



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:39 PM BST

PDB ID : 5KOZ  
Title : Structure function studies of R. palustris RubisCO (K192C mutant; CABP-bound)  
Authors : Arbing, M.A.; North, J.A.; Satagopan, S.; Tabita, F.R.  
Deposited on : 2016-07-01  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

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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	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

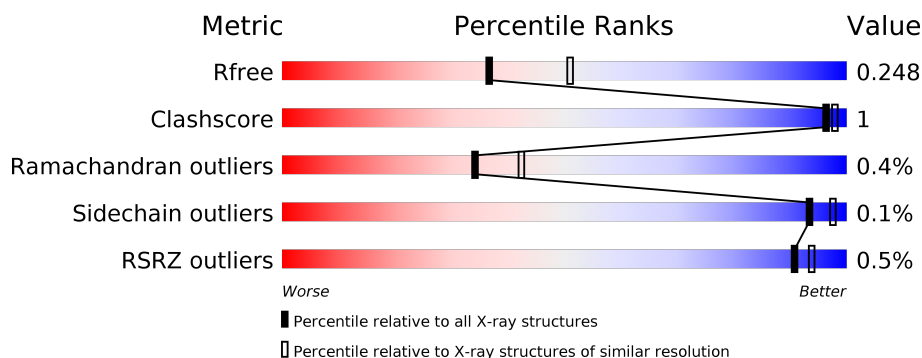
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	B	481	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	C	481	<div> <div></div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	D	481	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	E	481	<div> <div></div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	F	481	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	481	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>92%</div><div><div></div><div></div><div></div></div><div>• 5%</div></div></div>
1	H	481	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>92%</div><div><div></div><div></div><div></div></div><div>• 5%</div></div></div>
1	I	481	<div><div><div></div><div><div></div><div></div><div></div></div><div>93%</div><div><div></div><div></div><div></div></div><div>• 5%</div></div></div>
1	J	481	<div><div><div></div><div><div></div><div></div><div></div></div><div>93%</div><div><div></div><div></div><div></div></div><div>• 5%</div></div></div>
1	K	481	<div><div><div></div><div><div></div><div></div><div></div></div><div>92%</div><div><div></div><div></div><div></div></div><div>• 5%</div></div></div>
1	L	481	<div><div><div></div><div><div></div><div></div><div></div></div><div>92%</div><div><div></div><div></div><div></div></div><div>• 5%</div></div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 83751 atoms, of which 39714 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
			6752	2205	3284	599	644	20			
1	B	455	Total	C	H	N	O	S	0	0	0
			6738	2200	3275	599	644	20			
1	C	457	Total	C	H	N	O	S	0	1	0
			6797	2228	3290	608	651	20			
1	D	456	Total	C	H	N	O	S	0	0	0
			6808	2223	3310	605	650	20			
1	E	455	Total	C	H	N	O	S	0	1	0
			6828	2218	3336	608	646	20			
1	F	455	Total	C	H	N	O	S	0	0	0
			6743	2199	3284	600	640	20			
1	G	455	Total	C	H	N	O	S	0	0	0
			6798	2215	3313	600	650	20			
1	H	455	Total	C	H	N	O	S	0	0	0
			6780	2207	3309	602	642	20			
1	I	455	Total	C	H	N	O	S	0	0	0
			6758	2206	3283	602	647	20			
1	J	455	Total	C	H	N	O	S	0	0	0
			6788	2213	3308	604	643	20			
1	K	456	Total	C	H	N	O	S	0	0	0
			6811	2219	3321	605	646	20			
1	L	455	Total	C	H	N	O	S	0	0	0
			6771	2211	3293	603	644	20			

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	192	CYS	LYS	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	192	CYS	LYS	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	192	CYS	LYS	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	192	CYS	LYS	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	192	CYS	LYS	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	192	CYS	LYS	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	192	CYS	LYS	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	192	CYS	LYS	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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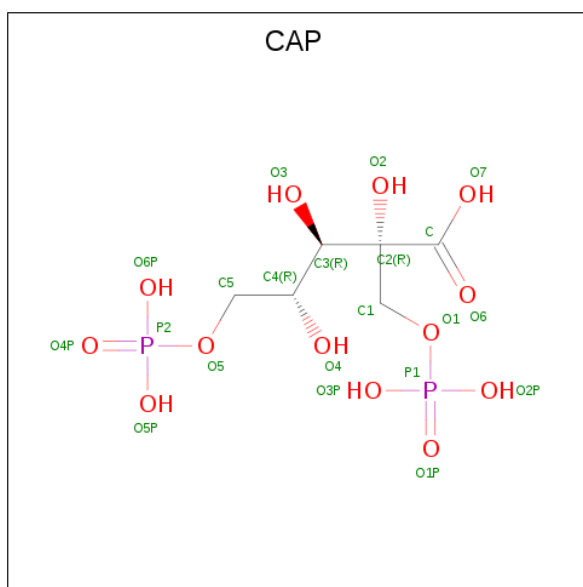
Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	HIS	-	expression tag	UNP Q6N0W9
I	-13	HIS	-	expression tag	UNP Q6N0W9
I	-12	HIS	-	expression tag	UNP Q6N0W9
I	-11	HIS	-	expression tag	UNP Q6N0W9
I	-10	HIS	-	expression tag	UNP Q6N0W9
I	-9	SER	-	expression tag	UNP Q6N0W9
I	-8	SER	-	expression tag	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	192	CYS	LYS	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	192	CYS	LYS	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	192	CYS	LYS	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	192	CYS	LYS	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>).

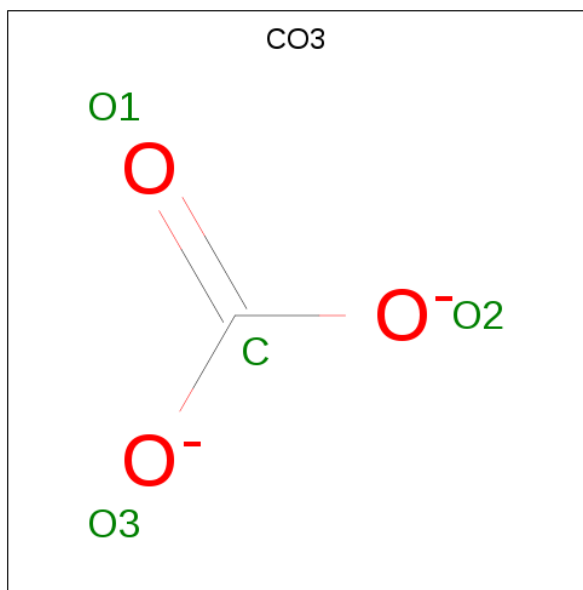


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	B	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	C	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	D	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	E	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	F	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	G	1	Total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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 1 3	0	0
4	B	1	Total C O 4 1 3	0	0
4	C	1	Total C O 4 1 3	0	0
4	D	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0
4	G	1	Total C O 4 1 3	0	0
4	H	1	Total C O 4 1 3	0	0
4	I	1	Total C O 4 1 3	0	0
4	J	1	Total C O 4 1 3	0	0
4	K	1	Total C O 4 1 3	0	0
4	L	1	Total C O 4 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	141	Total O 141 141	0	0
5	B	148	Total O 148 148	0	0
5	C	175	Total O 175 175	0	0
5	D	183	Total O 183 183	0	0
5	E	144	Total O 144 144	0	0
5	F	133	Total O 133 133	0	0
5	G	183	Total O 183 183	0	0
5	H	169	Total O 169 169	0	0

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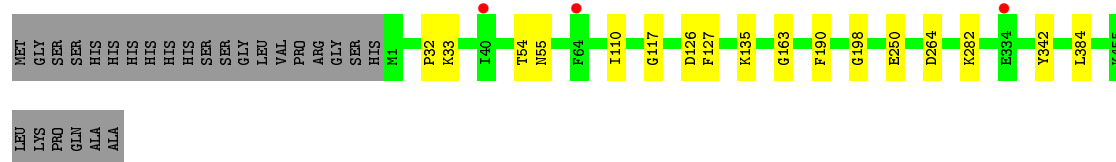
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	165	Total 165	O 165	0	0
5	J	178	Total 178	O 178	0	0
5	K	165	Total 165	O 165	0	0
5	L	175	Total 175	O 175	0	0

### 3 Residue-property plots

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



- Molecule 1: Ribulose biphosphate carboxylase



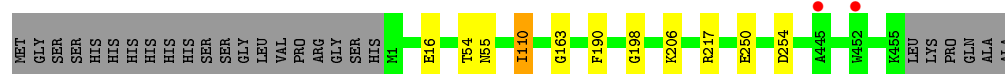
- Molecule 1: Ribulose biphosphate carboxylase



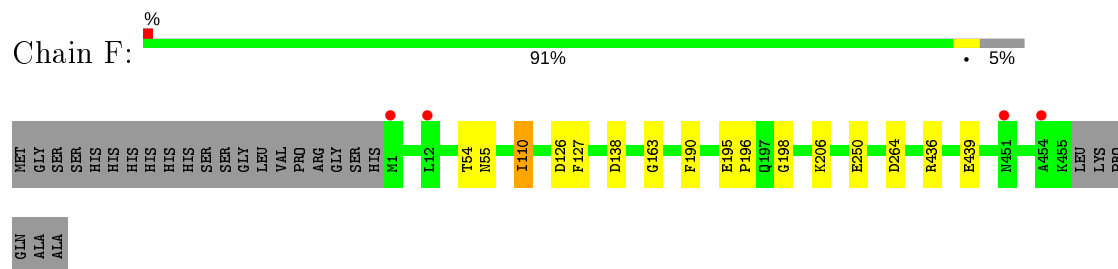
- Molecule 1: Ribulose biphosphate carboxylase



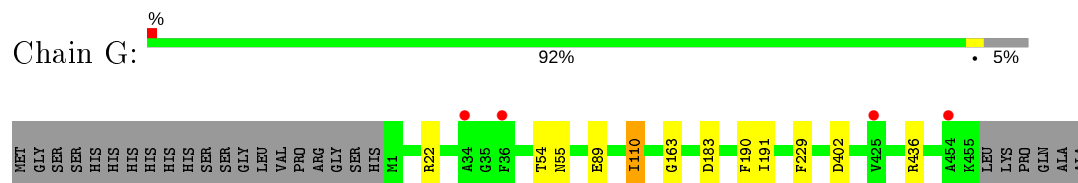
- Molecule 1: Ribulose biphosphate carboxylase



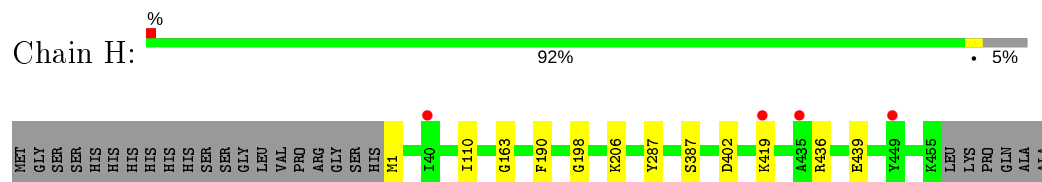
- Molecule 1: Ribulose biphosphate carboxylase



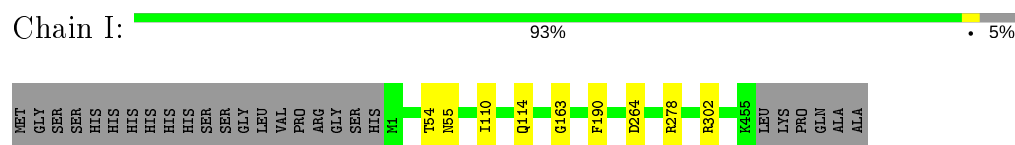
- Molecule 1: Ribulose biphosphate carboxylase



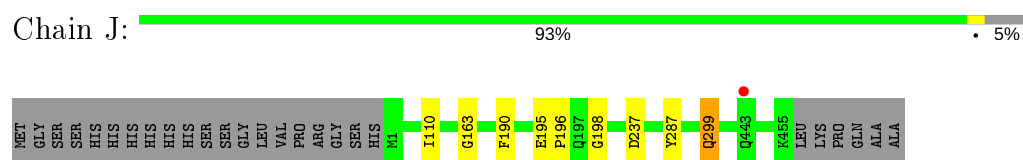
- Molecule 1: Ribulose biphosphate carboxylase



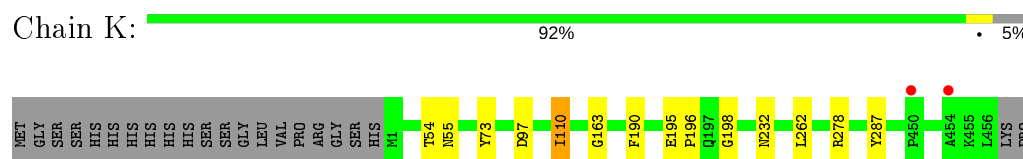
- Molecule 1: Ribulose biphosphate carboxylase



- 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	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.46Å 110.62Å 166.85Å 89.96° 101.77° 104.88°	Depositor
Resolution (Å)	11.49 – 2.30 87.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.4 (11.49-2.30) 92.5 (87.16-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, $R_{free}$	0.200 , 0.247 0.203 , 0.248	Depositor DCC
$R_{free}$ test set	20958 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	83751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.08 % 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 1.3536e-06. 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, CO3

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	0.25	0/3557	0.42	0/4822
1	B	0.25	0/3552	0.42	0/4816
1	C	0.25	0/3596	0.42	0/4873
1	D	0.26	0/3587	0.42	0/4860
1	E	0.26	0/3581	0.42	0/4851
1	F	0.25	0/3547	0.42	0/4809
1	G	0.25	0/3574	0.42	0/4843
1	H	0.25	0/3560	0.42	0/4826
1	I	0.26	0/3563	0.42	0/4829
1	J	0.26	0/3569	0.42	0/4836
1	K	0.26	0/3579	0.43	0/4849
1	L	0.26	0/3567	0.43	0/4834
All	All	0.26	0/42832	0.42	0/58048

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3468	3284	3299	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3463	3275	3286	5	0
1	C	3507	3290	3348	8	0
1	D	3498	3310	3349	7	0
1	E	3492	3336	3337	7	0
1	F	3459	3284	3297	10	0
1	G	3485	3313	3327	7	0
1	H	3471	3309	3311	8	0
1	I	3475	3283	3314	5	0
1	J	3480	3308	3330	4	0
1	K	3490	3321	3338	7	0
1	L	3478	3293	3324	7	0
2	A	21	9	8	0	0
2	B	21	9	7	0	0
2	C	21	9	8	0	0
2	D	21	9	8	0	0
2	E	21	9	9	0	0
2	F	21	9	9	0	0
2	G	21	9	7	0	0
2	H	21	9	7	0	0
2	I	21	9	8	0	0
2	J	21	9	7	0	0
2	K	21	9	8	0	0
2	L	21	9	8	1	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	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	141	0	0	4	0
5	B	148	0	0	1	0
5	C	175	0	0	2	0
5	D	183	0	0	1	0
5	E	144	0	0	1	0
5	F	133	0	0	1	0
5	G	183	0	0	1	0
5	H	169	0	0	3	0
5	I	165	0	0	1	0
5	J	178	0	0	1	0
5	K	165	0	0	1	0
5	L	175	0	0	0	0
All	All	44037	39714	39954	78	0

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

All (78) 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:K:97:ASP:OD2	1:K:278:ARG:NH2	2.18	0.76
1:A:264:ASP:OD2	5:A:601:HOH:O	2.11	0.68
1:B:436:ARG:NH1	1:B:439:GLU:OE1	2.27	0.67
1:J:299:GLN:NE2	5:J:601:HOH:O	2.23	0.66
1:E:217[A]:ARG:NH2	1:E:254:ASP:OD1	2.27	0.65
1:K:73:TYR:O	5:K:1601:HOH:O	2.14	0.65
1:G:22:ARG:NH2	1:G:89:GLU:OE2	2.29	0.65
1:L:22:ARG:NH2	1:L:89:GLU:OE2	2.30	0.64
1:H:387:SER:OG	1:H:419:LYS:NZ	2.33	0.58
1:C:22:ARG:NH2	1:C:89:GLU:OE2	2.38	0.57
1:C:206:LYS:NZ	1:E:250:GLU:OE2	2.21	0.57
1:B:206:LYS:NZ	1:F:250:GLU:OE2	2.22	0.57
1:I:278:ARG:NH1	1:J:237:ASP:OD2	2.41	0.54
1:C:430:ASP:OD1	5:C:601:HOH:O	2.18	0.53
1:A:250:GLU:OE2	1:E:206:LYS:NZ	2.27	0.52
1:H:206:LYS:NZ	1:L:250:GLU:OE2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:GLN:O	1:I:302:ARG:NH2	2.43	0.51
1:E:16:GLU:O	5:E:601:HOH:O	2.19	0.50
1:F:264:ASP:OD2	5:F:601:HOH:O	2.19	0.49
1:C:54:THR:OG1	1:C:55:ASN:N	2.46	0.48
1:D:3:GLN:OE1	5:D:601:HOH:O	2.20	0.48
1:D:250:GLU:OE2	1:F:206:LYS:NZ	2.28	0.48
1:G:183:ASP:OD2	5:G:601:HOH:O	2.20	0.48
1:H:163:GLY:HA2	1:H:190:PHE:O	2.13	0.48
1:H:387:SER:OG	1:H:419:LYS:CE	2.62	0.48
1:A:33:LYS:NZ	5:A:610:HOH:O	2.39	0.48
1:E:163:GLY:HA2	1:E:190:PHE:O	2.14	0.47
1:I:163:GLY:HA2	1:I:190:PHE:O	2.14	0.47
1:A:33:LYS:NZ	1:A:117:GLY:O	2.45	0.47
1:E:54:THR:OG1	1:E:55:ASN:N	2.47	0.47
1:D:163:GLY:HA2	1:D:190:PHE:O	2.15	0.46
1:C:278:ARG:NH1	1:D:237:ASP:OD2	2.48	0.46
1:H:436:ARG:NH1	1:H:439:GLU:OE1	2.49	0.46
1:C:436:ARG:NH1	1:C:439:GLU:OE1	2.49	0.46
1:K:232:ASN:HA	1:K:262:LEU:HB3	1.98	0.45
1:A:135:LYS:NZ	5:A:607:HOH:O	2.46	0.45
1:A:342:TYR:OH	1:A:384:LEU:O	2.31	0.45
1:K:163:GLY:HA2	1:K:190:PHE:O	2.17	0.45
1:D:22:ARG:NH2	1:D:89:GLU:OE2	2.50	0.45
1:L:163:GLY:HA2	1:L:190:PHE:O	2.15	0.45
1:H:419:LYS:NZ	5:H:619:HOH:O	2.49	0.45
1:F:126:ASP:OD1	1:F:127:PHE:N	2.51	0.44
1:G:163:GLY:HA2	1:G:190:PHE:O	2.18	0.44
1:A:163:GLY:HA2	1:A:190:PHE:O	2.18	0.44
1:D:68:VAL:O	1:D:68:VAL:CG1	2.66	0.43
1:F:163:GLY:HA2	1:F:190:PHE:O	2.19	0.43
1:I:54:THR:OG1	1:I:55:ASN:N	2.50	0.43
1:C:163:GLY:HA2	1:C:190:PHE:O	2.17	0.43
1:H:1:MET:N	5:H:614:HOH:O	2.47	0.43
1:C:135:LYS:NZ	5:C:618:HOH:O	2.44	0.43
1:L:25:LEU:O	1:L:127:PHE:HA	2.19	0.43
1:L:169:LYS:NZ	2:L:500:CAP:O7	2.52	0.43
1:A:32:PRO:O	5:A:602:HOH:O	2.21	0.43
1:G:110:ILE:HG23	1:G:110:ILE:O	2.19	0.43
1:A:282:LYS:HE3	1:F:138:ASP:HA	2.01	0.42
1:B:163:GLY:HA2	1:B:190:PHE:O	2.19	0.42
1:F:436:ARG:NH1	1:F:439:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:54:THR:OG1	1:K:55:ASN:N	2.51	0.42
1:J:195:GLU:N	1:J:196:PRO:CD	2.84	0.41
1:K:195:GLU:N	1:K:196:PRO:CD	2.83	0.41
1:I:264:ASP:OD2	5:I:601:HOH:O	2.21	0.41
1:A:54:THR:OG1	1:A:55:ASN:N	2.53	0.41
1:B:381:PHE:HB3	1:B:418:TRP:CE2	2.56	0.41
1:L:110:ILE:O	1:L:110:ILE:HG23	2.21	0.41
1:A:126:ASP:OD1	1:A:127:PHE:N	2.54	0.41
1:H:402:ASP:O	5:H:601:HOH:O	2.22	0.41
1:G:191:ILE:O	1:G:229:PHE:HA	2.21	0.41
1:L:195:GLU:N	1:L:196:PRO:CD	2.84	0.41
1:D:110:ILE:HG23	1:D:110:ILE:O	2.21	0.40
1:G:54:THR:OG1	1:G:55:ASN:N	2.51	0.40
1:K:110:ILE:O	1:K:110:ILE:HG23	2.21	0.40
1:B:189:ASP:OD1	5:B:601:HOH:O	2.22	0.40
1:F:110:ILE:O	1:F:110:ILE:HG23	2.21	0.40
1:E:110:ILE:HG23	1:E:110:ILE:O	2.21	0.40
1:F:195:GLU:N	1:F:196:PRO:CD	2.84	0.40
1:F:54:THR:OG1	1:F:55:ASN:N	2.53	0.40
1:G:402:ASP:OD2	1:G:436:ARG:HD3	2.21	0.40
1:J:163:GLY:HA2	1:J:190:PHE:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	453/481 (94%)	440 (97%)	11 (2%)	2 (0%)	34 42
1	B	453/481 (94%)	439 (97%)	13 (3%)	1 (0%)	47 58
1	C	456/481 (95%)	439 (96%)	16 (4%)	1 (0%)	47 58
1	D	454/481 (94%)	436 (96%)	16 (4%)	2 (0%)	34 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	454/481 (94%)	442 (97%)	10 (2%)	2 (0%)	34	42
1	F	453/481 (94%)	438 (97%)	13 (3%)	2 (0%)	34	42
1	G	453/481 (94%)	440 (97%)	12 (3%)	1 (0%)	47	58
1	H	453/481 (94%)	437 (96%)	14 (3%)	2 (0%)	34	42
1	I	453/481 (94%)	438 (97%)	14 (3%)	1 (0%)	47	58
1	J	453/481 (94%)	436 (96%)	15 (3%)	2 (0%)	34	42
1	K	454/481 (94%)	436 (96%)	16 (4%)	2 (0%)	34	42
1	L	453/481 (94%)	440 (97%)	11 (2%)	2 (0%)	34	42
All	All	5442/5772 (94%)	5261 (97%)	161 (3%)	20 (0%)	34	42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	110	ILE
1	G	110	ILE
1	C	110	ILE
1	I	110	ILE
1	D	110	ILE
1	H	110	ILE
1	K	110	ILE
1	A	110	ILE
1	B	110	ILE
1	E	110	ILE
1	E	198	GLY
1	L	110	ILE
1	L	198	GLY
1	A	198	GLY
1	D	198	GLY
1	F	198	GLY
1	J	110	ILE
1	J	198	GLY
1	K	198	GLY
1	H	198	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	340/373 (91%)	340 (100%)	0	100	100
1	B	339/373 (91%)	338 (100%)	1 (0%)	92	97
1	C	346/373 (93%)	346 (100%)	0	100	100
1	D	347/373 (93%)	347 (100%)	0	100	100
1	E	344/373 (92%)	344 (100%)	0	100	100
1	F	339/373 (91%)	339 (100%)	0	100	100
1	G	345/373 (92%)	345 (100%)	0	100	100
1	H	341/373 (91%)	340 (100%)	1 (0%)	92	97
1	I	343/373 (92%)	343 (100%)	0	100	100
1	J	343/373 (92%)	341 (99%)	2 (1%)	86	94
1	K	344/373 (92%)	343 (100%)	1 (0%)	92	97
1	L	343/373 (92%)	342 (100%)	1 (0%)	92	97
All	All	4114/4476 (92%)	4108 (100%)	6 (0%)	93	97

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

Mol	Chain	Res	Type
1	B	287	TYR
1	H	287	TYR
1	J	287	TYR
1	J	299	GLN
1	K	287	TYR
1	L	287	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	C	500	3	15,20,20	0.74	0	20,31,31	0.83	0
2	CAP	A	500	3	15,20,20	0.74	0	20,31,31	0.81	0
2	CAP	F	500	3	15,20,20	0.72	0	20,31,31	0.75	0
4	CO3	J	502	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	I	502	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	L	502	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	B	502	3	0,3,3	0.00	-	0,3,3	0.00	-
2	CAP	L	500	3	15,20,20	0.72	0	20,31,31	0.84	0
2	CAP	I	500	3	15,20,20	0.74	0	20,31,31	0.77	0
2	CAP	E	500	3	15,20,20	0.75	0	20,31,31	0.65	0
4	CO3	G	502	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	D	502	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	C	502	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	H	502	3	0,3,3	0.00	-	0,3,3	0.00	-
2	CAP	J	500	3	15,20,20	0.74	0	20,31,31	0.75	0
2	CAP	B	500	3	15,20,20	0.74	0	20,31,31	0.89	0
2	CAP	G	500	3	15,20,20	0.73	0	20,31,31	0.79	0
2	CAP	D	500	3	15,20,20	0.73	0	20,31,31	0.67	0
2	CAP	H	500	3	15,20,20	0.73	0	20,31,31	0.85	1 (5%)
4	CO3	A	502	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	K	502	3	0,3,3	0.00	-	0,3,3	0.00	-
2	CAP	K	500	3	15,20,20	0.72	0	20,31,31	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CO3	F	502	3	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	E	502	3	0,3,3	0.00	-	0,3,3	0.00	-

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	500	3	-	3/23/29/29	-
2	CAP	C	500	3	-	2/23/29/29	-
2	CAP	A	500	3	-	2/23/29/29	-
2	CAP	F	500	3	-	3/23/29/29	-
2	CAP	J	500	3	-	3/23/29/29	-
2	CAP	L	500	3	-	2/23/29/29	-
2	CAP	B	500	3	-	3/23/29/29	-
2	CAP	K	500	3	-	3/23/29/29	-
2	CAP	H	500	3	-	3/23/29/29	-
2	CAP	I	500	3	-	4/23/29/29	-
2	CAP	G	500	3	-	2/23/29/29	-
2	CAP	D	500	3	-	3/23/29/29	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	CAP	O3-C3-C4	2.17	113.77	109.13

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	CAP	O3-C3-C4-O4
2	A	500	CAP	O3-C3-C4-O4
2	F	500	CAP	O3-C3-C4-O4
2	L	500	CAP	O3-C3-C4-O4
2	I	500	CAP	O3-C3-C4-O4
2	J	500	CAP	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	B	500	CAP	O3-C3-C4-O4
2	G	500	CAP	O3-C3-C4-O4
2	H	500	CAP	O3-C3-C4-O4
2	K	500	CAP	O3-C3-C4-O4
2	C	500	CAP	O2-C2-C3-C4
2	A	500	CAP	O2-C2-C3-C4
2	F	500	CAP	O2-C2-C3-C4
2	L	500	CAP	O2-C2-C3-C4
2	I	500	CAP	O2-C2-C3-C4
2	E	500	CAP	O2-C2-C3-C4
2	J	500	CAP	O2-C2-C3-C4
2	B	500	CAP	O2-C2-C3-C4
2	G	500	CAP	O2-C2-C3-C4
2	D	500	CAP	O2-C2-C3-C4
2	H	500	CAP	O2-C2-C3-C4
2	K	500	CAP	O2-C2-C3-C4
2	B	500	CAP	C5-O5-P2-O4P
2	K	500	CAP	O4-C4-C5-O5
2	E	500	CAP	O3-C3-C4-O4
2	D	500	CAP	O3-C3-C4-O4
2	F	500	CAP	O4-C4-C5-O5
2	I	500	CAP	O4-C4-C5-O5
2	E	500	CAP	O4-C4-C5-O5
2	J	500	CAP	O4-C4-C5-O5
2	I	500	CAP	C2-C3-C4-O4
2	D	500	CAP	O4-C4-C5-O5
2	H	500	CAP	O4-C4-C5-O5

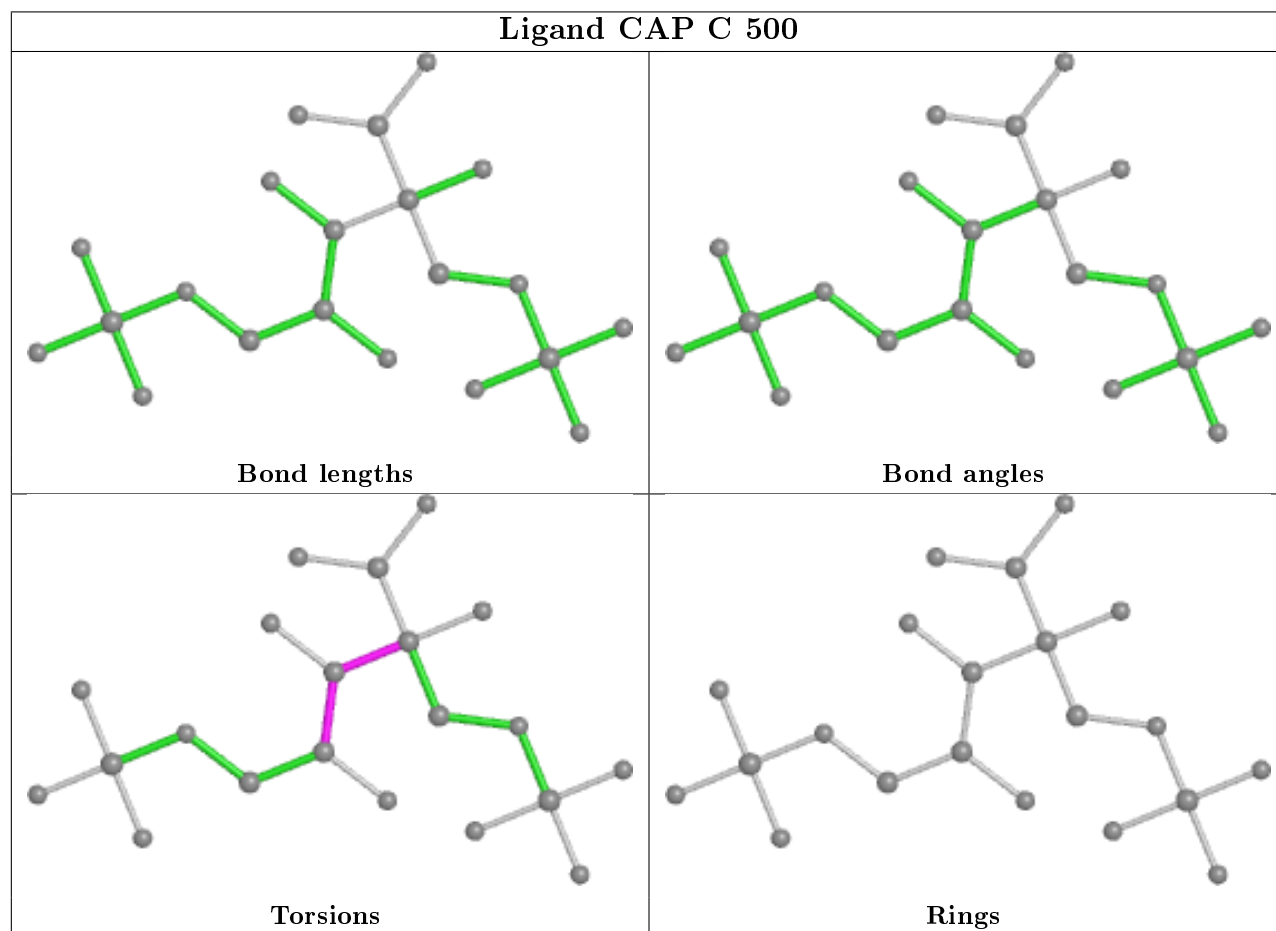
There are no ring outliers.

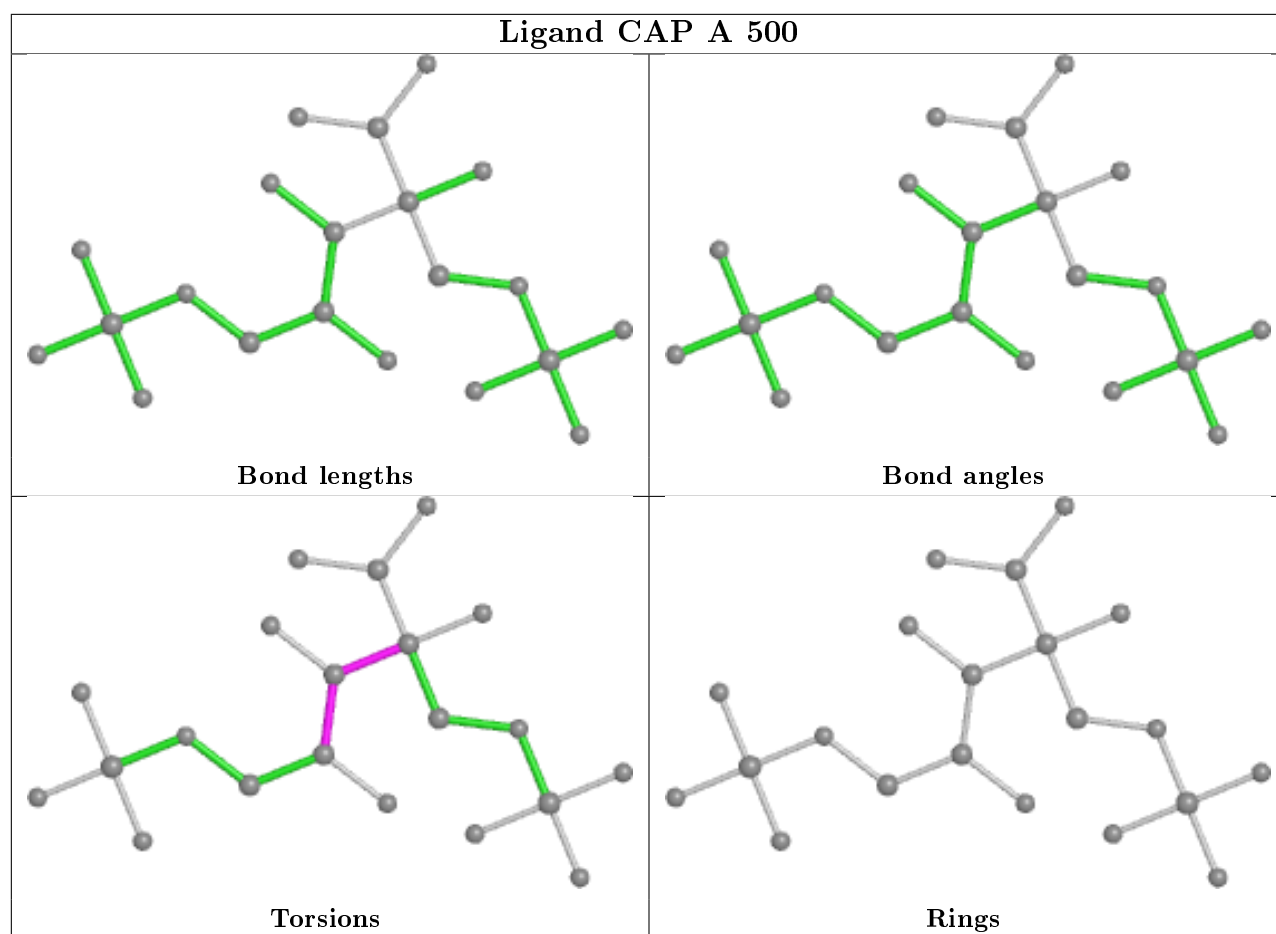
1 monomer is involved in 1 short contact:

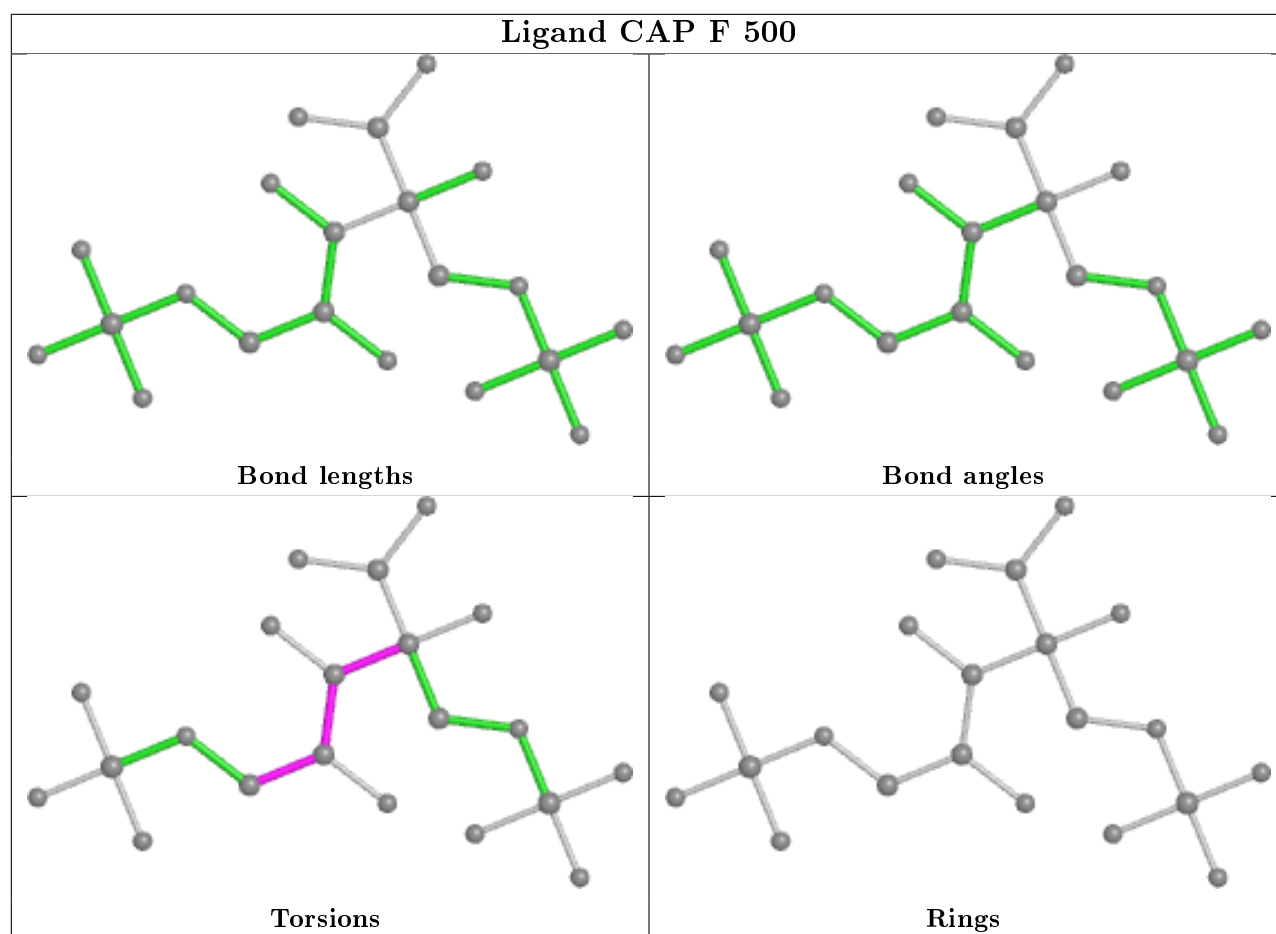
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	500	CAP	1	0

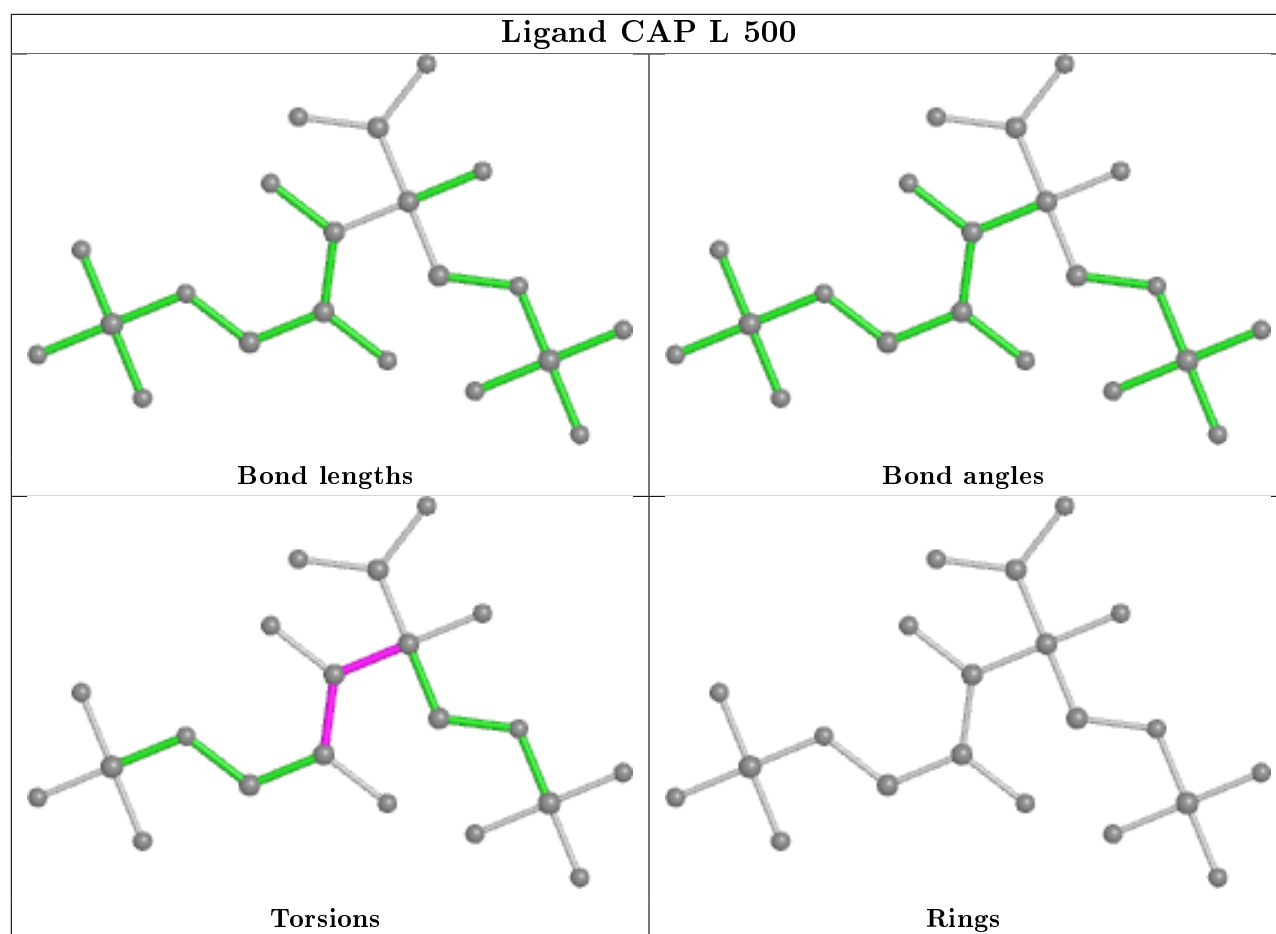
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

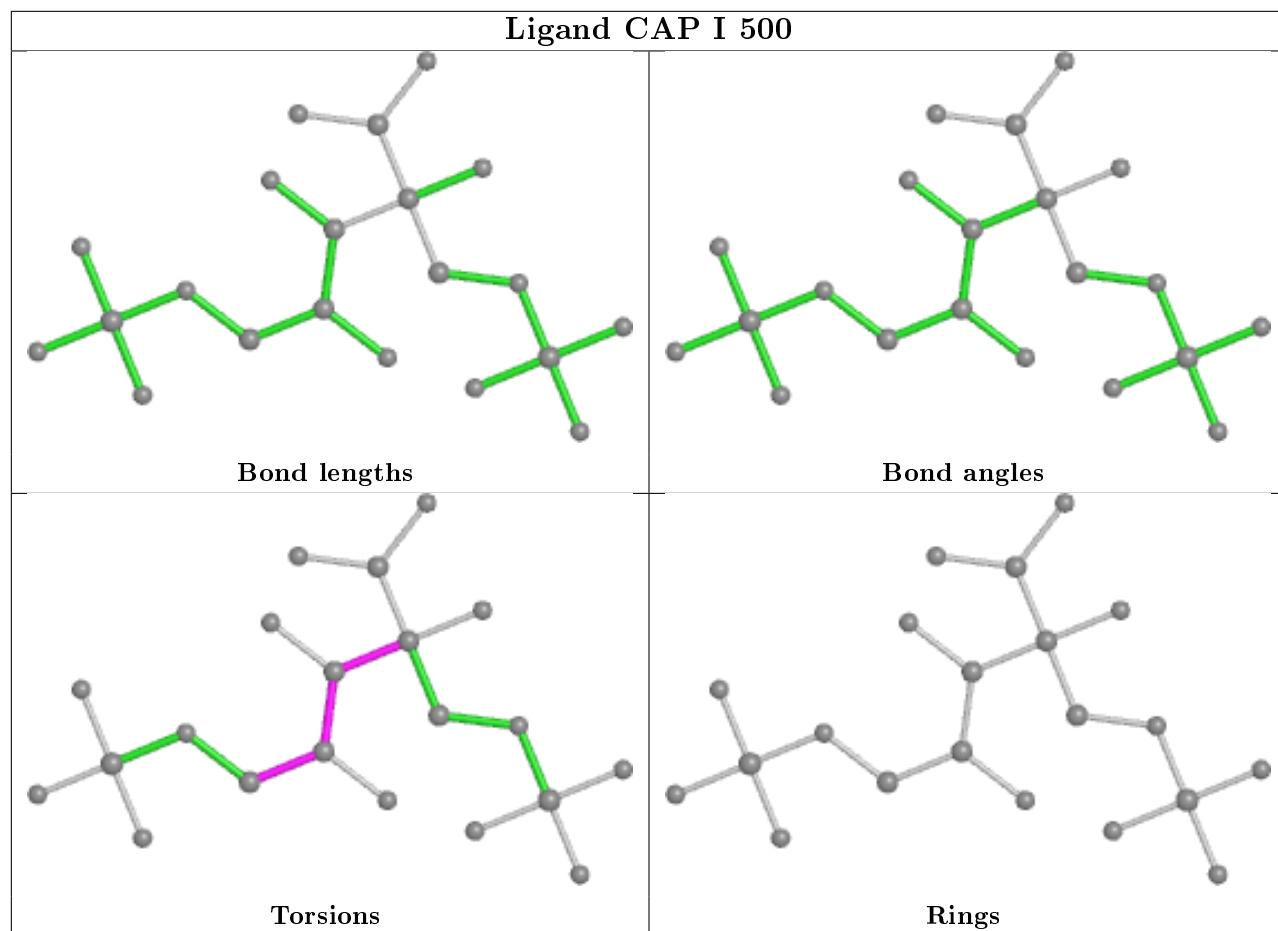


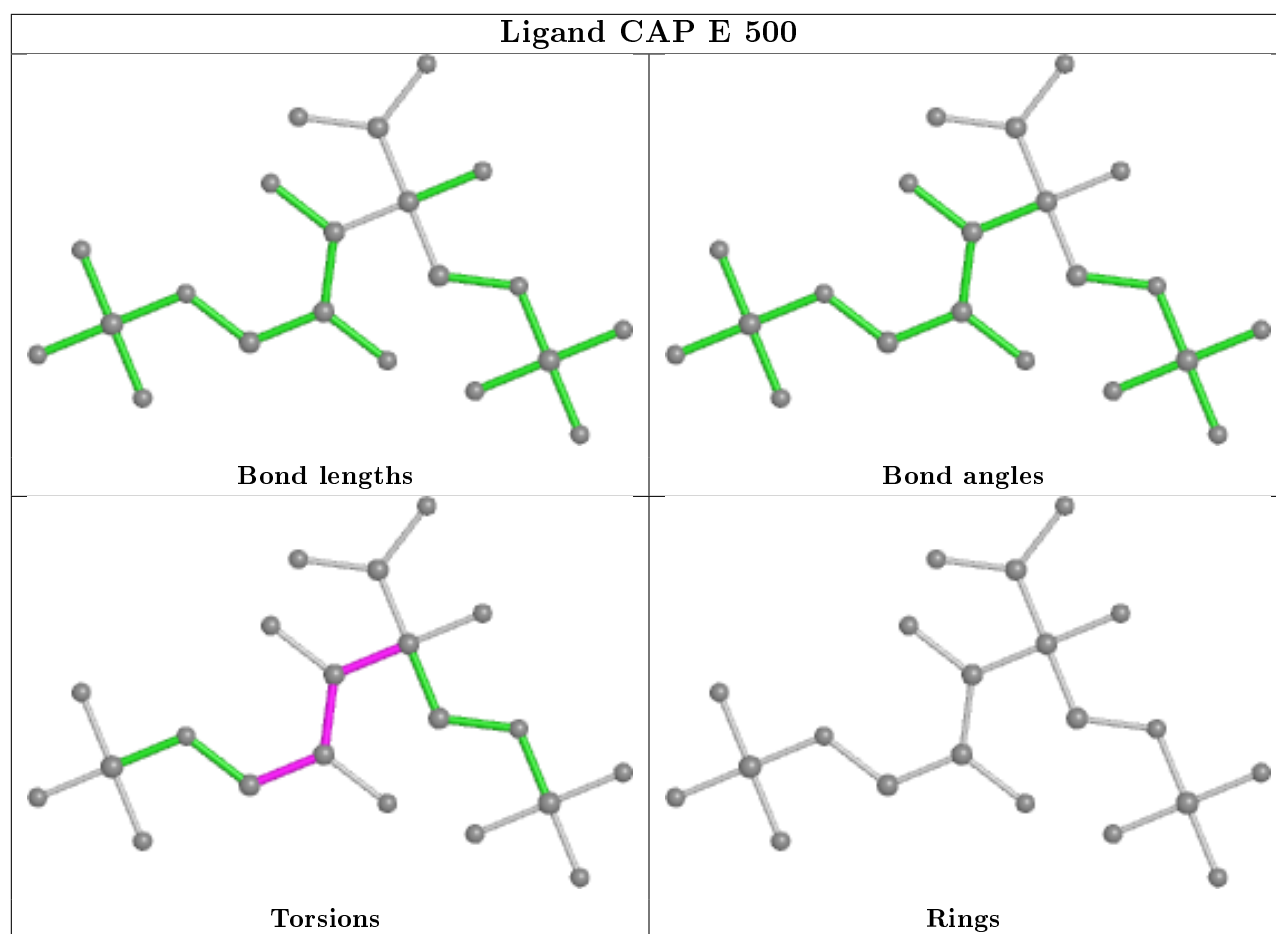


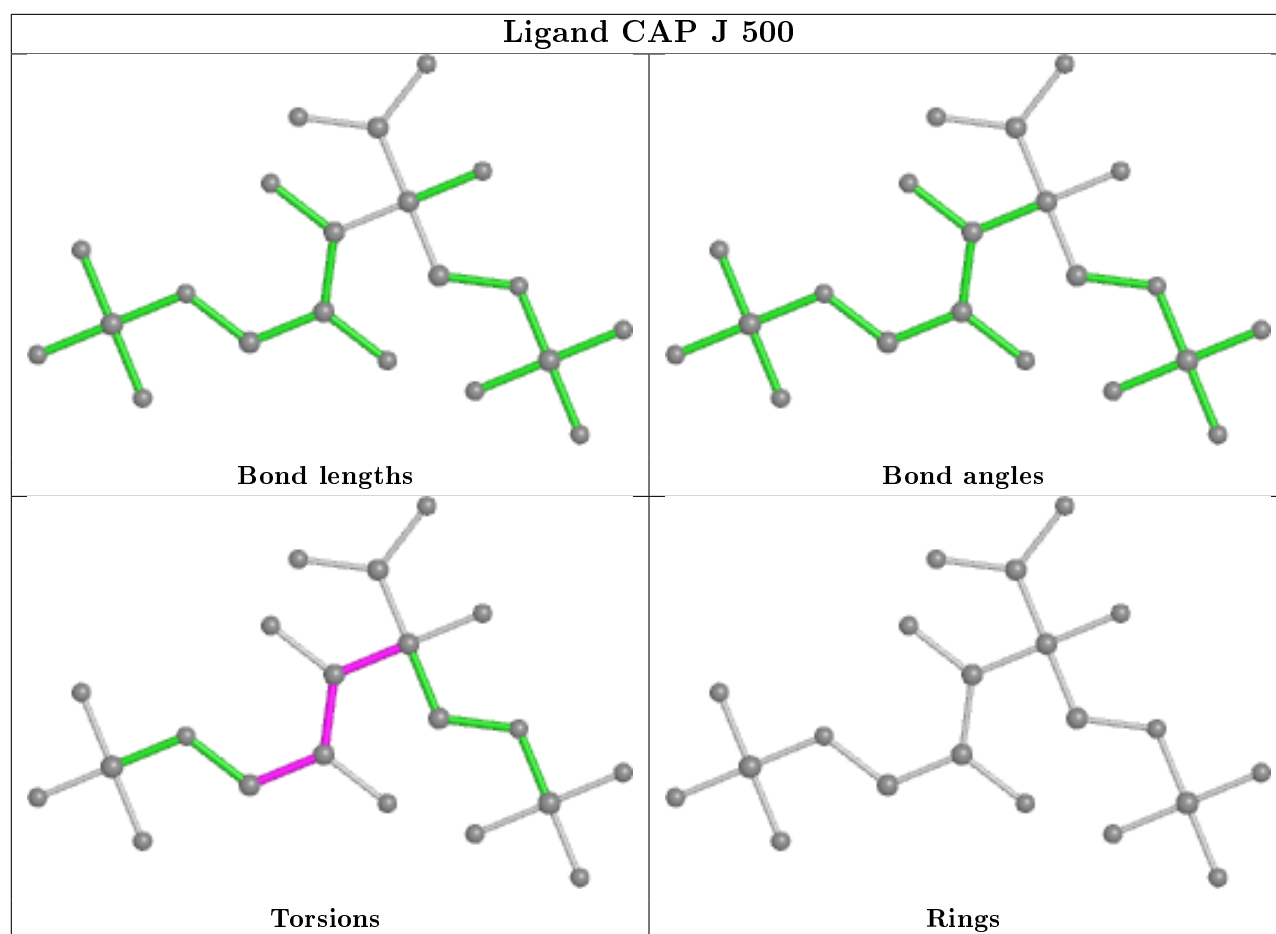


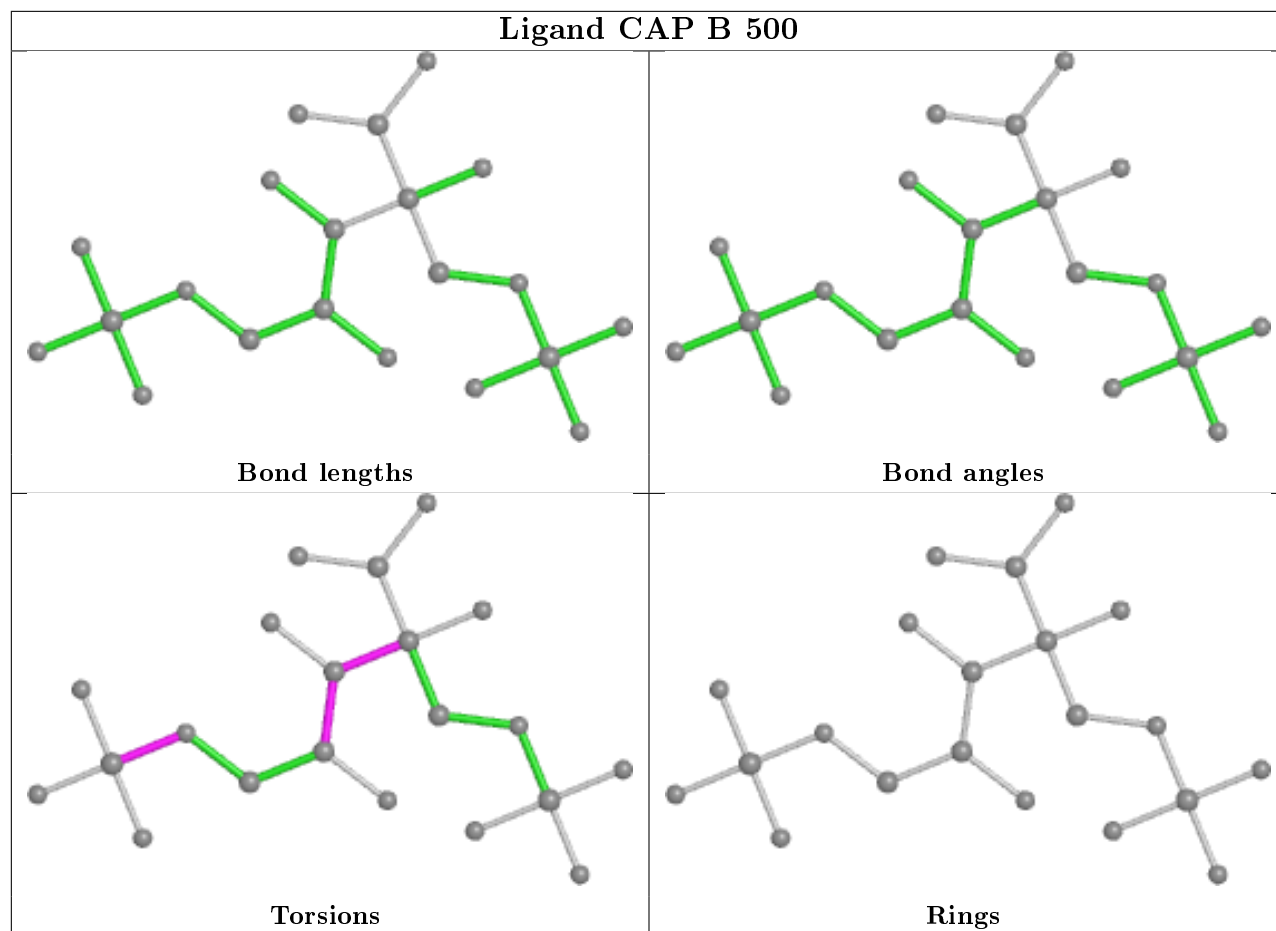


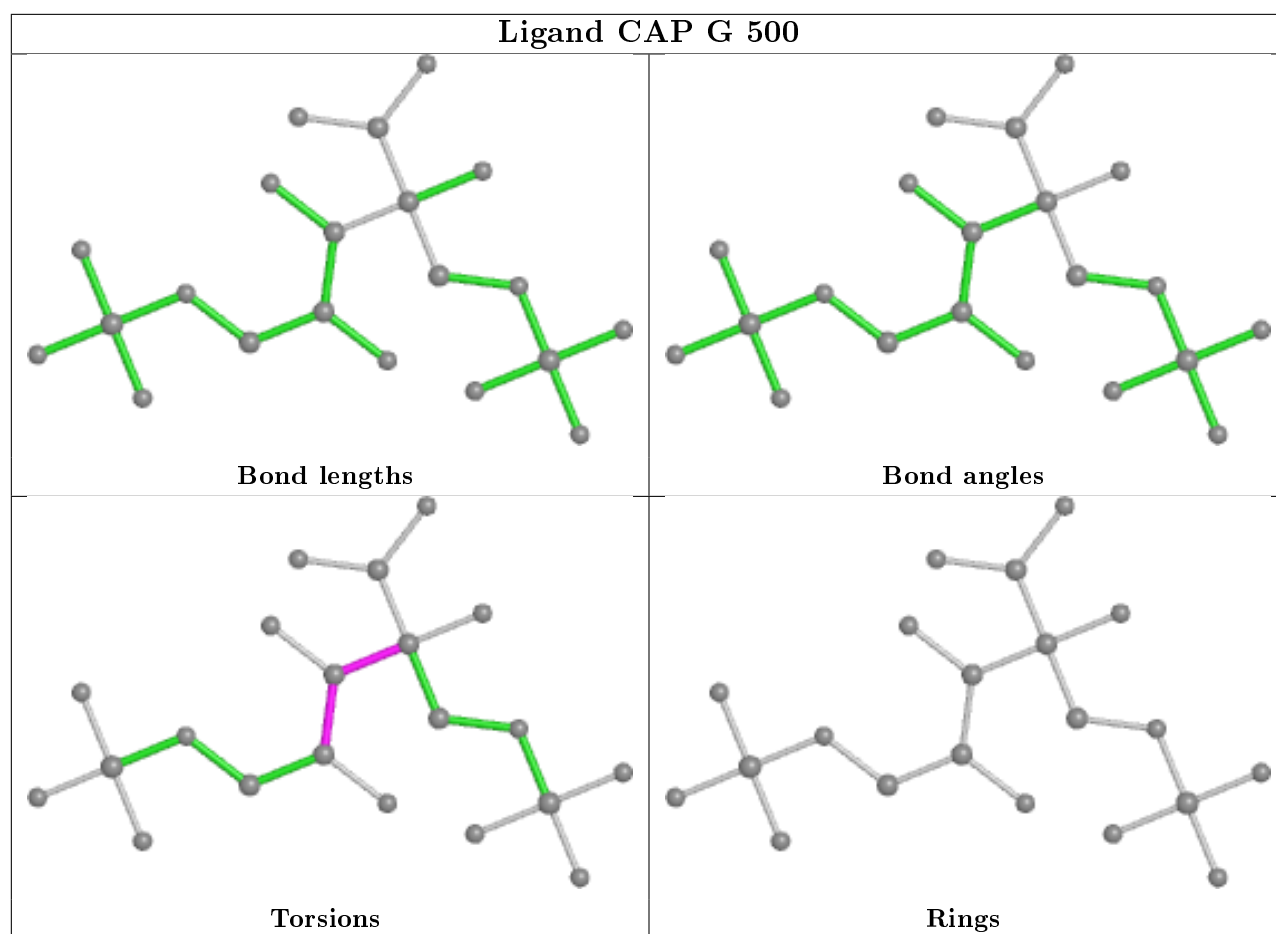


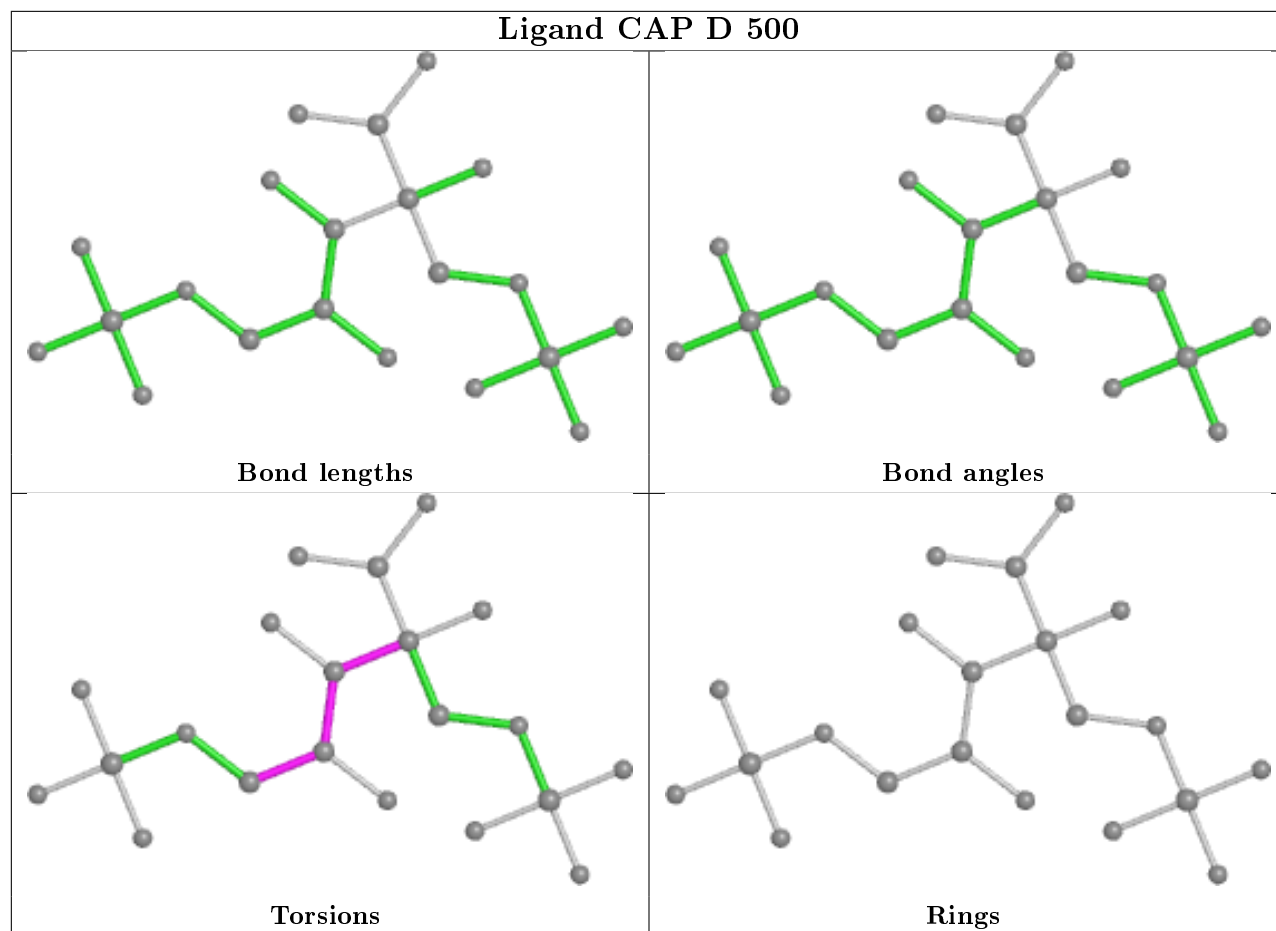


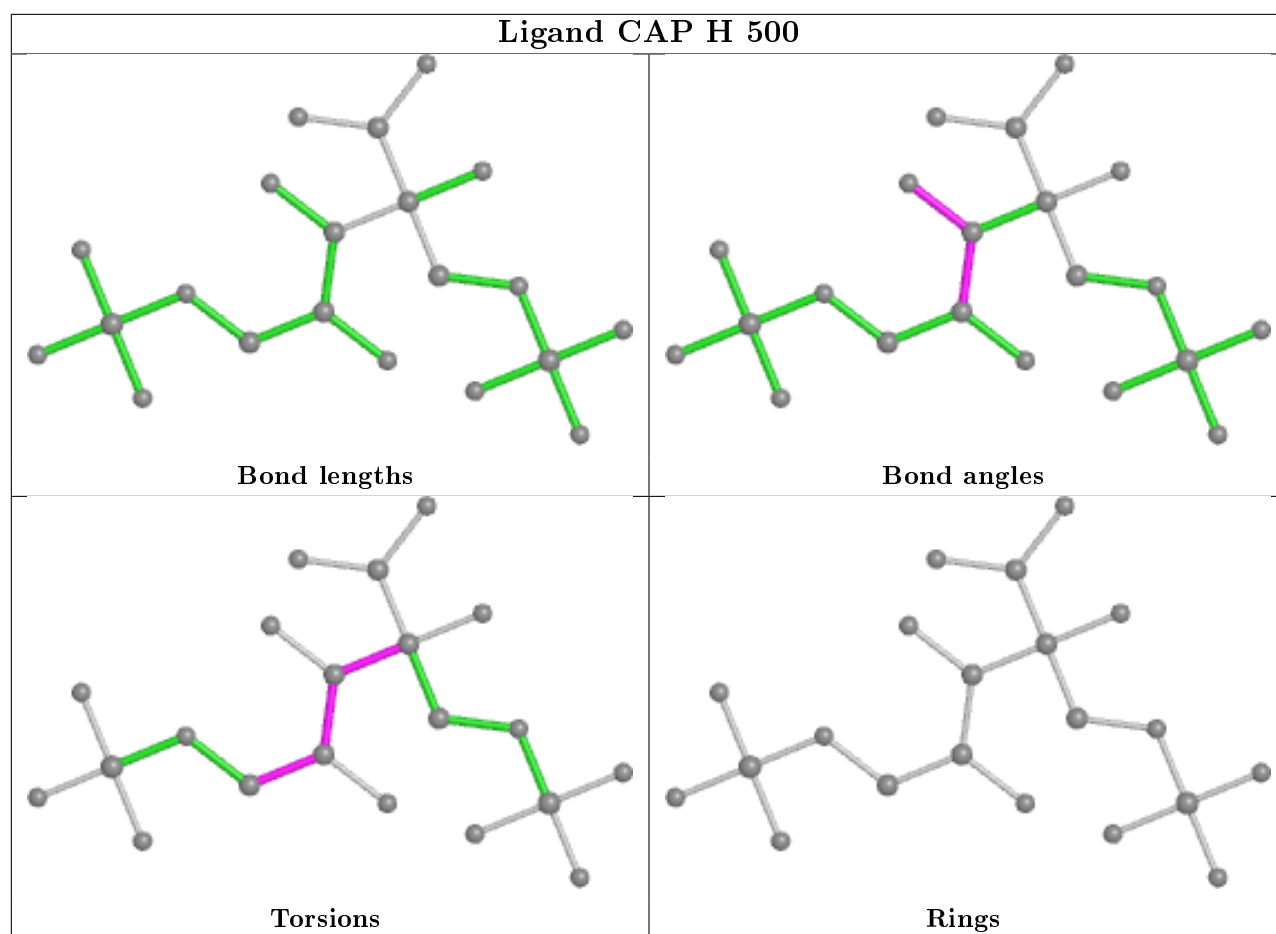


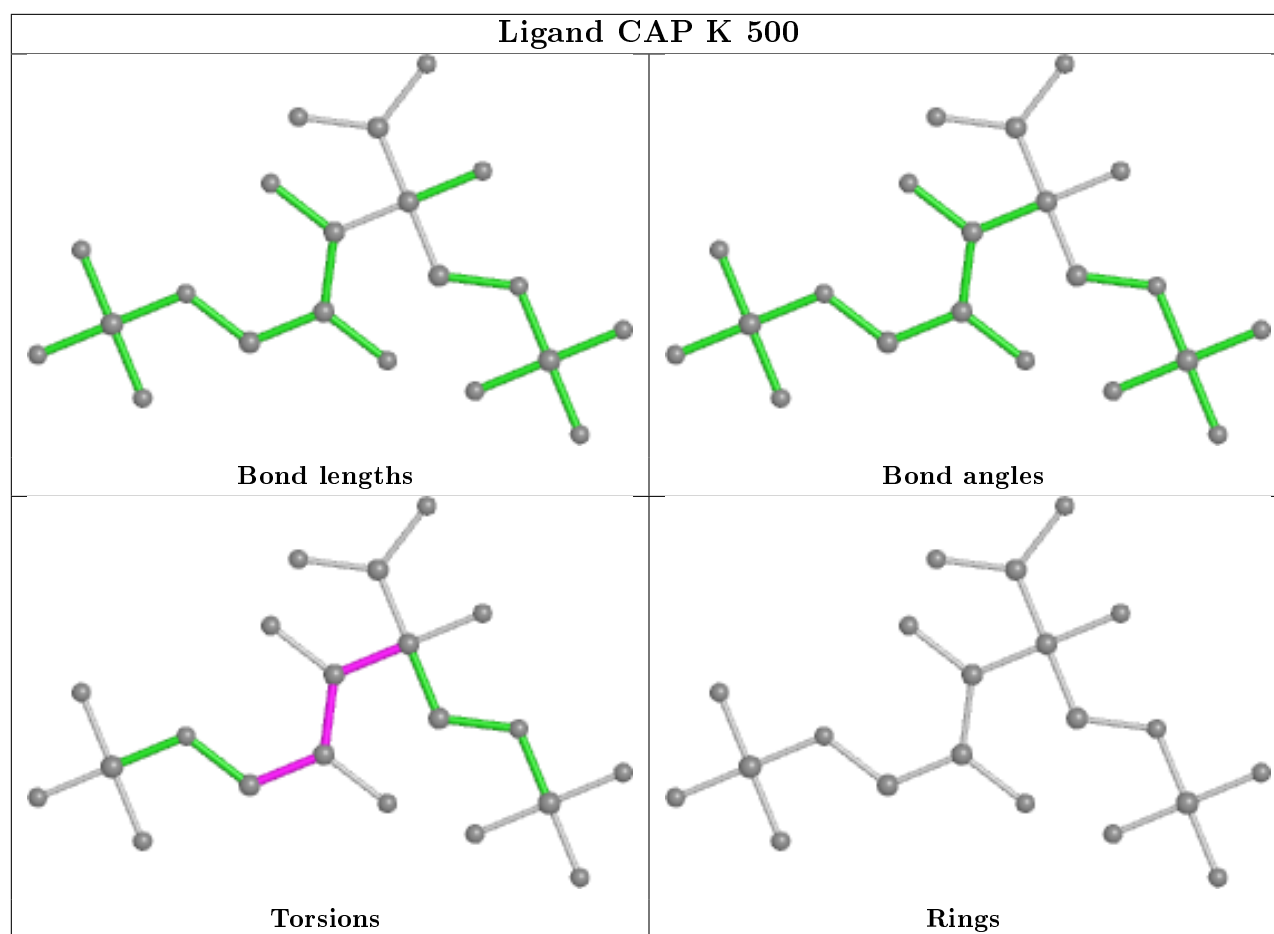












## 5.7 Other polymers [i](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	0.11	3 (0%) 87 91	33, 45, 64, 84	0
1	B	455/481 (94%)	0.16	5 (1%) 80 85	32, 43, 65, 89	0
1	C	457/481 (95%)	-0.03	1 (0%) 95 96	24, 35, 55, 94	0
1	D	456/481 (94%)	-0.04	3 (0%) 87 91	25, 36, 53, 77	0
1	E	455/481 (94%)	0.06	2 (0%) 92 95	28, 40, 59, 83	0
1	F	455/481 (94%)	0.03	4 (0%) 84 88	29, 42, 68, 98	0
1	G	455/481 (94%)	0.02	4 (0%) 84 88	22, 36, 55, 72	0
1	H	455/481 (94%)	0.05	4 (0%) 84 88	24, 37, 57, 81	0
1	I	455/481 (94%)	0.03	0 100 100	25, 39, 62, 85	0
1	J	455/481 (94%)	-0.02	1 (0%) 95 96	27, 37, 55, 86	0
1	K	456/481 (94%)	0.01	2 (0%) 92 95	22, 35, 57, 82	0
1	L	455/481 (94%)	-0.04	1 (0%) 95 96	21, 34, 53, 76	0
All	All	5464/5772 (94%)	0.03	30 (0%) 91 94	21, 38, 59, 98	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	36	PHE	4.5
1	K	454	ALA	4.0
1	K	450	PRO	3.4
1	H	419	LYS	3.4
1	E	452	TRP	3.3
1	H	449	TYR	3.2
1	G	425	VAL	3.2
1	B	404	GLY	3.0
1	D	425	VAL	2.7
1	L	449	TYR	2.7
1	E	445	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	40	ILE	2.6
1	H	435	ALA	2.6
1	A	40	ILE	2.6
1	F	454	ALA	2.5
1	B	422	ALA	2.4
1	A	334	GLU	2.3
1	J	443	GLN	2.3
1	B	375	LEU	2.3
1	B	449	TYR	2.3
1	D	90	LEU	2.2
1	F	1	MET	2.2
1	G	454	ALA	2.1
1	D	454	ALA	2.1
1	F	12	LEU	2.0
1	C	420	GLN	2.0
1	A	64	PHE	2.0
1	F	451	ASN	2.0
1	B	173	ARG	2.0
1	G	34	ALA	2.0

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

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

## 6.3 Carbohydrates [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( $\text{\AA}^2$ )	Q<0.9
3	MG	K	501	1/1	0.80	0.06	37,37,37,37	0
3	MG	A	501	1/1	0.91	0.11	44,44,44,44	0
4	CO3	I	502	4/4	0.93	0.22	39,45,46,47	0
3	MG	D	501	1/1	0.94	0.07	35,35,35,35	0

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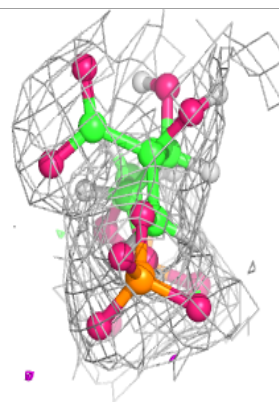
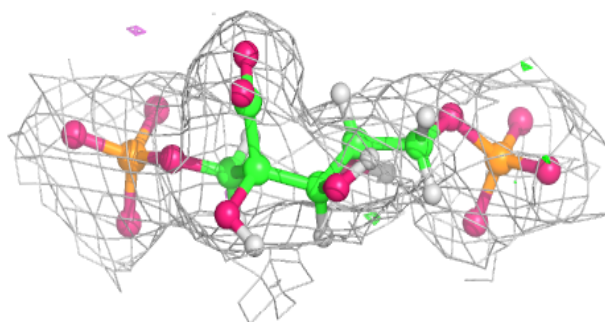
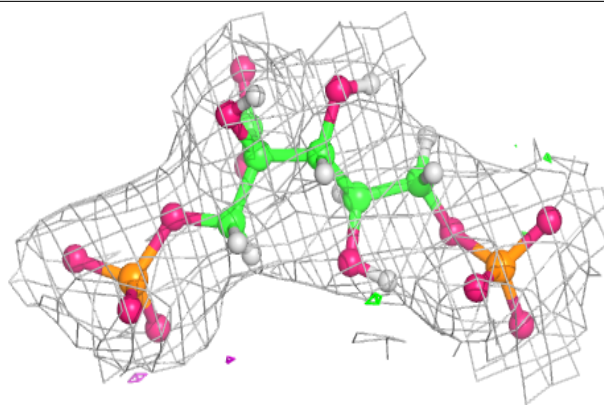
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	J	501	1/1	0.94	0.07	44,44,44,44	0
3	MG	F	501	1/1	0.94	0.13	38,38,38,38	0
4	CO3	J	502	4/4	0.95	0.17	35,38,38,42	0
4	CO3	B	502	4/4	0.95	0.21	41,42,43,43	0
4	CO3	A	502	4/4	0.95	0.20	53,54,54,55	0
4	CO3	C	502	4/4	0.95	0.13	34,38,38,40	0
3	MG	E	501	1/1	0.95	0.05	45,45,45,45	0
2	CAP	A	500	21/21	0.96	0.11	38,43,52,52	0
2	CAP	I	500	21/21	0.96	0.13	31,37,43,44	0
4	CO3	G	502	4/4	0.96	0.12	32,34,35,36	0
4	CO3	D	502	4/4	0.96	0.15	41,42,42,43	0
2	CAP	F	500	21/21	0.96	0.14	32,37,45,47	0
2	CAP	B	500	21/21	0.96	0.12	40,45,53,53	0
2	CAP	K	500	21/21	0.96	0.13	27,34,40,42	0
4	CO3	F	502	4/4	0.96	0.17	35,35,36,39	0
4	CO3	E	502	4/4	0.96	0.17	37,39,41,42	0
4	CO3	L	502	4/4	0.97	0.12	30,31,31,33	0
2	CAP	H	500	21/21	0.97	0.11	35,40,49,49	0
3	MG	L	501	1/1	0.97	0.08	32,32,32,32	0
2	CAP	E	500	21/21	0.97	0.13	37,44,52,53	0
3	MG	H	501	1/1	0.97	0.04	43,43,43,43	0
2	CAP	G	500	21/21	0.97	0.10	32,34,41,42	0
3	MG	C	501	1/1	0.97	0.07	36,36,36,36	0
2	CAP	D	500	21/21	0.97	0.10	26,31,38,42	0
2	CAP	C	500	21/21	0.97	0.13	28,30,34,36	0
3	MG	G	501	1/1	0.97	0.05	32,32,32,32	0
2	CAP	L	500	21/21	0.97	0.14	24,30,37,38	0
4	CO3	K	502	4/4	0.98	0.14	37,38,39,39	0
3	MG	B	501	1/1	0.98	0.06	44,44,44,44	0
4	CO3	H	502	4/4	0.98	0.21	53,62,64,65	0
2	CAP	J	500	21/21	0.98	0.11	32,38,46,51	0
3	MG	I	501	1/1	0.99	0.09	39,39,39,39	0

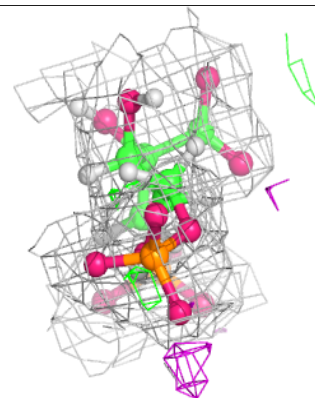
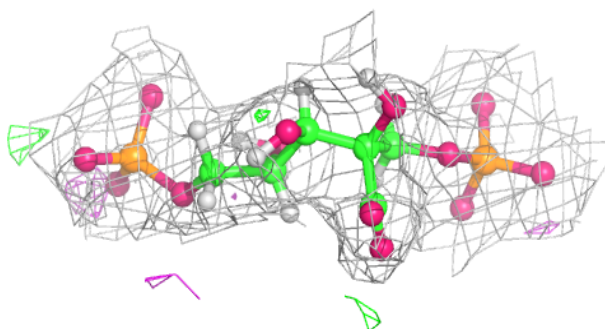
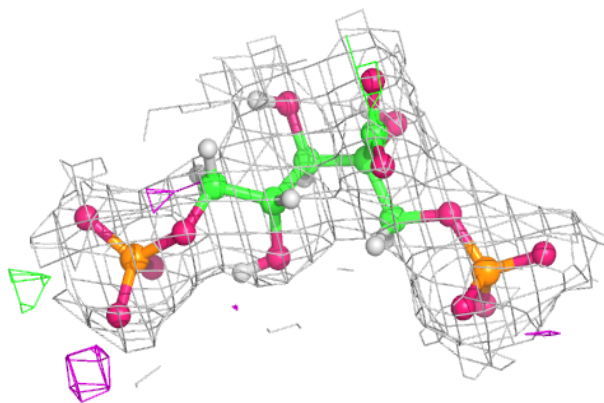
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CAP 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)

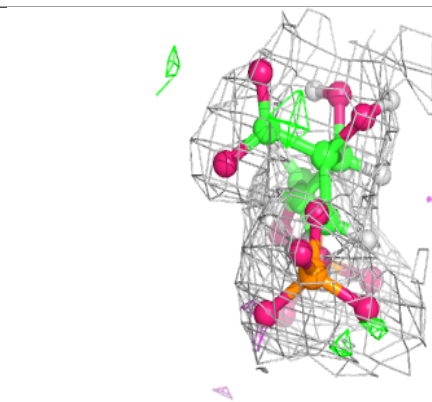
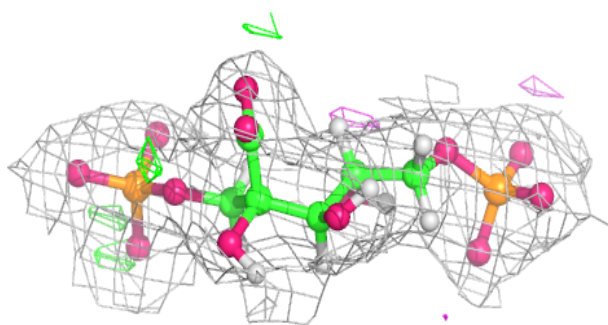
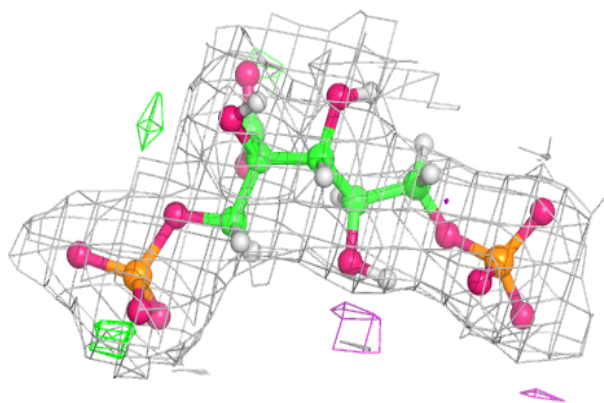
**Electron density around CAP I 500:**

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

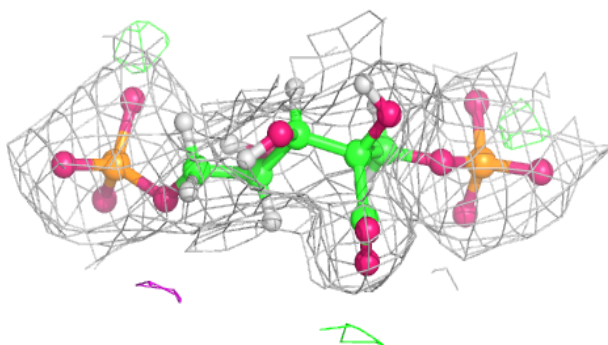
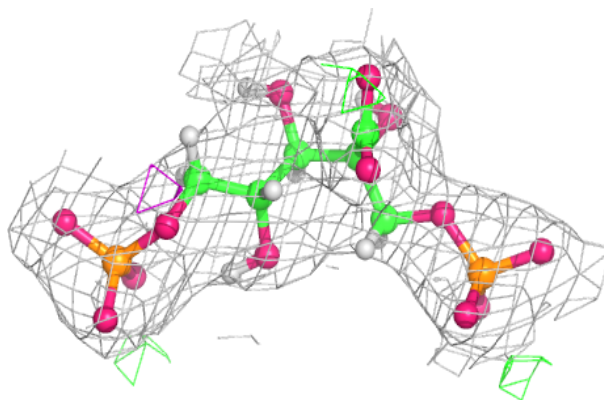


**Electron density around CAP F 500:**

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

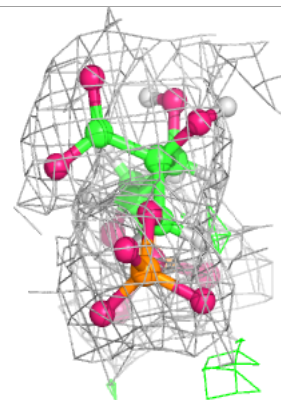
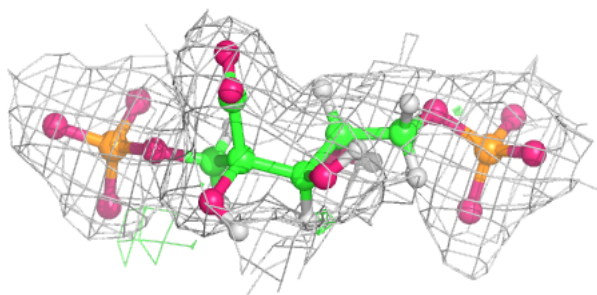
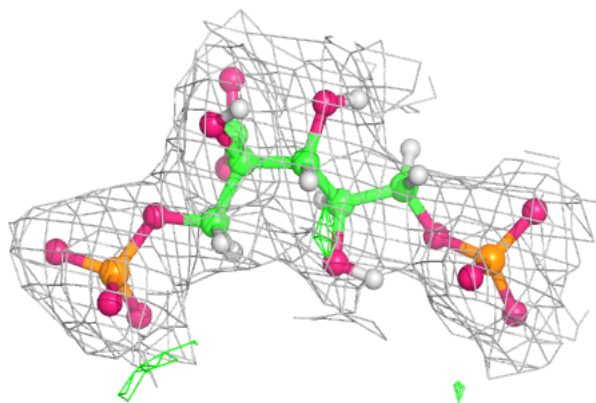
**Electron density around CAP B 500:**

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

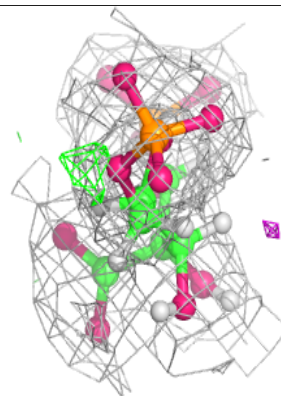
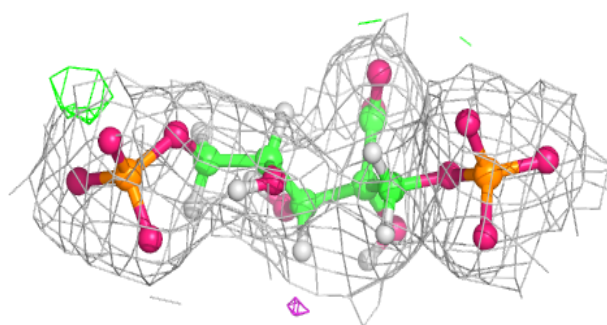
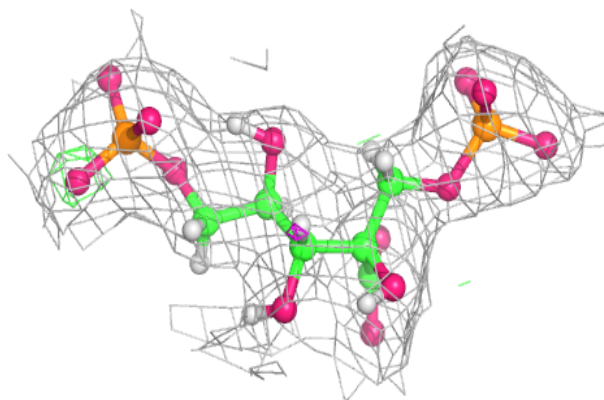


**Electron density around CAP K 500:**

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

**Electron density around CAP H 500:**

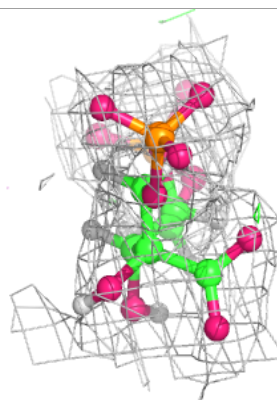
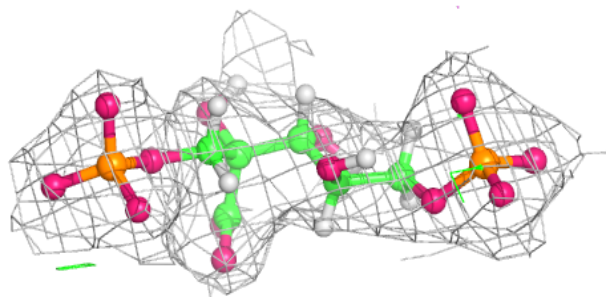
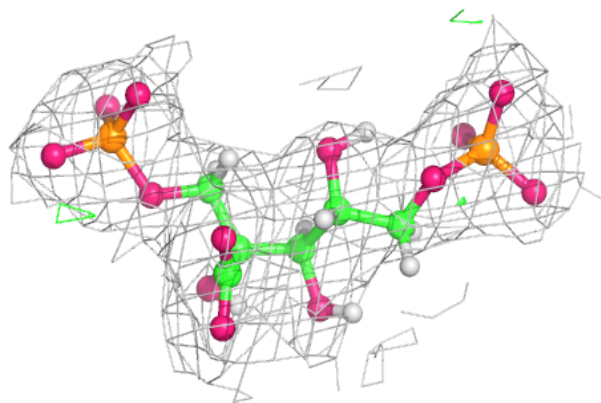
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



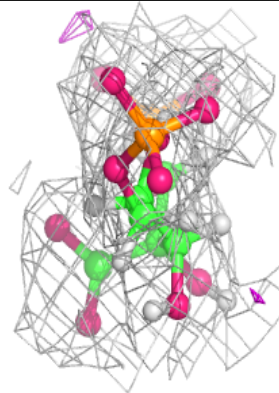
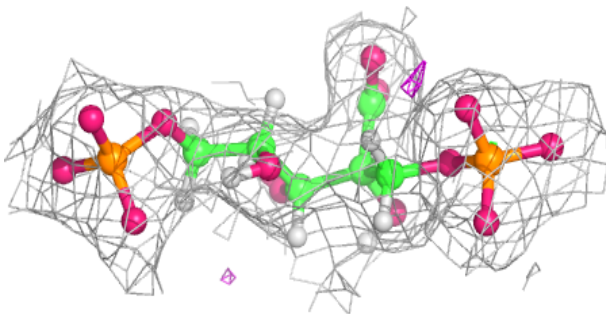
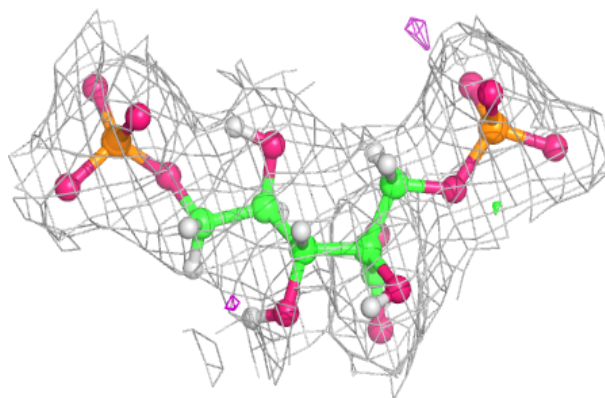


**Electron density around CAP E 500:**

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

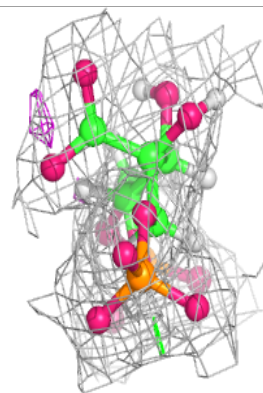
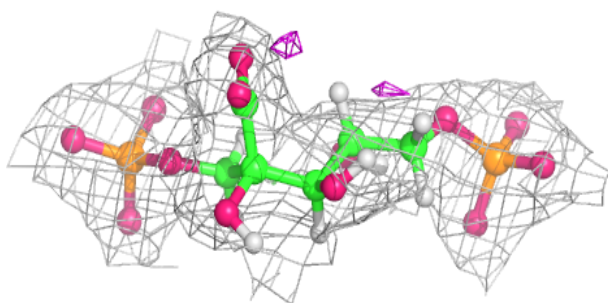
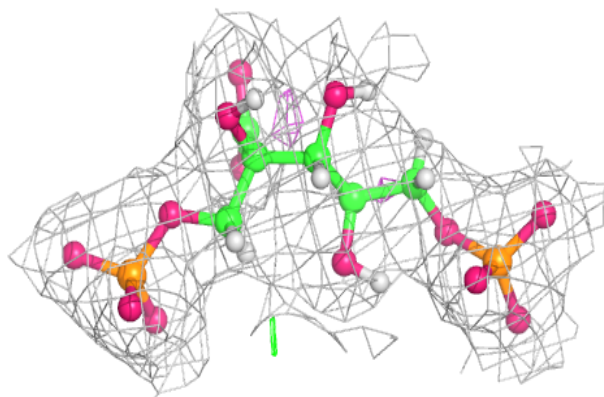
**Electron density around CAP G 500:**

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

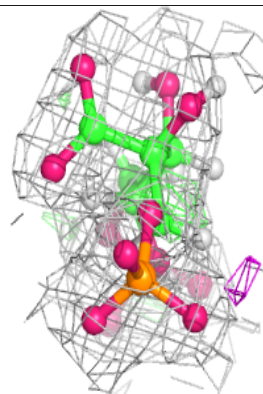
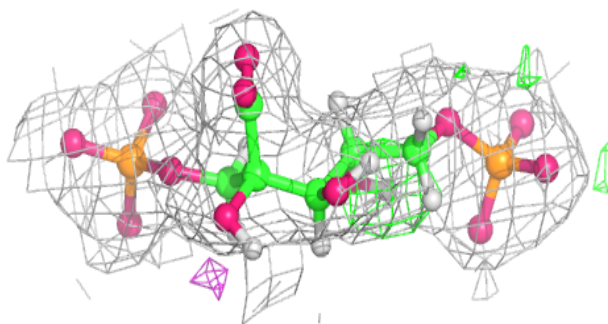
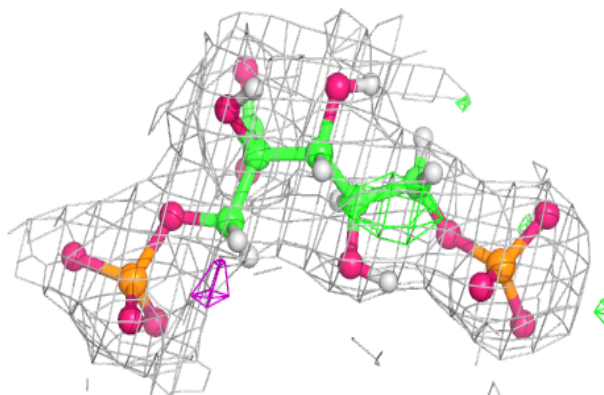


**Electron density around CAP D 500:**

$2mF_o-DF_c$  (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:**

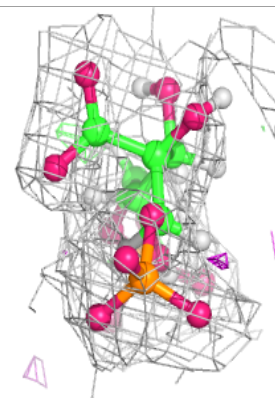
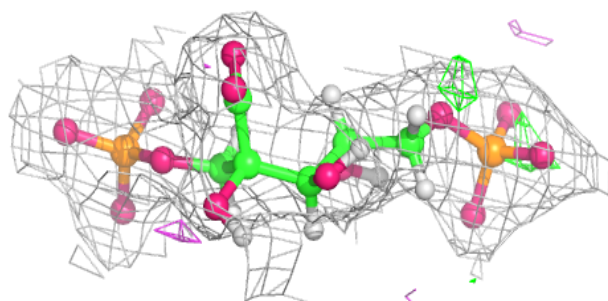
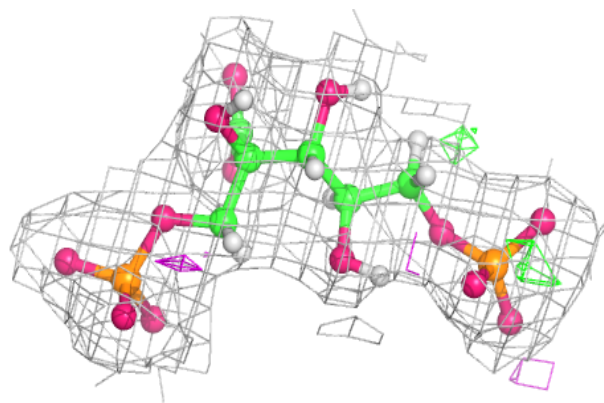
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



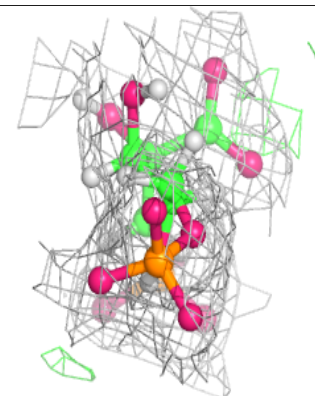
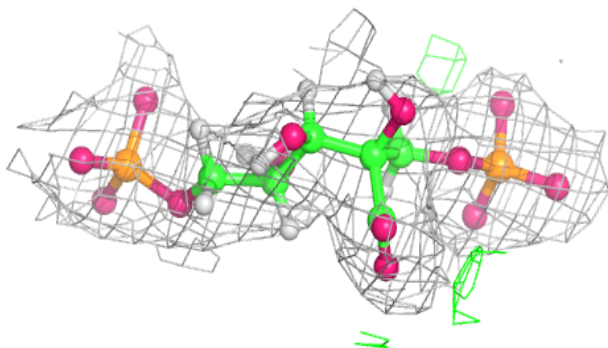
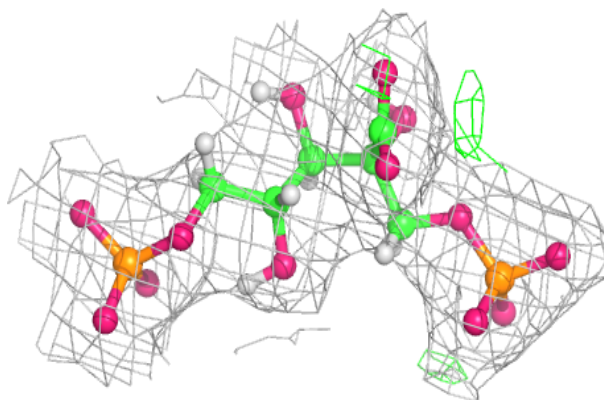


**Electron density around CAP L 500:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.