



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 02:38 PM UTC

PDB ID : 3KDO / pdb\_00003kdo  
Title : Crystal structure of Type III Rubisco SP6 mutant complexed with 2-CABP  
Authors : Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.  
Deposited on : 2009-10-23  
Resolution : 2.36 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 ⓘ](#)) were used in the production of this report:

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

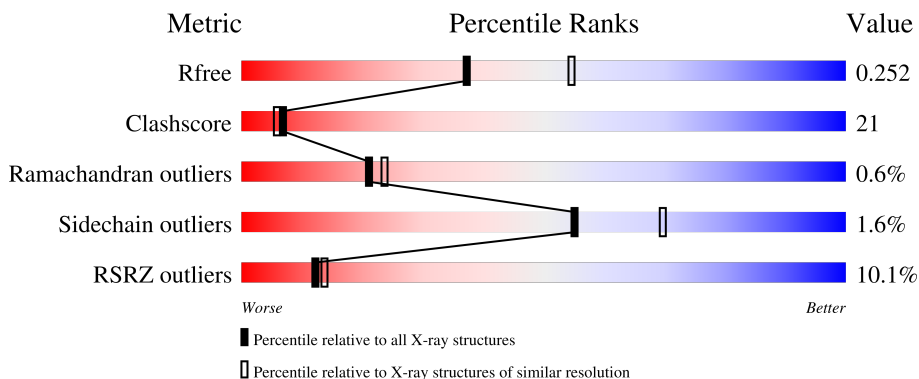
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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.




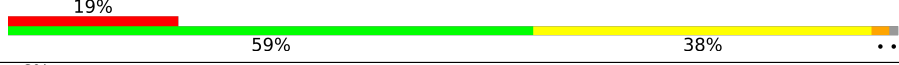


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	

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Mol	Chain	Length	Quality of chain
1	F	444	 4% 69% 28% ..
1	G	444	 4% 69% 28% ..
1	H	444	 19% 59% 38% ..
1	I	444	 6% 69% 29% .
1	J	444	 10% 69% 29% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36065 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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3341	2146	569	616	10	0	0	0
1	B	438	3391	2179	575	627	10	0	0	0
1	C	440	3420	2196	580	634	10	0	0	0
1	D	437	3419	2195	582	632	10	0	0	0
1	E	440	3418	2198	582	628	10	0	0	0
1	F	437	3415	2195	581	629	10	0	0	0
1	G	437	3423	2200	582	631	10	0	0	0
1	H	438	3382	2178	574	620	10	0	0	0
1	I	438	3410	2190	582	628	10	0	0	0
1	J	438	3415	2195	581	629	10	0	0	0

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	GLU	GLY	engineered mutation	UNP O93627
A	327	ARG	LYS	engineered mutation	UNP O93627
A	328	ASP	TRP	engineered mutation	UNP O93627
A	329	ILE	ASP	engineered mutation	UNP O93627
A	330	THR	VAL	engineered mutation	UNP O93627
A	331	LEU	ILE	engineered mutation	UNP O93627
A	332	GLY	GLN	engineered mutation	UNP O93627
A	333	PHE	ASN	engineered mutation	UNP O93627
A	334	VAL	ALA	engineered mutation	UNP O93627

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Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ASP	ARG	engineered mutation	UNP O93627
A	336	LEU	ILE	engineered mutation	UNP O93627
B	326	GLU	GLY	engineered mutation	UNP O93627
B	327	ARG	LYS	engineered mutation	UNP O93627
B	328	ASP	TRP	engineered mutation	UNP O93627
B	329	ILE	ASP	engineered mutation	UNP O93627
B	330	THR	VAL	engineered mutation	UNP O93627
B	331	LEU	ILE	engineered mutation	UNP O93627
B	332	GLY	GLN	engineered mutation	UNP O93627
B	333	PHE	ASN	engineered mutation	UNP O93627
B	334	VAL	ALA	engineered mutation	UNP O93627
B	335	ASP	ARG	engineered mutation	UNP O93627
B	336	LEU	ILE	engineered mutation	UNP O93627
C	326	GLU	GLY	engineered mutation	UNP O93627
C	327	ARG	LYS	engineered mutation	UNP O93627
C	328	ASP	TRP	engineered mutation	UNP O93627
C	329	ILE	ASP	engineered mutation	UNP O93627
C	330	THR	VAL	engineered mutation	UNP O93627
C	331	LEU	ILE	engineered mutation	UNP O93627
C	332	GLY	GLN	engineered mutation	UNP O93627
C	333	PHE	ASN	engineered mutation	UNP O93627
C	334	VAL	ALA	engineered mutation	UNP O93627
C	335	ASP	ARG	engineered mutation	UNP O93627
C	336	LEU	ILE	engineered mutation	UNP O93627
D	326	GLU	GLY	engineered mutation	UNP O93627
D	327	ARG	LYS	engineered mutation	UNP O93627
D	328	ASP	TRP	engineered mutation	UNP O93627
D	329	ILE	ASP	engineered mutation	UNP O93627
D	330	THR	VAL	engineered mutation	UNP O93627
D	331	LEU	ILE	engineered mutation	UNP O93627
D	332	GLY	GLN	engineered mutation	UNP O93627
D	333	PHE	ASN	engineered mutation	UNP O93627
D	334	VAL	ALA	engineered mutation	UNP O93627
D	335	ASP	ARG	engineered mutation	UNP O93627
D	336	LEU	ILE	engineered mutation	UNP O93627
E	326	GLU	GLY	engineered mutation	UNP O93627
E	327	ARG	LYS	engineered mutation	UNP O93627
E	328	ASP	TRP	engineered mutation	UNP O93627
E	329	ILE	ASP	engineered mutation	UNP O93627
E	330	THR	VAL	engineered mutation	UNP O93627
E	331	LEU	ILE	engineered mutation	UNP O93627
E	332	GLY	GLN	engineered mutation	UNP O93627

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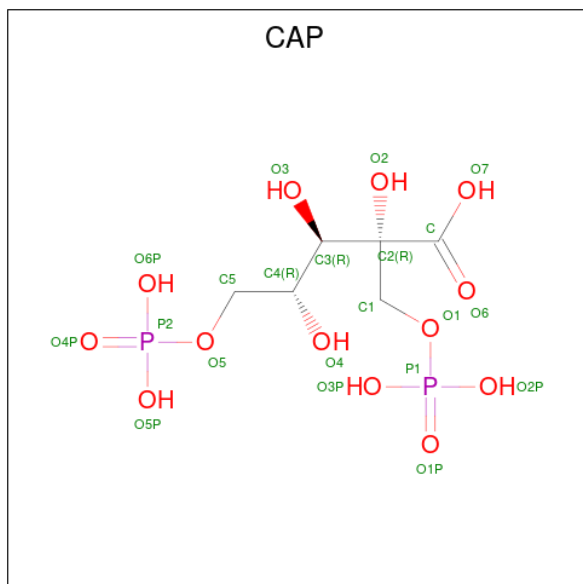
Chain	Residue	Modelled	Actual	Comment	Reference
E	333	PHE	ASN	engineered mutation	UNP O93627
E	334	VAL	ALA	engineered mutation	UNP O93627
E	335	ASP	ARG	engineered mutation	UNP O93627
E	336	LEU	ILE	engineered mutation	UNP O93627
F	326	GLU	GLY	engineered mutation	UNP O93627
F	327	ARG	LYS	engineered mutation	UNP O93627
F	328	ASP	TRP	engineered mutation	UNP O93627
F	329	ILE	ASP	engineered mutation	UNP O93627
F	330	THR	VAL	engineered mutation	UNP O93627
F	331	LEU	ILE	engineered mutation	UNP O93627
F	332	GLY	GLN	engineered mutation	UNP O93627
F	333	PHE	ASN	engineered mutation	UNP O93627
F	334	VAL	ALA	engineered mutation	UNP O93627
F	335	ASP	ARG	engineered mutation	UNP O93627
F	336	LEU	ILE	engineered mutation	UNP O93627
G	326	GLU	GLY	engineered mutation	UNP O93627
G	327	ARG	LYS	engineered mutation	UNP O93627
G	328	ASP	TRP	engineered mutation	UNP O93627
G	329	ILE	ASP	engineered mutation	UNP O93627
G	330	THR	VAL	engineered mutation	UNP O93627
G	331	LEU	ILE	engineered mutation	UNP O93627
G	332	GLY	GLN	engineered mutation	UNP O93627
G	333	PHE	ASN	engineered mutation	UNP O93627
G	334	VAL	ALA	engineered mutation	UNP O93627
G	335	ASP	ARG	engineered mutation	UNP O93627
G	336	LEU	ILE	engineered mutation	UNP O93627
H	326	GLU	GLY	engineered mutation	UNP O93627
H	327	ARG	LYS	engineered mutation	UNP O93627
H	328	ASP	TRP	engineered mutation	UNP O93627
H	329	ILE	ASP	engineered mutation	UNP O93627
H	330	THR	VAL	engineered mutation	UNP O93627
H	331	LEU	ILE	engineered mutation	UNP O93627
H	332	GLY	GLN	engineered mutation	UNP O93627
H	333	PHE	ASN	engineered mutation	UNP O93627
H	334	VAL	ALA	engineered mutation	UNP O93627
H	335	ASP	ARG	engineered mutation	UNP O93627
H	336	LEU	ILE	engineered mutation	UNP O93627
I	326	GLU	GLY	engineered mutation	UNP O93627
I	327	ARG	LYS	engineered mutation	UNP O93627
I	328	ASP	TRP	engineered mutation	UNP O93627
I	329	ILE	ASP	engineered mutation	UNP O93627
I	330	THR	VAL	engineered mutation	UNP O93627

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Chain	Residue	Modelled	Actual	Comment	Reference
I	331	LEU	ILE	engineered mutation	UNP O93627
I	332	GLY	GLN	engineered mutation	UNP O93627
I	333	PHE	ASN	engineered mutation	UNP O93627
I	334	VAL	ALA	engineered mutation	UNP O93627
I	335	ASP	ARG	engineered mutation	UNP O93627
I	336	LEU	ILE	engineered mutation	UNP O93627
J	326	GLU	GLY	engineered mutation	UNP O93627
J	327	ARG	LYS	engineered mutation	UNP O93627
J	328	ASP	TRP	engineered mutation	UNP O93627
J	329	ILE	ASP	engineered mutation	UNP O93627
J	330	THR	VAL	engineered mutation	UNP O93627
J	331	LEU	ILE	engineered mutation	UNP O93627
J	332	GLY	GLN	engineered mutation	UNP O93627
J	333	PHE	ASN	engineered mutation	UNP O93627
J	334	VAL	ALA	engineered mutation	UNP O93627
J	335	ASP	ARG	engineered mutation	UNP O93627
J	336	LEU	ILE	engineered mutation	UNP O93627

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			21	6	13	2		
2	D	1	Total	C	O	P	0	0
			21	6	13	2		
2	E	1	Total	C	O	P	0	0
			21	6	13	2		
2	F	1	Total	C	O	P	0	0
			21	6	13	2		
2	G	1	Total	C	O	P	0	0
			21	6	13	2		
2	H	1	Total	C	O	P	0	0
			21	6	13	2		
2	I	1	Total	C	O	P	0	0
			21	6	13	2		
2	J	1	Total	C	O	P	0	0
			21	6	13	2		

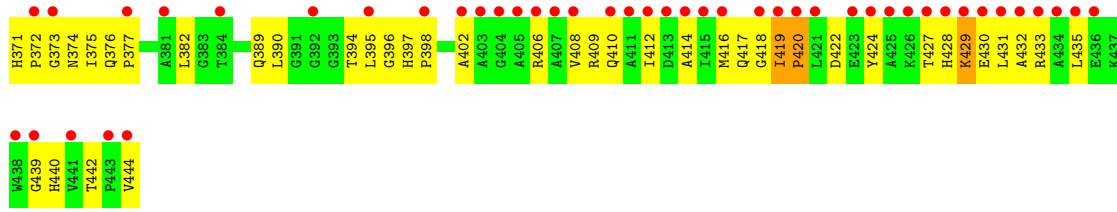
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

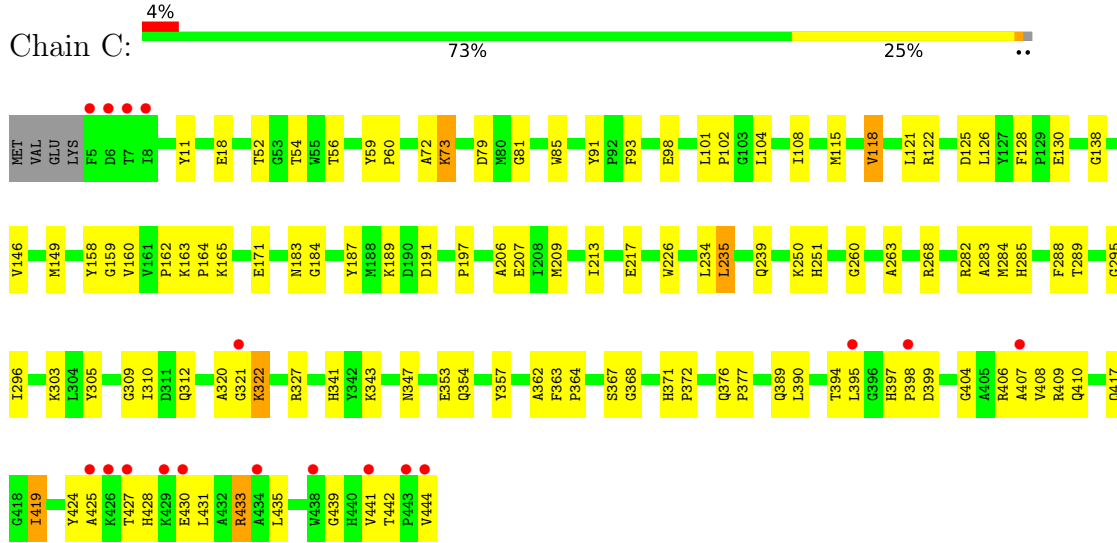
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	97	Total O 97 97	0	0
4	B	175	Total O 175 175	0	0
4	C	226	Total O 226 226	0	0
4	D	239	Total O 239 239	0	0
4	E	197	Total O 197 197	0	0
4	F	179	Total O 179 179	0	0
4	G	174	Total O 174 174	0	0
4	H	123	Total O 123 123	0	0
4	I	192	Total O 192 192	0	0
4	J	209	Total O 209 209	0	0

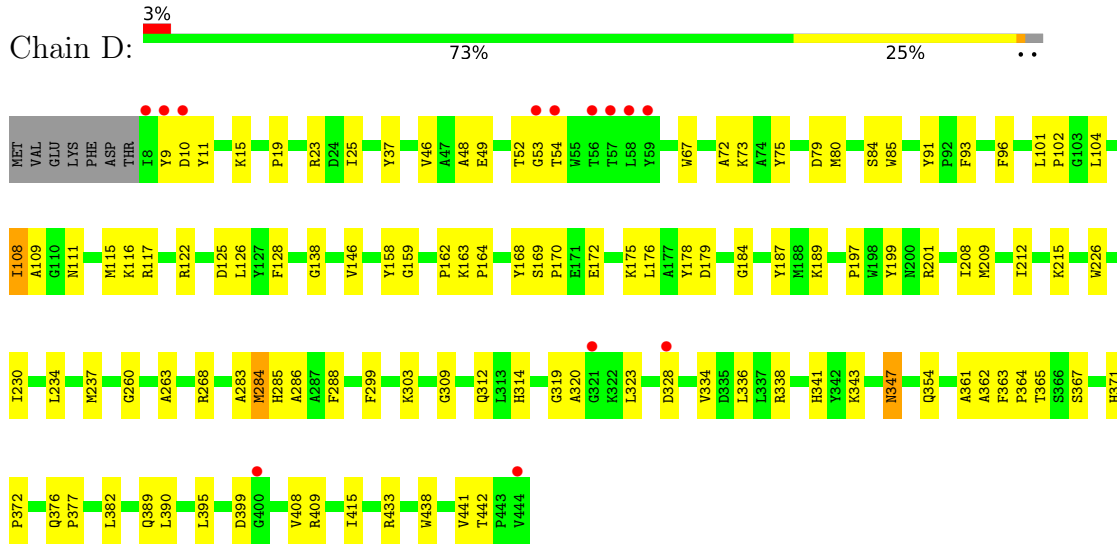




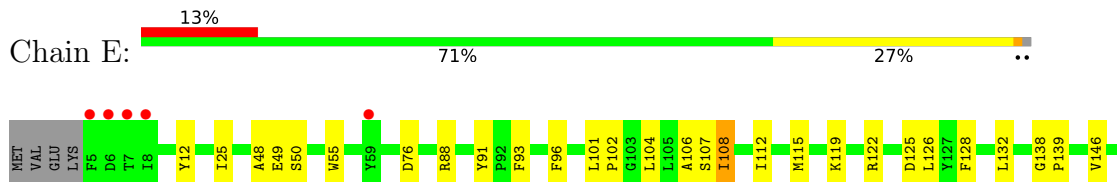
● Molecule 1: Ribulose biphosphate carboxylase

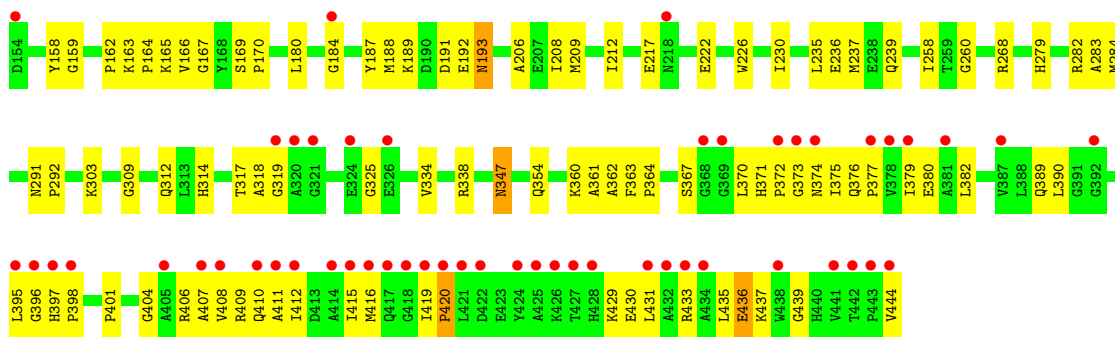


● Molecule 1: Ribulose biphosphate carboxylase

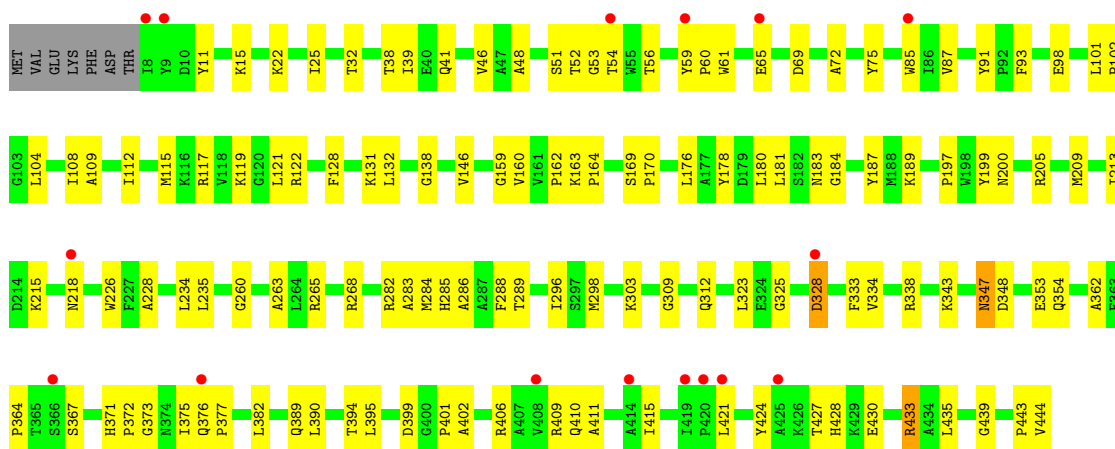


● Molecule 1: Ribulose biphosphate carboxylase

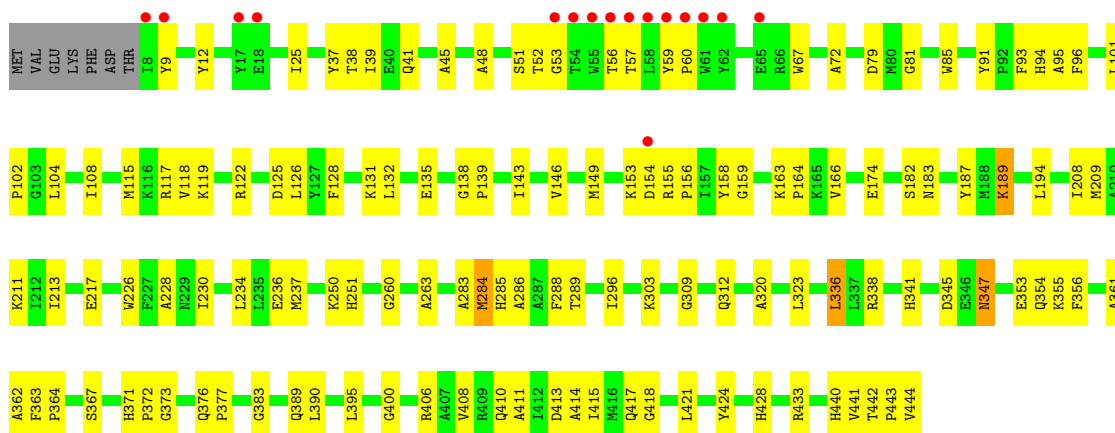




• Molecule 1: Ribulose biphosphate carboxylase

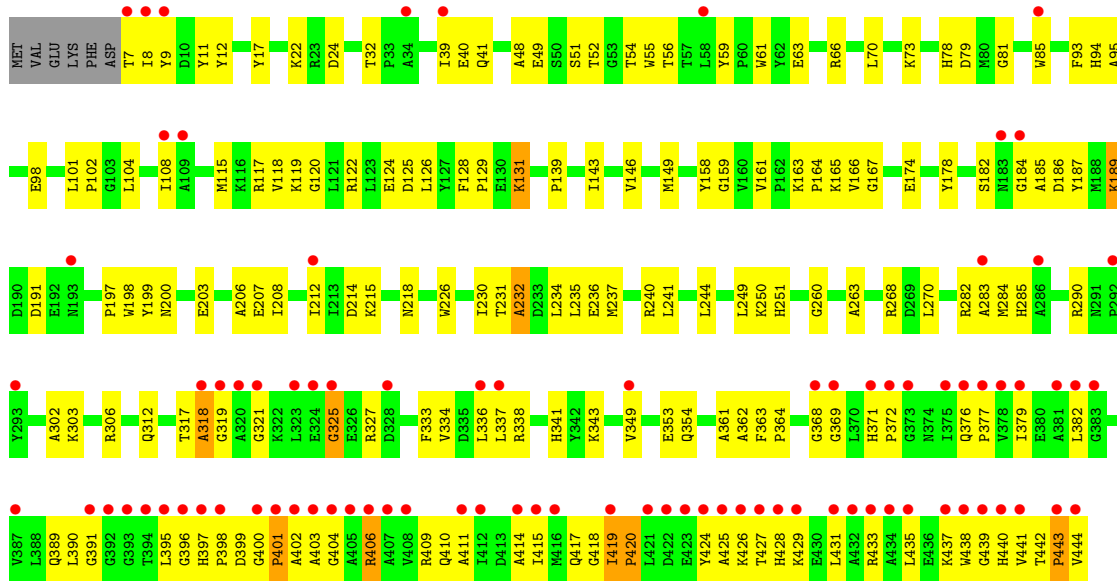


• Molecule 1: Ribulose biphosphate carboxylase

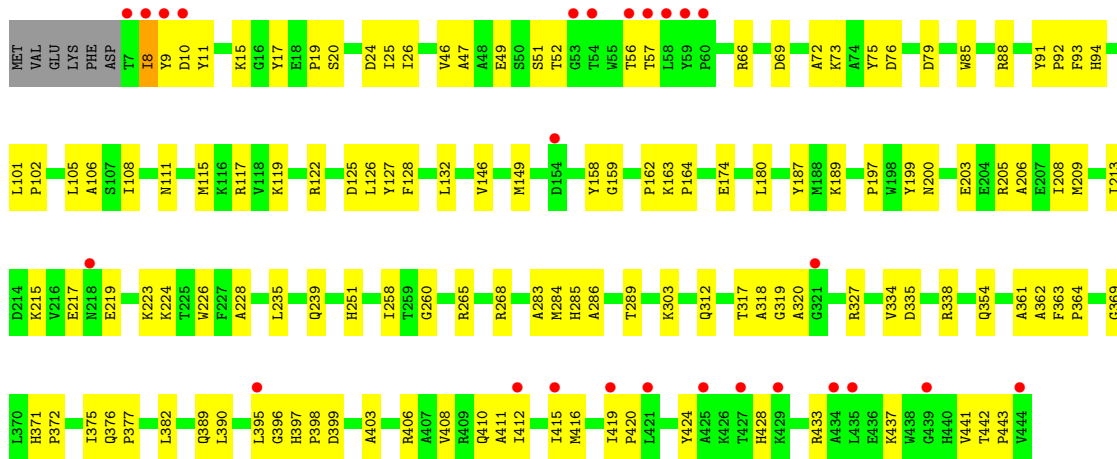


• Molecule 1: Ribulose biphosphate carboxylase

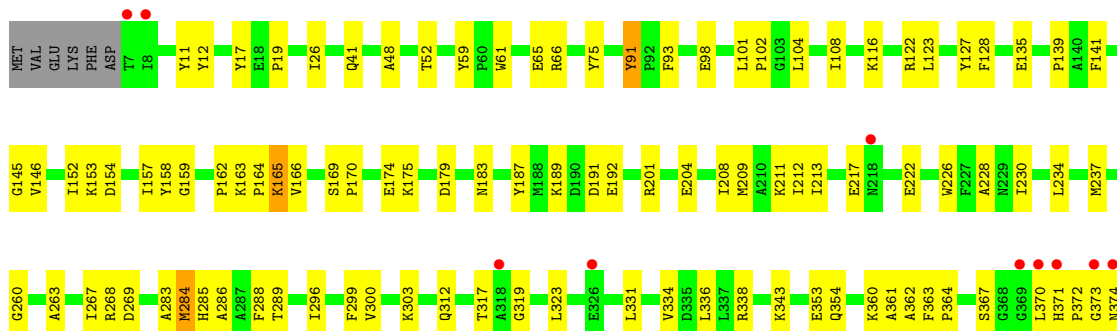


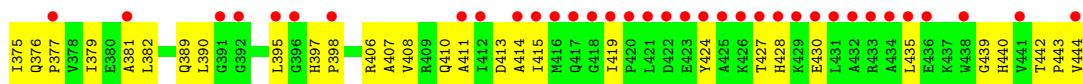


• Molecule 1: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.48Å 246.57Å 134.83Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	38.46 – 2.36 38.46 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.46-2.36) 99.3 (38.46-2.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.219 , 0.264 0.213 , 0.252	Depositor DCC
$R_{free}$ test set	12530 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	36065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: KCX, CAP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/3415	0.66	0/4642
1	B	0.29	0/3467	0.66	0/4712
1	C	0.30	0/3496	0.66	0/4750
1	D	0.30	0/3494	0.67	0/4739
1	E	0.29	0/3494	0.67	0/4744
1	F	0.29	0/3491	0.67	0/4738
1	G	0.29	0/3499	0.68	2/4747 (0.0%)
1	H	0.28	0/3458	0.67	0/4700
1	I	0.29	0/3485	0.66	0/4730
1	J	0.29	0/3491	0.67	0/4738
All	All	0.29	0/34790	0.67	2/47240 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	400	GLY	CA-C-N	5.31	124.77	119.24
1	G	400	GLY	C-N-CA	5.31	124.77	119.24

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	3341	0	3185	232	0
1	B	3391	0	3252	163	0
1	C	3420	0	3289	127	0
1	D	3419	0	3317	106	0
1	E	3418	0	3303	125	0
1	F	3415	0	3313	134	0
1	G	3423	0	3328	136	0
1	H	3382	0	3257	216	0
1	I	3410	0	3301	118	0
1	J	3415	0	3310	148	0
2	A	21	0	8	0	0
2	B	21	0	7	1	0
2	C	21	0	9	1	0
2	D	21	0	8	0	0
2	E	21	0	8	2	0
2	F	21	0	8	0	0
2	G	21	0	8	1	0
2	H	21	0	8	0	0
2	I	21	0	8	0	0
2	J	21	0	7	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	97	0	0	12	0
4	B	175	0	0	11	0
4	C	226	0	0	7	0
4	D	239	0	0	5	0
4	E	197	0	0	9	0
4	F	179	0	0	9	0
4	G	174	0	0	9	0
4	H	123	0	0	6	0
4	I	192	0	0	8	0
4	J	209	0	0	15	0
All	All	36065	0	32934	1432	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 21.

The worst 5 of 1432 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:H:397:HIS:ND1	1:H:398:PRO:HD2	1.29	1.44
1:H:397:HIS:CG	1:H:398:PRO:HD2	1.61	1.32
1:H:397:HIS:ND1	1:H:398:PRO:CD	2.06	1.18
1:I:72:ALA:O	1:I:73:LYS:HD2	1.43	1.17
1:A:149:MET:HE3	1:A:250:LYS:HD2	1.25	1.17

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	433/444 (98%)	386 (89%)	40 (9%)	7 (2%)	<b>7</b> <b>6</b>
1	B	435/444 (98%)	408 (94%)	25 (6%)	2 (0%)	24 27
1	C	437/444 (98%)	420 (96%)	16 (4%)	1 (0%)	43 52
1	D	434/444 (98%)	415 (96%)	18 (4%)	1 (0%)	43 52
1	E	437/444 (98%)	410 (94%)	25 (6%)	2 (0%)	24 27
1	F	434/444 (98%)	414 (95%)	19 (4%)	1 (0%)	43 52
1	G	434/444 (98%)	415 (96%)	18 (4%)	1 (0%)	43 52
1	H	435/444 (98%)	389 (89%)	39 (9%)	7 (2%)	<b>7</b> <b>6</b>
1	I	435/444 (98%)	415 (95%)	18 (4%)	2 (0%)	24 27
1	J	435/444 (98%)	414 (95%)	20 (5%)	1 (0%)	43 52
All	All	4349/4440 (98%)	4086 (94%)	238 (6%)	25 (1%)	21 24

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	426	LYS

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	429	LYS
1	A	34	ALA
1	A	82	ASP
1	A	117	ARG

### 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	321/356 (90%)	317 (99%)	4 (1%)	63	77
1	B	331/356 (93%)	325 (98%)	6 (2%)	51	66
1	C	336/356 (94%)	328 (98%)	8 (2%)	43	57
1	D	339/356 (95%)	334 (98%)	5 (2%)	57	72
1	E	335/356 (94%)	329 (98%)	6 (2%)	51	66
1	F	338/356 (95%)	330 (98%)	8 (2%)	43	57
1	G	340/356 (96%)	336 (99%)	4 (1%)	63	77
1	H	329/356 (92%)	322 (98%)	7 (2%)	47	61
1	I	336/356 (94%)	333 (99%)	3 (1%)	70	82
1	J	337/356 (95%)	333 (99%)	4 (1%)	63	77
All	All	3342/3560 (94%)	3287 (98%)	55 (2%)	55	70

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	363	PHE
1	F	347	ASN
1	J	363	PHE
1	I	149	MET
1	F	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	347	ASN
1	G	440	HIS
1	J	239	GLN
1	F	354	GLN
1	G	347	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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KCX	B	189	1,3	10,11,12	0.91	0	6,12,14	1.48	1 (16%)
1	KCX	E	189	1,3	10,11,12	0.91	0	6,12,14	1.45	1 (16%)
1	KCX	C	189	1,3	10,11,12	0.91	0	6,12,14	1.24	1 (16%)
1	KCX	J	189	1,3	10,11,12	0.89	0	6,12,14	1.48	1 (16%)
1	KCX	A	189	1,3	10,11,12	0.91	0	6,12,14	1.51	1 (16%)
1	KCX	I	189	1,3	10,11,12	0.93	0	6,12,14	1.26	1 (16%)
1	KCX	D	189	1,3	10,11,12	0.89	0	6,12,14	1.40	1 (16%)
1	KCX	F	189	1,3	10,11,12	0.86	0	6,12,14	1.52	1 (16%)
1	KCX	G	189	1,3	10,11,12	0.91	0	6,12,14	1.33	1 (16%)
1	KCX	H	189	1,3	10,11,12	0.91	0	6,12,14	1.37	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	189	1,3	-	0/9/10/12	-
1	KCX	E	189	1,3	-	0/9/10/12	-
1	KCX	C	189	1,3	-	1/9/10/12	-
1	KCX	J	189	1,3	-	1/9/10/12	-
1	KCX	A	189	1,3	-	0/9/10/12	-
1	KCX	I	189	1,3	-	0/9/10/12	-
1	KCX	D	189	1,3	-	0/9/10/12	-
1	KCX	F	189	1,3	-	0/9/10/12	-
1	KCX	G	189	1,3	-	0/9/10/12	-
1	KCX	H	189	1,3	-	0/9/10/12	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	189	KCX	OQ1-CX-NZ	-3.40	119.75	124.92
1	J	189	KCX	OQ1-CX-NZ	-3.36	119.81	124.92
1	A	189	KCX	OQ1-CX-NZ	-3.35	119.83	124.92
1	B	189	KCX	OQ1-CX-NZ	-3.31	119.89	124.92
1	E	189	KCX	OQ1-CX-NZ	-3.28	119.94	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	189	KCX	C-CA-CB-CG
1	J	189	KCX	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	189	KCX	1	0
1	H	189	KCX	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CAP	F	600	3	18,20,20	0.90	0	23,31,31	1.01	1 (4%)
2	CAP	B	600	3	18,20,20	0.89	0	23,31,31	1.06	1 (4%)
2	CAP	C	600	3	18,20,20	0.90	0	23,31,31	1.02	1 (4%)
2	CAP	A	600	3	18,20,20	0.92	0	23,31,31	1.04	1 (4%)
2	CAP	G	600	3	18,20,20	0.89	0	23,31,31	1.05	1 (4%)
2	CAP	J	600	3	18,20,20	0.92	0	23,31,31	1.07	1 (4%)
2	CAP	E	600	3	18,20,20	0.93	0	23,31,31	1.08	1 (4%)
2	CAP	H	600	3	18,20,20	0.89	0	23,31,31	1.05	1 (4%)
2	CAP	D	600	3	18,20,20	0.90	0	23,31,31	1.07	1 (4%)
2	CAP	I	600	3	18,20,20	0.88	0	23,31,31	1.01	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	F	600	3	-	6/29/29/29	-
2	CAP	B	600	3	-	7/29/29/29	-
2	CAP	C	600	3	-	7/29/29/29	-
2	CAP	A	600	3	-	6/29/29/29	-
2	CAP	G	600	3	-	6/29/29/29	-
2	CAP	J	600	3	-	8/29/29/29	-
2	CAP	E	600	3	-	6/29/29/29	-
2	CAP	H	600	3	-	8/29/29/29	-
2	CAP	D	600	3	-	6/29/29/29	-
2	CAP	I	600	3	-	6/29/29/29	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	CAP	O7-C-C2	3.65	120.17	114.06
2	G	600	CAP	O7-C-C2	3.63	120.14	114.06
2	H	600	CAP	O7-C-C2	3.63	120.13	114.06
2	E	600	CAP	O7-C-C2	3.63	120.13	114.06
2	B	600	CAP	O7-C-C2	3.58	120.06	114.06

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

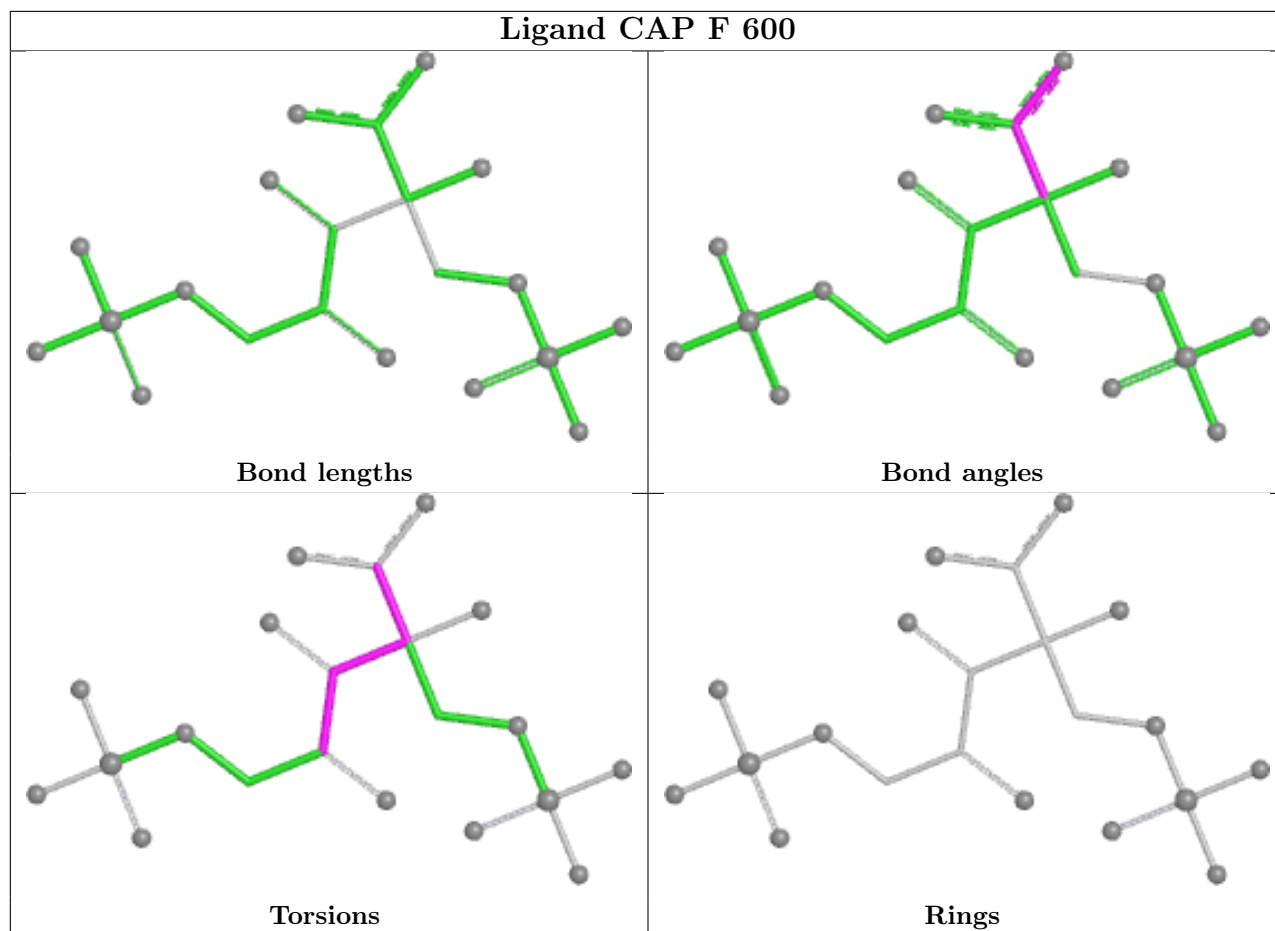
Mol	Chain	Res	Type	Atoms
2	A	600	CAP	O6-C-C2-C1
2	A	600	CAP	O7-C-C2-C1
2	A	600	CAP	O6-C-C2-O2
2	A	600	CAP	O7-C-C2-O2
2	A	600	CAP	O3-C3-C4-O4

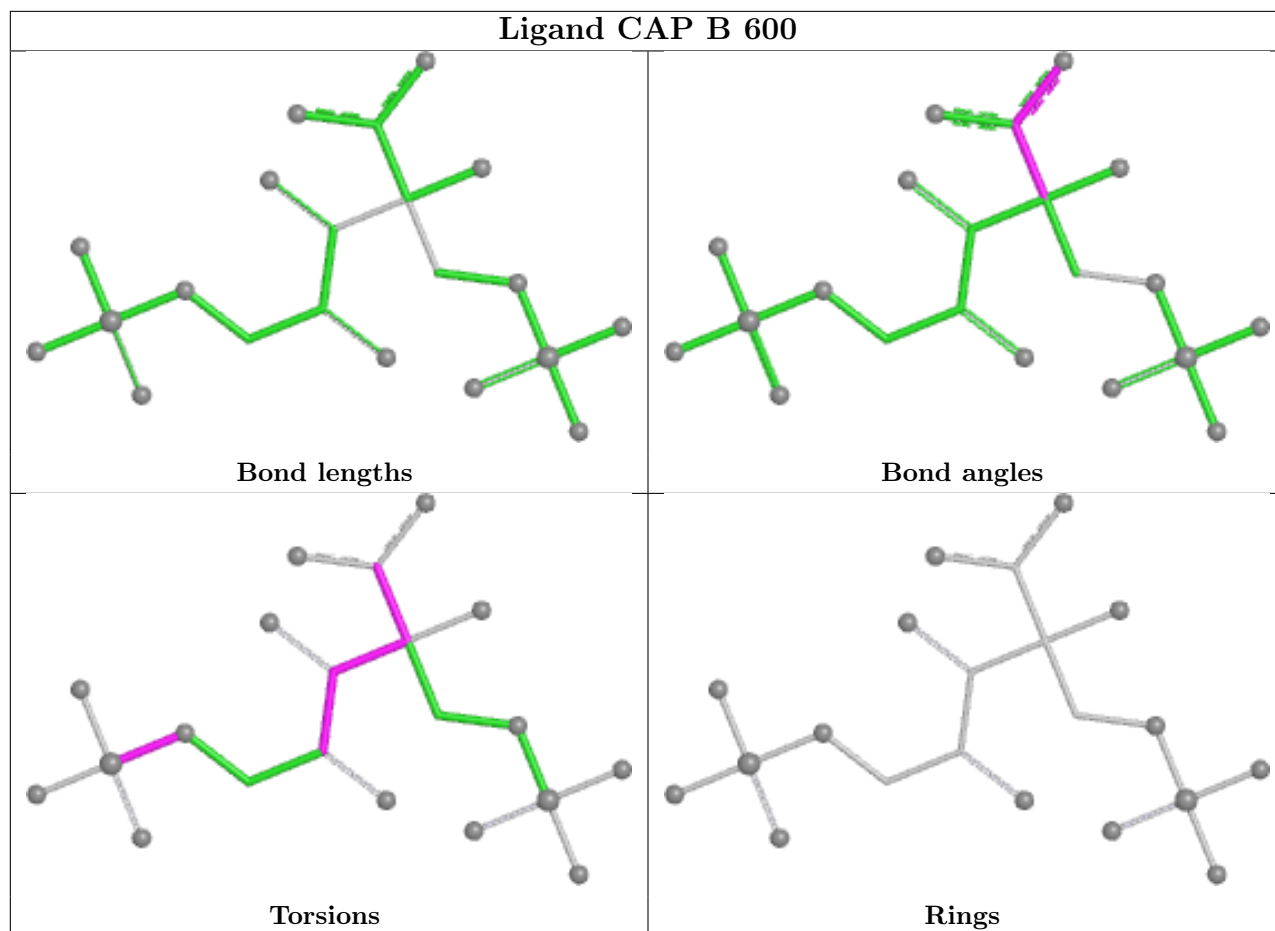
There are no ring outliers.

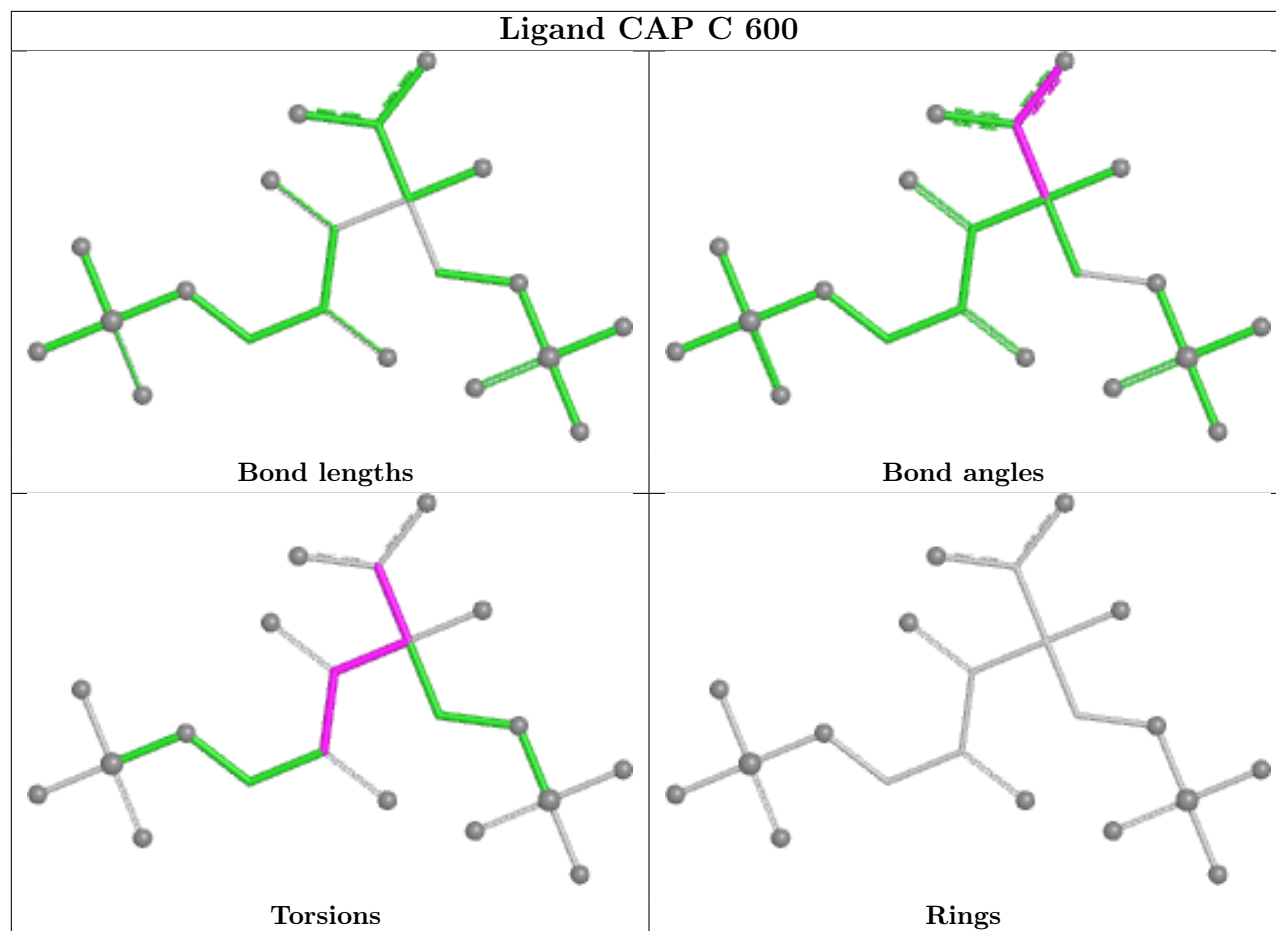
4 monomers are involved in 5 short contacts:

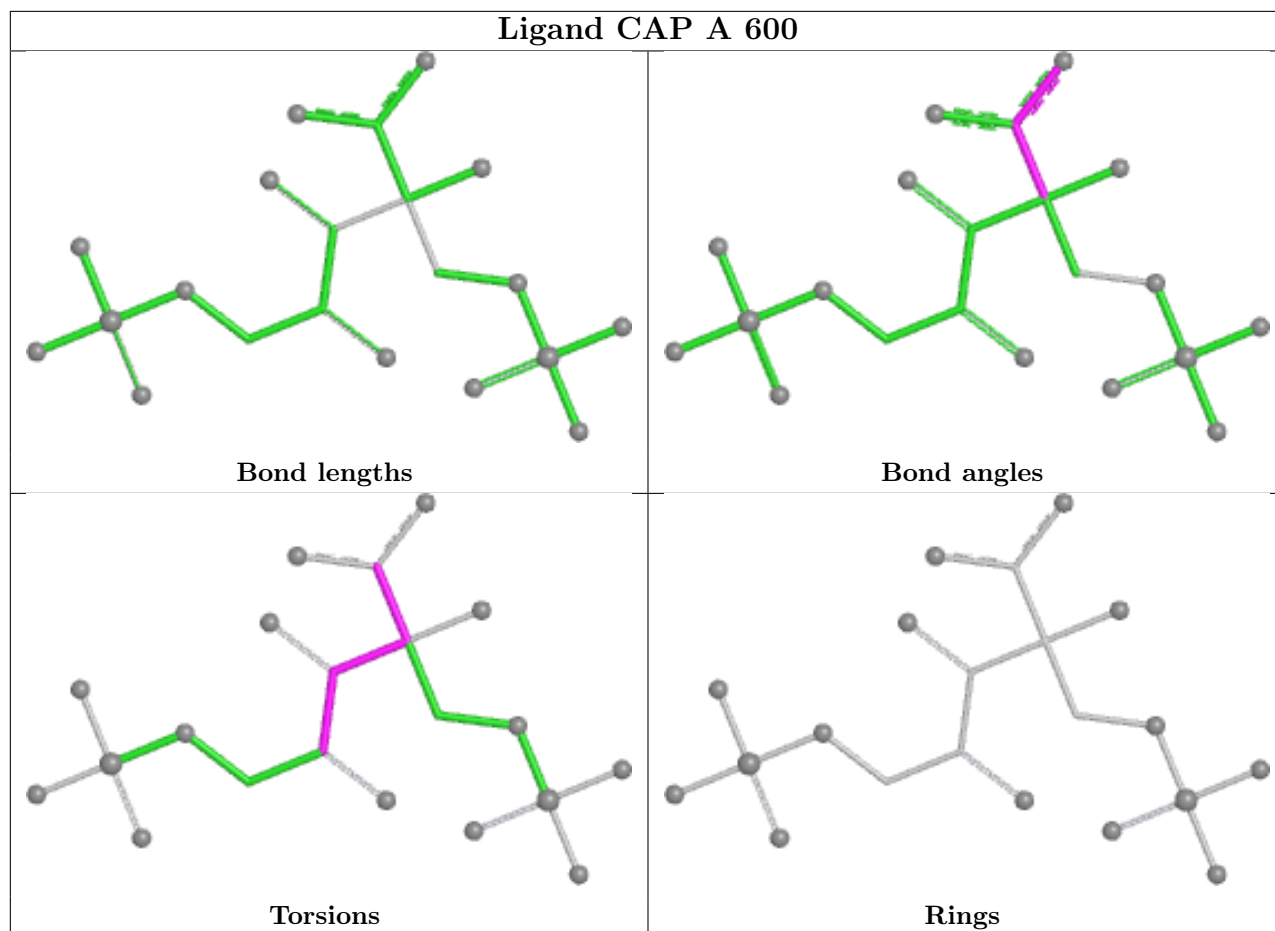
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	CAP	1	0
2	C	600	CAP	1	0
2	G	600	CAP	1	0
2	E	600	CAP	2	0

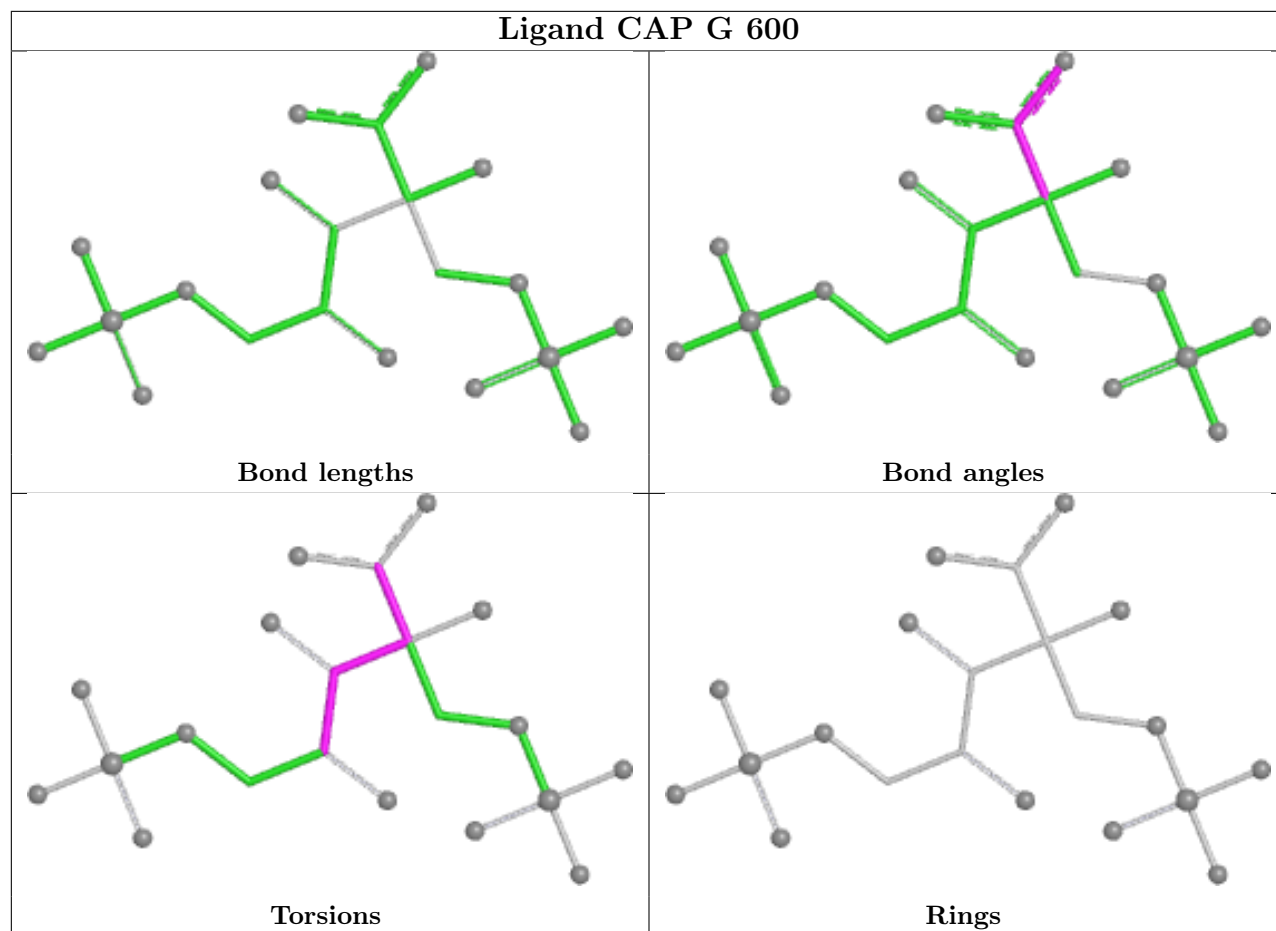
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

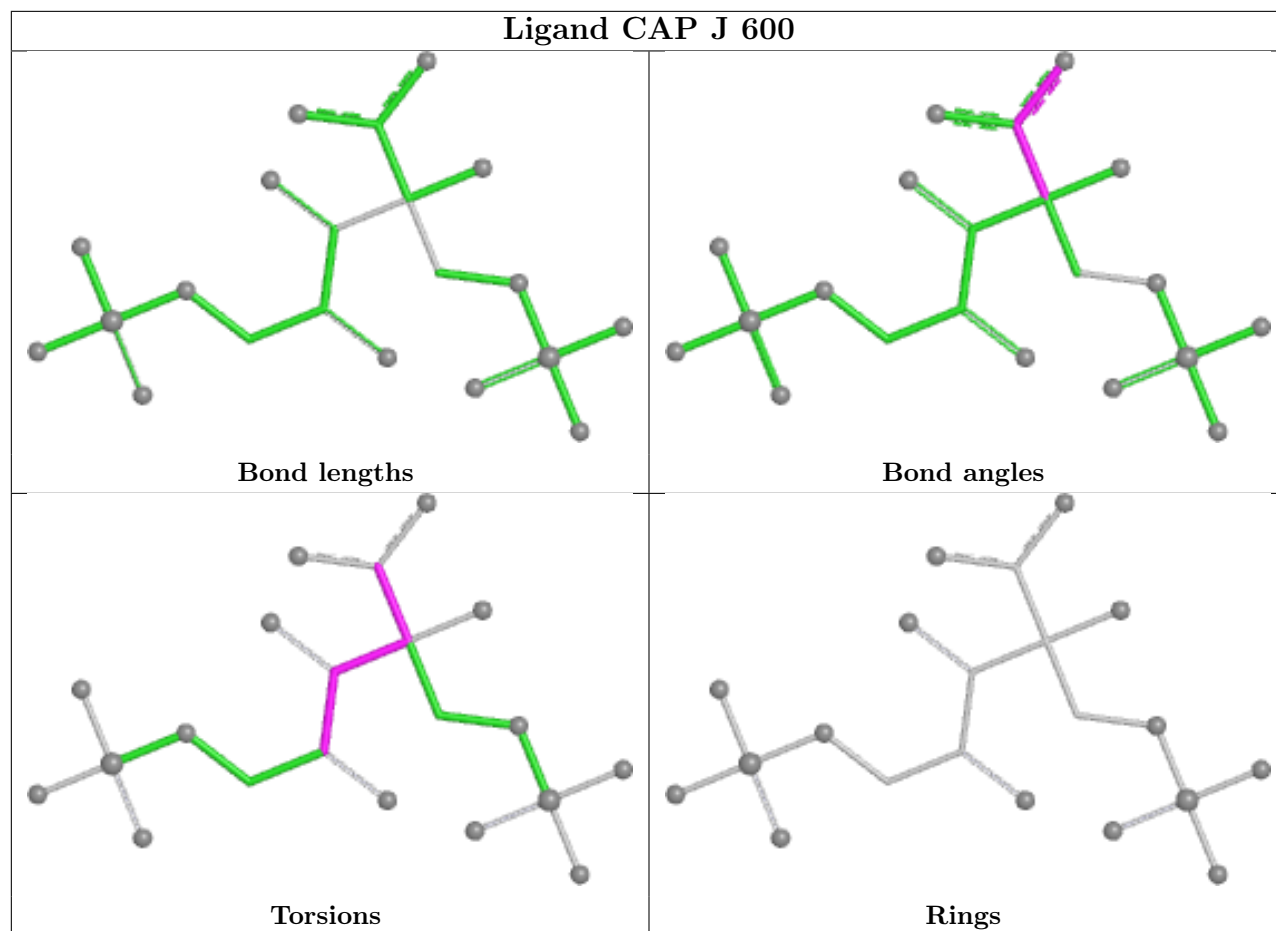


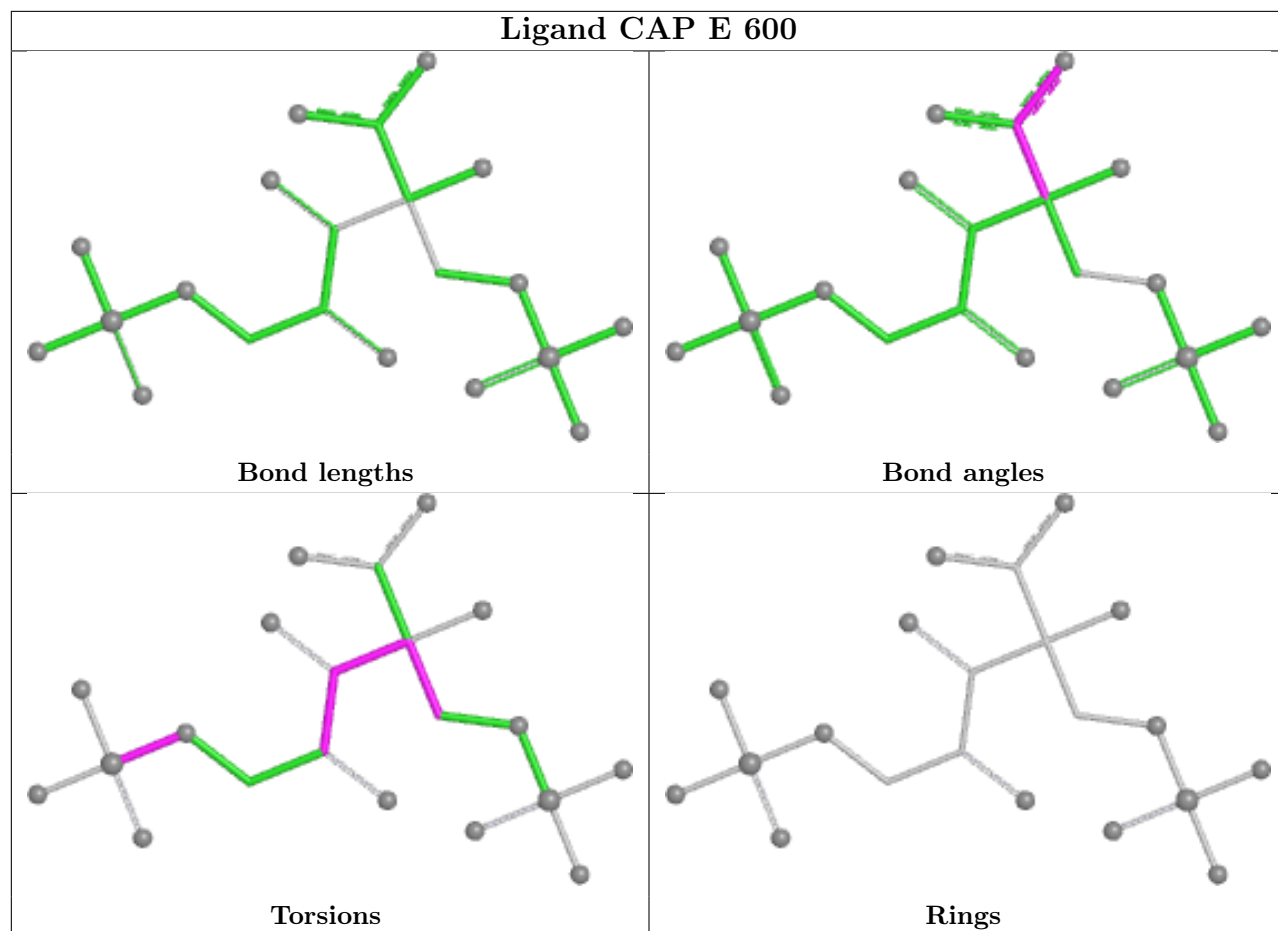


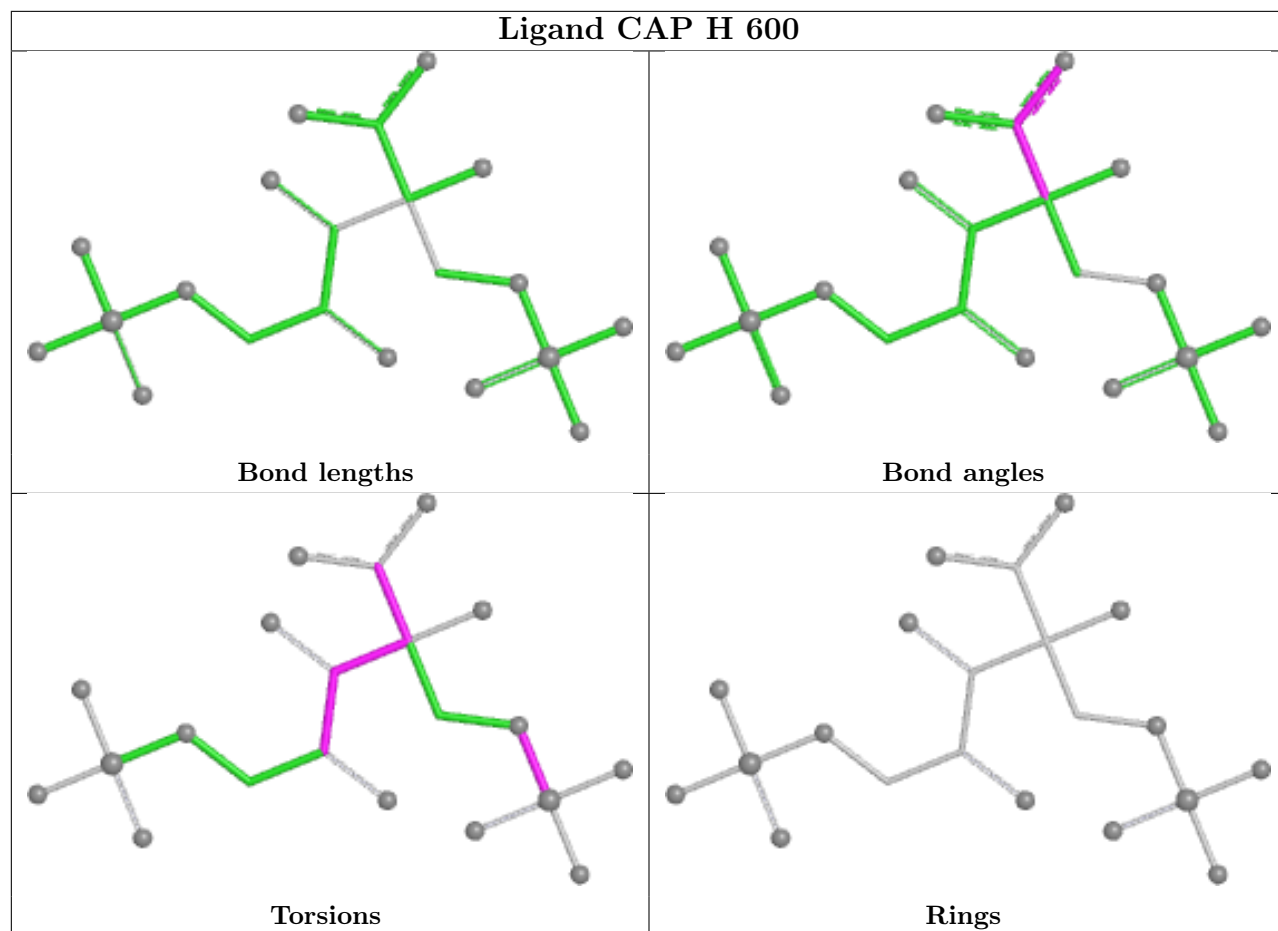


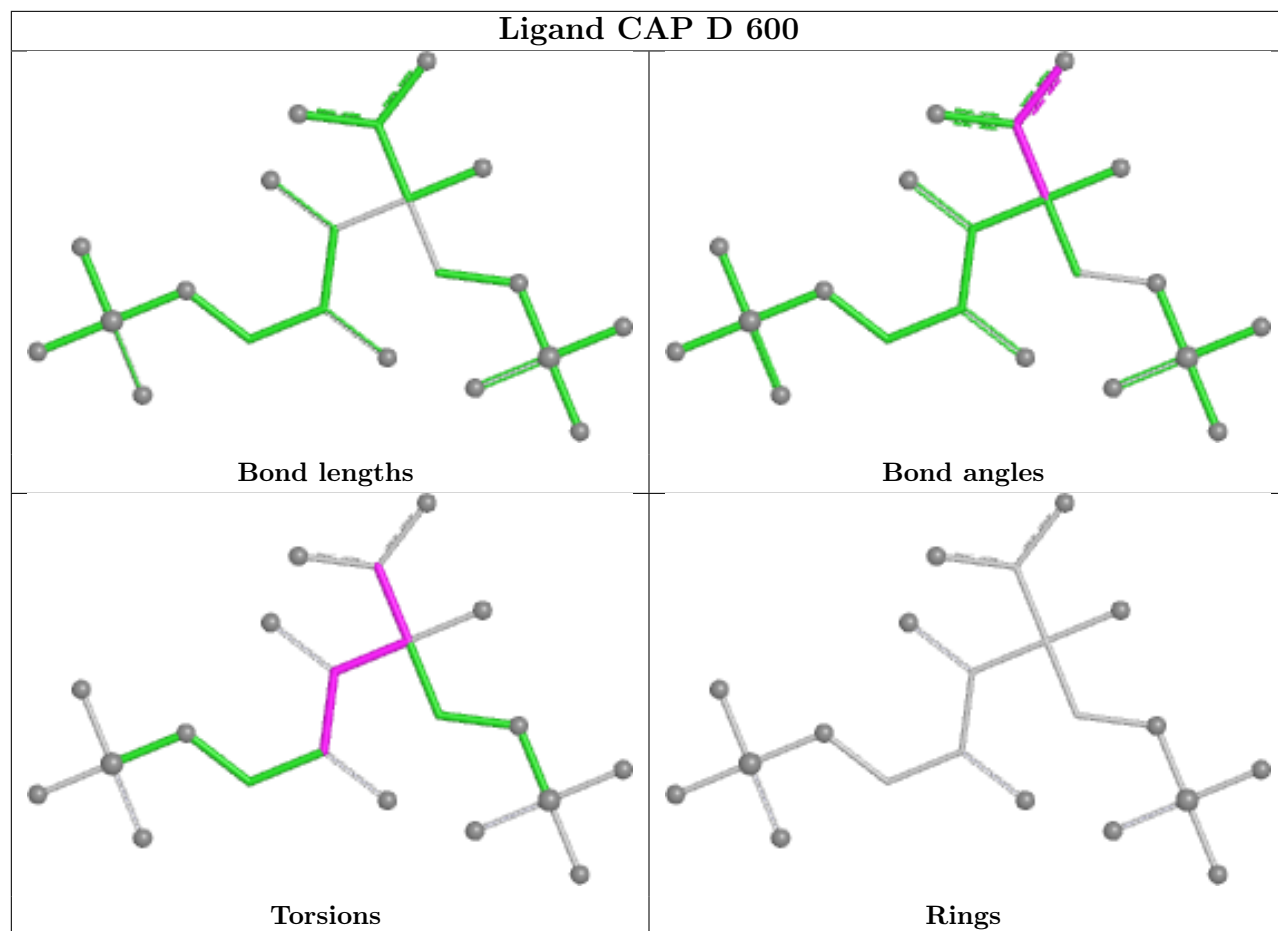


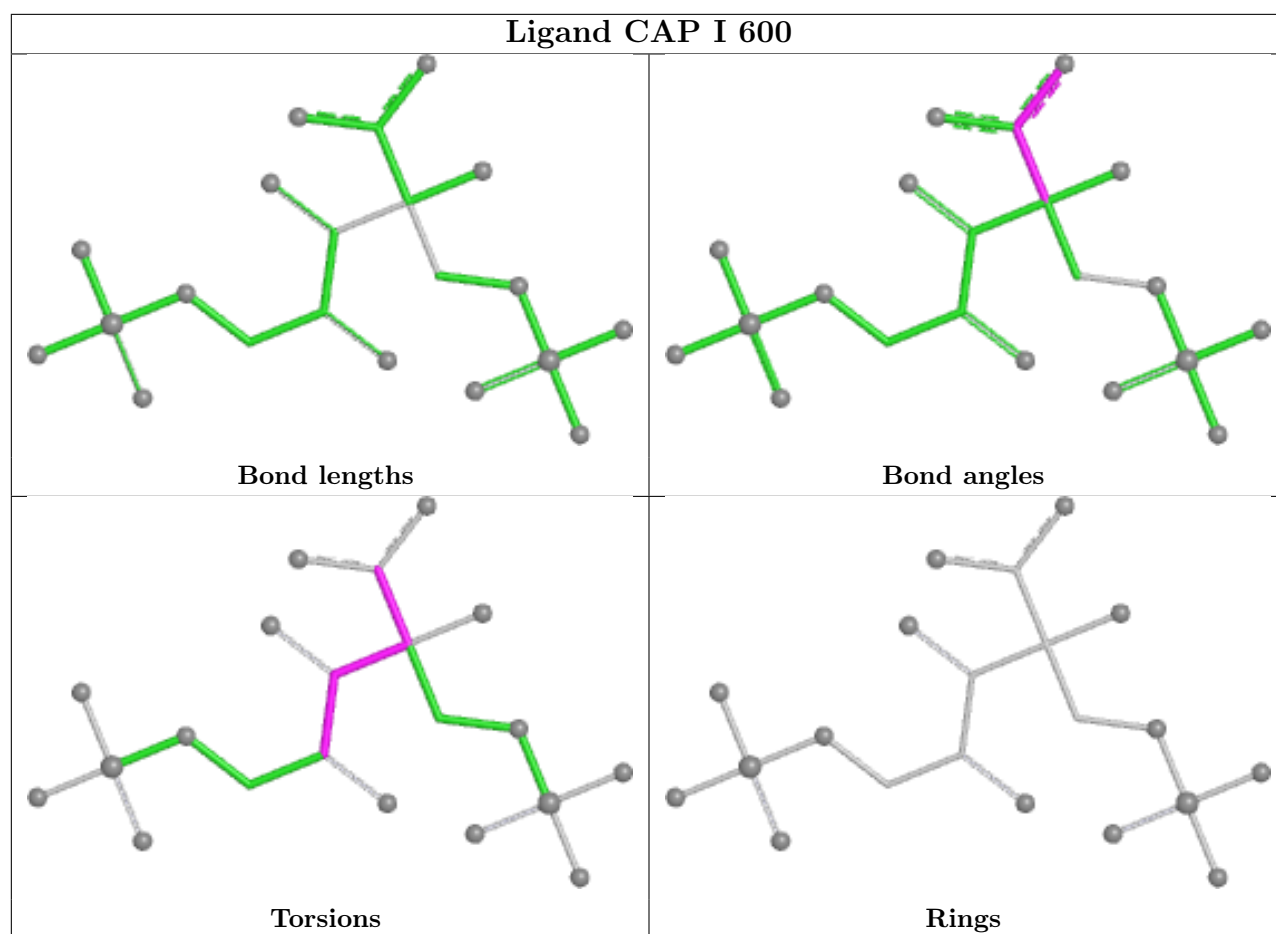












## 5.7 Other polymers [i](#)

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	435/444 (97%)	1.39	108 (24%) 2 1	28, 41, 56, 60	0
1	B	437/444 (98%)	0.71	56 (12%) 7 9	19, 32, 62, 65	0
1	C	439/444 (98%)	0.36	18 (4%) 41 47	17, 27, 49, 52	0
1	D	436/444 (98%)	0.17	13 (2%) 52 59	16, 24, 35, 42	0
1	E	439/444 (98%)	0.61	57 (12%) 7 8	18, 28, 58, 60	0
1	F	436/444 (98%)	0.43	16 (3%) 45 51	18, 29, 45, 51	0
1	G	436/444 (98%)	0.44	16 (3%) 45 51	18, 31, 44, 48	0
1	H	437/444 (98%)	1.17	86 (19%) 3 3	27, 37, 66, 66	0
1	I	437/444 (98%)	0.40	26 (5%) 28 32	17, 28, 47, 53	0
1	J	437/444 (98%)	0.53	45 (10%) 12 13	16, 25, 59, 60	0
All	All	4369/4440 (98%)	0.62	441 (10%) 12 14	16, 30, 52, 66	0

The worst 5 of 441 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	421	LEU	7.3
1	A	59	TYR	6.5
1	J	434	ALA	5.9
1	D	54	THR	5.9
1	E	415	ILE	5.4

### 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
1	KCX	H	189	12/13	0.94	0.09	35,36,37,37	0
1	KCX	B	189	12/13	0.95	0.08	30,31,32,33	0
1	KCX	C	189	12/13	0.96	0.07	24,24,24,24	0
1	KCX	E	189	12/13	0.96	0.07	22,23,24,24	0
1	KCX	A	189	12/13	0.96	0.07	33,33,33,34	0
1	KCX	I	189	12/13	0.96	0.07	24,25,26,26	0
1	KCX	J	189	12/13	0.96	0.07	22,23,23,24	0
1	KCX	G	189	12/13	0.97	0.07	21,21,22,23	0
1	KCX	F	189	12/13	0.97	0.06	22,22,22,22	0
1	KCX	D	189	12/13	0.98	0.06	16,18,19,19	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, 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.

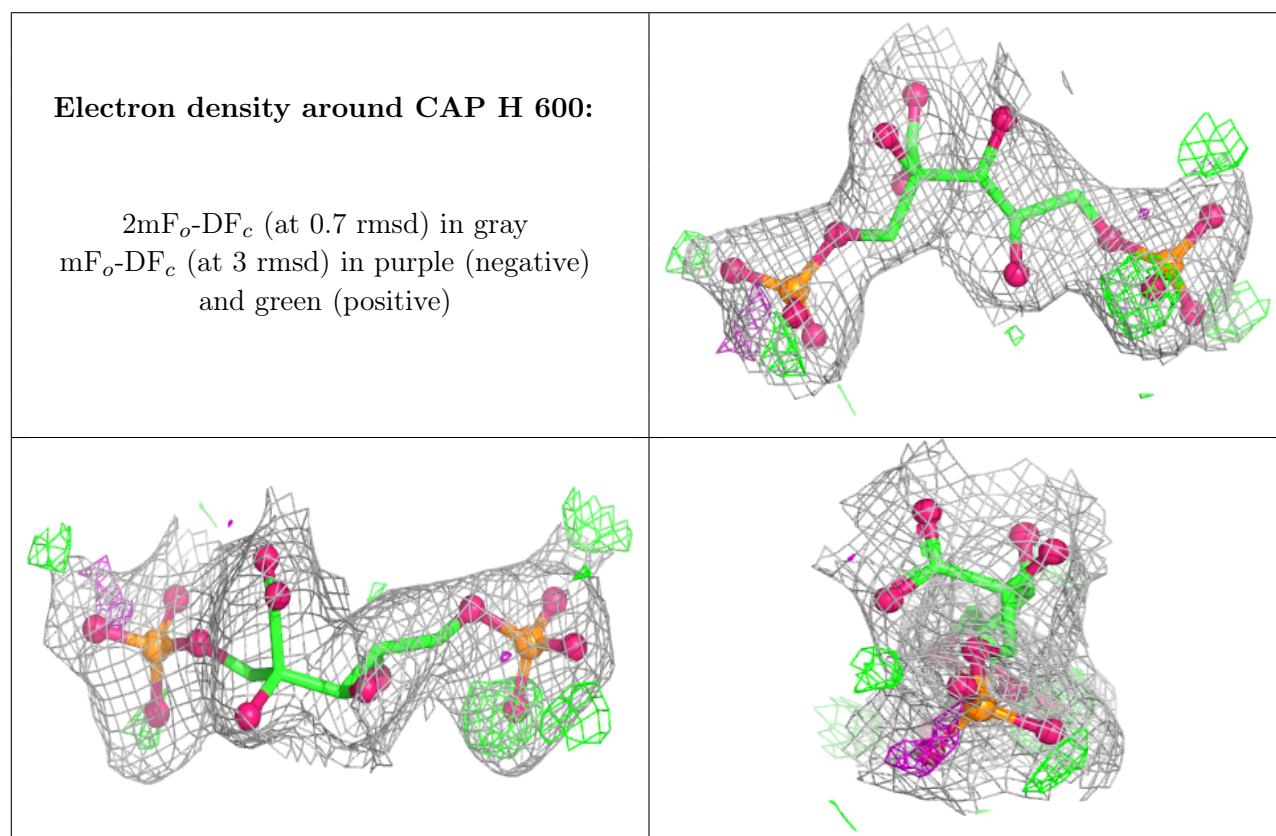
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CAP	H	600	21/21	0.86	0.13	41,42,42,43	0
2	CAP	E	600	21/21	0.89	0.14	31,37,40,41	0
2	CAP	A	600	21/21	0.92	0.11	36,38,38,39	0
3	MG	H	500	1/1	0.92	0.07	37,37,37,37	0
2	CAP	J	600	21/21	0.93	0.11	31,35,38,38	0
3	MG	C	500	1/1	0.94	0.06	28,28,28,28	0
2	CAP	C	600	21/21	0.95	0.09	30,31,32,32	0
2	CAP	B	600	21/21	0.96	0.08	31,35,36,37	0
2	CAP	G	600	21/21	0.97	0.07	22,25,26,26	0
2	CAP	F	600	21/21	0.97	0.07	22,24,24,25	0
2	CAP	I	600	21/21	0.97	0.06	18,21,21,22	0
2	CAP	D	600	21/21	0.98	0.06	16,20,21,21	0
3	MG	B	500	1/1	0.98	0.03	31,31,31,31	0
3	MG	D	500	1/1	0.99	0.03	15,15,15,15	0
3	MG	E	500	1/1	0.99	0.09	26,26,26,26	0
3	MG	G	500	1/1	0.99	0.03	20,20,20,20	0
3	MG	A	500	1/1	0.99	0.03	28,28,28,28	0
3	MG	I	500	1/1	0.99	0.04	20,20,20,20	0
3	MG	J	500	1/1	0.99	0.02	19,19,19,19	0

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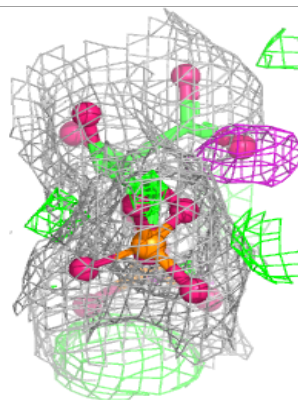
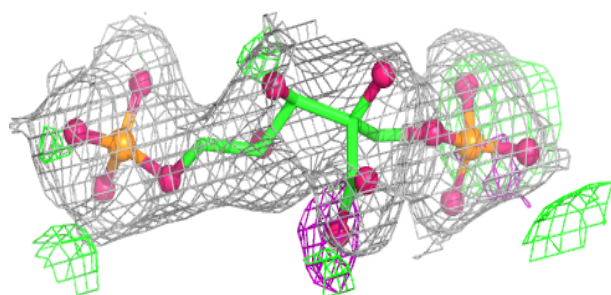
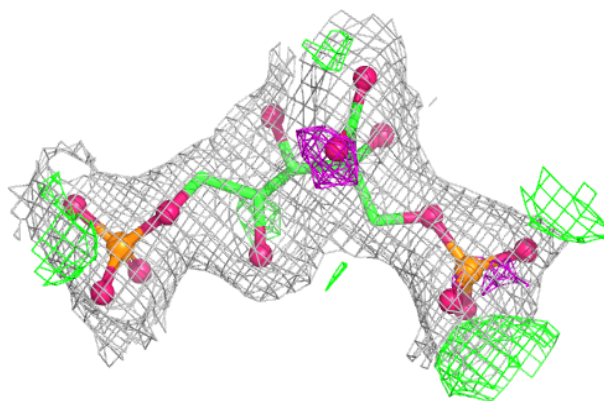
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	F	500	1/1	1.00	0.01	25,25,25,25	0

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.

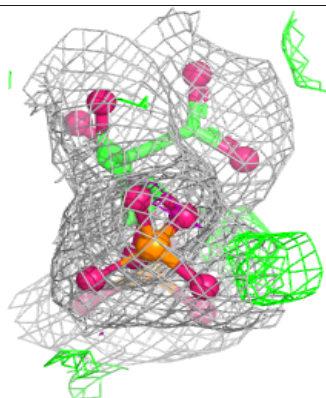
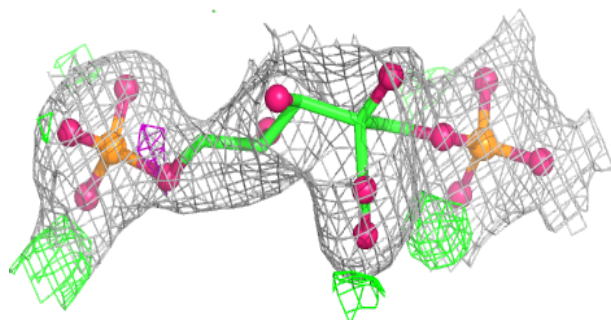
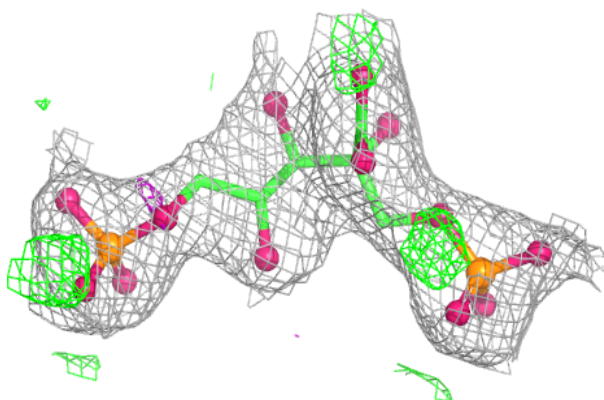


**Electron density around CAP E 600:**

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

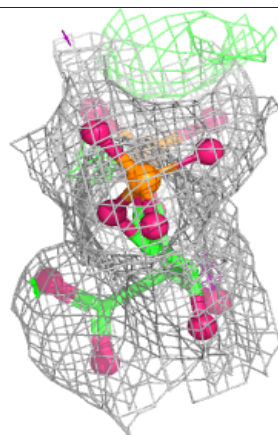
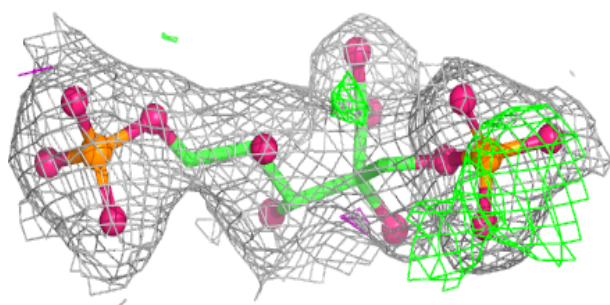
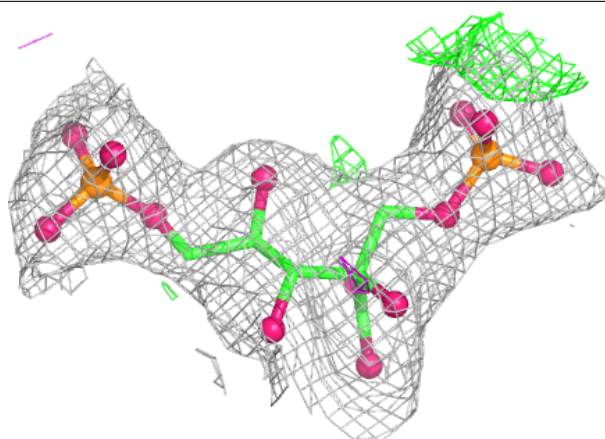
**Electron density around CAP A 600:**

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

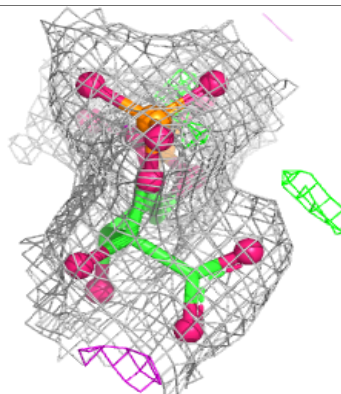
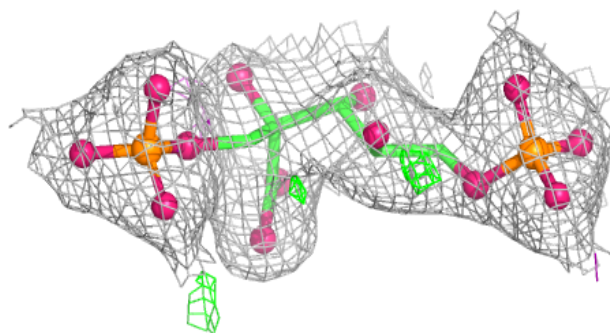
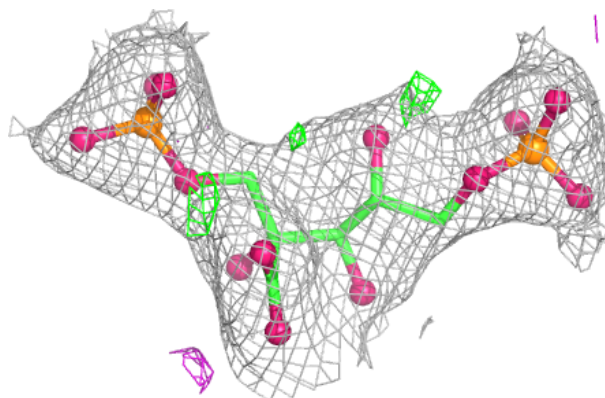


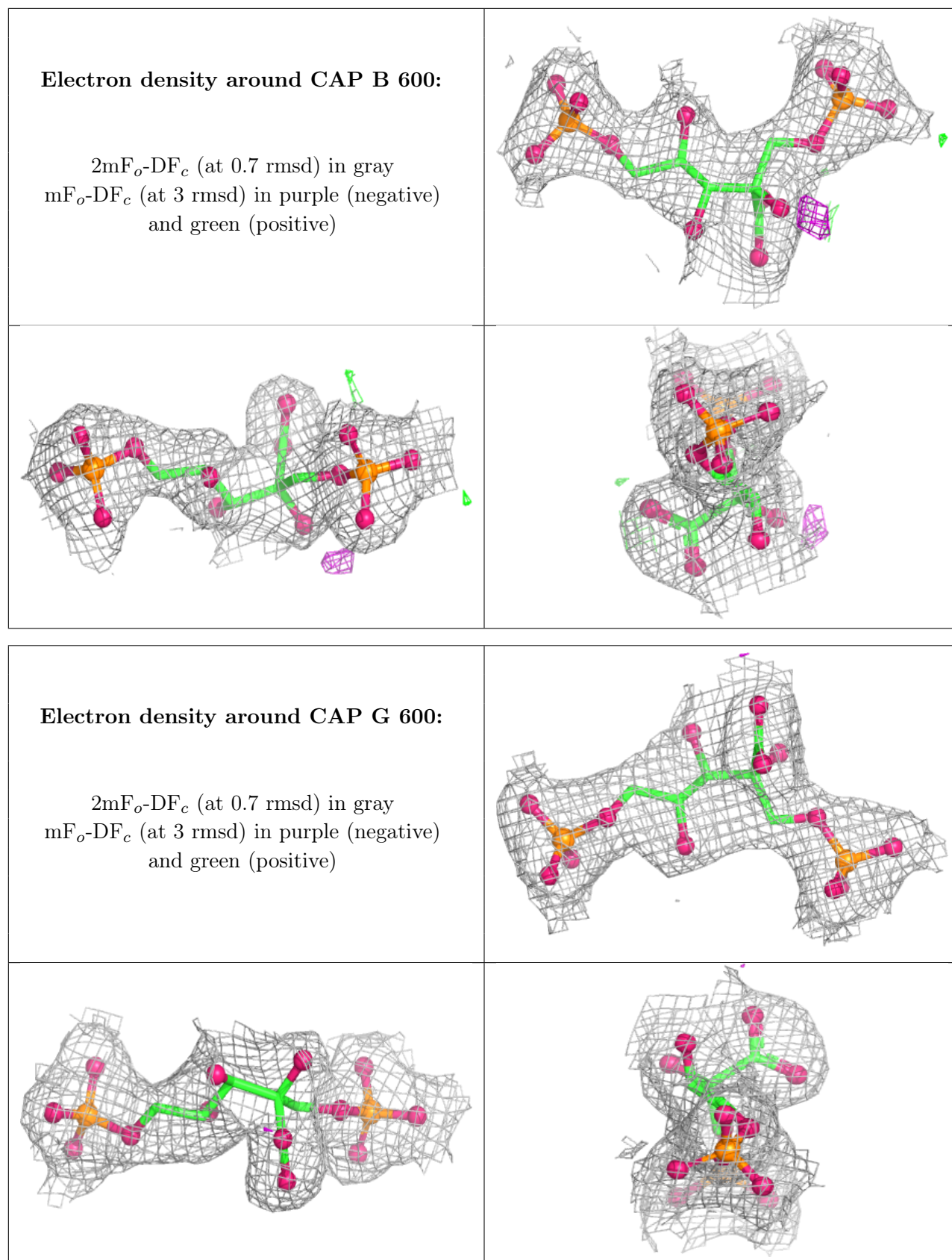
**Electron density around CAP J 600:**

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

**Electron density around CAP C 600:**

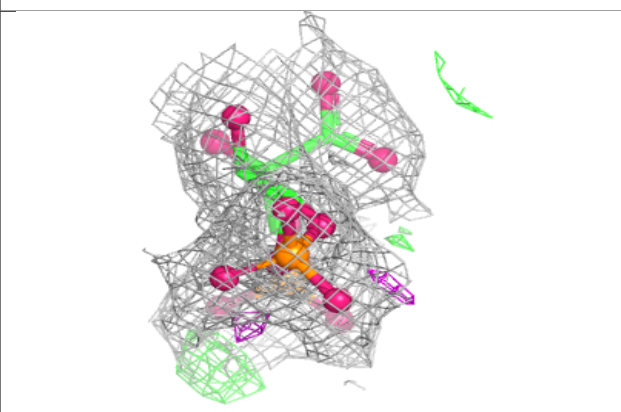
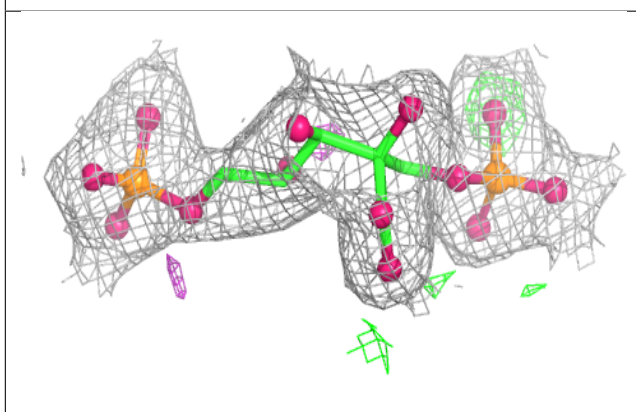
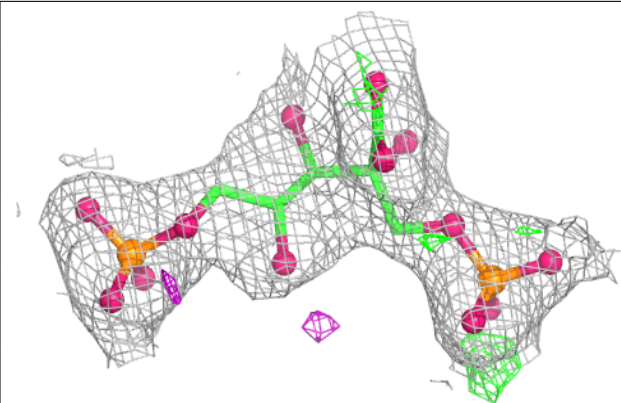
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



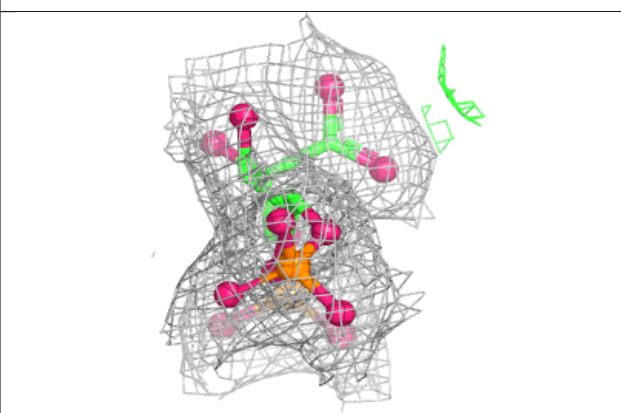
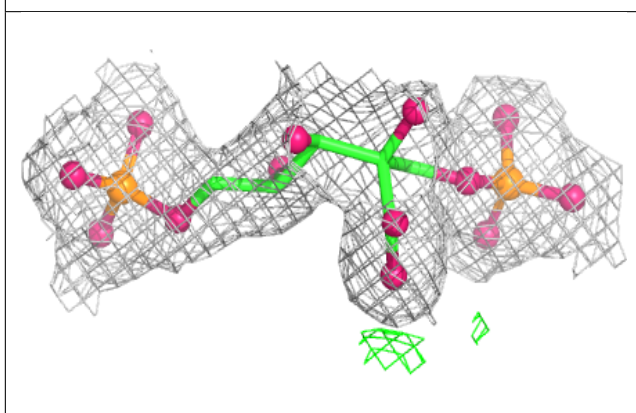
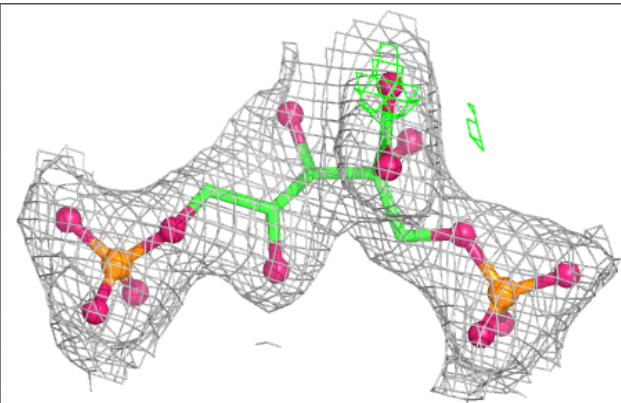


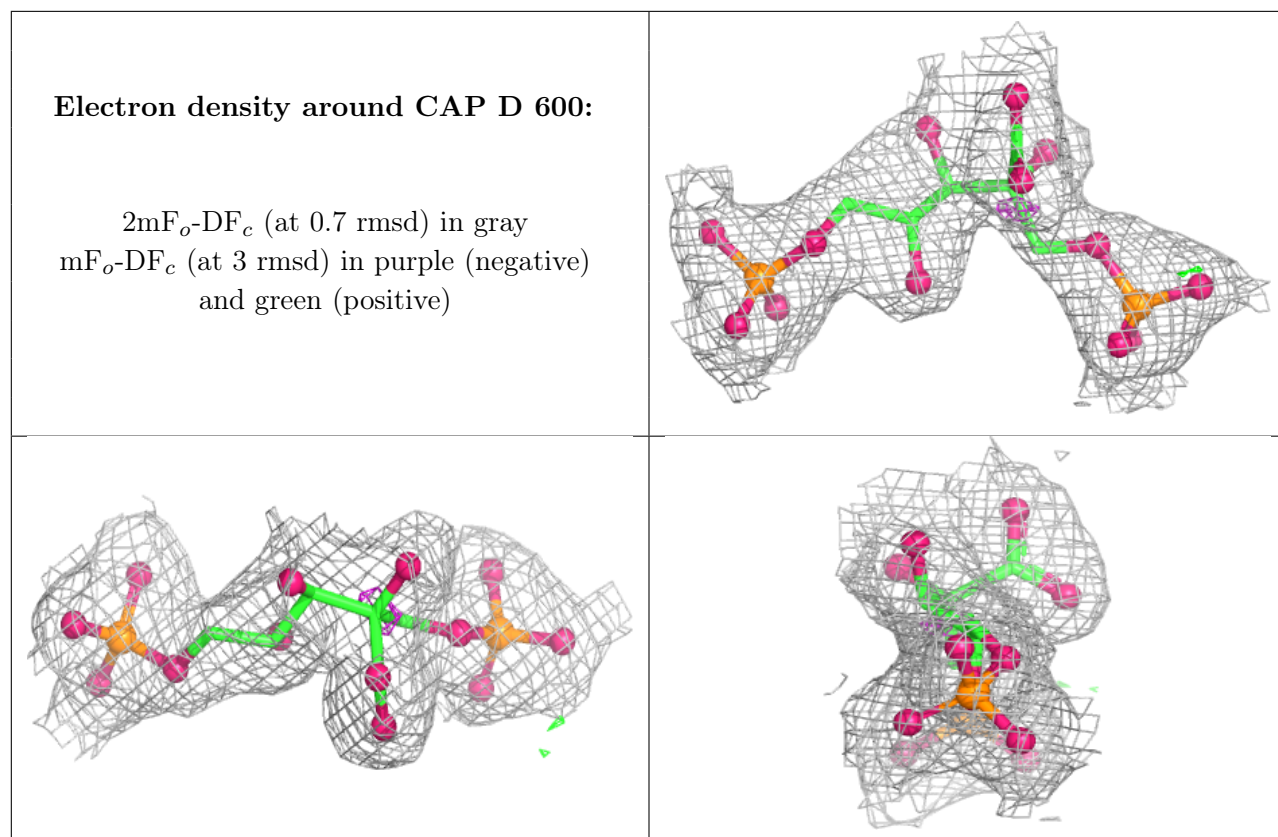
**Electron density around CAP F 600:**

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

**Electron density around CAP I 600:**

$2mF_o-DF_c$  (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.