



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 08:16 am BST

PDB ID : 2V68  
Title : Crystal structure of Chlamydomonas reinhardtii Rubisco with large- subunit mutations V331A, T342I  
Authors : Karkehabadi, S.; Satagopan, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.  
Deposited on : 2007-07-13  
Resolution : 2.30 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 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 : 2.11  
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) : 2.11

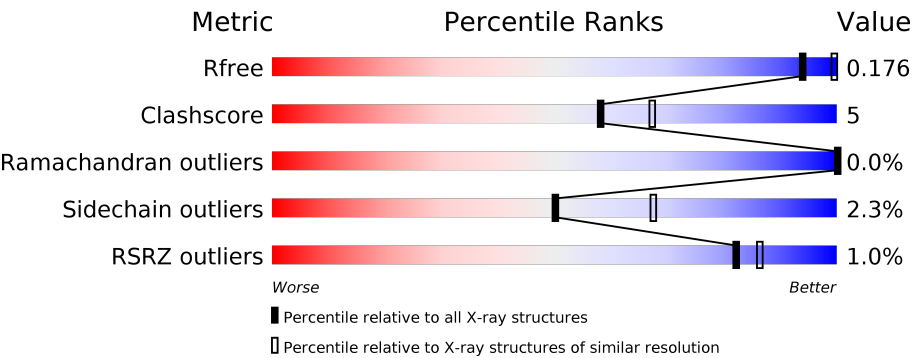
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



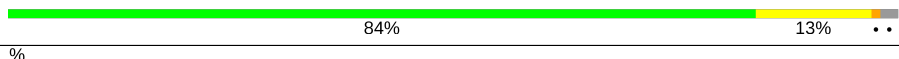
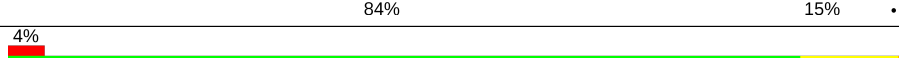
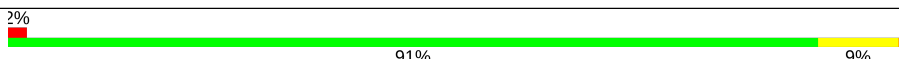
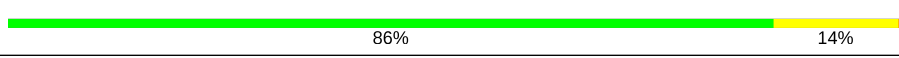

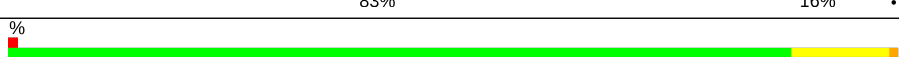

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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></div><div>87%11%.</div></div>
1	B	475	<div><div>%</div><div>86%12%..</div></div>
1	C	475	<div><div>%</div><div>88%10%..</div></div>
1	D	475	<div><div>%</div><div>87%11%.</div></div>
1	E	475	<div><div>%</div><div>87%12%.</div></div>
1	F	475	<div><div>2%</div><div>87%11%..</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	475	 89% 9% •
1	H	475	 84% 13% ••
2	I	140	 84% 15% •
2	J	140	 89% 11% •
2	K	140	 91% 9% •
2	L	140	 86% 14% •
2	M	140	 84% 15% •
2	N	140	 83% 16% •
2	O	140	 88% 11% •
2	P	140	 86% 14%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40965 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	466	Total	C	N	O	S	0	3	0
			3644	2303	642	675	24			
1	B	467	Total	C	N	O	S	0	4	0
			3651	2306	643	678	24			
1	C	467	Total	C	N	O	S	0	3	0
			3649	2306	643	676	24			
1	D	465	Total	C	N	O	S	0	3	0
			3640	2301	641	674	24			
1	E	466	Total	C	N	O	S	0	3	0
			3643	2303	642	674	24			
1	F	467	Total	C	N	O	S	0	4	0
			3653	2308	643	678	24			
1	G	466	Total	C	N	O	S	0	3	0
			3643	2302	642	675	24			
1	H	466	Total	C	N	O	S	0	3	0
			3644	2303	642	675	24			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	conflict	UNP P00877
A	331	ALA	VAL	engineered mutation	UNP P00877
A	342	ILE	THR	engineered mutation	UNP P00877
B	46	PRO	LEU	conflict	UNP P00877
B	331	ALA	VAL	engineered mutation	UNP P00877
B	342	ILE	THR	engineered mutation	UNP P00877
C	46	PRO	LEU	conflict	UNP P00877
C	331	ALA	VAL	engineered mutation	UNP P00877
C	342	ILE	THR	engineered mutation	UNP P00877
D	46	PRO	LEU	conflict	UNP P00877
D	331	ALA	VAL	engineered mutation	UNP P00877
D	342	ILE	THR	engineered mutation	UNP P00877

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	46	PRO	LEU	conflict	UNP P00877
E	331	ALA	VAL	engineered mutation	UNP P00877
E	342	ILE	THR	engineered mutation	UNP P00877
F	46	PRO	LEU	conflict	UNP P00877
F	331	ALA	VAL	engineered mutation	UNP P00877
F	342	ILE	THR	engineered mutation	UNP P00877
G	46	PRO	LEU	conflict	UNP P00877
G	331	ALA	VAL	engineered mutation	UNP P00877
G	342	ILE	THR	engineered mutation	UNP P00877
H	46	PRO	LEU	conflict	UNP P00877
H	331	ALA	VAL	engineered mutation	UNP P00877
H	342	ILE	THR	engineered mutation	UNP P00877

- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
2	J	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
2	K	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	L	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
2	M	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			
2	N	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	O	140	Total	C	N	O	S	0	1	0
			1145	740	190	203	12			
2	P	140	Total	C	N	O	S	0	0	0
			1143	739	190	203	11			

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

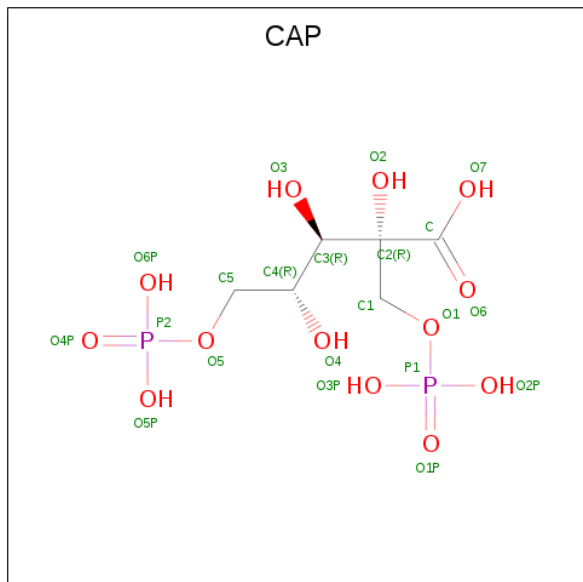
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	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	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

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



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

*Continued on next page...*

*Continued from previous page...*

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

- 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	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			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	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	E	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0
5	G	1	Total 4	C 2	O 2	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	I	1	Total 4	C 2	O 2	0	0
5	I	1	Total 4	C 2	O 2	0	0
5	J	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	L	1	Total 4	C 2	O 2	0	0
5	M	1	Total 4	C 2	O 2	0	0
5	N	1	Total 4	C 2	O 2	0	0
5	N	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	P	1	Total 4	C 2	O 2	0	0

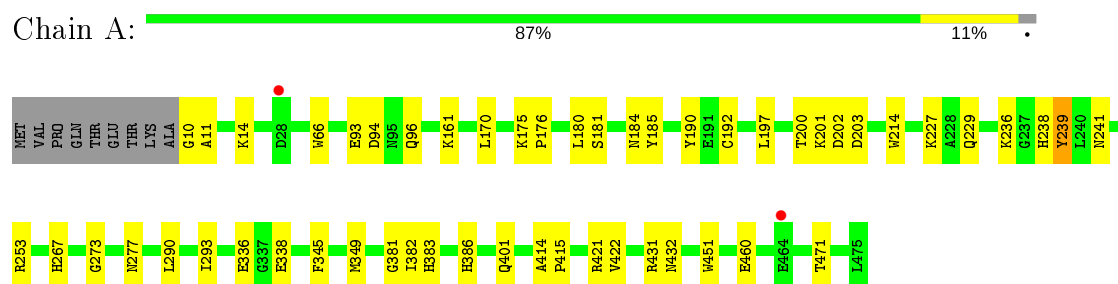
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	237	Total 237	O 237	0	0
6	B	216	Total 216	O 216	0	0
6	C	233	Total 233	O 233	0	0
6	D	211	Total 211	O 211	0	0
6	E	225	Total 225	O 225	0	0
6	F	211	Total 211	O 211	0	0
6	G	221	Total 221	O 221	0	0
6	H	234	Total 234	O 234	0	0
6	I	58	Total 58	O 58	0	0
6	J	57	Total 57	O 57	0	0
6	K	62	Total 62	O 62	0	0
6	L	78	Total 78	O 78	0	0
6	M	62	Total 62	O 62	0	0
6	N	58	Total 58	O 58	0	0
6	O	56	Total 56	O 56	0	0
6	P	57	Total 57	O 57	0	0

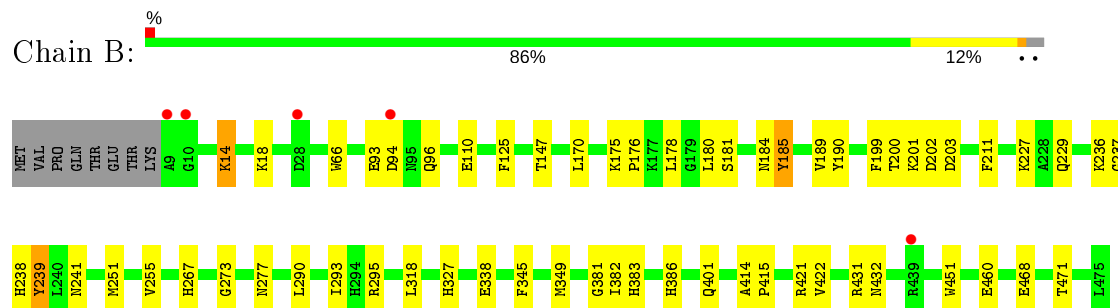
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

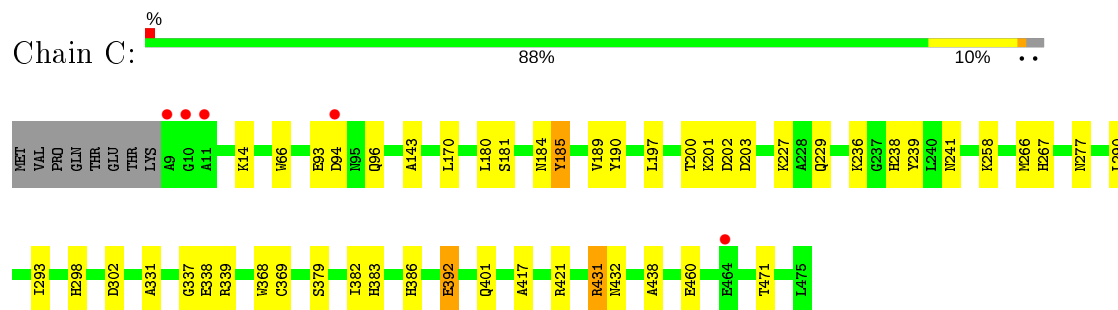
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



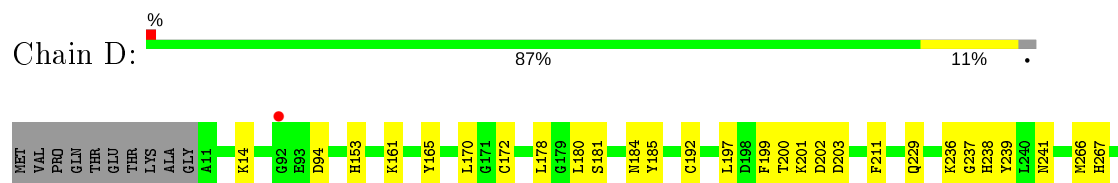
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



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

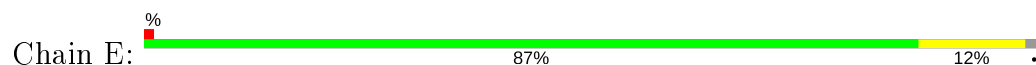


#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

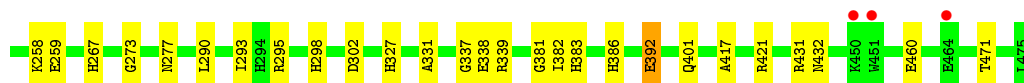
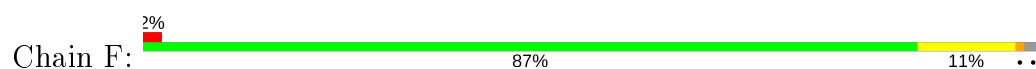




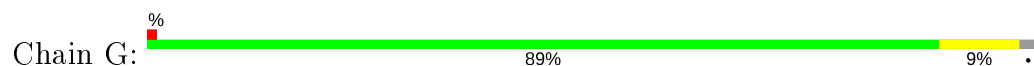
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



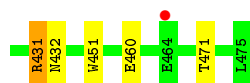
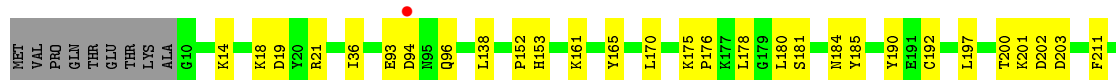
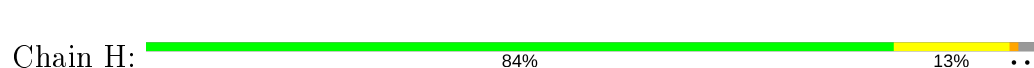
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



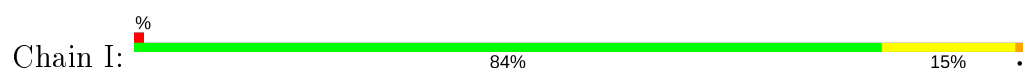
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



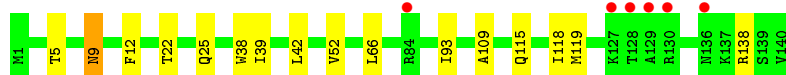
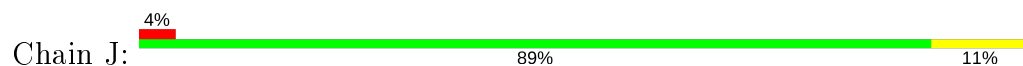
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



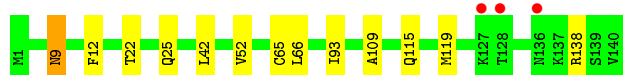
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



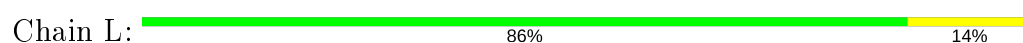
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



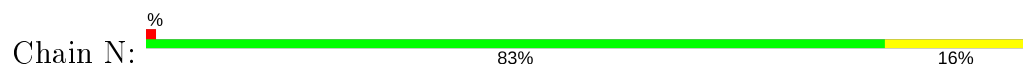
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



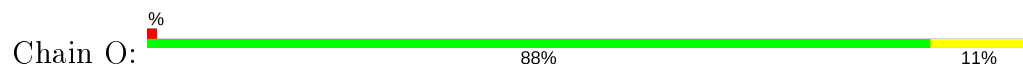
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



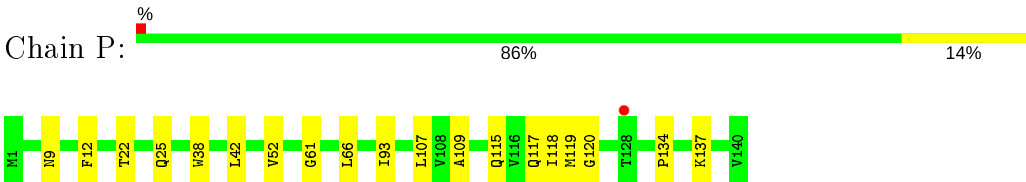
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.42Å 178.24Å 122.76Å 90.00° 117.72° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.71 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.30) 98.5 (29.71-2.22)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.203 0.173 , 0.176	Depositor DCC
$R_{free}$ test set	10093 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.010 for h,-k,-h-l 0.009 for -h-l,-k,l 0.105 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	40965	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, MME, 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	0.51	0/3698	0.57	0/4996
1	B	0.56	0/3712	0.59	0/5015
1	C	0.55	0/3703	0.61	0/5003
1	D	0.56	1/3694 (0.0%)	0.61	0/4991
1	E	0.55	0/3697	0.60	0/4996
1	F	0.55	0/3712	0.60	0/5015
1	G	0.55	0/3698	0.61	0/4996
1	H	0.56	0/3698	0.62	0/4996
2	I	0.49	0/1166	0.57	0/1584
2	J	0.53	0/1166	0.60	0/1584
2	K	0.54	0/1174	0.61	0/1594
2	L	0.54	0/1166	0.63	0/1584
2	M	0.53	0/1166	0.60	0/1584
2	N	0.53	0/1174	0.59	0/1594
2	O	0.53	0/1174	0.59	0/1594
2	P	0.55	0/1166	0.61	0/1584
All	All	0.54	1/38964 (0.0%)	0.60	0/52710

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	172	CYS	CB-SG	-5.89	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3644	0	3551	38	0
1	B	3651	0	3550	44	0
1	C	3649	0	3556	36	0
1	D	3640	0	3548	37	0
1	E	3643	0	3551	39	0
1	F	3653	0	3558	40	0
1	G	3643	0	3547	32	0
1	H	3644	0	3551	43	0
2	I	1143	0	1122	13	0
2	J	1143	0	1122	12	0
2	K	1145	0	1123	9	0
2	L	1143	0	1122	14	0
2	M	1143	0	1122	15	0
2	N	1145	0	1123	19	0
2	O	1145	0	1123	10	0
2	P	1143	0	1122	12	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
4	A	21	0	7	0	0
4	B	21	0	7	0	0
4	C	21	0	7	0	0
4	D	21	0	8	0	0
4	E	21	0	7	0	0
4	F	21	0	7	0	0
4	G	21	0	7	0	0
4	H	21	0	7	0	0
5	A	20	0	30	1	0
5	B	16	0	24	3	0
5	C	20	0	30	0	0
5	D	16	0	24	2	0
5	E	12	0	18	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	24	0	36	1	0
5	G	12	0	18	2	0
5	H	24	0	36	1	0
5	I	8	0	12	0	0
5	J	8	0	12	0	0
5	K	8	0	12	1	0
5	L	4	0	6	0	0
5	M	4	0	6	1	0
5	N	8	0	12	3	0
5	O	8	0	12	0	0
5	P	4	0	6	0	0
6	A	237	0	0	1	0
6	B	216	0	0	4	0
6	C	233	0	0	2	0
6	D	211	0	0	2	0
6	E	225	0	0	2	0
6	F	211	0	0	4	0
6	G	221	0	0	2	0
6	H	234	0	0	1	0
6	I	58	0	0	0	0
6	J	57	0	0	0	0
6	K	62	0	0	1	0
6	L	78	0	0	2	0
6	M	62	0	0	0	0
6	N	58	0	0	1	0
6	O	56	0	0	0	0
6	P	57	0	0	0	0
All	All	40965	0	37742	367	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 5.

The worst 5 of 367 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:A:267:HIS:HD2	1:A:277:ASN:HD22	1.06	0.99
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.05	0.98
1:D:267:HIS:HD2	1:D:277:ASN:HD22	1.08	0.98
1:F:267:HIS:HD2	1:F:277:ASN:HD22	1.12	0.97
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.00	0.97

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	462/475 (97%)	448 (97%)	13 (3%)	1 (0%)	47	58
1	B	464/475 (98%)	452 (97%)	12 (3%)	0	100	100
1	C	463/475 (98%)	449 (97%)	14 (3%)	0	100	100
1	D	461/475 (97%)	447 (97%)	14 (3%)	0	100	100
1	E	462/475 (97%)	449 (97%)	12 (3%)	1 (0%)	47	58
1	F	464/475 (98%)	449 (97%)	15 (3%)	0	100	100
1	G	462/475 (97%)	450 (97%)	12 (3%)	0	100	100
1	H	462/475 (97%)	450 (97%)	12 (3%)	0	100	100
2	I	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
2	J	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
2	K	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
2	L	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
2	M	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
2	N	139/140 (99%)	133 (96%)	6 (4%)	0	100	100
2	O	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
2	P	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
All	All	4807/4920 (98%)	4655 (97%)	150 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	11	ALA
1	A	11	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/375 (99%)	363 (98%)	7 (2%)	57	73
1	B	371/375 (99%)	364 (98%)	7 (2%)	57	73
1	C	370/375 (99%)	362 (98%)	8 (2%)	52	69
1	D	370/375 (99%)	363 (98%)	7 (2%)	57	73
1	E	370/375 (99%)	363 (98%)	7 (2%)	57	73
1	F	371/375 (99%)	363 (98%)	8 (2%)	52	69
1	G	370/375 (99%)	362 (98%)	8 (2%)	52	69
1	H	370/375 (99%)	361 (98%)	9 (2%)	49	66
2	I	122/122 (100%)	118 (97%)	4 (3%)	38	53
2	J	122/122 (100%)	119 (98%)	3 (2%)	47	65
2	K	123/122 (101%)	120 (98%)	3 (2%)	49	66
2	L	122/122 (100%)	119 (98%)	3 (2%)	47	65
2	M	122/122 (100%)	118 (97%)	4 (3%)	38	53
2	N	123/122 (101%)	120 (98%)	3 (2%)	49	66
2	O	123/122 (101%)	118 (96%)	5 (4%)	30	43
2	P	122/122 (100%)	119 (98%)	3 (2%)	47	65
All	All	3941/3976 (99%)	3852 (98%)	89 (2%)	50	67

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	239	TYR
1	G	241	ASN
2	O	12	PHE
1	F	241	ASN
1	G	94	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	267	HIS
1	G	401	GLN
2	O	8	ASN
1	F	304	GLN
1	G	238	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 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	SMC	B	256	1	5,6,7	0.53	0	2,6,8	0.62	0
1	SMC	H	256	1	5,6,7	0.71	0	2,6,8	0.41	0
1	HYP	G	104	1	6,8,9	0.63	0	5,10,12	1.23	0
1	KCX	C	201	1,3	7,11,12	0.90	0	4,12,14	0.45	0
1	HYP	E	151	1	6,8,9	0.71	0	5,10,12	1.19	0
1	HYP	A	151	1	6,8,9	0.66	0	5,10,12	1.47	0
1	SMC	D	369	1	5,6,7	0.81	0	2,6,8	1.00	0
1	SMC	F	369	1	5,6,7	0.93	0	2,6,8	0.50	0
1	KCX	A	201	1,3	7,11,12	1.14	1 (14%)	4,12,14	0.30	0
1	KCX	H	201	1,3	7,11,12	0.82	0	4,12,14	0.52	0
1	HYP	F	151	1	6,8,9	0.74	0	5,10,12	1.51	1 (20%)
1	HYP	C	104	1	6,8,9	0.47	0	5,10,12	1.01	0
1	KCX	E	201	1,3	7,11,12	1.10	1 (14%)	4,12,14	0.98	0
1	SMC	D	256	1	5,6,7	1.05	1 (20%)	2,6,8	1.64	1 (50%)
1	SMC	E	369	1	5,6,7	0.77	0	2,6,8	1.07	0
2	MME	I	1	2	7,8,9	2.80	1 (14%)	5,8,10	1.23	1 (20%)
1	KCX	B	201	1,3	7,11,12	0.94	0	4,12,14	0.29	0
2	MME	N	1	2	7,8,9	2.87	1 (14%)	5,8,10	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	B	151	1	6,8,9	0.55	0	5,10,12	1.60	1 (20%)
1	SMC	C	256	1	5,6,7	0.93	0	2,6,8	1.11	0
1	HYP	A	104	1	6,8,9	0.60	0	5,10,12	1.09	0
1	HYP	D	104	1	6,8,9	0.63	0	5,10,12	0.97	0
1	SMC	B	369	1	5,6,7	0.69	0	2,6,8	0.90	0
1	HYP	H	104	1	6,8,9	0.56	0	5,10,12	1.10	0
1	HYP	G	151	1	6,8,9	0.42	0	5,10,12	1.40	0
1	SMC	A	369	1	5,6,7	0.94	0	2,6,8	0.50	0
1	SMC	C	369	1	5,6,7	0.81	0	2,6,8	0.51	0
1	SMC	H	369	1	5,6,7	0.90	0	2,6,8	0.39	0
1	HYP	H	151	1	6,8,9	0.70	0	5,10,12	1.46	1 (20%)
1	SMC	A	256	1	5,6,7	0.78	0	2,6,8	0.98	0
2	MME	O	1	2	7,8,9	2.90	1 (14%)	5,8,10	1.21	1 (20%)
1	HYP	D	151	1	6,8,9	0.59	0	5,10,12	1.38	1 (20%)
1	KCX	F	201	1,3	7,11,12	0.76	0	4,12,14	0.46	0
1	HYP	F	104	1	6,8,9	0.59	0	5,10,12	1.08	0
1	HYP	B	104	1	6,8,9	0.65	0	5,10,12	1.00	0
1	HYP	E	104	1	6,8,9	0.68	0	5,10,12	1.10	0
2	MME	P	1	2	7,8,9	2.81	1 (14%)	5,8,10	1.30	1 (20%)
2	MME	K	1	2	7,8,9	2.79	1 (14%)	5,8,10	1.36	1 (20%)
1	SMC	F	256	1	5,6,7	0.74	0	2,6,8	0.30	0
1	HYP	C	151	1	6,8,9	0.71	0	5,10,12	1.58	1 (20%)
1	KCX	G	201	1,3	7,11,12	1.21	1 (14%)	4,12,14	0.50	0
1	SMC	E	256	1	5,6,7	0.93	0	2,6,8	1.18	0
1	SMC	G	369	1	5,6,7	1.08	0	2,6,8	0.53	0
1	SMC	G	256	1	5,6,7	0.56	0	2,6,8	0.45	0
2	MME	L	1	2	7,8,9	2.70	1 (14%)	5,8,10	1.09	0
2	MME	M	1	2	7,8,9	2.74	1 (14%)	5,8,10	1.33	1 (20%)
2	MME	J	1	2	7,8,9	2.84	1 (14%)	5,8,10	1.24	1 (20%)
1	KCX	D	201	1,3	7,11,12	1.22	1 (14%)	4,12,14	0.41	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	SMC	B	256	1	-	0/3/5/7	-
1	SMC	H	256	1	-	0/3/5/7	-
1	HYP	G	104	1	-	0/0/11/13	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	201	1,3	-	0/7/10/12	-
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	SMC	D	369	1	-	1/3/5/7	-
1	SMC	F	369	1	-	1/3/5/7	-
1	KCX	A	201	1,3	-	0/7/10/12	-
1	KCX	H	201	1,3	-	0/7/10/12	-
1	HYP	F	151	1	-	0/0/11/13	0/1/1/1
1	HYP	C	104	1	-	0/0/11/13	0/1/1/1
1	KCX	E	201	1,3	-	1/7/10/12	-
1	SMC	D	256	1	-	0/3/5/7	-
1	SMC	E	369	1	-	1/3/5/7	-
2	MME	I	1	2	-	3/5/8/10	-
1	KCX	B	201	1,3	-	0/7/10/12	-
2	MME	N	1	2	-	3/5/8/10	-
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	SMC	C	256	1	-	0/3/5/7	-
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	HYP	D	104	1	-	0/0/11/13	0/1/1/1
1	SMC	B	369	1	-	1/3/5/7	-
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	HYP	G	151	1	-	0/0/11/13	0/1/1/1
1	SMC	A	369	1	-	1/3/5/7	-
1	SMC	C	369	1	-	1/3/5/7	-
1	SMC	H	369	1	-	1/3/5/7	-
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	SMC	A	256	1	-	0/3/5/7	-
2	MME	O	1	2	-	2/5/8/10	-
1	HYP	D	151	1	-	0/0/11/13	0/1/1/1
1	KCX	F	201	1,3	-	0/7/10/12	-
1	HYP	F	104	1	-	0/0/11/13	0/1/1/1
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
2	MME	P	1	2	-	2/5/8/10	-
2	MME	K	1	2	-	2/5/8/10	-
1	SMC	F	256	1	-	0/3/5/7	-
1	HYP	C	151	1	-	0/0/11/13	0/1/1/1
1	KCX	G	201	1,3	-	0/7/10/12	-
1	SMC	E	256	1	-	0/3/5/7	-
1	SMC	G	369	1	-	1/3/5/7	-
1	SMC	G	256	1	-	0/3/5/7	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MME	L	1	2	-	3/5/8/10	-
2	MME	M	1	2	-	3/5/8/10	-
2	MME	J	1	2	-	3/5/8/10	-
1	KCX	D	201	1,3	-	0/7/10/12	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1	MME	CM-N	-7.34	1.27	1.46
2	P	1	MME	CM-N	-7.27	1.27	1.46
2	I	1	MME	CM-N	-7.26	1.27	1.46
2	J	1	MME	CM-N	-7.25	1.27	1.46
2	N	1	MME	CM-N	-7.21	1.27	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	MME	CM-N-CA	2.35	120.96	113.64
1	B	151	HYP	O-C-CA	-2.33	118.67	124.78
1	C	151	HYP	CG-CB-CA	-2.32	101.03	103.96
2	K	1	MME	CM-N-CA	2.31	120.83	113.64
1	D	256	SMC	CS-SG-CB	2.26	105.45	101.30

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	MME	C-CA-CB-CG
2	O	1	MME	CB-CG-SD-CE
2	L	1	MME	CB-CG-SD-CE
2	J	1	MME	CB-CG-SD-CE
2	K	1	MME	CB-CG-SD-CE

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	201	KCX	1	0
1	A	201	KCX	1	0
1	H	201	KCX	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	201	KCX	1	0
1	B	201	KCX	1	0
1	C	369	SMC	1	0
1	H	369	SMC	1	0
1	F	201	KCX	1	0
1	D	201	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 65 ligands modelled in this entry, 8 are monoatomic - leaving 57 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	K	1142	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	A	1483	-	3,3,3	0.48	0	2,2,2	0.41	0
5	EDO	H	1476	-	3,3,3	0.80	0	2,2,2	0.14	0
5	EDO	F	1482	-	3,3,3	0.60	0	2,2,2	0.11	0
5	EDO	B	1481	-	3,3,3	0.47	0	2,2,2	0.05	0
5	EDO	M	1141	-	3,3,3	0.49	0	2,2,2	0.11	0
5	EDO	B	1480	-	3,3,3	0.73	0	2,2,2	0.12	0
5	EDO	D	1478	-	3,3,3	0.55	0	2,2,2	0.08	0
4	CAP	A	477	3	15,20,20	0.97	0	20,31,31	0.62	0
4	CAP	B	477	3	15,20,20	0.97	1 (6%)	20,31,31	0.82	0
5	EDO	G	1480	-	3,3,3	0.47	0	2,2,2	0.25	0
5	EDO	N	1142	-	3,3,3	0.52	0	2,2,2	0.07	0
5	EDO	H	1482	-	3,3,3	0.53	0	2,2,2	0.17	0
5	EDO	D	1480	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	H	1478	-	3,3,3	0.42	0	2,2,2	0.26	0
5	EDO	F	1483	-	3,3,3	0.56	0	2,2,2	0.35	0
5	EDO	C	1478	-	3,3,3	0.54	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	O	1142	-	3,3,3	0.50	0	2,2,2	0.40	0
5	EDO	A	1482	-	3,3,3	0.66	0	2,2,2	0.22	0
5	EDO	D	1477	-	3,3,3	0.66	0	2,2,2	0.07	0
5	EDO	E	1478	-	3,3,3	0.53	0	2,2,2	0.24	0
5	EDO	I	1141	-	3,3,3	0.54	0	2,2,2	0.18	0
5	EDO	F	1479	-	3,3,3	0.48	0	2,2,2	0.16	0
5	EDO	D	1481	-	3,3,3	0.58	0	2,2,2	0.18	0
5	EDO	F	1484	-	3,3,3	0.63	0	2,2,2	0.06	0
5	EDO	F	1481	-	3,3,3	0.52	0	2,2,2	0.28	0
5	EDO	F	1480	-	3,3,3	0.51	0	2,2,2	0.28	0
5	EDO	A	1484	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	C	1481	-	3,3,3	0.61	0	2,2,2	0.17	0
5	EDO	H	1480	-	3,3,3	0.60	0	2,2,2	0.07	0
4	CAP	H	477	3	15,20,20	0.85	0	20,31,31	0.57	0
5	EDO	C	1482	-	3,3,3	0.65	0	2,2,2	0.23	0
5	EDO	G	1478	-	3,3,3	0.43	0	2,2,2	0.19	0
5	EDO	C	1477	-	3,3,3	0.52	0	2,2,2	0.22	0
5	EDO	E	1476	-	3,3,3	0.63	0	2,2,2	0.05	0
5	EDO	A	1477	-	3,3,3	0.48	0	2,2,2	0.29	0
5	EDO	B	1477	-	3,3,3	0.78	0	2,2,2	0.14	0
5	EDO	N	1141	-	3,3,3	0.61	0	2,2,2	0.13	0
5	EDO	K	1141	-	3,3,3	0.53	0	2,2,2	0.32	0
5	EDO	L	1141	-	3,3,3	0.53	0	2,2,2	0.17	0
5	EDO	H	1481	-	3,3,3	0.52	0	2,2,2	0.24	0
4	CAP	C	477	3	15,20,20	0.79	0	20,31,31	0.70	0
5	EDO	P	1141	-	3,3,3	0.50	0	2,2,2	0.28	0
4	CAP	E	477	3	15,20,20	0.71	0	20,31,31	0.91	0
5	EDO	J	1142	-	3,3,3	0.45	0	2,2,2	0.23	0
5	EDO	J	1141	-	3,3,3	0.49	0	2,2,2	0.25	0
5	EDO	H	1483	-	3,3,3	0.66	0	2,2,2	0.12	0
5	EDO	C	1480	-	3,3,3	0.64	0	2,2,2	0.09	0
5	EDO	B	1479	-	3,3,3	0.50	0	2,2,2	0.25	0
4	CAP	D	477	3	15,20,20	0.77	0	20,31,31	0.70	0
5	EDO	O	1141	-	3,3,3	0.42	0	2,2,2	0.32	0
5	EDO	E	1480	-	3,3,3	0.58	0	2,2,2	0.15	0
4	CAP	F	477	3	15,20,20	0.66	0	20,31,31	0.74	0
4	CAP	G	477	3	15,20,20	0.83	0	20,31,31	0.71	0
5	EDO	G	1476	-	3,3,3	0.65	0	2,2,2	0.17	0
5	EDO	A	1481	-	3,3,3	0.75	0	2,2,2	0.06	0
5	EDO	I	1142	-	3,3,3	0.64	0	2,2,2	0.21	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	K	1142	-	-	0/1/1/1	-
5	EDO	A	1483	-	-	1/1/1/1	-
5	EDO	H	1476	-	-	0/1/1/1	-
5	EDO	F	1482	-	-	0/1/1/1	-
5	EDO	B	1481	-	-	0/1/1/1	-
5	EDO	M	1141	-	-	1/1/1/1	-
5	EDO	B	1480	-	-	0/1/1/1	-
5	EDO	D	1478	-	-	1/1/1/1	-
4	CAP	A	477	3	-	3/23/29/29	-
4	CAP	B	477	3	-	4/23/29/29	-
5	EDO	G	1480	-	-	1/1/1/1	-
5	EDO	N	1142	-	-	0/1/1/1	-
5	EDO	H	1482	-	-	0/1/1/1	-
5	EDO	D	1480	-	-	1/1/1/1	-
5	EDO	H	1478	-	-	0/1/1/1	-
5	EDO	F	1483	-	-	1/1/1/1	-
5	EDO	C	1478	-	-	1/1/1/1	-
5	EDO	O	1142	-	-	1/1/1/1	-
5	EDO	A	1482	-	-	0/1/1/1	-
5	EDO	D	1477	-	-	0/1/1/1	-
5	EDO	E	1478	-	-	1/1/1/1	-
5	EDO	I	1141	-	-	1/1/1/1	-
5	EDO	F	1479	-	-	0/1/1/1	-
5	EDO	D	1481	-	-	1/1/1/1	-
5	EDO	F	1484	-	-	0/1/1/1	-
5	EDO	F	1481	-	-	0/1/1/1	-
5	EDO	F	1480	-	-	0/1/1/1	-
5	EDO	A	1484	-	-	1/1/1/1	-
5	EDO	C	1481	-	-	0/1/1/1	-
5	EDO	H	1480	-	-	0/1/1/1	-
4	CAP	H	477	3	-	3/23/29/29	-
5	EDO	C	1482	-	-	1/1/1/1	-
5	EDO	G	1478	-	-	1/1/1/1	-
5	EDO	C	1477	-	-	0/1/1/1	-
5	EDO	E	1476	-	-	0/1/1/1	-
5	EDO	A	1477	-	-	0/1/1/1	-
5	EDO	B	1477	-	-	0/1/1/1	-
5	EDO	N	1141	-	-	1/1/1/1	-
5	EDO	K	1141	-	-	0/1/1/1	-
5	EDO	L	1141	-	-	1/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	H	1481	-	-	1/1/1/1	-
4	CAP	C	477	3	-	3/23/29/29	-
5	EDO	P	1141	-	-	1/1/1/1	-
4	CAP	E	477	3	-	5/23/29/29	-
5	EDO	J	1142	-	-	0/1/1/1	-
5	EDO	J	1141	-	-	1/1/1/1	-
5	EDO	H	1483	-	-	0/1/1/1	-
5	EDO	C	1480	-	-	1/1/1/1	-
5	EDO	B	1479	-	-	1/1/1/1	-
4	CAP	D	477	3	-	3/23/29/29	-
5	EDO	O	1141	-	-	0/1/1/1	-
5	EDO	E	1480	-	-	0/1/1/1	-
4	CAP	F	477	3	-	3/23/29/29	-
4	CAP	G	477	3	-	3/23/29/29	-
5	EDO	G	1476	-	-	0/1/1/1	-
5	EDO	A	1481	-	-	1/1/1/1	-
5	EDO	I	1142	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	477	CAP	C4-C3	-2.39	1.51	1.54

There are no bond angle outliers.

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

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

There are no ring outliers.

10 monomers are involved in 15 short contacts:

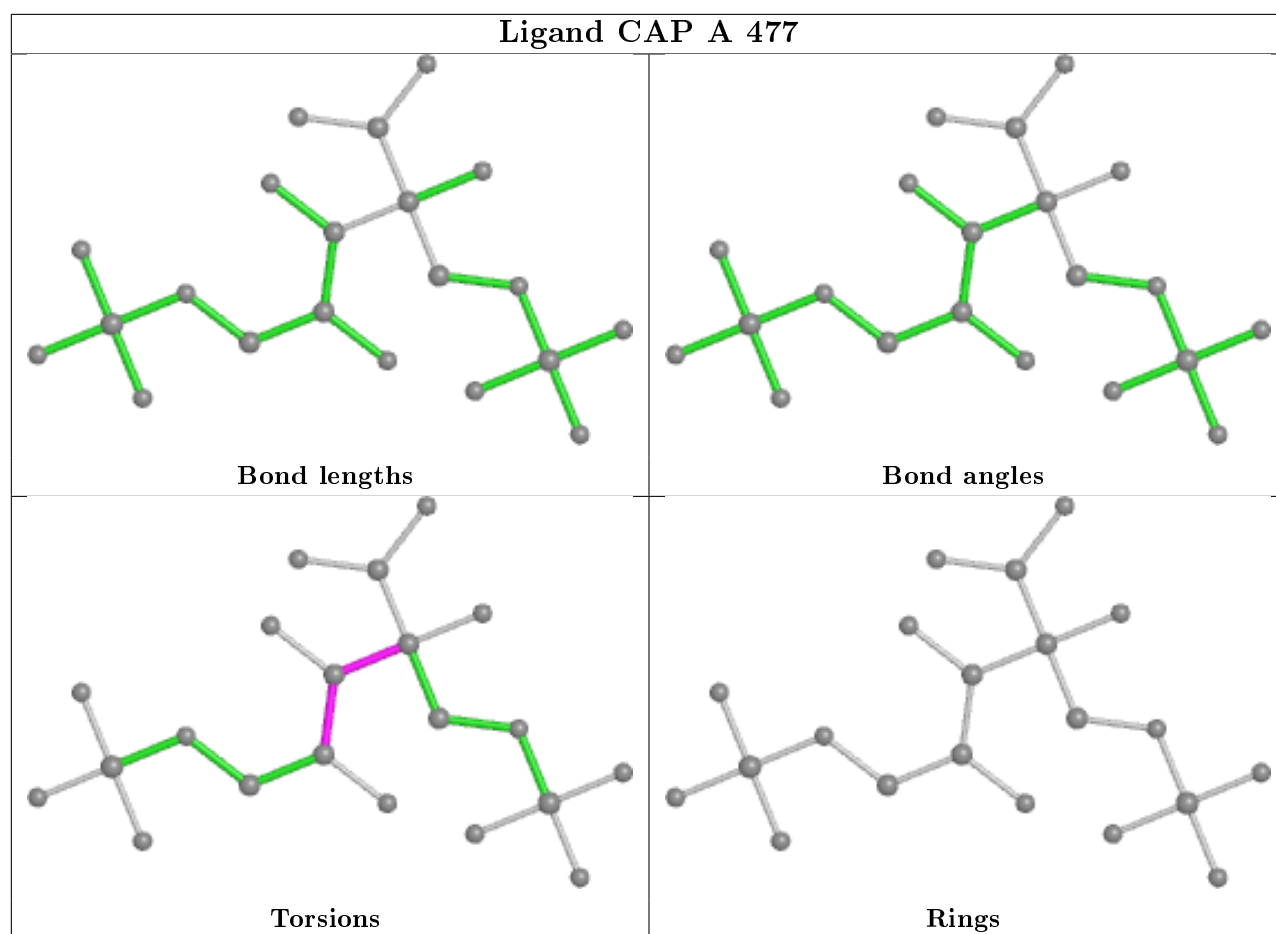
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1142	EDO	1	0
5	B	1481	EDO	1	0

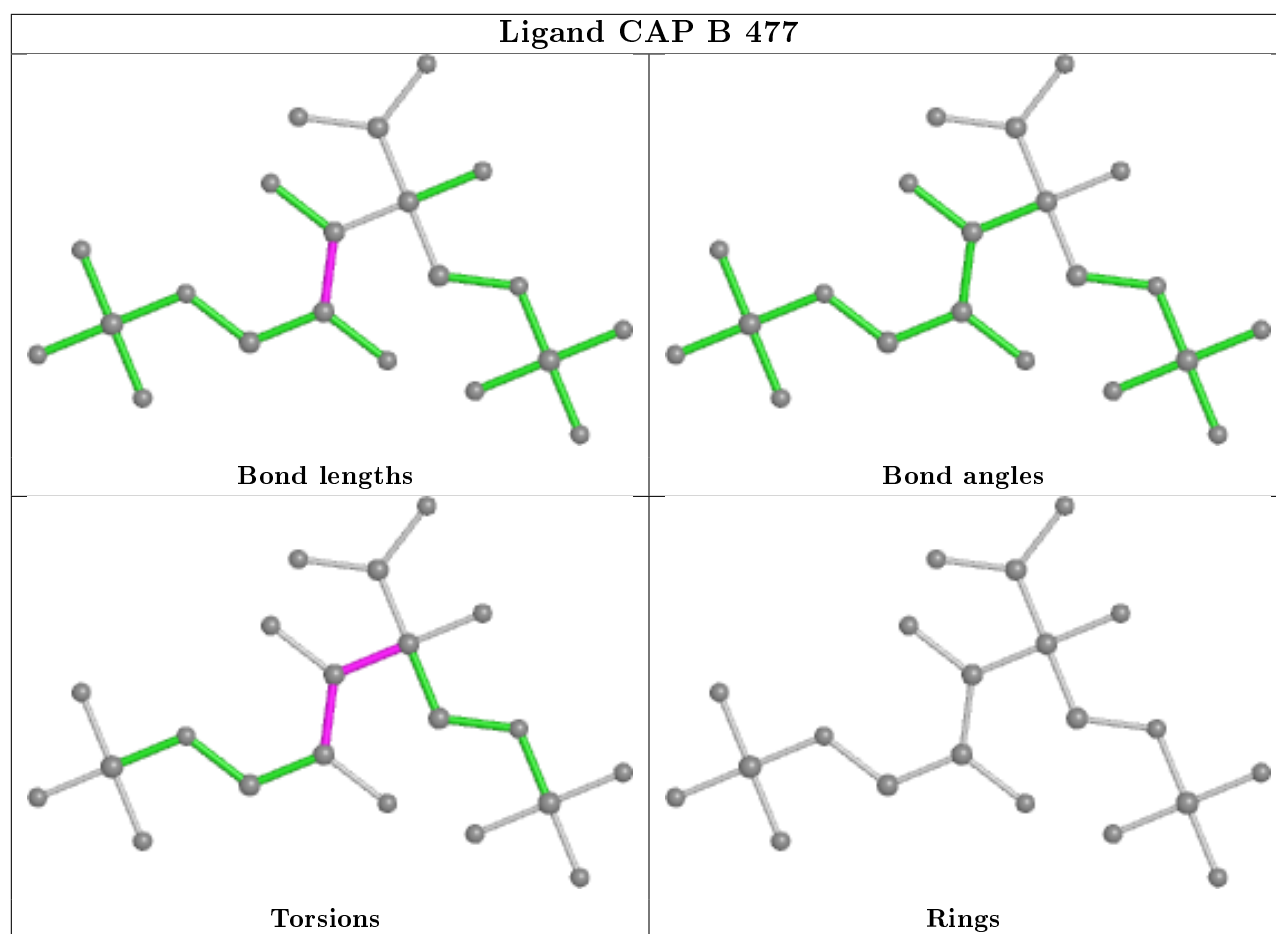
*Continued on next page...*

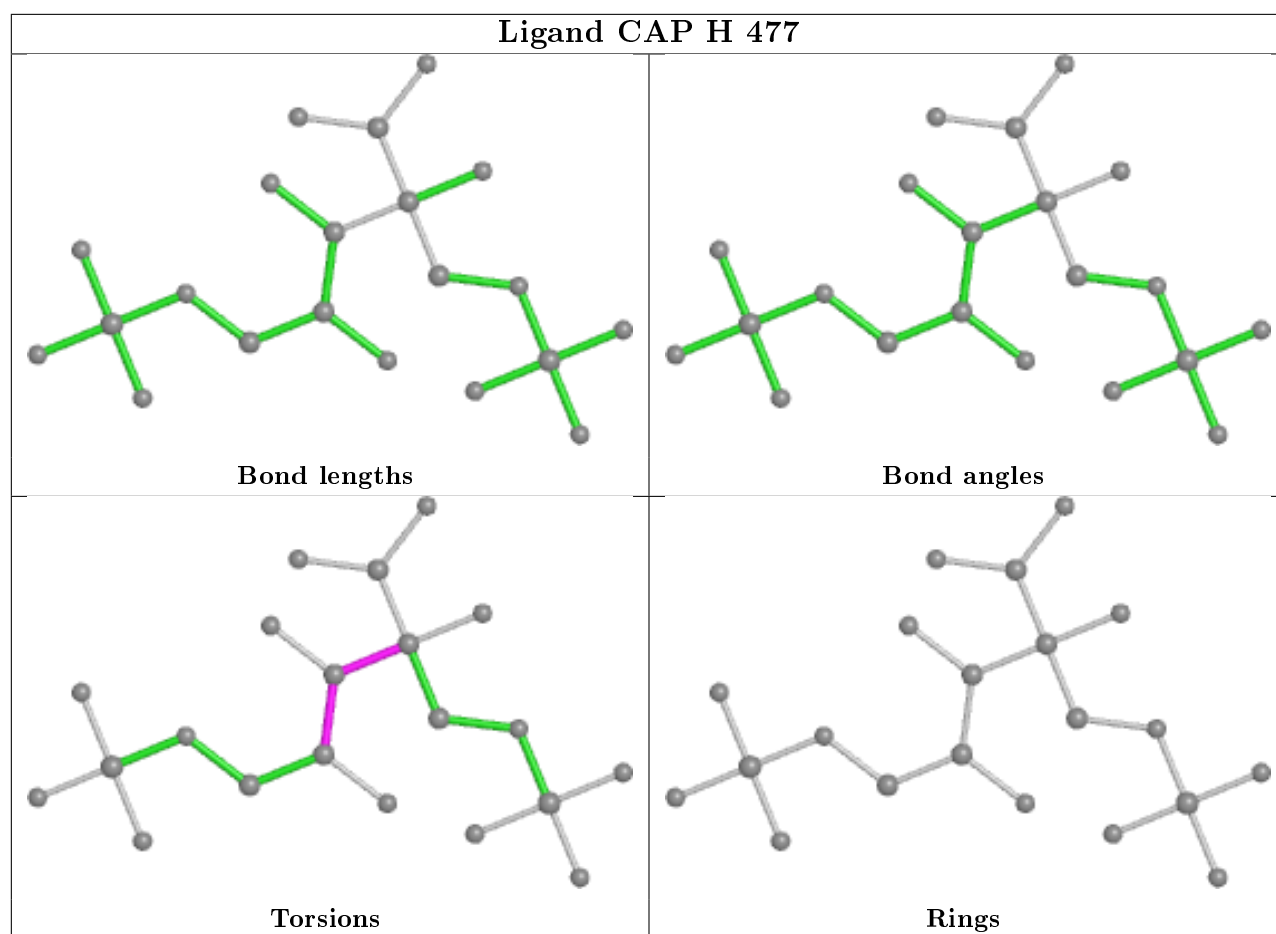
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1141	EDO	1	0
5	D	1478	EDO	2	0
5	G	1480	EDO	2	0
5	H	1482	EDO	1	0
5	F	1484	EDO	1	0
5	A	1484	EDO	1	0
5	N	1141	EDO	3	0
5	B	1479	EDO	2	0

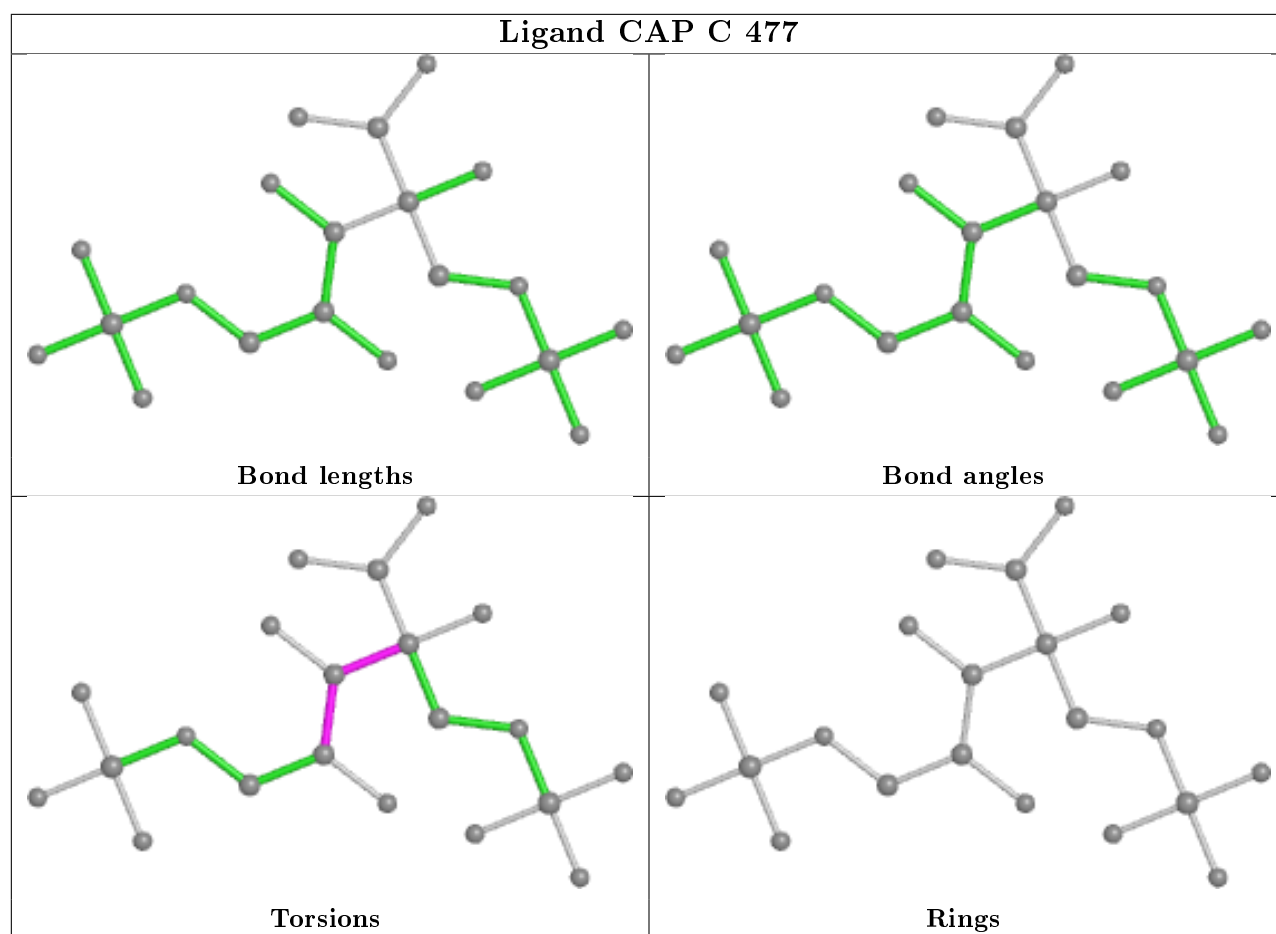
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

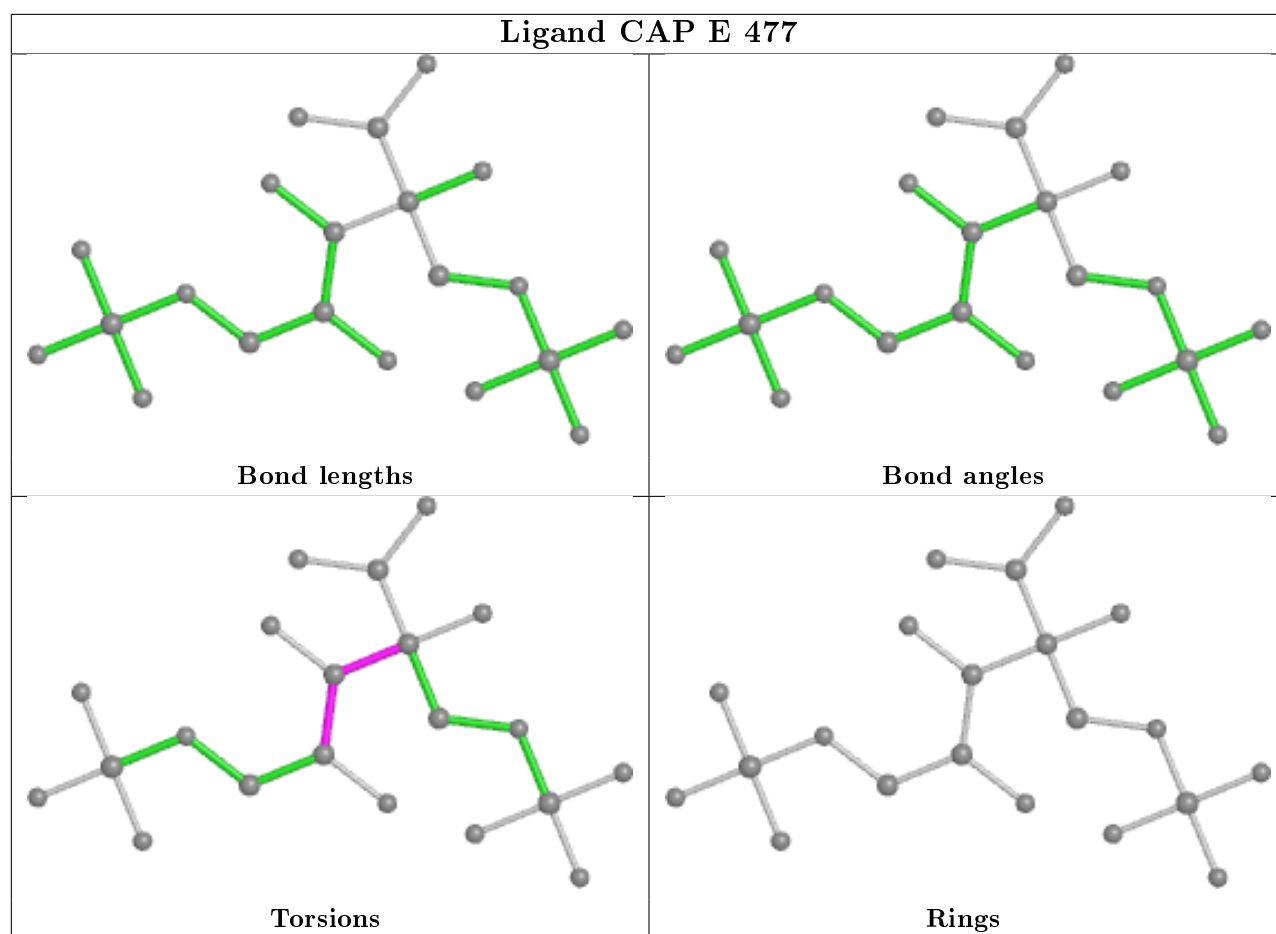


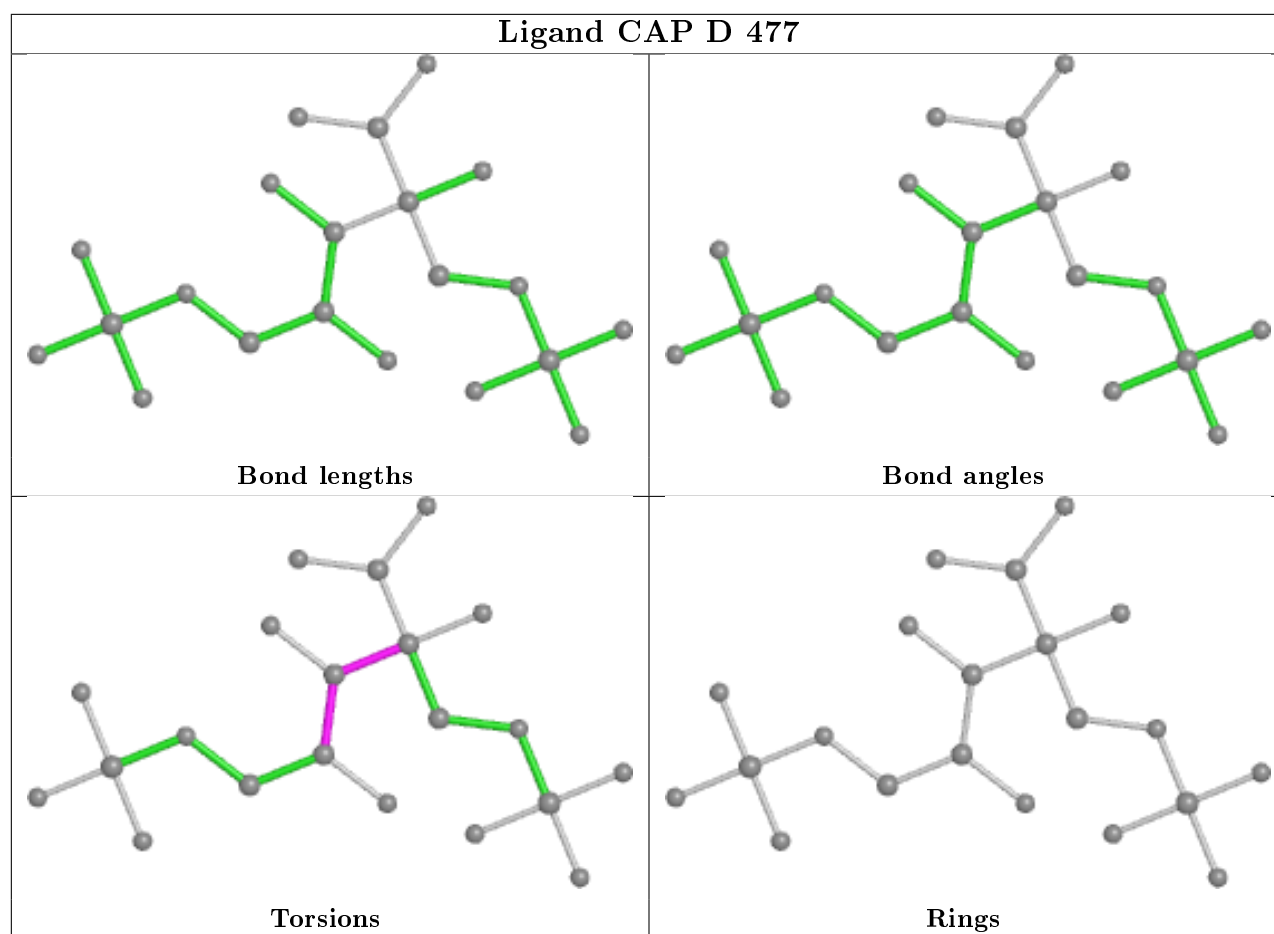


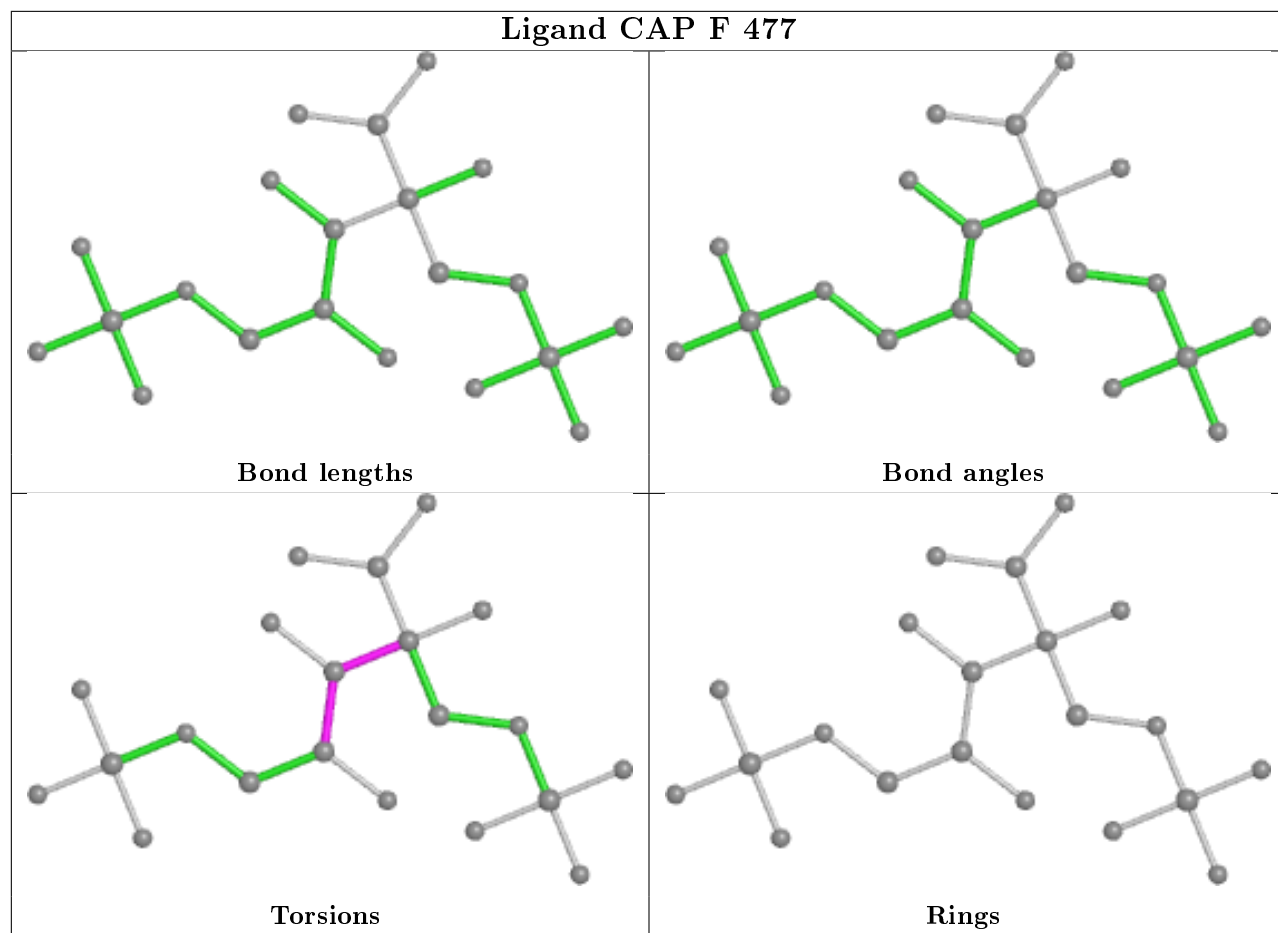


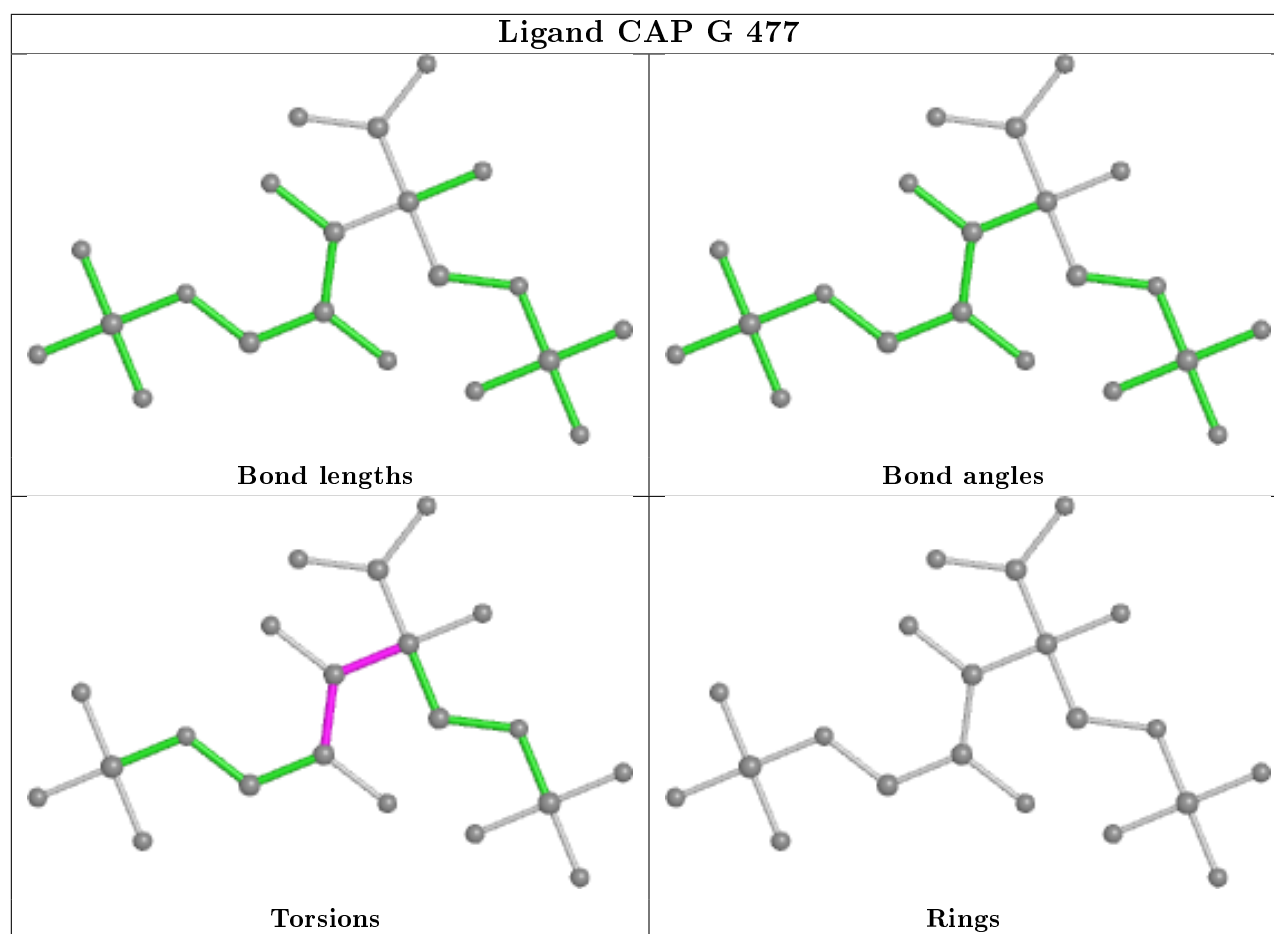












## 5.7 Other polymers [i](#)

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	461/475 (97%)	-0.40	2 (0%) 92 95	11, 16, 31, 40	0
1	B	462/475 (97%)	-0.38	5 (1%) 80 85	11, 16, 31, 42	0
1	C	462/475 (97%)	-0.43	5 (1%) 80 85	11, 16, 31, 41	0
1	D	460/475 (96%)	-0.38	4 (0%) 84 88	11, 16, 31, 42	0
1	E	461/475 (97%)	-0.40	6 (1%) 77 81	11, 16, 31, 40	0
1	F	462/475 (97%)	-0.41	8 (1%) 70 76	11, 16, 31, 44	1 (0%)
1	G	461/475 (97%)	-0.42	3 (0%) 87 91	11, 16, 31, 40	0
1	H	461/475 (97%)	-0.45	2 (0%) 92 95	11, 16, 31, 40	0
2	I	139/140 (99%)	-0.15	2 (1%) 75 80	12, 22, 34, 37	1 (0%)
2	J	139/140 (99%)	0.00	6 (4%) 35 42	13, 22, 36, 40	1 (0%)
2	K	139/140 (99%)	-0.20	3 (2%) 62 69	12, 22, 35, 37	1 (0%)
2	L	139/140 (99%)	-0.40	0 100 100	13, 22, 34, 36	0
2	M	139/140 (99%)	-0.40	0 100 100	13, 22, 34, 36	0
2	N	139/140 (99%)	-0.24	1 (0%) 87 91	12, 22, 36, 40	0
2	O	139/140 (99%)	-0.17	2 (1%) 75 80	12, 22, 34, 37	1 (0%)
2	P	139/140 (99%)	-0.18	1 (0%) 87 91	13, 22, 34, 37	0
All	All	4802/4920 (97%)	-0.36	50 (1%) 82 86	11, 17, 32, 44	5 (0%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	127	LYS	4.1
1	B	10	GLY	4.0
1	F	11	ALA	3.9
1	C	10	GLY	3.8
1	E	92	GLY	3.6

## 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
2	MME	K	1	9/10	0.90	0.15	26,27,31,33	0
1	HYP	H	151	8/9	0.91	0.12	12,13,13,13	0
2	MME	M	1	9/10	0.92	0.15	26,27,30,33	0
2	MME	J	1	9/10	0.92	0.14	26,26,31,33	0
1	HYP	A	104	8/9	0.93	0.09	13,14,14,14	0
2	MME	P	1	9/10	0.93	0.14	25,26,32,33	0
1	HYP	F	104	8/9	0.94	0.08	13,14,14,14	0
1	HYP	A	151	8/9	0.94	0.11	12,13,13,13	0
2	MME	L	1	9/10	0.94	0.12	26,27,31,33	0
2	MME	N	1	9/10	0.94	0.15	26,27,31,33	0
1	SMC	A	256	7/8	0.94	0.09	10,12,13,13	0
1	KCX	C	201	12/13	0.95	0.10	12,13,14,14	0
2	MME	O	1	9/10	0.95	0.09	26,27,31,33	0
1	HYP	E	104	8/9	0.95	0.09	13,14,14,14	0
1	SMC	C	369	7/8	0.95	0.09	16,16,17,19	0
1	HYP	E	151	8/9	0.95	0.09	12,13,13,13	0
1	HYP	C	104	8/9	0.95	0.08	13,14,14,15	0
1	HYP	H	104	8/9	0.96	0.08	13,14,14,15	0
1	SMC	A	369	7/8	0.96	0.09	16,16,17,19	0
1	KCX	B	201	12/13	0.96	0.11	12,13,14,14	0
1	SMC	E	256	7/8	0.96	0.09	10,12,13,13	0
1	KCX	A	201	12/13	0.96	0.10	12,13,13,14	0
1	SMC	G	369	7/8	0.96	0.08	16,16,17,19	0
1	HYP	D	151	8/9	0.96	0.09	12,13,13,13	0
1	KCX	D	201	12/13	0.96	0.11	12,13,13,14	0
1	KCX	E	201	12/13	0.97	0.10	12,13,13,14	0
1	SMC	H	256	7/8	0.97	0.08	11,12,12,13	0
1	SMC	E	369	7/8	0.97	0.07	16,16,18,19	0
2	MME	I	1	9/10	0.97	0.09	26,26,31,33	0
1	SMC	D	369	7/8	0.97	0.08	16,16,18,19	0
1	KCX	F	201	12/13	0.97	0.09	12,13,14,15	0
1	HYP	G	104	8/9	0.97	0.08	13,13,14,14	0
1	HYP	B	104	8/9	0.97	0.07	13,13,14,14	0
1	KCX	H	201	12/13	0.97	0.12	12,13,13,14	0
1	HYP	B	151	8/9	0.97	0.06	13,13,13,14	0
1	SMC	F	256	7/8	0.97	0.08	11,12,13,14	0
1	KCX	G	201	12/13	0.97	0.13	12,13,13,14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SMC	C	256	7/8	0.97	0.08	10,12,12,13	0
1	SMC	D	256	7/8	0.97	0.07	9,12,12,13	0
1	HYP	F	151	8/9	0.97	0.09	13,13,13,14	0
1	HYP	D	104	8/9	0.97	0.07	13,13,14,14	0
1	SMC	F	369	7/8	0.97	0.10	16,17,18,19	0
1	HYP	G	151	8/9	0.97	0.08	13,13,13,14	0
1	SMC	G	256	7/8	0.98	0.08	10,12,13,13	0
1	SMC	B	256	7/8	0.98	0.08	10,12,12,13	0
1	HYP	C	151	8/9	0.98	0.07	13,13,14,14	0
1	SMC	H	369	7/8	0.98	0.06	16,16,17,19	0
1	SMC	B	369	7/8	0.98	0.09	16,16,17,19	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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	I	1142	4/4	0.62	0.29	41,42,42,43	0
5	EDO	N	1141	4/4	0.69	0.21	30,32,34,35	0
5	EDO	C	1482	4/4	0.70	0.27	33,38,38,38	0
5	EDO	F	1481	4/4	0.71	0.29	41,41,41,42	0
5	EDO	H	1483	4/4	0.76	0.25	39,42,42,43	0
5	EDO	F	1484	4/4	0.79	0.19	24,26,28,29	0
5	EDO	E	1480	4/4	0.79	0.20	42,43,43,44	0
5	EDO	A	1482	4/4	0.80	0.16	31,32,32,33	0
5	EDO	B	1480	4/4	0.82	0.18	29,30,31,32	0
5	EDO	L	1141	4/4	0.82	0.19	47,47,48,48	0
5	EDO	C	1477	4/4	0.83	0.22	38,38,39,40	0
5	EDO	H	1480	4/4	0.85	0.15	35,38,39,39	0
5	EDO	F	1479	4/4	0.86	0.18	36,36,37,37	0
5	EDO	M	1141	4/4	0.86	0.22	33,34,34,36	0
5	EDO	P	1141	4/4	0.86	0.20	48,50,51,52	0
5	EDO	O	1142	4/4	0.88	0.20	31,32,34,36	0
5	EDO	D	1478	4/4	0.88	0.20	35,36,38,38	0

*Continued on next page...*



*Continued from previous page...*

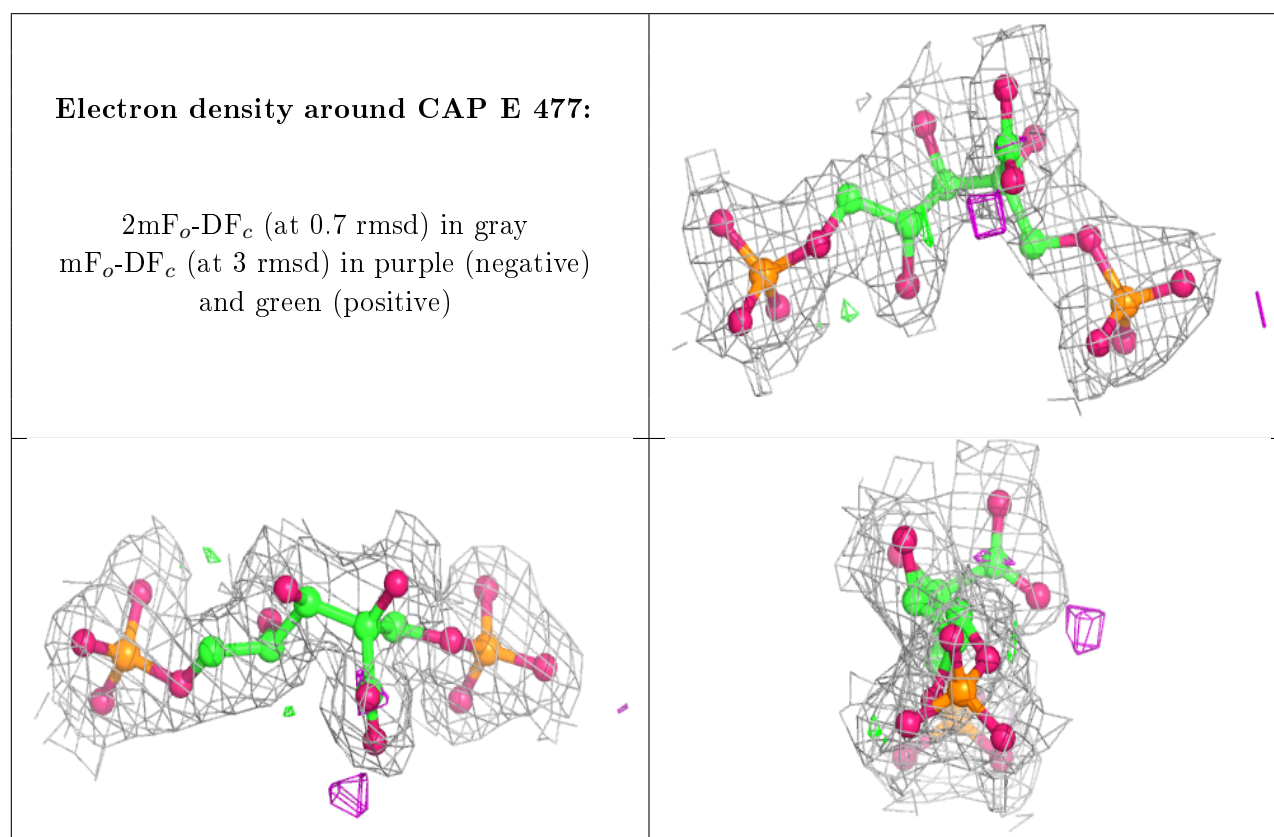
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	I	1141	4/4	0.88	0.19	35,35,35,35	0
5	EDO	J	1142	4/4	0.89	0.23	26,28,32,33	0
5	EDO	C	1481	4/4	0.89	0.18	27,30,30,30	0
5	EDO	B	1477	4/4	0.90	0.14	16,16,18,18	0
5	EDO	H	1476	4/4	0.90	0.13	17,20,21,21	0
5	EDO	K	1141	4/4	0.90	0.20	30,32,34,35	0
5	EDO	G	1480	4/4	0.91	0.14	38,38,38,39	0
5	EDO	D	1481	4/4	0.91	0.12	32,33,34,34	0
5	EDO	E	1476	4/4	0.91	0.16	22,22,24,25	0
5	EDO	A	1481	4/4	0.91	0.12	21,21,22,23	0
5	EDO	D	1477	4/4	0.92	0.15	20,21,21,22	0
5	EDO	C	1480	4/4	0.92	0.16	20,24,24,25	0
5	EDO	H	1481	4/4	0.92	0.21	39,40,41,41	0
5	EDO	A	1484	4/4	0.92	0.18	41,43,43,45	0
5	EDO	K	1142	4/4	0.93	0.11	40,40,40,41	0
5	EDO	F	1480	4/4	0.93	0.20	35,37,37,37	0
5	EDO	N	1142	4/4	0.93	0.09	25,26,26,28	0
5	EDO	J	1141	4/4	0.93	0.14	28,29,30,31	0
5	EDO	H	1482	4/4	0.93	0.10	21,21,22,22	0
5	EDO	H	1478	4/4	0.93	0.16	29,30,31,31	0
5	EDO	C	1478	4/4	0.93	0.12	27,27,28,28	0
5	EDO	F	1482	4/4	0.93	0.21	28,30,32,34	0
5	EDO	O	1141	4/4	0.94	0.15	32,33,34,37	0
5	EDO	A	1477	4/4	0.94	0.20	21,22,23,24	0
5	EDO	G	1476	4/4	0.94	0.11	20,20,23,23	0
5	EDO	B	1479	4/4	0.94	0.15	33,33,34,35	0
5	EDO	F	1483	4/4	0.95	0.10	21,23,26,27	0
5	EDO	D	1480	4/4	0.95	0.09	24,28,28,29	0
5	EDO	G	1478	4/4	0.95	0.11	25,25,25,25	0
4	CAP	E	477	21/21	0.96	0.10	14,16,17,19	0
5	EDO	A	1483	4/4	0.96	0.08	19,20,20,23	0
5	EDO	E	1478	4/4	0.96	0.09	23,25,26,26	0
4	CAP	D	477	21/21	0.97	0.11	14,16,17,18	0
4	CAP	B	477	21/21	0.98	0.10	14,16,18,19	0
4	CAP	C	477	21/21	0.98	0.08	13,16,18,19	0
3	MG	C	476	1/1	0.98	0.06	14,14,14,14	0
3	MG	D	476	1/1	0.98	0.04	14,14,14,14	0
5	EDO	B	1481	4/4	0.98	0.09	20,21,21,24	0
4	CAP	A	477	21/21	0.98	0.12	14,16,17,18	0
4	CAP	F	477	21/21	0.98	0.08	14,16,17,19	0
4	CAP	G	477	21/21	0.98	0.09	14,16,17,18	0
3	MG	A	476	1/1	0.98	0.10	14,14,14,14	0

*Continued on next page...*

*Continued from previous page...*

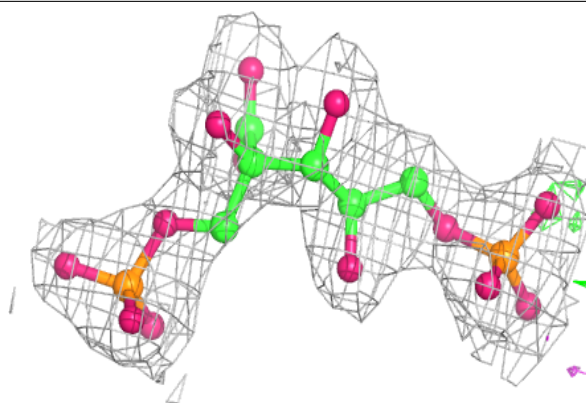
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	H	476	1/1	0.98	0.08	14,14,14,14	0
3	MG	E	476	1/1	0.98	0.06	14,14,14,14	0
3	MG	B	476	1/1	0.99	0.07	14,14,14,14	0
3	MG	G	476	1/1	0.99	0.16	14,14,14,14	0
4	CAP	H	477	21/21	0.99	0.10	14,16,17,19	0
3	MG	F	476	1/1	0.99	0.09	13,13,13,13	0

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

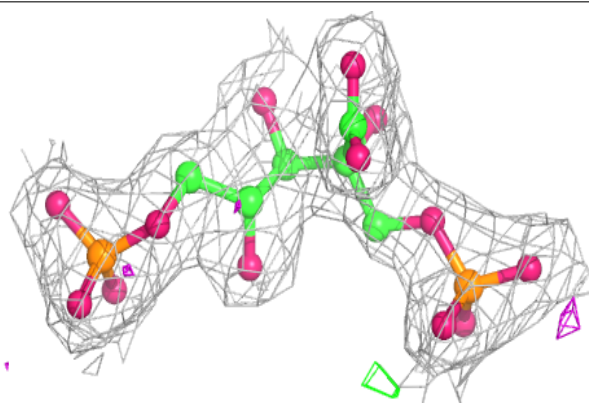


**Electron density around CAP D 477:**

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

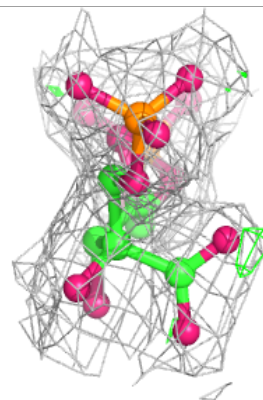
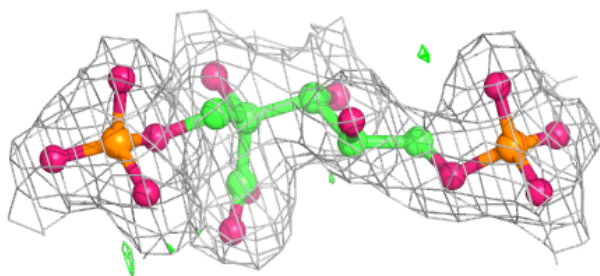
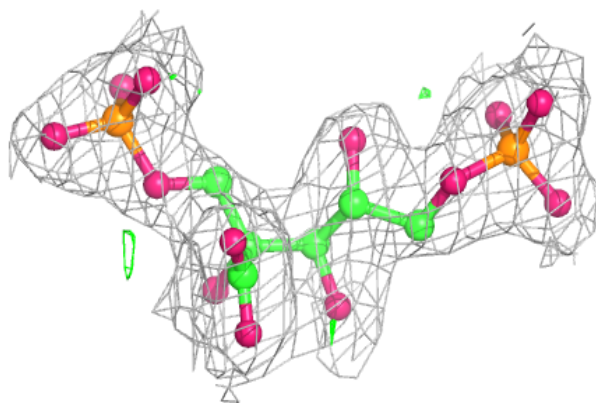
**Electron density around CAP B 477:**

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

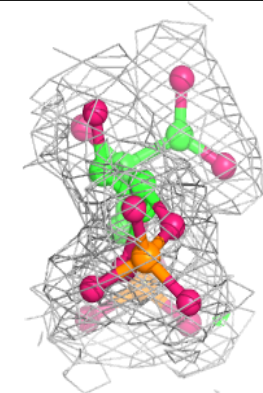
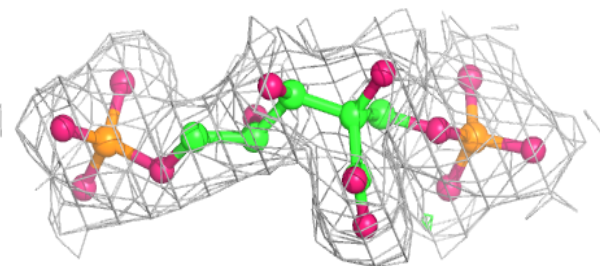
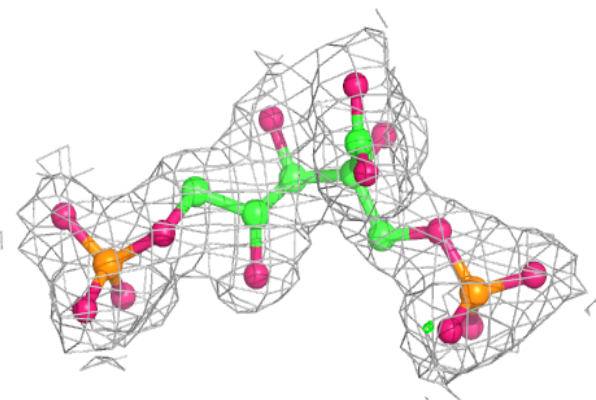


**Electron density around CAP C 477:**

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

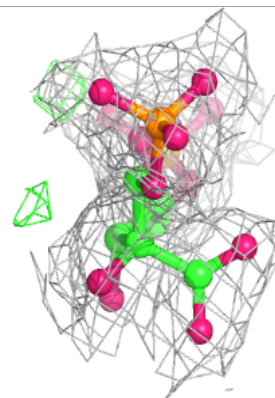
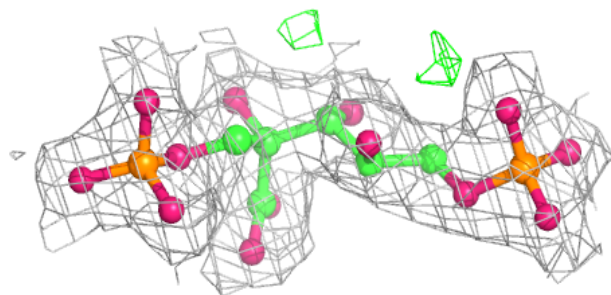
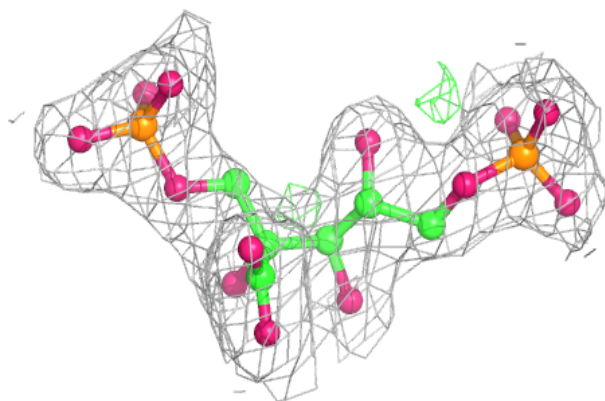
**Electron density around CAP A 477:**

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

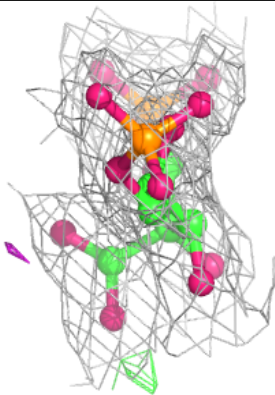
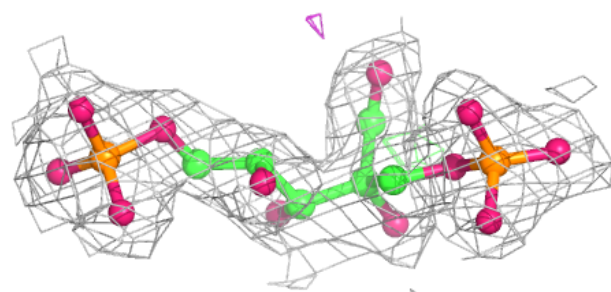
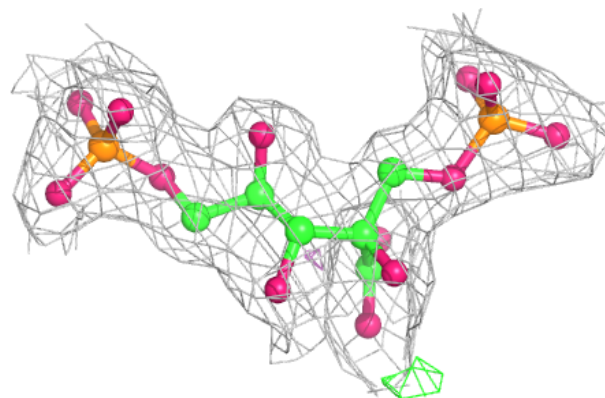


**Electron density around CAP F 477:**

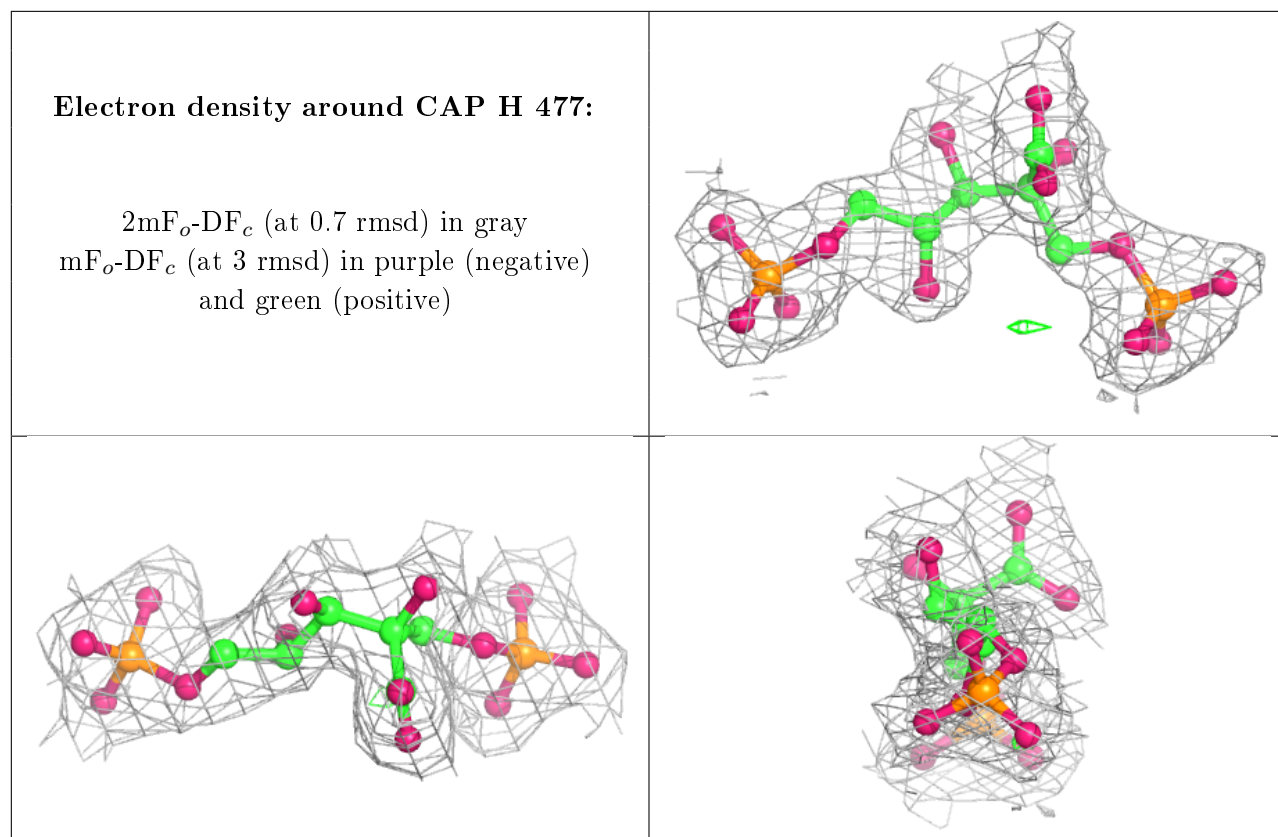
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CAP G 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.