



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 2, 2025 – 01:23 am BST

PDB ID : 1UPP / pdb_00001upp
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)

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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

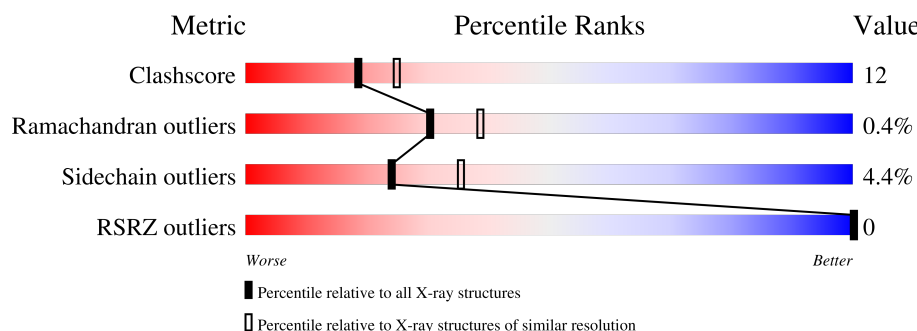
1 Overall quality at a glance

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))
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 $\leq 5\%$. 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	
1	C	475	
1	E	475	
1	G	475	
2	I	123	
2	J	123	

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Mol	Chain	Length	Quality of chain
2	K	123	<div><div></div><div>60%</div><div>36%</div><div>••</div></div>
2	L	123	<div><div></div><div>59%</div><div>36%</div><div>5%•</div></div>

2 Entry composition

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 BIPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3656	2319	640	679	18			
1	C	467	Total	C	N	O	S	0	0	0
			3656	2319	640	679	18			
1	E	467	Total	C	N	O	S	0	0	0
			3656	2319	640	679	18			
1	G	467	Total	C	N	O	S	0	0	0
			3656	2319	640	679	18			

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

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

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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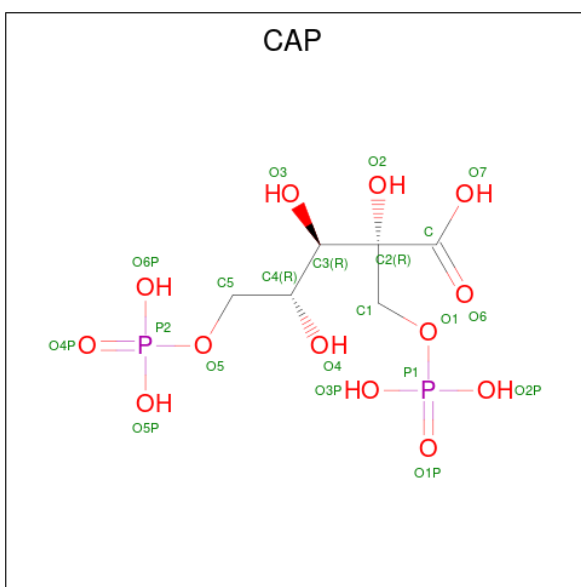
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Chain	Residue	Modelled	Actual	Comment	Reference
J	2	GLN	LYS	conflict	UNP Q43832
J	6	ILE	THR	conflict	UNP Q43832
J	7	LEU	GLN	conflict	UNP Q43832
J	9	LEU	MET	conflict	UNP Q43832
J	11	LYS	ARG	conflict	UNP Q43832
J	109	GLU	GLN	conflict	UNP Q43832
J	113	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 (CCD ID: CA) (formula: Ca).

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 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

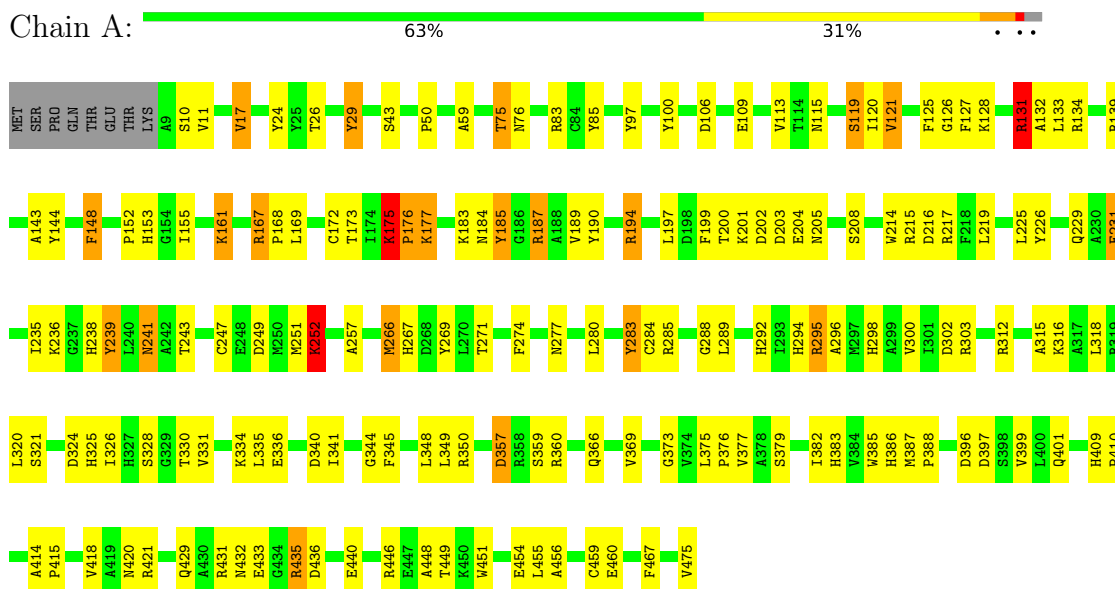
- Molecule 5 is water.

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

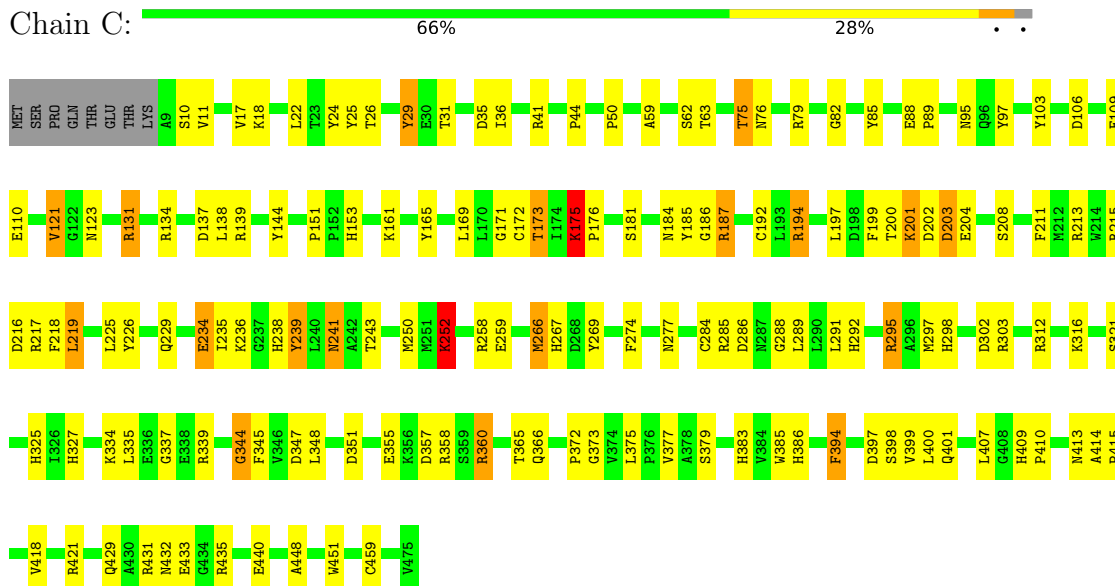
3 Residue-property plots

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.

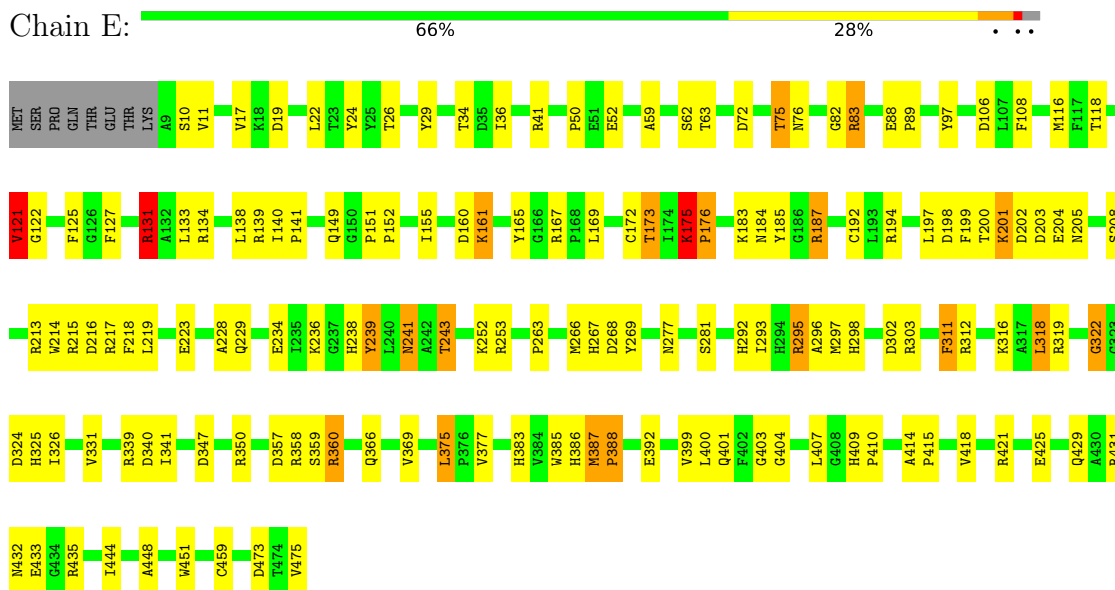
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



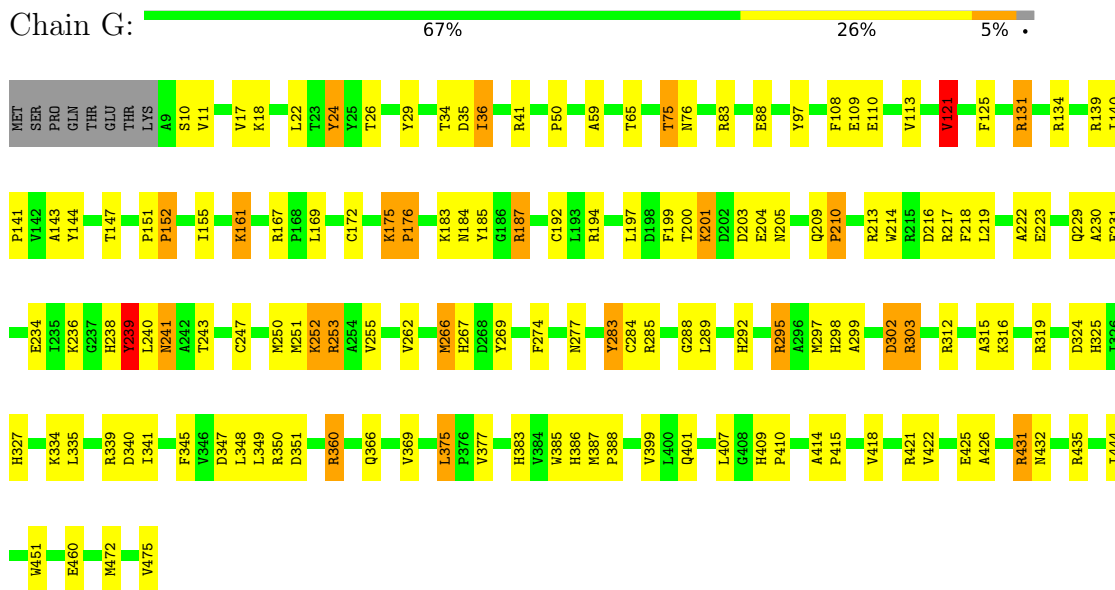
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



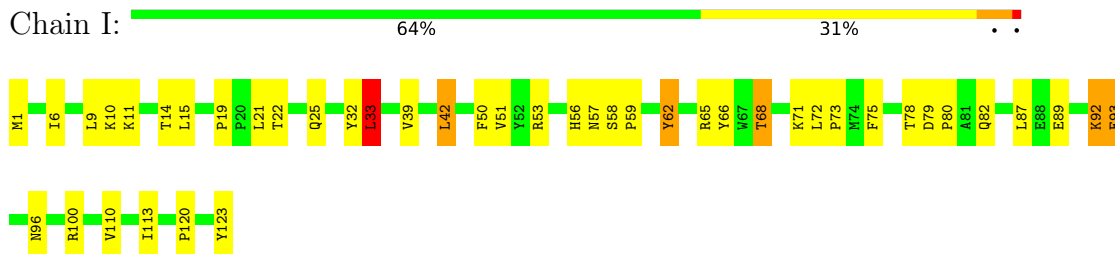
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

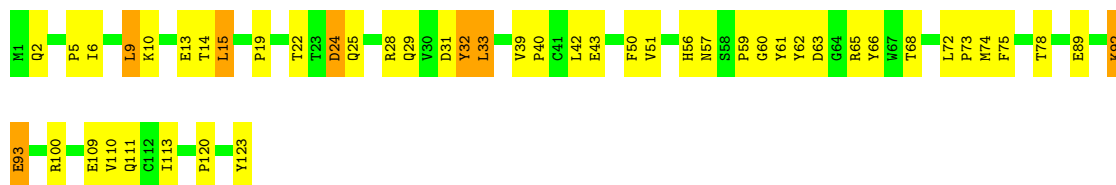


- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN



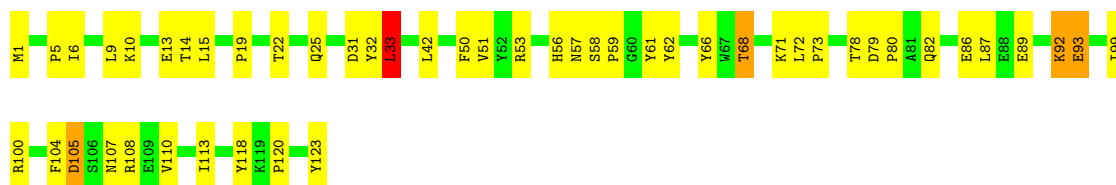
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain J:  61% 33% 6%



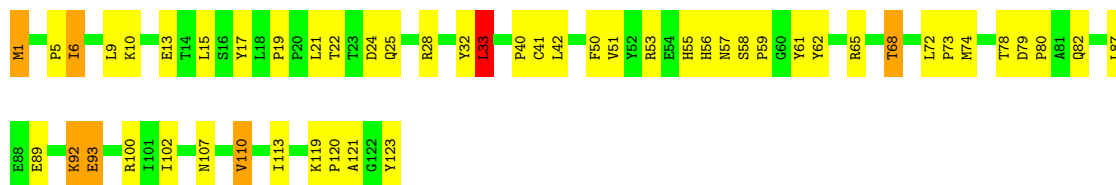
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain K:  60% 36% 4%



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain L:  59% 36% 5%



4 Data and refinement statistics

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 – 2.30 100.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	76.1 (100.00-2.30) 76.8 (100.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (Å ²)	18.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 1.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.459 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19504	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: KCX, CAP, CA

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(°)	Ideal(°)
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

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%)	22	27
1	C	464/475 (98%)	445 (96%)	18 (4%)	1 (0%)	44	55
1	E	464/475 (98%)	437 (94%)	24 (5%)	3 (1%)	22	27
1	G	464/475 (98%)	439 (95%)	24 (5%)	1 (0%)	44	55
2	I	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	J	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	16	20
2	K	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
2	L	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	16	20
All	All	2340/2392 (98%)	2209 (94%)	121 (5%)	10 (0%)	30	39

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 ⓘ

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%)	29	43
1	C	378/386 (98%)	364 (96%)	14 (4%)	29	43
1	E	378/386 (98%)	361 (96%)	17 (4%)	23	34
1	G	378/386 (98%)	366 (97%)	12 (3%)	34	50
2	I	112/112 (100%)	105 (94%)	7 (6%)	15	21
2	J	112/112 (100%)	105 (94%)	7 (6%)	15	21
2	K	112/112 (100%)	105 (94%)	7 (6%)	15	21
2	L	112/112 (100%)	104 (93%)	8 (7%)	12	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1960/1992 (98%)	1874 (96%)	86 (4%)	24	35

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

Mol	Chain	Res	Type
2	I	33	LEU
2	K	33	LEU
2	I	57	ASN
2	J	56	HIS
2	K	78	THR

Sometimes 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	241	ASN
1	G	184	ASN
2	L	107	ASN
2	J	57	ASN
1	E	267	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	3,1	9,11,12	1.43	2 (22%)	5,12,14	6.21	3 (60%)
1	KCX	A	201	3,1	9,11,12	1.41	1 (11%)	5,12,14	3.89	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	C	201	3,1	9,11,12	1.27	1 (11%)	5,12,14	1.93	1 (20%)
1	KCX	E	201	3,1	9,11,12	1.46	1 (11%)	5,12,14	4.04	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	G	201	3,1	-	2/9/10/12	-
1	KCX	A	201	3,1	-	0/9/10/12	-
1	KCX	C	201	3,1	-	1/9/10/12	-
1	KCX	E	201	3,1	-	3/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	201	KCX	OQ1-CX	3.63	1.28	1.21
1	A	201	KCX	OQ1-CX	2.70	1.26	1.21
1	G	201	KCX	OQ1-CX	2.67	1.26	1.21
1	C	201	KCX	OQ1-CX	2.26	1.25	1.21
1	G	201	KCX	CB-CA	2.03	1.56	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	201	KCX	CE-NZ-CX	12.62	142.15	121.89
1	E	201	KCX	OQ1-CX-NZ	7.16	136.05	124.96
1	A	201	KCX	CE-NZ-CX	6.68	132.61	121.89
1	A	201	KCX	OQ1-CX-NZ	5.45	133.40	124.96
1	G	201	KCX	OQ1-CX-NZ	5.24	133.08	124.96

There are no chirality outliers.

5 of 6 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	E	201	KCX	OQ1-CX-NZ-CE
1	G	201	KCX	OQ1-CX-NZ-CE
1	E	201	KCX	OQ2-CX-NZ-CE

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	C	477	3	17,20,20	1.92	5 (29%)	22,31,31	2.35	9 (40%)
4	CAP	G	477	3	17,20,20	1.87	3 (17%)	22,31,31	2.24	9 (40%)
4	CAP	E	477	3	17,20,20	1.78	3 (17%)	22,31,31	2.65	9 (40%)
4	CAP	A	477	3	17,20,20	1.75	4 (23%)	22,31,31	2.44	8 (36%)

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	C	477	3	-	9/29/29/29	-
4	CAP	G	477	3	-	6/29/29/29	-
4	CAP	E	477	3	-	7/29/29/29	-
4	CAP	A	477	3	-	14/29/29/29	-

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
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 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	477	CAP	O4-C4-C3	-6.13	96.53	108.78
4	A	477	CAP	O7-C-O6	-5.60	105.99	123.82
4	A	477	CAP	O4-C4-C3	-5.46	97.87	108.78
4	C	477	CAP	O7-C-O6	-5.01	107.90	123.82
4	E	477	CAP	P2-O5-C5	4.80	131.51	118.30

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

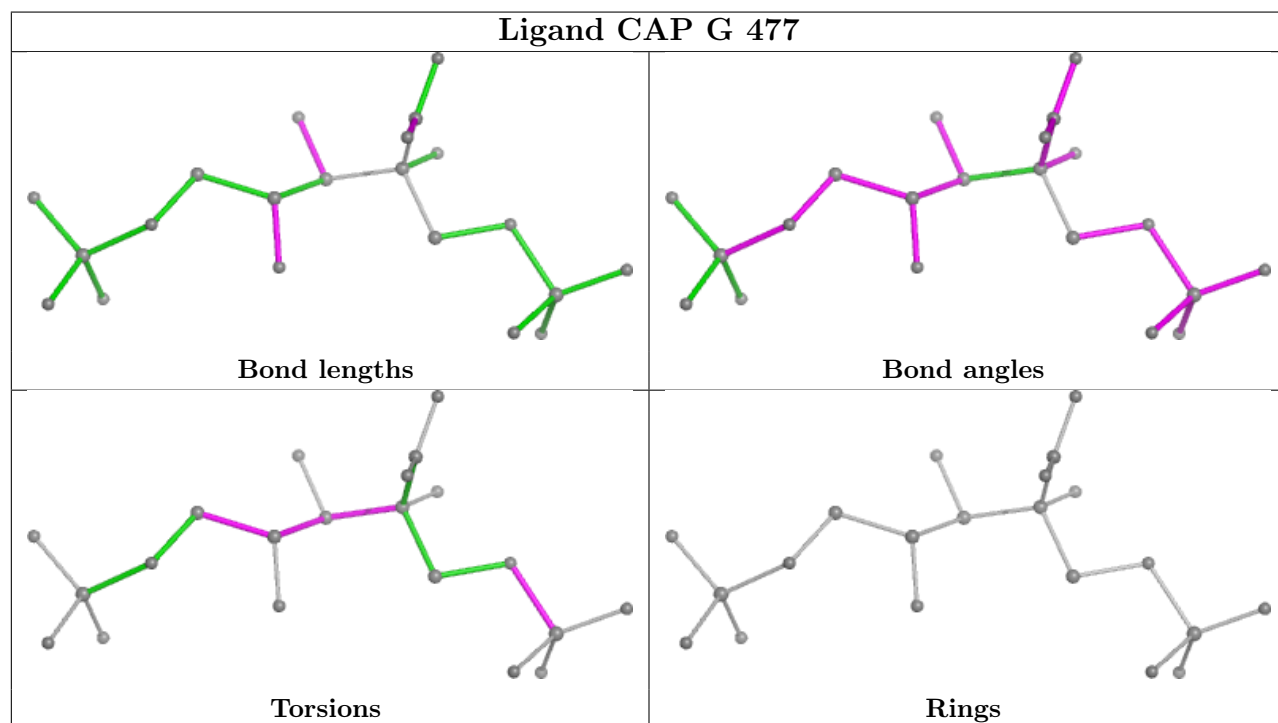
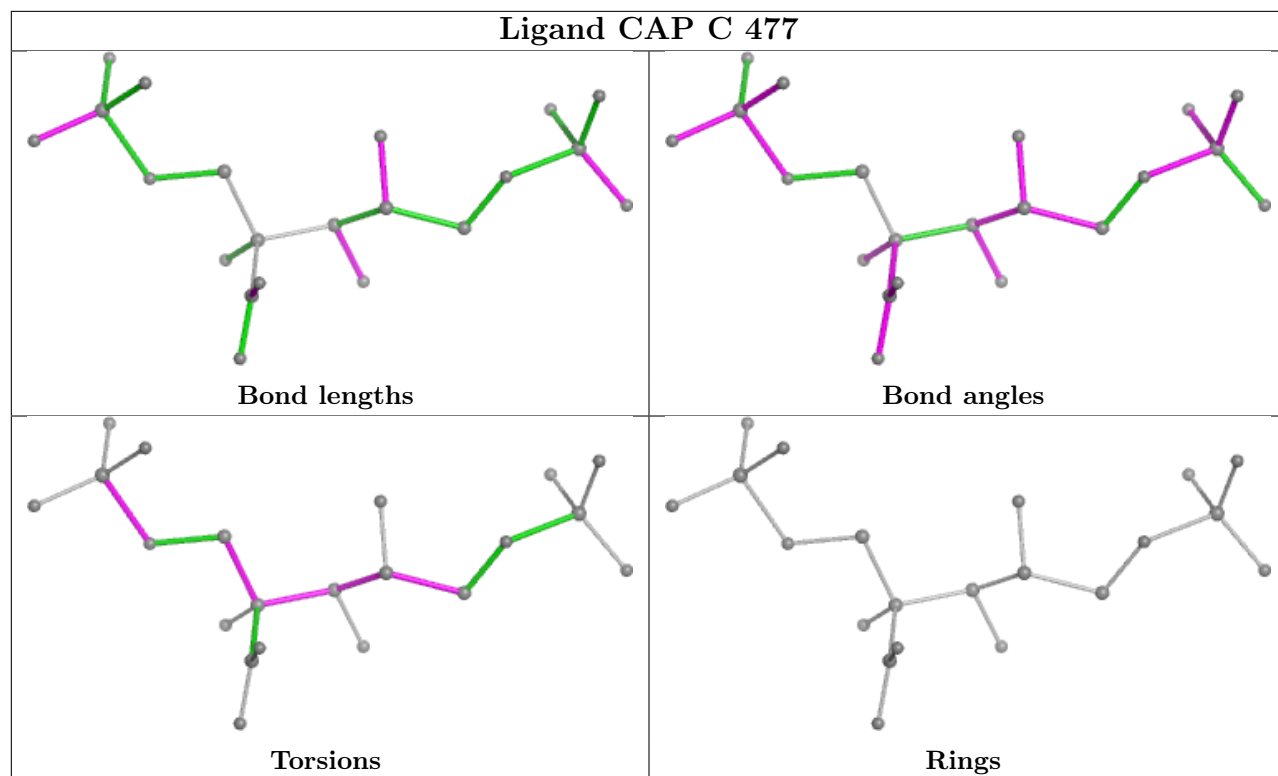
Mol	Chain	Res	Type	Atoms
4	A	477	CAP	O6-C-C2-C3
4	A	477	CAP	O6-C-C2-O2
4	A	477	CAP	C2-C3-C4-O4
4	A	477	CAP	O3-C3-C4-O4
4	A	477	CAP	O4-C4-C5-O5

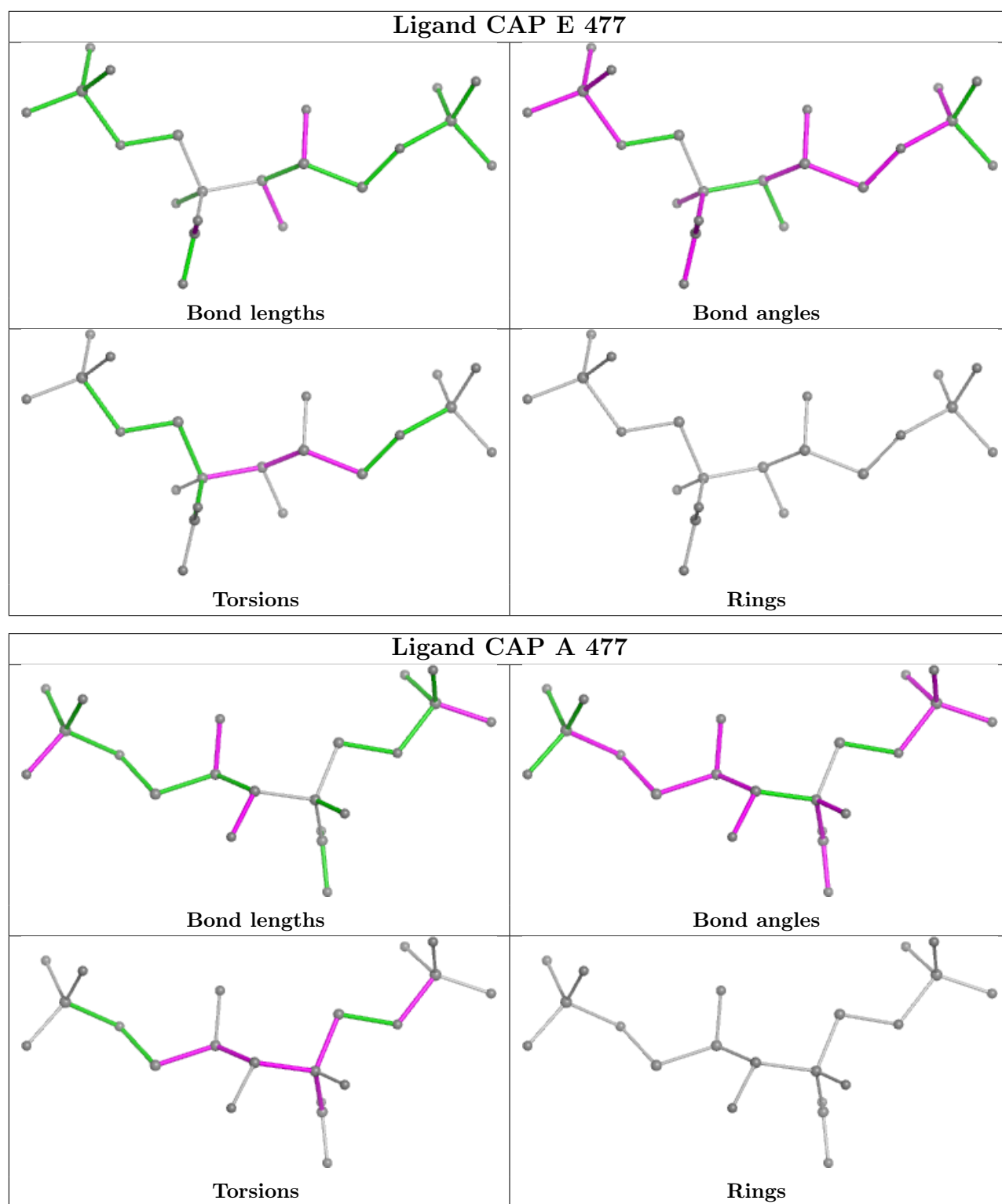
There are no ring outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	466/475 (98%)	-1.60	0 100 100	11, 20, 44, 85	0
1	C	466/475 (98%)	-1.58	0 100 100	11, 20, 44, 85	0
1	E	466/475 (98%)	-1.59	0 100 100	11, 20, 44, 85	0
1	G	466/475 (98%)	-1.61	0 100 100	11, 20, 45, 85	0
2	I	123/123 (100%)	-1.48	0 100 100	12, 32, 53, 67	0
2	J	123/123 (100%)	-1.48	0 100 100	12, 32, 53, 67	0
2	K	123/123 (100%)	-1.45	0 100 100	11, 32, 53, 67	0
2	L	123/123 (100%)	-1.46	0 100 100	12, 32, 53, 67	0
All	All	2356/2392 (98%)	-1.57	0 100 100	11, 21, 48, 85	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	KCX	C	201	12/13	0.99	0.03	12,15,18,18	0
1	KCX	G	201	12/13	0.99	0.03	12,14,18,18	0
1	KCX	E	201	12/13	1.00	0.02	13,14,18,19	0
1	KCX	A	201	12/13	1.00	0.02	13,14,18,18	0

6.3 Carbohydrates [i](#)

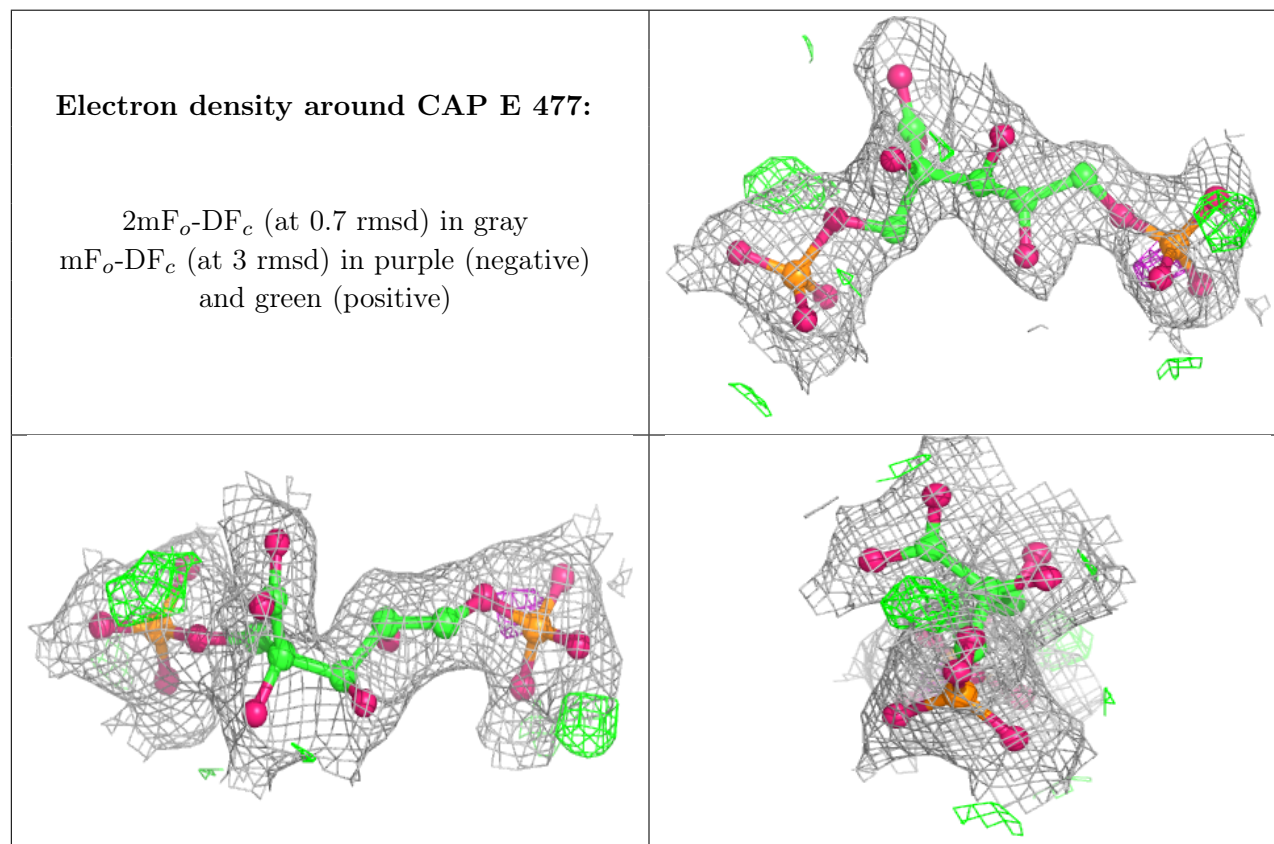
There are no monosaccharides in this entry.

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.

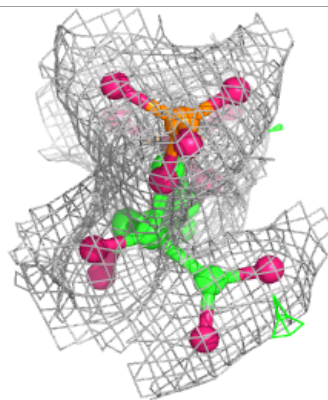
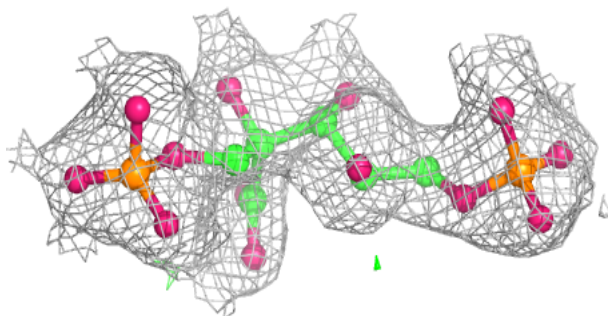
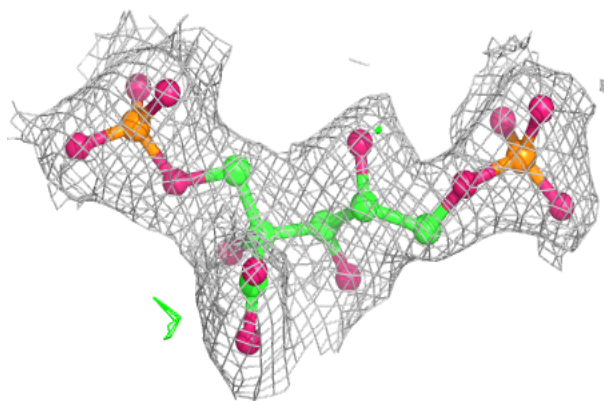
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	C	476	1/1	0.99	0.02	38,38,38,38	0
4	CAP	E	477	21/21	0.99	0.03	15,19,22,23	0
3	CA	E	476	1/1	1.00	0.04	36,36,36,36	0
3	CA	G	476	1/1	1.00	0.02	36,36,36,36	0
4	CAP	A	477	21/21	1.00	0.03	16,18,22,23	0
4	CAP	C	477	21/21	1.00	0.03	15,19,22,23	0
3	CA	A	476	1/1	1.00	0.02	38,38,38,38	0
4	CAP	G	477	21/21	1.00	0.02	15,19,23,24	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.

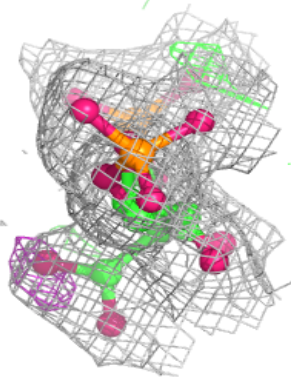
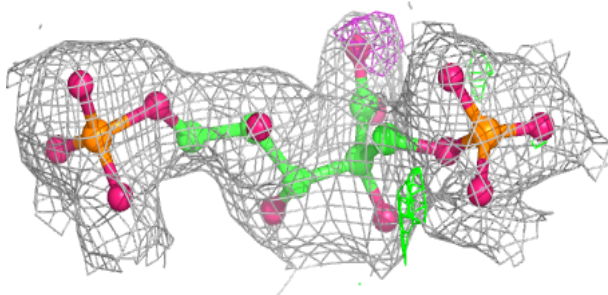
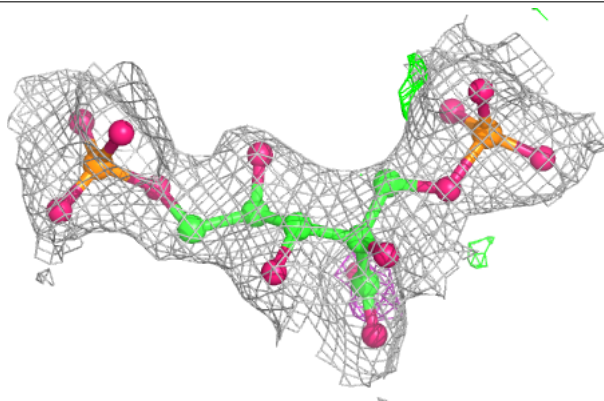


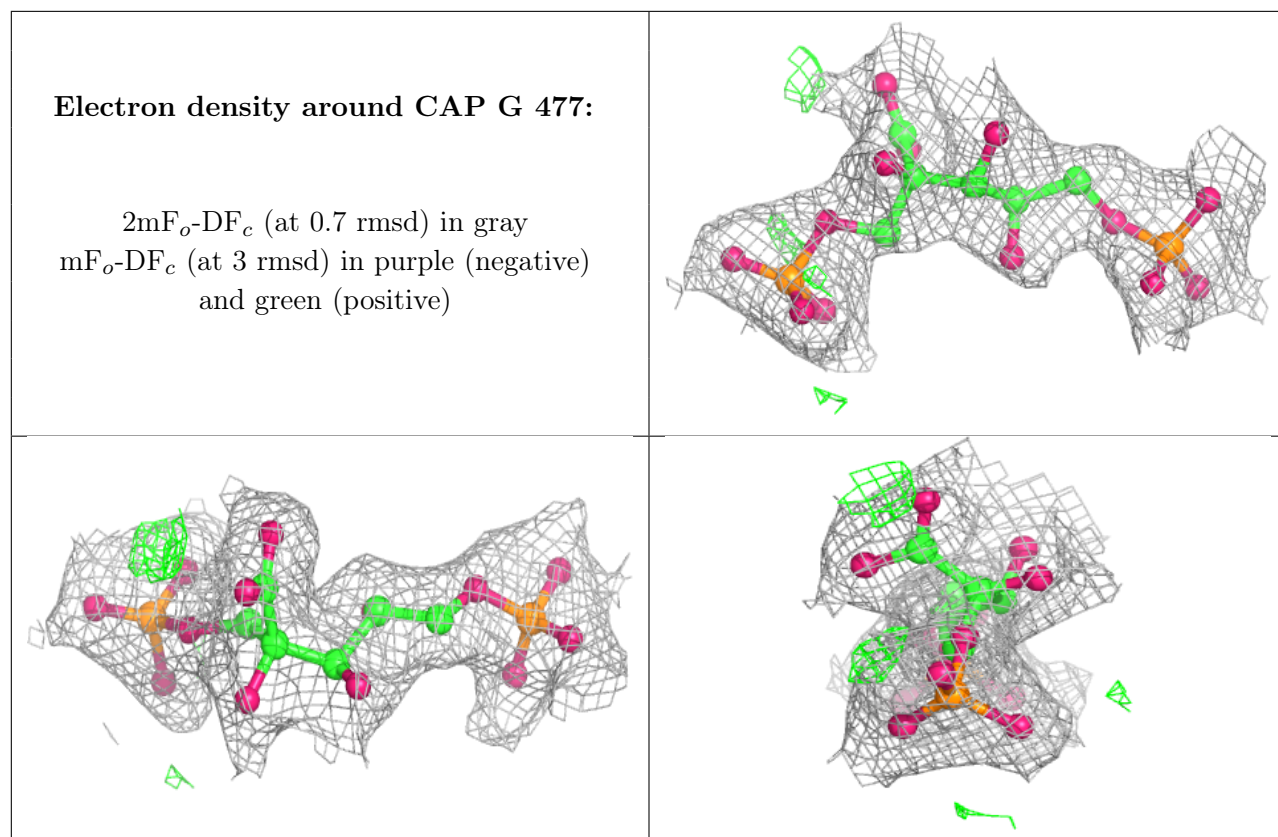
Electron density around CAP A 477:

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

**Electron density around CAP C 477:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.