



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 11:45 am GMT

PDB ID : 1UZH  
Title : A CHIMERIC CHLAMYDOMONAS, SYNECHOCOCCUS RUBISCO ENZYME  
Authors : Karkehabadi, S.; Spreitzer, R.J.; Andersson, I.  
Deposited on : 2004-03-12  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

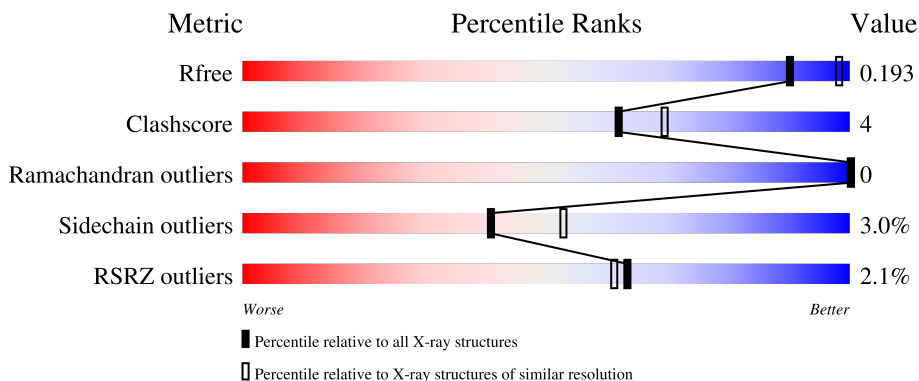
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	 88% 9% ..
1	B	475	 88% 9% .
1	E	475	 89% 9% .
1	H	475	 88% 10% ..
1	K	475	 89% 8% ..

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Mol	Chain	Length	Quality of chain
1	O	475	 % 90% 8% ..
1	R	475	 % 88% 10% ..
1	V	475	 2% 88% 10% ..
2	C	122	 2% 82% 16% .
2	F	122	 5% 84% 14% .
2	I	122	 3% 82% 16% .
2	J	122	 8% 84% 14% .
2	M	122	 6% 87% 11% .
2	P	122	 3% 81% 17% .
2	T	122	 7% 83% 16% .
2	W	122	 9% 85% 13% .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 40557 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
			Total	C	N	O	S			
1	A	465	3640	2300	641	675	24	0	3	0
1	B	467	3647	2305	642	676	24	0	3	0
1	E	469	3665	2315	646	680	24	0	3	0
1	H	469	3665	2315	646	680	24	0	3	0
1	K	469	3673	2321	646	682	24	0	5	0
1	O	469	3661	2313	646	678	24	0	2	0
1	R	469	3662	2314	646	678	24	0	2	0
1	V	469	3664	2316	645	679	24	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	conflict	UNP P00877
B	46	PRO	LEU	conflict	UNP P00877
E	46	PRO	LEU	conflict	UNP P00877
H	46	PRO	LEU	conflict	UNP P00877
K	46	PRO	LEU	conflict	UNP P00877
O	46	PRO	LEU	conflict	UNP P00877
R	46	PRO	LEU	conflict	UNP P00877
V	46	PRO	LEU	conflict	UNP P00877

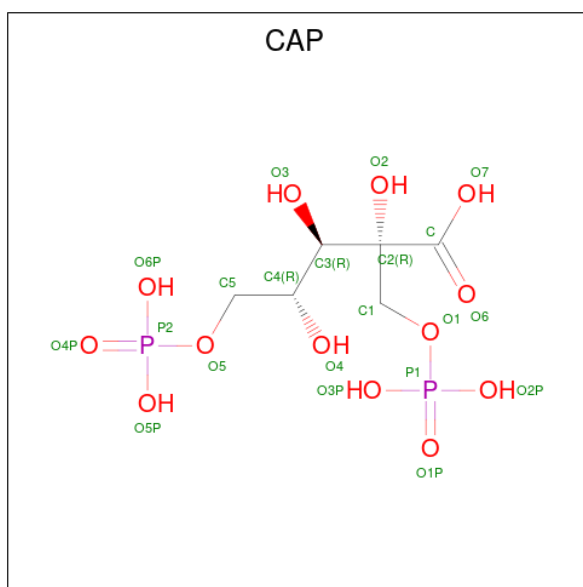
- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	122	Total	C	N	O	S	0	2	0
			1009	654	167	178	10			
2	F	122	Total	C	N	O	S	0	2	0
			1014	660	166	177	11			
2	I	122	Total	C	N	O	S	0	1	0
			1006	653	166	177	10			
2	J	122	Total	C	N	O	S	0	1	0
			1006	653	166	176	11			
2	M	122	Total	C	N	O	S	0	2	0
			1007	653	166	177	11			
2	P	122	Total	C	N	O	S	0	3	0
			1010	654	167	178	11			
2	T	122	Total	C	N	O	S	0	2	0
			1014	660	166	177	11			
2	W	122	Total	C	N	O	S	0	2	0
			1007	653	166	177	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: C<sub>6</sub>H<sub>14</sub>O<sub>13</sub>P<sub>2</sub>).



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: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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	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	B	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
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 C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	K	1	Total C O 4 2 2	0	0
5	M	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 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	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	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	294	Total O 294 294	0	0
6	B	317	Total O 317 317	0	0
6	C	61	Total O 61 61	0	0
6	E	292	Total O 292 292	0	0

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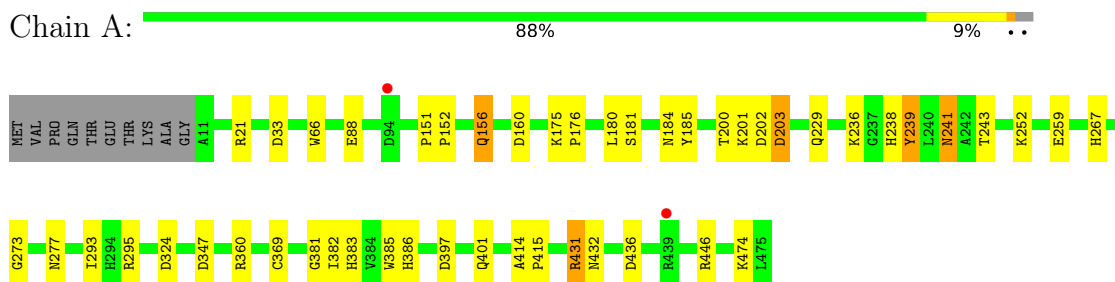
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	F	70	Total 70	O 70	0	0
6	H	288	Total 288	O 288	0	0
6	I	66	Total 66	O 66	0	0
6	J	57	Total 57	O 57	0	0
6	K	279	Total 279	O 279	0	0
6	M	56	Total 56	O 56	0	0
6	O	286	Total 286	O 286	0	0
6	P	55	Total 55	O 55	0	0
6	R	307	Total 307	O 307	0	0
6	T	73	Total 73	O 73	0	0
6	V	281	Total 281	O 281	0	0
6	W	49	Total 49	O 49	0	0

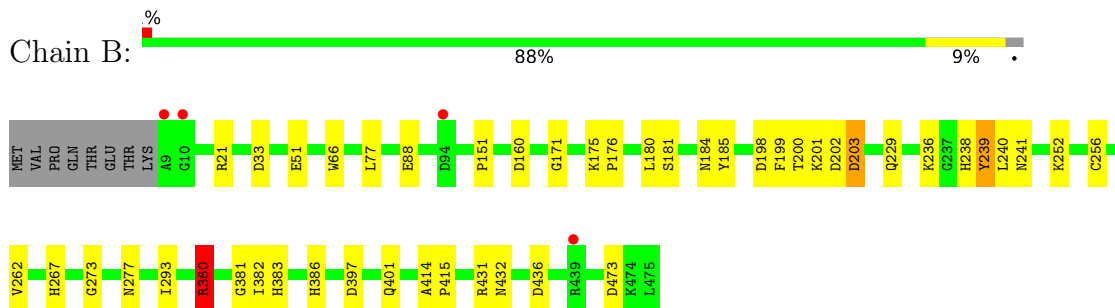
### 3 Residue-property plots

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.

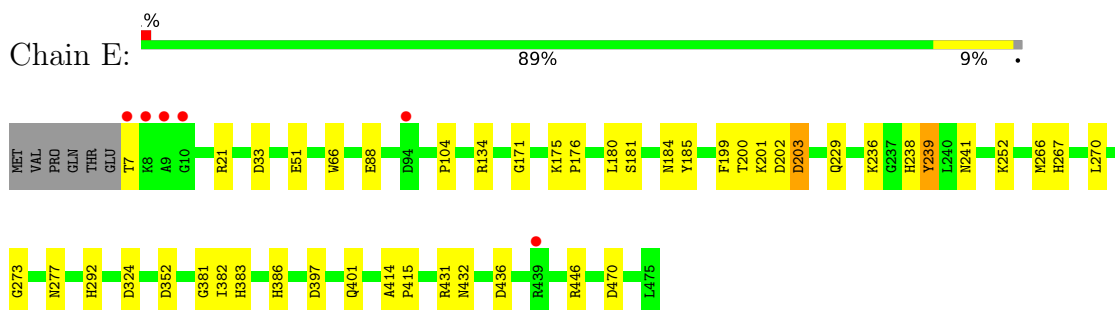
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



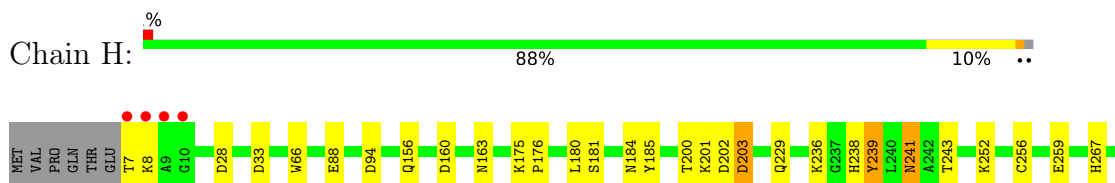
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

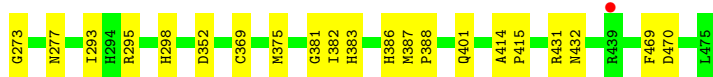


- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

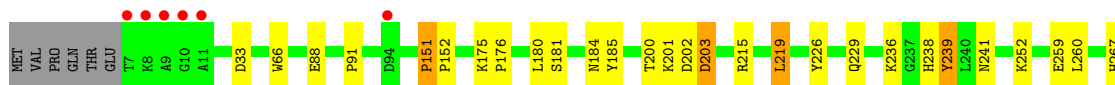
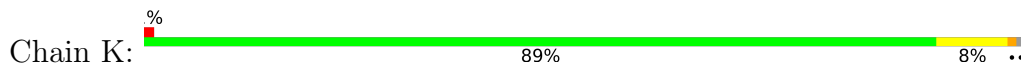


- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN





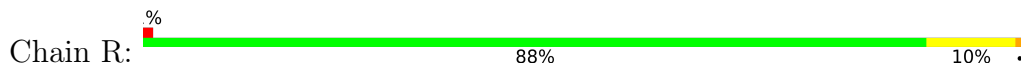
● Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



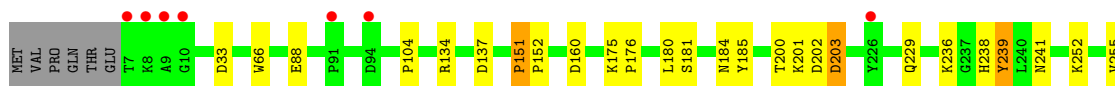
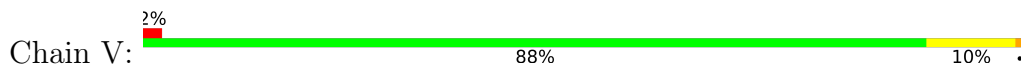
● Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN



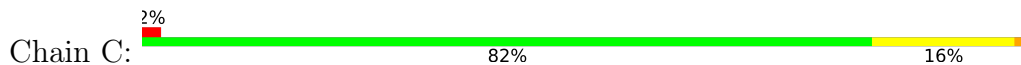
● Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

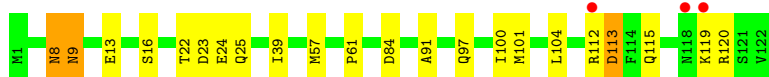


● Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

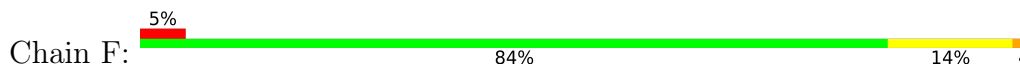


● Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

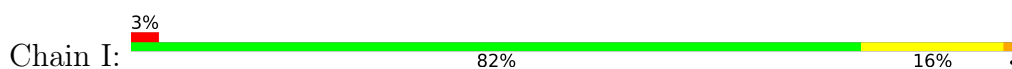




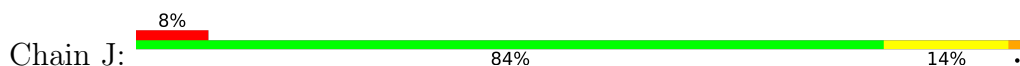
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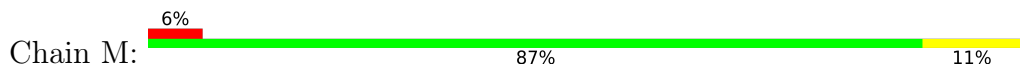
- Molecule 2: RIBULOSE BIPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BIPHOSPHATE CARBOXYLASE SMALL CHAIN



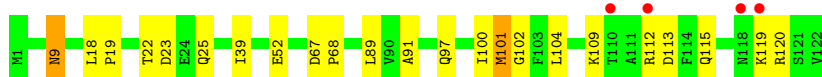
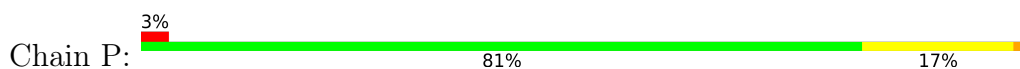
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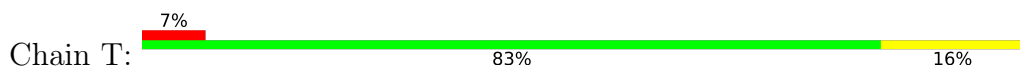
- Molecule 2: RIBULOSE BIPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BIPHOSPHATE CARBOXYLASE SMALL CHAIN

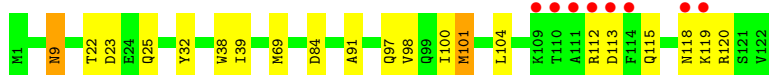


- Molecule 2: RIBULOSE BIPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BIPHOSPHATE CARBOXYLASE SMALL CHAIN

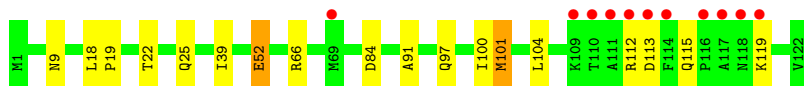
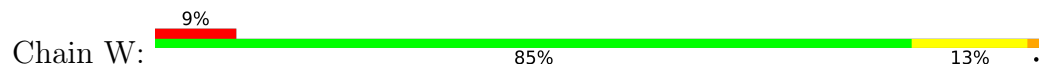


- Molecule 2: RIBULOSE BIPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BIPHOSPHATE CARBOXYLASE SMALL CHAIN





- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 2, RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.82Å 223.97Å 111.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.88 – 2.19	Depositor EDS
% Data completeness (in resolution range)	89.3 (30.00-2.20) 88.6 (29.88-2.19)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.160 , 0.193 0.162 , 0.193	Depositor DCC
$R_{free}$ test set	12581 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtrriage
Anisotropy	0.326	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.026 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	40557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, EDO, SMC, KCX, HYP, 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	0.61	0/3695	0.75	6/4993 (0.1%)
1	B	0.62	0/3704	0.80	13/5005 (0.3%)
1	E	0.61	0/3720	0.76	7/5026 (0.1%)
1	H	0.60	0/3720	0.76	7/5026 (0.1%)
1	K	0.62	0/3736	0.75	5/5048 (0.1%)
1	O	0.60	0/3711	0.76	3/5014 (0.1%)
1	R	0.60	0/3711	0.76	10/5014 (0.2%)
1	V	0.61	0/3718	0.75	9/5024 (0.2%)
2	C	0.61	0/1049	0.71	3/1426 (0.2%)
2	F	0.59	0/1056	0.69	2/1435 (0.1%)
2	I	0.60	0/1041	0.69	2/1415 (0.1%)
2	J	0.61	0/1043	0.70	2/1417 (0.1%)
2	M	0.61	0/1049	0.72	1/1425 (0.1%)
2	P	0.60	0/1057	0.72	2/1436 (0.1%)
2	T	0.61	0/1056	0.70	3/1435 (0.2%)
2	W	0.60	0/1049	0.70	2/1425 (0.1%)
All	All	0.61	0/38115	0.75	77/51564 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (77) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360[A]	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	B	360[B]	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	P	113	ASP	CB-CG-OD2	7.29	124.86	118.30
2	M	113	ASP	CB-CG-OD2	7.11	124.70	118.30
2	C	113	ASP	CB-CG-OD2	6.93	124.53	118.30
1	B	360[A]	ARG	CD-NE-CZ	6.91	133.27	123.60
1	B	360[B]	ARG	CD-NE-CZ	6.91	133.27	123.60
2	W	113	ASP	CB-CG-OD2	6.85	124.46	118.30
2	F	113	ASP	CB-CG-OD2	6.82	124.44	118.30
2	T	113	ASP	CB-CG-OD2	6.81	124.43	118.30
1	H	203	ASP	CB-CG-OD2	6.52	124.17	118.30
2	J	113	ASP	CB-CG-OD2	6.52	124.17	118.30
1	O	203	ASP	CB-CG-OD2	6.45	124.11	118.30
1	V	203	ASP	CB-CG-OD2	6.41	124.07	118.30
2	I	113	ASP	CB-CG-OD2	6.41	124.07	118.30
1	V	33	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	160	ASP	CB-CG-OD2	6.21	123.89	118.30
2	P	23	ASP	CB-CG-OD2	6.12	123.81	118.30
1	V	352	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	203	ASP	CB-CG-OD2	6.01	123.70	118.30
1	R	324	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	436	ASP	CB-CG-OD2	5.93	123.64	118.30
1	E	324	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	160	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	324	ASP	CB-CG-OD2	5.73	123.45	118.30
2	J	23	ASP	CB-CG-OD2	5.70	123.43	118.30
1	H	352	ASP	CB-CG-OD2	5.65	123.38	118.30
1	V	436	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	33	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	397	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	203	ASP	CB-CG-OD2	5.54	123.29	118.30
1	H	33	ASP	CB-CG-OD2	5.52	123.27	118.30
1	R	473	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	470	ASP	CB-CG-OD2	5.48	123.23	118.30
1	R	160	ASP	CB-CG-OD2	5.48	123.23	118.30
1	K	33[A]	ASP	CB-CG-OD2	5.48	123.23	118.30
1	K	33[B]	ASP	CB-CG-OD2	5.48	123.23	118.30
1	R	28	ASP	CB-CG-OD2	5.46	123.22	118.30
2	I	23	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	397	ASP	CB-CG-OD2	5.43	123.19	118.30
1	V	324	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	360[A]	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	360[B]	ARG	NE-CZ-NH1	-5.40	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	23	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	352	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	33	ASP	CB-CG-OD2	5.38	123.14	118.30
1	R	397	ASP	CB-CG-OD2	5.37	123.13	118.30
1	R	72	ASP	CB-CG-OD2	5.36	123.13	118.30
1	K	203	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	198	ASP	CB-CG-OD2	5.32	123.08	118.30
1	R	352	ASP	CB-CG-OD2	5.30	123.07	118.30
1	K	473	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	473	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	28	ASP	CB-CG-OD2	5.29	123.06	118.30
2	C	84	ASP	CB-CG-OD2	5.28	123.05	118.30
2	T	84	ASP	CB-CG-OD2	5.26	123.03	118.30
1	V	160	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	436	ASP	CB-CG-OD2	5.19	122.97	118.30
1	R	470	ASP	CB-CG-OD2	5.18	122.96	118.30
1	H	160	ASP	CB-CG-OD2	5.17	122.95	118.30
2	T	23	ASP	CB-CG-OD2	5.14	122.93	118.30
2	W	84	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	470	ASP	CB-CG-OD2	5.11	122.90	118.30
1	R	203	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	33	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	397	ASP	CB-CG-OD2	5.09	122.88	118.30
1	V	351	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	436	ASP	CB-CG-OD2	5.08	122.87	118.30
1	R	86	ASP	CB-CG-OD2	5.07	122.86	118.30
1	K	324	ASP	CB-CG-OD2	5.07	122.86	118.30
1	V	137	ASP	CB-CG-OD2	5.06	122.86	118.30
1	O	397	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	203	ASP	CB-CG-OD2	5.04	122.84	118.30
1	H	94	ASP	CB-CG-OD2	5.04	122.84	118.30
1	V	286	ASP	CB-CG-OD2	5.04	122.83	118.30
2	C	23	ASP	CB-CG-OD2	5.01	122.81	118.30
1	O	137	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	360[A]	ARG	Sidechain
1	B	360[B]	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3640	0	3542	34	0
1	B	3647	0	3550	31	0
1	E	3665	0	3570	30	0
1	H	3665	0	3570	37	0
1	K	3673	0	3581	33	0
1	O	3661	0	3568	30	0
1	R	3662	0	3572	32	0
1	V	3664	0	3575	32	0
2	C	1009	0	986	13	0
2	F	1014	0	989	13	0
2	I	1006	0	984	13	0
2	J	1006	0	984	15	0
2	M	1007	0	985	11	0
2	P	1010	0	987	13	0
2	T	1014	0	989	14	0
2	W	1007	0	985	12	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	8	0	0
4	B	21	0	7	0	0
4	E	21	0	8	0	0
4	H	21	0	8	1	0
4	K	21	0	8	0	0
4	O	21	0	8	0	0
4	R	21	0	9	0	0
4	V	21	0	7	0	0
5	A	20	0	30	0	0
5	B	24	0	36	2	0
5	C	4	0	6	0	0
5	E	20	0	30	2	0
5	F	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	24	0	36	3	0
5	J	4	0	6	1	0
5	K	20	0	30	0	0
5	M	4	0	6	0	0
5	O	20	0	30	1	0
5	P	4	0	6	0	0
5	R	20	0	30	2	0
5	T	4	0	6	0	0
5	V	24	0	36	0	0
5	W	4	0	6	0	0
6	A	294	0	0	7	0
6	B	317	0	0	5	0
6	C	61	0	0	1	0
6	E	292	0	0	1	0
6	F	70	0	0	2	0
6	H	288	0	0	11	0
6	I	66	0	0	1	0
6	J	57	0	0	4	0
6	K	279	0	0	6	0
6	M	56	0	0	1	0
6	O	286	0	0	2	0
6	P	55	0	0	1	0
6	R	307	0	0	7	0
6	T	73	0	0	2	0
6	V	281	0	0	5	0
6	W	49	0	0	3	0
All	All	40557	0	36780	326	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 4.

All (326) 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:H:375:MET:HG2	6:H:2185:HOH:O	1.31	1.28
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.04	0.99
1:V:255:VAL:O	1:V:259[B]:GLU:HG2	1.63	0.97
2:P:97:GLN:HE21	1:R:184:ASN:HD22	1.10	0.97
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.03	0.96
1:B:184:ASN:HD22	2:F:97:GLN:HE21	1.08	0.95
1:K:267:HIS:HD2	1:K:277:ASN:HD22	0.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:HIS:HD2	1:A:277:ASN:HD22	0.97	0.94
1:R:267:HIS:HD2	1:R:277:ASN:HD22	0.97	0.93
1:H:375:MET:CG	6:H:2185:HOH:O	2.00	0.93
1:E:267:HIS:HD2	1:E:277:ASN:HD22	0.96	0.93
1:O:267:HIS:HD2	1:O:277:ASN:HD22	0.98	0.93
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.01	0.91
1:H:184:ASN:HD22	2:W:97:GLN:HE21	1.18	0.90
1:E:184:ASN:HD22	2:J:97:GLN:HE21	1.15	0.89
1:V:460:GLU:HB3	6:V:2259:HOH:O	1.71	0.89
1:R:435:ARG:HG3	6:R:2266:HOH:O	1.72	0.89
1:K:259[B]:GLU:CG	6:K:2157:HOH:O	2.19	0.89
1:R:267:HIS:CD2	1:R:277:ASN:HD22	1.90	0.88
2:F:52:GLU:HG3	6:F:2035:HOH:O	1.72	0.88
1:E:267:HIS:CD2	1:E:277:ASN:HD22	1.88	0.88
2:M:97:GLN:HE21	1:O:184:ASN:HD22	1.20	0.87
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.89	0.87
1:O:267:HIS:CD2	1:O:277:ASN:HD22	1.91	0.87
2:C:97:GLN:HE21	1:V:184:ASN:HD22	1.20	0.86
1:A:184:ASN:HD22	2:T:97:GLN:HE21	1.19	0.86
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.24	0.85
1:O:431:ARG:HH21	1:O:432:ASN:HD21	1.23	0.85
1:E:270:LEU:O	5:E:1480:EDO:H22	1.75	0.85
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.93	0.84
1:K:267:HIS:CD2	1:K:277:ASN:HD22	1.90	0.84
1:V:431:ARG:HH21	1:V:432:ASN:HD21	1.21	0.84
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.22	0.83
1:R:431:ARG:HH21	1:R:432:ASN:HD21	1.25	0.83
1:A:21:ARG:NH1	6:A:2015:HOH:O	1.89	0.83
1:E:383:HIS:H	1:E:386:HIS:HD2	1.27	0.82
1:V:383:HIS:H	1:V:386:HIS:HD2	1.27	0.82
1:H:375:MET:SD	6:H:2185:HOH:O	2.38	0.81
2:I:97:GLN:HE21	1:K:184:ASN:HD22	1.26	0.81
1:E:21:ARG:CZ	1:E:51[B]:GLU:HG3	2.10	0.81
1:O:383:HIS:H	1:O:386:HIS:HD2	1.30	0.80
1:A:383:HIS:H	1:A:386:HIS:HD2	1.30	0.79
1:K:431:ARG:HH21	1:K:432:ASN:HD21	1.28	0.79
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.27	0.79
1:H:267:HIS:CD2	1:H:277:ASN:HD22	1.95	0.79
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.30	0.78
1:K:383:HIS:H	1:K:386:HIS:HD2	1.29	0.77
1:V:267:HIS:CD2	1:V:277:ASN:HD22	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:383:HIS:H	1:R:386:HIS:HD2	1.30	0.76
1:E:21:ARG:NH2	1:E:51[A]:GLU:OE1	2.19	0.76
1:B:383:HIS:H	1:B:386:HIS:HD2	1.32	0.75
2:W:52:GLU:HG3	6:W:2023:HOH:O	1.85	0.75
1:E:267:HIS:HD2	1:E:277:ASN:ND2	1.80	0.74
1:O:267:HIS:HD2	1:O:277:ASN:ND2	1.82	0.74
1:K:259[B]:GLU:HG2	6:K:2157:HOH:O	1.84	0.74
1:K:259[B]:GLU:HG3	6:K:2157:HOH:O	1.83	0.73
2:C:22:THR:H	2:C:25:GLN:HE21	1.35	0.73
1:H:383:HIS:H	1:H:386:HIS:HD2	1.38	0.72
1:B:21:ARG:NH2	1:B:51:GLU:OE1	2.23	0.71
1:E:21:ARG:NH1	1:E:51[B]:GLU:HG3	2.07	0.70
1:A:267:HIS:HD2	1:A:277:ASN:ND2	1.82	0.70
2:W:22:THR:H	2:W:25:GLN:HE21	1.40	0.70
2:M:22:THR:H	2:M:25:GLN:HE21	1.40	0.68
5:R:1480:EDO:H11	6:R:2195:HOH:O	1.95	0.67
1:K:267:HIS:HD2	1:K:277:ASN:ND2	1.83	0.67
2:F:22:THR:H	2:F:25:GLN:HE21	1.41	0.67
1:H:375:MET:CE	6:H:2185:HOH:O	2.42	0.67
1:O:202:ASP:OD1	1:O:238:HIS:HE1	1.78	0.67
2:I:22:THR:H	2:I:25:GLN:HE21	1.44	0.66
1:H:267:HIS:HD2	1:H:277:ASN:ND2	1.87	0.65
2:J:22:THR:H	2:J:25:GLN:HE21	1.44	0.64
2:T:22:THR:H	2:T:25:GLN:HE21	1.43	0.64
1:K:202:ASP:OD1	1:K:238:HIS:HE1	1.81	0.64
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.81	0.64
2:P:22:THR:H	2:P:25:GLN:HE21	1.45	0.64
1:K:200:THR:OG1	1:K:238:HIS:HD2	1.80	0.63
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.82	0.63
2:F:115:GLN:HE21	2:F:119:LYS:HB3	1.64	0.62
2:T:115:GLN:HE21	2:T:119:LYS:HB3	1.65	0.62
2:W:66:ARG:HD2	6:W:2030:HOH:O	2.00	0.62
2:J:115:GLN:HE21	2:J:119:LYS:HB3	1.65	0.62
1:R:202:ASP:OD1	1:R:238:HIS:HE1	1.83	0.62
2:C:97:GLN:NE2	1:V:181:SER:H	1.98	0.61
1:H:469:PHE:CZ	5:H:1480:EDO:H22	2.35	0.61
1:R:267:HIS:HD2	1:R:277:ASN:ND2	1.82	0.61
2:I:115:GLN:HE21	2:I:119:LYS:HB3	1.66	0.61
2:M:115:GLN:HE21	2:M:119:LYS:HB3	1.65	0.61
1:B:184:ASN:HD22	2:F:97:GLN:NE2	1.91	0.61
1:K:383:HIS:H	1:K:386:HIS:CD2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:115:GLN:HE21	2:P:119:LYS:HB3	1.66	0.60
2:C:97:GLN:HE22	1:V:180:LEU:HA	1.66	0.60
2:M:97:GLN:HE22	1:O:180:LEU:HA	1.66	0.59
2:W:115:GLN:HE21	2:W:119:LYS:HB3	1.66	0.59
2:C:115:GLN:HE21	2:C:119:LYS:HB3	1.67	0.59
1:B:181:SER:H	2:F:97:GLN:NE2	2.01	0.59
1:O:200:THR:OG1	1:O:238:HIS:HD2	1.85	0.59
1:R:200:THR:OG1	1:R:238:HIS:HD2	1.84	0.59
1:K:91:PRO:HA	6:K:2053:HOH:O	2.02	0.58
2:I:97:GLN:HE22	1:K:180:LEU:HA	1.67	0.58
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.86	0.58
1:H:66:TRP:CD1	1:R:381:GLY:HA2	2.38	0.58
6:H:2110:HOH:O	2:J:53:PHE:HD1	1.86	0.58
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.85	0.58
1:E:383:HIS:H	1:E:386:HIS:CD2	2.16	0.57
1:H:181:SER:H	2:W:97:GLN:NE2	2.03	0.57
1:V:200:THR:OG1	1:V:238:HIS:HD2	1.87	0.57
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.87	0.57
2:C:24:GLU:HB2	6:C:2020:HOH:O	2.04	0.57
1:A:383:HIS:H	1:A:386:HIS:CD2	2.17	0.57
2:W:66:ARG:HD3	6:W:2031:HOH:O	2.04	0.57
1:O:383:HIS:H	1:O:386:HIS:CD2	2.17	0.56
1:V:202:ASP:OD1	1:V:238:HIS:HE1	1.89	0.56
1:O:239:TYR:HE2	1:O:401:GLN:HE22	1.52	0.56
1:A:180:LEU:HA	2:T:97:GLN:HE22	1.70	0.56
1:A:181:SER:H	2:T:97:GLN:NE2	2.03	0.56
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.88	0.56
1:O:66:TRP:CD1	1:V:381:GLY:HA2	2.41	0.56
1:R:229:GLN:HE21	1:R:236:LYS:H	1.51	0.56
1:H:469:PHE:HZ	5:H:1480:EDO:H22	1.71	0.56
1:R:383:HIS:H	1:R:386:HIS:CD2	2.19	0.56
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.54	0.56
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.87	0.55
1:V:239:TYR:HE2	1:V:401:GLN:HE22	1.54	0.55
1:B:383:HIS:H	1:B:386:HIS:CD2	2.19	0.55
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.55	0.55
2:C:22:THR:H	2:C:25:GLN:NE2	2.04	0.55
2:T:118:ASN:HA	6:T:2067:HOH:O	2.06	0.55
1:E:180:LEU:HA	2:J:97:GLN:HE22	1.72	0.54
1:H:180:LEU:HA	2:W:97:GLN:HE22	1.72	0.54
2:P:97:GLN:NE2	1:R:181:SER:H	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.90	0.54
1:R:239:TYR:HE2	1:R:401:GLN:HE22	1.54	0.54
1:K:229:GLN:HE21	1:K:236:LYS:H	1.55	0.54
1:K:226:TYR:HB2	6:K:2137:HOH:O	2.08	0.54
2:M:22:THR:H	2:M:25:GLN:NE2	2.05	0.54
2:J:109:LYS:CG	6:J:2041:HOH:O	2.55	0.54
2:M:97:GLN:NE2	1:O:181:SER:H	2.06	0.54
1:H:229:GLN:HE21	1:H:236:LYS:H	1.54	0.54
1:V:450:LYS:HE3	6:V:2253:HOH:O	2.08	0.54
1:H:163:ASN:HB3	6:H:2109:HOH:O	2.07	0.53
1:H:267:HIS:HE1	6:R:2181:HOH:O	1.90	0.53
2:W:22:THR:H	2:W:25:GLN:NE2	2.06	0.53
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.42	0.53
1:E:66:TRP:CD1	1:K:381:GLY:HA2	2.44	0.53
1:E:181:SER:H	2:J:97:GLN:NE2	2.07	0.53
1:O:229:GLN:HE21	1:O:236:LYS:H	1.57	0.52
1:R:435:ARG:NE	6:R:2266:HOH:O	2.33	0.52
1:B:229:GLN:HE21	1:B:236:LYS:H	1.55	0.52
1:K:239:TYR:HE2	1:K:401:GLN:HE22	1.57	0.52
1:K:383:HIS:N	1:K:386:HIS:HD2	2.05	0.52
1:R:435:ARG:CG	6:R:2266:HOH:O	2.43	0.52
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.57	0.52
1:V:383:HIS:H	1:V:386:HIS:CD2	2.18	0.52
2:J:22:THR:H	2:J:25:GLN:NE2	2.07	0.52
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.45	0.52
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.58	0.51
1:O:336:GLU:O	5:O:1480:EDO:H12	2.10	0.51
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.93	0.51
1:E:229:GLN:HE21	1:E:236:LYS:H	1.57	0.51
2:I:22:THR:H	2:I:25:GLN:NE2	2.06	0.51
1:O:435:ARG:HG3	6:O:2254:HOH:O	2.10	0.51
2:P:22:THR:H	2:P:25:GLN:NE2	2.09	0.51
2:J:91:ALA:HB3	2:J:101:MET:HG2	1.93	0.50
2:T:22:THR:H	2:T:25:GLN:NE2	2.08	0.50
1:E:381:GLY:HA2	1:K:66:TRP:CD1	2.47	0.50
1:H:163:ASN:ND2	6:H:2110:HOH:O	2.44	0.50
2:P:97:GLN:HE22	1:R:180:LEU:HA	1.76	0.50
6:A:2176:HOH:O	1:B:267:HIS:HE1	1.94	0.50
1:B:180:LEU:HA	2:F:97:GLN:HE22	1.76	0.50
1:E:383:HIS:N	1:E:386:HIS:HD2	2.04	0.50
1:A:474:LYS:HE3	6:A:2282:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:109:LYS:HG2	6:P:2037:HOH:O	2.12	0.49
1:V:229:GLN:HE21	1:V:236:LYS:H	1.59	0.49
2:I:97:GLN:NE2	1:K:181:SER:H	2.10	0.49
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.47	0.49
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.94	0.49
1:B:360[B]:ARG:NH2	6:B:2233:HOH:O	2.45	0.49
1:O:414:ALA:HB3	1:O:415:PRO:HD3	1.94	0.49
1:H:431:ARG:HH21	1:H:432:ASN:ND2	2.03	0.49
1:A:229:GLN:HE21	1:A:236:LYS:H	1.59	0.49
1:A:383:HIS:N	1:A:386:HIS:HD2	2.05	0.49
5:B:1481:EDO:H11	6:B:2316:HOH:O	2.12	0.49
2:J:39:ILE:O	2:J:91:ALA:HA	2.13	0.49
2:T:32[A]:TYR:HD2	2:T:101:MET:CE	2.26	0.48
2:J:109:LYS:HG2	6:J:2041:HOH:O	2.13	0.48
1:O:381:GLY:HA2	1:V:66:TRP:CD1	2.47	0.48
1:B:383:HIS:N	1:B:386:HIS:HD2	2.06	0.48
2:C:13:GLU:O	2:C:16[A]:SER:OG	2.22	0.48
1:E:431:ARG:HH21	1:E:432:ASN:ND2	2.00	0.48
1:V:457:ALA:O	1:V:461[A]:VAL:HG23	2.14	0.48
2:F:22:THR:H	2:F:25:GLN:NE2	2.11	0.48
1:O:273:GLY:HA3	1:V:273:GLY:HA3	1.96	0.48
1:O:277:ASN:HD21	1:O:293:ILE:HD12	1.79	0.48
1:O:156[A]:GLN:HG3	2:T:98:VAL:HB	1.96	0.48
2:I:109:LYS:HE2	6:I:2048:HOH:O	2.14	0.47
2:F:39:ILE:O	2:F:91:ALA:HA	2.13	0.47
1:V:414:ALA:HB3	1:V:415:PRO:HD3	1.96	0.47
1:A:175:LYS:HA	1:A:176:PRO:C	2.35	0.47
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.96	0.47
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.95	0.47
6:O:2165:HOH:O	1:V:267:HIS:HE1	1.97	0.47
2:J:39:ILE:HG12	5:J:1123:EDO:H11	1.97	0.47
1:K:414:ALA:HB3	1:K:415:PRO:HD3	1.97	0.47
1:A:156[A]:GLN:HG3	2:I:98:VAL:HB	1.97	0.46
1:R:414:ALA:HB3	1:R:415:PRO:HD3	1.97	0.46
1:V:431:ARG:HH21	1:V:432:ASN:ND2	2.02	0.46
1:E:270:LEU:O	5:E:1480:EDO:C2	2.56	0.46
1:K:219[A]:LEU:HD12	1:K:260:LEU:HD21	1.97	0.46
1:H:383:HIS:H	1:H:386:HIS:CD2	2.24	0.46
1:B:277:ASN:HD21	1:B:293:ILE:HD12	1.80	0.46
2:I:39:ILE:O	2:I:91:ALA:HA	2.16	0.46
1:A:474:LYS:CE	6:A:2282:HOH:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:GLY:HA3	1:R:273:GLY:HA3	1.98	0.46
1:O:383:HIS:N	1:O:386:HIS:HD2	2.05	0.46
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.96	0.45
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.51	0.45
1:E:446:ARG:HD3	6:E:2258:HOH:O	2.17	0.45
2:C:9:ASN:HD21	2:C:120:ARG:HG2	1.80	0.45
1:H:295:ARG:HG3	1:H:298:HIS:CD2	2.52	0.45
1:E:175:LYS:HA	1:E:176:PRO:C	2.37	0.45
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.52	0.45
6:H:2165:HOH:O	1:R:267:HIS:HE1	1.99	0.45
1:R:18:LYS:O	5:R:1477:EDO:H21	2.16	0.45
1:R:386:HIS:HE1	6:R:2210:HOH:O	1.98	0.45
5:H:1481:EDO:H11	6:H:2173:HOH:O	2.16	0.45
1:K:382:ILE:HA	1:K:386:HIS:CD2	2.52	0.45
2:T:39:ILE:O	2:T:91:ALA:HA	2.16	0.44
1:V:175:LYS:HA	1:V:176:PRO:C	2.37	0.44
1:E:267:HIS:HE1	6:K:2161:HOH:O	2.00	0.44
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.52	0.44
2:F:9:ASN:HD21	2:F:120:ARG:HG2	1.83	0.44
1:A:446:ARG:HD3	6:A:2265:HOH:O	2.17	0.44
1:H:383:HIS:N	1:H:386:HIS:HD2	2.10	0.44
1:B:184:ASN:ND2	2:F:97:GLN:HE21	1.93	0.44
2:I:91:ALA:HB3	2:I:101:MET:HG2	2.00	0.44
1:V:435:ARG:HD3	6:V:2246:HOH:O	2.17	0.44
1:K:175:LYS:HA	1:K:176:PRO:C	2.38	0.44
2:M:9:ASN:HD21	2:M:120:ARG:HG2	1.83	0.44
1:R:347:ASP:OD2	1:R:360[B]:ARG:NH2	2.37	0.44
1:A:295:ARG:HG2	6:A:2287:HOH:O	2.18	0.44
2:T:9:ASN:HD21	2:T:120:ARG:HG2	1.83	0.43
2:J:109:LYS:HD3	6:J:2054:HOH:O	2.17	0.43
1:E:273:GLY:HA3	1:K:273:GLY:HA3	1.98	0.43
1:A:347:ASP:OD2	1:A:360[B]:ARG:NH2	2.38	0.43
1:H:277:ASN:HD21	1:H:293:ILE:HD12	1.83	0.43
1:H:163:ASN:CG	6:H:2110:HOH:O	2.56	0.43
1:H:175:LYS:HA	1:H:176:PRO:C	2.39	0.43
1:R:431:ARG:HH21	1:R:432:ASN:ND2	2.05	0.43
2:T:91:ALA:HB3	2:T:101:MET:HG2	2.00	0.43
1:A:267:HIS:HE1	6:A:2160:HOH:O	2.02	0.43
1:K:151:HYP:HA	1:K:152:PRO:HD3	1.94	0.43
1:K:200:THR:OG1	1:K:238:HIS:CD2	2.68	0.43
2:C:13:GLU:O	2:C:16[B]:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:241:ASN:ND2	1:H:243:THR:H	2.16	0.43
1:H:381:GLY:HA2	1:R:66:TRP:CD1	2.54	0.43
2:P:18:LEU:HB3	2:P:19:PRO:HD2	2.00	0.43
1:R:32:ARG:HD2	6:R:2033:HOH:O	2.17	0.43
2:C:39:ILE:O	2:C:91:ALA:HA	2.19	0.43
1:V:383:HIS:CE1	1:V:385:TRP:HB2	2.54	0.43
1:O:431:ARG:HE	1:O:432:ASN:HD22	1.67	0.42
2:P:91:ALA:HB3	2:P:101:MET:HG2	2.01	0.42
1:O:175:LYS:HA	1:O:176:PRO:C	2.39	0.42
1:A:151:HYP:HA	1:A:152:PRO:HD3	1.95	0.42
1:B:240:LEU:HD12	1:B:262:VAL:HG21	2.01	0.42
1:K:215:ARG:O	1:K:219[B]:LEU:HG	2.19	0.42
1:B:200:THR:O	1:B:238:HIS:HA	2.18	0.42
1:K:293:ILE:HG13	1:K:318:LEU:HD21	2.00	0.42
1:V:450:LYS:CE	6:V:2253:HOH:O	2.65	0.42
1:B:51:GLU:HG3	6:B:2044:HOH:O	2.18	0.42
2:C:8[B]:ASN:HD22	2:C:113:ASP:HA	1.83	0.42
1:K:200:THR:O	1:K:238:HIS:HA	2.20	0.42
1:H:201:KCX:OQ1	4:H:477:CAP:O3	2.38	0.42
2:J:9:ASN:ND2	6:J:2004:HOH:O	2.53	0.42
2:T:69:MET:HE3	6:T:2045:HOH:O	2.19	0.42
1:B:175:LYS:HA	1:B:176:PRO:C	2.40	0.42
2:I:9:ASN:HD21	2:I:120:ARG:HG2	1.85	0.42
2:P:39:ILE:O	2:P:91:ALA:HA	2.19	0.42
1:R:331:VAL:HA	1:R:337:GLY:O	2.20	0.42
2:T:32[A]:TYR:CE2	2:T:38:TRP:HZ3	2.38	0.42
1:K:292:HIS:HA	1:K:325:HIS:HB2	2.02	0.41
1:O:431:ARG:HE	1:O:432:ASN:ND2	2.18	0.41
1:A:241:ASN:HD22	1:A:243:THR:H	1.68	0.41
2:M:18:LEU:HB3	2:M:19:PRO:HD2	2.02	0.41
2:P:89:LEU:O	2:P:102:GLY:HA2	2.19	0.41
2:W:39:ILE:O	2:W:91:ALA:HA	2.20	0.41
1:V:368:TRP:O	1:V:369:SMC:C	2.68	0.41
1:B:77:LEU:HD12	1:B:77:LEU:HA	1.94	0.41
2:F:89:LEU:O	2:F:102:GLY:HA2	2.20	0.41
2:P:67:ASP:HA	2:P:68:PRO:HD2	1.91	0.41
1:B:386:HIS:HE1	6:B:2204:HOH:O	2.03	0.41
2:P:9:ASN:HD21	2:P:120:ARG:HG2	1.85	0.41
1:A:277:ASN:HD21	1:A:293:ILE:HD12	1.85	0.41
2:I:39:ILE:HA	2:I:40:PRO:HD3	1.95	0.41
1:R:383:HIS:N	1:R:386:HIS:HD2	2.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:151:HYP:HA	1:V:152:PRO:HD3	1.94	0.41
2:W:18:LEU:HB3	2:W:19:PRO:HD2	2.01	0.41
2:F:69:MET:HE3	6:F:2048:HOH:O	2.21	0.41
2:I:18:LEU:HB3	2:I:19:PRO:HD2	2.02	0.41
1:K:431:ARG:HH21	1:K:432:ASN:ND2	2.07	0.41
2:M:97:GLN:NE2	1:O:184:ASN:HD22	2.01	0.41
1:R:175:LYS:HA	1:R:176:PRO:C	2.41	0.41
2:J:89:LEU:O	2:J:102:GLY:HA2	2.20	0.41
2:M:39:ILE:O	2:M:91:ALA:HA	2.20	0.41
1:O:382:ILE:HA	1:O:386:HIS:CD2	2.56	0.41
1:R:200:THR:OG1	1:R:238:HIS:CD2	2.69	0.41
2:C:57:MET:SD	2:C:61:PRO:HD3	2.61	0.41
1:O:200:THR:O	1:O:238:HIS:HA	2.21	0.41
2:W:91:ALA:HB3	2:W:101:MET:HG2	2.03	0.41
1:H:386:HIS:HE1	6:H:2264:HOH:O	2.04	0.41
1:R:383:HIS:CE1	1:R:385:TRP:HB2	2.56	0.41
1:B:171:GLY:HA2	1:B:199:PHE:O	2.22	0.40
1:H:387:MET:HB3	1:H:388:PRO:HD3	2.03	0.40
1:R:457:ALA:O	1:R:461:VAL:HG22	2.21	0.40
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.55	0.40
1:V:379:SER:HB2	1:V:401:GLN:HB2	2.03	0.40
1:A:200:THR:OG1	1:A:238:HIS:CD2	2.68	0.40
1:A:241:ASN:ND2	1:A:243:THR:H	2.20	0.40
1:O:379:SER:HB2	1:O:401:GLN:HB2	2.02	0.40
1:V:267:HIS:HD2	1:V:277:ASN:ND2	1.89	0.40
5:B:1481:EDO:H22	6:B:2192:HOH:O	2.21	0.40
1:E:171:GLY:HA2	1:E:199:PHE:O	2.21	0.40
1:E:266:MET:HA	1:E:292:HIS:O	2.21	0.40
2:M:112:ARG:HB3	6:M:2054:HOH:O	2.22	0.40
1:V:386:HIS:HE1	6:V:2190:HOH:O	2.03	0.40
1:O:225:ILE:HD11	1:O:238:HIS:HB3	2.03	0.40

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	461/475 (97%)	448 (97%)	13 (3%)	0	100	100
1	B	463/475 (98%)	449 (97%)	14 (3%)	0	100	100
1	E	465/475 (98%)	451 (97%)	14 (3%)	0	100	100
1	H	465/475 (98%)	452 (97%)	13 (3%)	0	100	100
1	K	467/475 (98%)	454 (97%)	13 (3%)	0	100	100
1	O	464/475 (98%)	451 (97%)	13 (3%)	0	100	100
1	R	464/475 (98%)	450 (97%)	14 (3%)	0	100	100
1	V	465/475 (98%)	453 (97%)	12 (3%)	0	100	100
2	C	122/122 (100%)	115 (94%)	7 (6%)	0	100	100
2	F	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	I	121/122 (99%)	117 (97%)	4 (3%)	0	100	100
2	J	121/122 (99%)	116 (96%)	5 (4%)	0	100	100
2	M	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	P	123/122 (101%)	117 (95%)	6 (5%)	0	100	100
2	T	122/122 (100%)	117 (96%)	5 (4%)	0	100	100
2	W	122/122 (100%)	116 (95%)	6 (5%)	0	100	100
All	All	4689/4776 (98%)	4540 (97%)	149 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	371/376 (99%)	360 (97%)	11 (3%)	41	53
1	B	371/376 (99%)	365 (98%)	6 (2%)	62	76
1	E	373/376 (99%)	365 (98%)	8 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	373/376 (99%)	361 (97%)	12 (3%)	39	50
1	K	375/376 (100%)	366 (98%)	9 (2%)	49	62
1	O	372/376 (99%)	363 (98%)	9 (2%)	49	62
1	R	372/376 (99%)	362 (97%)	10 (3%)	44	57
1	V	373/376 (99%)	366 (98%)	7 (2%)	57	71
2	C	111/109 (102%)	104 (94%)	7 (6%)	18	20
2	F	111/109 (102%)	105 (95%)	6 (5%)	22	26
2	I	110/109 (101%)	102 (93%)	8 (7%)	14	15
2	J	110/109 (101%)	104 (94%)	6 (6%)	21	26
2	M	111/109 (102%)	106 (96%)	5 (4%)	27	34
2	P	112/109 (103%)	106 (95%)	6 (5%)	22	26
2	T	111/109 (102%)	106 (96%)	5 (4%)	27	34
2	W	111/109 (102%)	105 (95%)	6 (5%)	22	26
All	All	3867/3880 (100%)	3746 (97%)	121 (3%)	41	51

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLU
1	A	156[A]	GLN
1	A	156[B]	GLN
1	A	185	TYR
1	A	203	ASP
1	A	239	TYR
1	A	241	ASN
1	A	252	LYS
1	A	259[A]	GLU
1	A	259[B]	GLU
1	A	431	ARG
1	B	88	GLU
1	B	185	TYR
1	B	203	ASP
1	B	239	TYR
1	B	241	ASN
1	B	252	LYS
2	C	8[A]	ASN
2	C	8[B]	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	9	ASN
2	C	100	ILE
2	C	101	MET
2	C	104	LEU
2	C	112	ARG
1	E	7	THR
1	E	88	GLU
1	E	134	ARG
1	E	185	TYR
1	E	203	ASP
1	E	239	TYR
1	E	241	ASN
1	E	252	LYS
2	F	9	ASN
2	F	52	GLU
2	F	100	ILE
2	F	101	MET
2	F	104	LEU
2	F	112	ARG
1	H	7	THR
1	H	8	LYS
1	H	88	GLU
1	H	156[A]	GLN
1	H	156[B]	GLN
1	H	185	TYR
1	H	203	ASP
1	H	239	TYR
1	H	241	ASN
1	H	252	LYS
1	H	259[A]	GLU
1	H	259[B]	GLU
2	I	9	ASN
2	I	16[A]	SER
2	I	16[B]	SER
2	I	52	GLU
2	I	100	ILE
2	I	101	MET
2	I	104	LEU
2	I	112	ARG
2	J	9	ASN
2	J	52	GLU
2	J	100	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	101	MET
2	J	104	LEU
2	J	112	ARG
1	K	88	GLU
1	K	185	TYR
1	K	203	ASP
1	K	219[A]	LEU
1	K	219[B]	LEU
1	K	239	TYR
1	K	241	ASN
1	K	252	LYS
1	K	431	ARG
2	M	9	ASN
2	M	100	ILE
2	M	101	MET
2	M	104	LEU
2	M	112	ARG
1	O	7	THR
1	O	88	GLU
1	O	134	ARG
1	O	185	TYR
1	O	203	ASP
1	O	239	TYR
1	O	241	ASN
1	O	252	LYS
1	O	431	ARG
2	P	9	ASN
2	P	52	GLU
2	P	100	ILE
2	P	101	MET
2	P	104	LEU
2	P	112	ARG
1	R	7	THR
1	R	8	LYS
1	R	88	GLU
1	R	185	TYR
1	R	203	ASP
1	R	239	TYR
1	R	241	ASN
1	R	252	LYS
1	R	431	ARG
1	R	461	VAL

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Mol	Chain	Res	Type
2	T	9	ASN
2	T	100	ILE
2	T	101	MET
2	T	104	LEU
2	T	112	ARG
1	V	88	GLU
1	V	134	ARG
1	V	185	TYR
1	V	203	ASP
1	V	239	TYR
1	V	241	ASN
1	V	252	LYS
2	W	9	ASN
2	W	52	GLU
2	W	100	ILE
2	W	101	MET
2	W	104	LEU
2	W	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	163	ASN
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN
1	A	304	GLN
1	A	386	HIS
1	A	401	GLN
1	A	432	ASN
1	B	153	HIS
1	B	163	ASN
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	386	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	401	GLN
1	B	432	ASN
2	C	9	ASN
2	C	25	GLN
2	C	29	GLN
2	C	97	GLN
2	C	115	GLN
1	E	153	HIS
1	E	163	ASN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN
1	E	304	GLN
1	E	386	HIS
1	E	401	GLN
1	E	432	ASN
2	F	9	ASN
2	F	25	GLN
2	F	29	GLN
2	F	97	GLN
2	F	115	GLN
1	H	153	HIS
1	H	163	ASN
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	304	GLN
1	H	386	HIS
1	H	401	GLN
1	H	432	ASN
2	I	8	ASN
2	I	9	ASN
2	I	25	GLN
2	I	29	GLN
2	I	97	GLN
2	I	115	GLN
2	J	8	ASN
2	J	9	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	25	GLN
2	J	29	GLN
2	J	97	GLN
2	J	115	GLN
1	K	153	HIS
1	K	229	GLN
1	K	238	HIS
1	K	241	ASN
1	K	267	HIS
1	K	277	ASN
1	K	304	GLN
1	K	386	HIS
1	K	401	GLN
1	K	432	ASN
2	M	8	ASN
2	M	9	ASN
2	M	25	GLN
2	M	29	GLN
2	M	97	GLN
2	M	115	GLN
1	O	153	HIS
1	O	163	ASN
1	O	229	GLN
1	O	238	HIS
1	O	241	ASN
1	O	267	HIS
1	O	277	ASN
1	O	304	GLN
1	O	386	HIS
1	O	401	GLN
1	O	432	ASN
2	P	9	ASN
2	P	25	GLN
2	P	29	GLN
2	P	97	GLN
2	P	115	GLN
1	R	153	HIS
1	R	163	ASN
1	R	229	GLN
1	R	238	HIS
1	R	241	ASN
1	R	267	HIS

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Mol	Chain	Res	Type
1	R	277	ASN
1	R	304	GLN
1	R	386	HIS
1	R	401	GLN
1	R	432	ASN
2	T	9	ASN
2	T	25	GLN
2	T	29	GLN
2	T	97	GLN
2	T	115	GLN
1	V	153	HIS
1	V	163	ASN
1	V	229	GLN
1	V	238	HIS
1	V	241	ASN
1	V	267	HIS
1	V	277	ASN
1	V	304	GLN
1	V	386	HIS
1	V	401	GLN
1	V	432	ASN
2	W	9	ASN
2	W	25	GLN
2	W	29	GLN
2	W	97	GLN
2	W	115	GLN

### 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	HYP	A	151	1	6,8,9	0.57	0	5,10,12	1.41	0
1	SMC	V	369	1	5,6,7	1.17	1 (20%)	2,6,8	0.77	0
1	SMC	B	369	1	5,6,7	0.79	0	2,6,8	0.95	0
1	SMC	B	256	1	5,6,7	0.56	0	2,6,8	1.90	1 (50%)
1	HYP	R	104	1	6,8,9	0.45	0	5,10,12	1.22	0
1	SMC	R	369	1	5,6,7	1.34	1 (20%)	2,6,8	0.78	0
1	SMC	V	256	1	5,6,7	1.23	1 (20%)	2,6,8	0.51	0
1	KCX	H	201	3,1	9,11,12	1.02	0	5,12,14	1.11	0
1	HYP	A	104	1	6,8,9	0.65	0	5,10,12	1.12	0
1	HYP	K	104	1	6,8,9	0.25	0	5,10,12	1.02	0
1	KCX	O	201	3,1	9,11,12	0.81	0	5,12,14	1.10	1 (20%)
1	HYP	O	151	1	6,8,9	0.77	0	5,10,12	1.36	0
1	KCX	R	201	3,1	9,11,12	1.00	0	5,12,14	0.99	1 (20%)
1	HYP	H	151	1	6,8,9	0.62	0	5,10,12	1.34	0
1	KCX	E	201	3,1	9,11,12	1.25	1 (11%)	5,12,14	0.72	0
1	SMC	A	369	1	5,6,7	1.38	1 (20%)	2,6,8	1.71	1 (50%)
1	SMC	K	369	1	5,6,7	0.49	0	2,6,8	0.37	0
1	SMC	K	256	1	5,6,7	0.84	0	2,6,8	0.45	0
1	HYP	H	104	1	6,8,9	0.60	0	5,10,12	1.05	0
1	HYP	O	104	1	6,8,9	0.50	0	5,10,12	0.88	0
1	SMC	A	256	1	5,6,7	0.84	0	2,6,8	1.56	0
1	HYP	B	104	1	6,8,9	0.46	0	5,10,12	0.77	0
1	SMC	H	369	1	5,6,7	1.19	1 (20%)	2,6,8	1.19	0
1	HYP	B	151	1	6,8,9	0.81	0	5,10,12	1.21	1 (20%)
1	SMC	H	256	1	5,6,7	0.66	0	2,6,8	1.85	1 (50%)
1	KCX	B	201	3,1	9,11,12	1.03	0	5,12,14	1.06	1 (20%)
1	SMC	O	256	1	5,6,7	0.83	0	2,6,8	0.92	0
1	KCX	V	201	3,1	9,11,12	0.96	0	5,12,14	1.36	1 (20%)
1	HYP	E	104	1	6,8,9	0.58	0	5,10,12	1.73	2 (40%)
1	HYP	K	151	1	6,8,9	0.71	0	5,10,12	1.39	1 (20%)
1	SMC	O	369	1	5,6,7	0.82	0	2,6,8	0.47	0
1	HYP	V	151	1	6,8,9	0.32	0	5,10,12	1.45	1 (20%)
1	HYP	R	151	1	6,8,9	0.61	0	5,10,12	1.28	0
1	KCX	K	201	3,1	9,11,12	0.89	1 (11%)	5,12,14	0.79	0
1	HYP	E	151	1	6,8,9	0.48	0	5,10,12	1.27	0
1	SMC	E	369	1	5,6,7	0.60	0	2,6,8	0.35	0
1	SMC	R	256	1	5,6,7	0.97	0	2,6,8	0.92	0
1	KCX	A	201	3,1	9,11,12	1.01	0	5,12,14	1.19	1 (20%)
1	SMC	E	256	1	5,6,7	0.90	0	2,6,8	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	HYP	V	104	1	6,8,9	0.44	0	5,10,12	1.40	1 (20%)

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	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	SMC	V	369	1	-	1/3/5/7	-
1	SMC	B	369	1	-	1/3/5/7	-
1	SMC	B	256	1	-	0/3/5/7	-
1	HYP	R	104	1	-	0/0/11/13	0/1/1/1
1	SMC	R	369	1	-	1/3/5/7	-
1	SMC	V	256	1	-	0/3/5/7	-
1	KCX	H	201	3,1	-	0/9/10/12	-
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	HYP	K	104	1	-	0/0/11/13	0/1/1/1
1	KCX	O	201	3,1	-	0/9/10/12	-
1	HYP	O	151	1	-	0/0/11/13	0/1/1/1
1	KCX	R	201	3,1	-	0/9/10/12	-
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	KCX	E	201	3,1	-	0/9/10/12	-
1	SMC	A	369	1	-	1/3/5/7	-
1	SMC	K	369	1	-	1/3/5/7	-
1	SMC	K	256	1	-	0/3/5/7	-
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	HYP	O	104	1	-	0/0/11/13	0/1/1/1
1	SMC	A	256	1	-	0/3/5/7	-
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	SMC	H	369	1	-	1/3/5/7	-
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	SMC	H	256	1	-	0/3/5/7	-
1	KCX	B	201	3,1	-	0/9/10/12	-
1	SMC	O	256	1	-	0/3/5/7	-
1	KCX	V	201	3,1	-	0/9/10/12	-
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	HYP	K	151	1	-	0/0/11/13	0/1/1/1
1	SMC	O	369	1	-	1/3/5/7	-
1	HYP	V	151	1	-	0/0/11/13	0/1/1/1
1	HYP	R	151	1	-	0/0/11/13	0/1/1/1
1	KCX	K	201	3,1	-	0/9/10/12	-

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	SMC	CB-SG	2.76	1.84	1.80
1	R	369	SMC	CB-SG	2.67	1.84	1.80
1	V	256	SMC	CB-SG	2.48	1.84	1.80
1	E	201	KCX	OQ1-CX	2.48	1.26	1.21
1	H	369	SMC	CB-SG	2.25	1.83	1.80
1	K	201	KCX	CE-NZ	2.11	1.51	1.46
1	V	369	SMC	CB-SG	2.09	1.83	1.80

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	201	KCX	OQ1-CX-NZ	-2.93	120.41	124.96
1	E	104	HYP	OD1-CG-CD	-2.74	104.36	110.35
1	B	256	SMC	CA-CB-SG	-2.68	109.70	114.04
1	E	104	HYP	CB-CG-CD	2.48	106.30	103.27
1	V	104	HYP	O-C-CA	-2.41	118.45	124.78
1	H	256	SMC	CA-CB-SG	-2.34	110.25	114.04
1	B	201	KCX	OQ1-CX-NZ	-2.27	121.44	124.96
1	A	201	KCX	OQ1-CX-NZ	-2.27	121.44	124.96
1	O	201	KCX	OQ1-CX-NZ	-2.22	121.51	124.96
1	A	369	SMC	CS-SG-CB	-2.08	97.48	101.30
1	V	151	HYP	O-C-CA	-2.06	119.39	124.78
1	R	201	KCX	OQ1-CX-NZ	-2.05	121.78	124.96
1	B	151	HYP	CG-CB-CA	-2.04	101.38	103.96
1	K	151	HYP	OD1-CG-CD	-2.03	105.91	110.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	369	SMC	N-CA-CB-SG

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

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	151	HYP	1	0
1	V	369	SMC	1	0
1	H	201	KCX	1	0
1	K	151	HYP	1	0
1	V	151	HYP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 8 are monoatomic - leaving 58 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	O	477	3	17,20,20	1.07	2 (11%)	22,31,31	1.23	2 (9%)
5	EDO	K	1480	-	3,3,3	0.31	0	2,2,2	0.26	0
4	CAP	H	477	3	17,20,20	1.16	2 (11%)	22,31,31	0.86	0
5	EDO	A	1479	-	3,3,3	0.37	0	2,2,2	0.17	0
5	EDO	A	1480	-	3,3,3	0.33	0	2,2,2	0.66	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CAP	R	477	3	17,20,20	1.10	2 (11%)	22,31,31	1.07	2 (9%)
5	EDO	O	1477	-	3,3,3	0.28	0	2,2,2	0.33	0
5	EDO	T	1123	-	3,3,3	0.27	0	2,2,2	0.59	0
5	EDO	E	1478	-	3,3,3	0.26	0	2,2,2	0.42	0
4	CAP	E	477	3	17,20,20	1.23	2 (11%)	22,31,31	1.17	2 (9%)
5	EDO	H	1477	-	3,3,3	0.36	0	2,2,2	0.10	0
4	CAP	B	477	3	17,20,20	0.99	2 (11%)	22,31,31	1.17	2 (9%)
5	EDO	F	1123	-	3,3,3	0.32	0	2,2,2	0.79	0
5	EDO	K	1476	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	R	1478	-	3,3,3	0.31	0	2,2,2	0.20	0
5	EDO	B	1477	-	3,3,3	0.36	0	2,2,2	0.14	0
5	EDO	V	1476	-	3,3,3	0.42	0	2,2,2	0.14	0
5	EDO	H	1479	-	3,3,3	0.28	0	2,2,2	0.33	0
5	EDO	O	1480	-	3,3,3	0.43	0	2,2,2	0.47	0
5	EDO	O	1479	-	3,3,3	0.38	0	2,2,2	0.24	0
5	EDO	J	1123	-	3,3,3	0.26	0	2,2,2	0.57	0
5	EDO	K	1479	-	3,3,3	0.35	0	2,2,2	0.10	0
5	EDO	V	1478	-	3,3,3	0.28	0	2,2,2	0.22	0
5	EDO	K	1477	-	3,3,3	0.32	0	2,2,2	0.21	0
5	EDO	P	1123	-	3,3,3	0.30	0	2,2,2	0.22	0
5	EDO	A	1476	-	3,3,3	0.31	0	2,2,2	0.27	0
5	EDO	V	1477	-	3,3,3	0.35	0	2,2,2	0.18	0
5	EDO	V	1480	-	3,3,3	0.29	0	2,2,2	0.11	0
5	EDO	V	1481	-	3,3,3	0.37	0	2,2,2	0.28	0
5	EDO	E	1476	-	3,3,3	0.33	0	2,2,2	0.10	0
5	EDO	B	1480	-	3,3,3	0.39	0	2,2,2	0.09	0
5	EDO	E	1477	-	3,3,3	0.27	0	2,2,2	0.19	0
5	EDO	W	1123	-	3,3,3	0.27	0	2,2,2	0.39	0
4	CAP	V	477	3	17,20,20	1.17	2 (11%)	22,31,31	1.02	1 (4%)
5	EDO	M	1123	-	3,3,3	0.28	0	2,2,2	0.38	0
5	EDO	A	1477	-	3,3,3	0.27	0	2,2,2	0.14	0
5	EDO	E	1479	-	3,3,3	0.37	0	2,2,2	0.22	0
5	EDO	E	1480	-	3,3,3	0.34	0	2,2,2	0.19	0
5	EDO	K	1478	-	3,3,3	0.26	0	2,2,2	0.59	0
5	EDO	B	1476	-	3,3,3	0.35	0	2,2,2	0.46	0
5	EDO	R	1477	-	3,3,3	0.33	0	2,2,2	0.09	0
4	CAP	K	477	3	17,20,20	1.14	2 (11%)	22,31,31	1.31	1 (4%)
5	EDO	O	1476	-	3,3,3	0.34	0	2,2,2	0.16	0
5	EDO	B	1478	-	3,3,3	0.28	0	2,2,2	0.37	0
5	EDO	R	1476	-	3,3,3	0.40	0	2,2,2	0.20	0
5	EDO	C	1123	-	3,3,3	0.27	0	2,2,2	0.57	0
5	EDO	B	1479	-	3,3,3	0.33	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	H	1476	-	3,3,3	0.38	0	2,2,2	0.11	0
5	EDO	R	1479	-	3,3,3	0.33	0	2,2,2	0.18	0
4	CAP	A	477	3	17,20,20	1.21	2 (11%)	22,31,31	1.11	1 (4%)
5	EDO	R	1480	-	3,3,3	0.35	0	2,2,2	0.31	0
5	EDO	H	1478	-	3,3,3	0.24	0	2,2,2	0.04	0
5	EDO	O	1478	-	3,3,3	0.27	0	2,2,2	0.32	0
5	EDO	H	1481	-	3,3,3	0.35	0	2,2,2	0.23	0
5	EDO	V	1479	-	3,3,3	0.35	0	2,2,2	0.09	0
5	EDO	H	1480	-	3,3,3	0.34	0	2,2,2	0.30	0
5	EDO	B	1481	-	3,3,3	0.33	0	2,2,2	0.12	0
5	EDO	A	1478	-	3,3,3	0.31	0	2,2,2	0.21	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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	O	477	3	-	9/29/29/29	-
5	EDO	K	1480	-	-	0/1/1/1	-
4	CAP	H	477	3	-	8/29/29/29	-
5	EDO	A	1479	-	-	0/1/1/1	-
5	EDO	A	1480	-	-	1/1/1/1	-
4	CAP	R	477	3	-	7/29/29/29	-
5	EDO	O	1477	-	-	1/1/1/1	-
5	EDO	T	1123	-	-	0/1/1/1	-
5	EDO	E	1478	-	-	0/1/1/1	-
4	CAP	E	477	3	-	10/29/29/29	-
5	EDO	H	1477	-	-	0/1/1/1	-
4	CAP	B	477	3	-	7/29/29/29	-
5	EDO	F	1123	-	-	0/1/1/1	-
5	EDO	K	1476	-	-	0/1/1/1	-
5	EDO	R	1478	-	-	0/1/1/1	-
5	EDO	B	1477	-	-	0/1/1/1	-
5	EDO	V	1476	-	-	1/1/1/1	-
5	EDO	H	1479	-	-	0/1/1/1	-
5	EDO	O	1480	-	-	1/1/1/1	-
5	EDO	O	1479	-	-	0/1/1/1	-
5	EDO	J	1123	-	-	0/1/1/1	-
5	EDO	K	1479	-	-	1/1/1/1	-
5	EDO	V	1478	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	K	1477	-	-	0/1/1/1	-
5	EDO	P	1123	-	-	0/1/1/1	-
5	EDO	A	1476	-	-	1/1/1/1	-
5	EDO	V	1477	-	-	0/1/1/1	-
5	EDO	V	1480	-	-	0/1/1/1	-
5	EDO	V	1481	-	-	1/1/1/1	-
5	EDO	E	1476	-	-	0/1/1/1	-
5	EDO	B	1480	-	-	0/1/1/1	-
5	EDO	E	1477	-	-	1/1/1/1	-
5	EDO	W	1123	-	-	0/1/1/1	-
4	CAP	V	477	3	-	8/29/29/29	-
5	EDO	M	1123	-	-	0/1/1/1	-
5	EDO	A	1477	-	-	1/1/1/1	-
5	EDO	E	1479	-	-	1/1/1/1	-
5	EDO	E	1480	-	-	1/1/1/1	-
5	EDO	K	1478	-	-	0/1/1/1	-
5	EDO	B	1476	-	-	1/1/1/1	-
5	EDO	R	1477	-	-	1/1/1/1	-
4	CAP	K	477	3	-	7/29/29/29	-
5	EDO	O	1476	-	-	0/1/1/1	-
5	EDO	B	1478	-	-	1/1/1/1	-
5	EDO	R	1476	-	-	0/1/1/1	-
5	EDO	C	1123	-	-	1/1/1/1	-
5	EDO	B	1479	-	-	0/1/1/1	-
5	EDO	H	1476	-	-	1/1/1/1	-
5	EDO	R	1479	-	-	0/1/1/1	-
4	CAP	A	477	3	-	9/29/29/29	-
5	EDO	R	1480	-	-	0/1/1/1	-
5	EDO	H	1478	-	-	1/1/1/1	-
5	EDO	O	1478	-	-	0/1/1/1	-
5	EDO	H	1481	-	-	0/1/1/1	-
5	EDO	V	1479	-	-	1/1/1/1	-
5	EDO	H	1480	-	-	1/1/1/1	-
5	EDO	B	1481	-	-	0/1/1/1	-
5	EDO	A	1478	-	-	0/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	477	CAP	O6-C	3.13	1.32	1.22
4	A	477	CAP	O6-C	3.00	1.31	1.22
4	E	477	CAP	O6-C	2.96	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	477	CAP	O6-C	2.96	1.31	1.22
4	R	477	CAP	O7-C	2.94	1.41	1.30
4	K	477	CAP	O6-C	2.85	1.31	1.22
4	A	477	CAP	O7-C	2.75	1.40	1.30
4	R	477	CAP	O6-C	2.70	1.30	1.22
4	B	477	CAP	O6-C	2.58	1.30	1.22
4	K	477	CAP	O7-C	2.58	1.39	1.30
4	V	477	CAP	O7-C	2.58	1.39	1.30
4	H	477	CAP	O7-C	2.56	1.39	1.30
4	E	477	CAP	O7-C	2.46	1.39	1.30
4	V	477	CAP	O6-C	2.42	1.29	1.22
4	B	477	CAP	O7-C	2.40	1.39	1.30
4	O	477	CAP	O7-C	2.16	1.38	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	477	CAP	O2-C2-C	-4.06	101.55	108.97
4	O	477	CAP	O2-C2-C	-3.39	102.78	108.97
4	B	477	CAP	O2-C2-C	-3.09	103.32	108.97
4	A	477	CAP	O2-C2-C	-2.96	103.57	108.97
4	E	477	CAP	O6P-P2-O5	2.70	113.91	106.73
4	E	477	CAP	O2-C2-C	-2.42	104.55	108.97
4	V	477	CAP	O2-C2-C	-2.41	104.57	108.97
4	R	477	CAP	O7-C-O6	-2.22	116.75	123.82
4	O	477	CAP	O3-C3-C4	2.12	113.67	109.13
4	B	477	CAP	O4-C4-C5	-2.11	105.17	109.92
4	R	477	CAP	O5-P2-O4P	2.02	112.13	106.47

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	477	CAP	O6-C-C2-C1
4	A	477	CAP	O7-C-C2-C1
4	A	477	CAP	O6-C-C2-O2
4	A	477	CAP	O7-C-C2-O2
4	A	477	CAP	C2-C3-C4-O4
4	A	477	CAP	O3-C3-C4-O4
4	B	477	CAP	O6-C-C2-C1
4	B	477	CAP	O7-C-C2-C1
4	B	477	CAP	O6-C-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	477	CAP	O7-C-C2-O2
4	B	477	CAP	C2-C3-C4-O4
4	B	477	CAP	O3-C3-C4-O4
4	E	477	CAP	O6-C-C2-C1
4	E	477	CAP	O7-C-C2-C1
4	E	477	CAP	O6-C-C2-O2
4	E	477	CAP	O7-C-C2-O2
4	E	477	CAP	C2-C3-C4-O4
4	E	477	CAP	O3-C3-C4-O4
4	H	477	CAP	O6-C-C2-C1
4	H	477	CAP	O7-C-C2-C1
4	H	477	CAP	O6-C-C2-O2
4	H	477	CAP	O7-C-C2-O2
4	H	477	CAP	C2-C3-C4-O4
4	H	477	CAP	O3-C3-C4-O4
4	K	477	CAP	O6-C-C2-C1
4	K	477	CAP	O7-C-C2-C1
4	K	477	CAP	O6-C-C2-O2
4	K	477	CAP	O7-C-C2-O2
4	K	477	CAP	C2-C3-C4-O4
4	K	477	CAP	O3-C3-C4-O4
4	O	477	CAP	O6-C-C2-C1
4	O	477	CAP	O7-C-C2-C1
4	O	477	CAP	O6-C-C2-O2
4	O	477	CAP	O7-C-C2-O2
4	O	477	CAP	C2-C3-C4-O4
4	O	477	CAP	O3-C3-C4-O4
4	R	477	CAP	O6-C-C2-C1
4	R	477	CAP	O7-C-C2-C1
4	R	477	CAP	O6-C-C2-O2
4	R	477	CAP	O7-C-C2-O2
4	R	477	CAP	C2-C3-C4-O4
4	R	477	CAP	O3-C3-C4-O4
4	V	477	CAP	O6-C-C2-C1
4	V	477	CAP	O7-C-C2-C1
4	V	477	CAP	O6-C-C2-O2
4	V	477	CAP	O7-C-C2-O2
4	V	477	CAP	C2-C3-C4-O4
4	V	477	CAP	O3-C3-C4-O4
5	C	1123	EDO	O1-C1-C2-O2
5	A	1480	EDO	O1-C1-C2-O2
5	H	1478	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	V	1481	EDO	O1-C1-C2-O2
4	A	477	CAP	O2-C2-C3-C4
4	B	477	CAP	O2-C2-C3-C4
4	E	477	CAP	O2-C2-C3-C4
4	H	477	CAP	O2-C2-C3-C4
4	K	477	CAP	O2-C2-C3-C4
4	O	477	CAP	O2-C2-C3-C4
4	R	477	CAP	O2-C2-C3-C4
4	V	477	CAP	O2-C2-C3-C4
5	E	1477	EDO	O1-C1-C2-O2
5	O	1480	EDO	O1-C1-C2-O2
5	V	1478	EDO	O1-C1-C2-O2
4	E	477	CAP	C2-C3-C4-C5
4	H	477	CAP	C2-C3-C4-C5
4	O	477	CAP	C2-C3-C4-C5
5	A	1477	EDO	O1-C1-C2-O2
5	B	1478	EDO	O1-C1-C2-O2
5	E	1480	EDO	O1-C1-C2-O2
5	H	1480	EDO	O1-C1-C2-O2
5	K	1479	EDO	O1-C1-C2-O2
5	R	1477	EDO	O1-C1-C2-O2
5	B	1476	EDO	O1-C1-C2-O2
5	H	1476	EDO	O1-C1-C2-O2
4	A	477	CAP	C4-C5-O5-P2
5	A	1476	EDO	O1-C1-C2-O2
5	O	1477	EDO	O1-C1-C2-O2
5	V	1479	EDO	O1-C1-C2-O2
4	E	477	CAP	C4-C5-O5-P2
4	O	477	CAP	C4-C5-O5-P2
5	E	1479	EDO	O1-C1-C2-O2
5	V	1476	EDO	O1-C1-C2-O2
4	E	477	CAP	O3-C3-C4-C5
4	A	477	CAP	C2-C3-C4-C5
4	V	477	CAP	C2-C3-C4-C5

There are no ring outliers.

9 monomers are involved in 12 short contacts:

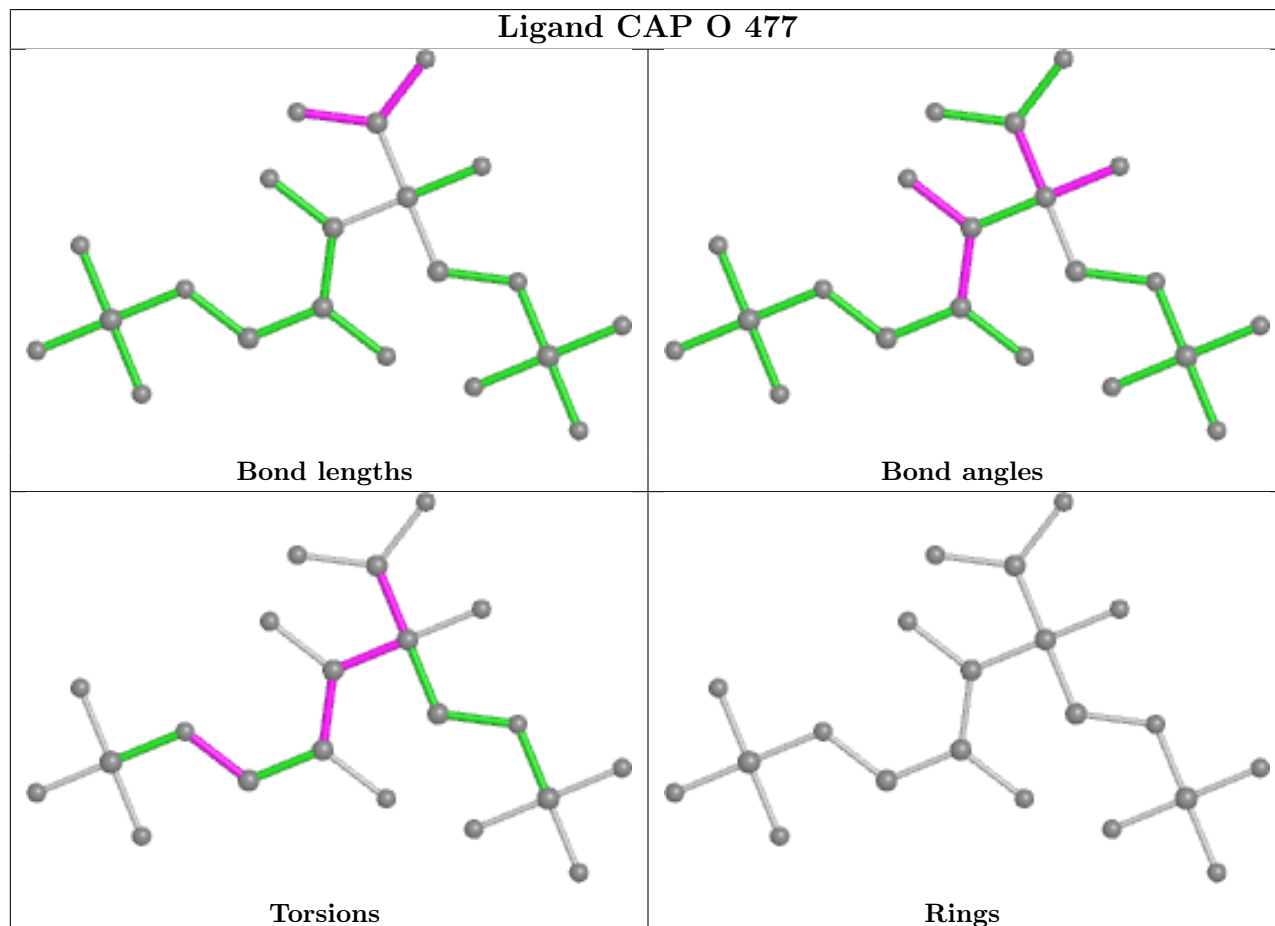
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	477	CAP	1	0
5	O	1480	EDO	1	0
5	J	1123	EDO	1	0

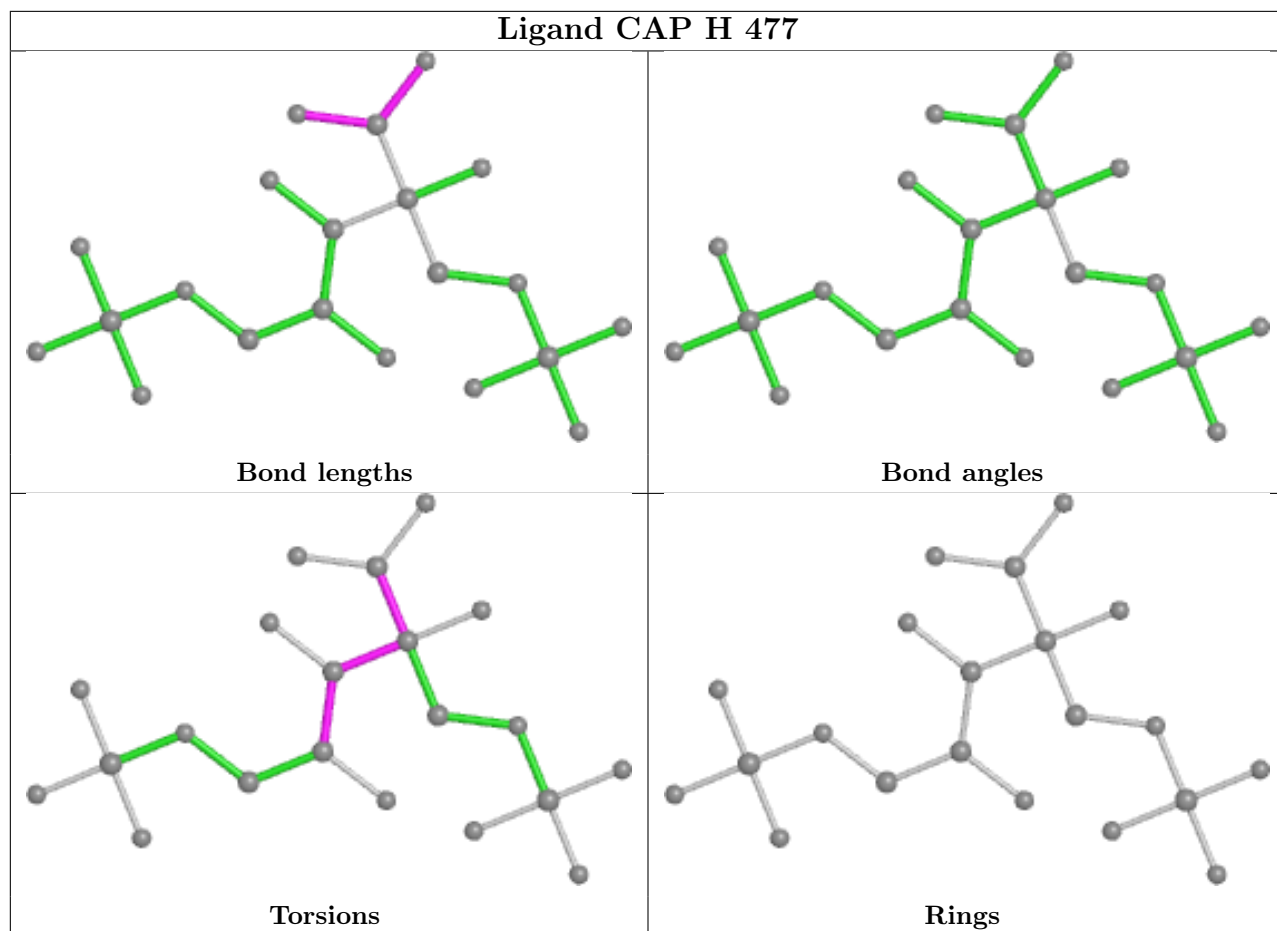
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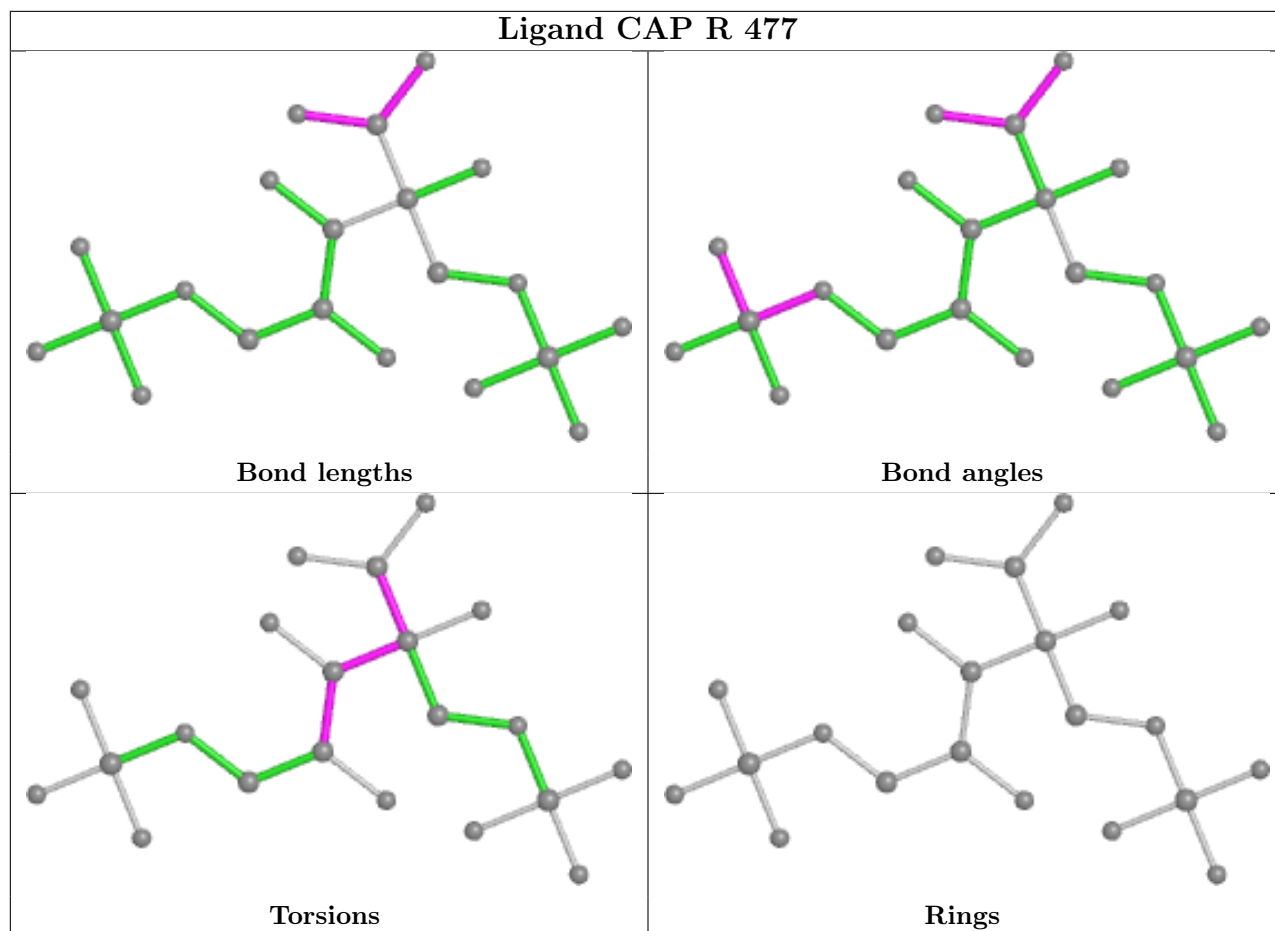
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1480	EDO	2	0
5	R	1477	EDO	1	0
5	R	1480	EDO	1	0
5	H	1481	EDO	1	0
5	H	1480	EDO	2	0
5	B	1481	EDO	2	0

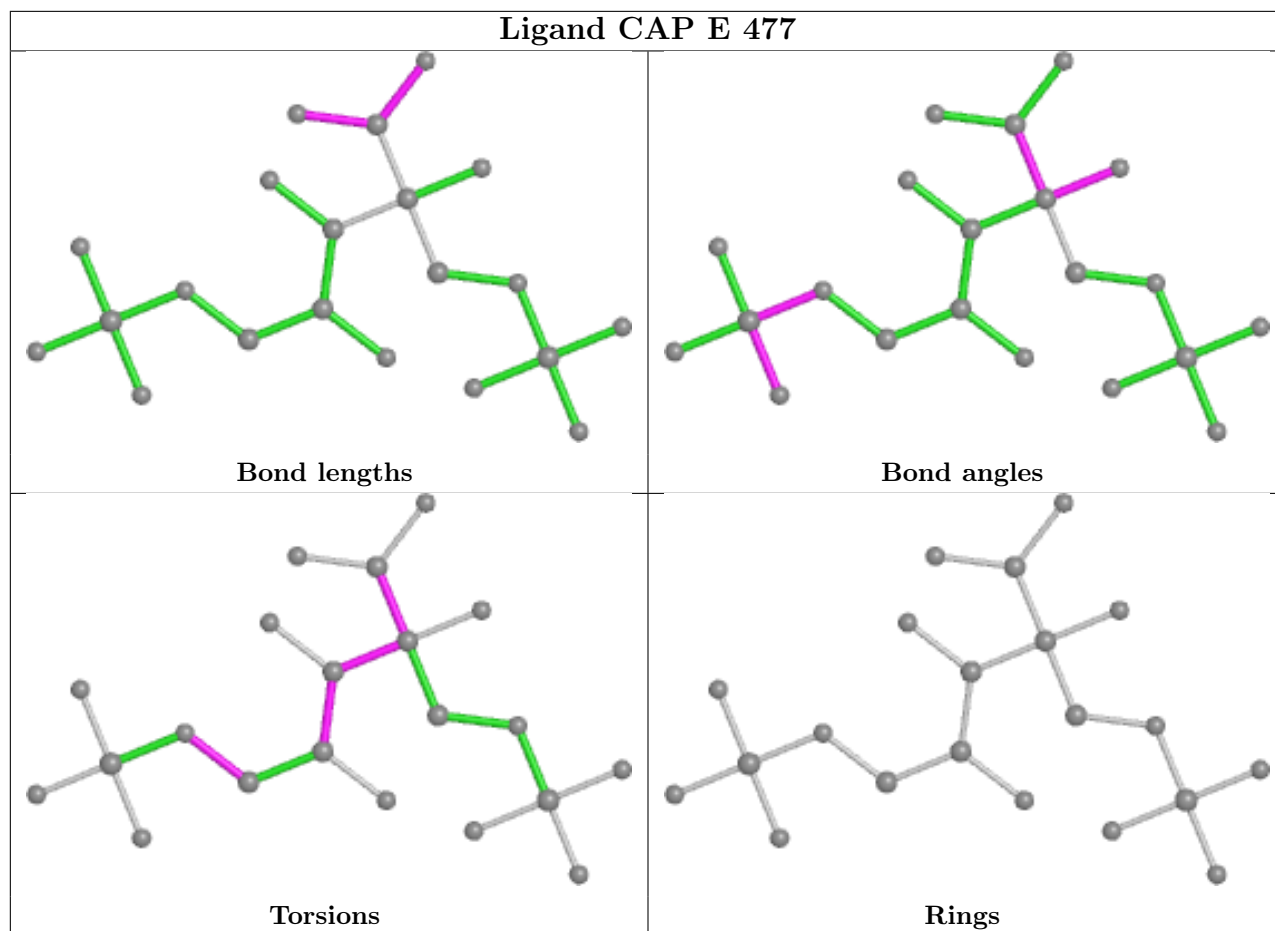
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

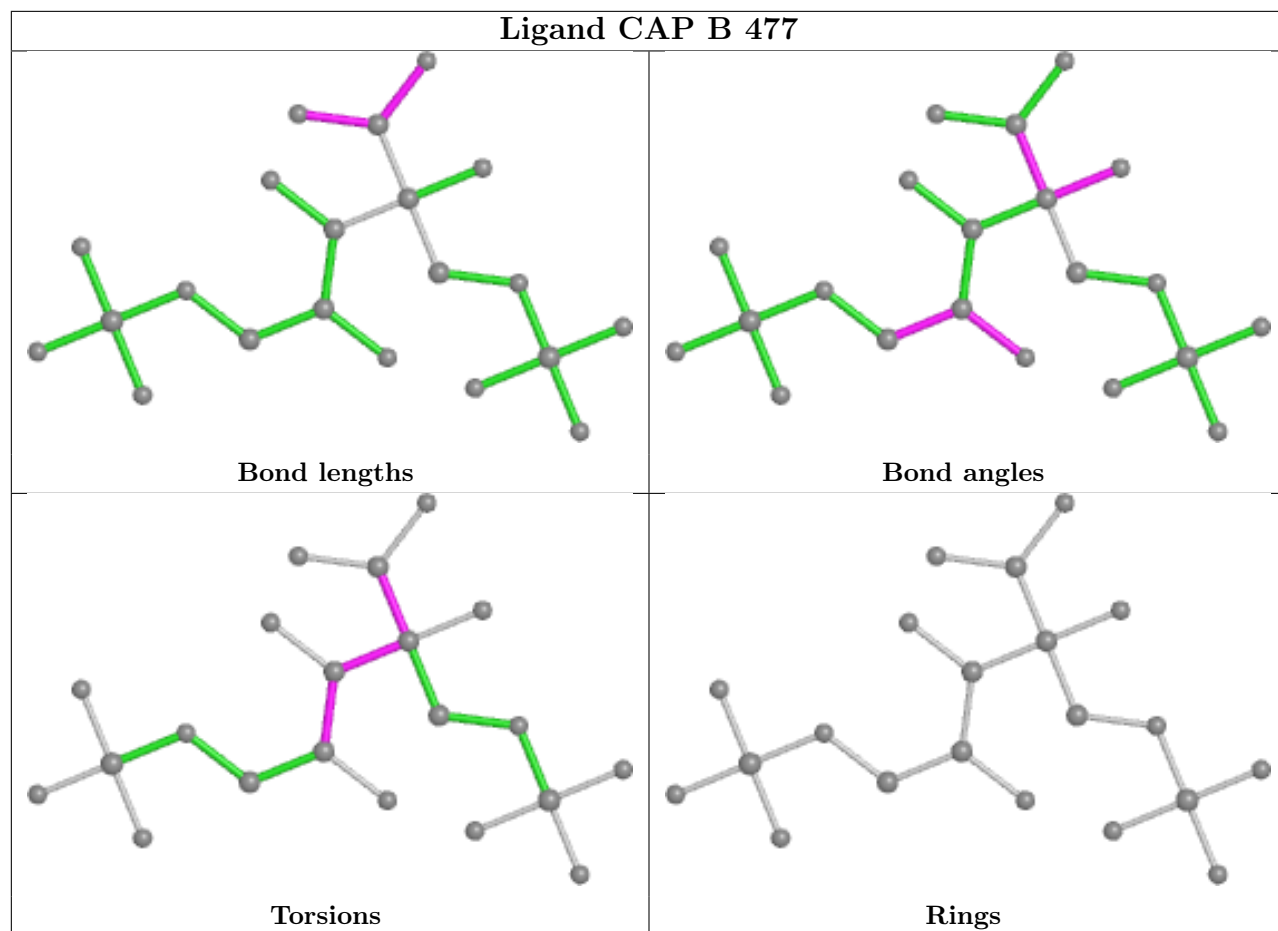


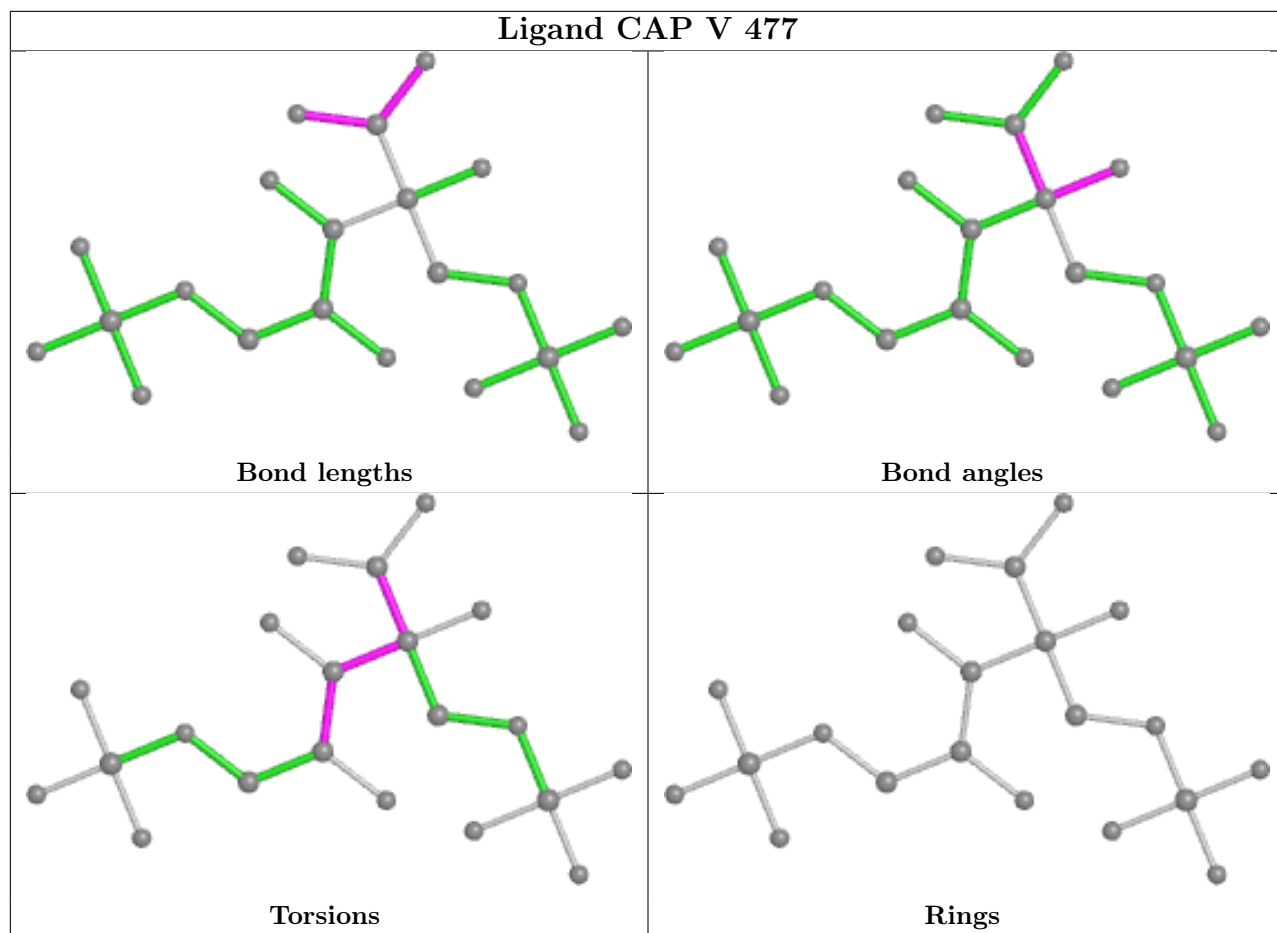


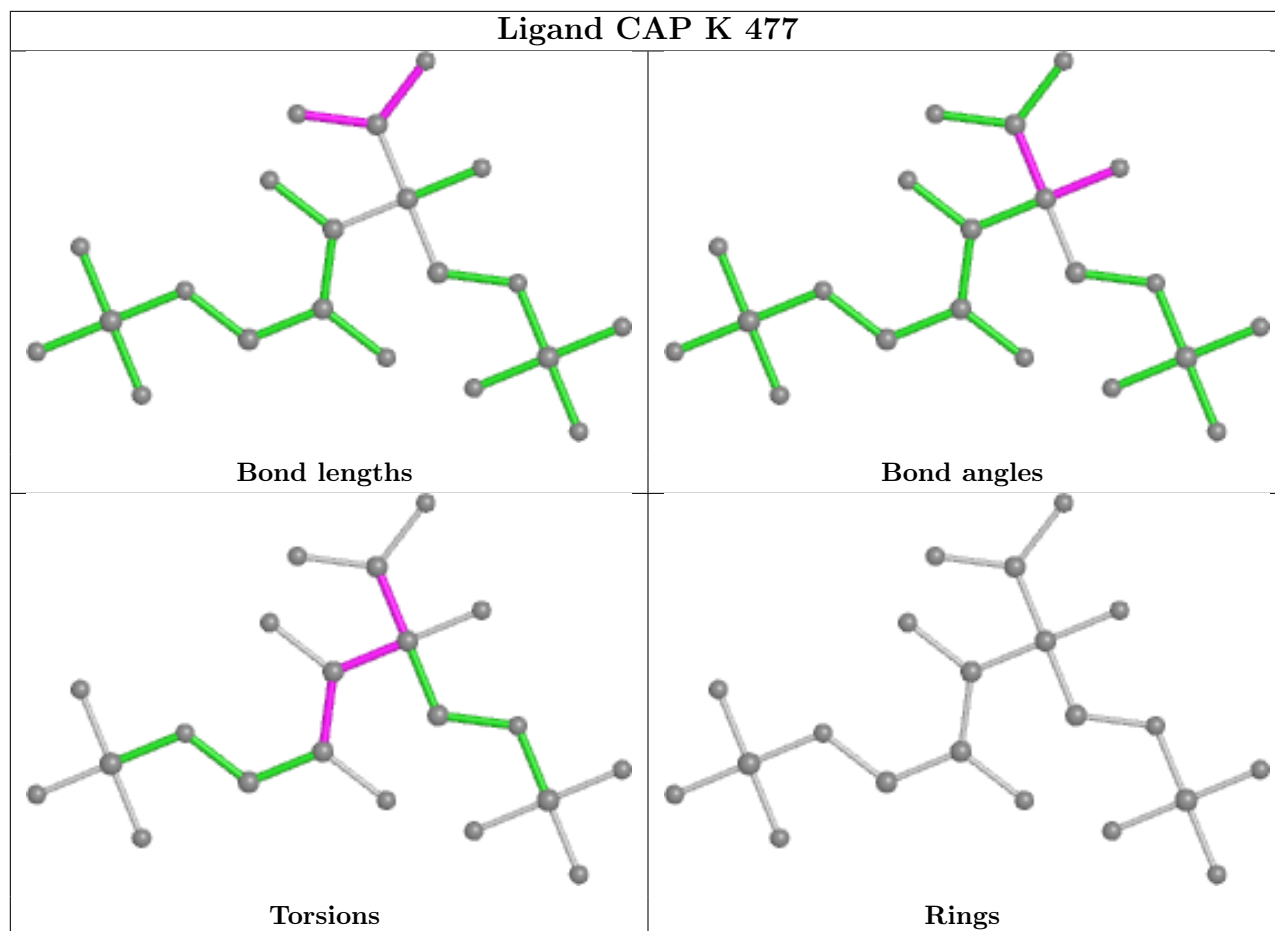


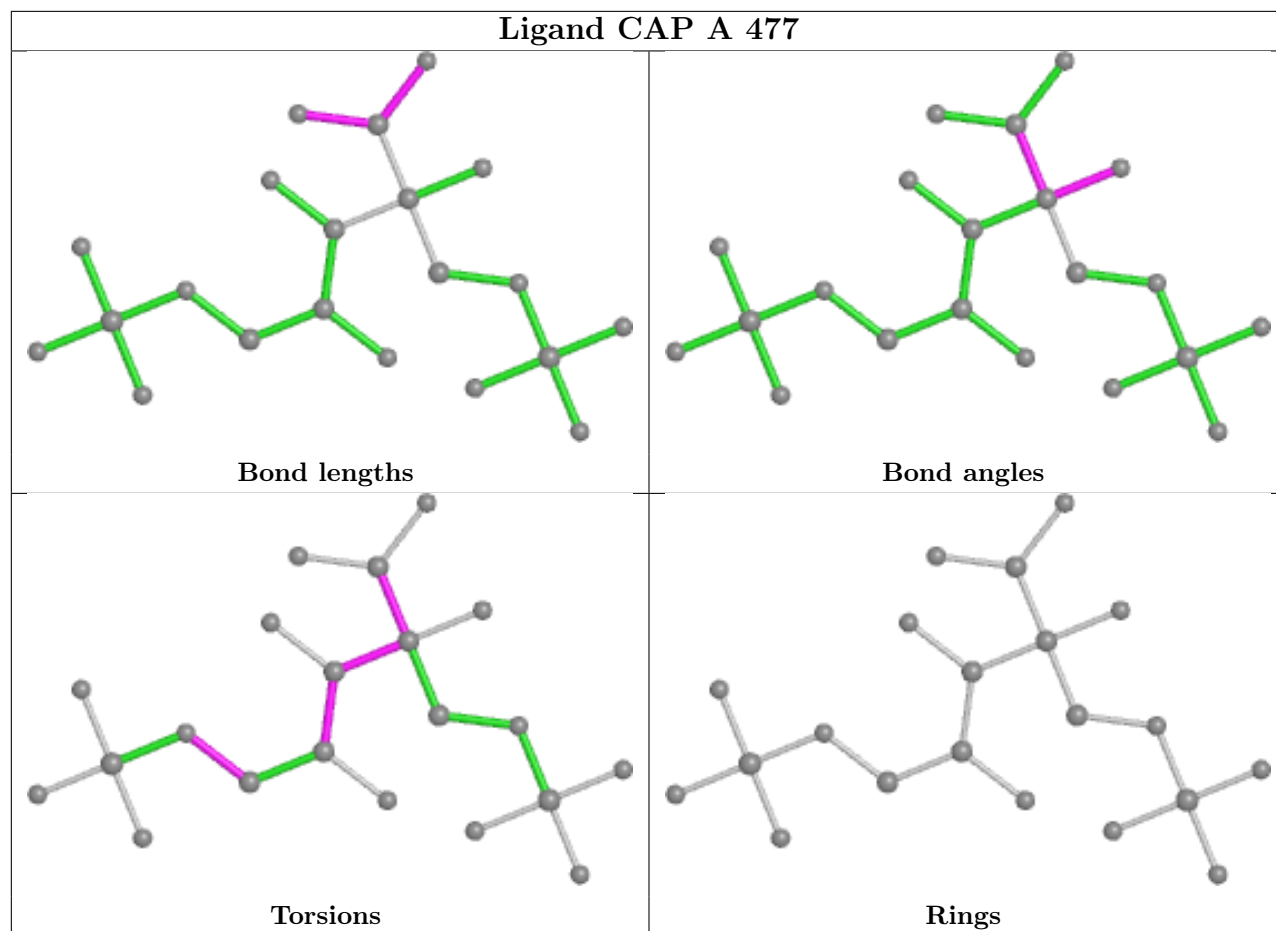












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	460/475 (96%)	-0.81	2 (0%) 92 91	13, 19, 34, 49	0
1	B	462/475 (97%)	-0.77	4 (0%) 84 83	12, 19, 34, 66	0
1	E	464/475 (97%)	-0.80	6 (1%) 77 75	13, 19, 35, 76	0
1	H	464/475 (97%)	-0.81	5 (1%) 80 79	13, 19, 35, 72	0
1	K	464/475 (97%)	-0.75	7 (1%) 73 72	13, 19, 35, 81	0
1	O	464/475 (97%)	-0.80	5 (1%) 80 79	13, 19, 35, 80	0
1	R	464/475 (97%)	-0.80	6 (1%) 77 75	12, 19, 35, 84	0
1	V	464/475 (97%)	-0.77	8 (1%) 70 68	13, 19, 35, 80	0
2	C	122/122 (100%)	-0.33	3 (2%) 57 55	18, 27, 58, 69	0
2	F	122/122 (100%)	-0.28	6 (4%) 29 28	18, 27, 58, 69	1 (0%)
2	I	122/122 (100%)	-0.38	4 (3%) 46 44	18, 27, 58, 69	1 (0%)
2	J	122/122 (100%)	-0.19	10 (8%) 11 10	18, 27, 58, 69	1 (0%)
2	M	122/122 (100%)	-0.23	7 (5%) 23 22	18, 27, 58, 69	1 (0%)
2	P	122/122 (100%)	-0.34	4 (3%) 46 44	18, 27, 58, 69	0
2	T	122/122 (100%)	-0.28	8 (6%) 18 17	18, 27, 58, 69	0
2	W	122/122 (100%)	-0.06	11 (9%) 9 8	18, 27, 58, 69	1 (0%)
All	All	4682/4776 (98%)	-0.68	96 (2%) 63 61	12, 20, 41, 84	5 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	112	ARG	8.5
1	E	9	ALA	6.5
2	W	111	ALA	6.4
2	T	112	ARG	6.0
2	J	112	ARG	5.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	W	112	ARG	5.3
1	B	10	GLY	5.0
1	O	10	GLY	4.9
2	M	111	ALA	4.9
1	B	9	ALA	4.8
1	O	8	LYS	4.8
2	W	110	THR	4.4
2	F	112	ARG	4.4
1	K	8	LYS	4.4
2	P	112	ARG	4.3
2	J	118	ASN	4.1
2	C	118	ASN	4.1
2	C	112	ARG	4.1
1	V	9	ALA	4.1
2	F	110	THR	4.0
2	I	112	ARG	3.9
2	T	118	ASN	3.9
2	T	110	THR	3.8
1	O	7	THR	3.8
2	J	114	PHE	3.8
2	I	118	ASN	3.8
2	T	113	ASP	3.7
1	V	7	THR	3.7
2	W	118	ASN	3.6
1	H	8	LYS	3.6
2	J	116	PRO	3.5
1	H	7	THR	3.5
2	J	117	ALA	3.4
1	E	8	LYS	3.3
2	M	118	ASN	3.3
1	O	9	ALA	3.2
1	V	10	GLY	3.2
2	J	119	LYS	3.2
2	W	117	ALA	3.2
1	H	9	ALA	3.1
1	K	9	ALA	3.1
1	K	10	GLY	3.1
2	I	114	PHE	3.1
1	V	8	LYS	3.0
1	R	8	LYS	3.0
1	E	10	GLY	3.0
2	P	119	LYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	T	119	LYS	3.0
2	J	110	THR	3.0
2	J	111	ALA	2.9
1	B	94	ASP	2.9
1	R	92	GLY	2.9
2	W	109	LYS	2.9
1	R	10	GLY	2.8
2	P	118	ASN	2.8
1	B	439	ARG	2.7
1	R	9	ALA	2.7
1	K	439	ARG	2.6
1	R	7	THR	2.6
2	F	114	PHE	2.6
2	F	119	LYS	2.6
1	V	439	ARG	2.5
2	W	114	PHE	2.5
2	M	119	LYS	2.5
2	M	110	THR	2.5
2	W	116	PRO	2.5
2	T	111	ALA	2.5
2	J	113	ASP	2.4
1	V	226	TYR	2.4
1	H	439	ARG	2.4
1	O	94	ASP	2.4
1	E	94	ASP	2.4
2	J	109	LYS	2.4
1	K	94	ASP	2.4
2	P	110	THR	2.3
2	M	117	ALA	2.3
1	K	7	THR	2.3
2	M	114	PHE	2.3
2	C	119	LYS	2.2
2	W	113	ASP	2.2
1	K	11	ALA	2.2
1	A	94	ASP	2.2
2	W	119	LYS	2.2
2	I	110	THR	2.2
1	V	94	ASP	2.2
2	F	118	ASN	2.2
2	T	114	PHE	2.2
1	A	439	ARG	2.1
1	E	7	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	439	ARG	2.1
2	T	109	LYS	2.1
2	F	113	ASP	2.1
2	W	69	MET	2.1
1	H	10	GLY	2.0
1	E	439	ARG	2.0
1	V	91	PRO	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	HYP	B	151	8/9	0.95	0.09	13,15,16,16	0
1	HYP	A	104	8/9	0.96	0.12	14,16,18,18	0
1	SMC	A	256	7/8	0.97	0.07	14,14,16,18	0
1	HYP	A	151	8/9	0.97	0.07	13,15,16,16	0
1	HYP	E	151	8/9	0.97	0.06	14,15,16,16	0
1	KCX	E	201	12/13	0.97	0.09	13,15,16,17	0
1	HYP	H	104	8/9	0.97	0.07	14,16,17,18	0
1	SMC	H	369	7/8	0.97	0.07	17,17,19,21	0
1	KCX	K	201	12/13	0.97	0.10	13,15,16,16	0
1	HYP	R	104	8/9	0.97	0.07	14,16,18,18	0
1	KCX	R	201	12/13	0.97	0.11	13,15,16,16	0
1	SMC	R	369	7/8	0.97	0.06	17,17,19,21	0
1	HYP	V	104	8/9	0.97	0.06	14,16,17,18	0
1	KCX	V	201	12/13	0.97	0.08	13,14,16,17	0
1	KCX	A	201	12/13	0.98	0.10	13,15,16,16	0
1	KCX	H	201	12/13	0.98	0.08	13,15,16,17	0
1	SMC	H	256	7/8	0.98	0.08	14,14,16,18	0
1	KCX	B	201	12/13	0.98	0.10	13,15,16,17	0
1	HYP	K	104	8/9	0.98	0.06	14,16,17,18	0
1	HYP	K	151	8/9	0.98	0.06	14,15,16,16	0
1	SMC	B	256	7/8	0.98	0.08	14,14,16,19	0
1	HYP	O	104	8/9	0.98	0.05	14,16,17,18	0
1	KCX	O	201	12/13	0.98	0.08	13,15,16,16	0
1	SMC	O	256	7/8	0.98	0.07	14,14,16,19	0
1	SMC	B	369	7/8	0.98	0.08	17,17,18,20	0
1	HYP	R	151	8/9	0.98	0.07	14,14,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	HYP	E	104	8/9	0.98	0.07	14,16,17,18	0
1	SMC	A	369	7/8	0.98	0.07	17,17,18,21	0
1	HYP	B	104	8/9	0.98	0.07	14,15,17,17	0
1	HYP	V	151	8/9	0.98	0.07	14,15,15,16	0
1	SMC	E	369	7/8	0.98	0.06	17,17,19,21	0
1	SMC	E	256	7/8	0.99	0.07	14,14,16,19	0
1	HYP	O	151	8/9	0.99	0.06	14,15,16,16	0
1	SMC	R	256	7/8	0.99	0.06	14,15,16,18	0
1	HYP	H	151	8/9	0.99	0.07	14,15,16,16	0
1	SMC	K	256	7/8	0.99	0.07	14,14,16,18	0
1	SMC	O	369	7/8	0.99	0.07	17,17,18,20	0
1	SMC	K	369	7/8	0.99	0.06	16,17,19,21	0
1	SMC	V	256	7/8	0.99	0.07	14,15,16,18	0
1	SMC	V	369	7/8	0.99	0.05	17,17,19,21	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	V	1481	4/4	0.76	0.25	34,40,43,48	0
5	EDO	O	1480	4/4	0.83	0.22	29,36,41,46	0
5	EDO	H	1480	4/4	0.87	0.23	39,51,53,53	0
5	EDO	H	1481	4/4	0.87	0.15	42,45,46,49	0
5	EDO	A	1480	4/4	0.90	0.17	38,40,41,44	0
5	EDO	W	1123	4/4	0.90	0.14	33,38,38,45	0
5	EDO	A	1478	4/4	0.91	0.12	27,34,34,38	0
5	EDO	R	1478	4/4	0.92	0.10	32,32,33,34	0
5	EDO	B	1479	4/4	0.93	0.09	26,32,33,35	0
5	EDO	P	1123	4/4	0.93	0.17	29,31,36,37	0
5	EDO	K	1479	4/4	0.93	0.16	28,29,34,34	0
5	EDO	M	1123	4/4	0.93	0.16	30,38,38,43	0
5	EDO	O	1478	4/4	0.93	0.11	33,35,37,39	0
5	EDO	C	1123	4/4	0.94	0.16	25,29,34,38	0

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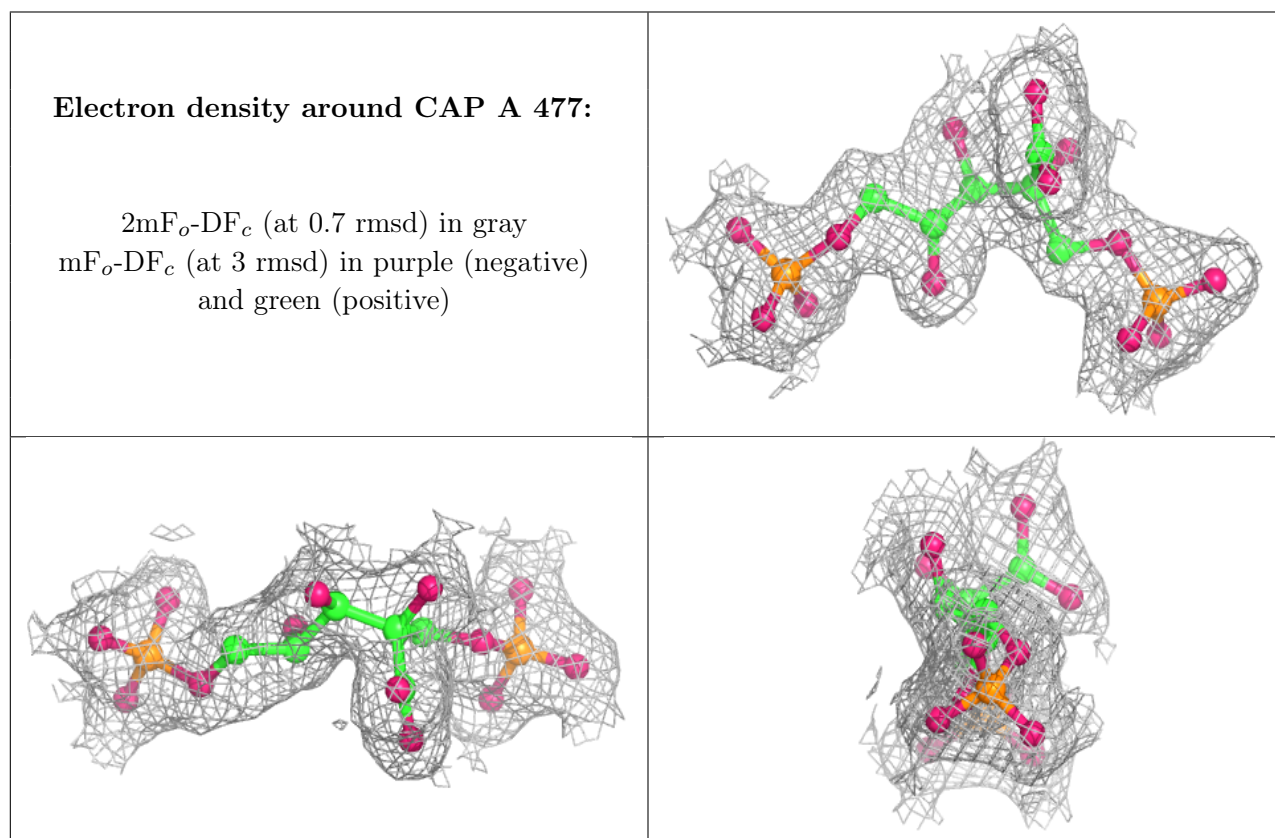
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	H	1479	4/4	0.94	0.10	28,28,32,37	0
5	EDO	K	1476	4/4	0.95	0.11	21,22,23,27	0
5	EDO	K	1478	4/4	0.95	0.11	31,31,32,34	0
5	EDO	R	1480	4/4	0.95	0.11	31,33,33,37	0
5	EDO	V	1476	4/4	0.95	0.16	21,21,27,30	0
5	EDO	V	1479	4/4	0.95	0.10	27,29,31,33	0
5	EDO	O	1479	4/4	0.95	0.15	24,26,32,33	0
5	EDO	E	1479	4/4	0.95	0.11	38,38,38,40	0
5	EDO	R	1476	4/4	0.96	0.09	19,21,23,23	0
5	EDO	K	1480	4/4	0.96	0.08	33,33,36,41	0
5	EDO	J	1123	4/4	0.96	0.18	35,39,43,46	0
5	EDO	T	1123	4/4	0.96	0.11	27,27,30,35	0
5	EDO	E	1478	4/4	0.96	0.08	34,34,35,37	0
5	EDO	K	1477	4/4	0.96	0.07	26,31,32,33	0
5	EDO	E	1480	4/4	0.96	0.11	29,31,32,32	0
5	EDO	F	1123	4/4	0.96	0.13	29,32,35,36	0
5	EDO	B	1481	4/4	0.97	0.10	30,35,37,38	0
5	EDO	O	1477	4/4	0.97	0.11	22,25,26,27	0
5	EDO	B	1478	4/4	0.97	0.09	21,23,27,29	0
5	EDO	H	1477	4/4	0.97	0.09	16,23,23,25	0
5	EDO	E	1476	4/4	0.97	0.08	21,22,24,28	0
5	EDO	B	1477	4/4	0.97	0.07	16,19,22,25	0
5	EDO	B	1480	4/4	0.97	0.14	22,33,34,35	0
3	MG	K	476	1/1	0.98	0.04	19,19,19,19	0
5	EDO	B	1476	4/4	0.98	0.30	2,3,3,6	4
3	MG	O	476	1/1	0.98	0.03	15,15,15,15	0
3	MG	V	476	1/1	0.98	0.05	16,16,16,16	0
5	EDO	R	1477	4/4	0.98	0.09	23,26,28,30	0
5	EDO	A	1476	4/4	0.98	0.05	22,22,24,27	0
5	EDO	R	1479	4/4	0.98	0.10	29,31,35,35	0
5	EDO	H	1476	4/4	0.98	0.33	2,5,5,10	4
5	EDO	A	1477	4/4	0.98	0.10	18,18,23,24	0
5	EDO	H	1478	4/4	0.98	0.11	24,26,28,29	0
5	EDO	V	1477	4/4	0.98	0.07	21,21,24,26	0
5	EDO	V	1478	4/4	0.98	0.11	23,27,30,31	0
5	EDO	O	1476	4/4	0.98	0.06	22,26,26,29	0
5	EDO	V	1480	4/4	0.98	0.12	24,27,29,30	0
3	MG	B	476	1/1	0.98	0.04	12,12,12,12	0
5	EDO	A	1479	4/4	0.98	0.12	15,25,26,27	0
3	MG	E	476	1/1	0.99	0.04	13,13,13,13	0
4	CAP	A	477	21/21	0.99	0.07	12,17,22,24	0
4	CAP	B	477	21/21	0.99	0.08	14,18,20,22	0

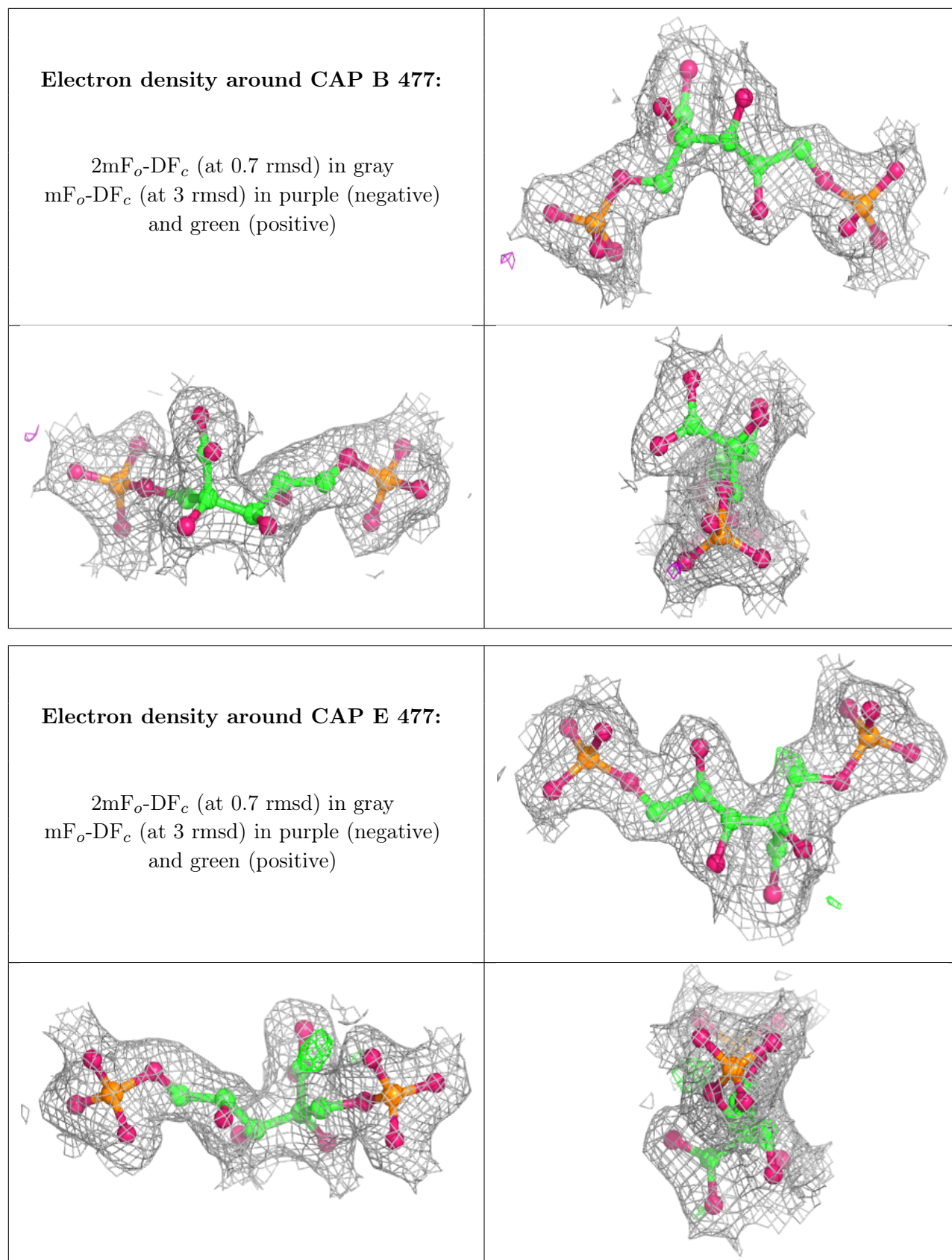
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CAP	E	477	21/21	0.99	0.07	15,19,22,24	0
4	CAP	H	477	21/21	0.99	0.07	16,20,23,28	0
4	CAP	K	477	21/21	0.99	0.07	13,16,21,24	0
4	CAP	O	477	21/21	0.99	0.06	12,17,20,24	0
4	CAP	R	477	21/21	0.99	0.07	11,16,20,26	0
4	CAP	V	477	21/21	0.99	0.07	16,18,22,23	0
3	MG	H	476	1/1	0.99	0.03	16,16,16,16	0
3	MG	R	476	1/1	0.99	0.04	11,11,11,11	0
5	EDO	E	1477	4/4	0.99	0.06	19,21,21,22	0
3	MG	A	476	1/1	1.00	0.04	17,17,17,17	0

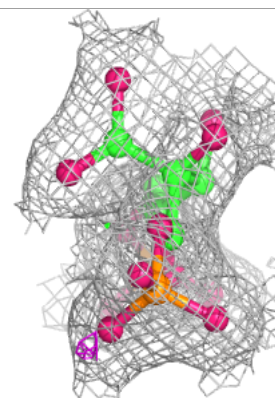
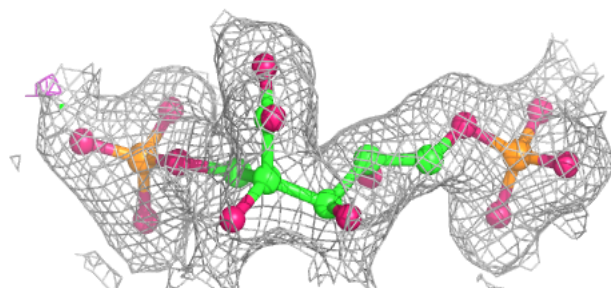
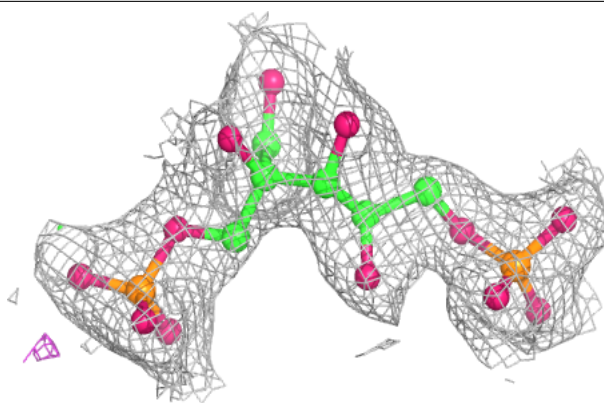
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



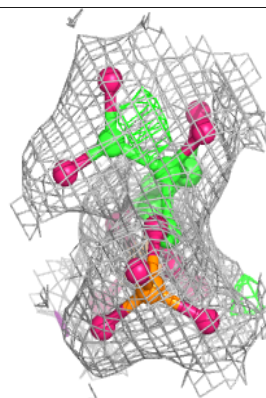
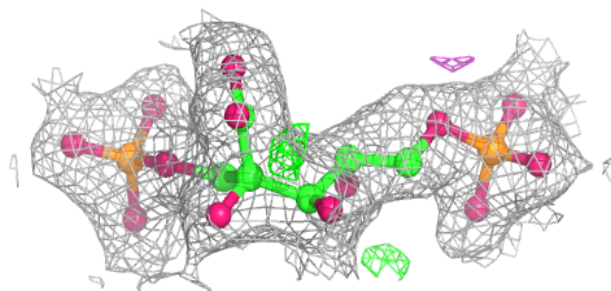
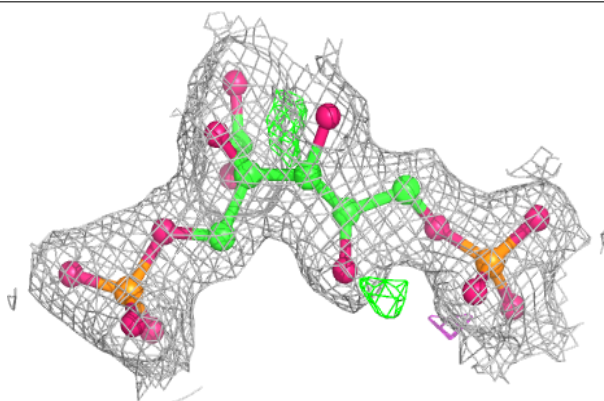


**Electron density around CAP H 477:**

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

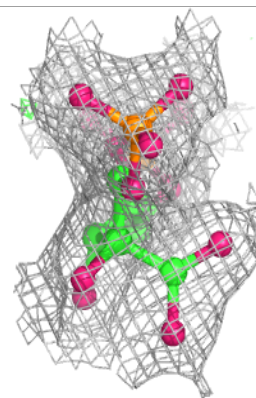
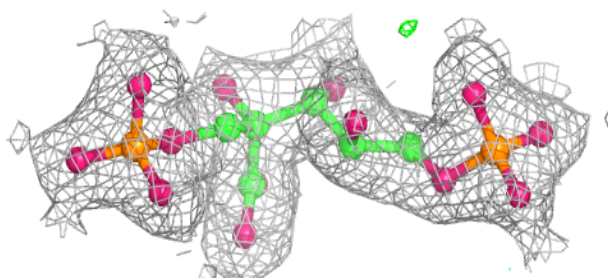
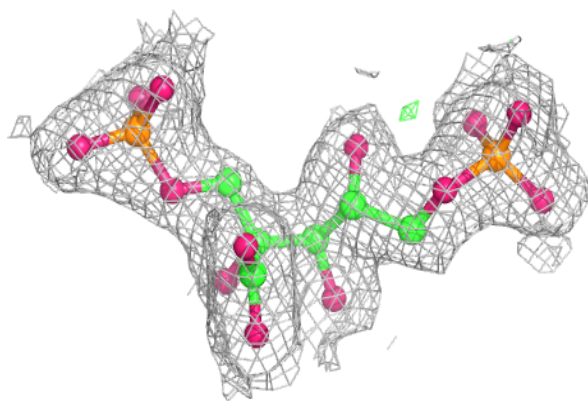
**Electron density around CAP K 477:**

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

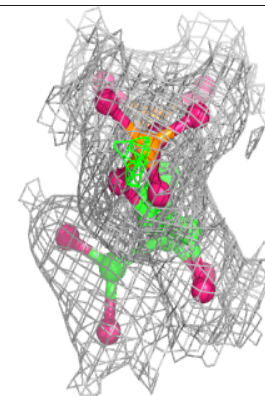
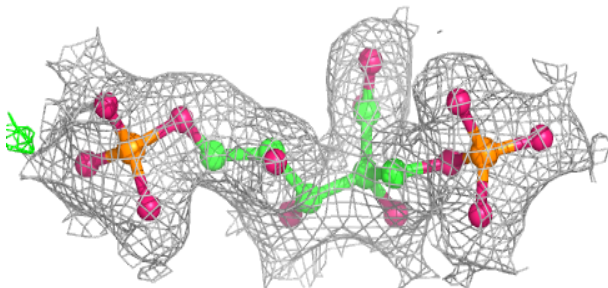
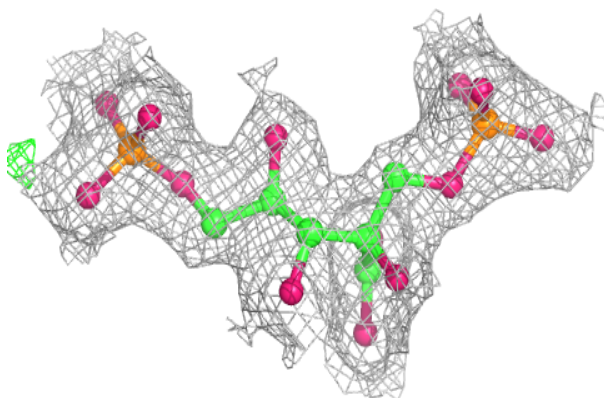


**Electron density around CAP O 477:**

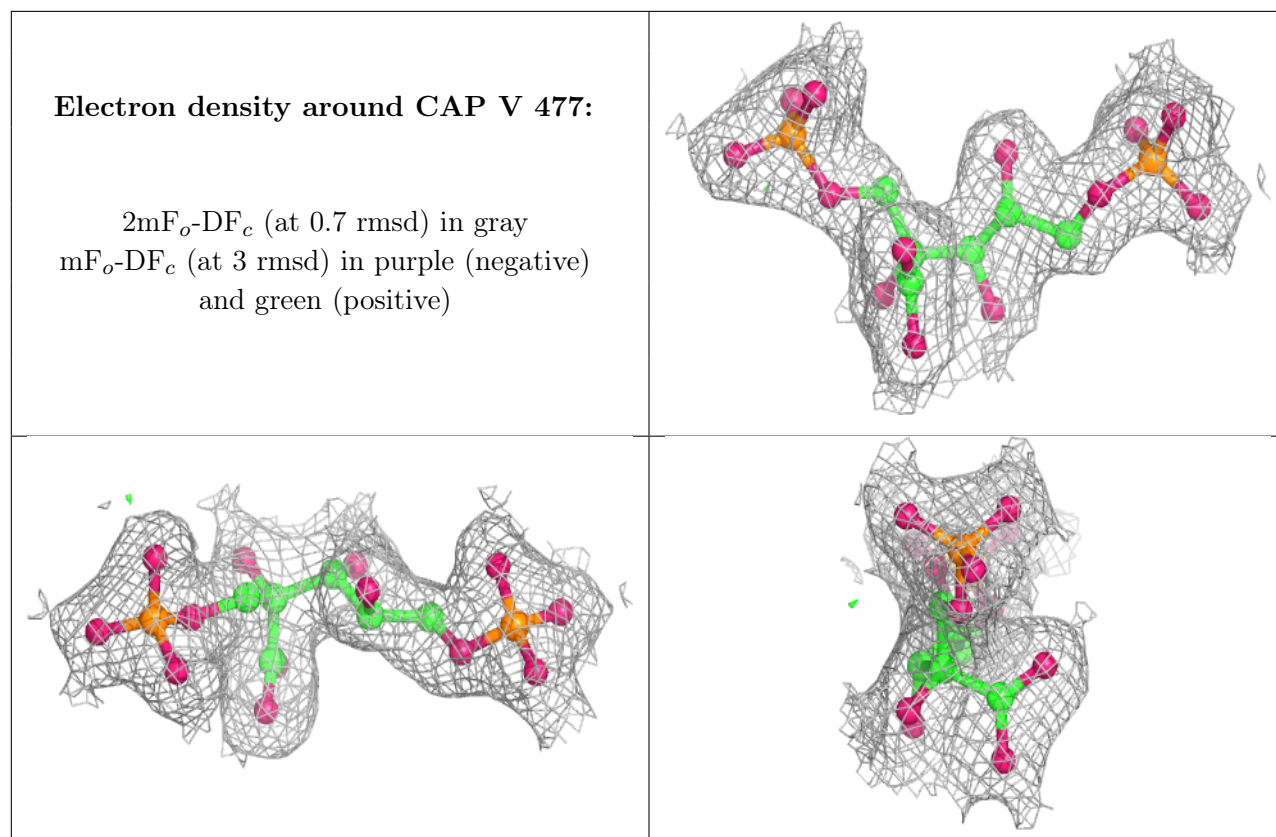
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CAP R 477:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.