



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 08:42 AM BST

PDB ID : 1UZH  
Title : A CHIMERIC CHLAMYDOMONAS, SYNECHOCOCCUS RUBISCO ENZYME  
Authors : Karkehabadi, S.; Spreitzer, R.J.; Andersson, I.  
Deposited on : 2004-03-12  
Resolution : 2.20 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

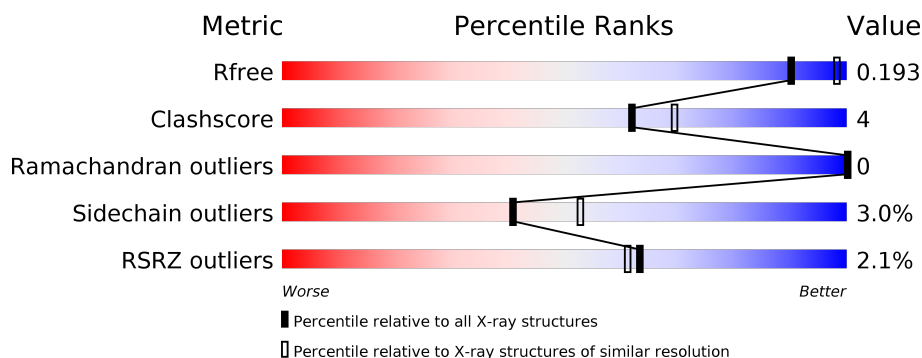
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	<div> <div style="width: 88%;"></div> <div style="width: 9%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> <div>88% 9% ..</div>
1	B	475	<div> <div style="width: 89%;"></div> <div style="width: 9%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>89% 9% ..</div>
1	E	475	<div> <div style="width: 89%;"></div> <div style="width: 9%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>89% 9% .</div>
1	H	475	<div> <div style="width: 88%;"></div> <div style="width: 10%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>88% 10% ..</div>
1	K	475	<div> <div style="width: 89%;"></div> <div style="width: 8%;"></div> <div style="width: 3%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>89% 8% ..</div>
1	O	475	<div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>91% 8% ..</div>

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Mol	Chain	Length	Quality of chain
1	R	475	<div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	V	475	<div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div>
2	C	122	<div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	F	122	<div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div>
2	I	122	<div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	J	122	<div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div>
2	M	122	<div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	P	122	<div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	T	122	<div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	W	122	<div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40557 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 BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	3	0
			3640	2300	641	675	24			
1	B	467	Total	C	N	O	S	0	3	0
			3647	2305	642	676	24			
1	E	469	Total	C	N	O	S	0	3	0
			3665	2315	646	680	24			
1	H	469	Total	C	N	O	S	0	3	0
			3665	2315	646	680	24			
1	K	469	Total	C	N	O	S	0	5	0
			3673	2321	646	682	24			
1	O	469	Total	C	N	O	S	0	2	0
			3661	2313	646	678	24			
1	R	469	Total	C	N	O	S	0	2	0
			3662	2314	646	678	24			
1	V	469	Total	C	N	O	S	0	3	0
			3664	2316	645	679	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	conflict	UNP P00877
B	46	PRO	LEU	conflict	UNP P00877
E	46	PRO	LEU	conflict	UNP P00877
H	46	PRO	LEU	conflict	UNP P00877
K	46	PRO	LEU	conflict	UNP P00877
O	46	PRO	LEU	conflict	UNP P00877
R	46	PRO	LEU	conflict	UNP P00877
V	46	PRO	LEU	conflict	UNP P00877

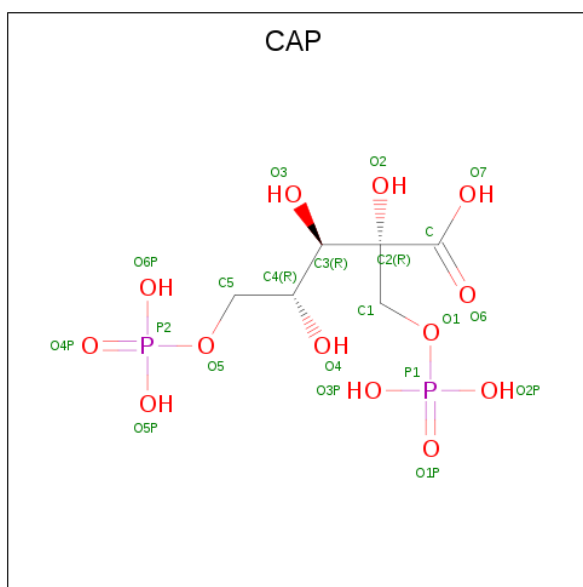
- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	122	Total	C	N	O	S	0	2	0
			1009	654	167	178	10			
2	F	122	Total	C	N	O	S	0	2	0
			1014	660	166	177	11			
2	I	122	Total	C	N	O	S	0	1	0
			1006	653	166	177	10			
2	J	122	Total	C	N	O	S	0	1	0
			1006	653	166	176	11			
2	M	122	Total	C	N	O	S	0	2	0
			1007	653	166	177	11			
2	P	122	Total	C	N	O	S	0	3	0
			1010	654	167	178	11			
2	T	122	Total	C	N	O	S	0	2	0
			1014	660	166	177	11			
2	W	122	Total	C	N	O	S	0	2	0
			1007	653	166	177	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	V	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		
3	R	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	H	1	Total	C	O	P	0	0
			21	6	13	2		
4	K	1	Total	C	O	P	0	0
			21	6	13	2		
4	O	1	Total	C	O	P	0	0
			21	6	13	2		
4	R	1	Total	C	O	P	0	0
			21	6	13	2		
4	V	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	K	1	Total 4	C 2	O 2	0	0
5	M	1	Total 4	C 2	O 2	0	0
5	O	1	Total 4	C 2	O 2	0	0
5	O	1	Total 4	C 2	O 2	0	0
5	O	1	Total 4	C 2	O 2	0	0
5	O	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	T	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	W	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	294	Total O 294 294	0	0
6	B	317	Total O 317 317	0	0
6	C	61	Total O 61 61	0	0
6	E	292	Total O 292 292	0	0

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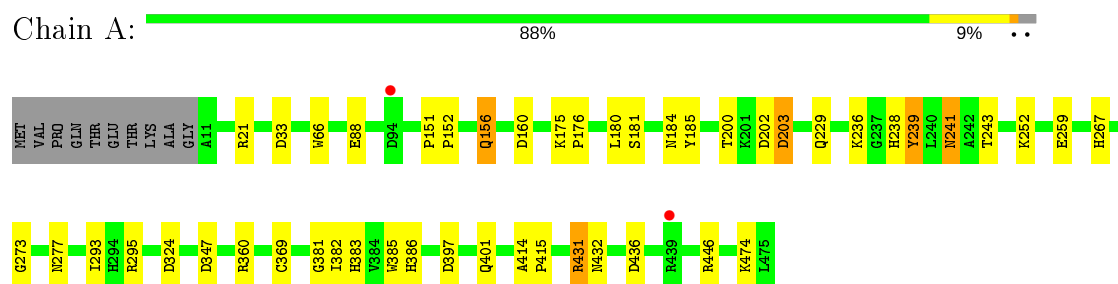
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	70	Total 70	O 70	0	0
6	H	288	Total 288	O 288	0	0
6	I	66	Total 66	O 66	0	0
6	J	57	Total 57	O 57	0	0
6	K	279	Total 279	O 279	0	0
6	M	56	Total 56	O 56	0	0
6	O	286	Total 286	O 286	0	0
6	P	55	Total 55	O 55	0	0
6	R	307	Total 307	O 307	0	0
6	T	73	Total 73	O 73	0	0
6	V	281	Total 281	O 281	0	0
6	W	49	Total 49	O 49	0	0

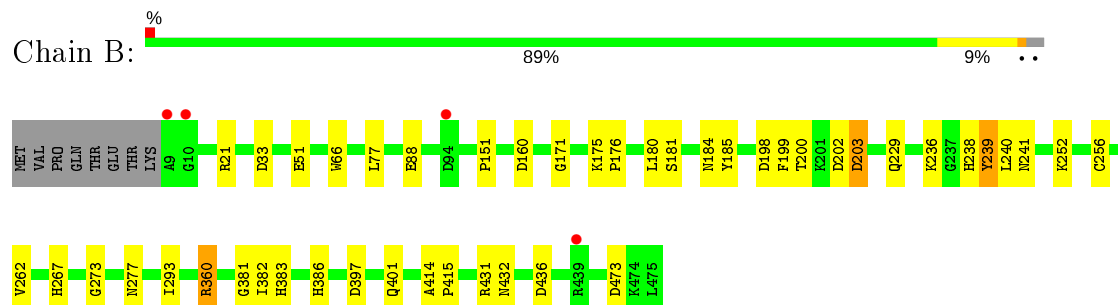
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

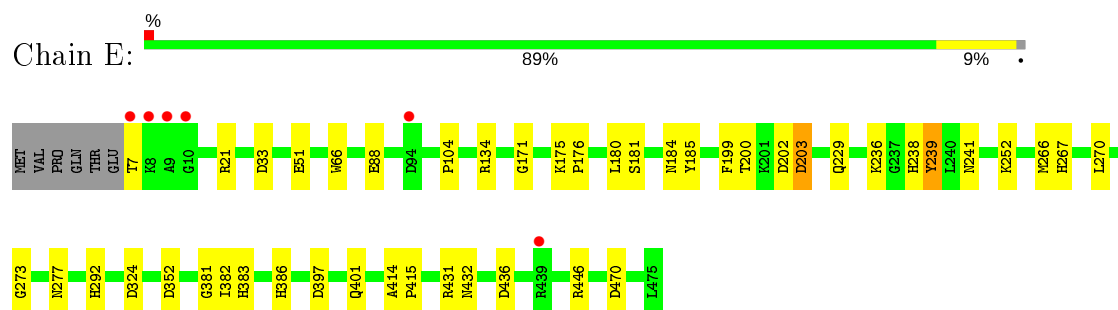
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



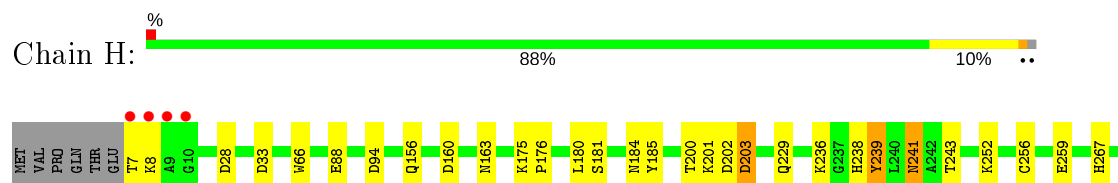
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

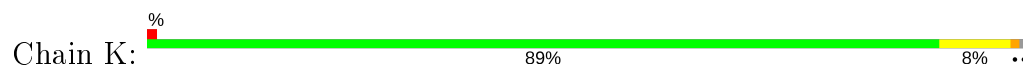


#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

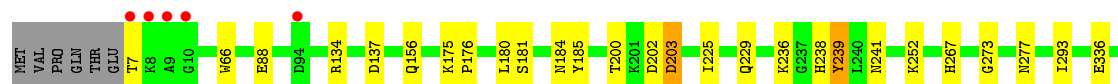




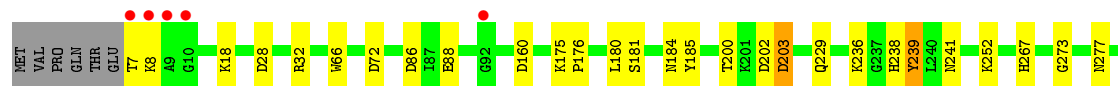
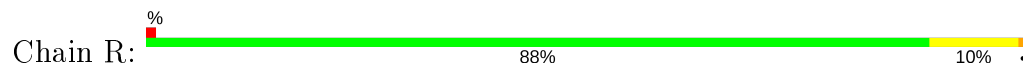
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



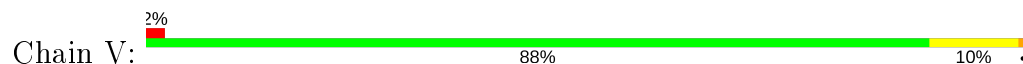
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



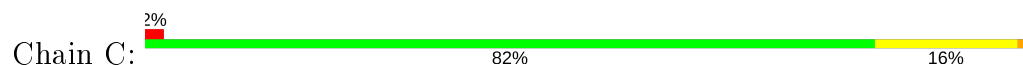
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

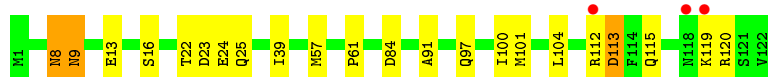


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

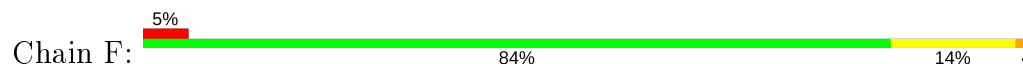


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

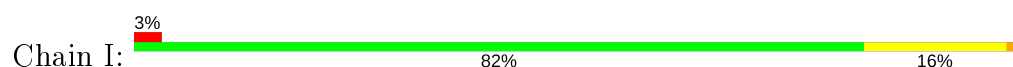




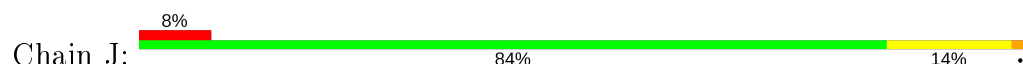
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN



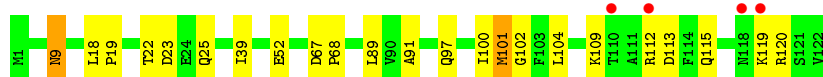
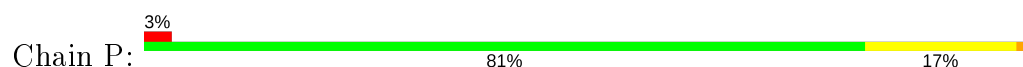
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN



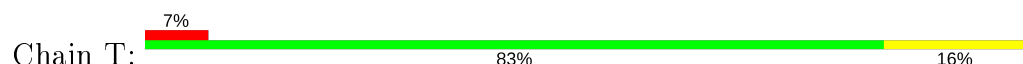
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

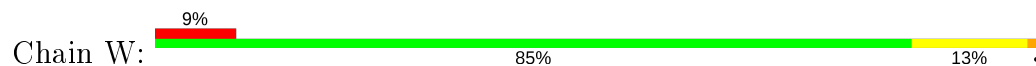


- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN





- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.82Å 223.97Å 111.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.88 – 2.19	Depositor EDS
% Data completeness (in resolution range)	89.3 (30.00-2.20) 88.6 (29.88-2.19)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.160 , 0.193 0.162 , 0.193	Depositor DCC
$R_{free}$ test set	12581 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	40557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.61	0/3695	0.75	6/4993 (0.1%)
1	B	0.62	0/3704	0.80	13/5005 (0.3%)
1	E	0.61	0/3720	0.76	7/5026 (0.1%)
1	H	0.60	0/3720	0.76	7/5026 (0.1%)
1	K	0.62	0/3736	0.75	5/5048 (0.1%)
1	O	0.60	0/3711	0.76	3/5014 (0.1%)
1	R	0.60	0/3711	0.76	10/5014 (0.2%)
1	V	0.61	0/3718	0.75	9/5024 (0.2%)
2	C	0.61	0/1049	0.71	3/1426 (0.2%)
2	F	0.59	0/1056	0.69	2/1435 (0.1%)
2	I	0.60	0/1041	0.69	2/1415 (0.1%)
2	J	0.61	0/1043	0.70	2/1417 (0.1%)
2	M	0.61	0/1049	0.72	1/1425 (0.1%)
2	P	0.60	0/1057	0.72	2/1436 (0.1%)
2	T	0.61	0/1056	0.70	3/1435 (0.2%)
2	W	0.60	0/1049	0.70	2/1425 (0.1%)
All	All	0.61	0/38115	0.75	77/51564 (0.1%)

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360[A]	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	B	360[B]	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	P	113	ASP	CB-CG-OD2	7.29	124.86	118.30
2	M	113	ASP	CB-CG-OD2	7.11	124.70	118.30
2	C	113	ASP	CB-CG-OD2	6.93	124.53	118.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3640	0	3542	34	0
1	B	3647	0	3550	31	0
1	E	3665	0	3570	30	0
1	H	3665	0	3570	37	0
1	K	3673	0	3581	33	0
1	O	3661	0	3568	30	0
1	R	3662	0	3572	32	0
1	V	3664	0	3575	32	0
2	C	1009	0	986	13	0
2	F	1014	0	989	13	0
2	I	1006	0	984	13	0
2	J	1006	0	984	15	0
2	M	1007	0	985	11	0
2	P	1010	0	987	13	0
2	T	1014	0	989	14	0
2	W	1007	0	985	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	A	21	0	8	0	0
4	B	21	0	7	0	0
4	E	21	0	8	0	0
4	H	21	0	8	1	0
4	K	21	0	8	0	0
4	O	21	0	8	0	0
4	R	21	0	9	0	0
4	V	21	0	7	0	0
5	A	20	0	30	0	0
5	B	24	0	36	2	0
5	C	4	0	6	0	0
5	E	20	0	30	2	0
5	F	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	24	0	36	3	0
5	J	4	0	6	1	0
5	K	20	0	30	0	0
5	M	4	0	6	0	0
5	O	20	0	30	1	0
5	P	4	0	6	0	0
5	R	20	0	30	2	0
5	T	4	0	6	0	0
5	V	24	0	36	0	0
5	W	4	0	6	0	0
6	A	294	0	0	7	0
6	B	317	0	0	5	0
6	C	61	0	0	1	0
6	E	292	0	0	1	0
6	F	70	0	0	2	0
6	H	288	0	0	11	0
6	I	66	0	0	1	0
6	J	57	0	0	4	0
6	K	279	0	0	6	0
6	M	56	0	0	1	0
6	O	286	0	0	2	0
6	P	55	0	0	1	0
6	R	307	0	0	7	0
6	T	73	0	0	2	0
6	V	281	0	0	5	0
6	W	49	0	0	3	0
All	All	40557	0	36780	326	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 4.

The worst 5 of 326 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:375:MET:HG2	6:H:2185:HOH:O	1.31	1.28
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.04	0.99
1:V:255:VAL:O	1:V:259[B]:GLU:HG2	1.63	0.97
2:P:97:GLN:HE21	1:R:184:ASN:HD22	1.10	0.97
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.03	0.96

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	448 (97%)	13 (3%)	0	100	100
1	B	463/475 (98%)	449 (97%)	14 (3%)	0	100	100
1	E	465/475 (98%)	451 (97%)	14 (3%)	0	100	100
1	H	465/475 (98%)	452 (97%)	13 (3%)	0	100	100
1	K	467/475 (98%)	454 (97%)	13 (3%)	0	100	100
1	O	464/475 (98%)	451 (97%)	13 (3%)	0	100	100
1	R	464/475 (98%)	450 (97%)	14 (3%)	0	100	100
1	V	465/475 (98%)	453 (97%)	12 (3%)	0	100	100
2	C	122/122 (100%)	115 (94%)	7 (6%)	0	100	100
2	F	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	I	121/122 (99%)	117 (97%)	4 (3%)	0	100	100
2	J	121/122 (99%)	116 (96%)	5 (4%)	0	100	100
2	M	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	P	123/122 (101%)	117 (95%)	6 (5%)	0	100	100
2	T	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	W	122/122 (100%)	116 (95%)	6 (5%)	0	100	100
All	All	4689/4776 (98%)	4540 (97%)	149 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/376 (99%)	360 (97%)	11 (3%)	41	53
1	B	371/376 (99%)	365 (98%)	6 (2%)	62	76
1	E	373/376 (99%)	365 (98%)	8 (2%)	53	67
1	H	373/376 (99%)	361 (97%)	12 (3%)	39	50
1	K	375/376 (100%)	366 (98%)	9 (2%)	49	62
1	O	372/376 (99%)	363 (98%)	9 (2%)	49	62
1	R	372/376 (99%)	362 (97%)	10 (3%)	44	57
1	V	373/376 (99%)	366 (98%)	7 (2%)	57	71
2	C	111/109 (102%)	104 (94%)	7 (6%)	18	20
2	F	111/109 (102%)	105 (95%)	6 (5%)	22	26
2	I	110/109 (101%)	102 (93%)	8 (7%)	14	15
2	J	110/109 (101%)	104 (94%)	6 (6%)	21	26
2	M	111/109 (102%)	106 (96%)	5 (4%)	27	34
2	P	112/109 (103%)	106 (95%)	6 (5%)	22	26
2	T	111/109 (102%)	106 (96%)	5 (4%)	27	34
2	W	111/109 (102%)	105 (95%)	6 (5%)	22	26
All	All	3867/3880 (100%)	3746 (97%)	121 (3%)	41	51

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	100	ILE
1	K	219[A]	LEU
1	V	203	ASP
2	I	104	LEU
2	J	101	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	97	GLN
1	K	304	GLN
1	V	277	ASN
2	J	8	ASN
1	K	153	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

40 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	K	104	1	6,8,9	0.25	0	5,10,12	1.02	0
1	SMC	E	369	1	5,6,7	0.60	0	2,6,8	0.35	0
1	HYP	A	151	1	6,8,9	0.57	0	5,10,12	1.41	0
1	SMC	B	256	1	5,6,7	0.56	0	2,6,8	1.90	1 (50%)
1	HYP	H	151	1	6,8,9	0.62	0	5,10,12	1.34	0
1	KCX	O	201	1,3	7,11,12	0.88	0	4,12,14	0.47	0
1	SMC	R	256	1	5,6,7	0.97	0	2,6,8	0.92	0
1	KCX	H	201	1,3	7,11,12	0.98	0	4,12,14	0.49	0
1	HYP	O	151	1	6,8,9	0.77	0	5,10,12	1.36	0
1	HYP	E	104	1	6,8,9	0.58	0	5,10,12	1.73	2 (40%)
1	SMC	V	369	1	5,6,7	1.17	1 (20%)	2,6,8	0.77	0
1	SMC	B	369	1	5,6,7	0.79	0	2,6,8	0.95	0
1	KCX	V	201	1,3	7,11,12	0.84	0	4,12,14	0.37	0
1	SMC	A	369	1	5,6,7	1.38	1 (20%)	2,6,8	1.71	1 (50%)
1	HYP	B	151	1	6,8,9	0.81	0	5,10,12	1.21	1 (20%)
1	KCX	R	201	1,3	7,11,12	1.08	0	4,12,14	0.59	0
1	SMC	K	369	1	5,6,7	0.49	0	2,6,8	0.37	0
1	HYP	V	151	1	6,8,9	0.32	0	5,10,12	1.45	1 (20%)
1	SMC	H	369	1	5,6,7	1.19	1 (20%)	2,6,8	1.19	0
1	HYP	A	104	1	6,8,9	0.65	0	5,10,12	1.12	0
1	HYP	K	151	1	6,8,9	0.71	0	5,10,12	1.39	1 (20%)
1	HYP	H	104	1	6,8,9	0.60	0	5,10,12	1.05	0
1	KCX	K	201	1,3	7,11,12	1.05	1 (14%)	4,12,14	0.44	0
1	KCX	E	201	1,3	7,11,12	1.08	0	4,12,14	0.47	0
1	SMC	K	256	1	5,6,7	0.84	0	2,6,8	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SMC	E	256	1	5,6,7	0.90	0	2,6,8	0.74	0
1	SMC	R	369	1	5,6,7	1.34	1 (20%)	2,6,8	0.78	0
1	SMC	O	369	1	5,6,7	0.82	0	2,6,8	0.47	0
1	SMC	A	256	1	5,6,7	0.84	0	2,6,8	1.56	0
1	HYP	O	104	1	6,8,9	0.50	0	5,10,12	0.88	0
1	SMC	H	256	1	5,6,7	0.66	0	2,6,8	1.85	1 (50%)
1	HYP	E	151	1	6,8,9	0.48	0	5,10,12	1.27	0
1	KCX	A	201	1,3	7,11,12	0.96	0	4,12,14	0.55	0
1	SMC	O	256	1	5,6,7	0.83	0	2,6,8	0.92	0
1	HYP	R	151	1	6,8,9	0.61	0	5,10,12	1.28	0
1	HYP	R	104	1	6,8,9	0.45	0	5,10,12	1.22	0
1	HYP	V	104	1	6,8,9	0.44	0	5,10,12	1.40	1 (20%)
1	KCX	B	201	1,3	7,11,12	1.05	0	4,12,14	0.56	0
1	SMC	V	256	1	5,6,7	1.23	1 (20%)	2,6,8	0.51	0
1	HYP	B	104	1	6,8,9	0.46	0	5,10,12	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	K	104	1	-	0/0/11/13	0/1/1/1
1	SMC	E	369	1	-	1/3/5/7	-
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	SMC	B	256	1	-	0/3/5/7	-
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	KCX	O	201	1,3	-	0/7/10/12	-
1	SMC	R	256	1	-	0/3/5/7	-
1	KCX	H	201	1,3	-	0/7/10/12	-
1	HYP	O	151	1	-	0/0/11/13	0/1/1/1
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	SMC	V	369	1	-	1/3/5/7	-
1	SMC	B	369	1	-	1/3/5/7	-
1	KCX	V	201	1,3	-	0/7/10/12	-
1	SMC	A	369	1	-	1/3/5/7	-
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	KCX	R	201	1,3	-	0/7/10/12	-
1	SMC	K	369	1	-	1/3/5/7	-
1	HYP	V	151	1	-	0/0/11/13	0/1/1/1
1	SMC	H	369	1	-	1/3/5/7	-
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	K	151	1	-	0/0/11/13	0/1/1/1
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	KCX	K	201	1,3	-	0/7/10/12	-
1	KCX	E	201	1,3	-	0/7/10/12	-
1	SMC	K	256	1	-	0/3/5/7	-
1	SMC	E	256	1	-	0/3/5/7	-
1	SMC	R	369	1	-	1/3/5/7	-
1	SMC	O	369	1	-	1/3/5/7	-
1	SMC	A	256	1	-	0/3/5/7	-
1	HYP	O	104	1	-	0/0/11/13	0/1/1/1
1	SMC	H	256	1	-	0/3/5/7	-
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	KCX	A	201	1,3	-	0/7/10/12	-
1	SMC	O	256	1	-	0/3/5/7	-
1	HYP	R	151	1	-	0/0/11/13	0/1/1/1
1	HYP	R	104	1	-	0/0/11/13	0/1/1/1
1	HYP	V	104	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	1,3	-	0/7/10/12	-
1	SMC	V	256	1	-	0/3/5/7	-
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	SMC	CB-SG	2.76	1.84	1.80
1	R	369	SMC	CB-SG	2.67	1.84	1.80
1	V	256	SMC	CB-SG	2.48	1.84	1.80
1	K	201	KCX	CE-NZ	2.46	1.51	1.45
1	H	369	SMC	CB-SG	2.25	1.83	1.80

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	104	HYP	OD1-CG-CD	-2.74	104.36	110.35
1	B	256	SMC	CA-CB-SG	-2.68	109.70	114.04
1	E	104	HYP	CB-CG-CD	2.48	106.30	103.27
1	V	104	HYP	O-C-CA	-2.41	118.45	124.78
1	H	256	SMC	CA-CB-SG	-2.34	110.25	114.04

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	369	SMC	N-CA-CB-SG
1	B	369	SMC	N-CA-CB-SG
1	K	369	SMC	N-CA-CB-SG
1	H	369	SMC	N-CA-CB-SG
1	O	369	SMC	N-CA-CB-SG

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	151	HYP	1	0
1	H	201	KCX	1	0
1	V	369	SMC	1	0
1	V	151	HYP	1	0
1	K	151	HYP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 8 are monoatomic - leaving 58 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	EDO	R	1480	-	3,3,3	0.35	0	2,2,2	0.31	0
5	EDO	K	1480	-	3,3,3	0.31	0	2,2,2	0.26	0
5	EDO	V	1476	-	3,3,3	0.42	0	2,2,2	0.14	0
5	EDO	E	1476	-	3,3,3	0.33	0	2,2,2	0.10	0
5	EDO	V	1477	-	3,3,3	0.35	0	2,2,2	0.18	0
5	EDO	J	1123	-	3,3,3	0.26	0	2,2,2	0.57	0
4	CAP	B	477	3	15,20,20	0.53	0	20,31,31	0.95	1 (5%)
4	CAP	K	477	3	15,20,20	0.72	0	20,31,31	0.99	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	R	1479	-	3,3,3	0.33	0	2,2,2	0.18	0
5	EDO	E	1479	-	3,3,3	0.37	0	2,2,2	0.22	0
5	EDO	O	1478	-	3,3,3	0.27	0	2,2,2	0.32	0
5	EDO	E	1477	-	3,3,3	0.27	0	2,2,2	0.19	0
5	EDO	B	1477	-	3,3,3	0.36	0	2,2,2	0.14	0
4	CAP	A	477	3	15,20,20	0.78	0	20,31,31	0.87	0
5	EDO	H	1476	-	3,3,3	0.38	0	2,2,2	0.11	0
5	EDO	M	1123	-	3,3,3	0.28	0	2,2,2	0.38	0
4	CAP	R	477	3	15,20,20	0.57	0	20,31,31	0.94	1 (5%)
5	EDO	B	1481	-	3,3,3	0.33	0	2,2,2	0.12	0
5	EDO	V	1481	-	3,3,3	0.37	0	2,2,2	0.28	0
5	EDO	O	1477	-	3,3,3	0.28	0	2,2,2	0.33	0
5	EDO	O	1476	-	3,3,3	0.34	0	2,2,2	0.16	0
5	EDO	R	1476	-	3,3,3	0.40	0	2,2,2	0.20	0
5	EDO	H	1477	-	3,3,3	0.36	0	2,2,2	0.10	0
5	EDO	R	1478	-	3,3,3	0.31	0	2,2,2	0.20	0
5	EDO	R	1477	-	3,3,3	0.33	0	2,2,2	0.09	0
5	EDO	A	1480	-	3,3,3	0.33	0	2,2,2	0.66	0
5	EDO	B	1480	-	3,3,3	0.39	0	2,2,2	0.09	0
5	EDO	V	1478	-	3,3,3	0.28	0	2,2,2	0.22	0
5	EDO	H	1478	-	3,3,3	0.24	0	2,2,2	0.04	0
5	EDO	K	1478	-	3,3,3	0.26	0	2,2,2	0.59	0
4	CAP	O	477	3	15,20,20	0.64	0	20,31,31	0.99	1 (5%)
5	EDO	A	1478	-	3,3,3	0.31	0	2,2,2	0.21	0
5	EDO	P	1123	-	3,3,3	0.30	0	2,2,2	0.22	0
5	EDO	V	1480	-	3,3,3	0.29	0	2,2,2	0.11	0
5	EDO	C	1123	-	3,3,3	0.27	0	2,2,2	0.57	0
5	EDO	T	1123	-	3,3,3	0.27	0	2,2,2	0.59	0
5	EDO	B	1479	-	3,3,3	0.33	0	2,2,2	0.28	0
5	EDO	K	1477	-	3,3,3	0.32	0	2,2,2	0.21	0
5	EDO	K	1479	-	3,3,3	0.35	0	2,2,2	0.10	0
5	EDO	K	1476	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	O	1479	-	3,3,3	0.38	0	2,2,2	0.24	0
5	EDO	H	1480	-	3,3,3	0.34	0	2,2,2	0.30	0
4	CAP	E	477	3	15,20,20	0.87	0	20,31,31	1.07	1 (5%)
4	CAP	V	477	3	15,20,20	0.86	0	20,31,31	0.88	0
5	EDO	W	1123	-	3,3,3	0.27	0	2,2,2	0.39	0
5	EDO	B	1476	-	3,3,3	0.35	0	2,2,2	0.46	0
5	EDO	F	1123	-	3,3,3	0.32	0	2,2,2	0.79	0
5	EDO	B	1478	-	3,3,3	0.28	0	2,2,2	0.37	0
5	EDO	E	1478	-	3,3,3	0.26	0	2,2,2	0.42	0
5	EDO	A	1477	-	3,3,3	0.27	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	O	1480	-	3,3,3	0.43	0	2,2,2	0.47	0
5	EDO	A	1476	-	3,3,3	0.31	0	2,2,2	0.27	0
5	EDO	H	1481	-	3,3,3	0.35	0	2,2,2	0.23	0
4	CAP	H	477	3	15,20,20	0.68	0	20,31,31	0.84	0
5	EDO	A	1479	-	3,3,3	0.37	0	2,2,2	0.17	0
5	EDO	E	1480	-	3,3,3	0.34	0	2,2,2	0.19	0
5	EDO	H	1479	-	3,3,3	0.28	0	2,2,2	0.33	0
5	EDO	V	1479	-	3,3,3	0.35	0	2,2,2	0.09	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	EDO	R	1480	-	-	0/1/1/1	-
5	EDO	K	1480	-	-	0/1/1/1	-
5	EDO	V	1476	-	-	1/1/1/1	-
5	EDO	E	1476	-	-	0/1/1/1	-
5	EDO	V	1477	-	-	0/1/1/1	-
5	EDO	J	1123	-	-	0/1/1/1	-
4	CAP	B	477	3	-	3/23/29/29	-
4	CAP	K	477	3	-	3/23/29/29	-
5	EDO	R	1479	-	-	0/1/1/1	-
5	EDO	E	1479	-	-	1/1/1/1	-
5	EDO	O	1478	-	-	0/1/1/1	-
5	EDO	E	1477	-	-	1/1/1/1	-
5	EDO	B	1477	-	-	0/1/1/1	-
4	CAP	A	477	3	-	5/23/29/29	-
5	EDO	H	1476	-	-	1/1/1/1	-
5	EDO	M	1123	-	-	0/1/1/1	-
4	CAP	R	477	3	-	3/23/29/29	-
5	EDO	B	1481	-	-	0/1/1/1	-
5	EDO	V	1481	-	-	1/1/1/1	-
5	EDO	O	1477	-	-	1/1/1/1	-
5	EDO	O	1476	-	-	0/1/1/1	-
5	EDO	R	1476	-	-	0/1/1/1	-
5	EDO	H	1477	-	-	0/1/1/1	-
5	EDO	R	1478	-	-	0/1/1/1	-
5	EDO	R	1477	-	-	1/1/1/1	-
5	EDO	A	1480	-	-	1/1/1/1	-
5	EDO	B	1480	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	V	1478	-	-	1/1/1/1	-
5	EDO	H	1478	-	-	1/1/1/1	-
5	EDO	K	1478	-	-	0/1/1/1	-
4	CAP	O	477	3	-	5/23/29/29	-
5	EDO	A	1478	-	-	0/1/1/1	-
5	EDO	P	1123	-	-	0/1/1/1	-
5	EDO	V	1480	-	-	0/1/1/1	-
5	EDO	C	1123	-	-	1/1/1/1	-
5	EDO	T	1123	-	-	0/1/1/1	-
5	EDO	B	1479	-	-	0/1/1/1	-
5	EDO	K	1477	-	-	0/1/1/1	-
5	EDO	K	1479	-	-	1/1/1/1	-
5	EDO	K	1476	-	-	0/1/1/1	-
5	EDO	O	1479	-	-	0/1/1/1	-
5	EDO	H	1480	-	-	1/1/1/1	-
4	CAP	E	477	3	-	6/23/29/29	-
4	CAP	V	477	3	-	4/23/29/29	-
5	EDO	W	1123	-	-	0/1/1/1	-
5	EDO	B	1476	-	-	1/1/1/1	-
5	EDO	F	1123	-	-	0/1/1/1	-
5	EDO	B	1478	-	-	1/1/1/1	-
5	EDO	E	1478	-	-	0/1/1/1	-
5	EDO	A	1477	-	-	1/1/1/1	-
5	EDO	O	1480	-	-	1/1/1/1	-
5	EDO	A	1476	-	-	1/1/1/1	-
5	EDO	H	1481	-	-	0/1/1/1	-
4	CAP	H	477	3	-	4/23/29/29	-
5	EDO	A	1479	-	-	0/1/1/1	-
5	EDO	E	1480	-	-	1/1/1/1	-
5	EDO	H	1479	-	-	0/1/1/1	-
5	EDO	V	1479	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	477	CAP	O6P-P2-O5	2.70	113.91	106.73
4	O	477	CAP	O3-C3-C4	2.12	113.67	109.13
4	B	477	CAP	O4-C4-C5	-2.11	105.17	109.92
4	R	477	CAP	O5-P2-O4P	2.02	112.13	106.47

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

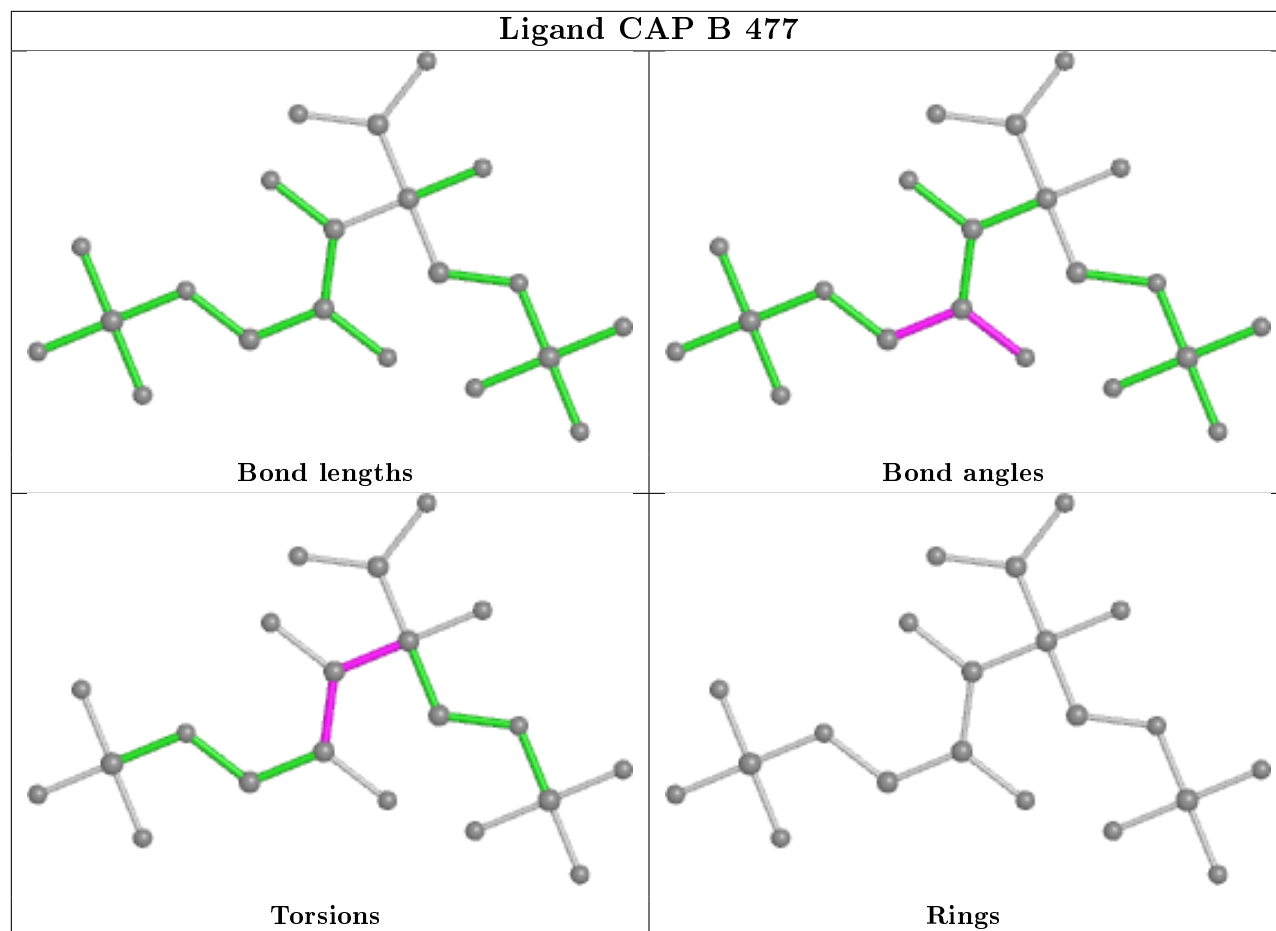
Mol	Chain	Res	Type	Atoms
4	B	477	CAP	C2-C3-C4-O4
4	B	477	CAP	O3-C3-C4-O4
4	K	477	CAP	C2-C3-C4-O4
4	K	477	CAP	O3-C3-C4-O4
4	A	477	CAP	C2-C3-C4-O4

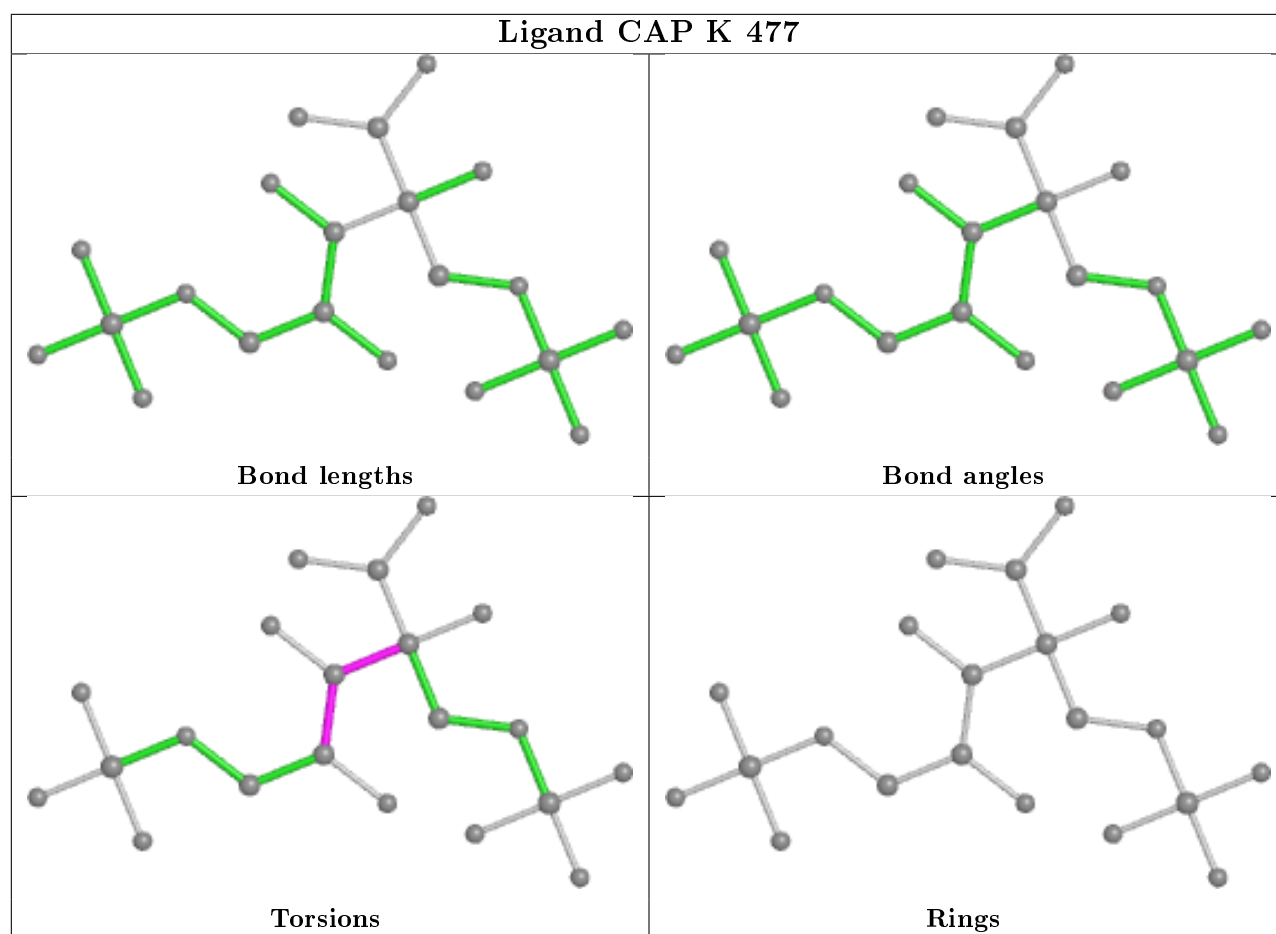
There are no ring outliers.

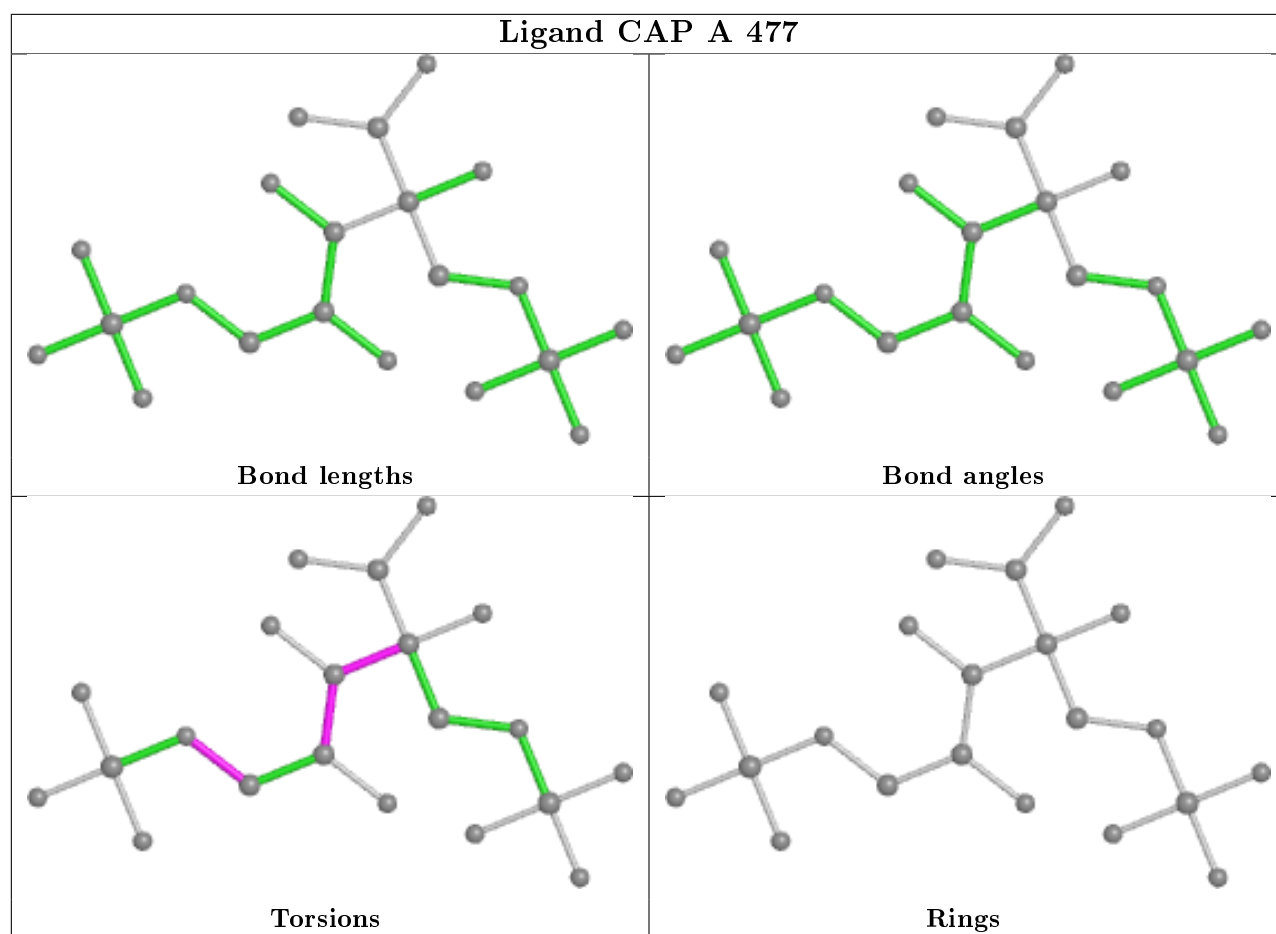
9 monomers are involved in 12 short contacts:

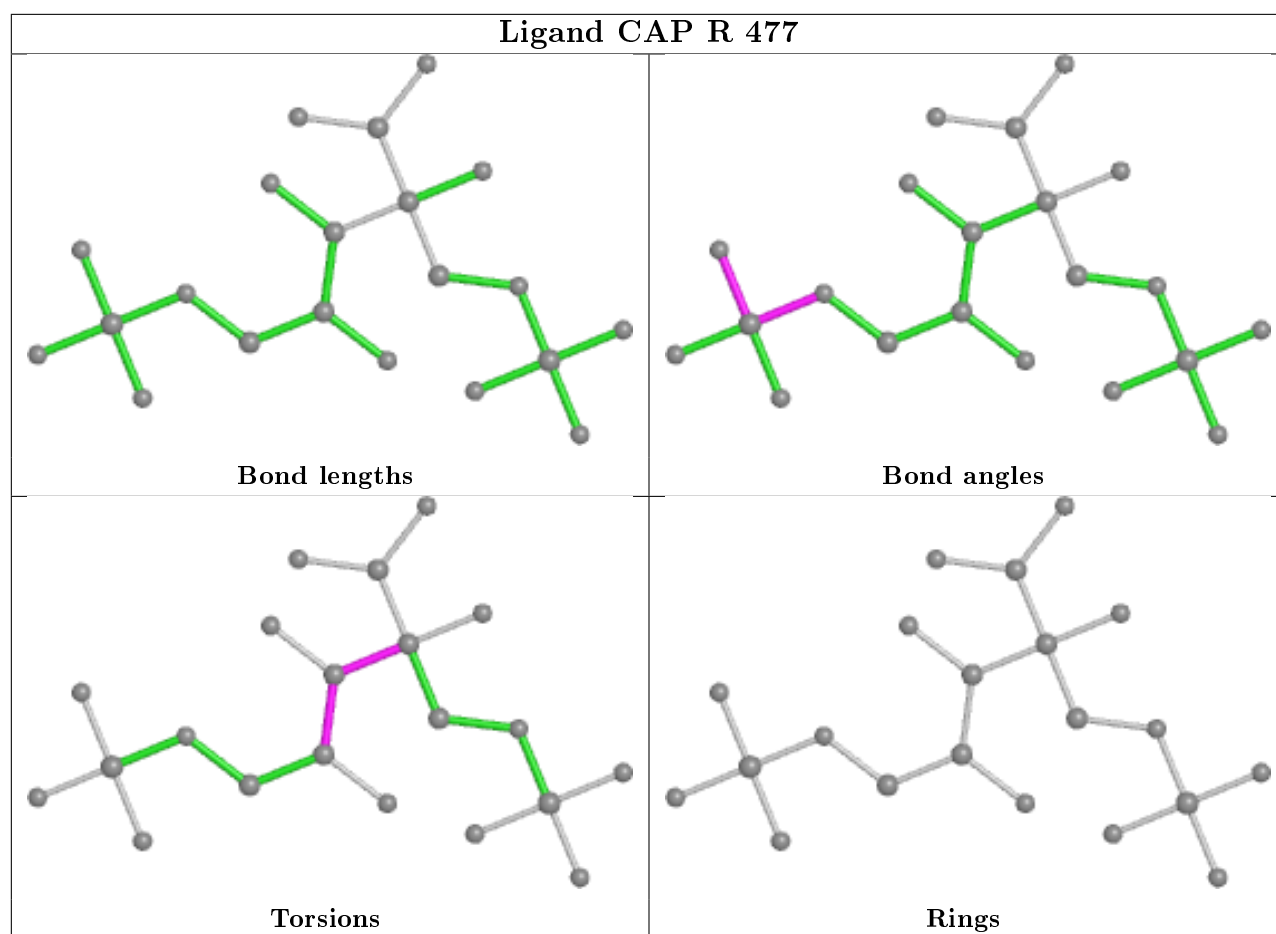
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1480	EDO	1	0
5	J	1123	EDO	1	0
5	B	1481	EDO	2	0
5	R	1477	EDO	1	0
5	H	1480	EDO	2	0
5	O	1480	EDO	1	0
5	H	1481	EDO	1	0
4	H	477	CAP	1	0
5	E	1480	EDO	2	0

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.

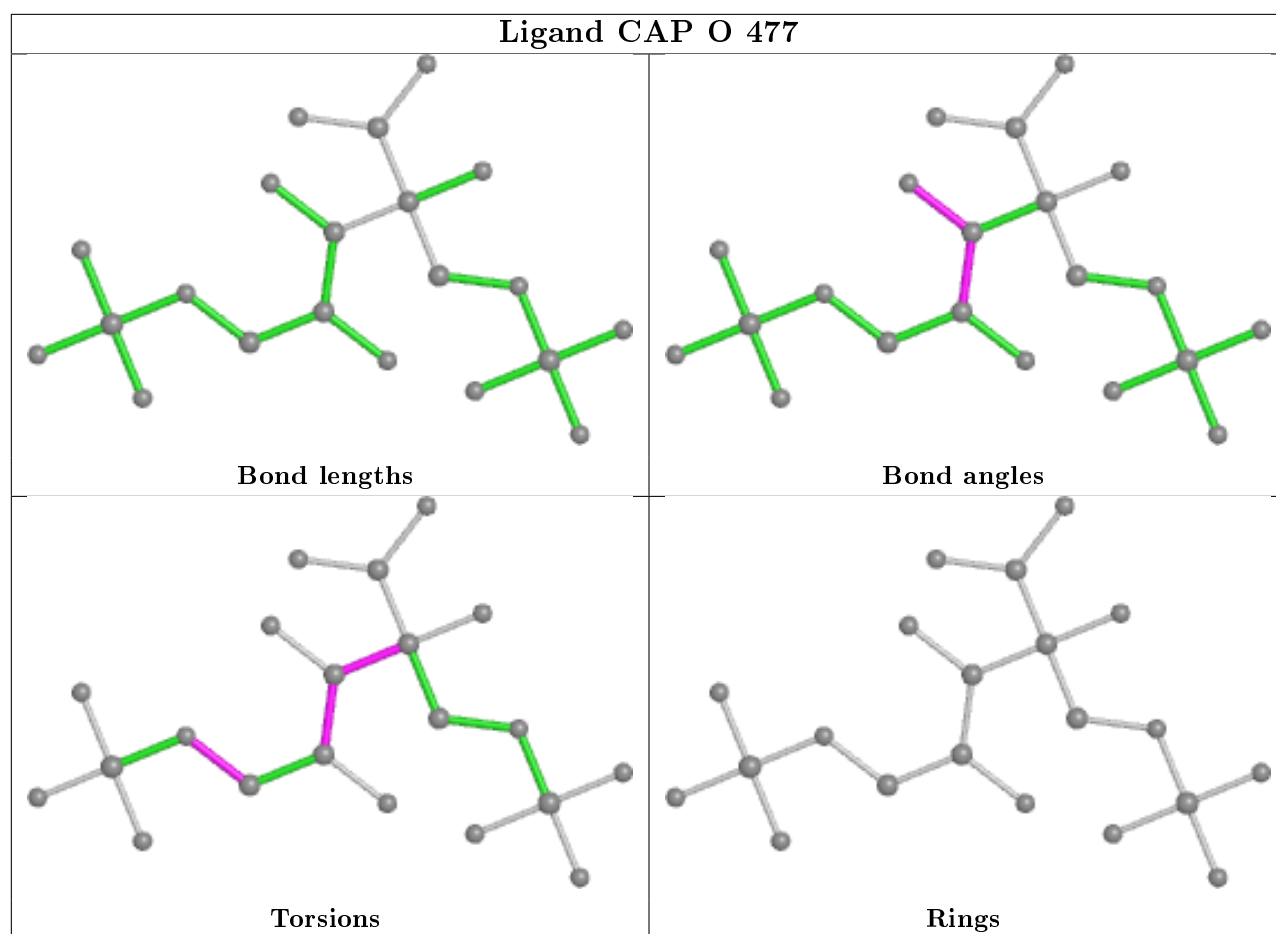


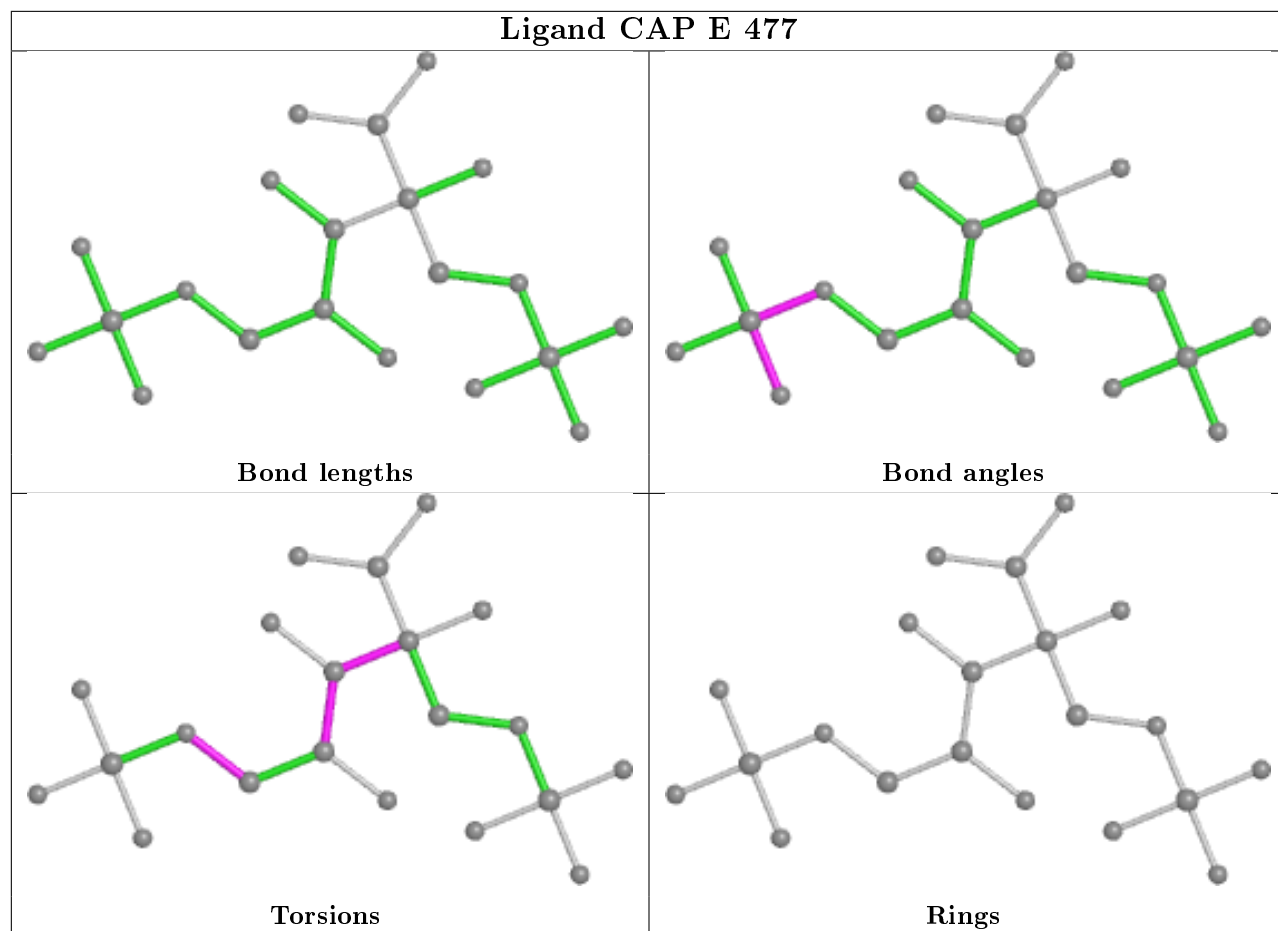


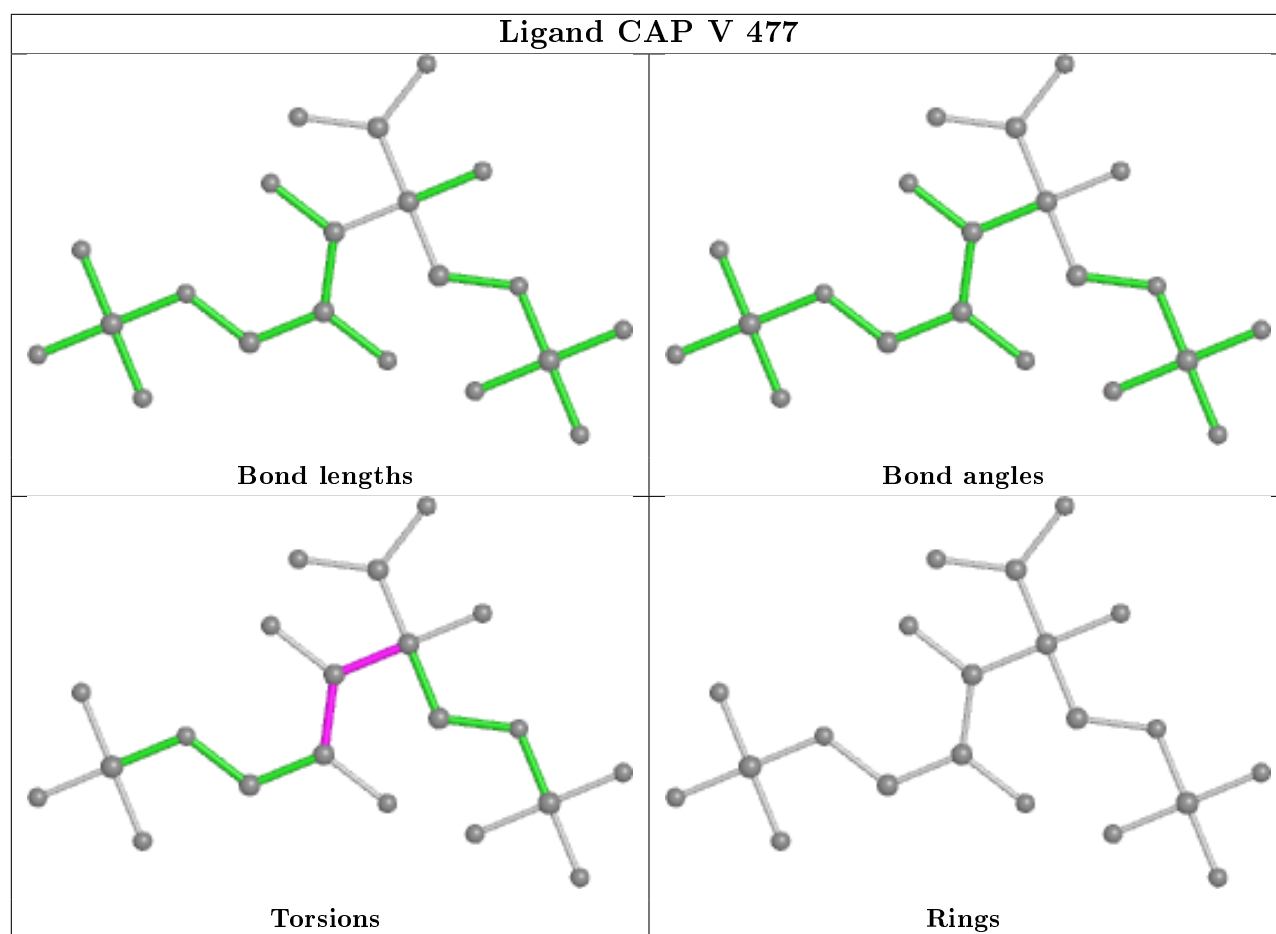


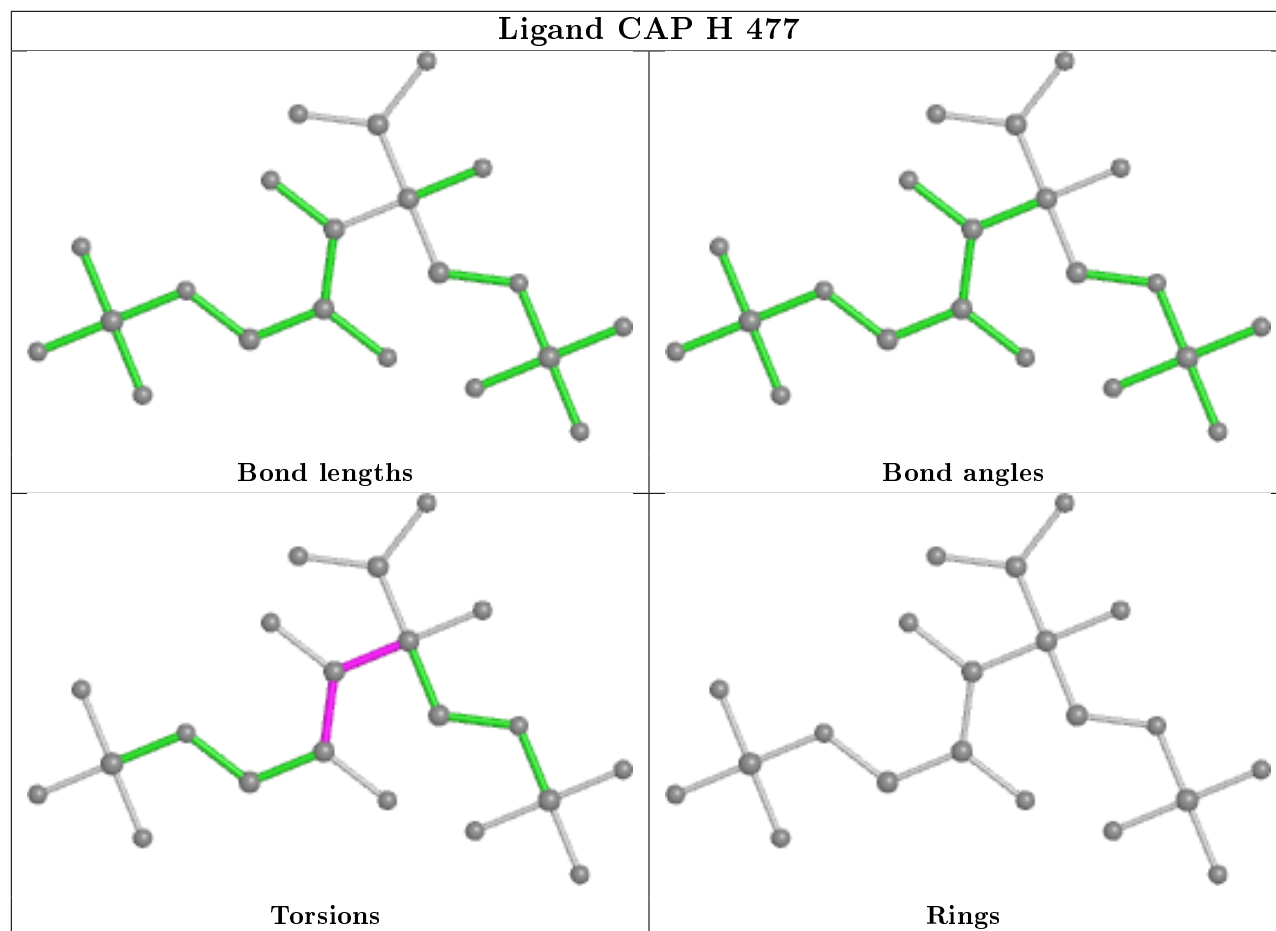












## 5.7 Other polymers [i](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	460/475 (96%)	-0.81	2 (0%) 92 91	13, 19, 34, 49	0
1	B	462/475 (97%)	-0.77	4 (0%) 84 83	12, 19, 34, 66	0
1	E	464/475 (97%)	-0.80	6 (1%) 77 75	13, 19, 35, 76	0
1	H	464/475 (97%)	-0.81	5 (1%) 80 79	13, 19, 35, 72	0
1	K	464/475 (97%)	-0.75	7 (1%) 73 72	13, 19, 35, 81	0
1	O	464/475 (97%)	-0.80	5 (1%) 80 79	13, 19, 35, 80	0
1	R	464/475 (97%)	-0.80	6 (1%) 77 75	12, 19, 35, 84	0
1	V	464/475 (97%)	-0.77	8 (1%) 70 68	13, 19, 35, 80	0
2	C	122/122 (100%)	-0.33	3 (2%) 57 55	18, 27, 58, 69	0
2	F	122/122 (100%)	-0.28	6 (4%) 29 28	18, 27, 58, 69	1 (0%)
2	I	122/122 (100%)	-0.38	4 (3%) 46 44	18, 27, 58, 69	1 (0%)
2	J	122/122 (100%)	-0.19	10 (8%) 11 10	18, 27, 58, 69	1 (0%)
2	M	122/122 (100%)	-0.23	7 (5%) 23 22	18, 27, 58, 69	1 (0%)
2	P	122/122 (100%)	-0.34	4 (3%) 46 44	18, 27, 58, 69	0
2	T	122/122 (100%)	-0.28	8 (6%) 18 17	18, 27, 58, 69	0
2	W	122/122 (100%)	-0.06	11 (9%) 9 8	18, 27, 58, 69	1 (0%)
All	All	4682/4776 (98%)	-0.68	96 (2%) 63 61	12, 20, 41, 84	5 (0%)

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	112	ARG	8.5
1	E	9	ALA	6.5
2	W	111	ALA	6.4
2	T	112	ARG	6.0
2	J	112	ARG	5.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	HYP	B	151	8/9	0.95	0.09	13,15,16,16	0
1	HYP	A	104	8/9	0.96	0.12	14,16,18,18	0
1	HYP	A	151	8/9	0.97	0.07	13,15,16,16	0
1	KCX	R	201	12/13	0.97	0.11	13,15,16,16	0
1	SMC	H	369	7/8	0.97	0.07	17,17,19,21	0
1	KCX	V	201	12/13	0.97	0.08	13,14,16,17	0
1	HYP	H	104	8/9	0.97	0.07	14,16,17,18	0
1	KCX	K	201	12/13	0.97	0.10	13,15,16,16	0
1	KCX	E	201	12/13	0.97	0.09	13,15,16,17	0
1	SMC	R	369	7/8	0.97	0.06	17,17,19,21	0
1	SMC	A	256	7/8	0.97	0.07	14,14,16,18	0
1	HYP	E	151	8/9	0.97	0.06	14,15,16,16	0
1	HYP	R	104	8/9	0.97	0.07	14,16,18,18	0
1	HYP	V	104	8/9	0.97	0.06	14,16,17,18	0
1	KCX	H	201	12/13	0.98	0.08	13,15,16,17	0
1	HYP	K	151	8/9	0.98	0.06	14,15,16,16	0
1	HYP	E	104	8/9	0.98	0.07	14,16,17,18	0
1	SMC	B	369	7/8	0.98	0.08	17,17,18,20	0
1	SMC	E	369	7/8	0.98	0.06	17,17,19,21	0
1	SMC	A	369	7/8	0.98	0.07	17,17,18,21	0
1	HYP	K	104	8/9	0.98	0.06	14,16,17,18	0
1	HYP	O	104	8/9	0.98	0.05	14,16,17,18	0
1	SMC	H	256	7/8	0.98	0.08	14,14,16,18	0
1	SMC	B	256	7/8	0.98	0.08	14,14,16,19	0
1	KCX	A	201	12/13	0.98	0.10	13,15,16,16	0
1	SMC	O	256	7/8	0.98	0.07	14,14,16,19	0
1	HYP	R	151	8/9	0.98	0.07	14,14,16,16	0
1	HYP	V	151	8/9	0.98	0.07	14,15,15,16	0
1	KCX	O	201	12/13	0.98	0.08	13,15,16,16	0
1	KCX	B	201	12/13	0.98	0.10	13,15,16,17	0
1	HYP	B	104	8/9	0.98	0.07	14,15,17,17	0
1	SMC	R	256	7/8	0.99	0.06	14,15,16,18	0
1	SMC	K	256	7/8	0.99	0.07	14,14,16,18	0
1	SMC	E	256	7/8	0.99	0.07	14,14,16,19	0
1	SMC	V	369	7/8	0.99	0.05	17,17,19,21	0
1	SMC	O	369	7/8	0.99	0.07	17,17,18,20	0
1	HYP	H	151	8/9	0.99	0.07	14,15,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SMC	K	369	7/8	0.99	0.06	16,17,19,21	0
1	SMC	V	256	7/8	0.99	0.07	14,15,16,18	0
1	HYP	O	151	8/9	0.99	0.06	14,15,16,16	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	EDO	V	1481	4/4	0.76	0.25	34,40,43,48	0
5	EDO	O	1480	4/4	0.83	0.22	29,36,41,46	0
5	EDO	H	1480	4/4	0.87	0.23	39,51,53,53	0
5	EDO	H	1481	4/4	0.87	0.15	42,45,46,49	0
5	EDO	W	1123	4/4	0.90	0.14	33,38,38,45	0
5	EDO	A	1480	4/4	0.90	0.17	38,40,41,44	0
5	EDO	A	1478	4/4	0.91	0.12	27,34,34,38	0
5	EDO	R	1478	4/4	0.92	0.10	32,32,33,34	0
5	EDO	K	1479	4/4	0.93	0.16	28,29,34,34	0
5	EDO	M	1123	4/4	0.93	0.16	30,38,38,43	0
5	EDO	O	1478	4/4	0.93	0.11	33,35,37,39	0
5	EDO	P	1123	4/4	0.93	0.17	29,31,36,37	0
5	EDO	B	1479	4/4	0.93	0.09	26,32,33,35	0
5	EDO	C	1123	4/4	0.94	0.16	25,29,34,38	0
5	EDO	H	1479	4/4	0.94	0.10	28,28,32,37	0
5	EDO	K	1478	4/4	0.95	0.11	31,31,32,34	0
5	EDO	E	1479	4/4	0.95	0.11	38,38,38,40	0
5	EDO	V	1476	4/4	0.95	0.16	21,21,27,30	0
5	EDO	R	1480	4/4	0.95	0.11	31,33,33,37	0
5	EDO	K	1476	4/4	0.95	0.11	21,22,23,27	0
5	EDO	O	1479	4/4	0.95	0.15	24,26,32,33	0
5	EDO	V	1479	4/4	0.95	0.10	27,29,31,33	0
5	EDO	R	1476	4/4	0.96	0.09	19,21,23,23	0
5	EDO	E	1478	4/4	0.96	0.08	34,34,35,37	0
5	EDO	K	1477	4/4	0.96	0.07	26,31,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	K	1480	4/4	0.96	0.08	33,33,36,41	0
5	EDO	F	1123	4/4	0.96	0.13	29,32,35,36	0
5	EDO	E	1480	4/4	0.96	0.11	29,31,32,32	0
5	EDO	J	1123	4/4	0.96	0.18	35,39,43,46	0
5	EDO	T	1123	4/4	0.96	0.11	27,27,30,35	0
5	EDO	E	1476	4/4	0.97	0.08	21,22,24,28	0
5	EDO	H	1477	4/4	0.97	0.09	16,23,23,25	0
5	EDO	B	1477	4/4	0.97	0.07	16,19,22,25	0
5	EDO	B	1481	4/4	0.97	0.10	30,35,37,38	0
5	EDO	O	1477	4/4	0.97	0.11	22,25,26,27	0
5	EDO	B	1480	4/4	0.97	0.14	22,33,34,35	0
5	EDO	B	1478	4/4	0.97	0.09	21,23,27,29	0
5	EDO	H	1478	4/4	0.98	0.11	24,26,28,29	0
5	EDO	V	1477	4/4	0.98	0.07	21,21,24,26	0
5	EDO	O	1476	4/4	0.98	0.06	22,26,26,29	0
3	MG	V	476	1/1	0.98	0.05	16,16,16,16	0
5	EDO	B	1476	4/4	0.98	0.30	2,3,3,6	4
3	MG	B	476	1/1	0.98	0.04	12,12,12,12	0
5	EDO	V	1480	4/4	0.98	0.12	24,27,29,30	0
5	EDO	A	1477	4/4	0.98	0.10	18,18,23,24	0
3	MG	K	476	1/1	0.98	0.04	19,19,19,19	0
3	MG	O	476	1/1	0.98	0.03	15,15,15,15	0
5	EDO	A	1476	4/4	0.98	0.05	22,22,24,27	0
5	EDO	H	1476	4/4	0.98	0.33	2,5,5,10	4
5	EDO	A	1479	4/4	0.98	0.12	15,25,26,27	0
5	EDO	R	1479	4/4	0.98	0.10	29,31,35,35	0
5	EDO	R	1477	4/4	0.98	0.09	23,26,28,30	0
5	EDO	V	1478	4/4	0.98	0.11	23,27,30,31	0
4	CAP	K	477	21/21	0.99	0.07	13,16,21,24	0
3	MG	H	476	1/1	0.99	0.03	16,16,16,16	0
4	CAP	A	477	21/21	0.99	0.07	12,17,22,24	0
4	CAP	B	477	21/21	0.99	0.08	14,18,20,22	0
4	CAP	E	477	21/21	0.99	0.07	15,19,22,24	0
3	MG	R	476	1/1	0.99	0.04	11,11,11,11	0
4	CAP	V	477	21/21	0.99	0.07	16,18,22,23	0
4	CAP	H	477	21/21	0.99	0.07	16,20,23,28	0
5	EDO	E	1477	4/4	0.99	0.06	19,21,21,22	0
4	CAP	R	477	21/21	0.99	0.07	11,16,20,26	0
3	MG	E	476	1/1	0.99	0.04	13,13,13,13	0
4	CAP	O	477	21/21	0.99	0.06	12,17,20,24	0
3	MG	A	476	1/1	1.00	0.04	17,17,17,17	0

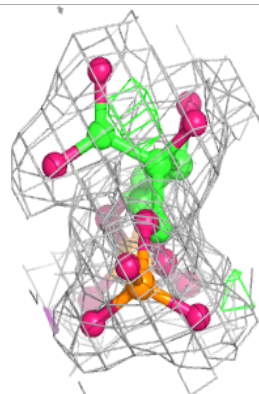
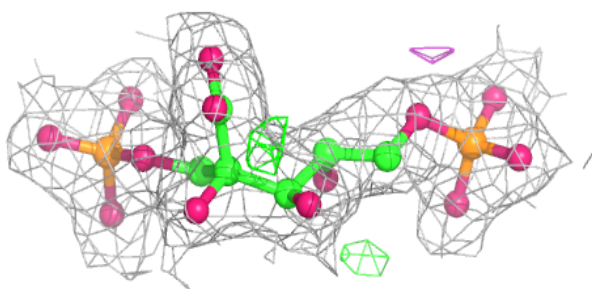
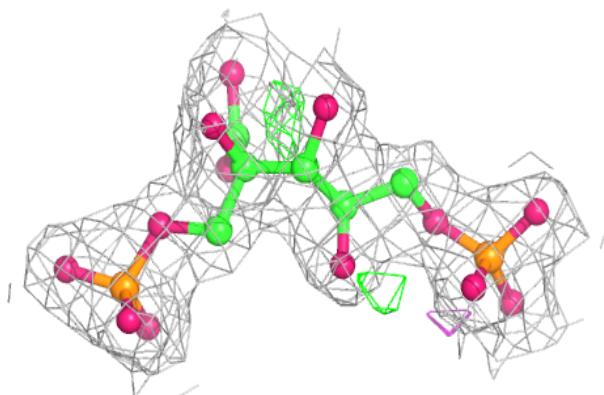
The following is a graphical depiction of the model fit to experimental electron density of all



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.

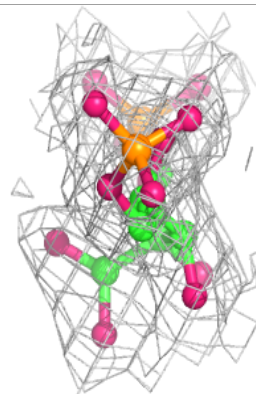
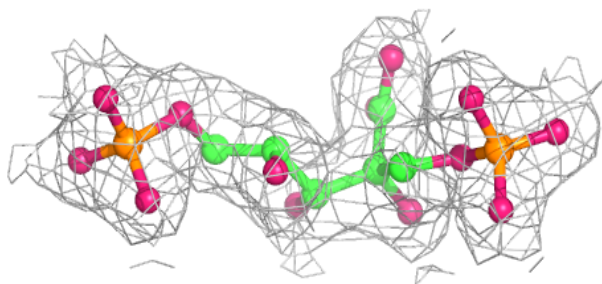
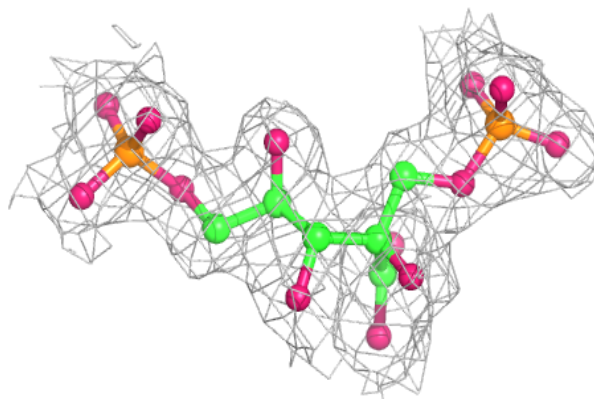
**Electron density around CAP K 477:**

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

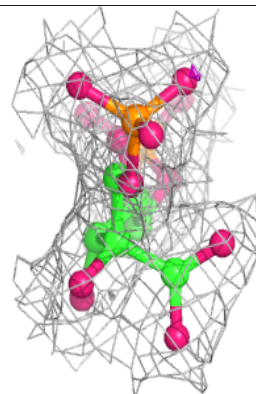
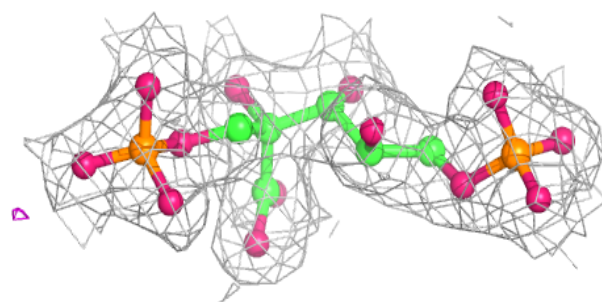
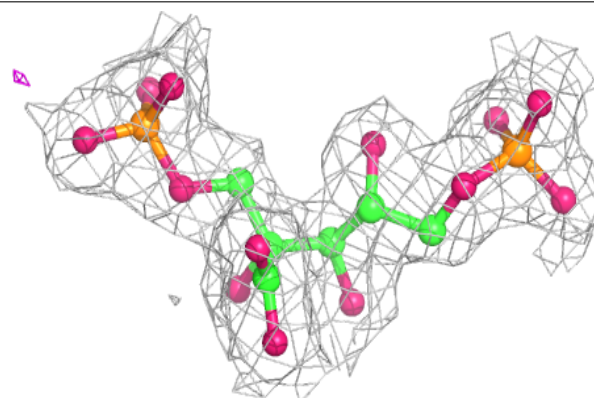


**Electron density around CAP A 477:**

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

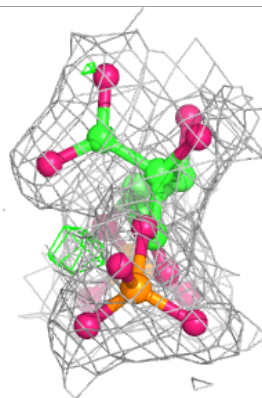
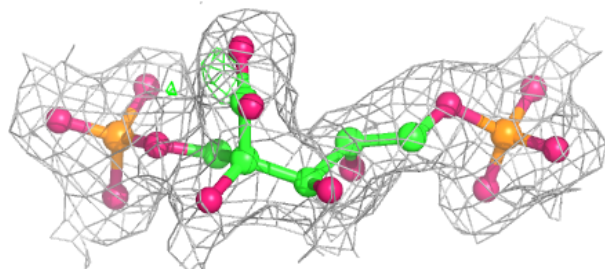
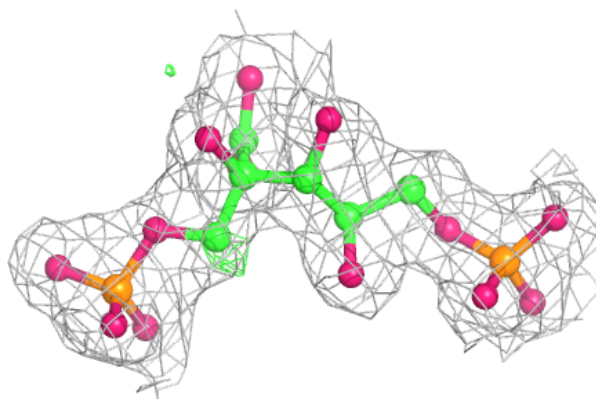
**Electron density around CAP B 477:**

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

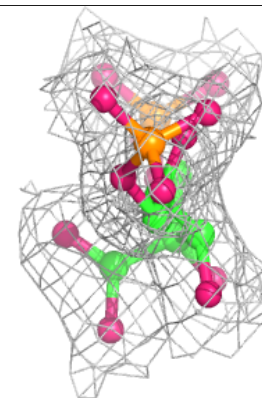
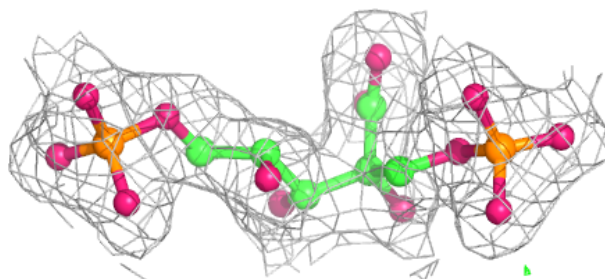
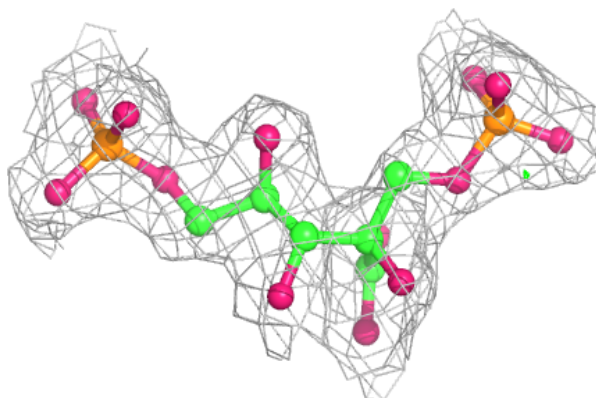


**Electron density around CAP E 477:**

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

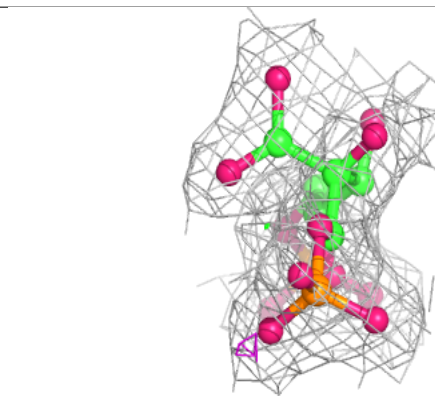
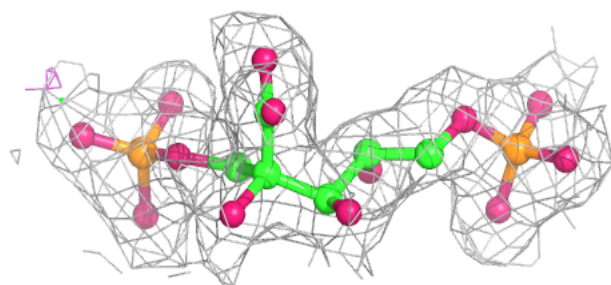
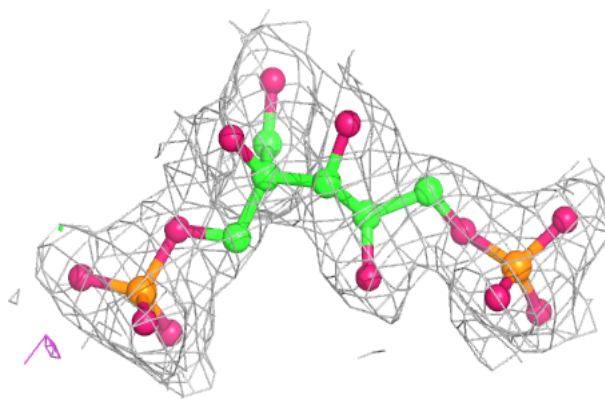
**Electron density around CAP V 477:**

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

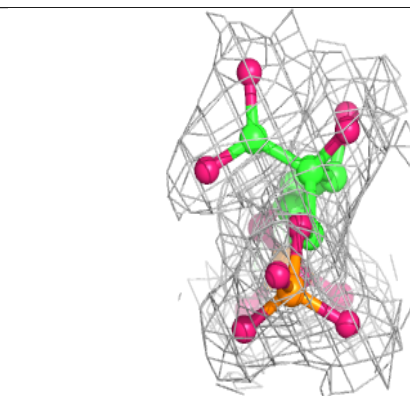
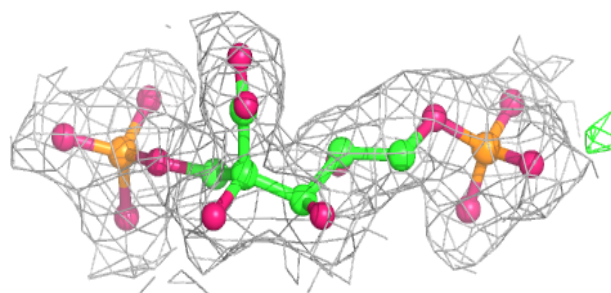
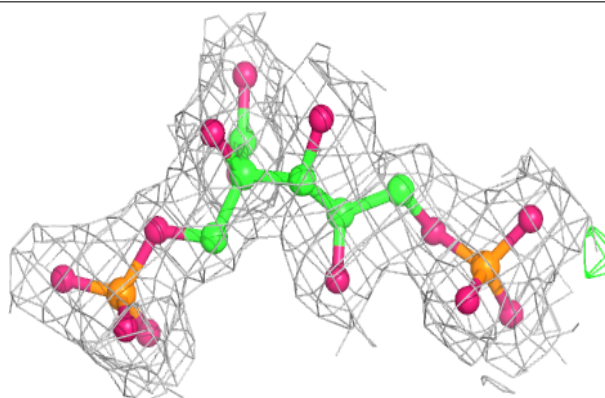


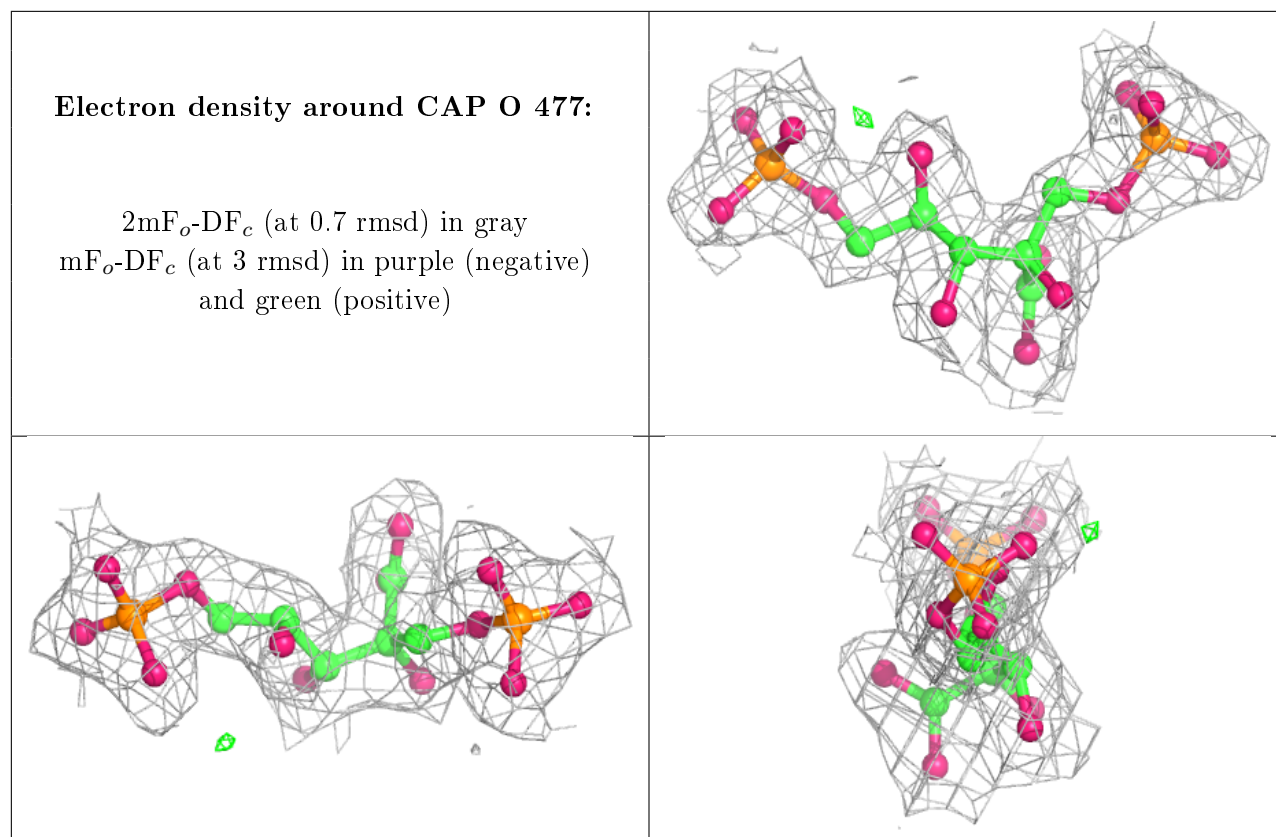
**Electron density around CAP H 477:**

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

**Electron density around CAP R 477:**

$2mF_o-DF_c$  (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.