



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 7, 2023 – 12:13 pm GMT

PDB ID : 1UZD
Title : Chlamydomonas, Spinach Chimeric Rubisco
Authors : Karkehabadi, S.; Spreitzer, R.J.; Andersson, I.
Deposited on : 2004-03-11
Resolution : 2.40 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

<https://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 : 2.36
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) : 2.36

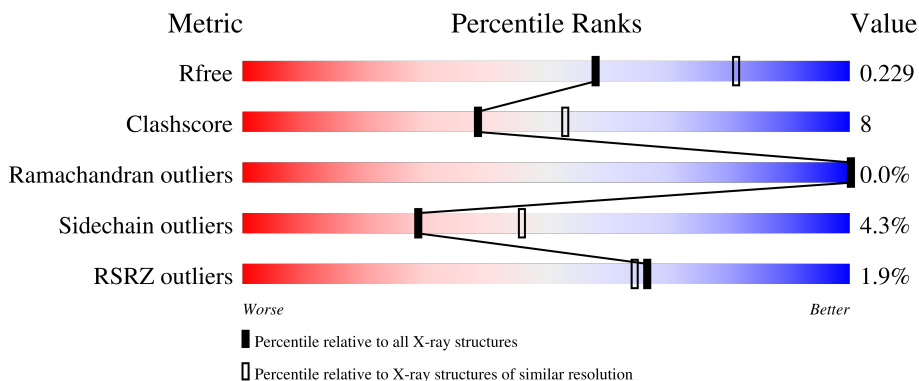
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



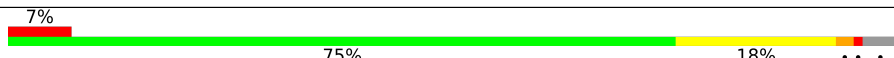

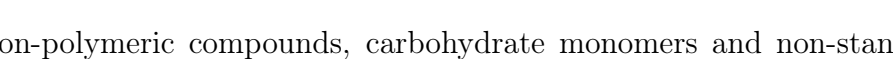
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	 85% 11% ..
1	B	475	 82% 14% ..
1	E	475	 83% 15% ..
1	H	475	 83% 14% ..
1	K	475	 86% 12% ..

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Mol	Chain	Length	Quality of chain	
1	O	475		83% 14% ..
1	R	475		82% 14% ..
1	V	475		82% 15% ..
2	C	134		77% 14% 5% .
2	F	134		75% 18% .. .
2	I	134		76% 16% . .
2	J	134		78% 15% . .
2	M	134		76% 16% . .
2	P	134		74% 18% . .
2	T	134		72% 20% . .
2	W	134		75% 19% .. .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	K	1482	-	-	-	X
5	EDO	O	1483	-	-	X	-
5	EDO	R	1484	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 40055 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
			Total	C	N	O	S			
1	A	465	Total 3637	C 2299	N 641	O 673	S 24	0	2	0
1	B	467	Total 3641	C 2302	N 640	O 675	S 24	0	1	0
1	E	465	Total 3640	C 2300	N 641	O 675	S 24	0	3	0
1	H	469	Total 3657	C 2312	N 643	O 678	S 24	0	1	0
1	K	469	Total 3669	C 2319	N 646	O 680	S 24	0	4	0
1	O	469	Total 3661	C 2313	N 646	O 678	S 24	0	2	0
1	R	465	Total 3637	C 2299	N 641	O 673	S 24	0	2	0
1	V	466	Total 3641	C 2301	N 642	O 674	S 24	0	2	0

- Molecule 2 is a protein called Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	129	Total 1070	C 694	N 182	O 184	S 10	0	1	0
2	F	129	Total 1083	C 703	N 183	O 186	S 11	0	4	0
2	I	129	Total 1073	C 695	N 183	O 185	S 10	0	2	0
2	J	129	Total 1072	C 695	N 182	O 184	S 11	0	2	0
2	M	129	Total 1070	C 694	N 182	O 184	S 10	0	1	0

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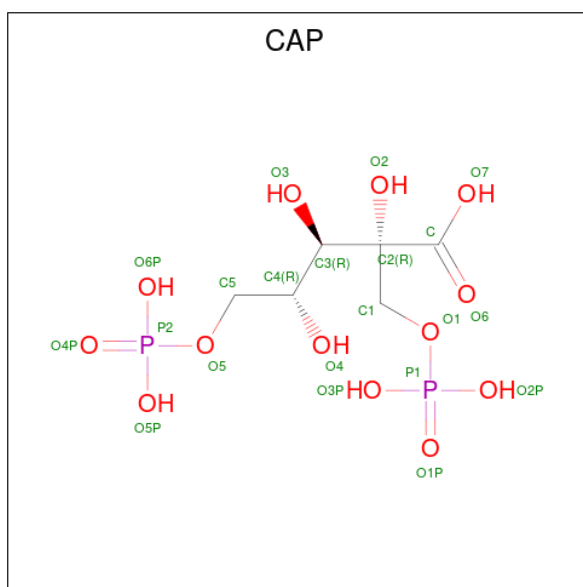
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	129	Total	C	N	O	S	0	1	0
			1070	694	182	184	10			
2	T	129	Total	C	N	O	S	0	2	0
			1078	701	182	185	10			
2	W	129	Total	C	N	O	S	0	3	0
			1073	695	182	185	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C₆H₁₄O₁₃P₂).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

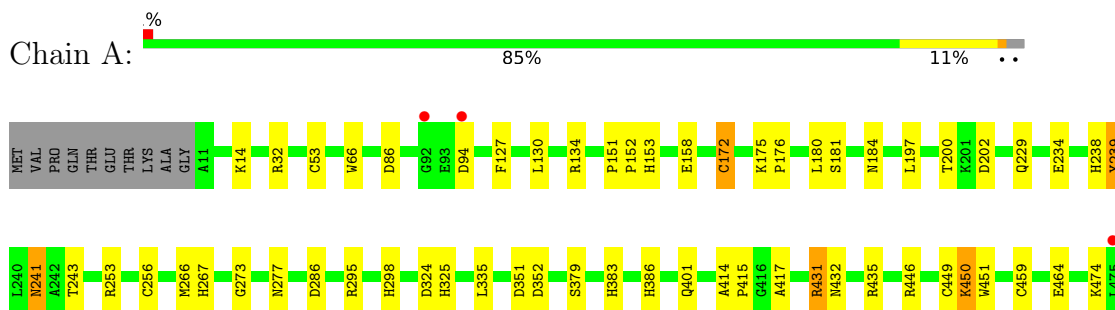
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	178	Total O 178 178	0	0
6	B	201	Total O 201 201	0	0
6	C	55	Total O 55 55	0	0
6	E	186	Total O 186 186	0	0
6	F	52	Total O 52 52	0	0
6	H	166	Total O 166 166	0	0
6	I	68	Total O 68 68	0	0
6	J	31	Total O 31 31	0	0
6	K	192	Total O 192 192	0	0
6	M	47	Total O 47 47	0	0
6	O	188	Total O 188 188	0	0
6	P	51	Total O 51 51	0	0
6	R	183	Total O 183 183	0	0
6	T	48	Total O 48 48	0	0
6	V	195	Total O 195 195	0	0
6	W	50	Total O 50 50	0	0

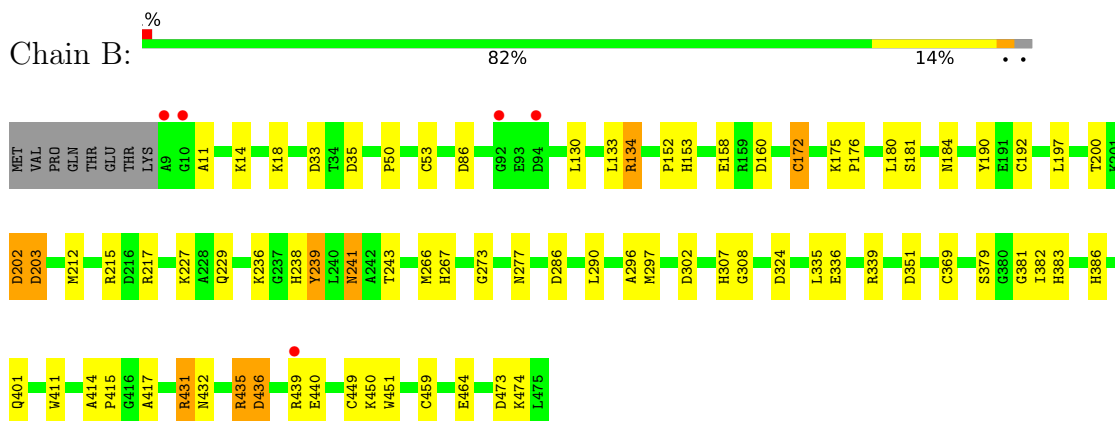
3 Residue-property plots [i](#)

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

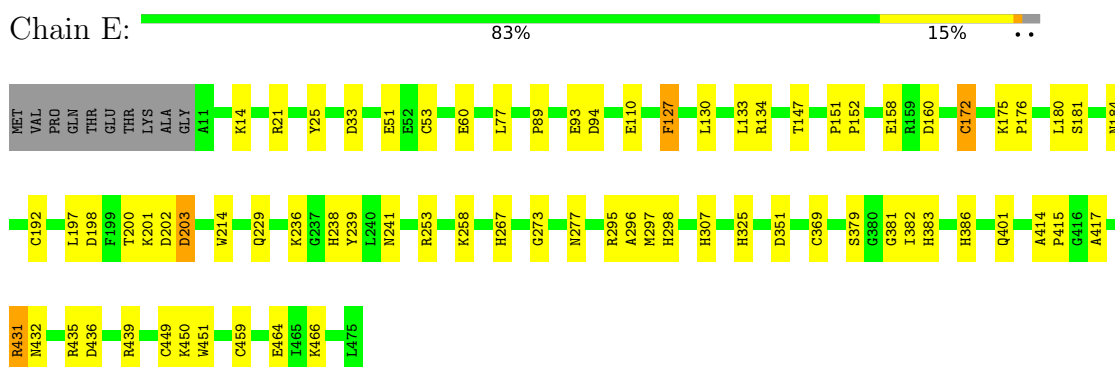
- Molecule 1: Ribulose biphosphate carboxylase large chain



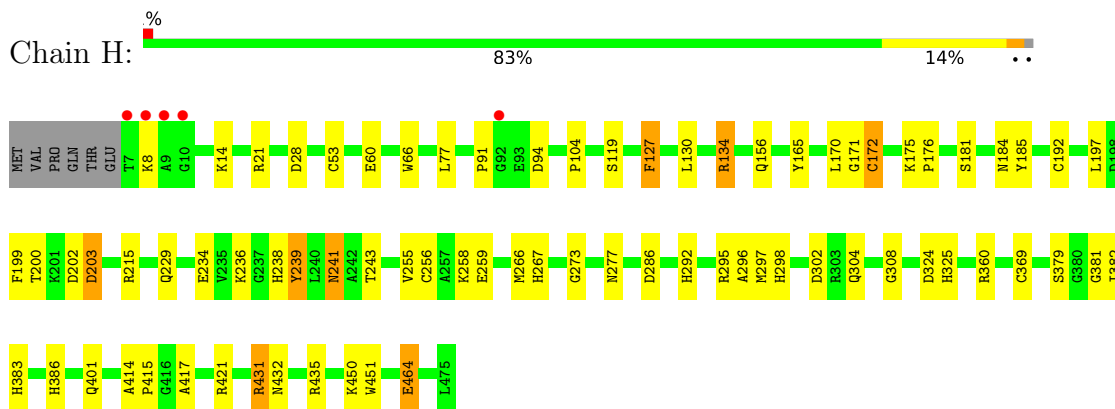
- Molecule 1: Ribulose biphosphate carboxylase large chain



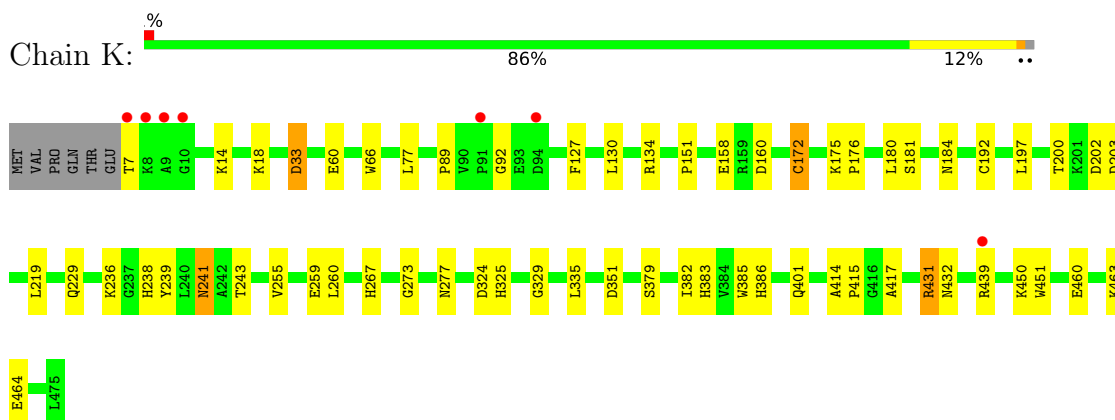
- Molecule 1: Ribulose biphosphate carboxylase large chain



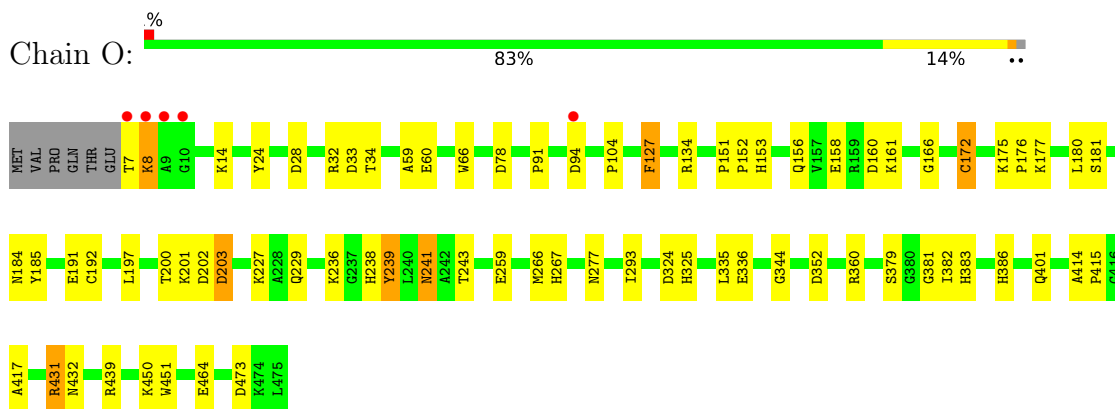
- Molecule 1: Ribulose biphosphate carboxylase large chain



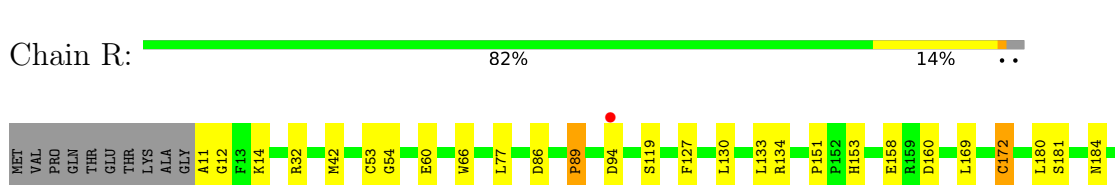
- Molecule 1: Ribulose biphosphate carboxylase large chain

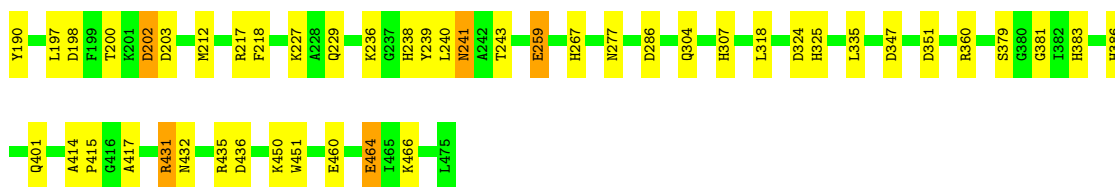


- Molecule 1: Ribulose biphosphate carboxylase large chain

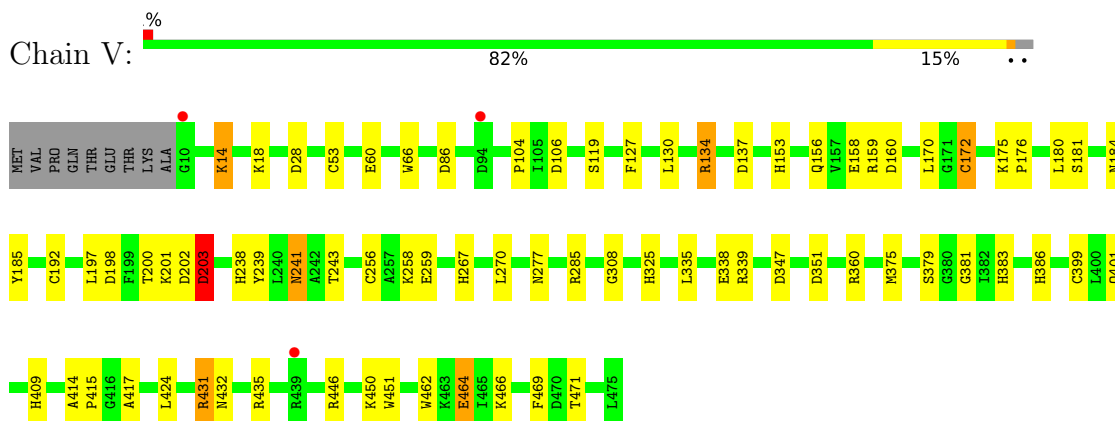


- Molecule 1: Ribulose biphosphate carboxylase large chain

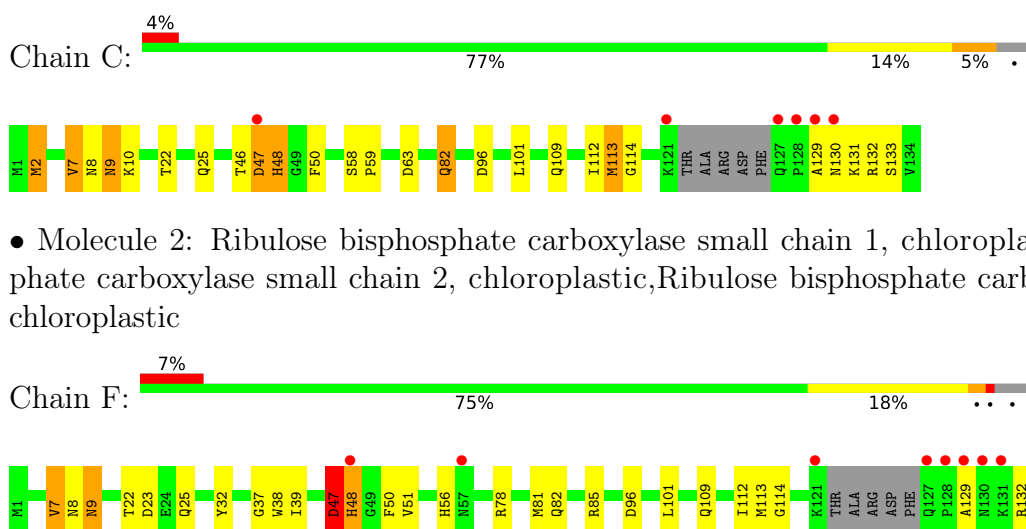




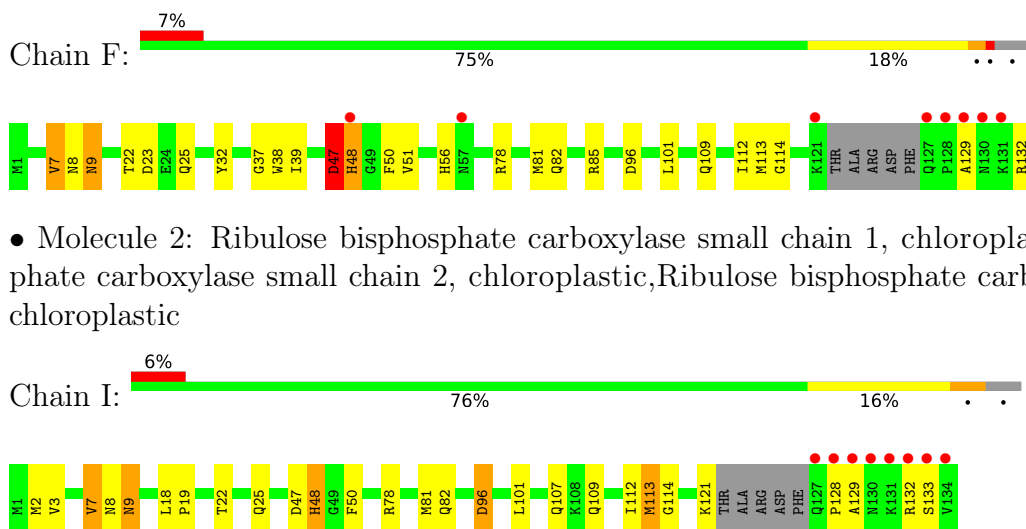
- Molecule 1: Ribulose biphosphate carboxylase large chain



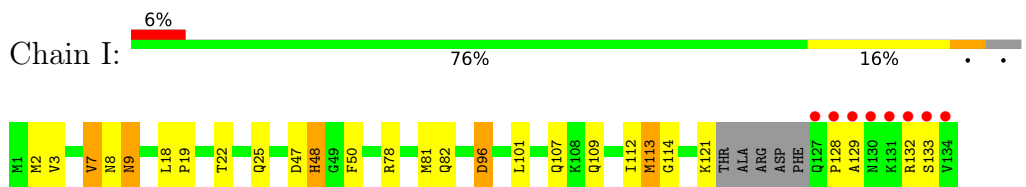
- Molecule 2: Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic



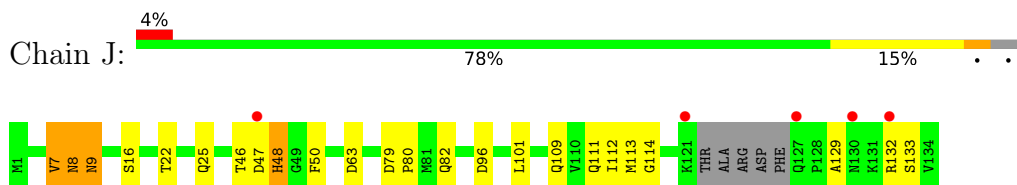
- Molecule 2: Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic



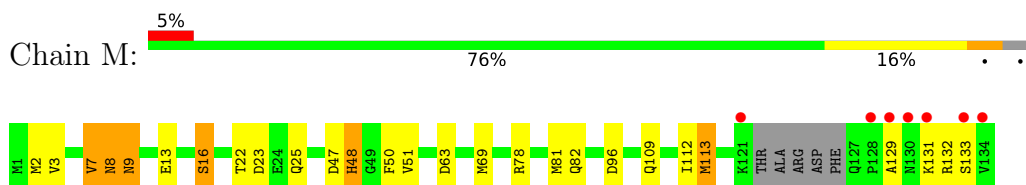
- Molecule 2: Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic



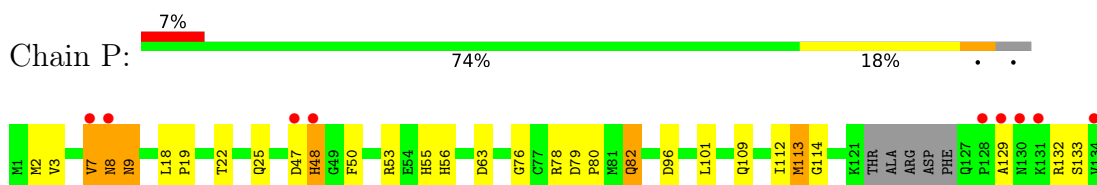
- Molecule 2: Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic



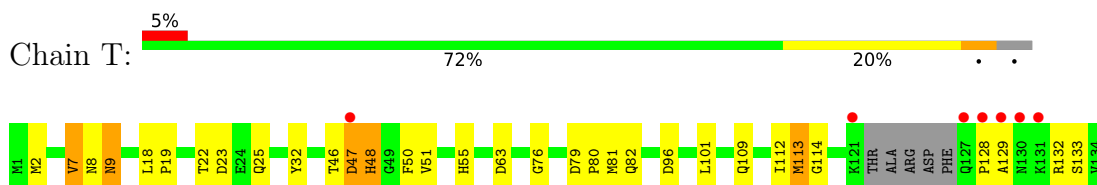
- Molecule 2: Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic



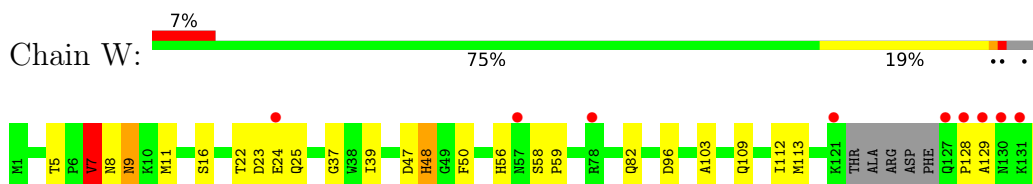
- Molecule 2: Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic



- Molecule 2: Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic



- Molecule 2: Ribulose biphosphate carboxylase small chain 1, chloroplastic, Ribulose biphosphate carboxylase small chain 2, chloroplastic, Ribulose biphosphate carboxylase small chain 1, chloroplastic



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	220.01Å 224.08Å 111.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.81 – 2.38	Depositor EDS
% Data completeness (in resolution range)	93.3 (50.00-2.40) 92.0 (49.81-2.38)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.39Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.230 0.190 , 0.229	Depositor DCC
R_{free} test set	10149 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtrriage
Anisotropy	0.402	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.037 for k,h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	40055	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, HYP, KCX, SMC, MG, CAP

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	0.66	0/3686	0.80	6/4981 (0.1%)
1	B	0.67	0/3684	0.80	11/4979 (0.2%)
1	E	0.66	0/3695	0.80	6/4993 (0.1%)
1	H	0.67	0/3700	0.81	6/5000 (0.1%)
1	K	0.68	0/3728	0.79	5/5037 (0.1%)
1	O	0.66	0/3711	0.81	8/5014 (0.2%)
1	R	0.67	0/3686	0.80	9/4981 (0.2%)
1	V	0.66	0/3690	0.81	7/4986 (0.1%)
2	C	0.66	0/1109	0.81	4/1506 (0.3%)
2	F	0.68	0/1138	0.78	2/1545 (0.1%)
2	I	0.65	0/1117	0.75	1/1517 (0.1%)
2	J	0.70	0/1117	0.77	3/1516 (0.2%)
2	M	0.65	0/1109	0.80	4/1506 (0.3%)
2	P	0.67	0/1109	0.76	4/1506 (0.3%)
2	T	0.66	0/1122	0.78	4/1524 (0.3%)
2	W	0.68	0/1123	0.77	3/1524 (0.2%)
All	All	0.67	0/38524	0.80	83/52115 (0.2%)

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
2	C	0	1
2	F	0	1
2	I	0	1
2	J	0	1
2	M	0	1
2	P	0	1
2	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	W	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	86	ASP	CB-CG-OD2	7.02	124.61	118.30
1	E	351	ASP	CB-CG-OD2	6.94	124.54	118.30
1	O	160	ASP	CB-CG-OD2	6.75	124.38	118.30
1	R	286	ASP	CB-CG-OD2	6.44	124.09	118.30
1	R	160	ASP	CB-CG-OD2	6.36	124.02	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	7	VAL	Peptide
2	F	7	VAL	Peptide
2	I	7	VAL	Peptide
2	J	7	VAL	Peptide
2	M	7	VAL	Peptide

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	3637	0	3546	41	0
1	B	3641	0	3549	52	0
1	E	3640	0	3544	56	0
1	H	3657	0	3569	50	0
1	K	3669	0	3583	43	0
1	O	3661	0	3570	49	0
1	R	3637	0	3546	54	0
1	V	3641	0	3549	57	0
2	C	1070	0	1035	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1083	0	1043	27	0
2	I	1073	0	1037	31	0
2	J	1072	0	1036	17	0
2	M	1070	0	1035	25	0
2	P	1070	0	1035	26	0
2	T	1078	0	1040	27	0
2	W	1073	0	1037	28	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	8	0	0
4	E	21	0	8	0	0
4	H	21	0	8	1	0
4	K	21	0	7	0	0
4	O	21	0	7	0	0
4	R	21	0	7	0	0
4	V	21	0	9	0	0
5	A	24	0	36	0	0
5	B	20	0	30	2	0
5	C	8	0	12	0	0
5	E	20	0	30	2	0
5	F	4	0	6	3	0
5	H	16	0	24	2	0
5	I	4	0	6	0	0
5	J	4	0	6	0	0
5	K	20	0	30	2	0
5	M	4	0	6	0	0
5	O	24	0	36	6	0
5	P	4	0	6	1	0
5	R	28	0	42	4	0
5	T	8	0	12	5	0
5	V	24	0	36	3	0
5	W	4	0	6	2	0
6	A	178	0	0	9	0
6	B	201	0	0	11	0
6	C	55	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	186	0	0	13	0
6	F	52	0	0	8	0
6	H	166	0	0	12	0
6	I	68	0	0	15	0
6	J	31	0	0	1	0
6	K	192	0	0	11	0
6	M	47	0	0	5	0
6	O	188	0	0	15	0
6	P	51	0	0	7	0
6	R	183	0	0	19	0
6	T	48	0	0	6	0
6	V	195	0	0	21	0
6	W	50	0	0	13	0
All	All	40055	0	37139	558	0

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 8.

The worst 5 of 558 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:107:GLN:HG3	6:I:2053:HOH:O	1.45	1.13
1:R:169:LEU:HB3	6:R:2077:HOH:O	1.51	1.10
2:P:8:ASN:HB2	6:P:2005:HOH:O	1.49	1.09
1:K:460:GLU:HB3	6:K:2174:HOH:O	1.56	1.04
1:K:267:HIS:CD2	1:K:277:ASN:HD22	1.76	1.03

There are no symmetry-related clashes.

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	460/475 (97%)	448 (97%)	12 (3%)	0	100	100
1	B	461/475 (97%)	446 (97%)	15 (3%)	0	100	100
1	E	461/475 (97%)	448 (97%)	13 (3%)	0	100	100
1	H	463/475 (98%)	450 (97%)	13 (3%)	0	100	100
1	K	466/475 (98%)	453 (97%)	13 (3%)	0	100	100
1	O	464/475 (98%)	449 (97%)	15 (3%)	0	100	100
1	R	460/475 (97%)	446 (97%)	14 (3%)	0	100	100
1	V	461/475 (97%)	449 (97%)	12 (3%)	0	100	100
2	C	126/134 (94%)	118 (94%)	8 (6%)	0	100	100
2	F	129/134 (96%)	120 (93%)	7 (5%)	2 (2%)	9	13
2	I	127/134 (95%)	118 (93%)	7 (6%)	2 (2%)	9	13
2	J	127/134 (95%)	121 (95%)	6 (5%)	0	100	100
2	M	126/134 (94%)	120 (95%)	6 (5%)	0	100	100
2	P	126/134 (94%)	118 (94%)	8 (6%)	0	100	100
2	T	127/134 (95%)	121 (95%)	6 (5%)	0	100	100
2	W	128/134 (96%)	121 (94%)	7 (6%)	0	100	100
All	All	4712/4872 (97%)	4546 (96%)	162 (3%)	4 (0%)	100	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	8[A]	ASN
2	F	8[B]	ASN
2	I	8[A]	ASN
2	I	8[B]	ASN

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	370/376 (98%)	357 (96%)	13 (4%)	36	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	369/376 (98%)	355 (96%)	14 (4%)	33	51
1	E	371/376 (99%)	358 (96%)	13 (4%)	36	55
1	H	371/376 (99%)	355 (96%)	16 (4%)	29	46
1	K	374/376 (100%)	363 (97%)	11 (3%)	42	62
1	O	372/376 (99%)	360 (97%)	12 (3%)	39	59
1	R	370/376 (98%)	357 (96%)	13 (4%)	36	55
1	V	370/376 (98%)	354 (96%)	16 (4%)	29	46
2	C	115/118 (98%)	107 (93%)	8 (7%)	15	24
2	F	118/118 (100%)	109 (92%)	9 (8%)	13	20
2	I	116/118 (98%)	109 (94%)	7 (6%)	19	31
2	J	116/118 (98%)	107 (92%)	9 (8%)	12	19
2	M	115/118 (98%)	105 (91%)	10 (9%)	10	15
2	P	115/118 (98%)	108 (94%)	7 (6%)	18	30
2	T	116/118 (98%)	107 (92%)	9 (8%)	12	19
2	W	117/118 (99%)	110 (94%)	7 (6%)	19	31
All	All	3895/3952 (99%)	3721 (96%)	174 (4%)	29	44

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	185	TYR
2	T	47	ASP
1	O	431	ARG
1	R	53	CYS
2	T	113	MET

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

Mol	Chain	Res	Type
2	J	25	GLN
1	V	229	GLN
2	M	9	ASN
1	V	153	HIS
2	W	9	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	H	201	1,3	9,11,12	1.02	0	5,12,14	0.97	0
1	HYP	R	151	1	6,8,9	0.59	0	5,10,12	1.58	2 (40%)
1	KCX	K	201	1,3	9,11,12	1.00	0	5,12,14	0.77	0
1	SMC	V	369	1	5,6,7	0.91	0	2,6,8	0.62	0
1	HYP	B	104	1	6,8,9	0.71	0	5,10,12	1.07	0
1	HYP	K	104	1	6,8,9	0.65	0	5,10,12	1.53	0
1	HYP	A	151	1	6,8,9	0.88	0	5,10,12	1.65	2 (40%)
1	HYP	K	151	1	6,8,9	0.55	0	5,10,12	1.69	2 (40%)
1	SMC	A	369	1	5,6,7	0.78	0	2,6,8	1.26	0
1	HYP	A	104	1	6,8,9	0.76	0	5,10,12	1.21	0
1	SMC	B	256	1	5,6,7	1.05	0	2,6,8	1.29	0
1	SMC	K	256	1	5,6,7	0.67	0	2,6,8	1.29	0
1	KCX	R	201	1,3	9,11,12	0.82	0	5,12,14	0.86	0
1	SMC	A	256	1	5,6,7	1.06	0	2,6,8	2.18	1 (50%)
1	SMC	K	369	1	5,6,7	0.62	0	2,6,8	1.45	0
1	KCX	V	201	1,3	9,11,12	1.10	0	5,12,14	1.76	1 (20%)
1	SMC	H	369	1	5,6,7	1.31	1 (20%)	2,6,8	1.12	0
1	KCX	O	201	1,3	9,11,12	1.00	0	5,12,14	1.50	1 (20%)
1	HYP	R	104	1	6,8,9	0.58	0	5,10,12	1.50	0
1	HYP	H	104	1	6,8,9	0.55	0	5,10,12	1.64	2 (40%)
1	SMC	E	369	1	5,6,7	0.98	1 (20%)	2,6,8	0.98	0
1	HYP	H	151	1	6,8,9	0.82	0	5,10,12	1.18	0
1	SMC	E	256	1	5,6,7	0.72	0	2,6,8	0.95	0
1	KCX	A	201	1,3	9,11,12	0.72	0	5,12,14	1.04	0
1	HYP	E	151	1	6,8,9	0.63	0	5,10,12	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	V	151	1	6,8,9	0.71	0	5,10,12	1.51	0
1	HYP	O	151	1	6,8,9	0.74	0	5,10,12	1.24	0
1	HYP	O	104	1	6,8,9	0.58	0	5,10,12	1.58	1 (20%)
1	KCX	B	201	1,3	9,11,12	1.01	0	5,12,14	0.65	0
1	HYP	V	104	1	6,8,9	0.67	0	5,10,12	1.39	1 (20%)
1	SMC	R	256	1	5,6,7	0.86	0	2,6,8	1.42	0
1	SMC	V	256	1	5,6,7	1.46	1 (20%)	2,6,8	0.67	0
1	SMC	O	256	1	5,6,7	0.82	0	2,6,8	0.55	0
1	HYP	B	151	1	6,8,9	0.64	0	5,10,12	1.13	0
1	KCX	E	201	1,3	9,11,12	0.97	0	5,12,14	0.97	1 (20%)
1	SMC	H	256	1	5,6,7	0.76	0	2,6,8	1.92	1 (50%)
1	SMC	R	369	1	5,6,7	0.95	0	2,6,8	0.97	0
1	HYP	E	104	1	6,8,9	0.95	0	5,10,12	1.16	0
1	SMC	B	369	1	5,6,7	1.35	1 (20%)	2,6,8	0.22	0
1	SMC	O	369	1	5,6,7	0.47	0	2,6,8	1.49	0

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

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	256	SMC	CB-SG	3.03	1.85	1.80
1	B	369	SMC	CB-SG	2.78	1.84	1.80
1	H	369	SMC	CB-SG	2.65	1.84	1.80
1	E	369	SMC	CB-SG	2.00	1.83	1.80

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	201	KCX	OQ1-CX-NZ	-3.74	119.15	124.96
1	O	201	KCX	OQ1-CX-NZ	-2.96	120.37	124.96
1	A	256	SMC	CA-CB-SG	-2.82	109.49	114.04
1	H	104	HYP	OD1-CG-CB	-2.41	104.08	110.03
1	R	151	HYP	CB-CG-CD	-2.35	100.39	103.27

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 8 are monoatomic - leaving 62 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	V	1478	-	3,3,3	0.53	0	2,2,2	0.53	0
4	CAP	H	1477	3	17,20,20	1.67	2 (11%)	22,31,31	0.91	1 (4%)
4	CAP	K	1477	3	17,20,20	1.65	1 (5%)	22,31,31	1.42	2 (9%)
5	EDO	K	1481	-	3,3,3	0.36	0	2,2,2	0.14	0
5	EDO	A	1483	-	3,3,3	0.47	0	2,2,2	0.17	0
5	EDO	O	1478	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	V	1482	-	3,3,3	0.28	0	2,2,2	0.33	0
5	EDO	E	1482	-	3,3,3	0.62	0	2,2,2	0.69	0
5	EDO	A	1479	-	3,3,3	0.31	0	2,2,2	0.26	0
5	EDO	R	1478	-	3,3,3	0.35	0	2,2,2	0.22	0
5	EDO	T	1136	-	3,3,3	0.34	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1482	-	3,3,3	0.37	0	2,2,2	0.28	0
5	EDO	R	1481	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	V	1483	-	3,3,3	0.44	0	2,2,2	0.23	0
5	EDO	W	1135	-	3,3,3	0.32	0	2,2,2	0.18	0
4	CAP	R	1477	3	17,20,20	1.68	2 (11%)	22,31,31	1.11	1 (4%)
5	EDO	O	1481	-	3,3,3	0.46	0	2,2,2	0.24	0
5	EDO	O	1480	-	3,3,3	0.36	0	2,2,2	0.18	0
5	EDO	A	1478	-	3,3,3	0.23	0	2,2,2	0.40	0
5	EDO	E	1479	-	3,3,3	0.37	0	2,2,2	0.41	0
5	EDO	V	1480	-	3,3,3	0.33	0	2,2,2	0.24	0
5	EDO	B	1482	-	3,3,3	0.41	0	2,2,2	0.45	0
5	EDO	A	1480	-	3,3,3	0.35	0	2,2,2	0.41	0
5	EDO	H	1478	-	3,3,3	0.48	0	2,2,2	0.08	0
5	EDO	K	1482	-	3,3,3	0.34	0	2,2,2	0.20	0
5	EDO	A	1481	-	3,3,3	0.31	0	2,2,2	0.46	0
5	EDO	J	1135	-	3,3,3	0.23	0	2,2,2	0.44	0
5	EDO	K	1480	-	3,3,3	0.38	0	2,2,2	0.11	0
5	EDO	B	1479	-	3,3,3	0.28	0	2,2,2	0.91	0
5	EDO	B	1480	-	3,3,3	0.32	0	2,2,2	0.17	0
5	EDO	I	1135	-	3,3,3	0.26	0	2,2,2	0.52	0
5	EDO	K	1479	-	3,3,3	0.36	0	2,2,2	0.69	0
4	CAP	B	1477	3	17,20,20	1.71	2 (11%)	22,31,31	1.14	3 (13%)
5	EDO	B	1481	-	3,3,3	0.32	0	2,2,2	0.35	0
5	EDO	P	1135	-	3,3,3	0.26	0	2,2,2	0.44	0
4	CAP	A	1477	3	17,20,20	1.60	1 (5%)	22,31,31	0.96	1 (4%)
5	EDO	R	1482	-	3,3,3	0.34	0	2,2,2	0.13	0
5	EDO	O	1482	-	3,3,3	0.23	0	2,2,2	0.37	0
5	EDO	M	1135	-	3,3,3	0.31	0	2,2,2	0.13	0
5	EDO	E	1478	-	3,3,3	0.39	0	2,2,2	0.13	0
5	EDO	R	1480	-	3,3,3	0.34	0	2,2,2	0.33	0
5	EDO	H	1479	-	3,3,3	0.38	0	2,2,2	0.58	0
5	EDO	R	1484	-	3,3,3	0.34	0	2,2,2	0.19	0
5	EDO	E	1480	-	3,3,3	0.27	0	2,2,2	0.36	0
5	EDO	F	1135	-	3,3,3	0.31	0	2,2,2	0.27	0
5	EDO	H	1481	-	3,3,3	0.25	0	2,2,2	0.33	0
4	CAP	E	1477	3	17,20,20	1.67	1 (5%)	22,31,31	1.44	5 (22%)
4	CAP	V	1477	3	17,20,20	1.76	2 (11%)	22,31,31	1.10	1 (4%)
5	EDO	E	1481	-	3,3,3	0.32	0	2,2,2	0.11	0
5	EDO	V	1479	-	3,3,3	0.39	0	2,2,2	0.14	0
5	EDO	V	1481	-	3,3,3	0.30	0	2,2,2	0.54	0
4	CAP	O	1477	3	17,20,20	1.64	2 (11%)	22,31,31	1.64	6 (27%)
5	EDO	B	1478	-	3,3,3	0.41	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	O	1479	-	3,3,3	0.33	0	2,2,2	0.55	0
5	EDO	K	1478	-	3,3,3	0.26	0	2,2,2	0.19	0
5	EDO	C	1135	-	3,3,3	0.30	0	2,2,2	0.39	0
5	EDO	R	1479	-	3,3,3	0.39	0	2,2,2	0.23	0
5	EDO	R	1483	-	3,3,3	0.53	0	2,2,2	0.58	0
5	EDO	O	1483	-	3,3,3	0.42	0	2,2,2	0.41	0
5	EDO	H	1480	-	3,3,3	0.29	0	2,2,2	0.24	0
5	EDO	C	1136	-	3,3,3	0.31	0	2,2,2	0.20	0
5	EDO	T	1135	-	3,3,3	0.37	0	2,2,2	0.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	V	1478	-	-	1/1/1/1	-
4	CAP	H	1477	3	-	10/29/29/29	-
4	CAP	K	1477	3	-	8/29/29/29	-
5	EDO	K	1481	-	-	0/1/1/1	-
5	EDO	A	1483	-	-	0/1/1/1	-
5	EDO	O	1478	-	-	0/1/1/1	-
5	EDO	V	1482	-	-	0/1/1/1	-
5	EDO	E	1482	-	-	0/1/1/1	-
5	EDO	A	1479	-	-	0/1/1/1	-
5	EDO	R	1478	-	-	0/1/1/1	-
5	EDO	T	1136	-	-	0/1/1/1	-
5	EDO	A	1482	-	-	1/1/1/1	-
5	EDO	R	1481	-	-	0/1/1/1	-
5	EDO	V	1483	-	-	1/1/1/1	-
5	EDO	W	1135	-	-	1/1/1/1	-
4	CAP	R	1477	3	-	7/29/29/29	-
5	EDO	O	1481	-	-	0/1/1/1	-
5	EDO	O	1480	-	-	1/1/1/1	-
5	EDO	A	1478	-	-	0/1/1/1	-
5	EDO	E	1479	-	-	1/1/1/1	-
5	EDO	V	1480	-	-	1/1/1/1	-
5	EDO	B	1482	-	-	1/1/1/1	-
5	EDO	A	1480	-	-	1/1/1/1	-
5	EDO	H	1478	-	-	0/1/1/1	-
5	EDO	K	1482	-	-	1/1/1/1	-
5	EDO	A	1481	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	J	1135	-	-	0/1/1/1	-
5	EDO	K	1480	-	-	1/1/1/1	-
5	EDO	B	1479	-	-	1/1/1/1	-
5	EDO	B	1480	-	-	0/1/1/1	-
5	EDO	I	1135	-	-	1/1/1/1	-
5	EDO	K	1479	-	-	1/1/1/1	-
4	CAP	B	1477	3	-	9/29/29/29	-
5	EDO	B	1481	-	-	1/1/1/1	-
5	EDO	P	1135	-	-	1/1/1/1	-
4	CAP	A	1477	3	-	6/29/29/29	-
5	EDO	R	1482	-	-	0/1/1/1	-
5	EDO	O	1482	-	-	1/1/1/1	-
5	EDO	M	1135	-	-	0/1/1/1	-
5	EDO	E	1478	-	-	0/1/1/1	-
5	EDO	R	1480	-	-	1/1/1/1	-
5	EDO	H	1479	-	-	0/1/1/1	-
5	EDO	R	1484	-	-	0/1/1/1	-
5	EDO	E	1480	-	-	0/1/1/1	-
5	EDO	F	1135	-	-	1/1/1/1	-
5	EDO	H	1481	-	-	1/1/1/1	-
4	CAP	E	1477	3	-	8/29/29/29	-
4	CAP	V	1477	3	-	7/29/29/29	-
5	EDO	E	1481	-	-	1/1/1/1	-
5	EDO	V	1479	-	-	0/1/1/1	-
5	EDO	V	1481	-	-	0/1/1/1	-
4	CAP	O	1477	3	-	9/29/29/29	-
5	EDO	B	1478	-	-	0/1/1/1	-
5	EDO	O	1479	-	-	0/1/1/1	-
5	EDO	K	1478	-	-	0/1/1/1	-
5	EDO	C	1135	-	-	1/1/1/1	-
5	EDO	R	1479	-	-	1/1/1/1	-
5	EDO	R	1483	-	-	0/1/1/1	-
5	EDO	O	1483	-	-	1/1/1/1	-
5	EDO	H	1480	-	-	1/1/1/1	-
5	EDO	C	1136	-	-	1/1/1/1	-
5	EDO	T	1135	-	-	1/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1477	CAP	O6-C	6.26	1.42	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	1477	CAP	O6-C	6.04	1.41	1.22
4	E	1477	CAP	O6-C	6.02	1.41	1.22
4	K	1477	CAP	O6-C	5.87	1.41	1.22
4	O	1477	CAP	O6-C	5.85	1.41	1.22

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1477	CAP	O2-C2-C	-4.39	100.94	108.97
4	O	1477	CAP	O2-C2-C	-3.12	103.28	108.97
4	E	1477	CAP	O4-C4-C5	-2.99	103.19	109.92
4	O	1477	CAP	O4-C4-C5	-2.98	103.21	109.92
4	O	1477	CAP	O4-C4-C3	-2.78	103.22	108.78

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

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

There are no ring outliers.

18 monomers are involved in 33 short contacts:

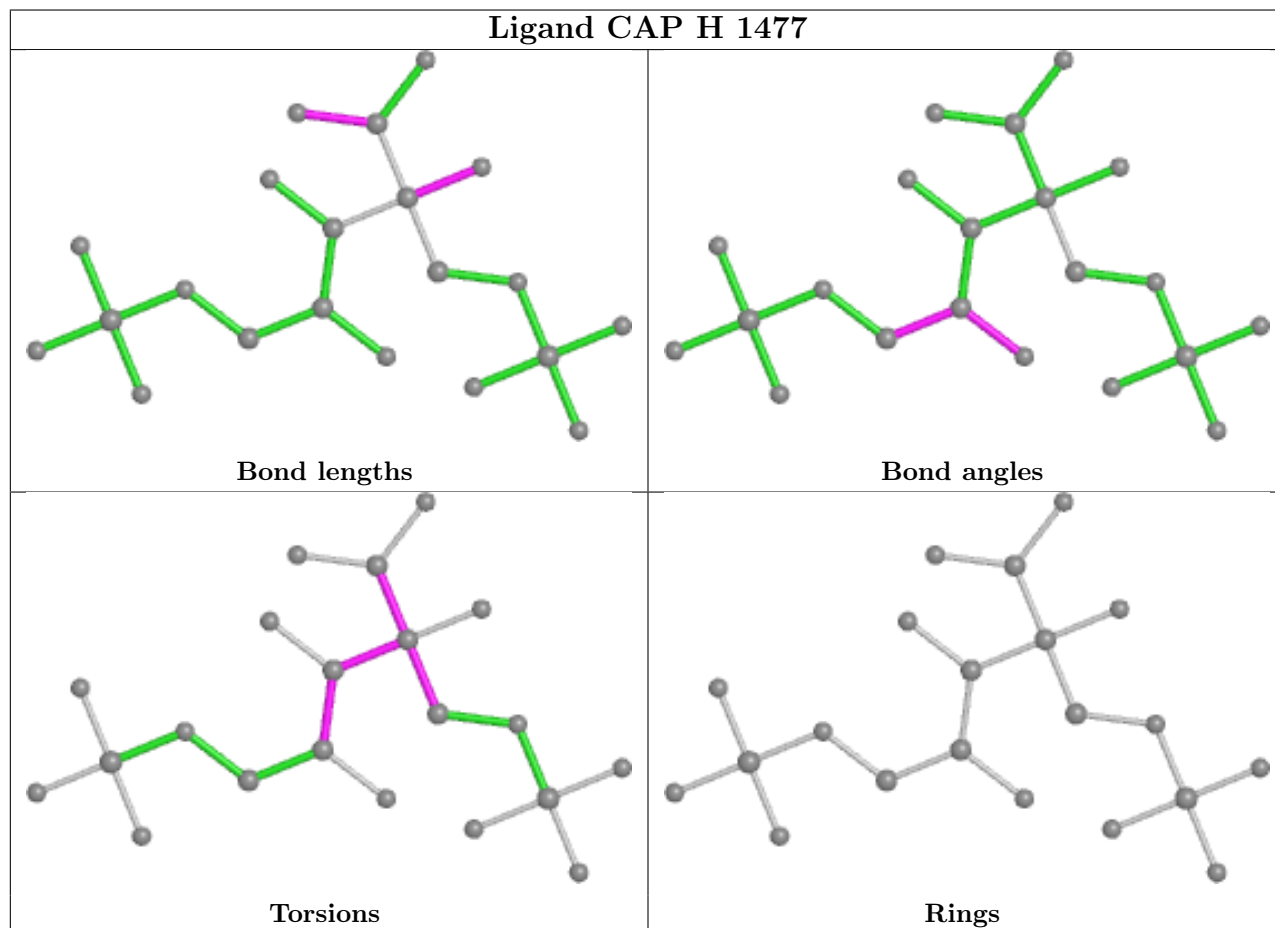
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	1478	EDO	1	0
4	H	1477	CAP	1	0
5	V	1482	EDO	1	0
5	T	1136	EDO	3	0
5	W	1135	EDO	2	0
5	V	1480	EDO	1	0
5	B	1482	EDO	1	0
5	H	1478	EDO	1	0
5	B	1479	EDO	1	0
5	K	1479	EDO	2	0
5	P	1135	EDO	1	0
5	R	1482	EDO	3	0
5	E	1480	EDO	2	0

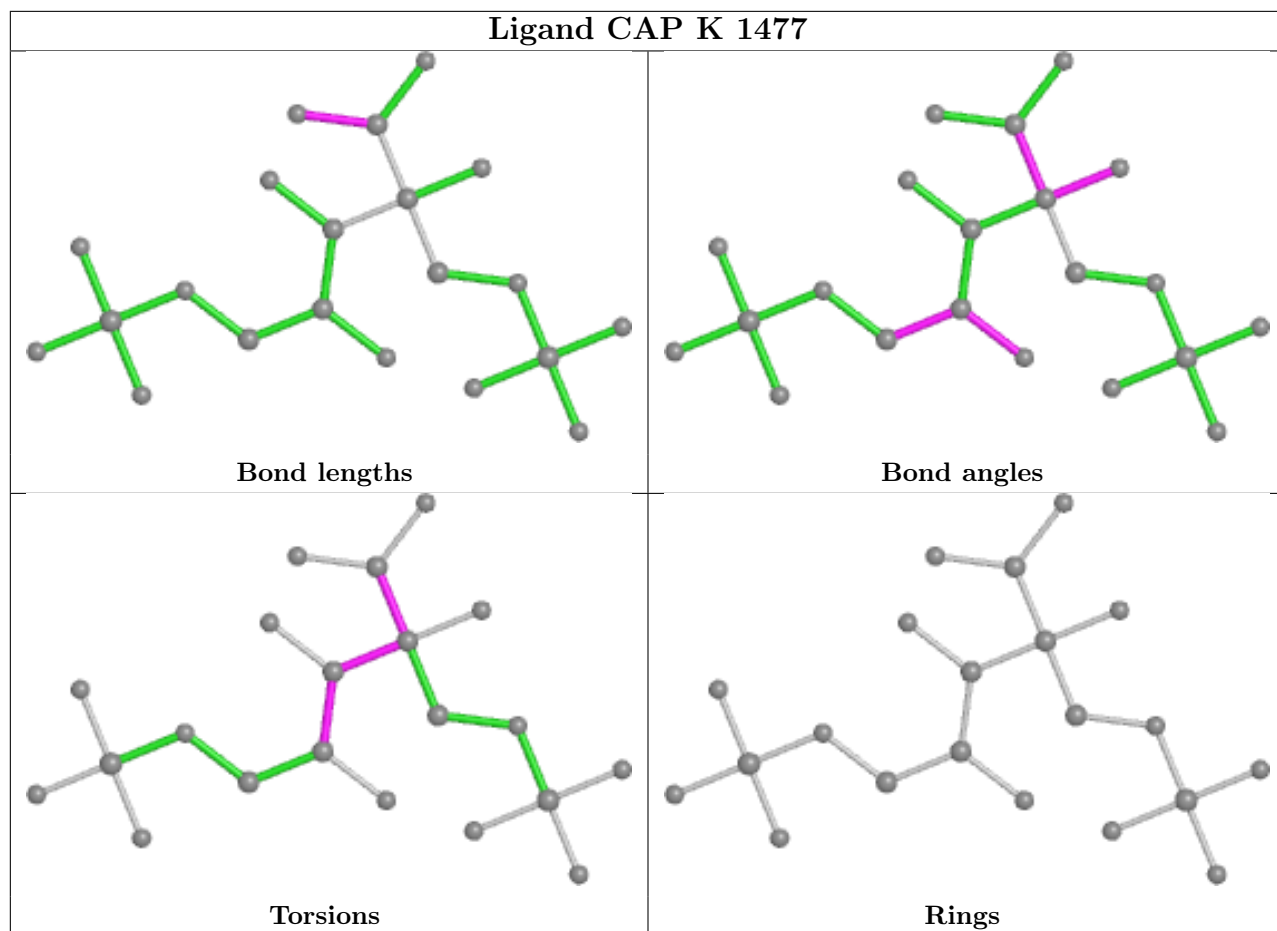
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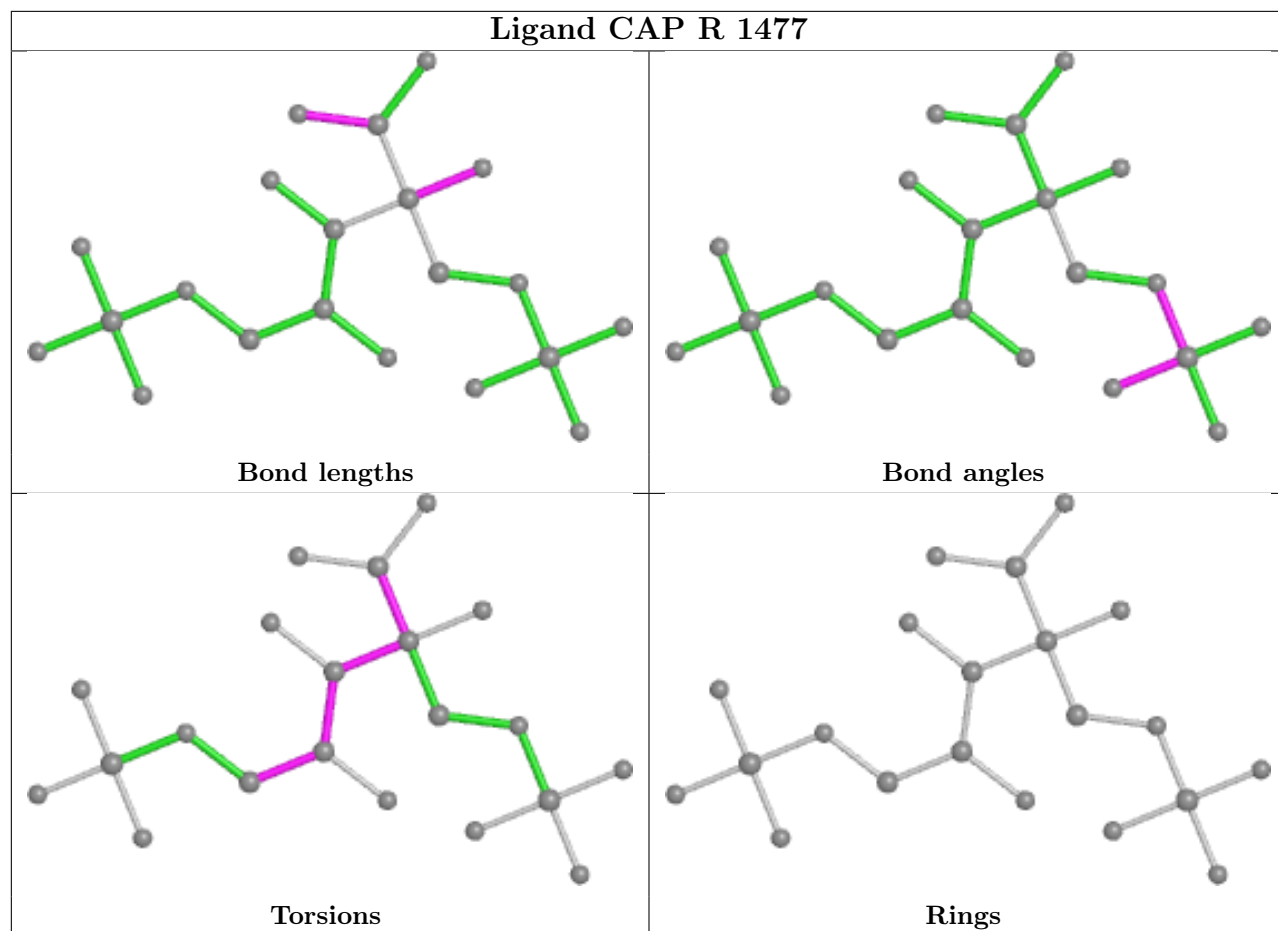
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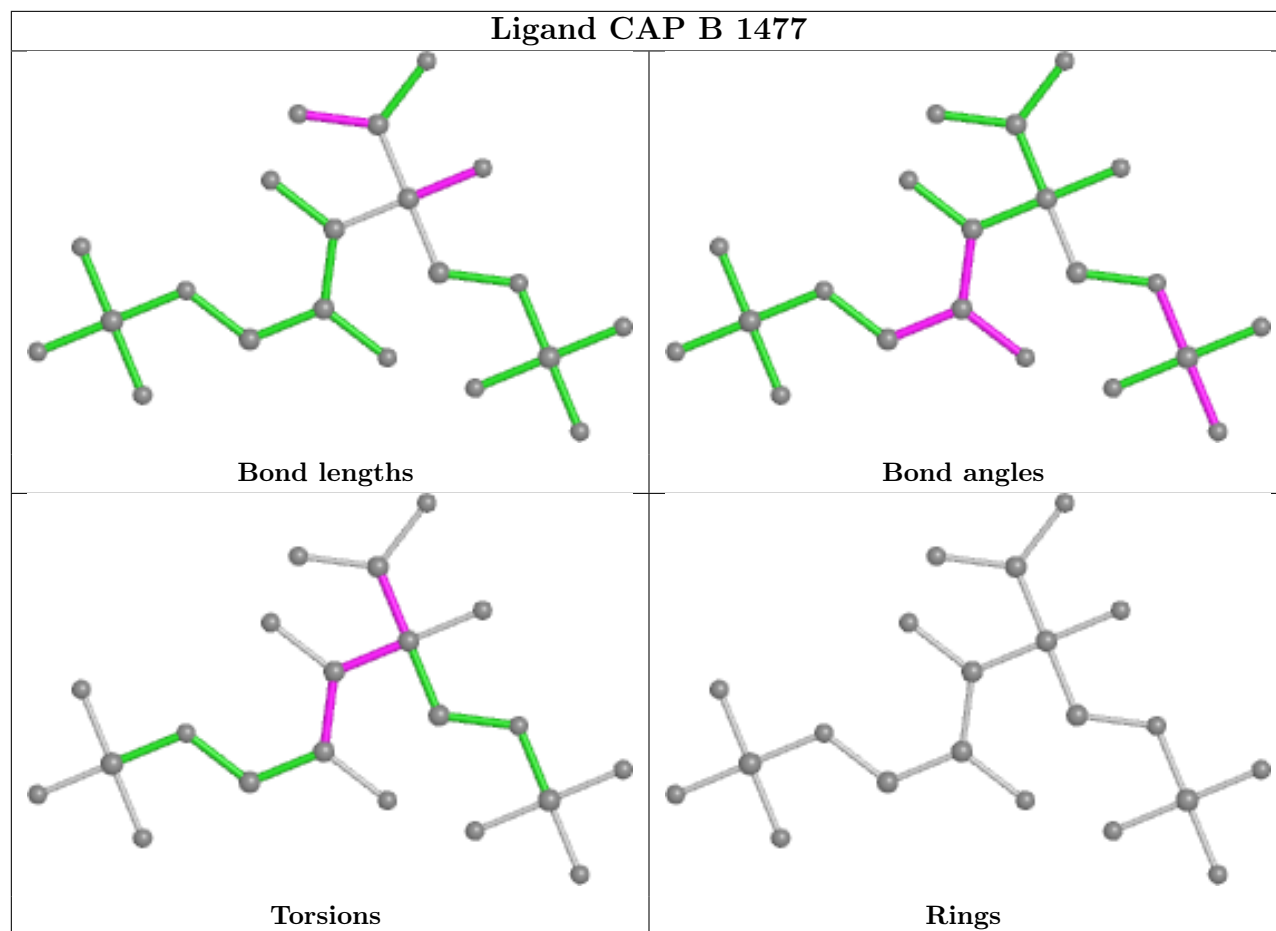
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1135	EDO	3	0
5	R	1483	EDO	1	0
5	O	1483	EDO	6	0
5	H	1480	EDO	1	0
5	T	1135	EDO	2	0

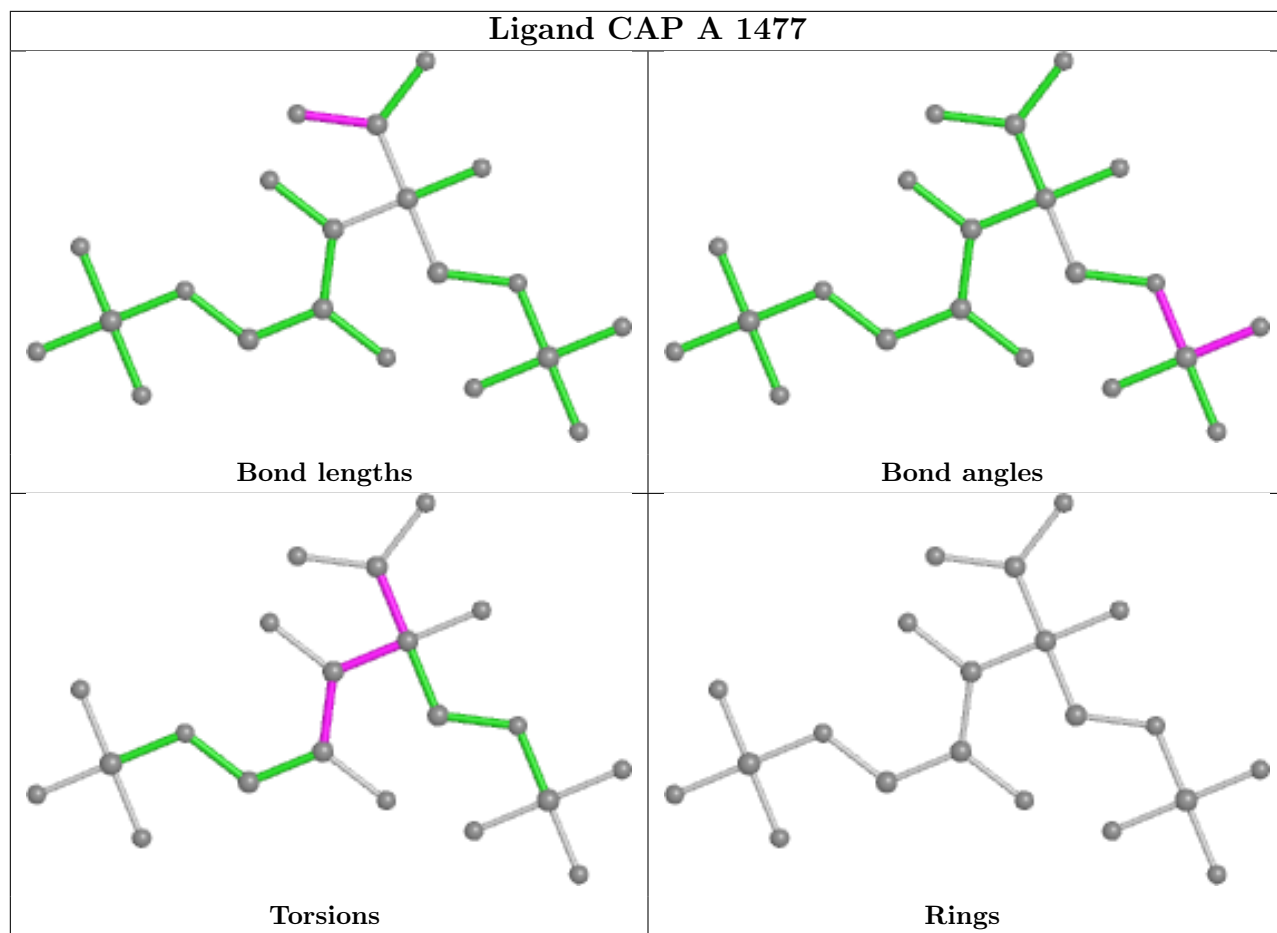
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

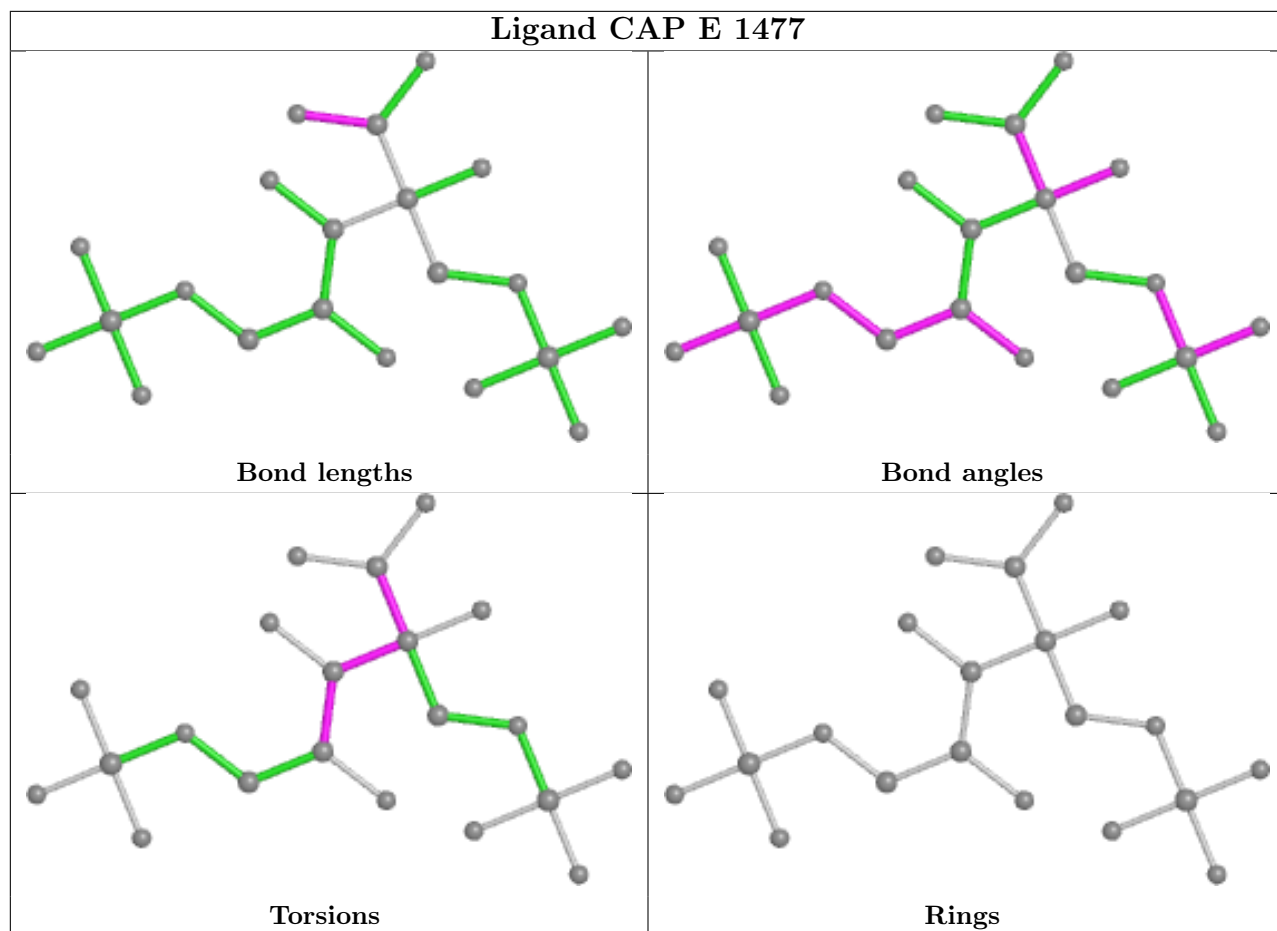


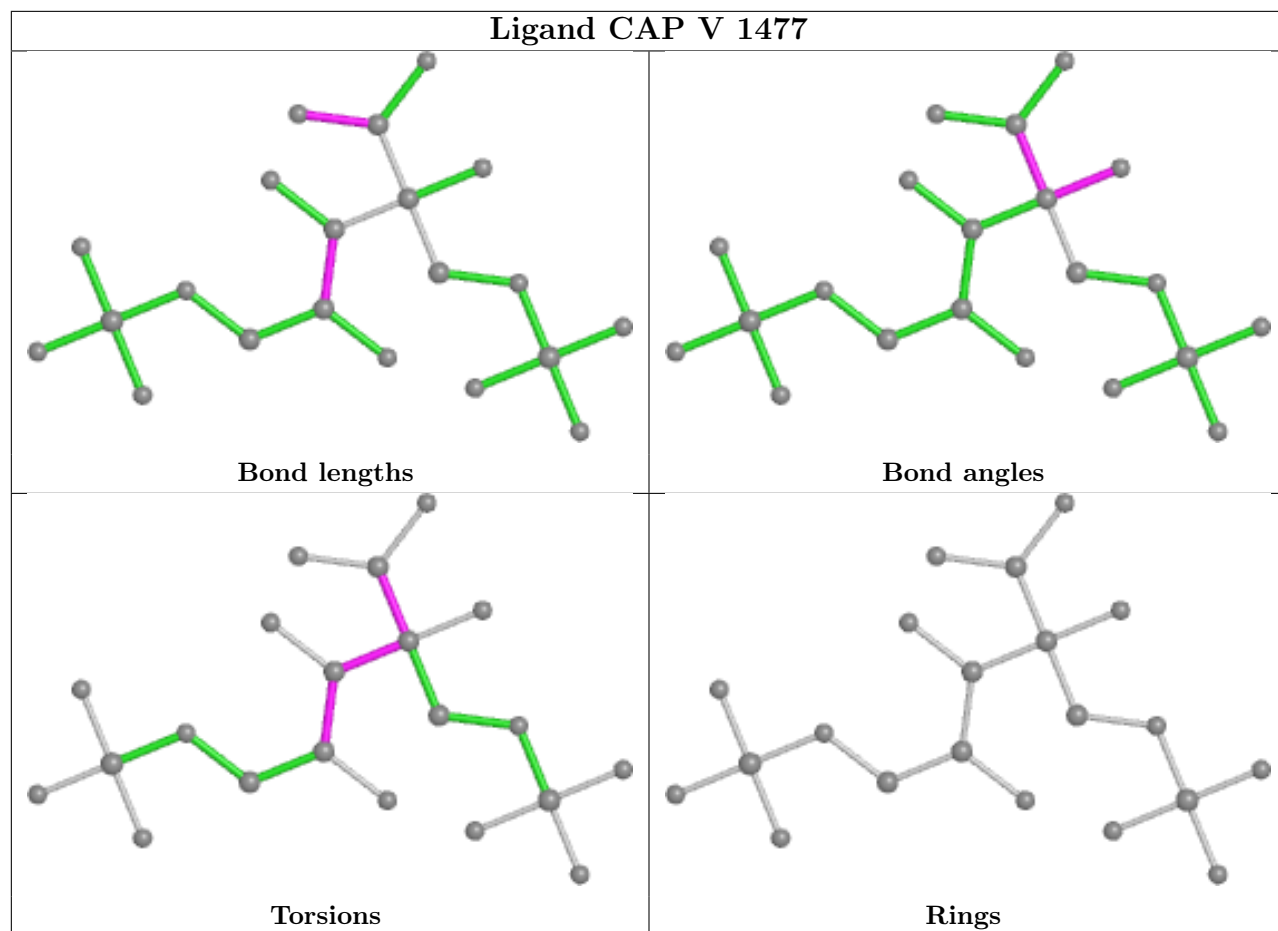


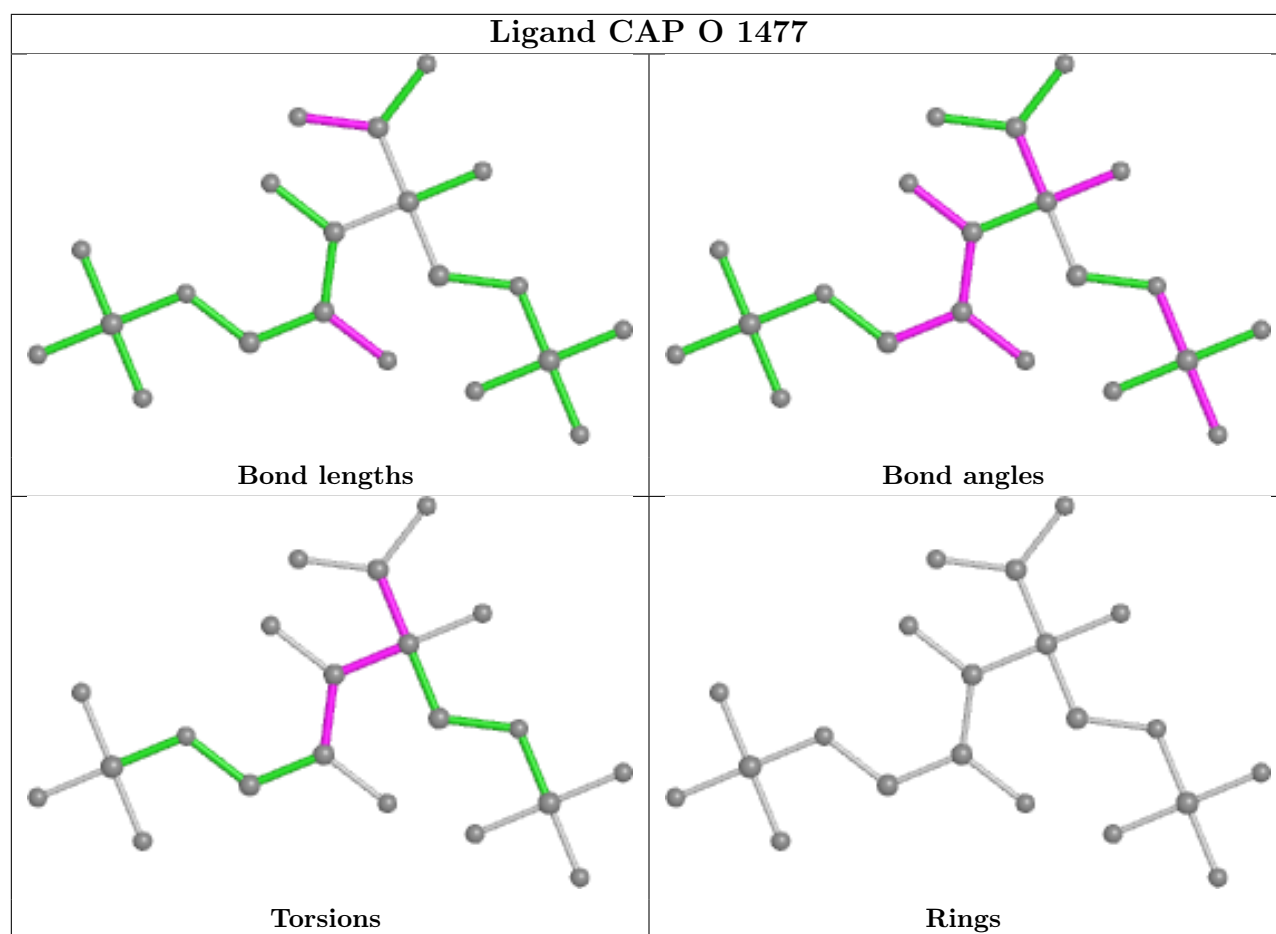












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	460/475 (96%)	-0.61	3 (0%) 87 86	9, 16, 32, 49	0
1	B	462/475 (97%)	-0.62	5 (1%) 80 79	9, 16, 33, 55	0
1	E	460/475 (96%)	-0.71	0 100 100	9, 16, 32, 49	0
1	H	464/475 (97%)	-0.63	5 (1%) 80 79	9, 16, 34, 70	0
1	K	464/475 (97%)	-0.63	7 (1%) 73 72	9, 16, 34, 66	0
1	O	464/475 (97%)	-0.62	5 (1%) 80 79	9, 16, 34, 66	0
1	R	460/475 (96%)	-0.66	1 (0%) 95 94	9, 16, 32, 49	0
1	V	461/475 (97%)	-0.59	3 (0%) 87 86	9, 16, 32, 49	0
2	C	129/134 (96%)	-0.06	6 (4%) 31 30	14, 25, 50, 58	0
2	F	129/134 (96%)	-0.07	10 (7%) 13 11	14, 25, 50, 58	0
2	I	129/134 (96%)	-0.25	8 (6%) 20 19	14, 25, 50, 58	0
2	J	129/134 (96%)	-0.11	5 (3%) 39 38	14, 26, 50, 58	0
2	M	129/134 (96%)	-0.13	7 (5%) 25 24	15, 25, 50, 58	0
2	P	129/134 (96%)	-0.16	9 (6%) 16 15	14, 25, 50, 58	0
2	T	129/134 (96%)	-0.21	7 (5%) 25 24	14, 25, 50, 58	0
2	W	129/134 (96%)	0.00	10 (7%) 13 11	14, 25, 50, 58	0
All	All	4727/4872 (97%)	-0.52	91 (1%) 66 64	9, 18, 38, 70	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	129	ALA	6.0
2	F	130	ASN	5.9
2	W	128	PRO	5.8
1	B	9	ALA	5.6
2	W	130	ASN	5.6

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	SMC	R	369	7/8	0.94	0.11	18,19,21,26	0
1	HYP	O	104	8/9	0.95	0.11	12,13,14,17	0
1	HYP	E	151	8/9	0.95	0.11	12,13,14,14	0
1	KCX	V	201	12/13	0.95	0.15	11,13,14,14	0
1	HYP	K	151	8/9	0.96	0.08	12,13,14,14	0
1	SMC	K	369	7/8	0.96	0.09	18,19,21,26	0
1	SMC	A	369	7/8	0.96	0.10	18,19,21,25	0
1	SMC	O	369	7/8	0.96	0.09	18,19,21,25	0
1	KCX	E	201	12/13	0.96	0.12	11,13,14,15	0
1	HYP	V	104	8/9	0.96	0.10	11,13,14,17	0
1	SMC	H	369	7/8	0.96	0.10	18,19,21,26	0
1	SMC	V	369	7/8	0.96	0.10	18,19,21,26	0
1	SMC	B	369	7/8	0.97	0.07	18,19,21,26	0
1	SMC	E	369	7/8	0.97	0.08	18,19,21,25	0
1	HYP	O	151	8/9	0.97	0.13	12,13,13,13	0
1	KCX	O	201	12/13	0.97	0.15	11,13,14,14	0
1	HYP	H	151	8/9	0.97	0.12	12,13,14,14	0
1	HYP	R	104	8/9	0.97	0.10	12,13,13,17	0
1	KCX	H	201	12/13	0.97	0.11	11,13,14,14	0
1	HYP	E	104	8/9	0.97	0.08	12,13,14,17	0
1	HYP	V	151	8/9	0.97	0.11	12,13,14,14	0
1	HYP	K	104	8/9	0.97	0.10	12,13,13,17	0
1	KCX	A	201	12/13	0.97	0.14	11,13,14,14	0
1	HYP	H	104	8/9	0.98	0.10	12,13,13,17	0
1	KCX	B	201	12/13	0.98	0.12	11,13,14,14	0
1	SMC	O	256	7/8	0.98	0.07	6,9,11,11	0
1	SMC	B	256	7/8	0.98	0.07	6,10,11,12	0
1	HYP	A	104	8/9	0.98	0.09	12,13,13,17	0
1	HYP	R	151	8/9	0.98	0.10	12,12,13,13	0
1	KCX	R	201	12/13	0.98	0.14	11,13,14,14	0
1	SMC	R	256	7/8	0.98	0.07	6,10,11,12	0
1	SMC	A	256	7/8	0.98	0.08	6,10,11,12	0
1	HYP	A	151	8/9	0.98	0.14	12,12,14,14	0
1	KCX	K	201	12/13	0.98	0.11	11,13,14,14	0
1	HYP	B	104	8/9	0.98	0.08	12,13,13,16	0
1	SMC	V	256	7/8	0.98	0.08	6,10,11,11	0
1	HYP	B	151	8/9	0.98	0.10	12,13,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SMC	H	256	7/8	0.99	0.05	6,10,11,11	0
1	SMC	K	256	7/8	0.99	0.07	6,9,11,11	0
1	SMC	E	256	7/8	0.99	0.07	6,10,11,11	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	R	1484	4/4	0.42	0.49	84,86,87,88	0
5	EDO	K	1482	4/4	0.62	0.43	62,66,68,69	0
5	EDO	K	1480	4/4	0.72	0.26	42,45,49,51	0
5	EDO	T	1135	4/4	0.74	0.29	56,57,60,62	0
5	EDO	R	1482	4/4	0.76	0.29	49,54,55,56	0
5	EDO	W	1135	4/4	0.80	0.20	40,41,45,47	0
5	EDO	V	1483	4/4	0.81	0.23	42,42,42,43	0
5	EDO	E	1478	4/4	0.82	0.20	43,45,45,47	0
5	EDO	C	1135	4/4	0.83	0.28	61,61,64,65	0
5	EDO	H	1481	4/4	0.83	0.23	40,43,43,49	0
5	EDO	O	1480	4/4	0.83	0.14	40,42,45,45	0
5	EDO	J	1135	4/4	0.83	0.16	37,39,43,50	0
5	EDO	P	1135	4/4	0.84	0.27	57,59,61,61	0
5	EDO	V	1478	4/4	0.86	0.28	28,30,32,32	0
5	EDO	E	1482	4/4	0.86	0.26	23,25,28,33	0
5	EDO	A	1480	4/4	0.86	0.23	30,31,32,34	0
5	EDO	B	1482	4/4	0.88	0.20	34,36,40,44	0
5	EDO	R	1481	4/4	0.88	0.18	28,34,35,37	0
5	EDO	I	1135	4/4	0.88	0.26	37,41,43,51	0
5	EDO	O	1483	4/4	0.88	0.26	28,42,43,48	0
5	EDO	A	1482	4/4	0.89	0.19	39,41,44,45	0
5	EDO	O	1482	4/4	0.89	0.18	40,41,43,44	0
5	EDO	R	1483	4/4	0.89	0.22	31,32,34,36	0
5	EDO	R	1480	4/4	0.89	0.20	41,43,45,47	0
5	EDO	V	1481	4/4	0.90	0.31	39,41,42,44	0

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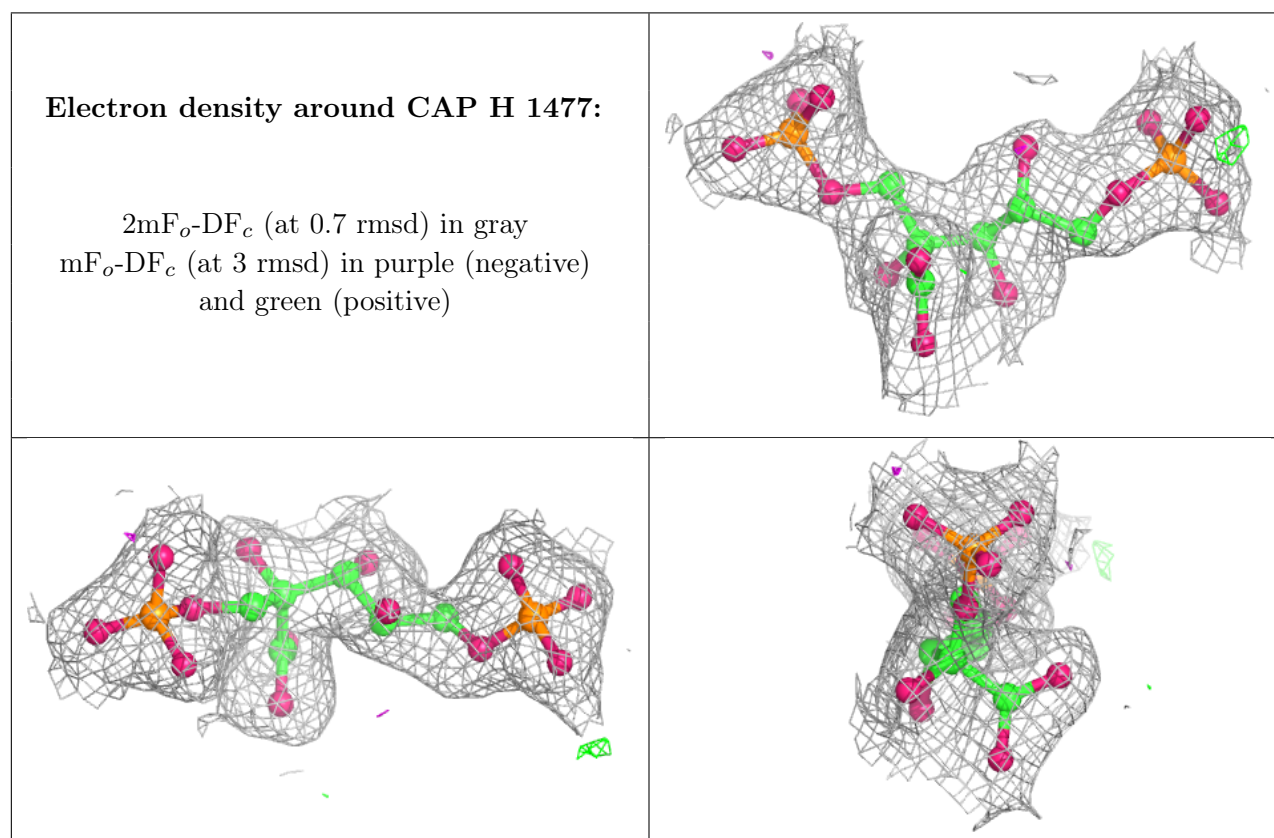
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	O	1478	4/4	0.90	0.16	21,32,33,36	0
5	EDO	A	1483	4/4	0.90	0.20	25,29,35,36	0
5	EDO	T	1136	4/4	0.91	0.13	38,41,45,45	0
5	EDO	F	1135	4/4	0.92	0.20	29,32,33,36	0
5	EDO	H	1478	4/4	0.92	0.15	25,27,31,32	0
5	EDO	B	1480	4/4	0.92	0.21	30,43,46,48	0
5	EDO	M	1135	4/4	0.92	0.16	29,32,33,34	0
5	EDO	B	1481	4/4	0.92	0.14	38,39,40,41	0
5	EDO	C	1136	4/4	0.93	0.14	26,32,35,40	0
5	EDO	A	1478	4/4	0.93	0.13	31,31,32,34	0
5	EDO	E	1481	4/4	0.93	0.23	30,36,40,44	0
5	EDO	B	1478	4/4	0.93	0.13	22,29,30,33	0
5	EDO	E	1480	4/4	0.94	0.26	40,44,45,52	0
5	EDO	V	1479	4/4	0.94	0.13	20,25,28,32	0
5	EDO	K	1481	4/4	0.94	0.20	22,33,35,37	0
3	MG	E	1476	1/1	0.94	0.10	29,29,29,29	0
5	EDO	K	1479	4/4	0.94	0.14	25,32,33,33	0
3	MG	H	1476	1/1	0.95	0.07	24,24,24,24	0
3	MG	K	1476	1/1	0.95	0.08	18,18,18,18	0
5	EDO	R	1478	4/4	0.95	0.13	27,29,31,35	0
5	EDO	V	1482	4/4	0.95	0.15	25,26,27,33	0
5	EDO	H	1479	4/4	0.95	0.13	21,26,27,30	0
5	EDO	K	1478	4/4	0.95	0.17	26,27,29,33	0
3	MG	B	1476	1/1	0.96	0.10	24,24,24,24	0
5	EDO	A	1481	4/4	0.96	0.12	36,38,44,48	0
5	EDO	R	1479	4/4	0.96	0.10	17,18,22,23	0
5	EDO	V	1480	4/4	0.96	0.11	9,16,18,26	0
5	EDO	O	1481	4/4	0.97	0.13	31,31,35,35	0
5	EDO	H	1480	4/4	0.97	0.18	55,55,58,59	0
5	EDO	O	1479	4/4	0.97	0.12	21,24,24,25	0
5	EDO	B	1479	4/4	0.97	0.08	16,16,19,20	0
5	EDO	E	1479	4/4	0.98	0.11	13,19,20,21	0
3	MG	V	1476	1/1	0.98	0.07	17,17,17,17	0
4	CAP	H	1477	21/21	0.98	0.09	7,17,21,25	0
4	CAP	O	1477	21/21	0.98	0.09	7,14,19,23	0
3	MG	A	1476	1/1	0.98	0.09	11,11,11,11	0
4	CAP	A	1477	21/21	0.99	0.08	9,14,21,25	0
5	EDO	A	1479	4/4	0.99	0.07	7,8,10,12	0
4	CAP	B	1477	21/21	0.99	0.10	7,11,17,21	0
4	CAP	E	1477	21/21	0.99	0.09	12,17,20,22	0
3	MG	R	1476	1/1	0.99	0.12	12,12,12,12	0
4	CAP	K	1477	21/21	0.99	0.09	7,14,21,29	0

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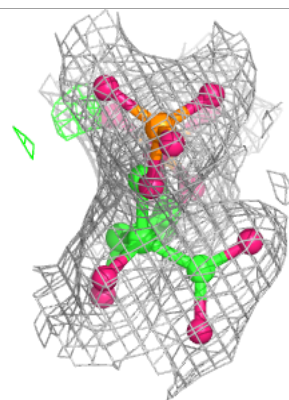
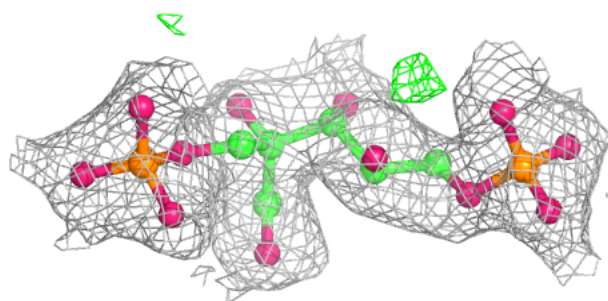
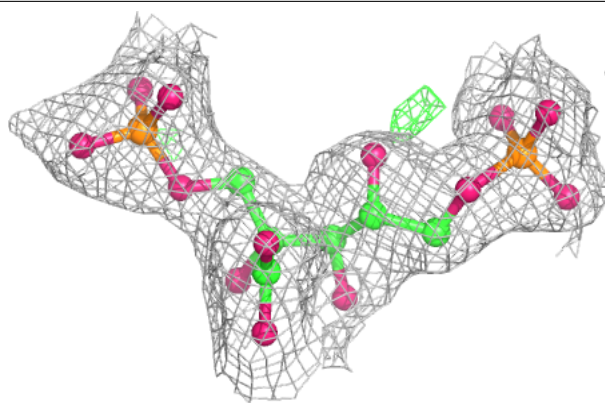
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	O	1476	1/1	0.99	0.10	13,13,13,13	0
4	CAP	R	1477	21/21	0.99	0.12	7,15,21,21	0
4	CAP	V	1477	21/21	0.99	0.10	6,16,19,22	0

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.

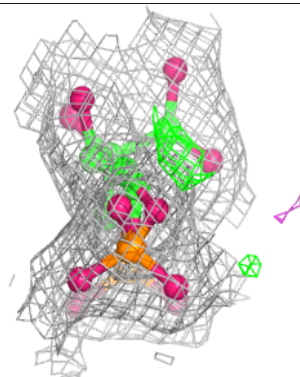
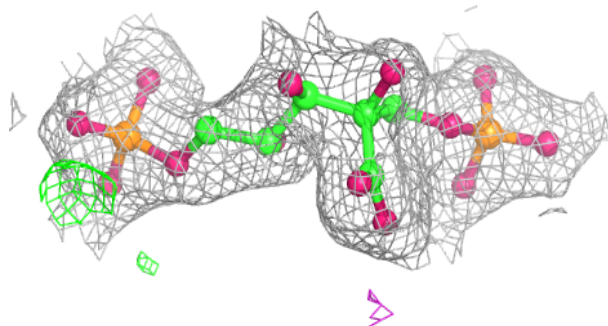
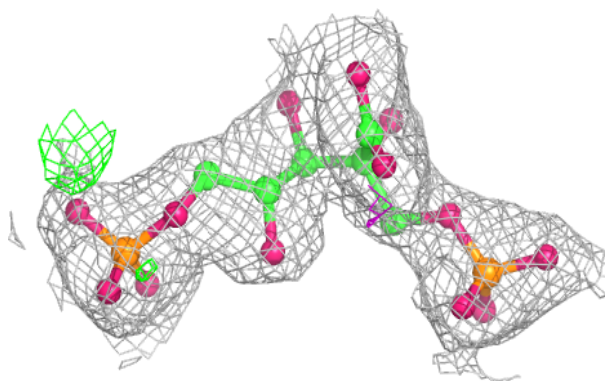


Electron density around CAP O 1477:

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

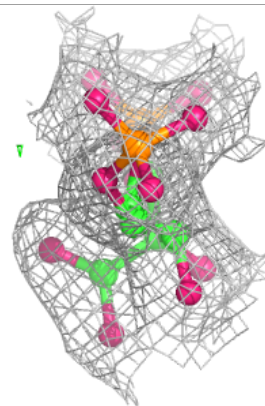
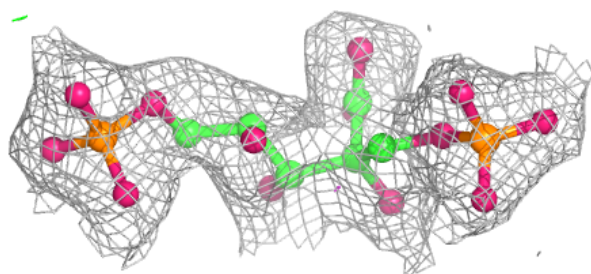
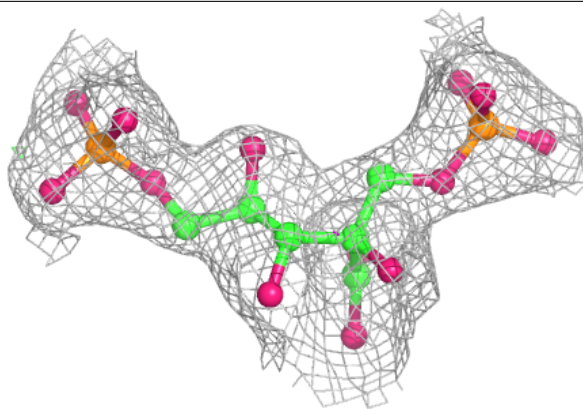
**Electron density around CAP A 1477:**

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

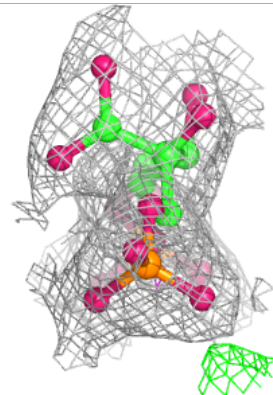
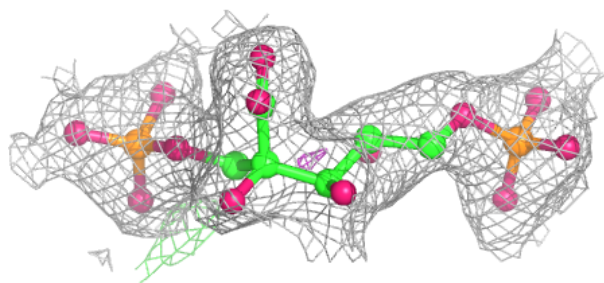
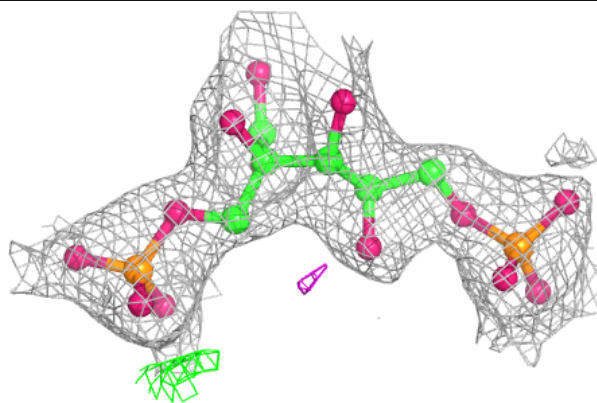


Electron density around CAP B 1477:

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

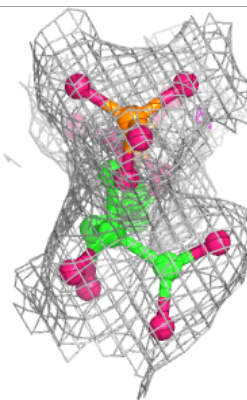
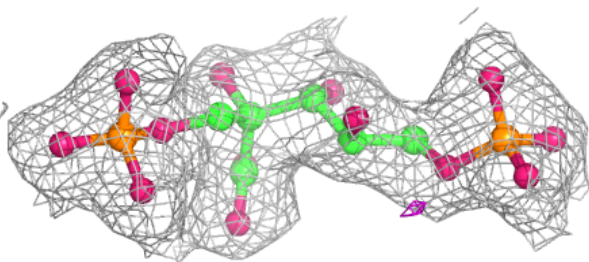
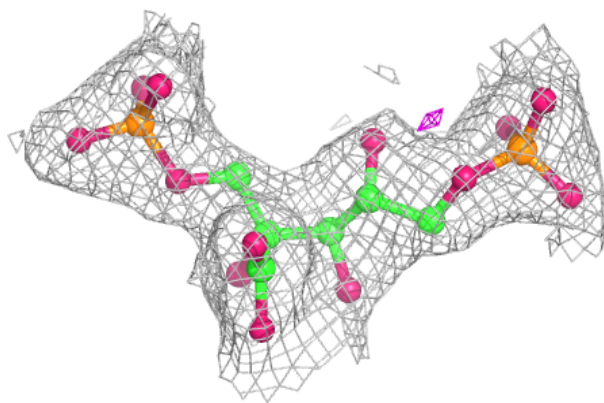
**Electron density around CAP E 1477:**

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

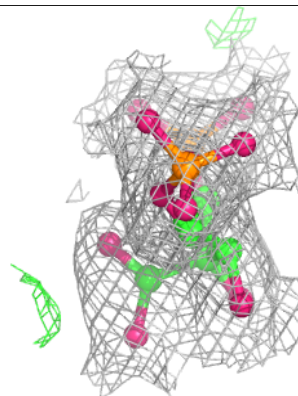
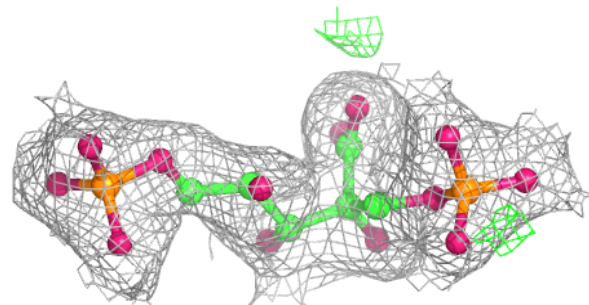
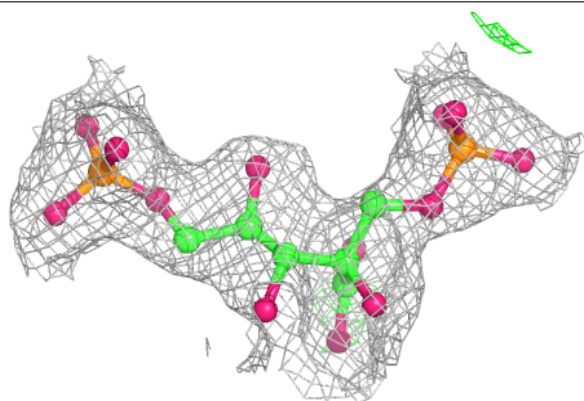


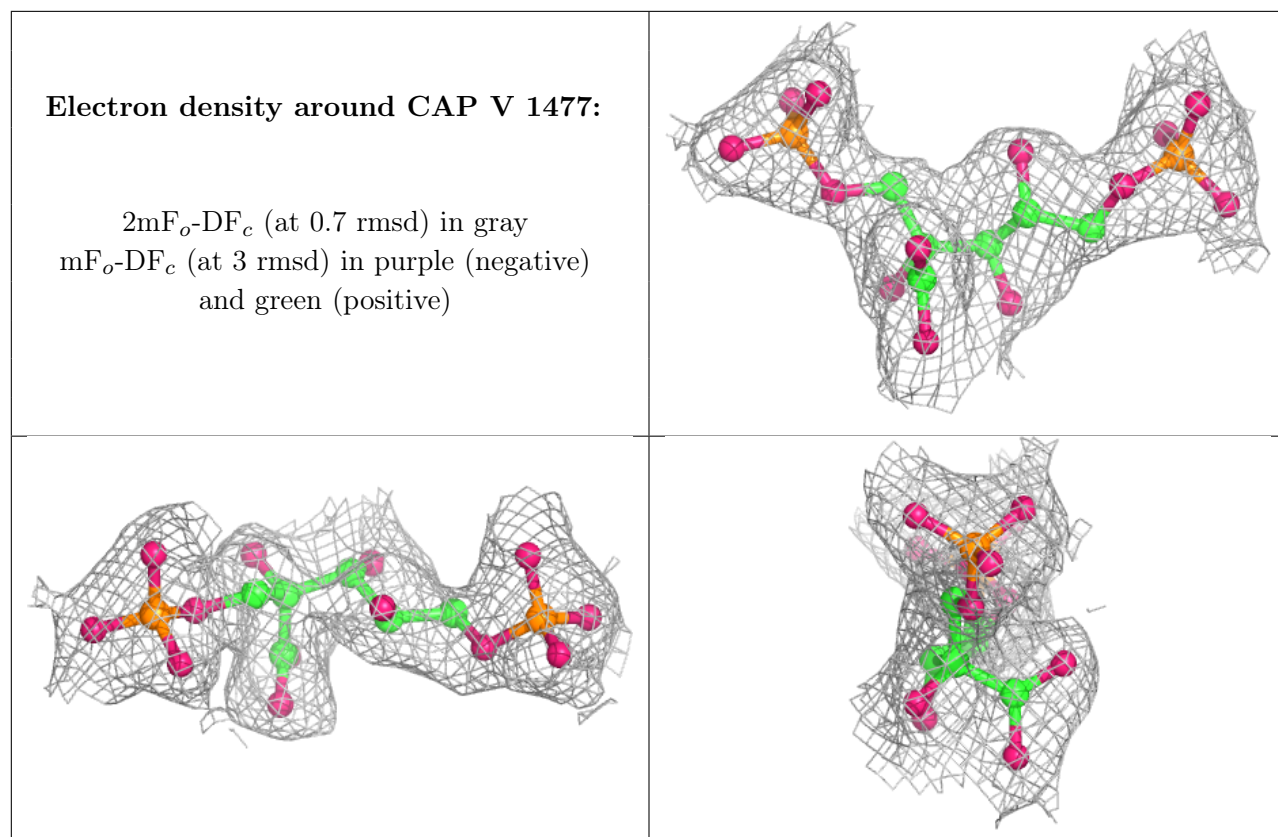
Electron density around CAP K 1477:

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

**Electron density around CAP R 1477:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.