



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:04 PM UTC

PDB ID : 1UWA / pdb_00001uwa
Title : L290F mutant rubisco from chlamydomonas
Authors : Karkehabadi, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on : 2004-02-03
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 ⓘ 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

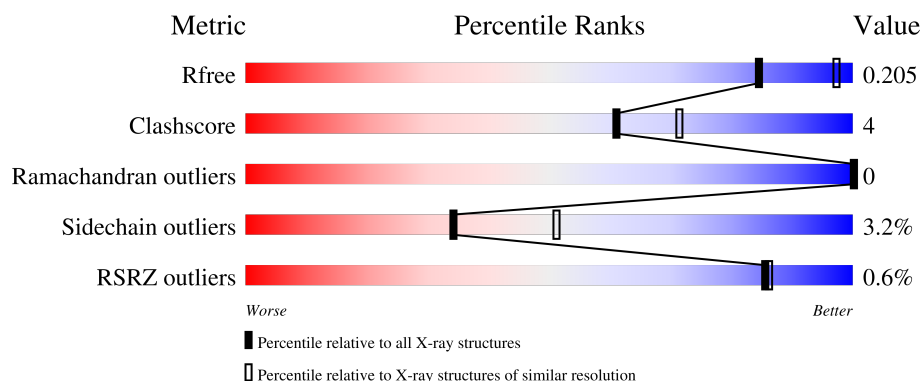
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	88%10% .
1	B	475	86%12% ..
1	E	475	% 88%10% ..
1	H	475	87%11% ..
1	K	475	% 88%10% ..

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Mol	Chain	Length	Quality of chain
1	O	475	 88% 10% ..
1	R	475	 87% 11% .
1	V	475	 88% 10% .
2	C	140	 86% 12% .
2	F	140	 87% 12% .
2	I	140	 4% 89% 10% .
2	J	140	 87% 12% .
2	M	140	 % 86% 14% .
2	P	140	 89% 10% .
2	T	140	 % 86% 13% .
2	W	140	 % 87% 12% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 41073 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	2	0
			3640	2302	641	673	24			
1	B	465	Total	C	N	O	S	0	3	0
			3643	2303	641	675	24			
1	E	469	Total	C	N	O	S	0	4	0
			3671	2319	646	682	24			
1	H	469	Total	C	N	O	S	0	4	0
			3674	2321	649	680	24			
1	K	469	Total	C	N	O	S	0	3	0
			3669	2319	646	680	24			
1	O	469	Total	C	N	O	S	0	4	0
			3672	2320	646	682	24			
1	R	465	Total	C	N	O	S	0	2	0
			3639	2302	641	672	24			
1	V	465	Total	C	N	O	S	0	1	0
			3635	2300	640	671	24			

There are 16 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	290	PHE	LEU	engineered mutation	UNP P00877
B	290	PHE	LEU	engineered mutation	UNP P00877
E	290	PHE	LEU	engineered mutation	UNP P00877
H	290	PHE	LEU	engineered mutation	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
K	290	PHE	LEU	engineered mutation	UNP P00877
O	290	PHE	LEU	engineered mutation	UNP P00877
R	290	PHE	LEU	engineered mutation	UNP P00877
V	290	PHE	LEU	engineered mutation	UNP P00877

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	140	Total	C	N	O	S	0	1	0
			1142	737	192	202	11			
2	F	140	Total	C	N	O	S	0	1	0
			1138	736	187	203	12			
2	I	140	Total	C	N	O	S	0	1	0
			1133	732	188	202	11			
2	J	140	Total	C	N	O	S	0	1	0
			1142	737	190	203	12			
2	M	140	Total	C	N	O	S	0	1	0
			1140	736	189	203	12			
2	P	140	Total	C	N	O	S	0	1	0
			1138	734	189	203	12			
2	T	140	Total	C	N	O	S	0	1	0
			1134	733	186	203	12			
2	W	140	Total	C	N	O	S	0	1	0
			1141	737	189	203	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
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

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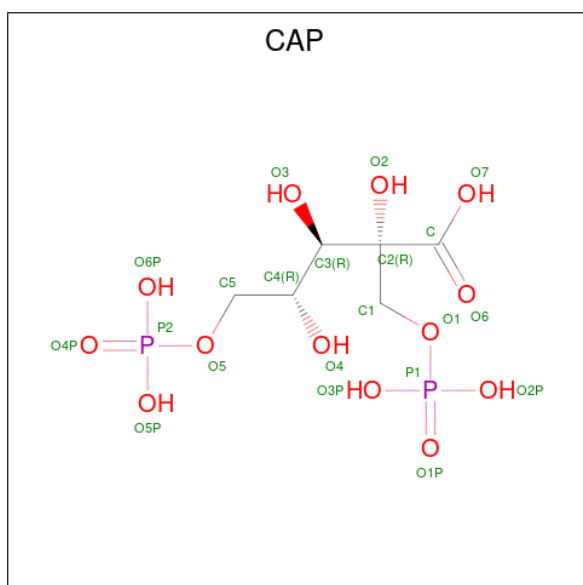
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Chain	Residue	Modelled	Actual	Comment	Reference
W	128	SER	THR	conflict	UNP P00873
W	132	TRP	PHE	conflict	UNP P00873

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

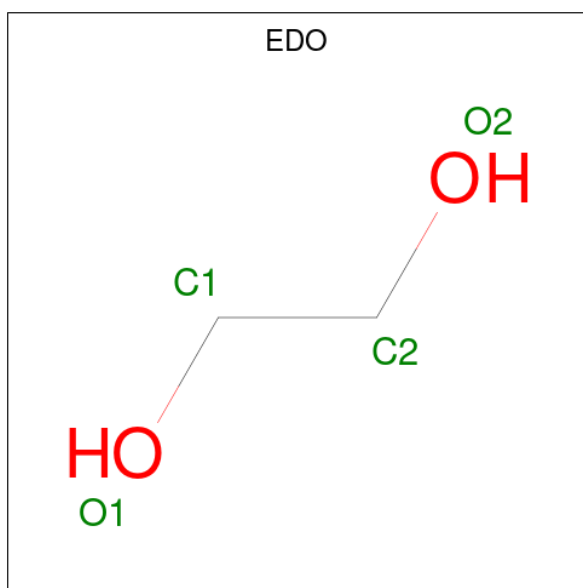
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	O	1	Total Mg 1 1	0	0
3	R	1	Total Mg 1 1	0	0
3	V	1	Total Mg 1 1	0	0

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



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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		

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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	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	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		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	253	Total O 253 253	0	0
6	B	252	Total O 252 252	0	0
6	C	47	Total O 47 47	0	0
6	E	253	Total O 253 253	0	0
6	F	49	Total O 49 49	0	0
6	H	195	Total O 195 195	0	0

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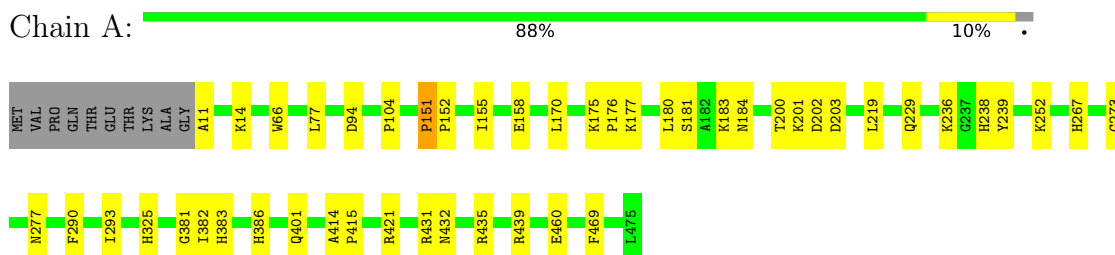
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	57	Total 57	O 57	0	0
6	J	45	Total 45	O 45	0	0
6	K	245	Total 245	O 245	0	0
6	M	63	Total 63	O 63	0	0
6	O	229	Total 229	O 229	0	0
6	P	60	Total 60	O 60	0	0
6	R	221	Total 221	O 221	0	0
6	T	52	Total 52	O 52	0	0
6	V	219	Total 219	O 219	0	0
6	W	70	Total 70	O 70	0	0

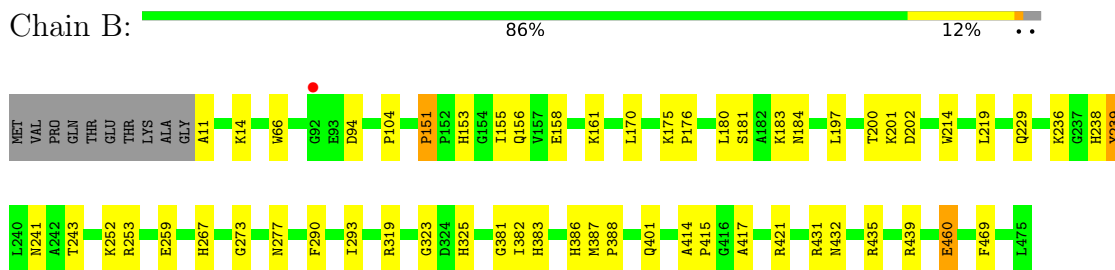
3 Residue-property plots [i](#)

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

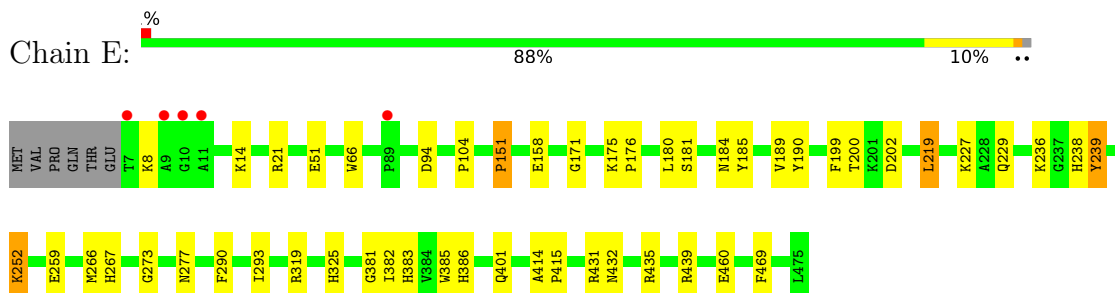
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



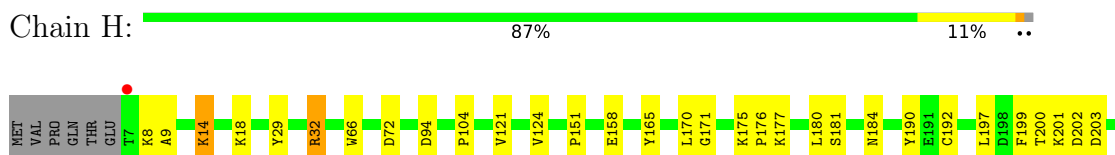
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

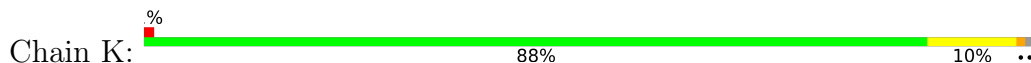


- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

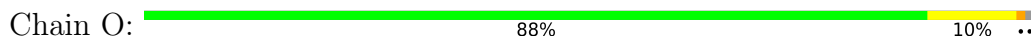




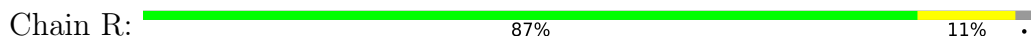
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



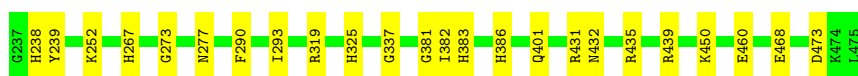
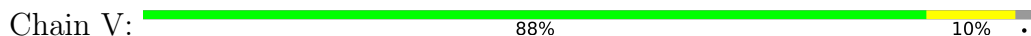
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



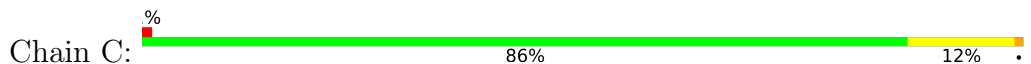
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

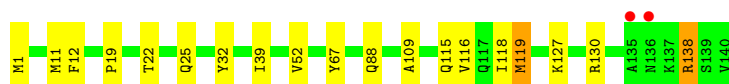


• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

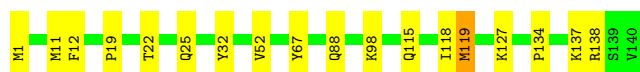
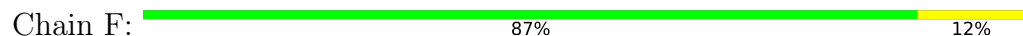


• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

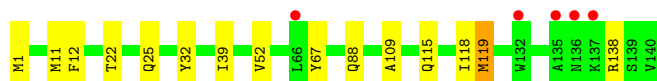
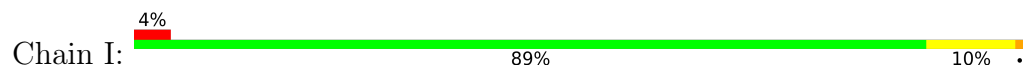




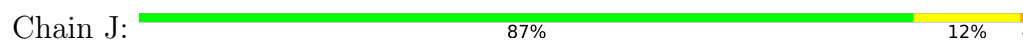
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



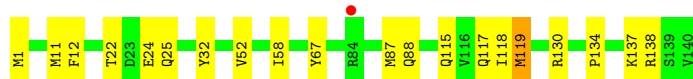
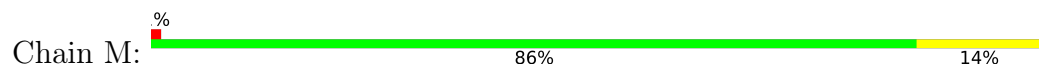
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



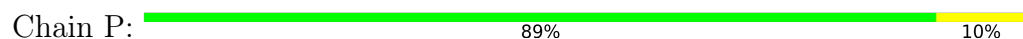
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



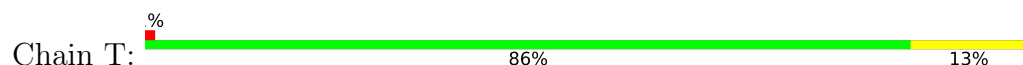
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



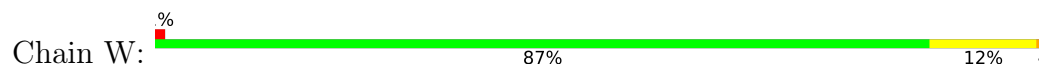
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1



- 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	120.98Å 177.71Å 122.66Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.30) 98.2 (30.00-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.171 , 0.205 0.170 , 0.205	Depositor DCC
R_{free} test set	12964 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.000 for h,-k,-h-l 0.000 for -h-l,-k,l 0.158 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	41073	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: HYP, KCX, CAP, MG, EDO, SMC

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	0.68	0/3690	0.89	1/4986 (0.0%)
1	B	0.66	0/3699	0.88	1/4998 (0.0%)
1	E	0.67	0/3733	0.88	0/5043
1	H	0.69	1/3735 (0.0%)	0.87	2/5045 (0.0%)
1	K	0.82	3/3722 (0.1%)	0.89	2/5025 (0.0%)
1	O	0.67	0/3733	0.88	1/5043 (0.0%)
1	R	0.67	0/3690	0.88	2/4986 (0.0%)
1	V	0.67	0/3680	0.86	1/4974 (0.0%)
2	C	0.67	1/1181 (0.1%)	0.98	3/1605 (0.2%)
2	F	0.67	0/1177	0.84	1/1600 (0.1%)
2	I	0.68	0/1172	0.84	0/1595
2	J	0.65	0/1181	0.81	0/1605
2	M	0.66	0/1179	0.84	0/1603
2	P	0.66	0/1177	0.82	0/1601
2	T	0.67	0/1173	0.83	1/1596 (0.1%)
2	W	0.64	0/1180	0.84	0/1604
All	All	0.69	5/39102 (0.0%)	0.87	15/52909 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	359	SER	C-N	28.09	1.82	1.34
2	C	19	PRO	CA-C	5.39	1.54	1.51
1	H	121	VAL	CA-CB	5.14	1.60	1.54
1	K	121	VAL	CA-CB	5.08	1.60	1.54
1	K	207	ASN	CA-C	5.05	1.54	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	138	ARG	NE-CZ-NH2	12.55	130.50	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	138	ARG	NE-CZ-NH1	-11.71	109.79	121.50
2	C	138	ARG	CD-NE-CZ	9.35	137.49	124.40
1	K	359	SER	O-C-N	-6.43	113.59	122.46
1	A	155	ILE	N-CA-C	5.94	116.12	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3640	0	3542	30	0
1	B	3643	0	3540	38	0
1	E	3671	0	3566	34	1
1	H	3674	0	3577	36	1
1	K	3669	0	3571	37	1
1	O	3672	0	3570	31	0
1	R	3639	0	3540	32	1
1	V	3635	0	3538	33	0
2	C	1142	0	1110	11	0
2	F	1138	0	1103	10	0
2	I	1133	0	1090	9	0
2	J	1142	0	1110	11	0
2	M	1140	0	1103	13	0
2	P	1138	0	1099	9	0
2	T	1134	0	1092	12	0
2	W	1141	0	1105	13	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	7	0	0
4	E	21	0	7	0	0
4	H	21	0	7	0	0
4	K	21	0	7	0	0
4	O	21	0	7	0	0
4	R	21	0	7	0	0
4	V	21	0	7	0	0
5	A	28	0	42	4	0
5	B	28	0	42	4	0
5	C	8	0	12	0	0
5	E	20	0	30	2	0
5	F	8	0	12	0	0
5	H	24	0	36	2	0
5	I	8	0	12	0	0
5	J	8	0	12	1	0
5	K	20	0	30	0	0
5	M	4	0	6	0	0
5	O	20	0	30	0	0
5	P	8	0	12	0	0
5	R	24	0	36	1	0
5	T	8	0	12	0	0
5	V	20	0	30	6	0
6	A	253	0	0	3	0
6	B	252	0	0	5	0
6	C	47	0	0	1	0
6	E	253	0	0	2	0
6	F	49	0	0	1	0
6	H	195	0	0	5	0
6	I	57	0	0	0	0
6	J	45	0	0	1	0
6	K	245	0	0	5	0
6	M	63	0	0	2	0
6	O	229	0	0	3	0
6	P	60	0	0	1	0
6	R	221	0	0	6	0
6	T	52	0	0	1	0
6	V	219	0	0	6	0
6	W	70	0	0	3	0
All	All	41073	0	37666	320	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 320 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:B:267:HIS:HD2	1:B:277:ASN:HD22	1.09	0.97
1:R:267:HIS:HD2	1:R:277:ASN:HD22	1.06	0.97
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.07	0.96
2:J:87:MET:HE3	6:J:315:HOH:O	1.64	0.96
1:K:267:HIS:HD2	1:K:277:ASN:HD22	1.12	0.95

All (2) 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:E:51[A]:GLU:OE2	1:K:439:ARG:NH2[1_554]	1.95	0.25
1:H:14:LYS:CE	1:R:460:GLU:OE1[2_547]	2.00	0.20

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/475 (97%)	446 (97%)	14 (3%)	0	100	100
1	B	461/475 (97%)	448 (97%)	13 (3%)	0	100	100
1	E	466/475 (98%)	452 (97%)	14 (3%)	0	100	100
1	H	466/475 (98%)	452 (97%)	14 (3%)	0	100	100
1	K	462/475 (97%)	449 (97%)	13 (3%)	0	100	100
1	O	466/475 (98%)	452 (97%)	14 (3%)	0	100	100
1	R	460/475 (97%)	446 (97%)	14 (3%)	0	100	100
1	V	459/475 (97%)	445 (97%)	14 (3%)	0	100	100
2	C	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
2	F	139/140 (99%)	133 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	139/140 (99%)	133 (96%)	6 (4%)	0	100	100
2	J	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
2	M	139/140 (99%)	134 (96%)	5 (4%)	0	100	100
2	P	139/140 (99%)	134 (96%)	5 (4%)	0	100	100
2	T	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
2	W	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
All	All	4812/4920 (98%)	4652 (97%)	160 (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	370/376 (98%)	363 (98%)	7 (2%)	50	69
1	B	371/376 (99%)	361 (97%)	10 (3%)	39	58
1	E	374/376 (100%)	365 (98%)	9 (2%)	43	62
1	H	374/376 (100%)	360 (96%)	14 (4%)	30	45
1	K	373/376 (99%)	364 (98%)	9 (2%)	43	62
1	O	374/376 (100%)	359 (96%)	15 (4%)	28	42
1	R	370/376 (98%)	363 (98%)	7 (2%)	50	69
1	V	369/376 (98%)	362 (98%)	7 (2%)	50	69
2	C	122/123 (99%)	114 (93%)	8 (7%)	15	21
2	F	122/123 (99%)	115 (94%)	7 (6%)	18	27
2	I	120/123 (98%)	114 (95%)	6 (5%)	22	33
2	J	123/123 (100%)	116 (94%)	7 (6%)	18	27
2	M	122/123 (99%)	115 (94%)	7 (6%)	18	27
2	P	122/123 (99%)	116 (95%)	6 (5%)	22	34
2	T	121/123 (98%)	115 (95%)	6 (5%)	22	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	122/123 (99%)	116 (95%)	6 (5%)	22	34
All	All	3949/3992 (99%)	3818 (97%)	131 (3%)	34	50

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	88	GLN
1	V	94	ASP
2	W	119	MET
1	H	239	TYR
1	H	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	9	ASN
1	V	238	HIS
1	K	432	ASN
1	V	229	GLN
2	W	8	ASN

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	SMC	E	369	1	5,6,7	0.67	0	3,6,8	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	H	201	3,1	10,11,12	0.90	0	6,12,14	1.40	1 (16%)
1	SMC	R	256	1	5,6,7	0.54	0	3,6,8	0.98	0
1	SMC	H	256	1	5,6,7	0.50	0	3,6,8	0.93	0
1	KCX	A	201	3,1	10,11,12	1.32	2 (20%)	6,12,14	0.78	0
1	HYP	E	151	1	7,8,9	1.06	1 (14%)	5,10,12	3.96	4 (80%)
1	HYP	K	104	1	7,8,9	0.88	0	5,10,12	3.62	3 (60%)
1	SMC	H	369	1	5,6,7	0.57	0	3,6,8	0.42	0
1	SMC	O	256	1	5,6,7	0.58	0	3,6,8	0.90	0
1	HYP	O	104	1	7,8,9	0.88	0	5,10,12	3.49	3 (60%)
1	SMC	A	369	1	5,6,7	0.76	0	3,6,8	0.71	0
1	SMC	V	256	1	5,6,7	0.58	0	3,6,8	0.65	0
1	HYP	K	151	1	7,8,9	1.17	1 (14%)	5,10,12	3.81	3 (60%)
1	SMC	E	256	1	5,6,7	0.74	0	3,6,8	0.81	0
1	HYP	B	151	1	7,8,9	1.30	1 (14%)	5,10,12	4.20	3 (60%)
1	HYP	A	151	1	7,8,9	1.03	1 (14%)	5,10,12	4.42	4 (80%)
1	KCX	E	201	3,1	10,11,12	1.06	0	6,12,14	0.76	0
1	KCX	O	201	3,1	10,11,12	1.11	0	6,12,14	1.00	1 (16%)
1	HYP	H	151	1	7,8,9	1.23	1 (14%)	5,10,12	4.42	4 (80%)
1	SMC	R	369	1	5,6,7	0.54	0	3,6,8	0.93	0
1	KCX	B	201	3,1	10,11,12	1.21	1 (10%)	6,12,14	0.62	0
1	SMC	B	256	1	5,6,7	0.89	0	3,6,8	0.89	0
1	SMC	O	369	1	5,6,7	0.66	0	3,6,8	1.42	1 (33%)
1	HYP	R	151	1	7,8,9	1.11	1 (14%)	5,10,12	3.61	3 (60%)
1	HYP	E	104	1	7,8,9	0.92	0	5,10,12	3.55	3 (60%)
1	SMC	A	256	1	5,6,7	0.73	0	3,6,8	0.59	0
1	SMC	B	369	1	5,6,7	0.60	0	3,6,8	0.67	0
1	HYP	R	104	1	6,7,9	0.81	0	7,8,12	1.40	2 (28%)
1	HYP	O	151	1	7,8,9	1.23	1 (14%)	5,10,12	4.28	3 (60%)
1	SMC	V	369	1	5,6,7	0.76	0	3,6,8	0.76	0
1	HYP	V	104	1	7,8,9	0.63	0	5,10,12	3.47	3 (60%)
1	KCX	V	201	3,1	10,11,12	0.77	0	6,12,14	0.83	0
1	KCX	K	201	3,1	10,11,12	0.93	0	6,12,14	1.18	1 (16%)
1	HYP	A	104	1	7,8,9	0.83	0	5,10,12	3.50	3 (60%)
1	HYP	V	151	1	7,8,9	1.31	1 (14%)	5,10,12	3.42	3 (60%)
1	SMC	K	256	1	5,6,7	0.88	0	3,6,8	0.96	0
1	SMC	K	369	1	5,6,7	0.88	0	3,6,8	0.36	0
1	HYP	B	104	1	7,8,9	1.03	0	5,10,12	3.55	3 (60%)
1	KCX	R	201	3,1	10,11,12	0.85	0	6,12,14	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	H	104	1	7,8,9	0.82	0	5,10,12	3.94	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	SMC	E	369	1	-	1/3/5/7	-
1	KCX	H	201	3,1	-	0/9/10/12	-
1	SMC	R	256	1	-	0/3/5/7	-
1	SMC	H	256	1	-	0/3/5/7	-
1	KCX	A	201	3,1	-	0/9/10/12	-
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	HYP	K	104	1	-	0/0/11/13	0/1/1/1
1	SMC	H	369	1	-	1/3/5/7	-
1	SMC	O	256	1	-	0/3/5/7	-
1	HYP	O	104	1	-	0/0/11/13	0/1/1/1
1	SMC	A	369	1	-	1/3/5/7	-
1	SMC	V	256	1	-	0/3/5/7	-
1	HYP	K	151	1	-	0/0/11/13	0/1/1/1
1	SMC	E	256	1	-	0/3/5/7	-
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	KCX	E	201	3,1	-	0/9/10/12	-
1	KCX	O	201	3,1	-	0/9/10/12	-
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	SMC	R	369	1	-	1/3/5/7	-
1	KCX	B	201	3,1	-	0/9/10/12	-
1	SMC	B	256	1	-	0/3/5/7	-
1	SMC	O	369	1	-	1/3/5/7	-
1	HYP	R	151	1	-	0/0/11/13	0/1/1/1
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	SMC	A	256	1	-	0/3/5/7	-
1	SMC	B	369	1	-	1/3/5/7	-
1	HYP	R	104	1	-	0/0/9/13	0/1/1/1
1	HYP	O	151	1	-	0/0/11/13	0/1/1/1
1	SMC	V	369	1	-	1/3/5/7	-
1	HYP	V	104	1	-	0/0/11/13	0/1/1/1
1	KCX	V	201	3,1	-	0/9/10/12	-
1	KCX	K	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	V	151	1	-	0/0/11/13	0/1/1/1
1	SMC	K	256	1	-	0/3/5/7	-
1	SMC	K	369	1	-	1/3/5/7	-
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

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	151	HYP	CA-N	-2.86	1.43	1.48
1	B	151	HYP	CA-N	-2.76	1.43	1.48
1	H	151	HYP	CA-N	-2.66	1.44	1.48
1	R	151	HYP	CA-N	-2.64	1.44	1.48
1	B	201	KCX	OQ1-CX	2.56	1.26	1.21

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	HYP	CB-CG-CD	6.71	110.63	103.16
1	H	104	HYP	CB-CG-CD	6.44	110.32	103.16
1	O	151	HYP	CB-CG-CD	6.37	110.25	103.16
1	H	151	HYP	OD1-CG-CD	-6.12	97.79	110.30
1	B	151	HYP	CB-CG-CD	5.95	109.78	103.16

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	151	HYP	1	0
1	K	151	HYP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	151	HYP	2	0
1	A	151	HYP	1	0
1	R	151	HYP	1	0
1	O	151	HYP	2	0
1	V	151	HYP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 8 are monoatomic - leaving 67 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	K	502	3	18,20,20	1.28	3 (16%)	23,31,31	1.02	1 (4%)
4	CAP	V	502	3	18,20,20	1.18	2 (11%)	23,31,31	1.06	2 (8%)
5	EDO	C	201	-	3,3,3	0.25	0	2,2,2	0.21	0
5	EDO	I	201	-	3,3,3	0.30	0	2,2,2	0.04	0
5	EDO	K	504	-	3,3,3	0.29	0	2,2,2	0.55	0
5	EDO	B	507	-	3,3,3	0.41	0	2,2,2	0.13	0
4	CAP	H	502	3	18,20,20	1.11	2 (11%)	23,31,31	1.03	2 (8%)
5	EDO	B	504	-	3,3,3	0.29	0	2,2,2	0.28	0
5	EDO	K	503	-	3,3,3	0.37	0	2,2,2	0.19	0
5	EDO	O	504	-	3,3,3	0.19	0	2,2,2	0.15	0
5	EDO	H	507	-	3,3,3	0.29	0	2,2,2	0.12	0
5	EDO	B	503	-	3,3,3	0.44	0	2,2,2	0.03	0
5	EDO	T	201	-	3,3,3	0.30	0	2,2,2	0.17	0
5	EDO	P	202	-	3,3,3	0.28	0	2,2,2	0.15	0
5	EDO	M	201	-	3,3,3	0.25	0	2,2,2	0.32	0
5	EDO	H	506	-	3,3,3	0.33	0	2,2,2	0.18	0
5	EDO	H	503	-	3,3,3	0.21	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	B	506	-	3,3,3	0.36	0	2,2,2	0.26	0
4	CAP	R	502	3	18,20,20	1.22	2 (11%)	23,31,31	1.08	1 (4%)
4	CAP	A	502	3	18,20,20	1.14	2 (11%)	23,31,31	1.00	0
5	EDO	E	505	-	3,3,3	0.31	0	2,2,2	0.38	0
5	EDO	H	505	-	3,3,3	0.32	0	2,2,2	0.17	0
5	EDO	I	202	-	3,3,3	0.24	0	2,2,2	0.44	0
5	EDO	A	506	-	3,3,3	0.34	0	2,2,2	0.15	0
5	EDO	B	505	-	3,3,3	0.28	0	2,2,2	0.26	0
4	CAP	B	502	3	18,20,20	1.19	2 (11%)	23,31,31	0.89	0
5	EDO	O	505	-	3,3,3	0.27	0	2,2,2	0.55	0
5	EDO	K	507	-	3,3,3	0.32	0	2,2,2	0.24	0
5	EDO	R	505	-	3,3,3	0.29	0	2,2,2	0.35	0
5	EDO	A	505	-	3,3,3	0.32	0	2,2,2	0.17	0
5	EDO	T	202	-	3,3,3	0.24	0	2,2,2	0.73	0
5	EDO	F	201	-	3,3,3	0.27	0	2,2,2	0.14	0
5	EDO	V	505	-	3,3,3	0.31	0	2,2,2	0.27	0
5	EDO	K	506	-	3,3,3	0.39	0	2,2,2	0.23	0
5	EDO	B	508	-	3,3,3	0.44	0	2,2,2	0.31	0
5	EDO	E	506	-	3,3,3	0.32	0	2,2,2	0.31	0
5	EDO	J	201	-	3,3,3	0.31	0	2,2,2	0.24	0
5	EDO	O	507	-	3,3,3	0.34	0	2,2,2	0.12	0
5	EDO	P	201	-	3,3,3	0.22	0	2,2,2	0.62	0
5	EDO	R	504	-	3,3,3	0.30	0	2,2,2	0.09	0
5	EDO	R	507	-	3,3,3	0.47	0	2,2,2	0.08	0
4	CAP	E	502	3	18,20,20	1.23	2 (11%)	23,31,31	1.18	2 (8%)
5	EDO	V	503	-	3,3,3	0.41	0	2,2,2	0.13	0
5	EDO	E	504	-	3,3,3	0.33	0	2,2,2	0.28	0
5	EDO	E	503	-	3,3,3	0.26	0	2,2,2	0.25	0
5	EDO	O	503	-	3,3,3	0.32	0	2,2,2	0.25	0
5	EDO	J	202	-	3,3,3	0.32	0	2,2,2	0.10	0
5	EDO	F	202	-	3,3,3	0.23	0	2,2,2	0.47	0
5	EDO	H	508	-	3,3,3	0.38	0	2,2,2	0.11	0
5	EDO	E	507	-	3,3,3	0.27	0	2,2,2	0.32	0
5	EDO	H	504	-	3,3,3	0.28	0	2,2,2	0.46	0
5	EDO	V	506	-	3,3,3	0.28	0	2,2,2	0.28	0
5	EDO	R	508	-	3,3,3	0.32	0	2,2,2	0.09	0
4	CAP	O	502	3	18,20,20	1.20	2 (11%)	23,31,31	1.01	1 (4%)
5	EDO	A	509	-	3,3,3	0.34	0	2,2,2	0.27	0
5	EDO	K	505	-	3,3,3	0.26	0	2,2,2	0.33	0
5	EDO	O	506	-	3,3,3	0.36	0	2,2,2	0.24	0
5	EDO	V	507	-	3,3,3	0.32	0	2,2,2	0.13	0
5	EDO	A	504	-	3,3,3	0.29	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	508	-	3,3,3	0.30	0	2,2,2	0.19	0
5	EDO	R	506	-	3,3,3	0.33	0	2,2,2	0.13	0
5	EDO	V	504	-	3,3,3	0.26	0	2,2,2	0.45	0
5	EDO	R	503	-	3,3,3	0.36	0	2,2,2	0.16	0
5	EDO	A	503	-	3,3,3	0.32	0	2,2,2	0.18	0
5	EDO	C	202	-	3,3,3	0.27	0	2,2,2	0.43	0
5	EDO	A	507	-	3,3,3	0.34	0	2,2,2	0.13	0
5	EDO	B	509	-	3,3,3	0.23	0	2,2,2	0.51	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
4	CAP	K	502	3	-	6/29/29/29	-
4	CAP	V	502	3	-	7/29/29/29	-
5	EDO	C	201	-	-	0/1/1/1	-
5	EDO	I	201	-	-	1/1/1/1	-
5	EDO	K	504	-	-	1/1/1/1	-
5	EDO	B	507	-	-	1/1/1/1	-
4	CAP	H	502	3	-	7/29/29/29	-
5	EDO	B	504	-	-	1/1/1/1	-
5	EDO	K	503	-	-	0/1/1/1	-
5	EDO	O	504	-	-	1/1/1/1	-
5	EDO	H	507	-	-	1/1/1/1	-
5	EDO	B	503	-	-	0/1/1/1	-
5	EDO	T	201	-	-	1/1/1/1	-
5	EDO	P	202	-	-	0/1/1/1	-
5	EDO	M	201	-	-	1/1/1/1	-
5	EDO	H	506	-	-	0/1/1/1	-
5	EDO	H	503	-	-	0/1/1/1	-
5	EDO	B	506	-	-	0/1/1/1	-
4	CAP	R	502	3	-	7/29/29/29	-
4	CAP	A	502	3	-	7/29/29/29	-
5	EDO	E	505	-	-	1/1/1/1	-
5	EDO	H	505	-	-	0/1/1/1	-
5	EDO	I	202	-	-	0/1/1/1	-
5	EDO	A	506	-	-	1/1/1/1	-
5	EDO	B	505	-	-	1/1/1/1	-
4	CAP	B	502	3	-	6/29/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	O	505	-	-	0/1/1/1	-
5	EDO	K	507	-	-	1/1/1/1	-
5	EDO	R	505	-	-	0/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	T	202	-	-	0/1/1/1	-
5	EDO	F	201	-	-	0/1/1/1	-
5	EDO	V	505	-	-	0/1/1/1	-
5	EDO	K	506	-	-	0/1/1/1	-
5	EDO	B	508	-	-	1/1/1/1	-
5	EDO	E	506	-	-	1/1/1/1	-
5	EDO	J	201	-	-	0/1/1/1	-
5	EDO	O	507	-	-	1/1/1/1	-
5	EDO	P	201	-	-	0/1/1/1	-
5	EDO	R	504	-	-	1/1/1/1	-
5	EDO	R	507	-	-	0/1/1/1	-
4	CAP	E	502	3	-	7/29/29/29	-
5	EDO	V	503	-	-	0/1/1/1	-
5	EDO	E	504	-	-	1/1/1/1	-
5	EDO	E	503	-	-	0/1/1/1	-
5	EDO	O	503	-	-	0/1/1/1	-
5	EDO	J	202	-	-	1/1/1/1	-
5	EDO	F	202	-	-	0/1/1/1	-
5	EDO	H	508	-	-	0/1/1/1	-
5	EDO	E	507	-	-	0/1/1/1	-
5	EDO	H	504	-	-	0/1/1/1	-
5	EDO	V	506	-	-	1/1/1/1	-
5	EDO	R	508	-	-	1/1/1/1	-
4	CAP	O	502	3	-	7/29/29/29	-
5	EDO	A	509	-	-	1/1/1/1	-
5	EDO	K	505	-	-	0/1/1/1	-
5	EDO	O	506	-	-	0/1/1/1	-
5	EDO	V	507	-	-	0/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	A	508	-	-	1/1/1/1	-
5	EDO	R	506	-	-	1/1/1/1	-
5	EDO	V	504	-	-	1/1/1/1	-
5	EDO	R	503	-	-	1/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	C	202	-	-	1/1/1/1	-
5	EDO	A	507	-	-	1/1/1/1	-
5	EDO	B	509	-	-	1/1/1/1	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	502	CAP	O6-C	3.40	1.32	1.22
4	V	502	CAP	O6-C	3.18	1.32	1.22
4	E	502	CAP	O6-C	3.16	1.32	1.22
4	K	502	CAP	O6-C	3.09	1.31	1.22
4	V	502	CAP	O7-C	3.08	1.41	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	502	CAP	O2-C2-C	-3.47	102.55	109.07
4	R	502	CAP	O2-C2-C	-3.30	102.87	109.07
4	V	502	CAP	O2-C2-C	-2.41	104.54	109.07
4	H	502	CAP	O2-C2-C	-2.24	104.86	109.07
4	V	502	CAP	O7-C-C2	2.23	117.78	114.06

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	CAP	O6-C-C2-C1
4	A	502	CAP	O7-C-C2-C1
4	A	502	CAP	O6-C-C2-O2
4	A	502	CAP	O7-C-C2-O2
4	A	502	CAP	O3-C3-C4-O4

There are no ring outliers.

13 monomers are involved in 20 short contacts:

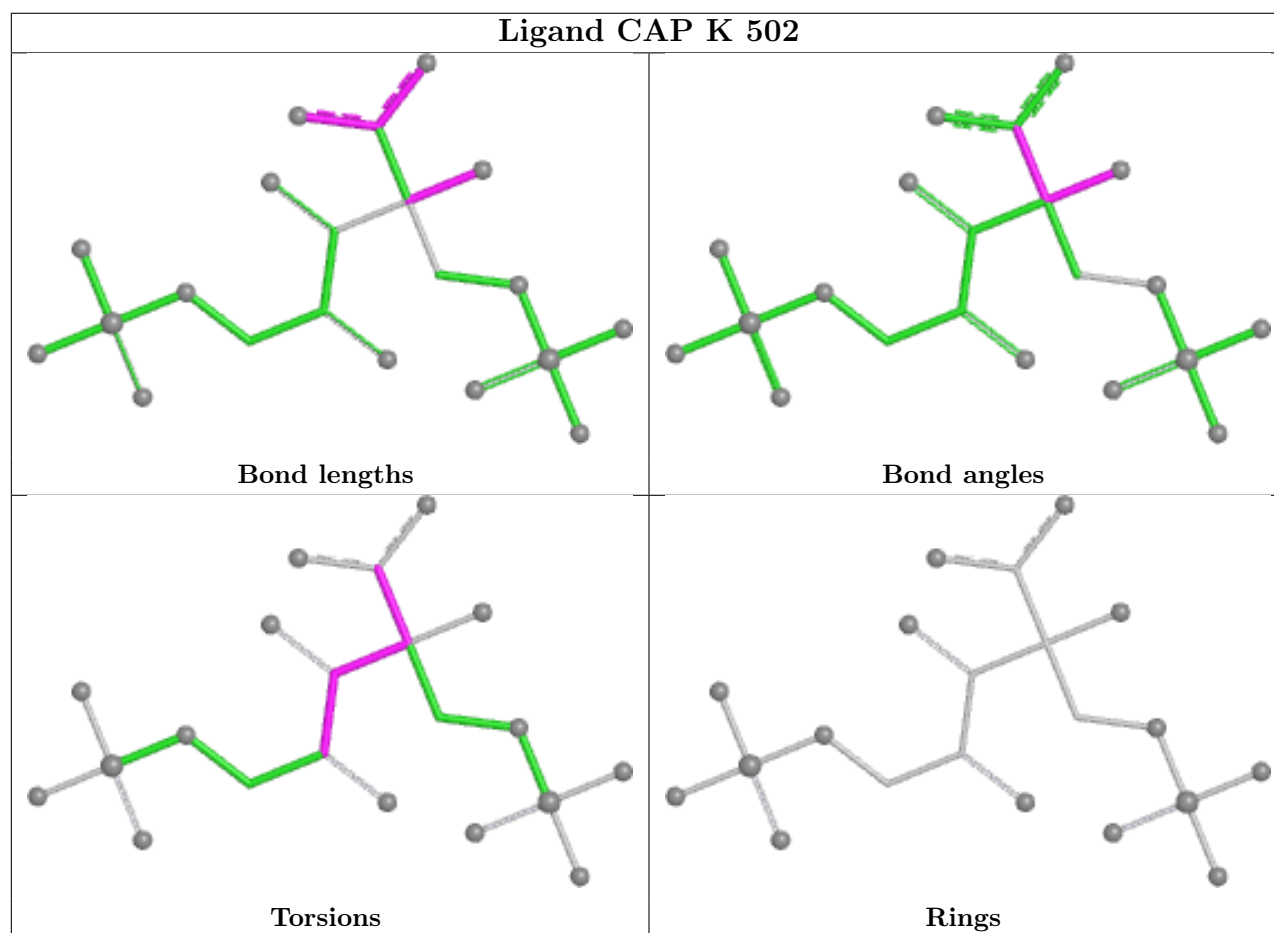
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	506	EDO	1	0
5	E	505	EDO	1	0
5	E	506	EDO	1	0
5	J	202	EDO	1	0
5	H	508	EDO	1	0
5	H	504	EDO	1	0
5	V	506	EDO	3	0
5	A	509	EDO	2	0
5	V	507	EDO	3	0
5	A	508	EDO	1	0
5	R	506	EDO	1	0

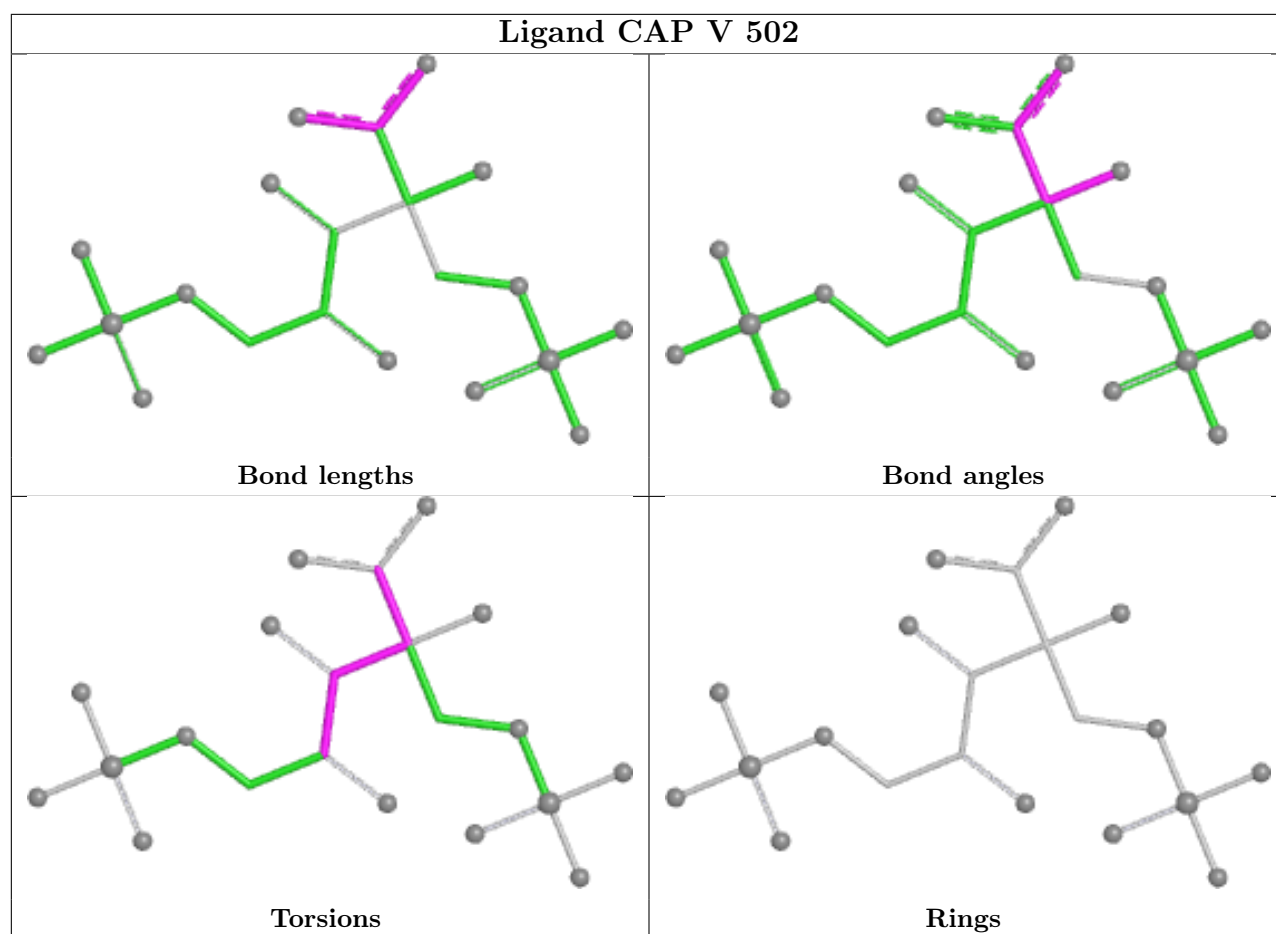
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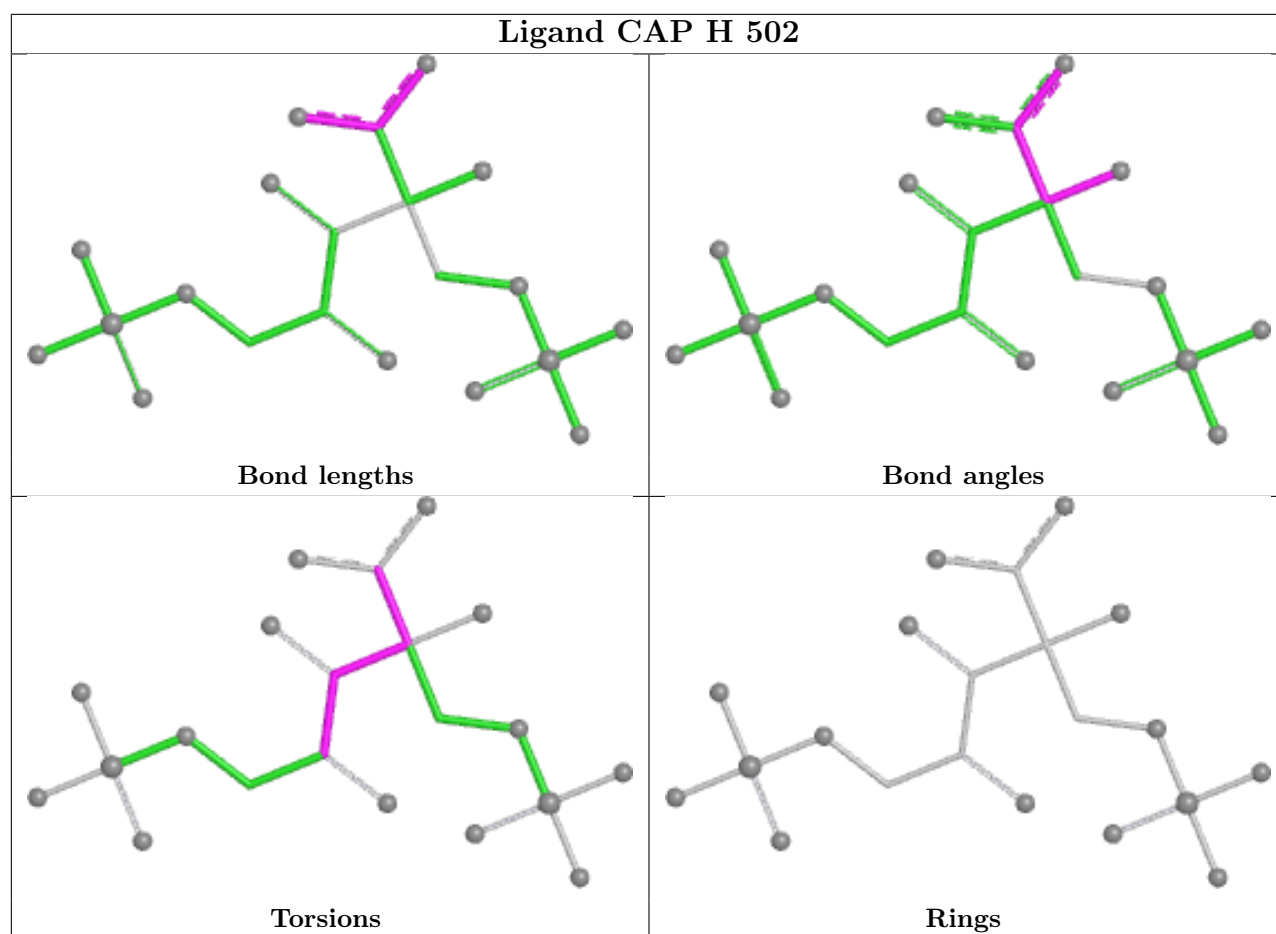
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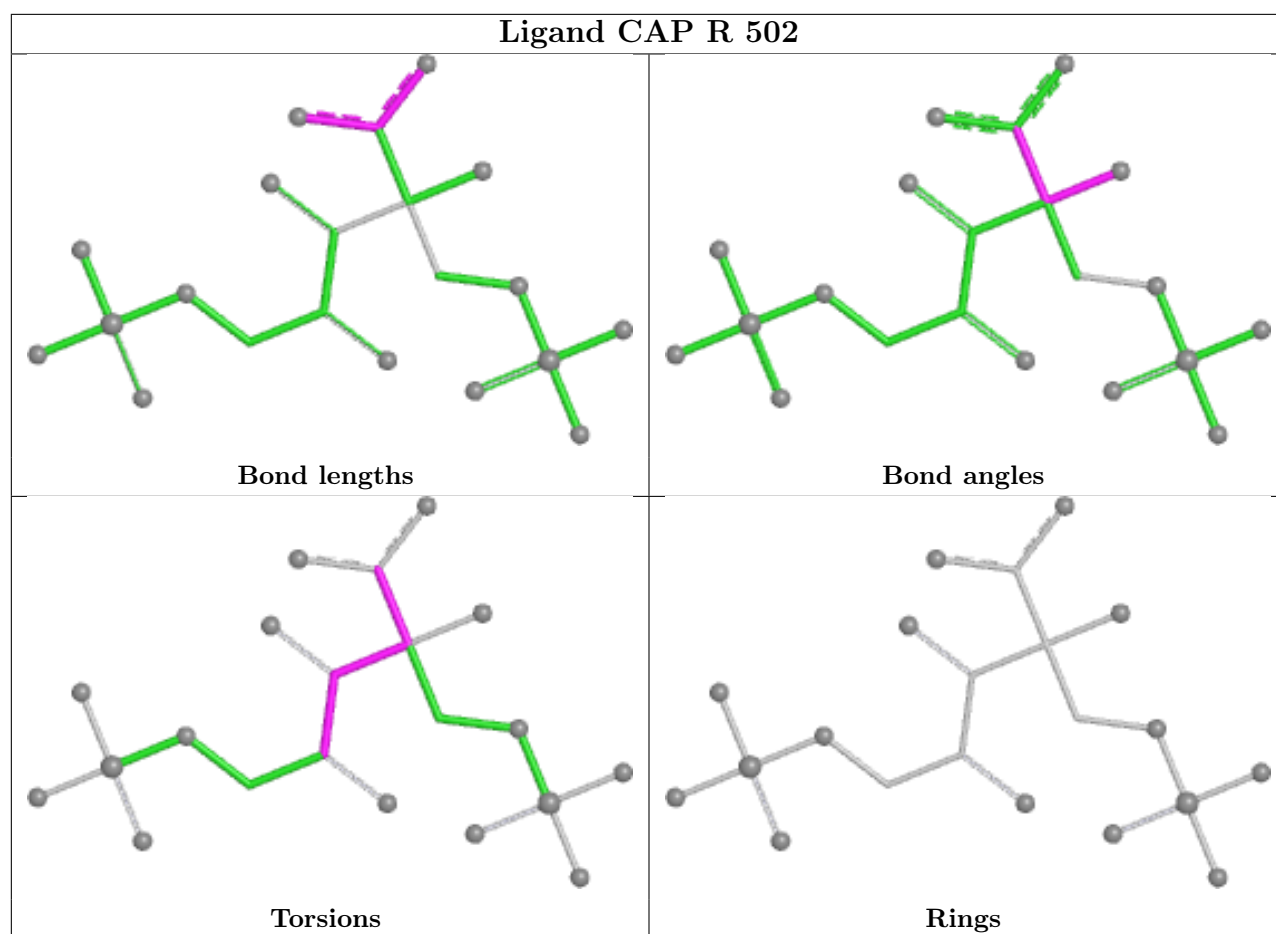
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	EDO	1	0
5	B	509	EDO	3	0

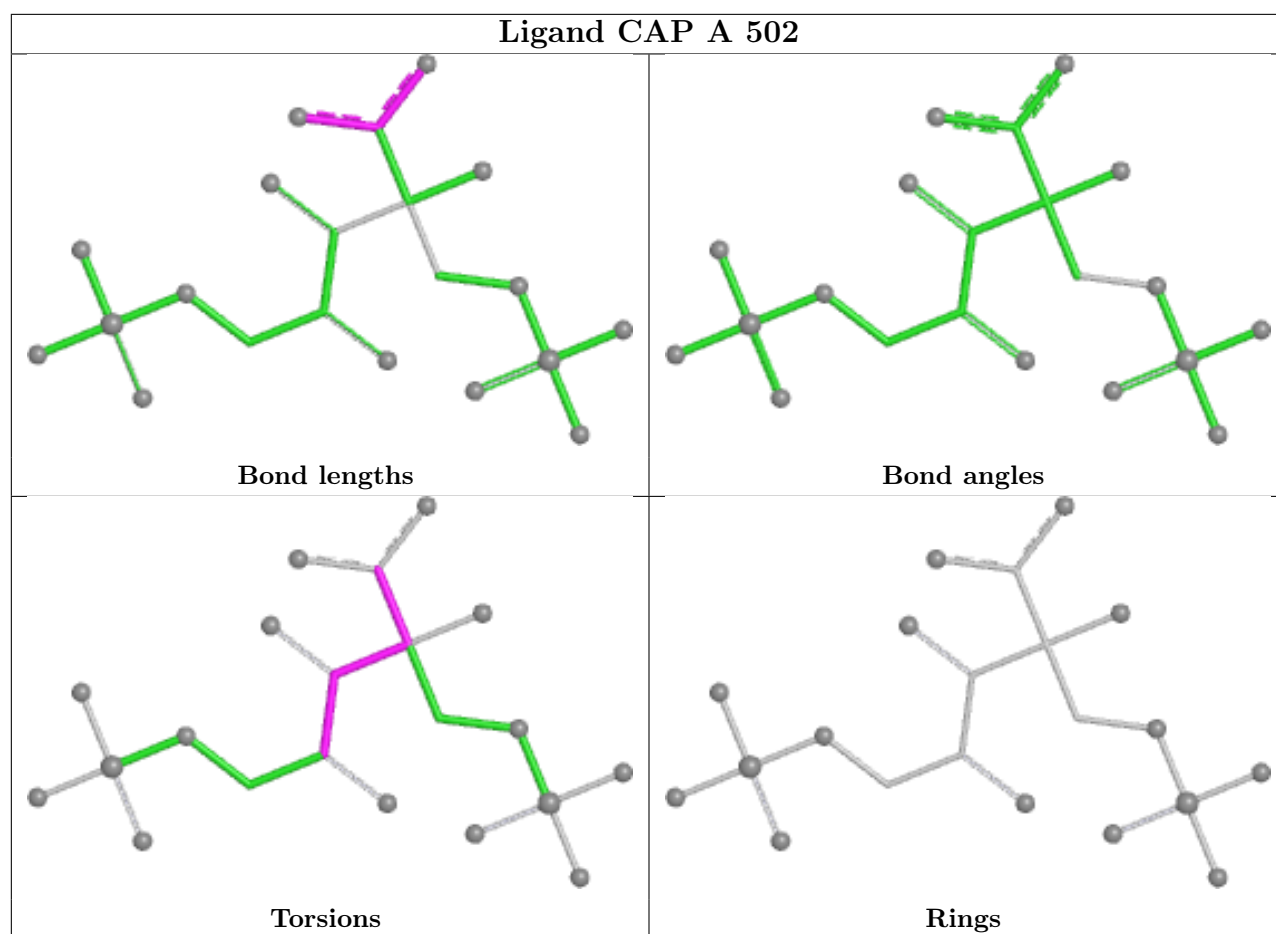
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

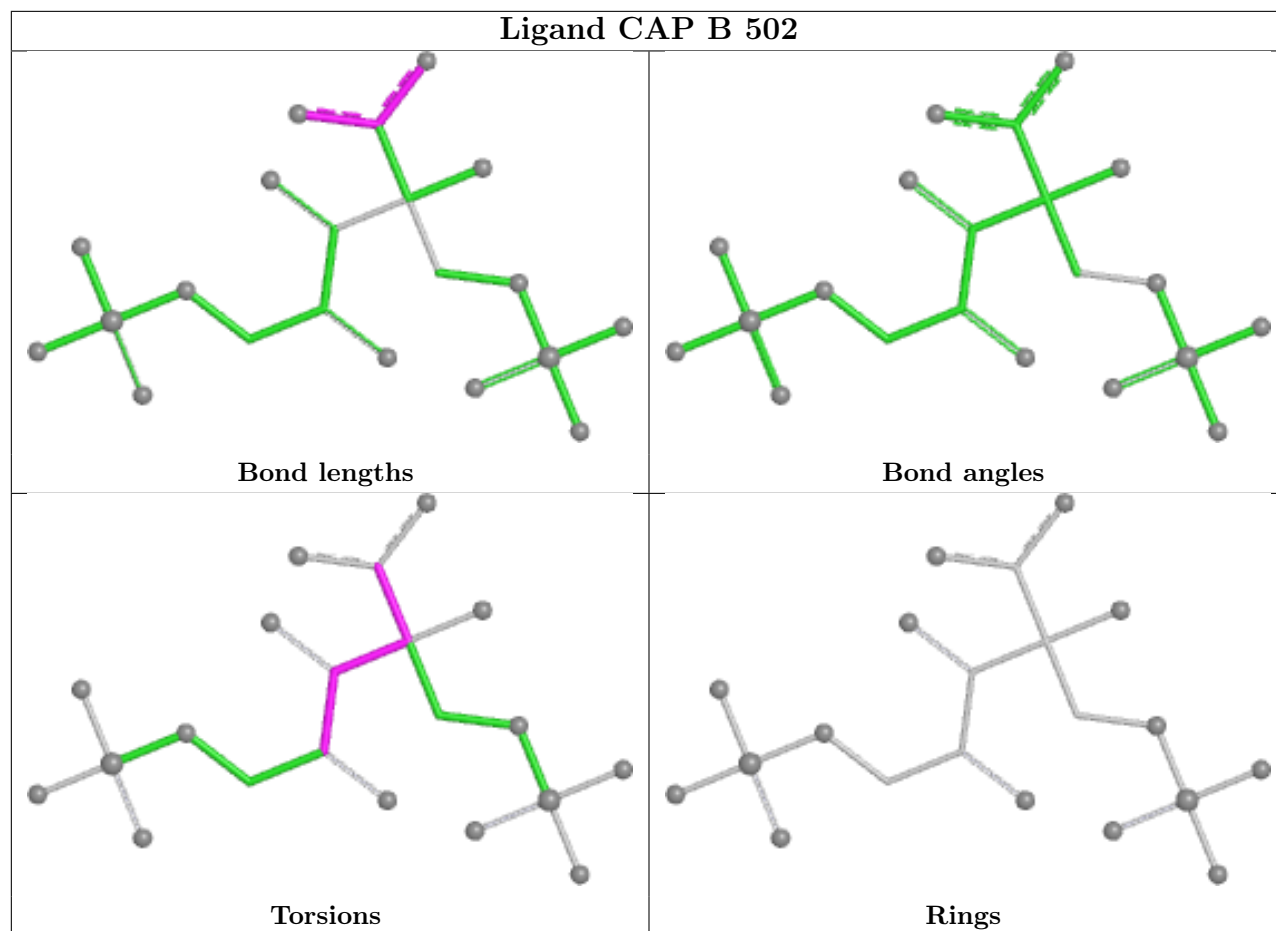




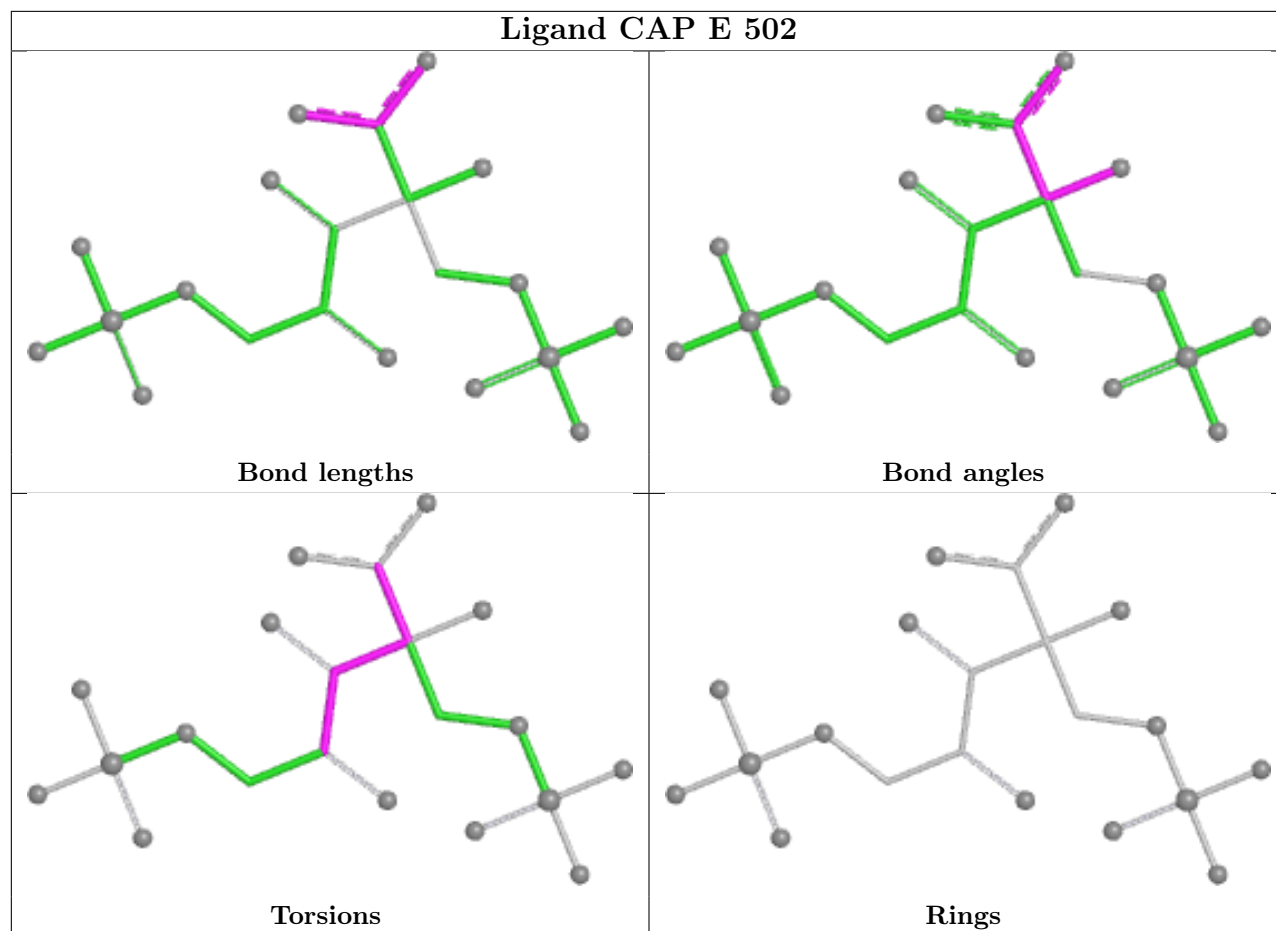


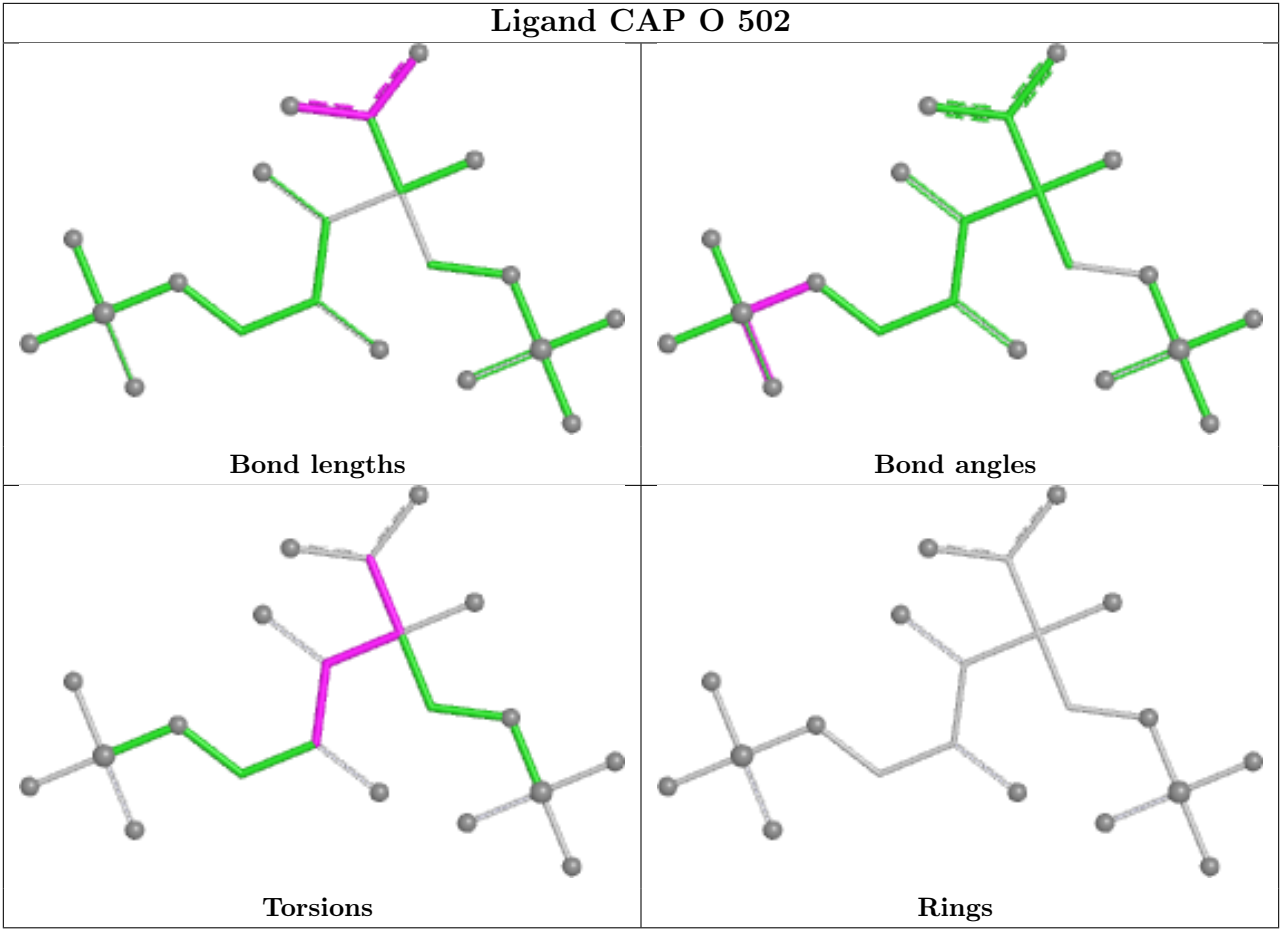






Ligand CAP E 502





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	K	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	360:ARG	C	361:GLY	N	2.35
1	K	359:SER	C	360:ARG	N	1.82

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%)	-0.37	0 100 100	20, 31, 46, 63	2 (0%)
1	B	460/475 (96%)	-0.40	1 (0%) 91 91	21, 31, 46, 63	3 (0%)
1	E	464/475 (97%)	-0.36	5 (1%) 78 79	21, 31, 47, 92	4 (0%)
1	H	464/475 (97%)	-0.31	2 (0%) 88 89	21, 31, 47, 95	4 (0%)
1	K	464/475 (97%)	-0.34	3 (0%) 85 86	21, 31, 47, 90	3 (0%)
1	O	464/475 (97%)	-0.35	2 (0%) 88 89	21, 31, 47, 87	4 (0%)
1	R	460/475 (96%)	-0.34	2 (0%) 88 89	20, 31, 46, 63	2 (0%)
1	V	460/475 (96%)	-0.33	2 (0%) 88 89	21, 31, 46, 63	1 (0%)
2	C	140/140 (100%)	0.10	2 (1%) 73 75	30, 40, 52, 64	1 (0%)
2	F	140/140 (100%)	-0.04	0 100 100	30, 40, 52, 60	1 (0%)
2	I	140/140 (100%)	0.17	5 (3%) 46 48	30, 40, 52, 56	1 (0%)
2	J	140/140 (100%)	0.01	0 100 100	30, 40, 52, 63	2 (1%)
2	M	140/140 (100%)	0.09	1 (0%) 84 85	30, 40, 52, 57	2 (1%)
2	P	140/140 (100%)	-0.01	0 100 100	30, 40, 52, 60	1 (0%)
2	T	140/140 (100%)	0.07	1 (0%) 84 85	30, 40, 52, 57	1 (0%)
2	W	140/140 (100%)	0.07	2 (1%) 73 75	30, 40, 52, 56	2 (1%)
All	All	4816/4920 (97%)	-0.26	28 (0%) 85 86	20, 32, 50, 95	34 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	89	PRO	4.8
1	K	439	ARG	4.5
1	V	92	GLY	3.8
2	I	136	ASN	3.6
2	I	137	LYS	3.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	R	104	7/9	0.77	0.09	26,28,30,30	0
1	HYP	B	151	8/9	0.89	0.09	24,27,29,30	0
1	HYP	H	104	8/9	0.91	0.08	26,29,30,30	0
1	HYP	O	104	8/9	0.91	0.08	26,28,30,30	0
1	HYP	O	151	8/9	0.91	0.07	24,28,29,30	0
1	HYP	E	104	8/9	0.91	0.08	26,28,30,30	0
1	HYP	A	151	8/9	0.92	0.07	24,28,29,30	0
1	HYP	V	104	8/9	0.92	0.07	26,28,30,30	0
1	HYP	V	151	8/9	0.92	0.07	24,28,29,30	0
1	HYP	B	104	8/9	0.93	0.08	26,28,30,30	0
1	HYP	R	151	8/9	0.93	0.08	24,28,29,30	0
1	HYP	E	151	8/9	0.94	0.07	24,28,29,30	0
1	KCX	B	201	12/13	0.94	0.07	23,26,28,29	0
1	SMC	H	369	7/8	0.94	0.08	28,31,32,37	0
1	HYP	K	151	8/9	0.94	0.06	24,28,29,30	0
1	KCX	A	201	12/13	0.94	0.06	23,26,28,29	0
1	HYP	K	104	8/9	0.95	0.05	26,29,30,30	0
1	SMC	E	369	7/8	0.95	0.08	28,30,32,37	0
1	SMC	K	369	7/8	0.95	0.07	28,30,32,37	0
1	KCX	H	201	12/13	0.96	0.05	23,26,28,29	0
1	KCX	E	201	12/13	0.96	0.06	23,26,28,29	0
1	HYP	A	104	8/9	0.96	0.06	26,28,30,30	0
1	SMC	B	369	7/8	0.96	0.07	28,30,32,36	0
1	KCX	R	201	12/13	0.96	0.06	23,26,28,29	0
1	SMC	R	369	7/8	0.96	0.06	28,30,32,37	0
1	KCX	K	201	12/13	0.96	0.06	23,26,28,29	0
1	HYP	H	151	8/9	0.96	0.05	24,28,29,30	0
1	KCX	V	201	12/13	0.96	0.06	23,26,28,29	0
1	SMC	V	256	7/8	0.96	0.07	27,29,30,31	0
1	SMC	V	369	7/8	0.96	0.06	28,30,32,37	0
1	KCX	O	201	12/13	0.97	0.05	23,26,28,29	0
1	SMC	O	369	7/8	0.97	0.06	28,30,32,36	0
1	SMC	A	369	7/8	0.97	0.05	28,30,32,37	0
1	SMC	A	256	7/8	0.97	0.06	27,29,29,31	0
1	SMC	B	256	7/8	0.97	0.06	27,28,29,30	0
1	SMC	R	256	7/8	0.97	0.06	27,29,29,31	0
1	SMC	O	256	7/8	0.98	0.05	27,29,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SMC	H	256	7/8	0.98	0.05	27,29,29,30	0
1	SMC	K	256	7/8	0.98	0.06	27,29,29,31	0
1	SMC	E	256	7/8	0.98	0.04	27,29,29,31	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	A	506	4/4	0.58	0.23	56,59,61,63	0
5	EDO	V	507	4/4	0.68	0.22	62,63,63,67	0
5	EDO	A	508	4/4	0.69	0.20	66,69,70,71	0
5	EDO	C	202	4/4	0.70	0.21	88,89,91,92	0
5	EDO	B	509	4/4	0.70	0.17	57,57,58,61	0
5	EDO	K	507	4/4	0.71	0.19	61,64,65,67	0
5	EDO	H	507	4/4	0.72	0.20	59,62,62,63	0
5	EDO	B	507	4/4	0.73	0.21	52,55,55,57	0
5	EDO	O	507	4/4	0.76	0.17	55,57,58,59	0
5	EDO	R	508	4/4	0.77	0.17	59,60,60,61	0
5	EDO	O	505	4/4	0.81	0.17	58,64,67,67	0
5	EDO	T	201	4/4	0.82	0.15	62,64,69,70	0
5	EDO	A	505	4/4	0.82	0.16	55,55,56,58	0
5	EDO	M	201	4/4	0.83	0.15	74,74,74,76	0
5	EDO	I	201	4/4	0.84	0.15	56,60,61,63	0
5	EDO	J	201	4/4	0.84	0.11	50,56,60,63	0
5	EDO	B	505	4/4	0.84	0.14	48,53,53,55	0
5	EDO	K	505	4/4	0.85	0.16	56,63,64,66	0
5	EDO	H	505	4/4	0.85	0.15	59,62,62,63	0
5	EDO	J	202	4/4	0.86	0.11	44,46,48,49	0
5	EDO	A	509	4/4	0.87	0.14	49,59,61,63	0
5	EDO	E	506	4/4	0.87	0.12	48,53,56,56	0
5	EDO	P	202	4/4	0.87	0.15	59,61,62,62	0
5	EDO	I	202	4/4	0.88	0.10	64,64,64,65	0
5	EDO	K	503	4/4	0.88	0.12	40,45,45,49	0

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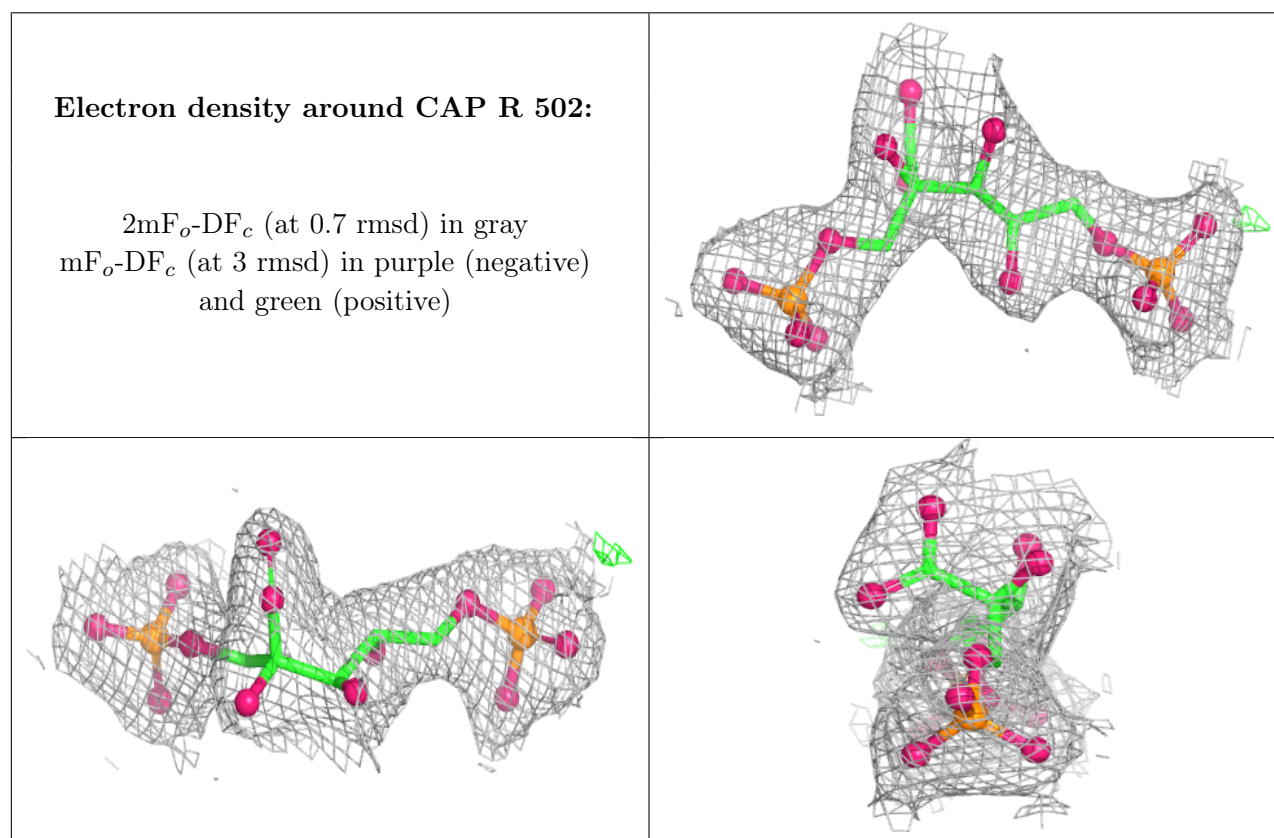
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	E	507	4/4	0.88	0.13	55,65,66,72	0
5	EDO	V	505	4/4	0.88	0.13	51,54,58,58	0
5	EDO	K	506	4/4	0.88	0.11	39,41,45,49	0
5	EDO	V	506	4/4	0.89	0.13	53,62,67,69	0
5	EDO	O	503	4/4	0.89	0.11	35,40,40,43	0
5	EDO	H	508	4/4	0.90	0.11	38,41,46,48	0
5	EDO	R	506	4/4	0.90	0.10	46,47,49,54	0
5	EDO	T	202	4/4	0.90	0.09	38,44,45,46	0
5	EDO	F	201	4/4	0.91	0.12	51,53,53,56	0
5	EDO	R	505	4/4	0.91	0.10	40,43,43,46	0
5	EDO	H	506	4/4	0.91	0.11	49,51,52,55	0
5	EDO	R	507	4/4	0.91	0.09	31,32,32,36	0
5	EDO	P	201	4/4	0.91	0.07	41,47,51,58	0
5	EDO	C	201	4/4	0.92	0.12	53,54,57,60	0
5	EDO	B	508	4/4	0.92	0.10	22,22,25,29	0
5	EDO	R	503	4/4	0.92	0.10	31,31,34,35	0
5	EDO	E	503	4/4	0.92	0.08	29,35,36,39	0
5	EDO	O	506	4/4	0.92	0.10	42,51,52,57	0
5	EDO	F	202	4/4	0.92	0.09	49,53,53,55	0
5	EDO	B	506	4/4	0.93	0.10	29,39,39,41	0
5	EDO	E	505	4/4	0.93	0.09	46,49,49,51	0
5	EDO	O	504	4/4	0.93	0.08	33,34,35,39	0
5	EDO	V	504	4/4	0.93	0.08	39,41,41,46	0
5	EDO	H	504	4/4	0.93	0.09	39,40,42,43	0
5	EDO	B	503	4/4	0.93	0.10	30,31,37,37	0
5	EDO	A	503	4/4	0.93	0.09	33,35,36,37	0
5	EDO	R	504	4/4	0.94	0.07	36,37,40,42	0
5	EDO	V	503	4/4	0.94	0.08	30,35,38,40	0
5	EDO	K	504	4/4	0.94	0.08	32,33,35,36	0
5	EDO	E	504	4/4	0.95	0.06	28,33,34,35	0
5	EDO	H	503	4/4	0.96	0.07	33,33,34,37	0
5	EDO	A	507	4/4	0.96	0.08	34,34,36,37	0
5	EDO	A	504	4/4	0.96	0.06	33,34,41,42	0
4	CAP	R	502	21/21	0.97	0.06	27,31,33,37	0
5	EDO	B	504	4/4	0.97	0.06	33,33,35,37	0
4	CAP	V	502	21/21	0.97	0.06	28,31,33,37	0
4	CAP	A	502	21/21	0.97	0.06	27,31,32,37	0
4	CAP	E	502	21/21	0.98	0.05	28,31,33,37	0
4	CAP	H	502	21/21	0.98	0.05	28,32,33,37	0
4	CAP	K	502	21/21	0.98	0.05	27,31,33,37	0
4	CAP	O	502	21/21	0.98	0.05	27,31,33,37	0
4	CAP	B	502	21/21	0.98	0.05	28,31,32,37	0

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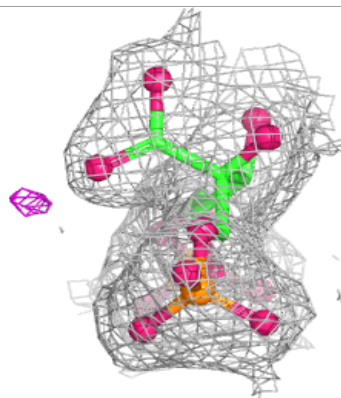
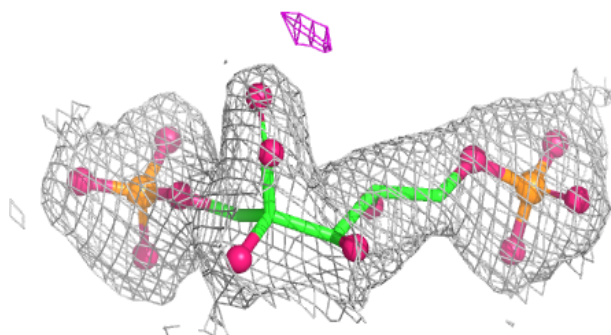
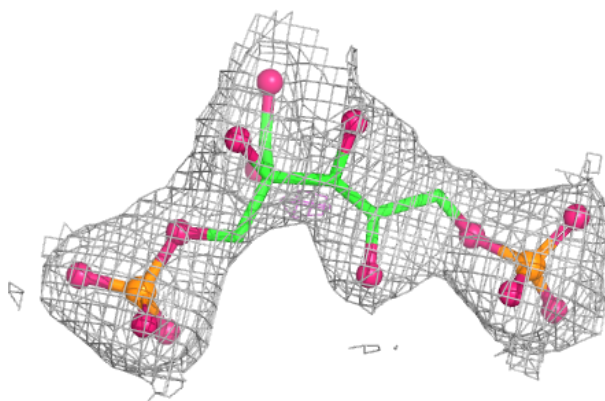
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	H	501	1/1	0.99	0.02	28,28,28,28	0
3	MG	K	501	1/1	0.99	0.02	27,27,27,27	0
3	MG	O	501	1/1	0.99	0.02	27,27,27,27	0
3	MG	R	501	1/1	0.99	0.02	28,28,28,28	0
3	MG	V	501	1/1	0.99	0.02	27,27,27,27	0
3	MG	A	501	1/1	0.99	0.03	27,27,27,27	0
3	MG	B	501	1/1	0.99	0.03	27,27,27,27	0
3	MG	E	501	1/1	0.99	0.06	27,27,27,27	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.

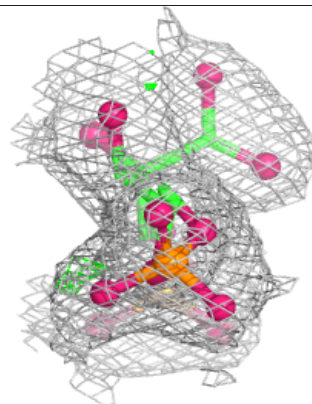
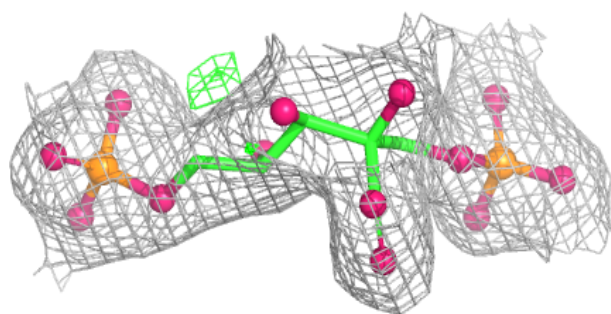
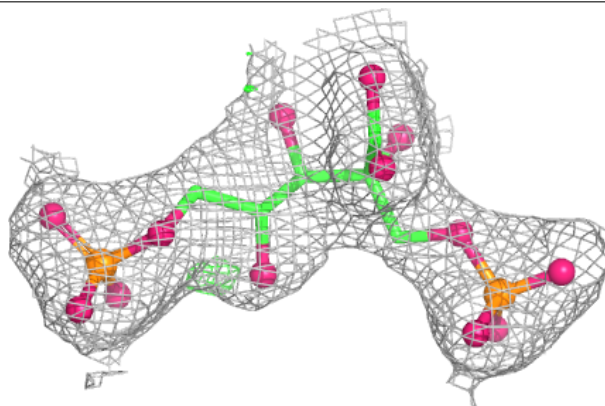


Electron density around CAP V 502:

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

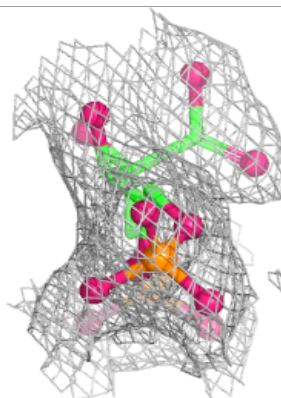
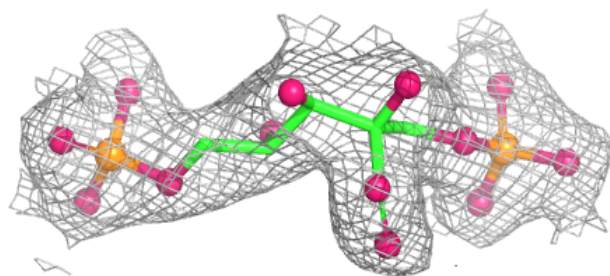
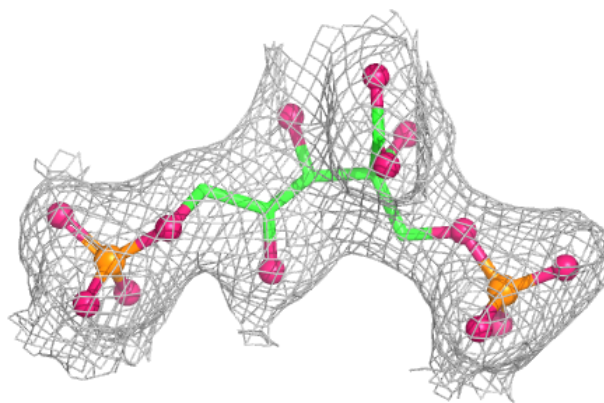
**Electron density around CAP A 502:**

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

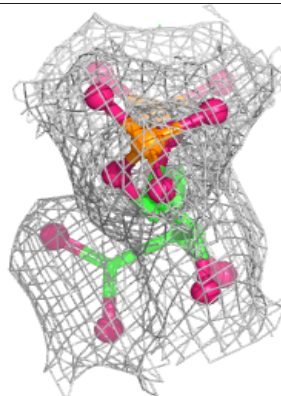
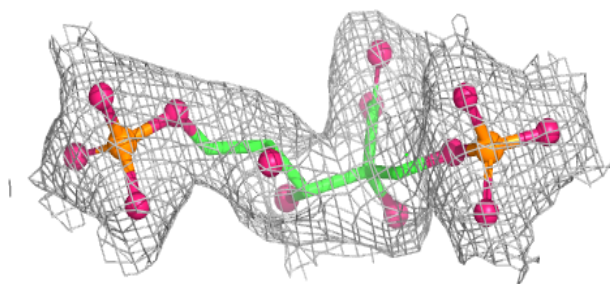
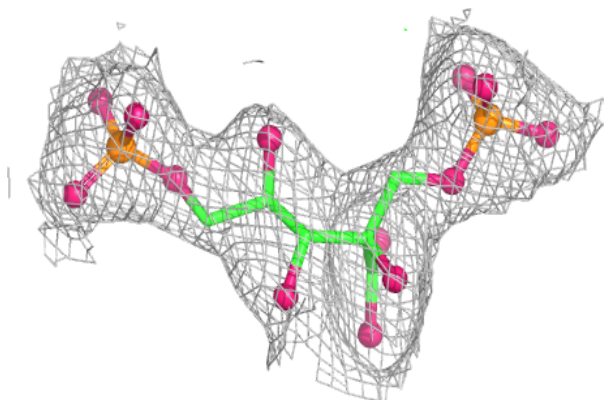


Electron density around CAP E 502:

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

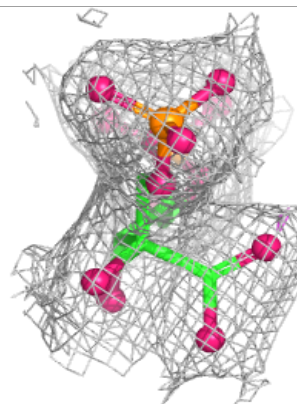
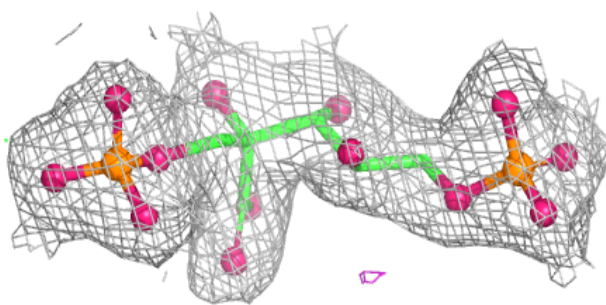
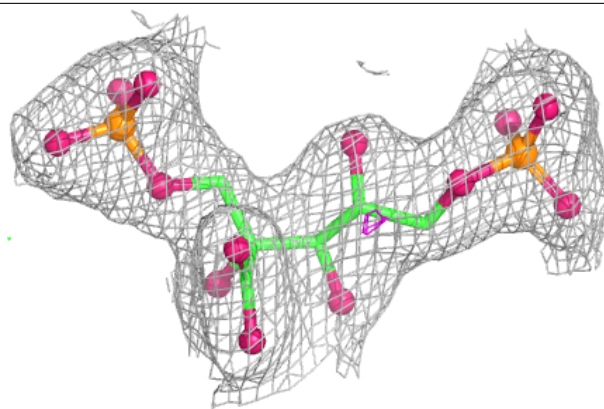
**Electron density around CAP H 502:**

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

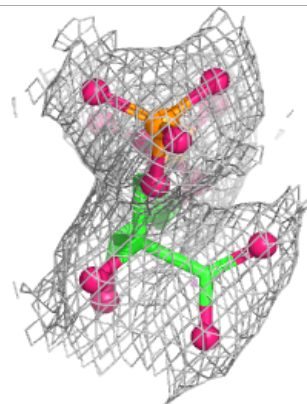
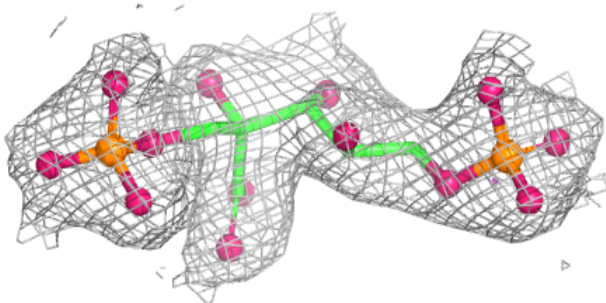
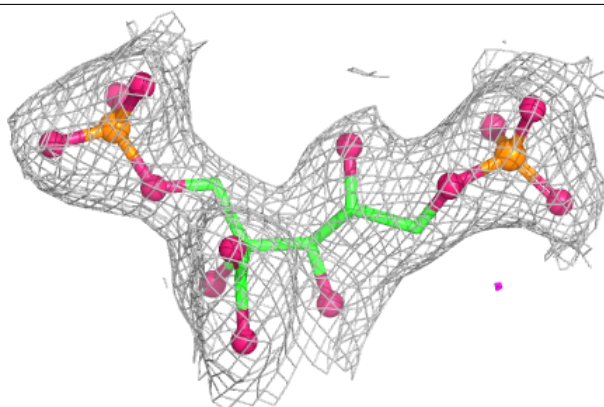


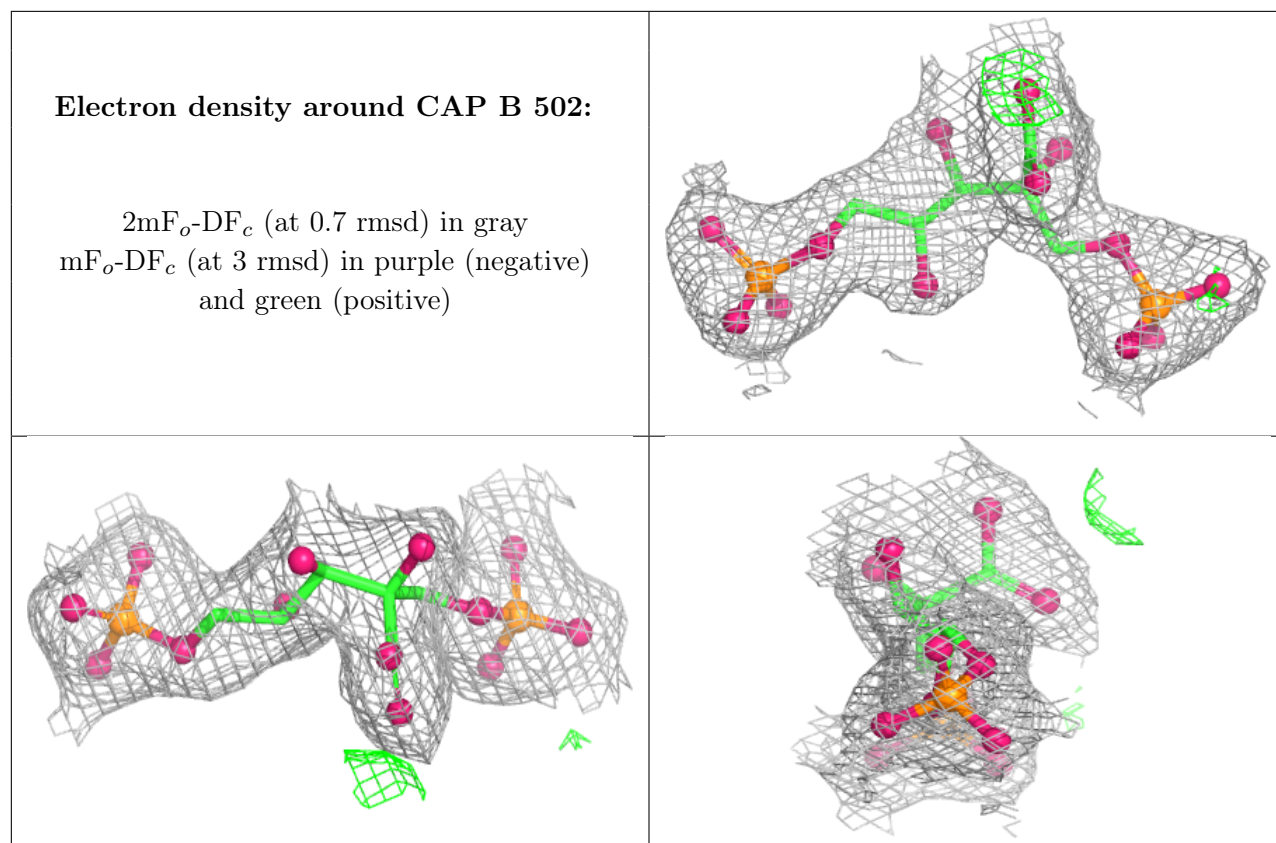
Electron density around CAP K 502:

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

**Electron density around CAP O 502:**

$2mF_o-DF_c$ (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.