



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:22 pm BST

PDB ID : 1UPM  
Title : ACTIVATED SPINACH RUBISCO COMPLEXED WITH 2-CARBOXYARABINITOL 2 BISPHOSPHAT AND CA<sup>2+</sup>.  
Authors : Karkehabadi, S.; Taylor, T.C.; Andersson, I.  
Deposited on : 2003-10-08  
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

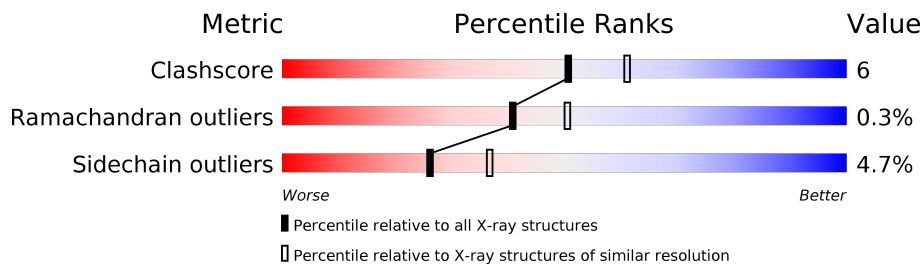
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	B	475	83% 13% ...
1	E	475	82% 13% ...
1	H	475	83% 12% ...
1	K	475	84% 11% ..
1	L	475	83% 12% ...
1	O	475	83% 13% ...
1	R	475	83% 13% ...
1	V	475	85% 11% ...
2	C	123	76% 18% 5% .

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	123	 80% 16% ..
2	I	123	 80% 15% 5%
2	M	123	 79% 18% .
2	P	123	 85% 12% .
2	S	123	 81% 14% 5%
2	T	123	 81% 15% .
2	W	123	 84% 13% ..

## 2 Entry composition [i](#)

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

There are 56 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*

*Continued from previous page...*

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

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

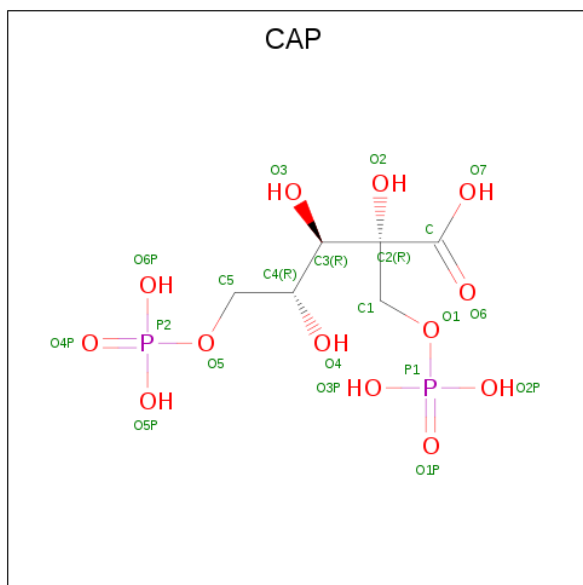
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	V	1	Total Ca 1 1	0	0
3	O	1	Total Ca 1 1	0	0
3	R	1	Total Ca 1 1	0	0

*Continued on next page...*

Continued from previous page...

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

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula:  $C_6H_{14}O_{13}P_2$ ).



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

- Molecule 5 is water.

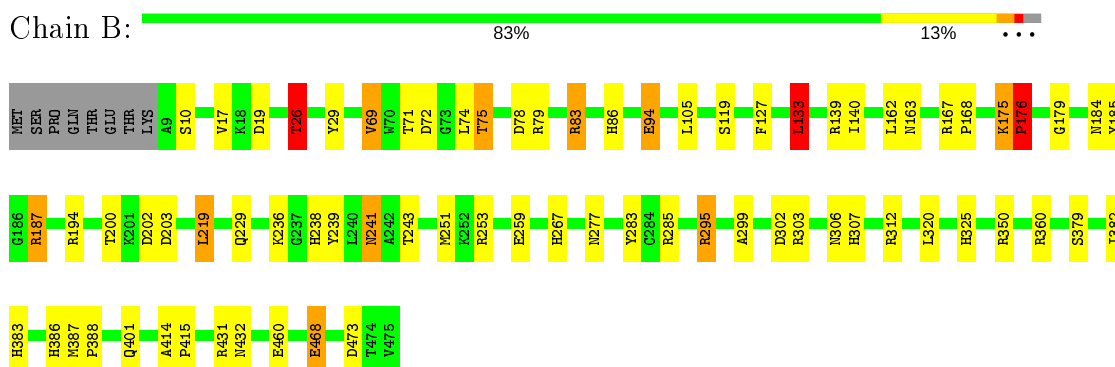
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	263	Total O 263 263	0	0
5	C	58	Total O 58 58	0	0
5	E	297	Total O 297 297	0	0
5	F	100	Total O 100 100	0	0
5	H	246	Total O 246 246	0	0
5	I	42	Total O 42 42	0	0
5	K	278	Total O 278 278	0	0
5	L	308	Total O 308 308	0	0
5	M	91	Total O 91 91	0	0
5	O	261	Total O 261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



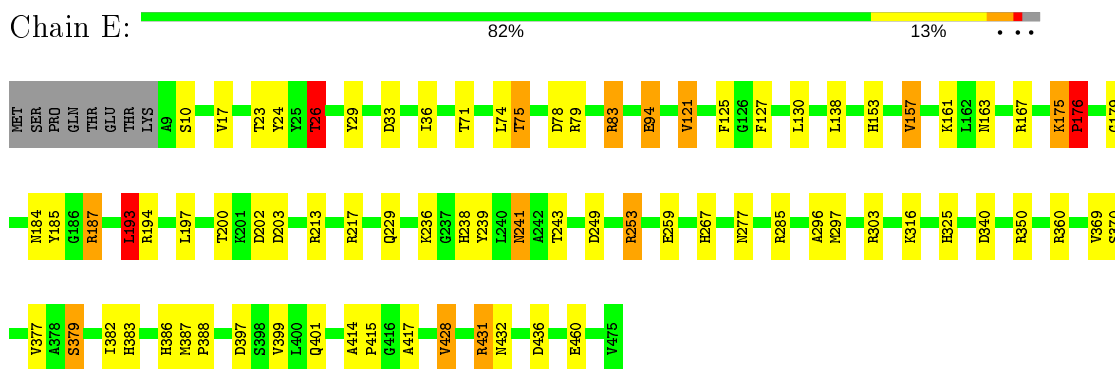
### 3 Residue-property plots [i](#)

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

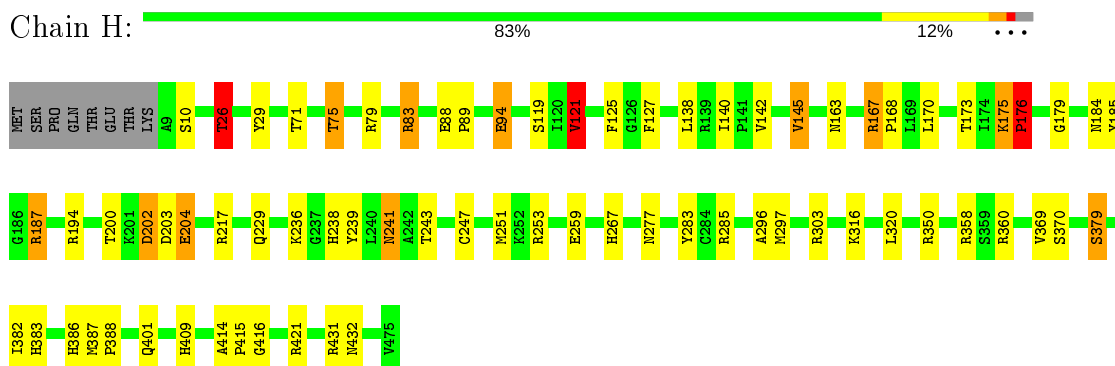
- Molecule 1: RIBULOSE BISPHTHOSPHATE CARBOXYLASE LARGE CHAIN



- Molecule 1: RIBULOSE BISPHTHOSPHATE CARBOXYLASE LARGE CHAIN

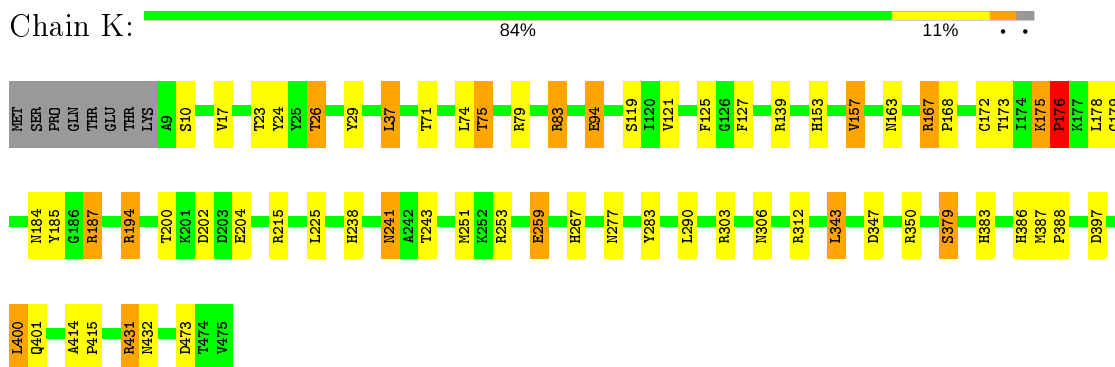


- Molecule 1: RIBULOSE BISPHTHOSPHATE CARBOXYLASE LARGE CHAIN



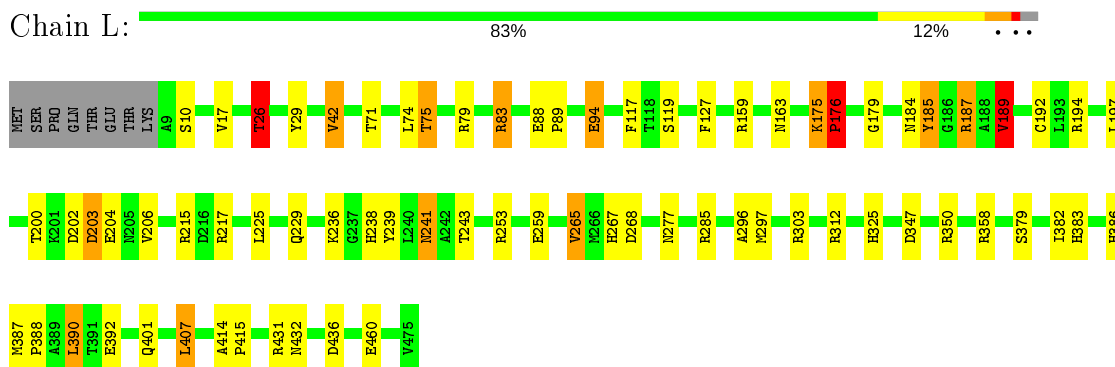
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain K:



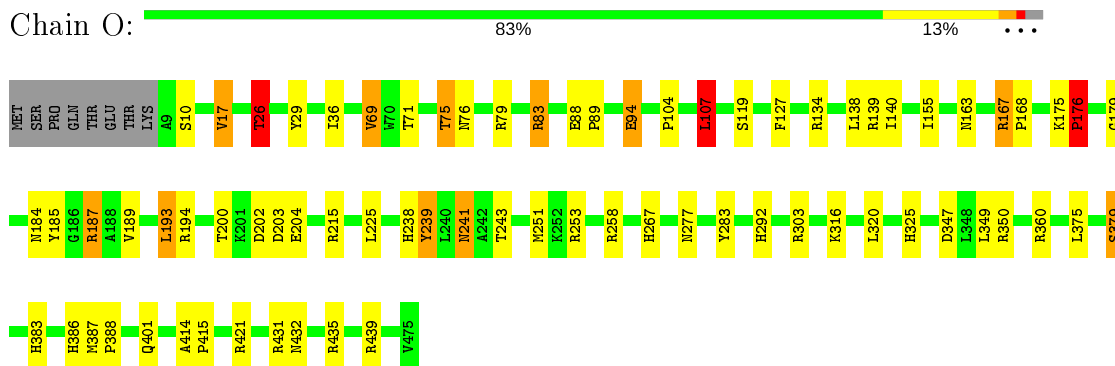
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain L:



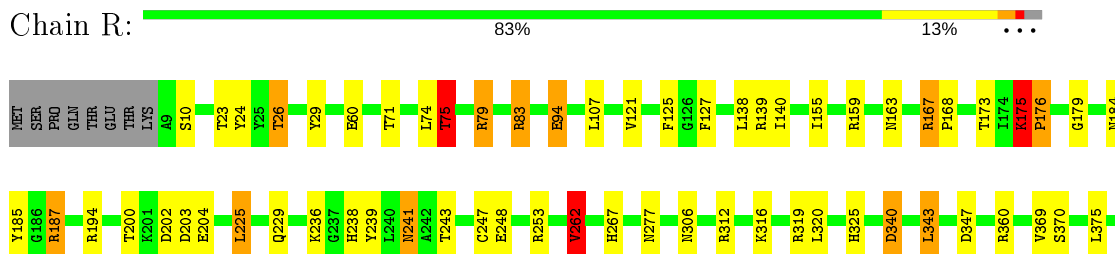
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain O:



- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

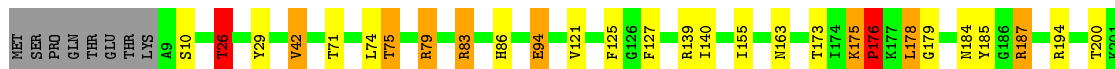
Chain R:





- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain V: 85% 11%



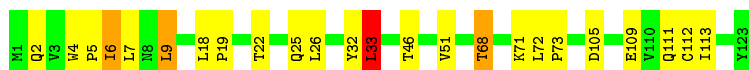
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain C: 76% 18% 5%



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain F: 80% 16%



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain I: 80% 15% 5%



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain M: 79% 18%




- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain P: 85% 12%




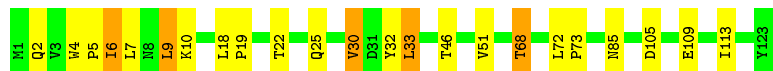
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain S:  81% 14% 5%




- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain T:  81% 15% .



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN

Chain W:  84% 13% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.60Å 220.94Å 116.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 98.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-2.30) 90.2 (98.33-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 2.29Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.230 , 0.200 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtrriage
Anisotropy	0.871	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	40436	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

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

<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: CA, CAP, KCX

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

All (2) bond length outliers are listed below:

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

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	176	PRO	CA-N-CD	-16.55	88.33	111.50
1	O	303	ARG	NE-CZ-NH1	12.19	126.40	120.30
1	L	187	ARG	NE-CZ-NH2	-12.03	114.28	120.30
1	O	187	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	L	285	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	K	253	ARG	NE-CZ-NH1	9.56	125.08	120.30
2	T	105	ASP	CB-CG-OD1	9.21	126.59	118.30
1	R	253	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	O	83	ARG	CD-NE-CZ	9.13	136.39	123.60
1	L	187	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	L	83	ARG	CD-NE-CZ	8.81	135.93	123.60
1	L	285	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	R	159	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	E	253	ARG	NE-CZ-NH2	-8.77	115.91	120.30
2	S	105	ASP	CB-CG-OD1	8.75	126.17	118.30
1	V	83	ARG	CD-NE-CZ	8.73	135.82	123.60
1	R	175	LYS	C-N-CD	-8.67	101.53	120.60
1	E	176	PRO	CA-N-CD	-8.66	99.38	111.50
1	R	187	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	L	176	PRO	CA-N-CD	-8.57	99.50	111.50
1	B	176	PRO	CA-N-CD	-8.44	99.68	111.50
1	K	350	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	B	83	ARG	CD-NE-CZ	8.40	135.36	123.60
1	L	407	LEU	CA-CB-CG	8.39	134.61	115.30
1	L	215	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	K	167	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	K	176	PRO	CA-N-CD	-8.32	99.85	111.50
1	R	83	ARG	CD-NE-CZ	8.16	135.03	123.60
1	R	159	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	V	176	PRO	CA-N-CD	-8.15	100.08	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	312	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	187	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	E	217	ARG	NE-CZ-NH2	7.95	124.27	120.30
1	O	176	PRO	CA-N-CD	-7.94	100.38	111.50
1	H	176	PRO	CA-N-CD	-7.93	100.40	111.50
1	R	83	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	R	319	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	V	253	ARG	CD-NE-CZ	7.71	134.40	123.60
1	E	203	ASP	CB-CG-OD2	7.70	125.23	118.30
1	H	350	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	M	105	ASP	CB-CG-OD1	7.67	125.21	118.30
1	H	350	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	253	ARG	CD-NE-CZ	7.63	134.28	123.60
1	E	83	ARG	CD-NE-CZ	7.62	134.27	123.60
1	K	83	ARG	CD-NE-CZ	7.56	134.19	123.60
1	R	325	HIS	CA-CB-CG	7.48	126.32	113.60
2	C	53	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	H	187	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	H	83	ARG	CD-NE-CZ	7.39	133.94	123.60
1	E	303	ARG	CD-NE-CZ	7.37	133.92	123.60
1	H	253	ARG	CD-NE-CZ	7.37	133.91	123.60
1	V	83	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	O	69	VAL	N-CA-CB	-7.31	95.42	111.50
1	O	350	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	H	83	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	L	217	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	B	219	LEU	CA-CB-CG	7.16	131.78	115.30
1	H	360	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	R	175	LYS	O-C-N	-7.12	107.57	121.10
1	V	303	ARG	CD-NE-CZ	7.07	133.50	123.60
1	R	262	VAL	N-CA-CB	-7.01	96.08	111.50
1	V	187	ARG	CD-NE-CZ	6.99	133.38	123.60
1	K	397	ASP	CB-CG-OD1	6.97	124.57	118.30
1	V	253	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	C	105	ASP	CB-CG-OD1	6.95	124.56	118.30
1	L	265	VAL	N-CA-CB	-6.89	96.34	111.50
2	C	110	VAL	CA-CB-CG1	6.87	121.20	110.90
1	H	217	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	R	203	ASP	CB-CG-OD2	6.82	124.44	118.30
1	B	285	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	69	VAL	N-CA-CB	-6.76	96.63	111.50
1	L	312	ARG	NE-CZ-NH2	-6.73	116.93	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	303	ARG	CD-NE-CZ	6.70	132.98	123.60
2	T	33	LEU	CA-CB-CG	6.69	130.68	115.30
1	K	303	ARG	CD-NE-CZ	6.68	132.95	123.60
1	R	176	PRO	N-CD-CG	-6.66	93.21	103.20
1	H	358	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	L	159	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	H	360	ARG	CD-NE-CZ	6.57	132.79	123.60
1	L	253	ARG	CD-NE-CZ	6.55	132.78	123.60
1	E	253	ARG	CD-NE-CZ	6.54	132.76	123.60
1	V	139	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	O	187	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	R	83	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	E	187	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	S	33	LEU	CA-CB-CG	6.43	130.08	115.30
1	V	79	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	P	105	ASP	CB-CG-OD1	6.41	124.07	118.30
1	V	259	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	O	360	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	187	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	B	83	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	259	GLU	OE1-CD-OE2	-6.33	115.70	123.30
1	E	350	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	I	105	ASP	CB-CG-OD1	6.33	124.00	118.30
1	O	215	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	R	253	ARG	CD-NE-CZ	6.30	132.43	123.60
1	B	303	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	R	312	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	R	262	VAL	CG1-CB-CG2	6.28	120.95	110.90
1	K	347	ASP	CB-CG-OD1	6.28	123.95	118.30
2	P	33	LEU	CA-CB-CG	6.27	129.72	115.30
1	H	187	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	W	33	LEU	CA-CB-CG	6.22	129.60	115.30
1	R	253	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	E	397	ASP	CB-CG-OD1	6.19	123.87	118.30
1	K	431	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	V	83	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	C	1	MET	N-CA-C	-6.16	94.37	111.00
1	K	194	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	H	167	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	K	350	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	R	347	ASP	CB-CG-OD1	6.10	123.79	118.30
1	L	259	GLU	OE1-CD-OE2	-6.08	116.01	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	33	LEU	CA-CB-CG	6.05	129.22	115.30
1	K	253	ARG	NE-CZ-NH2	-6.05	117.28	120.30
2	F	105	ASP	CB-CG-OD1	6.04	123.74	118.30
1	O	253	ARG	CD-NE-CZ	6.03	132.04	123.60
1	L	358	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	219	LEU	CB-CG-CD1	6.01	121.22	111.00
1	V	187	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	69	VAL	CB-CA-C	5.98	122.76	111.40
1	O	435	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	V	139	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	E	285	ARG	CD-NE-CZ	5.95	131.93	123.60
1	L	390	LEU	CB-CG-CD1	5.94	121.10	111.00
2	W	9	LEU	CB-CG-CD2	5.94	121.09	111.00
1	L	436	ASP	CB-CG-OD1	5.93	123.64	118.30
1	L	189	VAL	CA-CB-CG2	5.93	119.79	110.90
2	C	33	LEU	CA-CB-CG	5.91	128.89	115.30
2	I	9	LEU	CA-CB-CG	5.86	128.78	115.30
2	M	33	LEU	CA-CB-CG	5.86	128.78	115.30
1	H	145	VAL	CA-CB-CG2	5.86	119.69	110.90
1	R	397	ASP	CB-CG-OD1	5.86	123.57	118.30
2	I	42	LEU	CA-CB-CG	5.84	128.73	115.30
1	V	26	THR	CA-CB-CG2	5.84	120.58	112.40
1	L	203	ASP	CB-CG-OD2	5.84	123.55	118.30
1	B	19	ASP	CB-CG-OD1	5.83	123.55	118.30
2	T	9	LEU	CA-CB-CG	5.83	128.71	115.30
1	B	360	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	V	204	GLU	CG-CD-OE2	5.82	129.94	118.30
1	B	350	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	L	303	ARG	CD-NE-CZ	5.81	131.73	123.60
1	H	303	ARG	CD-NE-CZ	5.78	131.69	123.60
1	V	79	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	V	253	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	L	350	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	V	346	VAL	CA-CB-CG2	5.75	119.52	110.90
1	B	295	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	R	175	LYS	C-N-CA	5.72	146.03	122.00
1	L	26	THR	CA-CB-CG2	5.72	120.41	112.40
1	H	247	CYS	CA-CB-SG	-5.72	103.70	114.00
1	B	468	GLU	OE1-CD-OE2	-5.71	116.44	123.30
1	O	167	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	L	325	HIS	CA-CB-CG	5.71	123.30	113.60
1	V	42	VAL	CA-CB-CG1	5.71	119.46	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	202	ASP	CB-CG-OD1	5.70	123.43	118.30
1	L	215	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	303	ARG	CD-NE-CZ	5.67	131.54	123.60
1	L	176	PRO	N-CA-CB	5.67	110.11	103.30
1	L	83	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	133	LEU	CA-CB-CG	5.66	128.32	115.30
1	V	187	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	S	9	LEU	CB-CG-CD2	5.63	120.58	111.00
2	W	105	ASP	CB-CG-OD1	5.63	123.37	118.30
1	H	204	GLU	OE1-CD-OE2	-5.63	116.54	123.30
2	F	9	LEU	CA-CB-CG	5.63	128.25	115.30
1	O	134	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	R	360	ARG	CD-NE-CZ	5.63	131.48	123.60
1	E	203	ASP	CB-CG-OD1	-5.62	113.24	118.30
2	S	9	LEU	CA-CB-CG	5.61	128.21	115.30
1	E	431	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	E	253	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	L	42	VAL	CA-CB-CG1	5.54	119.22	110.90
1	E	193	LEU	CB-CG-CD1	5.53	120.41	111.00
1	H	259	GLU	OE1-CD-OE2	-5.48	116.73	123.30
2	T	9	LEU	CB-CG-CD2	5.47	120.30	111.00
1	E	157	VAL	CA-CB-CG2	5.47	119.10	110.90
1	V	234	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	K	400	LEU	CB-CG-CD1	5.45	120.26	111.00
1	L	265	VAL	CA-CB-CG1	5.45	119.07	110.90
1	O	139	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	O	107	LEU	CB-CG-CD1	5.42	120.22	111.00
1	V	285	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	H	26	THR	CA-CB-CG2	5.41	119.98	112.40
1	R	248	GLU	OE1-CD-OE2	-5.40	116.81	123.30
1	K	187	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	L	204	GLU	CG-CD-OE2	5.38	129.06	118.30
2	F	33	LEU	CA-CB-CG	5.38	127.67	115.30
1	V	203	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	325	HIS	CA-CB-CG	5.37	122.74	113.60
1	V	285	ARG	CD-NE-CZ	5.37	131.12	123.60
1	O	258	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	E	259	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	E	187	ARG	CD-NE-CZ	5.33	131.06	123.60
1	B	78	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	360	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	E	340	ASP	CB-CG-OD1	5.31	123.08	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	340	ASP	CB-CG-OD1	5.30	123.07	118.30
1	R	343	LEU	CB-CG-CD1	5.30	120.00	111.00
2	T	30	VAL	CA-CB-CG2	5.29	118.84	110.90
1	K	303	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	K	204	GLU	CG-CD-OE2	5.27	128.84	118.30
1	E	436	ASP	CB-CG-OD1	5.26	123.03	118.30
1	H	121	VAL	N-CA-CB	-5.25	99.94	111.50
1	O	239	TYR	CB-CG-CD1	5.25	124.15	121.00
1	O	421	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	K	157	VAL	CA-CB-CG2	5.24	118.77	110.90
1	E	285	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	O	69	VAL	CG1-CB-CG2	5.22	119.26	110.90
1	L	42	VAL	CA-CB-CG2	5.22	118.73	110.90
1	H	421	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	E	428	VAL	CA-CB-CG2	5.21	118.71	110.90
1	O	69	VAL	CB-CA-C	5.20	121.28	111.40
1	O	347	ASP	CB-CG-OD1	5.20	122.98	118.30
1	R	247	CYS	CA-CB-SG	-5.19	104.65	114.00
1	V	312	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	H	253	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	O	253	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	E	26	THR	CA-CB-CG2	5.15	119.61	112.40
1	O	204	GLU	CG-CD-OE2	5.14	128.58	118.30
1	O	26	THR	CA-CB-CG2	5.14	119.59	112.40
2	C	79	ASP	CB-CG-OD1	5.13	122.92	118.30
2	S	65	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	E	78	ASP	CB-CG-OD1	5.12	122.91	118.30
1	V	269	TYR	CA-CB-CG	5.12	123.14	113.40
2	C	9	LEU	CA-CB-CG	5.12	127.08	115.30
1	E	325	HIS	CA-CB-CG	5.12	122.30	113.60
1	B	133	LEU	CB-CG-CD2	5.12	119.70	111.00
1	L	117	PHE	CB-CG-CD1	5.11	124.38	120.80
1	R	139	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	R	75	THR	CB-CA-C	-5.08	97.87	111.60
1	K	259	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	E	167	ARG	CD-NE-CZ	5.06	130.69	123.60
1	R	167	ARG	CD-NE-CZ	5.06	130.69	123.60
1	B	312	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	H	285	ARG	CD-NE-CZ	5.06	130.69	123.60
1	L	268	ASP	CB-CG-OD1	5.06	122.85	118.30
1	E	213	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	K	253	ARG	CD-NE-CZ	5.05	130.67	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	350	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	26	THR	CA-CB-CG2	5.04	119.46	112.40
1	K	215	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	F	9	LEU	CB-CG-CD2	5.04	119.56	111.00
1	K	343	LEU	CB-CG-CD1	5.03	119.55	111.00
1	L	347	ASP	CB-CG-OD1	5.03	122.83	118.30
1	R	225	LEU	CA-CB-CG	5.01	126.83	115.30
2	P	9	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	72	ASP	CB-CG-OD1	5.01	122.81	118.30
2	S	79	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	175	LYS	Peptide
1	E	175	LYS	Peptide
1	H	175	LYS	Peptide
1	K	175	LYS	Peptide
1	L	175	LYS	Peptide
1	O	175	LYS	Peptide
1	R	175	LYS	Mainchain
1	V	175	LYS	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	B	3652	0	3560	40	1
1	E	3652	0	3560	44	0
1	H	3652	0	3560	40	0
1	K	3652	0	3560	37	0
1	L	3652	0	3560	33	0
1	O	3652	0	3560	39	1
1	R	3652	0	3560	41	0
1	V	3652	0	3560	37	0
2	C	1032	0	990	25	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1032	0	990	24	0
2	I	1032	0	990	26	0
2	M	1032	0	990	24	0
2	P	1032	0	990	19	0
2	S	1032	0	990	22	0
2	T	1032	0	990	20	0
2	W	1032	0	990	19	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	B	21	0	7	0	0
4	E	21	0	8	0	0
4	H	21	0	8	0	0
4	K	21	0	8	0	0
4	L	21	0	7	0	0
4	O	21	0	7	0	0
4	R	21	0	8	0	0
4	V	21	0	8	0	0
5	B	263	0	0	6	0
5	C	58	0	0	2	0
5	E	297	0	0	4	0
5	F	100	0	0	3	0
5	H	246	0	0	0	0
5	I	42	0	0	2	0
5	K	278	0	0	3	0
5	L	308	0	0	2	0
5	M	91	0	0	2	0
5	O	261	0	0	1	0
5	P	54	0	0	0	0
5	R	290	0	0	5	0
5	S	93	0	0	3	0
5	T	88	0	0	2	0
5	V	274	0	0	2	0
5	W	45	0	0	1	0
All	All	40436	0	36461	420	1

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

All (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:473:ASP:OD2	5:K:2273:HOH:O	1.71	1.08
2:C:22:THR:H	2:C:25:GLN:HE21	1.14	0.95
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.14	0.94
1:K:267:HIS:HD2	1:K:277:ASN:HD22	1.15	0.93
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.16	0.92
1:O:267:HIS:HD2	1:O:277:ASN:HD22	1.12	0.92
1:L:267:HIS:HD2	1:L:277:ASN:HD22	1.10	0.91
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.15	0.91
2:I:22:THR:H	2:I:25:GLN:HE21	1.19	0.91
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.19	0.89
1:R:267:HIS:HD2	1:R:277:ASN:HD22	1.19	0.89
2:T:22:THR:H	2:T:25:GLN:HE21	1.20	0.88
1:H:26:THR:HG21	1:H:83:ARG:HE	1.39	0.88
2:I:6:ILE:HG23	2:I:7:LEU:HD13	1.57	0.87
2:W:22:THR:H	2:W:25:GLN:HE21	1.22	0.86
1:B:26:THR:HG21	1:B:83:ARG:HE	1.40	0.86
2:C:6:ILE:HG23	2:C:7:LEU:HD13	1.57	0.85
2:P:22:THR:H	2:P:25:GLN:HE21	1.20	0.84
2:M:22:THR:H	2:M:25:GLN:HE21	1.24	0.84
2:S:22:THR:H	2:S:25:GLN:HE21	1.26	0.84
1:R:60:GLU:HB2	5:R:2042:HOH:O	1.77	0.84
1:R:26:THR:HG21	1:R:83:ARG:HE	1.43	0.84
1:V:26:THR:HG21	1:V:83:ARG:HE	1.42	0.84
1:K:26:THR:HG21	1:K:83:ARG:HE	1.43	0.83
1:L:26:THR:HG21	1:L:83:ARG:HE	1.42	0.83
1:O:414:ALA:HB3	1:O:415:PRO:HD3	1.62	0.80
1:O:26:THR:HG21	1:O:83:ARG:HE	1.43	0.80
1:V:414:ALA:HB3	1:V:415:PRO:HD3	1.63	0.80
1:E:26:THR:HG21	1:E:83:ARG:HE	1.46	0.80
1:O:267:HIS:CD2	1:O:277:ASN:HD22	1.98	0.79
1:L:392:GLU:HG3	5:L:2271:HOH:O	1.81	0.79
2:F:22:THR:H	2:F:25:GLN:HE21	1.26	0.79
1:H:379:SER:HB2	1:H:401:GLN:HB2	1.65	0.78
1:V:379:SER:HB2	1:V:401:GLN:HB2	1.64	0.78
1:K:153:HIS:HB3	1:K:157:VAL:HG22	1.66	0.78
1:R:414:ALA:HB3	1:R:415:PRO:HD3	1.65	0.77
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.66	0.77
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.68	0.76
2:F:7:LEU:HD21	2:M:46:THR:OG1	1.85	0.75
1:B:267:HIS:CD2	1:B:277:ASN:HD22	2.02	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:46:THR:OG1	2:P:7:LEU:HD21	1.86	0.75
2:S:46:THR:OG1	2:T:7:LEU:HD21	1.87	0.74
1:B:379:SER:HB2	1:B:401:GLN:HB2	1.70	0.74
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.69	0.74
1:V:267:HIS:CD2	1:V:277:ASN:HD22	2.01	0.74
1:R:379:SER:HB2	1:R:401:GLN:HB2	1.69	0.74
1:H:267:HIS:CD2	1:H:277:ASN:HD22	2.05	0.73
2:M:14:THR:O	2:M:15:LEU:HB2	1.88	0.72
1:E:153:HIS:HB3	1:E:157:VAL:HG22	1.72	0.72
1:K:267:HIS:CD2	1:K:277:ASN:HD22	2.03	0.72
1:R:267:HIS:CD2	1:R:277:ASN:HD22	2.05	0.72
2:T:7:LEU:HD12	5:T:2013:HOH:O	1.89	0.72
1:K:414:ALA:HB3	1:K:415:PRO:HD3	1.72	0.71
1:L:414:ALA:HB3	1:L:415:PRO:HD3	1.72	0.71
1:O:379:SER:HB2	1:O:401:GLN:HB2	1.71	0.70
1:E:267:HIS:CD2	1:E:277:ASN:HD22	2.04	0.70
1:L:267:HIS:CD2	1:L:277:ASN:HD22	2.02	0.70
1:V:431:ARG:HH21	1:V:432:ASN:HD21	1.40	0.69
1:K:26:THR:HG23	1:K:29:TYR:HB2	1.74	0.69
1:V:26:THR:HG23	1:V:29:TYR:HB2	1.75	0.69
2:W:32:TYR:HE2	2:W:113:ILE:HD11	1.57	0.69
1:E:379:SER:HB2	1:E:401:GLN:HB2	1.74	0.69
1:K:431:ARG:HH21	1:K:432:ASN:HD21	1.41	0.69
2:M:32:TYR:HE2	2:M:113:ILE:HD11	1.58	0.68
1:R:431:ARG:HH21	1:R:432:ASN:HD21	1.42	0.68
2:M:6:ILE:HG21	5:T:2042:HOH:O	1.93	0.67
1:H:383:HIS:H	1:H:386:HIS:HD2	1.41	0.67
2:C:22:THR:H	2:C:25:GLN:NE2	1.89	0.67
1:L:379:SER:HB2	1:L:401:GLN:HB2	1.75	0.67
1:K:379:SER:HB2	1:K:401:GLN:HB2	1.77	0.66
1:O:383:HIS:H	1:O:386:HIS:HD2	1.43	0.66
1:O:17:VAL:HA	5:O:2006:HOH:O	1.95	0.66
2:S:32:TYR:HE2	2:S:113:ILE:HD11	1.60	0.66
1:E:383:HIS:H	1:E:386:HIS:HD2	1.41	0.66
2:F:32:TYR:HE2	2:F:113:ILE:HD11	1.60	0.66
2:M:32:TYR:CE2	2:M:113:ILE:HD11	2.31	0.66
1:O:193:LEU:HD13	1:O:200:THR:HG23	1.78	0.65
2:C:32:TYR:CE2	2:C:113:ILE:HD11	2.32	0.65
1:L:26:THR:HG23	1:L:29:TYR:HB2	1.79	0.65
5:C:2030:HOH:O	2:I:6:ILE:HG21	1.96	0.65
2:C:32:TYR:HE2	2:C:113:ILE:HD11	1.62	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:32:TYR:HE2	2:T:113:ILE:HD11	1.62	0.64
2:S:32:TYR:CE2	2:S:113:ILE:HD11	2.32	0.64
2:W:22:THR:H	2:W:25:GLN:NE2	1.94	0.64
1:E:33:ASP:HB2	5:E:2031:HOH:O	1.98	0.64
1:O:26:THR:HG23	1:O:29:TYR:HB2	1.80	0.64
2:W:32:TYR:CE2	2:W:113:ILE:HD11	2.31	0.64
2:F:7:LEU:HD12	5:F:2019:HOH:O	1.97	0.64
1:H:26:THR:HG23	1:H:29:TYR:HB2	1.79	0.64
1:R:26:THR:HG23	1:R:29:TYR:HB2	1.80	0.63
1:R:383:HIS:H	1:R:386:HIS:HD2	1.45	0.63
2:F:32:TYR:CE2	2:F:113:ILE:HD11	2.33	0.63
2:I:32:TYR:CE2	2:I:113:ILE:HD11	2.34	0.63
5:F:2050:HOH:O	2:S:6:ILE:HG21	1.99	0.63
1:B:26:THR:HG23	1:B:29:TYR:HB2	1.81	0.63
2:C:6:ILE:CG2	2:C:7:LEU:HD13	2.28	0.62
2:F:22:THR:H	2:F:25:GLN:NE2	1.96	0.62
2:I:32:TYR:HE2	2:I:113:ILE:HD11	1.62	0.62
2:I:6:ILE:CG2	2:I:7:LEU:HD13	2.28	0.62
1:E:26:THR:HG23	1:E:29:TYR:HB2	1.81	0.62
1:O:431:ARG:HH21	1:O:432:ASN:HD21	1.45	0.62
2:M:7:LEU:HD21	2:T:46:THR:OG1	2.00	0.62
2:T:32:TYR:CE2	2:T:113:ILE:HD11	2.35	0.62
1:K:306:ASN:HB3	5:K:2074:HOH:O	1.99	0.61
1:L:431:ARG:HH21	1:L:432:ASN:HD21	1.46	0.61
2:S:22:THR:H	2:S:25:GLN:NE2	1.97	0.61
1:V:383:HIS:H	1:V:386:HIS:HD2	1.46	0.61
2:F:6:ILE:HG21	5:M:2048:HOH:O	2.01	0.61
2:F:7:LEU:HD11	2:M:46:THR:HG21	1.82	0.61
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.49	0.61
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.49	0.61
1:K:71:THR:OG1	1:O:176:PRO:HD2	2.01	0.60
1:E:460:GLU:HG2	5:E:2282:HOH:O	1.99	0.60
2:S:46:THR:HG21	2:T:7:LEU:HD11	1.82	0.60
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.49	0.60
2:I:46:THR:HG21	2:P:7:LEU:HD11	1.84	0.60
2:C:7:LEU:HD11	2:W:46:THR:OG1	2.02	0.60
2:P:22:THR:H	2:P:25:GLN:NE2	1.98	0.59
1:O:104:PRO:HD2	1:O:107:LEU:HD22	1.85	0.59
2:F:46:THR:OG1	2:S:7:LEU:HD21	2.03	0.59
2:P:32:TYR:CE2	2:P:113:ILE:HD11	2.37	0.59
2:F:68:THR:HG21	2:S:6:ILE:HD11	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:342:THR:O	1:V:346:VAL:HG13	2.03	0.59
2:F:6:ILE:HD11	2:M:68:THR:HG21	1.85	0.58
1:K:37:LEU:HB2	1:K:139:ARG:HB3	1.84	0.58
2:P:46:THR:OG1	2:W:7:LEU:HD21	2.03	0.58
2:T:22:THR:H	2:T:25:GLN:NE2	1.96	0.58
1:K:176:PRO:HD2	1:O:71:THR:OG1	2.03	0.58
1:E:193:LEU:HD13	1:E:200:THR:HG23	1.85	0.58
2:M:22:THR:H	2:M:25:GLN:NE2	1.99	0.58
2:P:32:TYR:HE2	2:P:113:ILE:HD11	1.68	0.58
2:F:6:ILE:CD1	2:M:68:THR:HG21	2.34	0.57
1:V:94:GLU:CD	1:V:94:GLU:H	2.08	0.57
2:M:14:THR:HG22	2:M:15:LEU:HD13	1.85	0.57
1:K:200:THR:OG1	1:K:238:HIS:HD2	1.88	0.56
1:E:71:THR:OG1	1:H:176:PRO:HD2	2.05	0.56
1:L:383:HIS:H	1:L:386:HIS:HD2	1.52	0.56
1:B:383:HIS:H	1:B:386:HIS:HD2	1.53	0.56
1:E:377:VAL:HB	1:E:399:VAL:HB	1.86	0.56
2:F:68:THR:HG21	2:S:6:ILE:CD1	2.36	0.56
1:O:94:GLU:CD	1:O:94:GLU:H	2.09	0.55
2:I:22:THR:H	2:I:25:GLN:NE2	1.97	0.55
2:I:72:LEU:HB3	2:I:73:PRO:HD2	1.88	0.55
1:O:202:ASP:OD1	1:O:238:HIS:HE1	1.89	0.55
2:M:7:LEU:HD12	5:M:2017:HOH:O	2.04	0.55
1:H:142:VAL:HA	1:H:145:VAL:HG13	1.89	0.55
1:R:306:ASN:HB3	5:R:2067:HOH:O	2.07	0.54
1:B:71:THR:OG1	1:L:176:PRO:HD2	2.07	0.54
1:K:259:GLU:HB2	5:K:2155:HOH:O	2.08	0.54
1:B:75:THR:HG21	1:L:179:GLY:O	2.07	0.54
1:L:387:MET:HB3	1:L:388:PRO:HD3	1.89	0.54
2:I:68:THR:HG21	2:P:6:ILE:CD1	2.37	0.54
1:L:200:THR:OG1	1:L:238:HIS:HD2	1.92	0.53
2:P:68:THR:HG21	2:W:6:ILE:HD11	1.89	0.53
1:E:194:ARG:NH1	2:F:6:ILE:HD12	2.24	0.53
2:W:6:ILE:HG22	2:W:7:LEU:HG	1.90	0.53
2:F:6:ILE:HG22	2:F:7:LEU:HG	1.90	0.53
2:S:68:THR:HG21	2:T:6:ILE:CD1	2.39	0.53
2:S:7:LEU:HD12	5:S:2015:HOH:O	2.08	0.53
1:V:194:ARG:NH1	2:W:6:ILE:HD12	2.23	0.53
1:K:383:HIS:H	1:K:386:HIS:HD2	1.56	0.52
2:C:6:ILE:HG21	5:W:2021:HOH:O	2.08	0.52
2:P:109:GLU:OE1	1:R:75:THR:HG23	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:200:THR:OG1	1:O:238:HIS:HD2	1.91	0.52
2:P:68:THR:HG21	2:W:6:ILE:CD1	2.39	0.52
1:B:179:GLY:O	1:L:75:THR:HG21	2.09	0.52
2:T:72:LEU:HB3	2:T:73:PRO:HD2	1.91	0.52
2:C:68:THR:HG21	2:I:6:ILE:HD11	1.92	0.52
1:K:94:GLU:CD	1:K:94:GLU:H	2.13	0.52
1:L:75:THR:HG23	2:W:109:GLU:OE1	2.10	0.52
2:C:68:THR:HG21	2:I:6:ILE:CD1	2.39	0.52
1:E:369:VAL:O	1:E:370:SER:HB2	2.09	0.52
2:C:6:ILE:CD1	2:W:68:THR:HG21	2.40	0.52
1:H:194:ARG:NH1	2:I:6:ILE:HD12	2.25	0.52
1:H:431:ARG:HE	1:H:432:ASN:ND2	2.08	0.52
5:R:2149:HOH:O	2:T:10:LYS:HE3	2.10	0.52
1:V:86:HIS:HD2	5:V:2068:HOH:O	1.93	0.52
1:E:241:ASN:ND2	1:E:243:THR:H	2.08	0.51
1:B:75:THR:HG23	2:F:109:GLU:OE1	2.10	0.51
1:R:229:GLN:HE21	1:R:236:LYS:H	1.56	0.51
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.94	0.51
1:B:94:GLU:H	1:B:94:GLU:CD	2.13	0.51
1:R:202:ASP:OD1	1:R:238:HIS:HE1	1.94	0.51
2:S:6:ILE:HG22	2:S:7:LEU:HG	1.92	0.51
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.94	0.51
1:K:179:GLY:O	1:O:75:THR:HG21	2.11	0.51
1:V:229:GLN:HE21	1:V:236:LYS:H	1.56	0.51
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.94	0.51
2:P:109:GLU:HG3	1:R:74:LEU:O	2.10	0.51
2:T:6:ILE:HG22	2:T:7:LEU:HG	1.93	0.51
1:R:94:GLU:H	1:R:94:GLU:CD	2.14	0.50
1:B:229:GLN:HE21	1:B:236:LYS:H	1.57	0.50
2:C:72:LEU:HB3	2:C:73:PRO:HD2	1.93	0.50
1:H:241:ASN:HD22	1:H:243:THR:H	1.58	0.50
1:R:179:GLY:O	1:V:75:THR:HG21	2.11	0.50
1:B:176:PRO:HD2	1:L:71:THR:OG1	2.11	0.50
1:V:200:THR:OG1	1:V:238:HIS:HD2	1.94	0.50
1:K:387:MET:HB3	1:K:388:PRO:HD3	1.94	0.50
2:C:7:LEU:HD21	2:W:46:THR:HG21	1.93	0.50
2:W:72:LEU:HB3	2:W:73:PRO:HD2	1.94	0.50
1:O:75:THR:HG23	2:T:109:GLU:OE1	2.11	0.50
2:M:6:ILE:CD1	2:T:68:THR:HG21	2.41	0.50
1:B:133:LEU:O	1:B:307:HIS:HA	2.12	0.49
1:H:369:VAL:O	1:H:370:SER:HB2	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:75:THR:HG21	1:O:179:GLY:O	2.12	0.49
2:S:68:THR:HG21	2:T:6:ILE:HD11	1.94	0.49
1:E:387:MET:HB3	1:E:388:PRO:HD3	1.93	0.49
1:R:200:THR:OG1	1:R:238:HIS:HD2	1.94	0.49
1:E:241:ASN:HD22	1:E:243:THR:H	1.59	0.49
1:H:94:GLU:CD	1:H:94:GLU:H	2.15	0.49
2:C:22:THR:N	2:C:25:GLN:HE21	1.96	0.49
2:P:72:LEU:HB3	2:P:73:PRO:HD2	1.93	0.49
1:V:431:ARG:HE	1:V:432:ASN:ND2	2.10	0.49
1:R:431:ARG:HE	1:R:432:ASN:ND2	2.10	0.49
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.95	0.49
1:B:241:ASN:HD22	1:B:243:THR:H	1.60	0.48
1:H:387:MET:HB3	1:H:388:PRO:HD3	1.94	0.48
1:L:94:GLU:H	1:L:94:GLU:CD	2.15	0.48
2:F:112:CYS:O	2:F:113:ILE:HD13	2.13	0.48
2:M:6:ILE:HD11	2:T:68:THR:HG21	1.94	0.48
1:O:155:ILE:HG12	1:O:375:LEU:HD13	1.94	0.48
1:R:75:THR:HG21	1:V:179:GLY:O	2.12	0.48
1:E:184:ASN:HD22	1:E:187:ARG:HH11	1.61	0.48
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.97	0.48
2:I:18:LEU:HB3	2:I:19:PRO:HD2	1.94	0.48
1:V:155:ILE:HG12	1:V:375:LEU:HD13	1.95	0.48
2:C:108:ARG:HB3	2:C:110:VAL:HG13	1.95	0.48
1:E:176:PRO:HD2	1:H:71:THR:OG1	2.13	0.48
1:V:202:ASP:OD1	1:V:238:HIS:HE1	1.97	0.48
1:O:292:HIS:HA	1:O:325:HIS:HB2	1.95	0.48
2:F:111:GLN:HG3	5:F:2092:HOH:O	2.14	0.48
1:B:194:ARG:NH1	2:C:6:ILE:HD12	2.29	0.47
1:E:94:GLU:H	1:E:94:GLU:CD	2.17	0.47
2:I:68:THR:HG21	2:P:6:ILE:HD11	1.95	0.47
1:R:176:PRO:HD2	1:V:71:THR:OG1	2.14	0.47
2:M:72:LEU:HB3	2:M:73:PRO:HD2	1.95	0.47
1:O:431:ARG:HE	1:O:432:ASN:ND2	2.12	0.47
1:R:241:ASN:HD22	1:R:243:THR:H	1.61	0.47
2:T:18:LEU:HB3	2:T:19:PRO:HD2	1.97	0.47
1:V:383:HIS:N	1:V:386:HIS:HD2	2.12	0.47
1:L:202:ASP:OD1	1:L:238:HIS:HE1	1.97	0.47
1:R:71:THR:OG1	1:V:176:PRO:HD2	2.14	0.47
1:B:383:HIS:N	1:B:386:HIS:HD2	2.13	0.47
1:L:194:ARG:NH1	2:S:6:ILE:HD12	2.30	0.47
1:L:431:ARG:HE	1:L:432:ASN:ND2	2.12	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:GLU:OE1	1:E:75:THR:HG23	2.14	0.47
2:I:116:ILE:HG22	5:I:2042:HOH:O	2.14	0.47
2:W:18:LEU:HB3	2:W:19:PRO:HD2	1.97	0.47
2:F:72:LEU:HB3	2:F:73:PRO:HD2	1.97	0.47
1:O:383:HIS:N	1:O:386:HIS:HD2	2.10	0.47
1:V:241:ASN:HD22	1:V:243:THR:H	1.63	0.47
1:E:431:ARG:HE	1:E:432:ASN:ND2	2.12	0.47
2:M:6:ILE:HG22	2:M:7:LEU:HG	1.96	0.47
1:B:74:LEU:O	2:F:109:GLU:HG3	2.16	0.46
1:K:202:ASP:OD1	1:K:238:HIS:HE1	1.98	0.46
1:O:194:ARG:NH1	2:P:6:ILE:HD12	2.30	0.46
1:V:387:MET:HB3	1:V:388:PRO:HD3	1.97	0.46
2:W:22:THR:N	2:W:25:GLN:HE21	2.02	0.46
5:E:2169:HOH:O	1:H:267:HIS:HE1	1.98	0.46
1:E:179:GLY:O	1:H:75:THR:HG21	2.15	0.46
2:I:109:GLU:HG3	1:K:74:LEU:O	2.16	0.46
1:K:167:ARG:HG3	1:K:168:PRO:O	2.15	0.46
1:R:121:VAL:HG22	1:R:125:PHE:CE1	2.50	0.46
1:B:306:ASN:HB3	5:B:2070:HOH:O	2.15	0.46
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.97	0.46
1:E:138:LEU:O	1:E:316:LYS:NZ	2.46	0.46
1:H:167:ARG:HG3	1:H:168:PRO:O	2.15	0.46
2:I:7:LEU:HB2	5:I:2004:HOH:O	2.15	0.46
2:P:6:ILE:HG22	2:P:7:LEU:HG	1.96	0.46
1:V:184:ASN:ND2	1:V:187:ARG:HH11	2.13	0.46
1:H:241:ASN:ND2	1:H:243:THR:H	2.13	0.46
1:B:473:ASP:HB2	5:B:2175:HOH:O	2.16	0.46
1:K:383:HIS:N	1:K:386:HIS:HD2	2.14	0.46
2:S:2:GLN:HG2	5:S:2004:HOH:O	2.15	0.46
1:K:175:LYS:HD3	1:K:175:LYS:HA	1.87	0.45
1:O:383:HIS:H	1:O:386:HIS:CD2	2.30	0.45
1:V:121:VAL:HG22	1:V:125:PHE:CE1	2.51	0.45
1:R:107:LEU:HD22	1:V:178:LEU:HD23	1.99	0.45
1:K:431:ARG:HE	1:K:432:ASN:ND2	2.15	0.45
1:H:383:HIS:N	1:H:386:HIS:HD2	2.11	0.45
1:V:241:ASN:ND2	1:V:243:THR:H	2.14	0.45
1:B:86:HIS:HD2	5:B:2067:HOH:O	1.99	0.45
2:C:109:GLU:HG3	1:E:74:LEU:O	2.16	0.45
1:H:140:ILE:HD13	1:H:320:LEU:HD11	1.98	0.45
2:S:72:LEU:HB3	2:S:73:PRO:HD2	1.99	0.45
1:H:138:LEU:O	1:H:316:LYS:NZ	2.48	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:TYR:O	1:L:189:VAL:HG13	2.17	0.45
1:O:138:LEU:O	1:O:316:LYS:NZ	2.49	0.45
1:R:387:MET:HB3	1:R:388:PRO:HD3	1.99	0.45
1:E:184:ASN:ND2	1:E:187:ARG:HH11	2.15	0.45
1:L:192:CYS:HB3	1:L:197:LEU:HD12	1.99	0.45
1:B:460:GLU:HG2	5:B:2249:HOH:O	2.17	0.45
1:B:241:ASN:ND2	1:B:243:THR:H	2.14	0.44
1:O:167:ARG:HG3	1:O:168:PRO:O	2.16	0.44
1:O:241:ASN:HD22	1:O:243:THR:H	1.65	0.44
2:C:6:ILE:HD11	2:W:68:THR:HG21	1.99	0.44
1:E:229:GLN:HE21	1:E:236:LYS:H	1.65	0.44
1:K:121:VAL:HG22	1:K:125:PHE:CE1	2.53	0.44
1:R:194:ARG:NH1	2:T:6:ILE:HD12	2.31	0.44
1:K:251:MET:HE1	1:K:283:TYR:CD1	2.52	0.44
1:V:414:ALA:CB	1:V:415:PRO:HD3	2.42	0.44
1:B:139:ARG:C	1:B:139:ARG:HD2	2.37	0.44
1:O:251:MET:HE1	1:O:283:TYR:CD1	2.52	0.44
1:R:184:ASN:HD22	1:R:187:ARG:HH11	1.66	0.44
1:R:383:HIS:N	1:R:386:HIS:HD2	2.13	0.44
5:C:2026:HOH:O	2:I:7:LEU:HD22	2.18	0.44
1:E:383:HIS:H	1:E:386:HIS:CD2	2.30	0.44
1:H:184:ASN:ND2	1:H:187:ARG:HH11	2.16	0.44
1:O:140:ILE:HD13	1:O:320:LEU:HD11	2.00	0.44
2:C:33:LEU:HB2	2:C:113:ILE:HG13	1.99	0.44
1:H:383:HIS:H	1:H:386:HIS:CD2	2.30	0.44
2:S:109:GLU:HG3	1:V:74:LEU:O	2.18	0.44
1:B:184:ASN:ND2	1:B:187:ARG:HH11	2.16	0.44
1:E:75:THR:HG21	1:H:179:GLY:O	2.18	0.44
1:R:369:VAL:O	1:R:370:SER:HB2	2.18	0.44
2:T:4:TRP:HA	2:T:5:PRO:HD3	1.88	0.43
1:B:251:MET:HE1	1:B:283:TYR:CD1	2.53	0.43
1:H:229:GLN:HE21	1:H:236:LYS:H	1.65	0.43
1:O:387:MET:N	1:O:388:PRO:CD	2.81	0.43
1:V:173:THR:HB	1:V:175:LYS:HE2	2.00	0.43
1:K:178:LEU:HD12	1:O:107:LEU:HG	2.01	0.43
2:S:18:LEU:HB3	2:S:19:PRO:HD2	2.01	0.43
1:B:431:ARG:HE	1:B:432:ASN:ND2	2.17	0.43
1:K:184:ASN:ND2	1:K:187:ARG:HH11	2.16	0.43
1:R:140:ILE:HD13	1:R:320:LEU:HD11	2.01	0.43
2:C:18:LEU:HB3	2:C:19:PRO:HD2	1.99	0.43
1:L:296:ALA:O	1:L:297:MET:CB	2.66	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:387:MET:HB3	1:O:388:PRO:HD3	2.00	0.43
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.53	0.43
1:O:75:THR:HG22	1:O:76:ASN:H	1.84	0.43
1:B:386:HIS:HE1	5:B:2185:HOH:O	2.00	0.43
2:C:46:THR:OG1	2:I:7:LEU:HD11	2.18	0.43
1:E:161:LYS:HG3	5:E:2106:HOH:O	2.19	0.43
2:I:79:ASP:HA	2:I:80:PRO:HD2	1.88	0.43
2:I:109:GLU:OE1	1:K:75:THR:HG23	2.19	0.43
1:R:267:HIS:HE1	5:V:2171:HOH:O	2.02	0.43
5:S:2051:HOH:O	2:T:6:ILE:HG12	2.18	0.43
2:I:46:THR:HG1	2:P:7:LEU:HD21	1.81	0.43
1:E:414:ALA:CB	1:E:415:PRO:HD3	2.43	0.43
1:K:184:ASN:HD22	1:K:187:ARG:HH11	1.67	0.43
1:R:167:ARG:HG3	1:R:168:PRO:O	2.19	0.42
1:B:175:LYS:HD3	1:B:175:LYS:HA	1.90	0.42
1:E:36:ILE:N	1:E:36:ILE:HD12	2.34	0.42
1:L:383:HIS:N	1:L:386:HIS:HD2	2.15	0.42
2:M:18:LEU:HB3	2:M:19:PRO:HD2	2.00	0.42
1:V:369:VAL:O	1:V:370:SER:HB2	2.19	0.42
1:B:299:ALA:HA	1:B:302:ASP:OD1	2.20	0.42
1:E:383:HIS:N	1:E:386:HIS:HD2	2.13	0.42
1:H:121:VAL:HG22	1:H:125:PHE:CE1	2.54	0.42
1:H:88:GLU:HA	1:H:89:PRO:HD2	1.96	0.42
1:O:241:ASN:ND2	1:O:243:THR:H	2.18	0.42
1:H:173:THR:HB	1:H:175:LYS:HE2	2.01	0.42
1:R:262:VAL:HG13	5:R:2164:HOH:O	2.19	0.42
2:C:11:LYS:HG3	2:C:17:TYR:CZ	2.55	0.42
1:E:175:LYS:HD3	1:E:175:LYS:HA	1.85	0.42
1:R:241:ASN:ND2	1:R:243:THR:H	2.17	0.42
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.55	0.42
1:K:194:ARG:NH1	2:M:6:ILE:HD12	2.34	0.42
1:B:167:ARG:HG3	1:B:168:PRO:O	2.20	0.42
1:B:140:ILE:HD13	1:B:320:LEU:HD11	2.01	0.41
2:C:81:ALA:O	2:C:85:ASN:HB2	2.20	0.41
1:H:75:THR:HG23	2:M:109:GLU:OE1	2.20	0.41
1:K:241:ASN:ND2	1:K:243:THR:H	2.18	0.41
1:V:140:ILE:HD13	1:V:320:LEU:HD11	2.02	0.41
1:O:184:ASN:ND2	1:O:187:ARG:HH11	2.18	0.41
1:R:23:THR:HB	1:R:24:TYR:CD2	2.55	0.41
1:H:251:MET:HE1	1:H:283:TYR:CD1	2.55	0.41
2:W:5:PRO:HB2	2:W:9:LEU:HD13	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.55	0.41
1:H:296:ALA:O	1:H:297:MET:CB	2.67	0.41
1:O:36:ILE:HD12	1:O:36:ILE:N	2.36	0.41
2:S:109:GLU:OE1	1:V:75:THR:HG23	2.20	0.41
2:I:81:ALA:O	2:I:85:ASN:HB2	2.20	0.41
1:R:382:ILE:HA	1:R:386:HIS:CD2	2.55	0.41
2:F:71:LYS:HB3	2:S:1:MET:SD	2.60	0.41
1:R:340:ASP:HB2	5:R:2198:HOH:O	2.19	0.41
1:K:23:THR:HB	1:K:24:TYR:CD2	2.55	0.41
1:L:88:GLU:HA	1:L:89:PRO:HD2	1.95	0.41
1:O:189:VAL:HG13	1:O:193:LEU:HD22	2.02	0.41
1:O:88:GLU:HA	1:O:89:PRO:HD2	1.97	0.41
2:P:79:ASP:HA	2:P:80:PRO:HD2	1.89	0.41
1:V:241:ASN:ND2	1:V:243:THR:OG1	2.49	0.41
2:C:4:TRP:HA	2:C:5:PRO:HD3	1.89	0.41
1:E:23:THR:HB	1:E:24:TYR:CD2	2.56	0.41
1:L:382:ILE:HA	1:L:386:HIS:CD2	2.56	0.41
2:P:18:LEU:HB3	2:P:19:PRO:HD2	2.03	0.41
1:E:296:ALA:O	1:E:297:MET:CB	2.69	0.41
1:L:184:ASN:ND2	1:L:187:ARG:HH11	2.18	0.41
1:H:184:ASN:HD22	1:H:187:ARG:HH11	1.69	0.41
2:I:4:TRP:HA	2:I:5:PRO:HD3	1.88	0.41
2:S:81:ALA:O	2:S:85:ASN:HB2	2.21	0.41
2:F:4:TRP:HA	2:F:5:PRO:HD3	1.93	0.41
2:M:4:TRP:HA	2:M:5:PRO:HD3	1.90	0.41
1:R:79:ARG:HG3	1:R:79:ARG:HH11	1.86	0.41
1:V:383:HIS:H	1:V:386:HIS:CD2	2.33	0.41
1:E:121:VAL:HG22	1:E:125:PHE:CE1	2.56	0.40
1:H:175:LYS:HA	1:H:175:LYS:HD3	1.87	0.40
1:L:460:GLU:HG2	5:L:2294:HOH:O	2.20	0.40
1:R:155:ILE:HG12	1:R:375:LEU:HD13	2.03	0.40
1:V:251:MET:HE1	1:V:283:TYR:CD1	2.57	0.40
1:B:295:ARG:HG2	5:B:2262:HOH:O	2.21	0.40
1:K:173:THR:HB	1:K:175:LYS:HE2	2.03	0.40
1:L:175:LYS:HD3	1:L:175:LYS:HA	1.84	0.40
2:F:18:LEU:HB3	2:F:19:PRO:HD2	2.02	0.40
1:H:409:HIS:CD2	1:H:416:GLY:HA2	2.57	0.40
1:L:241:ASN:HD22	1:L:243:THR:H	1.69	0.40
1:L:387:MET:N	1:L:388:PRO:CD	2.84	0.40
1:L:74:LEU:O	2:W:109:GLU:HG3	2.21	0.40
2:M:22:THR:N	2:M:25:GLN:HE21	2.05	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:138:LEU:O	1:R:316:LYS:NZ	2.51	0.40
1:B:387:MET:N	1:B:388:PRO:CD	2.84	0.40
1:E:197:LEU:HG	1:E:417:ALA:HB1	2.04	0.40
1:E:249:ASP:O	1:E:253:ARG:HG3	2.21	0.40
2:F:33:LEU:C	2:F:33:LEU:HD12	2.42	0.40
1:K:139:ARG:C	1:K:139:ARG:HD2	2.42	0.40
2:M:81:ALA:O	2:M:85:ASN:HB2	2.21	0.40
1:R:173:THR:HB	1:R:175:LYS:HE2	2.03	0.40
1:B:241:ASN:ND2	1:B:243:THR:OG1	2.53	0.40
1:L:229:GLN:HE21	1:L:236:LYS:H	1.69	0.40
2:M:112:CYS:O	2:M:113:ILE:HD13	2.21	0.40

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

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

## 5.3 Torsion angles [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	B	464/475 (98%)	440 (95%)	22 (5%)	2 (0%)	34	42
1	E	464/475 (98%)	438 (94%)	24 (5%)	2 (0%)	34	42
1	H	464/475 (98%)	445 (96%)	17 (4%)	2 (0%)	34	42
1	K	464/475 (98%)	443 (96%)	18 (4%)	3 (1%)	25	31
1	L	464/475 (98%)	444 (96%)	18 (4%)	2 (0%)	34	42
1	O	464/475 (98%)	442 (95%)	20 (4%)	2 (0%)	34	42
1	R	464/475 (98%)	442 (95%)	21 (4%)	1 (0%)	47	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	464/475 (98%)	441 (95%)	21 (4%)	2 (0%)	34	42
2	C	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	F	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	I	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
2	M	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	P	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	S	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	T	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	W	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
All	All	4680/4784 (98%)	4454 (95%)	210 (4%)	16 (0%)	41	50

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	SER
1	B	176	PRO
1	E	10	SER
1	E	176	PRO
1	H	10	SER
1	H	176	PRO
1	K	10	SER
1	K	176	PRO
1	L	10	SER
1	L	176	PRO
1	O	10	SER
1	O	176	PRO
1	R	10	SER
1	V	10	SER
1	V	176	PRO
1	K	172	CYS

### 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	B	377/386 (98%)	360 (96%)	17 (4%)	27	39
1	E	377/386 (98%)	362 (96%)	15 (4%)	31	44
1	H	377/386 (98%)	362 (96%)	15 (4%)	31	44
1	K	377/386 (98%)	361 (96%)	16 (4%)	30	42
1	L	377/386 (98%)	358 (95%)	19 (5%)	24	34
1	O	377/386 (98%)	359 (95%)	18 (5%)	25	36
1	R	377/386 (98%)	364 (97%)	13 (3%)	37	51
1	V	377/386 (98%)	364 (97%)	13 (3%)	37	51
2	C	112/112 (100%)	104 (93%)	8 (7%)	14	19
2	F	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	I	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	M	112/112 (100%)	104 (93%)	8 (7%)	14	19
2	P	112/112 (100%)	107 (96%)	5 (4%)	27	39
2	S	112/112 (100%)	105 (94%)	7 (6%)	18	24
2	T	112/112 (100%)	104 (93%)	8 (7%)	14	19
2	W	112/112 (100%)	105 (94%)	7 (6%)	18	24
All	All	3912/3984 (98%)	3729 (95%)	183 (5%)	26	37

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	VAL
1	B	26	THR
1	B	69	VAL
1	B	75	THR
1	B	79	ARG
1	B	94	GLU
1	B	105	LEU
1	B	119	SER
1	B	127	PHE
1	B	133	LEU
1	B	162	LEU
1	B	163	ASN
1	B	185	TYR
1	B	203	ASP
1	B	219	LEU
1	B	239	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	241	ASN
2	C	2	GLN
2	C	6	ILE
2	C	7	LEU
2	C	9	LEU
2	C	33	LEU
2	C	51	VAL
2	C	68	THR
2	C	85	ASN
1	E	17	VAL
1	E	26	THR
1	E	75	THR
1	E	79	ARG
1	E	94	GLU
1	E	121	VAL
1	E	127	PHE
1	E	130	LEU
1	E	163	ASN
1	E	185	TYR
1	E	193	LEU
1	E	239	TYR
1	E	241	ASN
1	E	379	SER
1	E	428	VAL
2	F	2	GLN
2	F	6	ILE
2	F	9	LEU
2	F	26	LEU
2	F	33	LEU
2	F	51	VAL
2	F	68	THR
1	H	26	THR
1	H	75	THR
1	H	79	ARG
1	H	94	GLU
1	H	119	SER
1	H	121	VAL
1	H	127	PHE
1	H	163	ASN
1	H	170	LEU
1	H	185	TYR
1	H	203	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	204	GLU
1	H	239	TYR
1	H	241	ASN
1	H	379	SER
2	I	2	GLN
2	I	6	ILE
2	I	7	LEU
2	I	9	LEU
2	I	33	LEU
2	I	42	LEU
2	I	68	THR
1	K	17	VAL
1	K	26	THR
1	K	37	LEU
1	K	75	THR
1	K	79	ARG
1	K	94	GLU
1	K	119	SER
1	K	127	PHE
1	K	163	ASN
1	K	185	TYR
1	K	225	LEU
1	K	241	ASN
1	K	290	LEU
1	K	343	LEU
1	K	379	SER
1	K	400	LEU
1	L	17	VAL
1	L	26	THR
1	L	42	VAL
1	L	75	THR
1	L	79	ARG
1	L	94	GLU
1	L	119	SER
1	L	127	PHE
1	L	163	ASN
1	L	185	TYR
1	L	189	VAL
1	L	203	ASP
1	L	206	VAL
1	L	225	LEU
1	L	239	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	241	ASN
1	L	265	VAL
1	L	390	LEU
1	L	407	LEU
2	M	2	GLN
2	M	6	ILE
2	M	9	LEU
2	M	15	LEU
2	M	21	LEU
2	M	33	LEU
2	M	51	VAL
2	M	68	THR
1	O	17	VAL
1	O	26	THR
1	O	69	VAL
1	O	75	THR
1	O	79	ARG
1	O	94	GLU
1	O	107	LEU
1	O	119	SER
1	O	127	PHE
1	O	163	ASN
1	O	185	TYR
1	O	193	LEU
1	O	203	ASP
1	O	225	LEU
1	O	239	TYR
1	O	241	ASN
1	O	349	LEU
1	O	379	SER
2	P	6	ILE
2	P	9	LEU
2	P	33	LEU
2	P	51	VAL
2	P	68	THR
1	R	26	THR
1	R	75	THR
1	R	79	ARG
1	R	94	GLU
1	R	127	PHE
1	R	163	ASN
1	R	185	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	R	204	GLU
1	R	225	LEU
1	R	239	TYR
1	R	241	ASN
1	R	262	VAL
1	R	343	LEU
2	S	2	GLN
2	S	6	ILE
2	S	9	LEU
2	S	33	LEU
2	S	51	VAL
2	S	68	THR
2	S	85	ASN
2	T	2	GLN
2	T	6	ILE
2	T	9	LEU
2	T	30	VAL
2	T	33	LEU
2	T	51	VAL
2	T	68	THR
2	T	85	ASN
1	V	26	THR
1	V	42	VAL
1	V	75	THR
1	V	79	ARG
1	V	94	GLU
1	V	127	PHE
1	V	163	ASN
1	V	178	LEU
1	V	185	TYR
1	V	239	TYR
1	V	241	ASN
1	V	346	VAL
1	V	379	SER
2	W	2	GLN
2	W	6	ILE
2	W	9	LEU
2	W	33	LEU
2	W	34	LEU
2	W	51	VAL
2	W	68	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such

sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	86	HIS
1	B	153	HIS
1	B	156	GLN
1	B	163	ASN
1	B	184	ASN
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	282	HIS
1	B	304	GLN
1	B	386	HIS
1	B	401	GLN
1	B	432	ASN
2	C	25	GLN
2	C	29	GLN
2	C	82	GLN
1	E	153	HIS
1	E	156	GLN
1	E	184	ASN
1	E	207	ASN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN
1	E	282	HIS
1	E	304	GLN
1	E	386	HIS
1	E	401	GLN
1	E	420	ASN
1	E	432	ASN
1	E	442	ASN
2	F	25	GLN
2	F	29	GLN
2	F	55	HIS
2	F	82	GLN
1	H	153	HIS
1	H	156	GLN
1	H	163	ASN
1	H	184	ASN

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	282	HIS
1	H	304	GLN
1	H	386	HIS
1	H	401	GLN
1	H	432	ASN
2	I	25	GLN
2	I	29	GLN
2	I	82	GLN
1	K	153	HIS
1	K	156	GLN
1	K	163	ASN
1	K	184	ASN
1	K	229	GLN
1	K	238	HIS
1	K	241	ASN
1	K	267	HIS
1	K	277	ASN
1	K	282	HIS
1	K	304	GLN
1	K	386	HIS
1	K	401	GLN
1	K	432	ASN
1	K	442	ASN
1	L	153	HIS
1	L	156	GLN
1	L	163	ASN
1	L	184	ASN
1	L	207	ASN
1	L	229	GLN
1	L	238	HIS
1	L	241	ASN
1	L	267	HIS
1	L	277	ASN
1	L	282	HIS
1	L	304	GLN
1	L	386	HIS
1	L	420	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	432	ASN
2	M	25	GLN
2	M	29	GLN
2	M	82	GLN
1	O	153	HIS
1	O	156	GLN
1	O	163	ASN
1	O	184	ASN
1	O	207	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	25	GLN
2	P	29	GLN
2	P	82	GLN
1	R	86	HIS
1	R	153	HIS
1	R	156	GLN
1	R	163	ASN
1	R	184	ASN
1	R	229	GLN
1	R	238	HIS
1	R	241	ASN
1	R	267	HIS
1	R	282	HIS
1	R	304	GLN
1	R	386	HIS
1	R	401	GLN
1	R	432	ASN
1	R	442	ASN
2	S	25	GLN
2	S	29	GLN
2	S	82	GLN
2	T	25	GLN
2	T	29	GLN
2	T	82	GLN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	V	86	HIS
1	V	153	HIS
1	V	156	GLN
1	V	163	ASN
1	V	184	ASN
1	V	229	GLN
1	V	238	HIS
1	V	241	ASN
1	V	267	HIS
1	V	282	HIS
1	V	304	GLN
1	V	386	HIS
1	V	401	GLN
1	V	420	ASN
1	V	432	ASN
1	V	442	ASN
2	W	25	GLN
2	W	29	GLN
2	W	82	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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KCX	B	201	1,3	7,11,12	0.41	0	4,12,14	1.19	1 (25%)
1	KCX	O	201	1,3	7,11,12	0.53	0	4,12,14	1.18	1 (25%)
1	KCX	K	201	1,3	7,11,12	0.61	0	4,12,14	1.01	0
1	KCX	E	201	1,3	7,11,12	0.58	0	4,12,14	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KCX	V	201	1,3	7,11,12	0.62	0	4,12,14	1.71	1 (25%)
1	KCX	L	201	1,3	7,11,12	0.77	0	4,12,14	0.86	0
1	KCX	R	201	1,3	7,11,12	0.58	0	4,12,14	0.43	0
1	KCX	H	201	1,3	7,11,12	0.49	0	4,12,14	1.04	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	201	1,3	-	1/7/10/12	-
1	KCX	O	201	1,3	-	0/7/10/12	-
1	KCX	K	201	1,3	-	0/7/10/12	-
1	KCX	E	201	1,3	-	0/7/10/12	-
1	KCX	V	201	1,3	-	0/7/10/12	-
1	KCX	L	201	1,3	-	0/7/10/12	-
1	KCX	R	201	1,3	-	0/7/10/12	-
1	KCX	H	201	1,3	-	0/7/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	201	KCX	CE-NZ-CX	3.08	128.17	122.95
1	O	201	KCX	CE-NZ-CX	2.27	126.80	122.95
1	H	201	KCX	CE-NZ-CX	2.04	126.40	122.95
1	B	201	KCX	CE-NZ-CX	2.04	126.40	122.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CAP	H	477	3	15,20,20	1.85	4 (26%)	20,31,31	1.85	8 (40%)
4	CAP	K	477	3	15,20,20	2.03	7 (46%)	20,31,31	2.18	8 (40%)
4	CAP	B	477	3	15,20,20	1.96	5 (33%)	20,31,31	2.07	5 (25%)
4	CAP	E	477	3	15,20,20	1.90	5 (33%)	20,31,31	1.83	6 (30%)
4	CAP	V	477	3	15,20,20	1.89	5 (33%)	20,31,31	1.91	6 (30%)
4	CAP	R	477	3	15,20,20	1.78	4 (26%)	20,31,31	1.92	7 (35%)
4	CAP	L	477	3	15,20,20	2.16	6 (40%)	20,31,31	2.00	7 (35%)
4	CAP	O	477	3	15,20,20	2.01	5 (33%)	20,31,31	1.93	8 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	H	477	3	-	4/23/29/29	-
4	CAP	K	477	3	-	5/23/29/29	-
4	CAP	B	477	3	-	4/23/29/29	-
4	CAP	E	477	3	-	4/23/29/29	-
4	CAP	V	477	3	-	4/23/29/29	-
4	CAP	R	477	3	-	5/23/29/29	-
4	CAP	L	477	3	-	5/23/29/29	-
4	CAP	O	477	3	-	4/23/29/29	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	477	CAP	O4-C4	-4.38	1.34	1.43
4	L	477	CAP	O4-C4	-4.22	1.34	1.43
4	V	477	CAP	O4-C4	-4.05	1.34	1.43
4	R	477	CAP	O4-C4	-3.98	1.34	1.43
4	B	477	CAP	O4-C4	-3.89	1.35	1.43
4	E	477	CAP	O4-C4	-3.81	1.35	1.43
4	O	477	CAP	O2-C2	-3.76	1.37	1.43
4	L	477	CAP	O2-C2	-3.63	1.37	1.43
4	K	477	CAP	O2-C2	-3.62	1.37	1.43
4	K	477	CAP	O4-C4	-3.62	1.35	1.43
4	E	477	CAP	O2-C2	-3.52	1.37	1.43
4	V	477	CAP	O2-C2	-3.52	1.37	1.43
4	O	477	CAP	O4-C4	-3.51	1.35	1.43
4	B	477	CAP	O2-C2	-3.08	1.38	1.43
4	O	477	CAP	O3-C3	-3.07	1.36	1.42
4	L	477	CAP	O3-C3	-3.04	1.36	1.42
4	B	477	CAP	O3-C3	-2.99	1.36	1.42
4	R	477	CAP	O2-C2	-2.94	1.38	1.43
4	R	477	CAP	O3-C3	-2.94	1.36	1.42
4	K	477	CAP	O3-C3	-2.93	1.36	1.42
4	L	477	CAP	C4-C3	2.85	1.56	1.54
4	K	477	CAP	P2-O4P	2.81	1.59	1.50
4	H	477	CAP	O2-C2	-2.81	1.38	1.43
4	H	477	CAP	O3-C3	-2.78	1.37	1.42
4	O	477	CAP	P2-O4P	2.66	1.59	1.50
4	E	477	CAP	O3-C3	-2.62	1.37	1.42
4	O	477	CAP	C4-C3	2.58	1.56	1.54
4	V	477	CAP	O3-C3	-2.56	1.37	1.42
4	B	477	CAP	C4-C3	2.52	1.56	1.54
4	L	477	CAP	P2-O4P	2.48	1.58	1.50
4	E	477	CAP	P2-O6P	-2.44	1.45	1.54
4	K	477	CAP	P2-O6P	-2.39	1.45	1.54
4	H	477	CAP	C4-C3	2.35	1.56	1.54
4	R	477	CAP	P2-O6P	-2.23	1.46	1.54
4	V	477	CAP	P2-O6P	-2.20	1.46	1.54
4	E	477	CAP	C4-C3	2.19	1.56	1.54
4	L	477	CAP	P2-O6P	-2.16	1.46	1.54
4	V	477	CAP	C4-C3	2.15	1.56	1.54
4	K	477	CAP	C4-C3	2.13	1.56	1.54
4	K	477	CAP	P2-O5P	-2.05	1.46	1.54
4	B	477	CAP	P2-O5P	-2.05	1.46	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	477	CAP	O3-C3-C4	-4.97	98.48	109.13
4	L	477	CAP	P2-O5-C5	4.56	130.86	118.30
4	H	477	CAP	O4-C4-C3	-4.27	100.24	108.78
4	K	477	CAP	O6P-P2-O5P	4.22	123.78	107.64
4	V	477	CAP	P2-O5-C5	4.12	129.64	118.30
4	B	477	CAP	P2-O5-C5	4.07	129.50	118.30
4	K	477	CAP	P2-O5-C5	4.02	129.37	118.30
4	V	477	CAP	O4-C4-C3	-3.90	100.99	108.78
4	O	477	CAP	P2-O5-C5	3.80	128.77	118.30
4	K	477	CAP	O4-C4-C3	-3.75	101.29	108.78
4	O	477	CAP	O4-C4-C3	-3.70	101.39	108.78
4	E	477	CAP	O3-C3-C4	-3.63	101.36	109.13
4	R	477	CAP	O3-C3-C4	-3.57	101.47	109.13
4	E	477	CAP	P2-O5-C5	3.56	128.10	118.30
4	R	477	CAP	P2-O5-C5	3.54	128.05	118.30
4	O	477	CAP	O3-C3-C4	-3.48	101.68	109.13
4	L	477	CAP	O4-C4-C3	-3.42	101.94	108.78
4	R	477	CAP	O3P-P1-O1	-3.42	97.64	106.73
4	B	477	CAP	O3P-P1-O1	-3.15	98.36	106.73
4	V	477	CAP	O3-C3-C4	-3.14	102.40	109.13
4	H	477	CAP	O3-C3-C4	-3.11	102.47	109.13
4	B	477	CAP	O4-C4-C3	-3.10	102.58	108.78
4	L	477	CAP	O6P-P2-O5P	3.04	119.26	107.64
4	K	477	CAP	O3P-P1-O1	-3.03	98.67	106.73
4	K	477	CAP	O3-C3-C4	-2.86	103.01	109.13
4	L	477	CAP	O5-C5-C4	2.83	116.92	109.36
4	L	477	CAP	O3-C3-C4	-2.82	103.09	109.13
4	V	477	CAP	O3P-P1-O2P	2.80	118.34	107.64
4	K	477	CAP	C5-C4-C3	2.78	117.62	111.94
4	R	477	CAP	C5-C4-C3	2.72	117.51	111.94
4	R	477	CAP	O4-C4-C3	-2.71	103.36	108.78
4	O	477	CAP	O5-C5-C4	2.67	116.50	109.36
4	E	477	CAP	O4-C4-C3	-2.61	103.56	108.78
4	E	477	CAP	O3P-P1-O1	-2.56	99.92	106.73
4	H	477	CAP	O3P-P1-O1P	2.53	120.59	110.68
4	H	477	CAP	P2-O5-C5	2.48	125.13	118.30
4	L	477	CAP	O1-P1-O1P	2.48	113.43	106.47
4	K	477	CAP	O4-C4-C5	-2.46	104.39	109.92
4	H	477	CAP	O3P-P1-O1	-2.45	100.21	106.73
4	H	477	CAP	O5-C5-C4	2.40	115.78	109.36
4	O	477	CAP	C5-C4-C3	2.36	116.77	111.94
4	O	477	CAP	O5P-P2-O5	2.32	112.90	106.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	477	CAP	O6P-P2-O5P	2.29	116.41	107.64
4	H	477	CAP	O3P-P1-O2P	2.25	116.24	107.64
4	V	477	CAP	C5-C4-C3	2.23	116.49	111.94
4	H	477	CAP	C5-C4-C3	2.22	116.48	111.94
4	B	477	CAP	O6P-P2-O5P	2.19	115.99	107.64
4	K	477	CAP	O5-P2-O4P	-2.14	100.46	106.47
4	E	477	CAP	O6P-P2-O5P	2.13	115.78	107.64
4	R	477	CAP	O3P-P1-O2P	2.12	115.74	107.64
4	E	477	CAP	C5-C4-C3	2.11	116.26	111.94
4	R	477	CAP	O3P-P1-O1P	2.09	118.85	110.68
4	O	477	CAP	O3P-P1-O1	-2.05	101.27	106.73
4	V	477	CAP	O3P-P1-O1	-2.01	101.39	106.73
4	L	477	CAP	O3P-P1-O1	-2.00	101.41	106.73

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	477	CAP	C2-C3-C4-O4
4	H	477	CAP	O3-C3-C4-O4
4	K	477	CAP	C2-C3-C4-O4
4	K	477	CAP	O3-C3-C4-O4
4	B	477	CAP	C2-C3-C4-O4
4	B	477	CAP	O3-C3-C4-O4
4	E	477	CAP	C2-C3-C4-O4
4	E	477	CAP	O3-C3-C4-O4
4	V	477	CAP	C2-C3-C4-O4
4	V	477	CAP	O3-C3-C4-O4
4	R	477	CAP	C2-C3-C4-O4
4	R	477	CAP	O3-C3-C4-O4
4	L	477	CAP	C2-C3-C4-O4
4	L	477	CAP	O3-C3-C4-O4
4	O	477	CAP	C2-C3-C4-O4
4	O	477	CAP	O3-C3-C4-O4
4	H	477	CAP	O2-C2-C3-C4
4	K	477	CAP	O2-C2-C3-C4
4	B	477	CAP	O2-C2-C3-C4
4	E	477	CAP	O2-C2-C3-C4
4	V	477	CAP	O2-C2-C3-C4
4	R	477	CAP	O2-C2-C3-C4
4	L	477	CAP	O2-C2-C3-C4
4	O	477	CAP	O2-C2-C3-C4

*Continued on next page...*



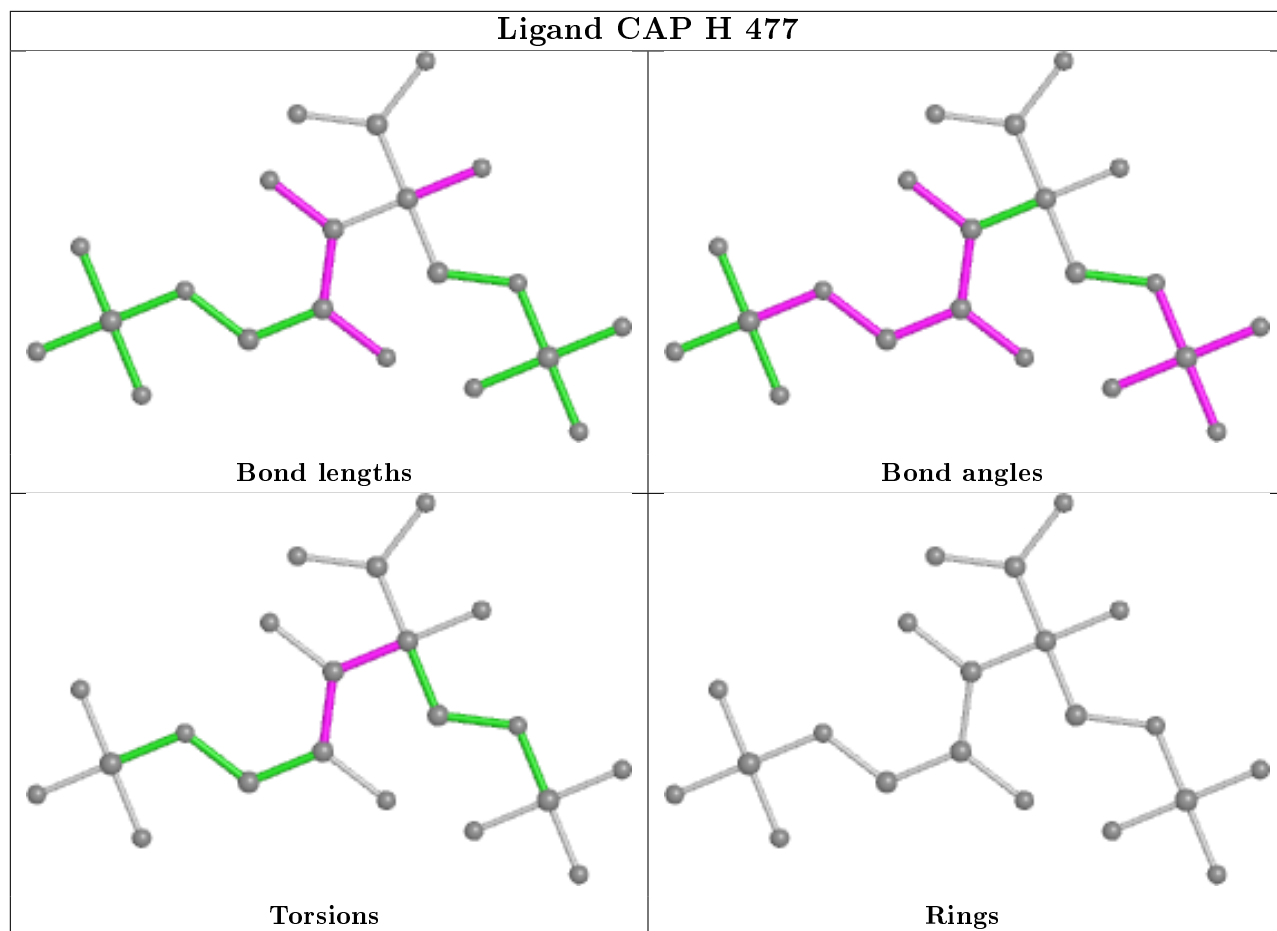
*Continued from previous page...*

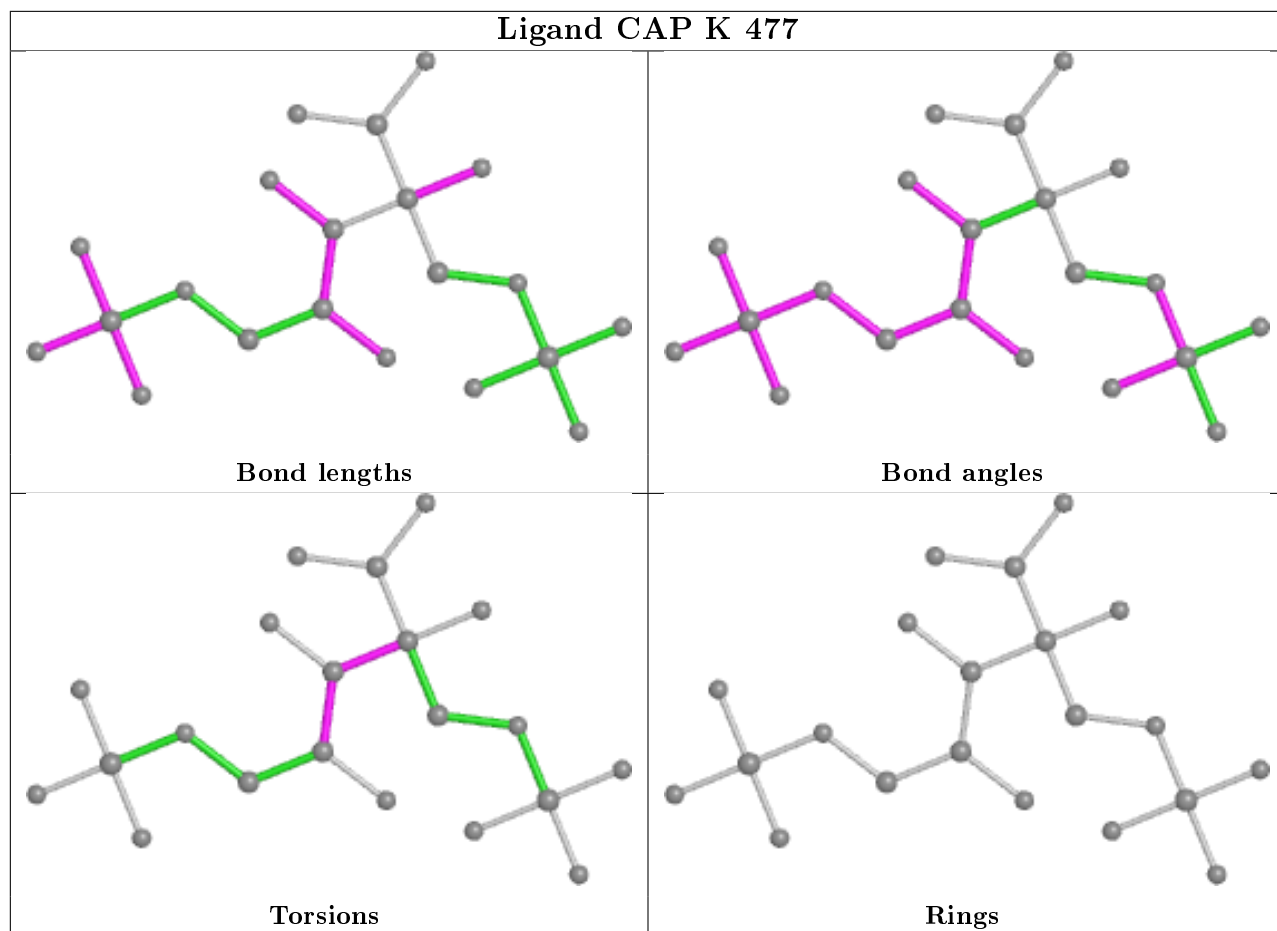
Mol	Chain	Res	Type	Atoms
4	K	477	CAP	C2-C3-C4-C5
4	B	477	CAP	C2-C3-C4-C5
4	E	477	CAP	C2-C3-C4-C5
4	R	477	CAP	C2-C3-C4-C5
4	L	477	CAP	C2-C3-C4-C5
4	O	477	CAP	C2-C3-C4-C5
4	L	477	CAP	C4-C5-O5-P2
4	K	477	CAP	O3-C3-C4-C5
4	R	477	CAP	O3-C3-C4-C5
4	H	477	CAP	C2-C3-C4-C5
4	V	477	CAP	C2-C3-C4-C5

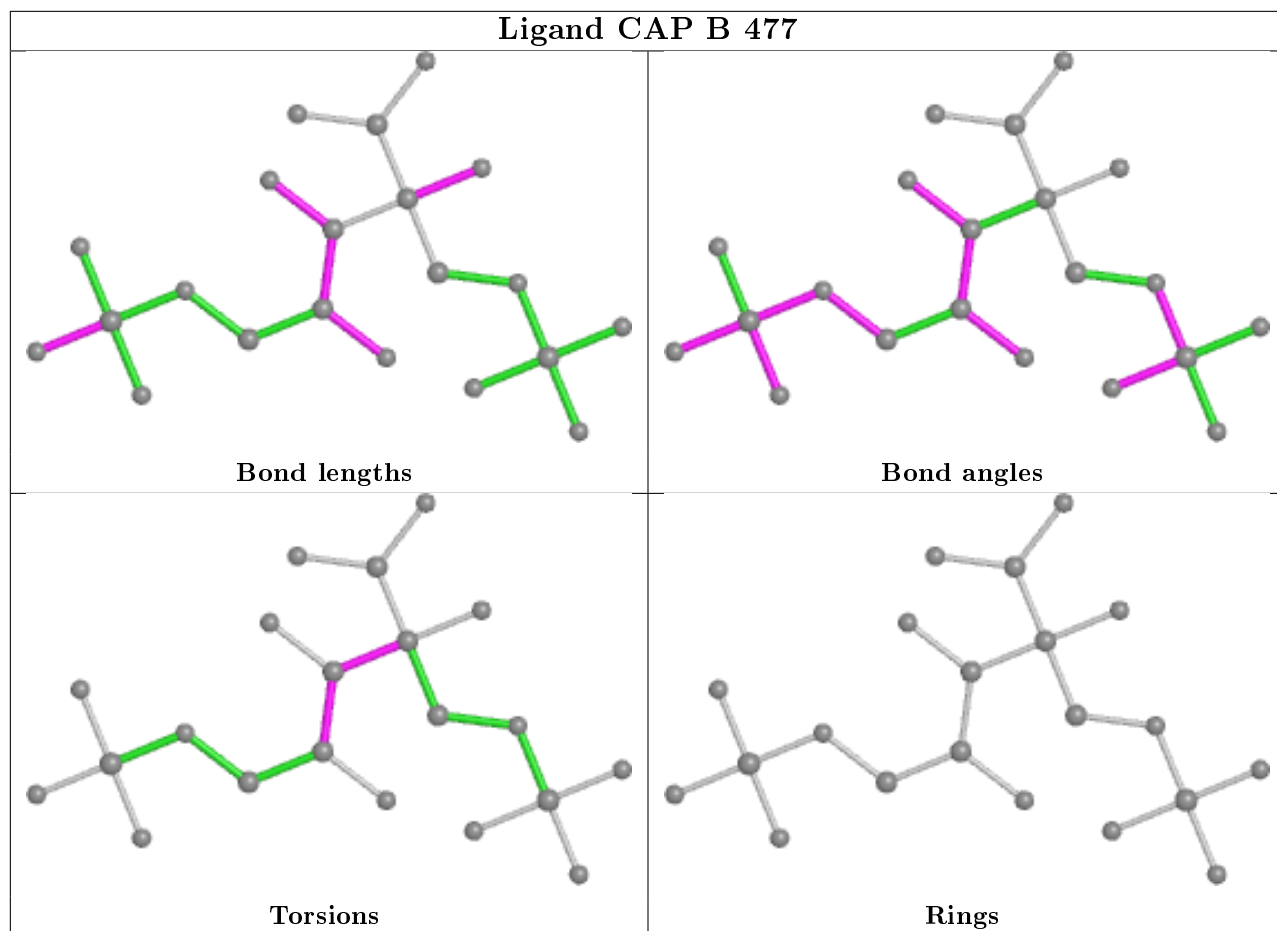
There are no ring outliers.

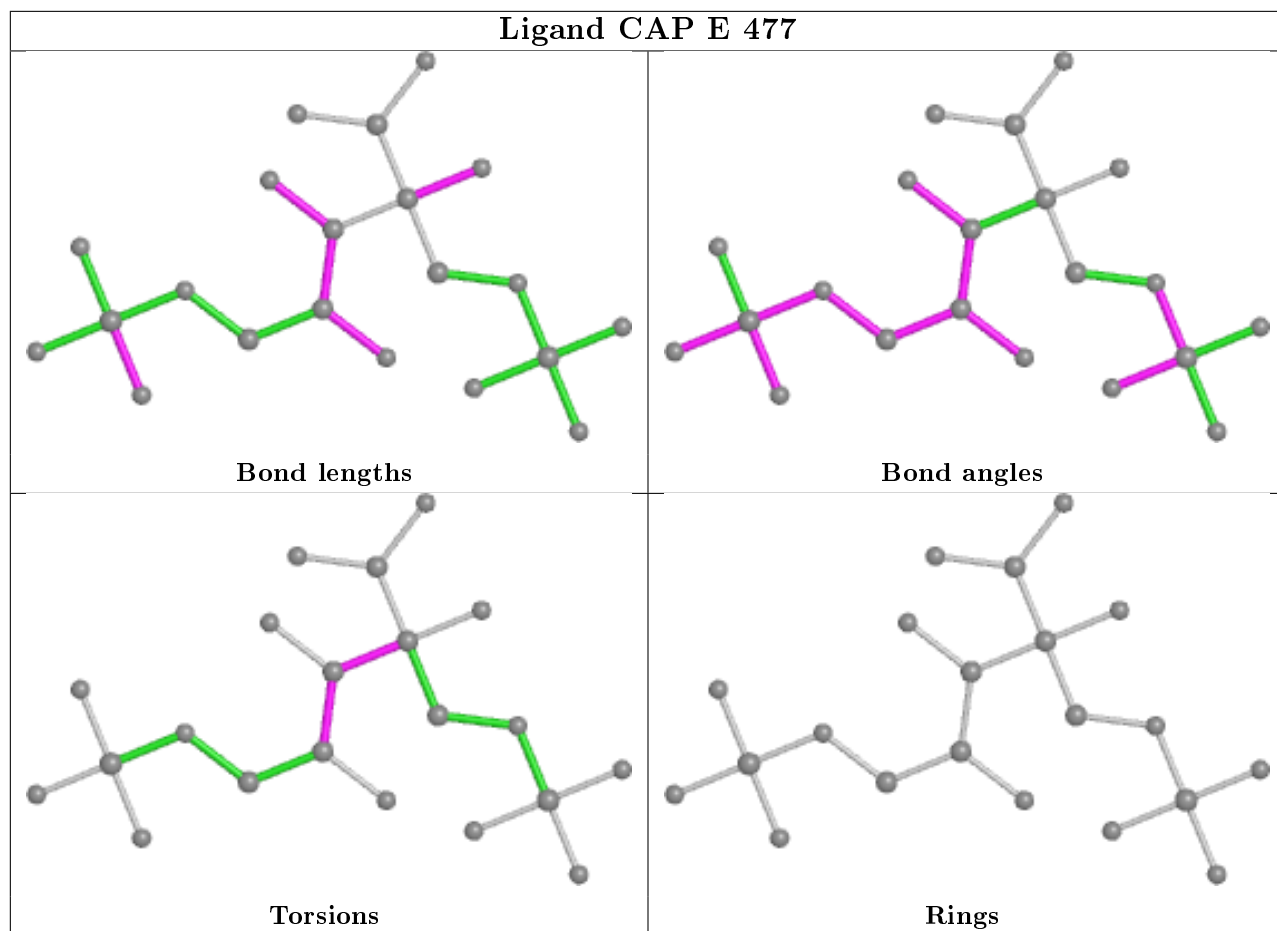
No monomer is involved in short contacts.

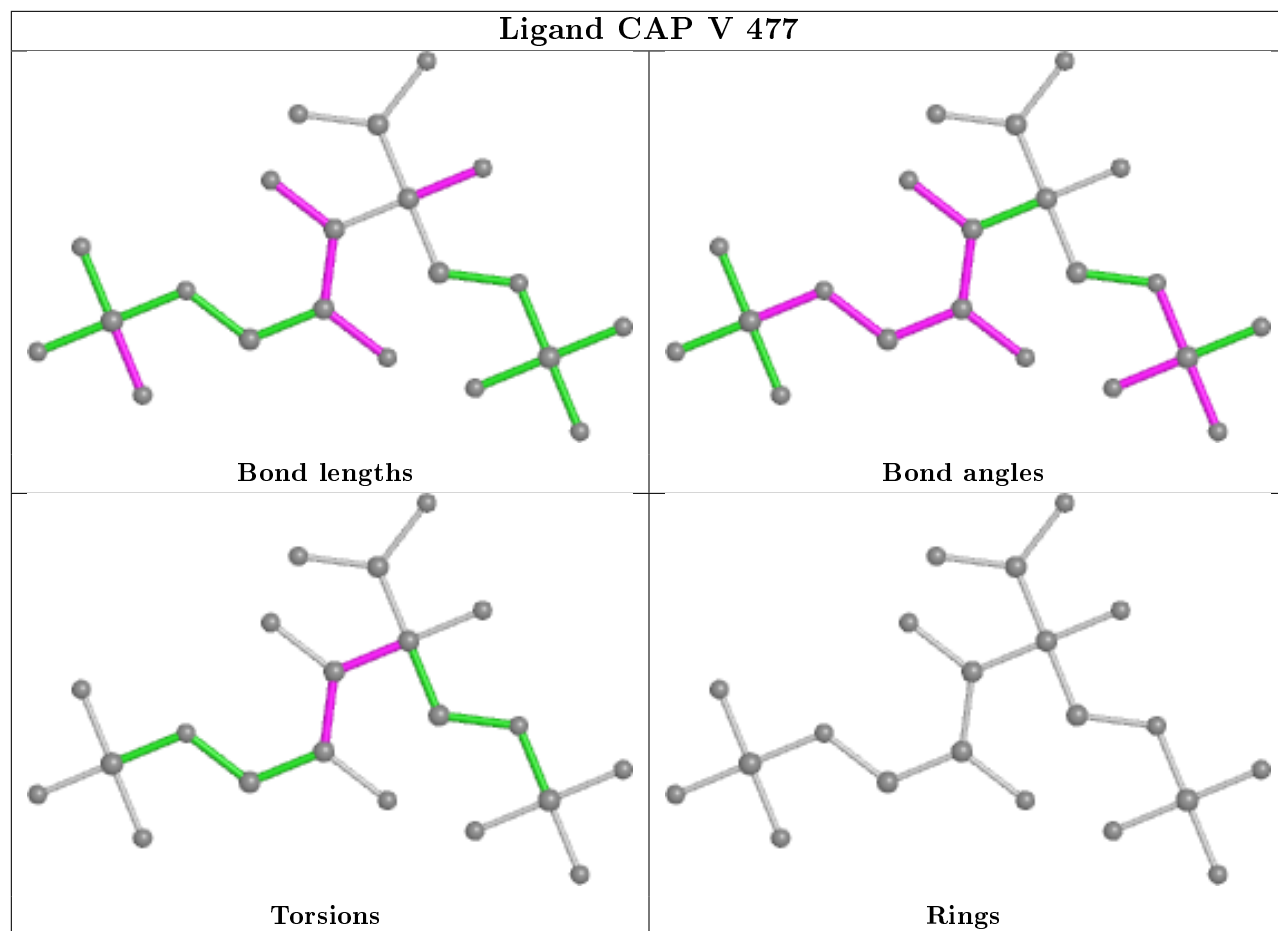
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

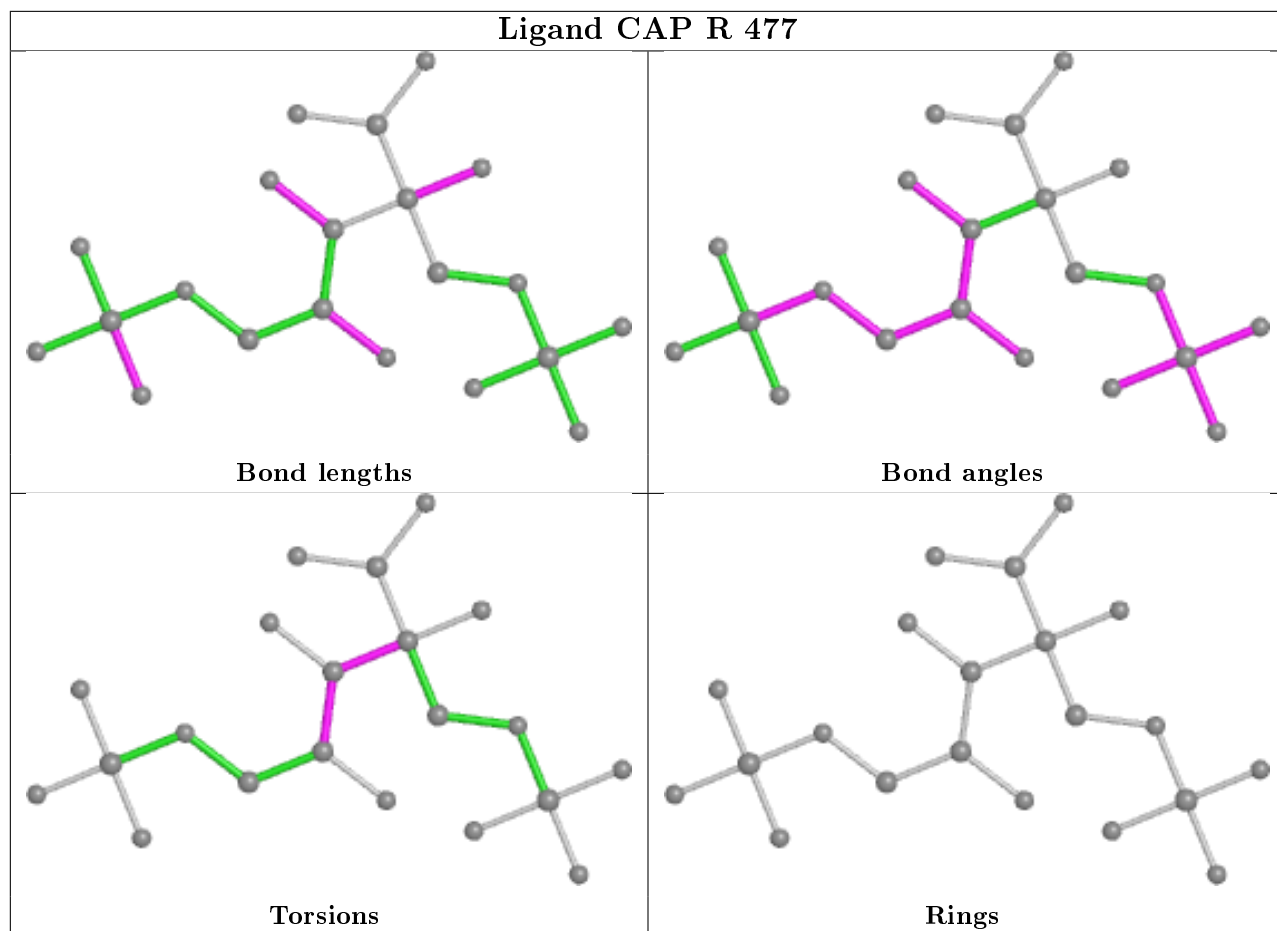


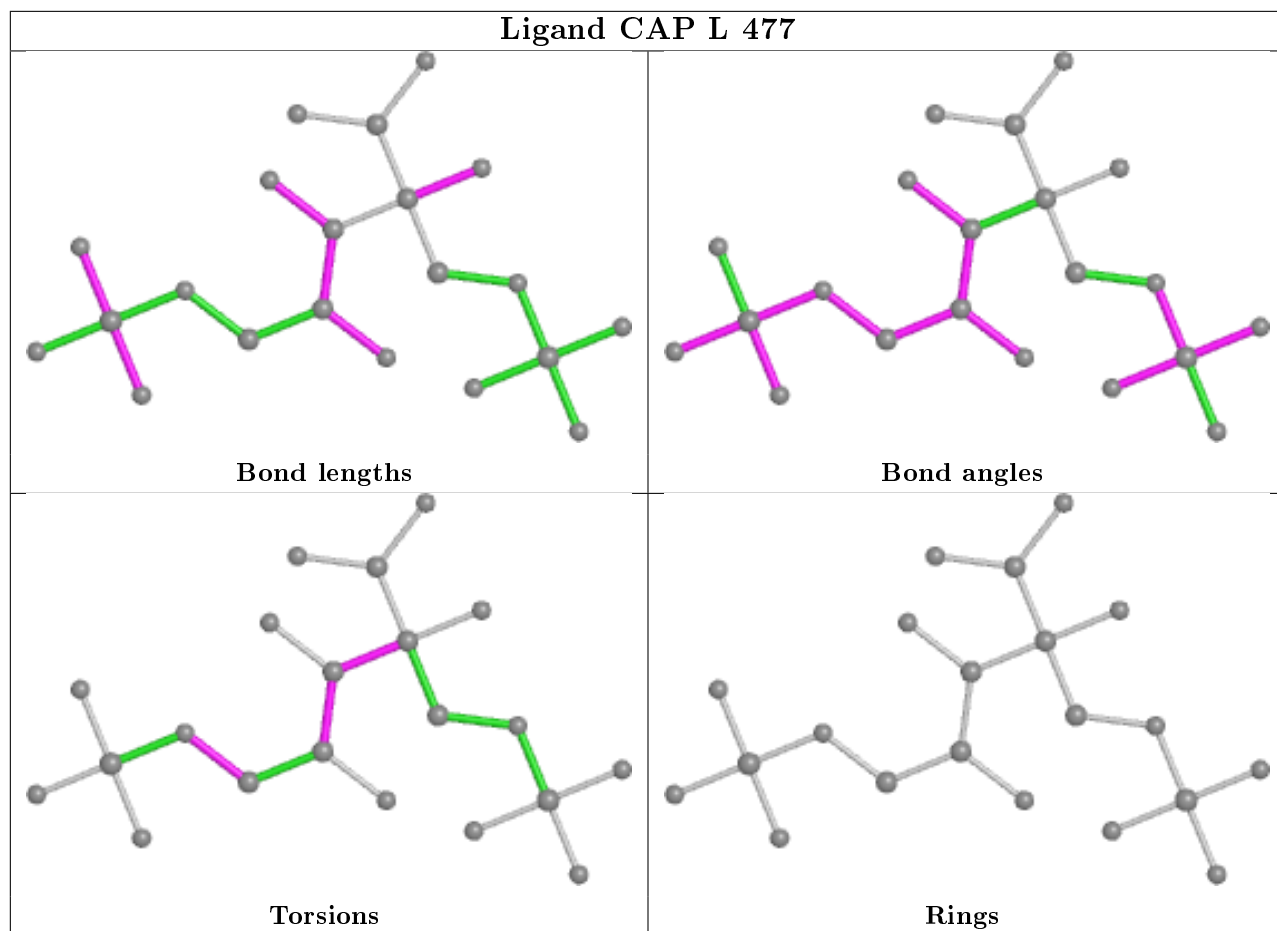




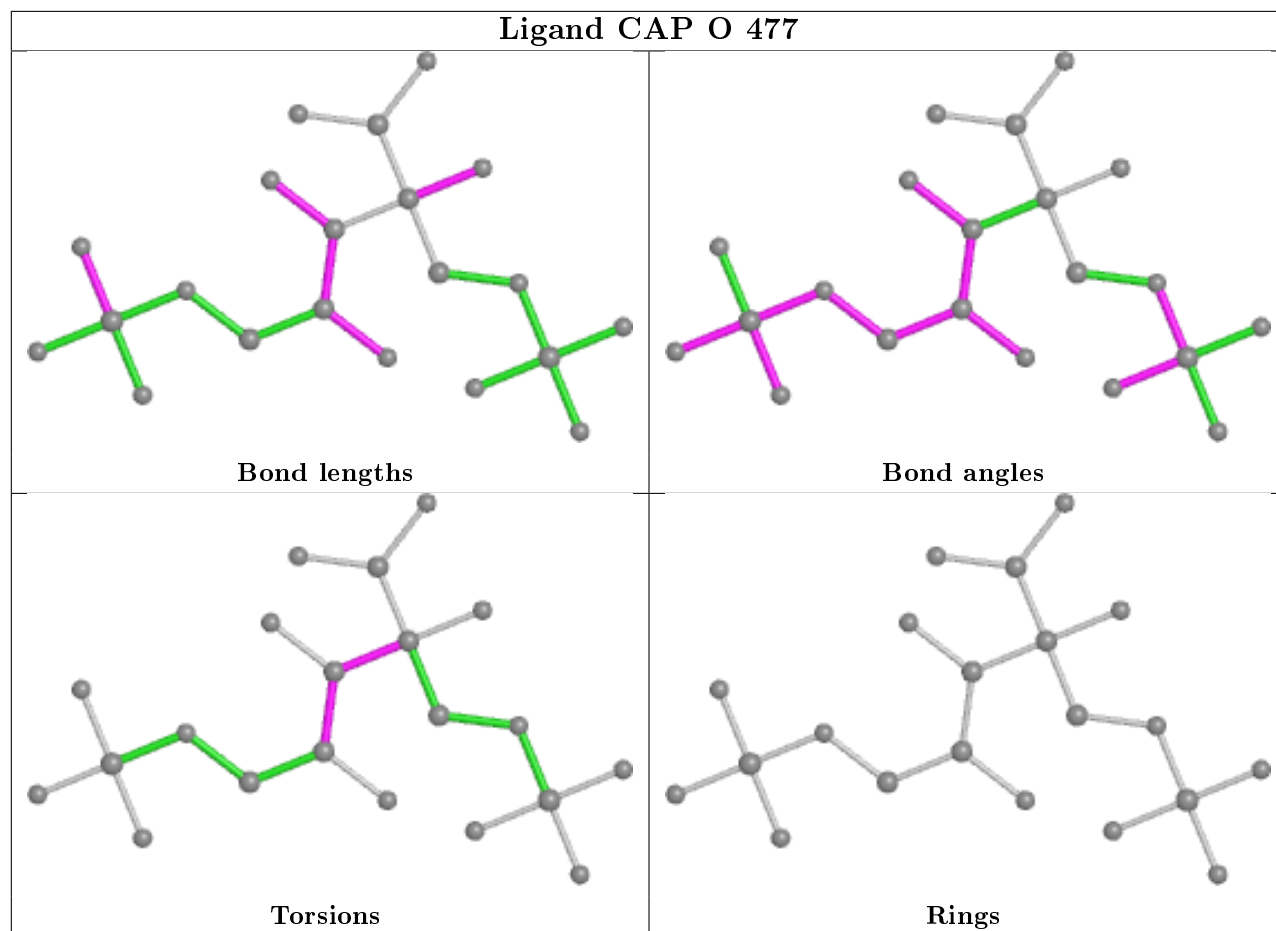












## 5.7 Other polymers [i](#)

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](#)

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

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

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

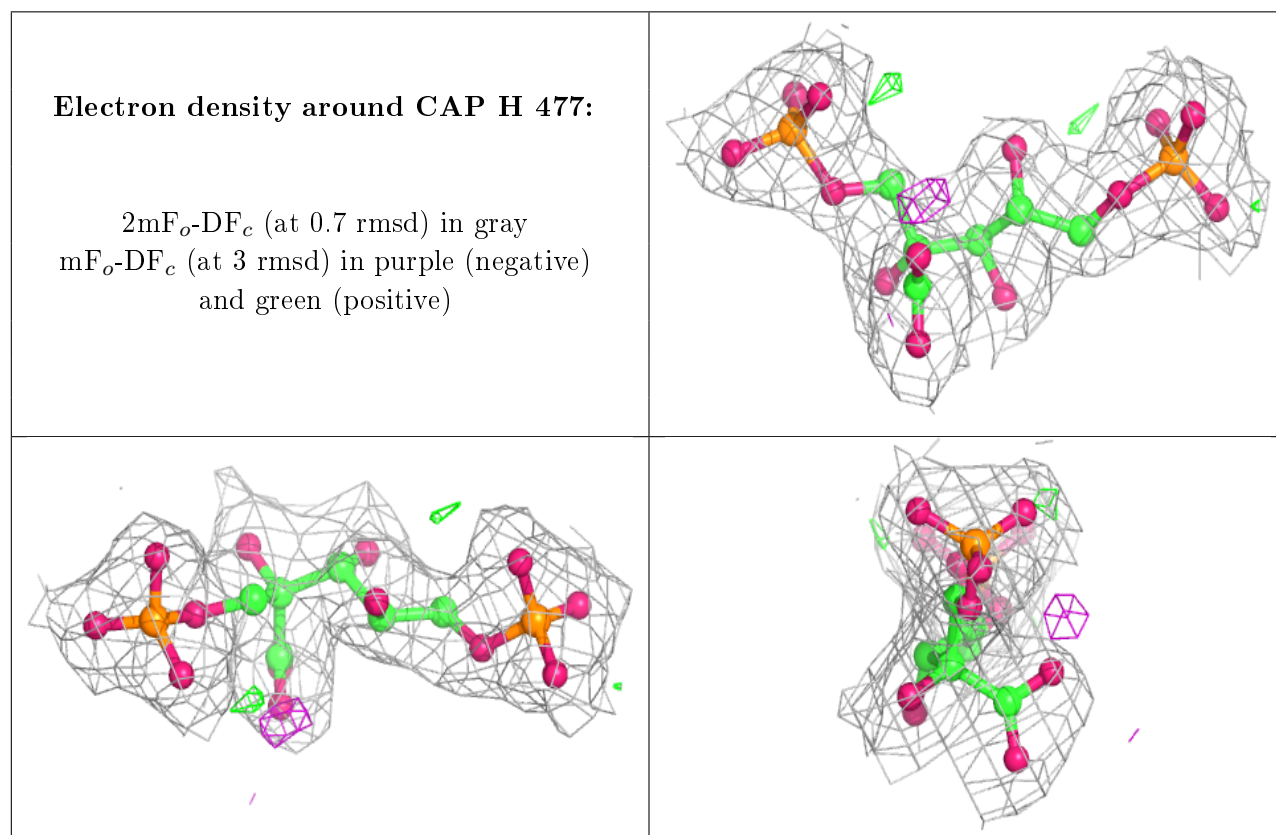
### 6.3 Carbohydrates [i](#)

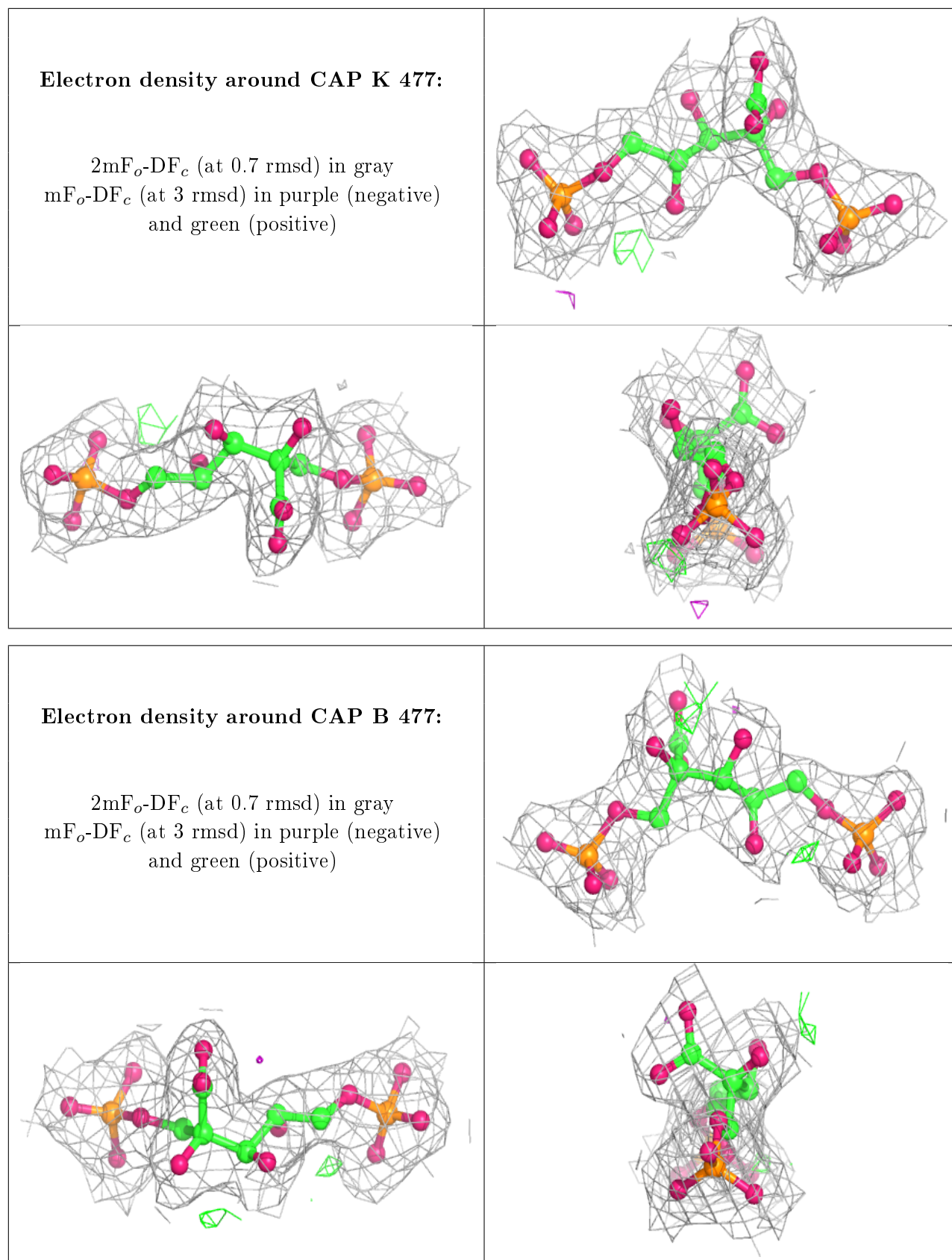
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

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

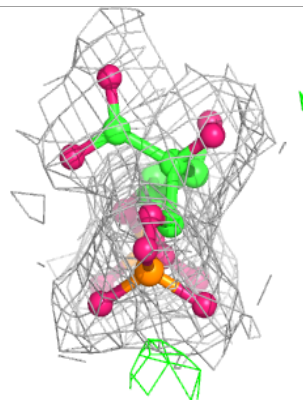
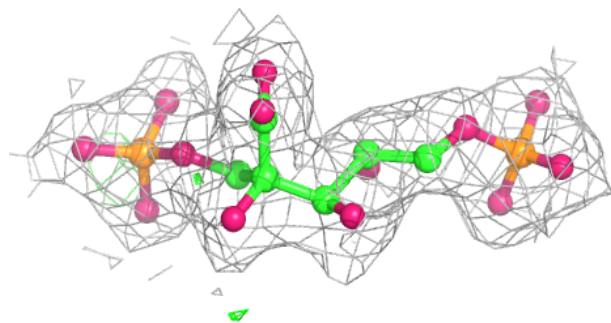
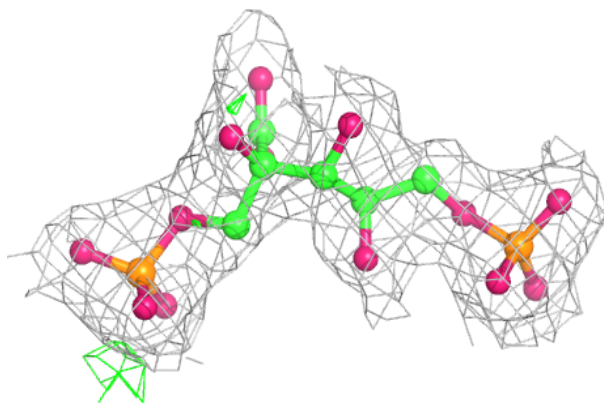
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



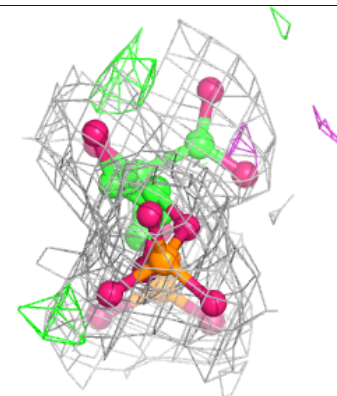
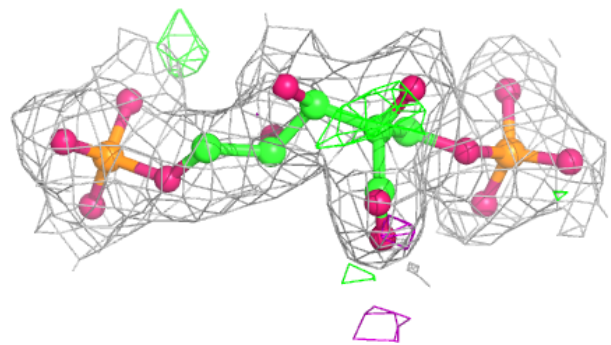
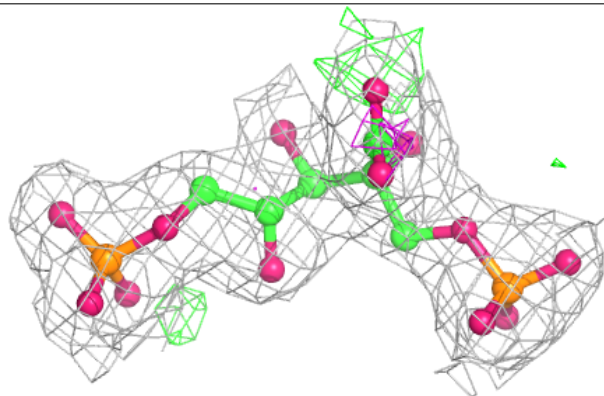


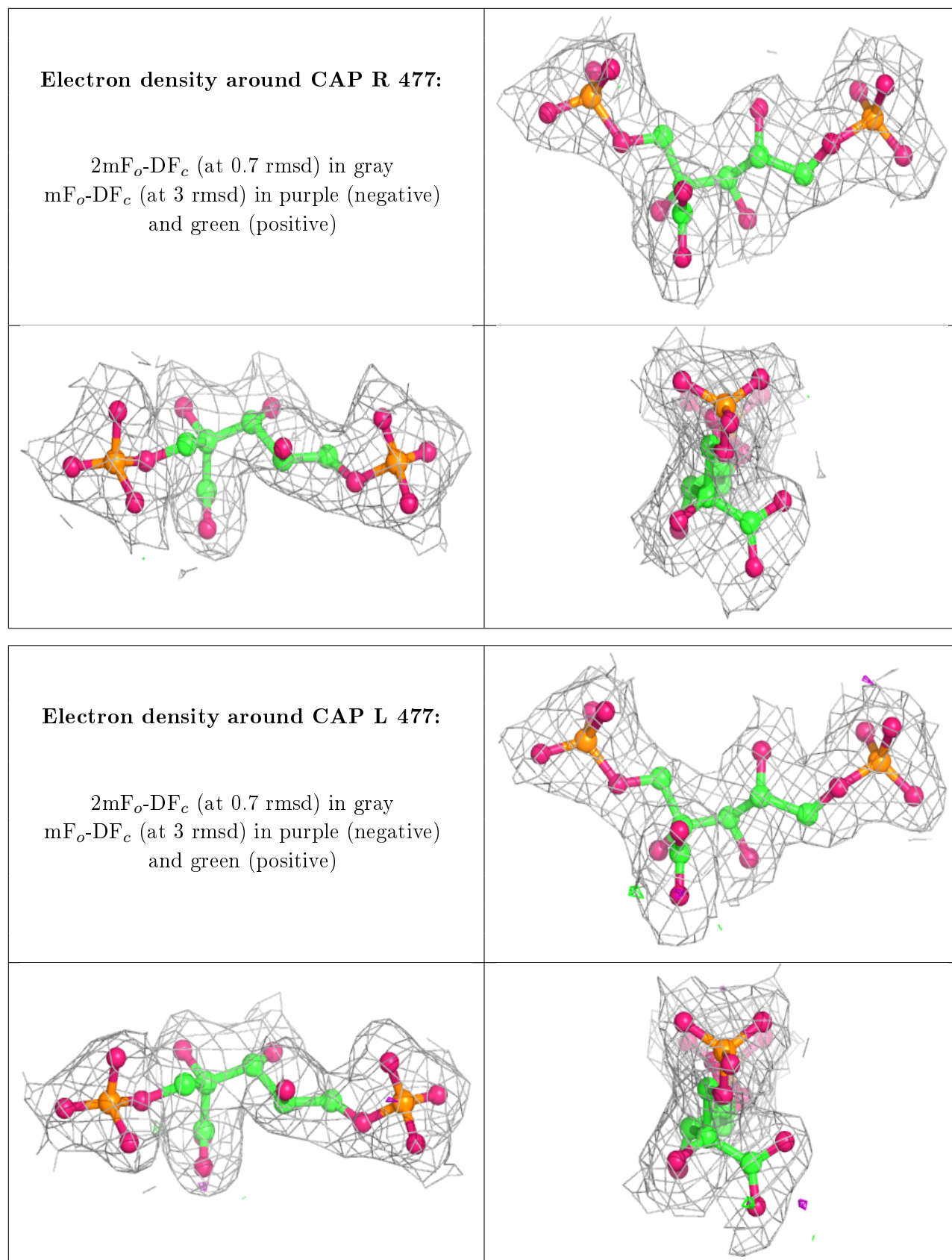
**Electron density around CAP E 477:**

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

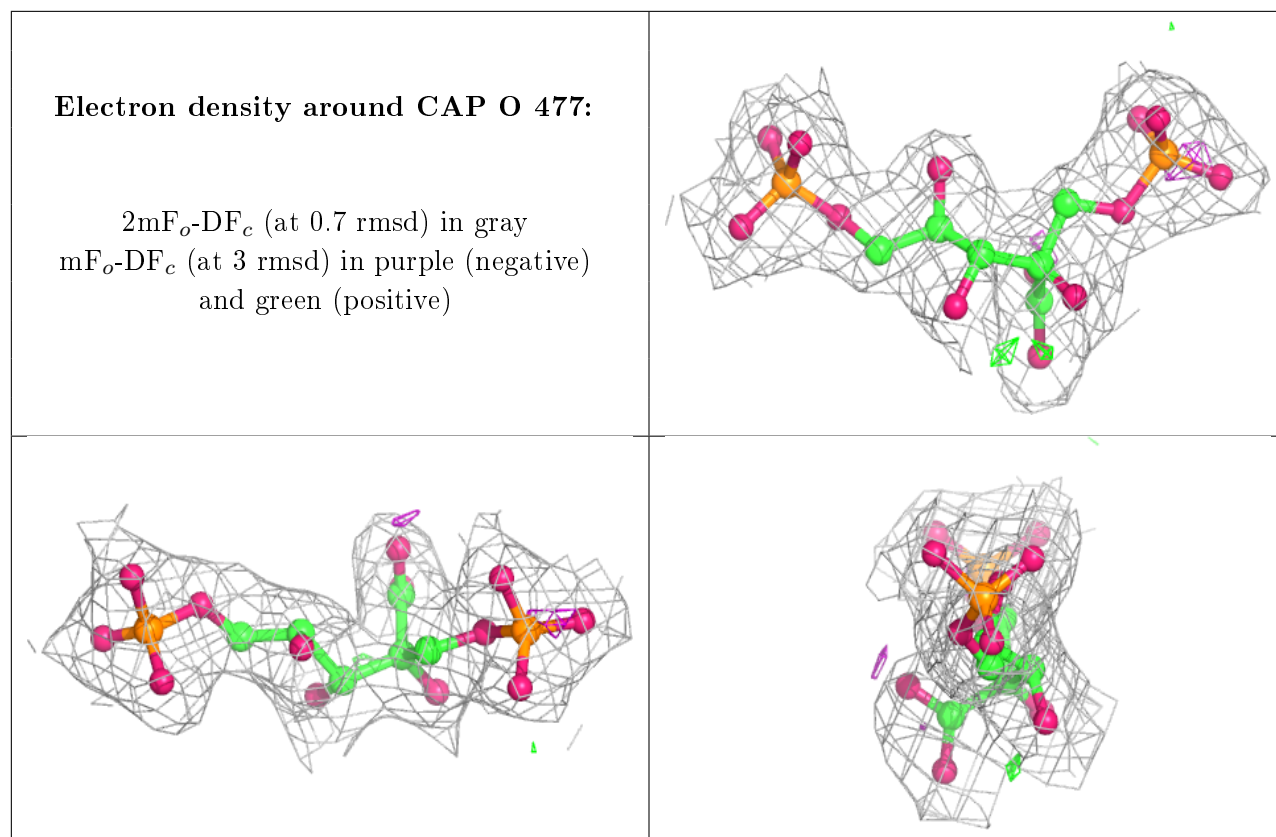
**Electron density around CAP V 477:**

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









## 6.5 Other polymers [i](#)

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