wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 12:01 am BST

PDB ID	:	1UPP
Title	:	SPINACH RUBISCO IN COMPLEX WITH 2-CARBOXYARABINITOL 2 BISPHOSPHATE and Calcium.
Authors	:	Karkehabadi, S.; Taylor, T.C.; Andersson, I.
Deposited on	:	2003-10-09
Resolution	:	2.30 Å(reported)

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

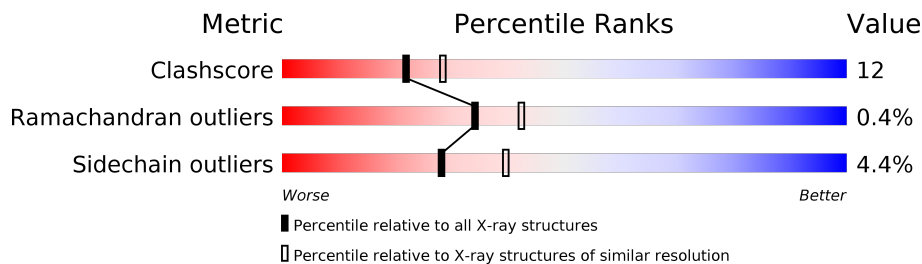|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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		12
Ramachandran outliers		0.4%
Sidechain outliers		4.4%

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	475	63% ... 30% · · ·
1	C	475	66% ... 28% · ·
1	E	475	66% ... 28% · · ·
1	G	475	67% ... 26% · ·
2	I	123	64% ... 31% · ·
2	J	123	61% ... 33% 6%
2	K	123	60% ... 36% · ·
2	L	123	59% ... 36% 5% ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19504 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	467	Total 3656	C 2319	N 640	O 679	S 18	0	0	0
1	C	467	Total 3656	C 2319	N 640	O 679	S 18	0	0	0
1	E	467	Total 3656	C 2319	N 640	O 679	S 18	0	0	0
1	G	467	Total 3656	C 2319	N 640	O 679	S 18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	123	Total 1032	C 673	N 167	O 185	S 7	0	0	0
2	J	123	Total 1032	C 673	N 167	O 185	S 7	0	0	0
2	K	123	Total 1032	C 673	N 167	O 185	S 7	0	0	0
2	L	123	Total 1032	C 673	N 167	O 185	S 7	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	2	GLN	LYS	conflict	UNP Q43832
J	6	ILE	THR	conflict	UNP Q43832
J	7	LEU	GLN	conflict	UNP Q43832
J	9	LEU	MET	conflict	UNP Q43832
J	11	LYS	ARG	conflict	UNP Q43832
J	109	GLU	GLN	conflict	UNP Q43832
J	113	ILE	VAL	conflict	UNP Q43832
K	2	GLN	LYS	conflict	UNP Q43832
K	6	ILE	THR	conflict	UNP Q43832
K	7	LEU	GLN	conflict	UNP Q43832
K	9	LEU	MET	conflict	UNP Q43832
K	11	LYS	ARG	conflict	UNP Q43832
K	109	GLU	GLN	conflict	UNP Q43832
K	113	ILE	VAL	conflict	UNP Q43832
L	2	GLN	LYS	conflict	UNP Q43832
L	6	ILE	THR	conflict	UNP Q43832
L	7	LEU	GLN	conflict	UNP Q43832
L	9	LEU	MET	conflict	UNP Q43832
L	11	LYS	ARG	conflict	UNP Q43832
L	109	GLU	GLN	conflict	UNP Q43832
L	113	ILE	VAL	conflict	UNP Q43832

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).
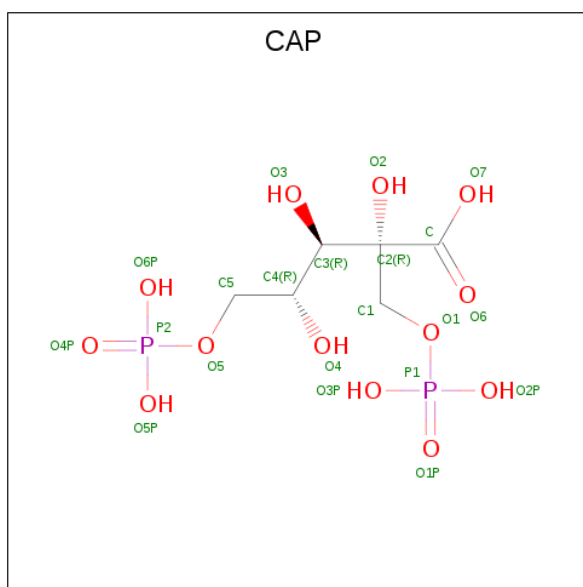
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 21	C 6	O 13	P 2	0	0
4	C	1	Total 21	C 6	O 13	P 2	0	0
4	E	1	Total 21	C 6	O 13	P 2	0	0
4	G	1	Total 21	C 6	O 13	P 2	0	0

- Molecule 5 is water.

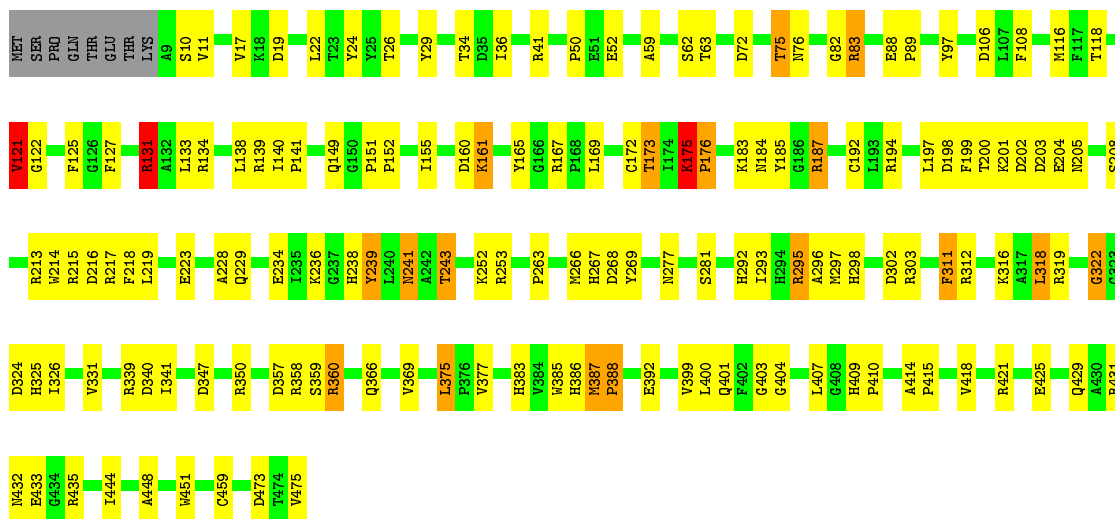| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total 112	O 112	0	0
5	C	121	Total 121	O 121	0	0
5	E	132	Total 132	O 132	0	0
5	G	133	Total 133	O 133	0	0
5	I	34	Total 34	O 34	0	0
5	J	44	Total 44	O 44	0	0
5	K	41	Total 41	O 41	0	0
5	L	47	Total 47	O 47	0	0

3 Residue-property plots ⓘ

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

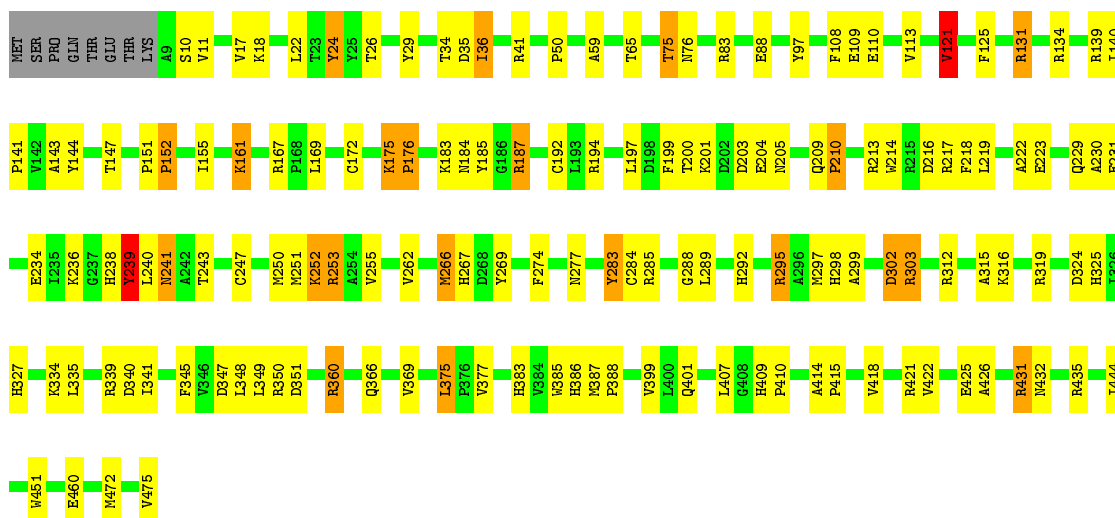- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain A:

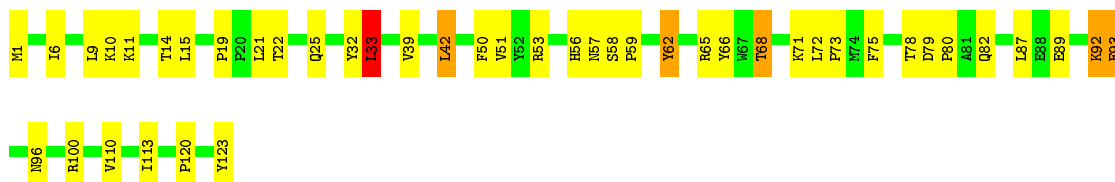- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain C:

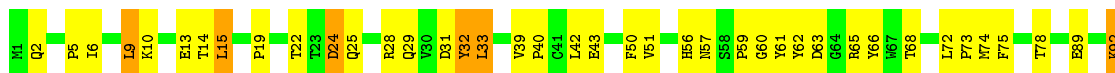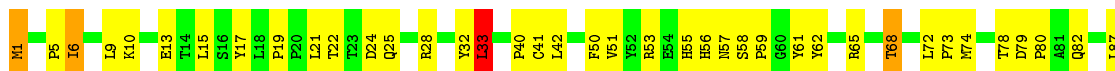- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain E:

66%　　　　28%

MET SER PRO THR GLU THR LYS A9 S10 V11 V17 K18 D19 L22 T23 Y24 Y25 T26 Y29 T34 D35 I36 R41 P50 E51 E52 A59 S62 T63 D72 T75 N76 G82 R83 E88 P89 Y97 D106 L107 F108 M116 F117 T118

V121 G122 F125 G126 F127 R131 A132 L133 R134 L138 R139 I140 P141 Q149 G150 P151 P152 I155 D160 K161 Y165 G166 R167 P168 L169 C172 T173 I174 K175 P176 K183 N184 Y185 G186 R187 C192 L193 R194 L197 D198 F199 T200 K201 D202 D203 E204 N205 S208

R213 W214 R215 D216 R217 F218 L219 E223 A228 Q229 E234 I235 K236 G237 H238 Y239 L240 N241 A242 T243 K252 R253 P263 M266 H267 D268 Y269 N277 S281 H292 I293 R294 A296 M297 H298 D302 R303 F311 R312 K316 A317 L318 R319 G322 G323

D324 H325 I326 V331 R339 D340 I341 D347 R350 D357 R358 S359 R360 Q366 V369 L375 P376 V377 H383 V384 W385 H386 M387 P388 E392 V399 L400 Q401 F402 G403 G404 L407 G408 H409 P410 A414 P415 V418 R421 E425 Q429 A430 R431

N432 E433 G434 R435 I444 A448 W451 C459 D473 T474 V475

• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain G:

67%　　　　26%

MET SER PRO THR GLU THR LYS A9 S10 V11 V17 K18 L22 T23 Y24 Y25 T26 Y29 T34 D35 I36 R41 P50 A59 T65 T75 N76 R83 E88 Y97 F108 E109 E110 V113 V121 F125 R131 R134 R139 I140

P141 V142 A143 Y144 T147 P151 P152 I155 K161 R167 P168 L169 C172 K175 P176 K183 N184 Y185 G186 R187 C192 L193 R194 L197 D198 F199 T200 K201 D202 D203 E204 N205 Q209 P210 R213 W214 R215 D216 R217 F218 L219 A222 E223 Q229 A230 E231

E234 I235 K236 G237 H238 Y239 L240 N241 A242 T243 C247 M250 M251 K252 R253 A254 V255 V262 M266 H267 D268 Y269 F274 N277 Y283 C284 R285 G288 L289 H292 R295 A296 M297 H298 A299 D302 R303 R312 A315 K316 R319 D324 H325 I326

H327 K334 L335 R339 D340 I341 F345 V346 D347 L348 I349 R350 D351 R360 Q366 V369 L375 P376 V377 H383 V384 W385 H386 M387 P388 V399 L400 Q401 L407 G408 H409 P410 A414 P415 V418 R421 V422 E425 A426 R431 N432 R435 I444

W451 E460 M472 V475

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain I:

64%　　　　31%

M1 I6 L9 K10 K11 T14 L15 P19 P20 L21 T22 Q25 Y32 L33 V39 L42 F50 V51 Y52 R53 H56 N57 S58 P59 Y62 R65 Y66 W67 T68 K71 L72 P73 M74 F75 T78 D79 P80 A81 Q82 L87 E88 E89 K92 E93

N96 R100 V110 I113 P120 Y123

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain J:

61%　　　　33%　　6%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

M1 Q2 P5 I6 L9 K10 E13 T14 L15 P19 T22 T23 D24 Q25 R28 Q29 V30 D31 Y32 L33 V39 P40 C41 L42 E43 F50 V51 H56 N57 S58 P59 G60 Y61 Y62 D63 G64 R65 Y66 W67 T68 L72 P73 M74 F75 T78 E89 K92

E93 R100 E109 V110 Q111 C112 I113 P120 Y123

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain K: 60% 36% • •

M1 P5 I6 L9 K10 E13 T14 L15 P19 T22 Q25 D31 Y32 L33 L42 F50 V51 Y52 R53 H56 N57 S58 P59 G60 Y61 Y62 Y66 W67 T68 K71 L72 P73 T78 D79 P80 A81 Q82 E86 L87 E88 E89 K92 E93 I99

R100 F104 D105 S106 N107 R108 E109 V110 I113 I118 Y118 K119 P120 Y123

• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain L: 59% 36% 5% •

M1 P5 I6 L9 K10 E13 T14 L15 S16 Y17 L18 P19 P20 L21 T22 T23 D24 Q25 R28 Y32 L33 P40 C41 L42 F50 V51 Y52 R53 E54 H55 H56 N57 S58 P59 G60 Y61 Y62 R65 T68 L72 P73 M74 T78 D79 P80 A81 Q82 L87

E88 E89 K92 E93 R100 I101 I102 N107 V110 I113 K119 P120 A121 G122 Y123

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	155.88Å 156.25Å 199.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 78.12 – 2.09	Depositor EDS
% Data completeness (in resolution range)	76.1 (100.00-2.30) 75.8 (78.12-2.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.307 0.254 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å²)	18.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 17.9	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.459 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19504	wwPDB-VP
Average B, all atoms (Å²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5694e-04.*

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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	A	0.87	1/3733 (0.0%)	1.75	75/5064 (1.5%)
1	C	0.84	2/3733 (0.1%)	1.84	77/5064 (1.5%)
1	E	0.86	0/3733	1.79	78/5064 (1.5%)
1	G	0.84	0/3733	1.70	69/5064 (1.4%)
2	I	0.69	0/1067	1.49	10/1453 (0.7%)
2	J	0.70	0/1067	1.53	21/1453 (1.4%)
2	K	0.66	0/1067	1.49	11/1453 (0.8%)
2	L	0.68	0/1067	1.45	8/1453 (0.6%)
All	All	0.82	3/19200 (0.0%)	1.71	349/26068 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	E	0	2
1	G	0	3
2	I	0	1
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176	PRO	N-CD	7.58	1.58	1.47
1	C	181	SER	CB-OG	5.80	1.49	1.42
1	A	43	SER	CB-OG	5.35	1.49	1.42

The worst 5 of 349 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	312	ARG	NE-CZ-NH1	19.65	130.12	120.30
1	C	312	ARG	NE-CZ-NH2	-17.11	111.75	120.30
2	K	100	ARG	NE-CZ-NH2	-16.34	112.13	120.30
1	C	176	PRO	CA-N-CD	-16.10	88.96	111.50
1	C	303	ARG	NE-CZ-NH1	15.75	128.18	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	LYS	Peptide
1	A	330	THR	Mainchain
1	C	175	LYS	Mainchain
1	E	175	LYS	Peptide
1	E	243	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3656	0	3565	94	0
1	C	3656	0	3565	80	0
1	E	3656	0	3564	76	0
1	G	3656	0	3564	79	0
2	I	1032	0	990	35	0
2	J	1032	0	990	32	0
2	K	1032	0	990	36	0
2	L	1032	0	990	38	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	21	0	7	0	0
4	C	21	0	6	1	0
4	E	21	0	7	0	0
4	G	21	0	7	0	0
5	A	112	0	0	13	0
5	C	121	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	132	0	0	11	0
5	G	133	0	0	10	3
5	I	34	0	0	1	0
5	J	44	0	0	3	0
5	K	41	0	0	6	0
5	L	47	0	0	6	0
All	All	19504	0	18245	439	4

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 12.

The worst 5 of 439 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:G:303:ARG:HG3	5:G:2084:HOH:O	1.58	1.03
2:K:22:THR:H	2:K:25:GLN:HE21	1.06	1.02
1:A:177:LYS:CD	5:A:2040:HOH:O	2.10	0.97
2:J:29:GLN:HB2	5:J:2016:HOH:O	1.67	0.95
2:J:22:THR:H	2:J:25:GLN:HE21	0.98	0.94

All (4) 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)
5:G:2077:HOH:O	5:G:2077:HOH:O[3_555]	1.65	0.55
5:G:2081:HOH:O	5:G:2081:HOH:O[3_555]	1.89	0.31
2:L:24:ASP:OD1	2:L:28:ARG:NH2[4_555]	2.05	0.15
5:G:2086:HOH:O	5:G:2086:HOH:O[3_555]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/475 (98%)	439 (95%)	22 (5%)	3 (1%)	25	31
1	C	464/475 (98%)	445 (96%)	18 (4%)	1 (0%)	47	58
1	E	464/475 (98%)	437 (94%)	24 (5%)	3 (1%)	25	31
1	G	464/475 (98%)	439 (95%)	24 (5%)	1 (0%)	47	58
2	I	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	J	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	19	23
2	K	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
2	L	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	19	23
All	All	2340/2392 (98%)	2209 (94%)	121 (5%)	10 (0%)	34	42

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	PRO
1	E	176	PRO
1	G	176	PRO
1	C	344	GLY
2	J	15	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/386 (98%)	364 (96%)	14 (4%)	34	48
1	C	378/386 (98%)	364 (96%)	14 (4%)	34	48
1	E	378/386 (98%)	361 (96%)	17 (4%)	27	39
1	G	378/386 (98%)	366 (97%)	12 (3%)	39	54
2	I	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	J	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	K	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	L	112/112 (100%)	104 (93%)	8 (7%)	14	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1960/1992 (98%)	1874 (96%)	86 (4%)	28 39

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	185	TYR
1	G	36	ILE
2	L	33	LEU
1	E	239	TYR
1	E	387	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	156	GLN
1	E	304	GLN
2	K	25	GLN
1	E	184	ASN
1	E	238	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	G	201	1,3	7,11,12	1.14	1 (14%)	4,12,14	5.82	2 (50%)
1	KCX	E	201	1,3	7,11,12	0.79	0	4,12,14	2.42	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	KCX	C	201	1,3	7,11,12	1.16	0	4,12,14	1.81	1 (25%)
1	KCX	A	201	1,3	7,11,12	1.08	0	4,12,14	2.93	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	G	201	1,3	-	1/7/10/12	-
1	KCX	E	201	1,3	-	1/7/10/12	-
1	KCX	C	201	1,3	-	1/7/10/12	-
1	KCX	A	201	1,3	-	0/7/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	201	KCX	CB-CA	2.03	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	201	KCX	CE-NZ-CX	11.34	142.15	122.95
1	A	201	KCX	CE-NZ-CX	5.71	132.61	122.95
1	E	201	KCX	CE-NZ-CX	4.09	129.87	122.95
1	C	201	KCX	CE-NZ-CX	3.01	128.04	122.95
1	G	201	KCX	CD-CG-CB	-2.18	105.92	113.62

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	201	KCX	O-C-CA-CB
1	E	201	KCX	CD-CE-NZ-CX
1	G	201	KCX	CD-CE-NZ-CX

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	201	KCX	3	0
1	C	201	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	G	477	3	15,20,20	1.96	3 (20%)	20,31,31	1.98	7 (35%)
4	CAP	A	477	3	15,20,20	1.79	4 (26%)	20,31,31	2.11	6 (30%)
4	CAP	C	477	3	15,20,20	2.04	5 (33%)	20,31,31	2.09	7 (35%)
4	CAP	E	477	3	15,20,20	1.81	3 (20%)	20,31,31	2.42	7 (35%)

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	G	477	3	-	6/23/29/29	-
4	CAP	A	477	3	-	8/23/29/29	-
4	CAP	C	477	3	-	9/23/29/29	-
4	CAP	E	477	3	-	7/23/29/29	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	477	CAP	O4-C4	-5.38	1.32	1.43

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	477	CAP	O3-C3	-4.38	1.34	1.42
4	E	477	CAP	O3-C3	-4.11	1.34	1.42
4	E	477	CAP	O4-C4	-3.75	1.35	1.43
4	A	477	CAP	O4-C4	-3.71	1.35	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	477	CAP	O4-C4-C3	-6.13	96.53	108.78
4	A	477	CAP	O4-C4-C3	-5.46	97.87	108.78
4	E	477	CAP	P2-O5-C5	4.80	131.51	118.30
4	C	477	CAP	O4-C4-C3	-4.70	99.39	108.78
4	G	477	CAP	O4-C4-C3	-4.34	100.11	108.78

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	477	CAP	C2-C3-C4-O4
4	E	477	CAP	O3-C3-C4-O4
4	E	477	CAP	O4-C4-C5-O5
4	G	477	CAP	C2-C3-C4-O4
4	G	477	CAP	O3-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	477	CAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 G 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP A 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP C 477

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP E 477

Bond lengths

Bond angles

Torsions

Rings
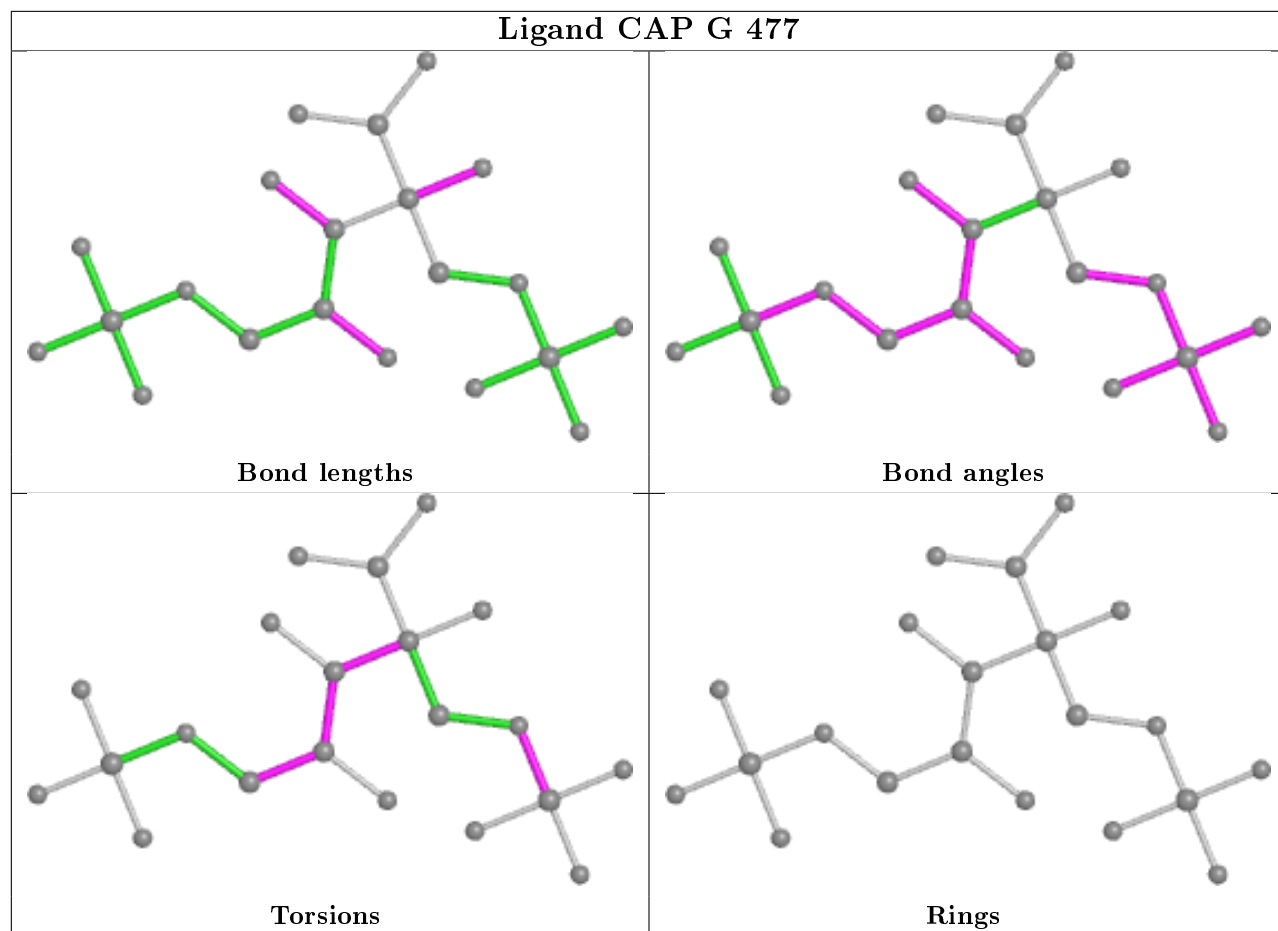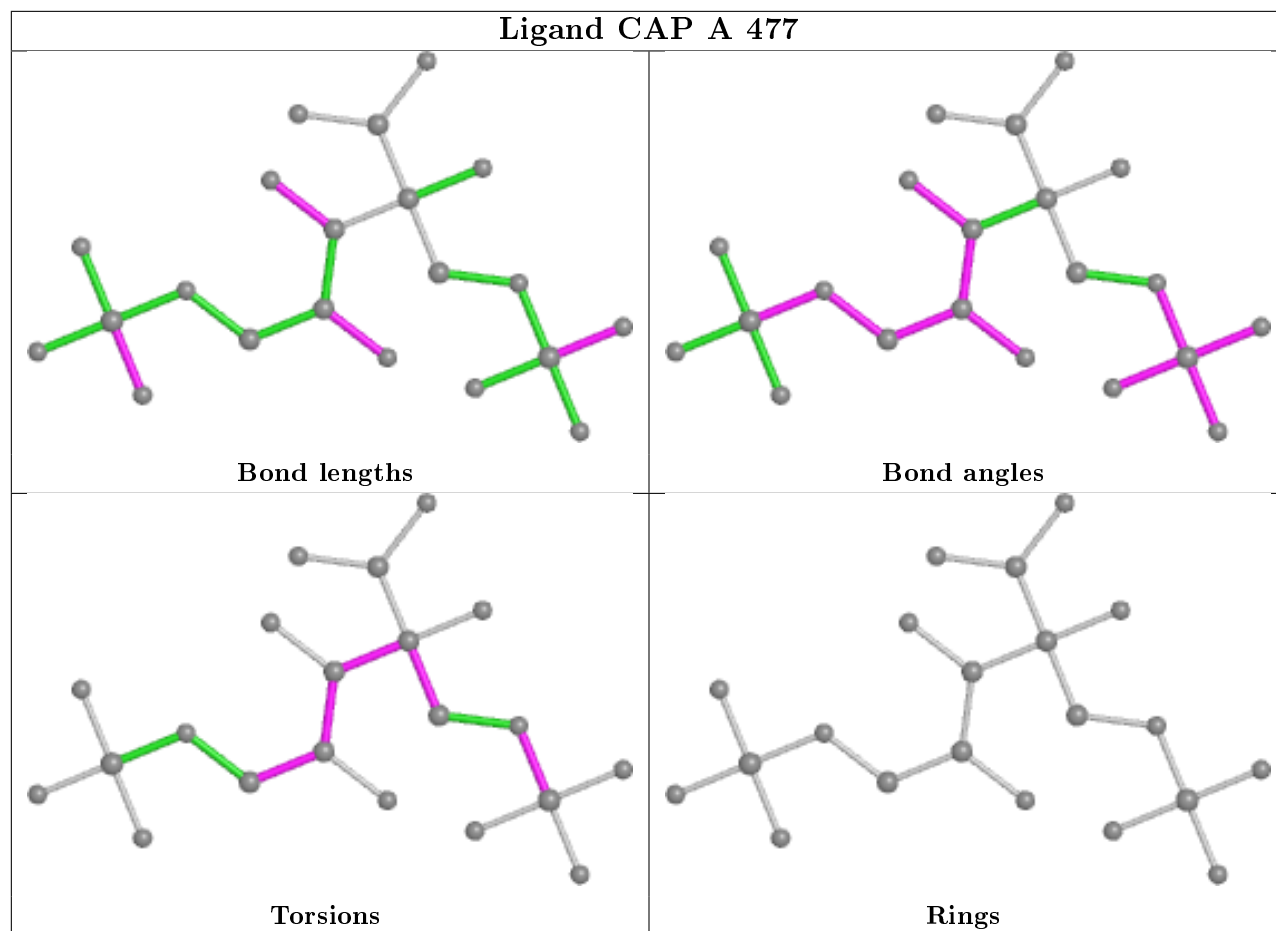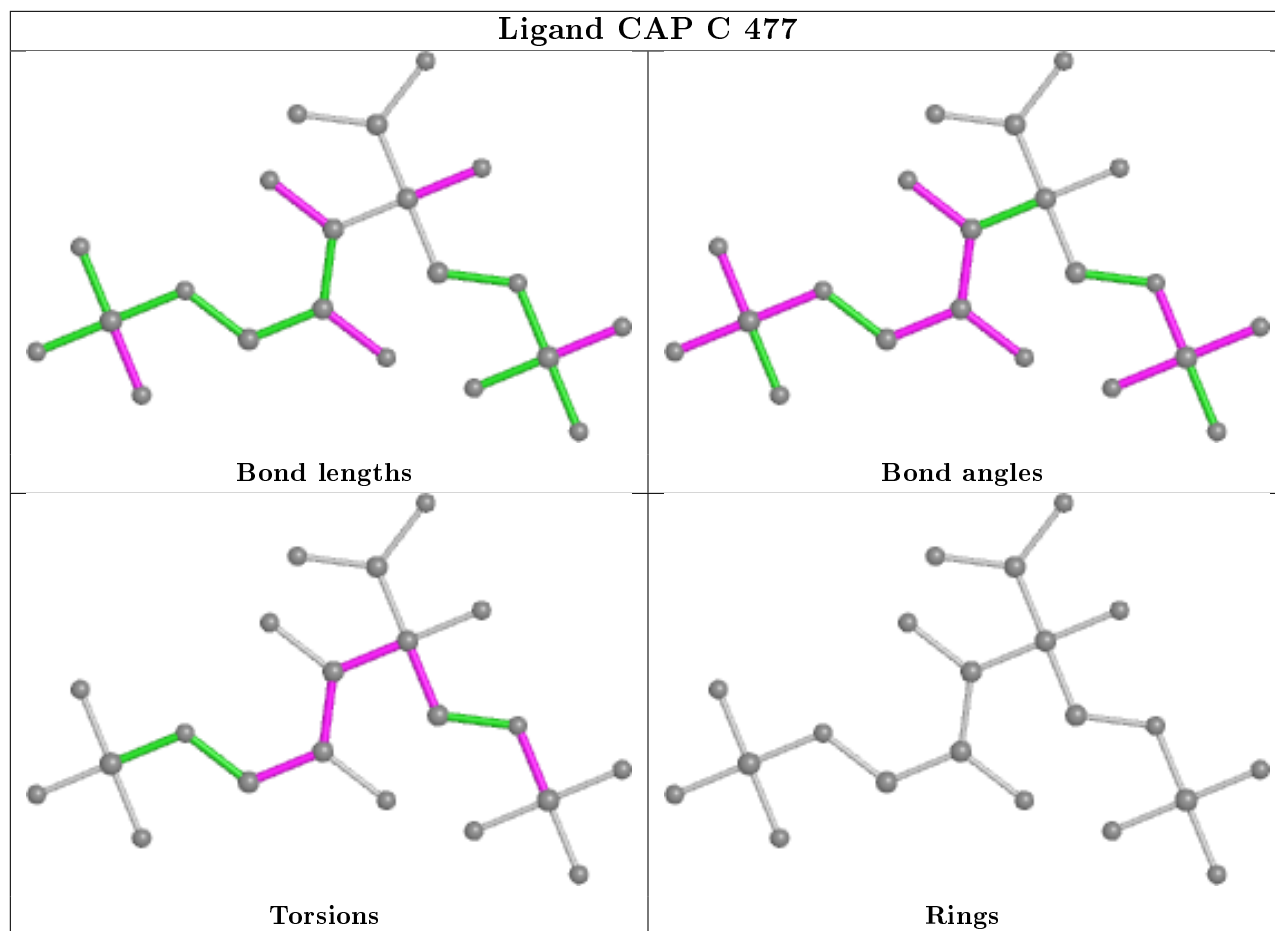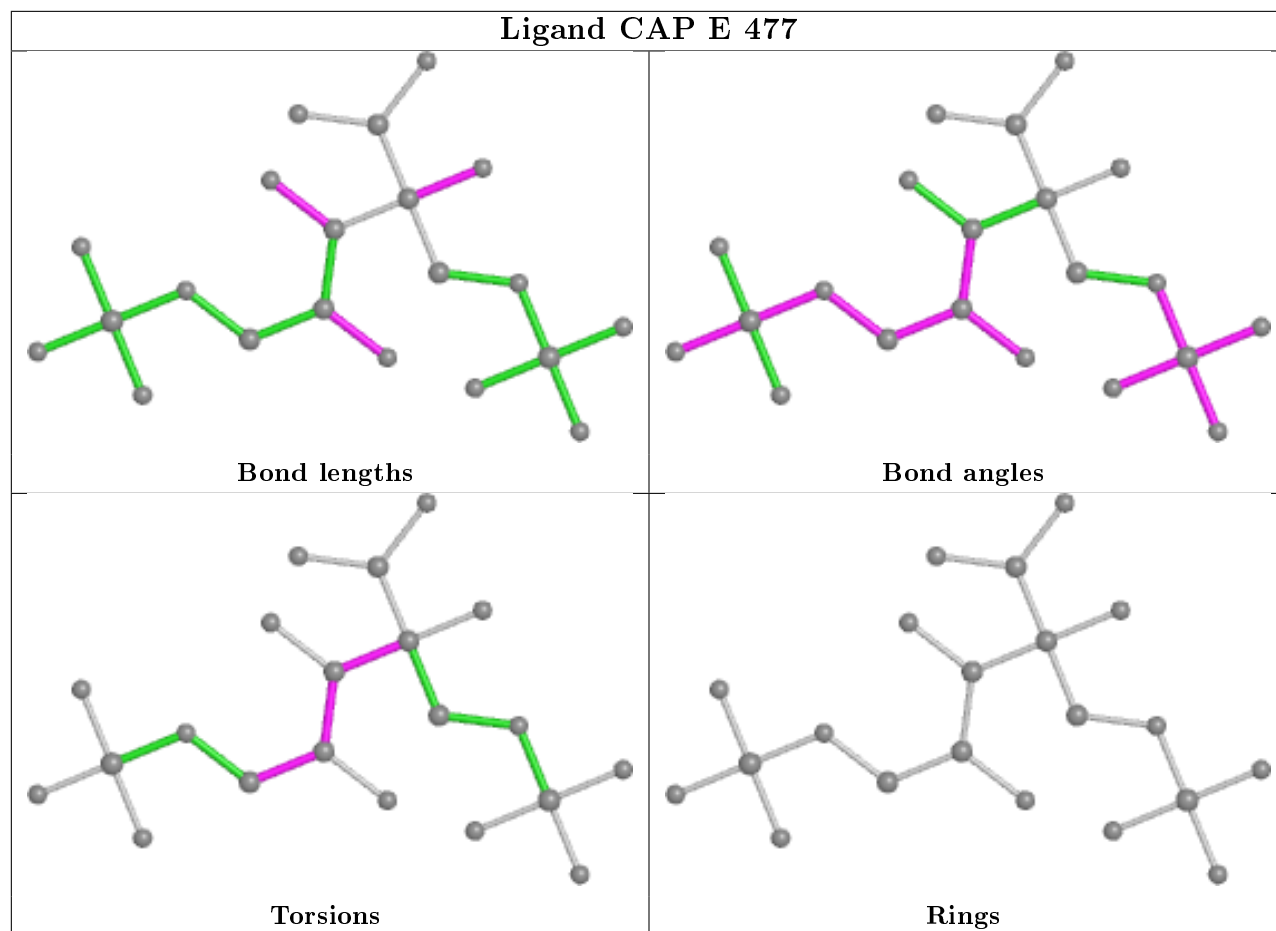
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

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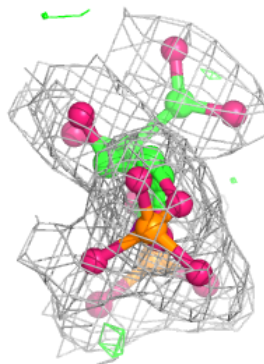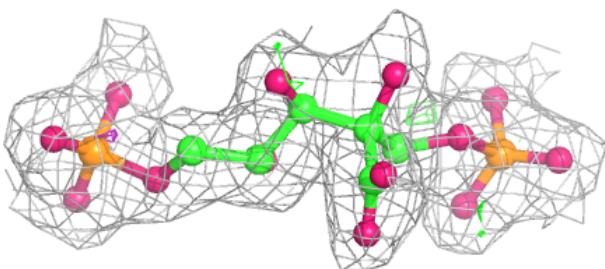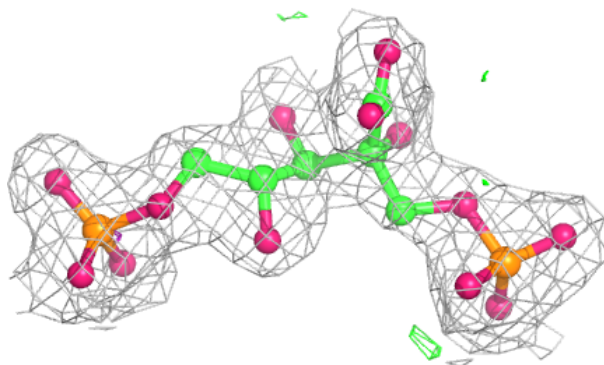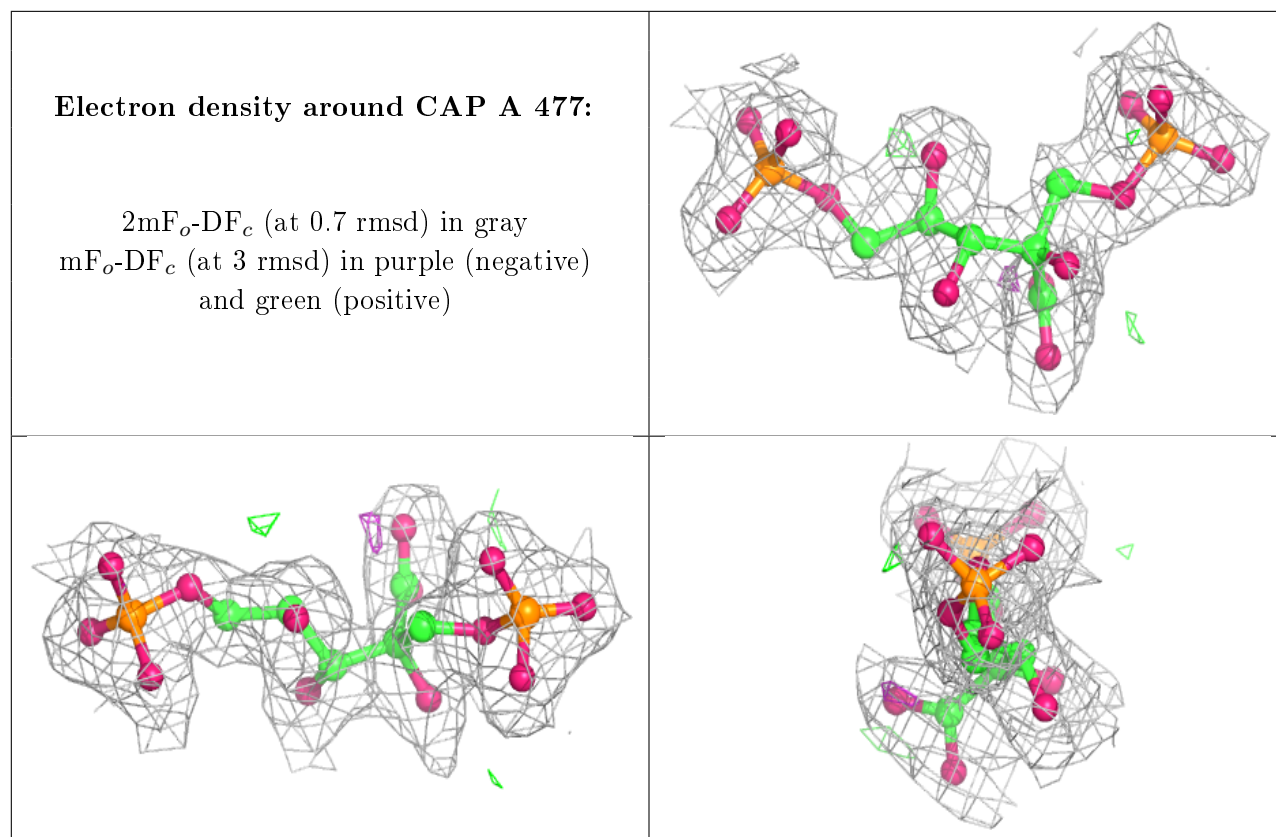

Electron density around CAP E 477:

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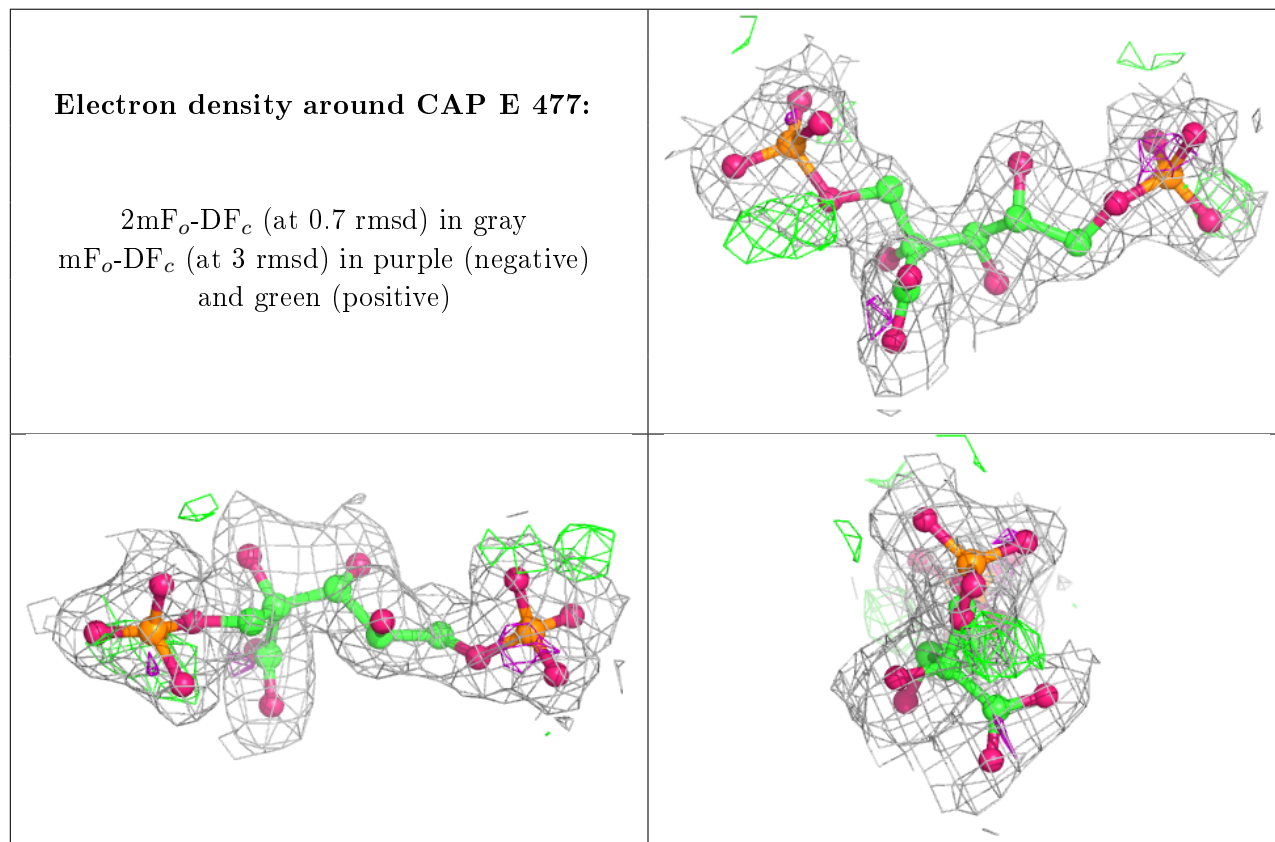
Electron density around CAP G 477:

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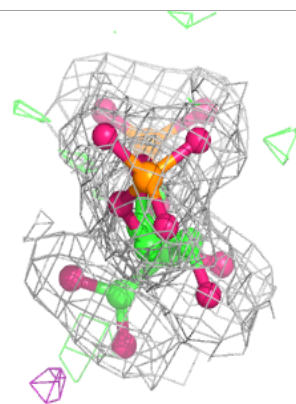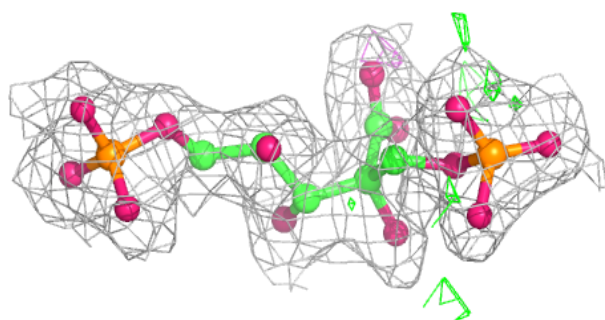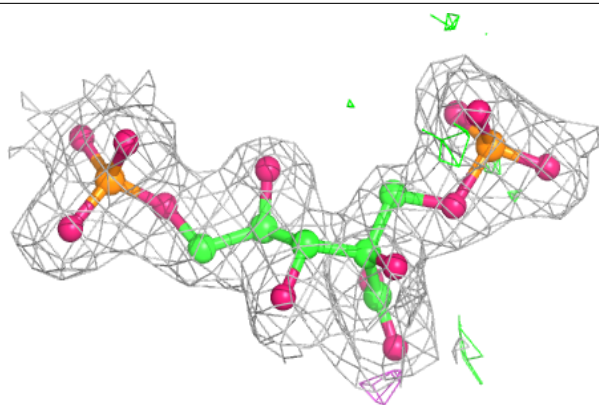
Electron density around CAP C 477:

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

Electron density around CAP A 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 ⓘ

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