



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2023 – 09:04 AM EDT

PDB ID : 1IR2  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

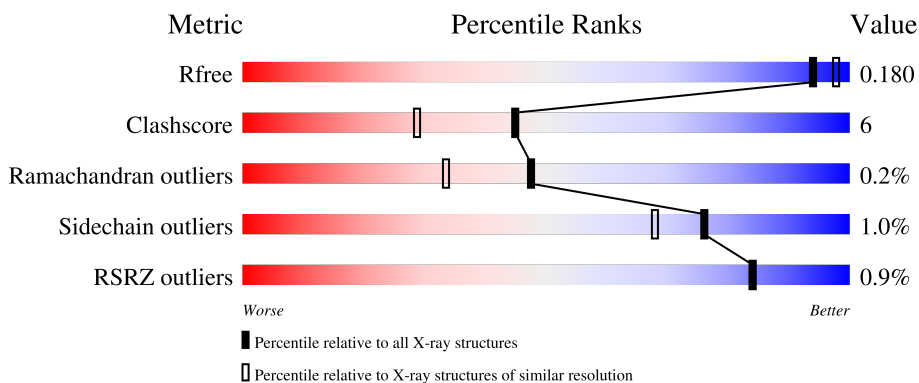
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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

Mol	Chain	Length	Quality of chain
1	A	475	 87% 11% ..
1	B	475	 83% 15% .
1	C	475	 83% 14% ..
1	D	475	 86% 12% .
1	E	475	 84% 13% ..



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Mol	Chain	Length	Quality of chain
1	F	475	85% 12% .
1	G	475	85% 13% ..
1	H	475	84% 13% ..
1	S	475	83% 14% .
1	T	475	83% 14% ..
1	U	475	82% 16% ..
1	V	475	83% 15% ..
1	W	475	84% 14% ..
1	X	475	84% 14% ..
1	Y	475	80% 17% ..
1	Z	475	85% 12% ..
2	1	140	80% 18% .
2	2	140	78% 21% .
2	3	140	76% 21% .
2	4	140	83% 16% .
2	5	140	83% 16% .
2	6	140	81% 19% .
2	7	140	84% 15% .
2	8	140	79% 19% .
2	I	140	83% 16% .
2	J	140	76% 22% .
2	K	140	76% 21% .
2	L	140	80% 18% .
2	M	140	77% 23%
2	N	140	82% 16% .

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Mol	Chain	Length	Quality of chain
2	O	140	 83% 17%
2	P	140	 % 79% 20% .

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

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

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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

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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
			Total	C	N	O	S			
2	I	140	1145	739	191	204	11	0	0	0
2	J	140	1145	739	191	204	11	0	0	0
2	K	140	1145	739	191	204	11	0	0	0
2	L	140	1145	739	191	204	11	0	0	0
2	M	140	1145	739	191	204	11	0	0	0
2	N	140	1145	739	191	204	11	0	0	0
2	O	140	1145	739	191	204	11	0	0	0
2	P	140	1145	739	191	204	11	0	0	0
2	1	140	1145	739	191	204	11	0	0	0
2	2	140	1145	739	191	204	11	0	0	0
2	3	140	1145	739	191	204	11	0	0	0
2	4	140	1145	739	191	204	11	0	0	0
2	5	140	1145	739	191	204	11	0	0	0

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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 (three-letter code: MG) (formula: Mg).

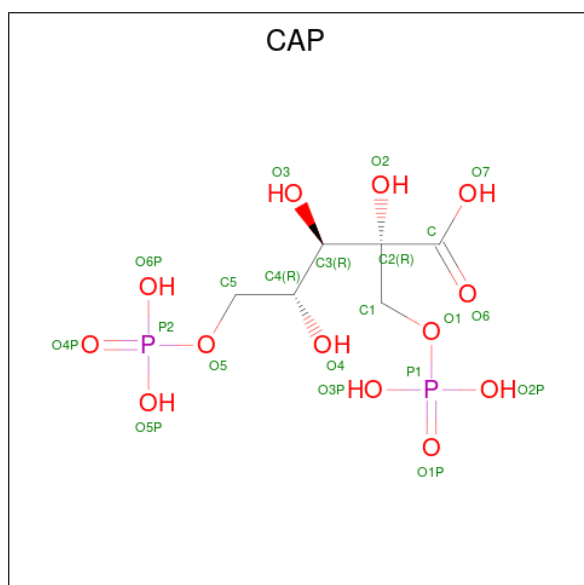
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

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

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula:  $C_6H_{14}O_{13}P_2$ ).



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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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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

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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		

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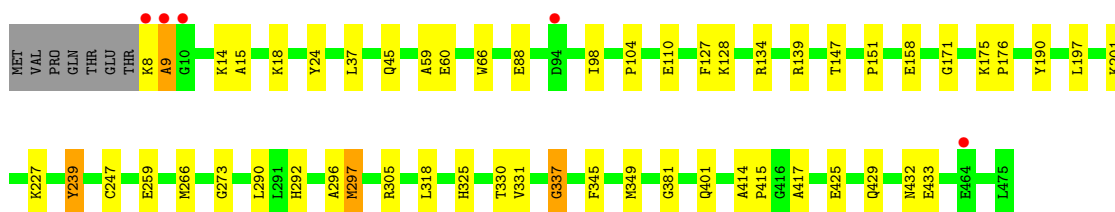
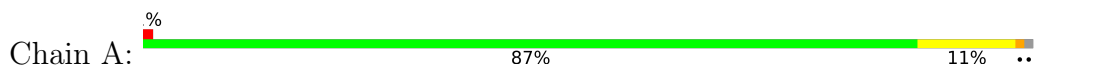
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	452	Total 452	O 452	0	0
6	P	200	Total 200	O 200	0	0
6	S	425	Total 425	O 425	0	0
6	1	173	Total 173	O 173	0	0
6	T	426	Total 426	O 426	0	0
6	2	173	Total 173	O 173	0	0
6	U	427	Total 427	O 427	0	0
6	3	170	Total 170	O 170	0	0
6	V	456	Total 456	O 456	0	0
6	4	174	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



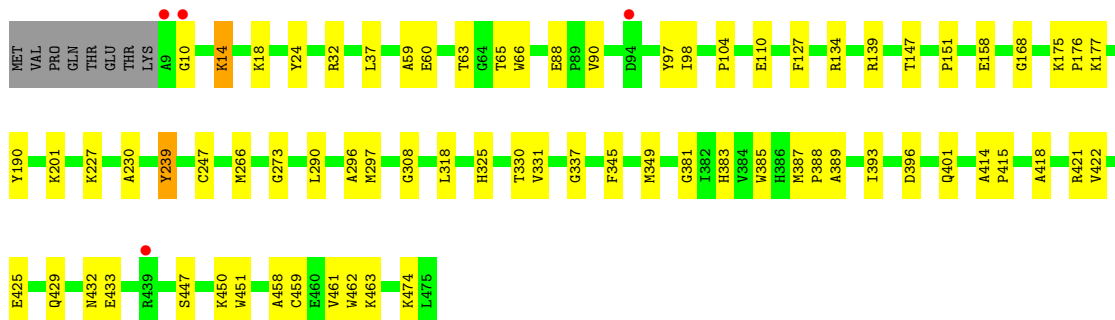
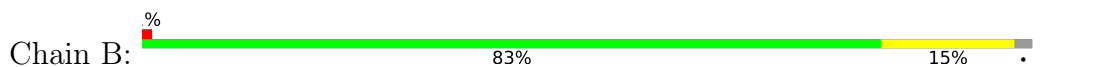
### 3 Residue-property plots [i](#)

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.

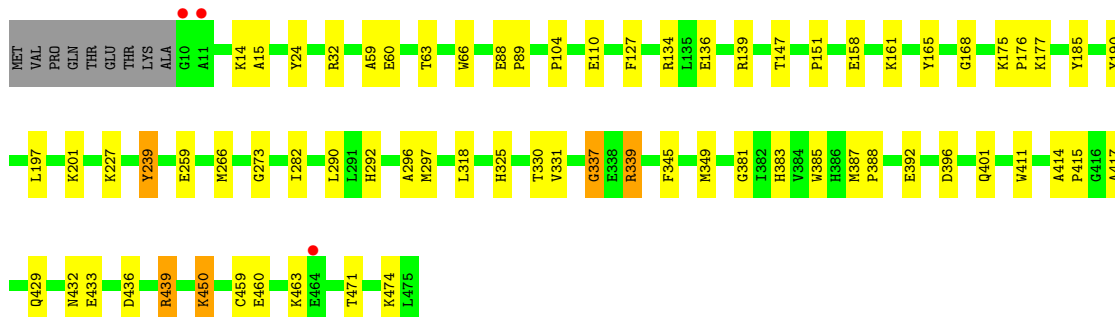
- Molecule 1: Large subunit of Rubisco



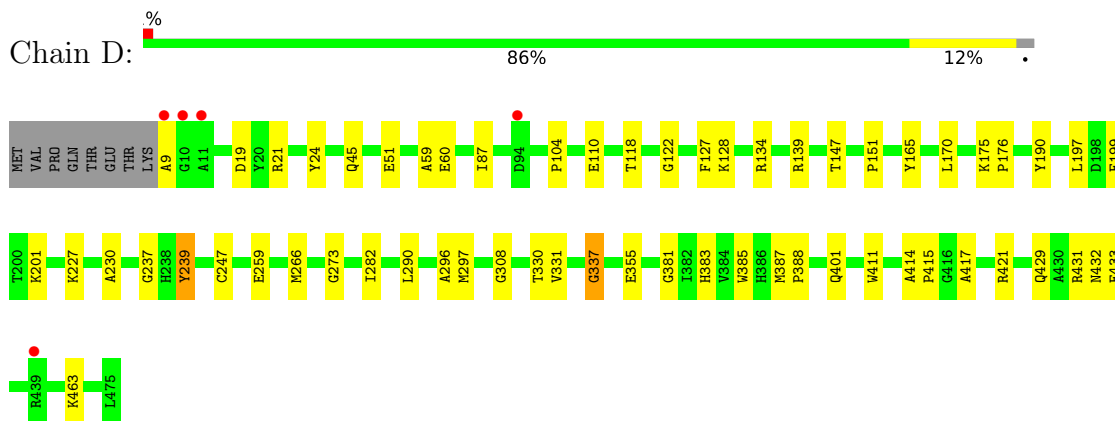
- Molecule 1: Large subunit of Rubisco



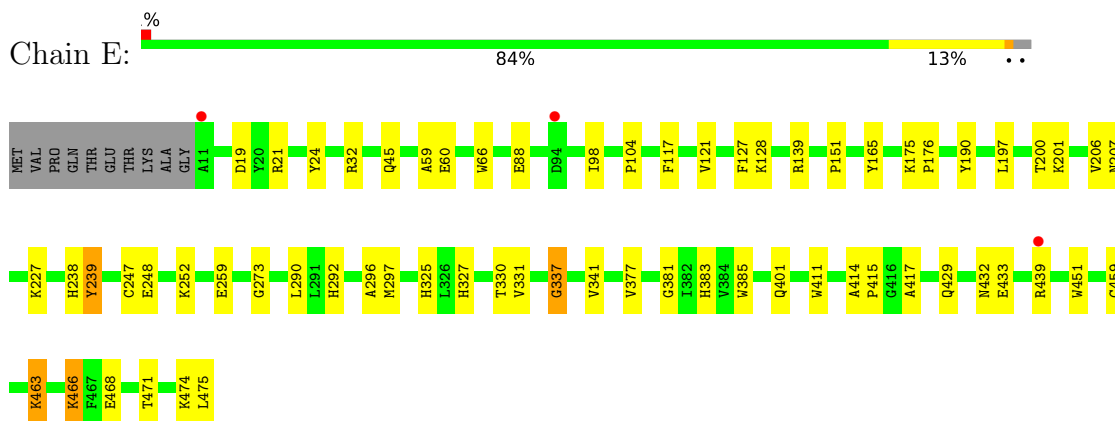
- Molecule 1: Large subunit of Rubisco



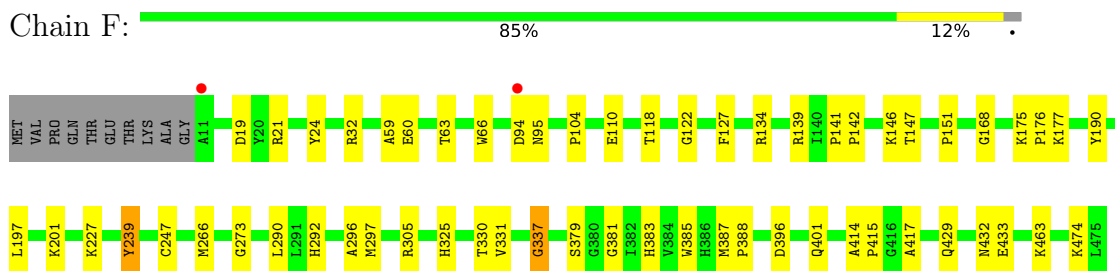
- Molecule 1: Large subunit of Rubisco



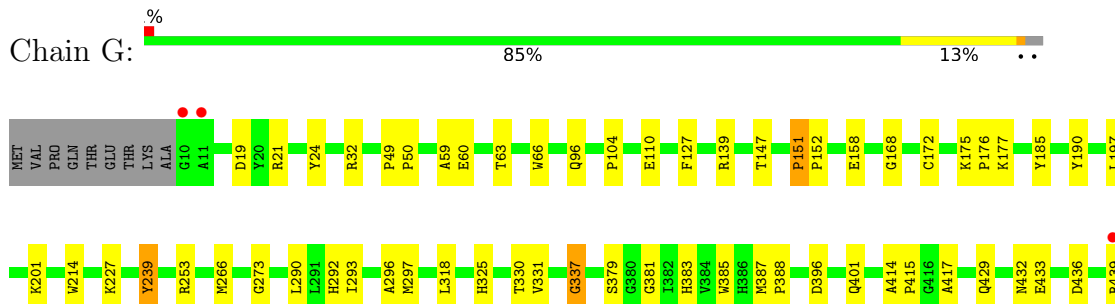
- Molecule 1: Large subunit of Rubisco



- Molecule 1: Large subunit of Rubisco

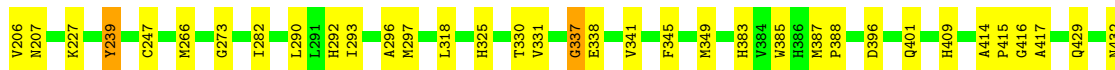
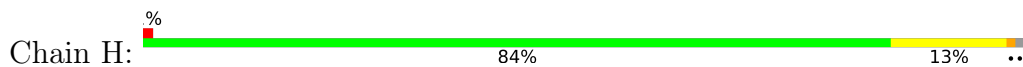


- Molecule 1: Large subunit of Rubisco

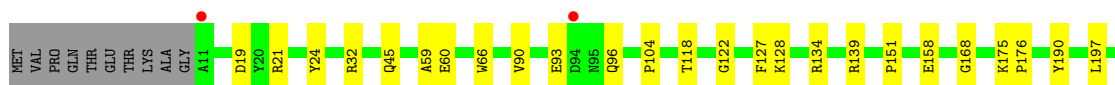
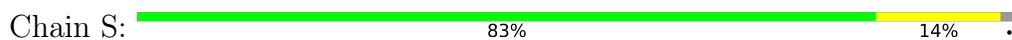




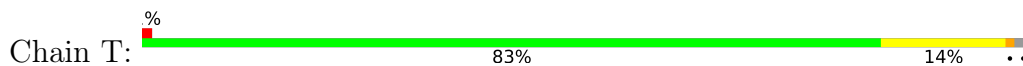
- Molecule 1: Large subunit of Rubisco



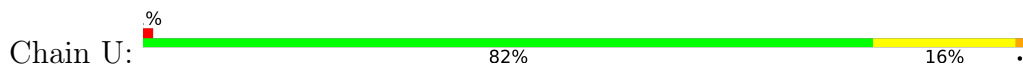
- Molecule 1: Large subunit of Rubisco

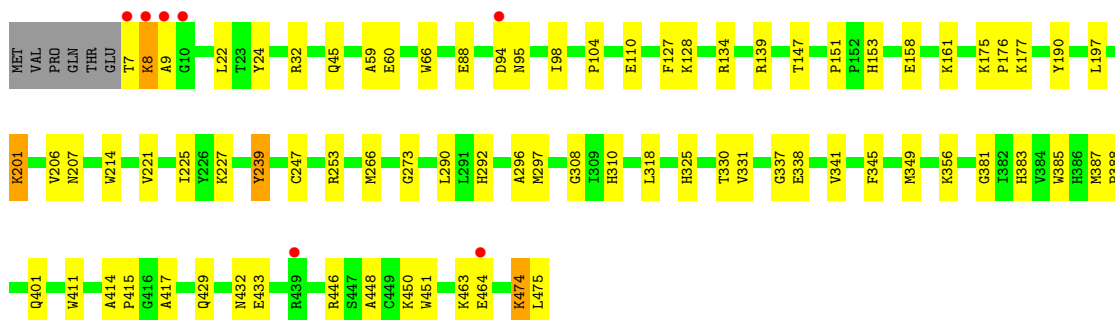


- Molecule 1: Large subunit of Rubisco

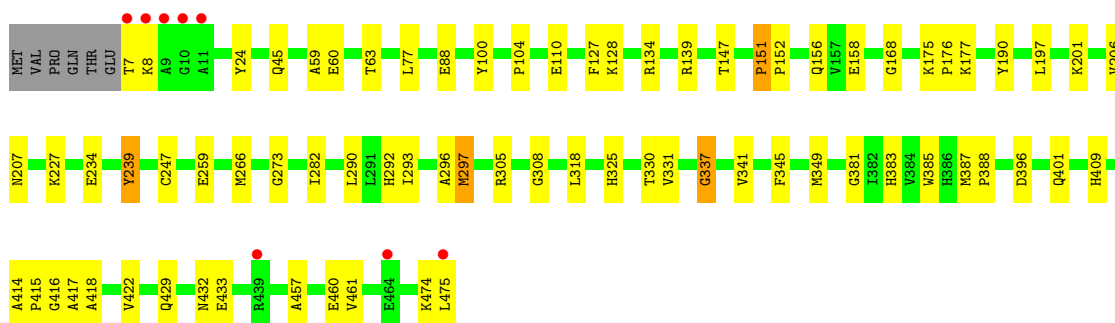
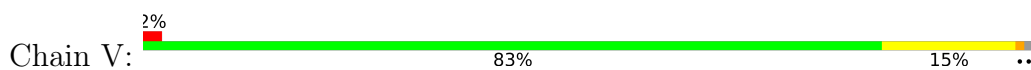


- Molecule 1: Large subunit of Rubisco

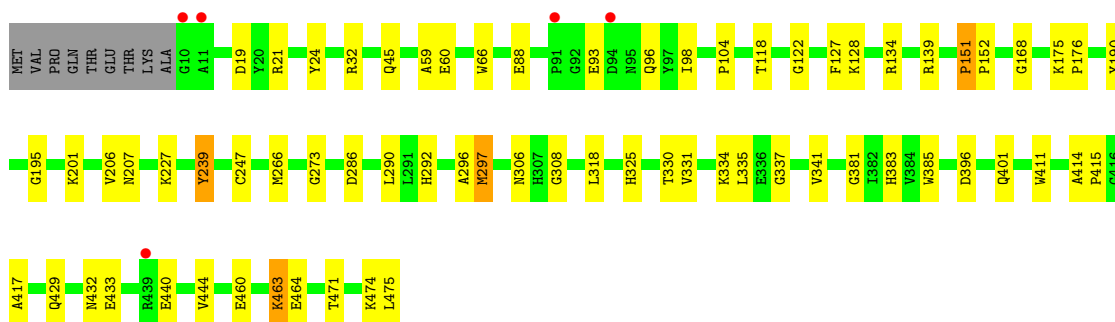
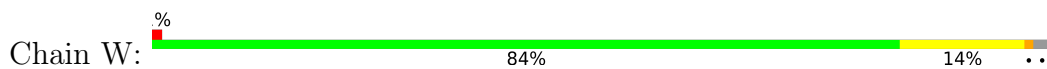




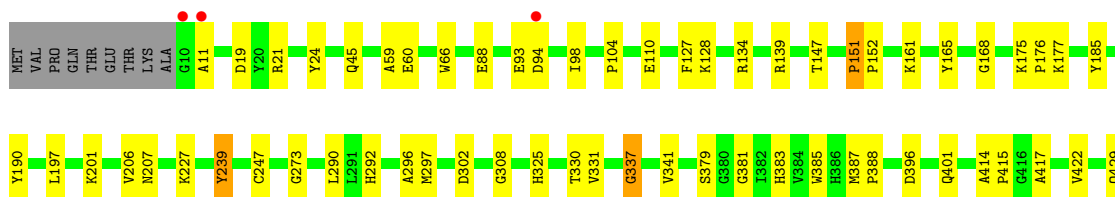
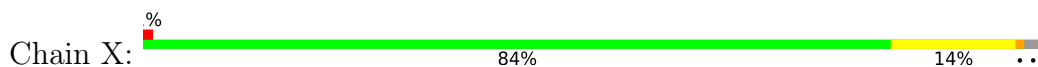
- Molecule 1: Large subunit of Rubisco



- Molecule 1: Large subunit of Rubisco

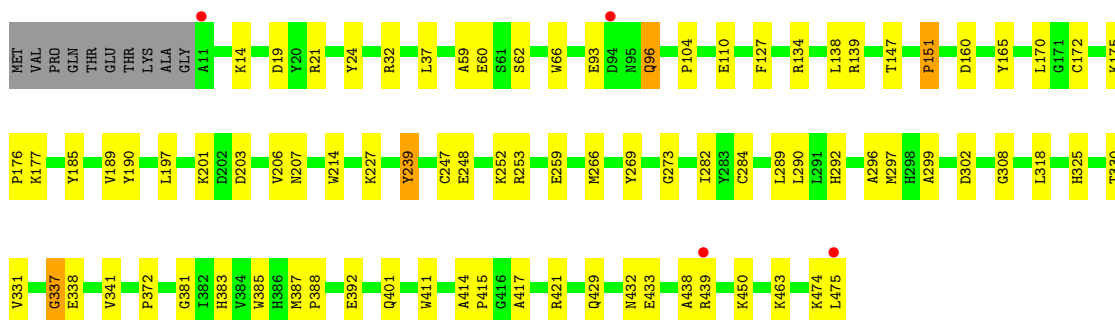
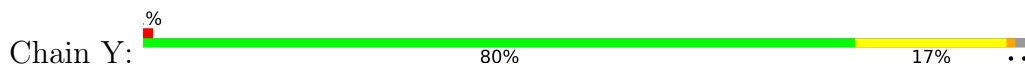


- Molecule 1: Large subunit of Rubisco

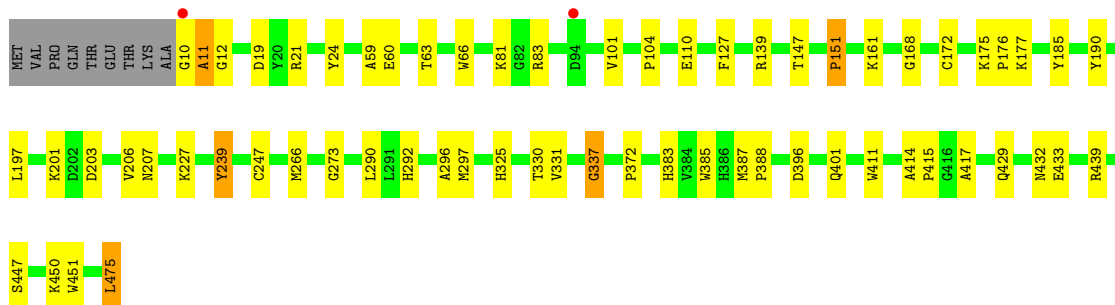
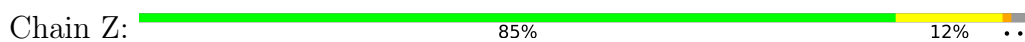




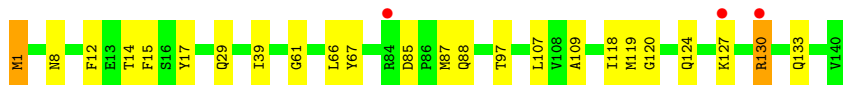
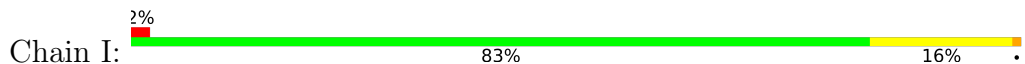
● Molecule 1: Large subunit of Rubisco



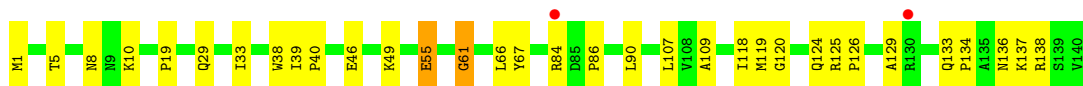
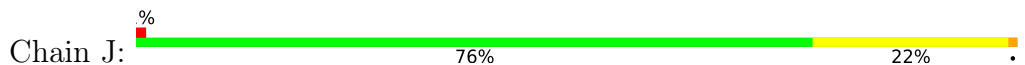
● Molecule 1: Large subunit of Rubisco



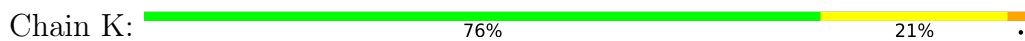
● Molecule 2: Small subunit of Rubisco



● Molecule 2: Small subunit of Rubisco

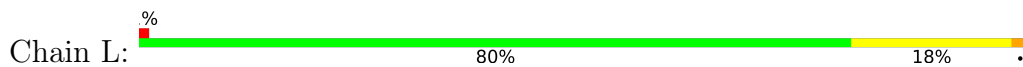


● Molecule 2: Small subunit of Rubisco

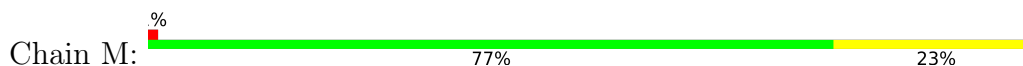




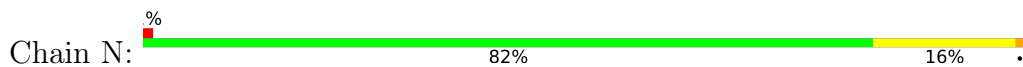
- Molecule 2: Small subunit of Rubisco



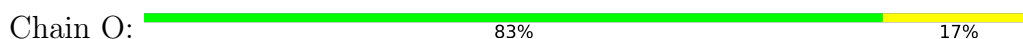
- Molecule 2: Small subunit of Rubisco



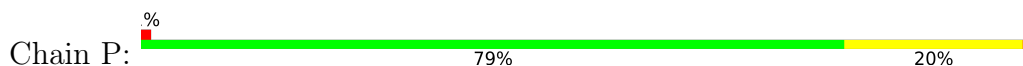
- Molecule 2: Small subunit of Rubisco



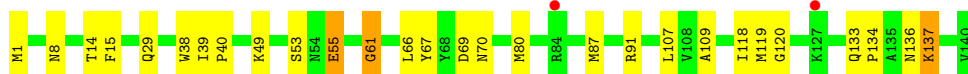
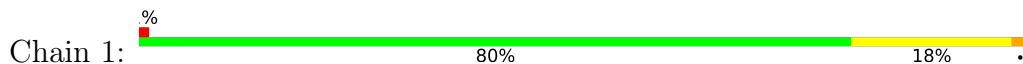
- Molecule 2: Small subunit of Rubisco



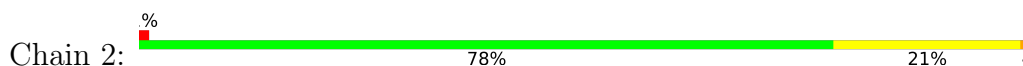
- Molecule 2: Small subunit of Rubisco

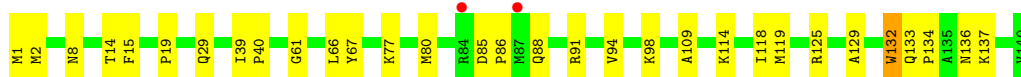


- Molecule 2: Small subunit of Rubisco

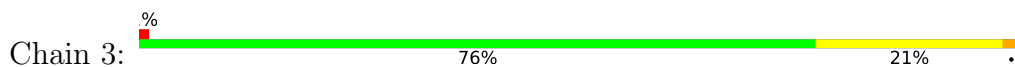


- Molecule 2: Small subunit of Rubisco

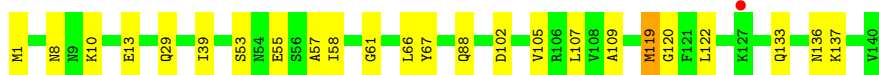
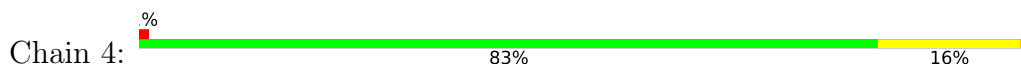




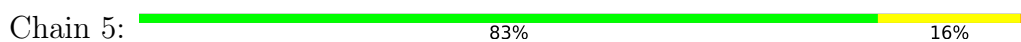
- Molecule 2: Small subunit of Rubisco



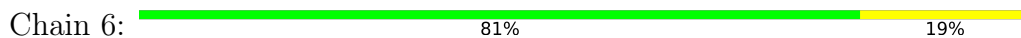
- Molecule 2: Small subunit of Rubisco



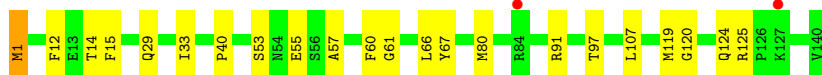
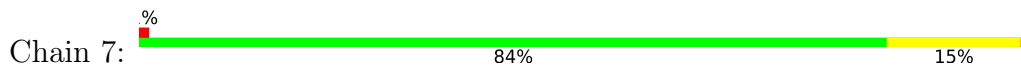
- Molecule 2: Small subunit of Rubisco



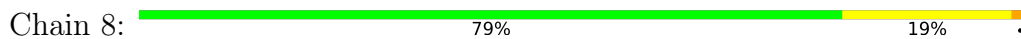
- Molecule 2: Small subunit of Rubisco



- Molecule 2: Small subunit of Rubisco



- Molecule 2: Small subunit of Rubisco



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.17Å 174.75Å 222.27Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	39.89 – 1.84 40.02 – 1.84	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.89-1.84) 90.7 (40.02-1.84)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.84Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.152 , 0.181 0.150 , 0.180	Depositor DCC
$R_{free}$ test set	37921 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.2	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	87087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage'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.*

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

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



## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/3684	0.60	0/4978
1	B	0.30	0/3675	0.61	0/4967
1	C	0.31	0/3670	0.61	0/4960
1	D	0.31	0/3675	0.61	0/4967
1	E	0.31	0/3666	0.62	0/4955
1	F	0.30	0/3666	0.60	0/4955
1	G	0.31	0/3670	0.61	0/4960
1	H	0.31	0/3684	0.62	0/4978
1	S	0.30	0/3666	0.61	0/4955
1	T	0.31	0/3670	0.61	0/4960
1	U	0.31	0/3691	0.61	0/4988
1	V	0.31	0/3691	0.62	0/4988
1	W	0.30	0/3670	0.60	0/4960
1	X	0.31	0/3670	0.60	0/4960
1	Y	0.31	0/3666	0.61	0/4955
1	Z	0.31	0/3670	0.61	0/4960
2	1	0.31	0/1169	0.60	1/1588 (0.1%)
2	2	0.30	0/1169	0.59	1/1588 (0.1%)
2	3	0.32	0/1169	0.60	1/1588 (0.1%)
2	4	0.32	0/1169	0.59	1/1588 (0.1%)
2	5	0.31	0/1169	0.61	1/1588 (0.1%)
2	6	0.31	0/1169	0.59	1/1588 (0.1%)
2	7	0.32	0/1169	0.60	1/1588 (0.1%)
2	8	0.32	0/1169	0.61	1/1588 (0.1%)
2	I	0.31	0/1169	0.59	1/1588 (0.1%)
2	J	0.30	0/1169	0.59	1/1588 (0.1%)
2	K	0.31	0/1169	0.60	1/1588 (0.1%)
2	L	0.32	0/1169	0.60	1/1588 (0.1%)
2	M	0.31	0/1169	0.60	1/1588 (0.1%)
2	N	0.31	0/1169	0.59	1/1588 (0.1%)
2	O	0.32	0/1169	0.60	1/1588 (0.1%)
2	P	0.32	0/1169	0.60	1/1588 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.31	0/77488	0.61	16/104854 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	61	GLY	N-CA-C	-6.03	98.03	113.10
2	M	61	GLY	N-CA-C	-6.02	98.05	113.10
2	J	61	GLY	N-CA-C	-5.99	98.13	113.10
2	6	61	GLY	N-CA-C	-5.97	98.17	113.10
2	L	61	GLY	N-CA-C	-5.96	98.19	113.10

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3646	0	3559	36	0
1	B	3637	0	3546	50	0
1	C	3632	0	3541	48	0
1	D	3637	0	3546	48	0
1	E	3628	0	3538	41	0
1	F	3628	0	3538	39	0
1	G	3632	0	3541	37	0
1	H	3646	0	3559	42	0
1	S	3628	0	3538	47	0
1	T	3632	0	3541	44	0
1	U	3653	0	3566	65	0
1	V	3653	0	3566	47	0
1	W	3632	0	3541	46	0
1	X	3632	0	3541	39	0
1	Y	3628	0	3538	57	0
1	Z	3632	0	3541	44	0
2	1	1145	0	1119	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1145	0	1119	22	0
2	3	1145	0	1119	33	0
2	4	1145	0	1119	19	0
2	5	1145	0	1119	15	0
2	6	1145	0	1119	23	0
2	7	1145	0	1119	18	0
2	8	1145	0	1119	27	0
2	I	1145	0	1119	19	0
2	J	1145	0	1119	25	0
2	K	1145	0	1119	30	0
2	L	1145	0	1119	25	0
2	M	1145	0	1119	30	0
2	N	1145	0	1119	23	0
2	O	1145	0	1119	16	0
2	P	1145	0	1119	20	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

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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	1	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	4	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	3	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

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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	5	0
6	T	426	0	0	5	0
6	U	427	0	0	7	0
6	V	456	0	0	3	0
6	W	421	0	0	6	0
6	X	450	0	0	2	0
6	Y	426	0	0	7	0
6	Z	474	0	0	5	0
All	All	87087	0	75085	975	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 6.

The worst 5 of 975 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%)	34 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	460/475 (97%)	443 (96%)	16 (4%)	1 (0%)	47	33
1	C	459/475 (97%)	445 (97%)	13 (3%)	1 (0%)	47	33
1	D	460/475 (97%)	445 (97%)	14 (3%)	1 (0%)	47	33
1	E	458/475 (96%)	442 (96%)	15 (3%)	1 (0%)	47	33
1	F	458/475 (96%)	441 (96%)	16 (4%)	1 (0%)	47	33
1	G	459/475 (97%)	445 (97%)	13 (3%)	1 (0%)	47	33
1	H	461/475 (97%)	448 (97%)	11 (2%)	2 (0%)	34	20
1	S	458/475 (96%)	441 (96%)	16 (4%)	1 (0%)	47	33
1	T	459/475 (97%)	445 (97%)	12 (3%)	2 (0%)	34	20
1	U	462/475 (97%)	443 (96%)	17 (4%)	2 (0%)	34	20
1	V	462/475 (97%)	443 (96%)	17 (4%)	2 (0%)	34	20
1	W	459/475 (97%)	443 (96%)	15 (3%)	1 (0%)	47	33
1	X	459/475 (97%)	444 (97%)	13 (3%)	2 (0%)	34	20
1	Y	458/475 (96%)	444 (97%)	13 (3%)	1 (0%)	47	33
1	Z	459/475 (97%)	442 (96%)	15 (3%)	2 (0%)	34	20
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9560/9840 (97%)	9177 (96%)	360 (4%)	23 (0%)	47 33

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 [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	369/376 (98%)	367 (100%)	2 (0%)	88 85
1	B	368/376 (98%)	366 (100%)	2 (0%)	88 85
1	C	368/376 (98%)	363 (99%)	5 (1%)	67 55
1	D	368/376 (98%)	366 (100%)	2 (0%)	88 85
1	E	368/376 (98%)	364 (99%)	4 (1%)	73 64
1	F	368/376 (98%)	367 (100%)	1 (0%)	92 90
1	G	368/376 (98%)	363 (99%)	5 (1%)	67 55
1	H	369/376 (98%)	366 (99%)	3 (1%)	81 75
1	S	368/376 (98%)	367 (100%)	1 (0%)	92 90
1	T	368/376 (98%)	365 (99%)	3 (1%)	81 75
1	U	370/376 (98%)	367 (99%)	3 (1%)	81 75
1	V	370/376 (98%)	367 (99%)	3 (1%)	81 75
1	W	368/376 (98%)	364 (99%)	4 (1%)	73 64
1	X	368/376 (98%)	364 (99%)	4 (1%)	73 64
1	Y	368/376 (98%)	364 (99%)	4 (1%)	73 64
1	Z	368/376 (98%)	363 (99%)	5 (1%)	67 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	123/123 (100%)	121 (98%)	2 (2%)	62	49
2	2	123/123 (100%)	121 (98%)	2 (2%)	62	49
2	3	123/123 (100%)	121 (98%)	2 (2%)	62	49
2	4	123/123 (100%)	121 (98%)	2 (2%)	62	49
2	5	123/123 (100%)	122 (99%)	1 (1%)	81	75
2	6	123/123 (100%)	122 (99%)	1 (1%)	81	75
2	7	123/123 (100%)	122 (99%)	1 (1%)	81	75
2	8	123/123 (100%)	121 (98%)	2 (2%)	62	49
2	I	123/123 (100%)	121 (98%)	2 (2%)	62	49
2	J	123/123 (100%)	121 (98%)	2 (2%)	62	49
2	K	123/123 (100%)	120 (98%)	3 (2%)	49	32
2	L	123/123 (100%)	120 (98%)	3 (2%)	49	32
2	M	123/123 (100%)	121 (98%)	2 (2%)	62	49
2	N	123/123 (100%)	122 (99%)	1 (1%)	81	75
2	O	123/123 (100%)	122 (99%)	1 (1%)	81	75
2	P	123/123 (100%)	121 (98%)	2 (2%)	62	49
All	All	7862/7984 (98%)	7782 (99%)	80 (1%)	76	68

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	4	119	MET
1	Y	239	TYR
1	W	297	MET
1	X	185	TYR
1	Z	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	8	ASN
2	4	29	GLN
2	2	88	GLN
2	3	29	GLN
1	W	207	ASN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	B	151	1	6,8,9	1.06	0	5,10,12	1.34	1 (20%)
1	HYP	G	104	1	6,8,9	1.09	1 (16%)	5,10,12	1.59	1 (20%)
1	SMC	S	256	1	5,6,7	0.53	0	2,6,8	0.83	0
1	SMC	W	256	1	5,6,7	0.53	0	2,6,8	1.07	0
1	KCX	Y	201	3,1	9,11,12	0.91	0	5,12,14	1.57	2 (40%)
1	SMC	D	369	1	5,6,7	0.54	0	2,6,8	0.67	0
1	HYP	A	104	1	6,8,9	1.05	1 (16%)	5,10,12	1.67	1 (20%)
2	MME	J	1	2	7,8,9	1.96	1 (14%)	5,8,10	1.42	1 (20%)
1	HYP	T	151	1	6,8,9	1.03	0	5,10,12	1.28	1 (20%)
2	MME	8	1	2	7,8,9	1.96	1 (14%)	5,8,10	1.41	1 (20%)
1	HYP	E	104	1	6,8,9	1.10	0	5,10,12	1.46	1 (20%)
1	HYP	G	151	1	6,8,9	1.10	0	5,10,12	1.26	1 (20%)
1	HYP	H	104	1	6,8,9	1.05	0	5,10,12	1.57	1 (20%)
1	HYP	F	104	1	6,8,9	1.04	0	5,10,12	1.61	1 (20%)
2	MME	4	1	2	7,8,9	1.96	1 (14%)	5,8,10	1.43	1 (20%)
2	MME	N	1	2	7,8,9	1.94	1 (14%)	5,8,10	1.44	1 (20%)
1	SMC	T	369	1	5,6,7	0.65	0	2,6,8	0.48	0
1	SMC	B	256	1	5,6,7	0.54	0	2,6,8	1.14	0
1	SMC	C	256	1	5,6,7	0.52	0	2,6,8	0.62	0
1	KCX	B	201	3,1	9,11,12	0.80	0	5,12,14	1.56	2 (40%)
1	KCX	S	201	3,1	9,11,12	0.93	1 (11%)	5,12,14	1.61	2 (40%)
1	HYP	Y	151	1	6,8,9	1.02	0	5,10,12	1.30	1 (20%)
1	SMC	E	369	1	5,6,7	0.54	0	2,6,8	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SMC	Y	256	1	5,6,7	0.49	0	2,6,8	0.86	0
2	MME	5	1	2	7,8,9	1.94	1 (14%)	5,8,10	1.43	1 (20%)
1	SMC	D	256	1	5,6,7	0.53	0	2,6,8	0.90	0
1	HYP	S	151	1	6,8,9	1.08	0	5,10,12	1.33	1 (20%)
1	HYP	V	151	1	6,8,9	1.04	0	5,10,12	1.28	1 (20%)
1	HYP	T	104	1	6,8,9	1.06	0	5,10,12	1.46	1 (20%)
1	HYP	Z	104	1	6,8,9	1.01	0	5,10,12	1.48	1 (20%)
1	SMC	Z	256	1	5,6,7	0.55	0	2,6,8	0.98	0
1	HYP	C	104	1	6,8,9	1.11	1 (16%)	5,10,12	1.45	1 (20%)
1	SMC	G	256	1	5,6,7	0.52	0	2,6,8	0.84	0
1	SMC	S	369	1	5,6,7	0.53	0	2,6,8	0.44	0
1	SMC	H	256	1	5,6,7	0.50	0	2,6,8	0.84	0
1	KCX	W	201	3,1	9,11,12	0.91	0	5,12,14	1.66	2 (40%)
2	MME	3	1	2	7,8,9	1.95	1 (14%)	5,8,10	1.42	1 (20%)
1	SMC	A	256	1	5,6,7	0.47	0	2,6,8	0.81	0
1	SMC	V	256	1	5,6,7	0.53	0	2,6,8	1.10	0
1	HYP	W	151	1	6,8,9	1.04	0	5,10,12	1.31	1 (20%)
1	SMC	U	256	1	5,6,7	0.49	0	2,6,8	0.91	0
1	SMC	B	369	1	5,6,7	0.61	0	2,6,8	0.29	0
1	HYP	A	151	1	6,8,9	1.03	0	5,10,12	1.32	1 (20%)
1	SMC	Z	369	1	5,6,7	0.60	0	2,6,8	0.24	0
1	HYP	C	151	1	6,8,9	1.00	0	5,10,12	1.33	1 (20%)
1	SMC	C	369	1	5,6,7	0.50	0	2,6,8	1.01	0
1	KCX	U	201	3,1	9,11,12	0.86	0	5,12,14	1.63	2 (40%)
1	KCX	C	201	3,1	9,11,12	0.96	0	5,12,14	1.61	2 (40%)
1	SMC	X	369	1	5,6,7	0.53	0	2,6,8	0.51	0
1	KCX	H	201	3,1	9,11,12	0.92	0	5,12,14	1.69	2 (40%)
1	SMC	W	369	1	5,6,7	0.55	0	2,6,8	0.58	0
1	KCX	A	201	3,1	9,11,12	0.90	0	5,12,14	1.66	2 (40%)
2	MME	2	1	2	7,8,9	1.93	1 (14%)	5,8,10	1.39	1 (20%)
1	SMC	A	369	1	5,6,7	0.67	0	2,6,8	0.27	0
2	MME	L	1	2	7,8,9	1.96	1 (14%)	5,8,10	1.32	1 (20%)
1	KCX	D	201	3,1	9,11,12	0.92	1 (11%)	5,12,14	1.53	2 (40%)
1	HYP	H	151	1	6,8,9	1.01	0	5,10,12	1.34	1 (20%)
2	MME	7	1	2	7,8,9	1.95	1 (14%)	5,8,10	1.37	1 (20%)
1	SMC	U	369	1	5,6,7	0.61	0	2,6,8	0.44	0
1	HYP	Y	104	1	6,8,9	1.00	0	5,10,12	1.59	1 (20%)
1	SMC	H	369	1	5,6,7	0.60	0	2,6,8	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	D	151	1	6,8,9	1.04	0	5,10,12	1.32	1 (20%)
2	MME	O	1	2	7,8,9	1.94	1 (14%)	5,8,10	1.39	1 (20%)
2	MME	I	1	2	7,8,9	1.95	1 (14%)	5,8,10	1.38	1 (20%)
1	KCX	E	201	3,1	9,11,12	0.96	0	5,12,14	1.66	2 (40%)
1	SMC	Y	369	1	5,6,7	0.69	0	2,6,8	0.42	0
1	KCX	F	201	3,1	9,11,12	0.92	0	5,12,14	1.59	2 (40%)
1	HYP	V	104	1	6,8,9	1.07	1 (16%)	5,10,12	1.46	1 (20%)
1	HYP	X	104	1	6,8,9	1.12	1 (16%)	5,10,12	1.55	1 (20%)
1	SMC	T	256	1	5,6,7	0.54	0	2,6,8	1.04	0
1	KCX	V	201	3,1	9,11,12	0.97	0	5,12,14	1.59	2 (40%)
1	HYP	U	104	1	6,8,9	1.07	0	5,10,12	1.53	1 (20%)
1	HYP	X	151	1	6,8,9	1.04	0	5,10,12	1.25	1 (20%)
2	MME	P	1	2	7,8,9	1.95	1 (14%)	5,8,10	1.47	1 (20%)
1	HYP	S	104	1	6,8,9	1.04	0	5,10,12	1.60	1 (20%)
2	MME	6	1	2	7,8,9	1.96	1 (14%)	5,8,10	1.40	1 (20%)
1	HYP	U	151	1	6,8,9	1.06	0	5,10,12	1.28	1 (20%)
1	SMC	V	369	1	5,6,7	0.56	0	2,6,8	0.52	0
1	HYP	W	104	1	6,8,9	1.13	0	5,10,12	1.64	1 (20%)
1	SMC	F	256	1	5,6,7	0.51	0	2,6,8	0.83	0
1	SMC	X	256	1	5,6,7	0.52	0	2,6,8	0.93	0
2	MME	1	1	2	7,8,9	1.96	1 (14%)	5,8,10	1.35	1 (20%)
1	KCX	T	201	3,1	9,11,12	0.93	0	5,12,14	1.61	2 (40%)
1	KCX	Z	201	3,1	9,11,12	0.97	1 (11%)	5,12,14	1.59	2 (40%)
1	SMC	E	256	1	5,6,7	0.56	0	2,6,8	0.87	0
1	SMC	F	369	1	5,6,7	0.60	0	2,6,8	0.33	0
1	KCX	G	201	3,1	9,11,12	0.90	0	5,12,14	1.62	2 (40%)
2	MME	K	1	2	7,8,9	1.95	1 (14%)	5,8,10	1.38	1 (20%)
1	HYP	Z	151	1	6,8,9	1.13	1 (16%)	5,10,12	1.21	1 (20%)
1	SMC	G	369	1	5,6,7	0.51	0	2,6,8	0.53	0
1	HYP	F	151	1	6,8,9	1.01	0	5,10,12	1.29	1 (20%)
1	HYP	E	151	1	6,8,9	1.11	1 (16%)	5,10,12	1.29	1 (20%)
1	HYP	B	104	1	6,8,9	1.06	1 (16%)	5,10,12	1.49	1 (20%)
1	KCX	X	201	3,1	9,11,12	0.86	0	5,12,14	1.66	2 (40%)
2	MME	M	1	2	7,8,9	1.93	1 (14%)	5,8,10	1.41	1 (20%)
1	HYP	D	104	1	6,8,9	1.10	0	5,10,12	1.49	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. '2' means no outliers of that kind were identified.

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	X	256	1	-	0/3/5/7	-
2	MME	1	1	2	-	1/5/8/10	-
1	KCX	T	201	3,1	-	0/9/10/12	-
1	KCX	Z	201	3,1	-	0/9/10/12	-
1	SMC	E	256	1	-	0/3/5/7	-
1	SMC	F	369	1	-	1/3/5/7	-
1	KCX	G	201	3,1	-	0/9/10/12	-
2	MME	K	1	2	-	2/5/8/10	-
1	HYP	Z	151	1	-	0/0/11/13	0/1/1/1
1	SMC	G	369	1	-	1/3/5/7	-
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	KCX	X	201	3,1	-	0/9/10/12	-
2	MME	M	1	2	-	1/5/8/10	-
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	1	MME	CM-N	-5.08	1.33	1.46
2	J	1	MME	CM-N	-5.06	1.33	1.46
2	6	1	MME	CM-N	-5.04	1.33	1.46
2	P	1	MME	CM-N	-5.04	1.33	1.46
2	3	1	MME	CM-N	-5.03	1.33	1.46

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	KCX	OQ1-CX-NZ	-2.92	120.43	124.96
1	E	201	KCX	OQ1-CX-NZ	-2.88	120.50	124.96
1	X	201	KCX	OQ1-CX-NZ	-2.88	120.50	124.96
1	W	104	HYP	O-C-CA	-2.86	117.28	124.78
1	H	201	KCX	OQ1-CX-NZ	-2.84	120.56	124.96

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

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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.

16 monomers are involved in 17 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	C	607	-	5,5,5	0.93	0	5,5,5	0.36	0
5	GOL	E	609	-	5,5,5	0.96	0	5,5,5	0.41	0
5	GOL	H	619	-	5,5,5	0.95	0	5,5,5	0.29	0
5	GOL	B	610	-	5,5,5	0.95	0	5,5,5	0.37	0
5	GOL	T	614	-	5,5,5	0.95	0	5,5,5	0.30	0
5	GOL	V	616	-	5,5,5	0.95	0	5,5,5	0.32	0
5	GOL	D	616	-	5,5,5	0.98	0	5,5,5	0.44	0
5	GOL	T	606	-	5,5,5	0.94	0	5,5,5	0.34	0
5	GOL	B	606	-	5,5,5	1.01	0	5,5,5	0.41	0
5	GOL	S	605	-	5,5,5	0.94	0	5,5,5	0.32	0
5	GOL	F	602	-	5,5,5	0.94	0	5,5,5	0.33	0
4	CAP	W	501	3	17,20,20	1.19	2 (11%)	22,31,31	1.25	1 (4%)
4	CAP	T	501	3	17,20,20	1.19	1 (5%)	22,31,31	1.23	1 (4%)
5	GOL	G	603	-	5,5,5	0.95	0	5,5,5	0.33	0
5	GOL	S	609	-	5,5,5	0.90	0	5,5,5	0.36	0
5	GOL	Y	603	-	5,5,5	0.95	0	5,5,5	0.35	0
5	GOL	A	605	-	5,5,5	0.98	0	5,5,5	0.36	0
5	GOL	D	608	-	5,5,5	0.98	0	5,5,5	0.28	0
5	GOL	A	613	-	5,5,5	0.92	0	5,5,5	0.30	0
5	GOL	F	617	-	5,5,5	0.94	0	5,5,5	0.25	0
5	GOL	G	618	-	5,5,5	0.91	0	5,5,5	0.33	0
5	GOL	C	615	-	5,5,5	0.93	0	5,5,5	0.35	0
4	CAP	Z	501	3	17,20,20	1.15	1 (5%)	22,31,31	1.22	1 (4%)
5	GOL	G	611	-	5,5,5	0.99	0	5,5,5	0.40	0
5	GOL	U	607	-	5,5,5	0.96	0	5,5,5	0.33	0
5	GOL	H	612	-	5,5,5	0.96	0	5,5,5	0.37	0
4	CAP	H	501	3	17,20,20	1.14	1 (5%)	22,31,31	1.22	1 (4%)
4	CAP	F	501	3	17,20,20	1.23	2 (11%)	22,31,31	1.22	1 (4%)
5	GOL	Y	618	-	5,5,5	0.95	0	5,5,5	0.32	0
4	CAP	Y	501	3	17,20,20	1.17	1 (5%)	22,31,31	1.22	1 (4%)
4	CAP	E	501	3	17,20,20	1.17	2 (11%)	22,31,31	1.18	1 (4%)
4	CAP	X	501	3	17,20,20	1.13	1 (5%)	22,31,31	1.22	1 (4%)
5	GOL	Z	619	-	5,5,5	0.92	0	5,5,5	0.33	0
4	CAP	A	501	3	17,20,20	1.18	2 (11%)	22,31,31	1.20	1 (4%)
4	CAP	V	501	3	17,20,20	1.23	2 (11%)	22,31,31	1.23	2 (9%)
4	CAP	D	501	3	17,20,20	1.22	2 (11%)	22,31,31	1.20	1 (4%)
5	GOL	W	620	-	5,5,5	0.94	0	5,5,5	0.42	0
5	GOL	V	608	-	5,5,5	0.96	0	5,5,5	0.34	0
4	CAP	U	501	3	17,20,20	1.22	1 (5%)	22,31,31	1.23	2 (9%)
5	GOL	S	613	-	5,5,5	0.92	0	5,5,5	0.32	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	W	601	-	5,5,5	0.93	0	5,5,5	0.35	0
5	GOL	X	602	-	5,5,5	0.92	0	5,5,5	0.35	0
4	CAP	B	501	3	17,20,20	1.18	1 (5%)	22,31,31	1.23	1 (4%)
5	GOL	Z	604	-	5,5,5	0.92	0	5,5,5	0.35	0
5	GOL	X	610	-	5,5,5	0.95	0	5,5,5	0.38	0
5	GOL	E	620	-	5,5,5	0.93	0	5,5,5	0.31	0
4	CAP	C	501	3	17,20,20	1.25	2 (11%)	22,31,31	1.28	2 (9%)
5	GOL	X	617	-	5,5,5	0.94	0	5,5,5	0.29	0
5	GOL	E	601	-	5,5,5	0.93	0	5,5,5	0.34	0
5	GOL	Y	611	-	5,5,5	0.97	0	5,5,5	0.37	0
5	GOL	Z	612	-	5,5,5	0.98	0	5,5,5	0.36	0
4	CAP	G	501	3	17,20,20	1.14	1 (5%)	22,31,31	1.24	2 (9%)
4	CAP	S	501	3	17,20,20	1.30	2 (11%)	22,31,31	1.22	1 (4%)
5	GOL	B	614	-	5,5,5	0.91	0	5,5,5	0.27	0
5	GOL	U	615	-	5,5,5	0.92	0	5,5,5	0.32	0
5	GOL	H	604	-	5,5,5	0.99	0	5,5,5	0.27	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
5	GOL	C	607	-	-	1/4/4/4	-
5	GOL	E	609	-	-	0/4/4/4	-
5	GOL	H	619	-	-	0/4/4/4	-
5	GOL	B	610	-	-	0/4/4/4	-
5	GOL	T	614	-	-	0/4/4/4	-
5	GOL	V	616	-	-	2/4/4/4	-
5	GOL	D	616	-	-	4/4/4/4	-
5	GOL	T	606	-	-	0/4/4/4	-
5	GOL	B	606	-	-	2/4/4/4	-
5	GOL	S	605	-	-	0/4/4/4	-
5	GOL	F	602	-	-	0/4/4/4	-
4	CAP	W	501	3	-	12/29/29/29	-
4	CAP	T	501	3	-	12/29/29/29	-
5	GOL	G	603	-	-	0/4/4/4	-
5	GOL	S	609	-	-	0/4/4/4	-
5	GOL	Y	603	-	-	1/4/4/4	-
5	GOL	A	605	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	608	-	-	2/4/4/4	-
5	GOL	A	613	-	-	0/4/4/4	-
5	GOL	F	617	-	-	0/4/4/4	-
5	GOL	G	618	-	-	0/4/4/4	-
5	GOL	C	615	-	-	2/4/4/4	-
4	CAP	Z	501	3	-	11/29/29/29	-
5	GOL	G	611	-	-	0/4/4/4	-
5	GOL	U	607	-	-	0/4/4/4	-
5	GOL	H	612	-	-	0/4/4/4	-
4	CAP	H	501	3	-	12/29/29/29	-
4	CAP	F	501	3	-	12/29/29/29	-
5	GOL	Y	618	-	-	2/4/4/4	-
4	CAP	Y	501	3	-	12/29/29/29	-
4	CAP	E	501	3	-	12/29/29/29	-
4	CAP	X	501	3	-	12/29/29/29	-
5	GOL	Z	619	-	-	0/4/4/4	-
4	CAP	A	501	3	-	12/29/29/29	-
4	CAP	V	501	3	-	12/29/29/29	-
4	CAP	D	501	3	-	12/29/29/29	-
5	GOL	W	620	-	-	2/4/4/4	-
5	GOL	V	608	-	-	1/4/4/4	-
4	CAP	U	501	3	-	11/29/29/29	-
5	GOL	S	613	-	-	0/4/4/4	-
5	GOL	W	601	-	-	0/4/4/4	-
5	GOL	X	602	-	-	1/4/4/4	-
4	CAP	B	501	3	-	11/29/29/29	-
5	GOL	Z	604	-	-	1/4/4/4	-
5	GOL	X	610	-	-	0/4/4/4	-
5	GOL	E	620	-	-	0/4/4/4	-
4	CAP	C	501	3	-	12/29/29/29	-
5	GOL	X	617	-	-	0/4/4/4	-
5	GOL	E	601	-	-	0/4/4/4	-
5	GOL	Y	611	-	-	0/4/4/4	-
5	GOL	Z	612	-	-	0/4/4/4	-
4	CAP	G	501	3	-	12/29/29/29	-
4	CAP	S	501	3	-	12/29/29/29	-
5	GOL	B	614	-	-	0/4/4/4	-
5	GOL	U	615	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	H	604	-	-	0/4/4/4	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	501	CAP	C5-C4	3.04	1.56	1.51
4	V	501	CAP	C5-C4	3.02	1.56	1.51
4	S	501	CAP	C5-C4	2.99	1.56	1.51
4	C	501	CAP	C5-C4	2.99	1.56	1.51
4	U	501	CAP	C5-C4	2.92	1.55	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	CAP	C2-C3-C4	2.82	119.74	114.00
4	S	501	CAP	C2-C3-C4	2.76	119.62	114.00
4	W	501	CAP	C2-C3-C4	2.70	119.49	114.00
4	G	501	CAP	C2-C3-C4	2.63	119.35	114.00
4	A	501	CAP	C2-C3-C4	2.60	119.28	114.00

There are no chirality outliers.

5 of 212 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:

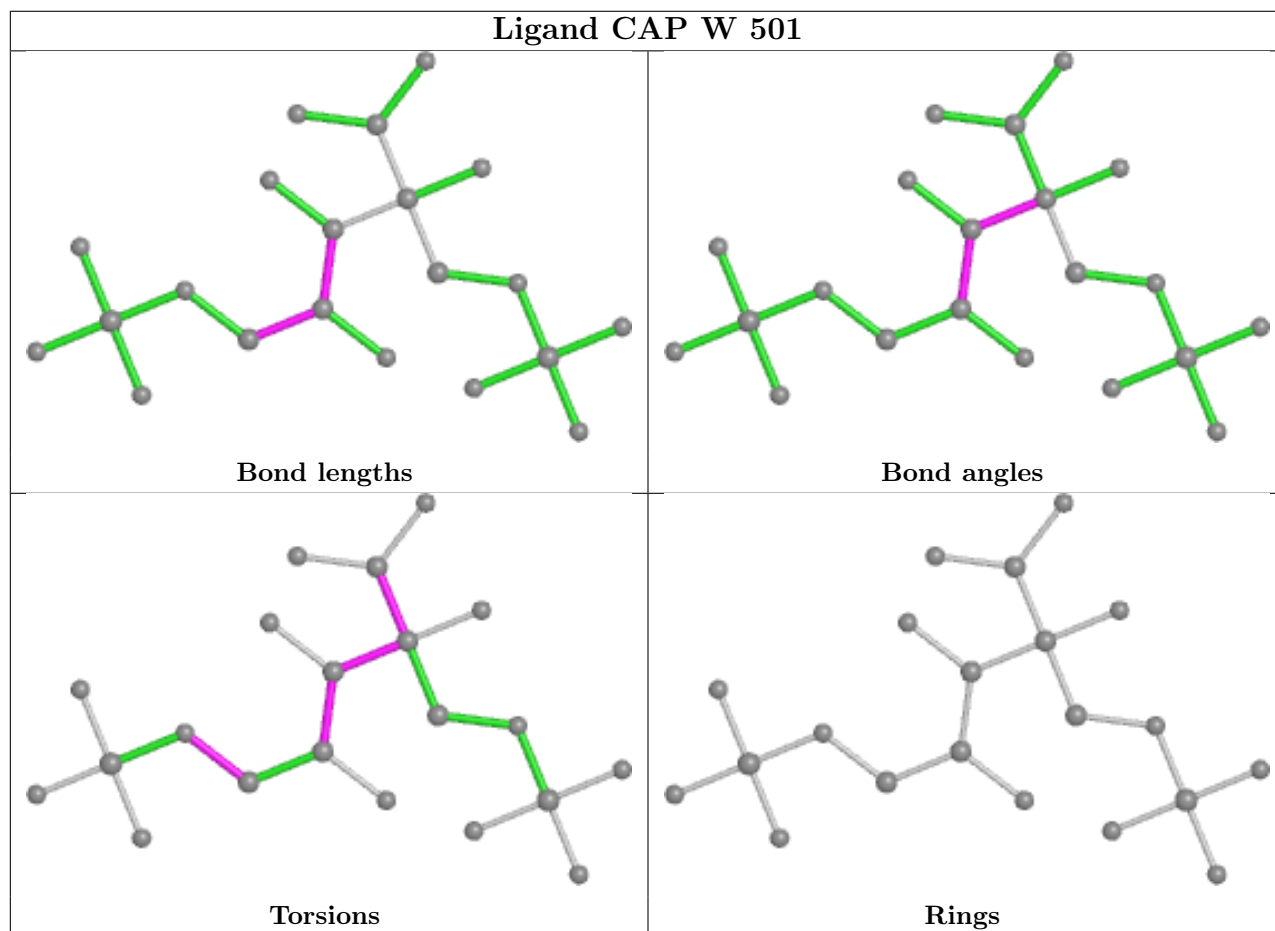
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	619	GOL	1	0
5	V	616	GOL	1	0
5	D	616	GOL	1	0
5	B	606	GOL	2	0
5	A	605	GOL	1	0
5	F	617	GOL	1	0
5	C	615	GOL	1	0

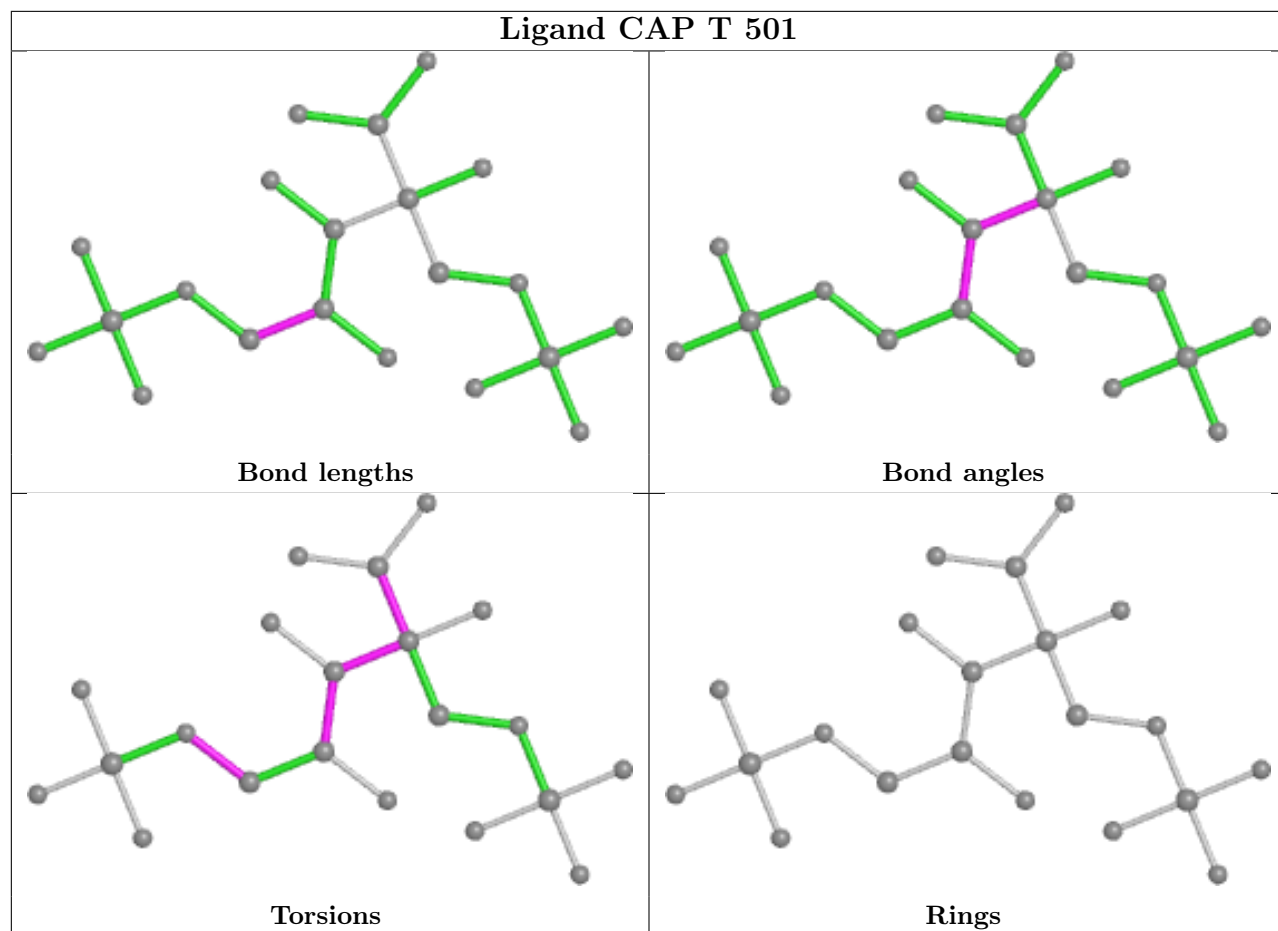
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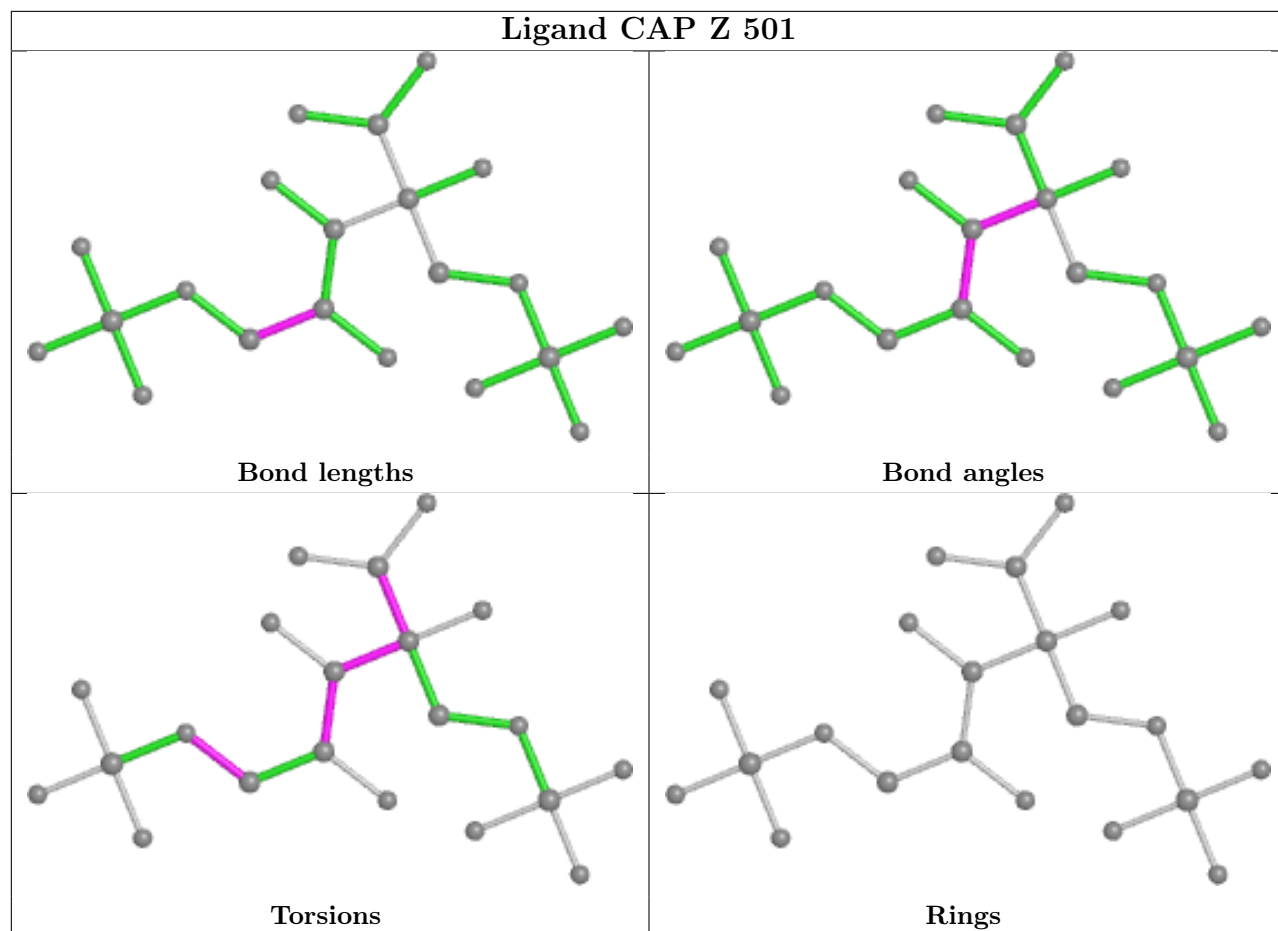
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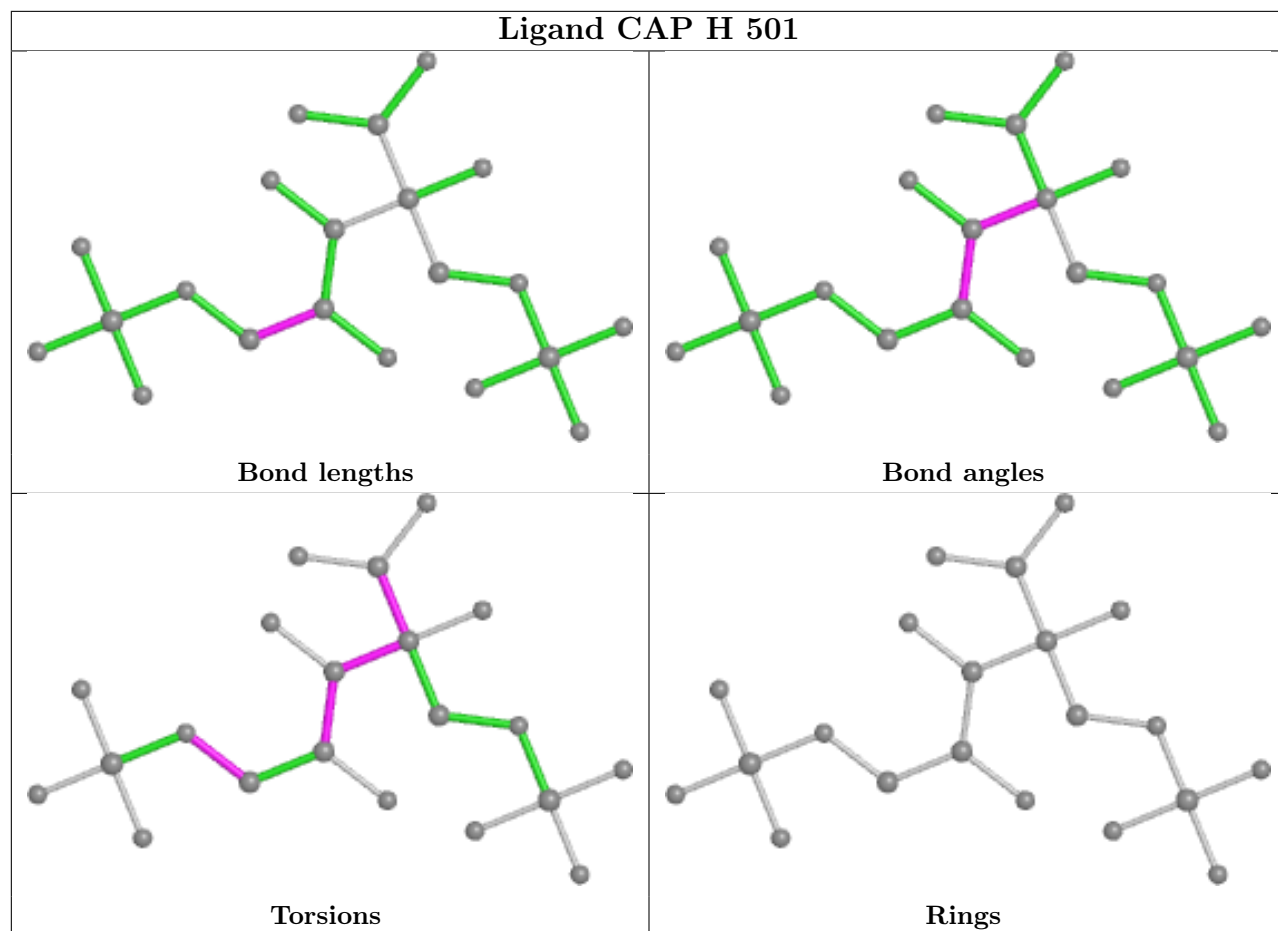
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	618	GOL	1	0
5	W	620	GOL	1	0

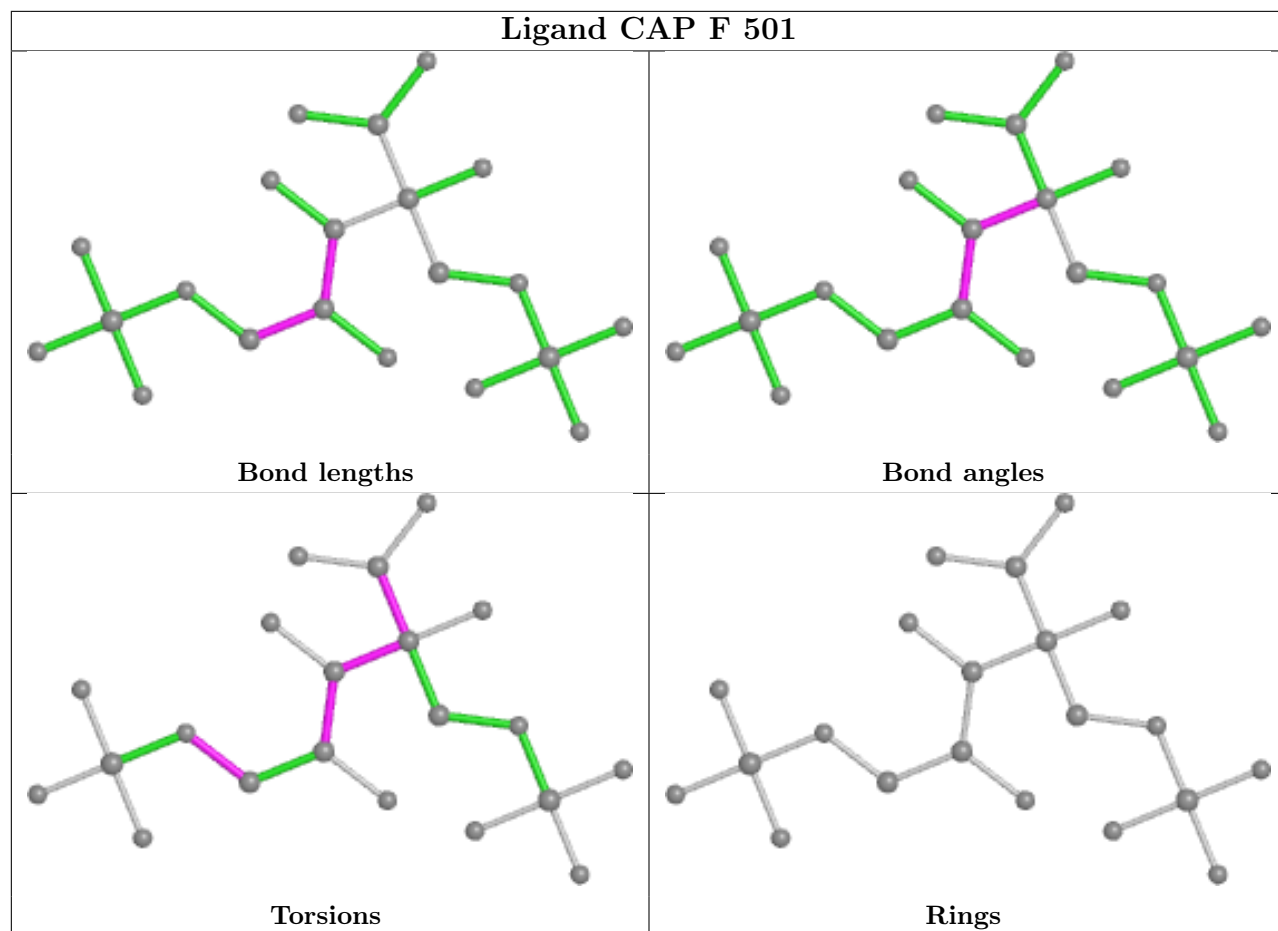
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



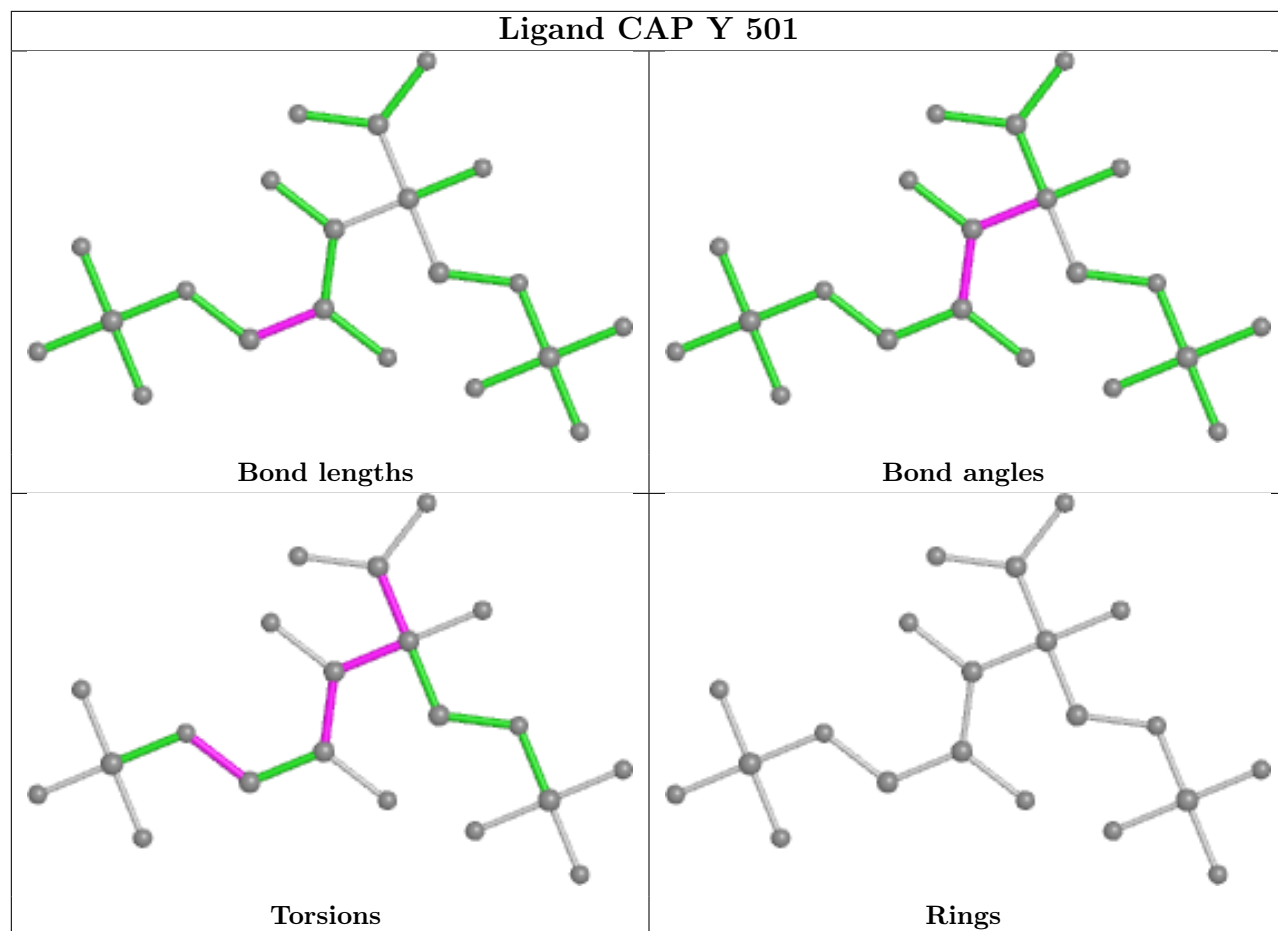


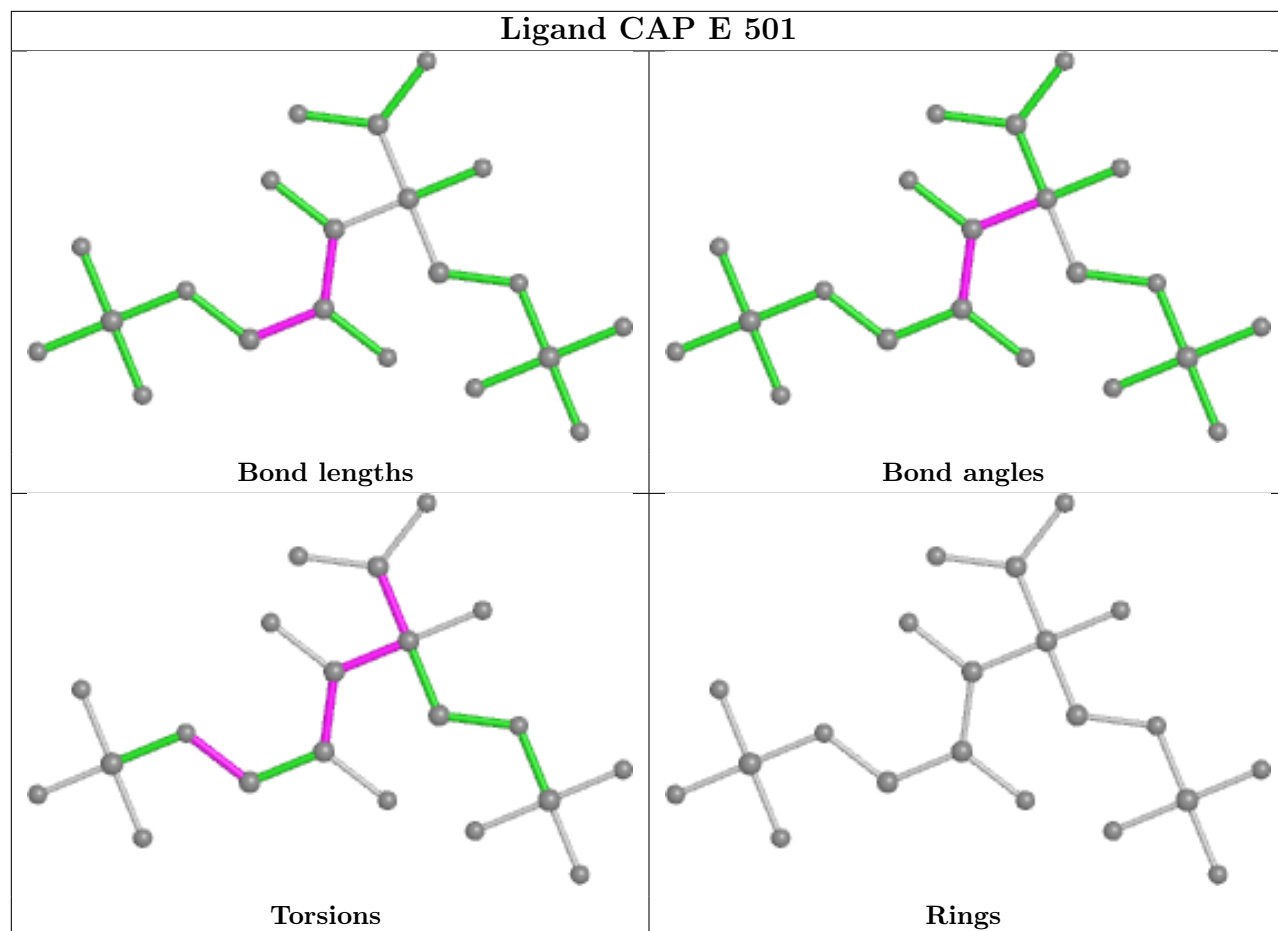


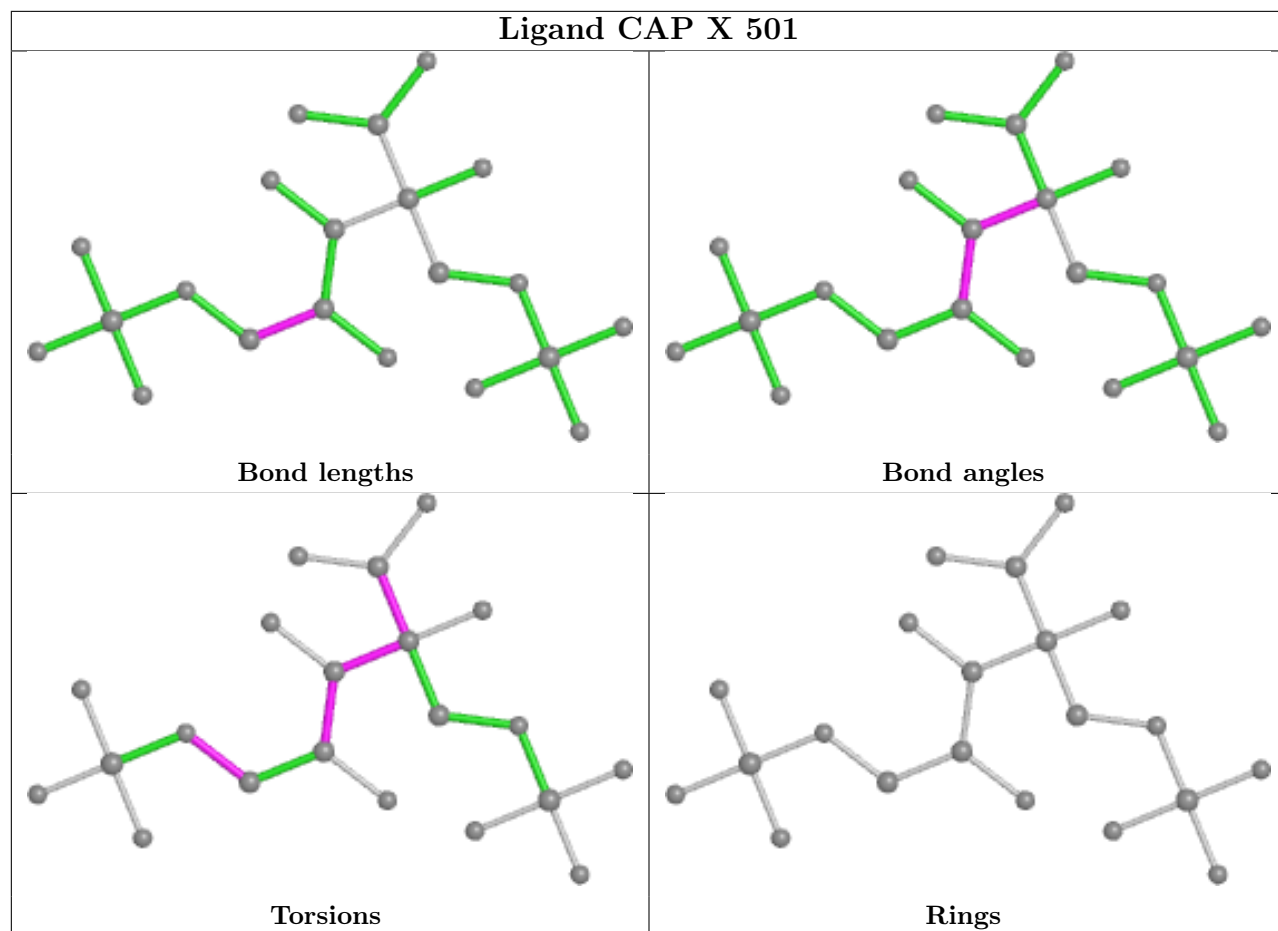


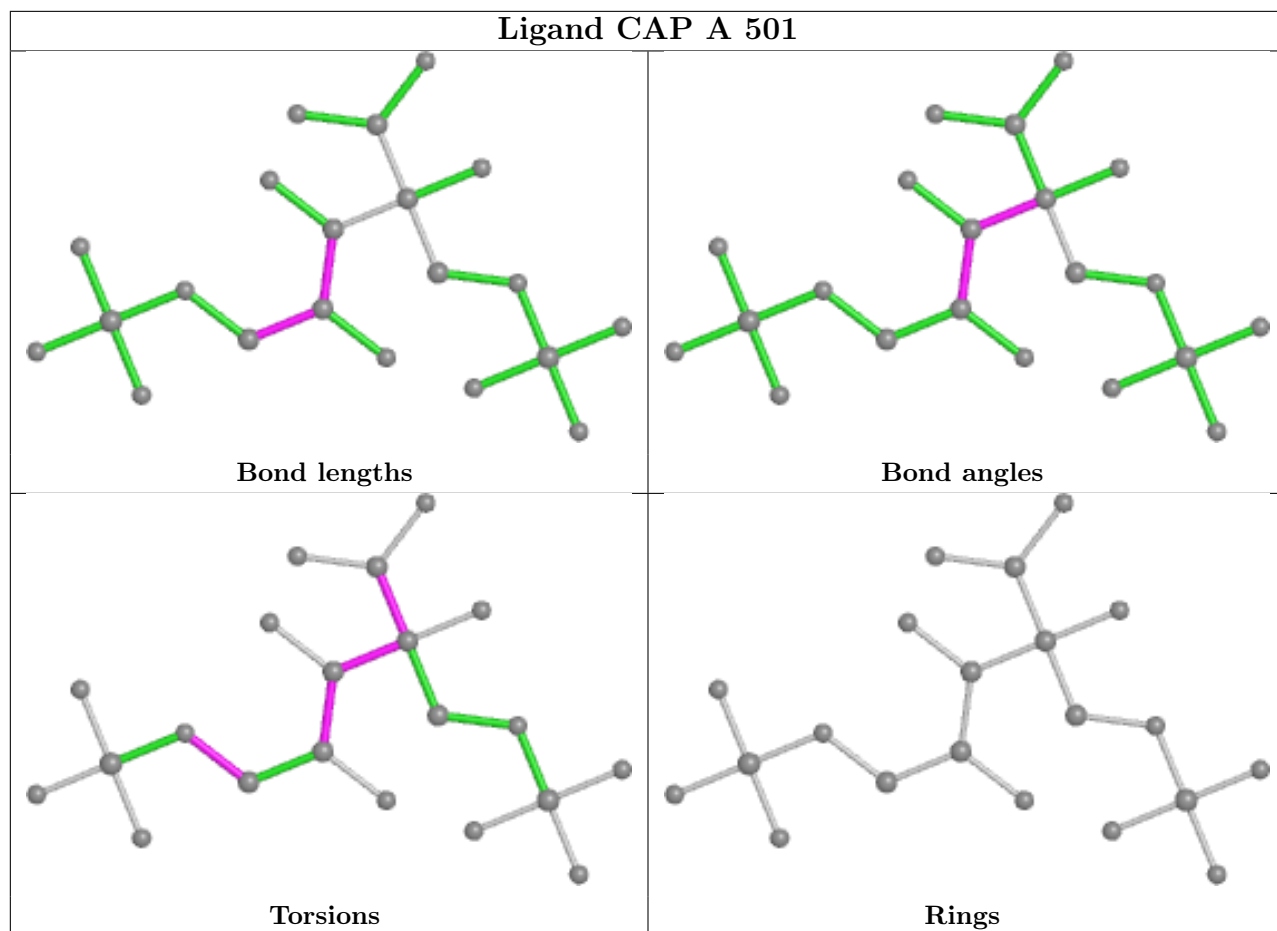


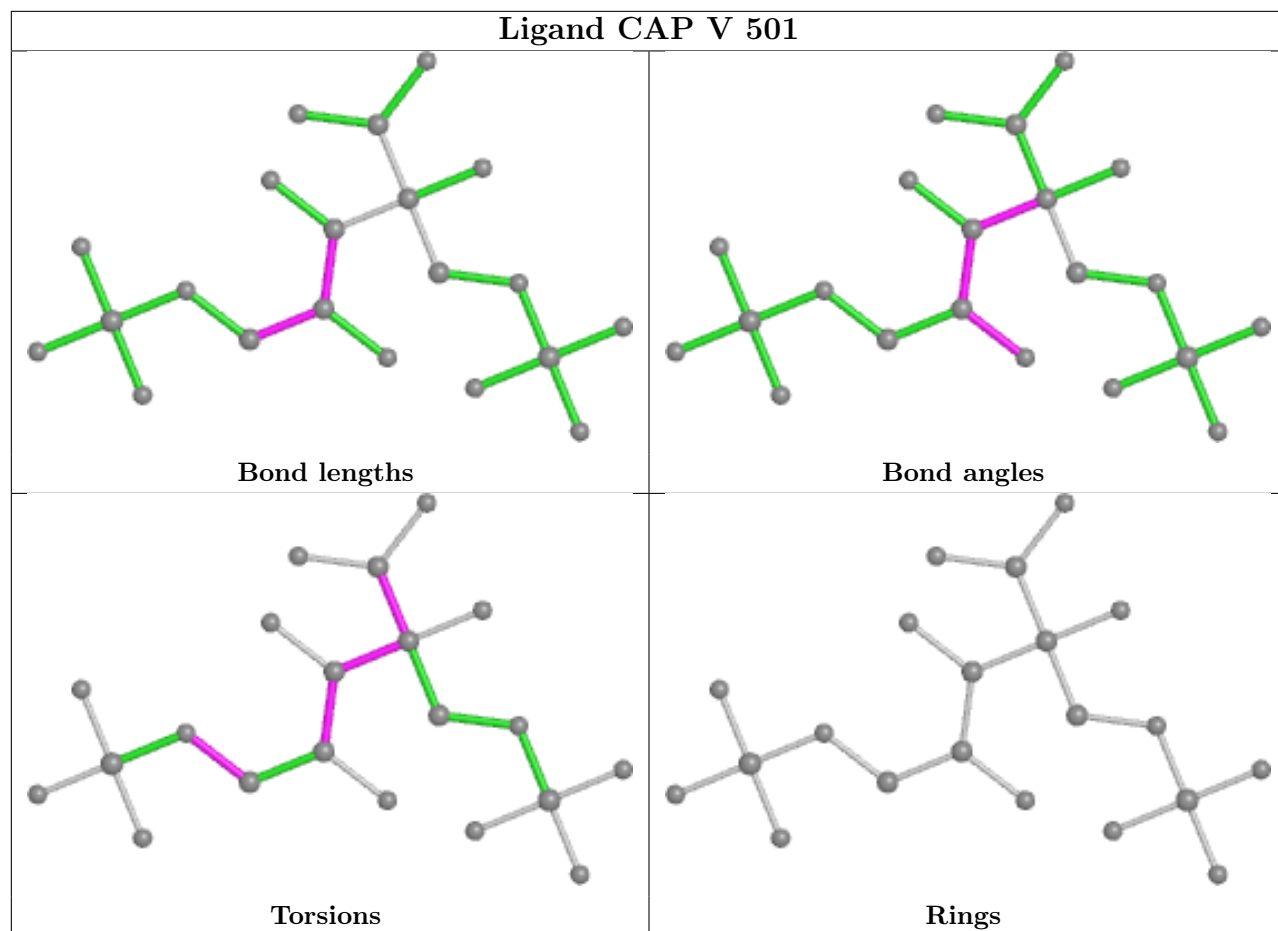


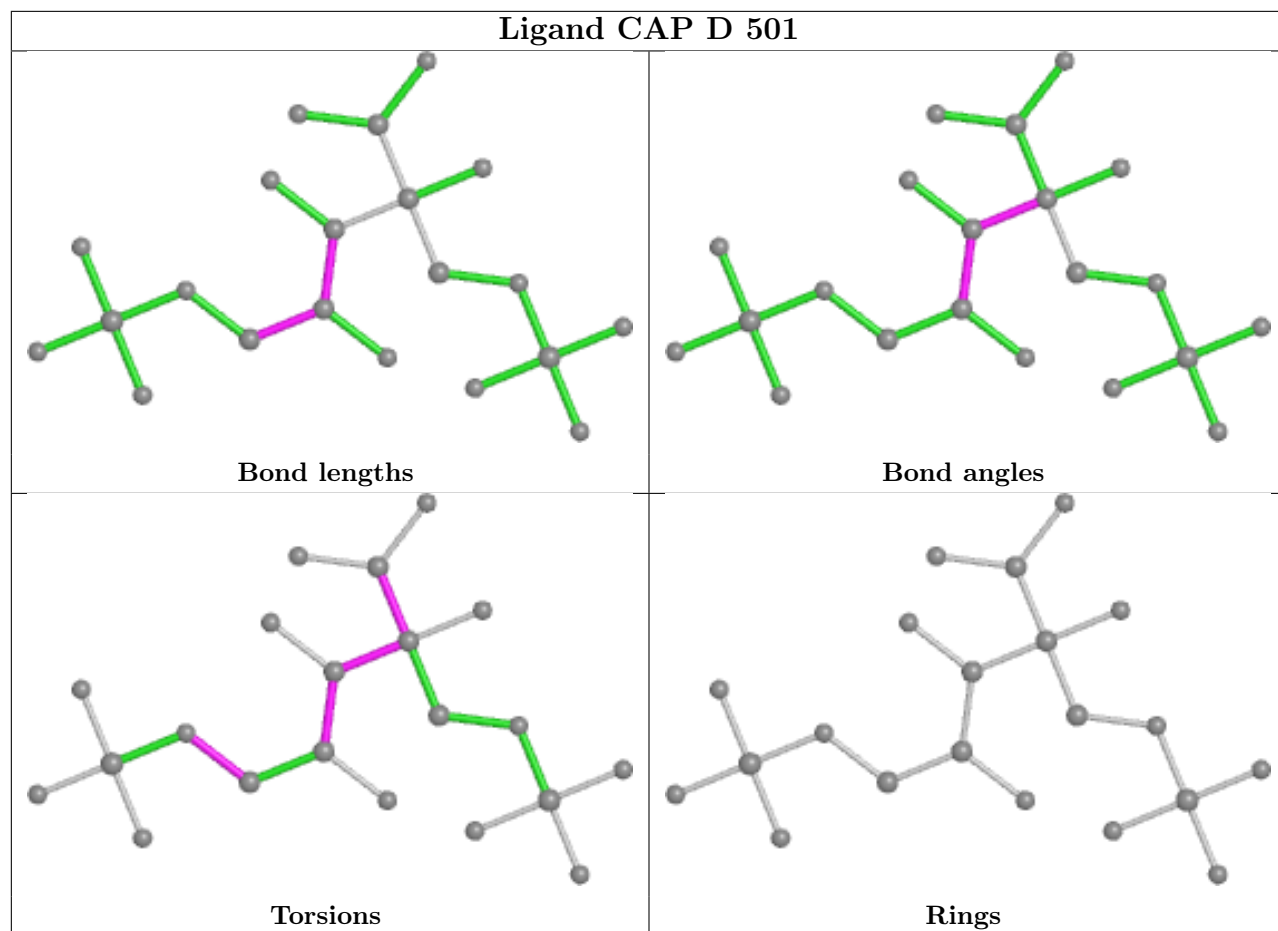


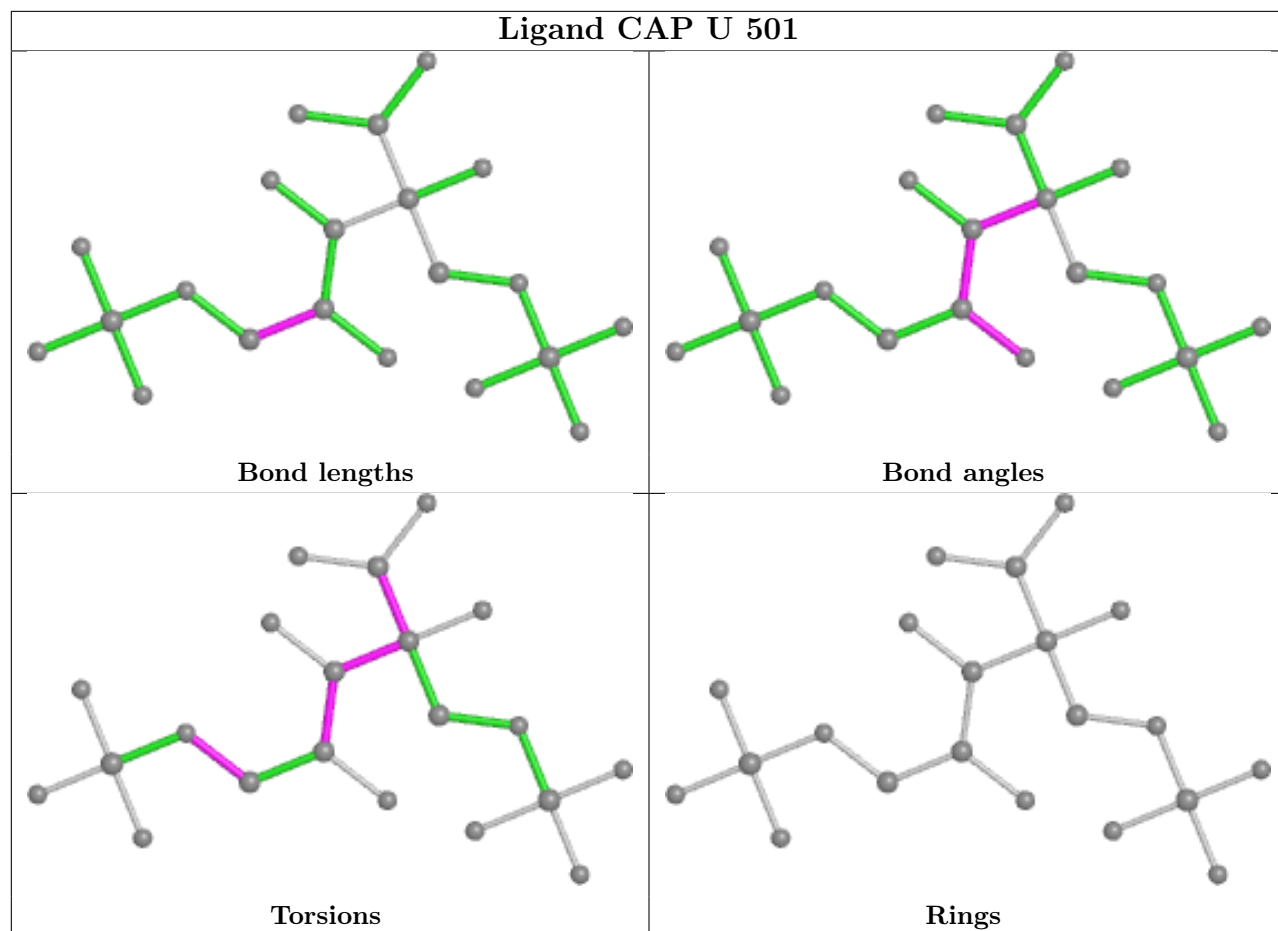


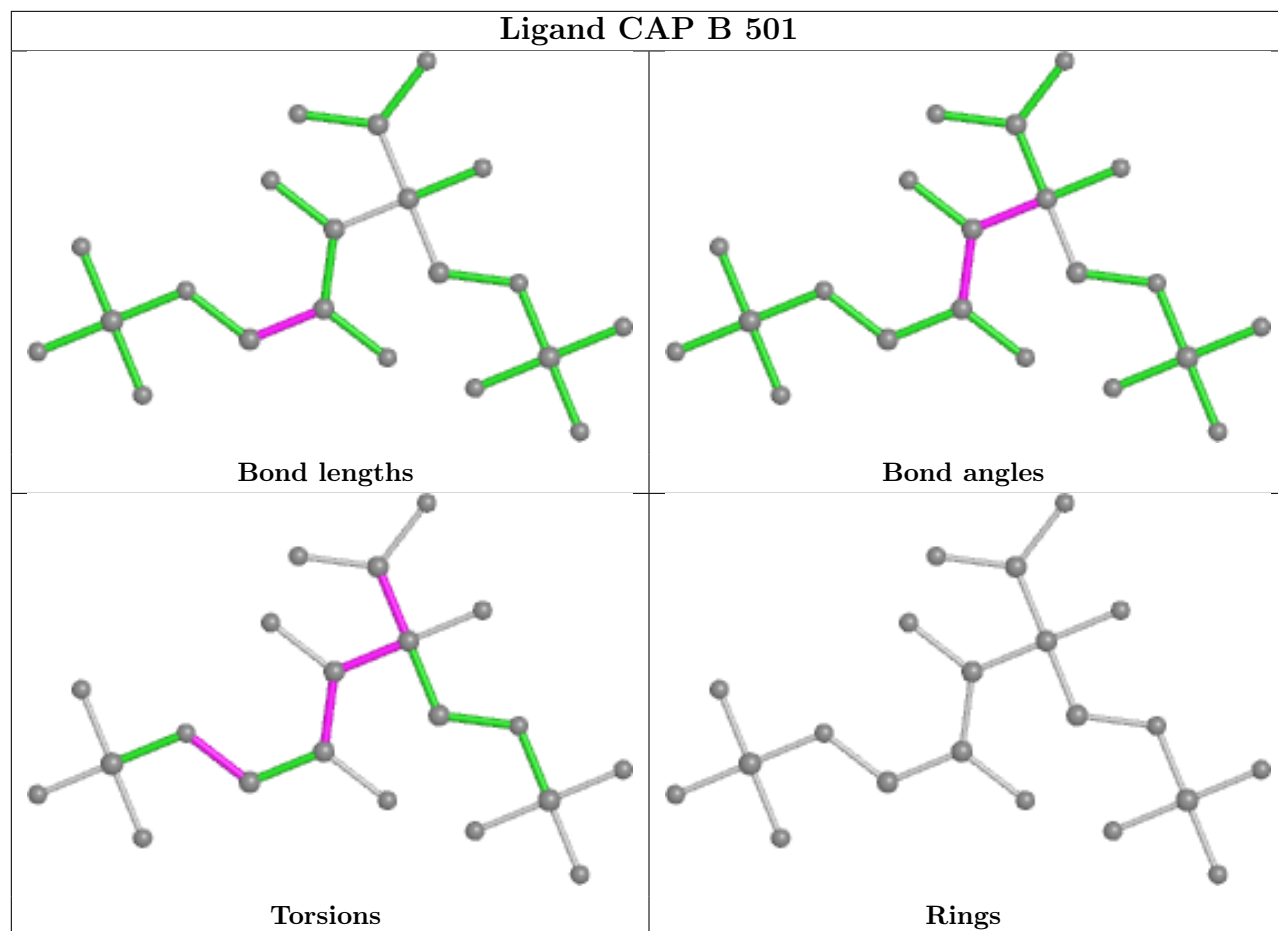




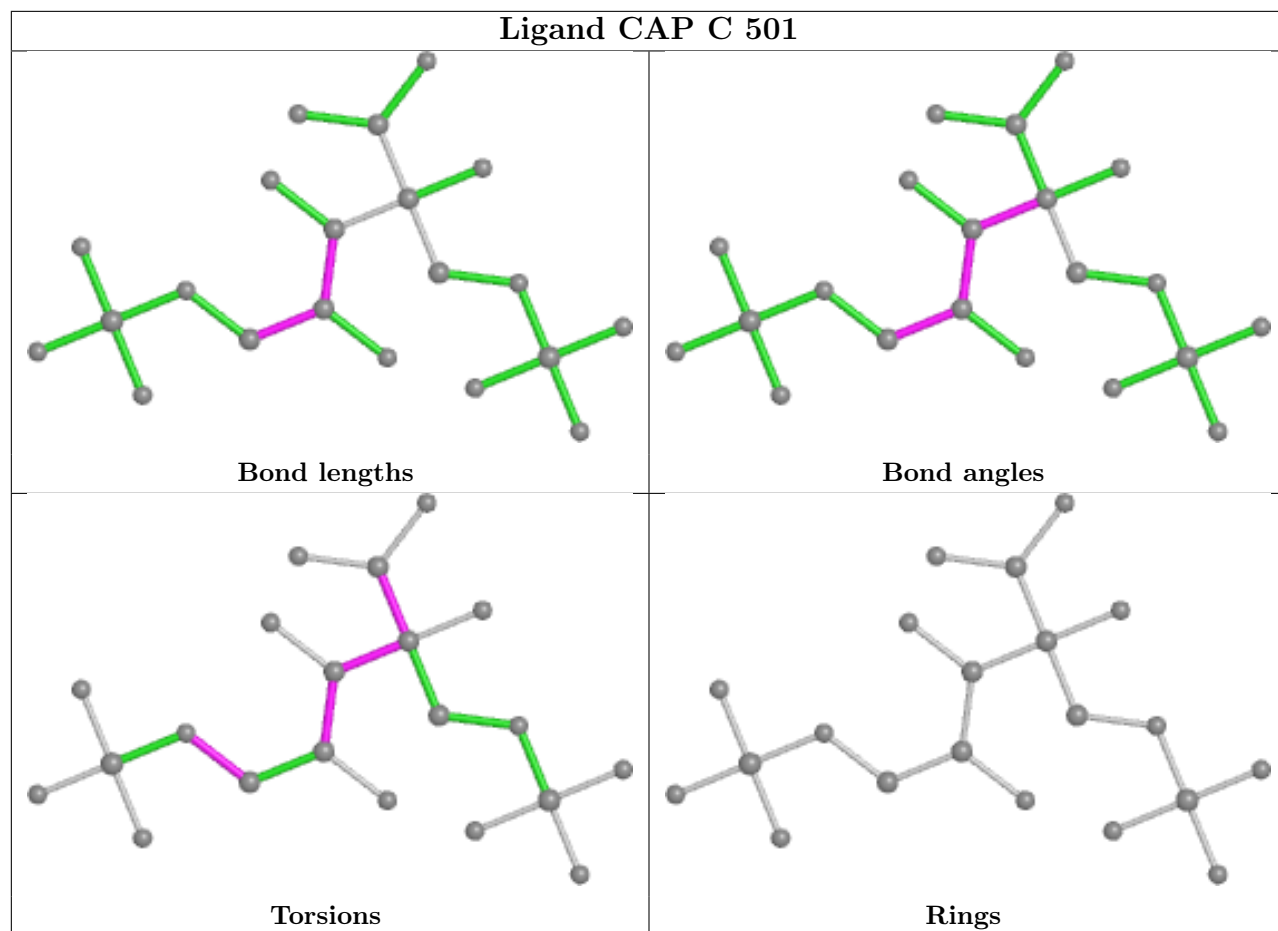


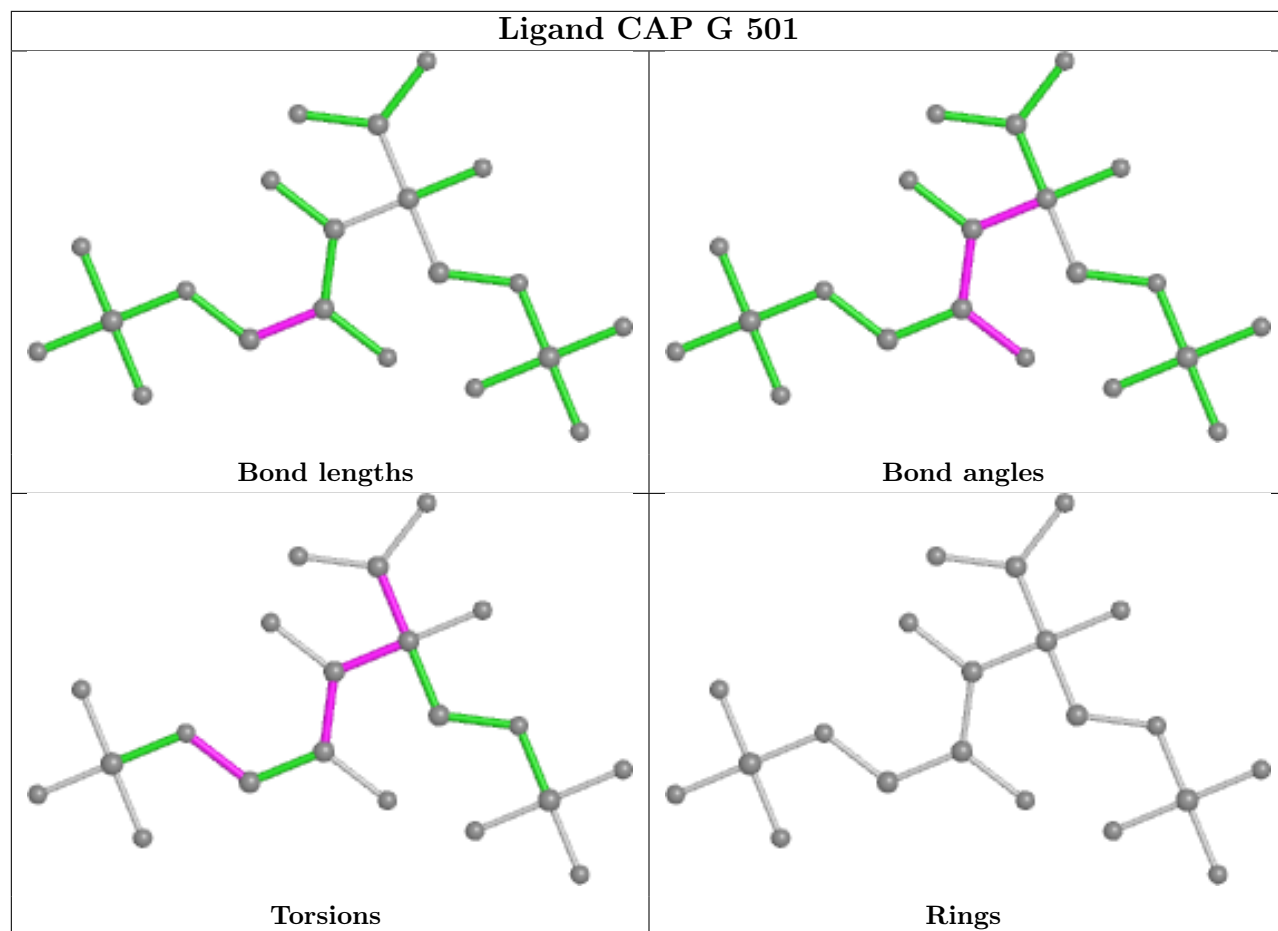


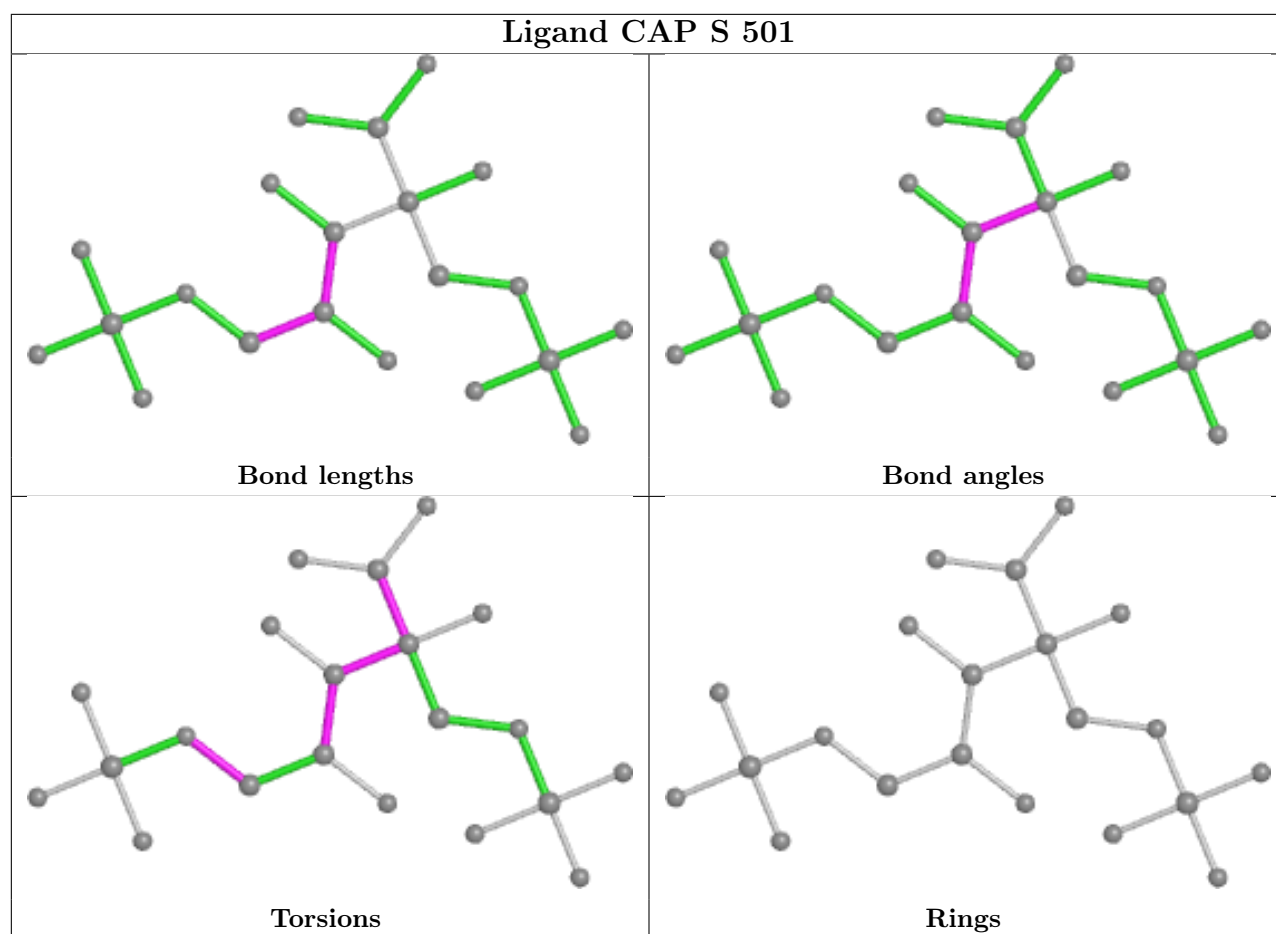












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	463/475 (97%)	-0.37	5 (1%) 80 80	5, 12, 27, 61	0
1	B	462/475 (97%)	-0.43	4 (0%) 84 84	7, 13, 28, 43	0
1	C	461/475 (97%)	-0.52	3 (0%) 87 87	6, 11, 24, 49	0
1	D	462/475 (97%)	-0.52	5 (1%) 80 80	6, 10, 23, 46	0
1	E	460/475 (96%)	-0.54	3 (0%) 87 87	6, 11, 24, 40	0
1	F	460/475 (96%)	-0.50	2 (0%) 92 92	7, 12, 24, 43	0
1	G	461/475 (97%)	-0.50	3 (0%) 87 87	6, 10, 24, 39	0
1	H	463/475 (97%)	-0.59	4 (0%) 84 84	4, 10, 22, 57	0
1	S	460/475 (96%)	-0.45	2 (0%) 92 92	6, 12, 27, 49	0
1	T	461/475 (97%)	-0.43	4 (0%) 84 84	6, 12, 27, 48	0
1	U	464/475 (97%)	-0.45	7 (1%) 73 73	6, 12, 27, 62	0
1	V	464/475 (97%)	-0.40	8 (1%) 70 69	5, 11, 26, 66	0
1	W	461/475 (97%)	-0.42	5 (1%) 80 80	6, 13, 29, 43	0
1	X	461/475 (97%)	-0.37	6 (1%) 77 77	6, 12, 27, 48	0
1	Y	460/475 (96%)	-0.46	4 (0%) 84 84	6, 11, 27, 45	0
1	Z	461/475 (97%)	-0.56	2 (0%) 92 92	5, 10, 23, 54	0
2	1	139/140 (99%)	-0.21	2 (1%) 75 75	8, 17, 30, 39	0
2	2	139/140 (99%)	-0.25	2 (1%) 75 75	9, 18, 31, 43	0
2	3	139/140 (99%)	-0.17	1 (0%) 87 87	9, 19, 34, 44	0
2	4	139/140 (99%)	-0.28	1 (0%) 87 87	9, 16, 30, 37	0
2	5	139/140 (99%)	-0.36	0 100 100	9, 16, 29, 38	0
2	6	139/140 (99%)	-0.23	0 100 100	9, 19, 33, 40	0
2	7	139/140 (99%)	-0.36	2 (1%) 75 75	8, 15, 28, 34	0
2	8	139/140 (99%)	-0.48	0 100 100	7, 14, 28, 34	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	I	139/140 (99%)	-0.22	3 (2%) 62 60	10, 18, 34, 45	0
2	J	139/140 (99%)	-0.19	2 (1%) 75 75	10, 20, 34, 42	0
2	K	139/140 (99%)	-0.26	0 100 100	8, 17, 31, 39	0
2	L	139/140 (99%)	-0.34	1 (0%) 87 87	9, 16, 30, 39	0
2	M	139/140 (99%)	-0.34	2 (1%) 75 75	8, 15, 31, 39	0
2	N	139/140 (99%)	-0.29	2 (1%) 75 75	8, 17, 29, 39	0
2	O	139/140 (99%)	-0.38	0 100 100	8, 14, 28, 36	0
2	P	139/140 (99%)	-0.40	2 (1%) 75 75	8, 14, 27, 37	0
All	All	9608/9840 (97%)	-0.43	87 (0%) 84 84	4, 12, 28, 66	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	10	GLY	8.6
1	T	10	GLY	8.4
1	D	9	ALA	7.8
1	X	10	GLY	7.2
1	V	7	THR	7.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MME	N	1	9/10	0.92	0.12	18,20,28,31	0
2	MME	L	1	9/10	0.93	0.13	18,24,30,30	0
2	MME	3	1	9/10	0.93	0.14	24,26,34,34	0
2	MME	4	1	9/10	0.93	0.12	24,25,30,30	0
2	MME	K	1	9/10	0.94	0.12	22,24,28,29	0
2	MME	J	1	9/10	0.94	0.12	20,23,31,31	0
2	MME	M	1	9/10	0.94	0.13	21,22,30,31	0
2	MME	8	1	9/10	0.94	0.14	21,24,27,30	0
2	MME	O	1	9/10	0.95	0.12	18,21,28,31	0
2	MME	1	1	9/10	0.95	0.11	21,23,24,25	0
2	MME	5	1	9/10	0.95	0.09	18,21,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	HYP	T	104	8/9	0.95	0.07	9,11,12,14	0
2	MME	2	1	9/10	0.96	0.09	21,23,27,27	0
1	KCX	A	201	12/13	0.96	0.14	7,9,10,11	0
1	KCX	V	201	12/13	0.96	0.14	8,9,11,11	0
1	HYP	E	104	8/9	0.96	0.07	7,9,10,10	0
2	MME	I	1	9/10	0.96	0.09	20,21,28,28	0
2	MME	6	1	9/10	0.96	0.10	20,21,26,27	0
2	MME	7	1	9/10	0.96	0.11	16,18,27,29	0
1	KCX	F	201	12/13	0.96	0.11	5,8,10,10	0
1	HYP	D	104	8/9	0.97	0.07	6,7,9,9	0
1	KCX	H	201	12/13	0.97	0.10	5,6,7,9	0
2	MME	P	1	9/10	0.97	0.10	17,21,25,25	0
1	HYP	S	104	8/9	0.97	0.07	11,12,13,14	0
1	KCX	S	201	12/13	0.97	0.12	5,8,8,11	0
1	HYP	B	104	8/9	0.97	0.06	8,11,11,13	0
1	KCX	B	201	12/13	0.97	0.10	7,10,11,12	0
1	HYP	T	151	8/9	0.97	0.07	6,7,8,9	0
1	HYP	E	151	8/9	0.97	0.08	8,9,10,10	0
1	HYP	U	104	8/9	0.97	0.06	9,9,9,9	0
1	KCX	E	201	12/13	0.97	0.08	6,8,10,11	0
1	HYP	V	104	8/9	0.97	0.07	8,9,10,10	0
1	HYP	A	104	8/9	0.97	0.07	10,11,12,14	0
1	HYP	F	151	8/9	0.97	0.08	11,11,12,12	0
1	HYP	W	104	8/9	0.97	0.07	10,11,11,12	0
1	KCX	W	201	12/13	0.97	0.10	9,10,12,12	0
1	KCX	C	201	12/13	0.97	0.10	7,9,11,11	0
1	HYP	X	104	8/9	0.97	0.07	10,10,11,11	0
1	HYP	X	151	8/9	0.97	0.07	7,9,10,10	0
1	KCX	X	201	12/13	0.97	0.10	7,8,10,10	0
1	HYP	A	151	8/9	0.97	0.07	8,8,9,11	0
1	KCX	Y	201	12/13	0.97	0.10	6,7,8,8	0
1	HYP	G	151	8/9	0.97	0.06	9,9,10,11	0
1	KCX	Z	201	12/13	0.97	0.10	4,7,8,9	0
1	KCX	G	201	12/13	0.97	0.13	5,7,8,9	0
1	HYP	H	104	8/9	0.98	0.05	6,7,8,9	0
1	HYP	H	151	8/9	0.98	0.07	5,5,6,6	0
1	HYP	V	151	8/9	0.98	0.06	7,7,9,9	0
1	HYP	B	151	8/9	0.98	0.07	9,10,11,12	0
1	HYP	F	104	8/9	0.98	0.05	8,10,12,14	0
1	HYP	D	151	8/9	0.98	0.07	4,7,8,8	0
1	HYP	W	151	8/9	0.98	0.07	5,8,9,9	0
1	HYP	S	151	8/9	0.98	0.07	7,8,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SMC	W	369	7/8	0.98	0.07	9,10,11,11	0
1	KCX	D	201	12/13	0.98	0.10	6,7,7,8	0
1	HYP	C	104	8/9	0.98	0.06	6,8,9,9	0
1	HYP	G	104	8/9	0.98	0.06	9,11,11,12	0
1	HYP	C	151	8/9	0.98	0.07	7,8,9,9	0
1	SMC	X	369	7/8	0.98	0.05	11,12,13,14	0
1	KCX	T	201	12/13	0.98	0.08	4,8,9,9	0
1	HYP	Y	104	8/9	0.98	0.06	10,11,11,12	0
1	HYP	Y	151	8/9	0.98	0.06	8,9,9,9	0
1	SMC	A	369	7/8	0.98	0.06	13,13,15,16	0
1	SMC	Y	369	7/8	0.98	0.05	11,12,13,14	0
1	SMC	B	369	7/8	0.98	0.06	12,13,13,14	0
1	HYP	Z	104	8/9	0.98	0.06	8,9,10,12	0
1	HYP	Z	151	8/9	0.98	0.06	6,7,8,9	0
1	HYP	U	151	8/9	0.98	0.07	7,9,9,9	0
1	KCX	U	201	12/13	0.98	0.12	8,10,11,11	0
1	SMC	V	256	7/8	0.99	0.04	6,6,7,8	0
1	SMC	V	369	7/8	0.99	0.05	10,10,12,14	0
1	SMC	C	256	7/8	0.99	0.05	7,8,9,10	0
1	SMC	C	369	7/8	0.99	0.05	8,10,12,12	0
1	SMC	S	256	7/8	0.99	0.05	4,6,7,7	0
1	SMC	S	369	7/8	0.99	0.04	10,10,12,12	0
1	SMC	W	256	7/8	0.99	0.05	8,9,9,10	0
1	SMC	E	256	7/8	0.99	0.05	6,7,8,8	0
1	SMC	E	369	7/8	0.99	0.04	8,9,10,11	0
1	SMC	G	256	7/8	0.99	0.06	5,6,8,8	0
1	SMC	G	369	7/8	0.99	0.06	11,11,13,13	0
1	SMC	T	256	7/8	0.99	0.05	6,6,7,8	0
1	SMC	X	256	7/8	0.99	0.05	7,7,9,11	0
1	SMC	T	369	7/8	0.99	0.05	11,12,13,15	0
1	SMC	D	256	7/8	0.99	0.05	5,7,8,10	0
1	SMC	D	369	7/8	0.99	0.05	8,9,10,10	0
1	SMC	B	256	7/8	0.99	0.05	7,8,9,9	0
1	SMC	A	256	7/8	0.99	0.05	7,8,8,8	0
1	SMC	Y	256	7/8	0.99	0.05	6,7,8,8	0
1	SMC	U	256	7/8	0.99	0.05	5,7,7,7	0
1	SMC	U	369	7/8	0.99	0.05	8,9,10,11	0
1	SMC	H	256	7/8	0.99	0.05	6,6,7,8	0
1	SMC	H	369	7/8	0.99	0.04	6,9,10,10	0
1	SMC	F	256	7/8	0.99	0.05	8,9,9,9	0
1	SMC	Z	256	7/8	0.99	0.04	6,7,7,8	0
1	SMC	Z	369	7/8	0.99	0.05	8,9,11,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SMC	F	369	7/8	0.99	0.04	10,11,12,13	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	H	604	6/6	0.71	0.20	25,30,33,34	0
5	GOL	H	619	6/6	0.80	0.17	29,32,34,34	0
5	GOL	Y	618	6/6	0.80	0.19	37,40,41,41	0
5	GOL	F	617	6/6	0.85	0.18	32,32,33,34	0
5	GOL	C	615	6/6	0.85	0.15	26,28,31,32	0
5	GOL	D	616	6/6	0.86	0.17	22,26,30,32	0
5	GOL	G	611	6/6	0.87	0.17	16,18,23,26	0
5	GOL	D	608	6/6	0.89	0.13	23,26,27,27	0
5	GOL	U	607	6/6	0.89	0.12	23,27,28,28	0
5	GOL	H	612	6/6	0.89	0.15	14,18,21,21	0
5	GOL	Z	612	6/6	0.89	0.17	17,19,22,23	0
5	GOL	E	609	6/6	0.90	0.14	14,17,20,22	0
5	GOL	E	620	6/6	0.90	0.14	22,26,28,28	0
5	GOL	S	609	6/6	0.90	0.18	23,25,28,32	0
5	GOL	A	605	6/6	0.90	0.13	26,27,29,30	0
5	GOL	V	616	6/6	0.90	0.14	25,27,29,30	0
5	GOL	W	620	6/6	0.90	0.14	34,36,36,37	0
5	GOL	Y	603	6/6	0.90	0.12	29,31,32,32	0
5	GOL	B	606	6/6	0.90	0.13	22,22,24,24	0
5	GOL	B	614	6/6	0.90	0.15	25,31,33,34	0
5	GOL	S	605	6/6	0.91	0.10	26,28,30,30	0
5	GOL	V	608	6/6	0.91	0.13	17,19,20,21	0
5	GOL	X	617	6/6	0.91	0.11	21,27,29,30	0
5	GOL	Y	611	6/6	0.92	0.15	19,21,22,23	0
5	GOL	S	613	6/6	0.92	0.12	23,25,25,26	0
5	GOL	Z	604	6/6	0.92	0.12	24,26,26,28	0
5	GOL	T	606	6/6	0.92	0.12	21,22,24,25	0

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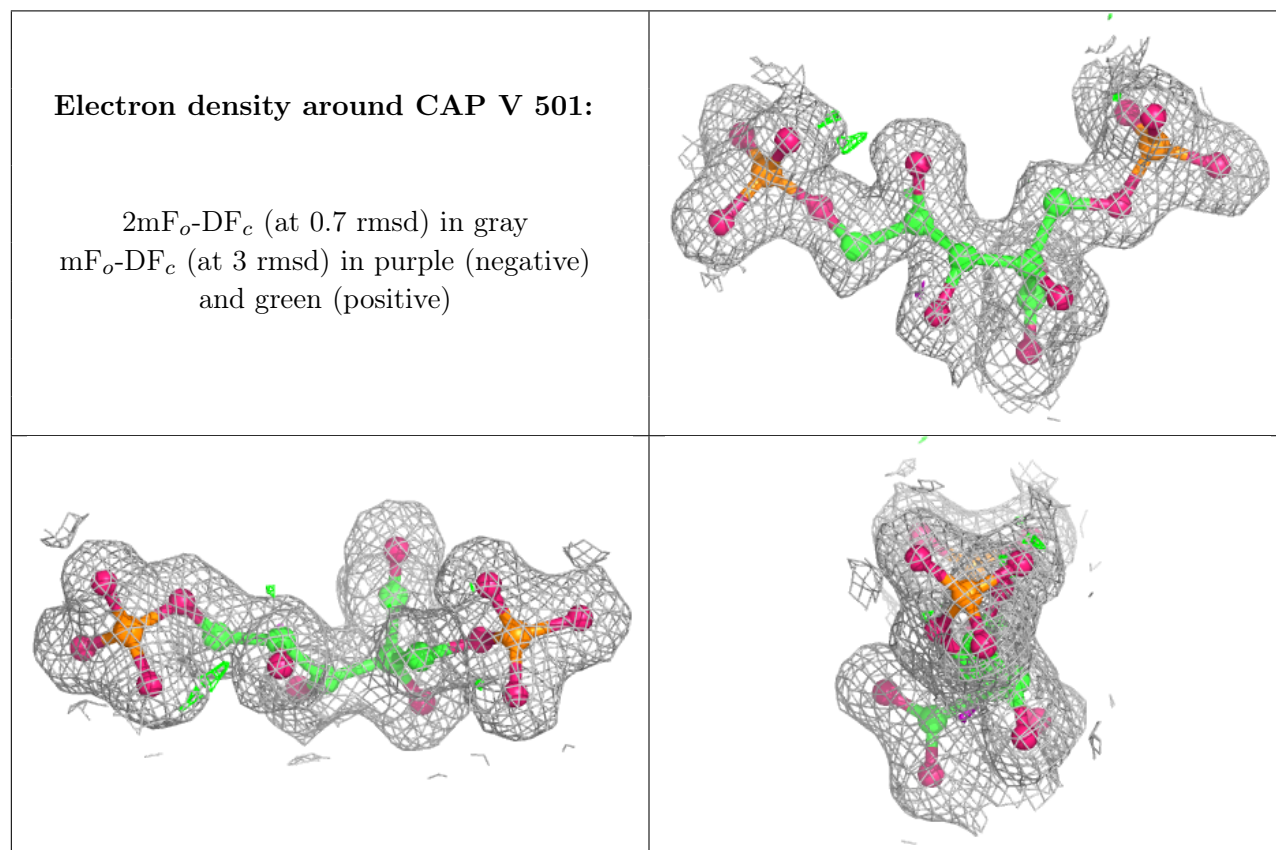
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	G	603	6/6	0.93	0.11	20,22,25,27	0
5	GOL	W	601	6/6	0.93	0.12	23,25,25,25	0
5	GOL	E	601	6/6	0.93	0.12	29,30,30,31	0
5	GOL	X	610	6/6	0.93	0.15	16,19,22,26	0
5	GOL	G	618	6/6	0.93	0.09	26,30,31,31	0
5	GOL	Z	619	6/6	0.93	0.09	19,24,25,26	0
5	GOL	A	613	6/6	0.94	0.10	25,29,30,30	0
5	GOL	C	607	6/6	0.94	0.09	23,24,26,27	0
5	GOL	T	614	6/6	0.94	0.08	22,27,29,29	0
5	GOL	F	602	6/6	0.94	0.07	22,24,25,27	0
5	GOL	B	610	6/6	0.95	0.13	18,20,21,23	0
5	GOL	U	615	6/6	0.95	0.08	20,23,25,27	0
5	GOL	X	602	6/6	0.96	0.09	19,20,22,22	0
4	CAP	V	501	21/21	0.98	0.09	8,10,11,12	0
4	CAP	W	501	21/21	0.98	0.08	9,11,15,17	0
4	CAP	X	501	21/21	0.98	0.10	8,11,13,14	0
4	CAP	Y	501	21/21	0.98	0.08	6,8,10,11	0
4	CAP	Z	501	21/21	0.98	0.07	7,9,10,11	0
3	MG	H	476	1/1	0.98	0.10	10,10,10,10	0
3	MG	U	476	1/1	0.98	0.09	11,11,11,11	0
4	CAP	A	501	21/21	0.98	0.10	7,10,11,14	0
4	CAP	B	501	21/21	0.98	0.07	10,12,15,17	0
4	CAP	C	501	21/21	0.98	0.09	8,10,11,13	0
4	CAP	E	501	21/21	0.98	0.07	8,11,11,12	0
4	CAP	F	501	21/21	0.98	0.08	9,11,13,15	0
4	CAP	S	501	21/21	0.98	0.10	10,12,12,13	0
4	CAP	T	501	21/21	0.98	0.07	6,10,11,12	0
4	CAP	U	501	21/21	0.98	0.09	11,13,14,16	0
3	MG	S	476	1/1	0.99	0.11	11,11,11,11	0
3	MG	T	476	1/1	0.99	0.05	12,12,12,12	0
4	CAP	G	501	21/21	0.99	0.08	6,8,10,11	0
4	CAP	H	501	21/21	0.99	0.08	6,8,9,11	0
3	MG	E	476	1/1	0.99	0.08	11,11,11,11	0
3	MG	V	476	1/1	0.99	0.10	12,12,12,12	0
3	MG	W	476	1/1	0.99	0.09	12,12,12,12	0
3	MG	X	476	1/1	0.99	0.11	13,13,13,13	0
3	MG	Y	476	1/1	0.99	0.08	11,11,11,11	0
3	MG	F	476	1/1	0.99	0.06	11,11,11,11	0
3	MG	G	476	1/1	0.99	0.11	11,11,11,11	0
3	MG	A	476	1/1	0.99	0.12	9,9,9,9	0
4	CAP	D	501	21/21	0.99	0.07	6,9,10,12	0
3	MG	D	476	1/1	1.00	0.09	9,9,9,9	0

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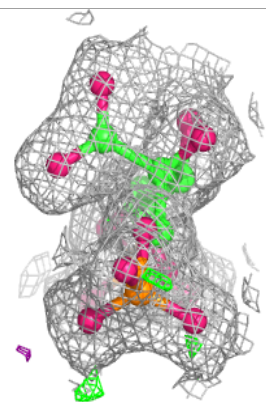
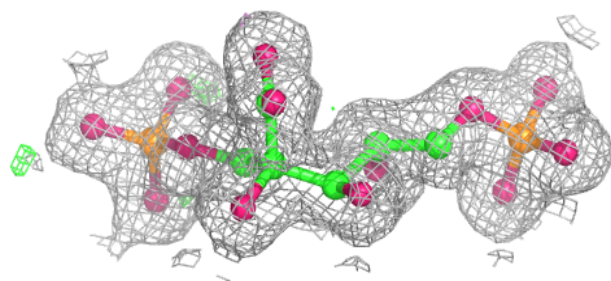
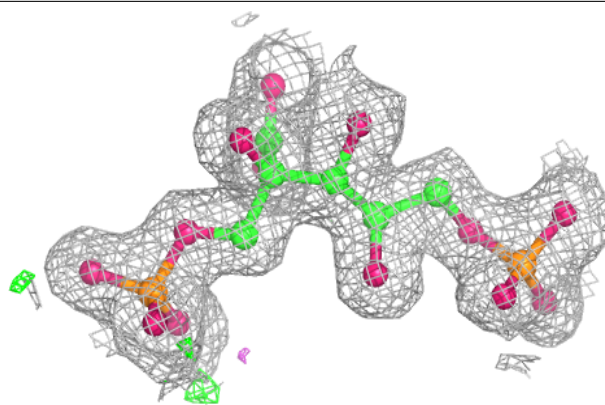
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	476	1/1	1.00	0.08	11,11,11,11	0
3	MG	C	476	1/1	1.00	0.10	13,13,13,13	0
3	MG	Z	476	1/1	1.00	0.09	9,9,9,9	0

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.

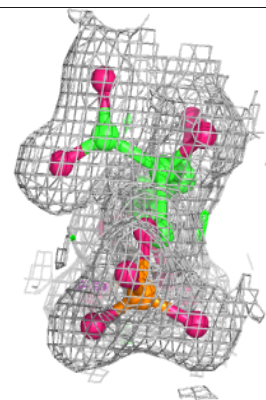
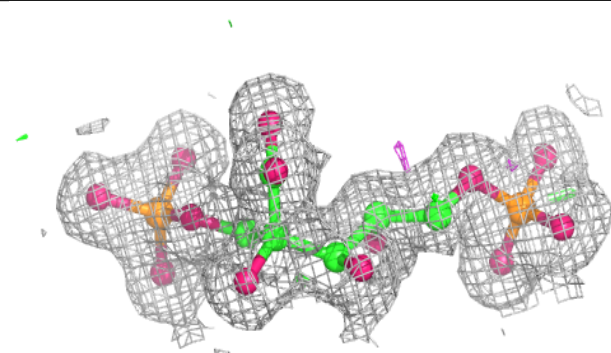
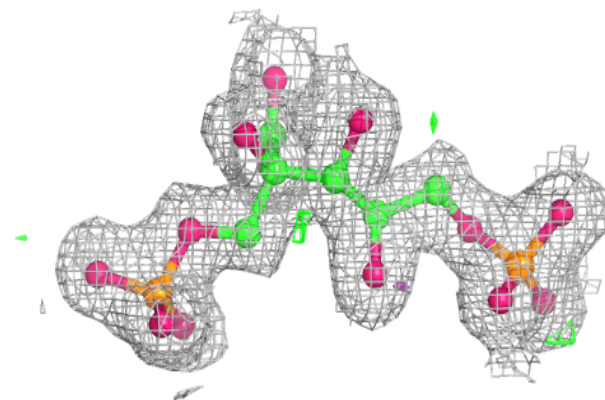


**Electron density around CAP W 501:**

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

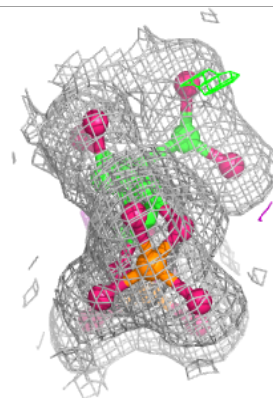
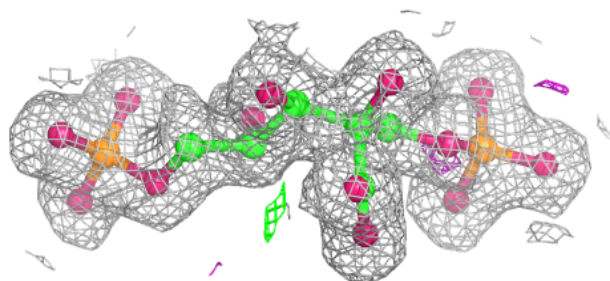
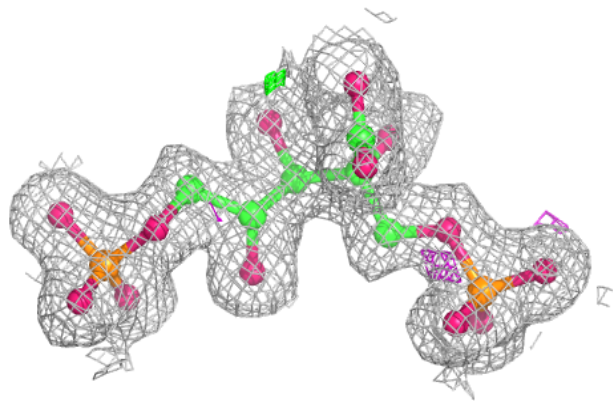
**Electron density around CAP X 501:**

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

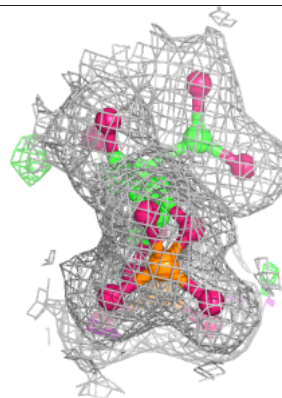
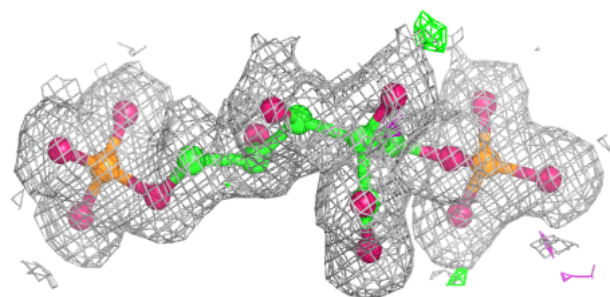
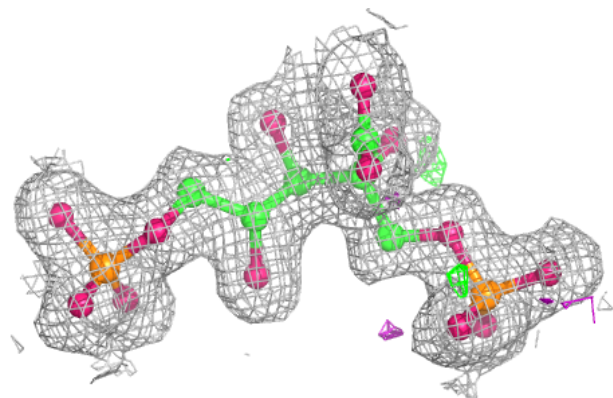


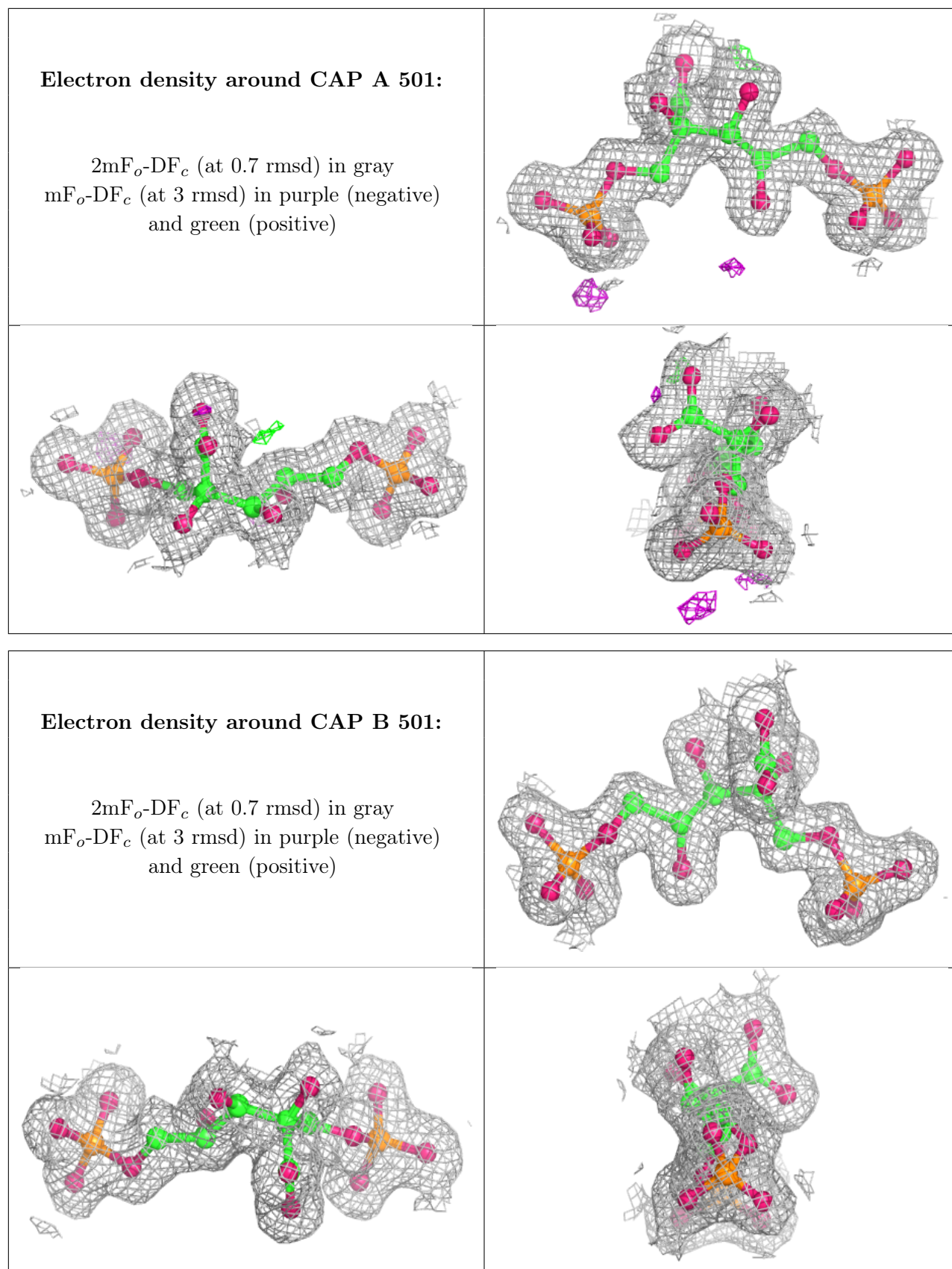
**Electron density around CAP Y 501:**

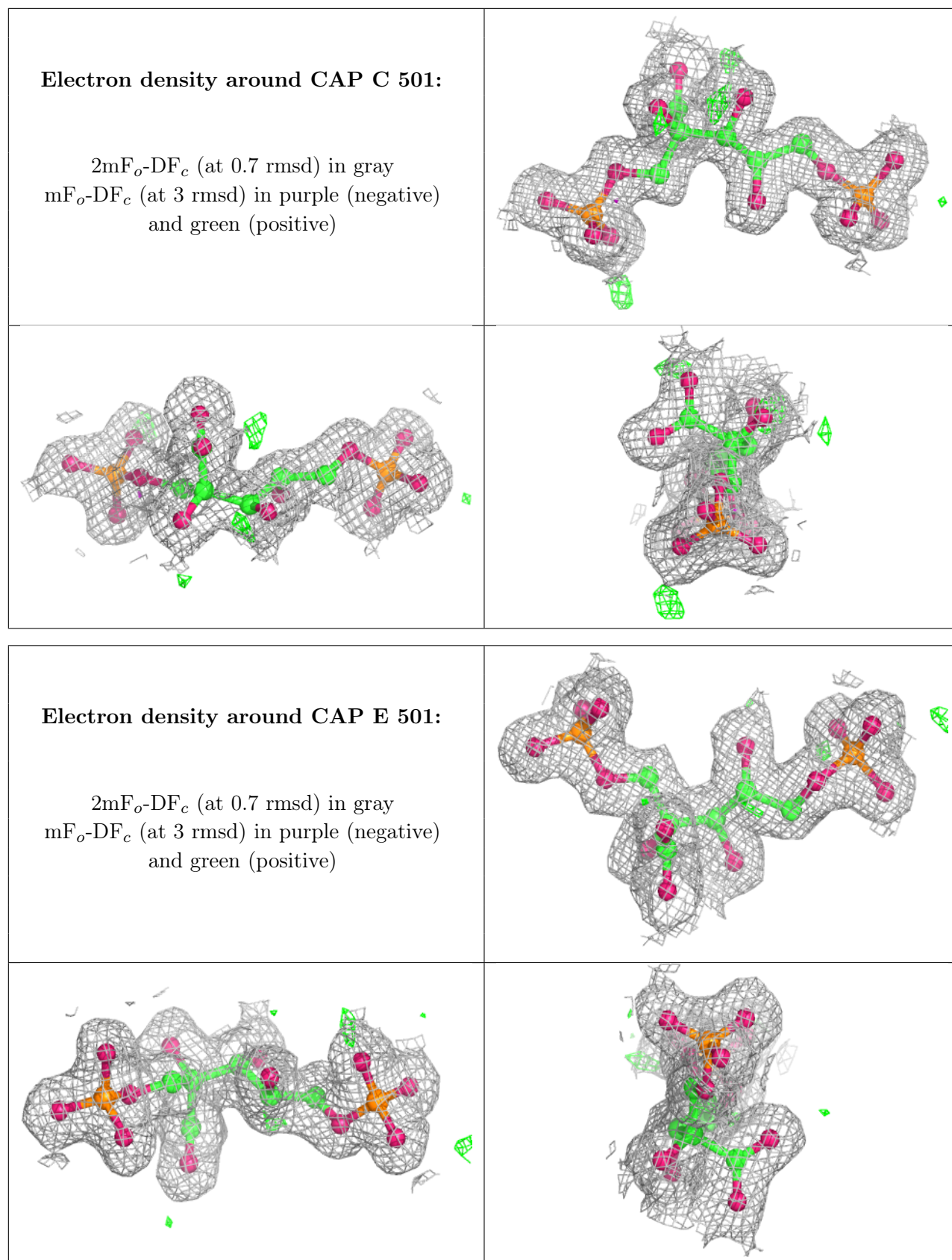
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)

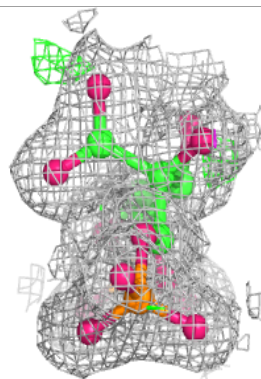
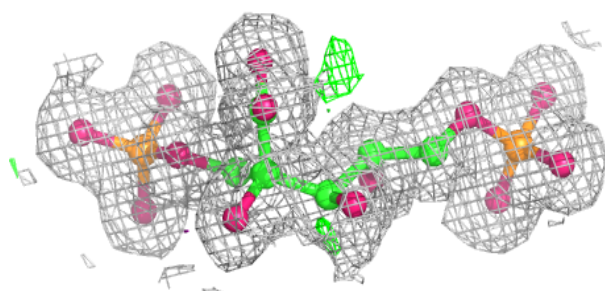
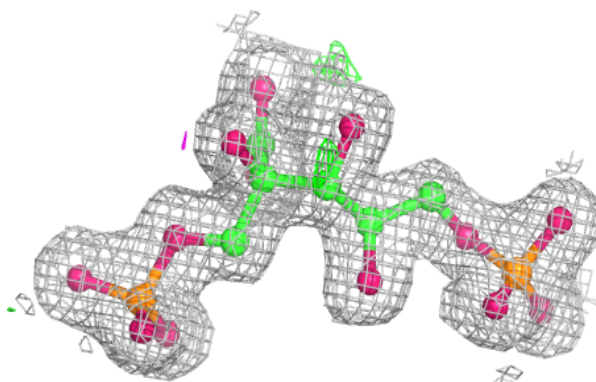




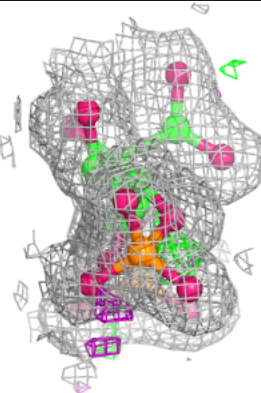
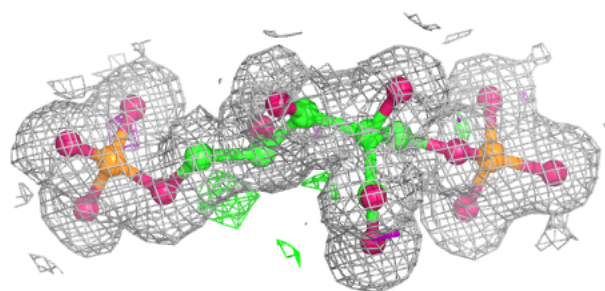
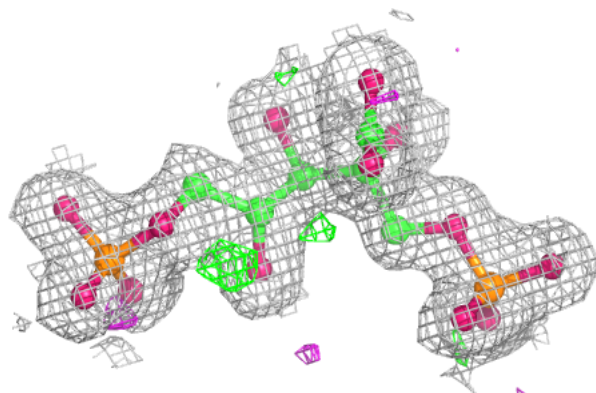


**Electron density around CAP F 501:**

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

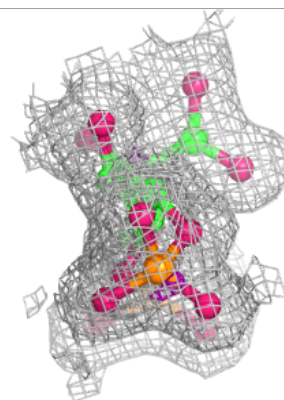
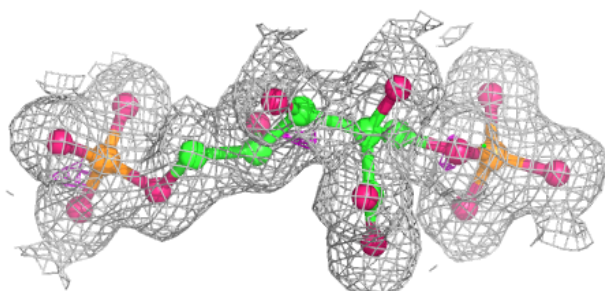
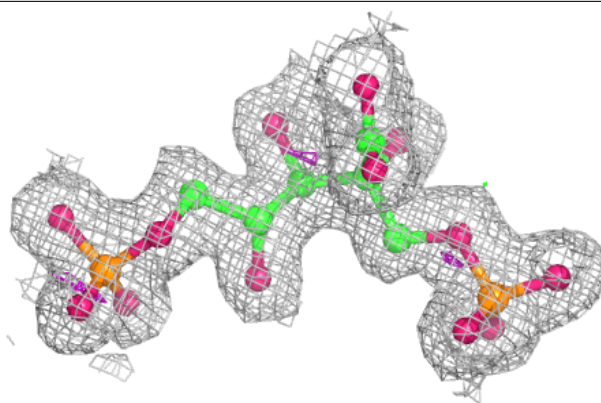
**Electron density around CAP S 501:**

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

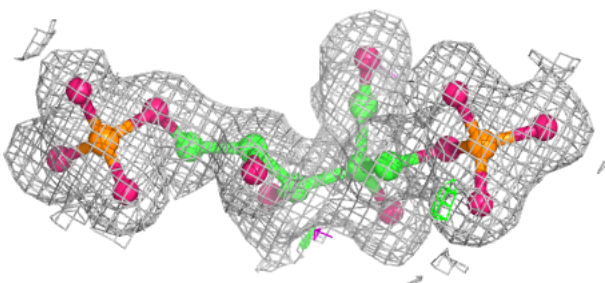
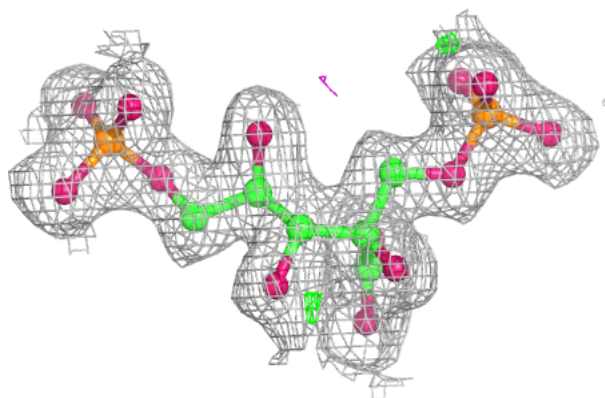


**Electron density around CAP T 501:**

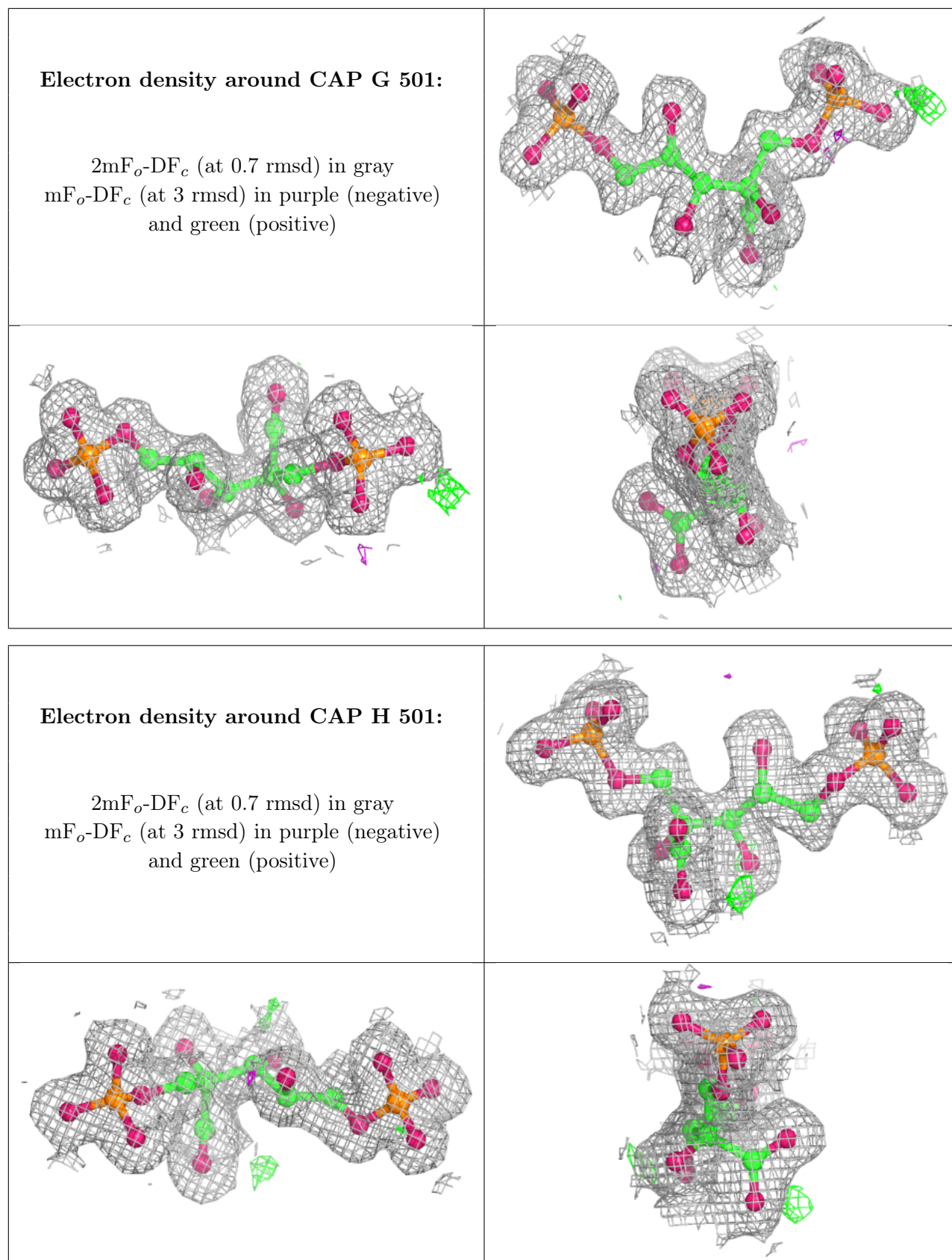
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

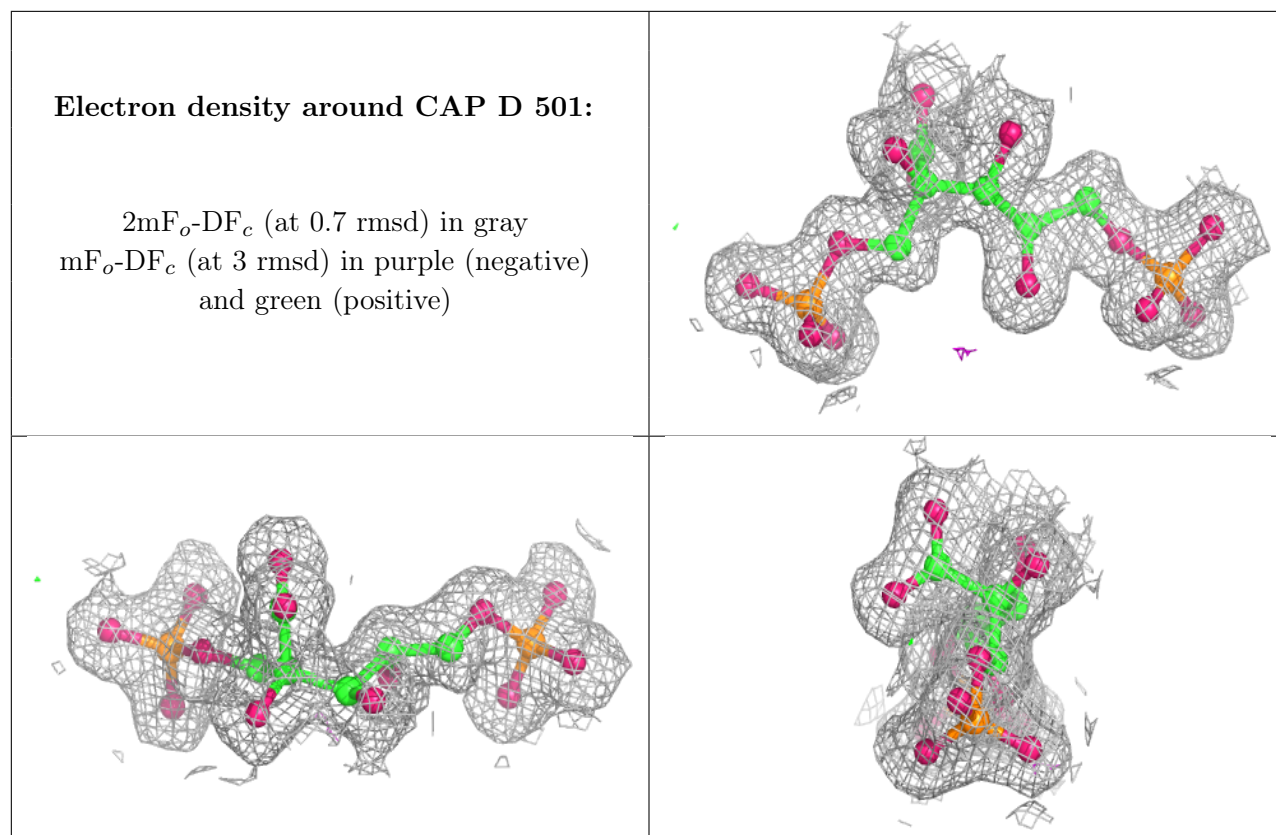
**Electron density around CAP U 501:**

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









## 6.5 Other polymers [i](#)

There are no such residues in this entry.