



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 11:37 am BST

PDB ID : 1RBL  
Title : STRUCTURE DETERMINATION AND REFINEMENT OF RIBULOSE 1,5  
BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE FROM SYNE-  
CHOCOCCUS PCC6301  
Authors : Newman, J.; Gutteridge, S.; Branden, C.-I.; Jones, T.A.  
Deposited on : 1993-05-12  
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 : 2.11  
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

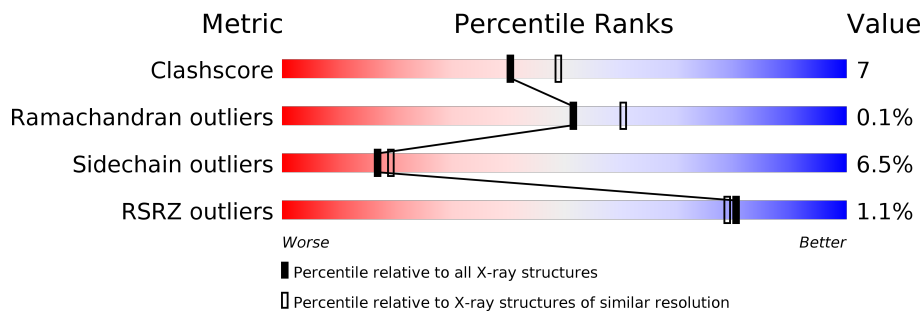
# 1 Overall quality at a glance

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))
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	467	 81% 15% ..
1	B	467	 81% 15% ..
1	C	467	 82% 14% ..
1	D	467	 82% 14% ..
1	E	467	 81% 15% ..
1	F	467	 81% 15% ..
1	G	467	 81% 15% ..

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Mol	Chain	Length	Quality of chain
1	H	467	 81% 15% ..
2	I	109	 3% 67% 30% ..
2	J	109	 5% 68% 28% ..
2	K	109	 3% 66% 30% ..
2	L	109	 6% 70% 27% ..
2	M	109	 2% 69% 26% ..
2	N	109	 2% 68% 29% ..
2	O	109	 6% 67% 29% ..
2	P	109	 5% 67% 30% ..

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 36988 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 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	B	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	C	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	D	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	E	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	F	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	G	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	H	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ARG	PRO	CONFLICT	UNP P00880
A	42	PHE	VAL	CONFLICT	UNP P00880
A	91	ALA	GLN	CONFLICT	UNP P00880
A	356	ALA	ARG	CONFLICT	UNP P00880
B	41	ARG	PRO	CONFLICT	UNP P00880
B	42	PHE	VAL	CONFLICT	UNP P00880
B	91	ALA	GLN	CONFLICT	UNP P00880
B	356	ALA	ARG	CONFLICT	UNP P00880
C	41	ARG	PRO	CONFLICT	UNP P00880
C	42	PHE	VAL	CONFLICT	UNP P00880
C	91	ALA	GLN	CONFLICT	UNP P00880
C	356	ALA	ARG	CONFLICT	UNP P00880

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Chain	Residue	Modelled	Actual	Comment	Reference
D	41	ARG	PRO	CONFLICT	UNP P00880
D	42	PHE	VAL	CONFLICT	UNP P00880
D	91	ALA	GLN	CONFLICT	UNP P00880
D	356	ALA	ARG	CONFLICT	UNP P00880
E	41	ARG	PRO	CONFLICT	UNP P00880
E	42	PHE	VAL	CONFLICT	UNP P00880
E	91	ALA	GLN	CONFLICT	UNP P00880
E	356	ALA	ARG	CONFLICT	UNP P00880
F	41	ARG	PRO	CONFLICT	UNP P00880
F	42	PHE	VAL	CONFLICT	UNP P00880
F	91	ALA	GLN	CONFLICT	UNP P00880
F	356	ALA	ARG	CONFLICT	UNP P00880
G	41	ARG	PRO	CONFLICT	UNP P00880
G	42	PHE	VAL	CONFLICT	UNP P00880
G	91	ALA	GLN	CONFLICT	UNP P00880
G	356	ALA	ARG	CONFLICT	UNP P00880
H	41	ARG	PRO	CONFLICT	UNP P00880
H	42	PHE	VAL	CONFLICT	UNP P00880
H	91	ALA	GLN	CONFLICT	UNP P00880
H	356	ALA	ARG	CONFLICT	UNP P00880

- Molecule 2 is a protein called RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	I	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	N	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	J	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	O	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	K	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	P	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	L	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			

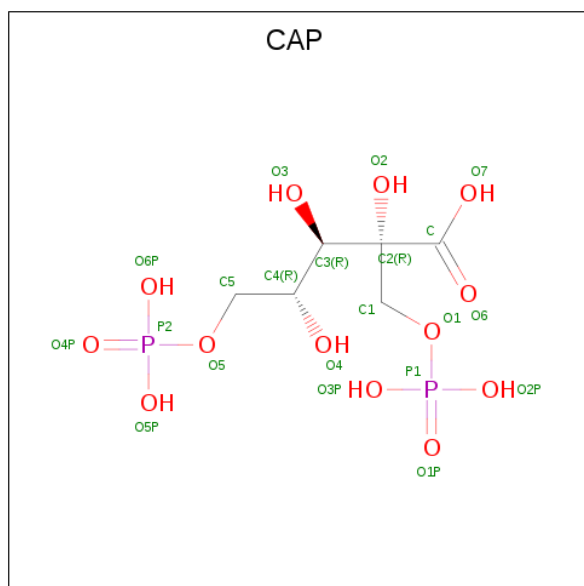
There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	76	ALA	ASP	CONFLICT	UNP P04716
M	78	ALA	LYS	CONFLICT	UNP P04716
M	79	ALA	SER	CONFLICT	UNP P04716
M	109	GLU	GLN	CONFLICT	UNP P04716
M	113	SER	VAL	CONFLICT	UNP P04716
I	76	ALA	ASP	CONFLICT	UNP P04716
I	78	ALA	LYS	CONFLICT	UNP P04716
I	79	ALA	SER	CONFLICT	UNP P04716
I	109	GLU	GLN	CONFLICT	UNP P04716
I	113	SER	VAL	CONFLICT	UNP P04716
N	76	ALA	ASP	CONFLICT	UNP P04716
N	78	ALA	LYS	CONFLICT	UNP P04716
N	79	ALA	SER	CONFLICT	UNP P04716
N	109	GLU	GLN	CONFLICT	UNP P04716
N	113	SER	VAL	CONFLICT	UNP P04716
J	76	ALA	ASP	CONFLICT	UNP P04716
J	78	ALA	LYS	CONFLICT	UNP P04716
J	79	ALA	SER	CONFLICT	UNP P04716
J	109	GLU	GLN	CONFLICT	UNP P04716
J	113	SER	VAL	CONFLICT	UNP P04716
O	76	ALA	ASP	CONFLICT	UNP P04716
O	78	ALA	LYS	CONFLICT	UNP P04716
O	79	ALA	SER	CONFLICT	UNP P04716
O	109	GLU	GLN	CONFLICT	UNP P04716
O	113	SER	VAL	CONFLICT	UNP P04716
K	76	ALA	ASP	CONFLICT	UNP P04716
K	78	ALA	LYS	CONFLICT	UNP P04716
K	79	ALA	SER	CONFLICT	UNP P04716
K	109	GLU	GLN	CONFLICT	UNP P04716
K	113	SER	VAL	CONFLICT	UNP P04716
P	76	ALA	ASP	CONFLICT	UNP P04716
P	78	ALA	LYS	CONFLICT	UNP P04716
P	79	ALA	SER	CONFLICT	UNP P04716
P	109	GLU	GLN	CONFLICT	UNP P04716
P	113	SER	VAL	CONFLICT	UNP P04716
L	76	ALA	ASP	CONFLICT	UNP P04716
L	78	ALA	LYS	CONFLICT	UNP P04716
L	79	ALA	SER	CONFLICT	UNP P04716
L	109	GLU	GLN	CONFLICT	UNP P04716
L	113	SER	VAL	CONFLICT	UNP P04716

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

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

- 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>).



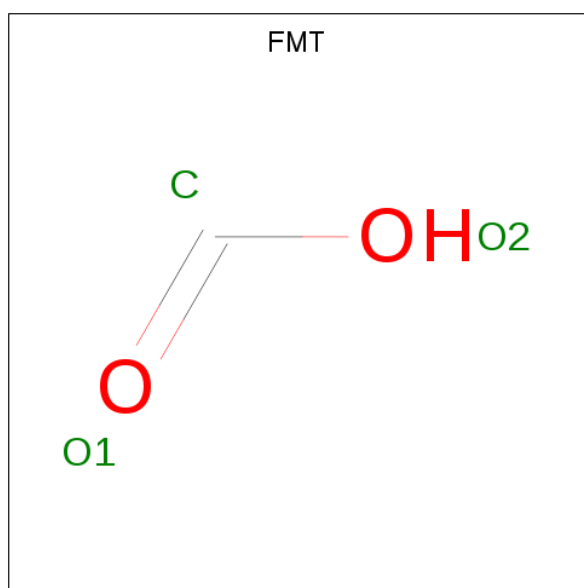
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 21 6 13 2	0	0
4	B	1	Total C O P 21 6 13 2	0	0
4	C	1	Total C O P 21 6 13 2	0	0

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

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		
5	E	1	Total	C	O	0	0
			3	1	2		
5	F	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			3	1	2		
5	H	1	Total	C	O	0	0
			3	1	2		

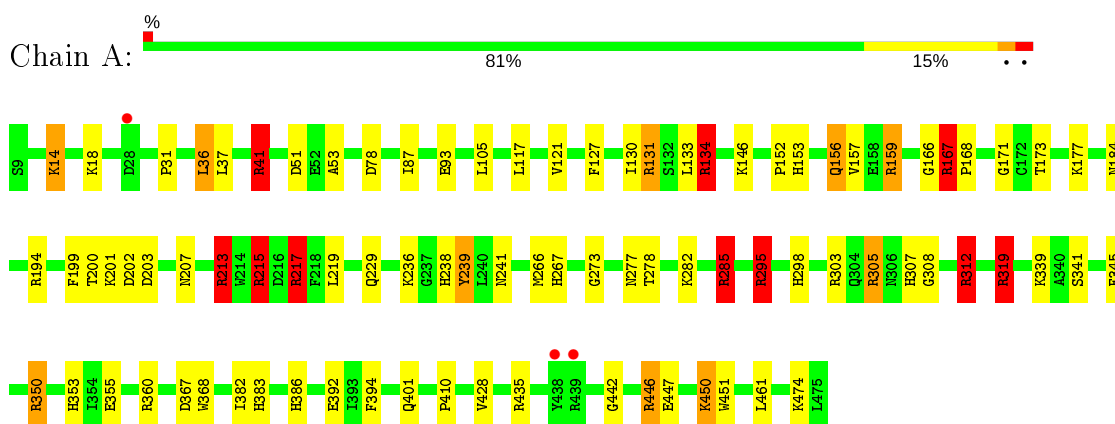
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	214	Total	O	0	0
			214	214		
6	M	53	Total	O	0	0
			53	53		
6	B	4	Total	O	0	0
			4	4		
6	C	9	Total	O	0	0
			9	9		
6	N	5	Total	O	0	0
			5	5		
6	D	3	Total	O	0	0
			3	3		
6	G	2	Total	O	0	0
			2	2		
6	P	2	Total	O	0	0
			2	2		

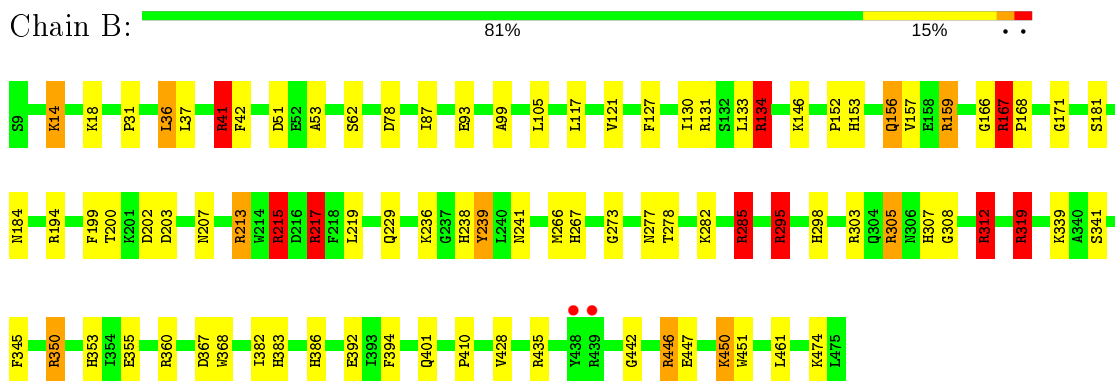
### 3 Residue-property plots

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.

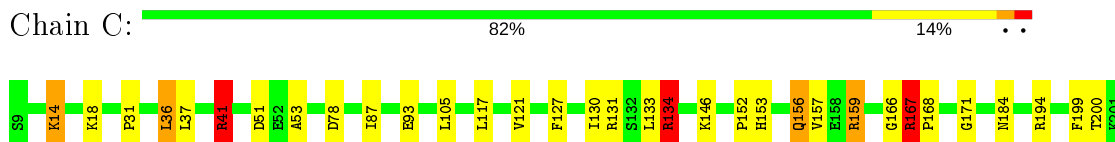
- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

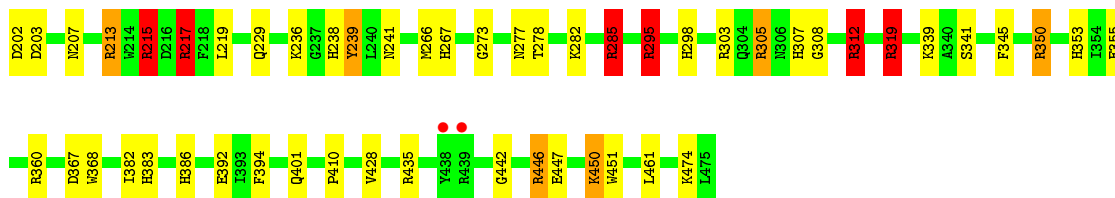


- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



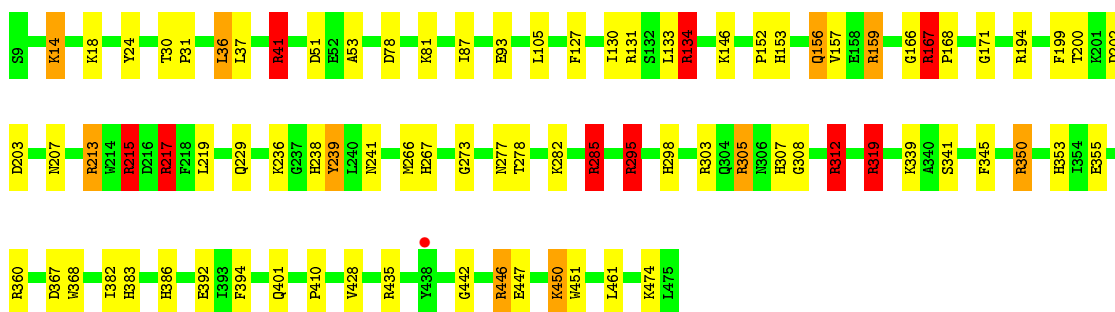
- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)





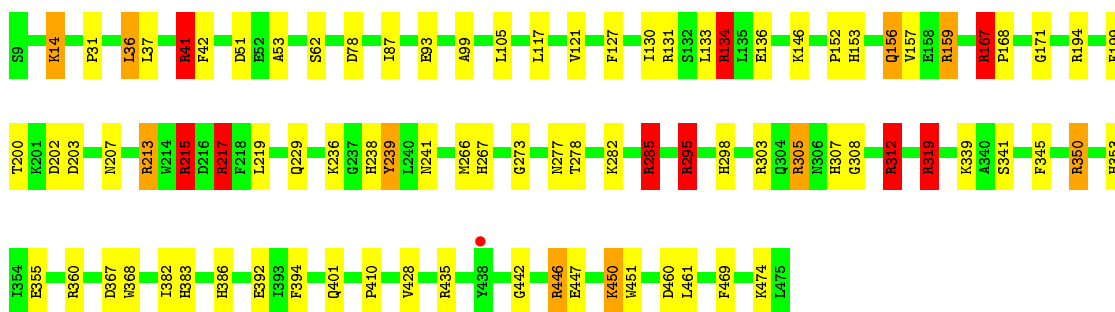
• Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain D: 82% 14% 4%



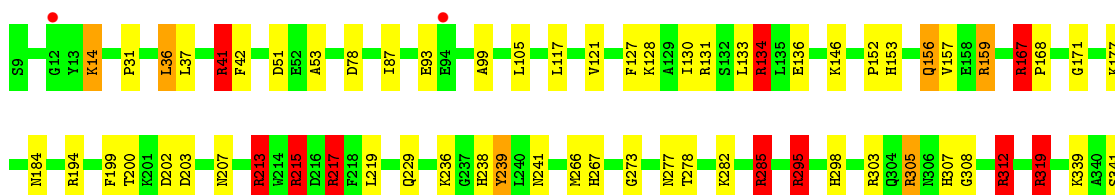
• Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

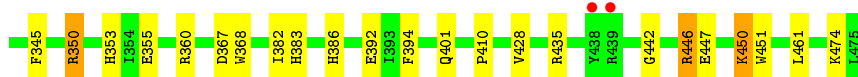
Chain E: 81% 15% 4%



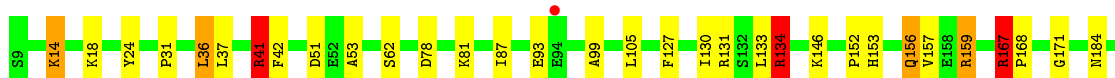
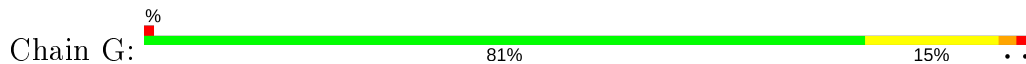
• Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain F: 81% 15% 4%

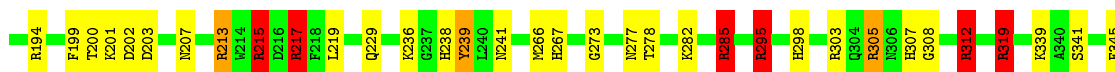
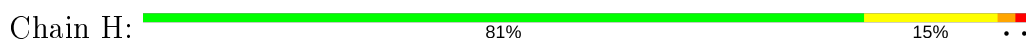




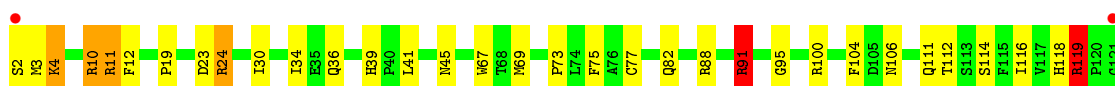
- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



- Molecule 2: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

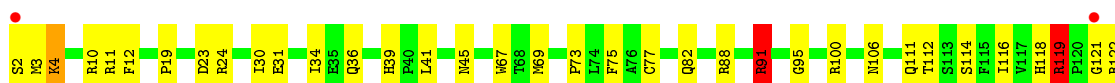


- Molecule 2: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)





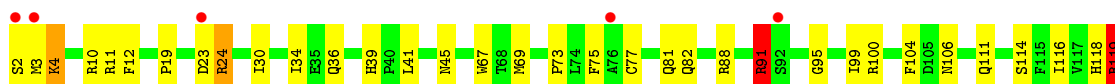
- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)



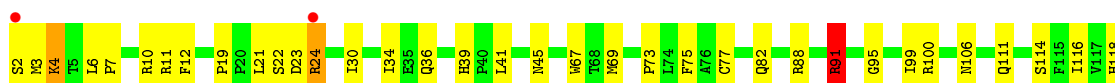
- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)





- Molecule 2: RIBULOSE 1,5 BISPHTHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)



- Molecule 2: RIBULOSE 1,5 BISPHTHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.90Å 111.90Å 199.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20 19.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20) 39.6 (19.99-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.96 (at 2.19Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.200 , (Not available) 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtrriage
Anisotropy	0.632	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 22.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	36988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0290e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, CAP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/3745	0.63	8/5071 (0.2%)
1	B	0.34	0/3745	0.63	8/5071 (0.2%)
1	C	0.34	0/3745	0.63	8/5071 (0.2%)
1	D	0.34	0/3745	0.63	8/5071 (0.2%)
1	E	0.34	0/3745	0.63	8/5071 (0.2%)
1	F	0.34	0/3745	0.63	9/5071 (0.2%)
1	G	0.34	0/3745	0.63	9/5071 (0.2%)
1	H	0.34	0/3745	0.63	8/5071 (0.2%)
2	I	0.38	0/936	0.59	1/1265 (0.1%)
2	J	0.38	0/936	0.59	1/1265 (0.1%)
2	K	0.37	0/936	0.59	1/1265 (0.1%)
2	L	0.38	0/936	0.59	1/1265 (0.1%)
2	M	0.37	0/936	0.59	1/1265 (0.1%)
2	N	0.38	0/936	0.59	1/1265 (0.1%)
2	O	0.37	0/936	0.59	1/1265 (0.1%)
2	P	0.38	0/936	0.59	1/1265 (0.1%)
All	All	0.35	0/37448	0.62	74/50688 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	B	0	17
1	C	0	17
1	D	0	17
1	E	0	17
1	F	0	17
1	G	0	17

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	17
2	I	0	5
2	J	0	5
2	K	0	5
2	L	0	5
2	M	0	5
2	N	0	5
2	O	0	5
2	P	0	5
All	All	0	176

There are no bond length outliers.

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	159	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	E	159	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	C	159	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	A	159	ARG	NE-CZ-NH1	-8.19	116.21	120.30
1	H	159	ARG	NE-CZ-NH1	-8.18	116.21	120.30

There are no chirality outliers.

5 of 176 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	134	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	167	ARG	Sidechain
1	A	41	ARG	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3653	0	3568	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3653	0	3568	54	0
1	C	3653	0	3568	48	0
1	D	3653	0	3568	49	0
1	E	3653	0	3568	50	4
1	F	3653	0	3568	49	0
1	G	3653	0	3568	48	0
1	H	3653	0	3568	52	0
2	I	909	0	865	20	2
2	J	909	0	865	18	2
2	K	909	0	865	20	28
2	L	909	0	865	18	4
2	M	909	0	865	22	1
2	N	909	0	865	18	1
2	O	909	0	865	19	28
2	P	909	0	865	20	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	21	0	9	1	0
4	B	21	0	9	1	0
4	C	21	0	9	1	0
4	D	21	0	9	1	0
4	E	21	0	9	1	0
4	F	21	0	9	1	0
4	G	21	0	9	1	0
4	H	21	0	9	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
5	E	3	0	0	0	0
5	F	3	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	0	0
6	A	214	0	0	5	0
6	B	4	0	0	0	0
6	C	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	3	0	0	0	0
6	G	2	0	0	0	0
6	M	53	0	0	3	0
6	N	5	0	0	0	0
6	P	2	0	0	0	0
All	All	36988	0	35536	518	35

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 518 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:C:295:ARG:HD2	4:C:476:CAP:O5P	1.74	0.88
1:A:295:ARG:HD2	4:A:476:CAP:O5P	1.74	0.88
1:G:295:ARG:HD2	4:G:476:CAP:O5P	1.74	0.87
1:E:295:ARG:HD2	4:E:476:CAP:O5P	1.74	0.87
1:B:295:ARG:HD2	4:B:476:CAP:O5P	1.74	0.86

The worst 5 of 35 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:ARG:CZ	2:K:22:SER:N[2_554]	0.87	1.33
2:O:24:ARG:NE	2:K:22:SER:N[2_554]	1.02	1.18
2:O:24:ARG:NE	2:K:21:LEU:C[2_554]	1.09	1.11
2:O:24:ARG:NH1	2:K:22:SER:CA[2_554]	1.10	1.10
2:O:24:ARG:CZ	2:K:22:SER:CA[2_554]	1.17	1.03

## 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	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	B	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	C	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	D	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	E	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	F	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	G	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	H	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
2	I	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
2	J	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17	16
2	K	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
2	L	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17	16
2	M	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
2	N	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17	16
2	O	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17	16
2	P	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
All	All	4576/4608 (99%)	4424 (97%)	148 (3%)	4 (0%)	51	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	3	MET
2	N	121	GLY
2	J	121	GLY
2	O	121	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/377 (100%)	355 (94%)	22 (6%)	20	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	377/377 (100%)	355 (94%)	22 (6%)	20	23
1	C	377/377 (100%)	355 (94%)	22 (6%)	20	23
1	D	377/377 (100%)	355 (94%)	22 (6%)	20	23
1	E	377/377 (100%)	355 (94%)	22 (6%)	20	23
1	F	377/377 (100%)	355 (94%)	22 (6%)	20	23
1	G	377/377 (100%)	355 (94%)	22 (6%)	20	23
1	H	377/377 (100%)	355 (94%)	22 (6%)	20	23
2	I	99/99 (100%)	90 (91%)	9 (9%)	9	9
2	J	99/99 (100%)	90 (91%)	9 (9%)	9	9
2	K	99/99 (100%)	90 (91%)	9 (9%)	9	9
2	L	99/99 (100%)	90 (91%)	9 (9%)	9	9
2	M	99/99 (100%)	90 (91%)	9 (9%)	9	9
2	N	99/99 (100%)	90 (91%)	9 (9%)	9	9
2	O	99/99 (100%)	90 (91%)	9 (9%)	9	9
2	P	99/99 (100%)	90 (91%)	9 (9%)	9	9
All	All	3808/3808 (100%)	3560 (94%)	248 (6%)	17	19

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	341	SER
1	E	241	ASN
1	H	219	LEU
2	J	4	LYS
1	E	36	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	401	GLN
1	E	353	HIS
1	H	277	ASN
2	J	45	ASN
1	E	156	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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
4	CAP	D	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.13	6 (30%)
4	CAP	F	476	3	15,20,20	2.13	7 (46%)	20,31,31	2.14	5 (25%)
5	FMT	D	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
4	CAP	G	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	5 (25%)
4	CAP	B	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	5 (25%)
5	FMT	G	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	H	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
4	CAP	H	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	5 (25%)
4	CAP	A	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	5 (25%)
4	CAP	C	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	6 (30%)
4	CAP	E	476	3	15,20,20	2.13	7 (46%)	20,31,31	2.14	6 (30%)
5	FMT	F	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-

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
4	CAP	D	476	3	-	6/23/29/29	-
4	CAP	B	476	3	-	6/23/29/29	-
4	CAP	F	476	3	-	6/23/29/29	-
4	CAP	H	476	3	-	6/23/29/29	-
4	CAP	A	476	3	-	6/23/29/29	-
4	CAP	C	476	3	-	6/23/29/29	-
4	CAP	E	476	3	-	6/23/29/29	-
4	CAP	G	476	3	-	6/23/29/29	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	476	CAP	P2-O5	-3.93	1.47	1.60
4	B	476	CAP	P2-O5	-3.93	1.47	1.60
4	G	476	CAP	P2-O5	-3.93	1.47	1.60
4	A	476	CAP	P2-O5	-3.92	1.47	1.60
4	H	476	CAP	P2-O5	-3.92	1.47	1.60

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	476	CAP	C5-C4-C3	5.27	122.71	111.94
4	H	476	CAP	C5-C4-C3	5.27	122.71	111.94
4	G	476	CAP	C5-C4-C3	5.26	122.69	111.94
4	C	476	CAP	C5-C4-C3	5.25	122.68	111.94
4	A	476	CAP	C5-C4-C3	5.25	122.67	111.94

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	476	CAP	C2-C3-C4-C5
4	F	476	CAP	C2-C3-C4-O4
4	F	476	CAP	O3-C3-C4-O4
4	G	476	CAP	C2-C3-C4-C5
4	G	476	CAP	C2-C3-C4-O4

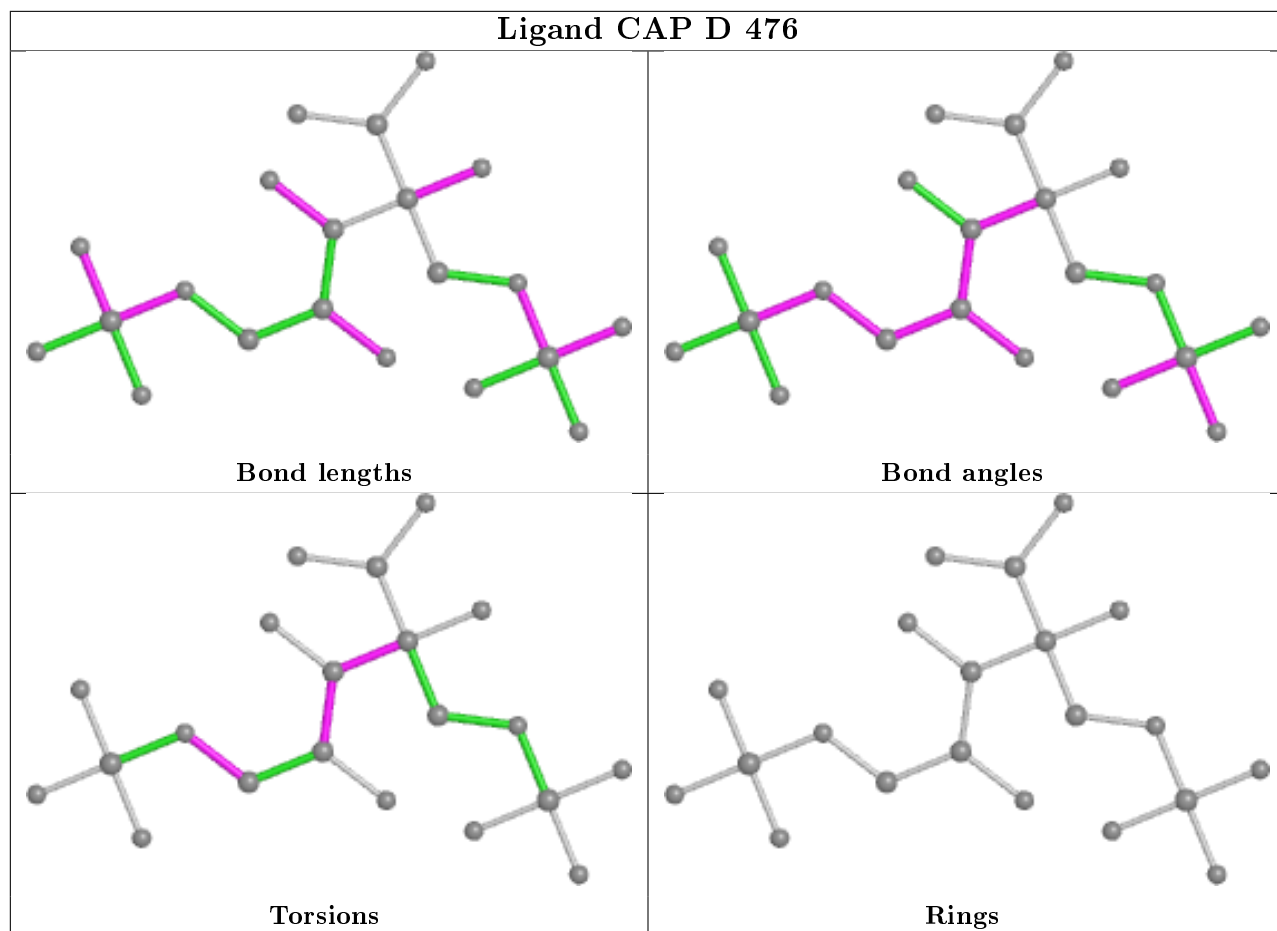
There are no ring outliers.

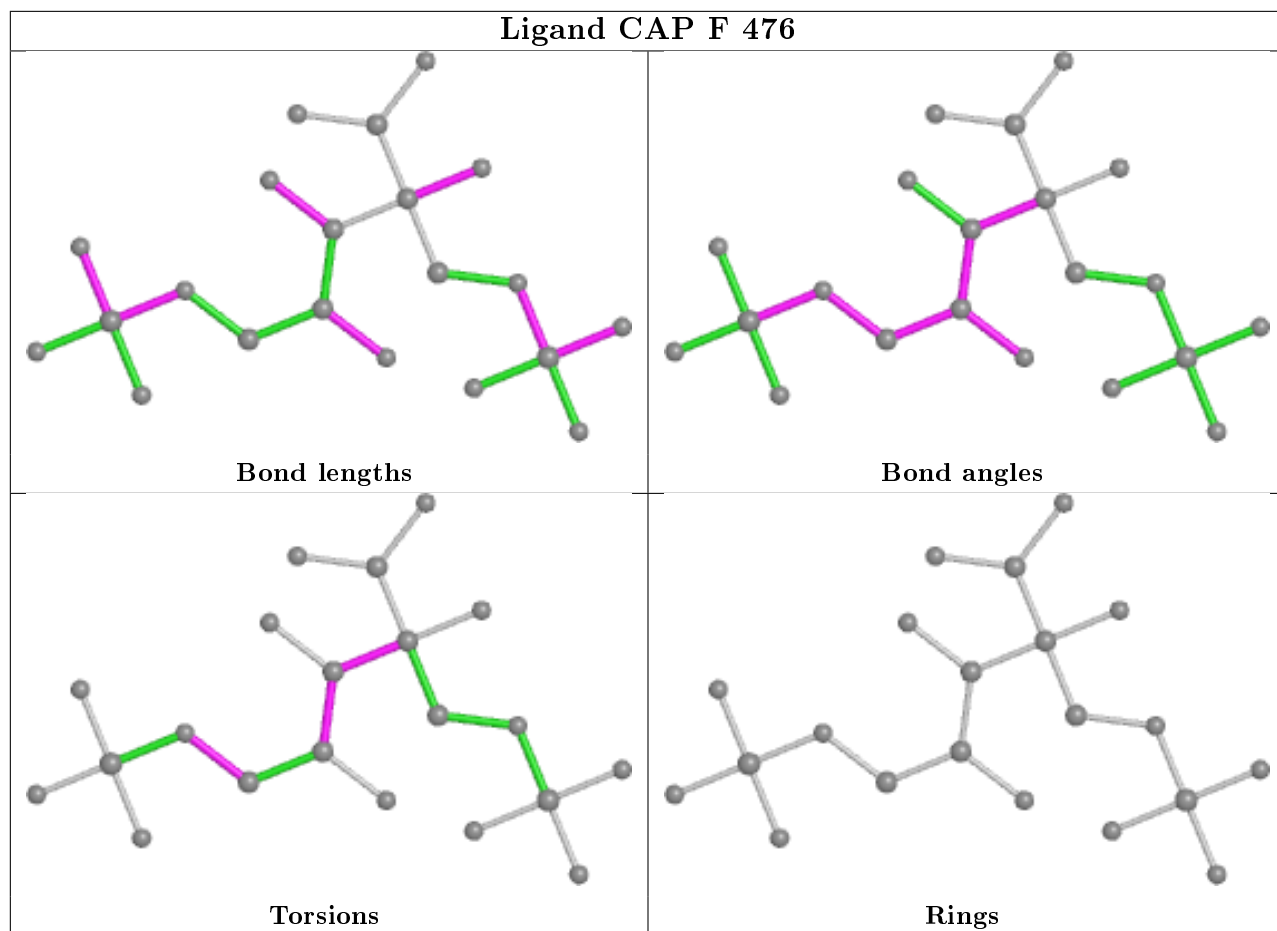
8 monomers are involved in 8 short contacts:

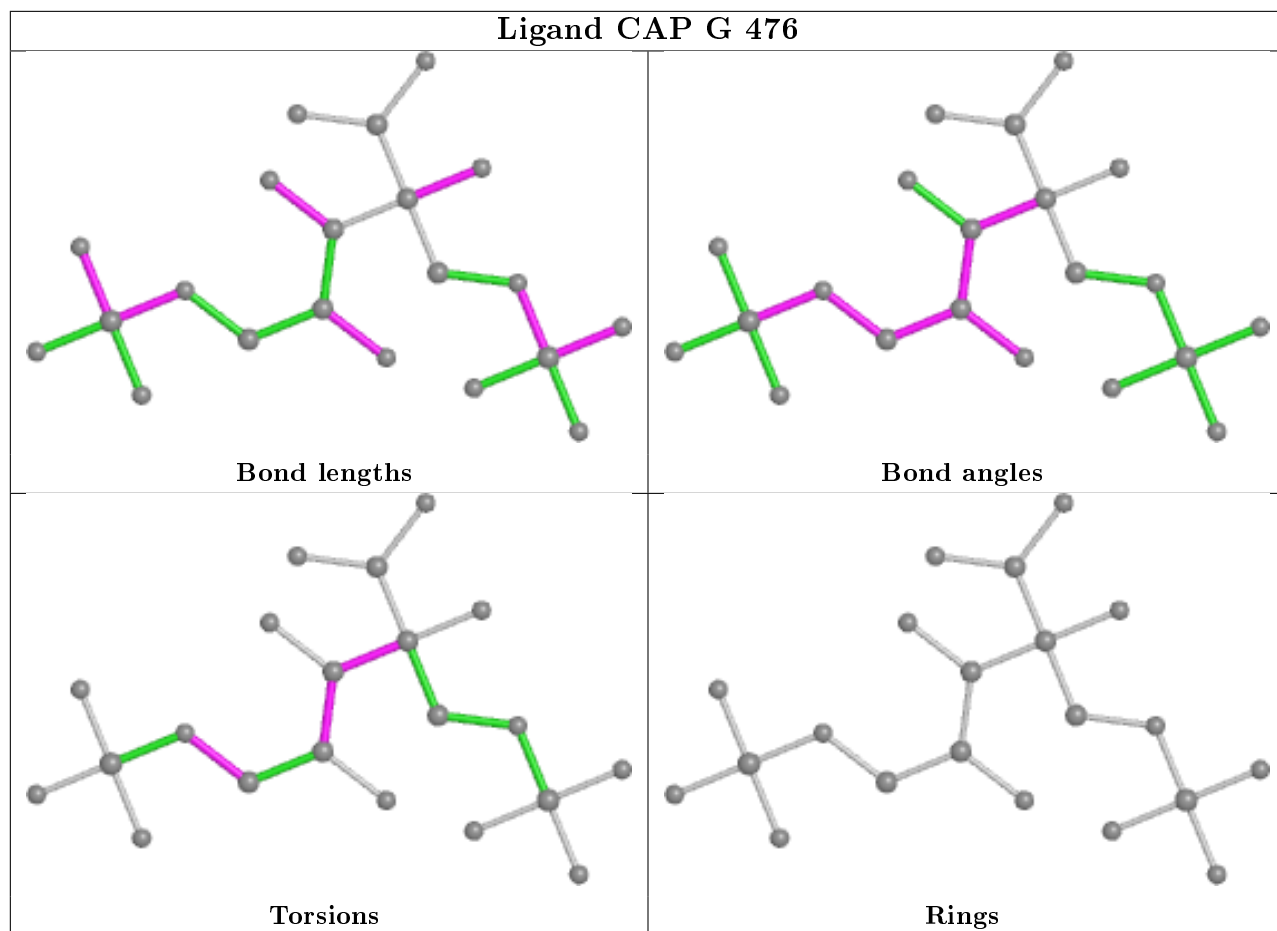
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	476	CAP	1	0
4	F	476	CAP	1	0
4	G	476	CAP	1	0
4	B	476	CAP	1	0
4	H	476	CAP	1	0
4	A	476	CAP	1	0
4	C	476	CAP	1	0
4	E	476	CAP	1	0

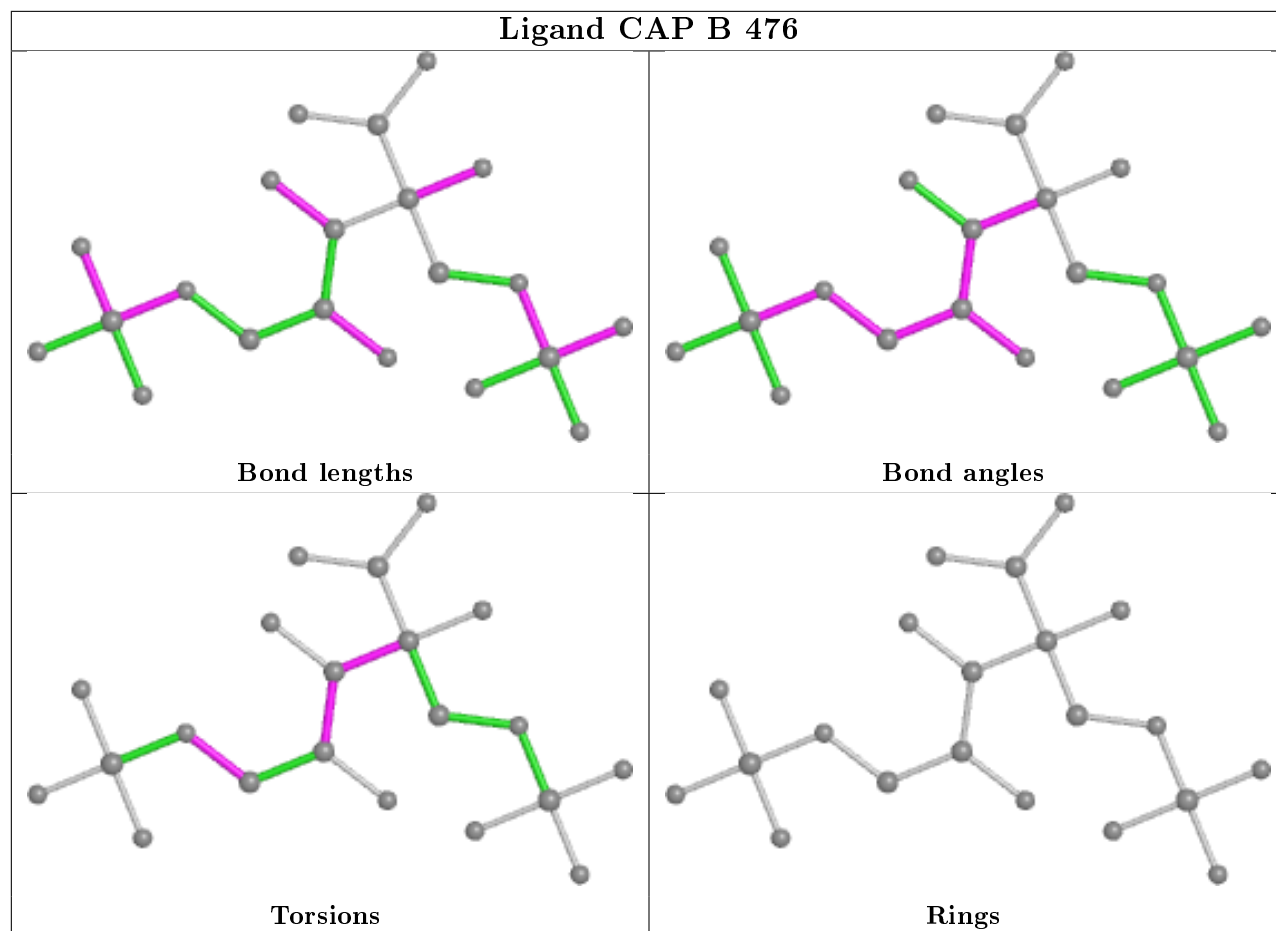
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

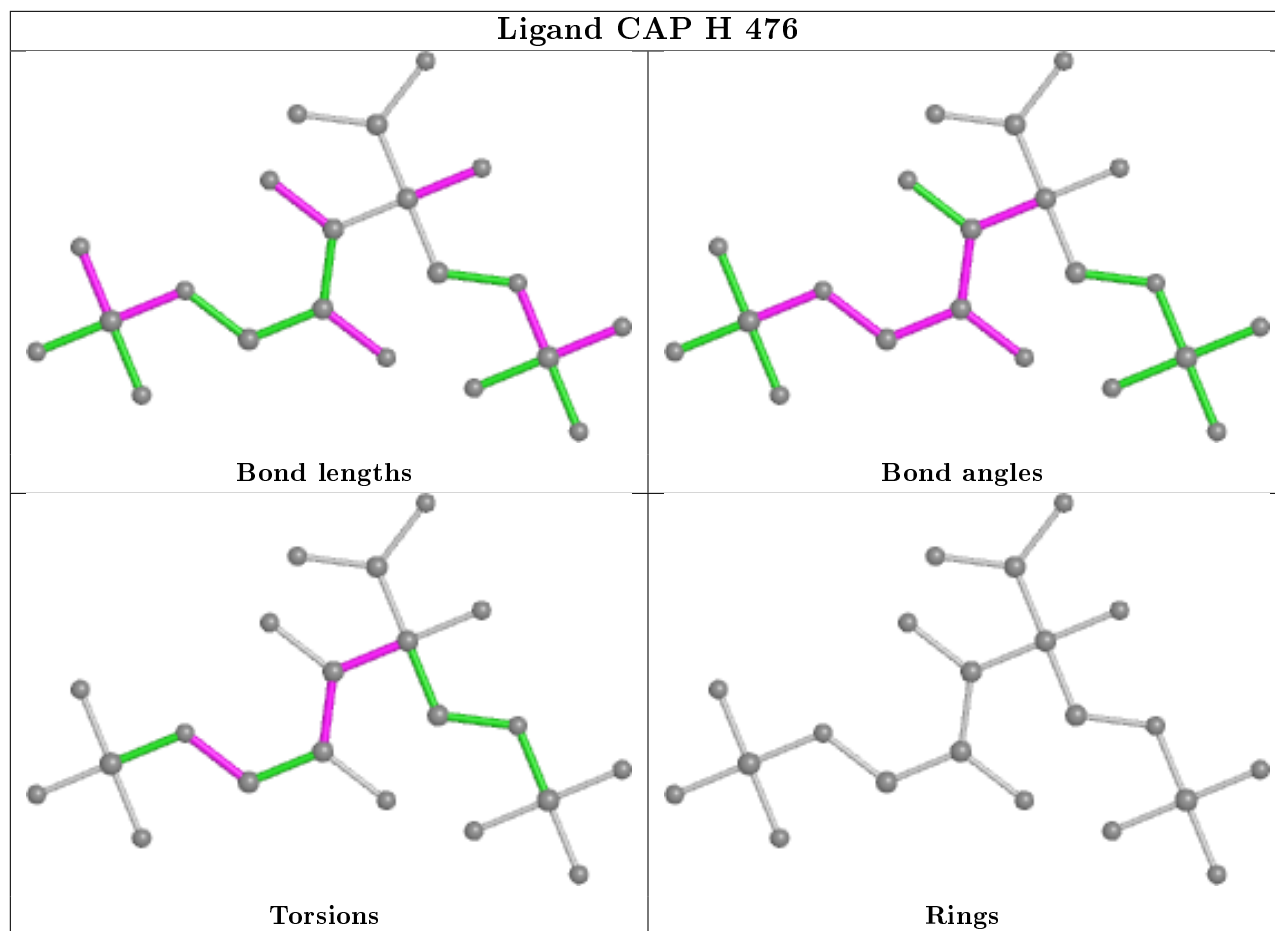


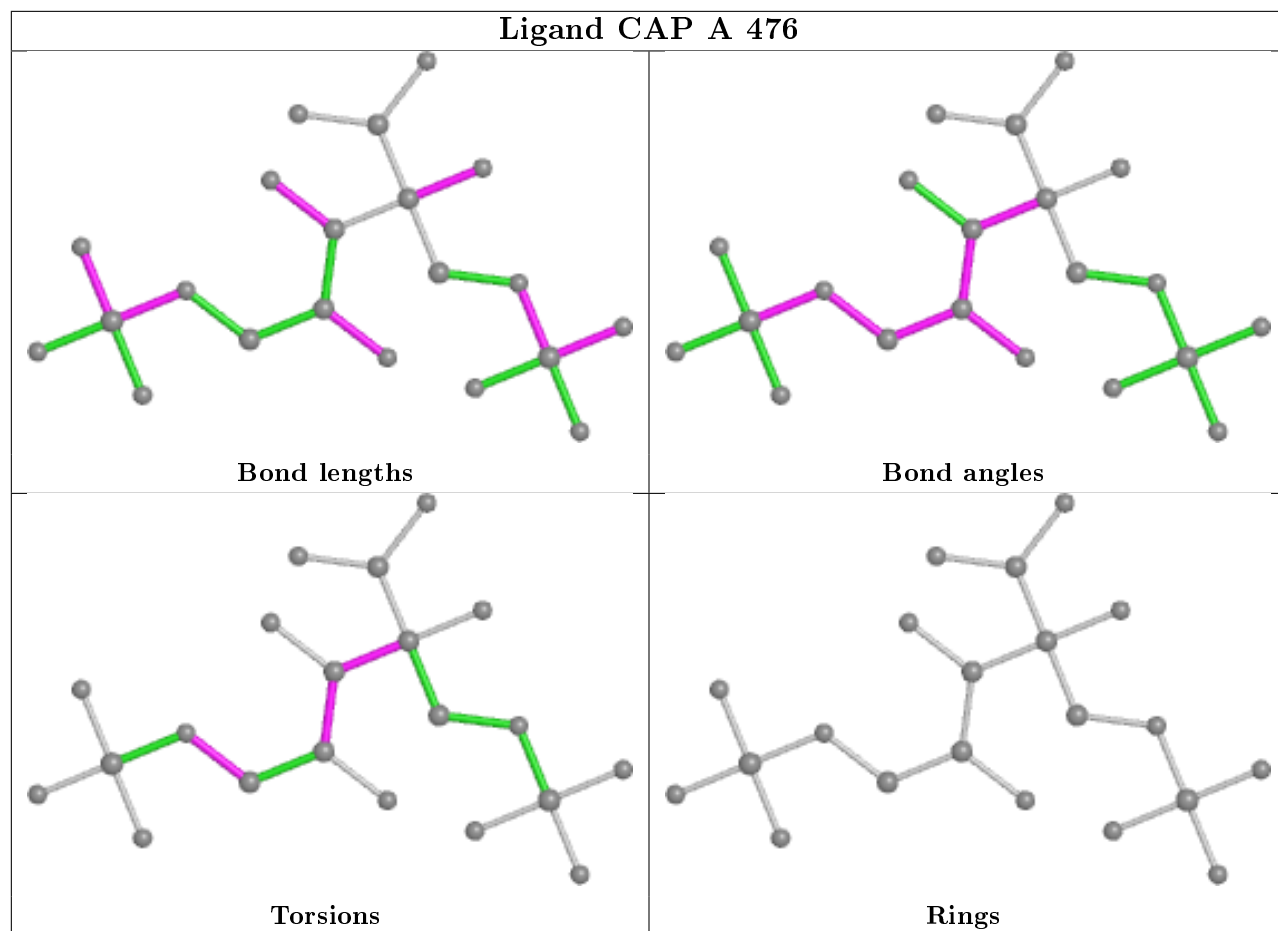


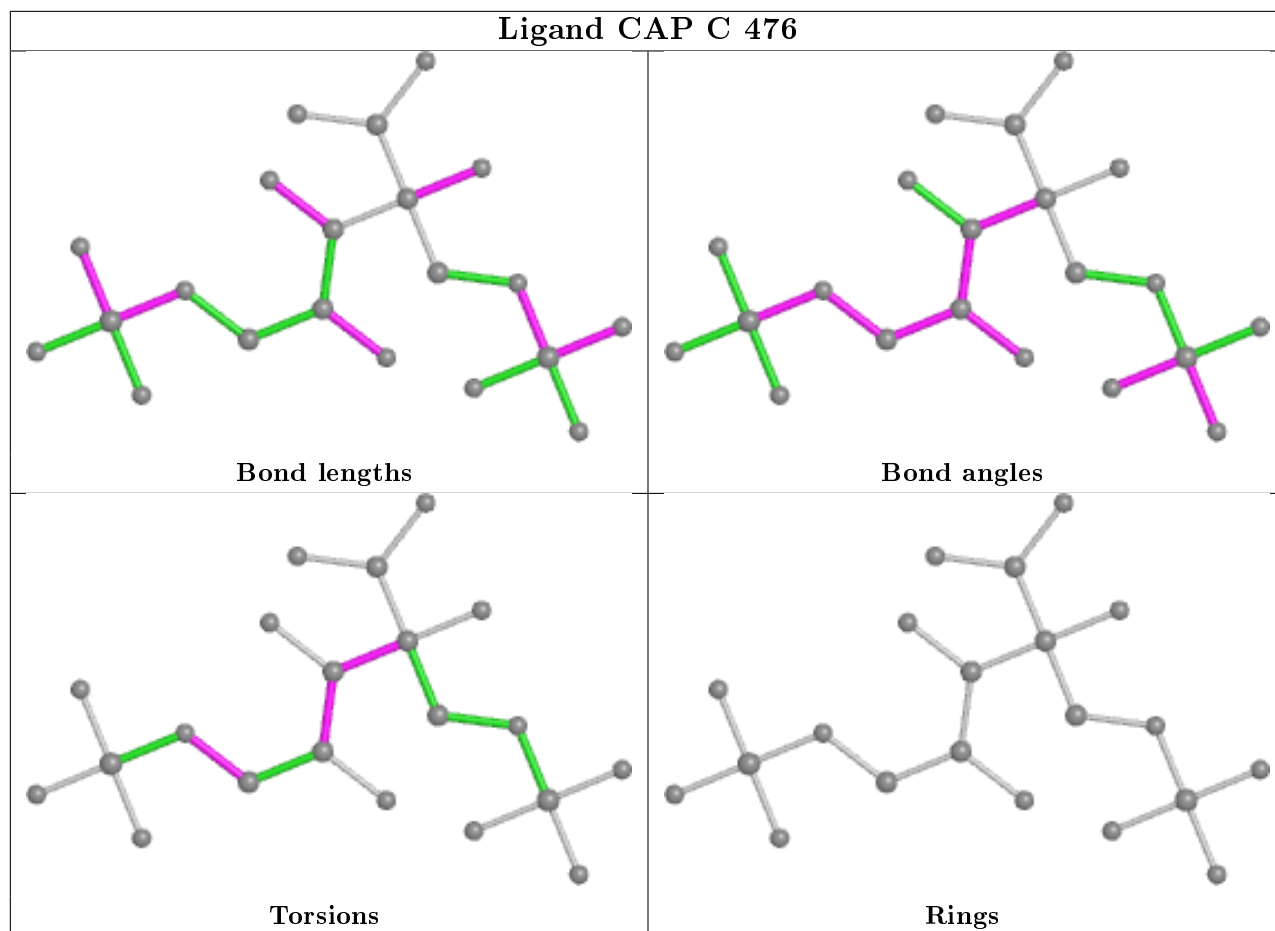


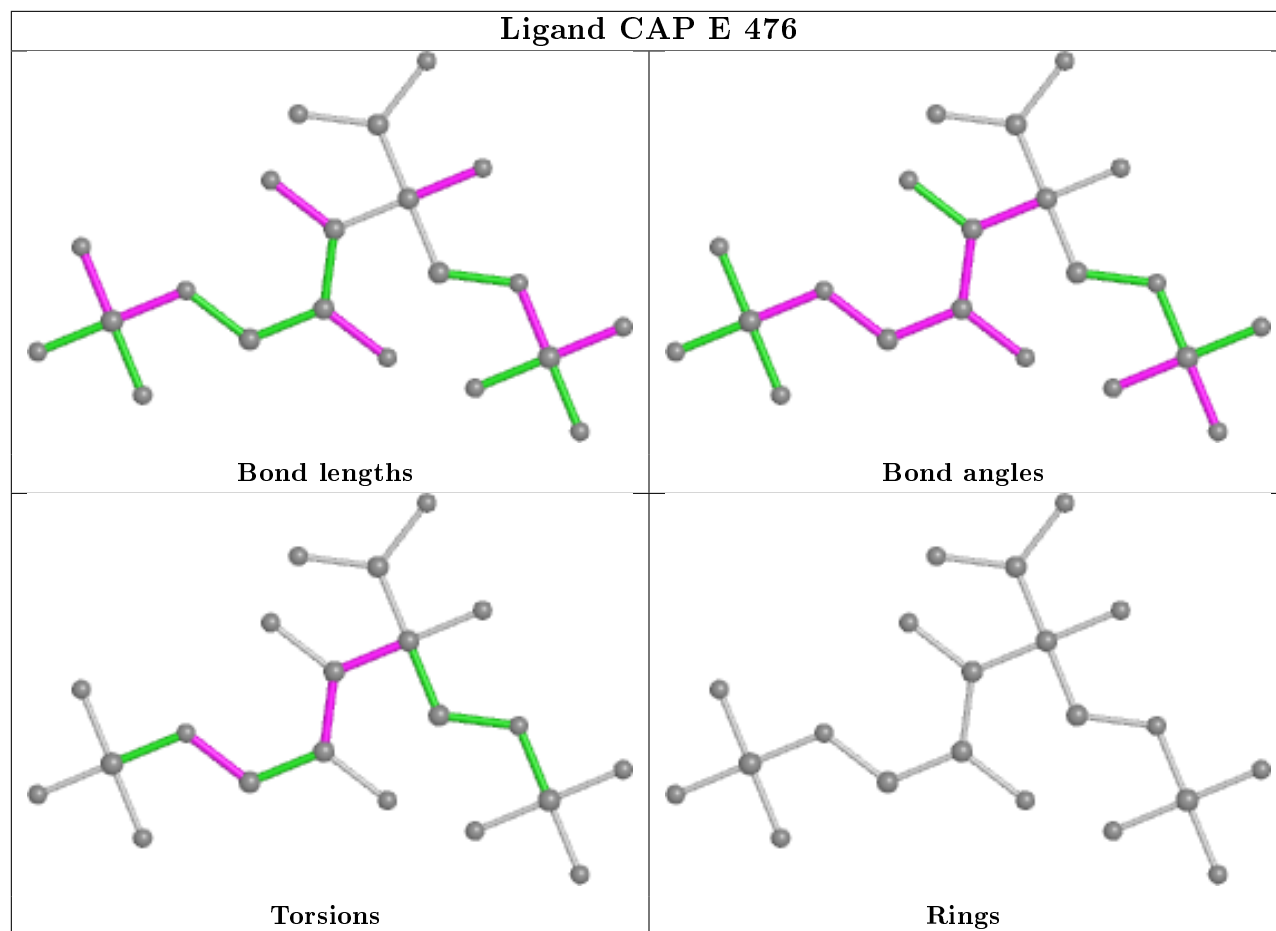












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	464/467 (99%)	-0.74	3 (0%) 89 88	11, 18, 36, 62	0
1	B	464/467 (99%)	-0.74	2 (0%) 92 91	11, 18, 36, 62	0
1	C	464/467 (99%)	-0.76	2 (0%) 92 91	11, 18, 36, 62	0
1	D	464/467 (99%)	-0.76	1 (0%) 95 94	11, 18, 36, 62	0
1	E	464/467 (99%)	-0.78	1 (0%) 95 94	11, 18, 36, 62	0
1	F	464/467 (99%)	-0.79	4 (0%) 84 83	11, 18, 36, 62	0
1	G	464/467 (99%)	-0.82	3 (0%) 89 88	11, 18, 36, 62	0
1	H	464/467 (99%)	-0.83	1 (0%) 95 94	11, 18, 36, 62	0
2	I	108/109 (99%)	-0.32	3 (2%) 53 51	16, 28, 60, 80	0
2	J	108/109 (99%)	-0.08	5 (4%) 32 31	16, 28, 60, 80	0
2	K	108/109 (99%)	-0.14	3 (2%) 53 51	16, 28, 60, 80	0
2	L	108/109 (99%)	-0.13	6 (5%) 24 23	16, 28, 60, 80	0
2	M	108/109 (99%)	-0.33	2 (1%) 66 65	16, 28, 60, 80	0
2	N	108/109 (99%)	-0.27	2 (1%) 66 65	16, 28, 60, 80	0
2	O	108/109 (99%)	-0.07	6 (5%) 24 23	16, 28, 60, 80	0
2	P	108/109 (99%)	-0.21	5 (4%) 32 31	16, 28, 60, 80	0
All	All	4576/4608 (99%)	-0.67	49 (1%) 80 79	11, 19, 45, 80	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	121	GLY	11.1
2	L	121	GLY	10.5
2	J	121	GLY	9.9
2	O	2	SER	9.6
2	M	121	GLY	8.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

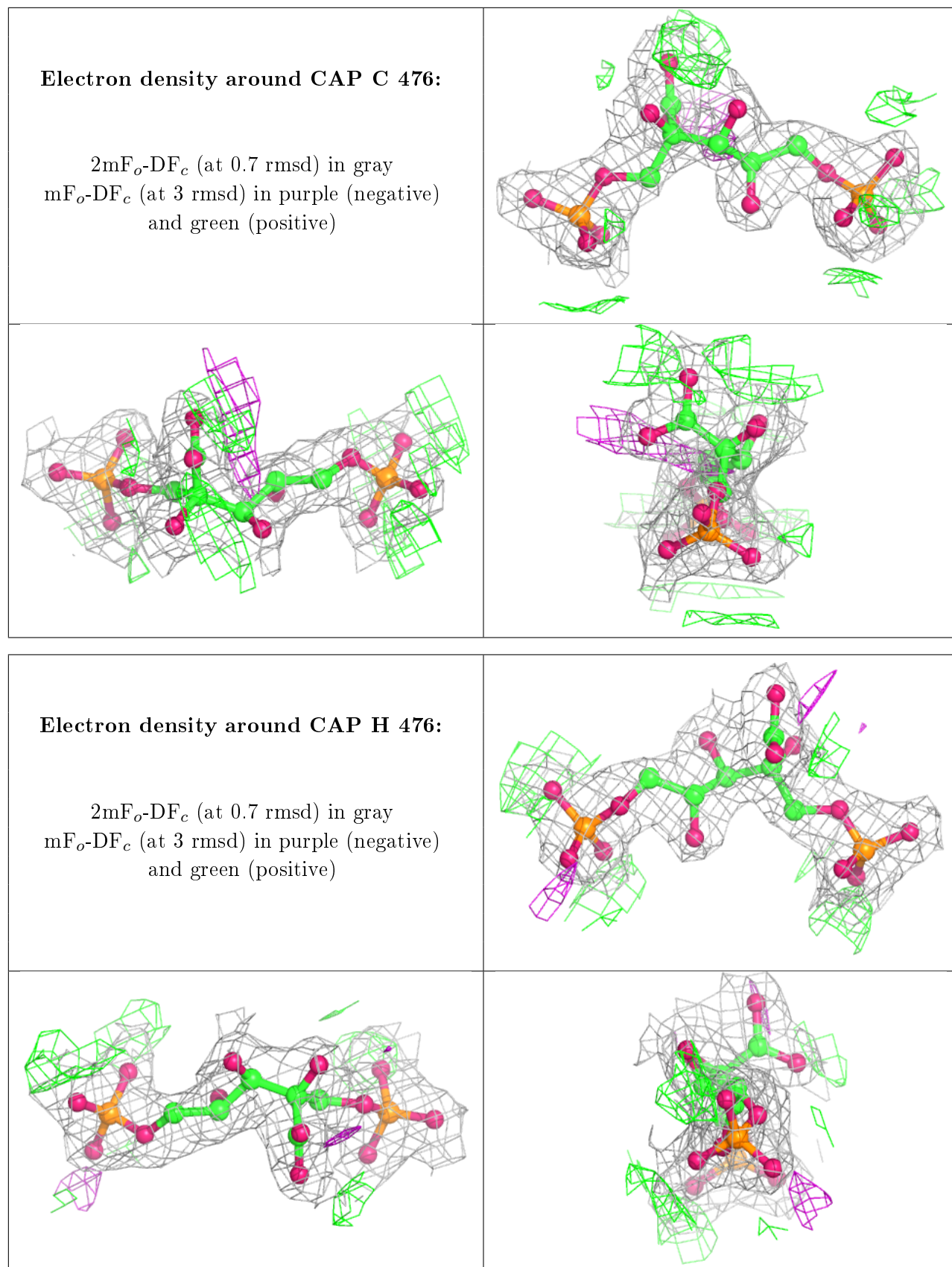
## 6.4 Ligands [i](#)

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
3	MG	F	477	1/1	0.92	0.14	19,19,19,19	0
3	MG	B	477	1/1	0.94	0.19	19,19,19,19	0
3	MG	D	477	1/1	0.94	0.09	19,19,19,19	0
3	MG	C	477	1/1	0.95	0.18	19,19,19,19	0
3	MG	E	477	1/1	0.95	0.16	19,19,19,19	0
5	FMT	E	478	3/3	0.96	0.09	13,13,14,15	0
4	CAP	C	476	21/21	0.97	0.09	13,16,20,21	0
3	MG	H	477	1/1	0.97	0.07	19,19,19,19	0
3	MG	G	477	1/1	0.97	0.12	19,19,19,19	0
4	CAP	H	476	21/21	0.97	0.08	13,16,20,21	0
4	CAP	E	476	21/21	0.97	0.09	13,16,20,21	0
3	MG	A	477	1/1	0.97	0.16	19,19,19,19	0
5	FMT	B	478	3/3	0.97	0.11	13,13,14,15	0
4	CAP	F	476	21/21	0.98	0.08	13,16,20,21	0
5	FMT	C	478	3/3	0.98	0.09	13,13,14,15	0
5	FMT	A	478	3/3	0.98	0.09	13,13,14,15	0
4	CAP	B	476	21/21	0.98	0.09	13,16,20,21	0
5	FMT	G	478	3/3	0.98	0.07	13,13,14,15	0
4	CAP	A	476	21/21	0.98	0.08	13,16,20,21	0
4	CAP	G	476	21/21	0.98	0.07	13,16,20,21	0
4	CAP	D	476	21/21	0.98	0.07	13,16,20,21	0
5	FMT	H	478	3/3	0.99	0.07	13,13,14,15	0
5	FMT	D	478	3/3	0.99	0.07	13,13,14,15	0
5	FMT	F	478	3/3	0.99	0.07	13,13,14,15	0

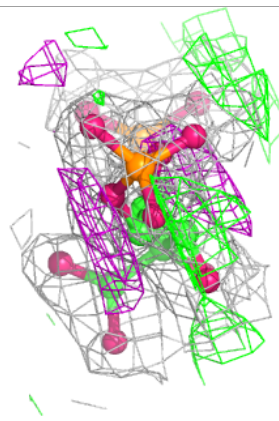
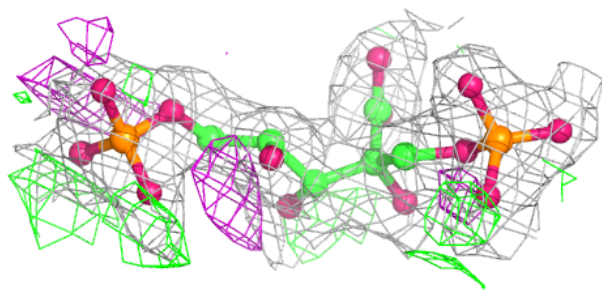
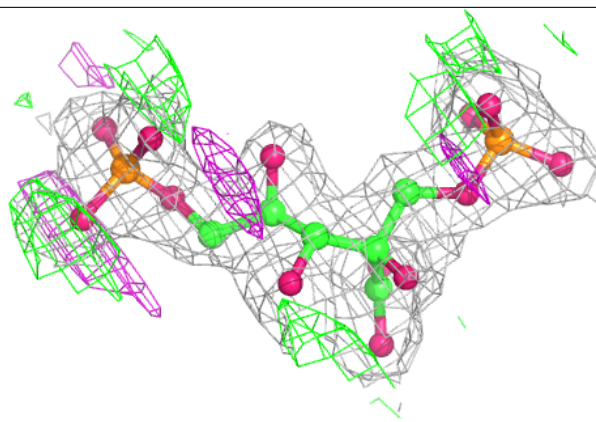
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

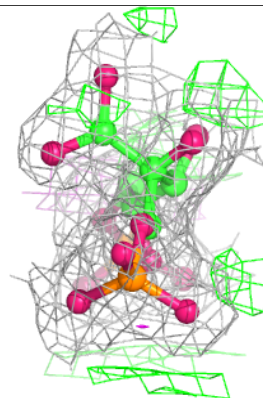
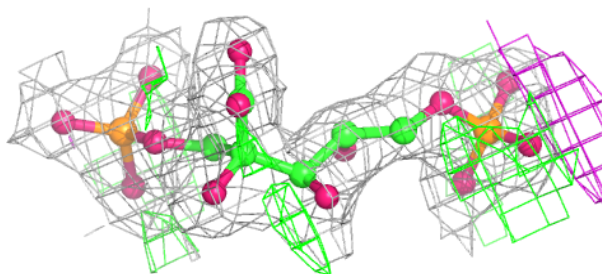
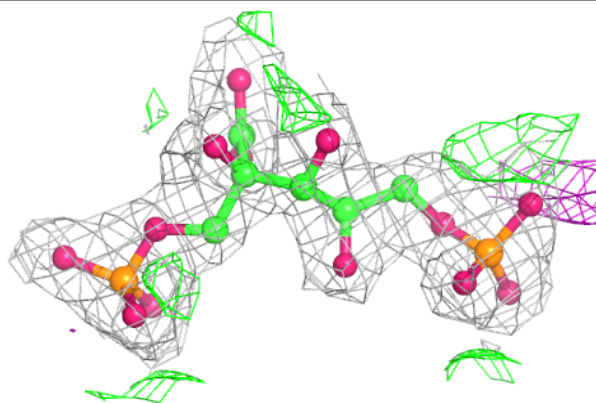


**Electron density around CAP E 476:**

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

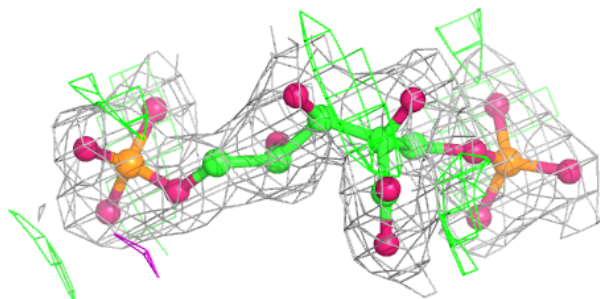
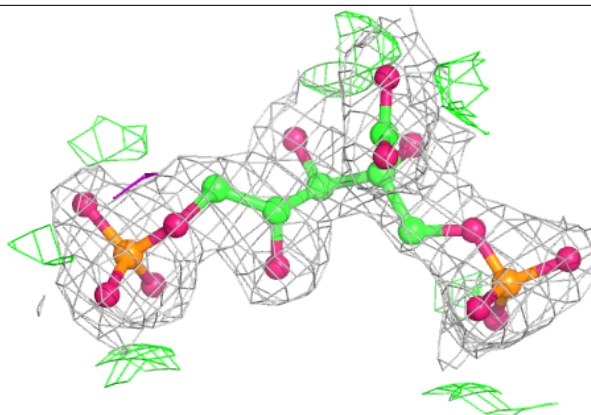
**Electron density around CAP F 476:**

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

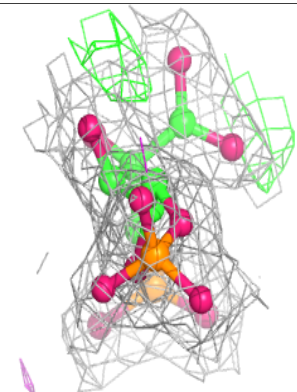
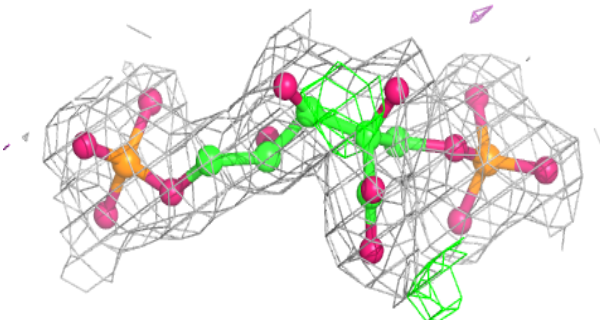
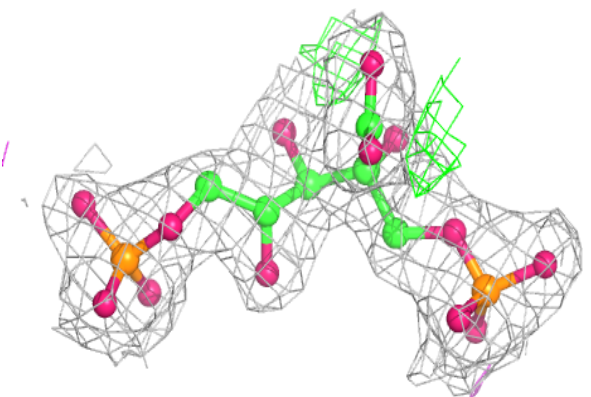


**Electron density around CAP B 476:**

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

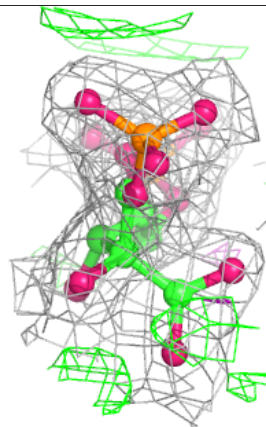
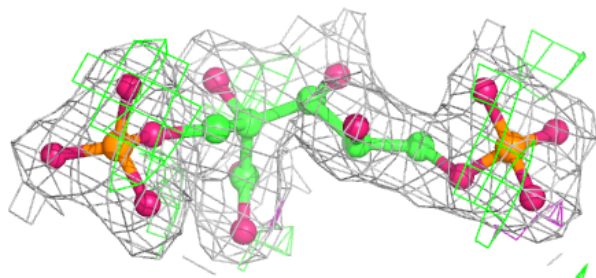
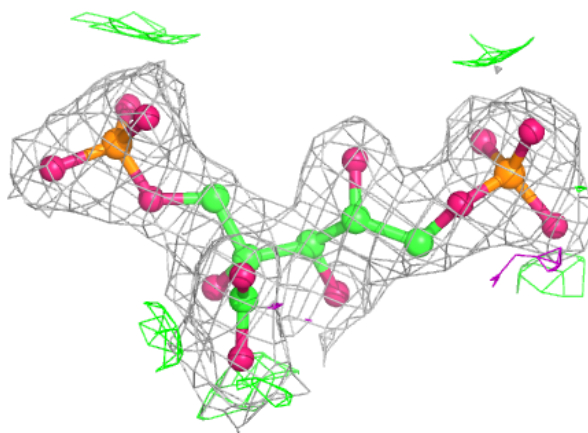
**Electron density around CAP A 476:**

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

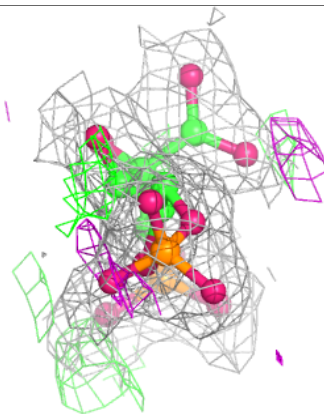
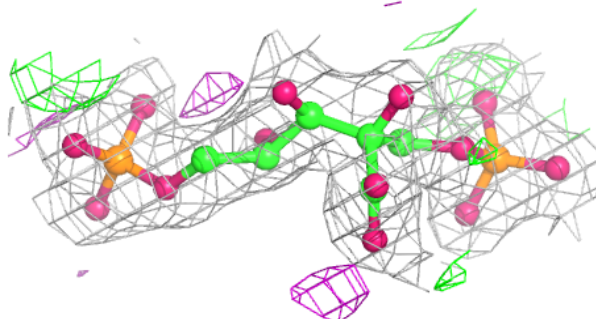
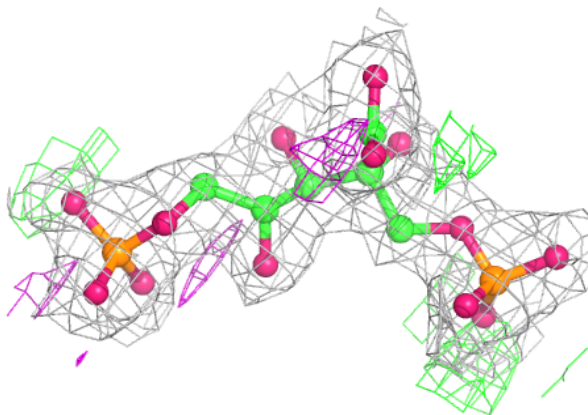


**Electron density around CAP G 476:**

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

**Electron density around CAP D 476:**

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



## 6.5 Other polymers

There are no such residues in this entry.