



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:02 PM UTC

PDB ID : 5HAT / pdb_00005hat
Title : Structure function studies of R. palustris RubisCO (S59F/M331A mutant; CABP-bound)
Authors : Arbing, M.A.; Leong, J.G.; Cascio, D.; Varaljay, V.A.; Satagopan, S.; North, J.A.; Tabita, F.R.
Deposited on : 2015-12-30
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

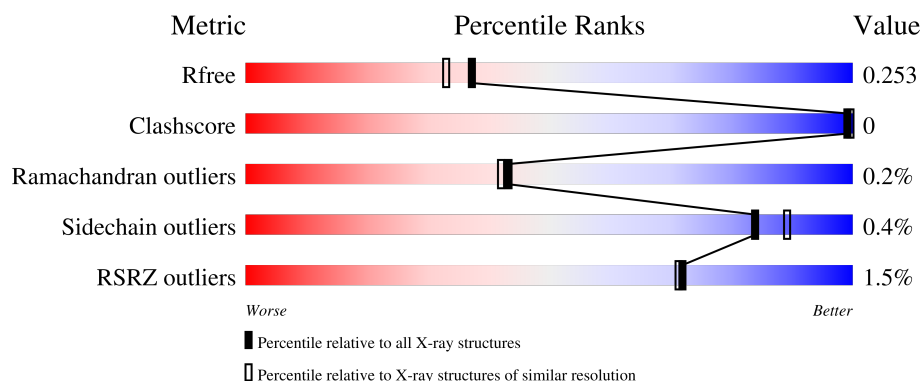
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	481	% 92% • 5%
1	B	481	2% 93% • 5%
1	C	481	2% 92% • 5%
1	D	481	% 92% • 5%

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Mol	Chain	Length	Quality of chain
1	E	481	% 93% • 5%
1	F	481	% 92% • 5%
1	G	481	% 92% • 5%
1	H	481	% 94% • 5%
1	I	481	2% 93% • 5%
1	J	481	2% 93% • 5%
1	K	481	2% 92% • 5%
1	L	481	2% 93% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 85482 atoms, of which 40451 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
			6867	2233	3357	607	652	18			
1	B	455	Total	C	H	N	O	S	0	0	0
			6868	2233	3358	607	652	18			
1	C	455	Total	C	H	N	O	S	0	0	0
			6855	2230	3352	607	648	18			
1	D	455	Total	C	H	N	O	S	0	0	0
			6884	2236	3367	609	654	18			
1	E	457	Total	C	H	N	O	S	0	0	0
			6911	2245	3381	611	656	18			
1	F	456	Total	C	H	N	O	S	0	0	0
			6873	2236	3359	608	652	18			
1	G	456	Total	C	H	N	O	S	0	0	0
			6876	2239	3358	608	653	18			
1	H	456	Total	C	H	N	O	S	0	0	0
			6897	2241	3375	609	654	18			
1	I	455	Total	C	H	N	O	S	0	0	0
			6862	2231	3358	607	648	18			
1	J	455	Total	C	H	N	O	S	0	0	0
			6871	2233	3361	609	650	18			
1	K	455	Total	C	H	N	O	S	0	0	0
			6836	2227	3336	603	652	18			
1	L	457	Total	C	H	N	O	S	0	0	0
			6906	2245	3381	610	652	18			

There are 264 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
A	331	ALA	MET	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
B	331	ALA	MET	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP Q6N0W9
C	-15	HIS	-	expression tag	UNP Q6N0W9
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
C	331	ALA	MET	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
D	331	ALA	MET	engineered mutation	UNP Q6N0W9
E	-19	MET	-	initiating methionine	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
E	331	ALA	MET	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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	331	ALA	MET	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
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
G	331	ALA	MET	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

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	HIS	-	expression tag	UNP Q6N0W9
H	59	PHE	SER	engineered mutation	UNP Q6N0W9
H	331	ALA	MET	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
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	59	PHE	SER	engineered mutation	UNP Q6N0W9
I	331	ALA	MET	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

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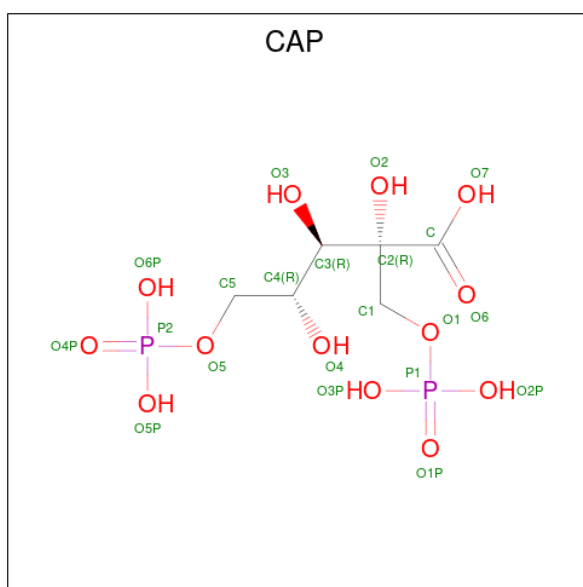
Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	expression tag	UNP Q6N0W9
J	-1	SER	-	expression tag	UNP Q6N0W9
J	0	HIS	-	expression tag	UNP Q6N0W9
J	59	PHE	SER	engineered mutation	UNP Q6N0W9
J	331	ALA	MET	engineered mutation	UNP Q6N0W9
K	-19	MET	-	initiating methionine	UNP Q6N0W9
K	-18	GLY	-	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
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
K	331	ALA	MET	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
L	331	ALA	MET	engineered mutation	UNP Q6N0W9

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: MG) (formula: Mg).

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

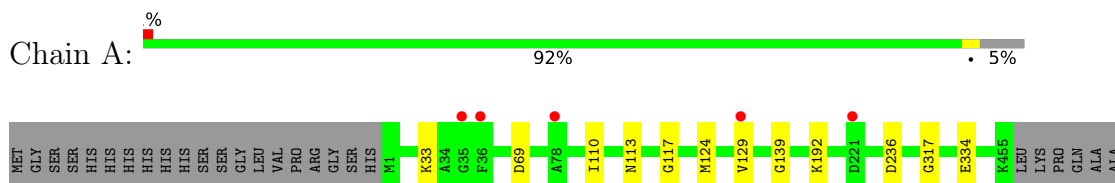
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total 222	O 222	0	0
4	B	185	Total 185	O 185	0	0
4	C	179	Total 179	O 179	0	0
4	D	228	Total 228	O 228	0	0
4	E	223	Total 223	O 223	0	0
4	F	249	Total 249	O 249	0	0
4	G	264	Total 264	O 264	0	0
4	H	229	Total 229	O 229	0	0
4	I	228	Total 228	O 228	0	0
4	J	201	Total 201	O 201	0	0
4	K	179	Total 179	O 179	0	0
4	L	217	Total 217	O 217	0	0

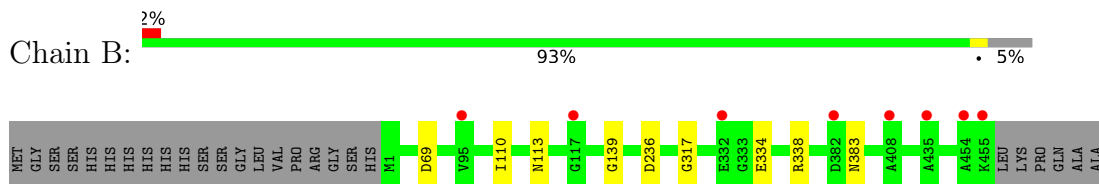
3 Residue-property plots [i](#)

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.

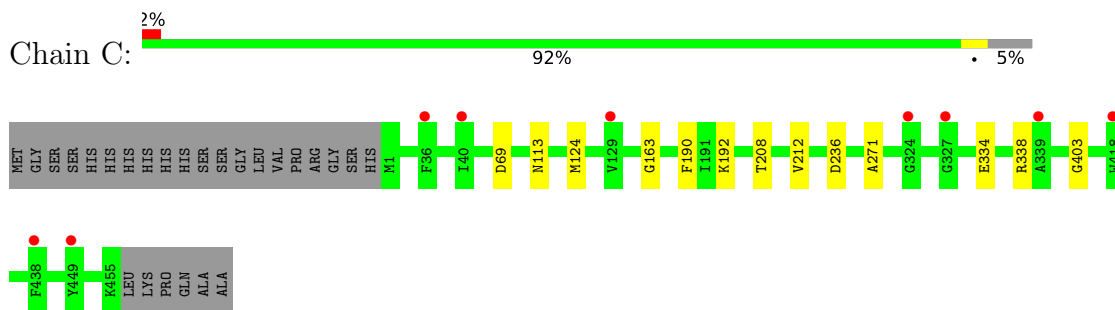
- Molecule 1: Ribulose biphosphate carboxylase



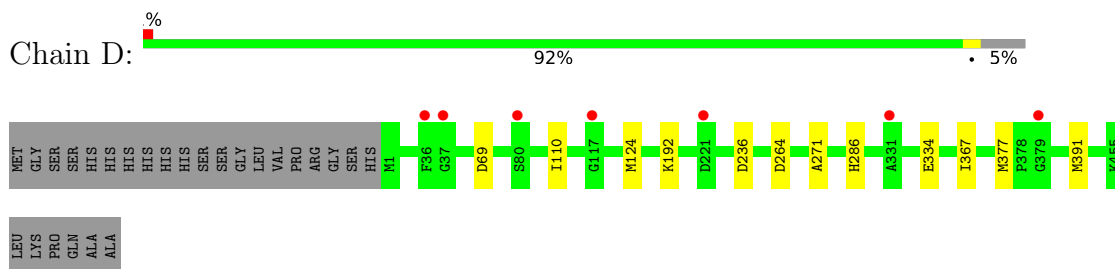
- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase

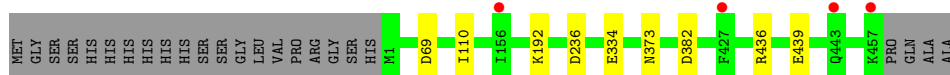


- Molecule 1: Ribulose biphosphate carboxylase

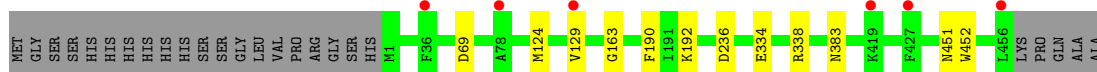
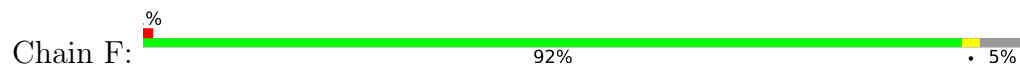


- Molecule 1: Ribulose biphosphate carboxylase

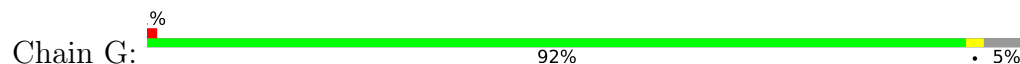




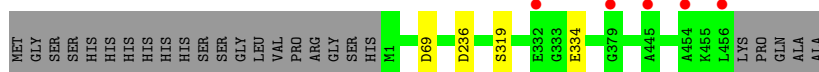
- Molecule 1: Ribulose biphosphate carboxylase



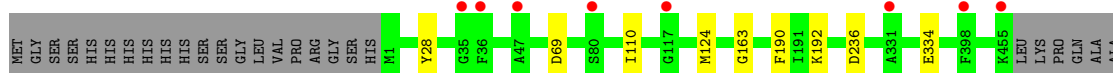
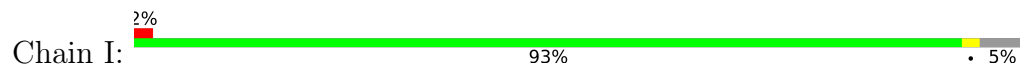
- Molecule 1: Ribulose biphosphate carboxylase



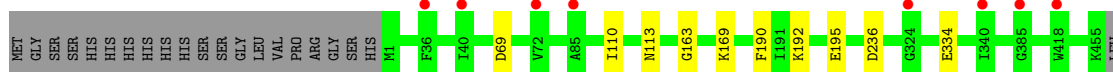
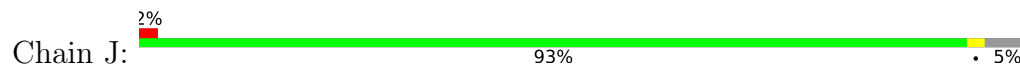
- Molecule 1: Ribulose biphosphate carboxylase



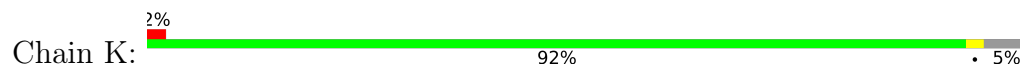
- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase



ALA
ALA

● Molecule 1: Ribulose biphosphate carboxylase



ALA
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.14Å 111.03Å 167.26Å 90.03° 101.69° 105.05°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (20.00-2.00) 91.0 (20.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.213 , 0.249 0.216 , 0.253	Depositor DCC
R_{free} test set	31836 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	85482	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 64.43 % 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 8.2929e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.87	1/3587 (0.0%)	1.07	4/4856 (0.1%)
1	B	0.83	0/3587	1.06	3/4856 (0.1%)
1	C	0.85	1/3580 (0.0%)	1.06	5/4847 (0.1%)
1	D	0.87	2/3594 (0.1%)	1.08	3/4865 (0.1%)
1	E	0.84	0/3607	1.07	4/4883 (0.1%)
1	F	0.88	1/3591 (0.0%)	1.09	5/4863 (0.1%)
1	G	0.88	1/3595 (0.0%)	1.08	3/4867 (0.1%)
1	H	0.86	0/3599	1.06	3/4872 (0.1%)
1	I	0.87	2/3581 (0.1%)	1.06	2/4848 (0.0%)
1	J	0.83	0/3587	1.05	3/4856 (0.1%)
1	K	0.83	0/3577	1.05	3/4845 (0.1%)
1	L	0.84	0/3602	1.07	3/4875 (0.1%)
All	All	0.86	8/43087 (0.0%)	1.07	41/58333 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	124	MET	SD-CE	-9.04	1.56	1.79
1	A	124	MET	SD-CE	-6.74	1.62	1.79
1	C	124	MET	SD-CE	-6.17	1.64	1.79
1	I	124	MET	SD-CE	-5.39	1.66	1.79
1	I	28	TYR	CA-C	-5.36	1.46	1.52
1	D	124	MET	SD-CE	-5.35	1.66	1.79
1	D	367	ILE	CG1-CD1	5.17	1.72	1.51
1	G	124	MET	SD-CE	-5.10	1.66	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	236	ASP	CA-CB-CG	7.89	120.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	451	ASN	CA-CB-CG	7.21	119.81	112.60
1	F	236	ASP	CA-CB-CG	6.60	119.20	112.60
1	K	236	ASP	CA-CB-CG	6.39	118.99	112.60
1	E	236	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	236	ASP	CA-CB-CG	6.18	118.78	112.60
1	L	236	ASP	CA-CB-CG	6.17	118.77	112.60
1	F	69	ASP	CA-CB-CG	6.16	118.76	112.60
1	B	69	ASP	CA-CB-CG	6.12	118.72	112.60
1	G	69	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	236	ASP	CA-CB-CG	5.99	118.58	112.60
1	D	69	ASP	CA-CB-CG	5.93	118.53	112.60
1	C	236	ASP	CA-CB-CG	5.92	118.52	112.60
1	G	236	ASP	CA-CB-CG	5.81	118.41	112.60
1	I	69	ASP	CA-CB-CG	5.68	118.28	112.60
1	J	69	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	236	ASP	CA-CB-CG	5.63	118.23	112.60
1	D	286	HIS	CA-CB-CG	5.63	119.43	113.80
1	K	69	ASP	CA-CB-CG	5.62	118.22	112.60
1	H	69	ASP	CA-CB-CG	5.56	118.16	112.60
1	E	69	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	69	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	129	VAL	CB-CA-C	5.34	116.45	110.52
1	L	69	ASP	CA-CB-CG	5.33	117.93	112.60
1	I	236	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	69	ASP	CA-CB-CG	5.31	117.91	112.60
1	E	373	ASN	CA-CB-CG	5.30	117.90	112.60
1	H	319	SER	N-CA-C	-5.28	105.57	112.23
1	J	113	ASN	CA-CB-CG	5.27	117.87	112.60
1	F	452	TRP	N-CA-C	5.22	117.37	111.11
1	A	113	ASN	CA-CB-CG	5.18	117.78	112.60
1	B	113	ASN	CA-CB-CG	5.18	117.78	112.60
1	F	129	VAL	CB-CA-C	5.15	116.23	110.52
1	C	403	GLY	CA-C-N	5.11	125.65	119.98
1	C	403	GLY	C-N-CA	5.11	125.65	119.98
1	J	236	ASP	CA-CB-CG	5.10	117.70	112.60
1	G	113	ASN	CA-CB-CG	5.07	117.67	112.60
1	L	450	PRO	N-CA-C	5.06	122.90	112.47
1	E	382	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	113	ASN	CA-CB-CG	5.03	117.62	112.60
1	K	193	ASN	CA-CB-CG	5.02	117.62	112.60

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	3510	3357	3369	2	0
1	B	3510	3358	3369	2	0
1	C	3503	3352	3363	4	0
1	D	3517	3367	3379	2	0
1	E	3530	3381	3392	1	0
1	F	3514	3359	3371	2	0
1	G	3518	3358	3380	2	0
1	H	3522	3375	3386	0	0
1	I	3504	3358	3369	1	0
1	J	3510	3361	3373	2	0
1	K	3500	3336	3347	2	0
1	L	3525	3381	3393	3	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	8	0	0
2	F	21	9	8	0	0
2	G	21	9	8	0	0
2	H	21	9	8	0	0
2	I	21	9	7	0	0
2	J	21	9	7	0	0
2	K	21	9	8	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	222	0	0	0	0
4	B	185	0	0	0	0
4	C	179	0	0	0	0
4	D	228	0	0	0	0
4	E	223	0	0	0	0
4	F	249	0	0	0	0
4	G	264	0	0	0	0
4	H	229	0	0	0	0
4	I	228	0	0	0	0
4	J	201	0	0	0	0
4	K	179	0	0	0	0
4	L	217	0	0	0	0
All	All	45031	40451	40581	21	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.

All (21) 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:F:338:ARG:NH2	1:F:383:ASN:OD1	2.25	0.67
1:B:338:ARG:NH1	1:B:383:ASN:OD1	2.43	0.52
1:J:169:LYS:NZ	1:J:195:GLU:OE2	2.41	0.49
1:E:436:ARG:NH1	1:E:439:GLU:OE1	2.48	0.44
1:D:377:MET:HG2	1:D:391:MET:SD	2.58	0.44
1:A:139:GLY:C	1:A:317:GLY:HA2	2.43	0.43
1:L:139:GLY:C	1:L:317:GLY:HA2	2.44	0.43
1:G:208:THR:O	1:G:212:VAL:HG23	2.20	0.42
1:B:139:GLY:C	1:B:317:GLY:HA2	2.45	0.42
1:K:436:ARG:NH1	1:K:439:GLU:OE1	2.50	0.42
1:L:163:GLY:HA2	1:L:190:PHE:O	2.20	0.42
1:A:33:LYS:HD2	1:A:117:GLY:O	2.21	0.41
1:L:389:LEU:C	1:L:389:LEU:HD12	2.45	0.41
1:C:163:GLY:HA2	1:C:190:PHE:O	2.21	0.41
1:F:163:GLY:HA2	1:F:190:PHE:O	2.21	0.41
1:G:163:GLY:HA2	1:G:190:PHE:O	2.21	0.41
1:I:163:GLY:HA2	1:I:190:PHE:O	2.21	0.41
1:C:271:ALA:HB3	1:D:271:ALA:HB3	2.03	0.41
1:J:163:GLY:HA2	1:J:190:PHE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:THR:O	1:C:212:VAL:HG23	2.21	0.40
1:C:338:ARG:NH2	1:K:446:ASP:OD2	2.54	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	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	43	42
1	B	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	43	42
1	C	452/481 (94%)	440 (97%)	12 (3%)	0	100	100
1	D	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	43	42
1	E	454/481 (94%)	441 (97%)	12 (3%)	1 (0%)	43	42
1	F	453/481 (94%)	442 (98%)	11 (2%)	0	100	100
1	G	453/481 (94%)	441 (97%)	11 (2%)	1 (0%)	43	42
1	H	453/481 (94%)	441 (97%)	12 (3%)	0	100	100
1	I	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	43	42
1	J	452/481 (94%)	438 (97%)	13 (3%)	1 (0%)	43	42
1	K	452/481 (94%)	441 (98%)	10 (2%)	1 (0%)	43	42
1	L	454/481 (94%)	441 (97%)	12 (3%)	1 (0%)	43	42
All	All	5431/5772 (94%)	5285 (97%)	137 (2%)	9 (0%)	43	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ILE
1	D	110	ILE

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Mol	Chain	Res	Type
1	L	110	ILE
1	B	110	ILE
1	G	110	ILE
1	I	110	ILE
1	K	110	ILE
1	E	110	ILE
1	J	110	ILE

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	347/371 (94%)	346 (100%)	1 (0%)	86	91
1	B	347/371 (94%)	346 (100%)	1 (0%)	86	91
1	C	345/371 (93%)	344 (100%)	1 (0%)	86	91
1	D	349/371 (94%)	347 (99%)	2 (1%)	78	85
1	E	350/371 (94%)	349 (100%)	1 (0%)	86	91
1	F	347/371 (94%)	346 (100%)	1 (0%)	86	91
1	G	348/371 (94%)	346 (99%)	2 (1%)	78	85
1	H	349/371 (94%)	348 (100%)	1 (0%)	86	91
1	I	346/371 (93%)	345 (100%)	1 (0%)	86	91
1	J	347/371 (94%)	346 (100%)	1 (0%)	86	91
1	K	345/371 (93%)	342 (99%)	3 (1%)	70	78
1	L	348/371 (94%)	347 (100%)	1 (0%)	86	91
All	All	4168/4452 (94%)	4152 (100%)	16 (0%)	84	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	GLU
1	B	334	GLU
1	C	334	GLU

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Mol	Chain	Res	Type
1	D	264	ASP
1	D	334	GLU
1	E	334	GLU
1	F	334	GLU
1	G	161	ILE
1	G	334	GLU
1	H	334	GLU
1	I	334	GLU
1	J	334	GLU
1	K	334	GLU
1	K	365	THR
1	K	455	LYS
1	L	334	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	383	ASN
1	D	157	ASN
1	E	157	ASN
1	F	157	ASN
1	F	316	GLN
1	G	175	GLN
1	H	383	ASN
1	J	157	ASN
1	K	23	HIS
1	L	157	ASN
1	L	383	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	D	192	1,3	10,11,12	1.77	1 (10%)	6,12,14	1.40	1 (16%)
1	KCX	K	192	1,3	10,11,12	3.12	2 (20%)	6,12,14	2.29	1 (16%)
1	KCX	C	192	1,3	10,11,12	1.45	2 (20%)	6,12,14	0.49	0
1	KCX	J	192	1,3	10,11,12	1.97	2 (20%)	6,12,14	1.25	1 (16%)
1	KCX	B	192	1,3	10,11,12	1.01	0	6,12,14	0.46	0
1	KCX	G	192	1,3	10,11,12	2.30	1 (10%)	6,12,14	1.37	1 (16%)
1	KCX	A	192	1,3	10,11,12	3.06	2 (20%)	6,12,14	2.00	2 (33%)
1	KCX	I	192	1,3	10,11,12	1.39	1 (10%)	6,12,14	0.58	0
1	KCX	L	192	1,3	10,11,12	1.27	1 (10%)	6,12,14	0.53	0
1	KCX	F	192	1,3	10,11,12	1.25	1 (10%)	6,12,14	0.43	0
1	KCX	E	192	1,3	10,11,12	2.44	2 (20%)	6,12,14	1.28	1 (16%)
1	KCX	H	192	1,3	10,11,12	1.24	0	6,12,14	0.43	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	D	192	1,3	-	0/9/10/12	-
1	KCX	K	192	1,3	-	0/9/10/12	-
1	KCX	C	192	1,3	-	0/9/10/12	-
1	KCX	J	192	1,3	-	0/9/10/12	-
1	KCX	B	192	1,3	-	0/9/10/12	-
1	KCX	G	192	1,3	-	0/9/10/12	-
1	KCX	A	192	1,3	-	2/9/10/12	-
1	KCX	I	192	1,3	-	0/9/10/12	-
1	KCX	L	192	1,3	-	0/9/10/12	-
1	KCX	F	192	1,3	-	0/9/10/12	-
1	KCX	E	192	1,3	-	0/9/10/12	-
1	KCX	H	192	1,3	-	0/9/10/12	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	192	KCX	OQ1-CX	9.27	1.38	1.21
1	A	192	KCX	OQ1-CX	8.45	1.37	1.21
1	G	192	KCX	OQ1-CX	6.51	1.33	1.21
1	E	192	KCX	OQ1-CX	6.34	1.33	1.21
1	J	192	KCX	OQ1-CX	4.42	1.29	1.21
1	D	192	KCX	OQ1-CX	4.39	1.29	1.21
1	A	192	KCX	CE-NZ	3.55	1.54	1.46
1	C	192	KCX	CE-NZ	3.06	1.53	1.46
1	J	192	KCX	CE-NZ	2.79	1.52	1.46
1	F	192	KCX	CE-NZ	2.78	1.52	1.46
1	E	192	KCX	CB-CA	2.62	1.57	1.53
1	I	192	KCX	CB-CA	2.60	1.57	1.53
1	L	192	KCX	CE-NZ	2.51	1.51	1.46
1	K	192	KCX	CE-NZ	2.35	1.51	1.46
1	C	192	KCX	CG-CB	2.04	1.60	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	192	KCX	OQ1-CX-NZ	-5.36	116.78	124.92
1	D	192	KCX	OQ1-CX-NZ	-3.23	120.01	124.92
1	G	192	KCX	OQ1-CX-NZ	-3.22	120.02	124.92
1	A	192	KCX	CD-CE-NZ	3.18	121.11	112.20
1	A	192	KCX	OQ1-CX-NZ	-3.16	120.13	124.92
1	E	192	KCX	OQ1-CX-NZ	-2.94	120.46	124.92
1	J	192	KCX	OQ1-CX-NZ	-2.90	120.52	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	192	KCX	CE-CD-CG-CB
1	A	192	KCX	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CAP	E	500	3	18,20,20	1.19	1 (5%)	23,31,31	1.69	8 (34%)
2	CAP	D	500	3	18,20,20	1.15	1 (5%)	23,31,31	1.85	5 (21%)
2	CAP	I	500	3	18,20,20	1.11	1 (5%)	23,31,31	1.84	7 (30%)
2	CAP	G	500	3	18,20,20	1.17	2 (11%)	23,31,31	1.72	6 (26%)
2	CAP	K	500	3	18,20,20	1.11	0	23,31,31	1.66	7 (30%)
2	CAP	L	500	3	18,20,20	1.14	0	23,31,31	1.64	7 (30%)
2	CAP	C	500	3	18,20,20	1.10	0	23,31,31	1.77	7 (30%)
2	CAP	A	500	3	18,20,20	0.97	0	23,31,31	1.76	6 (26%)
2	CAP	B	500	3	18,20,20	1.18	2 (11%)	23,31,31	1.85	6 (26%)
2	CAP	H	500	3	18,20,20	1.33	1 (5%)	23,31,31	1.81	7 (30%)
2	CAP	F	500	3	18,20,20	1.15	0	23,31,31	1.57	6 (26%)
2	CAP	J	500	3	18,20,20	1.19	1 (5%)	23,31,31	1.68	8 (34%)

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	-	7/29/29/29	-
2	CAP	D	500	3	-	9/29/29/29	-
2	CAP	I	500	3	-	7/29/29/29	-
2	CAP	G	500	3	-	7/29/29/29	-
2	CAP	K	500	3	-	8/29/29/29	-
2	CAP	L	500	3	-	7/29/29/29	-
2	CAP	C	500	3	-	8/29/29/29	-
2	CAP	A	500	3	-	8/29/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	B	500	3	-	7/29/29/29	-
2	CAP	H	500	3	-	8/29/29/29	-
2	CAP	F	500	3	-	8/29/29/29	-
2	CAP	J	500	3	-	8/29/29/29	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	CAP	C2-C	-3.00	1.50	1.53
2	B	500	CAP	C4-C3	-2.49	1.51	1.54
2	J	500	CAP	C2-C	-2.41	1.51	1.53
2	G	500	CAP	C2-C	-2.37	1.51	1.53
2	G	500	CAP	C4-C3	-2.31	1.51	1.54
2	I	500	CAP	C4-C3	-2.24	1.51	1.54
2	B	500	CAP	P2-O6P	-2.07	1.47	1.54
2	E	500	CAP	C2-C	-2.03	1.51	1.53
2	D	500	CAP	P1-O3P	-2.01	1.47	1.54

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	CAP	O7-C-C2	4.98	122.41	114.06
2	I	500	CAP	O7-C-C2	4.51	121.61	114.06
2	H	500	CAP	O7-C-C2	4.45	121.51	114.06
2	A	500	CAP	O7-C-C2	4.26	121.19	114.06
2	G	500	CAP	O7-C-C2	4.03	120.81	114.06
2	C	500	CAP	O7-C-C2	4.01	120.77	114.06
2	D	500	CAP	O5-P2-O4P	3.68	116.38	106.44
2	D	500	CAP	O2P-P1-O1	3.67	116.23	106.67
2	D	500	CAP	O5P-P2-O5	3.46	115.69	106.67
2	L	500	CAP	O7-C-C2	3.18	119.38	114.06
2	E	500	CAP	O7-C-C2	3.08	119.22	114.06
2	J	500	CAP	O7-C-C2	2.98	119.05	114.06
2	I	500	CAP	O3P-P1-O1	2.98	114.43	106.67
2	A	500	CAP	O3P-P1-O1	2.96	114.39	106.67
2	C	500	CAP	O3P-P1-O1	2.90	114.23	106.67
2	B	500	CAP	O5-P2-O4P	2.86	114.17	106.44
2	K	500	CAP	O2P-P1-O1	2.86	114.12	106.67
2	F	500	CAP	O7-C-C2	2.85	118.82	114.06
2	J	500	CAP	O6P-P2-O5	2.83	114.05	106.67
2	I	500	CAP	O5P-P2-O5	2.82	114.03	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	CAP	O5-P2-O4P	2.81	114.03	106.44
2	I	500	CAP	O6P-P2-O5	2.80	113.98	106.67
2	F	500	CAP	O6P-P2-O5	2.78	113.91	106.67
2	L	500	CAP	O2P-P1-O1	2.77	113.88	106.67
2	K	500	CAP	O7-C-C2	2.77	118.69	114.06
2	G	500	CAP	O6P-P2-O5	2.73	113.80	106.67
2	G	500	CAP	O2P-P1-O1	2.73	113.78	106.67
2	E	500	CAP	O1-P1-O1P	2.72	113.79	106.44
2	C	500	CAP	O6P-P2-O5	2.71	113.74	106.67
2	H	500	CAP	O3P-P1-O1	2.71	113.72	106.67
2	L	500	CAP	O6P-P2-O5	2.68	113.65	106.67
2	K	500	CAP	O1-P1-O1P	2.68	113.67	106.44
2	J	500	CAP	O3P-P1-O1	2.67	113.62	106.67
2	J	500	CAP	O1-P1-O1P	2.64	113.58	106.44
2	F	500	CAP	O5P-P2-O5	2.63	113.52	106.67
2	J	500	CAP	O2P-P1-O1	2.61	113.48	106.67
2	D	500	CAP	O7-C-C2	2.58	118.38	114.06
2	E	500	CAP	O2P-P1-O1	2.58	113.39	106.67
2	A	500	CAP	O5P-P2-O5	2.57	113.36	106.67
2	F	500	CAP	O3P-P1-O1	2.57	113.36	106.67
2	B	500	CAP	O3P-P1-O1	2.56	113.35	106.67
2	H	500	CAP	O2P-P1-O1	2.55	113.31	106.67
2	A	500	CAP	O2P-P1-O1	2.55	113.31	106.67
2	H	500	CAP	O5P-P2-O5	2.54	113.28	106.67
2	C	500	CAP	O5-P2-O4P	2.52	113.26	106.44
2	B	500	CAP	O1-P1-O1P	2.51	113.21	106.44
2	B	500	CAP	O2P-P1-O1	2.49	113.16	106.67
2	L	500	CAP	O5P-P2-O5	2.49	113.16	106.67
2	L	500	CAP	O3P-P1-O1	2.49	113.15	106.67
2	J	500	CAP	O5P-P2-O5	2.47	113.11	106.67
2	K	500	CAP	O6P-P2-O5	2.46	113.09	106.67
2	H	500	CAP	O1-P1-O1P	2.46	113.10	106.44
2	A	500	CAP	O6P-P2-O5	2.45	113.07	106.67
2	E	500	CAP	O6P-P2-O5	2.45	113.07	106.67
2	F	500	CAP	O1-P1-O1P	2.43	113.02	106.44
2	K	500	CAP	O3P-P1-O1	2.43	113.02	106.67
2	G	500	CAP	O5-P2-O4P	2.42	112.98	106.44
2	E	500	CAP	O3P-P1-O1	2.40	112.92	106.67
2	C	500	CAP	O5P-P2-O5	2.38	112.88	106.67
2	C	500	CAP	O1-P1-O1P	2.37	112.85	106.44
2	I	500	CAP	O2P-P1-O1	2.37	112.85	106.67
2	I	500	CAP	O5-P2-O4P	2.36	112.82	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	CAP	O5P-P2-O5	2.36	112.81	106.67
2	K	500	CAP	O5P-P2-O5	2.34	112.77	106.67
2	G	500	CAP	O3P-P1-O1	2.31	112.69	106.67
2	L	500	CAP	O5-P2-O4P	2.31	112.67	106.44
2	D	500	CAP	O1-P1-O1P	2.29	112.64	106.44
2	H	500	CAP	O5-P2-O4P	2.27	112.59	106.44
2	G	500	CAP	O1-P1-O1P	2.27	112.58	106.44
2	C	500	CAP	O2P-P1-O1	2.26	112.56	106.67
2	F	500	CAP	O2P-P1-O1	2.25	112.55	106.67
2	A	500	CAP	O5-P2-O4P	2.22	112.45	106.44
2	L	500	CAP	O1-P1-O1P	2.18	112.32	106.44
2	K	500	CAP	O5-P2-O4P	2.16	112.27	106.44
2	H	500	CAP	O6P-P2-O5	2.14	112.26	106.67
2	J	500	CAP	O3P-P1-O1P	-2.14	102.48	110.83
2	I	500	CAP	O1-P1-O1P	2.13	112.19	106.44
2	E	500	CAP	O2P-P1-O1P	-2.09	102.70	110.83
2	J	500	CAP	O5-P2-O4P	2.07	112.04	106.44
2	B	500	CAP	O6P-P2-O5	2.07	112.06	106.67

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	CAP	O6-C-C2-O2
2	A	500	CAP	O3-C3-C4-O4
2	B	500	CAP	O6-C-C2-O2
2	B	500	CAP	O3-C3-C4-O4
2	C	500	CAP	O6-C-C2-O2
2	C	500	CAP	O3-C3-C4-O4
2	D	500	CAP	O6-C-C2-C3
2	D	500	CAP	O6-C-C2-O2
2	E	500	CAP	O6-C-C2-C3
2	E	500	CAP	O6-C-C2-O2
2	E	500	CAP	O7-C-C2-O2
2	E	500	CAP	O3-C3-C4-O4
2	F	500	CAP	O6-C-C2-C3
2	F	500	CAP	O6-C-C2-O2
2	F	500	CAP	O7-C-C2-O2
2	F	500	CAP	O3-C3-C4-O4
2	G	500	CAP	O6-C-C2-O2
2	G	500	CAP	O3-C3-C4-O4
2	H	500	CAP	O6-C-C2-O2

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Mol	Chain	Res	Type	Atoms
2	H	500	CAP	O3-C3-C4-O4
2	I	500	CAP	O6-C-C2-O2
2	I	500	CAP	O3-C3-C4-O4
2	J	500	CAP	O6-C-C2-C3
2	J	500	CAP	O6-C-C2-O2
2	J	500	CAP	O7-C-C2-O2
2	J	500	CAP	O3-C3-C4-O4
2	K	500	CAP	O6-C-C2-C3
2	K	500	CAP	O6-C-C2-O2
2	K	500	CAP	O7-C-C2-O2
2	K	500	CAP	O3-C3-C4-O4
2	L	500	CAP	O6-C-C2-C3
2	L	500	CAP	O6-C-C2-O2
2	L	500	CAP	O7-C-C2-O2
2	L	500	CAP	O3-C3-C4-O4
2	E	500	CAP	O6-C-C2-C1
2	E	500	CAP	O7-C-C2-C1
2	F	500	CAP	O6-C-C2-C1
2	J	500	CAP	O6-C-C2-C1
2	K	500	CAP	O6-C-C2-C1
2	K	500	CAP	O7-C-C2-C1
2	L	500	CAP	O6-C-C2-C1
2	L	500	CAP	O7-C-C2-C1
2	D	500	CAP	O7-C-C2-O2
2	D	500	CAP	O6-C-C2-C1
2	D	500	CAP	O7-C-C2-C1
2	F	500	CAP	O7-C-C2-C1
2	J	500	CAP	O7-C-C2-C1
2	D	500	CAP	O3-C3-C4-O4
2	A	500	CAP	O6-C-C2-C3
2	B	500	CAP	O6-C-C2-C3
2	C	500	CAP	O6-C-C2-C3
2	G	500	CAP	O6-C-C2-C3
2	I	500	CAP	O6-C-C2-C3
2	G	500	CAP	O7-C-C2-O2
2	A	500	CAP	O2-C2-C3-C4
2	B	500	CAP	O2-C2-C3-C4
2	C	500	CAP	O2-C2-C3-C4
2	D	500	CAP	O2-C2-C3-C4
2	E	500	CAP	O2-C2-C3-C4
2	F	500	CAP	O2-C2-C3-C4
2	G	500	CAP	O2-C2-C3-C4

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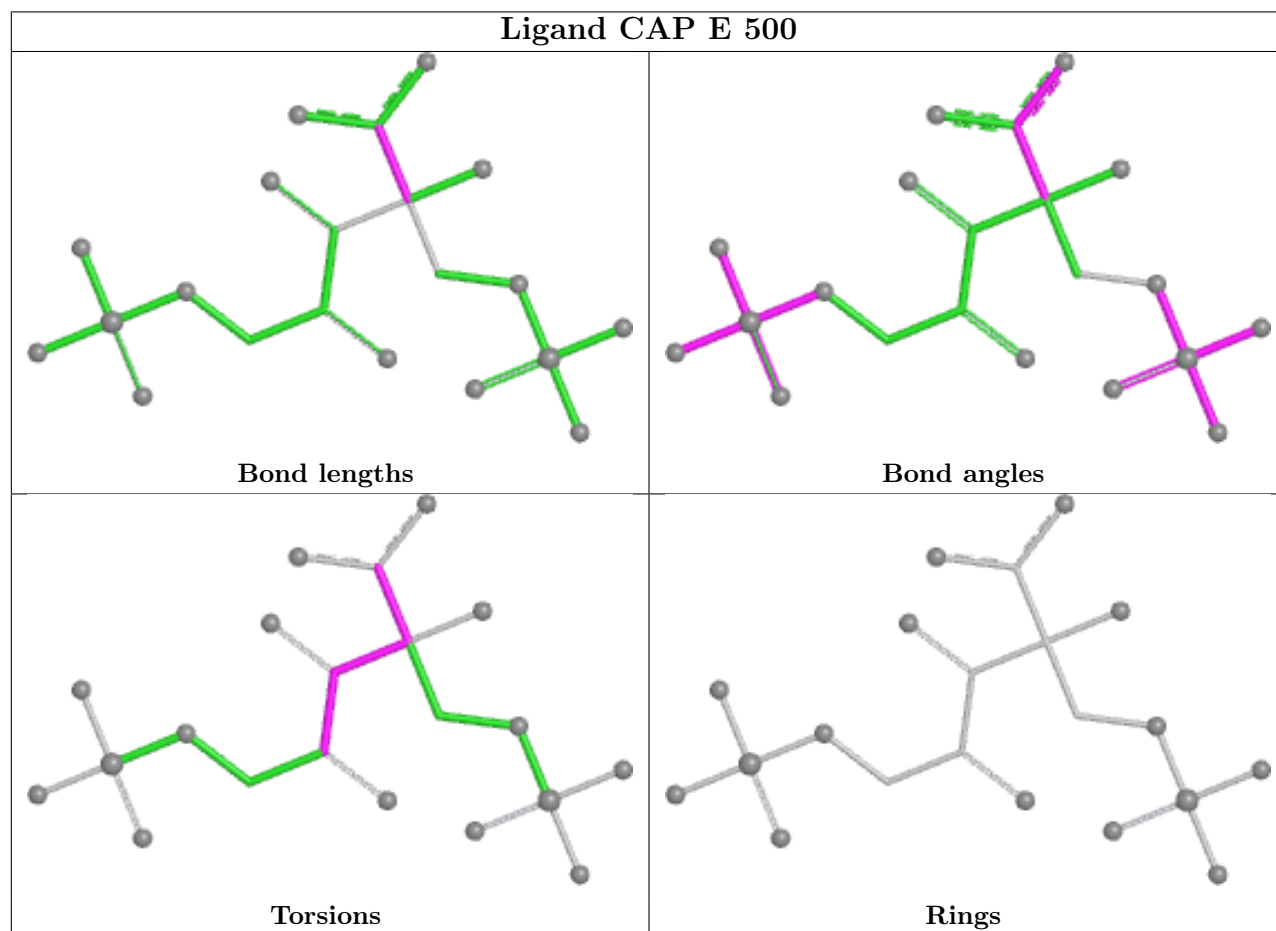
Mol	Chain	Res	Type	Atoms
2	H	500	CAP	O2-C2-C3-C4
2	I	500	CAP	O2-C2-C3-C4
2	J	500	CAP	O2-C2-C3-C4
2	K	500	CAP	O2-C2-C3-C4
2	L	500	CAP	O2-C2-C3-C4
2	H	500	CAP	O6-C-C2-C1
2	A	500	CAP	O7-C-C2-C3
2	B	500	CAP	O7-C-C2-C3
2	C	500	CAP	O7-C-C2-C3
2	D	500	CAP	O7-C-C2-C3
2	F	500	CAP	O7-C-C2-C3
2	G	500	CAP	O7-C-C2-C3
2	H	500	CAP	O7-C-C2-C3
2	I	500	CAP	O7-C-C2-C3
2	J	500	CAP	O7-C-C2-C3
2	K	500	CAP	O7-C-C2-C3
2	A	500	CAP	O7-C-C2-C1
2	B	500	CAP	O7-C-C2-C1
2	G	500	CAP	O7-C-C2-C1
2	H	500	CAP	O7-C-C2-C1
2	I	500	CAP	O7-C-C2-C1
2	A	500	CAP	O7-C-C2-O2
2	B	500	CAP	O7-C-C2-O2
2	C	500	CAP	O7-C-C2-O2
2	H	500	CAP	O7-C-C2-O2
2	I	500	CAP	O7-C-C2-O2
2	H	500	CAP	O6-C-C2-C3
2	D	500	CAP	C4-C5-O5-P2
2	A	500	CAP	O6-C-C2-C1
2	C	500	CAP	O7-C-C2-C1
2	C	500	CAP	O6-C-C2-C1

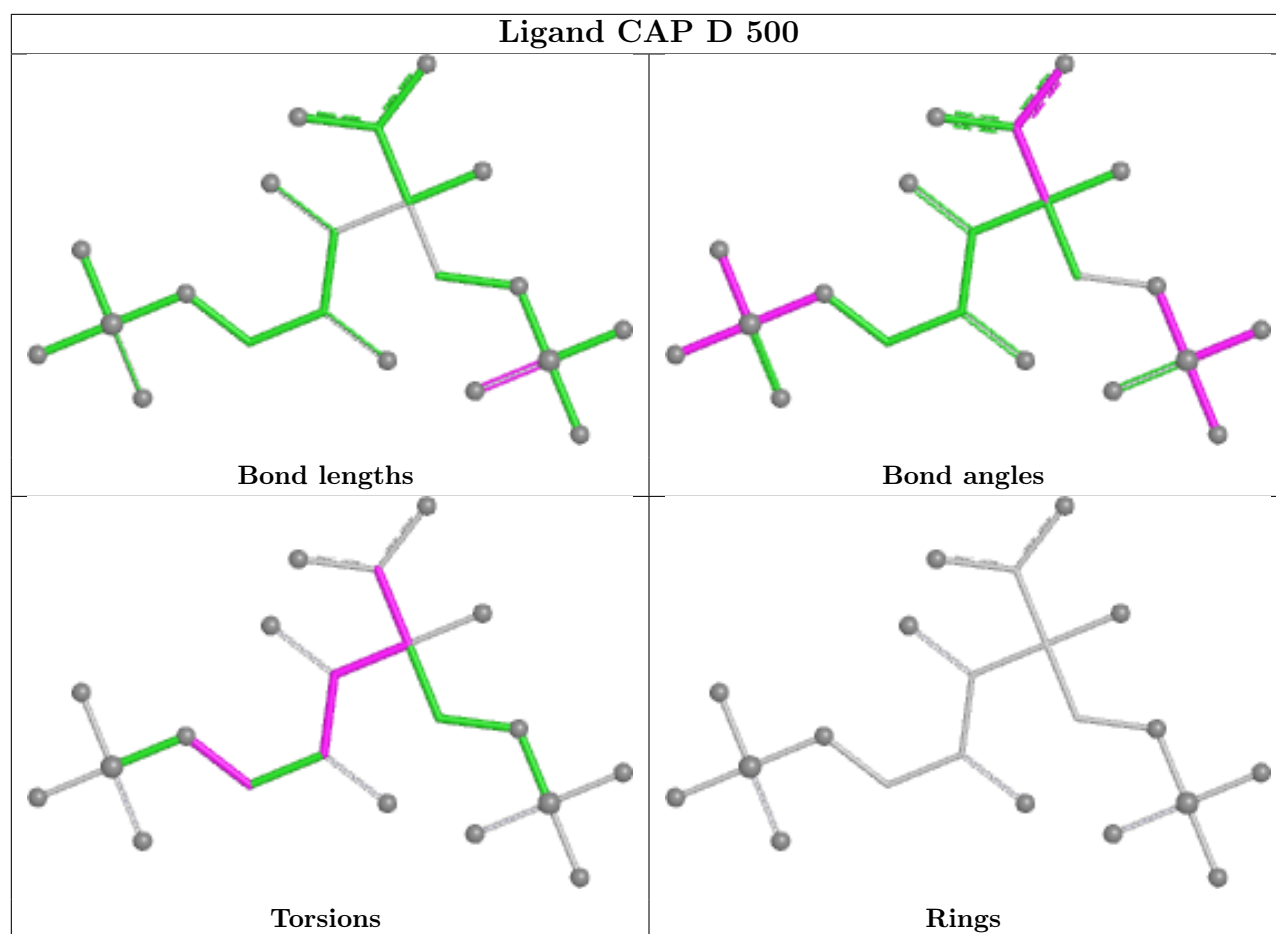
There are no ring outliers.

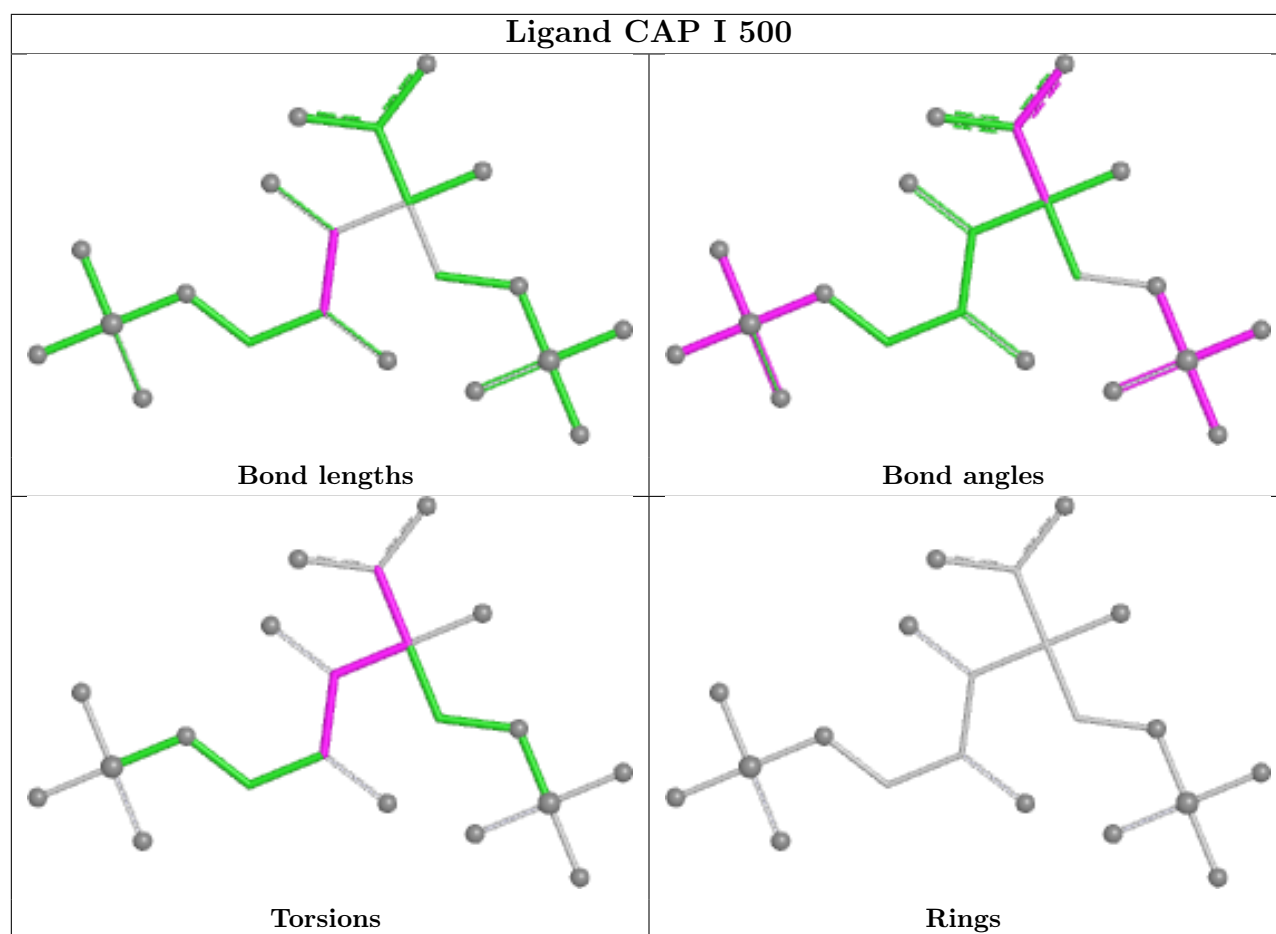
No monomer is involved in short contacts.

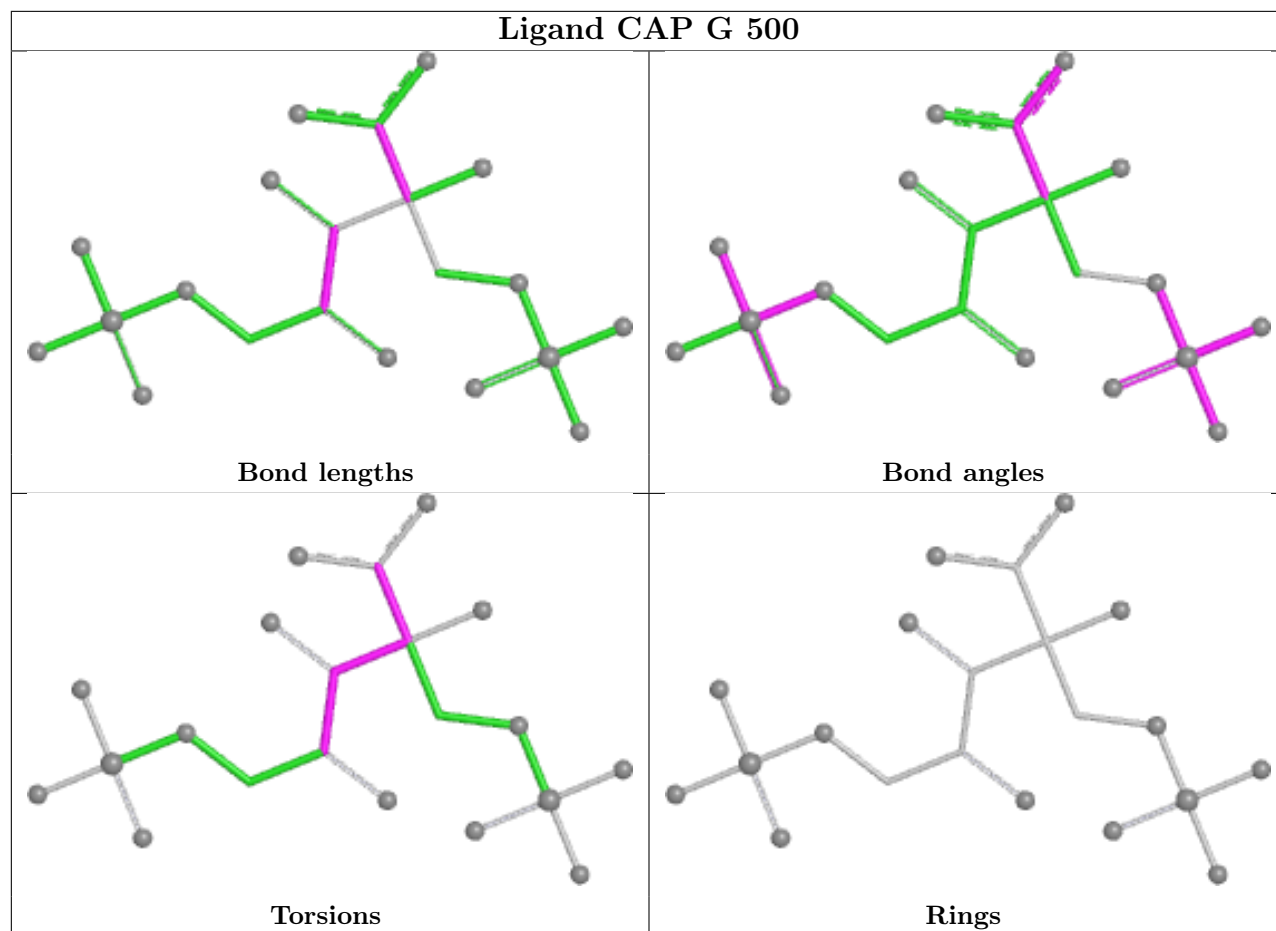
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

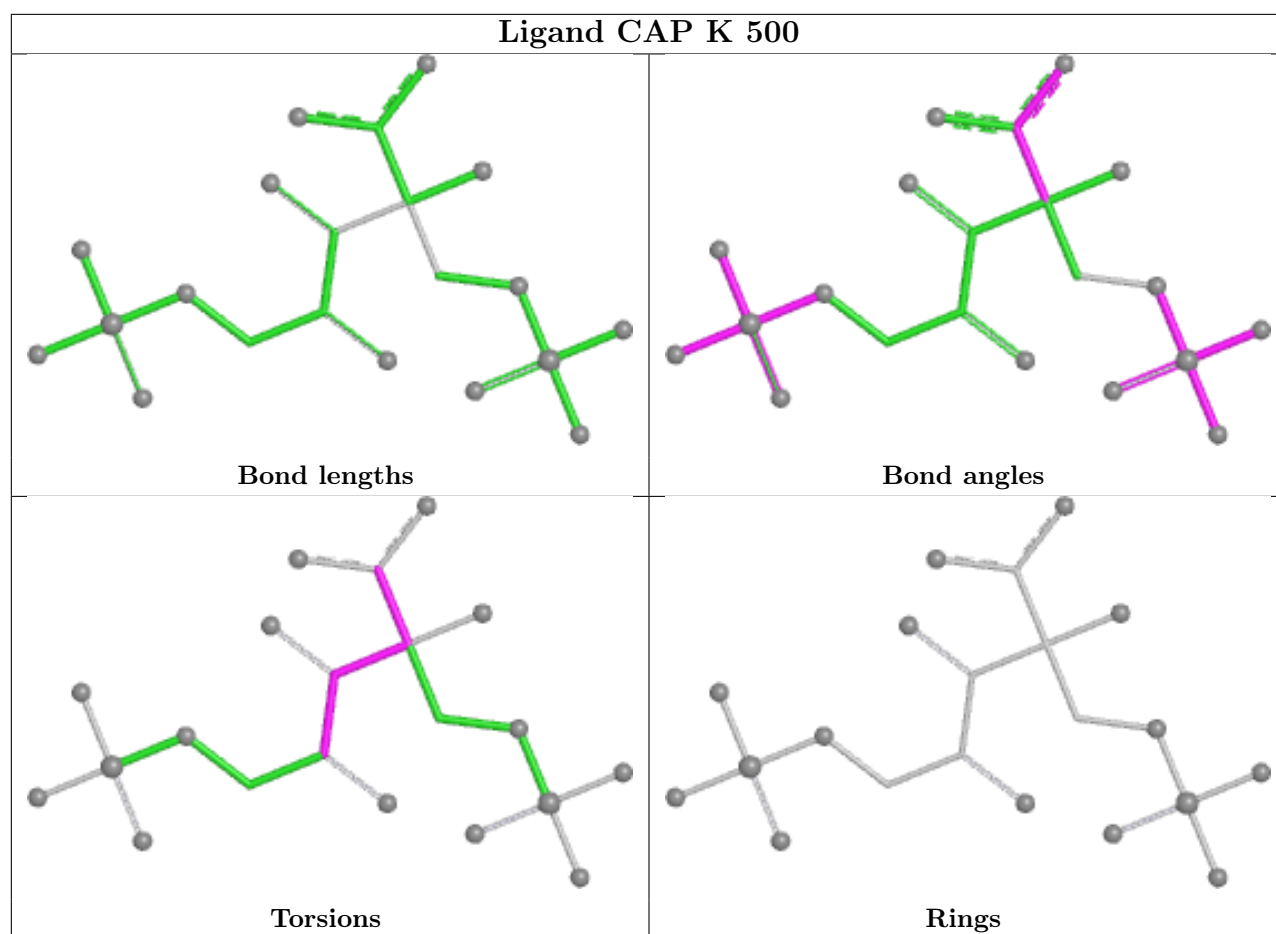
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

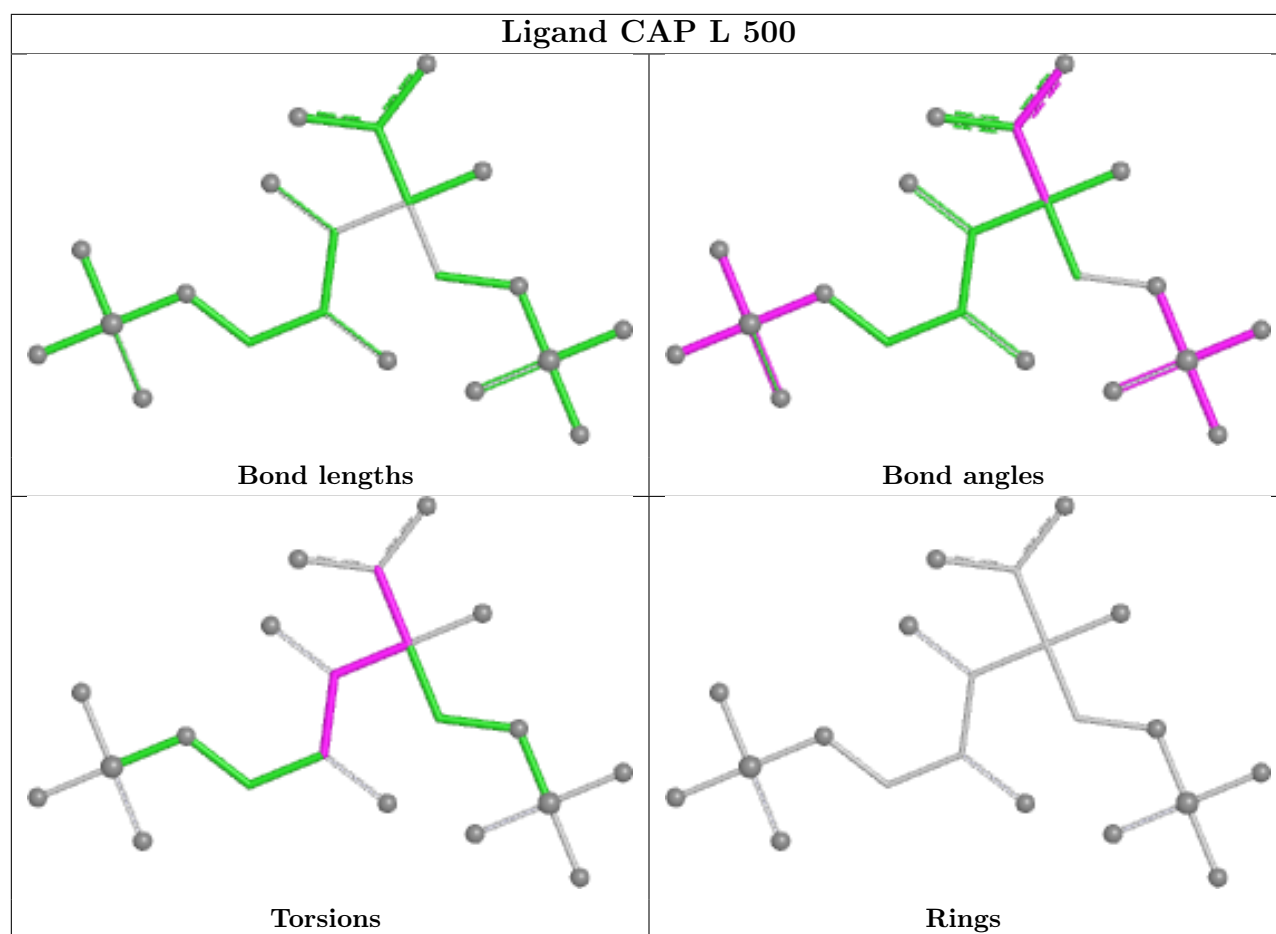


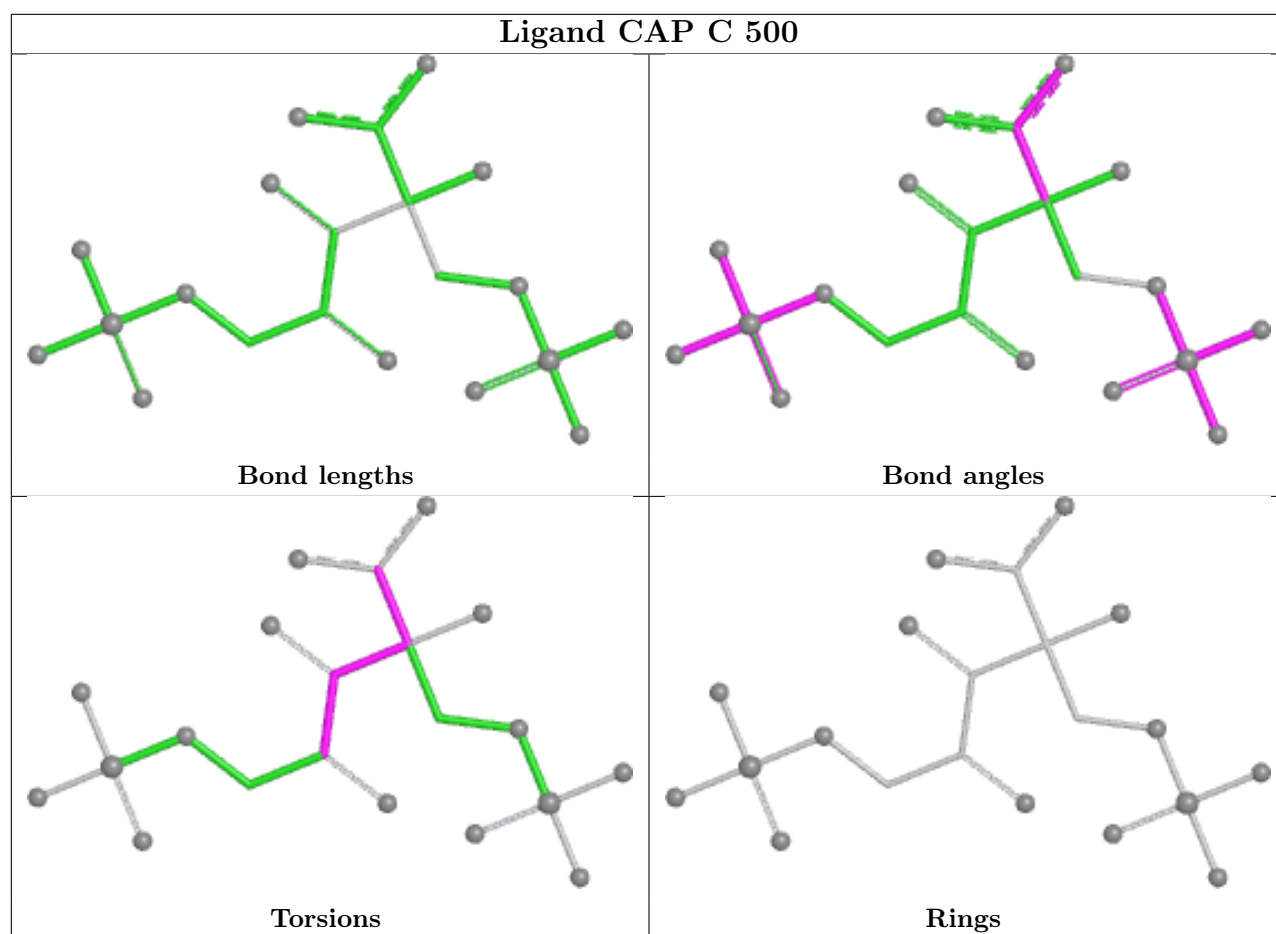


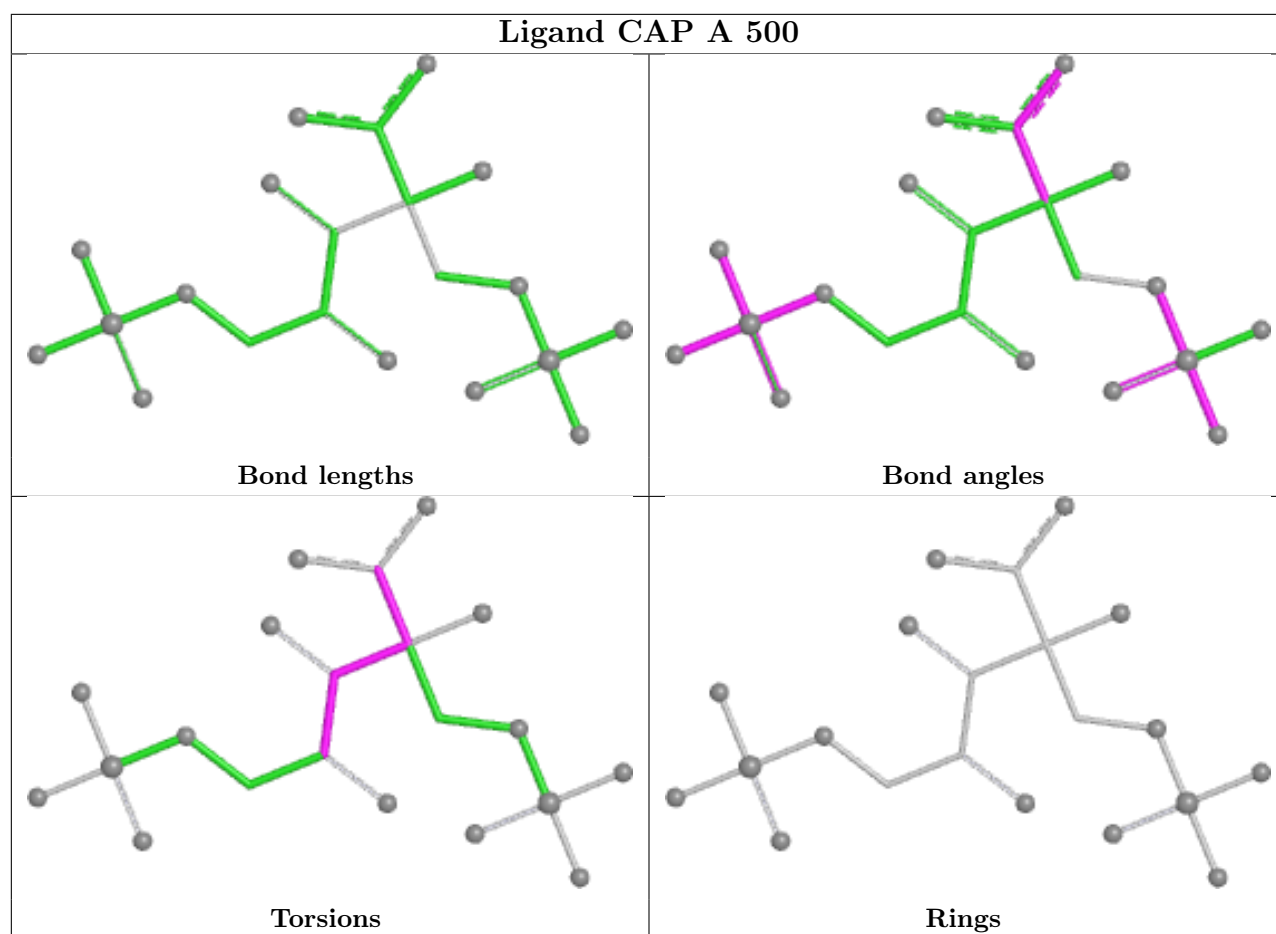


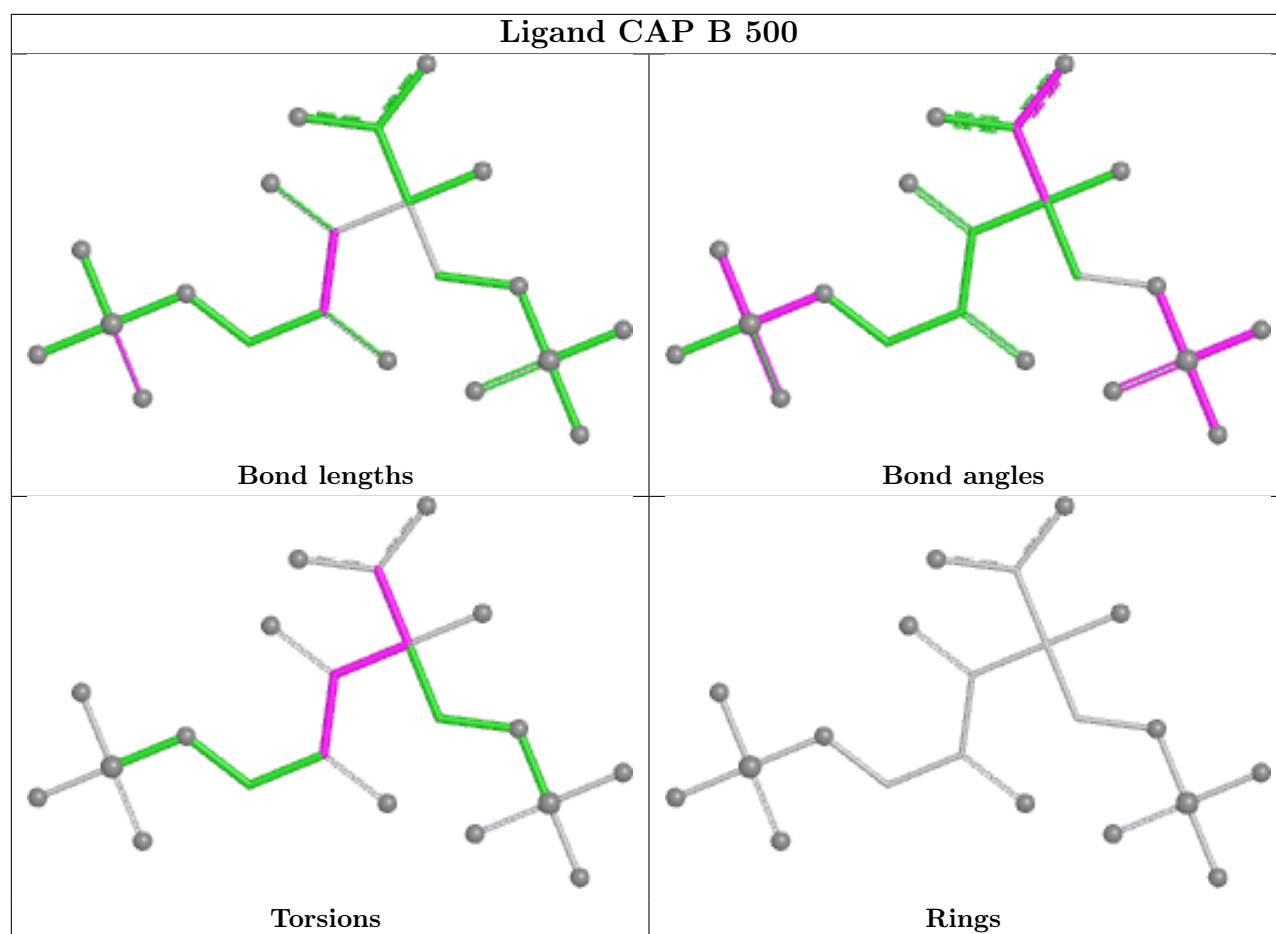


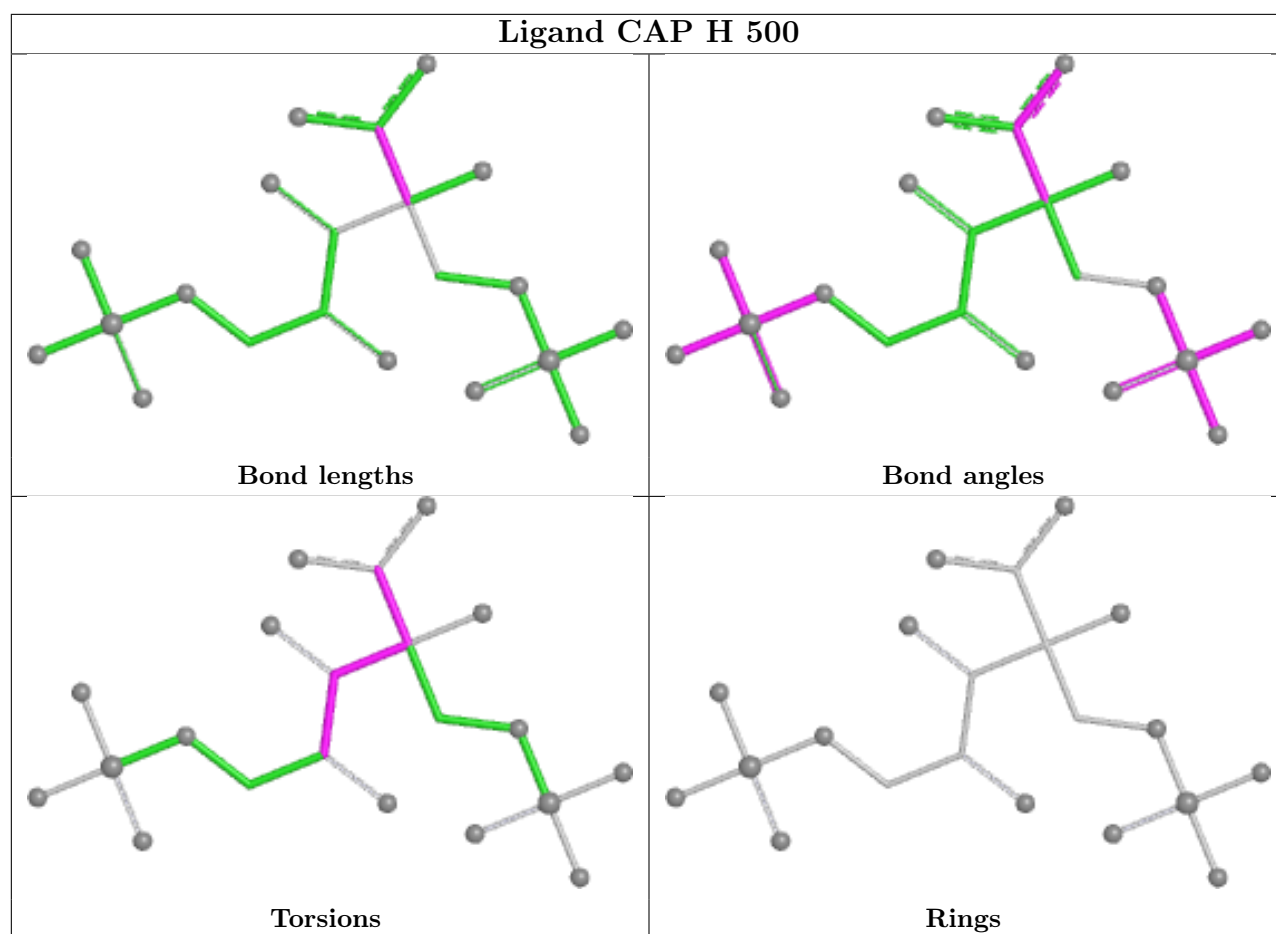


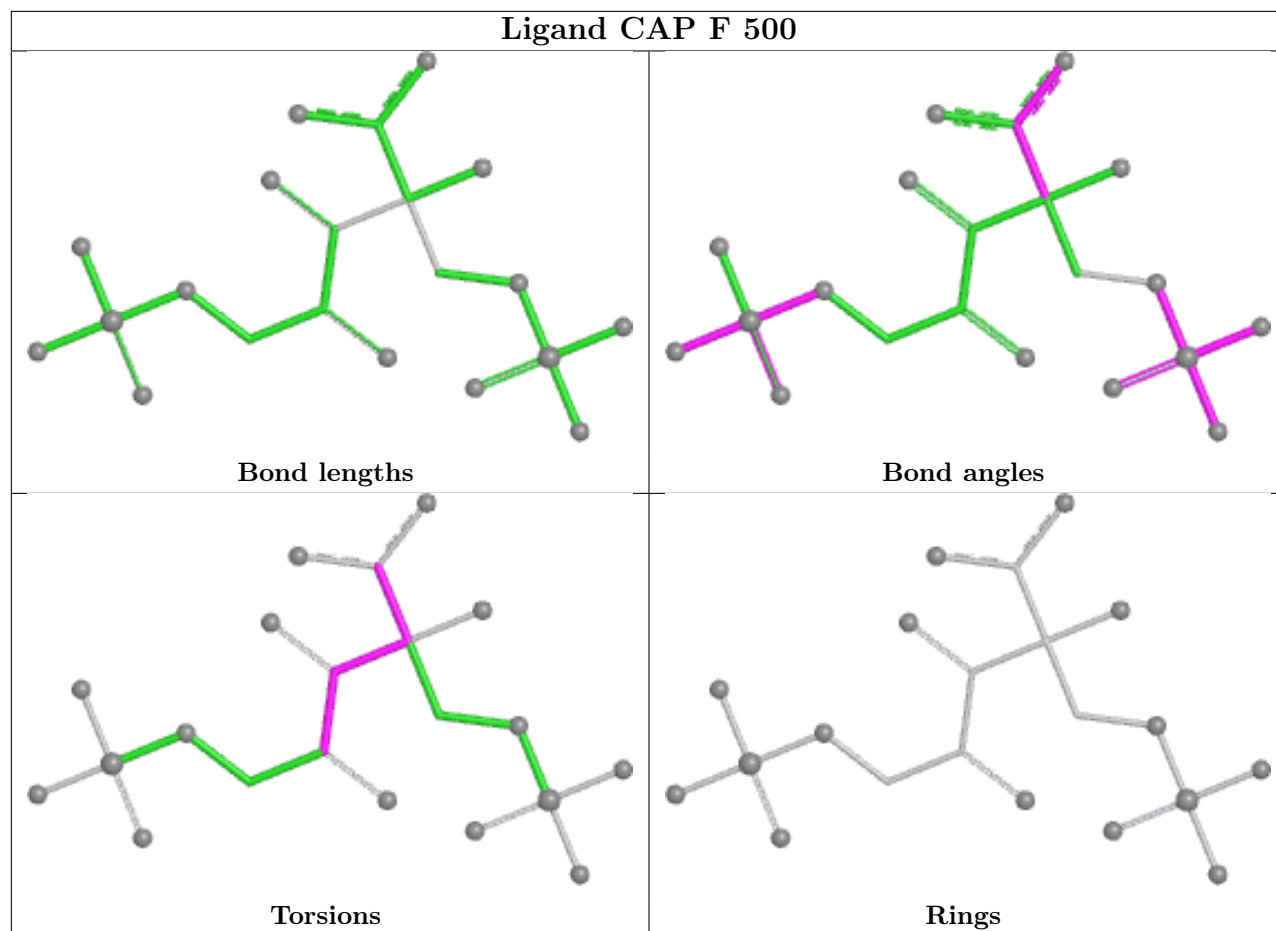


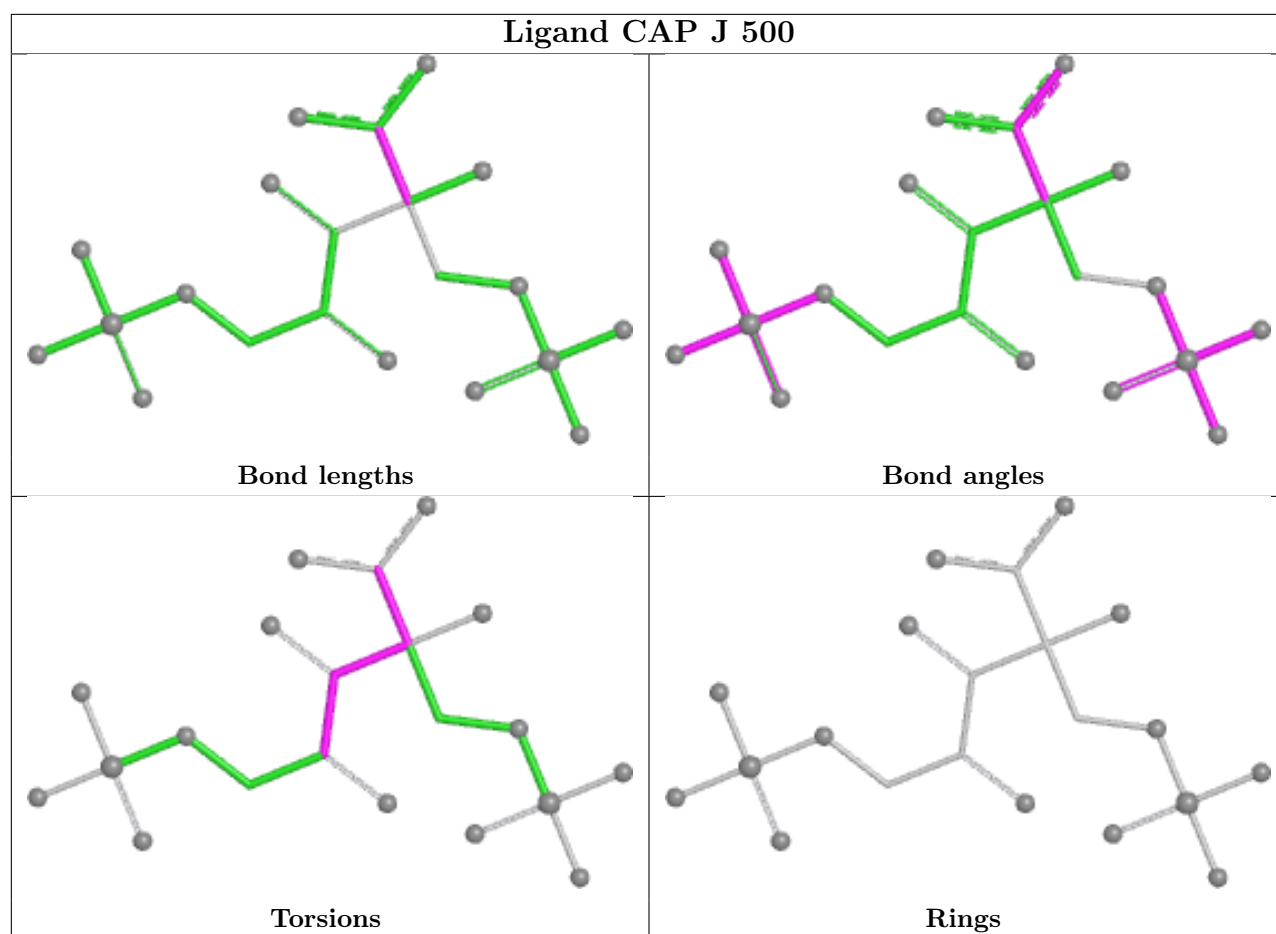












5.7 Other polymers [i](#)

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	454/481 (94%)	0.17	5 (1%) 78 77	27, 39, 58, 88	0
1	B	454/481 (94%)	0.20	8 (1%) 67 67	30, 41, 64, 136	0
1	C	454/481 (94%)	0.31	9 (1%) 65 64	31, 42, 65, 88	0
1	D	454/481 (94%)	0.29	7 (1%) 72 71	29, 41, 62, 111	0
1	E	456/481 (94%)	0.12	4 (0%) 81 80	28, 39, 59, 81	0
1	F	455/481 (94%)	0.16	6 (1%) 75 74	29, 38, 54, 74	0
1	G	455/481 (94%)	0.12	4 (0%) 81 80	27, 37, 54, 76	0
1	H	455/481 (94%)	0.09	5 (1%) 78 77	26, 37, 57, 89	0
1	I	454/481 (94%)	0.27	8 (1%) 67 67	27, 40, 65, 109	0
1	J	454/481 (94%)	0.39	8 (1%) 67 67	28, 41, 64, 84	0
1	K	454/481 (94%)	0.22	10 (2%) 62 61	29, 42, 67, 123	0
1	L	456/481 (94%)	0.23	8 (1%) 67 67	28, 41, 59, 92	0
All	All	5455/5772 (94%)	0.21	82 (1%) 72 71	26, 40, 61, 136	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	456	LEU	4.6
1	D	117	GLY	3.7
1	F	456	LEU	3.6
1	C	324	GLY	3.6
1	K	451	ASN	3.5
1	E	457	LYS	3.5
1	B	455	LYS	3.2
1	B	435	ALA	3.1
1	I	35	GLY	3.0
1	G	414	ALA	3.0
1	D	331	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	453	ARG	2.9
1	A	78	ALA	2.9
1	A	35	GLY	2.8
1	E	156	ILE	2.8
1	C	36	PHE	2.7
1	F	78	ALA	2.7
1	H	445	ALA	2.7
1	K	452	TRP	2.7
1	B	454	ALA	2.7
1	F	36	PHE	2.6
1	L	441	PHE	2.6
1	L	451	ASN	2.6
1	J	324	GLY	2.6
1	A	36	PHE	2.6
1	C	449	TYR	2.6
1	L	129	VAL	2.6
1	I	455	LYS	2.6
1	D	80	SER	2.6
1	J	36	PHE	2.6
1	C	327	GLY	2.6
1	L	221	ASP	2.6
1	J	418	TRP	2.6
1	H	454	ALA	2.5
1	D	36	PHE	2.5
1	I	36	PHE	2.5
1	L	81	LEU	2.5
1	B	408	ALA	2.5
1	K	455	LYS	2.5
1	B	117	GLY	2.5
1	K	37	GLY	2.5
1	K	430	ASP	2.4
1	G	36	PHE	2.4
1	C	40	ILE	2.4
1	H	332	GLU	2.4
1	B	382	ASP	2.4
1	J	85	ALA	2.4
1	A	129	VAL	2.4
1	H	456	LEU	2.3
1	L	457	LYS	2.3
1	F	427	PHE	2.3
1	I	331	ALA	2.3
1	K	448	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	80	SER	2.3
1	J	72	VAL	2.3
1	D	37	GLY	2.3
1	C	418	TRP	2.3
1	E	427	PHE	2.2
1	F	129	VAL	2.2
1	B	95	VAL	2.2
1	B	332	GLU	2.2
1	E	443	GLN	2.2
1	L	418	TRP	2.2
1	K	450	PRO	2.1
1	C	129	VAL	2.1
1	J	385	GLY	2.1
1	D	379	GLY	2.1
1	I	117	GLY	2.1
1	J	340	ILE	2.1
1	L	35	GLY	2.1
1	I	47	ALA	2.1
1	J	40	ILE	2.1
1	I	398	PHE	2.1
1	D	221	ASP	2.0
1	C	438	PHE	2.0
1	K	434	PHE	2.0
1	C	339	ALA	2.0
1	G	78	ALA	2.0
1	A	221	ASP	2.0
1	F	419	LYS	2.0
1	K	429	LYS	2.0
1	H	379	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KCX	J	192	12/13	0.83	0.12	34,36,38,39	0
1	KCX	C	192	12/13	0.88	0.12	33,34,37,38	0
1	KCX	A	192	12/13	0.89	0.10	32,33,38,38	0
1	KCX	D	192	12/13	0.91	0.10	31,34,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KCX	G	192	12/13	0.92	0.09	30,34,38,38	0
1	KCX	B	192	12/13	0.92	0.07	31,34,38,38	0
1	KCX	L	192	12/13	0.92	0.09	30,36,42,42	0
1	KCX	I	192	12/13	0.93	0.08	31,32,35,35	0
1	KCX	E	192	12/13	0.93	0.08	30,33,34,35	0
1	KCX	H	192	12/13	0.93	0.07	27,31,33,33	0
1	KCX	F	192	12/13	0.94	0.07	29,33,37,38	0
1	KCX	K	192	12/13	0.95	0.07	27,35,38,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

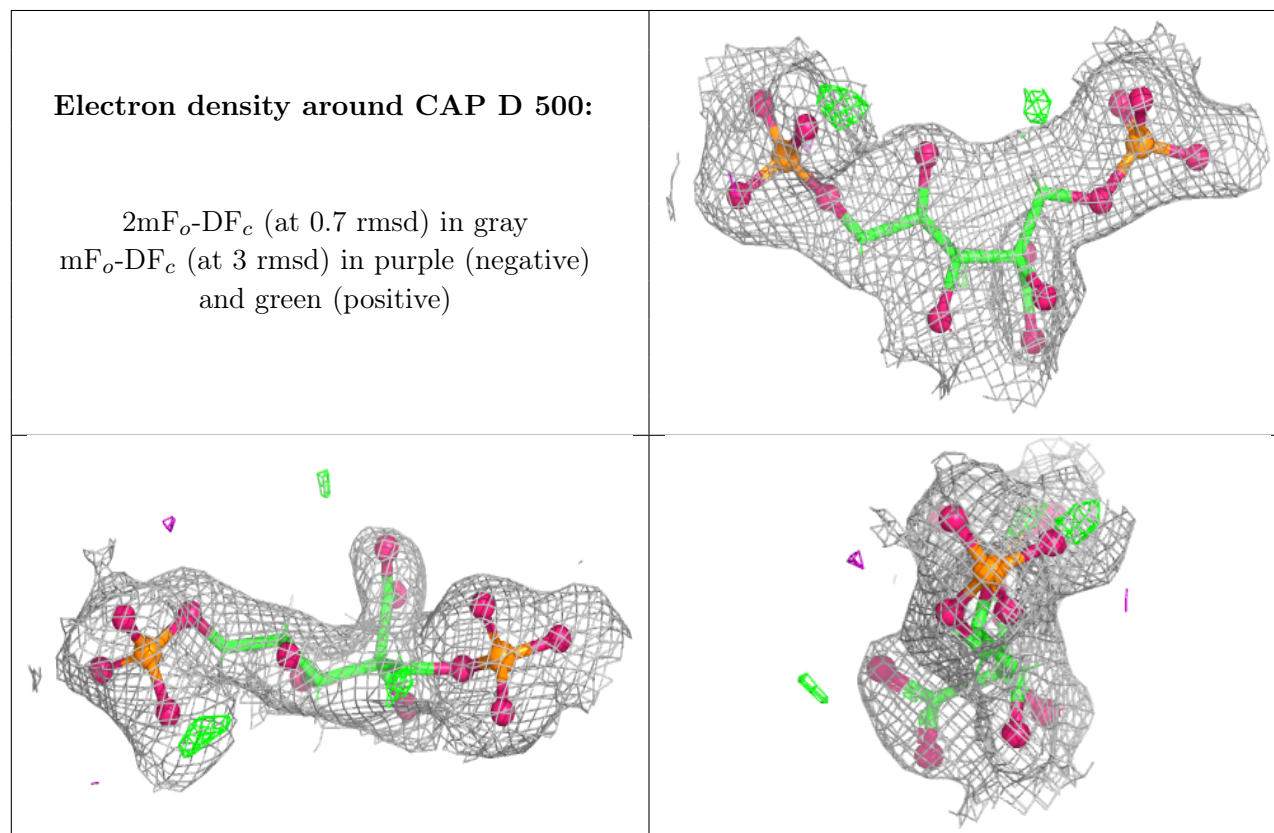
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CAP	D	500	21/21	0.91	0.08	29,38,42,43	0
2	CAP	C	500	21/21	0.92	0.09	39,44,49,51	0
2	CAP	J	500	21/21	0.93	0.09	32,45,49,51	0
2	CAP	B	500	21/21	0.94	0.08	31,38,44,44	0
2	CAP	A	500	21/21	0.94	0.08	33,38,45,53	0
2	CAP	G	500	21/21	0.95	0.07	28,35,41,42	0
2	CAP	H	500	21/21	0.95	0.07	27,34,38,42	0
2	CAP	I	500	21/21	0.95	0.07	35,40,45,49	0
2	CAP	E	500	21/21	0.95	0.08	33,38,45,47	0
2	CAP	L	500	21/21	0.95	0.07	35,43,48,49	0
2	CAP	K	500	21/21	0.96	0.07	31,38,42,43	0
2	CAP	F	500	21/21	0.96	0.06	33,41,44,46	0
3	MG	A	501	1/1	0.96	0.11	37,37,37,37	0
3	MG	D	501	1/1	0.96	0.04	44,44,44,44	0
3	MG	G	501	1/1	0.96	0.10	40,40,40,40	0
3	MG	I	501	1/1	0.96	0.05	38,38,38,38	0
3	MG	F	501	1/1	0.97	0.10	39,39,39,39	0
3	MG	J	501	1/1	0.97	0.05	38,38,38,38	0
3	MG	H	501	1/1	0.98	0.02	30,30,30,30	0
3	MG	C	501	1/1	0.98	0.03	40,40,40,40	0

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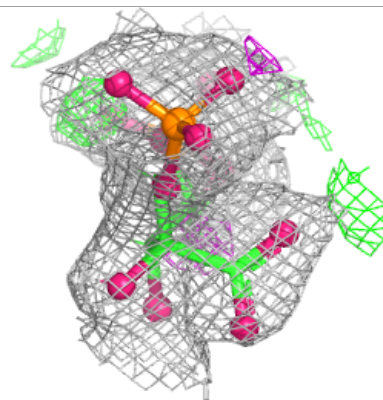
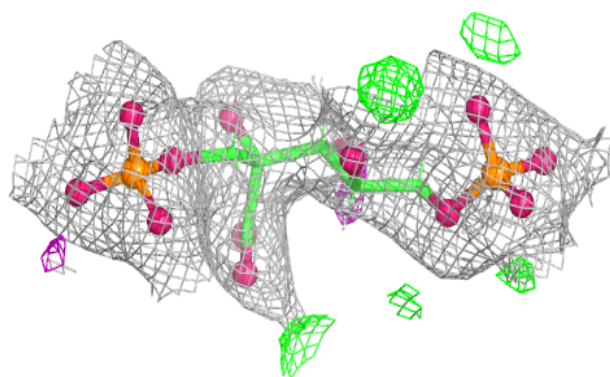
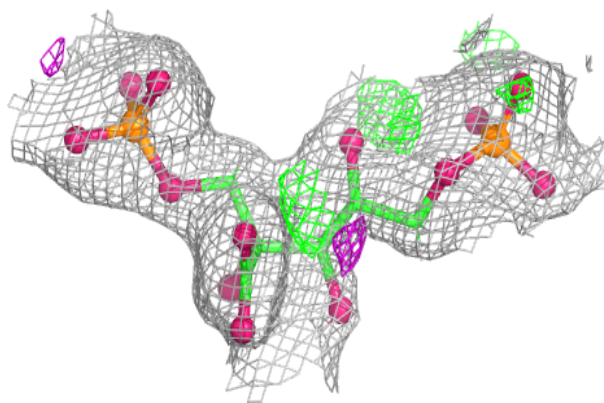
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	E	501	1/1	0.98	0.03	33,33,33,33	0
3	MG	L	501	1/1	0.98	0.09	41,41,41,41	0
3	MG	K	501	1/1	0.99	0.03	37,37,37,37	0
3	MG	B	501	1/1	0.99	0.03	33,33,33,33	0

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.

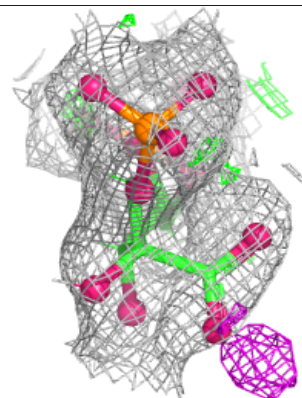
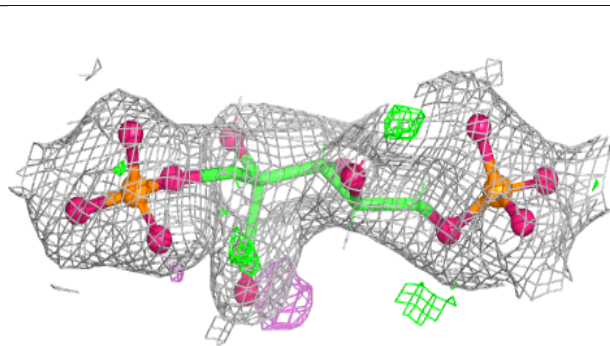
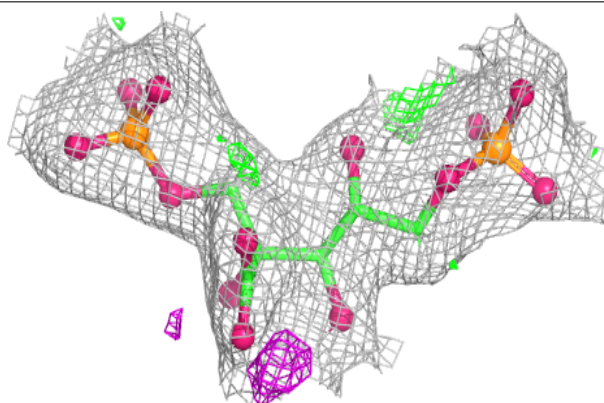


Electron density around CAP C 500:

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

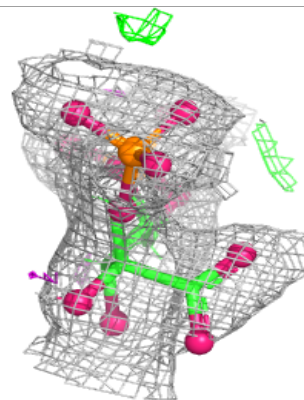
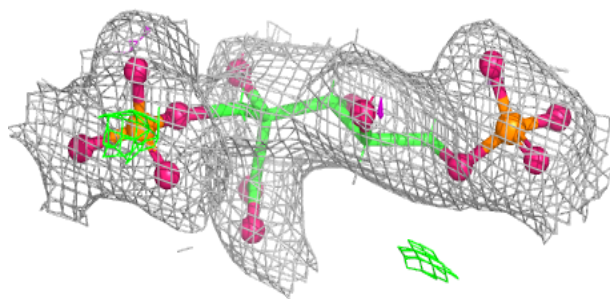
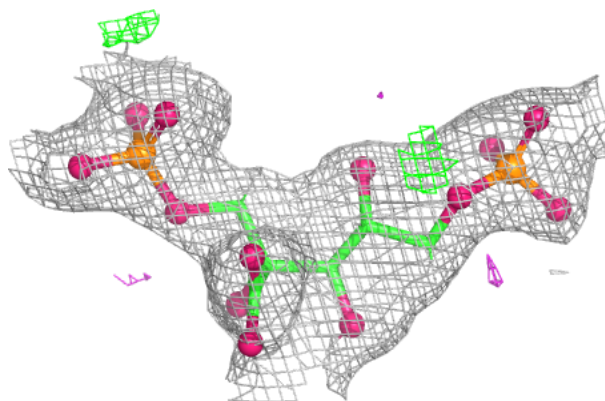
**Electron density around CAP J 500:**

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

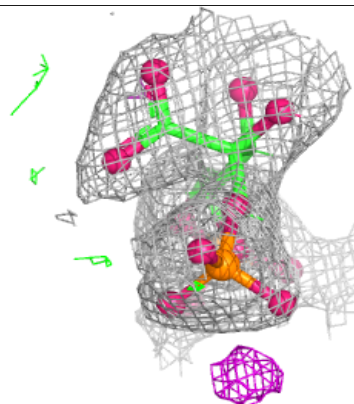
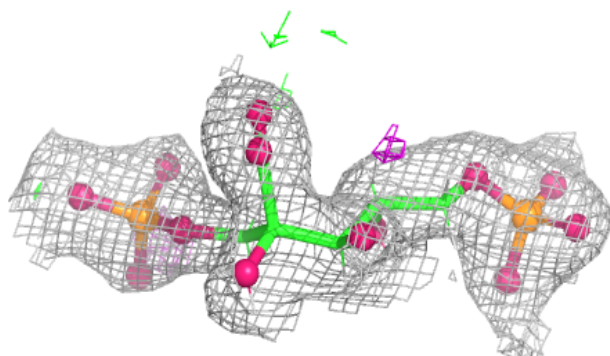
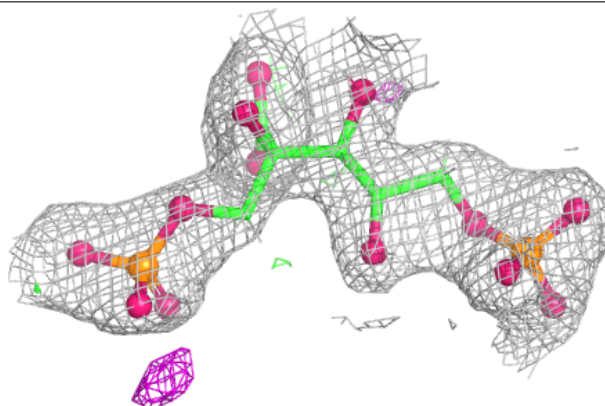


Electron density around CAP B 500:

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

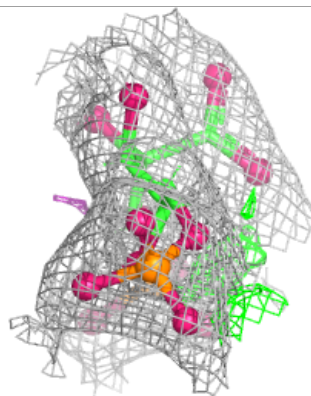
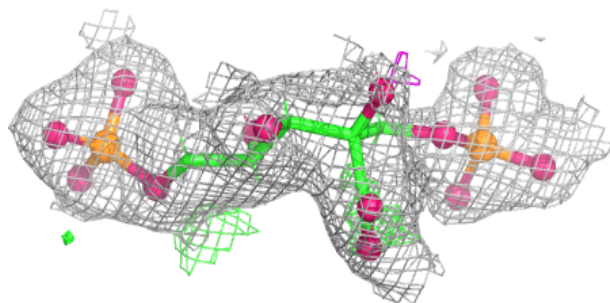
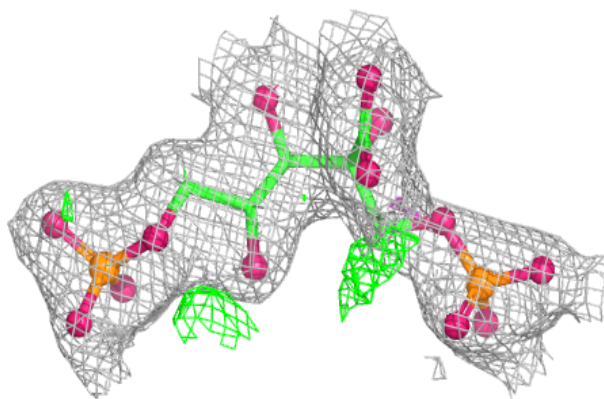
**Electron density around CAP A 500:**

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

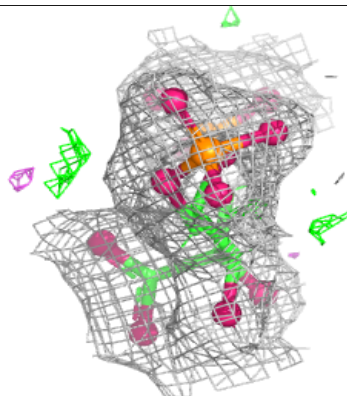
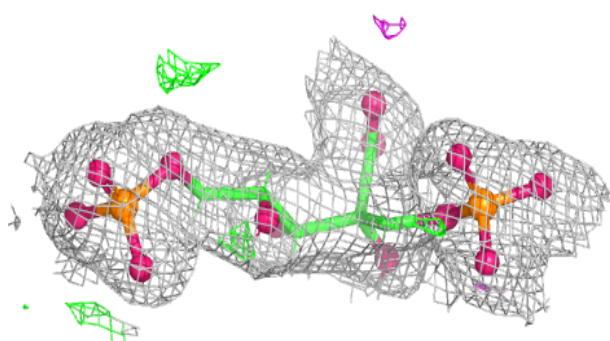
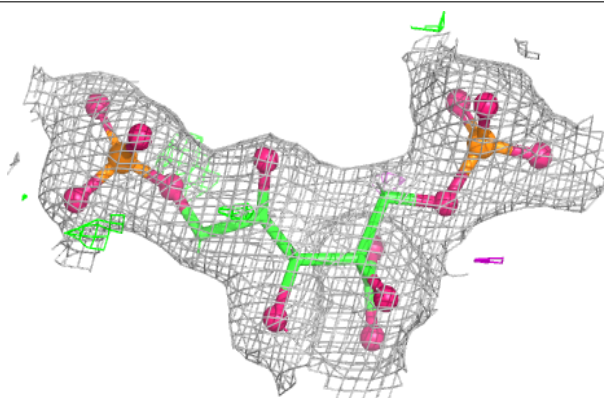


Electron density around CAP G 500:

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

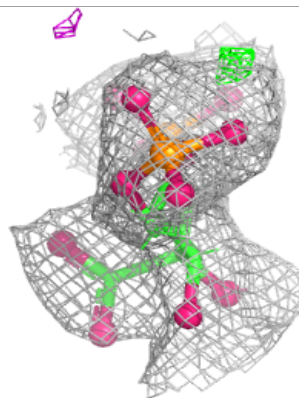
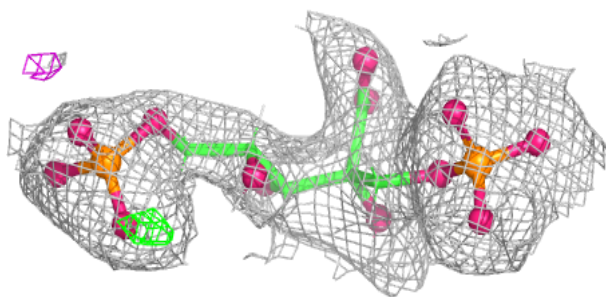
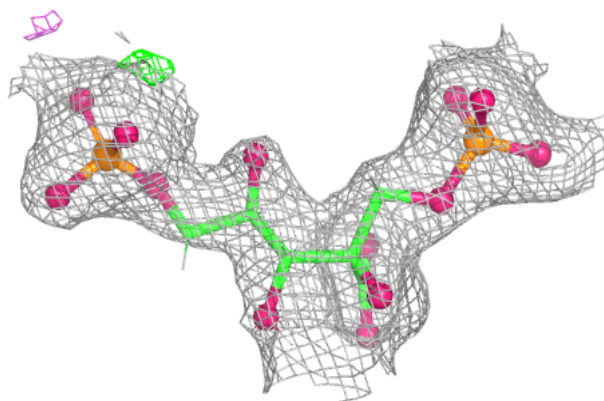
**Electron density around CAP H 500:**

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and green (positive)

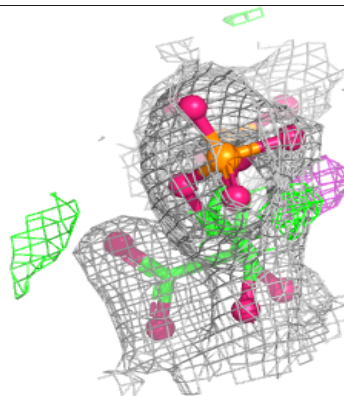
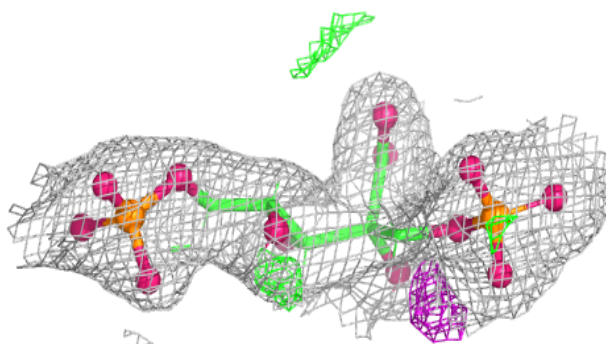
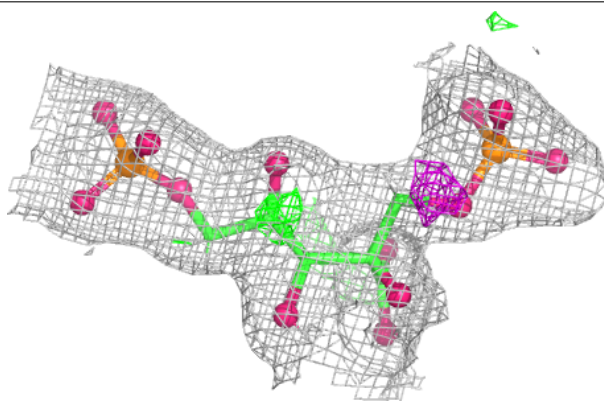


Electron density around CAP I 500:

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

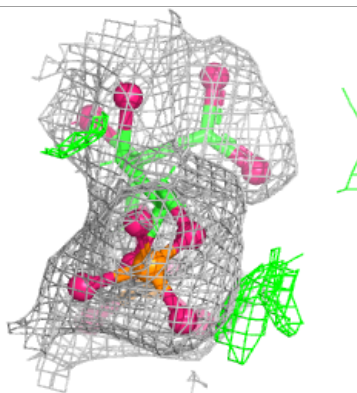
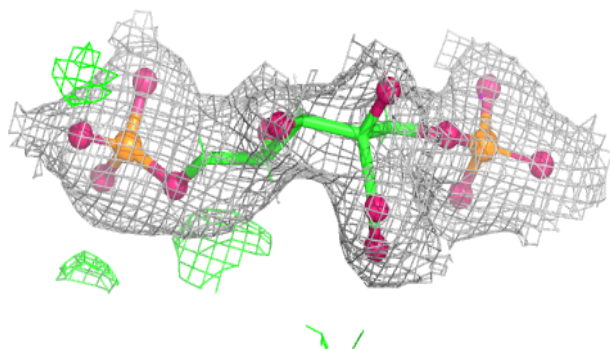
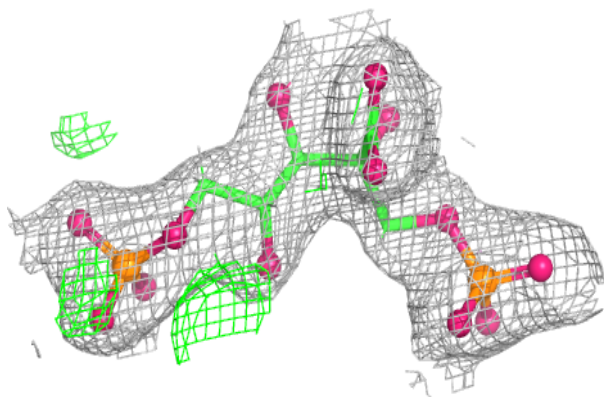
**Electron density around CAP E 500:**

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and green (positive)

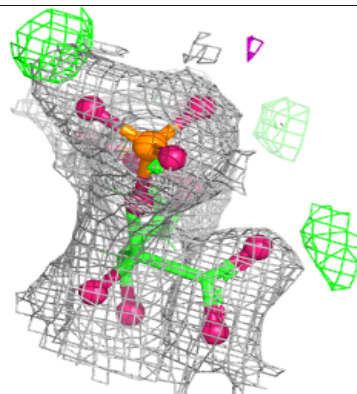
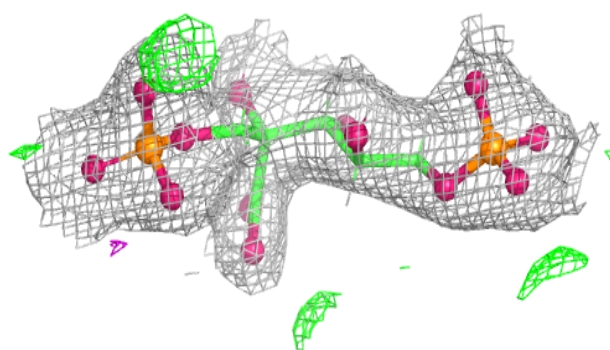
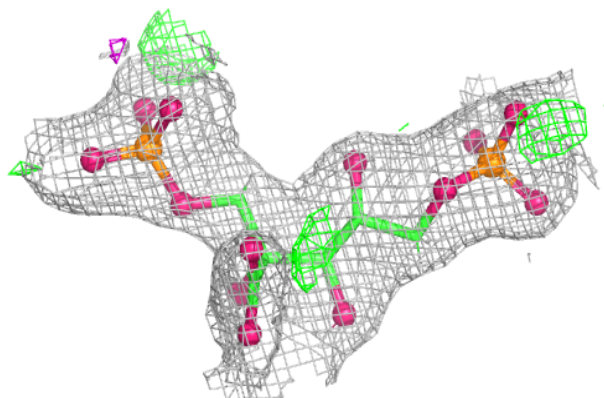


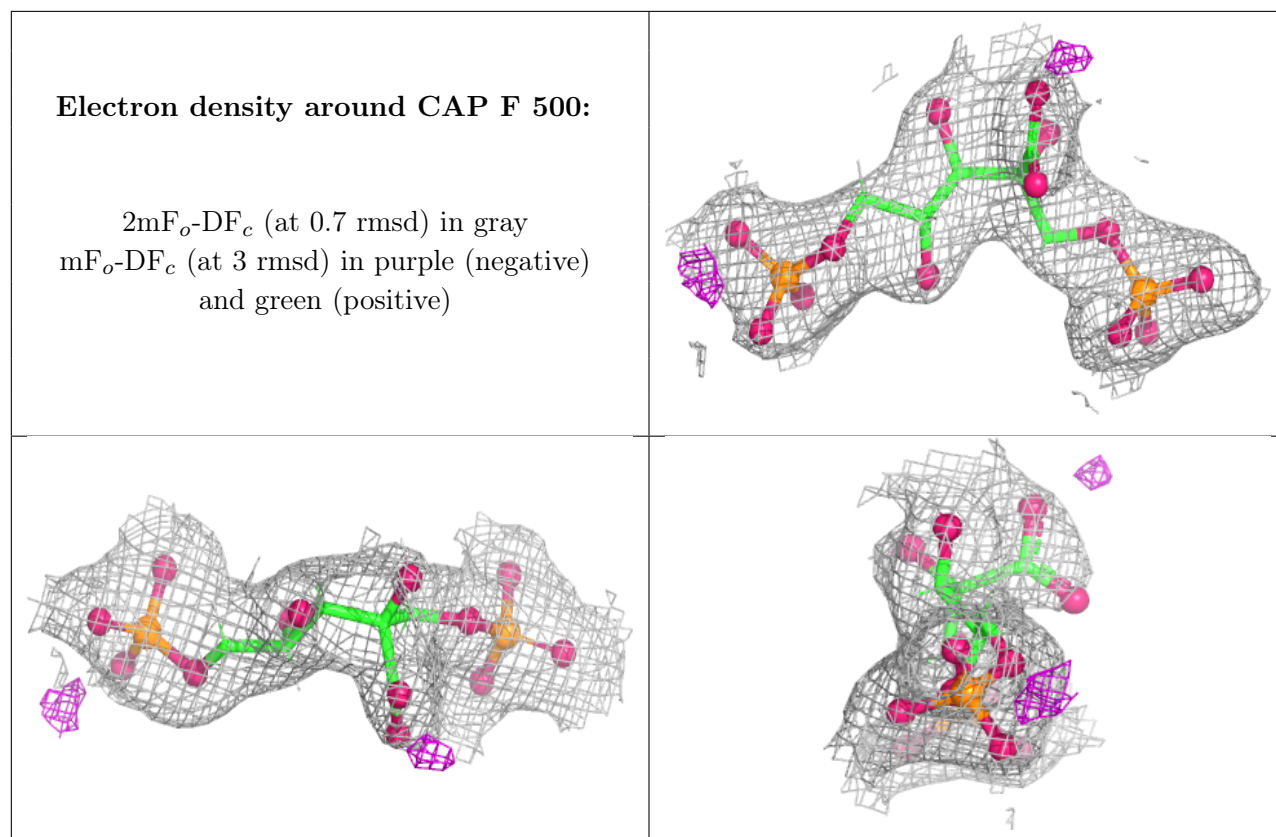
Electron density around CAP L 500:

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

**Electron density around CAP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.