



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 09:38 PM UTC

PDB ID : 1IR2 / pdb_00001ir2
Title : Crystal Structure of Activated Ribulose-1,5-bisphosphate Carboxylase/oxygenase (Rubisco) from Green alga, *Chlamydomonas reinhardtii* Complexed with 2-Carboxyarabinitol-1,5-bisphosphate (2-CABP)
Authors : Mizohata, E.; Matsumura, H.; Okano, Y.; Kumei, M.; Takuma, H.; Onodera, J.; Kato, K.; Shibata, N.; Inoue, T.; Yokota, A.; Kai, Y.
Deposited on : 2001-09-03
Resolution : 1.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) 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

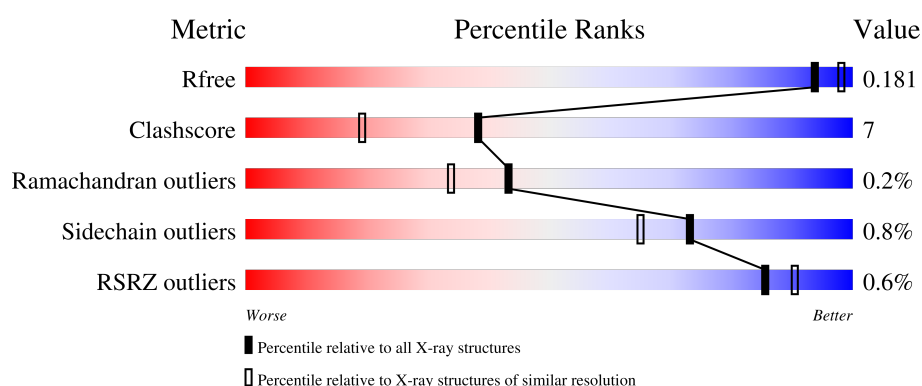
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.



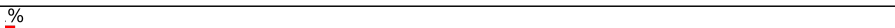
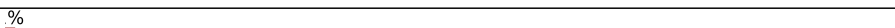
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	475	% 83% 15% ..
1	B	475	% 79% 18% ..
1	C	475	79% 17% ..
1	D	475	% 81% 16% ..
1	E	475	80% 17% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	475	 81% 16% ..
1	G	475	 81% 16% ..
1	H	475	 81% 17% ..
1	S	475	 79% 18% ..
1	T	475	 79% 18% ..
1	U	475	 79% 19% ..
1	V	475	 79% 19% ..
1	W	475	 79% 18% ..
1	X	475	 80% 16% ..
1	Y	475	 77% 19% ..
1	Z	475	 81% 15% ..
2	1	140	 79% 19% ..
2	2	140	 78% 21% .
2	3	140	 74% 22% .
2	4	140	 81% 18% .
2	5	140	 77% 20% .
2	6	140	 79% 19% .
2	7	140	 83% 14% .
2	8	140	 79% 18% .
2	I	140	 81% 16% .
2	J	140	 74% 24% .
2	K	140	 73% 23% .
2	L	140	 76% 20% .
2	M	140	 75% 22% .
2	N	140	 80% 16% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O	140	 78% 21% .
2	P	140	 76% 21% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 87087 atoms, of which 0 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 Large subunit of Rubisco.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3646	2306	641	675	24			
1	B	467	Total	C	N	O	S	0	0	0
			3637	2300	639	674	24			
1	C	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	D	467	Total	C	N	O	S	0	0	0
			3637	2300	639	674	24			
1	E	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	F	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	G	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	H	468	Total	C	N	O	S	0	0	0
			3646	2306	641	675	24			
1	S	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	T	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	U	469	Total	C	N	O	S	0	0	0
			3653	2310	642	677	24			
1	V	469	Total	C	N	O	S	0	0	0
			3653	2310	642	677	24			
1	W	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	X	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			
1	Y	465	Total	C	N	O	S	0	0	0
			3628	2295	637	672	24			
1	Z	466	Total	C	N	O	S	0	0	0
			3632	2297	638	673	24			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	SEE REMARK 999	UNP P00877
A	104	HYP	PRO	modified residue	UNP P00877
A	151	HYP	PRO	modified residue	UNP P00877
A	201	KCX	LYS	modified residue	UNP P00877
A	256	SMC	CYS	modified residue	UNP P00877
A	369	SMC	CYS	modified residue	UNP P00877
B	46	PRO	LEU	SEE REMARK 999	UNP P00877
B	104	HYP	PRO	modified residue	UNP P00877
B	151	HYP	PRO	modified residue	UNP P00877
B	201	KCX	LYS	modified residue	UNP P00877
B	256	SMC	CYS	modified residue	UNP P00877
B	369	SMC	CYS	modified residue	UNP P00877
C	46	PRO	LEU	SEE REMARK 999	UNP P00877
C	104	HYP	PRO	modified residue	UNP P00877
C	151	HYP	PRO	modified residue	UNP P00877
C	201	KCX	LYS	modified residue	UNP P00877
C	256	SMC	CYS	modified residue	UNP P00877
C	369	SMC	CYS	modified residue	UNP P00877
D	46	PRO	LEU	SEE REMARK 999	UNP P00877
D	104	HYP	PRO	modified residue	UNP P00877
D	151	HYP	PRO	modified residue	UNP P00877
D	201	KCX	LYS	modified residue	UNP P00877
D	256	SMC	CYS	modified residue	UNP P00877
D	369	SMC	CYS	modified residue	UNP P00877
E	46	PRO	LEU	SEE REMARK 999	UNP P00877
E	104	HYP	PRO	modified residue	UNP P00877
E	151	HYP	PRO	modified residue	UNP P00877
E	201	KCX	LYS	modified residue	UNP P00877
E	256	SMC	CYS	modified residue	UNP P00877
E	369	SMC	CYS	modified residue	UNP P00877
F	46	PRO	LEU	SEE REMARK 999	UNP P00877
F	104	HYP	PRO	modified residue	UNP P00877
F	151	HYP	PRO	modified residue	UNP P00877
F	201	KCX	LYS	modified residue	UNP P00877
F	256	SMC	CYS	modified residue	UNP P00877
F	369	SMC	CYS	modified residue	UNP P00877
G	46	PRO	LEU	SEE REMARK 999	UNP P00877
G	104	HYP	PRO	modified residue	UNP P00877
G	151	HYP	PRO	modified residue	UNP P00877
G	201	KCX	LYS	modified residue	UNP P00877
G	256	SMC	CYS	modified residue	UNP P00877
G	369	SMC	CYS	modified residue	UNP P00877

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	46	PRO	LEU	SEE REMARK 999	UNP P00877
H	104	HYP	PRO	modified residue	UNP P00877
H	151	HYP	PRO	modified residue	UNP P00877
H	201	KCX	LYS	modified residue	UNP P00877
H	256	SMC	CYS	modified residue	UNP P00877
H	369	SMC	CYS	modified residue	UNP P00877
S	46	PRO	LEU	SEE REMARK 999	UNP P00877
S	104	HYP	PRO	modified residue	UNP P00877
S	151	HYP	PRO	modified residue	UNP P00877
S	201	KCX	LYS	modified residue	UNP P00877
S	256	SMC	CYS	modified residue	UNP P00877
S	369	SMC	CYS	modified residue	UNP P00877
T	46	PRO	LEU	SEE REMARK 999	UNP P00877
T	104	HYP	PRO	modified residue	UNP P00877
T	151	HYP	PRO	modified residue	UNP P00877
T	201	KCX	LYS	modified residue	UNP P00877
T	256	SMC	CYS	modified residue	UNP P00877
T	369	SMC	CYS	modified residue	UNP P00877
U	46	PRO	LEU	SEE REMARK 999	UNP P00877
U	104	HYP	PRO	modified residue	UNP P00877
U	151	HYP	PRO	modified residue	UNP P00877
U	201	KCX	LYS	modified residue	UNP P00877
U	256	SMC	CYS	modified residue	UNP P00877
U	369	SMC	CYS	modified residue	UNP P00877
V	46	PRO	LEU	SEE REMARK 999	UNP P00877
V	104	HYP	PRO	modified residue	UNP P00877
V	151	HYP	PRO	modified residue	UNP P00877
V	201	KCX	LYS	modified residue	UNP P00877
V	256	SMC	CYS	modified residue	UNP P00877
V	369	SMC	CYS	modified residue	UNP P00877
W	46	PRO	LEU	SEE REMARK 999	UNP P00877
W	104	HYP	PRO	modified residue	UNP P00877
W	151	HYP	PRO	modified residue	UNP P00877
W	201	KCX	LYS	modified residue	UNP P00877
W	256	SMC	CYS	modified residue	UNP P00877
W	369	SMC	CYS	modified residue	UNP P00877
X	46	PRO	LEU	SEE REMARK 999	UNP P00877
X	104	HYP	PRO	modified residue	UNP P00877
X	151	HYP	PRO	modified residue	UNP P00877
X	201	KCX	LYS	modified residue	UNP P00877
X	256	SMC	CYS	modified residue	UNP P00877
X	369	SMC	CYS	modified residue	UNP P00877

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	46	PRO	LEU	SEE REMARK 999	UNP P00877
Y	104	HYP	PRO	modified residue	UNP P00877
Y	151	HYP	PRO	modified residue	UNP P00877
Y	201	KCX	LYS	modified residue	UNP P00877
Y	256	SMC	CYS	modified residue	UNP P00877
Y	369	SMC	CYS	modified residue	UNP P00877
Z	46	PRO	LEU	SEE REMARK 999	UNP P00877
Z	104	HYP	PRO	modified residue	UNP P00877
Z	151	HYP	PRO	modified residue	UNP P00877
Z	201	KCX	LYS	modified residue	UNP P00877
Z	256	SMC	CYS	modified residue	UNP P00877
Z	369	SMC	CYS	modified residue	UNP P00877

- Molecule 2 is a protein called Small subunit of Rubisco.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	J	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	K	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	L	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	M	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	N	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	O	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	P	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	1	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	2	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	3	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	4	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	5	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	6	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	7	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			
2	8	140	Total	C	N	O	S	0	0	0
			1145	739	191	204	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	MME	MET	modified residue	UNP P08475
J	1	MME	MET	modified residue	UNP P08475
K	1	MME	MET	modified residue	UNP P08475
L	1	MME	MET	modified residue	UNP P08475
M	1	MME	MET	modified residue	UNP P08475
N	1	MME	MET	modified residue	UNP P08475
O	1	MME	MET	modified residue	UNP P08475
P	1	MME	MET	modified residue	UNP P08475
1	1	MME	MET	modified residue	UNP P08475
2	1	MME	MET	modified residue	UNP P08475
3	1	MME	MET	modified residue	UNP P08475
4	1	MME	MET	modified residue	UNP P08475
5	1	MME	MET	modified residue	UNP P08475
6	1	MME	MET	modified residue	UNP P08475
7	1	MME	MET	modified residue	UNP P08475
8	1	MME	MET	modified residue	UNP P08475

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

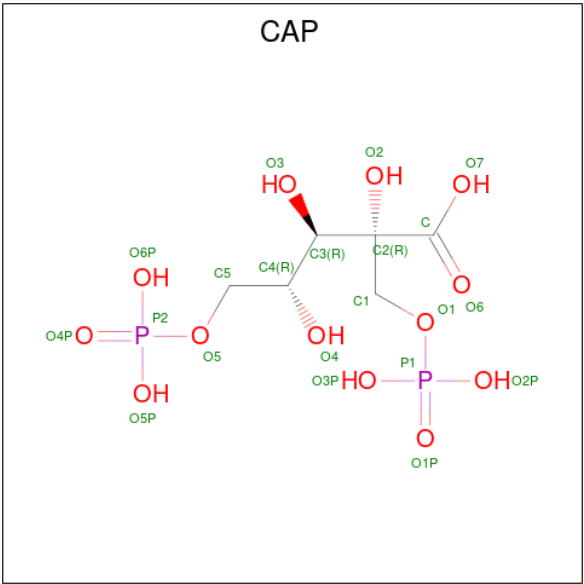
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	S	1	Total	Mg	0	0
			1	1		
3	T	1	Total	Mg	0	0
			1	1		
3	U	1	Total	Mg	0	0
			1	1		
3	V	1	Total	Mg	0	0
			1	1		
3	W	1	Total	Mg	0	0
			1	1		
3	X	1	Total	Mg	0	0
			1	1		
3	Y	1	Total	Mg	0	0
			1	1		
3	Z	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: C₆H₁₄O₁₃P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	C	1	Total	C	O	P	0	0
			21	6	13	2		
4	D	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	F	1	Total	C	O	P	0	0
			21	6	13	2		
4	G	1	Total	C	O	P	0	0
			21	6	13	2		
4	H	1	Total	C	O	P	0	0
			21	6	13	2		
4	S	1	Total	C	O	P	0	0
			21	6	13	2		
4	T	1	Total	C	O	P	0	0
			21	6	13	2		
4	U	1	Total	C	O	P	0	0
			21	6	13	2		
4	V	1	Total	C	O	P	0	0
			21	6	13	2		
4	W	1	Total	C	O	P	0	0
			21	6	13	2		
4	X	1	Total	C	O	P	0	0
			21	6	13	2		
4	Y	1	Total	C	O	P	0	0
			21	6	13	2		
4	Z	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	H	1	Total 6	C 3	O 3	0	0
5	H	1	Total 6	C 3	O 3	0	0
5	H	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	U	1	Total 6	C 3	O 3	0	0
5	U	1	Total 6	C 3	O 3	0	0
5	V	1	Total 6	C 3	O 3	0	0
5	V	1	Total 6	C 3	O 3	0	0
5	W	1	Total 6	C 3	O 3	0	0
5	W	1	Total 6	C 3	O 3	0	0
5	X	1	Total 6	C 3	O 3	0	0
5	X	1	Total 6	C 3	O 3	0	0
5	X	1	Total 6	C 3	O 3	0	0
5	Y	1	Total 6	C 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	Y	1	Total	C	O	0	0
			6	3	3		
5	Y	1	Total	C	O	0	0
			6	3	3		
5	Z	1	Total	C	O	0	0
			6	3	3		
5	Z	1	Total	C	O	0	0
			6	3	3		
5	Z	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	459	Total	O	0	0
			459	459		
6	I	172	Total	O	0	0
			172	172		
6	B	406	Total	O	0	0
			406	406		
6	J	170	Total	O	0	0
			170	170		
6	C	478	Total	O	0	0
			478	478		
6	K	187	Total	O	0	0
			187	187		
6	D	480	Total	O	0	0
			480	480		
6	L	186	Total	O	0	0
			186	186		
6	E	463	Total	O	0	0
			463	463		
6	M	181	Total	O	0	0
			181	181		
6	F	450	Total	O	0	0
			450	450		
6	N	186	Total	O	0	0
			186	186		
6	G	466	Total	O	0	0
			466	466		
6	O	179	Total	O	0	0
			179	179		

Continued on next page...

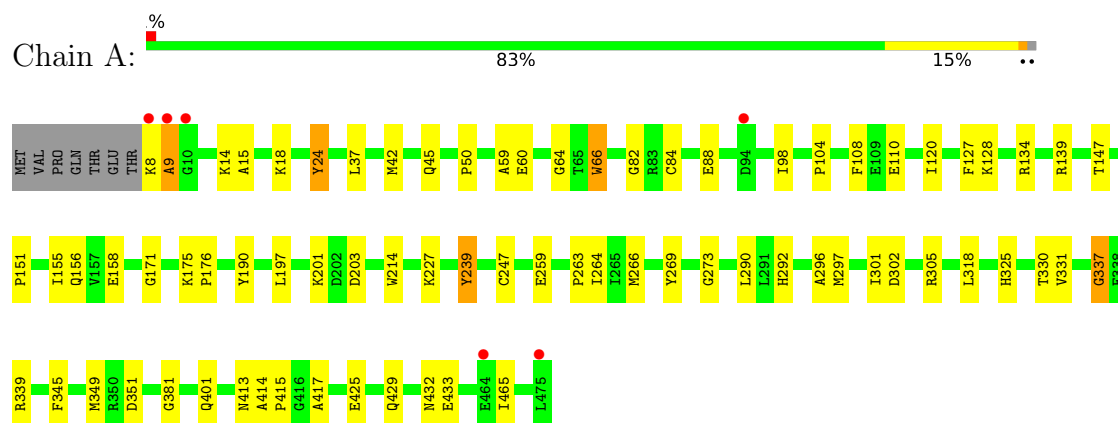
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	452	Total 452	O 452	0	0
6	P	200	Total 200	O 200	0	0
6	S	425	Total 425	O 425	0	0
6	1	173	Total 173	O 173	0	0
6	T	426	Total 426	O 426	0	0
6	2	173	Total 173	O 173	0	0
6	U	427	Total 427	O 427	0	0
6	3	170	Total 170	O 170	0	0
6	V	456	Total 456	O 456	0	0
6	4	174	Total 174	O 174	0	0
6	W	421	Total 421	O 421	0	0
6	5	174	Total 174	O 174	0	0
6	X	450	Total 450	O 450	0	0
6	6	146	Total 146	O 146	0	0
6	Y	426	Total 426	O 426	0	0
6	7	184	Total 184	O 184	0	0
6	Z	474	Total 474	O 474	0	0
6	8	185	Total 185	O 185	0	0

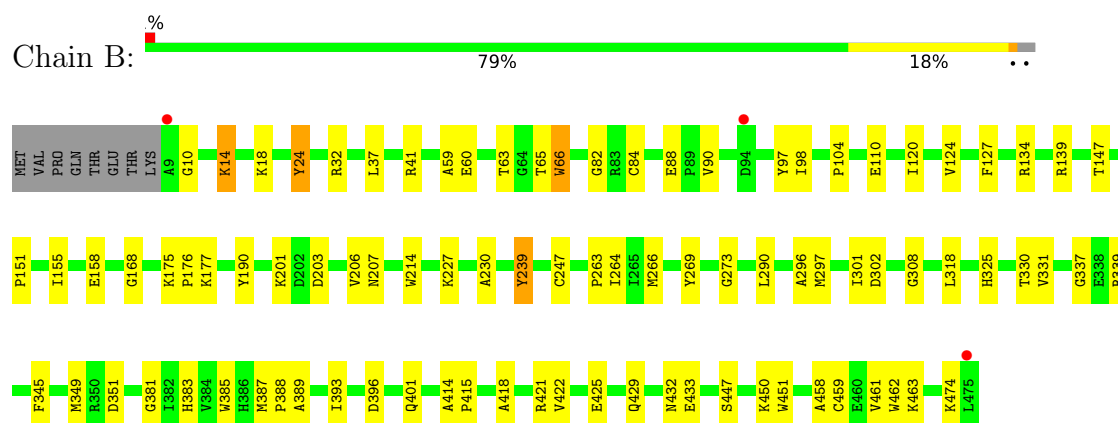
3 Residue-property plots [i](#)

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.

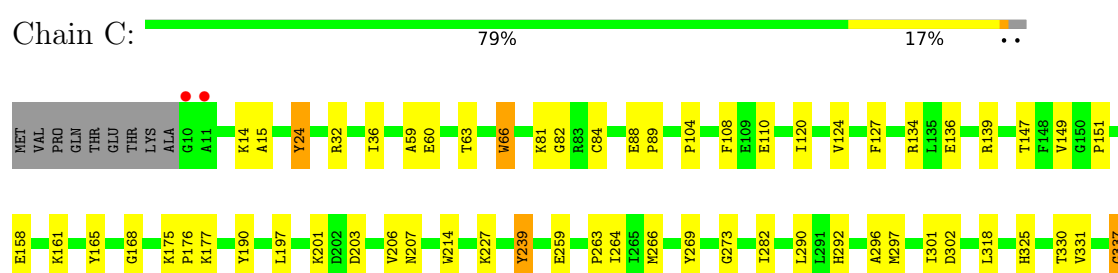
• Molecule 1: Large subunit of Rubisco



• Molecule 1: Large subunit of Rubisco

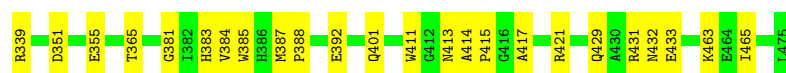
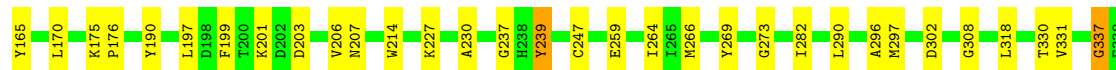
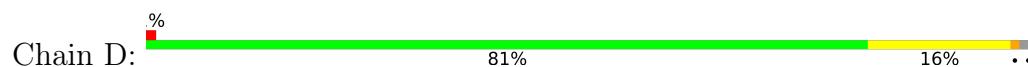


• Molecule 1: Large subunit of Rubisco

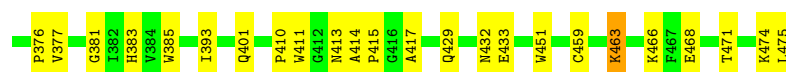
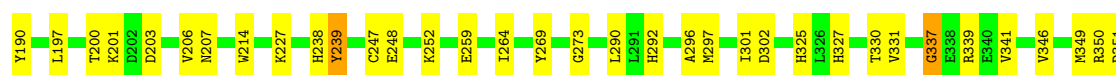
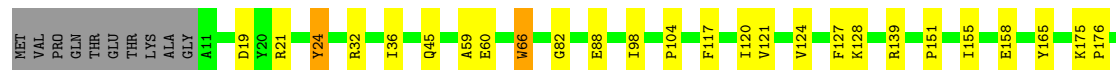
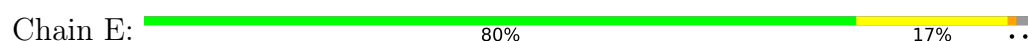




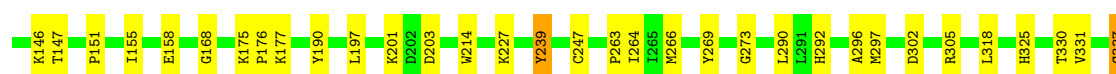
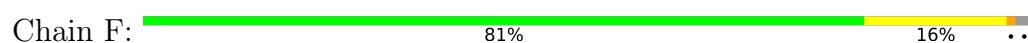
- Molecule 1: Large subunit of Rubisco



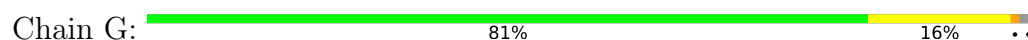
- Molecule 1: Large subunit of Rubisco

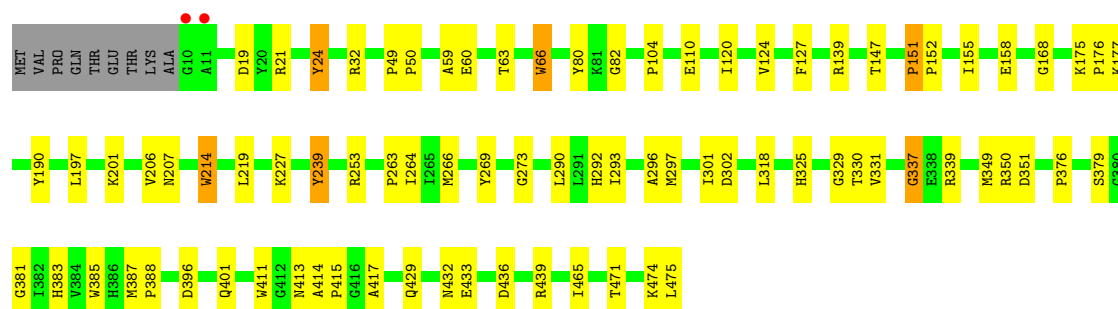


- Molecule 1: Large subunit of Rubisco

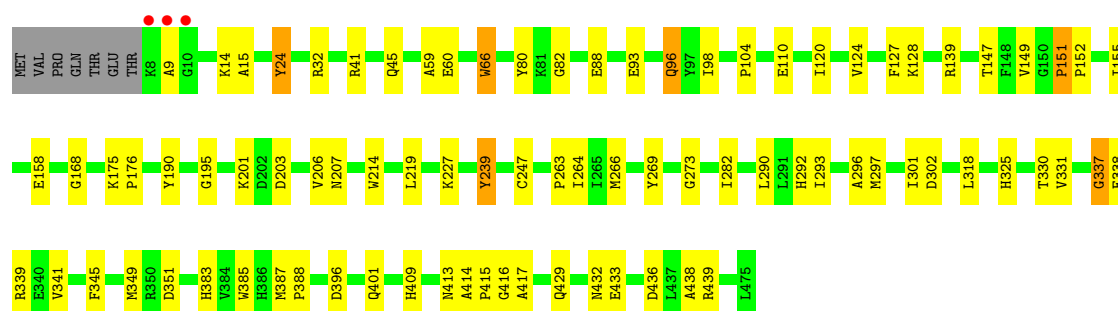
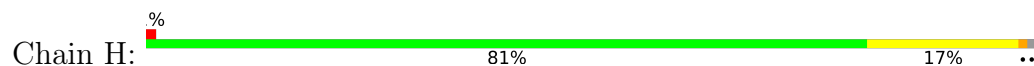


- Molecule 1: Large subunit of Rubisco

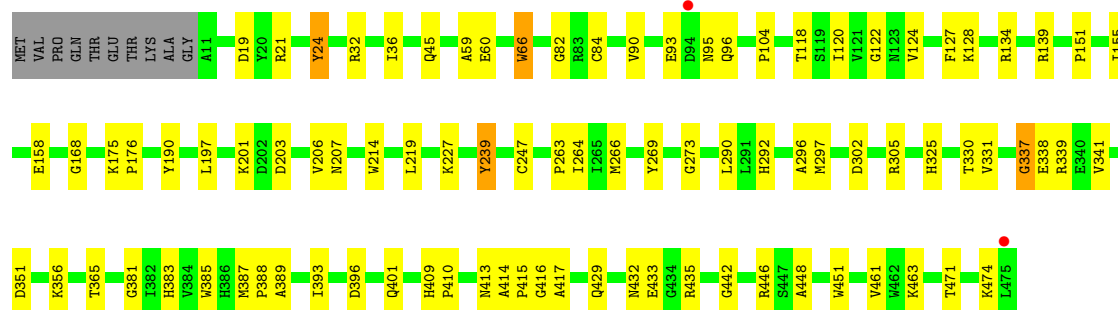
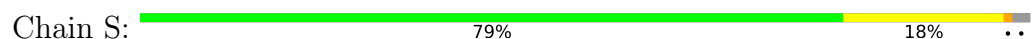




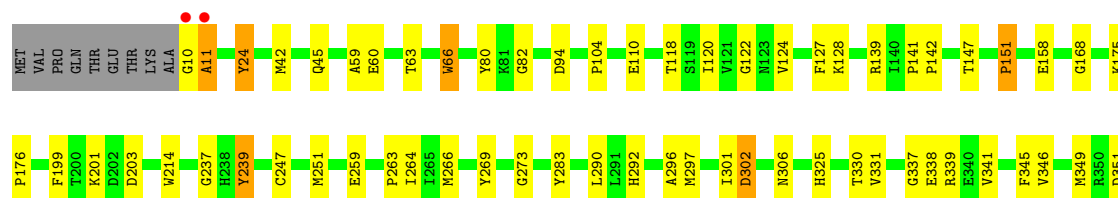
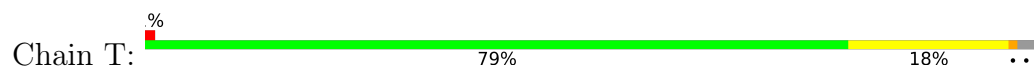
- Molecule 1: Large subunit of Rubisco



- Molecule 1: Large subunit of Rubisco

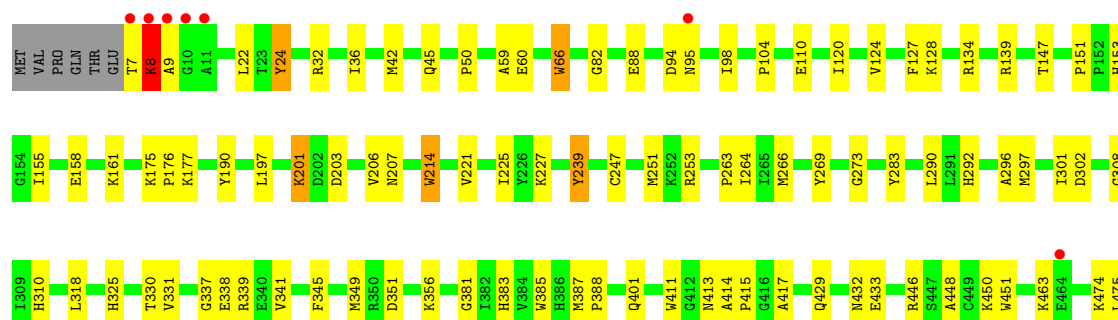
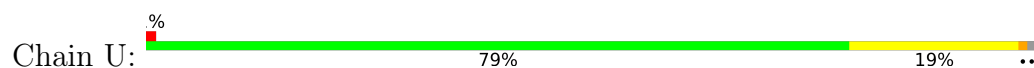


- Molecule 1: Large subunit of Rubisco

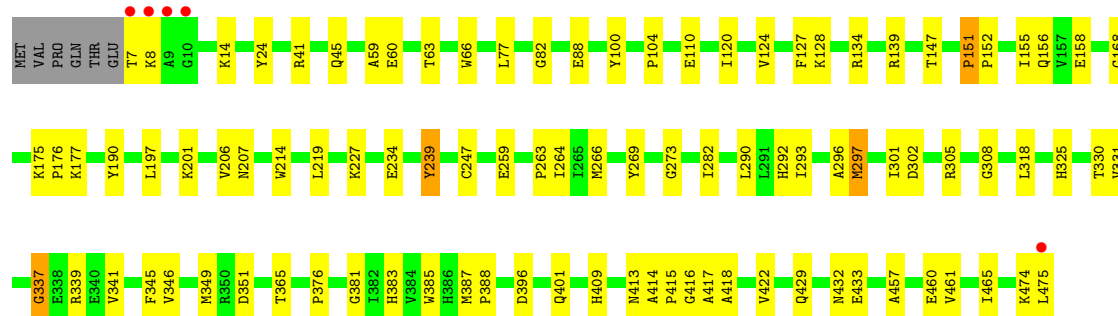
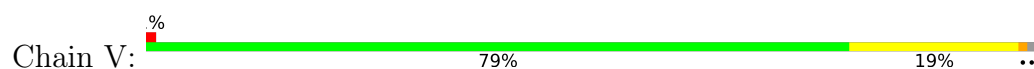




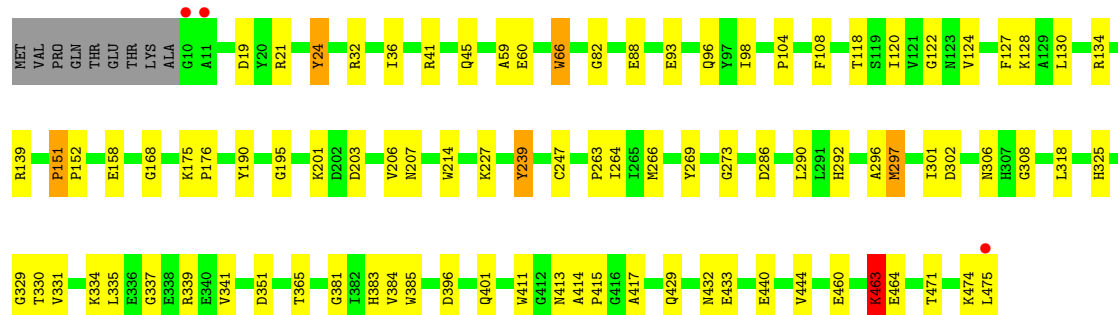
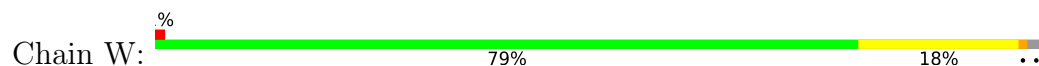
- Molecule 1: Large subunit of Rubisco



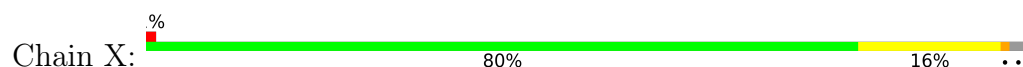
- Molecule 1: Large subunit of Rubisco

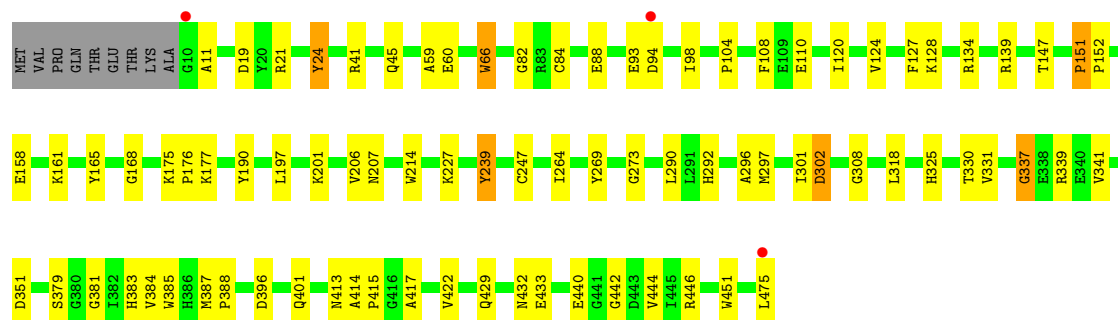


- Molecule 1: Large subunit of Rubisco

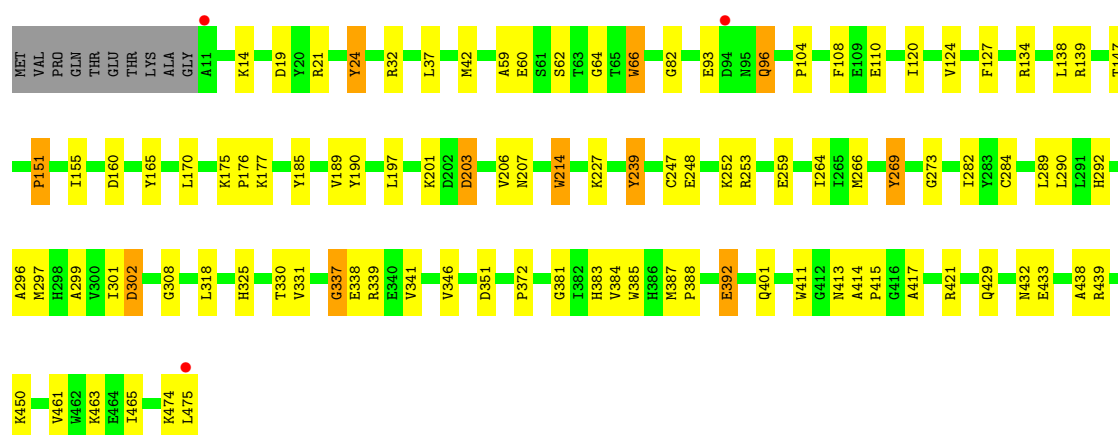
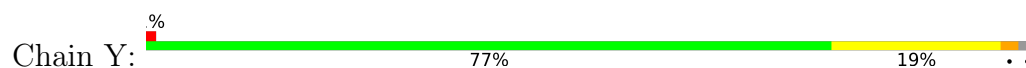


- Molecule 1: Large subunit of Rubisco

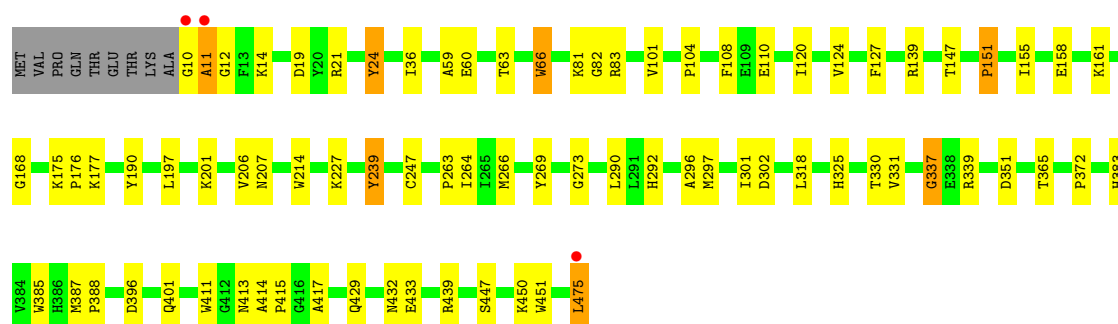
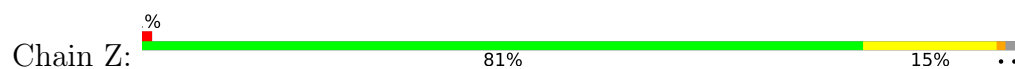




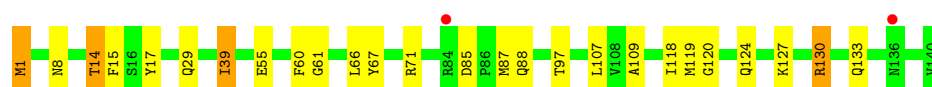
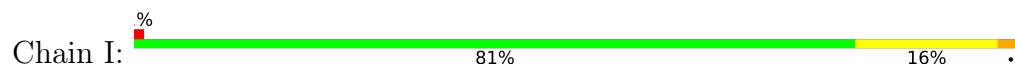
• Molecule 1: Large subunit of Rubisco



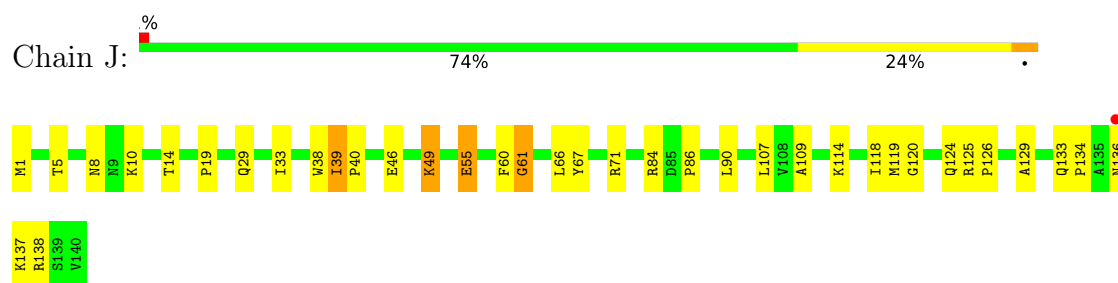
• Molecule 1: Large subunit of Rubisco



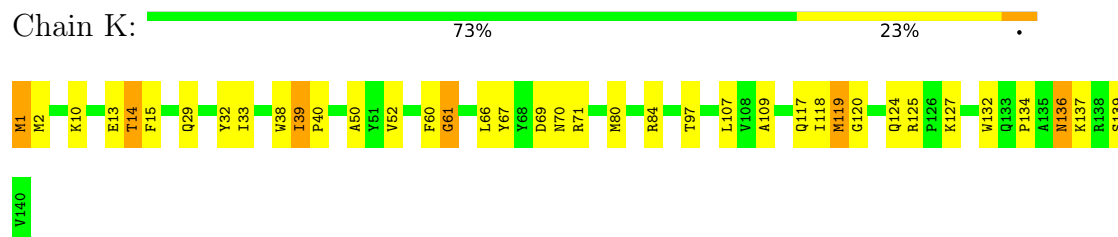
• Molecule 2: Small subunit of Rubisco



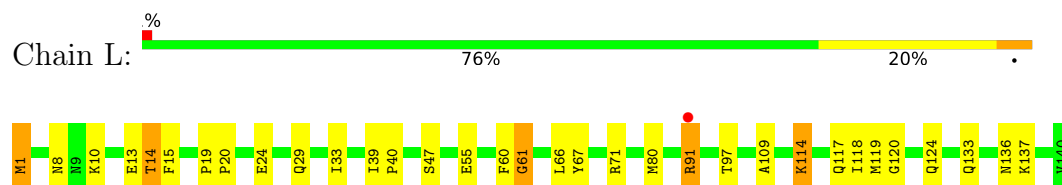
• Molecule 2: Small subunit of Rubisco



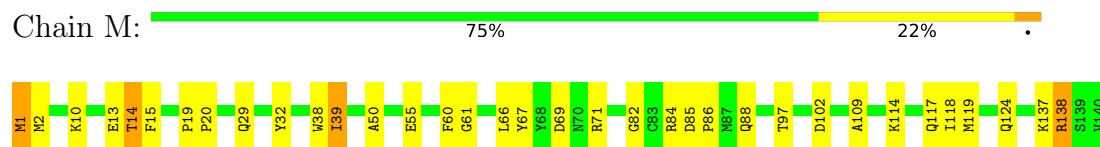
- Molecule 2: Small subunit of Rubisco



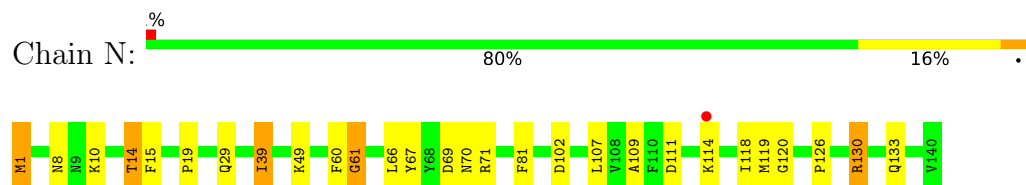
- Molecule 2: Small subunit of Rubisco



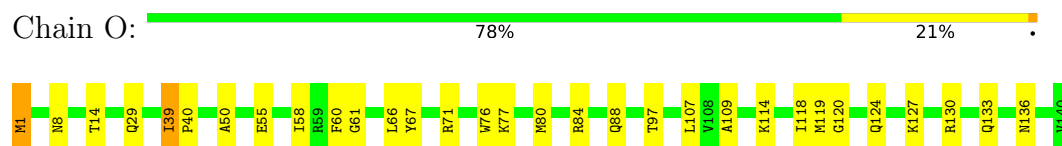
- Molecule 2: Small subunit of Rubisco



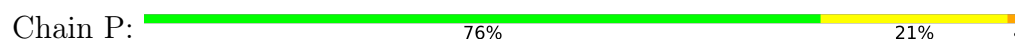
- Molecule 2: Small subunit of Rubisco



- Molecule 2: Small subunit of Rubisco



- Molecule 2: Small subunit of Rubisco





- Molecule 2: Small subunit of Rubisco

Chain 1: 79% 19% ..



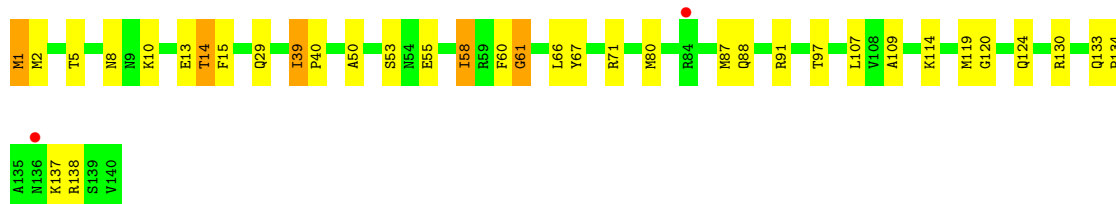
- Molecule 2: Small subunit of Rubisco

Chain 2: 78% 21% .



- Molecule 2: Small subunit of Rubisco

Chain 3: 74% 22% .



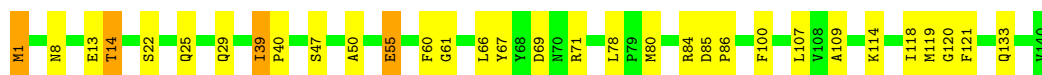
- Molecule 2: Small subunit of Rubisco

Chain 4: 81% 18% .



- Molecule 2: Small subunit of Rubisco

Chain 5: 77% 20% .



- Molecule 2: Small subunit of Rubisco

Chain 6: 79% 19% .



- Molecule 2: Small subunit of Rubisco

Chain 7:

83%

14%

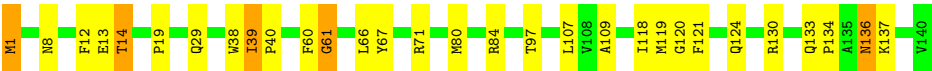


● Molecule 2: Small subunit of Rubisco

Chain 8:

79%

18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.17Å 174.75Å 222.27Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	39.89 – 1.84 39.89 – 1.84	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.89-1.84) 90.7 (39.89-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.84Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.152 , 0.181 0.152 , 0.181	Depositor DCC
R_{free} test set	37921 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	87087	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HYP, CAP, MME, KCX, SMC, 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	0.35	0/3684	0.93	19/4978 (0.4%)
1	B	0.35	0/3675	0.93	17/4967 (0.3%)
1	C	0.34	0/3670	0.94	22/4960 (0.4%)
1	D	0.35	0/3675	0.92	18/4967 (0.4%)
1	E	0.35	0/3666	0.94	19/4955 (0.4%)
1	F	0.34	0/3666	0.92	18/4955 (0.4%)
1	G	0.35	0/3670	0.93	19/4960 (0.4%)
1	H	0.35	0/3684	0.93	19/4978 (0.4%)
1	S	0.35	0/3666	0.93	18/4955 (0.4%)
1	T	0.35	0/3670	0.93	21/4960 (0.4%)
1	U	0.35	0/3691	0.92	18/4988 (0.4%)
1	V	0.35	0/3691	0.94	18/4988 (0.4%)
1	W	0.34	0/3670	0.92	22/4960 (0.4%)
1	X	0.35	0/3670	0.91	17/4960 (0.3%)
1	Y	0.35	0/3666	0.94	22/4955 (0.4%)
1	Z	0.36	0/3670	0.93	18/4960 (0.4%)
2	1	0.34	0/1169	0.94	7/1588 (0.4%)
2	2	0.35	0/1169	0.91	4/1588 (0.3%)
2	3	0.35	0/1169	0.95	7/1588 (0.4%)
2	4	0.34	0/1169	0.93	7/1588 (0.4%)
2	5	0.33	0/1169	0.97	10/1588 (0.6%)
2	6	0.34	0/1169	0.91	5/1588 (0.3%)
2	7	0.35	0/1169	0.94	6/1588 (0.4%)
2	8	0.35	0/1169	0.92	5/1588 (0.3%)
2	I	0.33	0/1169	0.92	6/1588 (0.4%)
2	J	0.33	0/1169	0.96	7/1588 (0.4%)
2	K	0.34	0/1169	0.92	6/1588 (0.4%)
2	L	0.33	0/1169	0.94	7/1588 (0.4%)
2	M	0.35	0/1169	0.94	7/1588 (0.4%)
2	N	0.34	0/1169	0.94	6/1588 (0.4%)
2	O	0.35	0/1169	0.96	8/1588 (0.5%)
2	P	0.35	0/1169	0.96	6/1588 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.35	0/77488	0.93	409/104854 (0.4%)

There are no bond length outliers.

The worst 5 of 409 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	61	GLY	N-CA-C	-10.01	98.13	112.55
2	1	61	GLY	N-CA-C	-9.97	98.20	112.55
2	N	61	GLY	N-CA-C	-9.91	98.28	112.55
2	I	61	GLY	N-CA-C	-9.72	98.56	112.55
2	2	61	GLY	N-CA-C	-9.31	99.15	112.55

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	3646	0	3559	39	0
1	B	3637	0	3546	52	0
1	C	3632	0	3541	49	0
1	D	3637	0	3546	50	0
1	E	3628	0	3538	45	0
1	F	3628	0	3538	43	0
1	G	3632	0	3541	41	0
1	H	3646	0	3559	45	0
1	S	3628	0	3538	50	0
1	T	3632	0	3541	48	0
1	U	3653	0	3566	70	0
1	V	3653	0	3566	48	0
1	W	3632	0	3541	48	0
1	X	3632	0	3541	41	0
1	Y	3628	0	3538	57	0
1	Z	3632	0	3541	50	0
2	1	1145	0	1119	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1145	0	1119	22	0
2	3	1145	0	1119	35	0
2	4	1145	0	1119	21	0
2	5	1145	0	1119	17	0
2	6	1145	0	1119	25	0
2	7	1145	0	1119	18	0
2	8	1145	0	1119	30	0
2	I	1145	0	1119	19	0
2	J	1145	0	1119	24	0
2	K	1145	0	1119	34	0
2	L	1145	0	1119	28	0
2	M	1145	0	1119	33	0
2	N	1145	0	1119	24	0
2	O	1145	0	1119	20	0
2	P	1145	0	1119	21	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	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
4	A	21	0	8	0	0
4	B	21	0	8	0	0
4	C	21	0	8	0	0
4	D	21	0	7	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	8	0	0
4	H	21	0	7	0	0
4	S	21	0	7	0	0
4	T	21	0	7	0	0
4	U	21	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	21	0	7	0	0
4	W	21	0	8	0	0
4	X	21	0	8	0	0
4	Y	21	0	8	0	0
4	Z	21	0	8	0	0
5	A	12	0	16	1	0
5	B	18	0	24	2	0
5	C	12	0	16	1	0
5	D	12	0	16	1	0
5	E	18	0	24	0	0
5	F	12	0	16	1	0
5	G	18	0	24	0	0
5	H	18	0	24	1	0
5	S	18	0	24	0	0
5	T	12	0	16	0	0
5	U	12	0	16	0	0
5	V	12	0	16	1	0
5	W	12	0	16	1	0
5	X	18	0	24	0	0
5	Y	18	0	24	1	0
5	Z	18	0	24	0	0
6	1	173	0	0	2	0
6	2	173	0	0	2	0
6	3	170	0	0	3	0
6	4	174	0	0	2	0
6	5	174	0	0	0	0
6	6	146	0	0	2	0
6	7	184	0	0	3	0
6	8	185	0	0	1	0
6	A	459	0	0	1	0
6	B	406	0	0	5	0
6	C	478	0	0	2	0
6	D	480	0	0	6	0
6	E	463	0	0	3	0
6	F	450	0	0	5	0
6	G	466	0	0	3	0
6	H	452	0	0	4	0
6	I	172	0	0	3	0
6	J	170	0	0	3	0
6	K	187	0	0	3	0
6	L	186	0	0	5	0
6	M	181	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	186	0	0	2	0
6	O	179	0	0	0	0
6	P	200	0	0	3	0
6	S	425	0	0	6	0
6	T	426	0	0	5	0
6	U	427	0	0	8	0
6	V	456	0	0	3	0
6	W	421	0	0	6	0
6	X	450	0	0	3	0
6	Y	426	0	0	7	0
6	Z	474	0	0	6	0
All	All	87087	0	75085	1041	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 7.

The worst 5 of 1041 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:U:8:LYS:HD2	2:8:84:ARG:HH11	1.07	1.10
1:U:8:LYS:HG2	1:U:9:ALA:H	1.00	1.08
1:A:247:CYS:HG	1:E:247:CYS:HG	1.07	0.96
1:U:8:LYS:HG2	1:U:9:ALA:N	1.84	0.92
1:D:247:CYS:HG	1:H:247:CYS:HG	1.11	0.92

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	461/475 (97%)	444 (96%)	15 (3%)	2 (0%)	30 18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	460/475 (97%)	443 (96%)	16 (4%)	1 (0%)	43	34
1	C	459/475 (97%)	445 (97%)	13 (3%)	1 (0%)	43	34
1	D	460/475 (97%)	445 (97%)	14 (3%)	1 (0%)	43	34
1	E	458/475 (96%)	442 (96%)	15 (3%)	1 (0%)	43	34
1	F	458/475 (96%)	441 (96%)	16 (4%)	1 (0%)	43	34
1	G	459/475 (97%)	445 (97%)	13 (3%)	1 (0%)	43	34
1	H	461/475 (97%)	448 (97%)	11 (2%)	2 (0%)	30	18
1	S	458/475 (96%)	441 (96%)	16 (4%)	1 (0%)	43	34
1	T	459/475 (97%)	445 (97%)	12 (3%)	2 (0%)	30	18
1	U	462/475 (97%)	443 (96%)	17 (4%)	2 (0%)	30	18
1	V	462/475 (97%)	443 (96%)	17 (4%)	2 (0%)	30	18
1	W	459/475 (97%)	443 (96%)	15 (3%)	1 (0%)	43	34
1	X	459/475 (97%)	444 (97%)	13 (3%)	2 (0%)	30	18
1	Y	458/475 (96%)	444 (97%)	13 (3%)	1 (0%)	43	34
1	Z	459/475 (97%)	442 (96%)	15 (3%)	2 (0%)	30	18
2	1	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	2	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
2	3	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	4	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	5	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	6	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
2	7	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	8	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
2	I	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	J	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	K	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
2	L	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
2	M	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	O	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
2	P	138/140 (99%)	130 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9560/9840 (97%)	9177 (96%)	360 (4%)	23 (0%)	43 34

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ALA
1	T	11	ALA
1	U	8	LYS
1	Z	11	ALA
1	X	11	ALA

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	369/376 (98%)	368 (100%)	1 (0%)	86 81
1	B	368/376 (98%)	366 (100%)	2 (0%)	81 75
1	C	368/376 (98%)	365 (99%)	3 (1%)	73 65
1	D	368/376 (98%)	364 (99%)	4 (1%)	65 54
1	E	368/376 (98%)	366 (100%)	2 (0%)	81 75
1	F	368/376 (98%)	367 (100%)	1 (0%)	86 81
1	G	368/376 (98%)	365 (99%)	3 (1%)	73 65
1	H	369/376 (98%)	366 (99%)	3 (1%)	73 65
1	S	368/376 (98%)	365 (99%)	3 (1%)	73 65
1	T	368/376 (98%)	366 (100%)	2 (0%)	81 75
1	U	370/376 (98%)	369 (100%)	1 (0%)	86 81
1	V	370/376 (98%)	365 (99%)	5 (1%)	59 45
1	W	368/376 (98%)	364 (99%)	4 (1%)	65 54
1	X	368/376 (98%)	365 (99%)	3 (1%)	73 65
1	Y	368/376 (98%)	364 (99%)	4 (1%)	65 54
1	Z	368/376 (98%)	366 (100%)	2 (0%)	81 75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	2	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	3	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	4	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	5	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	6	123/123 (100%)	123 (100%)	0	100	100
2	7	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	8	123/123 (100%)	121 (98%)	2 (2%)	55	39
2	I	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	J	123/123 (100%)	121 (98%)	2 (2%)	55	39
2	K	123/123 (100%)	120 (98%)	3 (2%)	43	25
2	L	123/123 (100%)	121 (98%)	2 (2%)	55	39
2	M	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	N	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	O	123/123 (100%)	122 (99%)	1 (1%)	73	65
2	P	123/123 (100%)	121 (98%)	2 (2%)	55	39
All	All	7862/7984 (98%)	7798 (99%)	64 (1%)	73	65

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	239	TYR
2	7	119	MET
1	G	239	TYR
1	G	219	LEU
1	Z	239	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
2	1	88	GLN
2	8	136	ASN
2	3	8	ASN
2	8	124	GLN
2	7	8	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

96 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	HYP	E	151	1	7,8,9	1.14	1 (14%)	5,10,12	1.33	1 (20%)
1	KCX	D	201	1,3	10,11,12	0.93	1 (10%)	6,12,14	1.39	1 (16%)
1	HYP	D	151	1	7,8,9	1.12	1 (14%)	5,10,12	1.36	1 (20%)
1	HYP	Y	104	1	7,8,9	1.05	0	5,10,12	1.70	1 (20%)
2	MME	5	1	2	7,8,9	2.07	1 (14%)	5,8,10	1.46	1 (20%)
1	KCX	U	201	1,3	10,11,12	0.87	0	6,12,14	1.48	2 (33%)
1	SMC	F	256	1	5,6,7	0.52	0	3,6,8	0.61	0
1	SMC	B	256	1	5,6,7	0.51	0	3,6,8	0.81	0
1	SMC	D	369	1	5,6,7	0.56	0	3,6,8	0.44	0
2	MME	M	1	2	7,8,9	2.06	1 (14%)	5,8,10	1.44	1 (20%)
1	HYP	V	104	1	7,8,9	1.12	1 (14%)	5,10,12	1.55	1 (20%)
1	KCX	W	201	1,3	10,11,12	0.91	0	6,12,14	1.50	2 (33%)
1	HYP	D	104	1	7,8,9	1.10	1 (14%)	5,10,12	1.60	1 (20%)
2	MME	O	1	2	7,8,9	2.07	1 (14%)	5,8,10	1.42	1 (20%)
1	SMC	C	369	1	5,6,7	0.51	0	3,6,8	0.59	0
2	MME	L	1	2	7,8,9	2.09	1 (14%)	5,8,10	1.34	1 (20%)
1	SMC	U	369	1	5,6,7	0.62	0	3,6,8	0.45	0
1	HYP	F	104	1	7,8,9	1.09	1 (14%)	5,10,12	1.72	1 (20%)
2	MME	K	1	2	7,8,9	2.08	1 (14%)	5,8,10	1.42	1 (20%)
1	HYP	B	104	1	7,8,9	1.12	1 (14%)	5,10,12	1.59	1 (20%)
1	SMC	T	256	1	5,6,7	0.49	0	3,6,8	0.66	0
2	MME	6	1	2	7,8,9	2.09	1 (14%)	5,8,10	1.44	1 (20%)
1	KCX	C	201	1,3	10,11,12	0.96	0	6,12,14	1.46	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	S	104	1	7,8,9	1.08	0	5,10,12	1.72	1 (20%)
1	HYP	T	104	1	7,8,9	1.10	0	5,10,12	1.54	1 (20%)
1	HYP	C	151	1	7,8,9	1.05	1 (14%)	5,10,12	1.36	1 (20%)
2	MME	7	1	2	7,8,9	2.08	1 (14%)	5,8,10	1.40	1 (20%)
1	SMC	H	369	1	5,6,7	0.61	0	3,6,8	0.46	0
1	HYP	U	151	1	7,8,9	1.10	0	5,10,12	1.33	1 (20%)
1	KCX	V	201	1,3	10,11,12	0.97	0	6,12,14	1.44	1 (16%)
1	HYP	F	151	1	7,8,9	1.04	0	5,10,12	1.32	1 (20%)
1	KCX	B	201	1,3	10,11,12	0.83	0	6,12,14	1.42	1 (16%)
1	HYP	Y	151	1	7,8,9	1.06	0	5,10,12	1.33	1 (20%)
1	SMC	C	256	1	5,6,7	0.52	0	3,6,8	0.50	0
1	KCX	H	201	1,3	10,11,12	0.91	0	6,12,14	1.52	2 (33%)
2	MME	N	1	2	7,8,9	2.07	1 (14%)	5,8,10	1.47	1 (20%)
1	HYP	H	151	1	7,8,9	1.05	1 (14%)	5,10,12	1.40	1 (20%)
1	HYP	X	104	1	7,8,9	1.15	1 (14%)	5,10,12	1.66	1 (20%)
1	HYP	G	104	1	7,8,9	1.15	1 (14%)	5,10,12	1.70	1 (20%)
1	SMC	V	256	1	5,6,7	0.48	0	3,6,8	0.85	0
1	SMC	Z	256	1	5,6,7	0.52	0	3,6,8	0.66	0
1	SMC	G	256	1	5,6,7	0.52	0	3,6,8	0.63	0
1	HYP	U	104	1	7,8,9	1.09	0	5,10,12	1.62	1 (20%)
1	KCX	T	201	1,3	10,11,12	0.93	0	6,12,14	1.46	2 (33%)
2	MME	I	1	2	7,8,9	2.08	1 (14%)	5,8,10	1.42	1 (20%)
1	HYP	S	151	1	7,8,9	1.14	0	5,10,12	1.35	1 (20%)
1	HYP	T	151	1	7,8,9	1.08	0	5,10,12	1.31	1 (20%)
1	HYP	H	104	1	7,8,9	1.10	0	5,10,12	1.67	1 (20%)
1	SMC	D	256	1	5,6,7	0.51	0	3,6,8	0.76	0
1	SMC	S	256	1	5,6,7	0.53	0	3,6,8	0.57	0
2	MME	3	1	2	7,8,9	2.08	1 (14%)	5,8,10	1.45	1 (20%)
1	SMC	T	369	1	5,6,7	0.67	0	3,6,8	0.43	0
2	MME	2	1	2	7,8,9	2.05	1 (14%)	5,8,10	1.42	1 (20%)
1	KCX	A	201	1,3	10,11,12	0.90	0	6,12,14	1.51	2 (33%)
1	SMC	Y	369	1	5,6,7	0.65	0	3,6,8	0.41	0
1	HYP	V	151	1	7,8,9	1.09	0	5,10,12	1.31	1 (20%)
1	SMC	W	256	1	5,6,7	0.55	0	3,6,8	0.58	0
2	MME	1	1	2	7,8,9	2.09	1 (14%)	5,8,10	1.38	1 (20%)
2	MME	P	1	2	7,8,9	2.08	1 (14%)	5,8,10	1.49	1 (20%)
2	MME	8	1	2	7,8,9	2.09	1 (14%)	5,8,10	1.44	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	A	151	1	7,8,9	1.09	0	5,10,12	1.36	1 (20%)
1	SMC	Z	369	1	5,6,7	0.58	0	3,6,8	0.36	0
1	HYP	E	104	1	7,8,9	1.13	1 (14%)	5,10,12	1.54	1 (20%)
1	SMC	U	256	1	5,6,7	0.49	0	3,6,8	0.64	0
1	KCX	Z	201	1,3	10,11,12	0.96	1 (10%)	6,12,14	1.44	1 (16%)
1	SMC	S	369	1	5,6,7	0.54	0	3,6,8	0.40	0
1	SMC	B	369	1	5,6,7	0.61	0	3,6,8	0.32	0
1	HYP	Z	151	1	7,8,9	1.21	1 (14%)	5,10,12	1.26	1 (20%)
1	SMC	Y	256	1	5,6,7	0.51	0	3,6,8	0.71	0
1	HYP	B	151	1	7,8,9	1.11	1 (14%)	5,10,12	1.37	1 (20%)
1	KCX	Y	201	1,3	10,11,12	0.92	0	6,12,14	1.43	1 (16%)
1	SMC	W	369	1	5,6,7	0.57	0	3,6,8	0.52	0
1	SMC	H	256	1	5,6,7	0.50	0	3,6,8	0.61	0
1	SMC	A	256	1	5,6,7	0.49	0	3,6,8	0.68	0
1	SMC	G	369	1	5,6,7	0.53	0	3,6,8	0.45	0
2	MME	J	1	2	7,8,9	2.09	1 (14%)	5,8,10	1.45	1 (20%)
1	KCX	E	201	1,3	10,11,12	0.95	0	6,12,14	1.50	2 (33%)
1	SMC	X	369	1	5,6,7	0.55	0	3,6,8	0.40	0
1	KCX	F	201	1,3	10,11,12	0.92	0	6,12,14	1.44	1 (16%)
1	HYP	C	104	1	7,8,9	1.14	1 (14%)	5,10,12	1.54	1 (20%)
1	HYP	W	151	1	7,8,9	1.11	0	5,10,12	1.35	1 (20%)
1	KCX	G	201	1,3	10,11,12	0.91	0	6,12,14	1.46	2 (33%)
1	HYP	G	151	1	7,8,9	1.15	1 (14%)	5,10,12	1.29	1 (20%)
1	KCX	X	201	1,3	10,11,12	0.88	0	6,12,14	1.50	2 (33%)
1	SMC	E	256	1	5,6,7	0.53	0	3,6,8	0.57	0
1	SMC	A	369	1	5,6,7	0.67	0	3,6,8	0.31	0
1	HYP	X	151	1	7,8,9	1.10	0	5,10,12	1.28	1 (20%)
1	SMC	F	369	1	5,6,7	0.61	0	3,6,8	0.39	0
1	SMC	V	369	1	5,6,7	0.56	0	3,6,8	0.43	0
1	HYP	Z	104	1	7,8,9	1.05	0	5,10,12	1.56	1 (20%)
1	KCX	S	201	1,3	10,11,12	0.94	1 (10%)	6,12,14	1.46	2 (33%)
1	HYP	W	104	1	7,8,9	1.15	1 (14%)	5,10,12	1.76	2 (40%)
1	SMC	X	256	1	5,6,7	0.51	0	3,6,8	0.65	0
1	SMC	E	369	1	5,6,7	0.56	0	3,6,8	0.39	0
1	HYP	A	104	1	7,8,9	1.09	1 (14%)	5,10,12	1.80	2 (40%)
2	MME	4	1	2	7,8,9	2.10	1 (14%)	5,8,10	1.46	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	KCX	D	201	1,3	-	0/9/10/12	-
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	HYP	Y	104	1	-	0/0/11/13	0/1/1/1
2	MME	5	1	2	-	2/5/8/10	-
1	KCX	U	201	1,3	-	0/9/10/12	-
1	SMC	F	256	1	-	0/3/5/7	-
1	SMC	B	256	1	-	0/3/5/7	-
1	SMC	D	369	1	-	2/3/5/7	-
2	MME	M	1	2	-	1/5/8/10	-
1	HYP	V	104	1	-	0/0/11/13	0/1/1/1
1	KCX	W	201	1,3	-	0/9/10/12	-
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
2	MME	O	1	2	-	1/5/8/10	-
1	SMC	C	369	1	-	1/3/5/7	-
2	MME	L	1	2	-	1/5/8/10	-
1	SMC	U	369	1	-	1/3/5/7	-
1	HYP	F	104	1	-	0/0/11/13	0/1/1/1
2	MME	K	1	2	-	2/5/8/10	-
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	SMC	T	256	1	-	0/3/5/7	-
2	MME	6	1	2	-	1/5/8/10	-
1	KCX	C	201	1,3	-	0/9/10/12	-
1	HYP	S	104	1	-	0/0/11/13	0/1/1/1
1	HYP	T	104	1	-	0/0/11/13	0/1/1/1
1	HYP	C	151	1	-	0/0/11/13	0/1/1/1
2	MME	7	1	2	-	3/5/8/10	-
1	SMC	H	369	1	-	1/3/5/7	-
1	HYP	U	151	1	-	0/0/11/13	0/1/1/1
1	KCX	V	201	1,3	-	0/9/10/12	-
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	1,3	-	0/9/10/12	-
1	HYP	Y	151	1	-	0/0/11/13	0/1/1/1
1	SMC	C	256	1	-	0/3/5/7	-
1	KCX	H	201	1,3	-	0/9/10/12	-
2	MME	N	1	2	-	1/5/8/10	-
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	HYP	X	104	1	-	0/0/11/13	0/1/1/1
1	HYP	G	104	1	-	0/0/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	V	256	1	-	0/3/5/7	-
1	SMC	Z	256	1	-	0/3/5/7	-
1	SMC	G	256	1	-	0/3/5/7	-
1	HYP	U	104	1	-	0/0/11/13	0/1/1/1
1	KCX	T	201	1,3	-	0/9/10/12	-
2	MME	I	1	2	-	3/5/8/10	-
1	HYP	S	151	1	-	0/0/11/13	0/1/1/1
1	HYP	T	151	1	-	0/0/11/13	0/1/1/1
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	SMC	D	256	1	-	0/3/5/7	-
1	SMC	S	256	1	-	0/3/5/7	-
2	MME	3	1	2	-	0/5/8/10	-
1	SMC	T	369	1	-	1/3/5/7	-
2	MME	2	1	2	-	3/5/8/10	-
1	KCX	A	201	1,3	-	0/9/10/12	-
1	SMC	Y	369	1	-	1/3/5/7	-
1	HYP	V	151	1	-	0/0/11/13	0/1/1/1
1	SMC	W	256	1	-	0/3/5/7	-
2	MME	1	1	2	-	1/5/8/10	-
2	MME	P	1	2	-	2/5/8/10	-
2	MME	8	1	2	-	1/5/8/10	-
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	SMC	Z	369	1	-	1/3/5/7	-
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	SMC	U	256	1	-	0/3/5/7	-
1	KCX	Z	201	1,3	-	0/9/10/12	-
1	SMC	S	369	1	-	1/3/5/7	-
1	SMC	B	369	1	-	1/3/5/7	-
1	HYP	Z	151	1	-	0/0/11/13	0/1/1/1
1	SMC	Y	256	1	-	0/3/5/7	-
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	KCX	Y	201	1,3	-	0/9/10/12	-
1	SMC	W	369	1	-	1/3/5/7	-
1	SMC	H	256	1	-	0/3/5/7	-
1	SMC	A	256	1	-	0/3/5/7	-
1	SMC	G	369	1	-	1/3/5/7	-
2	MME	J	1	2	-	3/5/8/10	-
1	KCX	E	201	1,3	-	0/9/10/12	-
1	SMC	X	369	1	-	1/3/5/7	-
1	KCX	F	201	1,3	-	0/9/10/12	-
1	HYP	C	104	1	-	0/0/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	W	151	1	-	0/0/11/13	0/1/1/1
1	KCX	G	201	1,3	-	0/9/10/12	-
1	HYP	G	151	1	-	0/0/11/13	0/1/1/1
1	KCX	X	201	1,3	-	0/9/10/12	-
1	SMC	E	256	1	-	0/3/5/7	-
1	SMC	A	369	1	-	1/3/5/7	-
1	HYP	X	151	1	-	0/0/11/13	0/1/1/1
1	SMC	F	369	1	-	1/3/5/7	-
1	SMC	V	369	1	-	2/3/5/7	-
1	HYP	Z	104	1	-	0/0/11/13	0/1/1/1
1	KCX	S	201	1,3	-	0/9/10/12	-
1	HYP	W	104	1	-	0/0/11/13	0/1/1/1
1	SMC	X	256	1	-	0/3/5/7	-
1	SMC	E	369	1	-	1/3/5/7	-
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
2	MME	4	1	2	-	1/5/8/10	-

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	1	MME	CM-N	-5.43	1.33	1.46
2	J	1	MME	CM-N	-5.41	1.33	1.46
2	6	1	MME	CM-N	-5.39	1.33	1.46
2	P	1	MME	CM-N	-5.38	1.33	1.46
2	3	1	MME	CM-N	-5.38	1.33	1.46

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	KCX	OQ1-CX-NZ	-2.96	120.43	124.92
1	W	104	HYP	O-C-CA	-2.91	117.28	124.77
1	E	201	KCX	OQ1-CX-NZ	-2.91	120.50	124.92
1	X	201	KCX	OQ1-CX-NZ	-2.91	120.50	124.92
1	H	201	KCX	OQ1-CX-NZ	-2.87	120.56	124.92

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	MME	C-CA-CB-CG
2	J	1	MME	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	369	SMC	C-CA-CB-SG
2	2	1	MME	C-CA-CB-CG
1	V	369	SMC	C-CA-CB-SG

There are no ring outliers.

19 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	1	MME	1	0
1	U	201	KCX	1	0
2	M	1	MME	1	0
2	O	1	MME	2	0
2	L	1	MME	1	0
2	K	1	MME	2	0
2	7	1	MME	2	0
1	Y	151	HYP	1	0
2	N	1	MME	1	0
1	H	151	HYP	1	0
2	I	1	MME	1	0
1	T	151	HYP	1	0
2	3	1	MME	1	0
1	V	151	HYP	1	0
2	8	1	MME	4	0
1	Z	151	HYP	1	0
1	W	151	HYP	1	0
1	G	151	HYP	1	0
1	X	151	HYP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 16 are monoatomic - leaving 56 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	$\# Z > 2$
5	GOL	B	606	-	5,5,5	1.04	0	5,5,5	0.43	0
5	GOL	H	604	-	5,5,5	1.02	0	5,5,5	0.30	0
4	CAP	W	501	3	18,20,20	1.62	3 (16%)	23,31,31	1.58	2 (8%)
5	GOL	B	610	-	5,5,5	0.98	0	5,5,5	0.41	0
5	GOL	W	601	-	5,5,5	0.96	0	5,5,5	0.39	0
4	CAP	S	501	3	18,20,20	1.65	3 (16%)	23,31,31	1.52	2 (8%)
4	CAP	B	501	3	18,20,20	1.55	3 (16%)	23,31,31	1.53	2 (8%)
5	GOL	H	619	-	5,5,5	0.99	0	5,5,5	0.33	0
5	GOL	S	605	-	5,5,5	0.97	0	5,5,5	0.36	0
5	GOL	Z	604	-	5,5,5	0.95	0	5,5,5	0.39	0
4	CAP	H	501	3	18,20,20	1.49	3 (16%)	23,31,31	1.53	2 (8%)
5	GOL	X	617	-	5,5,5	0.97	0	5,5,5	0.32	0
5	GOL	T	606	-	5,5,5	0.97	0	5,5,5	0.39	0
4	CAP	V	501	3	18,20,20	1.60	3 (16%)	23,31,31	1.56	3 (13%)
5	GOL	G	611	-	5,5,5	1.02	0	5,5,5	0.44	0
5	GOL	C	615	-	5,5,5	0.95	0	5,5,5	0.39	0
5	GOL	E	609	-	5,5,5	0.98	0	5,5,5	0.45	0
5	GOL	U	607	-	5,5,5	0.99	0	5,5,5	0.37	0
5	GOL	W	620	-	5,5,5	0.97	0	5,5,5	0.44	0
5	GOL	Y	611	-	5,5,5	1.00	0	5,5,5	0.42	0
4	CAP	F	501	3	18,20,20	1.58	3 (16%)	23,31,31	1.53	2 (8%)
5	GOL	B	614	-	5,5,5	0.93	0	5,5,5	0.30	0
5	GOL	F	602	-	5,5,5	0.97	0	5,5,5	0.38	0
5	GOL	S	609	-	5,5,5	0.93	0	5,5,5	0.40	0
5	GOL	Z	612	-	5,5,5	1.00	0	5,5,5	0.40	0
5	GOL	V	616	-	5,5,5	0.98	0	5,5,5	0.36	0
5	GOL	G	603	-	5,5,5	0.98	0	5,5,5	0.37	0
5	GOL	U	615	-	5,5,5	0.95	0	5,5,5	0.35	0
4	CAP	G	501	3	18,20,20	1.43	2 (11%)	23,31,31	1.56	3 (13%)
4	CAP	A	501	3	18,20,20	1.59	3 (16%)	23,31,31	1.53	2 (8%)
5	GOL	G	618	-	5,5,5	0.93	0	5,5,5	0.36	0
4	CAP	Y	501	3	18,20,20	1.55	3 (16%)	23,31,31	1.55	2 (8%)
5	GOL	F	617	-	5,5,5	0.97	0	5,5,5	0.27	0
5	GOL	A	613	-	5,5,5	0.95	0	5,5,5	0.33	0
4	CAP	X	501	3	18,20,20	1.58	2 (11%)	23,31,31	1.54	2 (8%)
5	GOL	A	605	-	5,5,5	1.01	0	5,5,5	0.38	0
5	GOL	E	620	-	5,5,5	0.96	0	5,5,5	0.34	0
4	CAP	E	501	3	18,20,20	1.58	3 (16%)	23,31,31	1.51	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	V	608	-	5,5,5	0.99	0	5,5,5	0.38	0
5	GOL	C	607	-	5,5,5	0.96	0	5,5,5	0.41	0
5	GOL	D	616	-	5,5,5	1.00	0	5,5,5	0.45	0
5	GOL	Y	618	-	5,5,5	0.98	0	5,5,5	0.36	0
5	GOL	E	601	-	5,5,5	0.96	0	5,5,5	0.39	0
5	GOL	H	612	-	5,5,5	0.99	0	5,5,5	0.42	0
5	GOL	Z	619	-	5,5,5	0.95	0	5,5,5	0.36	0
5	GOL	D	608	-	5,5,5	1.01	0	5,5,5	0.31	0
5	GOL	S	613	-	5,5,5	0.95	0	5,5,5	0.36	0
5	GOL	X	602	-	5,5,5	0.95	0	5,5,5	0.40	0
5	GOL	X	610	-	5,5,5	0.98	0	5,5,5	0.42	0
5	GOL	Y	603	-	5,5,5	0.98	0	5,5,5	0.39	0
5	GOL	T	614	-	5,5,5	0.98	0	5,5,5	0.33	0
4	CAP	T	501	3	18,20,20	1.56	2 (11%)	23,31,31	1.56	2 (8%)
4	CAP	Z	501	3	18,20,20	1.48	3 (16%)	23,31,31	1.54	2 (8%)
4	CAP	C	501	3	18,20,20	1.61	3 (16%)	23,31,31	1.62	3 (13%)
4	CAP	D	501	3	18,20,20	1.55	3 (16%)	23,31,31	1.50	2 (8%)
4	CAP	U	501	3	18,20,20	1.61	3 (16%)	23,31,31	1.53	3 (13%)

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
5	GOL	B	606	-	-	2/4/4/4	-
5	GOL	H	604	-	-	0/4/4/4	-
4	CAP	W	501	3	-	12/29/29/29	-
5	GOL	B	610	-	-	0/4/4/4	-
5	GOL	W	601	-	-	0/4/4/4	-
4	CAP	S	501	3	-	12/29/29/29	-
4	CAP	B	501	3	-	11/29/29/29	-
5	GOL	H	619	-	-	0/4/4/4	-
5	GOL	S	605	-	-	0/4/4/4	-
5	GOL	Z	604	-	-	1/4/4/4	-
4	CAP	H	501	3	-	12/29/29/29	-
5	GOL	X	617	-	-	0/4/4/4	-
5	GOL	T	606	-	-	0/4/4/4	-
4	CAP	V	501	3	-	12/29/29/29	-
5	GOL	G	611	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	615	-	-	2/4/4/4	-
5	GOL	E	609	-	-	0/4/4/4	-
5	GOL	U	607	-	-	0/4/4/4	-
5	GOL	W	620	-	-	3/4/4/4	-
5	GOL	Y	611	-	-	0/4/4/4	-
4	CAP	F	501	3	-	12/29/29/29	-
5	GOL	B	614	-	-	0/4/4/4	-
5	GOL	F	602	-	-	0/4/4/4	-
5	GOL	S	609	-	-	0/4/4/4	-
5	GOL	Z	612	-	-	0/4/4/4	-
5	GOL	V	616	-	-	2/4/4/4	-
5	GOL	G	603	-	-	1/4/4/4	-
5	GOL	U	615	-	-	0/4/4/4	-
4	CAP	G	501	3	-	12/29/29/29	-
4	CAP	A	501	3	-	12/29/29/29	-
5	GOL	G	618	-	-	0/4/4/4	-
4	CAP	Y	501	3	-	12/29/29/29	-
5	GOL	F	617	-	-	0/4/4/4	-
5	GOL	A	613	-	-	0/4/4/4	-
4	CAP	X	501	3	-	12/29/29/29	-
5	GOL	A	605	-	-	2/4/4/4	-
5	GOL	E	620	-	-	0/4/4/4	-
4	CAP	E	501	3	-	12/29/29/29	-
5	GOL	V	608	-	-	1/4/4/4	-
5	GOL	C	607	-	-	1/4/4/4	-
5	GOL	D	616	-	-	4/4/4/4	-
5	GOL	Y	618	-	-	2/4/4/4	-
5	GOL	E	601	-	-	0/4/4/4	-
5	GOL	H	612	-	-	0/4/4/4	-
5	GOL	Z	619	-	-	0/4/4/4	-
5	GOL	D	608	-	-	2/4/4/4	-
5	GOL	S	613	-	-	0/4/4/4	-
5	GOL	X	602	-	-	1/4/4/4	-
5	GOL	X	610	-	-	0/4/4/4	-
5	GOL	Y	603	-	-	1/4/4/4	-
5	GOL	T	614	-	-	0/4/4/4	-
4	CAP	T	501	3	-	12/29/29/29	-
4	CAP	Z	501	3	-	11/29/29/29	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	C	501	3	-	12/29/29/29	-
4	CAP	D	501	3	-	12/29/29/29	-
4	CAP	U	501	3	-	11/29/29/29	-

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	501	CAP	C2-C	4.70	1.58	1.53
4	W	501	CAP	C2-C	4.67	1.58	1.53
4	A	501	CAP	C2-C	4.52	1.58	1.53
4	E	501	CAP	C2-C	4.51	1.58	1.53
4	U	501	CAP	C2-C	4.47	1.58	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	CAP	O7-C-C2	4.61	121.78	114.06
4	W	501	CAP	O7-C-C2	4.54	121.67	114.06
4	T	501	CAP	O7-C-C2	4.52	121.62	114.06
4	V	501	CAP	O7-C-C2	4.50	121.60	114.06
4	X	501	CAP	O7-C-C2	4.45	121.52	114.06

There are no chirality outliers.

5 of 214 torsion outliers are listed below:

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

There are no ring outliers.

9 monomers are involved in 10 short contacts:

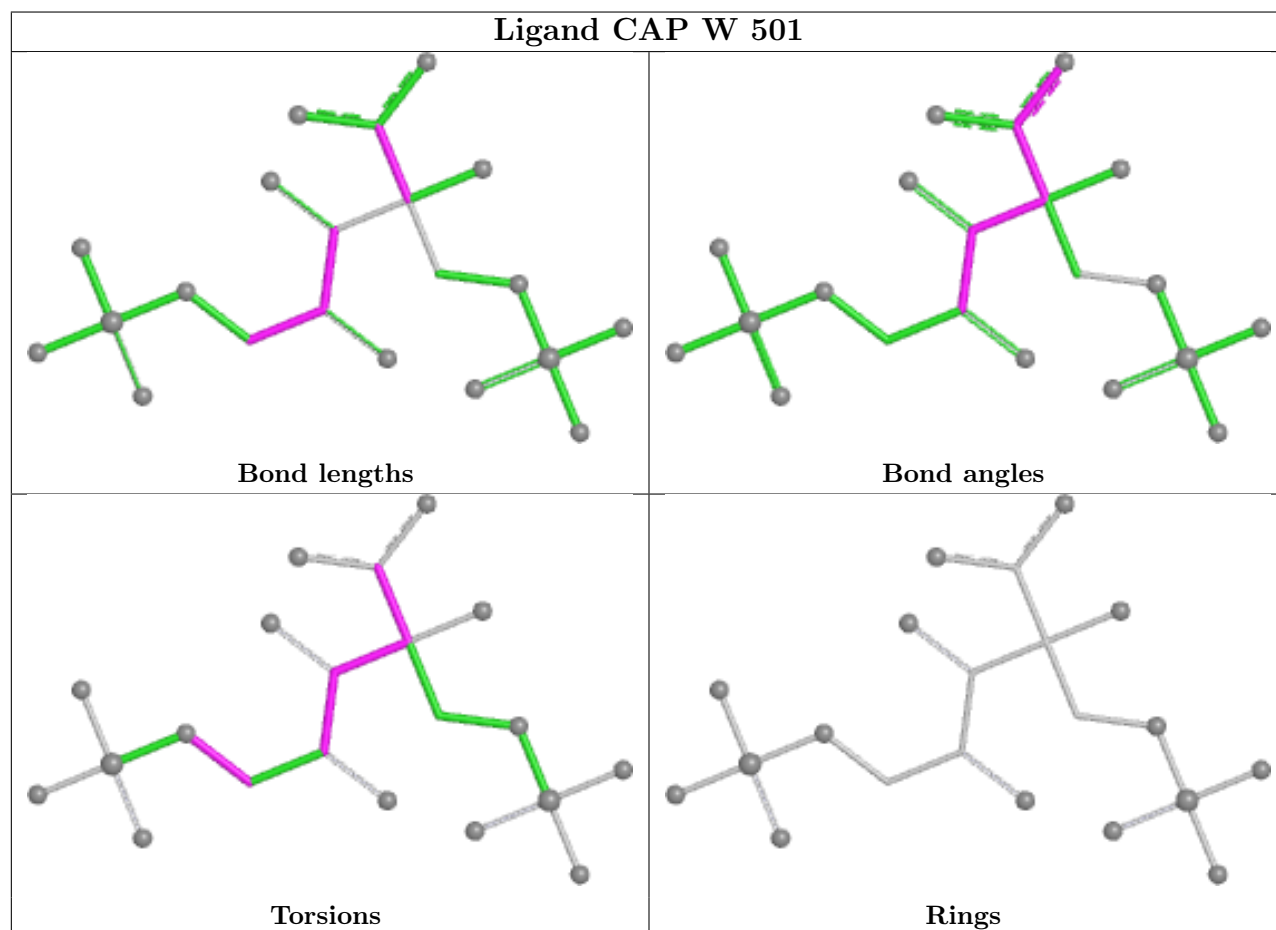
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606	GOL	2	0
5	H	619	GOL	1	0
5	C	615	GOL	1	0
5	W	620	GOL	1	0

Continued on next page...

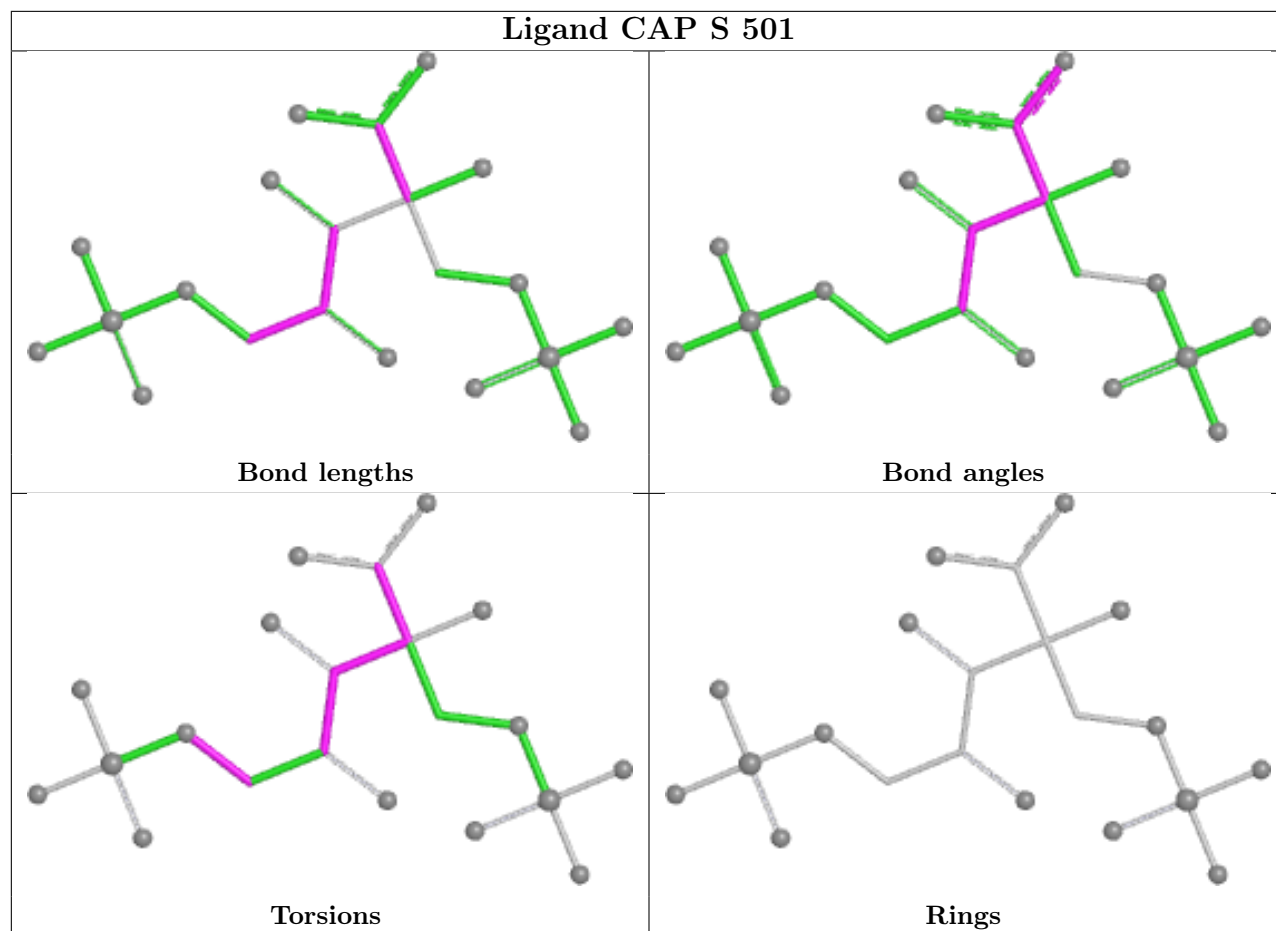
Continued from previous page...

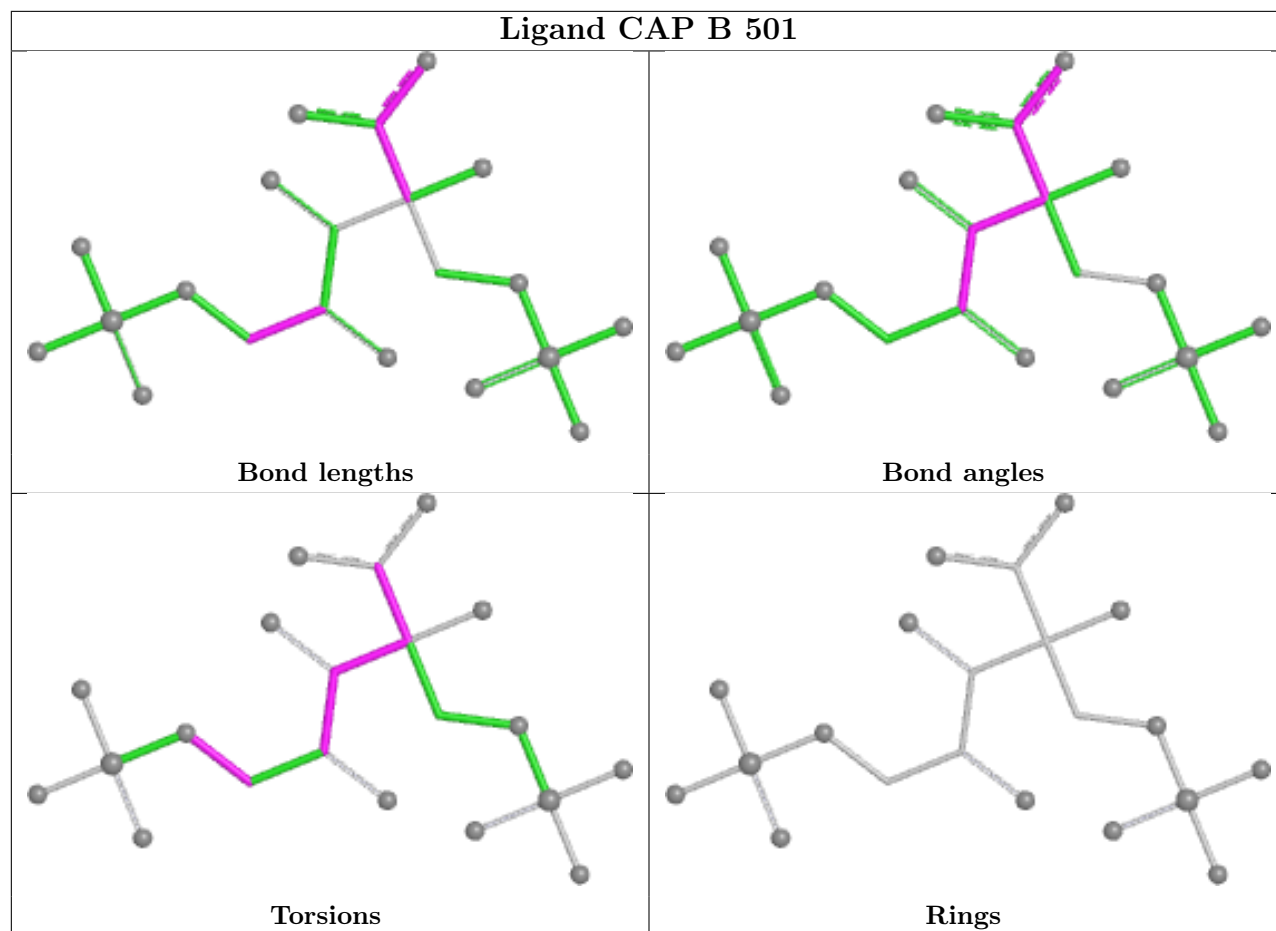
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	616	GOL	1	0
5	F	617	GOL	1	0
5	A	605	GOL	1	0
5	D	616	GOL	1	0
5	Y	618	GOL	1	0

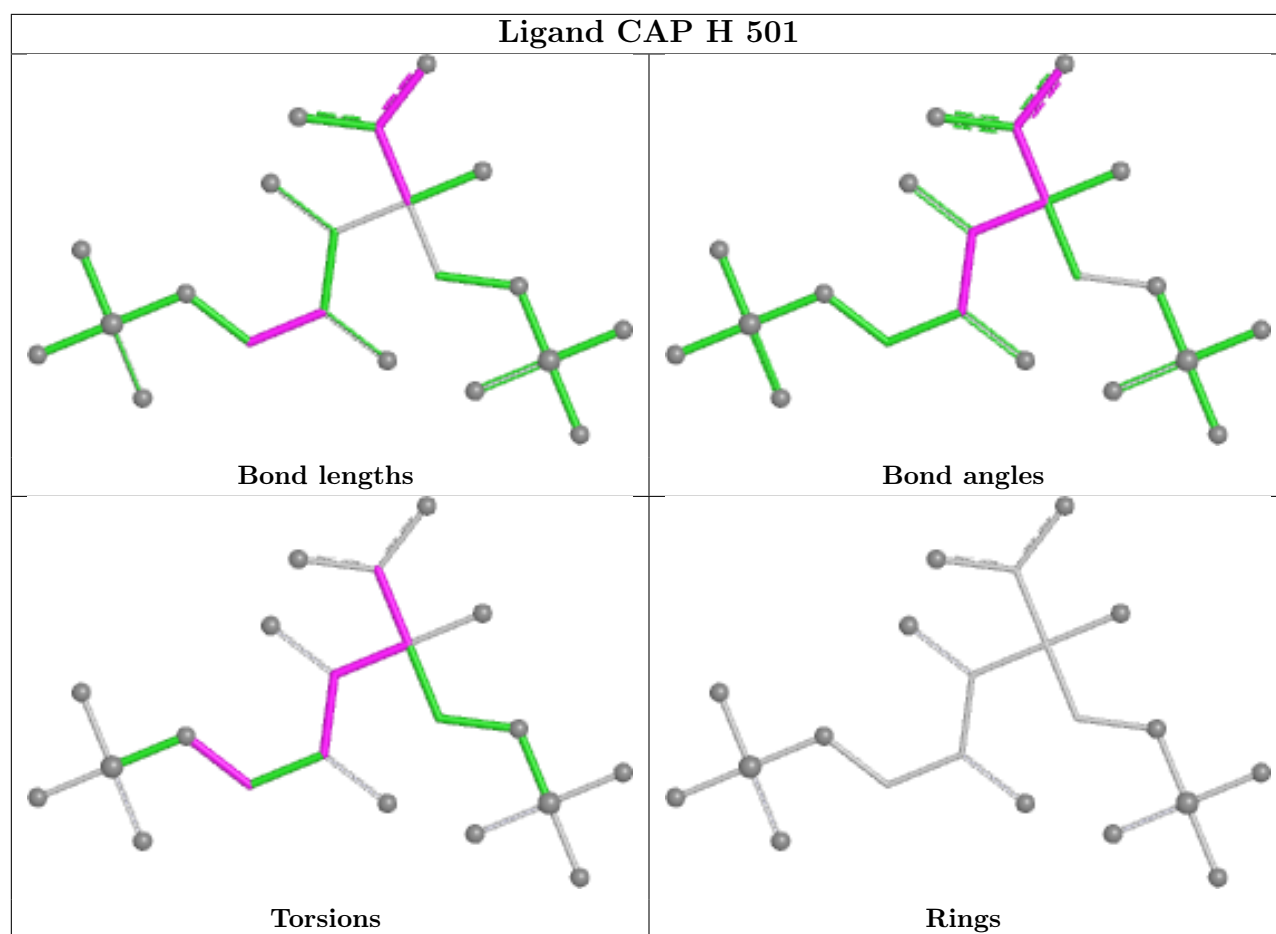
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

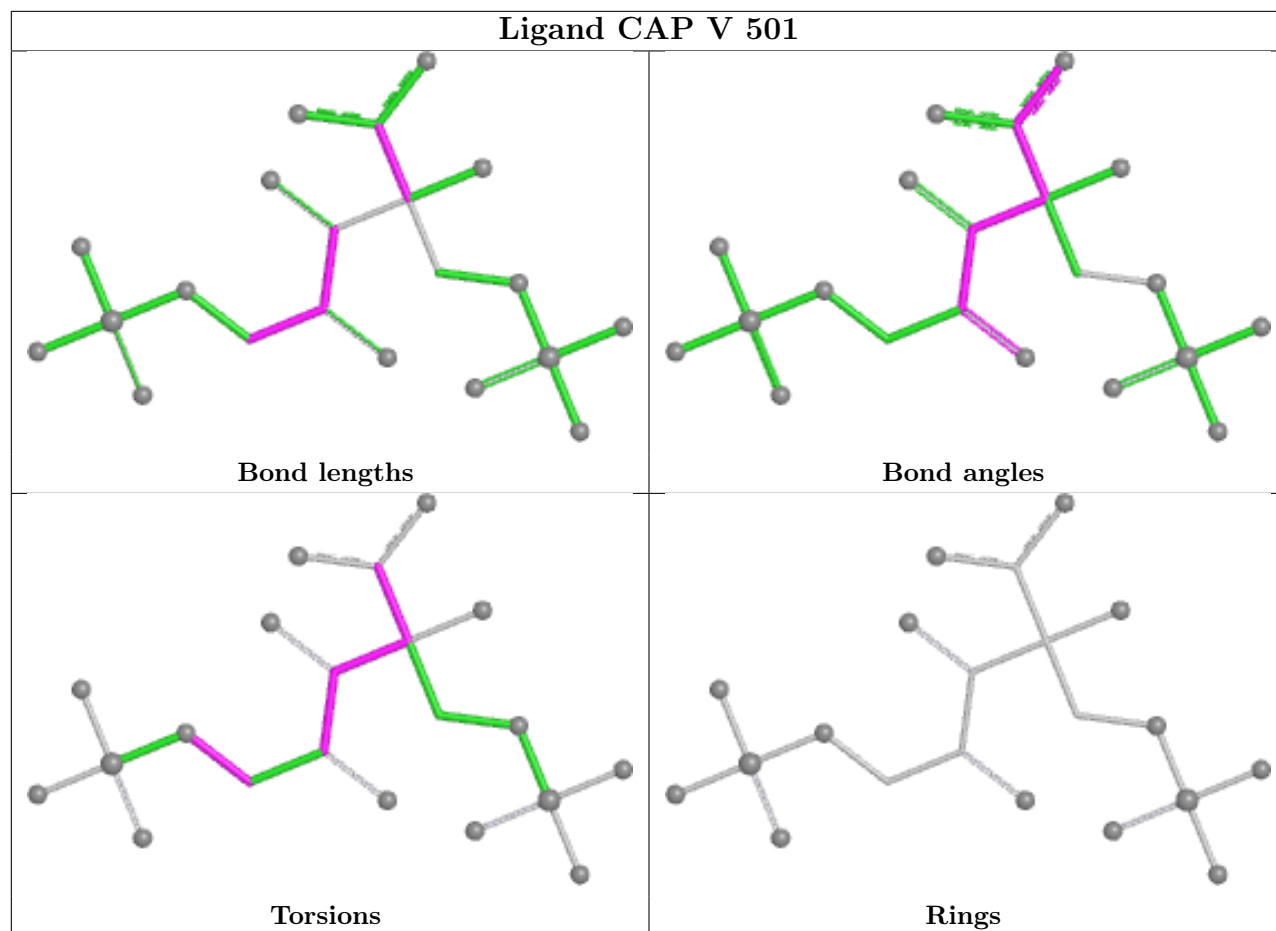


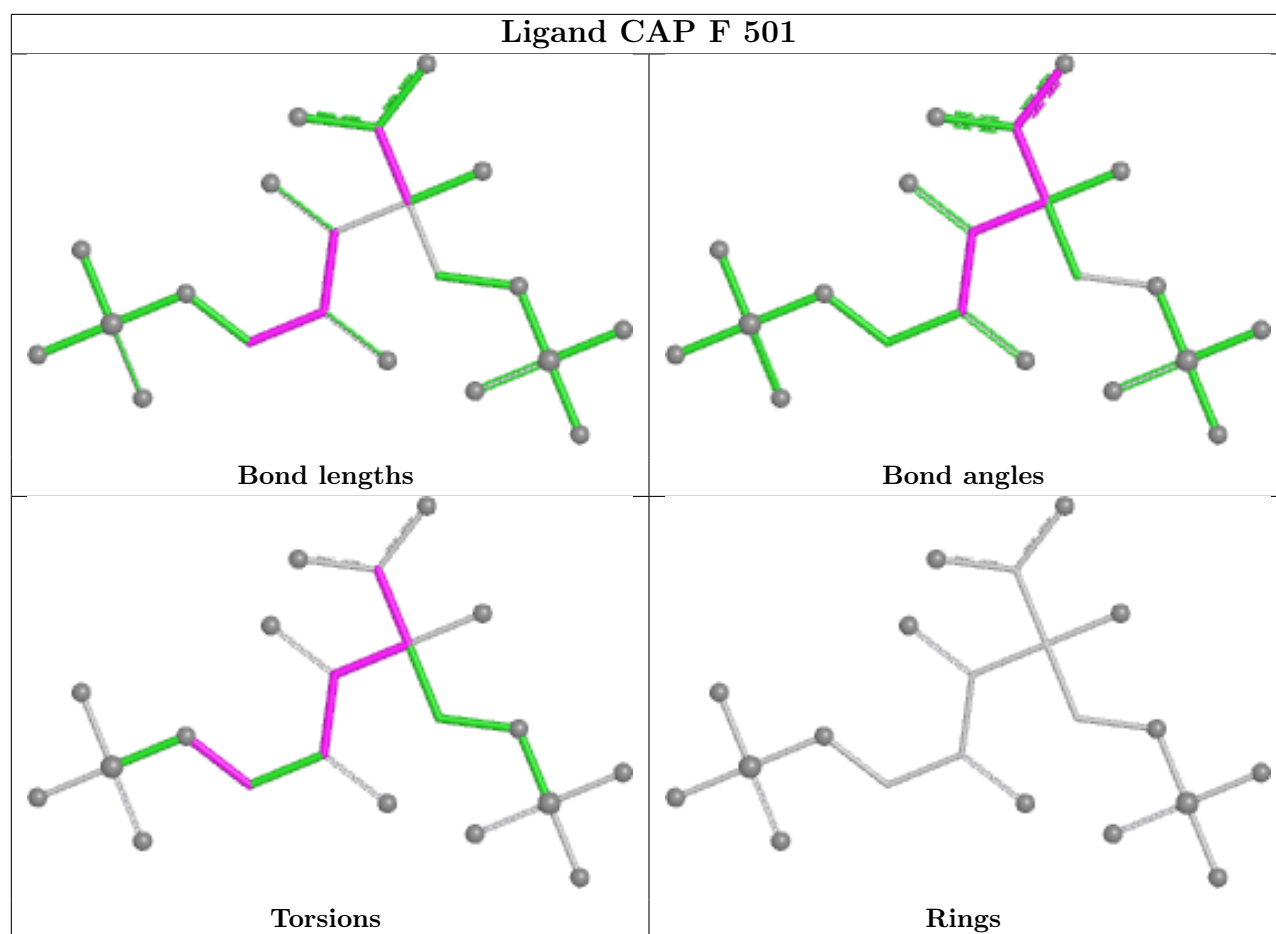
Ligand CAP S 501

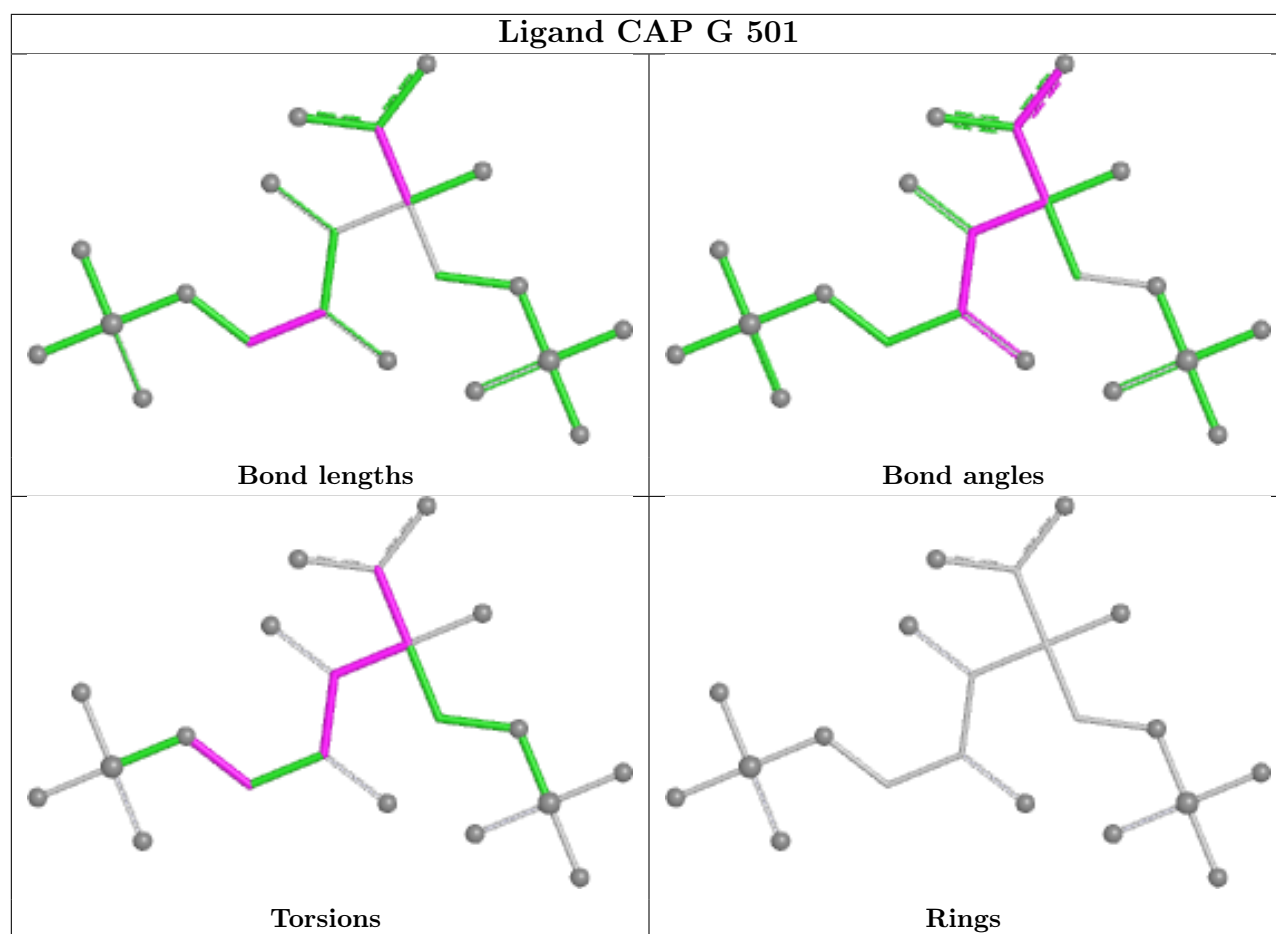


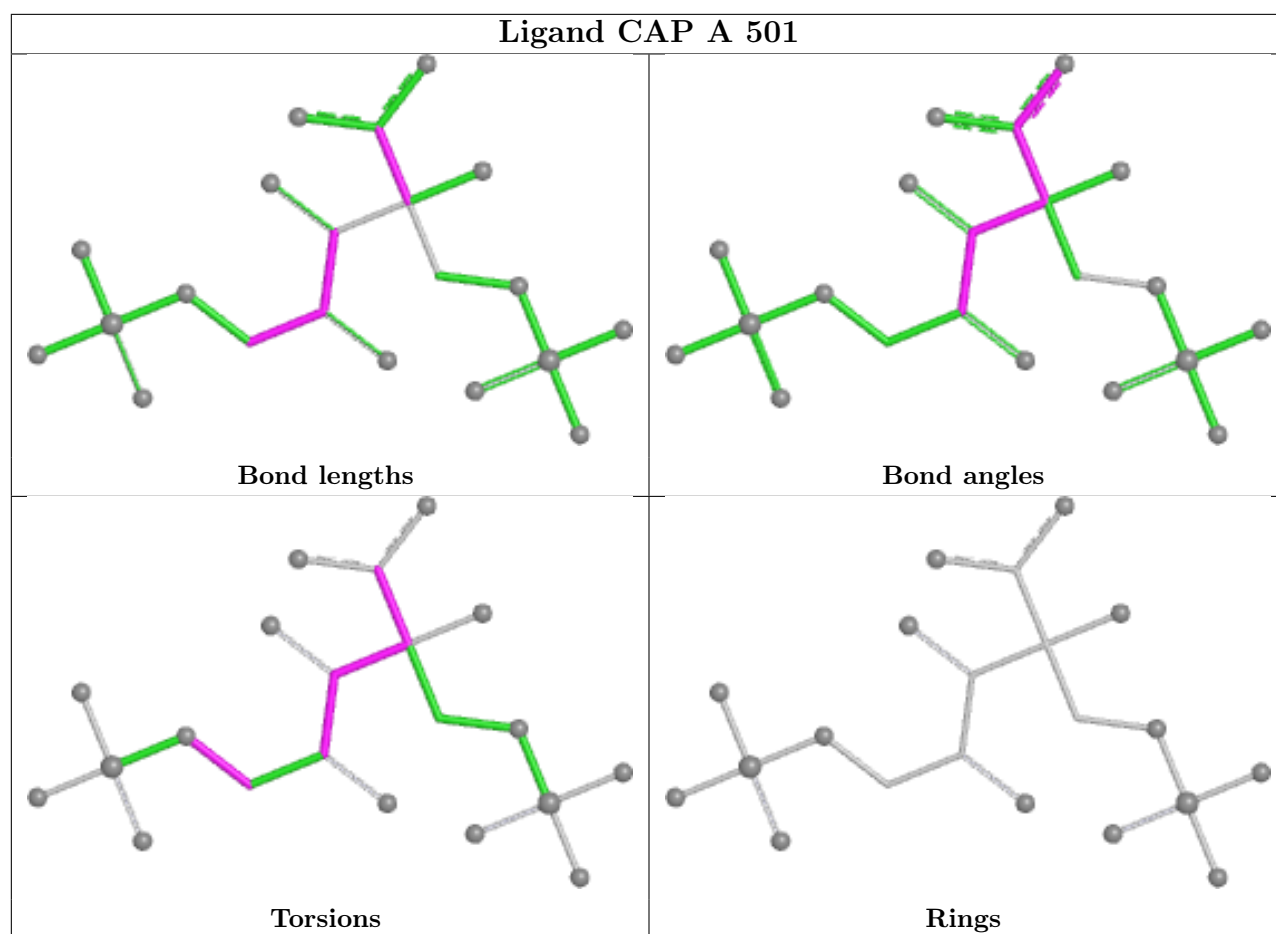


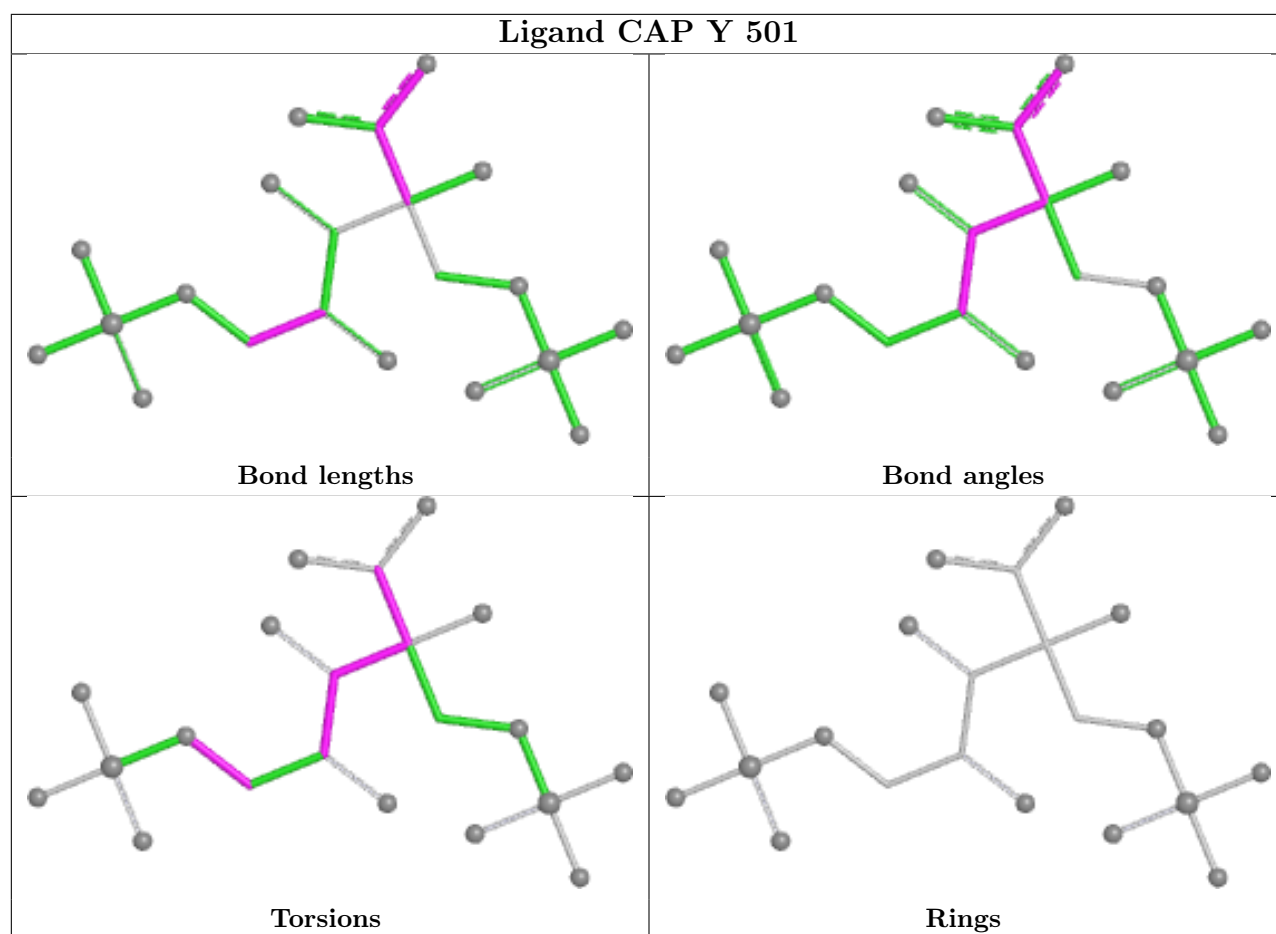


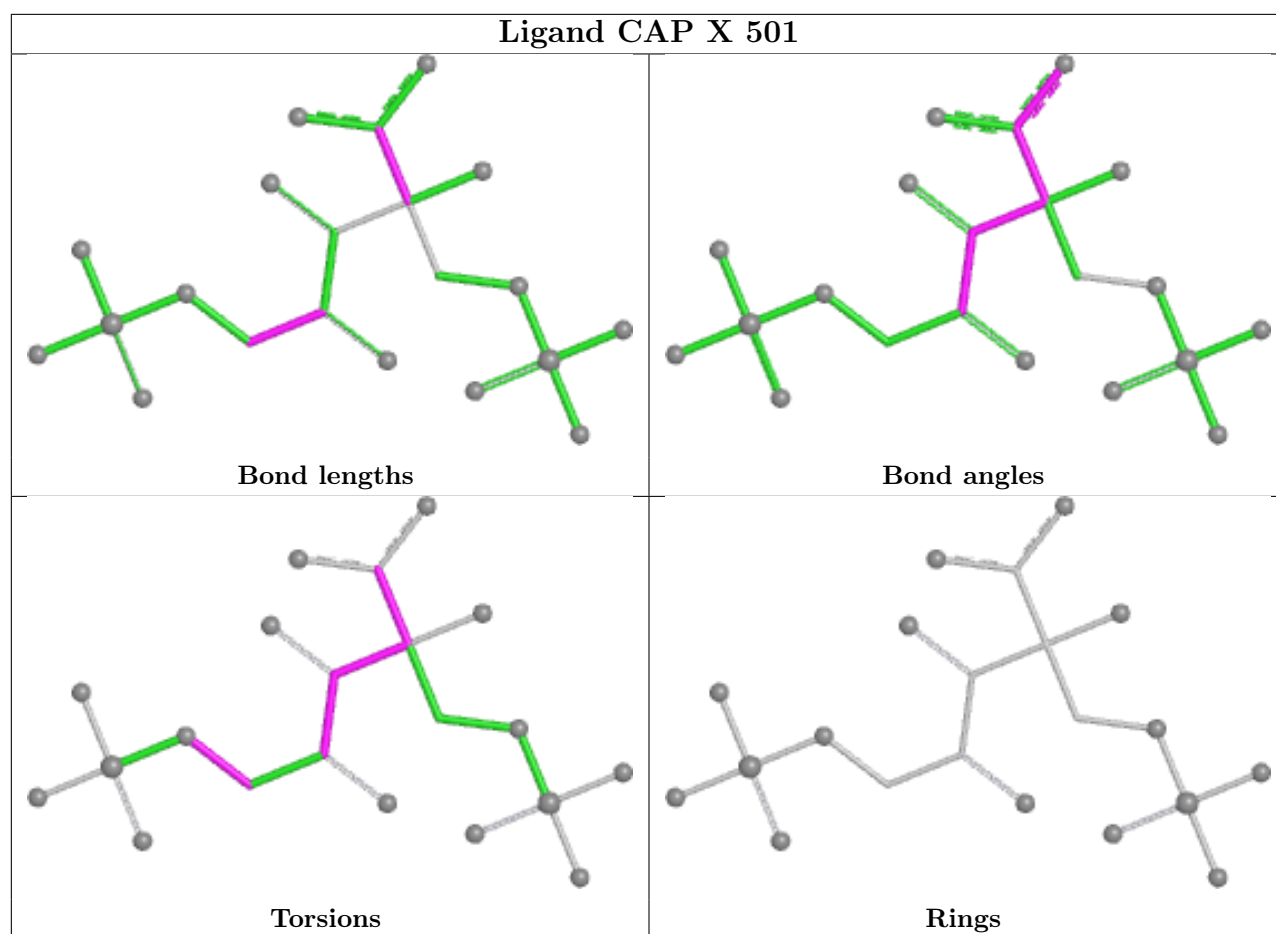


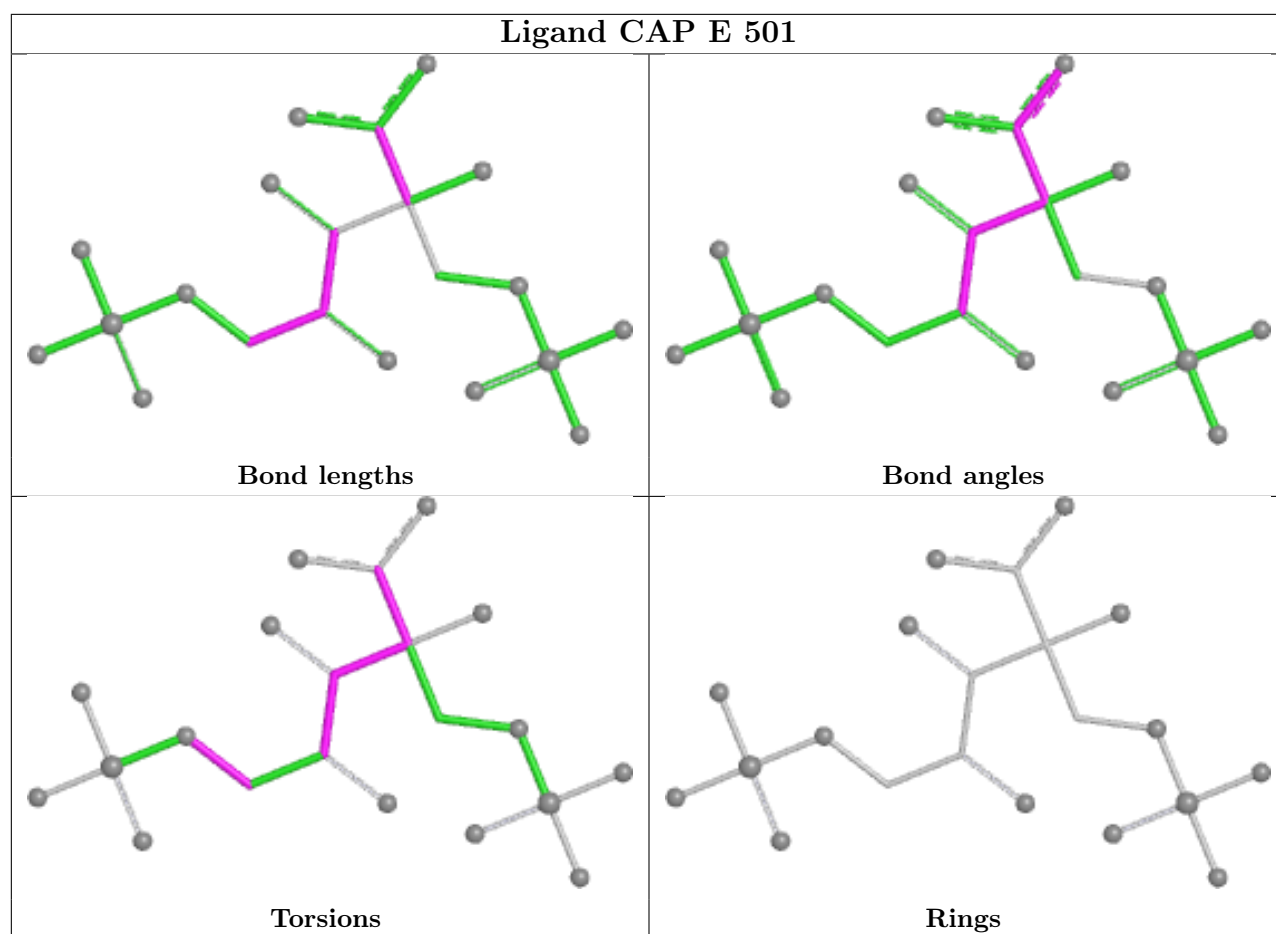


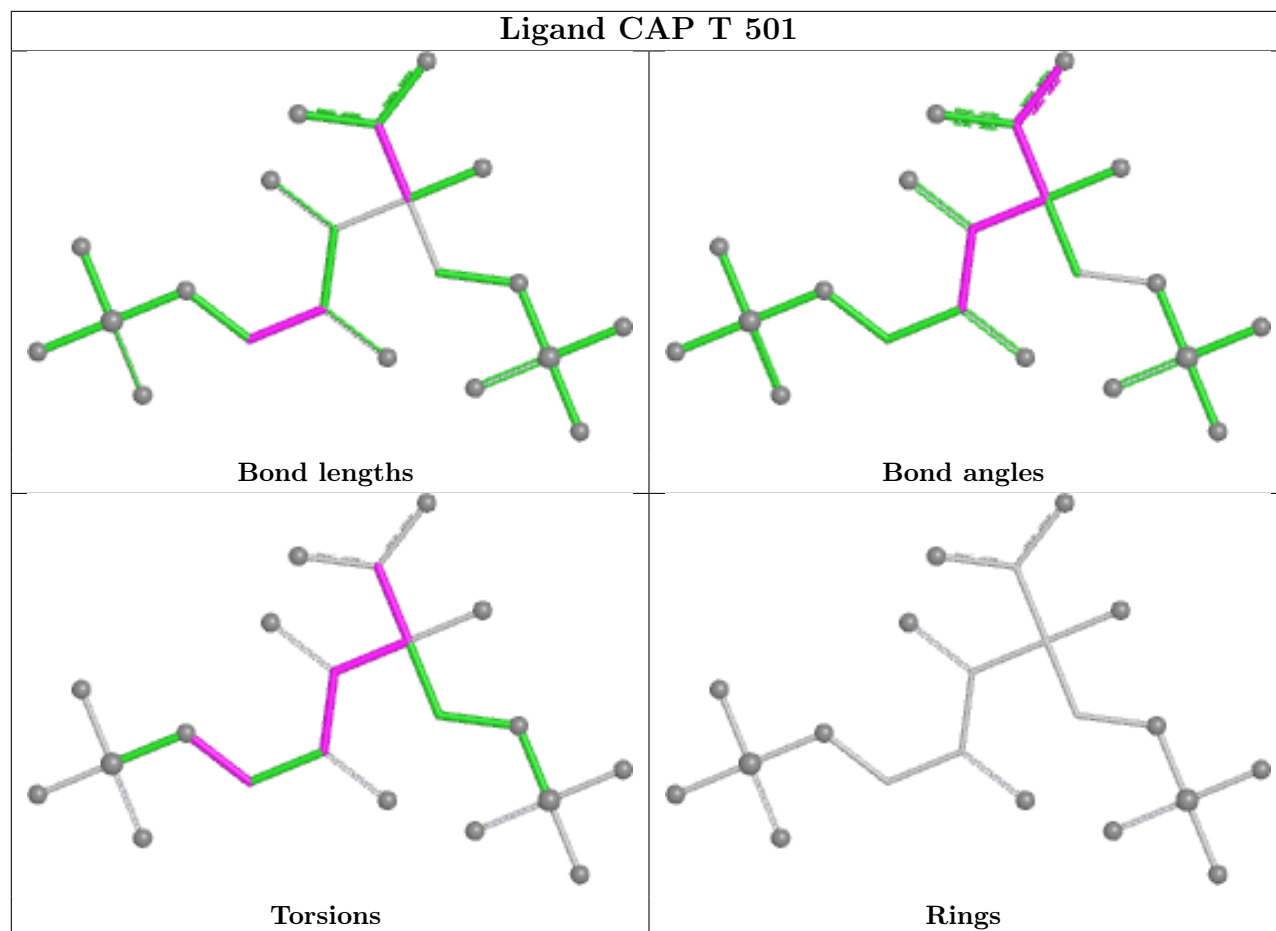




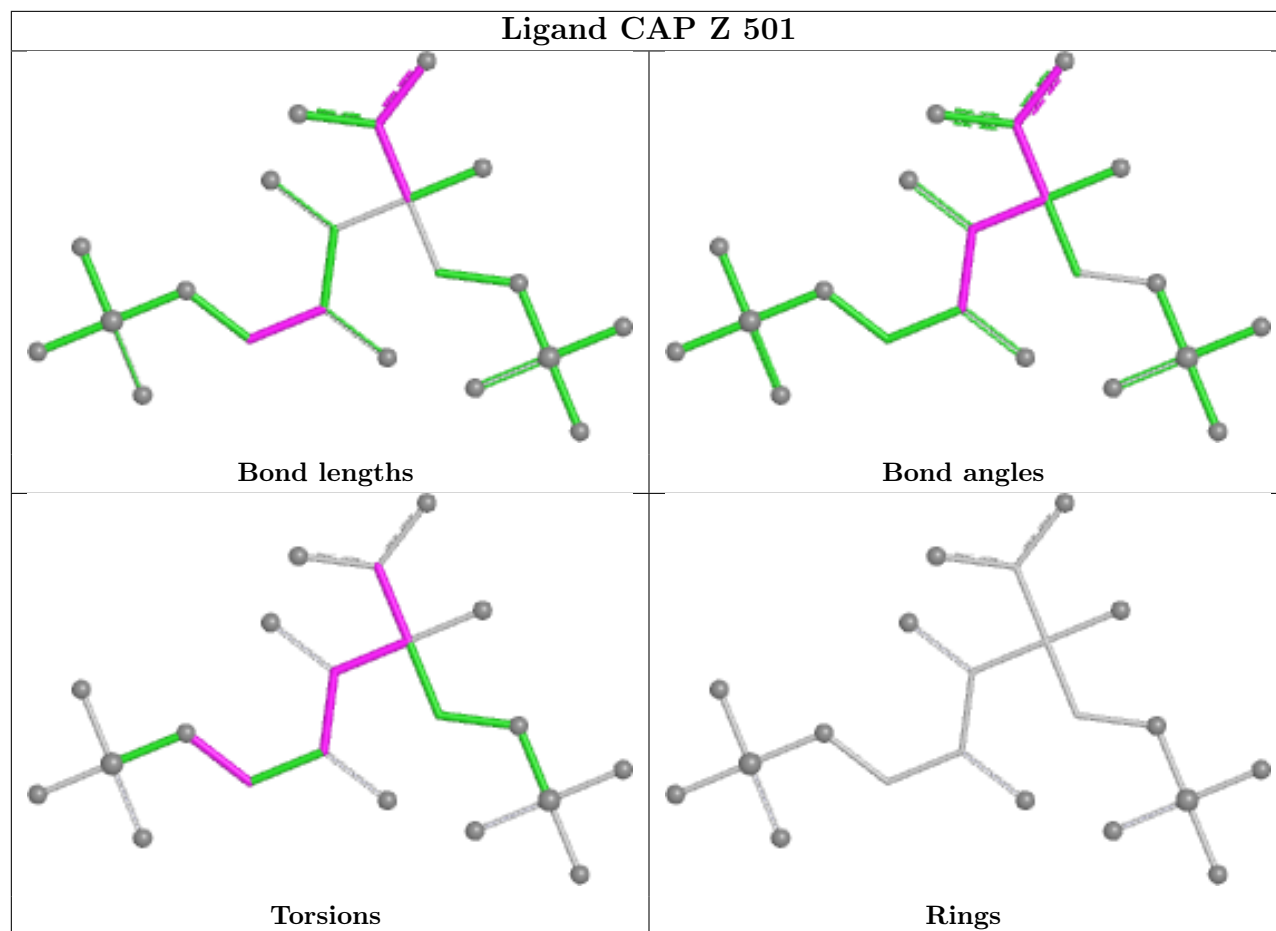


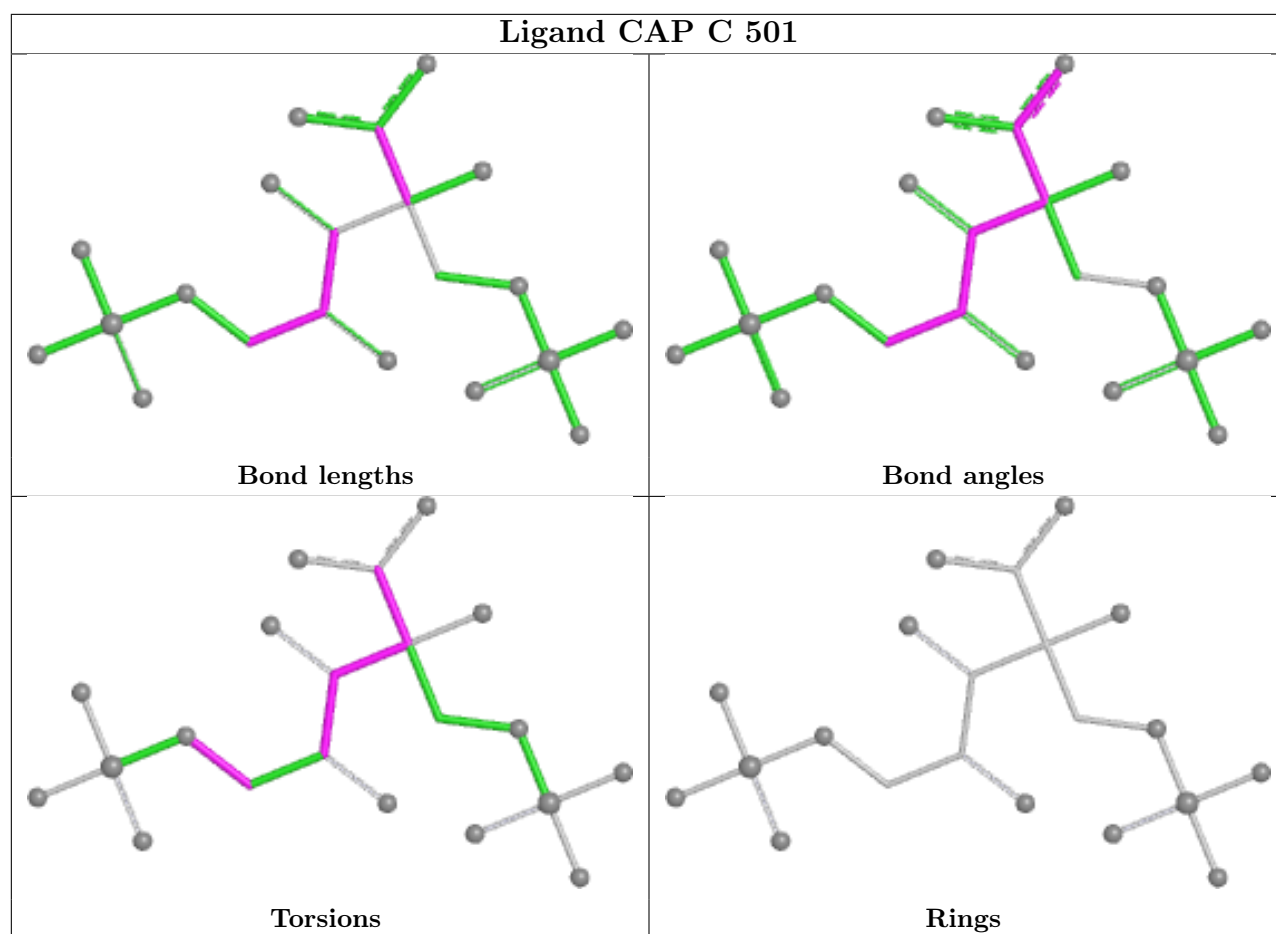


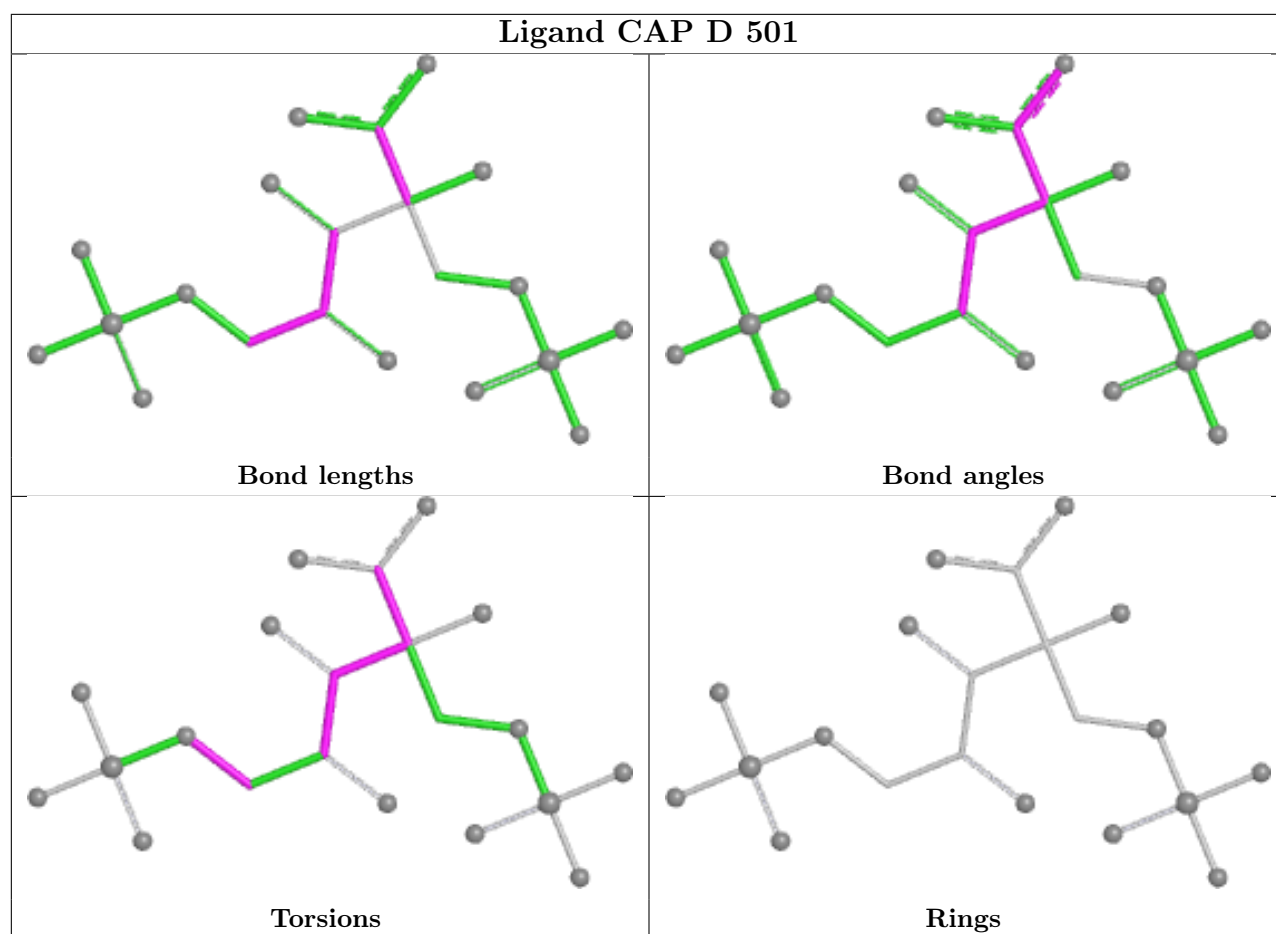


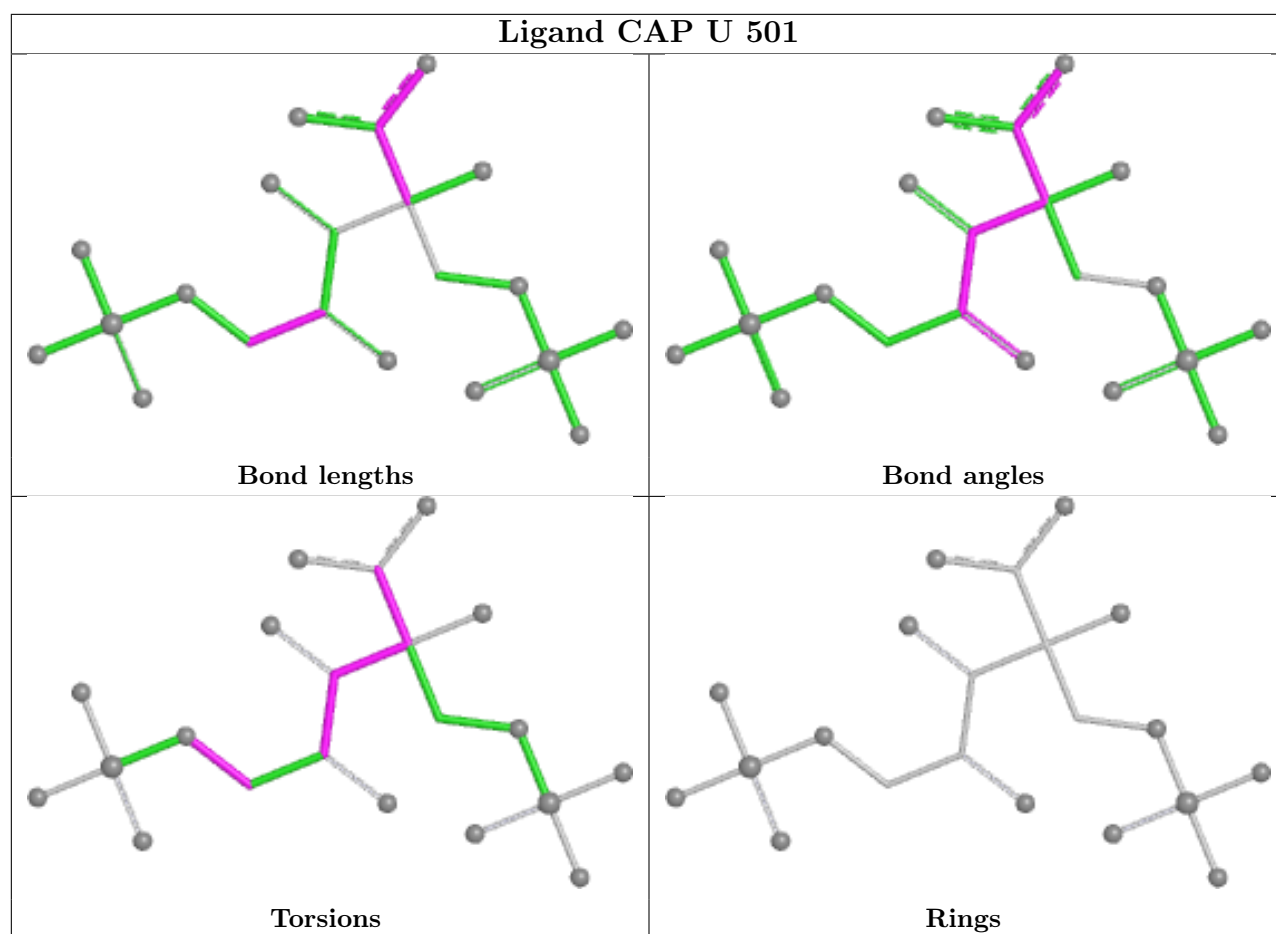


Ligand CAP Z 501









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	463/475 (97%)	-0.52	6 (1%) 75 82	5, 12, 27, 61	0
1	B	462/475 (97%)	-0.48	3 (0%) 85 90	7, 13, 28, 43	0
1	C	461/475 (97%)	-0.61	2 (0%) 88 93	6, 11, 24, 49	0
1	D	462/475 (97%)	-0.66	3 (0%) 85 90	6, 10, 23, 46	0
1	E	460/475 (96%)	-0.65	0 100 100	6, 11, 24, 40	0
1	F	460/475 (96%)	-0.56	2 (0%) 88 93	7, 12, 24, 43	0
1	G	461/475 (97%)	-0.63	2 (0%) 88 93	6, 10, 24, 39	0
1	H	463/475 (97%)	-0.67	3 (0%) 85 90	4, 10, 22, 57	0
1	S	460/475 (96%)	-0.50	2 (0%) 88 93	6, 12, 27, 49	0
1	T	461/475 (97%)	-0.50	3 (0%) 84 90	6, 12, 27, 48	0
1	U	464/475 (97%)	-0.50	7 (1%) 72 79	6, 12, 27, 62	0
1	V	464/475 (97%)	-0.55	5 (1%) 78 84	5, 11, 26, 66	0
1	W	461/475 (97%)	-0.50	3 (0%) 84 90	6, 13, 29, 43	0
1	X	461/475 (97%)	-0.52	3 (0%) 84 90	6, 12, 27, 48	0
1	Y	460/475 (96%)	-0.55	3 (0%) 84 90	6, 11, 27, 45	0
1	Z	461/475 (97%)	-0.67	3 (0%) 84 90	5, 10, 23, 54	0
2	1	139/140 (99%)	-0.20	0 100 100	8, 17, 30, 39	0
2	2	139/140 (99%)	-0.15	1 (0%) 84 90	9, 18, 31, 43	0
2	3	139/140 (99%)	-0.05	2 (1%) 73 81	9, 19, 34, 44	0
2	4	139/140 (99%)	-0.20	0 100 100	9, 16, 30, 37	0
2	5	139/140 (99%)	-0.27	0 100 100	9, 16, 29, 38	0
2	6	139/140 (99%)	-0.11	0 100 100	9, 19, 33, 40	0
2	7	139/140 (99%)	-0.26	0 100 100	8, 15, 28, 34	0
2	8	139/140 (99%)	-0.39	0 100 100	7, 14, 28, 34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	I	139/140 (99%)	-0.11	2 (1%) 73 81	10, 18, 34, 45	0
2	J	139/140 (99%)	-0.06	1 (0%) 84 90	10, 20, 34, 42	0
2	K	139/140 (99%)	-0.17	0 100 100	8, 17, 31, 39	0
2	L	139/140 (99%)	-0.25	1 (0%) 84 90	9, 16, 30, 39	0
2	M	139/140 (99%)	-0.25	0 100 100	8, 15, 31, 39	0
2	N	139/140 (99%)	-0.23	1 (0%) 84 90	8, 17, 29, 39	0
2	O	139/140 (99%)	-0.30	0 100 100	8, 14, 28, 36	0
2	P	139/140 (99%)	-0.35	0 100 100	8, 14, 27, 37	0
All	All	9608/9840 (97%)	-0.48	58 (0%) 85 90	4, 12, 28, 66	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	10	GLY	6.1
1	C	10	GLY	5.6
1	U	9	ALA	5.4
1	Z	10	GLY	5.2
1	V	7	THR	5.2

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MME	L	1	9/10	0.92	0.10	18,24,30,30	0
2	MME	N	1	9/10	0.92	0.11	18,20,28,31	0
2	MME	3	1	9/10	0.92	0.11	24,26,34,34	0
2	MME	M	1	9/10	0.93	0.09	21,22,30,31	0
2	MME	4	1	9/10	0.93	0.10	24,25,30,30	0
2	MME	8	1	9/10	0.93	0.11	21,24,27,30	0
2	MME	1	1	9/10	0.94	0.09	21,23,24,25	0
2	MME	K	1	9/10	0.94	0.09	22,24,28,29	0
2	MME	J	1	9/10	0.94	0.08	20,23,31,31	0
2	MME	O	1	9/10	0.94	0.09	18,21,28,31	0
1	HYP	T	104	8/9	0.95	0.06	9,11,12,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	HYP	W	104	8/9	0.95	0.06	10,11,11,12	0
2	MME	5	1	9/10	0.95	0.09	18,21,30,31	0
1	HYP	X	104	8/9	0.95	0.06	10,10,11,11	0
2	MME	6	1	9/10	0.95	0.09	20,21,26,27	0
2	MME	7	1	9/10	0.95	0.08	16,18,27,29	0
2	MME	I	1	9/10	0.95	0.07	20,21,28,28	0
1	KCX	S	201	12/13	0.96	0.05	5,8,8,11	0
1	HYP	E	151	8/9	0.96	0.05	8,9,10,10	0
1	HYP	A	104	8/9	0.96	0.05	10,11,12,14	0
1	HYP	T	151	8/9	0.96	0.05	6,7,8,9	0
2	MME	2	1	9/10	0.96	0.07	21,23,27,27	0
1	HYP	F	151	8/9	0.96	0.05	11,11,12,12	0
1	HYP	V	104	8/9	0.96	0.05	8,9,10,10	0
1	KCX	V	201	12/13	0.96	0.05	8,9,11,11	0
1	KCX	F	201	12/13	0.96	0.05	5,8,10,10	0
1	KCX	A	201	12/13	0.96	0.05	7,9,10,11	0
1	HYP	G	151	8/9	0.96	0.05	9,9,10,11	0
1	HYP	E	104	8/9	0.96	0.05	7,9,10,10	0
1	KCX	X	201	12/13	0.96	0.05	7,8,10,10	0
1	KCX	H	201	12/13	0.96	0.05	5,6,7,9	0
1	KCX	Y	201	12/13	0.96	0.05	6,7,8,8	0
2	MME	P	1	9/10	0.96	0.07	17,21,25,25	0
1	HYP	S	104	8/9	0.96	0.05	11,12,13,14	0
1	KCX	C	201	12/13	0.97	0.04	7,9,11,11	0
1	KCX	T	201	12/13	0.97	0.05	4,8,9,9	0
1	HYP	B	104	8/9	0.97	0.05	8,11,11,13	0
1	HYP	U	104	8/9	0.97	0.04	9,9,9,9	0
1	KCX	U	201	12/13	0.97	0.04	8,10,11,11	0
1	HYP	D	104	8/9	0.97	0.04	6,7,9,9	0
1	HYP	G	104	8/9	0.97	0.05	9,11,11,12	0
1	HYP	D	151	8/9	0.97	0.05	4,7,8,8	0
1	KCX	G	201	12/13	0.97	0.04	5,7,8,9	0
1	KCX	D	201	12/13	0.97	0.04	6,7,7,8	0
1	KCX	W	201	12/13	0.97	0.05	9,10,12,12	0
1	HYP	B	151	8/9	0.97	0.04	9,10,11,12	0
1	KCX	B	201	12/13	0.97	0.05	7,10,11,12	0
1	HYP	X	151	8/9	0.97	0.04	7,9,10,10	0
1	HYP	A	151	8/9	0.97	0.04	8,8,9,11	0
1	HYP	S	151	8/9	0.97	0.04	7,8,9,9	0
1	KCX	E	201	12/13	0.97	0.05	6,8,10,11	0
1	HYP	C	104	8/9	0.97	0.05	6,8,9,9	0
1	HYP	Z	104	8/9	0.97	0.05	8,9,10,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KCX	Z	201	12/13	0.97	0.05	4,7,8,9	0
1	HYP	F	104	8/9	0.97	0.04	8,10,12,14	0
1	SMC	W	369	7/8	0.98	0.06	9,10,11,11	0
1	HYP	H	151	8/9	0.98	0.04	5,5,6,6	0
1	HYP	C	151	8/9	0.98	0.04	7,8,9,9	0
1	SMC	A	369	7/8	0.98	0.05	13,13,15,16	0
1	HYP	V	151	8/9	0.98	0.04	7,7,9,9	0
1	SMC	X	369	7/8	0.98	0.04	11,12,13,14	0
1	SMC	F	256	7/8	0.98	0.04	8,9,9,9	0
1	HYP	Y	104	8/9	0.98	0.04	10,11,11,12	0
1	HYP	Y	151	8/9	0.98	0.04	8,9,9,9	0
1	SMC	V	369	7/8	0.98	0.04	10,10,12,14	0
1	SMC	B	369	7/8	0.98	0.05	12,13,13,14	0
1	HYP	H	104	8/9	0.98	0.04	6,7,8,9	0
1	HYP	Z	151	8/9	0.98	0.04	6,7,8,9	0
1	HYP	W	151	8/9	0.98	0.04	5,8,9,9	0
1	HYP	U	151	8/9	0.98	0.04	7,9,9,9	0
1	SMC	E	369	7/8	0.99	0.04	8,9,10,11	0
1	SMC	S	256	7/8	0.99	0.04	4,6,7,7	0
1	SMC	S	369	7/8	0.99	0.04	10,10,12,12	0
1	SMC	D	256	7/8	0.99	0.04	5,7,8,10	0
1	SMC	G	256	7/8	0.99	0.04	5,6,8,8	0
1	SMC	W	256	7/8	0.99	0.04	8,9,9,10	0
1	SMC	G	369	7/8	0.99	0.04	11,11,13,13	0
1	SMC	D	369	7/8	0.99	0.04	8,9,10,10	0
1	SMC	T	256	7/8	0.99	0.03	6,6,7,8	0
1	SMC	T	369	7/8	0.99	0.05	11,12,13,15	0
1	SMC	B	256	7/8	0.99	0.04	7,8,9,9	0
1	SMC	X	256	7/8	0.99	0.04	7,7,9,11	0
1	SMC	A	256	7/8	0.99	0.04	7,8,8,8	0
1	SMC	C	256	7/8	0.99	0.04	7,8,9,10	0
1	SMC	H	256	7/8	0.99	0.03	6,6,7,8	0
1	SMC	U	256	7/8	0.99	0.03	5,7,7,7	0
1	SMC	U	369	7/8	0.99	0.04	8,9,10,11	0
1	SMC	Y	256	7/8	0.99	0.04	6,7,8,8	0
1	SMC	Y	369	7/8	0.99	0.04	11,12,13,14	0
1	SMC	H	369	7/8	0.99	0.04	6,9,10,10	0
1	SMC	F	369	7/8	0.99	0.04	10,11,12,13	0
1	SMC	C	369	7/8	0.99	0.04	8,10,12,12	0
1	SMC	E	256	7/8	0.99	0.04	6,7,8,8	0
1	SMC	Z	256	7/8	0.99	0.04	6,7,7,8	0
1	SMC	Z	369	7/8	0.99	0.04	8,9,11,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SMC	V	256	7/8	0.99	0.04	6,6,7,8	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
5	GOL	H	604	6/6	0.78	0.17	25,30,33,34	0
5	GOL	H	619	6/6	0.79	0.16	29,32,34,34	0
5	GOL	C	615	6/6	0.82	0.14	26,28,31,32	0
5	GOL	Y	618	6/6	0.82	0.16	37,40,41,41	0
5	GOL	F	617	6/6	0.84	0.14	32,32,33,34	0
5	GOL	W	620	6/6	0.86	0.13	34,36,36,37	0
5	GOL	E	609	6/6	0.87	0.10	14,17,20,22	0
5	GOL	D	608	6/6	0.87	0.12	23,26,27,27	0
5	GOL	A	605	6/6	0.88	0.12	26,27,29,30	0
5	GOL	Y	603	6/6	0.88	0.11	29,31,32,32	0
5	GOL	U	607	6/6	0.88	0.10	23,27,28,28	0
5	GOL	S	609	6/6	0.89	0.12	23,25,28,32	0
5	GOL	G	611	6/6	0.89	0.12	16,18,23,26	0
5	GOL	V	616	6/6	0.89	0.11	25,27,29,30	0
5	GOL	B	606	6/6	0.89	0.10	22,22,24,24	0
5	GOL	H	612	6/6	0.89	0.11	14,18,21,21	0
5	GOL	D	616	6/6	0.89	0.12	22,26,30,32	0
5	GOL	X	617	6/6	0.90	0.10	21,27,29,30	0
5	GOL	B	614	6/6	0.90	0.12	25,31,33,34	0
5	GOL	V	608	6/6	0.90	0.10	17,19,20,21	0
5	GOL	Z	604	6/6	0.90	0.10	24,26,26,28	0
5	GOL	E	620	6/6	0.91	0.10	22,26,28,28	0
5	GOL	T	606	6/6	0.91	0.09	21,22,24,25	0
5	GOL	Y	611	6/6	0.91	0.10	19,21,22,23	0
5	GOL	W	601	6/6	0.91	0.09	23,25,25,25	0
5	GOL	S	605	6/6	0.91	0.09	26,28,30,30	0
5	GOL	Z	612	6/6	0.91	0.10	17,19,22,23	0

Continued on next page...

Continued from previous page...

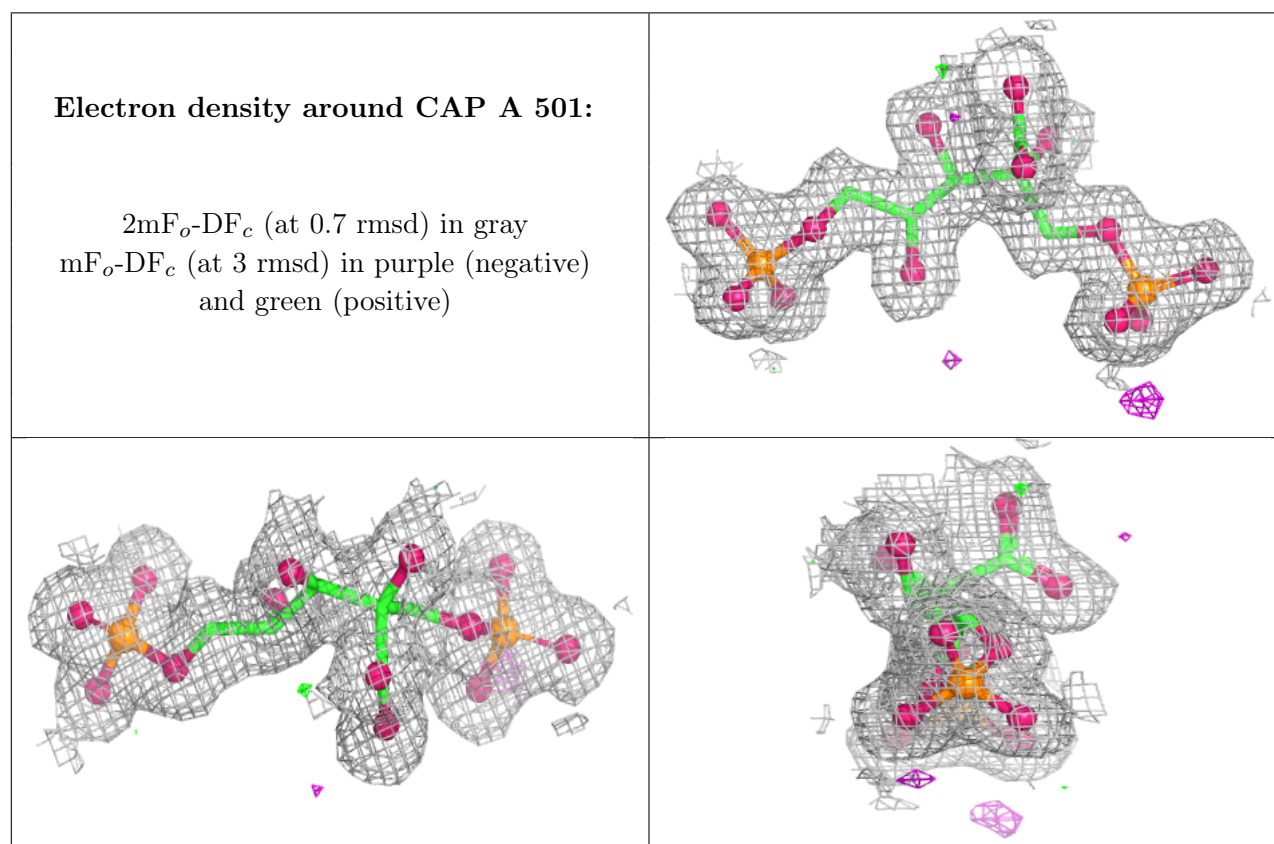
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	613	6/6	0.92	0.09	25,29,30,30	0
5	GOL	C	607	6/6	0.92	0.08	23,24,26,27	0
5	GOL	X	610	6/6	0.92	0.09	16,19,22,26	0
5	GOL	B	610	6/6	0.93	0.08	18,20,21,23	0
5	GOL	G	603	6/6	0.93	0.08	20,22,25,27	0
5	GOL	E	601	6/6	0.93	0.09	29,30,30,31	0
5	GOL	G	618	6/6	0.93	0.09	26,30,31,31	0
5	GOL	S	613	6/6	0.93	0.08	23,25,25,26	0
5	GOL	F	602	6/6	0.93	0.08	22,24,25,27	0
5	GOL	Z	619	6/6	0.93	0.08	19,24,25,26	0
5	GOL	T	614	6/6	0.94	0.07	22,27,29,29	0
5	GOL	U	615	6/6	0.95	0.07	20,23,25,27	0
5	GOL	X	602	6/6	0.95	0.07	19,20,22,22	0
4	CAP	A	501	21/21	0.98	0.04	7,10,11,14	0
4	CAP	B	501	21/21	0.98	0.04	10,12,15,17	0
4	CAP	C	501	21/21	0.98	0.04	8,10,11,13	0
4	CAP	E	501	21/21	0.98	0.04	8,11,11,12	0
4	CAP	F	501	21/21	0.98	0.04	9,11,13,15	0
4	CAP	G	501	21/21	0.98	0.04	6,8,10,11	0
4	CAP	S	501	21/21	0.98	0.05	10,12,12,13	0
4	CAP	T	501	21/21	0.98	0.04	6,10,11,12	0
4	CAP	U	501	21/21	0.98	0.04	11,13,14,16	0
4	CAP	V	501	21/21	0.98	0.04	8,10,11,12	0
4	CAP	W	501	21/21	0.98	0.04	9,11,15,17	0
4	CAP	X	501	21/21	0.98	0.04	8,11,13,14	0
4	CAP	Y	501	21/21	0.98	0.04	6,8,10,11	0
4	CAP	Z	501	21/21	0.98	0.04	7,9,10,11	0
3	MG	A	476	1/1	0.98	0.02	9,9,9,9	0
3	MG	F	476	1/1	0.98	0.02	11,11,11,11	0
3	MG	H	476	1/1	0.98	0.03	10,10,10,10	0
3	MG	S	476	1/1	0.98	0.03	11,11,11,11	0
3	MG	V	476	1/1	0.99	0.03	12,12,12,12	0
3	MG	W	476	1/1	0.99	0.02	12,12,12,12	0
3	MG	X	476	1/1	0.99	0.03	13,13,13,13	0
3	MG	Y	476	1/1	0.99	0.02	11,11,11,11	0
3	MG	B	476	1/1	0.99	0.02	11,11,11,11	0
3	MG	G	476	1/1	0.99	0.04	11,11,11,11	0
3	MG	C	476	1/1	0.99	0.03	13,13,13,13	0
4	CAP	D	501	21/21	0.99	0.04	6,9,10,12	0
3	MG	E	476	1/1	0.99	0.02	11,11,11,11	0
3	MG	T	476	1/1	0.99	0.02	12,12,12,12	0
3	MG	U	476	1/1	0.99	0.02	11,11,11,11	0

Continued on next page...

Continued from previous page...

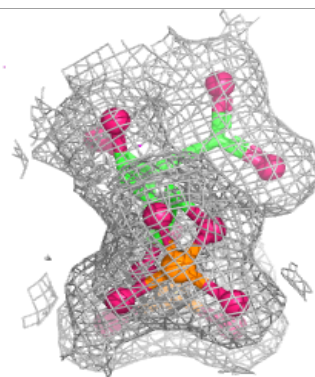
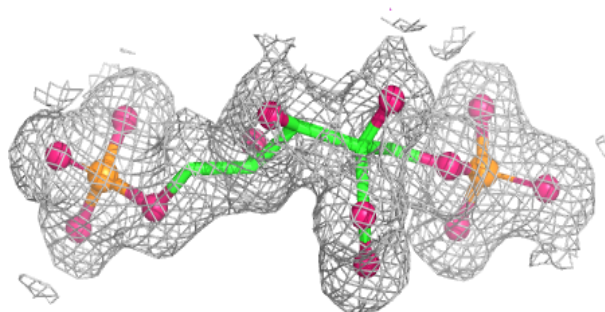
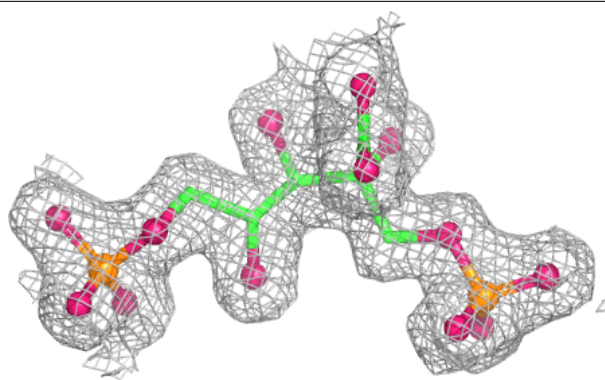
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CAP	H	501	21/21	0.99	0.04	6,8,9,11	0
3	MG	D	476	1/1	1.00	0.01	9,9,9,9	0
3	MG	Z	476	1/1	1.00	0.02	9,9,9,9	0

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.

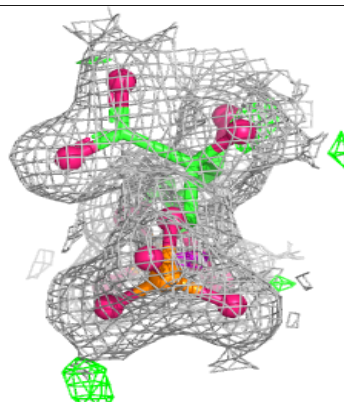
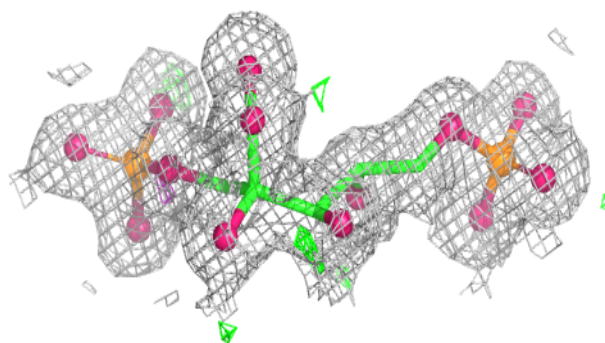
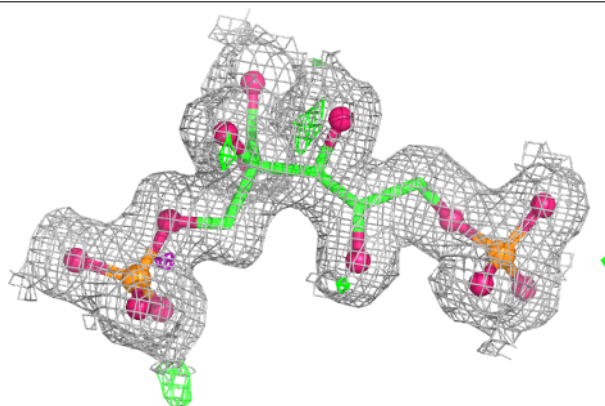


Electron density around CAP B 501:

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

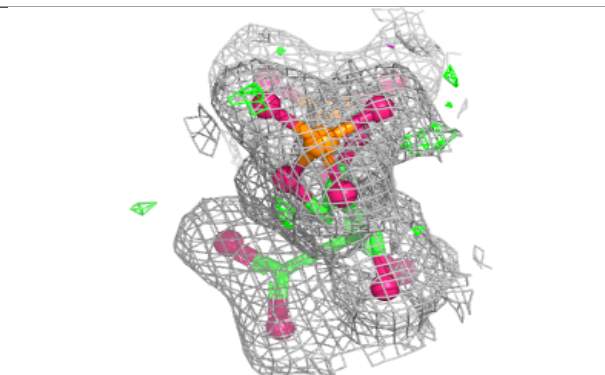
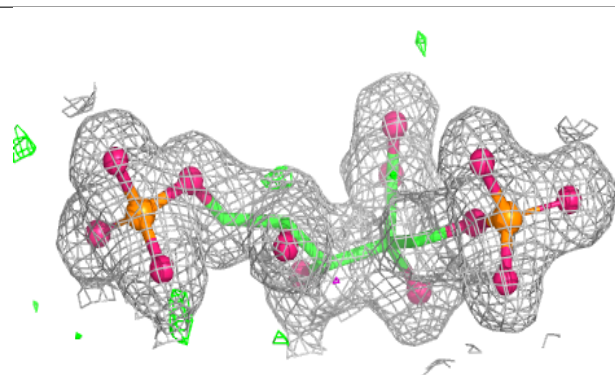
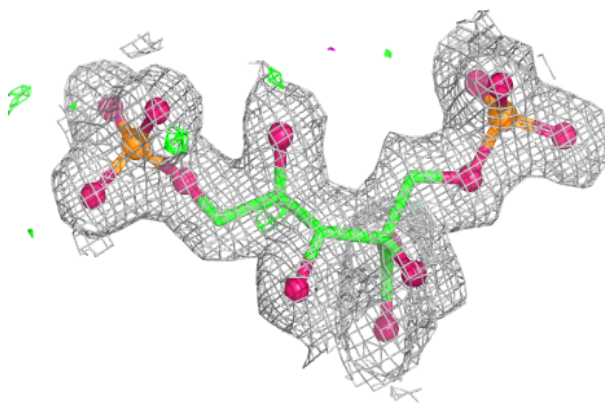
**Electron density around CAP C 501:**

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

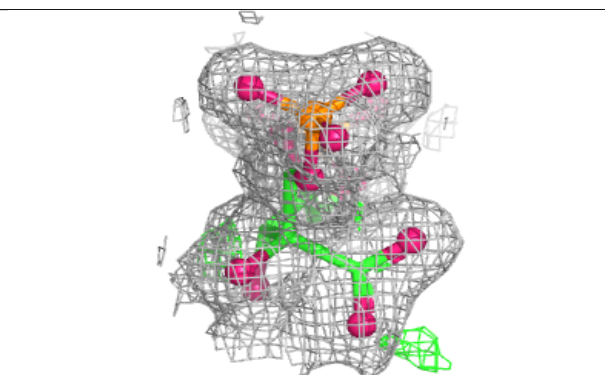
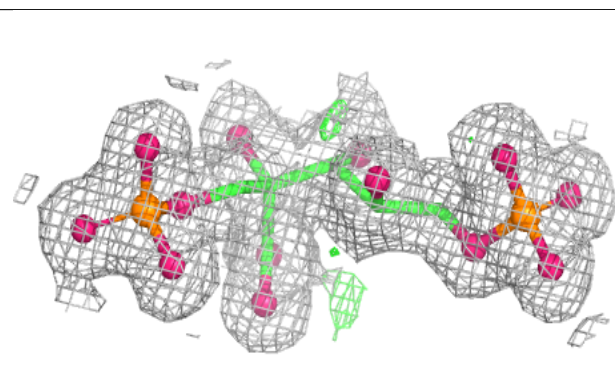
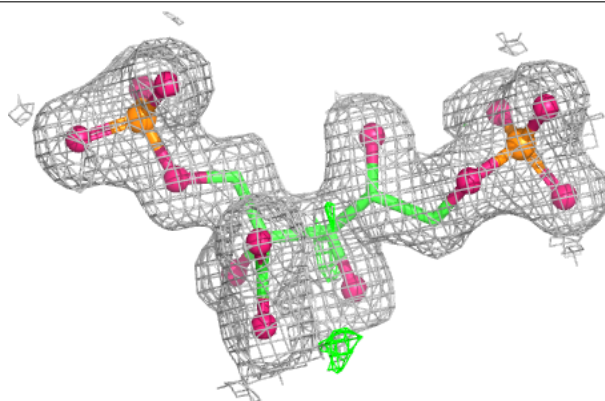


Electron density around CAP E 501:

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

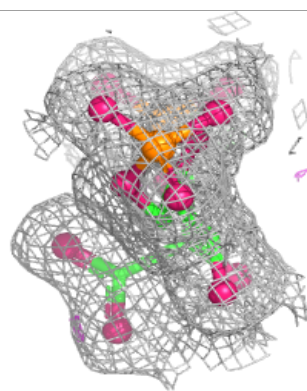
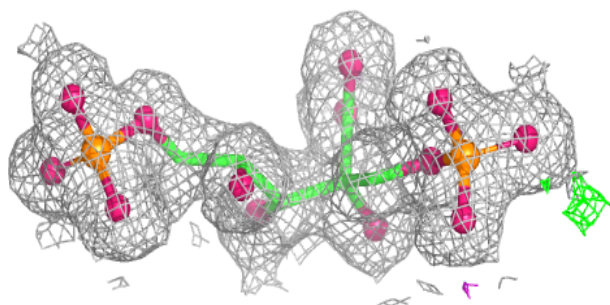
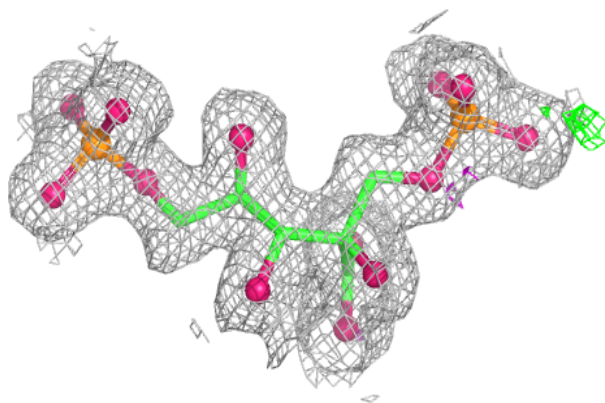
**Electron density around CAP F 501:**

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

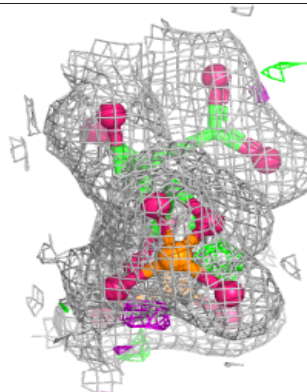
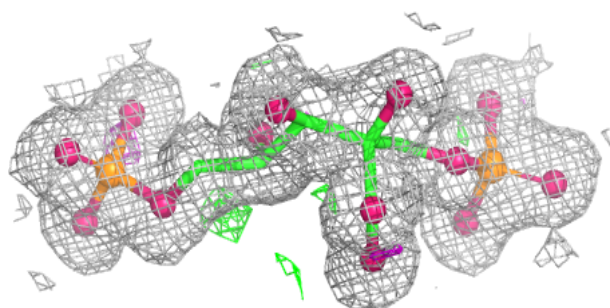
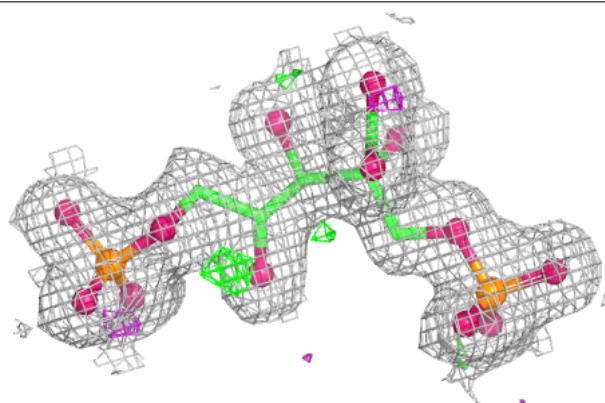


Electron density around CAP G 501:

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

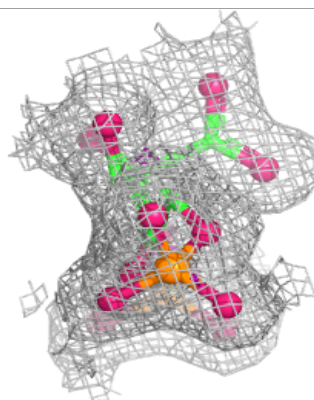
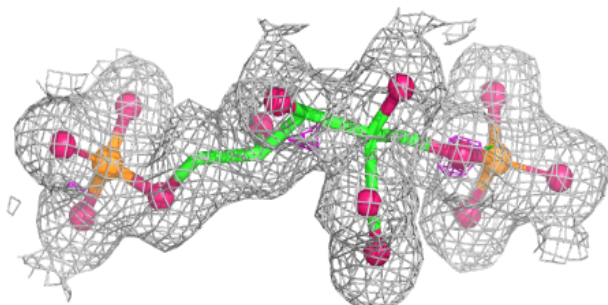
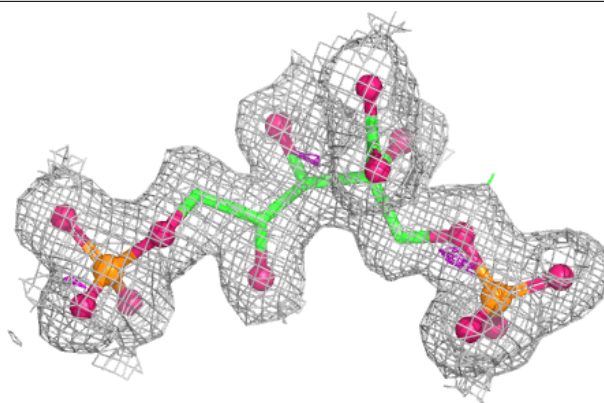
**Electron density around CAP S 501:**

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

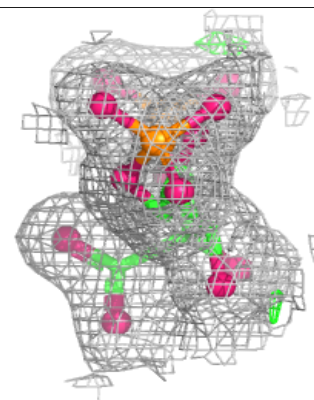
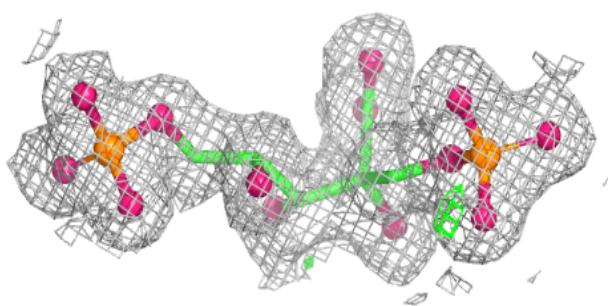
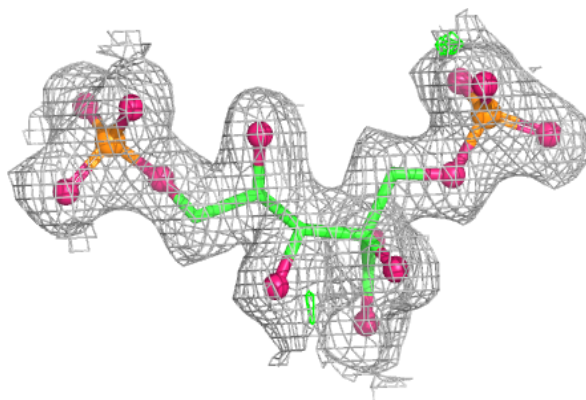


Electron density around CAP T 501:

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

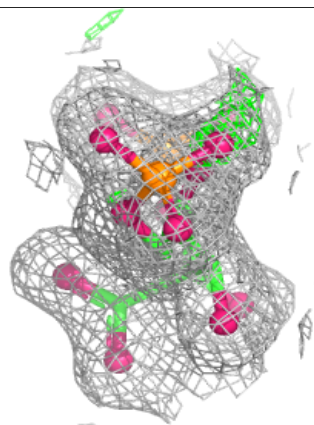
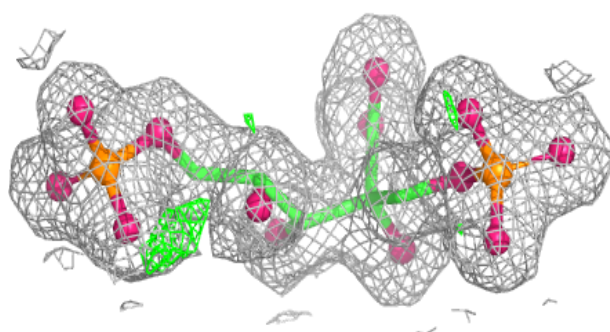
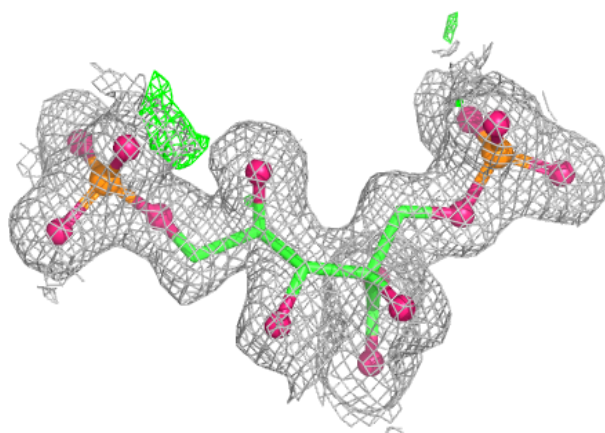
**Electron density around CAP U 501:**

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

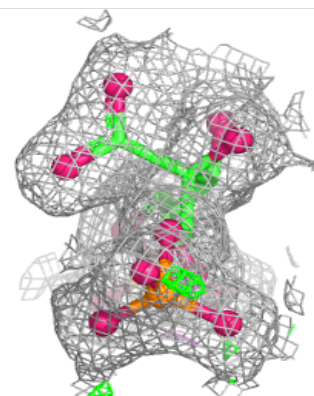
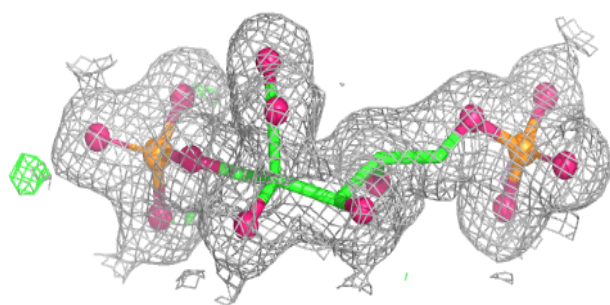
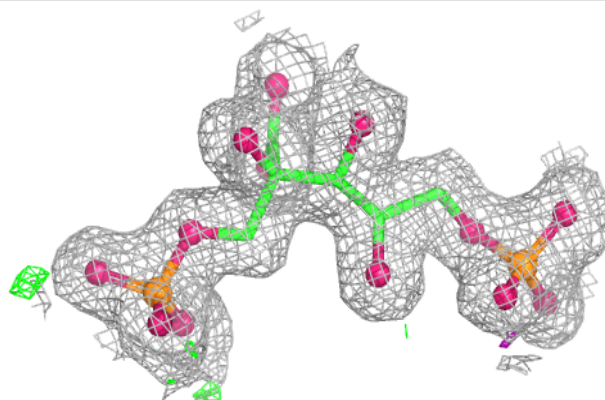


Electron density around CAP V 501:

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

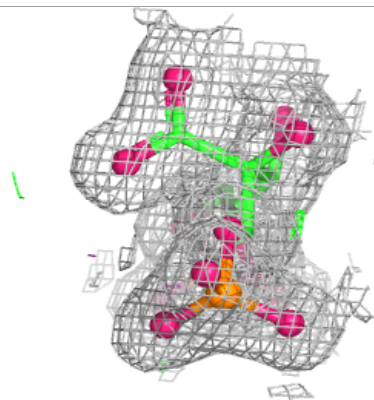
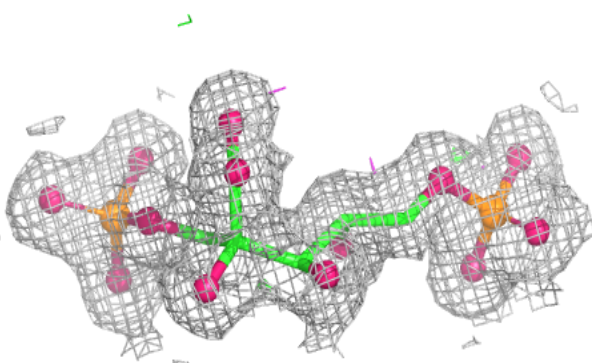
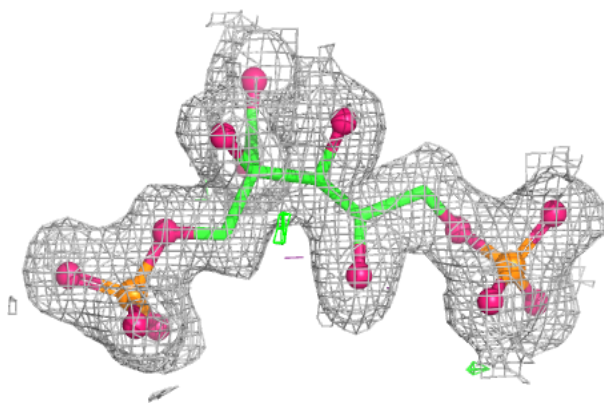
**Electron density around CAP W 501:**

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

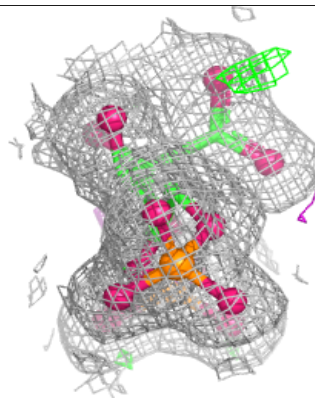
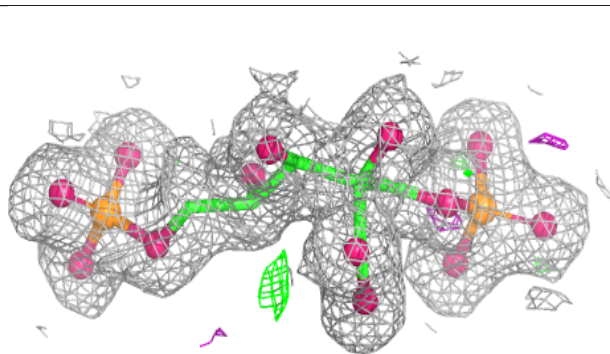
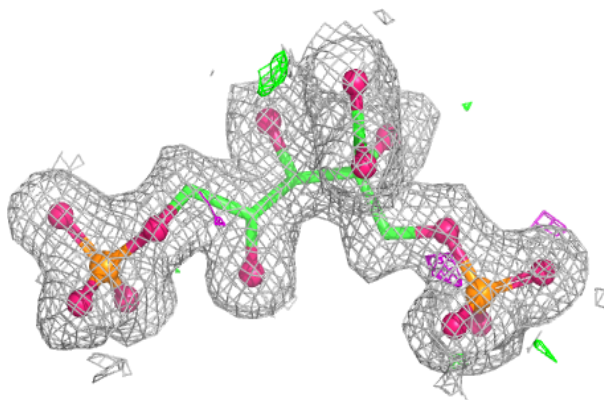


Electron density around CAP X 501:

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

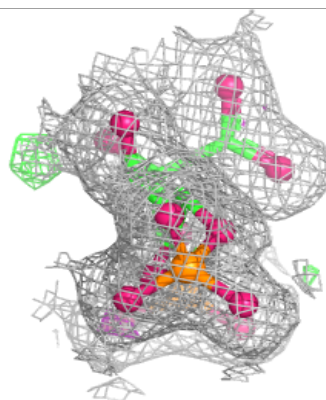
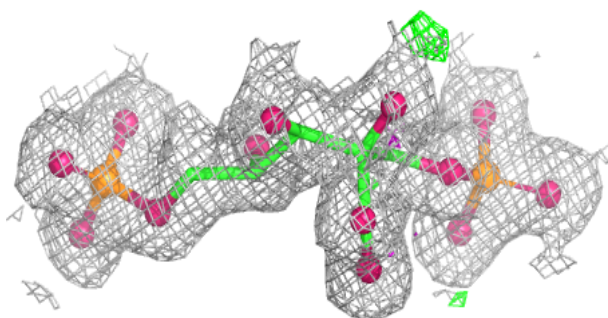
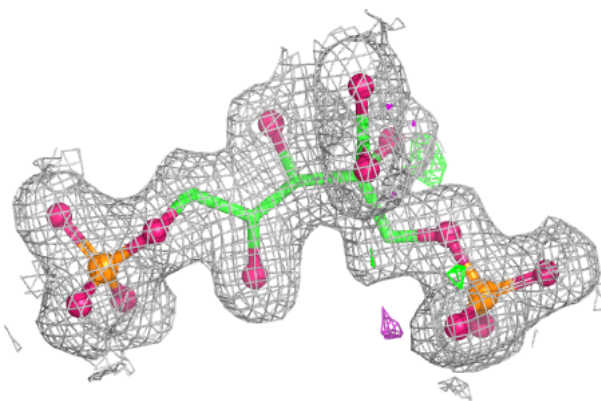
**Electron density around CAP Y 501:**

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

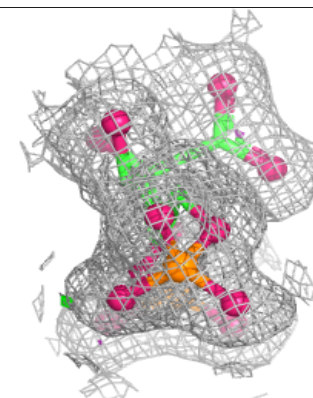
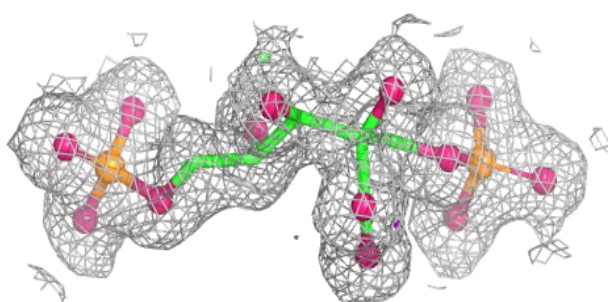
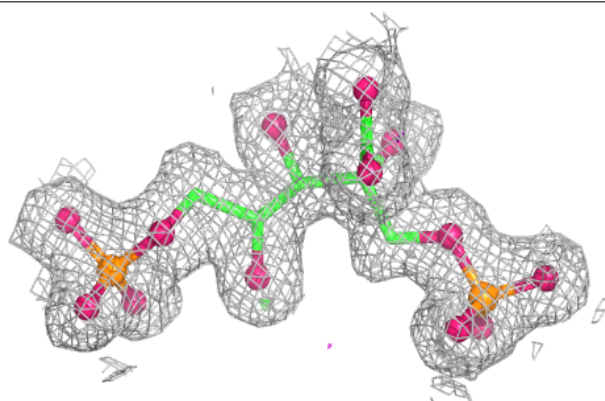


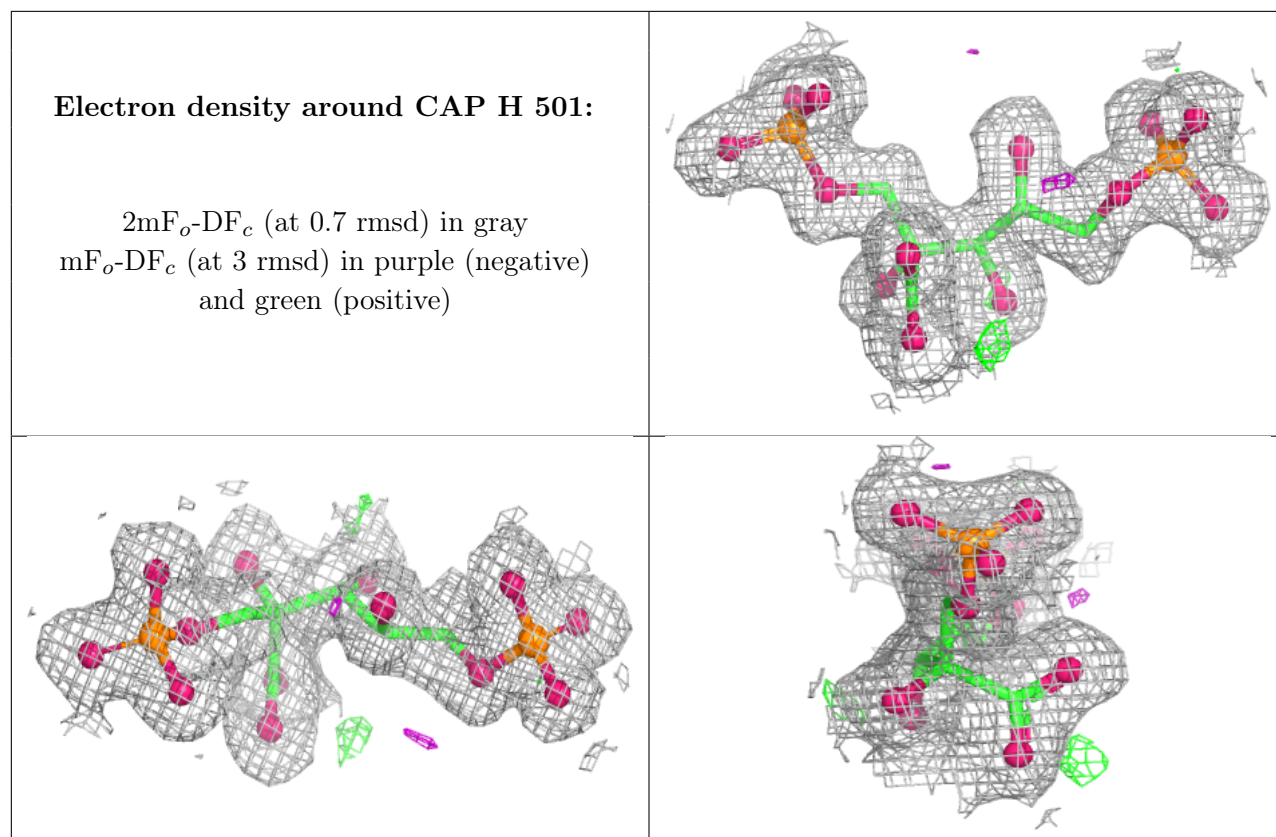
Electron density around CAP Z 501:

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

**Electron density around CAP D 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.