wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 05:22 pm BST

PDB ID	:	1UPM
Title	:	ACTIVATED SPINACH RUBISCO COMPLEXED WITH 2-CARBOXYARABINITOL 2 BISPHOSPHAT AND CA2+.
Authors	:	Karkehabadi, S.; Taylor, T.C.; Andersson, I.
Deposited on	:	2003-10-08
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

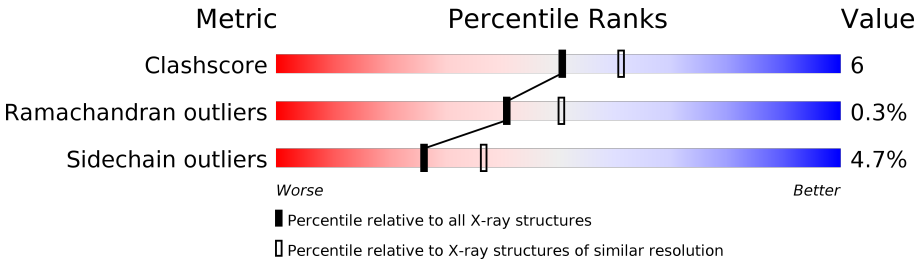
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	B	475	83% 13% • • •
1	E	475	82% 13% • • •
1	H	475	83% 12% • • •
1	K	475	84% 11% • •
1	L	475	83% 12% • • •
1	O	475	83% 13% • • •
1	R	475	83% 13% • • •
1	V	475	85% 11% • • •
2	C	123	76% 18% 5% •

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Mol	Chain	Length	Quality of chain
2	F	123	80% 16%
2	I	123	80% 15% 5%
2	M	123	79% 18%
2	P	123	85% 12%
2	S	123	81% 14% 5%
2	T	123	81% 15%
2	W	123	84% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 40436 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	B	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	E	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	H	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	K	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	L	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	O	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	R	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	V	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	F	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	I	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	M	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	P	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	T	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			
2	W	123	Total	C	N	O	S	0	0	0
			1032	673	167	185	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	GLN	LYS	conflict	UNP Q43832
S	6	ILE	THR	conflict	UNP Q43832
S	7	LEU	GLN	conflict	UNP Q43832
S	9	LEU	MET	conflict	UNP Q43832
S	11	LYS	ARG	conflict	UNP Q43832
S	109	GLU	GLN	conflict	UNP Q43832
S	113	ILE	VAL	conflict	UNP Q43832
C	2	GLN	LYS	conflict	UNP Q43832
C	6	ILE	THR	conflict	UNP Q43832
C	7	LEU	GLN	conflict	UNP Q43832
C	9	LEU	MET	conflict	UNP Q43832
C	11	LYS	ARG	conflict	UNP Q43832
C	109	GLU	GLN	conflict	UNP Q43832
C	113	ILE	VAL	conflict	UNP Q43832
F	2	GLN	LYS	conflict	UNP Q43832
F	6	ILE	THR	conflict	UNP Q43832
F	7	LEU	GLN	conflict	UNP Q43832
F	9	LEU	MET	conflict	UNP Q43832
F	11	LYS	ARG	conflict	UNP Q43832
F	109	GLU	GLN	conflict	UNP Q43832
F	113	ILE	VAL	conflict	UNP Q43832
I	2	GLN	LYS	conflict	UNP Q43832
I	6	ILE	THR	conflict	UNP Q43832
I	7	LEU	GLN	conflict	UNP Q43832
I	9	LEU	MET	conflict	UNP Q43832
I	11	LYS	ARG	conflict	UNP Q43832
I	109	GLU	GLN	conflict	UNP Q43832
I	113	ILE	VAL	conflict	UNP Q43832
M	2	GLN	LYS	conflict	UNP Q43832
M	6	ILE	THR	conflict	UNP Q43832
M	7	LEU	GLN	conflict	UNP Q43832
M	9	LEU	MET	conflict	UNP Q43832

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Chain	Residue	Modelled	Actual	Comment	Reference
M	11	LYS	ARG	conflict	UNP Q43832
M	109	GLU	GLN	conflict	UNP Q43832
M	113	ILE	VAL	conflict	UNP Q43832
P	2	GLN	LYS	conflict	UNP Q43832
P	6	ILE	THR	conflict	UNP Q43832
P	7	LEU	GLN	conflict	UNP Q43832
P	9	LEU	MET	conflict	UNP Q43832
P	11	LYS	ARG	conflict	UNP Q43832
P	109	GLU	GLN	conflict	UNP Q43832
P	113	ILE	VAL	conflict	UNP Q43832
T	2	GLN	LYS	conflict	UNP Q43832
T	6	ILE	THR	conflict	UNP Q43832
T	7	LEU	GLN	conflict	UNP Q43832
T	9	LEU	MET	conflict	UNP Q43832
T	11	LYS	ARG	conflict	UNP Q43832
T	109	GLU	GLN	conflict	UNP Q43832
T	113	ILE	VAL	conflict	UNP Q43832
W	2	GLN	LYS	conflict	UNP Q43832
W	6	ILE	THR	conflict	UNP Q43832
W	7	LEU	GLN	conflict	UNP Q43832
W	9	LEU	MET	conflict	UNP Q43832
W	11	LYS	ARG	conflict	UNP Q43832
W	109	GLU	GLN	conflict	UNP Q43832
W	113	ILE	VAL	conflict	UNP Q43832

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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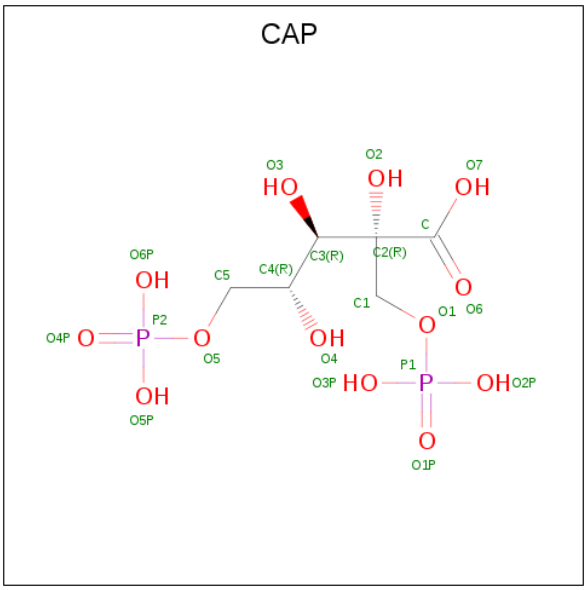
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total Ca 1 1	0	0

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



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

- Molecule 5 is water.

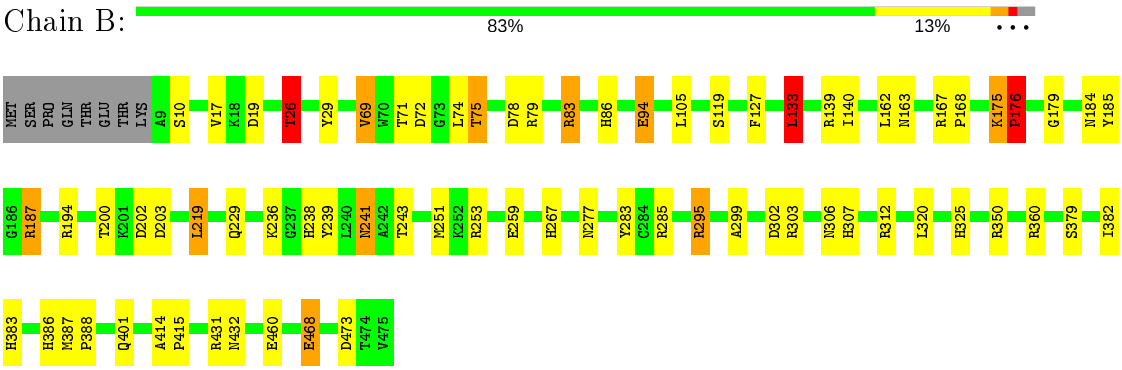
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	263	Total O 263 263	0	0
5	C	58	Total O 58 58	0	0
5	E	297	Total O 297 297	0	0
5	F	100	Total O 100 100	0	0
5	H	246	Total O 246 246	0	0
5	I	42	Total O 42 42	0	0
5	K	278	Total O 278 278	0	0
5	L	308	Total O 308 308	0	0
5	M	91	Total O 91 91	0	0
5	O	261	Total O 261 261	0	0
5	P	54	Total O 54 54	0	0
5	R	290	Total O 290 290	0	0
5	S	93	Total O 93 93	0	0
5	T	88	Total O 88 88	0	0
5	V	274	Total O 274 274	0	0
5	W	45	Total O 45 45	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. 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. 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.

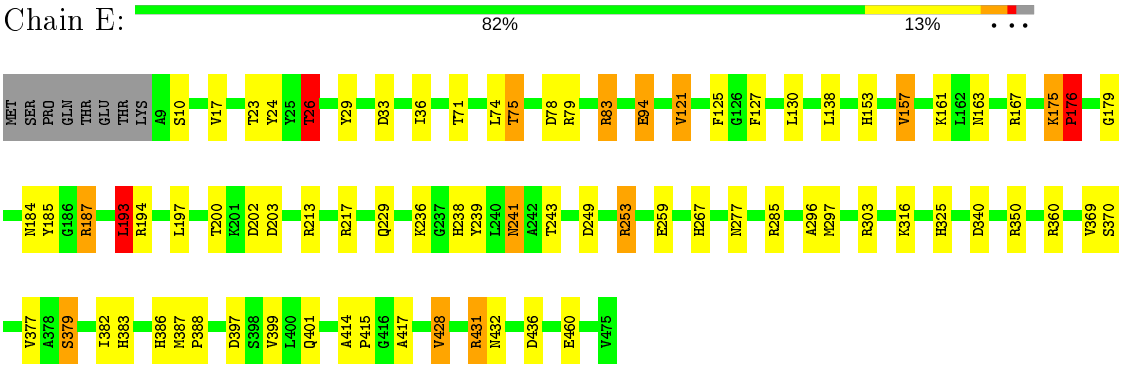
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain B:



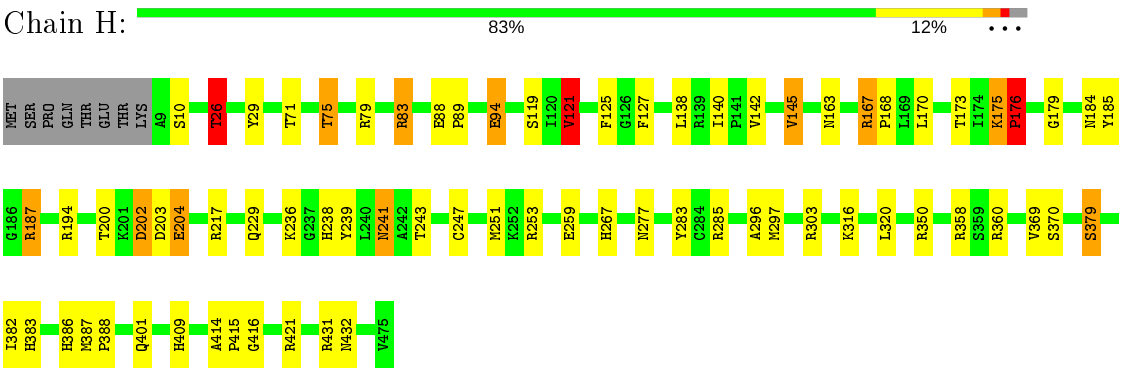
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain E:



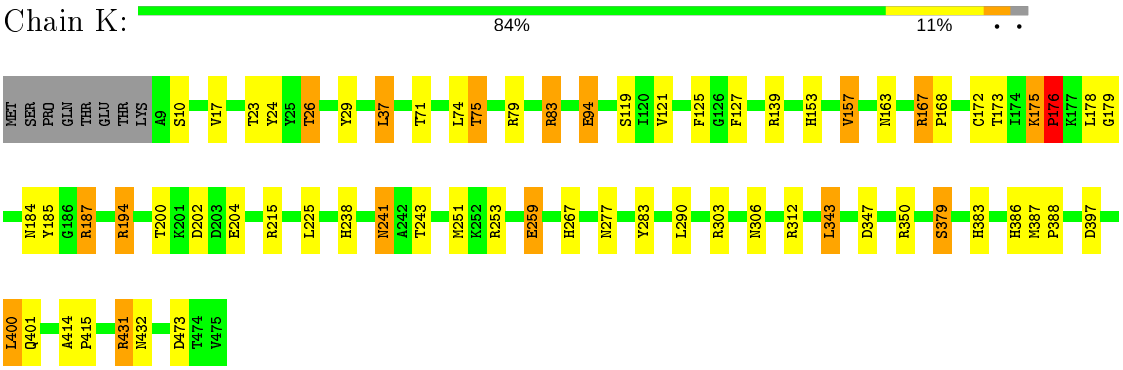
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain H:



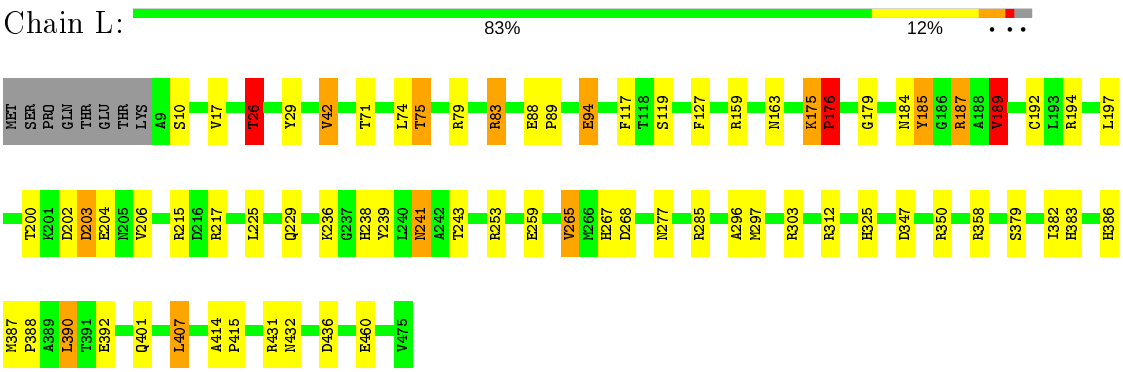
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain K:



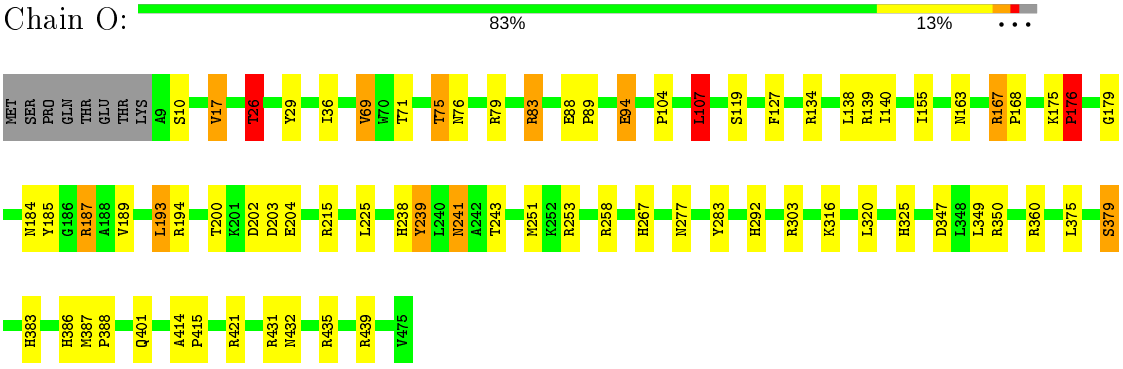
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain L:



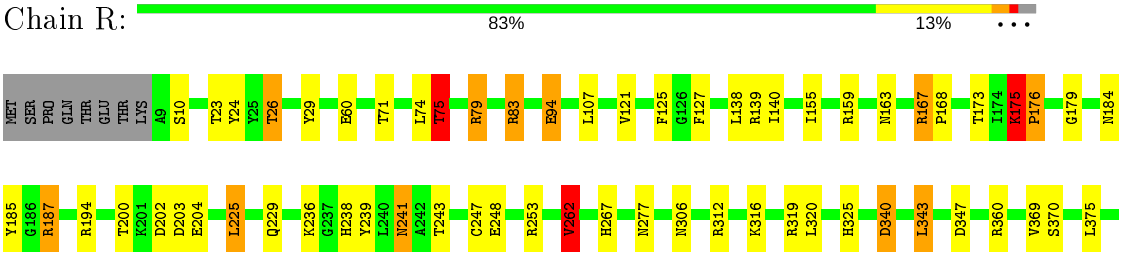
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain O:



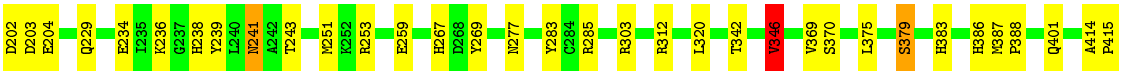
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain R:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain V:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain C:

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain F:

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

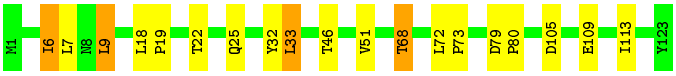
Chain I:

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain M:

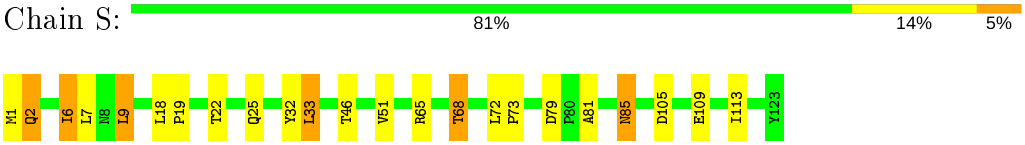
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain P:



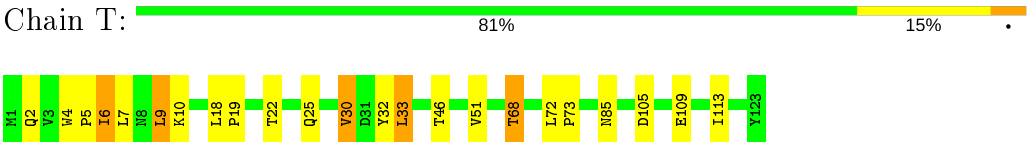
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain S:



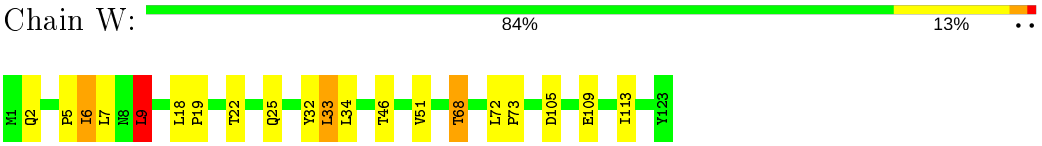
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain T:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	219.60Å 220.94Å 116.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 98.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-2.30) 90.2 (98.33-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.80 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.200 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.871	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40436	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, CAP, 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	B	0.53	0/3729	1.18	26/5057 (0.5%)
1	E	0.53	0/3729	1.18	29/5057 (0.6%)
1	H	0.52	0/3729	1.15	24/5057 (0.5%)
1	K	0.55	0/3729	1.22	22/5057 (0.4%)
1	L	0.55	0/3729	1.23	33/5057 (0.7%)
1	O	0.55	0/3729	1.21	25/5057 (0.5%)
1	R	0.56	1/3729 (0.0%)	1.22	31/5057 (0.6%)
1	V	0.52	0/3729	1.16	26/5057 (0.5%)
2	C	2.18	1/1067 (0.1%)	1.02	7/1453 (0.5%)
2	F	0.46	0/1067	1.03	4/1453 (0.3%)
2	I	0.44	0/1067	1.03	4/1453 (0.3%)
2	M	0.47	0/1067	1.02	2/1453 (0.1%)
2	P	0.42	0/1067	0.99	3/1453 (0.2%)
2	S	0.45	0/1067	1.06	6/1453 (0.4%)
2	T	0.44	0/1067	1.06	5/1453 (0.3%)
2	W	0.43	0/1067	0.99	3/1453 (0.2%)
All	All	0.63	2/38368 (0.0%)	1.16	250/52080 (0.5%)

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	B	0	1
1	E	0	1
1	H	0	1
1	K	0	1
1	L	0	1
1	O	0	1
1	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	V	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	MET	N-CA	69.94	2.86	1.46
1	R	176	PRO	N-CD	8.49	1.59	1.47

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	176	PRO	CA-N-CD	-16.55	88.33	111.50
1	O	303	ARG	NE-CZ-NH1	12.19	126.40	120.30
1	L	187	ARG	NE-CZ-NH2	-12.03	114.28	120.30
1	O	187	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	L	285	ARG	NE-CZ-NH1	9.71	125.15	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	175	LYS	Peptide
1	E	175	LYS	Peptide
1	H	175	LYS	Peptide
1	K	175	LYS	Peptide
1	L	175	LYS	Peptide

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	B	3652	0	3560	40	1
1	E	3652	0	3560	44	0
1	H	3652	0	3560	40	0
1	K	3652	0	3560	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3652	0	3560	33	0
1	O	3652	0	3560	39	1
1	R	3652	0	3560	41	0
1	V	3652	0	3560	37	0
2	C	1032	0	990	25	0
2	F	1032	0	990	24	0
2	I	1032	0	990	26	0
2	M	1032	0	990	24	0
2	P	1032	0	990	19	0
2	S	1032	0	990	22	0
2	T	1032	0	990	20	0
2	W	1032	0	990	19	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	B	21	0	7	0	0
4	E	21	0	8	0	0
4	H	21	0	8	0	0
4	K	21	0	8	0	0
4	L	21	0	7	0	0
4	O	21	0	7	0	0
4	R	21	0	8	0	0
4	V	21	0	8	0	0
5	B	263	0	0	6	0
5	C	58	0	0	2	0
5	E	297	0	0	4	0
5	F	100	0	0	3	0
5	H	246	0	0	0	0
5	I	42	0	0	2	0
5	K	278	0	0	3	0
5	L	308	0	0	2	0
5	M	91	0	0	2	0
5	O	261	0	0	1	0
5	P	54	0	0	0	0
5	R	290	0	0	5	0
5	S	93	0	0	3	0
5	T	88	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	274	0	0	2	0
5	W	45	0	0	1	0
All	All	40436	0	36461	420	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 420 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:K:473:ASP:OD2	5:K:2273:HOH:O	1.71	1.08
2:C:22:THR:H	2:C:25:GLN:HE21	1.14	0.95
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.14	0.94
1:K:267:HIS:HD2	1:K:277:ASN:HD22	1.15	0.93
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.16	0.92

All (1) 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)
1:B:468:GLU:OE1	1:O:439:ARG:NH1[4_456]	2.13	0.07

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	B	464/475 (98%)	440 (95%)	22 (5%)	2 (0%)	34 42
1	E	464/475 (98%)	438 (94%)	24 (5%)	2 (0%)	34 42
1	H	464/475 (98%)	445 (96%)	17 (4%)	2 (0%)	34 42
1	K	464/475 (98%)	443 (96%)	18 (4%)	3 (1%)	25 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	464/475 (98%)	444 (96%)	18 (4%)	2 (0%)	34	42
1	O	464/475 (98%)	442 (95%)	20 (4%)	2 (0%)	34	42
1	R	464/475 (98%)	442 (95%)	21 (4%)	1 (0%)	47	58
1	V	464/475 (98%)	441 (95%)	21 (4%)	2 (0%)	34	42
2	C	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	F	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	I	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	M	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	P	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	S	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	T	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	W	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
All	All	4680/4784 (98%)	4454 (95%)	210 (4%)	16 (0%)	41	50

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	SER
1	B	176	PRO
1	E	10	SER
1	E	176	PRO
1	H	10	SER

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	B	377/386 (98%)	360 (96%)	17 (4%)	27	39
1	E	377/386 (98%)	362 (96%)	15 (4%)	31	44
1	H	377/386 (98%)	362 (96%)	15 (4%)	31	44
1	K	377/386 (98%)	361 (96%)	16 (4%)	30	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	377/386 (98%)	358 (95%)	19 (5%)	24	34
1	O	377/386 (98%)	359 (95%)	18 (5%)	25	36
1	R	377/386 (98%)	364 (97%)	13 (3%)	37	51
1	V	377/386 (98%)	364 (97%)	13 (3%)	37	51
2	C	112/112 (100%)	104 (93%)	8 (7%)	14	19
2	F	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	I	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	M	112/112 (100%)	104 (93%)	8 (7%)	14	19
2	P	112/112 (100%)	107 (96%)	5 (4%)	27	39
2	S	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	T	112/112 (100%)	104 (93%)	8 (7%)	14	19
2	W	112/112 (100%)	105 (94%)	7 (6%)	18	24
All	All	3912/3984 (98%)	3729 (95%)	183 (5%)	26	37

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	343	LEU
1	L	390	LEU
1	V	163	ASN
1	L	17	VAL
1	L	127	PHE

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	K	304	GLN
1	L	304	GLN
1	V	267	HIS
1	K	401	GLN
1	L	184	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	B	201	1,3	7,11,12	0.41	0	4,12,14	1.19	1 (25%)
1	KCX	O	201	1,3	7,11,12	0.53	0	4,12,14	1.18	1 (25%)
1	KCX	K	201	1,3	7,11,12	0.61	0	4,12,14	1.01	0
1	KCX	E	201	1,3	7,11,12	0.58	0	4,12,14	0.77	0
1	KCX	V	201	1,3	7,11,12	0.62	0	4,12,14	1.71	1 (25%)
1	KCX	L	201	1,3	7,11,12	0.77	0	4,12,14	0.86	0
1	KCX	R	201	1,3	7,11,12	0.58	0	4,12,14	0.43	0
1	KCX	H	201	1,3	7,11,12	0.49	0	4,12,14	1.04	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	201	1,3	-	1/7/10/12	-
1	KCX	O	201	1,3	-	0/7/10/12	-
1	KCX	K	201	1,3	-	0/7/10/12	-
1	KCX	E	201	1,3	-	0/7/10/12	-
1	KCX	V	201	1,3	-	0/7/10/12	-
1	KCX	L	201	1,3	-	0/7/10/12	-
1	KCX	R	201	1,3	-	0/7/10/12	-
1	KCX	H	201	1,3	-	0/7/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	201	KCX	CE-NZ-CX	3.08	128.17	122.95
1	O	201	KCX	CE-NZ-CX	2.27	126.80	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	201	KCX	CE-NZ-CX	2.04	126.40	122.95
1	B	201	KCX	CE-NZ-CX	2.04	126.40	122.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	201	KCX	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	H	477	3	15,20,20	1.85	4 (26%)	20,31,31	1.85	8 (40%)
4	CAP	K	477	3	15,20,20	2.03	7 (46%)	20,31,31	2.18	8 (40%)
4	CAP	B	477	3	15,20,20	1.96	5 (33%)	20,31,31	2.07	5 (25%)
4	CAP	E	477	3	15,20,20	1.90	5 (33%)	20,31,31	1.83	6 (30%)
4	CAP	V	477	3	15,20,20	1.89	5 (33%)	20,31,31	1.91	6 (30%)
4	CAP	R	477	3	15,20,20	1.78	4 (26%)	20,31,31	1.92	7 (35%)
4	CAP	L	477	3	15,20,20	2.16	6 (40%)	20,31,31	2.00	7 (35%)
4	CAP	O	477	3	15,20,20	2.01	5 (33%)	20,31,31	1.93	8 (40%)

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	H	477	3	-	4/23/29/29	-
4	CAP	K	477	3	-	5/23/29/29	-
4	CAP	B	477	3	-	4/23/29/29	-
4	CAP	E	477	3	-	4/23/29/29	-
4	CAP	V	477	3	-	4/23/29/29	-
4	CAP	R	477	3	-	5/23/29/29	-
4	CAP	L	477	3	-	5/23/29/29	-
4	CAP	O	477	3	-	4/23/29/29	-

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	477	CAP	O4-C4	-4.38	1.34	1.43
4	L	477	CAP	O4-C4	-4.22	1.34	1.43
4	V	477	CAP	O4-C4	-4.05	1.34	1.43
4	R	477	CAP	O4-C4	-3.98	1.34	1.43
4	B	477	CAP	O4-C4	-3.89	1.35	1.43

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	477	CAP	O3-C3-C4	-4.97	98.48	109.13
4	L	477	CAP	P2-O5-C5	4.56	130.86	118.30
4	H	477	CAP	O4-C4-C3	-4.27	100.24	108.78
4	K	477	CAP	O6P-P2-O5P	4.22	123.78	107.64
4	V	477	CAP	P2-O5-C5	4.12	129.64	118.30

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

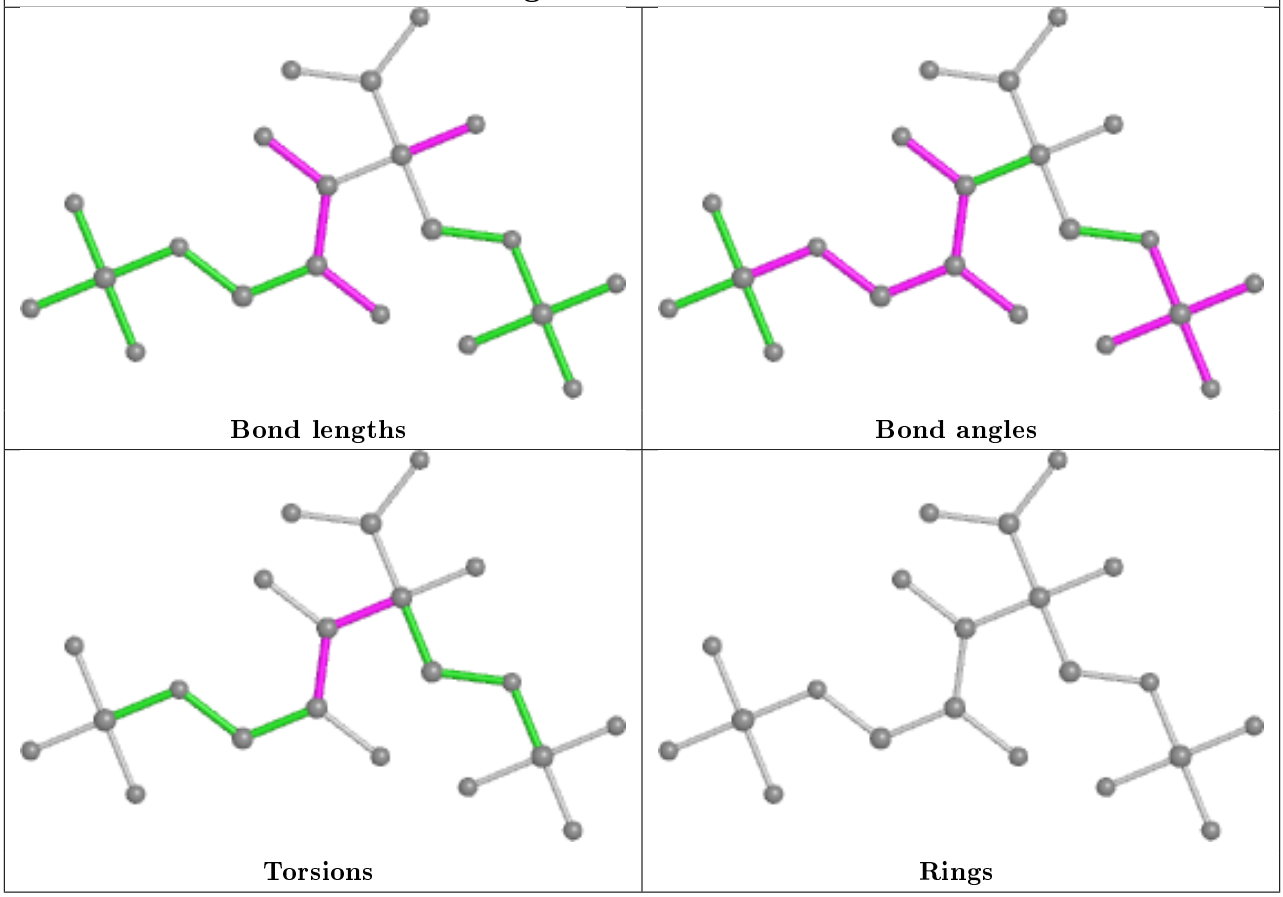
Mol	Chain	Res	Type	Atoms
4	H	477	CAP	C2-C3-C4-O4
4	H	477	CAP	O3-C3-C4-O4
4	K	477	CAP	C2-C3-C4-O4
4	K	477	CAP	O3-C3-C4-O4
4	B	477	CAP	C2-C3-C4-O4

There are no ring outliers.

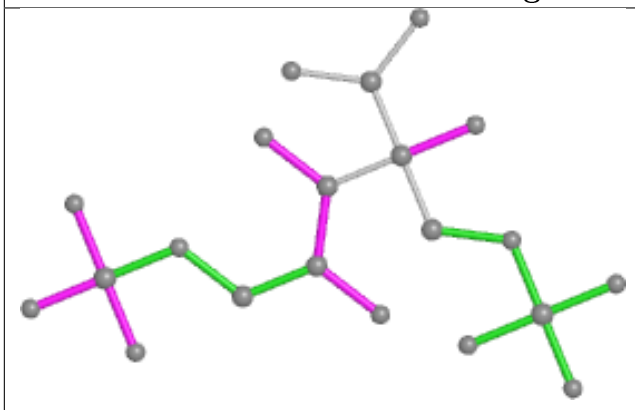
No monomer is involved in short contacts.

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 then 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.

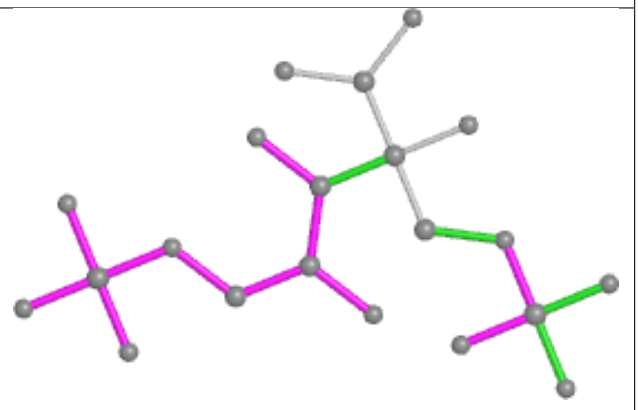
Ligand CAP H 477



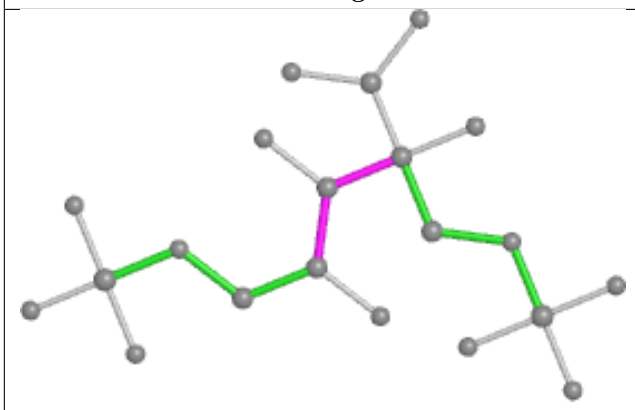
Ligand CAP K 477



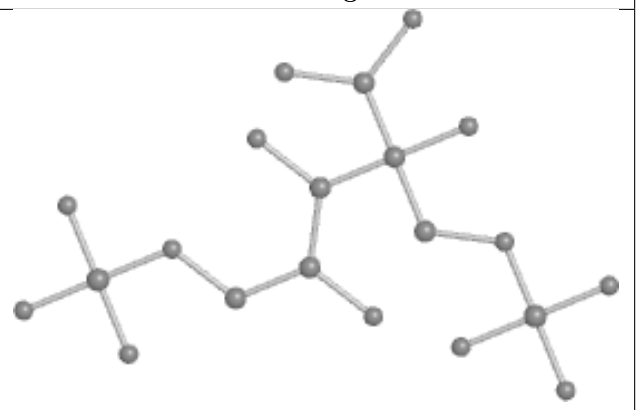
Bond lengths



Bond angles

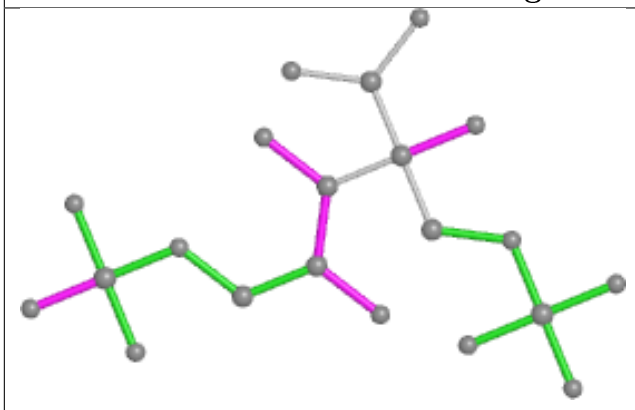


Torsions



Rings

Ligand CAP B 477



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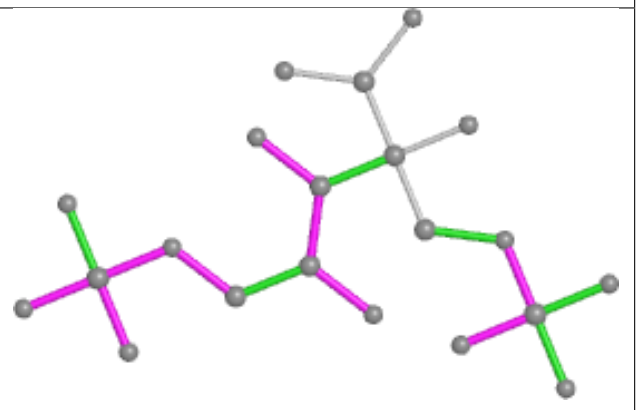

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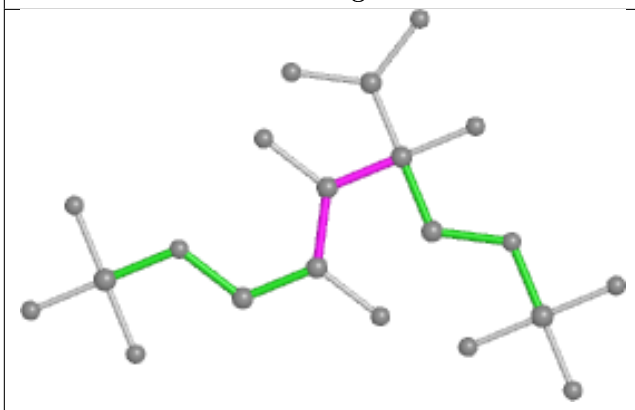

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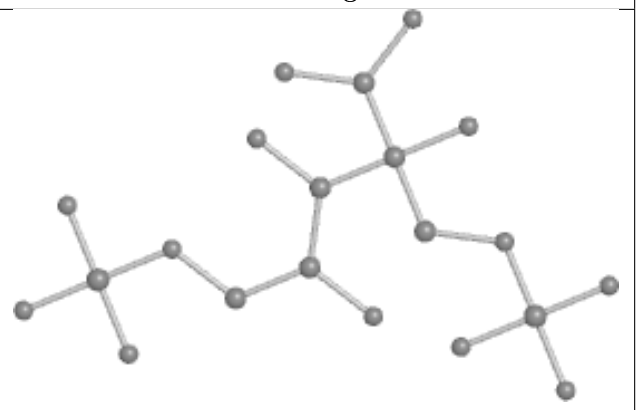
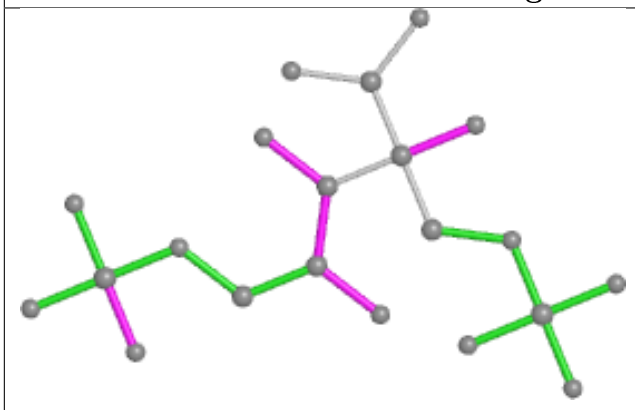
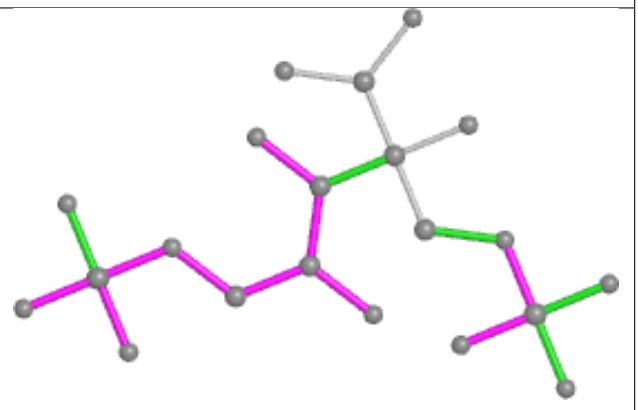


Rings

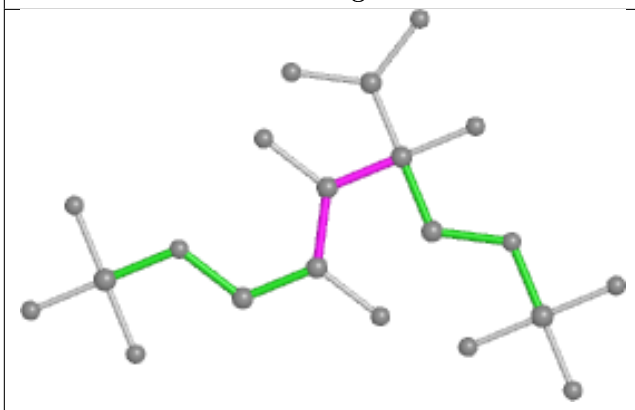
Ligand CAP E 477



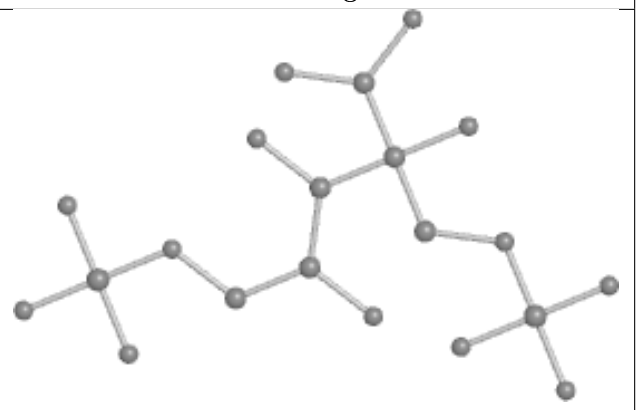
Bond lengths



Bond angles

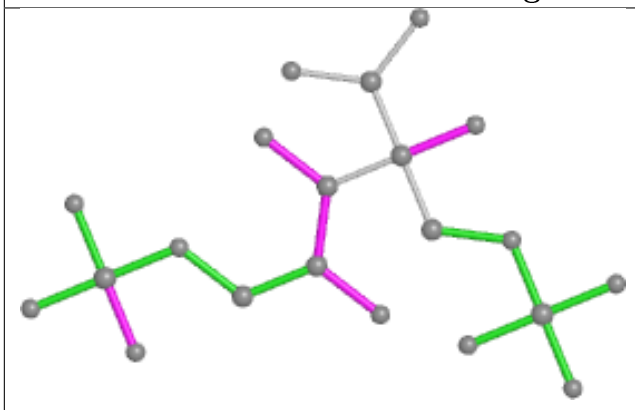


Torsions

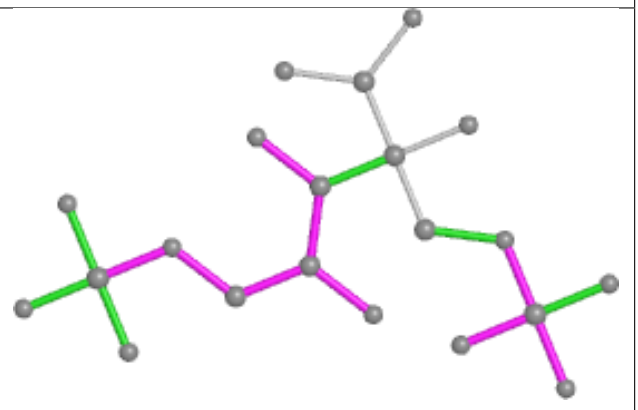


Rings

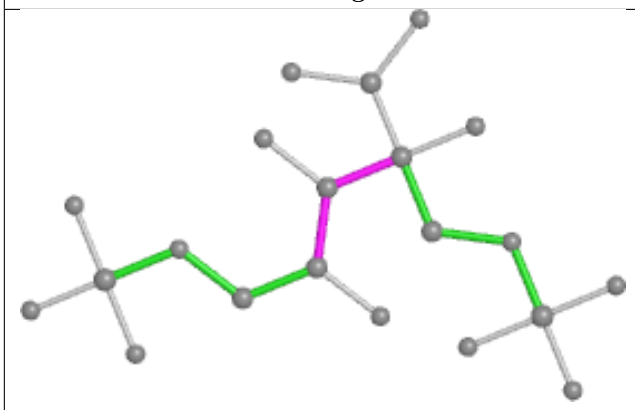
Ligand CAP V 477



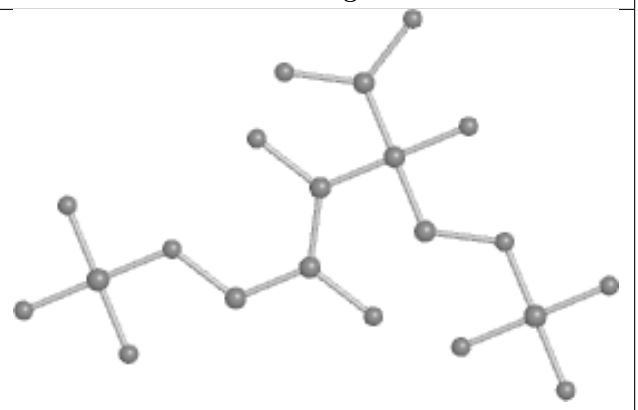
Bond lengths



Bond angles

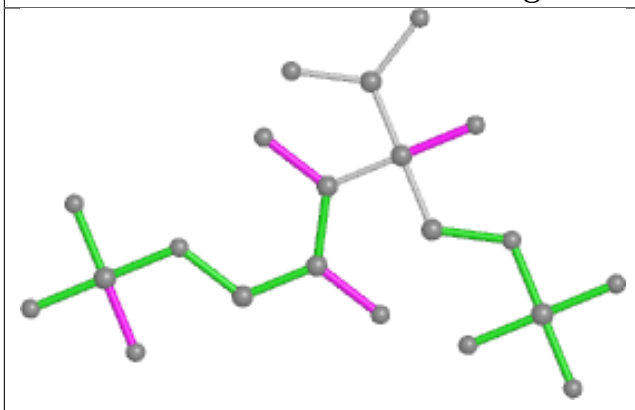


Torsions



Rings

Ligand CAP R 477



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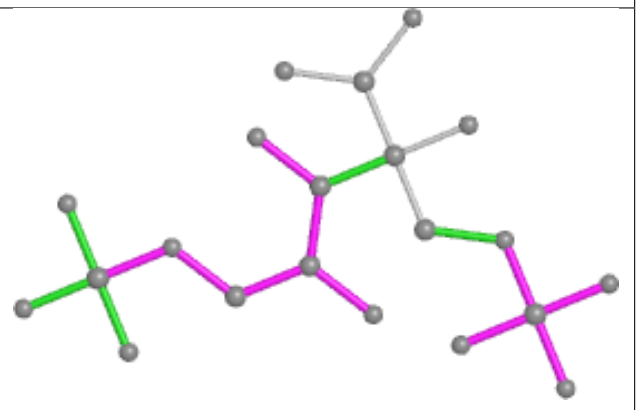
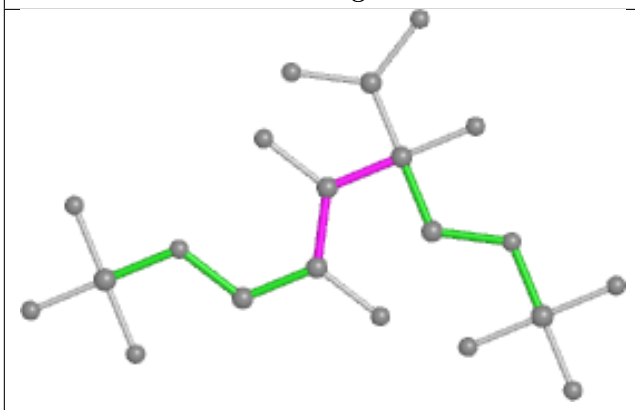
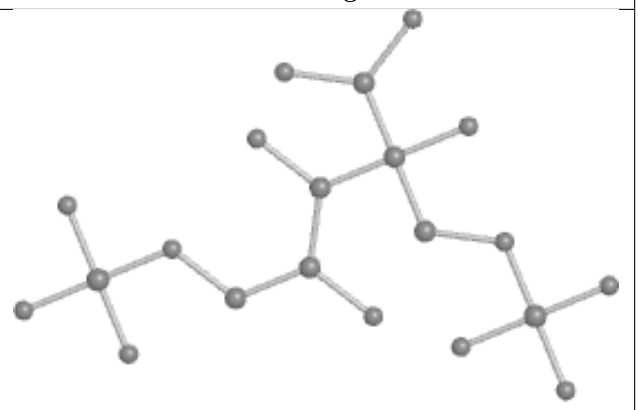


Bond angles

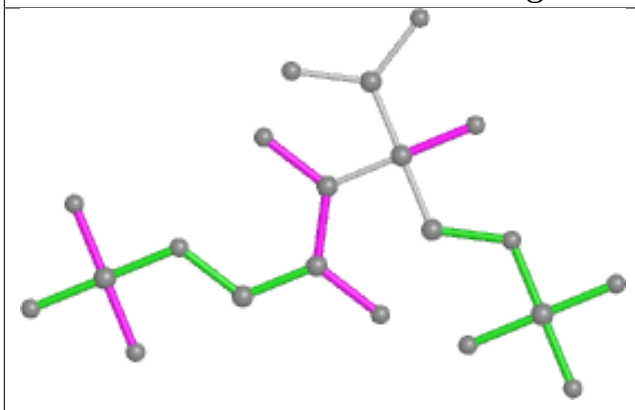


Torsions

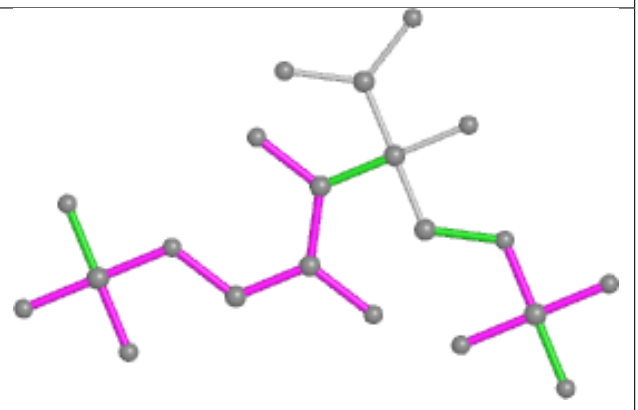


Rings

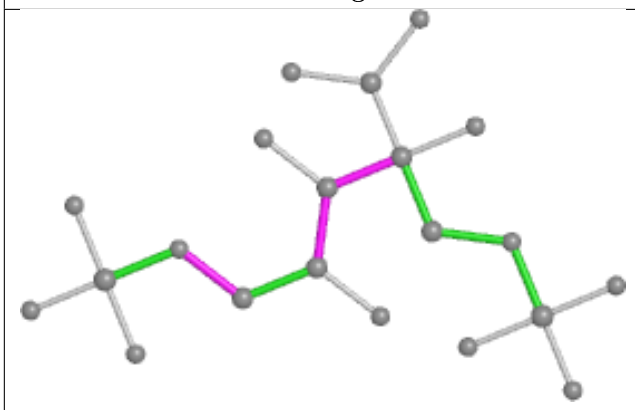
Ligand CAP L 477



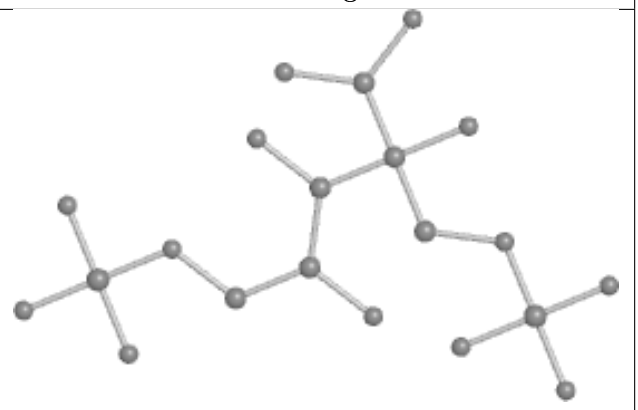
Bond lengths



Bond angles

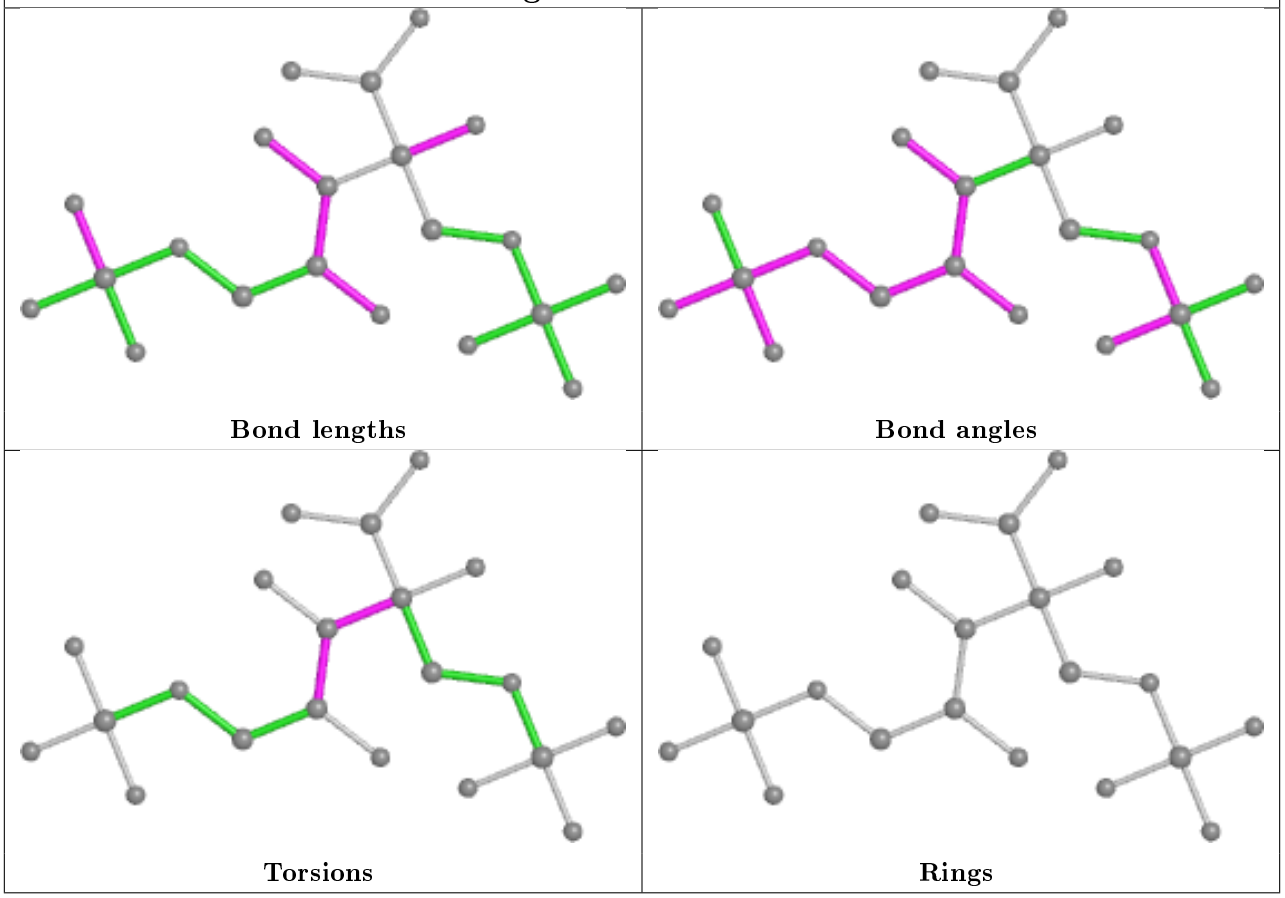


Torsions



Rings

Ligand CAP O 477



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

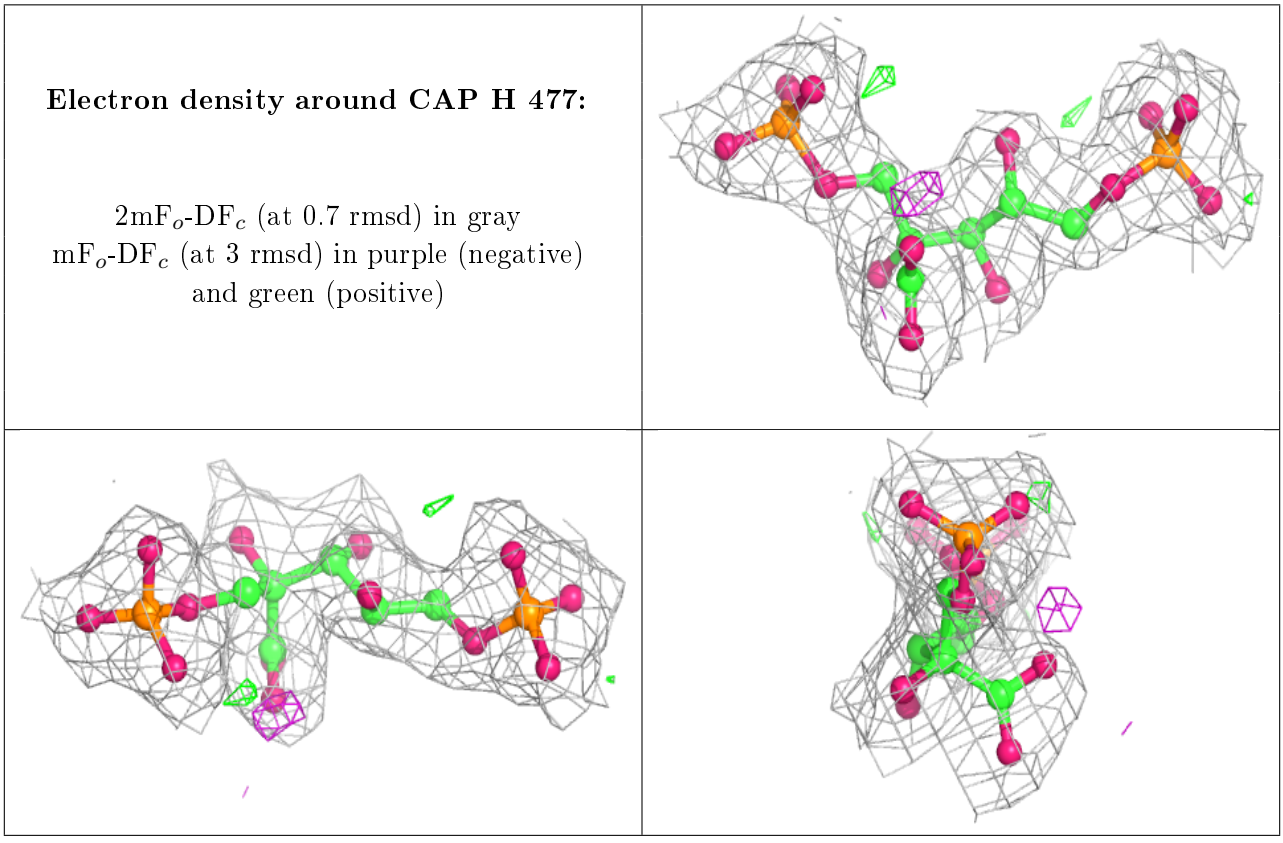
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

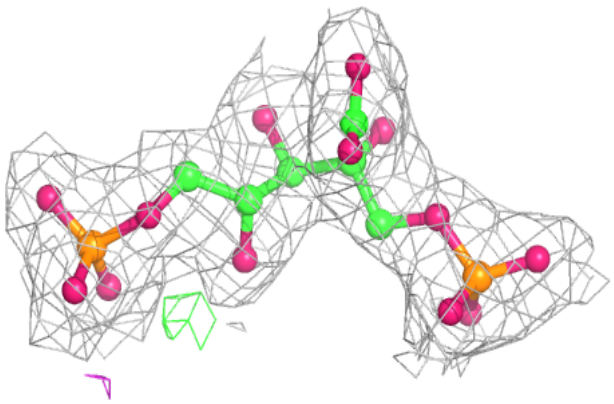
Electron density around CAP H 477:

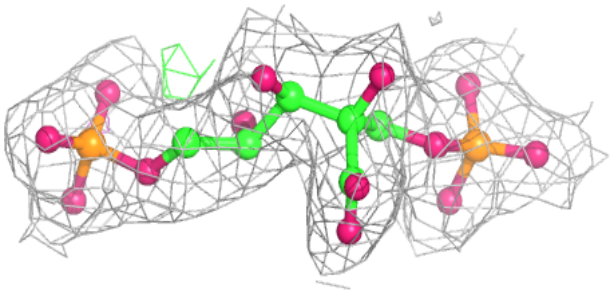
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

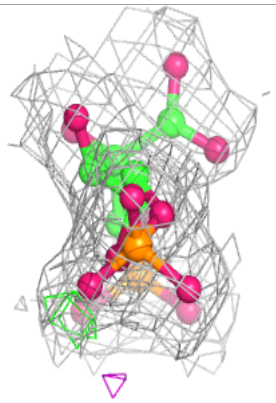


Electron density around CAP K 477:

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

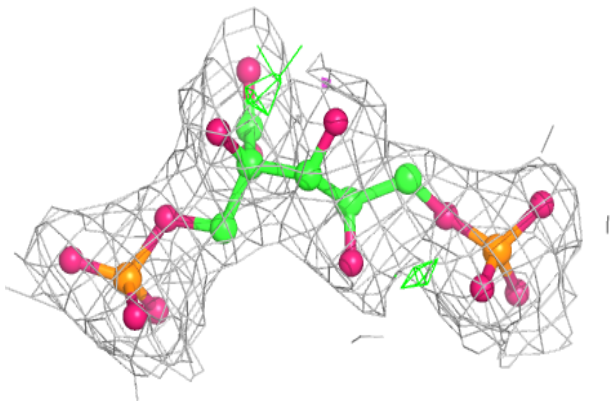


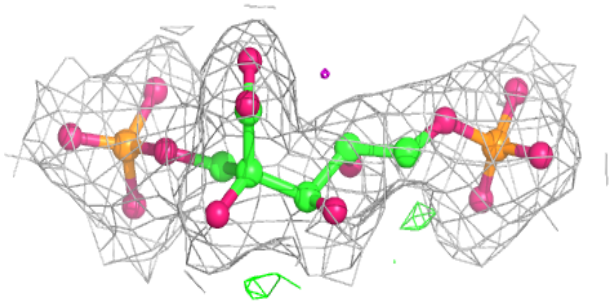


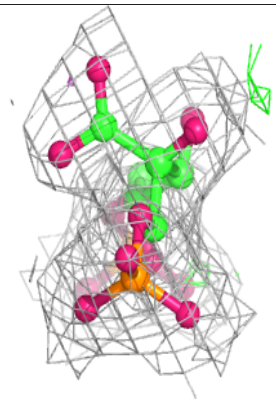


Electron density around CAP B 477:

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

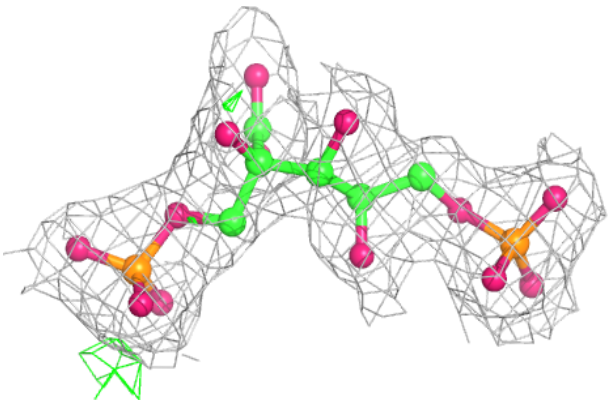


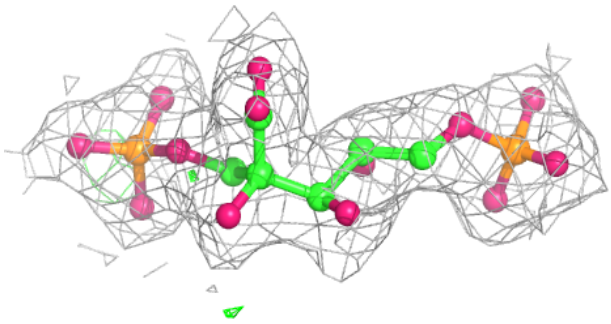


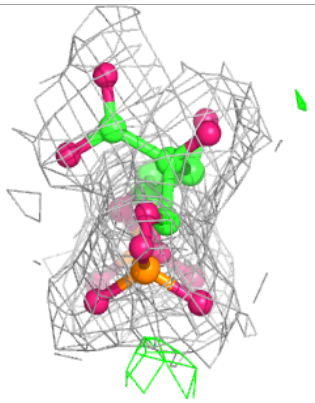


Electron density around CAP E 477:

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

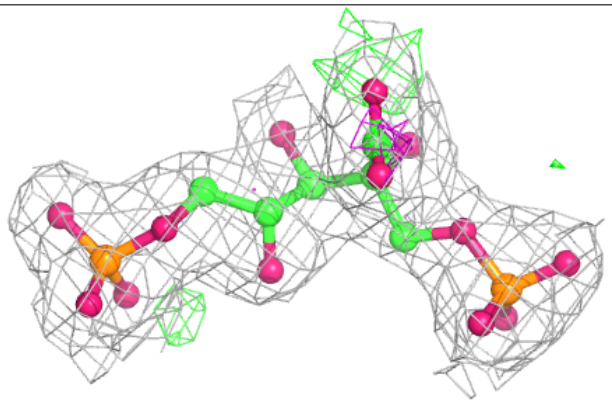


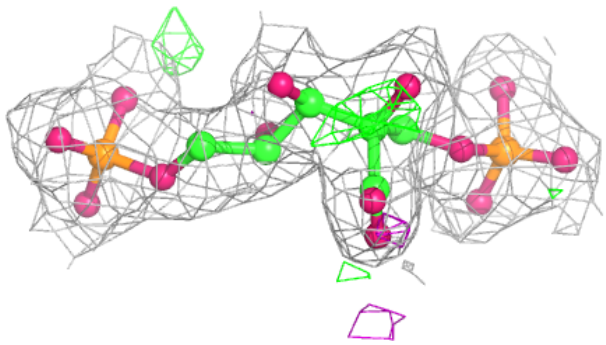


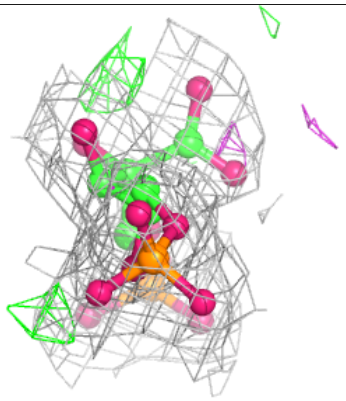


Electron density around CAP V 477:

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

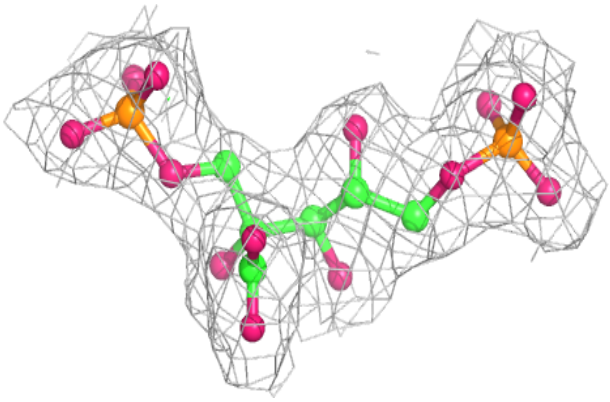


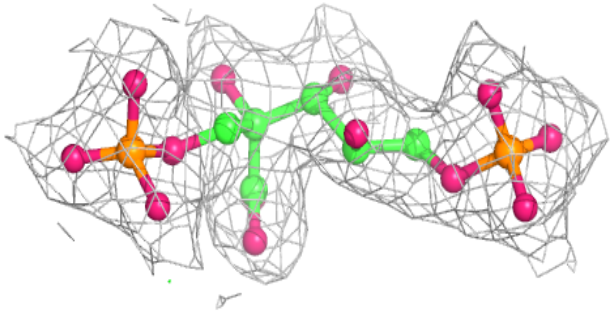


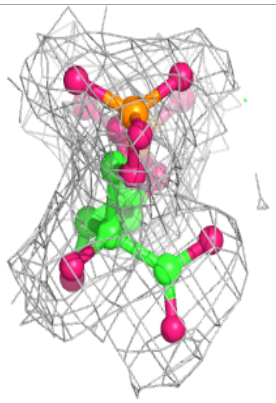


Electron density around CAP R 477:

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

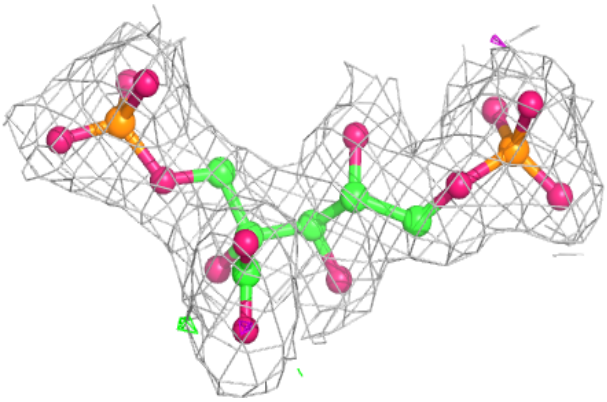


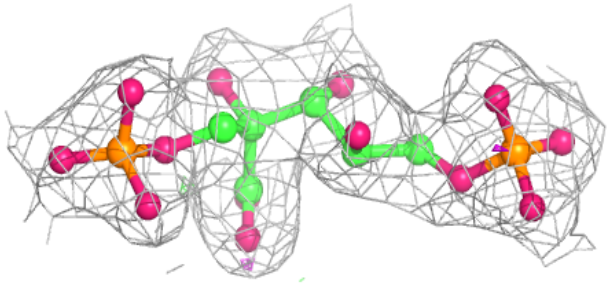


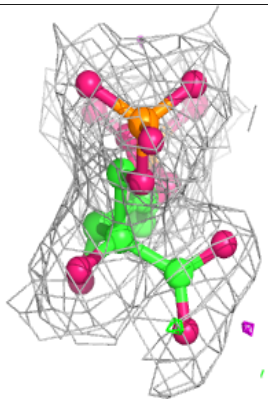


Electron density around CAP L 477:

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

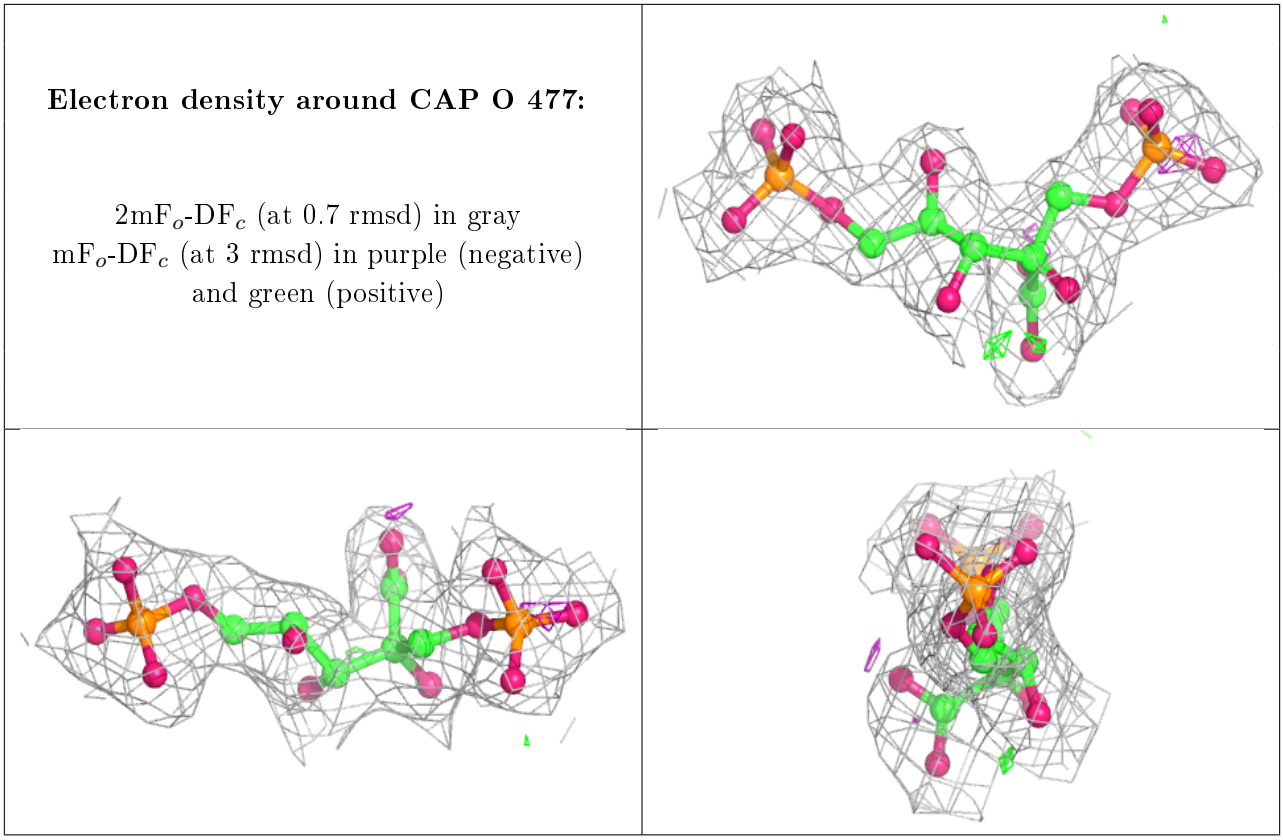






Electron density around CAP O 477:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.