wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 11:39 PM EST

PDB ID	:	5HAT
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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

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

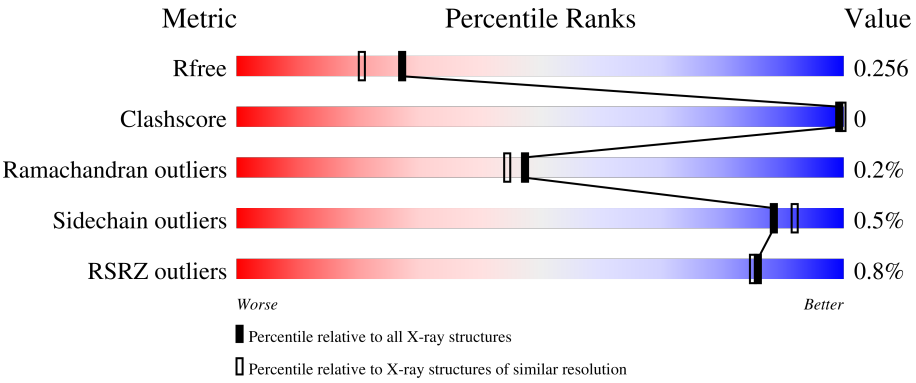
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	93% • 5%
1	B	481	% 94% • 5%
1	C	481	% 93% • 5%
1	D	481	% 93% • 5%

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Mol	Chain	Length	Quality of chain
1	E	481	94% • 5%
1	F	481	93% • 5%
1	G	481	93% • 5%
1	H	481	95% 5%
1	I	481	93% • 5%
1	J	481	93% • 5%
1	K	481	93% • 5%
1	L	481	94% • 5%

2 Entry composition (i)

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 bisphosphate 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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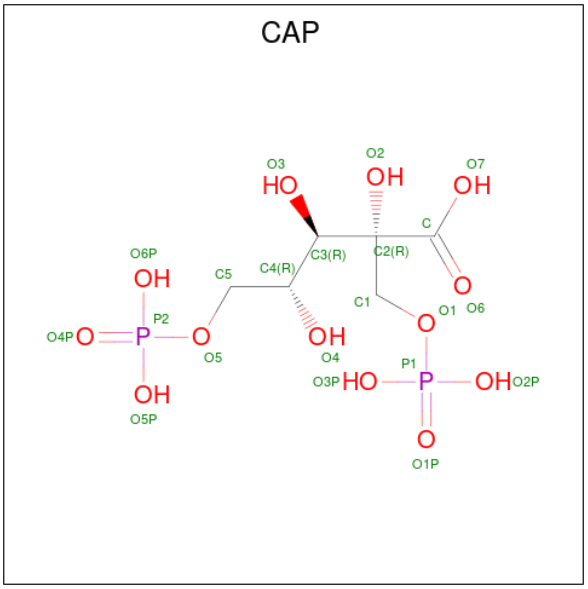
Chain	Residue	Modelled	Actual	Comment	Reference
L	-4	PRO	-	expression tag	UNP Q6N0W9
L	-3	ARG	-	expression tag	UNP Q6N0W9
L	-2	GLY	-	expression tag	UNP Q6N0W9
L	-1	SER	-	expression tag	UNP Q6N0W9
L	0	HIS	-	expression tag	UNP Q6N0W9
L	59	PHE	SER	engineered mutation	UNP Q6N0W9
L	331	ALA	MET	engineered mutation	UNP Q6N0W9

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: 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 (three-letter code: 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.

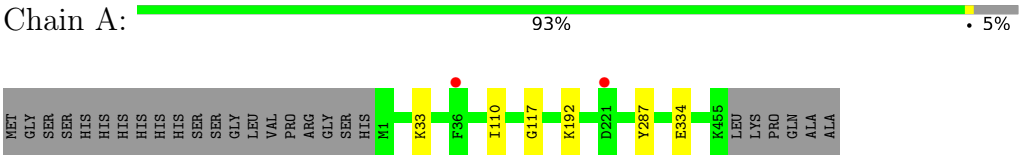
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	222	Total O 222 222	0	0
4	B	185	Total O 185 185	0	0
4	C	179	Total O 179 179	0	0
4	D	228	Total O 228 228	0	0
4	E	223	Total O 223 223	0	0
4	F	249	Total O 249 249	0	0
4	G	264	Total O 264 264	0	0
4	H	229	Total O 229 229	0	0
4	I	228	Total O 228 228	0	0
4	J	201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

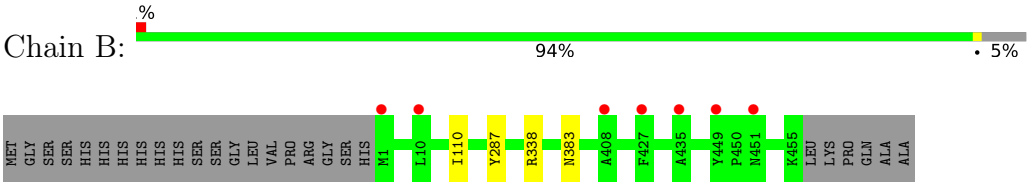
• Molecule 1: Ribulose bisphosphate carboxylase

Chain A:



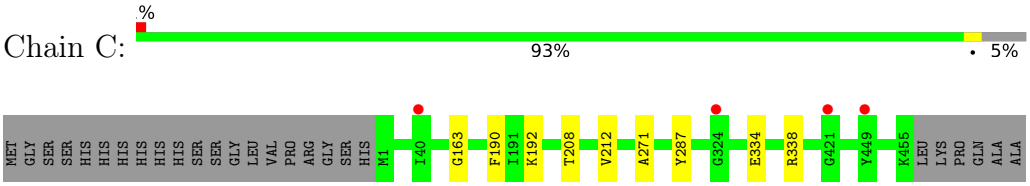
• Molecule 1: Ribulose bisphosphate carboxylase

Chain B:



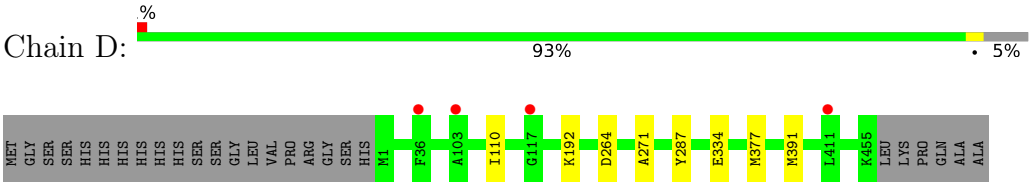
• Molecule 1: Ribulose bisphosphate carboxylase

Chain C:



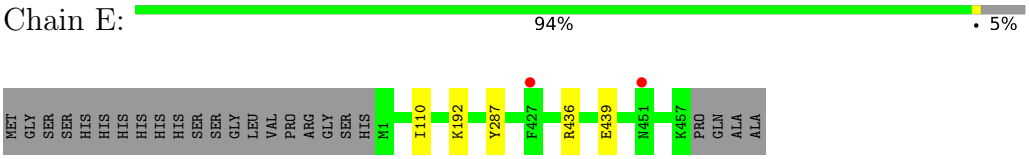
• Molecule 1: Ribulose bisphosphate carboxylase

Chain D:



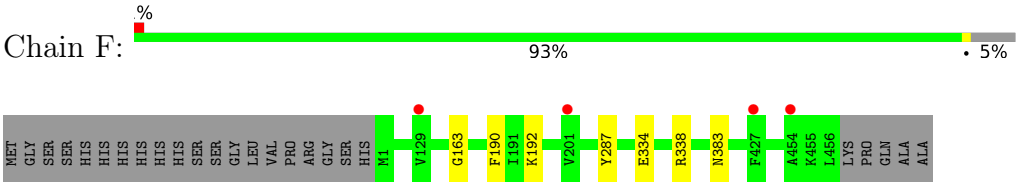
• Molecule 1: Ribulose bisphosphate carboxylase

Chain E:



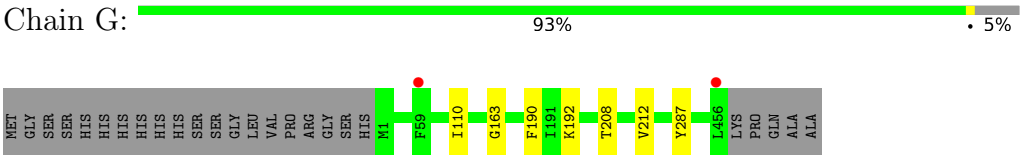
• Molecule 1: Ribulose bisphosphate carboxylase

Chain F:



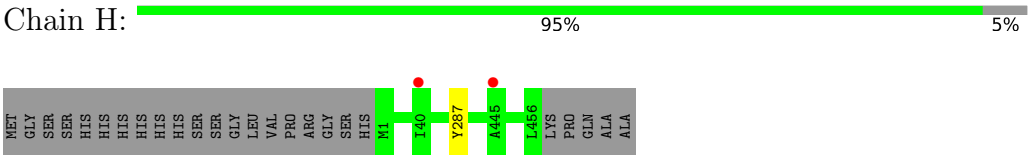
• Molecule 1: Ribulose bisphosphate carboxylase

Chain G:



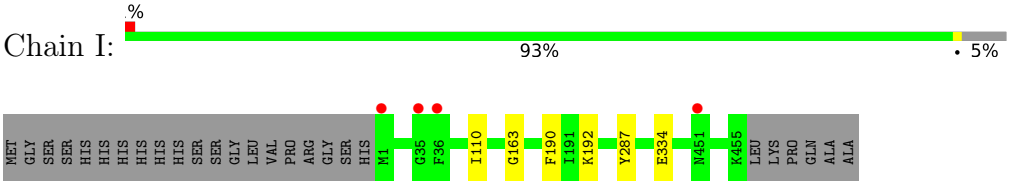
• Molecule 1: Ribulose bisphosphate carboxylase

Chain H:



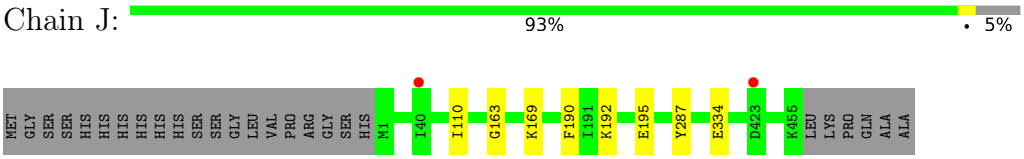
• Molecule 1: Ribulose bisphosphate carboxylase

Chain I:



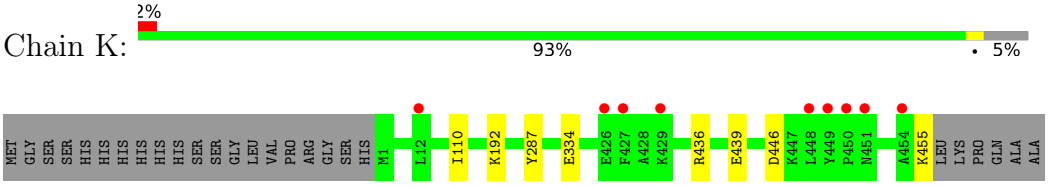
• Molecule 1: Ribulose bisphosphate carboxylase

Chain J:



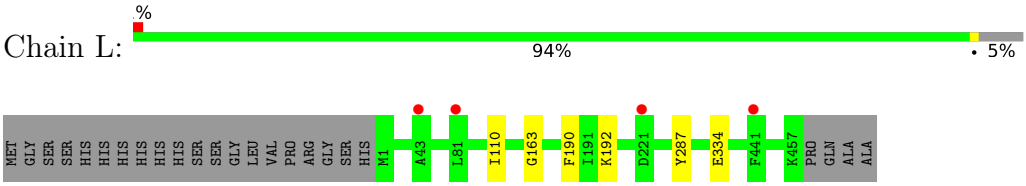
• Molecule 1: Ribulose bisphosphate carboxylase

Chain K:



• Molecule 1: Ribulose bisphosphate carboxylase

Chain L:



4 Data and refinement statistics (i)

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 91.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (20.00-2.00) 90.8 (91.97-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.213 , 0.249 0.222 , 0.256	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 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.51	0/3587	0.63	0/4856
1	B	0.49	0/3587	0.62	0/4856
1	C	0.49	0/3580	0.62	0/4847
1	D	0.51	0/3594	0.63	0/4865
1	E	0.49	0/3607	0.62	0/4883
1	F	0.53	0/3591	0.64	0/4863
1	G	0.53	0/3595	0.63	0/4867
1	H	0.51	0/3599	0.62	0/4872
1	I	0.51	0/3581	0.62	0/4848
1	J	0.48	0/3587	0.61	0/4856
1	K	0.48	0/3577	0.62	0/4845
1	L	0.50	0/3602	0.63	0/4875
All	All	0.50	0/43087	0.62	0/58333

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	3510	3357	3369	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3510	3358	3369	1	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	1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	17	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 17 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

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%)	47	44
1	B	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	47	44
1	C	452/481 (94%)	440 (97%)	12 (3%)	0	100	100
1	D	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	47	44
1	E	454/481 (94%)	441 (97%)	12 (3%)	1 (0%)	47	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	453/481 (94%)	442 (98%)	11 (2%)	0	100	100
1	G	453/481 (94%)	441 (97%)	11 (2%)	1 (0%)	47	44
1	H	453/481 (94%)	441 (97%)	12 (3%)	0	100	100
1	I	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	47	44
1	J	452/481 (94%)	438 (97%)	13 (3%)	1 (0%)	47	44
1	K	452/481 (94%)	441 (98%)	10 (2%)	1 (0%)	47	44
1	L	454/481 (94%)	441 (97%)	12 (3%)	1 (0%)	47	44
All	All	5431/5772 (94%)	5285 (97%)	137 (2%)	9 (0%)	47	44

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ILE
1	D	110	ILE
1	L	110	ILE
1	B	110	ILE
1	G	110	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/371 (94%)	345 (99%)	2 (1%)	86	90
1	B	347/371 (94%)	346 (100%)	1 (0%)	92	95
1	C	345/371 (93%)	343 (99%)	2 (1%)	86	90
1	D	349/371 (94%)	346 (99%)	3 (1%)	78	83
1	E	350/371 (94%)	349 (100%)	1 (0%)	92	95
1	F	347/371 (94%)	345 (99%)	2 (1%)	86	90
1	G	348/371 (94%)	347 (100%)	1 (0%)	92	95
1	H	349/371 (94%)	348 (100%)	1 (0%)	92	95
1	I	346/371 (93%)	344 (99%)	2 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	347/371 (94%)	345 (99%)	2 (1%)	86 90
1	K	345/371 (93%)	342 (99%)	3 (1%)	78 83
1	L	348/371 (94%)	346 (99%)	2 (1%)	86 90
All	All	4168/4452 (94%)	4146 (100%)	22 (0%)	88 92

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	334	GLU
1	K	287	TYR
1	J	334	GLU
1	K	334	GLU
1	D	287	TYR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	B	192	3,1	9,11,12	1.09	0	5,12,14	0.34	0
1	KCX	A	192	3,1	9,11,12	3.16	2 (22%)	5,12,14	2.13	2 (40%)
1	KCX	G	192	3,1	9,11,12	2.35	1 (11%)	5,12,14	1.43	1 (20%)
1	KCX	H	192	3,1	9,11,12	1.30	0	5,12,14	0.39	0
1	KCX	C	192	3,1	9,11,12	1.52	1 (11%)	5,12,14	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	KCX	E	192	3,1	9,11,12	2.54	2 (22%)	5,12,14	1.33	1 (20%)
1	KCX	F	192	3,1	9,11,12	1.34	2 (22%)	5,12,14	0.27	0
1	KCX	L	192	3,1	9,11,12	1.35	1 (11%)	5,12,14	0.46	0
1	KCX	J	192	3,1	9,11,12	2.01	2 (22%)	5,12,14	1.30	1 (20%)
1	KCX	D	192	3,1	9,11,12	1.81	1 (11%)	5,12,14	1.46	1 (20%)
1	KCX	K	192	3,1	9,11,12	3.24	2 (22%)	5,12,14	2.47	1 (20%)
1	KCX	I	192	3,1	9,11,12	1.50	1 (11%)	5,12,14	0.60	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	B	192	3,1	-	0/9/10/12	-
1	KCX	A	192	3,1	-	2/9/10/12	-
1	KCX	G	192	3,1	-	0/9/10/12	-
1	KCX	H	192	3,1	-	0/9/10/12	-
1	KCX	C	192	3,1	-	0/9/10/12	-
1	KCX	E	192	3,1	-	0/9/10/12	-
1	KCX	F	192	3,1	-	0/9/10/12	-
1	KCX	L	192	3,1	-	0/9/10/12	-
1	KCX	J	192	3,1	-	0/9/10/12	-
1	KCX	D	192	3,1	-	0/9/10/12	-
1	KCX	K	192	3,1	-	0/9/10/12	-
1	KCX	I	192	3,1	-	0/9/10/12	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	192	KCX	OQ1-CX	9.19	1.38	1.21
1	A	192	KCX	OQ1-CX	8.37	1.37	1.21
1	G	192	KCX	OQ1-CX	6.45	1.33	1.21
1	E	192	KCX	OQ1-CX	6.28	1.33	1.21
1	J	192	KCX	OQ1-CX	4.38	1.29	1.21

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	192	KCX	OQ1-CX-NZ	-5.27	116.78	124.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	192	KCX	OQ1-CX-NZ	-3.19	120.01	124.96
1	G	192	KCX	OQ1-CX-NZ	-3.18	120.02	124.96
1	A	192	KCX	OQ1-CX-NZ	-3.12	120.13	124.96
1	A	192	KCX	CD-CE-NZ	3.11	121.11	112.21

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CAP	H	500	3	17,20,20	1.13	0	22,31,31	1.48	6 (27%)
2	CAP	A	500	3	17,20,20	0.92	0	22,31,31	1.49	5 (22%)
2	CAP	B	500	3	17,20,20	1.16	2 (11%)	22,31,31	1.47	4 (18%)
2	CAP	L	500	3	17,20,20	1.09	0	22,31,31	1.49	6 (27%)
2	CAP	D	500	3	17,20,20	1.14	0	22,31,31	1.76	4 (18%)
2	CAP	G	500	3	17,20,20	1.04	1 (5%)	22,31,31	1.42	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CAP	F	500	3	17,20,20	1.09	0	22,31,31	1.44	5 (22%)
2	CAP	C	500	3	17,20,20	1.01	0	22,31,31	1.52	6 (27%)
2	CAP	I	500	3	17,20,20	1.08	1 (5%)	22,31,31	1.52	6 (27%)
2	CAP	K	500	3	17,20,20	1.09	0	22,31,31	1.54	6 (27%)
2	CAP	E	500	3	17,20,20	1.09	0	22,31,31	1.55	7 (31%)
2	CAP	J	500	3	17,20,20	1.05	0	22,31,31	1.53	6 (27%)

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	H	500	3	-	8/29/29/29	-
2	CAP	A	500	3	-	8/29/29/29	-
2	CAP	B	500	3	-	7/29/29/29	-
2	CAP	L	500	3	-	7/29/29/29	-
2	CAP	D	500	3	-	9/29/29/29	-
2	CAP	G	500	3	-	7/29/29/29	-
2	CAP	F	500	3	-	8/29/29/29	-
2	CAP	C	500	3	-	7/29/29/29	-
2	CAP	I	500	3	-	7/29/29/29	-
2	CAP	K	500	3	-	8/29/29/29	-
2	CAP	E	500	3	-	7/29/29/29	-
2	CAP	J	500	3	-	8/29/29/29	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	CAP	C4-C3	-2.49	1.51	1.54
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	-2.01	1.47	1.54

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	CAP	O2P-P1-O1	3.57	116.23	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	CAP	O5-P2-O4P	3.53	116.38	106.47
2	D	500	CAP	O5P-P2-O5	3.37	115.69	106.73
2	I	500	CAP	O3P-P1-O1	2.89	114.43	106.73
2	A	500	CAP	O3P-P1-O1	2.88	114.39	106.73

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

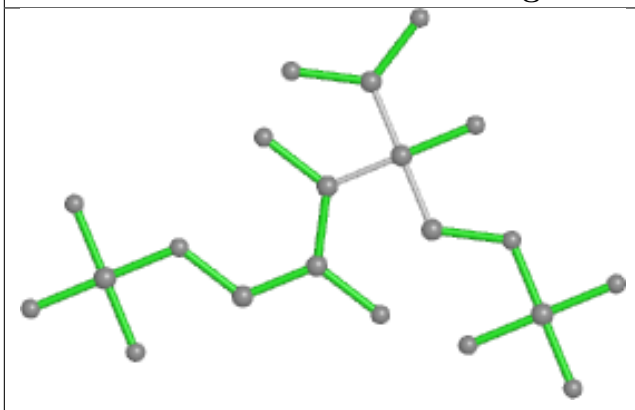
Mol	Chain	Res	Type	Atoms
2	A	500	CAP	O6-C-C2-C3
2	A	500	CAP	O6-C-C2-O2
2	A	500	CAP	O3-C3-C4-O4
2	B	500	CAP	O6-C-C2-C3
2	B	500	CAP	O6-C-C2-O2

There are no ring outliers.

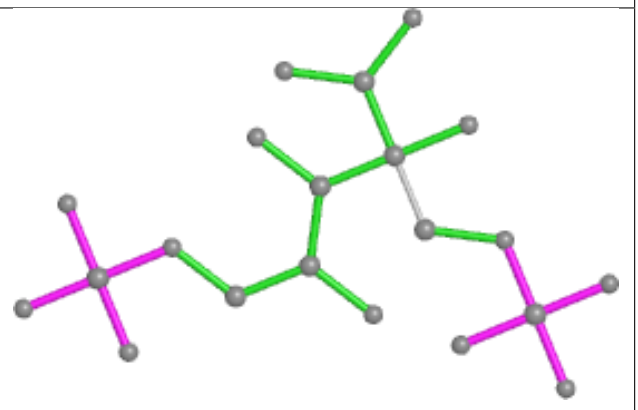
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

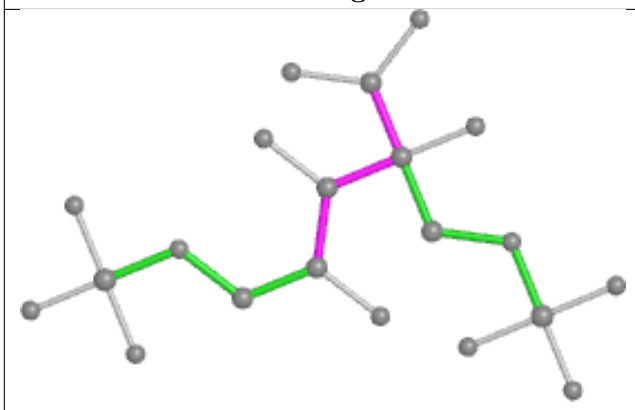
Ligand CAP H 500



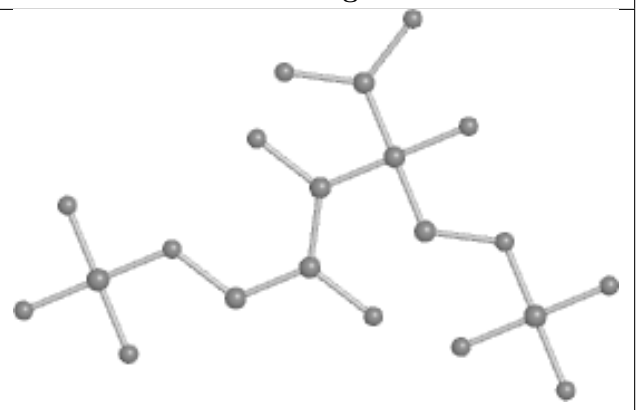
Bond lengths



Bond angles

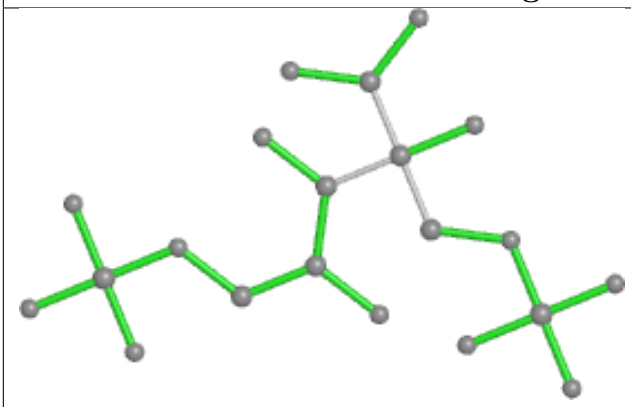


Torsions

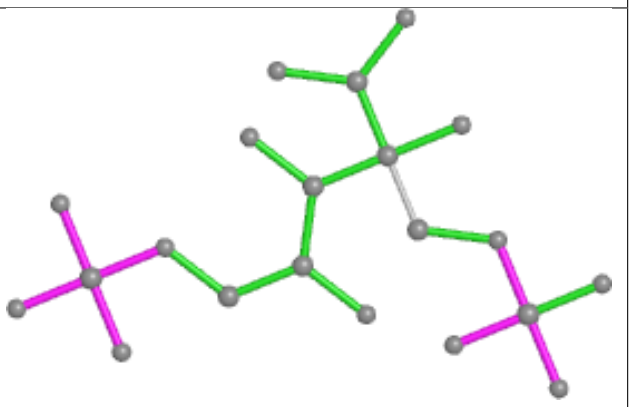


Rings

Ligand CAP A 500



Bond lengths



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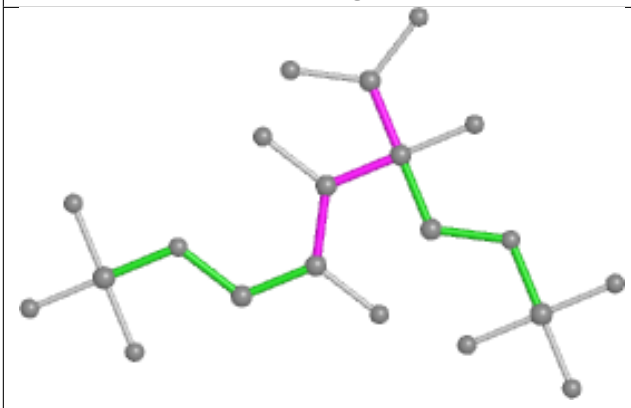

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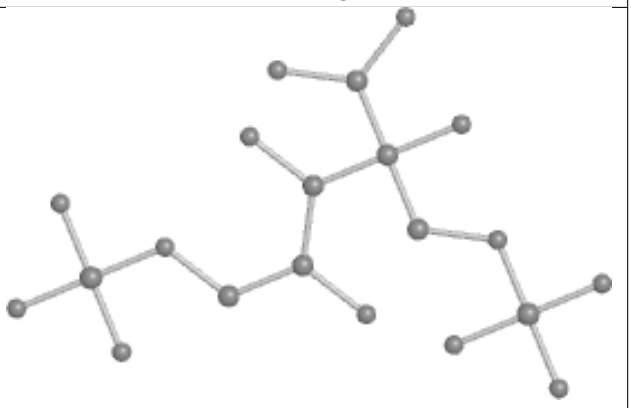
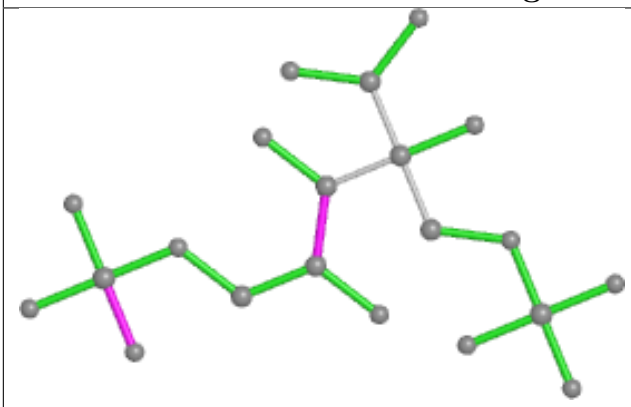


Rings

Ligand CAP B 500



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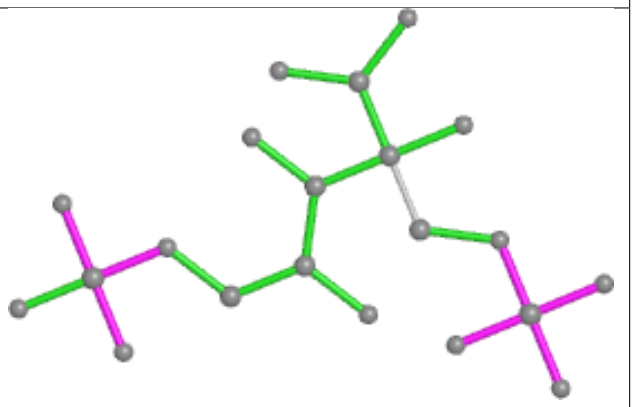
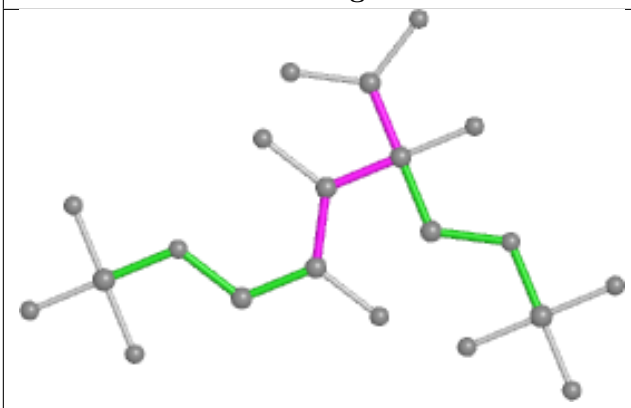


Bond angles



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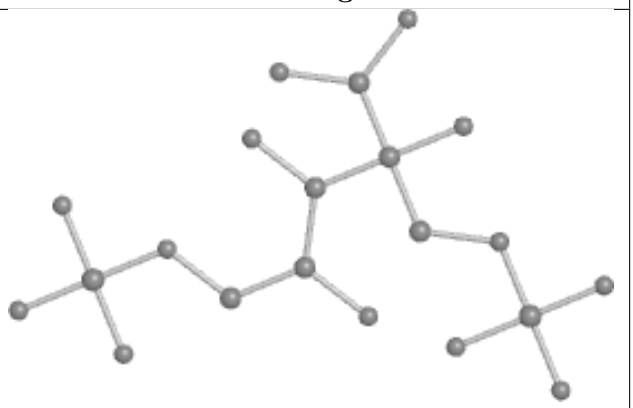
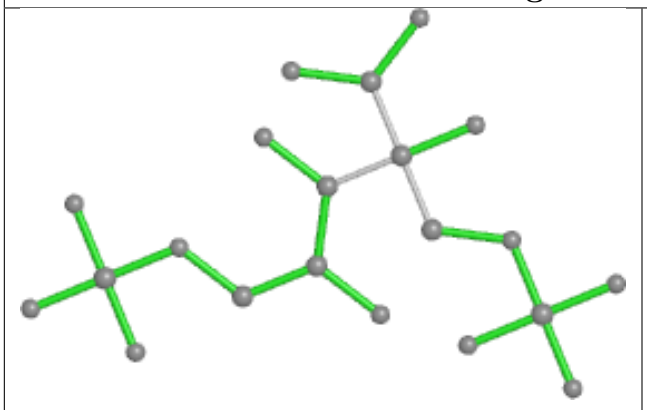


Rings

Ligand CAP L 500



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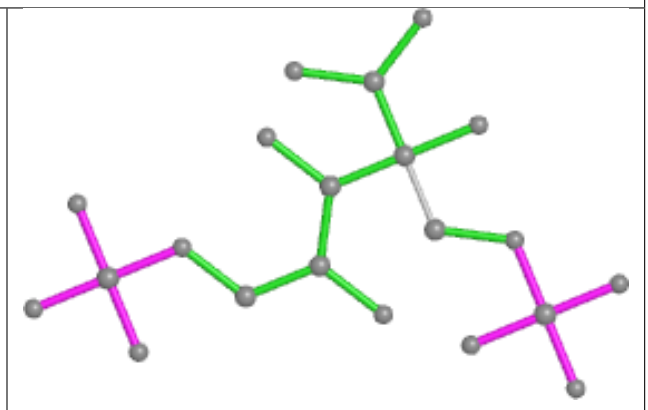
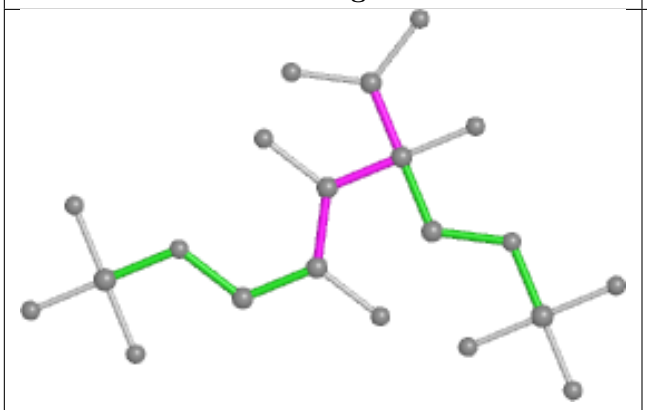


Bond angles



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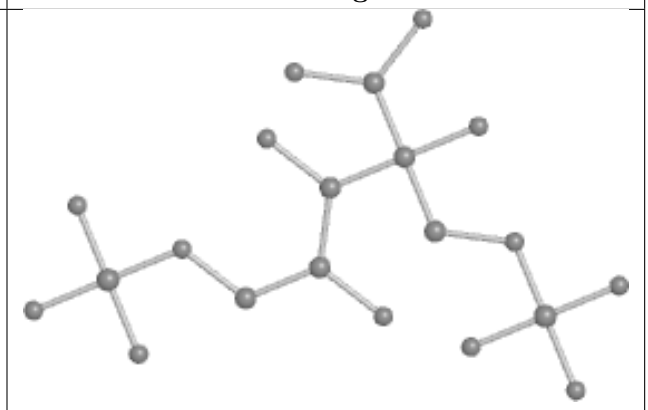
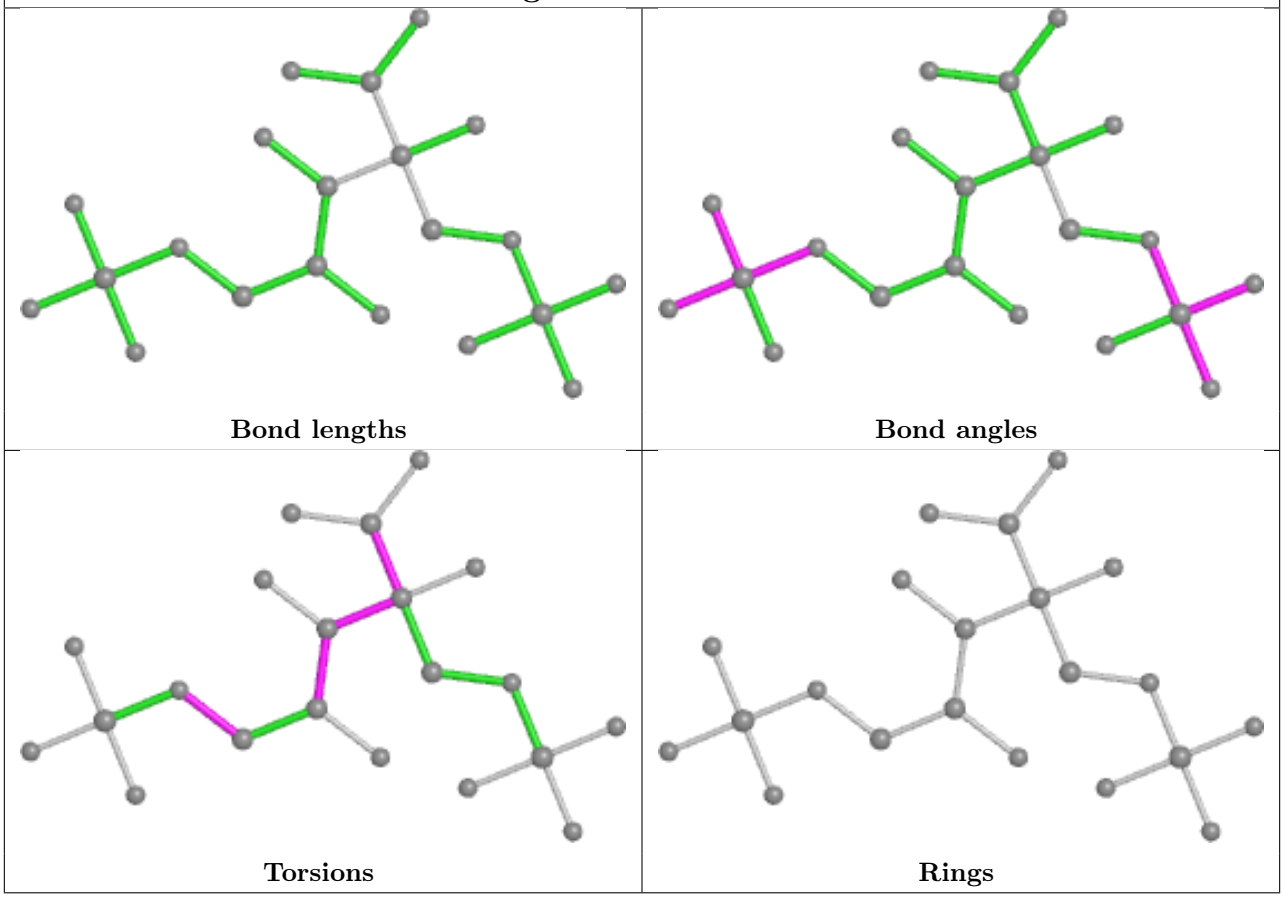
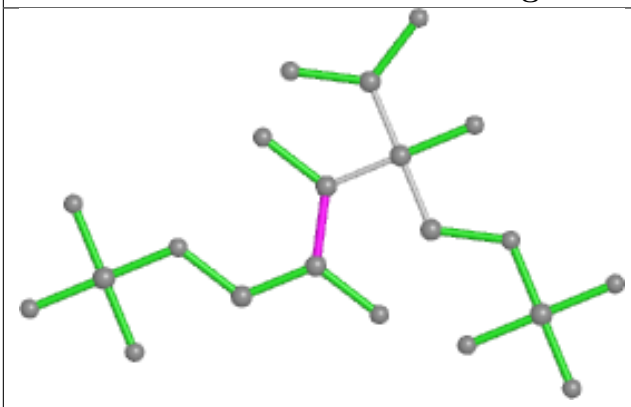


Rings

Ligand CAP D 500



Ligand CAP G 500



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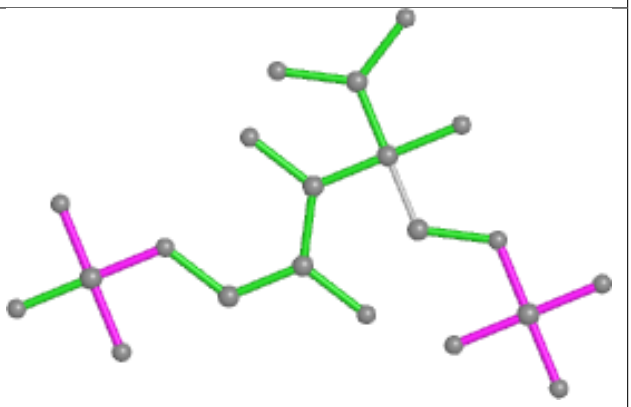
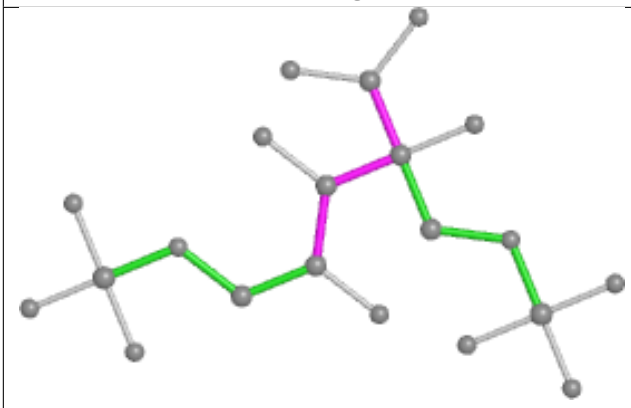


Bond angles



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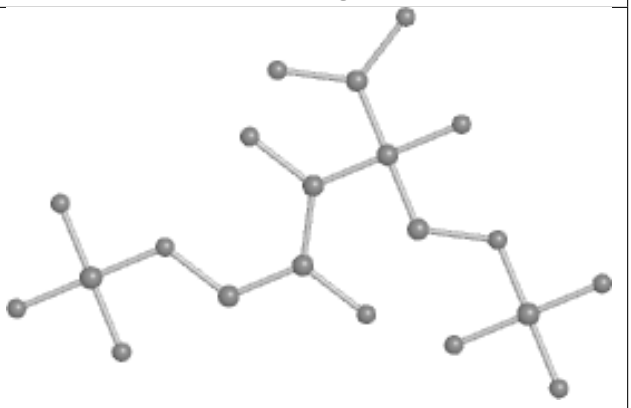

Rings

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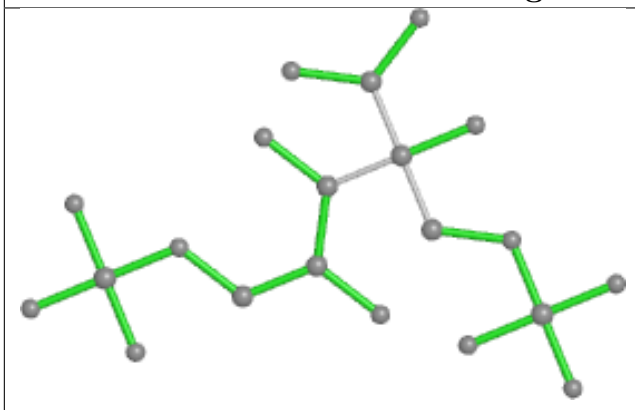

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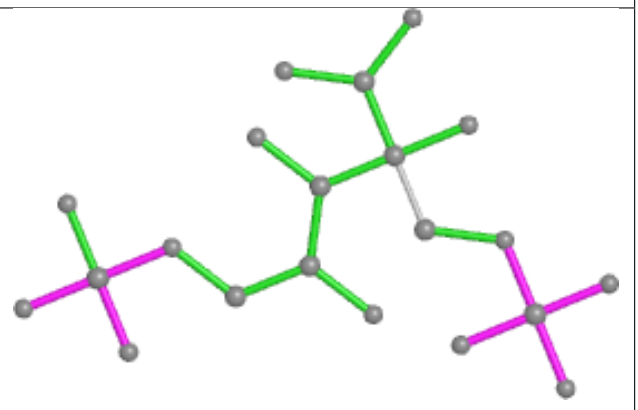
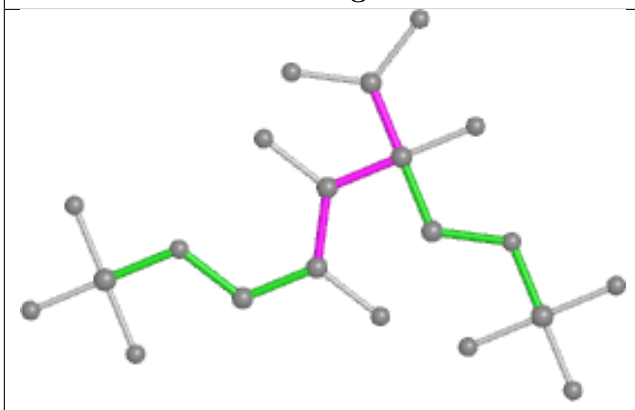


Bond angles



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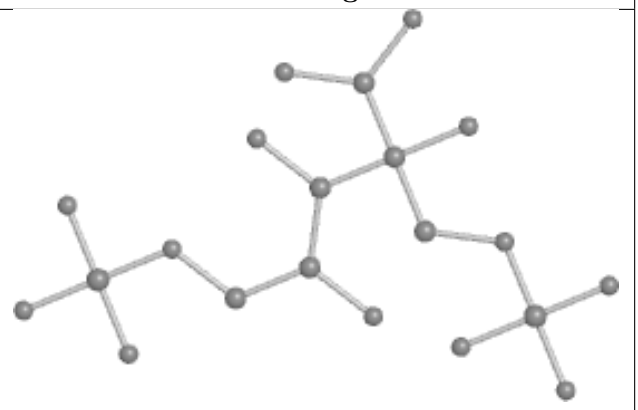
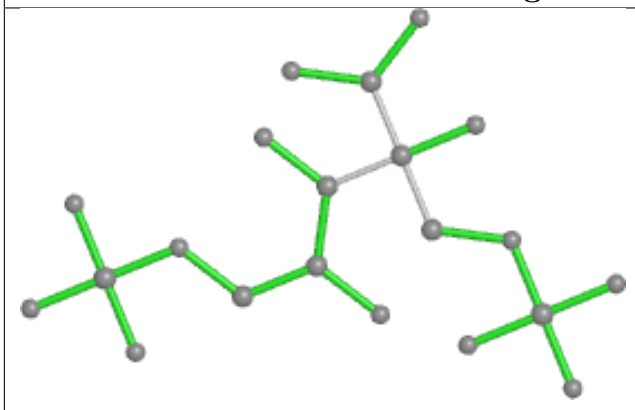


Rings

Ligand CAP C 500



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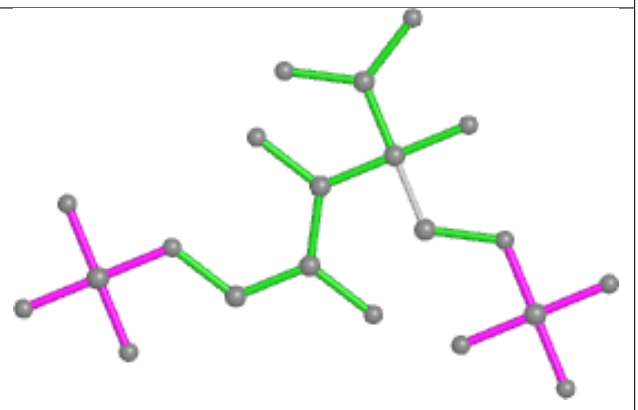
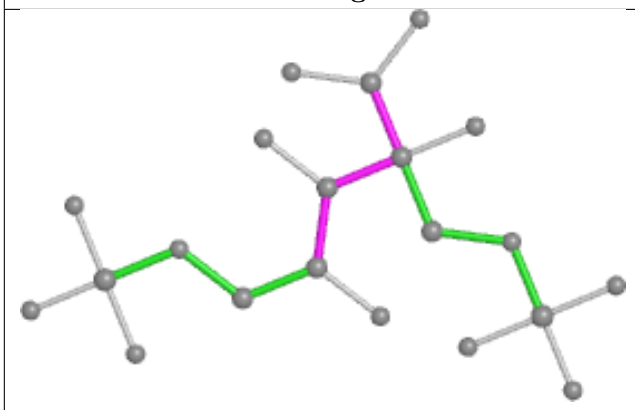
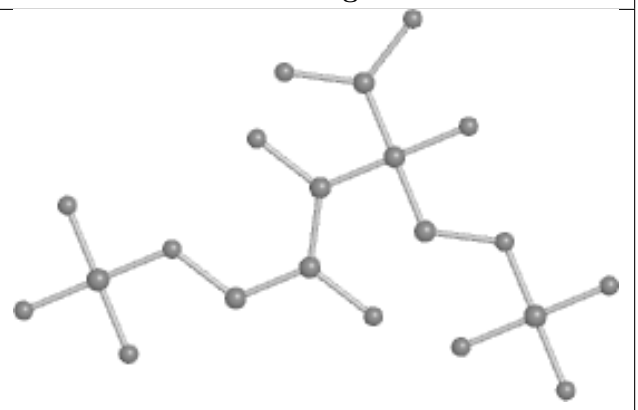


Bond angles

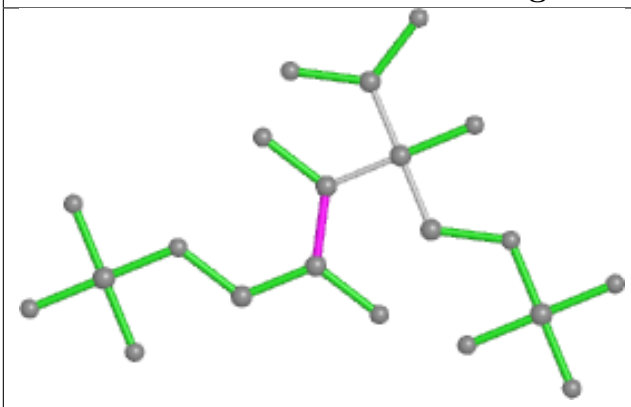


Torsions



Rings

Ligand CAP I 500



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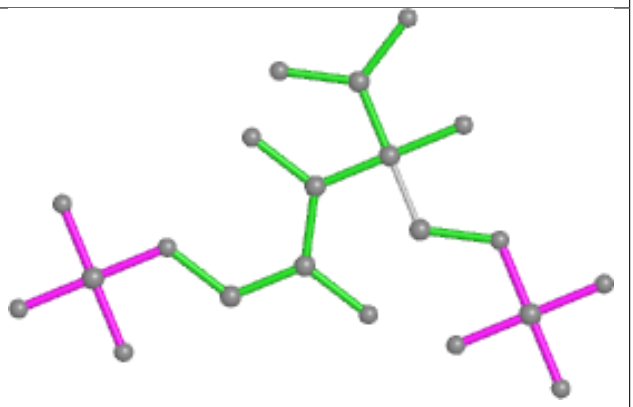
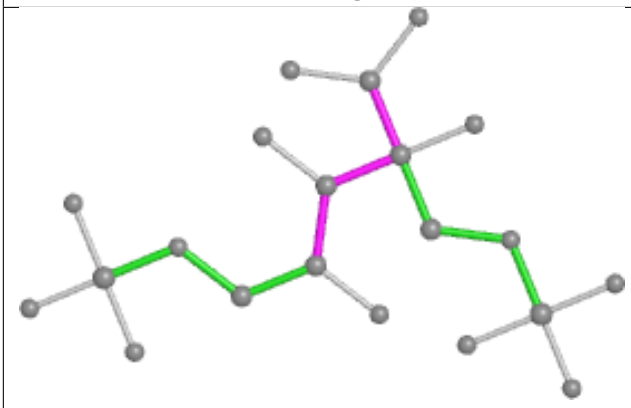
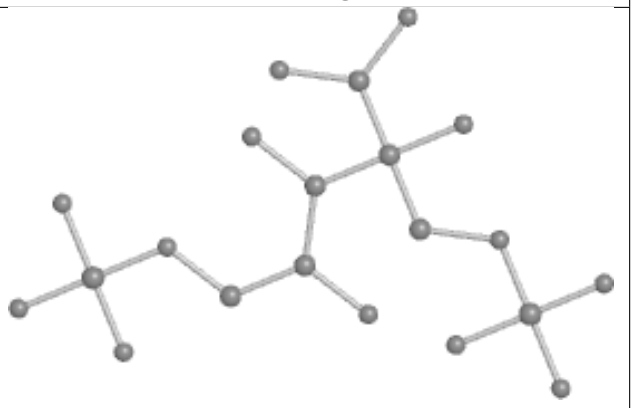


Bond angles

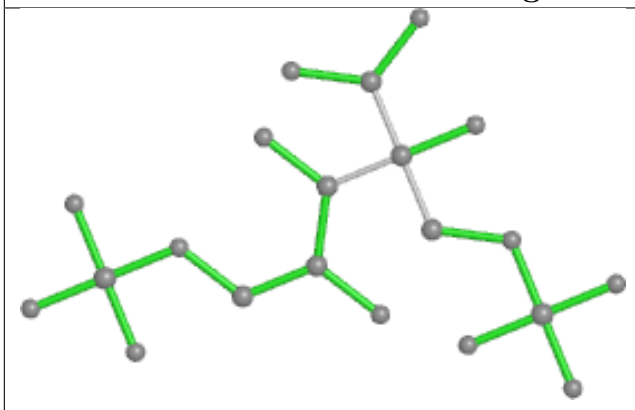


Torsions

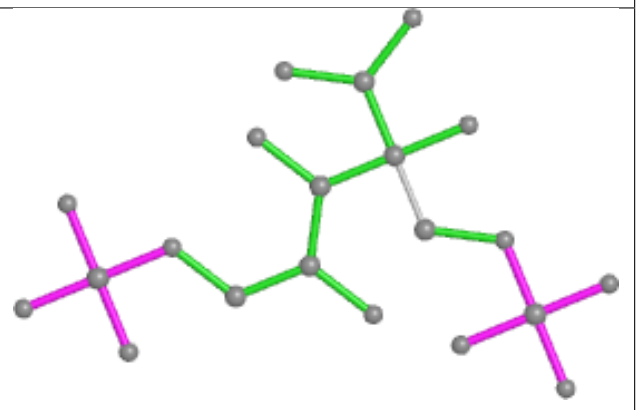


Rings

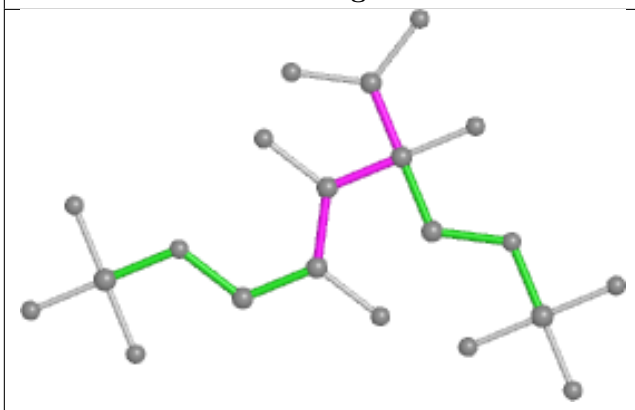
Ligand CAP K 500



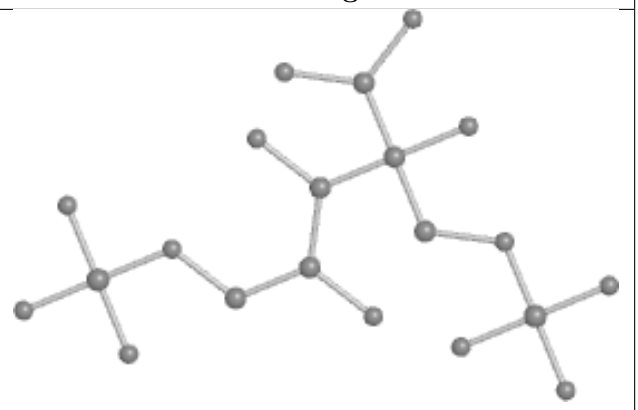
Bond lengths



Bond angles

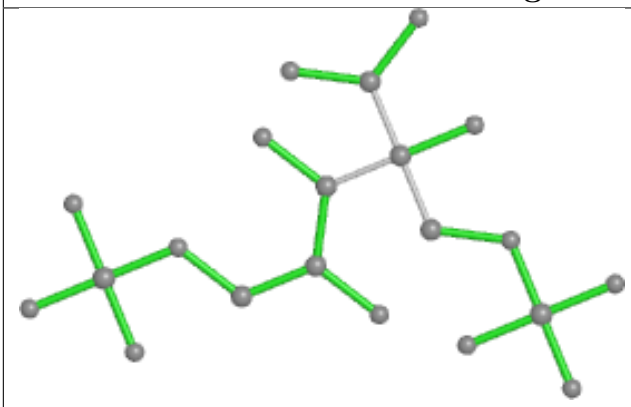


Torsions

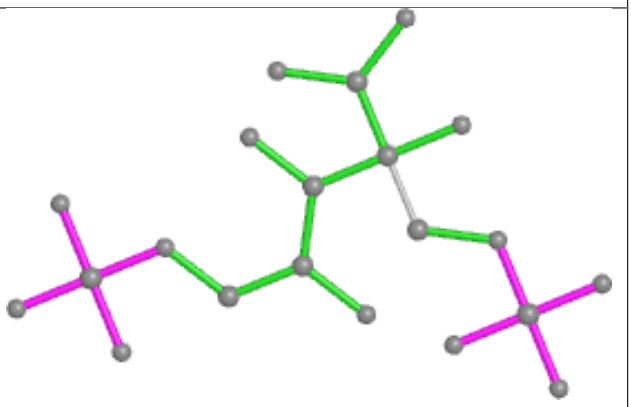


Rings

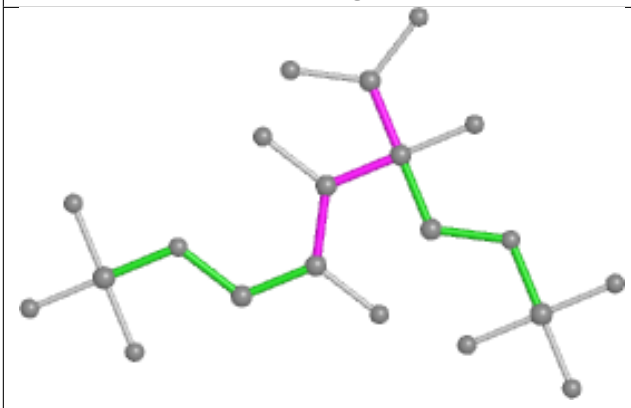
Ligand CAP E 500



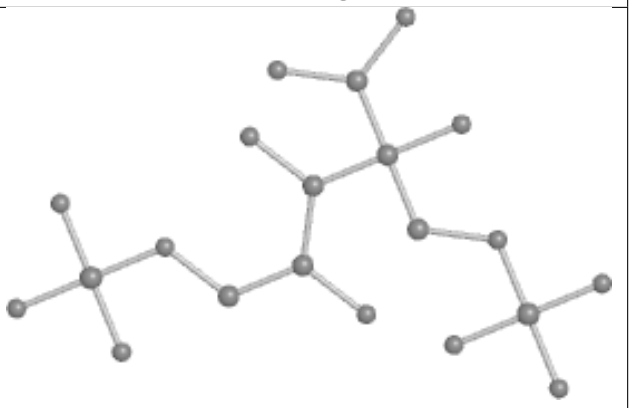
Bond lengths



Bond angles

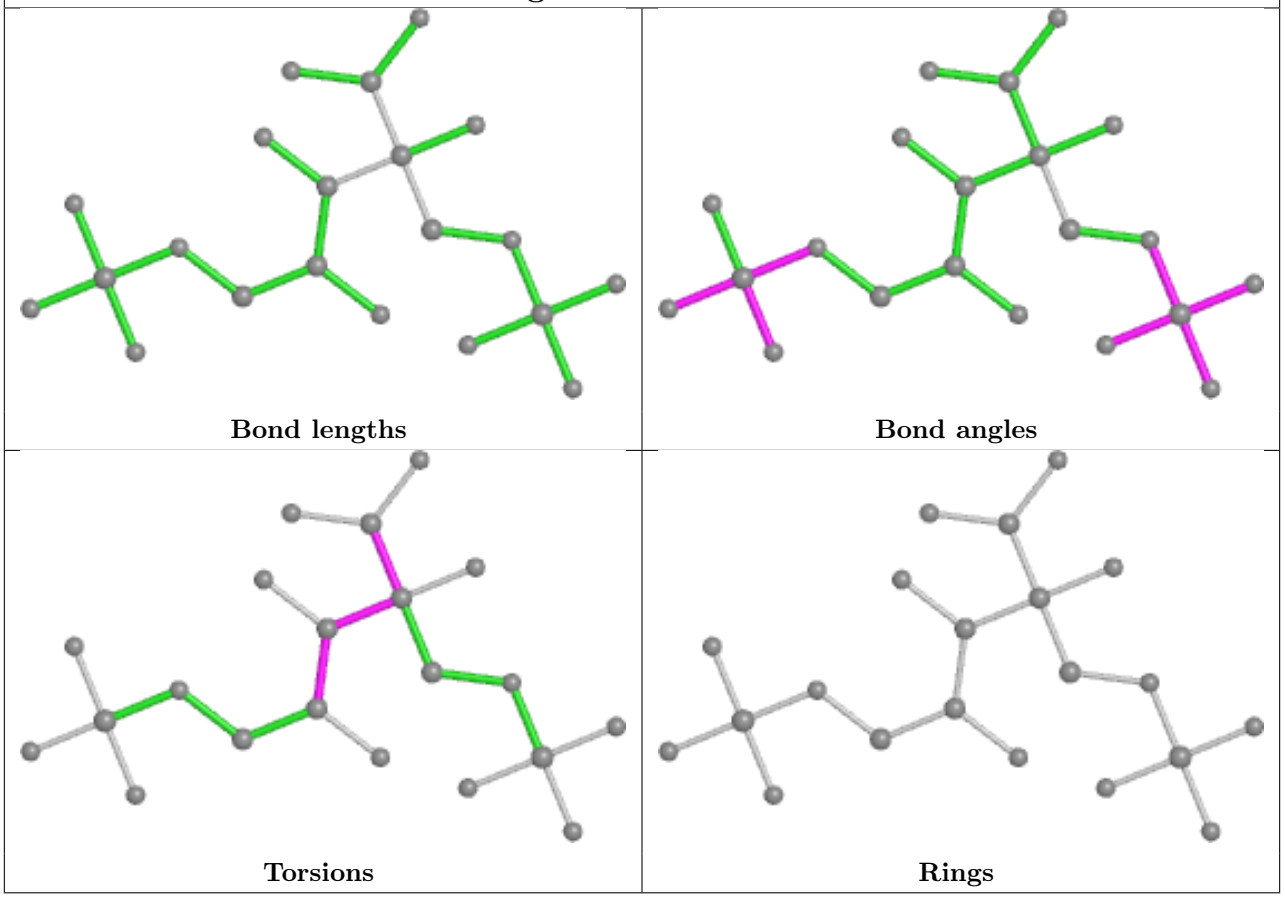


Torsions



Rings

Ligand CAP J 500



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	454/481 (94%)	-0.06	2 (0%)	92	92	28, 39, 57, 85	0
1	B	454/481 (94%)	0.05	7 (1%)	73	72	30, 41, 65, 125	0
1	C	454/481 (94%)	0.09	4 (0%)	84	83	31, 43, 65, 81	0
1	D	454/481 (94%)	0.05	4 (0%)	84	83	29, 41, 61, 105	0
1	E	456/481 (94%)	-0.02	2 (0%)	92	92	28, 39, 60, 81	0
1	F	455/481 (94%)	-0.03	4 (0%)	84	83	29, 38, 55, 74	0
1	G	455/481 (94%)	-0.04	2 (0%)	92	92	28, 37, 54, 76	0
1	H	455/481 (94%)	-0.04	2 (0%)	92	92	27, 37, 57, 82	0
1	I	454/481 (94%)	0.04	4 (0%)	84	83	29, 40, 60, 103	0
1	J	454/481 (94%)	0.10	2 (0%)	92	92	29, 42, 63, 82	0
1	K	454/481 (94%)	0.04	9 (1%)	65	63	30, 43, 67, 116	0
1	L	456/481 (94%)	0.00	4 (0%)	84	83	28, 40, 60, 85	0
All	All	5455/5772 (94%)	0.01	46 (0%)	86	85	27, 40, 61, 125	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	451	ASN	4.0
1	C	449	TYR	3.6
1	D	36	PHE	3.5
1	C	40	ILE	3.2
1	L	441	PHE	3.2

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	J	192	12/13	0.90	0.13	34,36,38,39	0
1	KCX	C	192	12/13	0.91	0.14	33,34,37,38	0
1	KCX	G	192	12/13	0.93	0.13	30,34,38,38	0
1	KCX	A	192	12/13	0.93	0.12	32,33,38,38	0
1	KCX	E	192	12/13	0.95	0.11	30,33,34,35	0
1	KCX	K	192	12/13	0.95	0.10	27,35,38,39	0
1	KCX	L	192	12/13	0.95	0.11	30,36,42,42	0
1	KCX	H	192	12/13	0.96	0.11	27,31,33,33	0
1	KCX	I	192	12/13	0.96	0.11	31,32,35,35	0
1	KCX	B	192	12/13	0.96	0.11	31,34,38,38	0
1	KCX	F	192	12/13	0.96	0.10	29,33,37,38	0
1	KCX	D	192	12/13	0.96	0.12	31,34,39,39	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	501	1/1	0.90	0.06	44,44,44,44	0
3	MG	A	501	1/1	0.94	0.08	37,37,37,37	0
2	CAP	D	500	21/21	0.94	0.11	29,38,42,43	0
2	CAP	C	500	21/21	0.95	0.12	39,44,49,51	0
2	CAP	E	500	21/21	0.96	0.13	33,38,45,47	0
2	CAP	I	500	21/21	0.96	0.12	35,40,45,49	0
2	CAP	J	500	21/21	0.96	0.11	32,45,49,51	0
2	CAP	K	500	21/21	0.96	0.12	31,38,42,43	0
2	CAP	L	500	21/21	0.96	0.11	35,43,48,49	0
2	CAP	A	500	21/21	0.96	0.11	33,38,45,53	0
2	CAP	B	500	21/21	0.96	0.12	31,38,44,44	0
2	CAP	F	500	21/21	0.97	0.12	33,41,44,46	0
2	CAP	G	500	21/21	0.97	0.11	28,35,41,42	0
2	CAP	H	500	21/21	0.97	0.12	27,34,38,42	0

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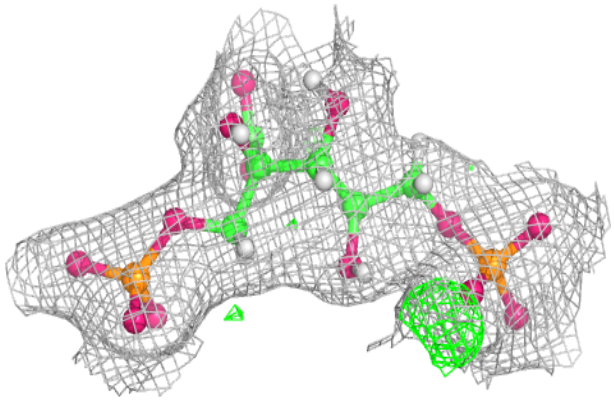
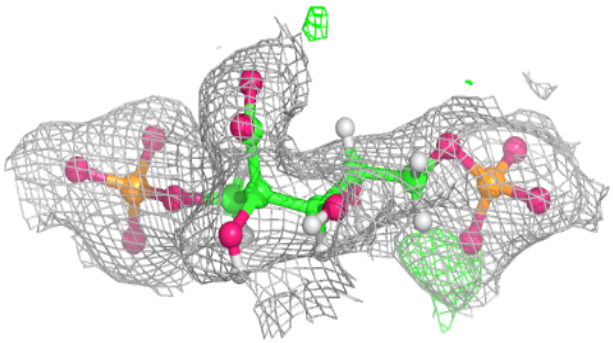
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	G	501	1/1	0.97	0.08	40,40,40,40	0
3	MG	I	501	1/1	0.97	0.07	38,38,38,38	0
3	MG	J	501	1/1	0.97	0.05	38,38,38,38	0
3	MG	L	501	1/1	0.97	0.06	41,41,41,41	0
3	MG	B	501	1/1	0.98	0.05	33,33,33,33	0
3	MG	E	501	1/1	0.98	0.07	33,33,33,33	0
3	MG	F	501	1/1	0.99	0.10	39,39,39,39	0
3	MG	C	501	1/1	0.99	0.08	40,40,40,40	0
3	MG	H	501	1/1	0.99	0.06	30,30,30,30	0
3	MG	K	501	1/1	1.00	0.08	37,37,37,37	0

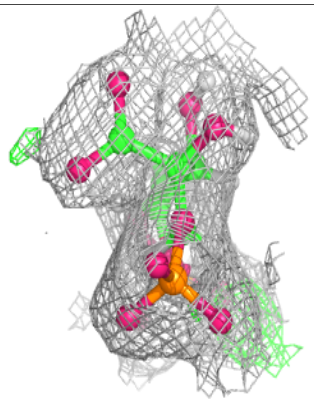
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAP 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)

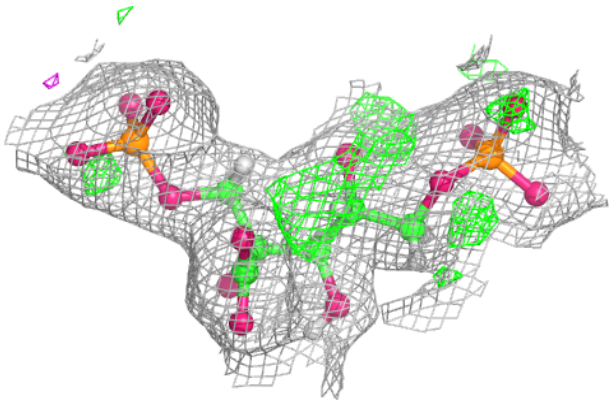


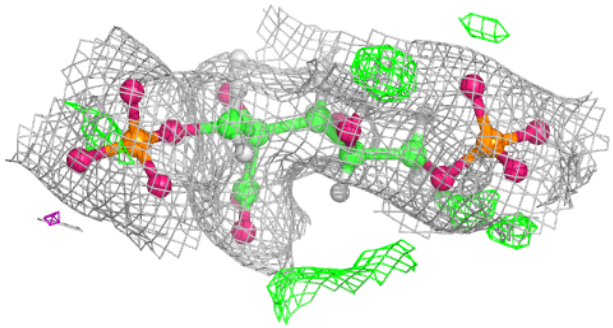


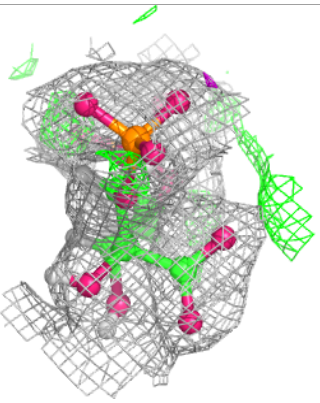


Electron density around CAP C 500:

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

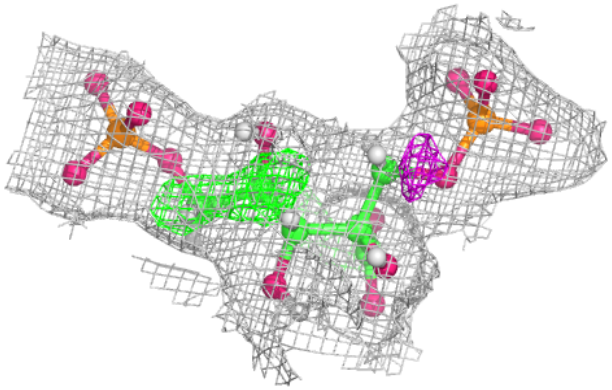


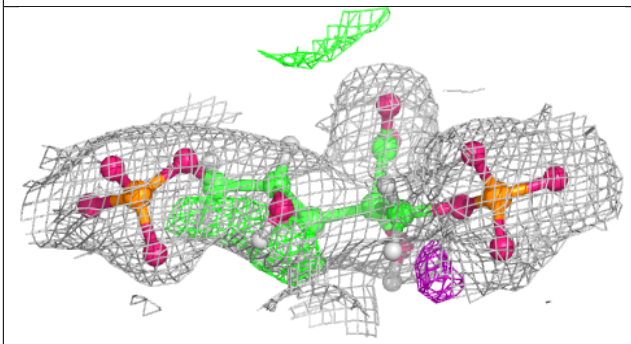


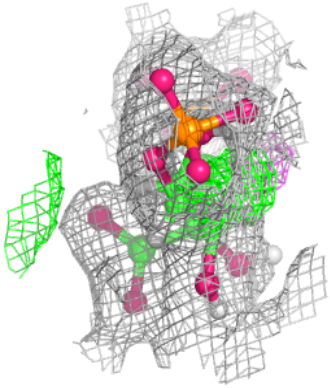


Electron density around CAP E 500:

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

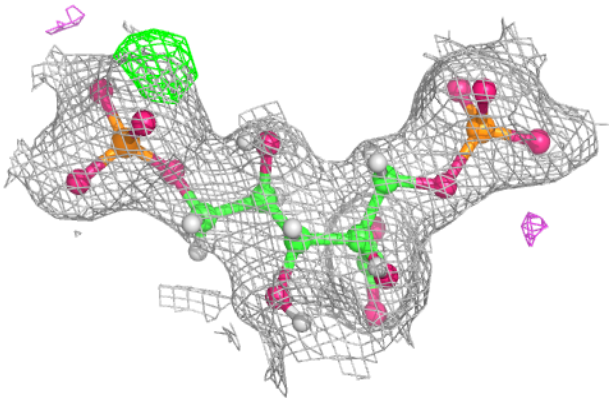


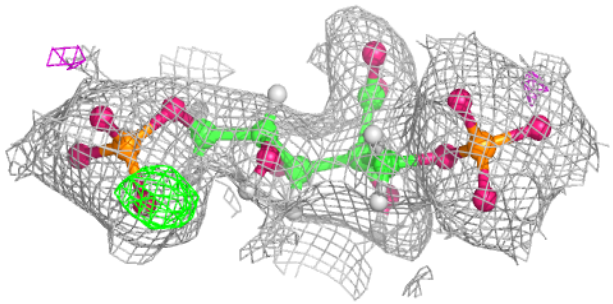


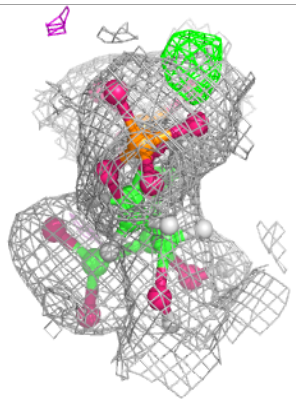


Electron density around CAP I 500:

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

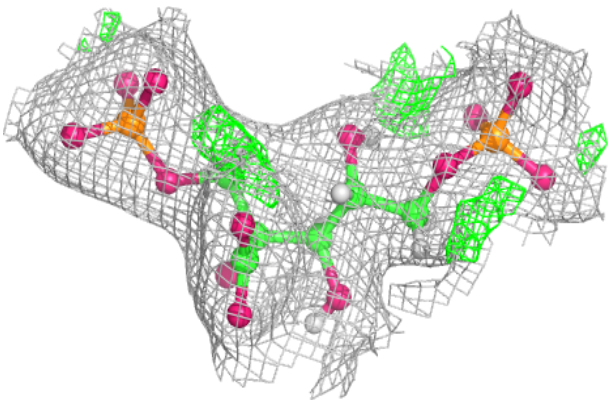


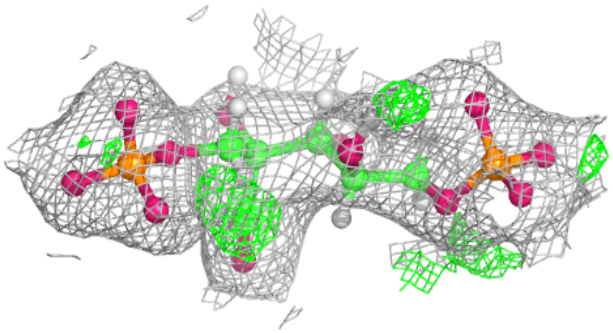


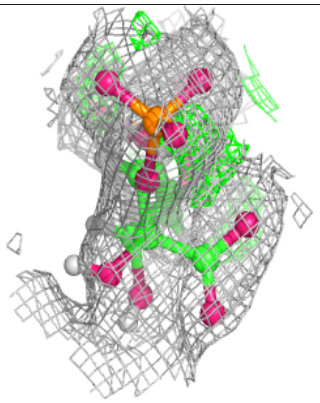


Electron density around CAP J 500:

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

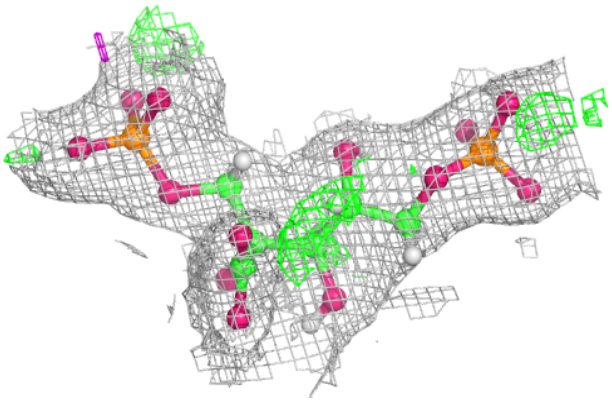


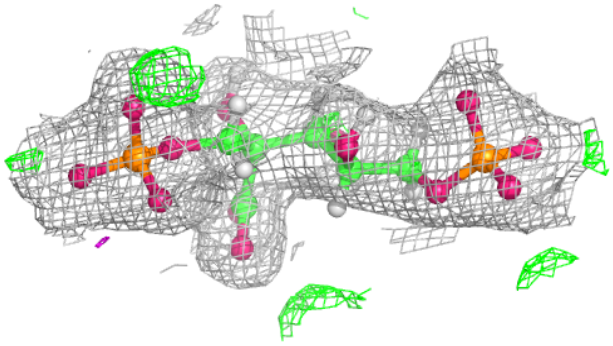


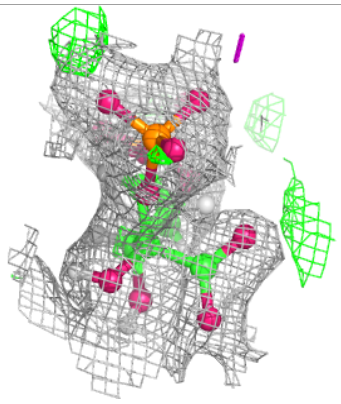


Electron density around CAP K 500:

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

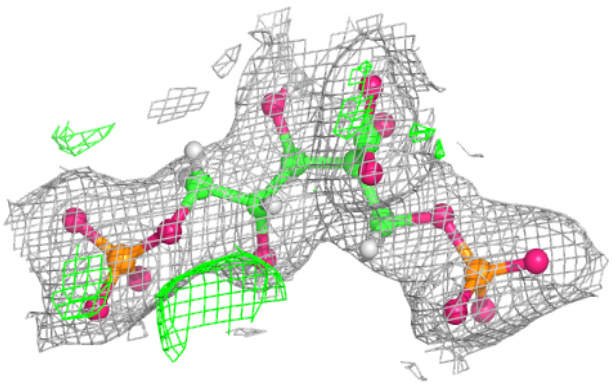


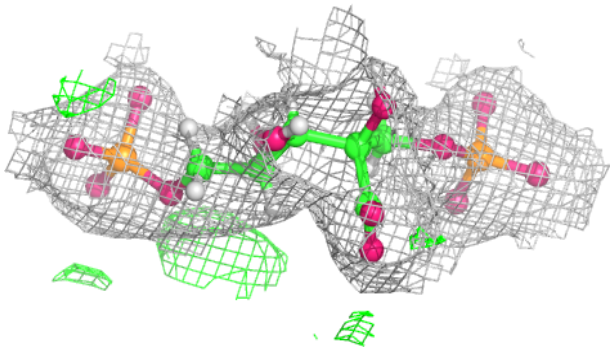


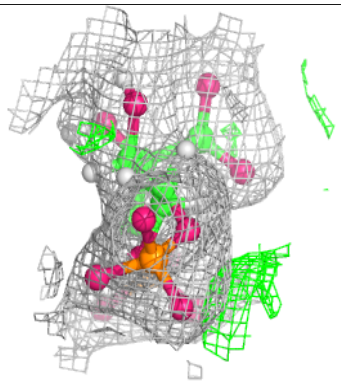


Electron density around CAP L 500:

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

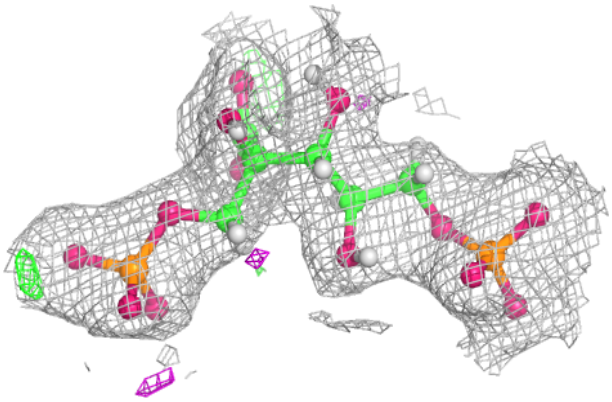


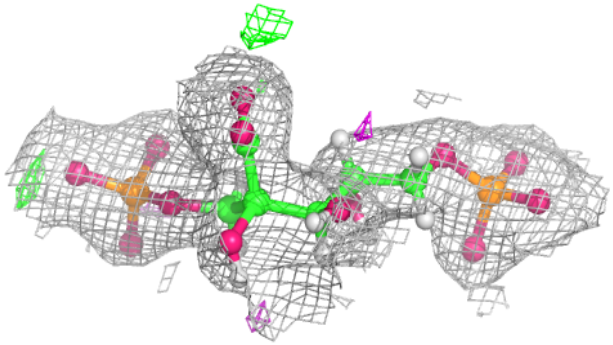


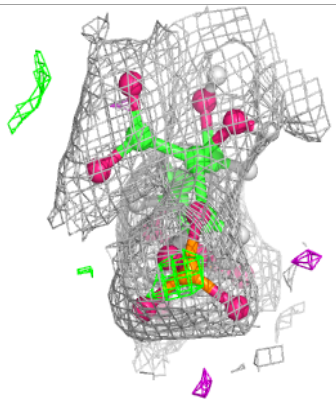


Electron density around CAP A 500:

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

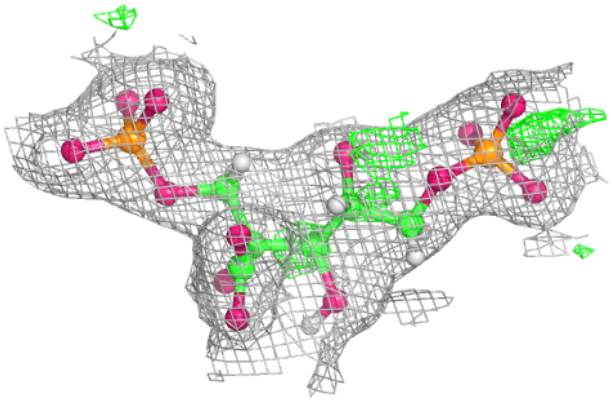


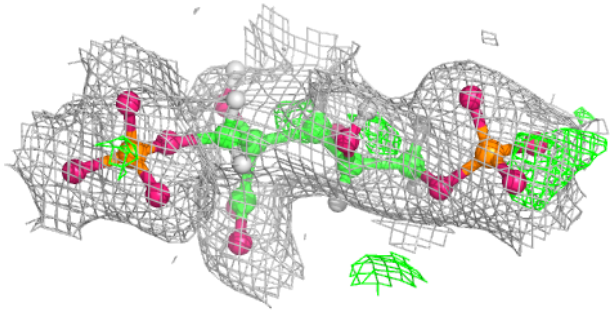


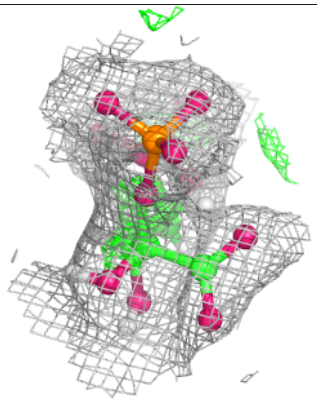


Electron density around CAP B 500:

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

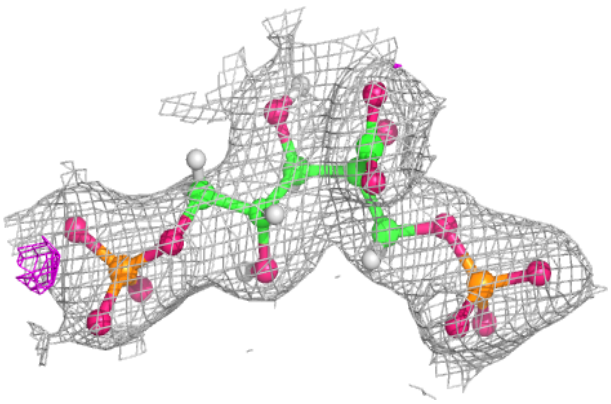


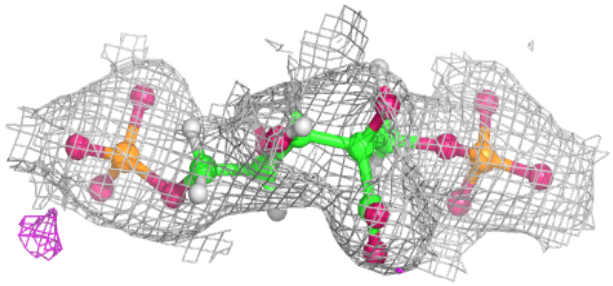


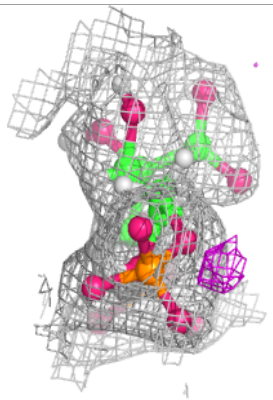


Electron density around CAP F 500:

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

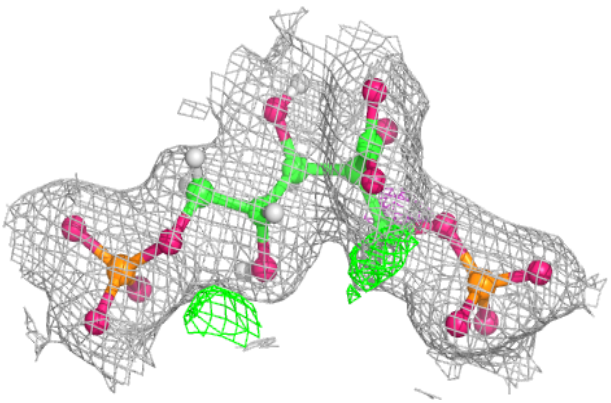


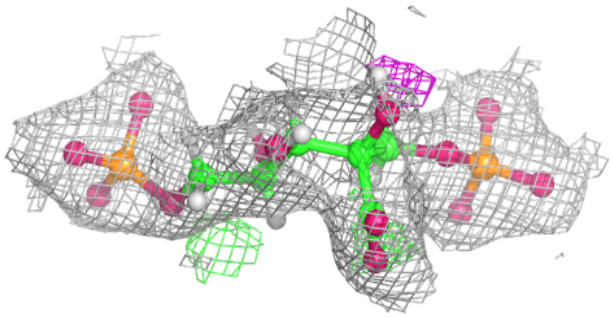


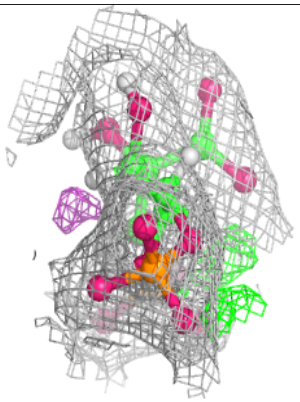


Electron density around CAP G 500:

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

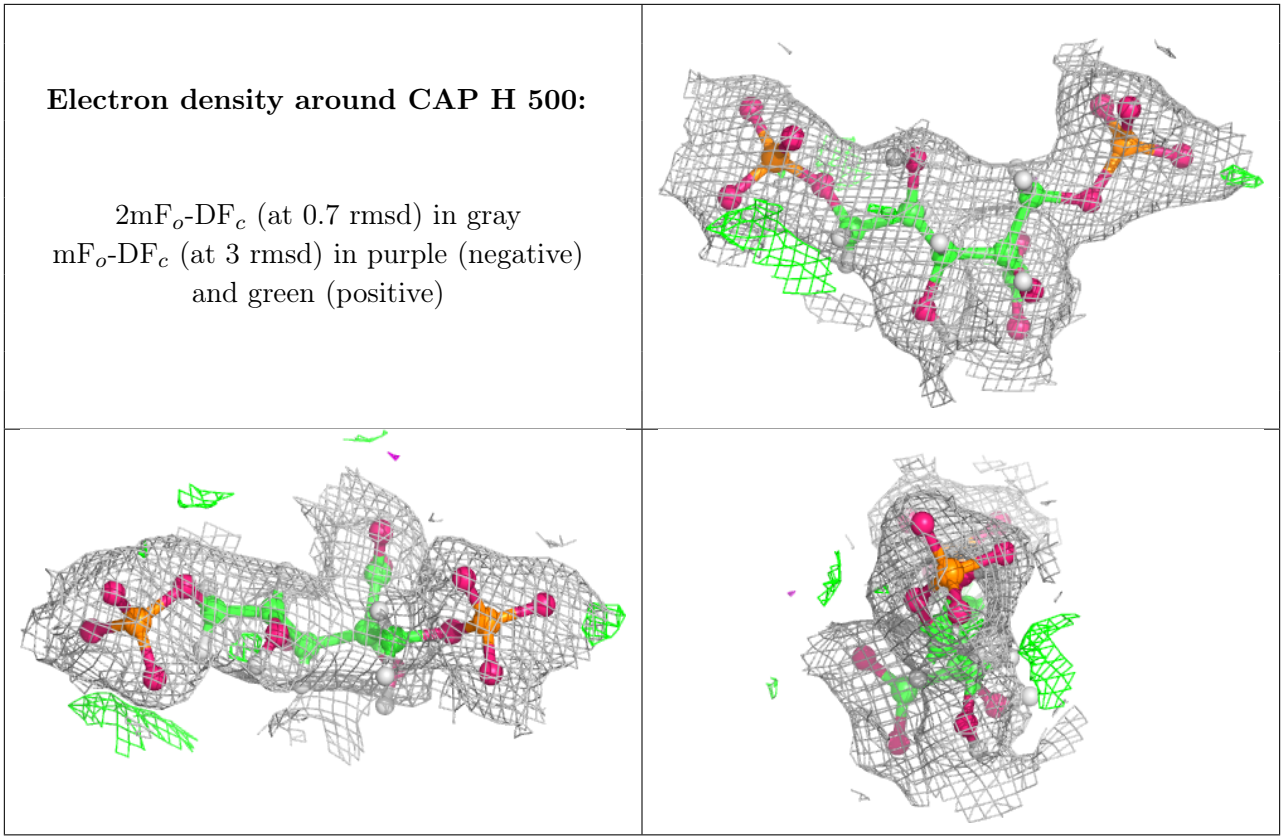






Electron density around CAP H 500:

$2mF_o$-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.