WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 1, 2025 – 11:49 pm BST

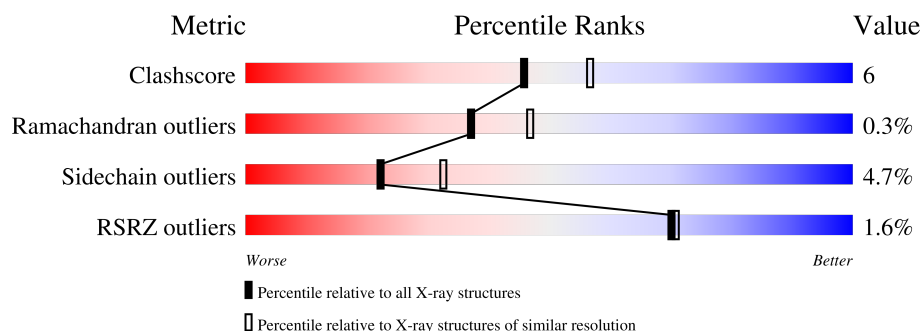|		
PDB ID	:	1UPM / pdb_00001upm
Title	:	ACTIVATED SPINACH RUBISCO COMPLEXED WITH 2-CARBOXYARABINITOL 2 BISPHOSPHAT AND CA2+.
Authors	:	Karkehabadi, S.; Taylor, T.C.; Andersson, I.
Deposited on	:	2003-10-08
Resolution	:	2.30 Å(reported)

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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	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		4.7%
RSRZ outliers		1.6%

Worse *Better*

▊ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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 <=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	B	475	.% 83% 13% ・・・
1	E	475	2% 81% 14% ・・・
1	H	475	.% 83% 13% ・・・
1	K	475	.% 84% 11% ・・
1	L	475	2% 83% 12% ・・・
1	O	475	.% 83% 13% ・・・

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Mol	Chain	Length	Quality of chain
1	R	475	2% 83% 13% •••
1	V	475	% 85% 11% •••
2	C	123	% 76% 18% 5% •
2	F	123	3% 80% 16% ••
2	I	123	80% 15% 5%
2	M	123	3% 79% 18% •
2	P	123	2% 85% 12% •
2	S	123	3% 81% 14% 5%
2	T	123	2% 81% 15% •
2	W	123	% 84% 13% ••

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 40436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	E	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	H	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	K	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	L	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	O	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	R	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			
1	V	467	Total	C	N	O	S	0	0	0
			3652	2316	640	678	18			

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

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

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

There are 56 discrepancies between the modelled and reference sequences:

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

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$).
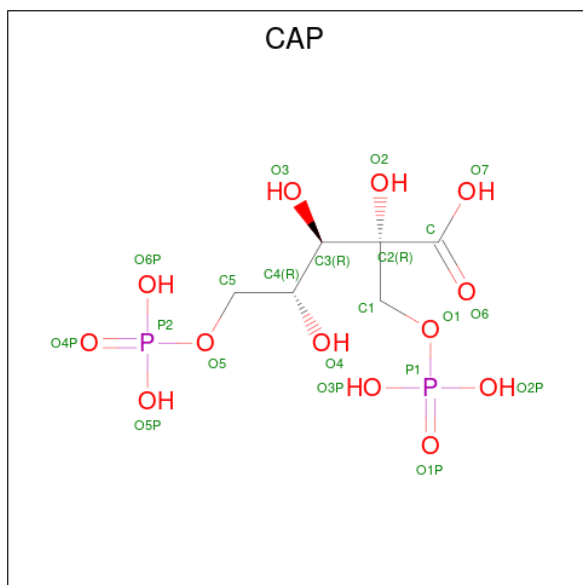
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 21	C 6	O 13	P 2	0	0
4	E	1	Total 21	C 6	O 13	P 2	0	0
4	H	1	Total 21	C 6	O 13	P 2	0	0
4	K	1	Total 21	C 6	O 13	P 2	0	0
4	L	1	Total 21	C 6	O 13	P 2	0	0
4	O	1	Total 21	C 6	O 13	P 2	0	0
4	R	1	Total 21	C 6	O 13	P 2	0	0
4	V	1	Total 21	C 6	O 13	P 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	263	Total 263	O 263	0	0
5	C	58	Total 58	O 58	0	0
5	E	297	Total 297	O 297	0	0
5	F	100	Total 100	O 100	0	0
5	H	246	Total 246	O 246	0	0
5	I	42	Total 42	O 42	0	0
5	K	278	Total 278	O 278	0	0
5	L	308	Total 308	O 308	0	0
5	M	91	Total 91	O 91	0	0
5	O	261	Total 261	O 261	0	0
5	P	54	Total 54	O 54	0	0
5	R	290	Total 290	O 290	0	0
5	S	93	Total 93	O 93	0	0
5	T	88	Total 88	O 88	0	0
5	V	274	Total 274	O 274	0	0
5	W	45	Total 45	O 45	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.
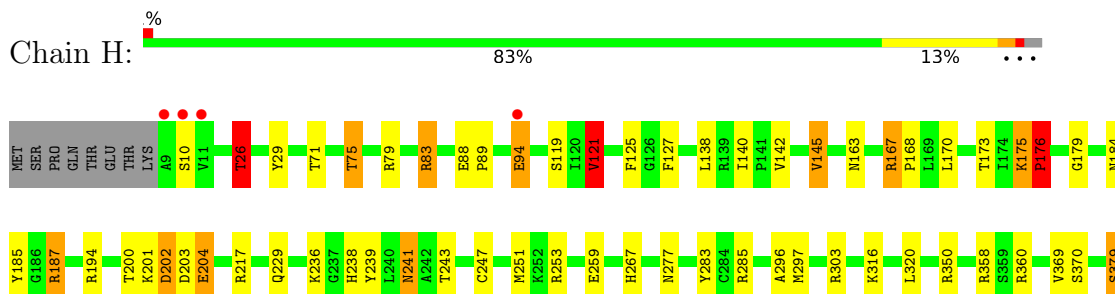
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

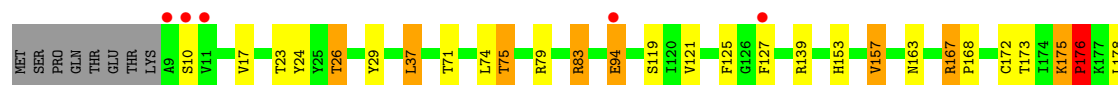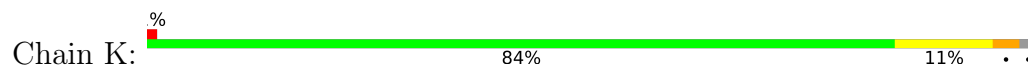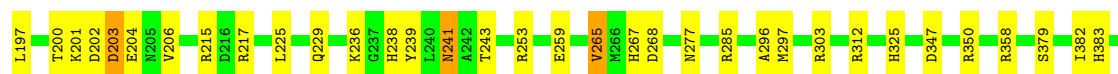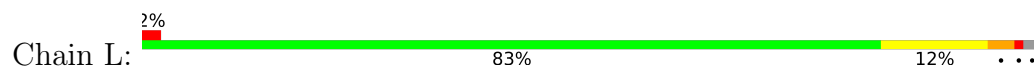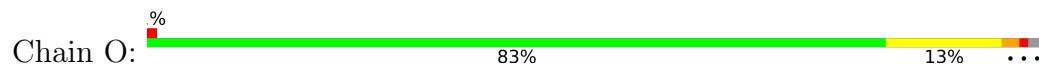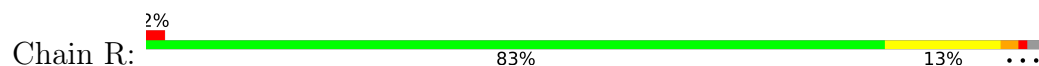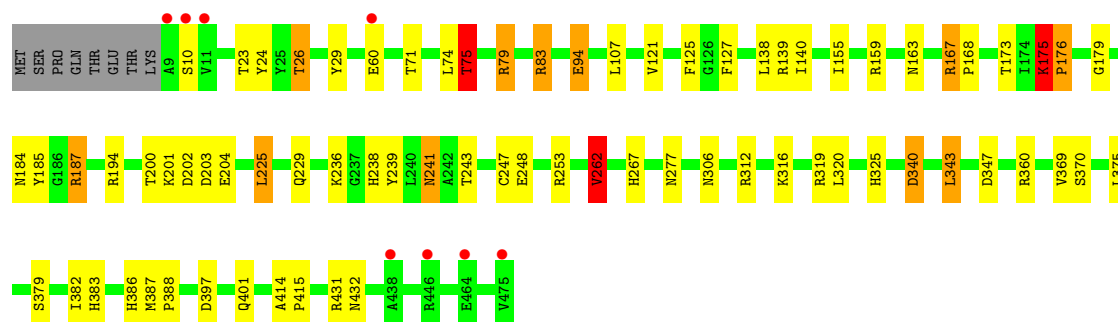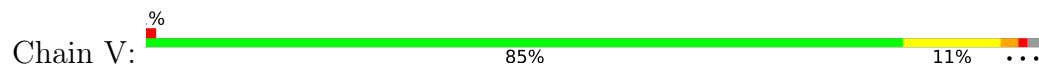• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

I382 H383 H386 M387 P388 Q401 H409 A414 P415 G416 R421 R431 N432 E464 V475

● Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain K:
%
84% 11% · ·

MET SER PRO GLN THR GLU THR LYS A9 S10 V11 V17 T23 Y24 Y25 T26 Y29 L37 T71 L74 T75 R79 R83 E94 S119 I120 V121 F125 G126 F127 R139 H153 V157 N163 R167 P168 C172 T173 I174 K175 P176 K177 L178

G179 N184 Y185 G186 R187 R194 T200 K201 D202 D203 E204 R215 L225 H238 N241 A242 T243 M251 K252 R253 E259 H267 N277 Y283 L290 R303 N306 R312 L343 D347 R350 S379 H383 H386 M387 P388 D397

L400 Q401 A414 P415 R431 N432 D473 T474 V475

● Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain L:
2%
83% 12% · · ·

MET SER PRO GLN THR GLU THR LYS A9 S10 V11 V17 T26 Y29 V42 T71 L74 T75 R79 R83 E88 P89 E94 F117 T118 S119 F127 R159 N163 K175 P176 G179 N184 Y185 G186 R187 A188 V189 C192 L193 R194

L197 T200 K201 D202 D203 E204 N205 V206 R215 D216 R217 L225 Q229 K236 G237 H238 Y239 L240 N241 A242 T243 R253 E259 V265 M266 H267 D268 N277 R285 A296 M297 R303 R312 H325 D347 R350 R358 S379 I382 H383

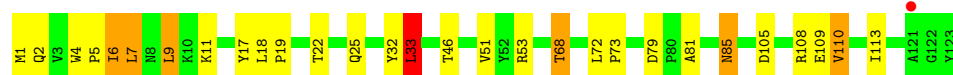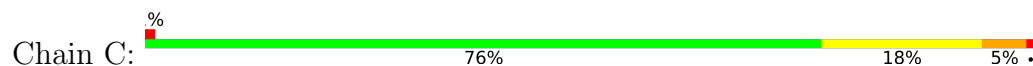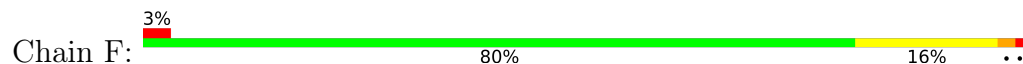H386 M387 P388 A389 L390 T391 E392 Q401 L407 A414 P415 R431 N432 D436 L437 A438 R439 R446 E460 E464 V475

● Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain O:
%
83% 13% · · ·

MET SER PRO GLN THR GLU THR LYS A9 S10 V11 V17 T26 Y29 I36 V69 W70 T71 T75 N76 R79 R83 E88 P89 E94 P104 L107 S119 F127 R134 L138 R139 I140 I155 N163 R167 P168 K175 P176

G179 N184 Y185 G186 R187 A188 V189 L193 R194 T200 K201 D202 D203 E204 R215 L225 H238 Y239 L240 N241 A242 T243 M251 K252 R253 R258 H267 N277 Y283 H292 R303 K316 L320 H325 D347 L348 L349 R350 R360 L375

S379 H383 H386 M387 P388 Q401 A414 P415 R421 R431 N432 R435 R439 R446 D473 T474 V475

● Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain R:
2%
83% 13% · · ·

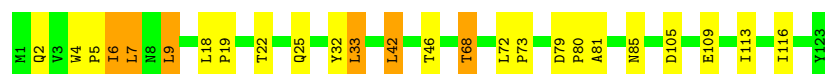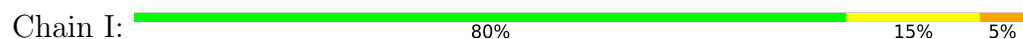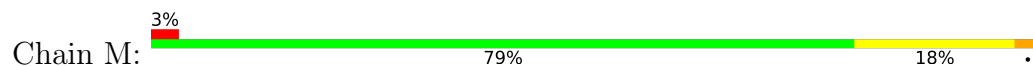• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain V:

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain C:

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain F:

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain I:

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain M:

● Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain P:

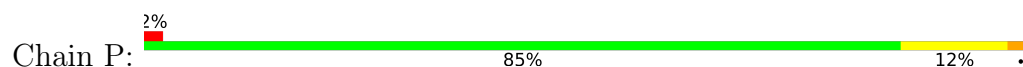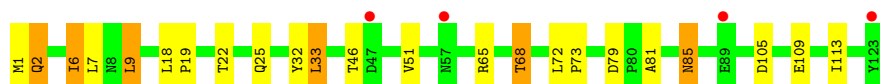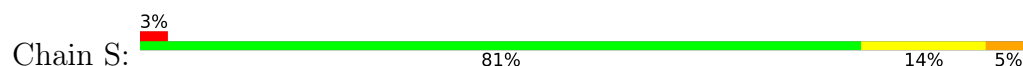● Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain S:

● Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain T:

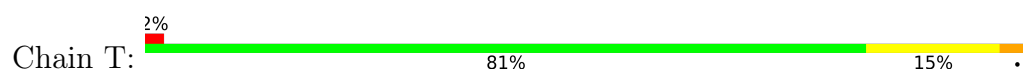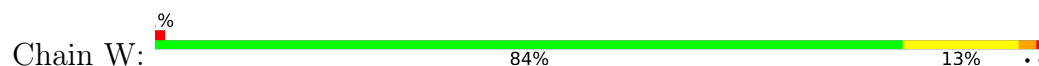● Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain W:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	219.60Å 220.94Å 116.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-2.30) 90.0 (20.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.80 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.200 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.871	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40436	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

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

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	H	0	1
1	K	0	1
1	L	0	1
1	O	0	1
1	R	0	1

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

All (2) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

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

5.2   Too-close contacts   ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3652	0	3560	40	1
1	E	3652	0	3560	44	0
1	H	3652	0	3560	40	0
1	K	3652	0	3560	37	0

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

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

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

The worst 5 of 420 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:473:ASP:OD2	5:K:2273:HOH:O	1.71	1.08
2:C:22:THR:H	2:C:25:GLN:HE21	1.14	0.95
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.14	0.94
1:K:267:HIS:HD2	1:K:277:ASN:HD22	1.15	0.93
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.16	0.92

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLU:OE1	1:O:439:ARG:NH1[4_456]	2.13	0.07

5.3 Torsion angles ⓘ

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	B	464/475 (98%)	440 (95%)	22 (5%)	2 (0%)	30	39
1	E	464/475 (98%)	438 (94%)	24 (5%)	2 (0%)	30	39
1	H	464/475 (98%)	445 (96%)	17 (4%)	2 (0%)	30	39
1	K	464/475 (98%)	443 (96%)	18 (4%)	3 (1%)	22	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	464/475 (98%)	444 (96%)	18 (4%)	2 (0%)	30	39
1	O	464/475 (98%)	442 (95%)	20 (4%)	2 (0%)	30	39
1	R	464/475 (98%)	442 (95%)	21 (4%)	1 (0%)	44	55
1	V	464/475 (98%)	441 (95%)	21 (4%)	2 (0%)	30	39
2	C	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	F	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	I	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	M	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	P	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	S	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	T	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	W	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
All	All	4680/4784 (98%)	4454 (95%)	210 (4%)	16 (0%)	37	47

5 of 16 Ramachandran outliers are listed below:

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

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	377/386 (98%)	360 (96%)	17 (4%)	23	34
1	E	377/386 (98%)	362 (96%)	15 (4%)	27	40
1	H	377/386 (98%)	362 (96%)	15 (4%)	27	40
1	K	377/386 (98%)	361 (96%)	16 (4%)	25	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	377/386 (98%)	358 (95%)	19 (5%)	20	30
1	O	377/386 (98%)	359 (95%)	18 (5%)	21	32
1	R	377/386 (98%)	364 (97%)	13 (3%)	32	47
1	V	377/386 (98%)	364 (97%)	13 (3%)	32	47
2	C	112/112 (100%)	104 (93%)	8 (7%)	12	17
2	F	112/112 (100%)	105 (94%)	7 (6%)	15	21
2	I	112/112 (100%)	105 (94%)	7 (6%)	15	21
2	M	112/112 (100%)	104 (93%)	8 (7%)	12	17
2	P	112/112 (100%)	107 (96%)	5 (4%)	23	34
2	S	112/112 (100%)	105 (94%)	7 (6%)	15	21
2	T	112/112 (100%)	104 (93%)	8 (7%)	12	17
2	W	112/112 (100%)	105 (94%)	7 (6%)	15	21
All	All	3912/3984 (98%)	3729 (95%)	183 (5%)	22	32

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

Mol	Chain	Res	Type
1	O	75	THR
1	R	225	LEU
1	O	119	SER
2	P	6	ILE
2	S	9	LEU

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

Mol	Chain	Res	Type
1	R	304	GLN
2	W	29	GLN
1	R	442	ASN
1	V	184	ASN
1	H	304	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	KCX	V	201	1,3	9,11,12	0.96	1 (11%)	5,12,14	2.18	2 (40%)
1	KCX	B	201	1,3	9,11,12	0.94	1 (11%)	5,12,14	1.67	2 (40%)
1	KCX	R	201	1,3	9,11,12	1.01	1 (11%)	5,12,14	0.96	0
1	KCX	O	201	1,3	9,11,12	0.97	1 (11%)	5,12,14	2.05	2 (40%)
1	KCX	L	201	1,3	9,11,12	1.11	1 (11%)	5,12,14	1.14	1 (20%)
1	KCX	K	201	1,3	9,11,12	0.92	1 (11%)	5,12,14	1.50	2 (40%)
1	KCX	H	201	1,3	9,11,12	1.06	1 (11%)	5,12,14	2.03	2 (40%)
1	KCX	E	201	1,3	9,11,12	0.91	1 (11%)	5,12,14	1.65	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	V	201	1,3	-	0/9/10/12	-
1	KCX	B	201	1,3	-	1/9/10/12	-
1	KCX	R	201	1,3	-	0/9/10/12	-
1	KCX	O	201	1,3	-	0/9/10/12	-
1	KCX	L	201	1,3	-	0/9/10/12	-
1	KCX	K	201	1,3	-	0/9/10/12	-
1	KCX	H	201	1,3	-	0/9/10/12	-
1	KCX	E	201	1,3	-	0/9/10/12	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	201	KCX	OQ1-CX	2.87	1.27	1.21
1	L	201	KCX	OQ1-CX	2.62	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	201	KCX	OQ1-CX	2.61	1.26	1.21
1	B	201	KCX	OQ1-CX	2.57	1.26	1.21
1	O	201	KCX	OQ1-CX	2.50	1.26	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	201	KCX	CE-NZ-CX	3.91	128.17	121.89
1	H	201	KCX	OQ1-CX-NZ	3.55	130.46	124.96
1	O	201	KCX	OQ1-CX-NZ	3.36	130.17	124.96
1	O	201	KCX	CE-NZ-CX	3.06	126.80	121.89
1	E	201	KCX	OQ1-CX-NZ	2.97	129.56	124.96

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	CAP	E	477	3	17,20,20	1.76	6 (35%)	22,31,31	1.94	7 (31%)
4	CAP	V	477	3	17,20,20	1.74	5 (29%)	22,31,31	2.02	7 (31%)
4	CAP	R	477	3	17,20,20	1.69	5 (29%)	22,31,31	1.96	8 (36%)
4	CAP	O	477	3	17,20,20	1.86	6 (35%)	22,31,31	1.96	9 (40%)
4	CAP	B	477	3	17,20,20	1.85	6 (35%)	22,31,31	2.09	6 (27%)
4	CAP	K	477	3	17,20,20	1.89	8 (47%)	22,31,31	2.18	9 (40%)
4	CAP	L	477	3	17,20,20	2.02	7 (41%)	22,31,31	2.03	8 (36%)
4	CAP	H	477	3	17,20,20	1.76	4 (23%)	22,31,31	1.99	9 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	E	477	3	-	10/29/29/29	-
4	CAP	V	477	3	-	10/29/29/29	-
4	CAP	R	477	3	-	11/29/29/29	-
4	CAP	O	477	3	-	10/29/29/29	-
4	CAP	B	477	3	-	10/29/29/29	-
4	CAP	K	477	3	-	9/29/29/29	-
4	CAP	L	477	3	-	11/29/29/29	-
4	CAP	H	477	3	-	10/29/29/29	-

The worst 5 of 47 bond length outliers are listed below:

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

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	477	CAP	O3-C3-C4	-4.97	98.48	109.13
4	L	477	CAP	P2-O5-C5	4.56	130.86	118.30

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

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	477	CAP	O6-C-C2-C3
4	B	477	CAP	O6-C-C2-O2
4	B	477	CAP	C2-C3-C4-O4
4	B	477	CAP	O3-C3-C4-O4
4	E	477	CAP	O6-C-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand CAP E 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP V 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP R 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP O 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP B 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP K 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP L 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP H 477

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	B	466/475 (98%)	-0.41	6 (1%)	74	75	13, 22, 42, 105	0
1	E	466/475 (98%)	-0.40	10 (2%)	63	64	13, 22, 42, 105	0
1	H	466/475 (98%)	-0.37	6 (1%)	74	75	14, 22, 42, 105	0
1	K	466/475 (98%)	-0.36	6 (1%)	74	75	13, 22, 42, 105	0
1	L	466/475 (98%)	-0.38	10 (2%)	63	64	13, 22, 42, 105	0
1	O	466/475 (98%)	-0.35	5 (1%)	77	78	13, 22, 42, 105	0
1	R	466/475 (98%)	-0.39	8 (1%)	69	69	13, 22, 42, 105	0
1	V	466/475 (98%)	-0.37	6 (1%)	74	75	13, 22, 42, 105	0
2	C	123/123 (100%)	-0.02	1 (0%)	82	83	19, 32, 51, 66	0
2	F	123/123 (100%)	0.10	4 (3%)	49	51	18, 32, 51, 66	0
2	I	123/123 (100%)	0.16	0	100	100	19, 32, 51, 66	0
2	M	123/123 (100%)	0.01	4 (3%)	49	51	18, 32, 51, 66	0
2	P	123/123 (100%)	0.05	2 (1%)	70	71	19, 32, 51, 66	0
2	S	123/123 (100%)	0.12	4 (3%)	49	51	18, 32, 51, 66	0
2	T	123/123 (100%)	-0.00	3 (2%)	59	61	18, 32, 51, 66	0
2	W	123/123 (100%)	-0.05	1 (0%)	82	83	19, 32, 51, 66	0
All	All	4712/4784 (98%)	-0.29	76 (1%)	70	71	13, 23, 48, 105	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	9	ALA	6.1
1	L	9	ALA	5.9
1	O	9	ALA	5.9
1	L	10	SER	5.2
1	V	9	ALA	5.0

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.
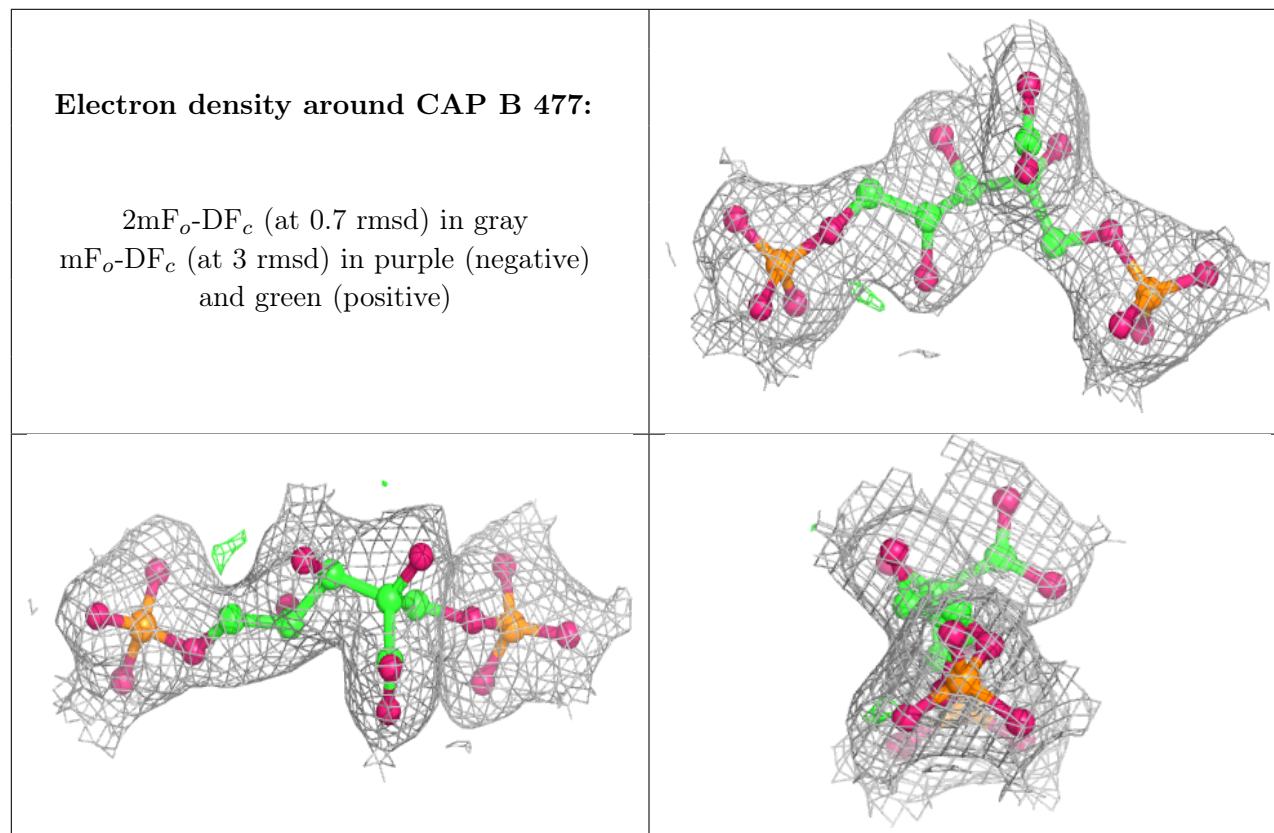
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	O	201	12/13	0.92	0.09	17,18,24,24	0
1	KCX	H	201	12/13	0.93	0.08	17,18,24,24	0
1	KCX	B	201	12/13	0.94	0.08	17,18,24,24	0
1	KCX	R	201	12/13	0.94	0.07	17,18,24,24	0
1	KCX	L	201	12/13	0.95	0.07	17,18,23,24	0
1	KCX	E	201	12/13	0.95	0.07	17,18,23,23	0
1	KCX	K	201	12/13	0.95	0.07	17,18,23,24	0
1	KCX	V	201	12/13	0.96	0.05	17,18,23,24	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	CA	K	476	1/1	0.94	0.06	42,42,42,42	0
3	CA	H	476	1/1	0.95	0.05	42,42,42,42	0
3	CA	B	476	1/1	0.95	0.06	42,42,42,42	0
3	CA	R	476	1/1	0.95	0.05	41,41,41,41	0
3	CA	V	476	1/1	0.95	0.11	42,42,42,42	0
3	CA	O	476	1/1	0.97	0.06	43,43,43,43	0
4	CAP	B	477	21/21	0.97	0.06	17,22,26,27	0
4	CAP	H	477	21/21	0.97	0.06	17,21,26,26	0
4	CAP	K	477	21/21	0.97	0.07	16,21,26,27	0
4	CAP	O	477	21/21	0.97	0.07	16,21,26,27	0
4	CAP	V	477	21/21	0.97	0.07	16,21,26,27	0
3	CA	L	476	1/1	0.98	0.06	42,42,42,42	0
4	CAP	L	477	21/21	0.98	0.06	16,21,26,26	0
4	CAP	E	477	21/21	0.98	0.06	16,21,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CAP	R	477	21/21	0.98	0.05	16,21,26,26	0
3	CA	E	476	1/1	0.98	0.04	42,42,42,42	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 B 477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
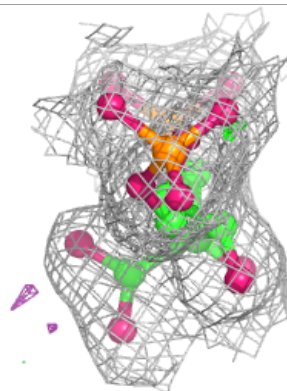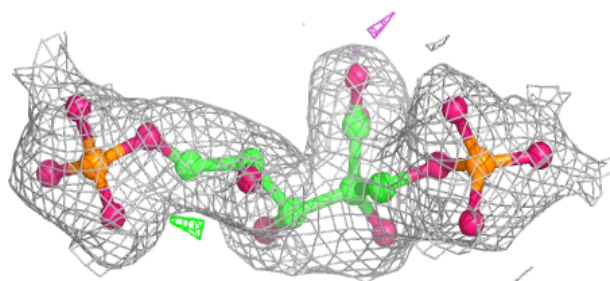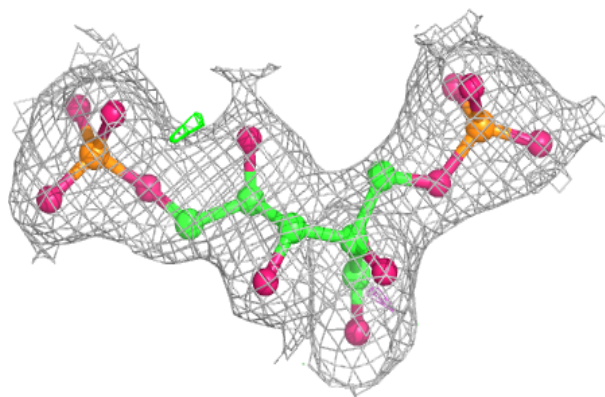
Electron density around CAP H 477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
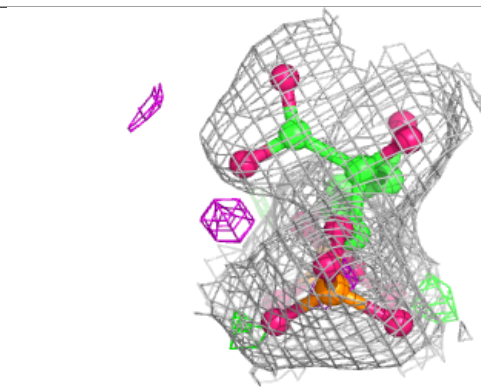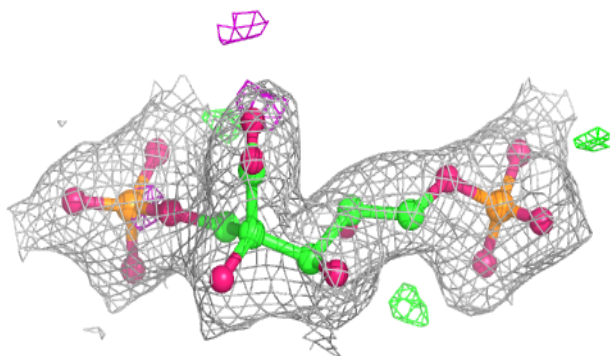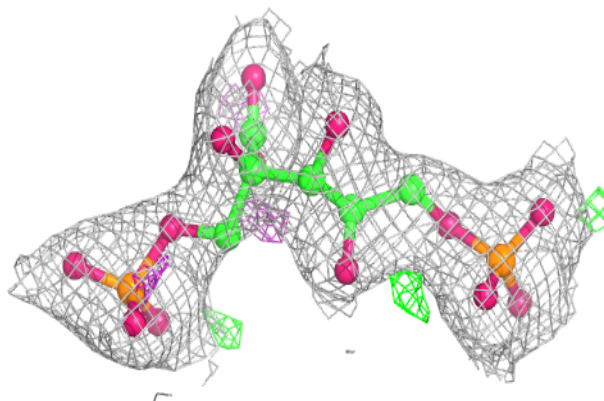
Electron density around CAP K 477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
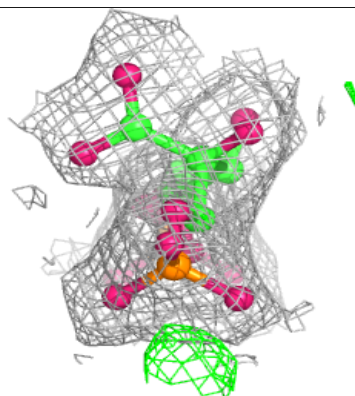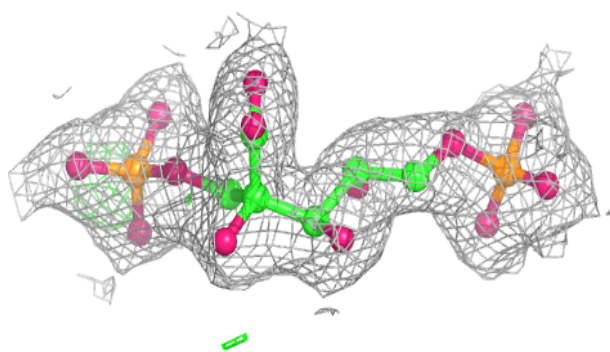mF_o-DF_c (at 3 rmsd) in purple (negative)
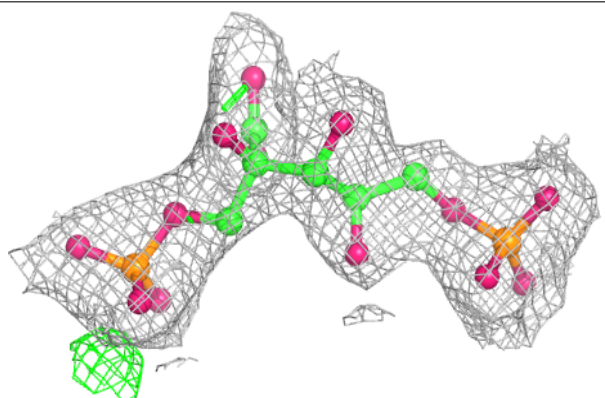and green (positive)
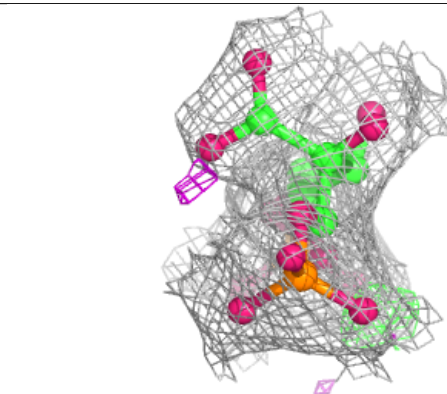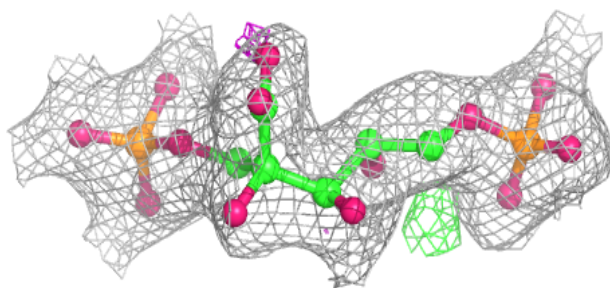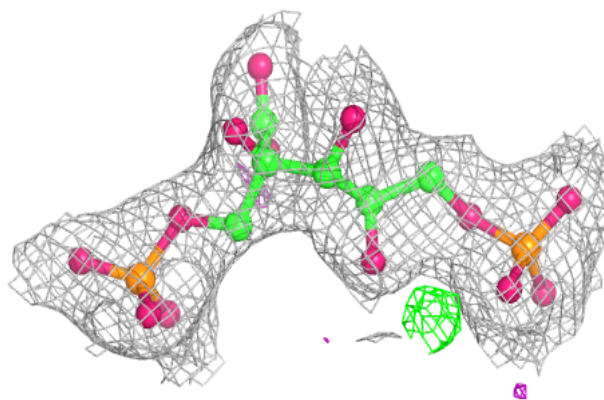
Electron density around CAP O 477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
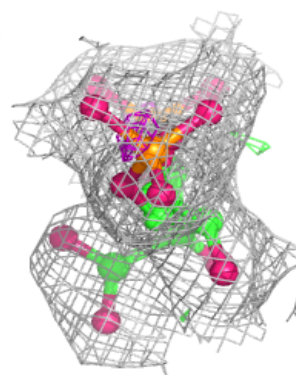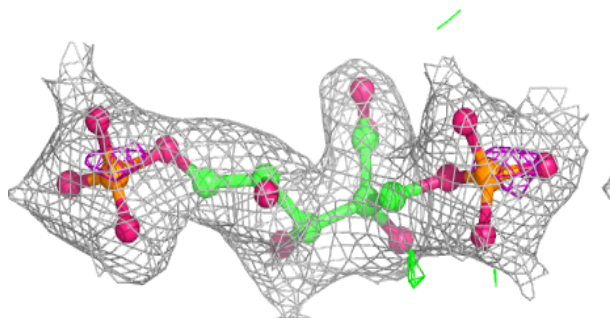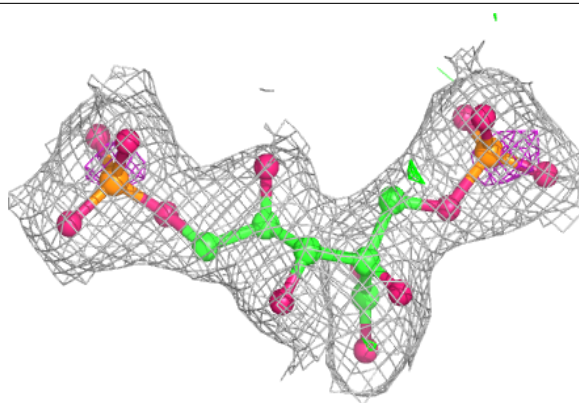
Electron density around CAP V 477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
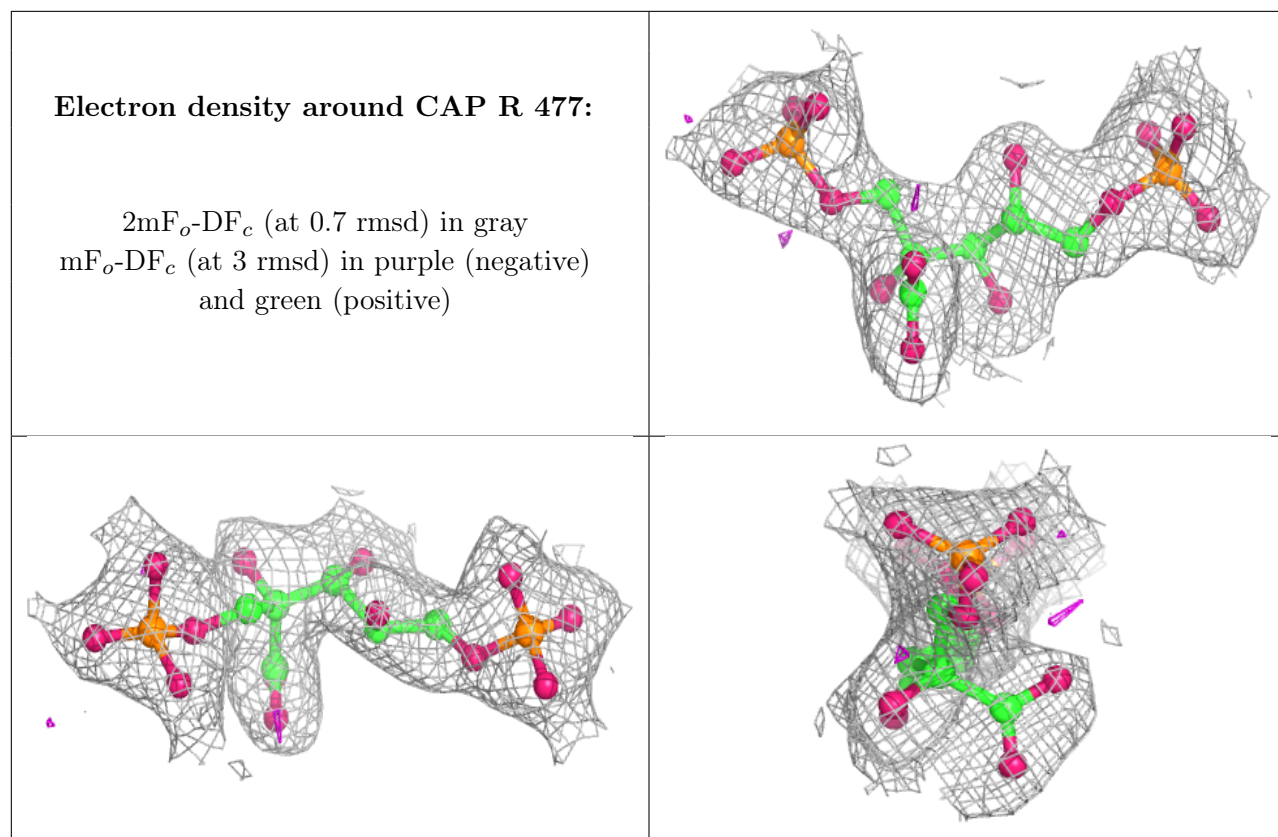mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
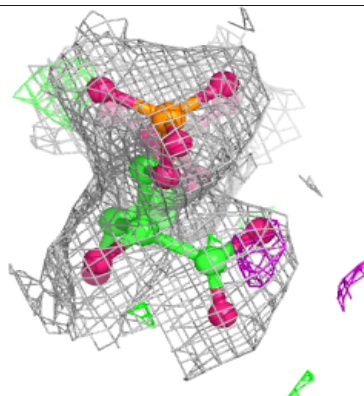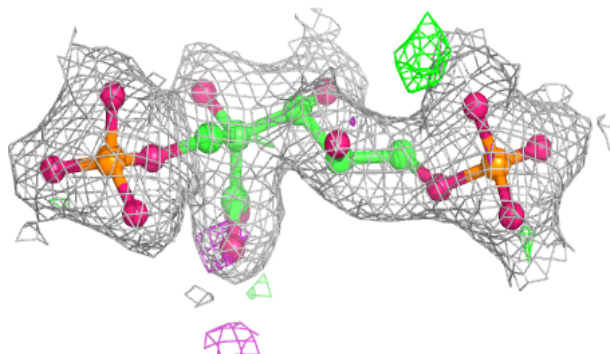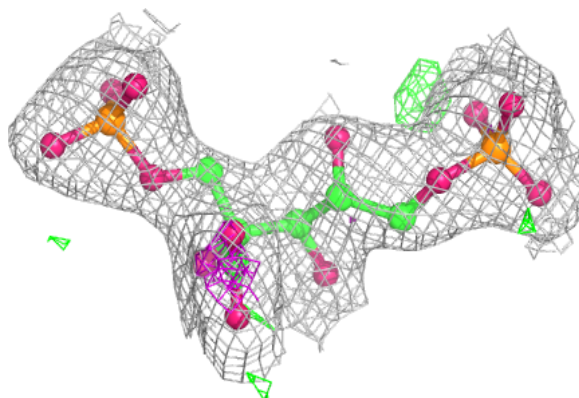
Electron density around CAP L 477:

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

Electron density around CAP E 477:

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

Electron density around CAP R 477:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.