



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 07:29 PM UTC

PDB ID : 1UW9 / pdb_00001uw9
Title : L290F-A222T chlamydomonas Rubisco mutant
Authors : Karkehabadi, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on : 2004-02-03
Resolution : 2.05 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

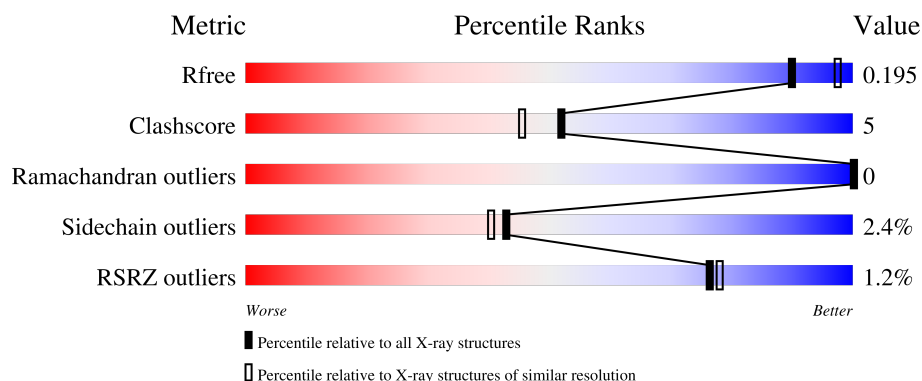
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



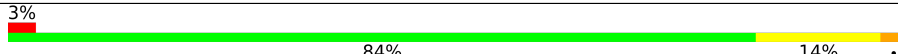
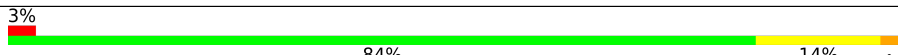
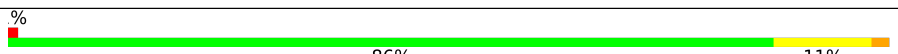
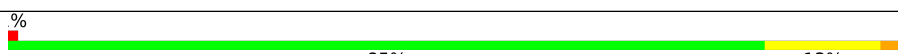
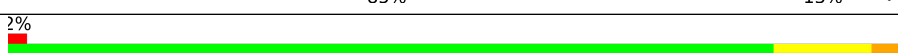
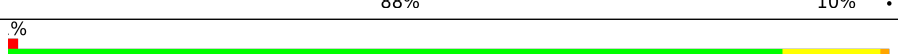
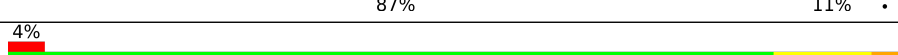
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	87% 11% ..
1	B	475	86% 11% .
1	E	475	87% 10% .
1	H	475	89% 10% .
1	K	475	88% 9% ..

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Mol	Chain	Length	Quality of chain	
1	O	475		..
1	R	475		.
1	V	475		.
2	C	140		.
2	F	140		..
2	I	140		.
2	J	140		.
2	M	140		.
2	P	140		.
2	T	140		.
2	W	140		.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1483	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 41674 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	4	0
			3646	2304	641	676	25			
1	B	467	Total	C	N	O	S	0	4	0
			3654	2309	642	677	26			
1	E	465	Total	C	N	O	S	0	4	0
			3646	2304	641	676	25			
1	H	469	Total	C	N	O	S	0	4	0
			3671	2319	646	681	25			
1	K	469	Total	C	N	O	S	0	6	0
			3679	2325	646	683	25			
1	O	469	Total	C	N	O	S	0	2	0
			3663	2315	645	678	25			
1	R	465	Total	C	N	O	S	0	3	0
			3643	2303	641	674	25			
1	V	466	Total	C	N	O	S	0	5	0
			3653	2309	642	677	25			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	conflict	UNP P00877
B	46	PRO	LEU	conflict	UNP P00877
E	46	PRO	LEU	conflict	UNP P00877
H	46	PRO	LEU	conflict	UNP P00877
K	46	PRO	LEU	conflict	UNP P00877
O	46	PRO	LEU	conflict	UNP P00877
R	46	PRO	LEU	conflict	UNP P00877
V	46	PRO	LEU	conflict	UNP P00877
A	222	THR	ALA	engineered mutation	UNP P00877
A	290	PHE	LEU	engineered mutation	UNP P00877
B	222	THR	ALA	engineered mutation	UNP P00877
B	290	PHE	LEU	engineered mutation	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
E	222	THR	ALA	engineered mutation	UNP P00877
E	290	PHE	LEU	engineered mutation	UNP P00877
H	222	THR	ALA	engineered mutation	UNP P00877
H	290	PHE	LEU	engineered mutation	UNP P00877
K	222	THR	ALA	engineered mutation	UNP P00877
K	290	PHE	LEU	engineered mutation	UNP P00877
O	222	THR	ALA	engineered mutation	UNP P00877
O	290	PHE	LEU	engineered mutation	UNP P00877
R	222	THR	ALA	engineered mutation	UNP P00877
R	290	PHE	LEU	engineered mutation	UNP P00877
V	222	THR	ALA	engineered mutation	UNP P00877
V	290	PHE	LEU	engineered mutation	UNP P00877

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	140	Total	C	N	O	S	0	2	0
			1149	741	192	205	11			
2	F	140	Total	C	N	O	S	0	2	0
			1154	747	191	204	12			
2	I	140	Total	C	N	O	S	0	1	0
			1146	740	191	204	11			
2	J	140	Total	C	N	O	S	0	2	0
			1154	747	191	204	12			
2	M	140	Total	C	N	O	S	0	2	0
			1147	740	191	204	12			
2	P	140	Total	C	N	O	S	0	3	0
			1150	741	192	205	12			
2	T	140	Total	C	N	O	S	0	3	0
			1157	748	192	205	12			
2	W	140	Total	C	N	O	S	0	2	0
			1147	740	191	204	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	128	SER	THR	conflict	UNP P00873
I	132	TRP	PHE	conflict	UNP P00873
C	128	SER	THR	conflict	UNP P00873
C	132	TRP	PHE	conflict	UNP P00873
F	128	SER	THR	conflict	UNP P00873
F	132	TRP	PHE	conflict	UNP P00873

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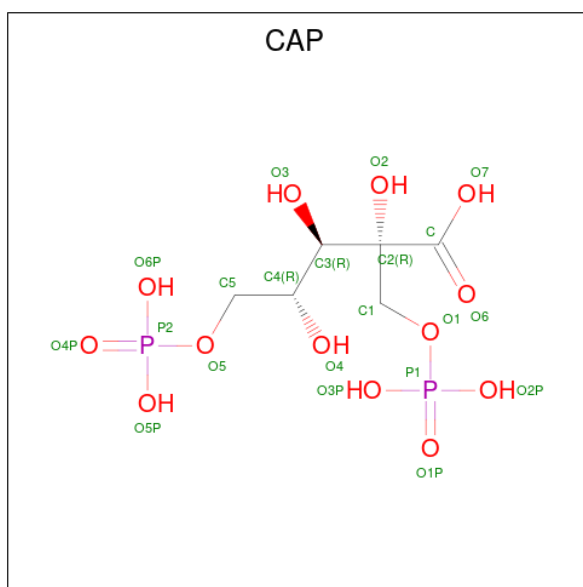
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Chain	Residue	Modelled	Actual	Comment	Reference
J	128	SER	THR	conflict	UNP P00873
J	132	TRP	PHE	conflict	UNP P00873
P	128	SER	THR	conflict	UNP P00873
P	132	TRP	PHE	conflict	UNP P00873
T	128	SER	THR	conflict	UNP P00873
T	132	TRP	PHE	conflict	UNP P00873
M	128	SER	THR	conflict	UNP P00873
M	132	TRP	PHE	conflict	UNP P00873
W	128	SER	THR	conflict	UNP P00873
W	132	TRP	PHE	conflict	UNP P00873

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

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

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: C₆H₁₄O₁₃P₂).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

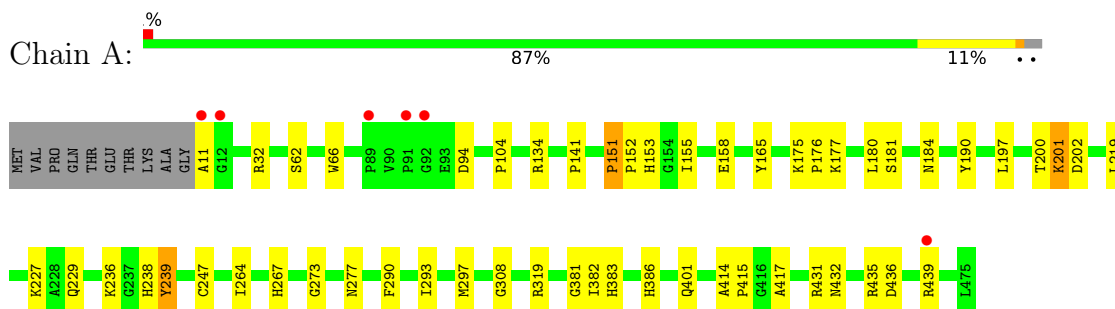
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	283	Total 283	O 283	0	0
6	B	276	Total 276	O 276	0	0
6	C	80	Total 80	O 80	0	0
6	E	285	Total 285	O 285	0	0
6	F	96	Total 96	O 96	0	0
6	H	271	Total 271	O 271	0	0
6	I	67	Total 67	O 67	0	0
6	J	74	Total 74	O 74	0	0
6	K	253	Total 253	O 253	0	0
6	M	87	Total 87	O 87	0	0
6	O	281	Total 281	O 281	0	0
6	P	60	Total 60	O 60	0	0
6	R	261	Total 261	O 261	0	0
6	T	76	Total 76	O 76	0	0
6	V	289	Total 289	O 289	0	0
6	W	80	Total 80	O 80	0	0

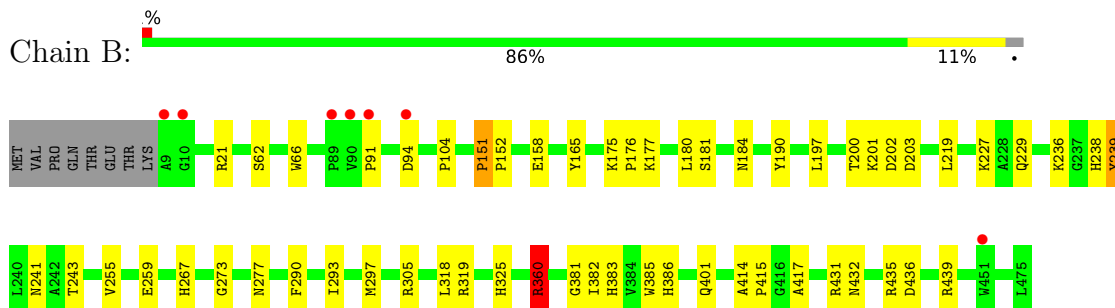
3 Residue-property plots

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

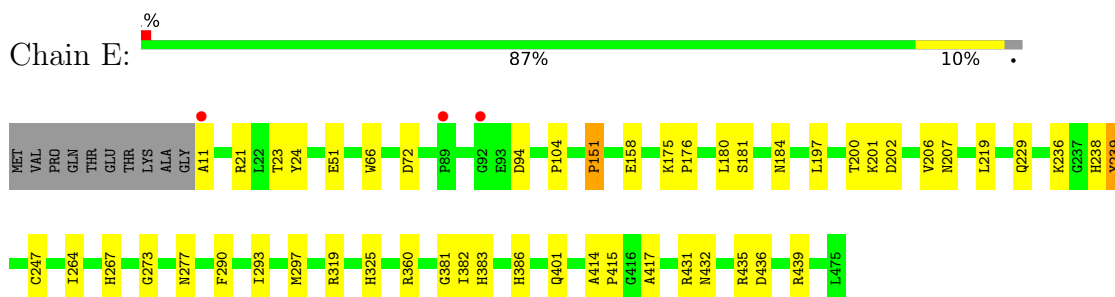
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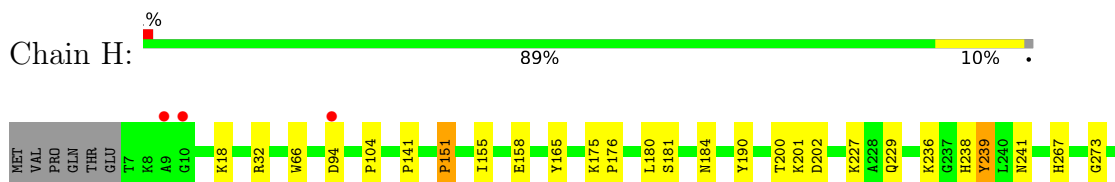
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

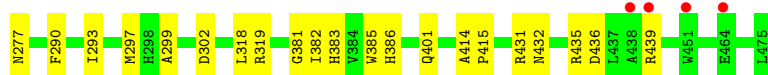


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

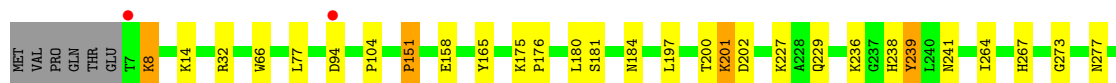
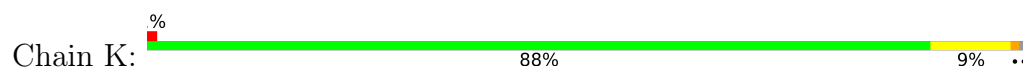


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

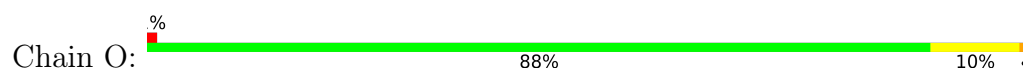




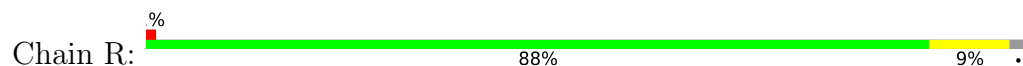
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



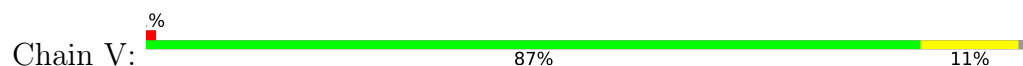
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



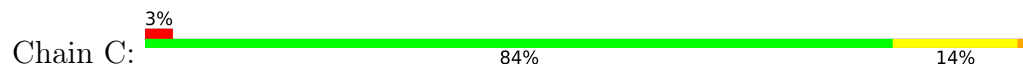
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

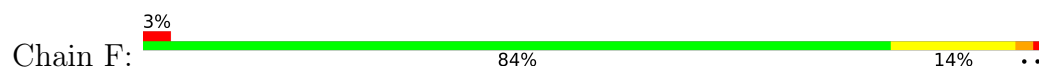


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

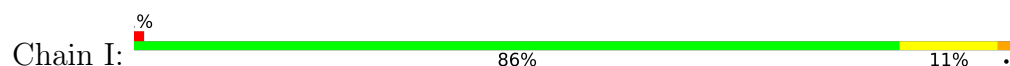




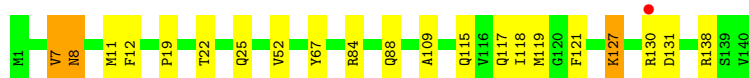
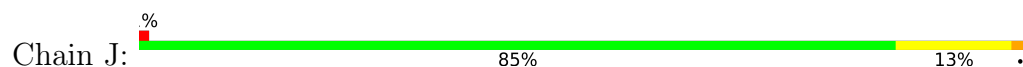
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



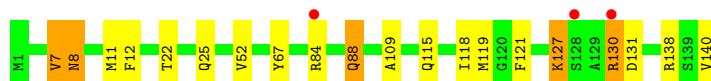
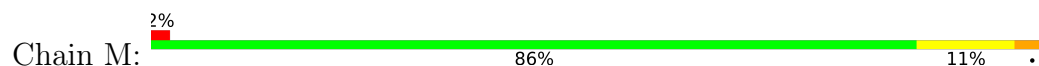
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



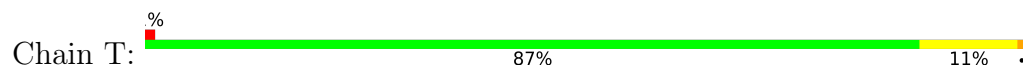
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



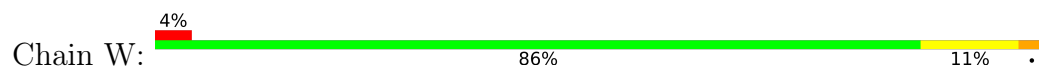
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

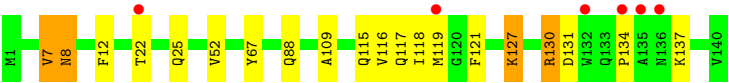


- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



- 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, α , β , γ	126.07Å 178.20Å 120.46Å 90.00° 120.35° 90.00°	Depositor
Resolution (Å)	20.00 – 2.05 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.05) 89.5 (20.00-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.194 0.166 , 0.195	Depositor DCC
R_{free} test set	11867 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	41674	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, SMC, KCX, HYP

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	0.56	0/3707	0.83	3/5009 (0.1%)
1	B	0.58	0/3722	0.85	2/5029 (0.0%)
1	E	0.56	0/3707	0.82	1/5009 (0.0%)
1	H	0.56	0/3732	0.83	2/5042 (0.0%)
1	K	0.54	0/3748	0.83	1/5064 (0.0%)
1	O	0.57	0/3714	0.83	1/5018 (0.0%)
1	R	0.57	0/3698	0.82	0/4997
1	V	0.56	0/3718	0.82	1/5024 (0.0%)
2	C	0.61	0/1191	0.91	5/1618 (0.3%)
2	F	0.58	0/1198	0.88	4/1627 (0.2%)
2	I	0.60	0/1183	0.88	3/1607 (0.2%)
2	J	0.57	0/1198	0.89	5/1627 (0.3%)
2	M	0.57	0/1191	0.88	3/1617 (0.2%)
2	P	0.58	0/1199	0.89	2/1628 (0.1%)
2	T	0.58	0/1206	0.89	2/1638 (0.1%)
2	W	0.59	0/1191	0.90	3/1617 (0.2%)
All	All	0.57	0/39303	0.84	38/53171 (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	B	0	2
2	C	0	1
2	F	0	1
2	I	0	1
2	J	0	1
2	M	0	1
2	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	1
2	W	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	8	ASN	N-CA-C	-10.19	92.88	108.67
2	F	8	ASN	N-CA-C	-10.15	92.06	108.41
2	I	8	ASN	N-CA-C	-10.04	93.10	108.67
2	P	8[A]	ASN	N-CA-C	-9.54	93.88	108.67
2	P	8[B]	ASN	N-CA-C	-9.54	93.88	108.67

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	360[A]	ARG	Sidechain
1	B	360[B]	ARG	Sidechain
2	C	7	VAL	Peptide
2	F	7	VAL	Peptide
2	I	7	VAL	Peptide

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	3646	0	3544	39	0
1	B	3654	0	3555	41	0
1	E	3646	0	3544	36	0
1	H	3671	0	3572	32	0
1	K	3679	0	3583	34	3
1	O	3663	0	3566	35	1
1	R	3643	0	3546	33	2
1	V	3653	0	3556	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1149	0	1123	20	0
2	F	1154	0	1126	23	0
2	I	1146	0	1121	14	0
2	J	1154	0	1126	15	0
2	M	1147	0	1122	22	0
2	P	1150	0	1124	15	0
2	T	1157	0	1128	15	0
2	W	1147	0	1122	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	7	0	0
4	E	21	0	7	0	0
4	O	42	0	15	0	0
4	R	42	0	15	0	0
4	V	21	0	7	0	0
5	A	24	0	36	4	0
5	B	20	0	30	0	0
5	C	8	0	12	0	0
5	E	20	0	30	4	0
5	H	24	0	36	2	0
5	I	4	0	6	1	0
5	J	8	0	12	1	0
5	K	20	0	30	1	0
5	M	8	0	12	0	0
5	O	24	0	36	0	0
5	P	8	0	12	0	0
5	R	16	0	24	1	0
5	T	8	0	12	1	0
5	V	20	0	30	0	0
5	W	8	0	12	0	0
6	A	283	0	0	7	0
6	B	276	0	0	5	0
6	C	80	0	0	3	0
6	E	285	0	0	7	0
6	F	96	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	271	0	0	3	0
6	I	67	0	0	0	0
6	J	74	0	0	2	0
6	K	253	0	0	2	0
6	M	87	0	0	4	0
6	O	281	0	0	4	0
6	P	60	0	0	0	0
6	R	261	0	0	4	0
6	T	76	0	0	4	0
6	V	289	0	0	3	0
6	W	80	0	0	0	0
All	All	41674	0	37846	392	3

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 392 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)
2:C:130:ARG:NH1	6:C:2073:HOH:O	1.79	1.12
1:K:267:HIS:HD2	1:K:277:ASN:HD22	1.05	1.02
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.04	1.00
1:A:267:HIS:HD2	1:A:277:ASN:HD22	0.99	0.97
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.02	0.94

All (3) 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:K:14:LYS:CE	1:R:460:GLU:OE2[2_646]	1.53	0.67
1:K:439:ARG:NH1	1:O:88:GLU:CG[1_556]	2.08	0.12
1:K:14:LYS:NZ	1:R:460:GLU:OE2[2_646]	2.09	0.11

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%)	451 (98%)	11 (2%)	0	100	100
1	B	465/475 (98%)	454 (98%)	11 (2%)	0	100	100
1	E	462/475 (97%)	448 (97%)	14 (3%)	0	100	100
1	H	466/475 (98%)	452 (97%)	14 (3%)	0	100	100
1	K	468/475 (98%)	454 (97%)	14 (3%)	0	100	100
1	O	464/475 (98%)	453 (98%)	11 (2%)	0	100	100
1	R	461/475 (97%)	450 (98%)	11 (2%)	0	100	100
1	V	464/475 (98%)	452 (97%)	12 (3%)	0	100	100
2	C	140/140 (100%)	132 (94%)	8 (6%)	0	100	100
2	F	140/140 (100%)	134 (96%)	6 (4%)	0	100	100
2	I	139/140 (99%)	134 (96%)	5 (4%)	0	100	100
2	J	140/140 (100%)	134 (96%)	6 (4%)	0	100	100
2	M	140/140 (100%)	135 (96%)	5 (4%)	0	100	100
2	P	141/140 (101%)	135 (96%)	6 (4%)	0	100	100
2	T	141/140 (101%)	137 (97%)	4 (3%)	0	100	100
2	W	140/140 (100%)	133 (95%)	7 (5%)	0	100	100
All	All	4833/4920 (98%)	4688 (97%)	145 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/377 (99%)	368 (99%)	5 (1%)	61	63
1	B	374/377 (99%)	366 (98%)	8 (2%)	47	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	373/377 (99%)	368 (99%)	5 (1%)	61	63
1	H	375/377 (100%)	370 (99%)	5 (1%)	61	63
1	K	377/377 (100%)	371 (98%)	6 (2%)	55	56
1	O	373/377 (99%)	366 (98%)	7 (2%)	50	50
1	R	372/377 (99%)	367 (99%)	5 (1%)	61	63
1	V	374/377 (99%)	370 (99%)	4 (1%)	65	68
2	C	125/123 (102%)	119 (95%)	6 (5%)	23	16
2	F	125/123 (102%)	118 (94%)	7 (6%)	19	12
2	I	124/123 (101%)	118 (95%)	6 (5%)	23	16
2	J	125/123 (102%)	119 (95%)	6 (5%)	23	16
2	M	125/123 (102%)	119 (95%)	6 (5%)	23	16
2	P	126/123 (102%)	120 (95%)	6 (5%)	23	16
2	T	126/123 (102%)	120 (95%)	6 (5%)	23	16
2	W	125/123 (102%)	119 (95%)	6 (5%)	23	16
All	All	3992/4000 (100%)	3898 (98%)	94 (2%)	43	40

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	118	ILE
2	P	127	LYS
2	M	130	ARG
1	O	297	MET
1	R	239	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
2	T	115	GLN
1	V	238	HIS
2	W	25	GLN
1	H	241	ASN
1	H	238	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	A	201	3,1	10,11,12	1.00	0	6,12,14	1.08	1 (16%)
1	SMC	A	369	1	5,6,7	0.66	0	3,6,8	0.73	0
1	SMC	A	256	1	5,6,7	0.77	0	3,6,8	0.52	0
1	SMC	H	256	1	5,6,7	0.68	0	3,6,8	0.80	0
1	KCX	H	201	3,1	10,11,12	0.97	0	6,12,14	0.96	1 (16%)
1	SMC	E	256	1	5,6,7	0.59	0	3,6,8	0.65	0
1	SMC	O	256	1	5,6,7	0.72	0	3,6,8	0.67	0
1	HYP	V	151	1	7,8,9	1.10	1 (14%)	5,10,12	3.92	4 (80%)
1	SMC	K	369	1	5,6,7	0.83	0	3,6,8	0.82	0
1	SMC	R	256	1	5,6,7	0.63	0	3,6,8	0.83	0
1	HYP	R	151	1	7,8,9	1.19	1 (14%)	5,10,12	3.95	4 (80%)
1	KCX	V	201	3,1	10,11,12	1.02	0	6,12,14	1.14	1 (16%)
1	HYP	E	151	1	7,8,9	1.10	1 (14%)	5,10,12	3.95	4 (80%)
1	SMC	K	256	1	5,6,7	0.95	0	3,6,8	0.83	0
1	KCX	O	201	3,1	10,11,12	1.03	0	6,12,14	0.96	0
1	SMC	R	369	1	5,6,7	0.74	0	3,6,8	0.83	0
1	KCX	E	201	3,1	10,11,12	1.13	0	6,12,14	1.04	1 (16%)
1	HYP	A	104	1	7,8,9	0.89	0	5,10,12	3.32	3 (60%)
1	HYP	B	104	1	7,8,9	0.80	0	5,10,12	3.16	3 (60%)
1	KCX	R	201	3,1	10,11,12	0.82	0	6,12,14	1.07	1 (16%)
1	HYP	H	104	1	7,8,9	0.96	1 (14%)	5,10,12	3.44	3 (60%)
1	KCX	K	201	3,1	10,11,12	1.03	0	6,12,14	1.23	1 (16%)
1	HYP	V	104	1	7,8,9	0.91	0	5,10,12	3.26	3 (60%)
1	HYP	O	104	1	7,8,9	0.90	0	5,10,12	3.25	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	K	151	1	7,8,9	1.11	1 (14%)	5,10,12	4.08	4 (80%)
1	SMC	B	256	1	5,6,7	0.77	0	3,6,8	0.53	0
1	SMC	B	369	1	5,6,7	0.59	0	3,6,8	0.78	0
1	HYP	R	104	1	7,8,9	0.82	0	5,10,12	3.55	3 (60%)
1	SMC	H	369	1	5,6,7	0.76	0	3,6,8	0.79	0
1	HYP	E	104	1	7,8,9	0.94	0	5,10,12	3.46	3 (60%)
1	HYP	H	151	1	7,8,9	1.08	0	5,10,12	3.98	4 (80%)
1	KCX	B	201	3,1	10,11,12	1.17	1 (10%)	6,12,14	0.92	0
1	HYP	O	151	1	7,8,9	1.19	1 (14%)	5,10,12	3.98	4 (80%)
1	SMC	V	256	1	5,6,7	0.82	0	3,6,8	0.64	0
1	SMC	E	369	1	5,6,7	0.92	0	3,6,8	0.97	0
1	HYP	K	104	1	7,8,9	0.86	0	5,10,12	3.39	3 (60%)
1	SMC	V	369	1	5,6,7	0.73	0	3,6,8	0.72	0
1	SMC	O	369	1	5,6,7	0.59	0	3,6,8	0.74	0
1	HYP	A	151	1	7,8,9	1.03	1 (14%)	5,10,12	4.35	4 (80%)
1	HYP	B	151	1	7,8,9	1.23	1 (14%)	5,10,12	3.85	3 (60%)

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	A	201	3,1	-	0/9/10/12	-
1	SMC	A	369	1	-	1/3/5/7	-
1	SMC	A	256	1	-	0/3/5/7	-
1	SMC	H	256	1	-	0/3/5/7	-
1	KCX	H	201	3,1	-	0/9/10/12	-
1	SMC	E	256	1	-	0/3/5/7	-
1	SMC	O	256	1	-	0/3/5/7	-
1	HYP	V	151	1	-	0/0/11/13	0/1/1/1
1	SMC	K	369	1	-	1/3/5/7	-
1	SMC	R	256	1	-	0/3/5/7	-
1	HYP	R	151	1	-	0/0/11/13	0/1/1/1
1	KCX	V	201	3,1	-	0/9/10/12	-
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	SMC	K	256	1	-	0/3/5/7	-
1	KCX	O	201	3,1	-	0/9/10/12	-
1	SMC	R	369	1	-	1/3/5/7	-
1	KCX	E	201	3,1	-	0/9/10/12	-
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	KCX	R	201	3,1	-	0/9/10/12	-
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	KCX	K	201	3,1	-	0/9/10/12	-
1	HYP	V	104	1	-	0/0/11/13	0/1/1/1
1	HYP	O	104	1	-	0/0/11/13	0/1/1/1
1	HYP	K	151	1	-	0/0/11/13	0/1/1/1
1	SMC	B	256	1	-	0/3/5/7	-
1	SMC	B	369	1	-	1/3/5/7	-
1	HYP	R	104	1	-	0/0/11/13	0/1/1/1
1	SMC	H	369	1	-	1/3/5/7	-
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	3,1	-	0/9/10/12	-
1	HYP	O	151	1	-	0/0/11/13	0/1/1/1
1	SMC	V	256	1	-	0/3/5/7	-
1	SMC	E	369	1	-	1/3/5/7	-
1	HYP	K	104	1	-	0/0/11/13	0/1/1/1
1	SMC	V	369	1	-	1/3/5/7	-
1	SMC	O	369	1	-	1/3/5/7	-
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	151	HYP	CA-N	-2.46	1.44	1.48
1	R	151	HYP	CA-N	-2.40	1.44	1.48
1	O	151	HYP	CA-N	-2.39	1.44	1.48
1	B	151	HYP	CA-N	-2.34	1.44	1.48
1	H	104	HYP	CA-N	-2.25	1.44	1.48

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	HYP	OD1-CG-CD	-6.11	97.81	110.30
1	A	151	HYP	CB-CG-CD	5.85	109.67	103.16
1	O	151	HYP	CB-CG-CD	5.69	109.49	103.16
1	E	151	HYP	CB-CG-CD	5.67	109.47	103.16
1	K	151	HYP	CB-CG-CD	5.63	109.43	103.16

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	201	KCX	1	0
1	V	151	HYP	2	0
1	R	151	HYP	1	0
1	E	151	HYP	1	0
1	K	201	KCX	1	0
1	K	151	HYP	1	0
1	H	151	HYP	1	0
1	O	151	HYP	1	0
1	A	151	HYP	2	0
1	B	151	HYP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 8 are monoatomic - leaving 63 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	A	1478	-	3,3,3	0.40	0	2,2,2	0.16	0
5	EDO	V	1479	-	3,3,3	0.29	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	H	1480	-	3,3,3	0.31	0	2,2,2	0.22	0
5	EDO	H	1478	-	3,3,3	0.34	0	2,2,2	0.39	0
5	EDO	R	1480	-	3,3,3	0.28	0	2,2,2	0.28	0
5	EDO	O	1481	-	3,3,3	0.31	0	2,2,2	0.25	0
5	EDO	P	1142	-	3,3,3	0.27	0	2,2,2	0.29	0
5	EDO	V	1482	-	3,3,3	0.26	0	2,2,2	0.24	0
4	CAP	R	1478	3	18,20,20	1.58	1 (5%)	23,31,31	1.53	3 (13%)
5	EDO	T	1141	-	3,3,3	0.28	0	2,2,2	0.23	0
5	EDO	R	1482	-	3,3,3	0.32	0	2,2,2	0.07	0
5	EDO	B	1480	-	3,3,3	0.30	0	2,2,2	0.24	0
5	EDO	A	1481	-	3,3,3	0.31	0	2,2,2	0.25	0
5	EDO	A	1483	-	3,3,3	0.31	0	2,2,2	0.19	0
4	CAP	O	1476	3	18,20,20	1.64	2 (11%)	23,31,31	1.33	3 (13%)
5	EDO	C	1141	-	3,3,3	0.28	0	2,2,2	0.14	0
5	EDO	E	1482	-	3,3,3	0.23	0	2,2,2	0.20	0
5	EDO	H	1479	-	3,3,3	0.30	0	2,2,2	0.07	0
5	EDO	O	1480	-	3,3,3	0.27	0	2,2,2	0.28	0
5	EDO	H	1481	-	3,3,3	0.28	0	2,2,2	0.28	0
5	EDO	O	1479	-	3,3,3	0.37	0	2,2,2	0.21	0
5	EDO	M	1142	-	3,3,3	0.29	0	2,2,2	0.26	0
5	EDO	A	1479	-	3,3,3	0.26	0	2,2,2	0.35	0
5	EDO	B	1479	-	3,3,3	0.31	0	2,2,2	0.44	0
4	CAP	V	1476	3	18,20,20	1.57	1 (5%)	23,31,31	1.62	3 (13%)
5	EDO	M	1141	-	3,3,3	0.25	0	2,2,2	0.22	0
5	EDO	E	1478	-	3,3,3	0.30	0	2,2,2	0.07	0
5	EDO	I	1141	-	3,3,3	0.25	0	2,2,2	0.28	0
5	EDO	V	1480	-	3,3,3	0.30	0	2,2,2	0.37	0
5	EDO	H	1482	-	3,3,3	0.27	0	2,2,2	0.21	0
4	CAP	E	1477	3	18,20,20	1.50	1 (5%)	23,31,31	1.57	3 (13%)
5	EDO	E	1479	-	3,3,3	0.25	0	2,2,2	0.30	0
5	EDO	R	1479	-	3,3,3	0.33	0	2,2,2	0.09	0
5	EDO	V	1478	-	3,3,3	0.34	0	2,2,2	0.22	0
4	CAP	B	1477	3	18,20,20	1.52	1 (5%)	23,31,31	1.65	3 (13%)
5	EDO	A	1480	-	3,3,3	0.27	0	2,2,2	0.39	0
5	EDO	E	1481	-	3,3,3	0.33	0	2,2,2	0.14	0
5	EDO	J	1141	-	3,3,3	0.28	0	2,2,2	0.23	0
5	EDO	K	1478	-	3,3,3	0.28	0	2,2,2	0.35	0
5	EDO	B	1478	-	3,3,3	0.39	0	2,2,2	0.14	0
4	CAP	A	1477	3	18,20,20	1.50	1 (5%)	23,31,31	1.62	3 (13%)
5	EDO	C	1142	-	3,3,3	0.29	0	2,2,2	0.49	0
5	EDO	K	1481	-	3,3,3	0.31	0	2,2,2	0.12	0
5	EDO	O	1484	-	3,3,3	0.30	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	P	1141	-	3,3,3	0.28	0	2,2,2	0.28	0
5	EDO	R	1481	-	3,3,3	0.32	0	2,2,2	0.38	0
5	EDO	T	1142	-	3,3,3	0.26	0	2,2,2	0.57	0
5	EDO	B	1481	-	3,3,3	0.28	0	2,2,2	0.33	0
4	CAP	O	1478	3	18,20,20	1.59	1 (5%)	23,31,31	1.53	3 (13%)
5	EDO	K	1480	-	3,3,3	0.33	0	2,2,2	0.07	0
5	EDO	O	1482	-	3,3,3	0.35	0	2,2,2	0.31	0
5	EDO	K	1479	-	3,3,3	0.26	0	2,2,2	0.38	0
5	EDO	H	1477	-	3,3,3	0.32	0	2,2,2	0.41	0
5	EDO	A	1482	-	3,3,3	0.25	0	2,2,2	0.20	0
5	EDO	W	1142	-	3,3,3	0.28	0	2,2,2	0.21	0
5	EDO	O	1483	-	3,3,3	0.28	0	2,2,2	0.47	0
5	EDO	K	1477	-	3,3,3	0.39	0	2,2,2	0.05	0
5	EDO	B	1482	-	3,3,3	0.28	0	2,2,2	0.40	0
5	EDO	E	1480	-	3,3,3	0.30	0	2,2,2	0.23	0
4	CAP	R	1476	3	18,20,20	1.50	1 (5%)	23,31,31	1.53	2 (8%)
5	EDO	J	1142	-	3,3,3	0.26	0	2,2,2	0.41	0
5	EDO	W	1141	-	3,3,3	0.29	0	2,2,2	0.12	0
5	EDO	V	1481	-	3,3,3	0.33	0	2,2,2	0.14	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	A	1478	-	-	0/1/1/1	-
5	EDO	V	1479	-	-	1/1/1/1	-
5	EDO	H	1480	-	-	0/1/1/1	-
5	EDO	H	1478	-	-	0/1/1/1	-
5	EDO	R	1480	-	-	1/1/1/1	-
5	EDO	O	1481	-	-	0/1/1/1	-
5	EDO	P	1142	-	-	0/1/1/1	-
5	EDO	V	1482	-	-	0/1/1/1	-
4	CAP	R	1478	3	-	11/29/29/29	-
5	EDO	T	1141	-	-	1/1/1/1	-
5	EDO	R	1482	-	-	1/1/1/1	-
5	EDO	B	1480	-	-	0/1/1/1	-
5	EDO	A	1481	-	-	0/1/1/1	-
5	EDO	A	1483	-	-	1/1/1/1	-
4	CAP	O	1476	3	-	10/29/29/29	-
5	EDO	C	1141	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	1482	-	-	1/1/1/1	-
5	EDO	H	1479	-	-	0/1/1/1	-
5	EDO	O	1480	-	-	0/1/1/1	-
5	EDO	H	1481	-	-	0/1/1/1	-
5	EDO	O	1479	-	-	0/1/1/1	-
5	EDO	M	1142	-	-	1/1/1/1	-
5	EDO	A	1479	-	-	1/1/1/1	-
5	EDO	B	1479	-	-	1/1/1/1	-
4	CAP	V	1476	3	-	8/29/29/29	-
5	EDO	M	1141	-	-	1/1/1/1	-
5	EDO	E	1478	-	-	0/1/1/1	-
5	EDO	I	1141	-	-	0/1/1/1	-
5	EDO	V	1480	-	-	0/1/1/1	-
5	EDO	H	1482	-	-	0/1/1/1	-
4	CAP	E	1477	3	-	9/29/29/29	-
5	EDO	E	1479	-	-	1/1/1/1	-
5	EDO	R	1479	-	-	0/1/1/1	-
5	EDO	V	1478	-	-	0/1/1/1	-
4	CAP	B	1477	3	-	9/29/29/29	-
5	EDO	A	1480	-	-	0/1/1/1	-
5	EDO	E	1481	-	-	0/1/1/1	-
5	EDO	J	1141	-	-	0/1/1/1	-
5	EDO	K	1478	-	-	1/1/1/1	-
5	EDO	B	1478	-	-	1/1/1/1	-
4	CAP	A	1477	3	-	9/29/29/29	-
5	EDO	C	1142	-	-	0/1/1/1	-
5	EDO	K	1481	-	-	0/1/1/1	-
5	EDO	O	1484	-	-	1/1/1/1	-
5	EDO	P	1141	-	-	0/1/1/1	-
5	EDO	R	1481	-	-	0/1/1/1	-
5	EDO	T	1142	-	-	0/1/1/1	-
5	EDO	B	1481	-	-	1/1/1/1	-
4	CAP	O	1478	3	-	10/29/29/29	-
5	EDO	K	1480	-	-	0/1/1/1	-
5	EDO	O	1482	-	-	0/1/1/1	-
5	EDO	K	1479	-	-	0/1/1/1	-
5	EDO	H	1477	-	-	1/1/1/1	-
5	EDO	A	1482	-	-	1/1/1/1	-
5	EDO	W	1142	-	-	0/1/1/1	-
5	EDO	O	1483	-	-	1/1/1/1	-
5	EDO	K	1477	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1482	-	-	0/1/1/1	-
5	EDO	E	1480	-	-	0/1/1/1	-
4	CAP	R	1476	3	-	9/29/29/29	-
5	EDO	J	1142	-	-	0/1/1/1	-
5	EDO	W	1141	-	-	1/1/1/1	-
5	EDO	V	1481	-	-	0/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	1478	CAP	O6-C	6.09	1.41	1.22
4	O	1478	CAP	O6-C	6.07	1.41	1.22
4	E	1477	CAP	O6-C	6.00	1.40	1.22
4	O	1476	CAP	O6-C	5.99	1.40	1.22
4	R	1476	CAP	O6-C	5.75	1.40	1.22

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	1476	CAP	O7-C-C2	5.91	123.95	114.06
4	R	1476	CAP	O7-C-C2	5.86	123.87	114.06
4	B	1477	CAP	O7-C-C2	5.79	123.76	114.06
4	A	1477	CAP	O7-C-C2	5.69	123.58	114.06
4	E	1477	CAP	O7-C-C2	5.55	123.36	114.06

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1477	CAP	O6-C-C2-O2
4	A	1477	CAP	C2-C3-C4-O4
4	A	1477	CAP	O3-C3-C4-O4
4	B	1477	CAP	O7-C-C2-C1
4	B	1477	CAP	O6-C-C2-O2

There are no ring outliers.

10 monomers are involved in 15 short contacts:

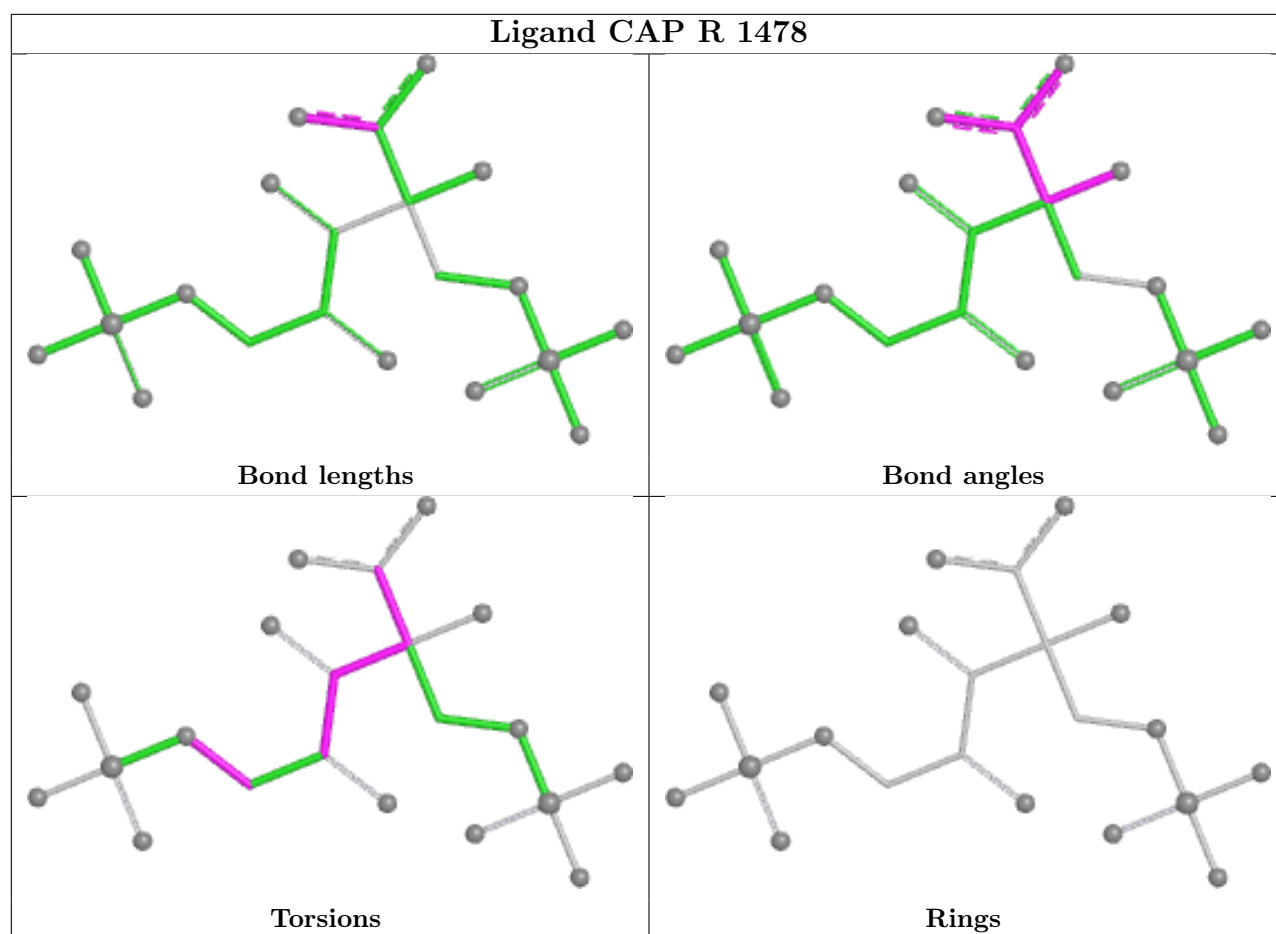
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	1141	EDO	1	0
5	R	1482	EDO	1	0

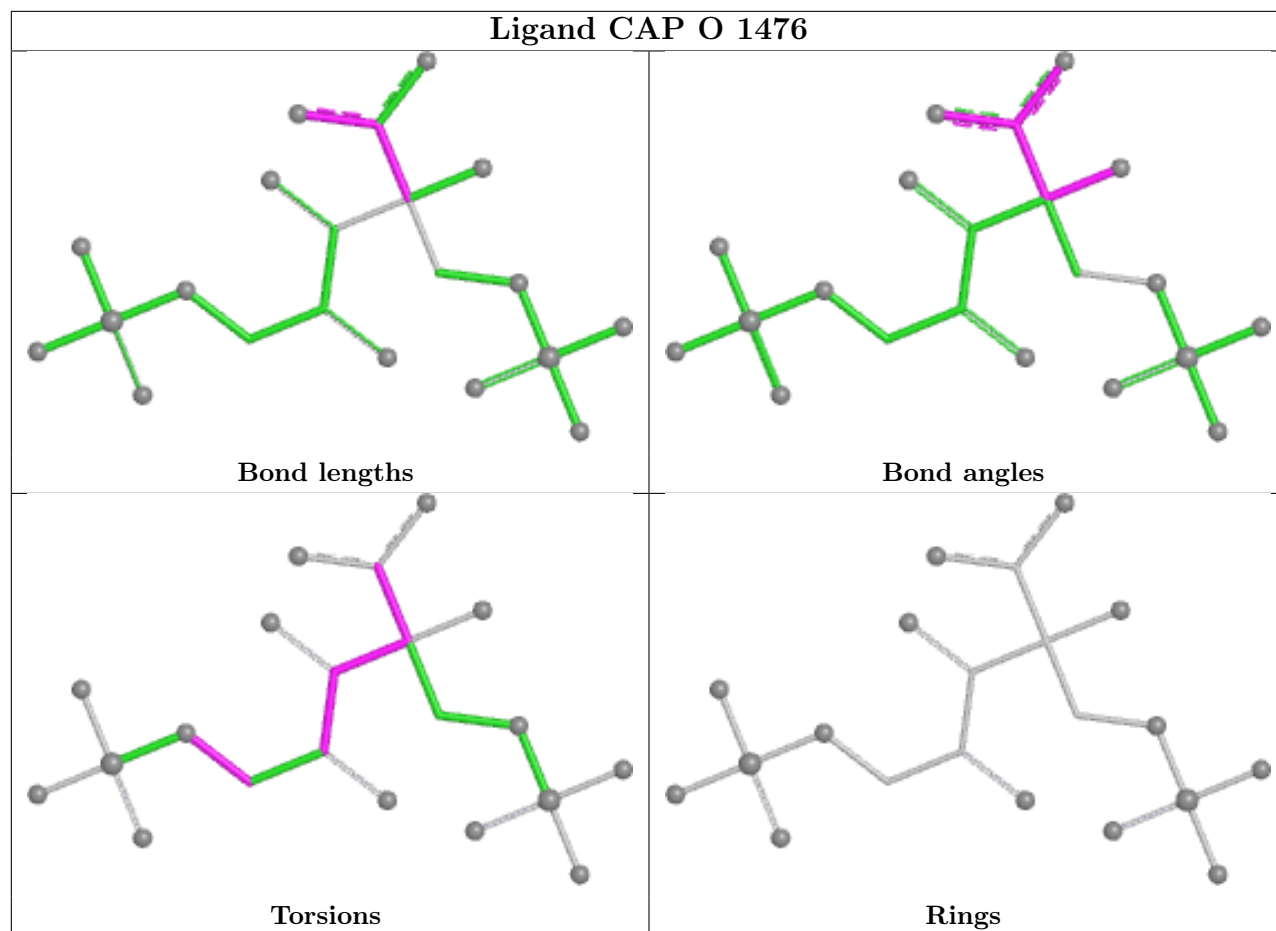
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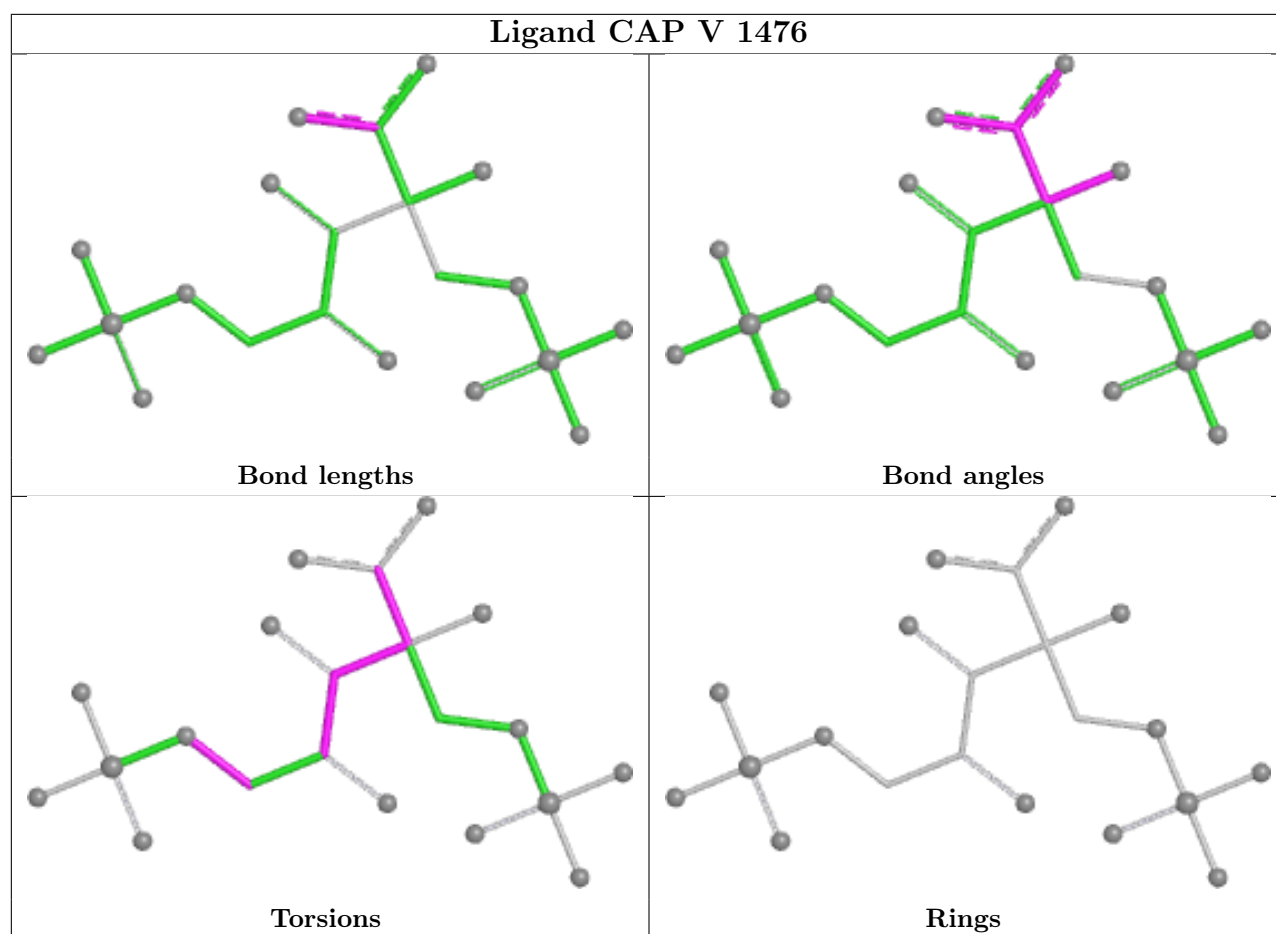
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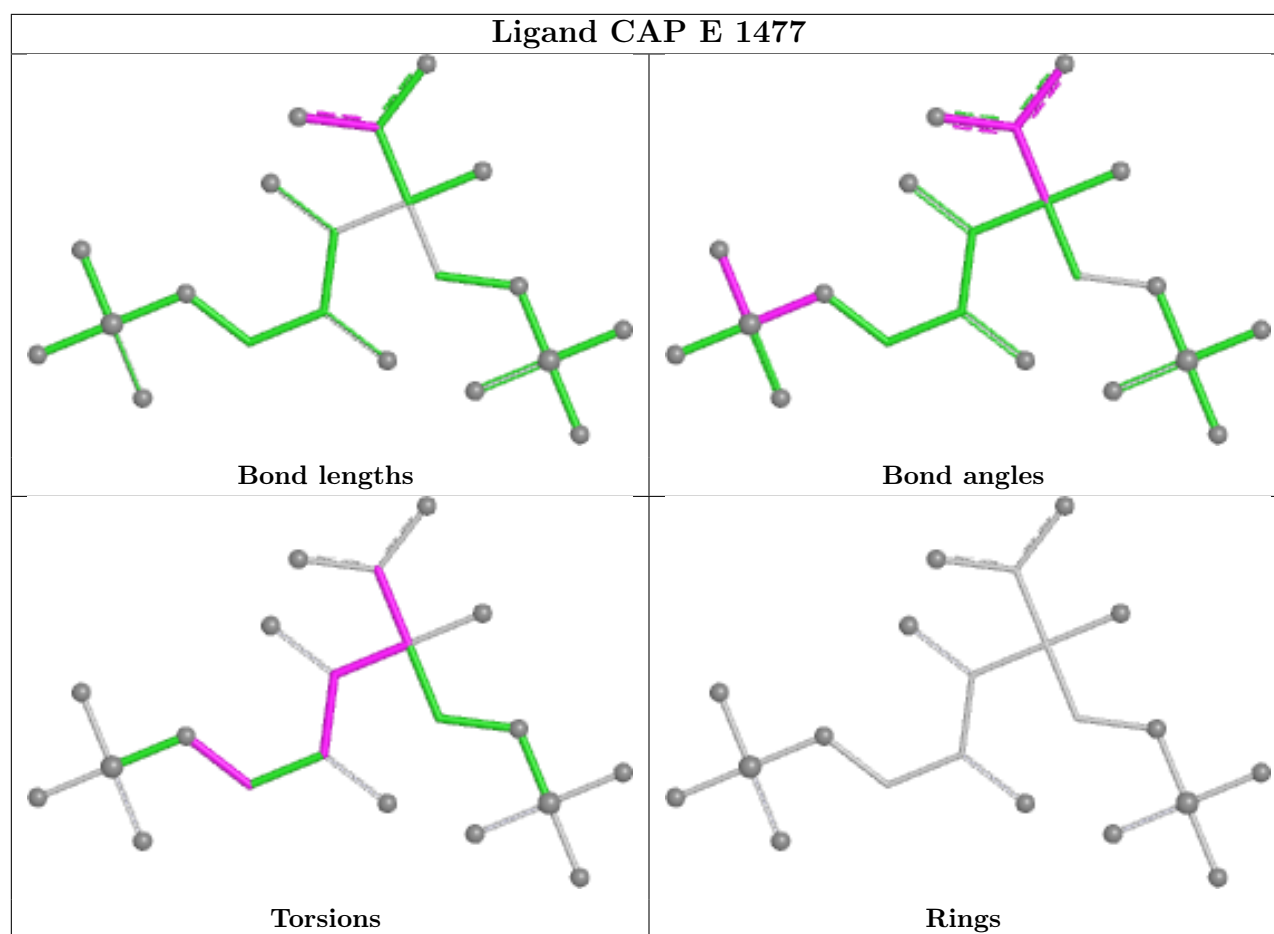
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1483	EDO	4	0
5	E	1482	EDO	3	0
5	H	1479	EDO	1	0
5	E	1478	EDO	1	0
5	I	1141	EDO	1	0
5	J	1141	EDO	1	0
5	H	1477	EDO	1	0
5	K	1477	EDO	1	0

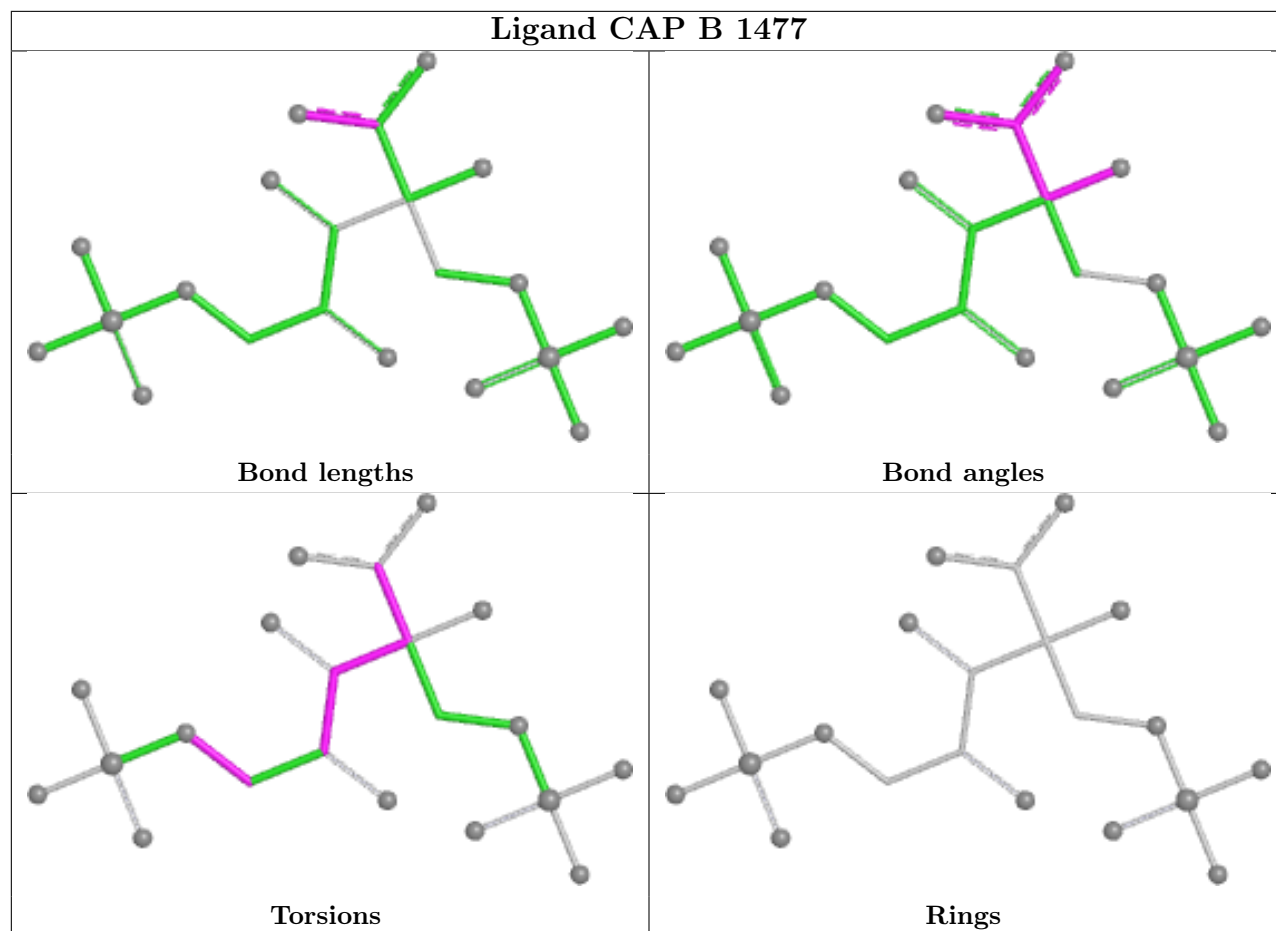
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

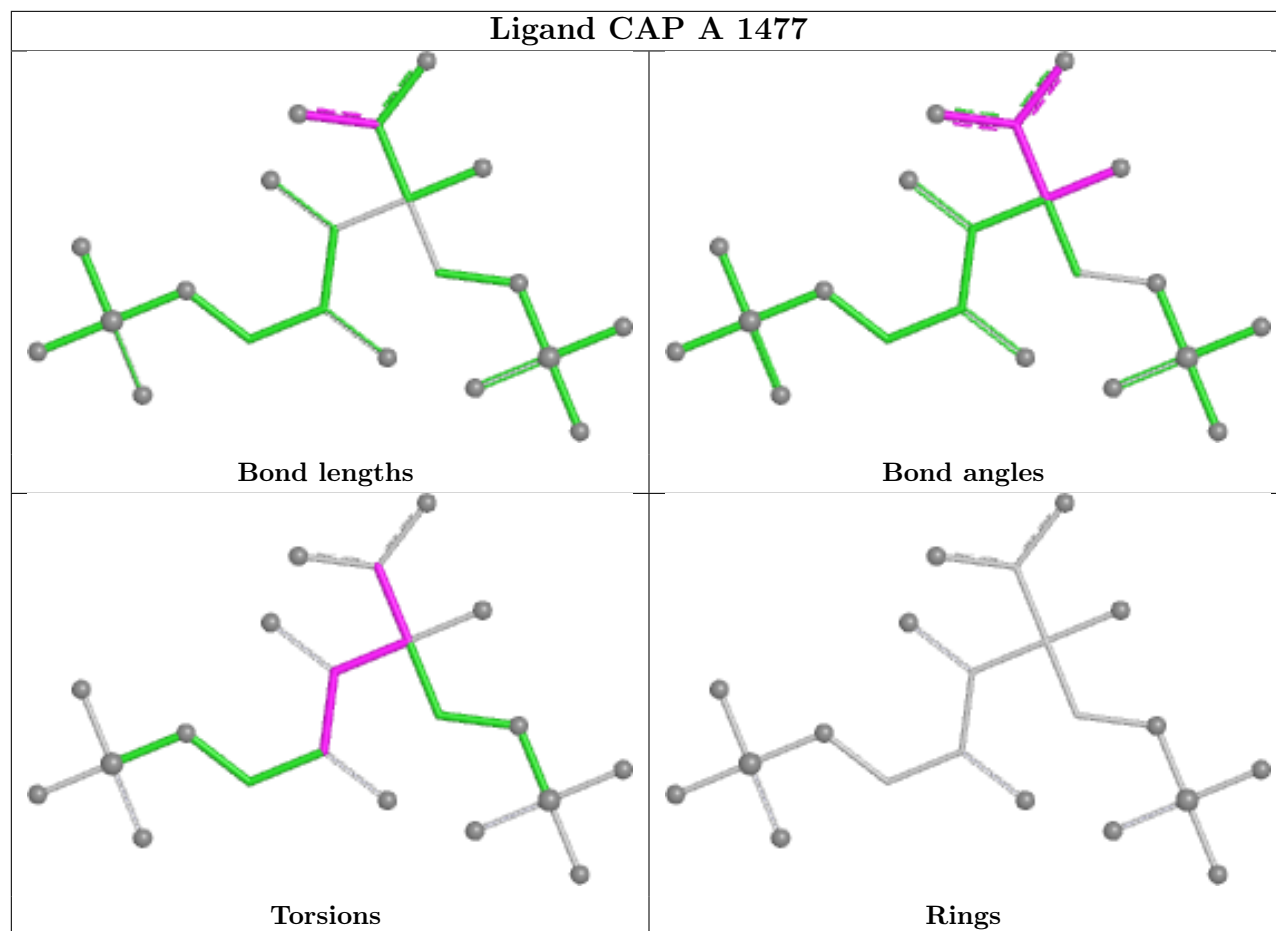


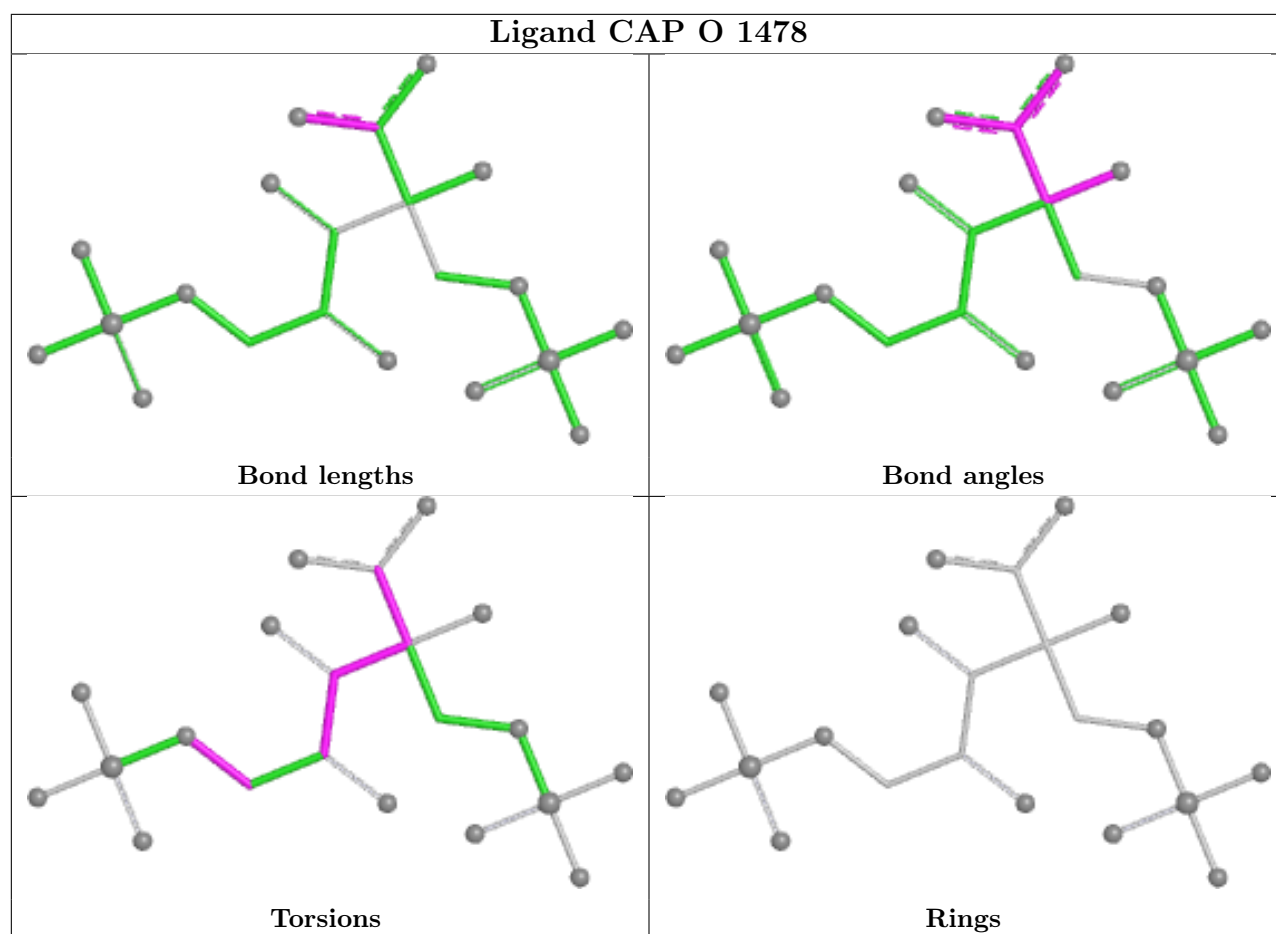


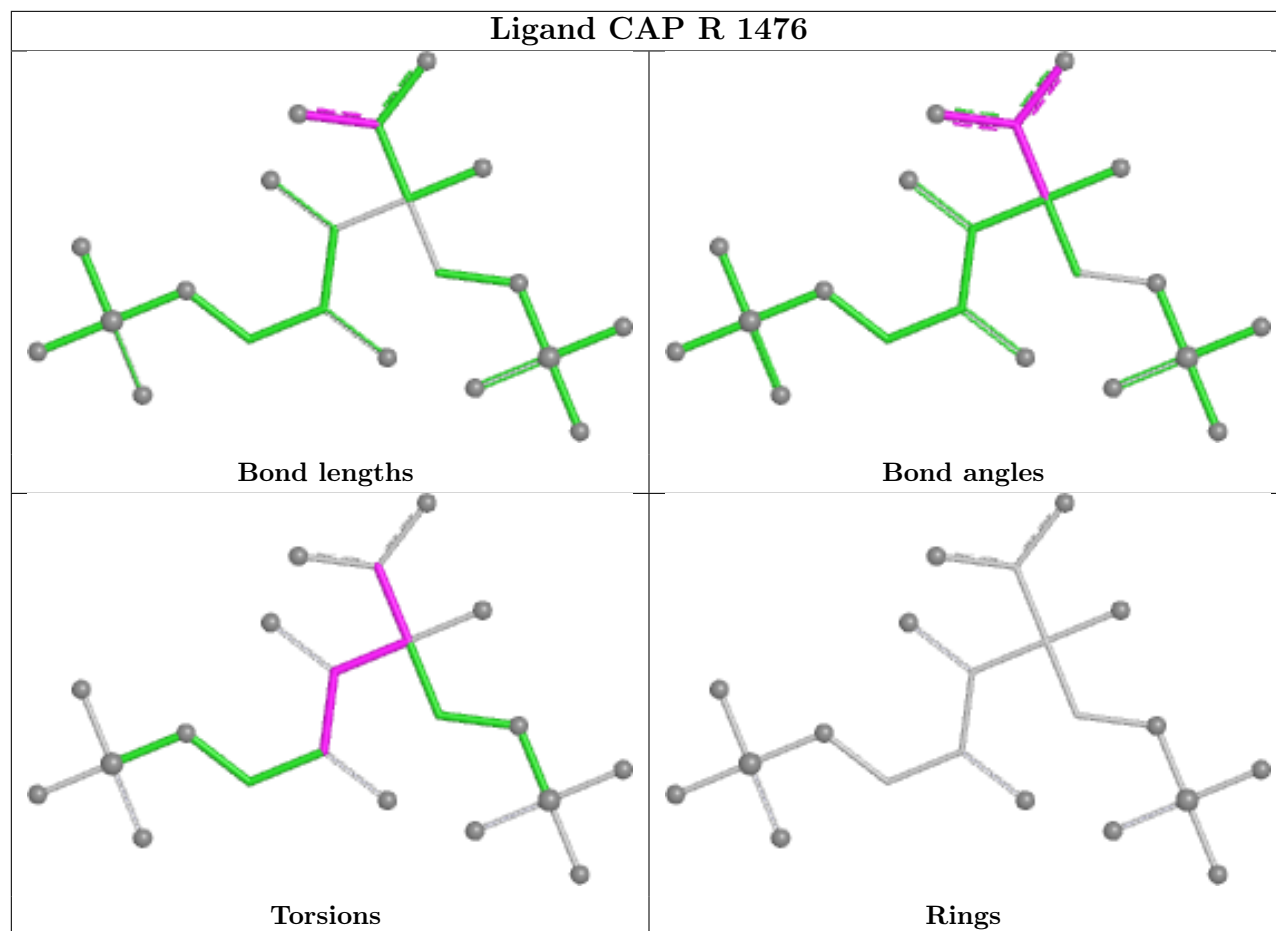












5.7 Other polymers [i](#)

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	460/475 (96%)	-0.52	6 (1%) 75 76	10, 15, 28, 43	4 (0%)
1	B	462/475 (97%)	-0.51	7 (1%) 72 73	9, 15, 28, 43	4 (0%)
1	E	460/475 (96%)	-0.51	3 (0%) 84 85	10, 15, 28, 43	4 (0%)
1	H	464/475 (97%)	-0.47	7 (1%) 72 73	9, 15, 29, 52	4 (0%)
1	K	464/475 (97%)	-0.49	3 (0%) 85 87	9, 15, 29, 52	6 (1%)
1	O	464/475 (97%)	-0.50	3 (0%) 85 87	12, 15, 29, 51	2 (0%)
1	R	460/475 (96%)	-0.50	3 (0%) 84 85	9, 15, 28, 43	3 (0%)
1	V	461/475 (97%)	-0.52	4 (0%) 81 83	9, 15, 28, 43	5 (1%)
2	C	140/140 (100%)	-0.08	4 (2%) 53 55	13, 20, 33, 41	2 (1%)
2	F	140/140 (100%)	-0.02	4 (2%) 53 55	12, 20, 33, 41	2 (1%)
2	I	140/140 (100%)	-0.06	1 (0%) 84 85	13, 20, 33, 41	1 (0%)
2	J	140/140 (100%)	-0.16	1 (0%) 84 85	12, 20, 33, 41	2 (1%)
2	M	140/140 (100%)	-0.04	3 (2%) 63 65	13, 20, 33, 41	2 (1%)
2	P	140/140 (100%)	-0.19	0 100 100	13, 20, 33, 41	3 (2%)
2	T	140/140 (100%)	-0.15	1 (0%) 84 85	12, 20, 33, 41	3 (2%)
2	W	140/140 (100%)	-0.07	6 (4%) 40 40	13, 20, 33, 41	2 (1%)
All	All	4815/4920 (97%)	-0.41	56 (1%) 76 78	9, 16, 30, 52	49 (1%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	10	GLY	8.2
1	H	439	ARG	5.8
2	F	130	ARG	5.6
2	M	130	ARG	4.8
1	V	11	ALA	4.2

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, 95th 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 ²)	Q<0.9
1	HYP	K	104	8/9	0.90	0.07	14,14,14,15	0
1	HYP	B	104	8/9	0.92	0.07	13,14,14,15	0
1	HYP	A	104	8/9	0.93	0.07	13,14,14,14	0
1	HYP	R	151	8/9	0.93	0.07	12,13,13,13	0
1	HYP	H	151	8/9	0.94	0.06	12,13,13,13	0
1	HYP	A	151	8/9	0.94	0.06	12,13,13,13	0
1	HYP	H	104	8/9	0.94	0.06	14,14,14,14	0
1	KCX	R	201	12/13	0.94	0.06	11,12,13,14	0
1	HYP	V	104	8/9	0.94	0.07	14,14,14,14	0
1	HYP	V	151	8/9	0.94	0.06	12,13,13,13	0
1	HYP	K	151	8/9	0.95	0.06	12,13,13,13	0
1	HYP	O	104	8/9	0.95	0.06	14,14,14,15	0
1	HYP	R	104	8/9	0.95	0.06	14,14,14,14	0
1	KCX	B	201	12/13	0.95	0.06	11,12,13,14	0
1	HYP	E	104	8/9	0.95	0.05	14,14,14,14	0
1	KCX	H	201	12/13	0.95	0.06	11,12,13,14	0
1	HYP	E	151	8/9	0.95	0.06	12,13,13,13	0
1	HYP	O	151	8/9	0.96	0.05	12,13,13,13	0
1	KCX	O	201	12/13	0.96	0.06	11,12,13,14	0
1	HYP	B	151	8/9	0.96	0.05	12,13,13,13	0
1	KCX	E	201	12/13	0.96	0.06	11,12,13,14	0
1	SMC	A	369	7/8	0.96	0.08	15,16,16,17	0
1	KCX	K	201	12/13	0.96	0.06	11,12,13,14	0
1	KCX	A	201	12/13	0.96	0.05	11,12,13,14	0
1	KCX	V	201	12/13	0.96	0.06	11,12,13,14	0
1	SMC	V	256	7/8	0.96	0.07	11,12,13,13	0
1	SMC	B	369	7/8	0.97	0.06	15,16,16,17	0
1	SMC	K	369	7/8	0.97	0.07	15,16,16,18	0
1	SMC	H	369	7/8	0.97	0.07	15,16,16,17	0
1	SMC	V	369	7/8	0.97	0.06	15,16,16,18	0
1	SMC	A	256	7/8	0.98	0.06	11,13,13,13	0
1	SMC	E	256	7/8	0.98	0.04	11,13,13,13	0
1	SMC	R	256	7/8	0.98	0.05	11,12,13,13	0
1	SMC	R	369	7/8	0.98	0.06	15,16,16,17	0
1	SMC	E	369	7/8	0.98	0.06	15,16,16,18	0
1	SMC	H	256	7/8	0.98	0.05	11,13,13,13	0
1	SMC	O	256	7/8	0.98	0.05	11,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SMC	O	369	7/8	0.98	0.07	15,16,16,17	0
1	SMC	K	256	7/8	0.98	0.05	11,13,13,13	0
1	SMC	B	256	7/8	0.99	0.04	11,13,13,13	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	K	1479	4/4	0.79	0.11	29,29,29,29	0
5	EDO	I	1141	4/4	0.82	0.15	39,42,43,45	0
5	EDO	M	1142	4/4	0.83	0.12	48,50,50,50	0
5	EDO	M	1141	4/4	0.84	0.14	42,42,43,43	0
5	EDO	H	1480	4/4	0.85	0.09	33,33,33,33	0
5	EDO	R	1481	4/4	0.86	0.09	22,23,25,26	0
5	EDO	W	1141	4/4	0.87	0.10	30,32,32,33	0
5	EDO	A	1480	4/4	0.88	0.09	31,31,31,32	0
5	EDO	T	1142	4/4	0.89	0.10	25,28,29,31	0
5	EDO	K	1481	4/4	0.89	0.11	28,29,30,30	0
5	EDO	A	1483	4/4	0.90	0.07	18,18,18,20	0
5	EDO	B	1480	4/4	0.90	0.08	26,27,27,27	0
5	EDO	K	1477	4/4	0.90	0.11	19,19,20,22	0
5	EDO	C	1141	4/4	0.90	0.09	25,28,28,33	0
5	EDO	E	1480	4/4	0.90	0.08	26,27,27,28	0
5	EDO	W	1142	4/4	0.90	0.10	36,38,39,39	0
5	EDO	O	1483	4/4	0.91	0.08	27,30,31,31	0
5	EDO	O	1484	4/4	0.91	0.07	24,24,25,26	0
5	EDO	B	1482	4/4	0.91	0.09	28,29,29,29	0
5	EDO	J	1141	4/4	0.92	0.08	32,33,33,34	0
5	EDO	T	1141	4/4	0.92	0.10	26,26,27,28	0
5	EDO	O	1481	4/4	0.92	0.07	23,25,25,26	0
5	EDO	V	1480	4/4	0.92	0.09	25,28,29,30	0
5	EDO	J	1142	4/4	0.92	0.11	31,33,35,37	0
5	EDO	A	1478	4/4	0.92	0.09	15,15,16,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	1482	4/4	0.93	0.07	25,25,27,28	0
5	EDO	P	1141	4/4	0.93	0.07	27,29,30,32	0
5	EDO	E	1479	4/4	0.93	0.08	25,27,27,27	0
5	EDO	A	1481	4/4	0.93	0.08	20,22,23,23	0
5	EDO	H	1477	4/4	0.93	0.07	17,18,18,19	0
5	EDO	O	1480	4/4	0.93	0.07	22,23,24,24	0
5	EDO	H	1479	4/4	0.93	0.08	26,28,29,30	0
5	EDO	K	1478	4/4	0.93	0.07	25,25,25,26	0
5	EDO	E	1482	4/4	0.94	0.07	21,21,21,21	0
5	EDO	O	1482	4/4	0.94	0.08	22,24,25,26	0
5	EDO	B	1478	4/4	0.94	0.07	13,13,14,15	0
5	EDO	V	1478	4/4	0.94	0.07	14,15,15,17	0
5	EDO	O	1479	4/4	0.94	0.06	15,16,16,17	0
5	EDO	H	1478	4/4	0.94	0.08	20,21,21,21	0
5	EDO	P	1142	4/4	0.94	0.09	28,30,32,34	0
5	EDO	R	1482	4/4	0.95	0.09	23,24,24,26	0
5	EDO	C	1142	4/4	0.95	0.06	25,25,26,27	0
5	EDO	B	1481	4/4	0.95	0.07	26,27,27,28	0
5	EDO	B	1479	4/4	0.95	0.06	21,21,21,22	0
5	EDO	V	1479	4/4	0.95	0.06	20,21,22,23	0
3	MG	H	1476	1/1	0.95	0.04	14,14,14,14	0
5	EDO	V	1482	4/4	0.95	0.07	25,25,26,27	0
5	EDO	H	1481	4/4	0.95	0.07	21,23,23,24	0
5	EDO	H	1482	4/4	0.95	0.08	30,30,30,31	0
5	EDO	K	1480	4/4	0.96	0.06	23,26,26,28	0
5	EDO	A	1479	4/4	0.96	0.06	21,21,22,23	0
5	EDO	R	1479	4/4	0.96	0.05	13,14,14,15	0
5	EDO	R	1480	4/4	0.96	0.06	18,19,20,21	0
3	MG	V	1477	1/1	0.96	0.04	13,13,13,13	0
5	EDO	E	1481	4/4	0.96	0.07	26,27,29,29	0
3	MG	K	1476	1/1	0.96	0.04	13,13,13,13	0
5	EDO	E	1478	4/4	0.97	0.05	15,16,17,18	0
3	MG	E	1476	1/1	0.97	0.03	14,14,14,14	0
5	EDO	V	1481	4/4	0.97	0.05	17,21,23,23	0
4	CAP	V	1476	21/21	0.98	0.04	10,13,14,15	0
3	MG	O	1477	1/1	0.98	0.03	13,13,13,13	0
3	MG	R	1477	1/1	0.98	0.02	12,12,12,12	0
3	MG	A	1476	1/1	0.98	0.03	17,17,17,17	0
4	CAP	E	1477	21/21	0.98	0.05	13,15,16,16	0
4	CAP	R	1476	21/21	0.98	0.04	14,16,16,17	0
4	CAP	R	1478	21/21	0.98	0.04	14,16,16,17	0
4	CAP	O	1476	21/21	0.99	0.03	10,13,13,16	0

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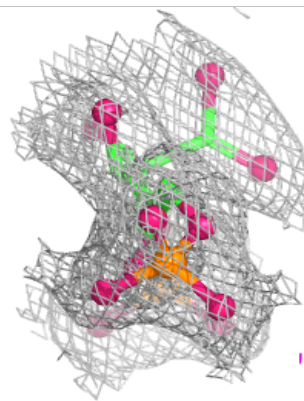
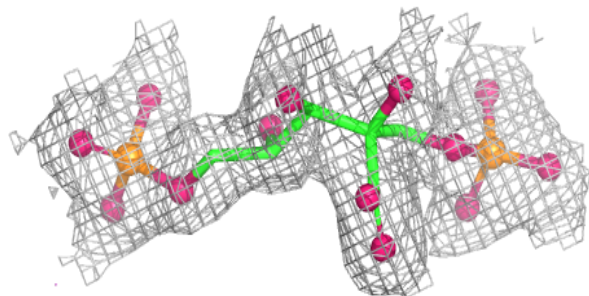
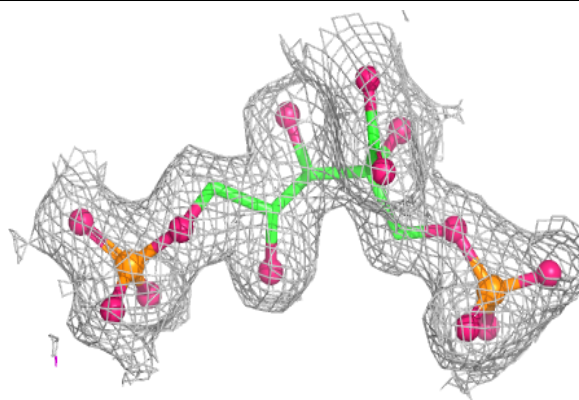
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CAP	O	1478	21/21	0.99	0.04	12,14,16,19	0
4	CAP	A	1477	21/21	0.99	0.04	11,14,15,16	0
4	CAP	B	1477	21/21	0.99	0.04	12,13,14,15	0
3	MG	B	1476	1/1	0.99	0.04	12,12,12,12	0

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.

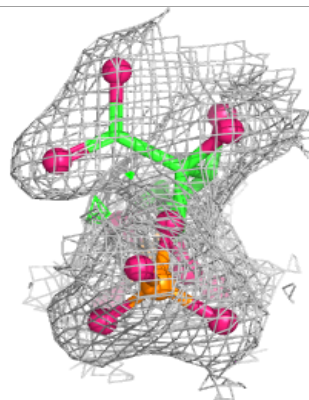
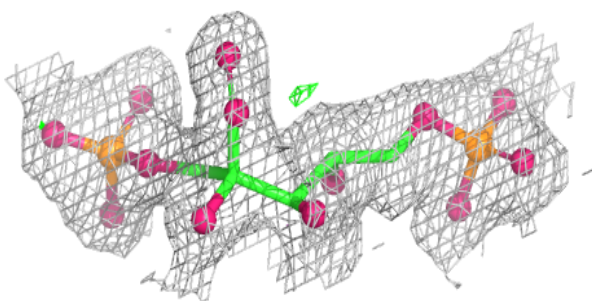
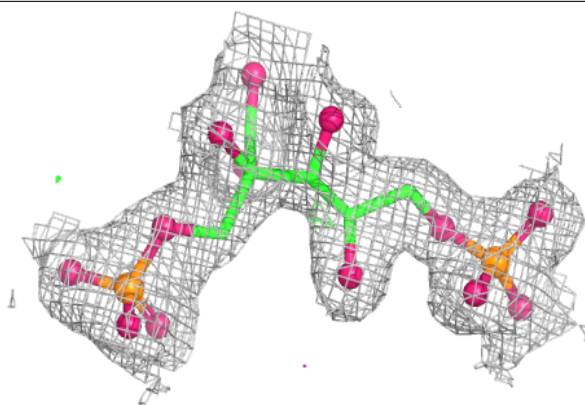
Electron density around CAP V 1476:

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

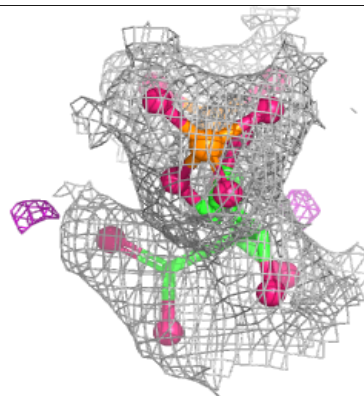
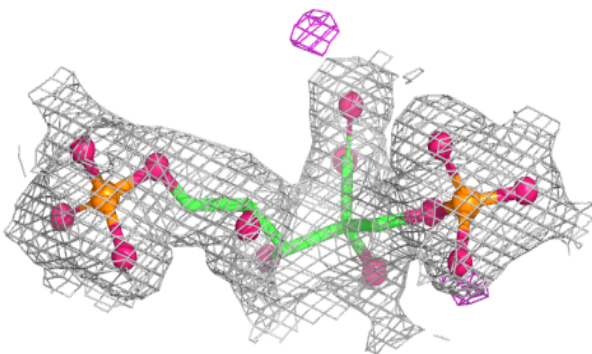
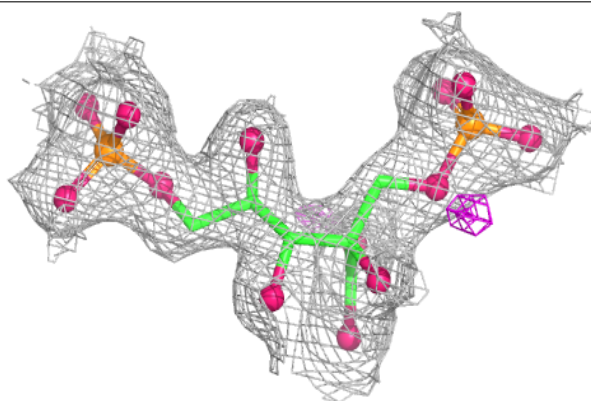


Electron density around CAP E 1477:

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

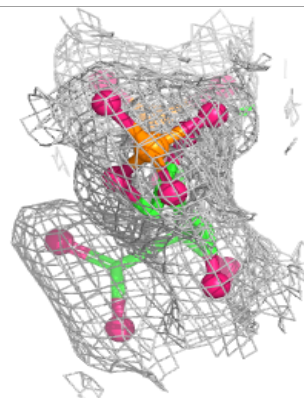
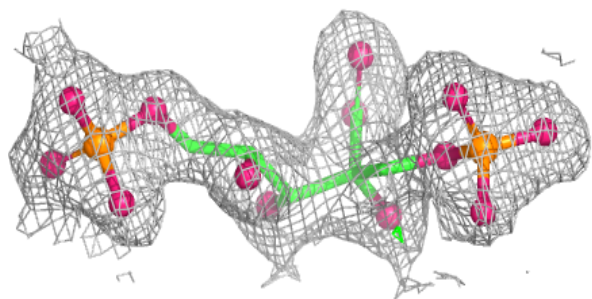
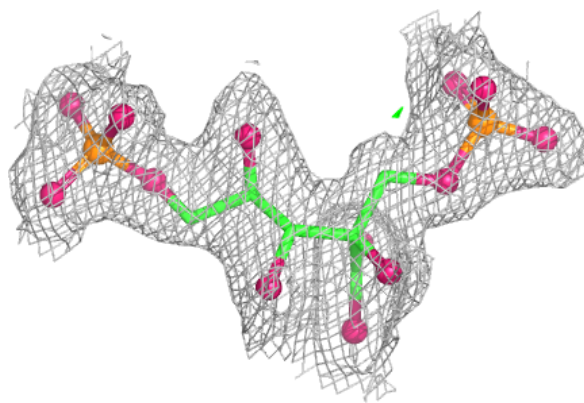
**Electron density around CAP R 1476:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

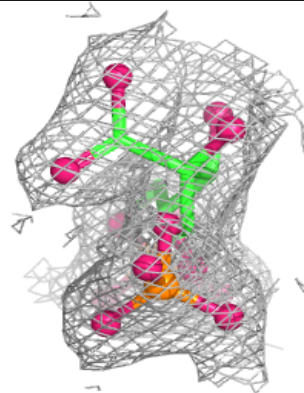
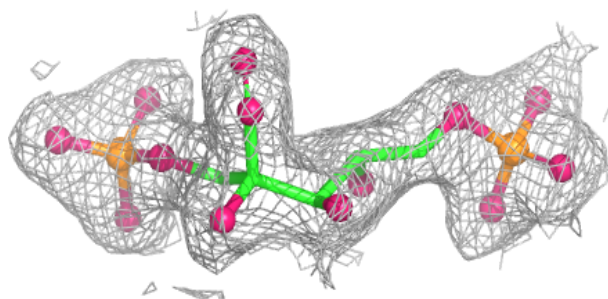
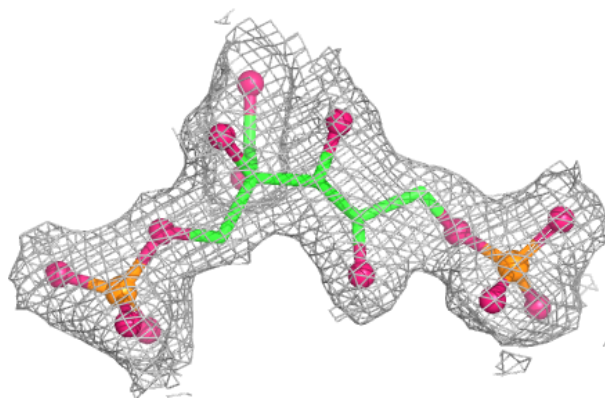


Electron density around CAP R 1478:

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

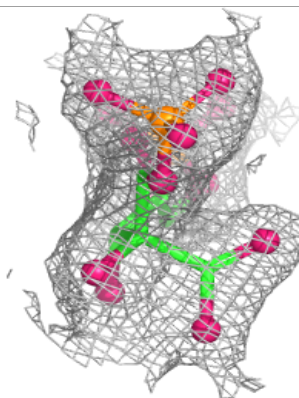
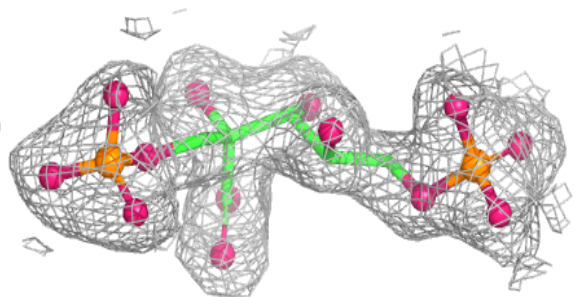
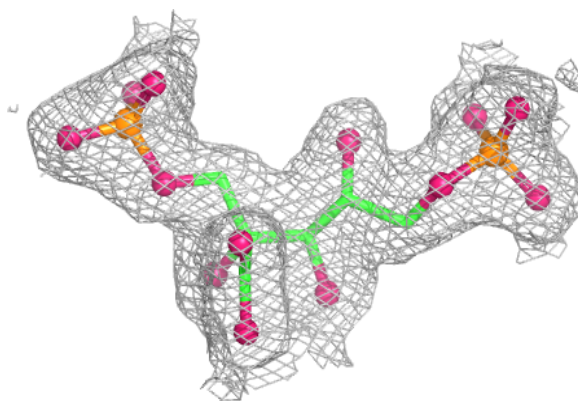
**Electron density around CAP O 1476:**

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

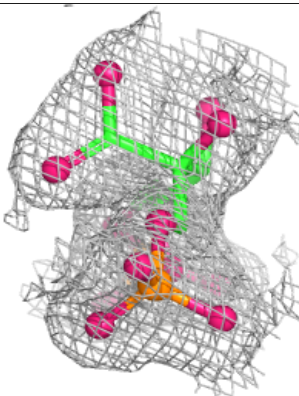
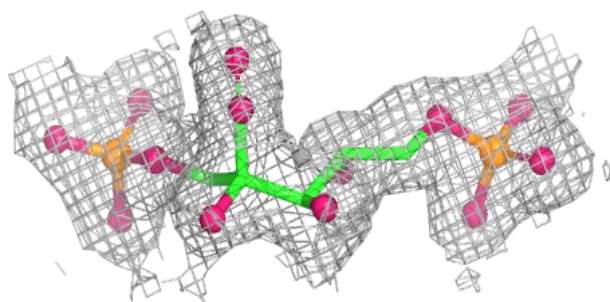
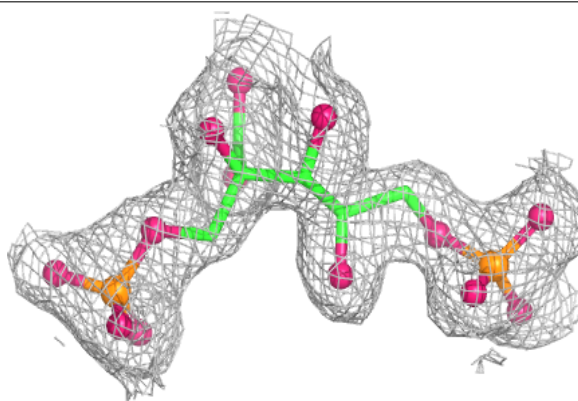


Electron density around CAP O 1478:

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

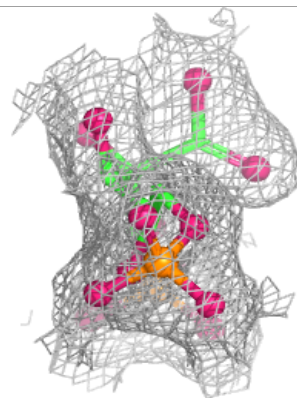
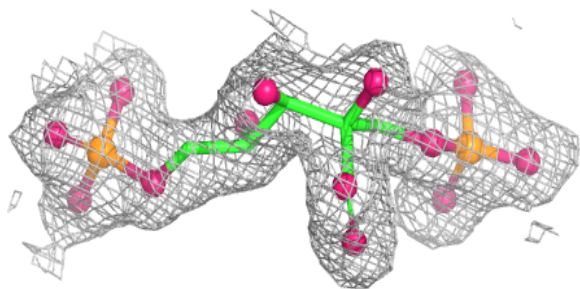
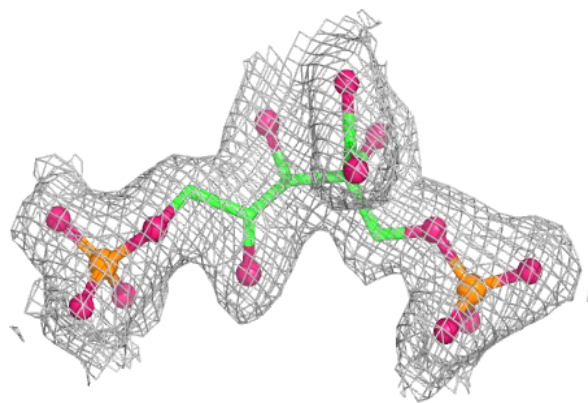
**Electron density around CAP A 1477:**

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



Electron density around CAP B 1477:

$2mF_o-DF_c$ (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.