



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:00 am BST

PDB ID : 1BWV  
Title : Activated Ribulose 1,5-Bisphosphate Carboxylase/Oxygenase (RUBISCO)  
Complexed with the Reaction Intermediate Analogue 2-Carboxyarabinitol 1,5-Bisphosphate  
Authors : Sugawara, H.; Yamamoto, H.; Shibata, N.; Inoue, T.; Miyake, C.; Yokota, A.; Kai, Y.  
Deposited on : 1998-09-29  
Resolution : 2.40 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.

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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 : 1.8.5 (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

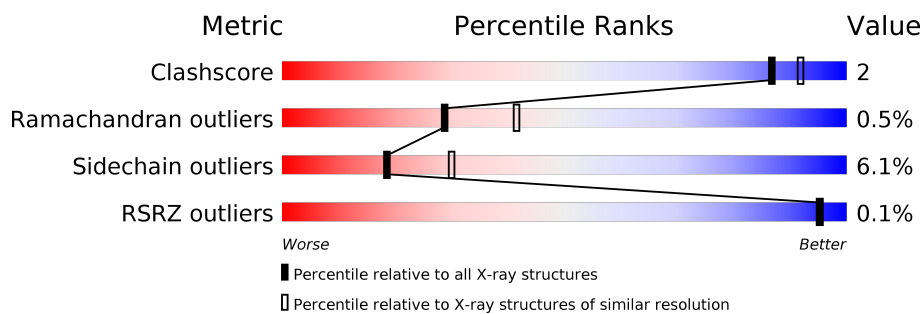
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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  $\leq 5\%$ . 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	493	
1	C	493	
1	E	493	
1	G	493	
2	S	138	
2	U	138	
2	W	138	

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Mol	Chain	Length	Quality of chain
2	Y	138	<div><div></div><div>86%</div><div>13%</div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20038 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 PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3709	2365	641	684	19			
1	C	472	Total	C	N	O	S	0	0	0
			3709	2365	641	684	19			
1	E	472	Total	C	N	O	S	0	0	0
			3709	2365	641	684	19			
1	G	472	Total	C	N	O	S	0	0	0
			3709	2365	641	684	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	KCX	LYS	MODIFIED RESIDUE	UNP O98949
C	201	KCX	LYS	MODIFIED RESIDUE	UNP O98949
E	201	KCX	LYS	MODIFIED RESIDUE	UNP O98949
G	201	KCX	LYS	MODIFIED RESIDUE	UNP O98949

- Molecule 2 is a protein called PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	138	Total	C	N	O	S	0	0	0
			1143	736	193	211	3			
2	U	138	Total	C	N	O	S	0	0	0
			1143	736	193	211	3			
2	W	138	Total	C	N	O	S	0	0	0
			1143	736	193	211	3			
2	Y	138	Total	C	N	O	S	0	0	0
			1143	736	193	211	3			

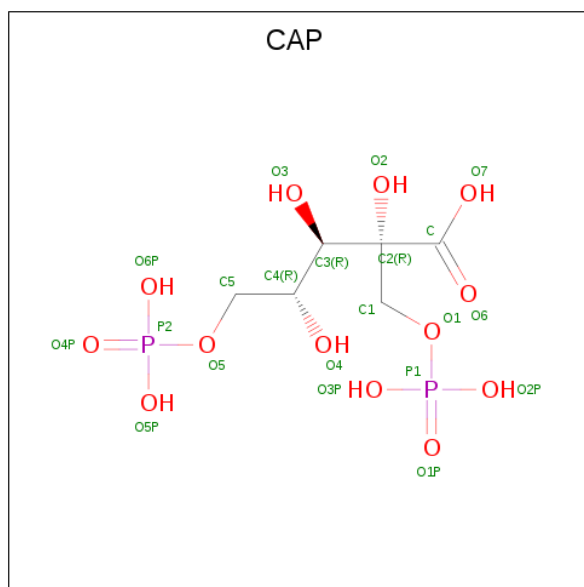
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	8	VAL	MET	CONFLICT	UNP O98950
U	8	VAL	MET	CONFLICT	UNP O98950
W	8	VAL	MET	CONFLICT	UNP O98950
Y	8	VAL	MET	CONFLICT	UNP O98950

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

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

- 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
4	A	1	Total C O P 21 6 13 2	0	0
4	C	1	Total C O P 21 6 13 2	0	0
4	E	1	Total C O P 21 6 13 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	O	P	0	0
			21	6	13	2		

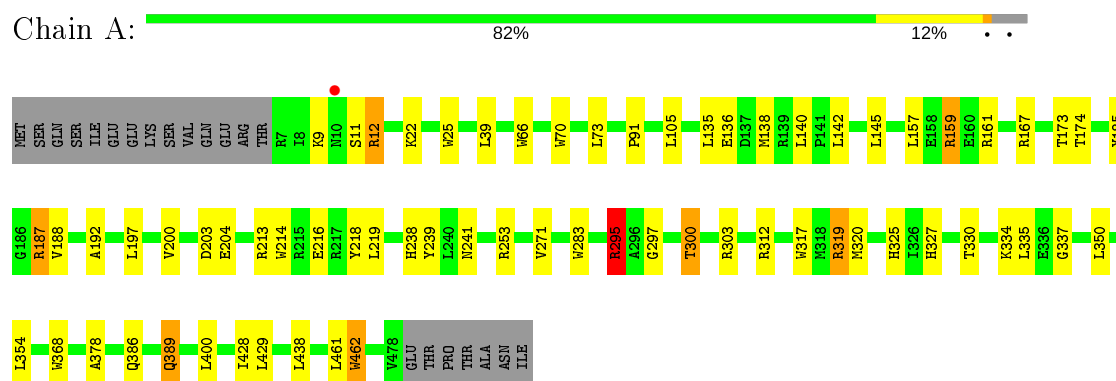
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total	O	0	0
			118	118		
5	S	26	Total	O	0	0
			26	26		
5	C	102	Total	O	0	0
			102	102		
5	U	30	Total	O	0	0
			30	30		
5	E	104	Total	O	0	0
			104	104		
5	W	24	Total	O	0	0
			24	24		
5	G	107	Total	O	0	0
			107	107		
5	Y	31	Total	O	0	0
			31	31		

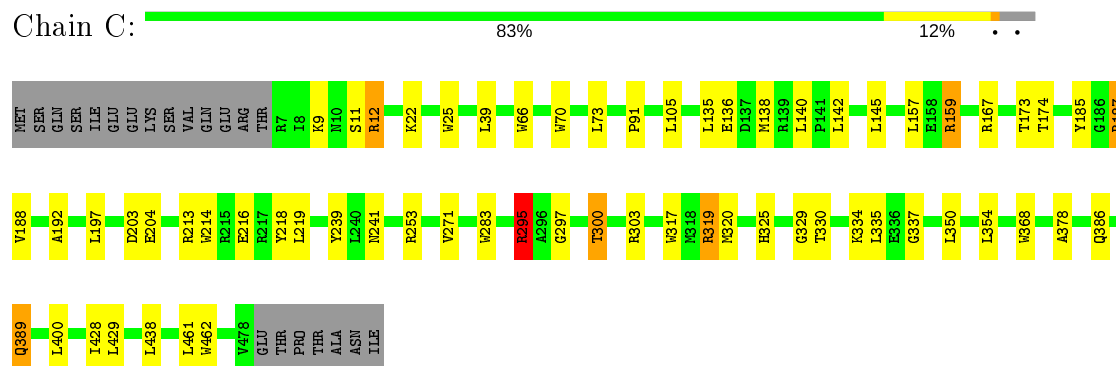
### 3 Residue-property plots [i](#)

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 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.

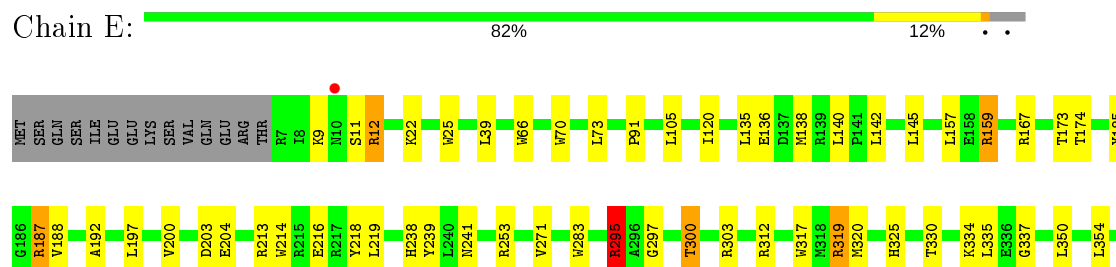
#### • Molecule 1: PROTEIN (RIBULOSE BISPHTHOSPHATE CARBOXYLASE)



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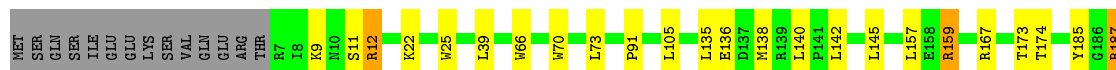
#### • Molecule 1: PROTEIN (RIBULOSE BISPHTHOSPHATE CARBOXYLASE)





• Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE)

Chain G: 82% 12% . .



• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE)

Chain S: 87% 12% .



• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE)

Chain U: 87% 11% .



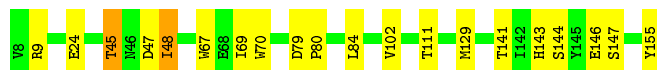
• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE)

Chain W: 89% 9% .



• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE)

Chain Y: 86% 13% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.07Å 117.07Å 319.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 39.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.0 (20.00-2.40) 86.5 (39.72-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.0	Depositor
R, $R_{free}$	0.163 , 0.197 0.161 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 3.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.70	1/3777 (0.0%)	1.26	38/5116 (0.7%)
1	C	0.69	1/3777 (0.0%)	1.26	35/5116 (0.7%)
1	E	0.69	1/3777 (0.0%)	1.26	37/5116 (0.7%)
1	G	0.73	1/3777 (0.0%)	1.27	35/5116 (0.7%)
2	S	0.66	0/1172	1.22	8/1583 (0.5%)
2	U	0.66	0/1172	1.23	9/1583 (0.6%)
2	W	0.66	0/1172	1.23	9/1583 (0.6%)
2	Y	0.66	0/1172	1.23	10/1583 (0.6%)
All	All	0.69	4/19796 (0.0%)	1.25	181/26796 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	204	GLU	CD-OE1	-19.10	1.04	1.25
1	A	204	GLU	CD-OE1	-14.95	1.09	1.25
1	C	204	GLU	CD-OE1	-13.52	1.10	1.25
1	E	204	GLU	CD-OE1	-13.08	1.11	1.25

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	E	187	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	66	TRP	CD1-CG-CD2	8.73	113.29	106.30
1	E	66	TRP	CD1-CG-CD2	8.66	113.23	106.30
1	C	187	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	G	66	TRP	CD1-CG-CD2	8.58	113.16	106.30
1	G	187	ARG	NE-CZ-NH1	8.55	124.58	120.30
2	U	70	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	C	66	TRP	CD1-CG-CD2	8.45	113.06	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	70	TRP	CD1-CG-CD2	8.44	113.05	106.30
2	W	70	TRP	CD1-CG-CD2	8.43	113.05	106.30
2	S	70	TRP	CD1-CG-CD2	8.37	113.00	106.30
1	A	368	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	E	368	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	G	368	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	E	283	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	C	368	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A	283	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	G	462	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	E	25	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	C	283	TRP	CD1-CG-CD2	7.92	112.64	106.30
2	U	70	TRP	CE2-CD2-CG	-7.91	100.97	107.30
2	S	70	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	A	66	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	A	462	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	E	214	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	C	462	TRP	CD1-CG-CD2	7.86	112.59	106.30
2	W	70	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	E	317	TRP	CD1-CG-CD2	7.84	112.58	106.30
2	Y	70	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	G	25	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	C	317	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	G	283	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	E	462	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	A	214	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	G	317	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	G	214	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	E	66	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	C	214	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	A	25	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	C	25	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	317	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	G	25	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	G	70	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	G	66	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	E	368	TRP	CE2-CD2-CG	-7.69	101.14	107.30
1	C	70	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	A	368	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	C	25	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	C	66	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	C	368	TRP	CE2-CD2-CG	-7.63	101.19	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	G	368	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	E	70	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	A	70	TRP	CD1-CG-CD2	7.57	112.36	106.30
2	U	67	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	A	25	TRP	CE2-CD2-CG	-7.49	101.31	107.30
2	Y	67	TRP	CD1-CG-CD2	7.48	112.29	106.30
1	C	283	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	G	70	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	G	283	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	A	214	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	462	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	C	70	TRP	CE2-CD2-CG	-7.41	101.37	107.30
2	S	67	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	A	283	TRP	CE2-CD2-CG	-7.41	101.38	107.30
1	E	214	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	E	462	TRP	CE2-CD2-CG	-7.40	101.38	107.30
2	W	67	TRP	CD1-CG-CD2	7.38	112.20	106.30
1	G	462	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	E	283	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	G	214	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	C	462	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	70	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	E	70	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	C	214	TRP	CE2-CD2-CG	-7.23	101.51	107.30
1	G	317	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	C	317	TRP	CE2-CD2-CG	-7.09	101.63	107.30
2	S	67	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	E	317	TRP	CE2-CD2-CG	-7.03	101.68	107.30
2	W	67	TRP	CE2-CD2-CG	-7.03	101.68	107.30
2	U	67	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	Y	67	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	317	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	E	187	ARG	NE-CZ-NH2	-6.63	116.98	120.30
2	U	9	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	187	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	W	9	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	E	159	ARG	NE-CZ-NH1	6.59	123.60	120.30
2	Y	9	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	A	159	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	C	187	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	G	187	ARG	NE-CZ-NH2	-6.39	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	9	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	12	ARG	CA-CB-CG	6.29	127.23	113.40
1	E	12	ARG	CA-CB-CG	6.28	127.22	113.40
1	G	159	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	G	12	ARG	CA-CB-CG	6.26	127.18	113.40
1	C	12	ARG	CA-CB-CG	6.26	127.17	113.40
2	U	9	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	S	9	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	159	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	Y	9	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	E	295	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	303	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	295	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	319	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	G	303	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	E	319	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	253	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	G	253	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	319	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	S	9	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	G	319	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	325	HIS	CA-CB-CG	5.69	123.27	113.60
1	G	295	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	C	295	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	G	325	HIS	CA-CB-CG	5.65	123.20	113.60
1	A	303	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	E	253	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	E	429	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	429	LEU	CA-CB-CG	5.55	128.07	115.30
1	G	429	LEU	CA-CB-CG	5.55	128.07	115.30
1	C	429	LEU	CA-CB-CG	5.55	128.07	115.30
1	E	325	HIS	CA-CB-CG	5.54	123.03	113.60
1	A	325	HIS	CA-CB-CG	5.54	123.01	113.60
1	E	25	TRP	CB-CG-CD1	-5.53	119.81	127.00
1	G	25	TRP	CG-CD2-CE3	5.53	138.87	133.90
1	E	173	THR	CA-CB-CG2	-5.52	104.67	112.40
1	C	253	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	25	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	C	25	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	A	253	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	253	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	E	218	TYR	CB-CG-CD2	-5.44	117.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	THR	CA-CB-CG2	-5.43	104.79	112.40
1	E	303	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	25	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	A	218	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	G	218	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	253	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	U	70	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	A	25	TRP	CG-CD2-CE3	5.39	138.75	133.90
2	Y	70	TRP	CG-CD2-CE3	5.37	138.74	133.90
1	C	25	TRP	CB-CG-CD1	-5.37	120.02	127.00
1	C	12	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	G	25	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	C	218	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	C	368	TRP	CG-CD2-CE3	5.35	138.71	133.90
1	C	173	THR	CA-CB-CG2	-5.32	104.95	112.40
1	E	368	TRP	CG-CD2-CE3	5.32	138.69	133.90
2	W	70	TRP	CG-CD2-CE3	5.31	138.68	133.90
2	S	70	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	G	253	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	70	TRP	CG-CD2-CE3	5.29	138.66	133.90
1	A	368	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	E	70	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	G	70	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	G	173	THR	CA-CB-CG2	-5.26	105.03	112.40
1	G	368	TRP	CG-CD2-CE3	5.26	138.64	133.90
1	C	70	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	A	66	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	E	312	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	G	12	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	U	9	ARG	N-CA-C	-5.16	97.07	111.00
2	Y	9	ARG	N-CA-C	-5.15	97.10	111.00
1	G	66	TRP	CG-CD1-NE1	-5.14	104.96	110.10
2	U	70	TRP	CG-CD1-NE1	-5.13	104.97	110.10
2	W	70	TRP	CG-CD1-NE1	-5.13	104.97	110.10
2	Y	70	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	E	66	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	C	66	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	70	TRP	CB-CG-CD1	-5.06	120.43	127.00
1	A	312	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	161	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	E	70	TRP	CB-CG-CD1	-5.03	120.46	127.00
2	W	70	TRP	CB-CG-CD1	-5.03	120.47	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	70	TRP	CB-CG-CD1	-5.02	120.48	127.00
1	A	12	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	E	12	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	Y	70	TRP	CB-CG-CD1	-5.00	120.50	127.00

There are no chirality outliers.

There are no planarity outliers.

## 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	3709	0	3688	17	0
1	C	3709	0	3688	15	0
1	E	3709	0	3688	16	0
1	G	3709	0	3688	16	0
2	S	1143	0	1131	5	0
2	U	1143	0	1131	6	0
2	W	1143	0	1131	4	0
2	Y	1143	0	1131	6	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	21	0	7	1	0
4	C	21	0	7	1	0
4	E	21	0	7	1	0
4	G	21	0	7	1	0
5	A	118	0	0	1	0
5	C	102	0	0	1	0
5	E	104	0	0	0	0
5	G	107	0	0	1	0
5	S	26	0	0	0	0
5	U	30	0	0	1	0
5	W	24	0	0	0	0
5	Y	31	0	0	0	0
All	All	20038	0	19304	81	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 2.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:GLY:O	1:G:300:THR:HB	2.00	0.62
1:C:297:GLY:O	1:C:300:THR:HB	2.00	0.62
1:A:297:GLY:O	1:A:300:THR:HB	2.00	0.61
1:E:297:GLY:O	1:E:300:THR:HB	2.00	0.61
1:G:140:LEU:HD13	1:G:320:MET:SD	2.41	0.60
1:A:140:LEU:HD13	1:A:320:MET:SD	2.41	0.60
1:E:140:LEU:HD13	1:E:320:MET:SD	2.41	0.59
1:C:140:LEU:HD13	1:C:320:MET:SD	2.42	0.59
1:E:192:ALA:HB1	1:E:197:LEU:HD12	1.86	0.57
1:A:192:ALA:HB1	1:A:197:LEU:HD12	1.86	0.57
1:C:192:ALA:HB1	1:C:197:LEU:HD12	1.87	0.56
1:A:39:LEU:HD23	1:A:136:GLU:HB2	1.88	0.55
1:E:39:LEU:HD23	1:E:136:GLU:HB2	1.88	0.55
1:G:192:ALA:HB1	1:G:197:LEU:HD12	1.87	0.54
1:G:39:LEU:HD23	1:G:136:GLU:HB2	1.89	0.53
1:C:39:LEU:HD23	1:C:136:GLU:HB2	1.89	0.53
1:C:330:THR:HG22	1:C:378:ALA:HB1	1.93	0.50
1:G:330:THR:HG22	1:G:378:ALA:HB1	1.93	0.50
1:E:330:THR:HG22	1:E:378:ALA:HB1	1.93	0.50
2:S:146:GLU:HG3	2:S:155:TYR:CE1	2.47	0.49
2:W:146:GLU:HG3	2:W:155:TYR:CE1	2.47	0.49
1:A:330:THR:HG22	1:A:378:ALA:HB1	1.93	0.49
2:Y:146:GLU:HG3	2:Y:155:TYR:CE1	2.48	0.48
2:U:146:GLU:HG3	2:U:155:TYR:CE1	2.48	0.48
1:E:135:LEU:HD21	1:E:138:MET:CE	2.44	0.48
1:G:135:LEU:HD21	1:G:138:MET:CE	2.44	0.47
2:W:45:THR:HB	2:W:47:ASP:H	1.79	0.47
1:C:135:LEU:HD21	1:C:138:MET:CE	2.44	0.47
1:E:334:LYS:HG3	1:E:335:LEU:HD22	1.97	0.47
1:E:174:THR:HG23	1:E:188:VAL:HG11	1.97	0.47
1:A:135:LEU:HD21	1:A:138:MET:CE	2.44	0.47
2:Y:45:THR:HB	2:Y:47:ASP:H	1.79	0.47
2:S:45:THR:HB	2:S:47:ASP:H	1.79	0.47
1:G:174:THR:HG23	1:G:188:VAL:HG11	1.96	0.46
1:A:174:THR:HG23	1:A:188:VAL:HG11	1.97	0.46
1:C:174:THR:HG23	1:C:188:VAL:HG11	1.97	0.46
1:A:334:LYS:HG3	1:A:335:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:102:VAL:HG13	2:Y:111:THR:HG23	1.98	0.45
2:U:45:THR:HB	2:U:47:ASP:H	1.80	0.45
2:Y:143:HIS:HE1	2:Y:147:SER:O	1.99	0.45
1:G:334:LYS:HG3	1:G:335:LEU:HD22	1.98	0.45
2:U:143:HIS:HE1	2:U:147:SER:O	1.99	0.45
2:S:143:HIS:HE1	2:S:147:SER:O	2.00	0.45
2:W:102:VAL:HG13	2:W:111:THR:HG23	1.99	0.45
1:A:462:TRP:HB2	5:A:582:HOH:O	2.17	0.44
1:C:334:LYS:HG3	1:C:335:LEU:HD22	1.98	0.44
2:U:102:VAL:HG13	2:U:111:THR:HG23	1.98	0.44
2:W:143:HIS:HE1	2:W:147:SER:O	2.00	0.44
2:S:79:ASP:HA	2:S:80:PRO:HD2	1.88	0.44
1:E:216:GLU:HG2	1:G:157:LEU:CD1	2.47	0.44
1:E:213:ARG:HB2	1:E:216:GLU:OE2	2.18	0.44
1:A:216:GLU:HG2	1:C:157:LEU:CD1	2.48	0.43
1:A:295:ARG:HD2	4:A:491:CAP:O4P	2.18	0.43
1:C:213:ARG:HB2	1:C:216:GLU:OE2	2.19	0.43
1:G:213:ARG:HB2	1:G:216:GLU:OE2	2.19	0.43
2:S:102:VAL:HG13	2:S:111:THR:HG23	1.99	0.43
1:A:213:ARG:HB2	1:A:216:GLU:OE2	2.18	0.43
1:A:386:GLN:O	1:A:389:GLN:HG2	2.19	0.43
1:G:329:GLY:HA2	5:G:564:HOH:O	2.19	0.43
1:E:295:ARG:HD2	4:E:491:CAP:O4P	2.18	0.42
1:E:159:ARG:NH2	1:E:167:ARG:O	2.53	0.42
1:C:295:ARG:HD2	4:C:491:CAP:O4P	2.20	0.42
1:C:386:GLN:O	1:C:389:GLN:HG2	2.20	0.42
1:G:386:GLN:O	1:G:389:GLN:HG2	2.20	0.42
1:A:157:LEU:CD1	1:G:216:GLU:HG2	2.50	0.42
1:E:200:VAL:O	1:E:238:HIS:HA	2.20	0.42
1:A:200:VAL:O	1:A:238:HIS:HA	2.20	0.42
1:E:386:GLN:O	1:E:389:GLN:HG2	2.19	0.42
1:A:159:ARG:NH2	1:A:167:ARG:O	2.53	0.41
2:U:24:GLU:HB2	5:U:534:HOH:O	2.20	0.41
1:C:216:GLU:HG2	1:E:157:LEU:CD1	2.50	0.41
1:G:159:ARG:NH2	1:G:167:ARG:O	2.53	0.41
1:E:120:ILE:HG21	1:E:138:MET:HE2	2.02	0.41
1:G:295:ARG:HD2	4:G:491:CAP:O4P	2.20	0.41
1:C:159:ARG:NH2	1:C:167:ARG:O	2.53	0.41
2:U:79:ASP:HA	2:U:80:PRO:HD2	1.88	0.41
2:Y:79:ASP:HA	2:Y:80:PRO:HD2	1.88	0.41
1:A:295:ARG:HG3	1:A:327:HIS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:129:MET:HB2	2:Y:141:THR:HB	2.03	0.40
1:C:329:GLY:HA2	5:C:564:HOH:O	2.22	0.40
1:G:200:VAL:O	1:G:238:HIS:HA	2.22	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	469/493 (95%)	451 (96%)	16 (3%)	2 (0%)	34	48
1	C	469/493 (95%)	451 (96%)	16 (3%)	2 (0%)	34	48
1	E	469/493 (95%)	452 (96%)	15 (3%)	2 (0%)	34	48
1	G	469/493 (95%)	451 (96%)	16 (3%)	2 (0%)	34	48
2	S	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	22	32
2	U	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	22	32
2	W	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	22	32
2	Y	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	22	32
All	All	2420/2524 (96%)	2317 (96%)	91 (4%)	12 (0%)	29	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	C	11	SER
1	E	11	SER
1	G	11	SER
2	S	48	ILE
2	U	48	ILE
2	W	48	ILE

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Mol	Chain	Res	Type
2	Y	48	ILE
1	A	337	GLY
1	C	337	GLY
1	E	337	GLY
1	G	337	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/402 (95%)	357 (94%)	25 (6%)	17	27
1	C	382/402 (95%)	357 (94%)	25 (6%)	17	27
1	E	382/402 (95%)	357 (94%)	25 (6%)	17	27
1	G	382/402 (95%)	357 (94%)	25 (6%)	17	27
2	S	126/126 (100%)	120 (95%)	6 (5%)	25	41
2	U	126/126 (100%)	120 (95%)	6 (5%)	25	41
2	W	126/126 (100%)	121 (96%)	5 (4%)	31	49
2	Y	126/126 (100%)	120 (95%)	6 (5%)	25	41
All	All	2032/2112 (96%)	1909 (94%)	123 (6%)	18	30

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	12	ARG
1	A	22	LYS
1	A	73	LEU
1	A	91	PRO
1	A	105	LEU
1	A	142	LEU
1	A	145	LEU
1	A	185	TYR
1	A	187	ARG

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Mol	Chain	Res	Type
1	A	203	ASP
1	A	219	LEU
1	A	239	TYR
1	A	241	ASN
1	A	271	VAL
1	A	295	ARG
1	A	300	THR
1	A	319	ARG
1	A	350	LEU
1	A	354	LEU
1	A	389	GLN
1	A	400	LEU
1	A	428	ILE
1	A	438	LEU
1	A	461	LEU
2	S	24	GLU
2	S	45	THR
2	S	48	ILE
2	S	69	ILE
2	S	84	LEU
2	S	144	SER
1	C	9	LYS
1	C	12	ARG
1	C	22	LYS
1	C	73	LEU
1	C	91	PRO
1	C	105	LEU
1	C	142	LEU
1	C	145	LEU
1	C	185	TYR
1	C	187	ARG
1	C	203	ASP
1	C	219	LEU
1	C	239	TYR
1	C	241	ASN
1	C	271	VAL
1	C	295	ARG
1	C	300	THR
1	C	319	ARG
1	C	350	LEU
1	C	354	LEU
1	C	389	GLN

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Mol	Chain	Res	Type
1	C	400	LEU
1	C	428	ILE
1	C	438	LEU
1	C	461	LEU
2	U	24	GLU
2	U	45	THR
2	U	48	ILE
2	U	69	ILE
2	U	84	LEU
2	U	144	SER
1	E	9	LYS
1	E	12	ARG
1	E	22	LYS
1	E	73	LEU
1	E	91	PRO
1	E	105	LEU
1	E	142	LEU
1	E	145	LEU
1	E	185	TYR
1	E	187	ARG
1	E	203	ASP
1	E	219	LEU
1	E	239	TYR
1	E	241	ASN
1	E	271	VAL
1	E	295	ARG
1	E	300	THR
1	E	319	ARG
1	E	350	LEU
1	E	354	LEU
1	E	389	GLN
1	E	400	LEU
1	E	428	ILE
1	E	438	LEU
1	E	461	LEU
2	W	24	GLU
2	W	45	THR
2	W	48	ILE
2	W	69	ILE
2	W	144	SER
1	G	9	LYS
1	G	12	ARG

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Mol	Chain	Res	Type
1	G	22	LYS
1	G	73	LEU
1	G	91	PRO
1	G	105	LEU
1	G	142	LEU
1	G	145	LEU
1	G	185	TYR
1	G	187	ARG
1	G	203	ASP
1	G	219	LEU
1	G	239	TYR
1	G	241	ASN
1	G	271	VAL
1	G	295	ARG
1	G	300	THR
1	G	319	ARG
1	G	350	LEU
1	G	354	LEU
1	G	389	GLN
1	G	400	LEU
1	G	428	ILE
1	G	438	LEU
1	G	461	LEU
2	Y	24	GLU
2	Y	45	THR
2	Y	48	ILE
2	Y	69	ILE
2	Y	84	LEU
2	Y	144	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	255	ASN
2	S	88	ASN
2	S	143	HIS
1	C	241	ASN
1	C	255	ASN
2	U	88	ASN
2	U	143	HIS
1	E	241	ASN

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Mol	Chain	Res	Type
1	E	255	ASN
2	W	12	GLN
2	W	88	ASN
1	G	241	ASN
1	G	255	ASN
2	Y	88	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KCX	C	201	1,3	7,11,12	0.60	0	4,12,14	1.07	0
1	KCX	A	201	1,3	7,11,12	0.63	0	4,12,14	1.51	1 (25%)
1	KCX	G	201	1,3	7,11,12	0.65	0	4,12,14	0.93	0
1	KCX	E	201	1,3	7,11,12	0.62	0	4,12,14	0.99	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	KCX	CG-CD-CE	2.07	123.35	113.56

There are no chirality outliers.

There are no torsion outliers.

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CAP	C	491	3	15,20,20	1.67	1 (6%)	20,31,31	1.14	2 (10%)
4	CAP	E	491	3	15,20,20	1.09	1 (6%)	20,31,31	1.49	3 (15%)
4	CAP	G	491	3	15,20,20	1.55	1 (6%)	20,31,31	1.13	2 (10%)
4	CAP	A	491	3	15,20,20	1.02	0	20,31,31	1.39	4 (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
4	CAP	C	491	3	-	5/23/29/29	-
4	CAP	E	491	3	-	3/23/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAP	G	491	3	-	5/23/29/29	-
4	CAP	A	491	3	-	4/23/29/29	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	491	CAP	C4-C3	-5.14	1.49	1.54
4	G	491	CAP	C4-C3	-4.63	1.49	1.54
4	E	491	CAP	O4-C4	-2.15	1.38	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	491	CAP	O4-C4-C3	-3.73	101.32	108.78
4	A	491	CAP	O4-C4-C3	-3.14	102.52	108.78
4	A	491	CAP	C2-C3-C4	-2.56	108.80	114.00
4	C	491	CAP	O5P-P2-O4P	2.41	120.10	110.68
4	E	491	CAP	O5P-P2-O4P	2.36	119.93	110.68
4	G	491	CAP	O5P-P2-O4P	2.34	119.86	110.68
4	A	491	CAP	O5P-P2-O4P	2.33	119.79	110.68
4	E	491	CAP	O2P-P1-O1P	2.18	119.20	110.68
4	A	491	CAP	O2P-P1-O1P	2.15	119.08	110.68
4	G	491	CAP	O2P-P1-O1P	2.07	118.79	110.68
4	C	491	CAP	O2P-P1-O1P	2.07	118.77	110.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	491	CAP	C2-C3-C4-O4
4	C	491	CAP	O3-C3-C4-O4
4	A	491	CAP	C2-C3-C4-O4
4	A	491	CAP	O3-C3-C4-O4
4	E	491	CAP	C2-C3-C4-O4
4	E	491	CAP	O3-C3-C4-O4
4	G	491	CAP	C2-C3-C4-O4
4	G	491	CAP	O3-C3-C4-O4
4	C	491	CAP	O2-C2-C3-C4
4	A	491	CAP	O2-C2-C3-C4
4	E	491	CAP	O2-C2-C3-C4
4	G	491	CAP	O2-C2-C3-C4

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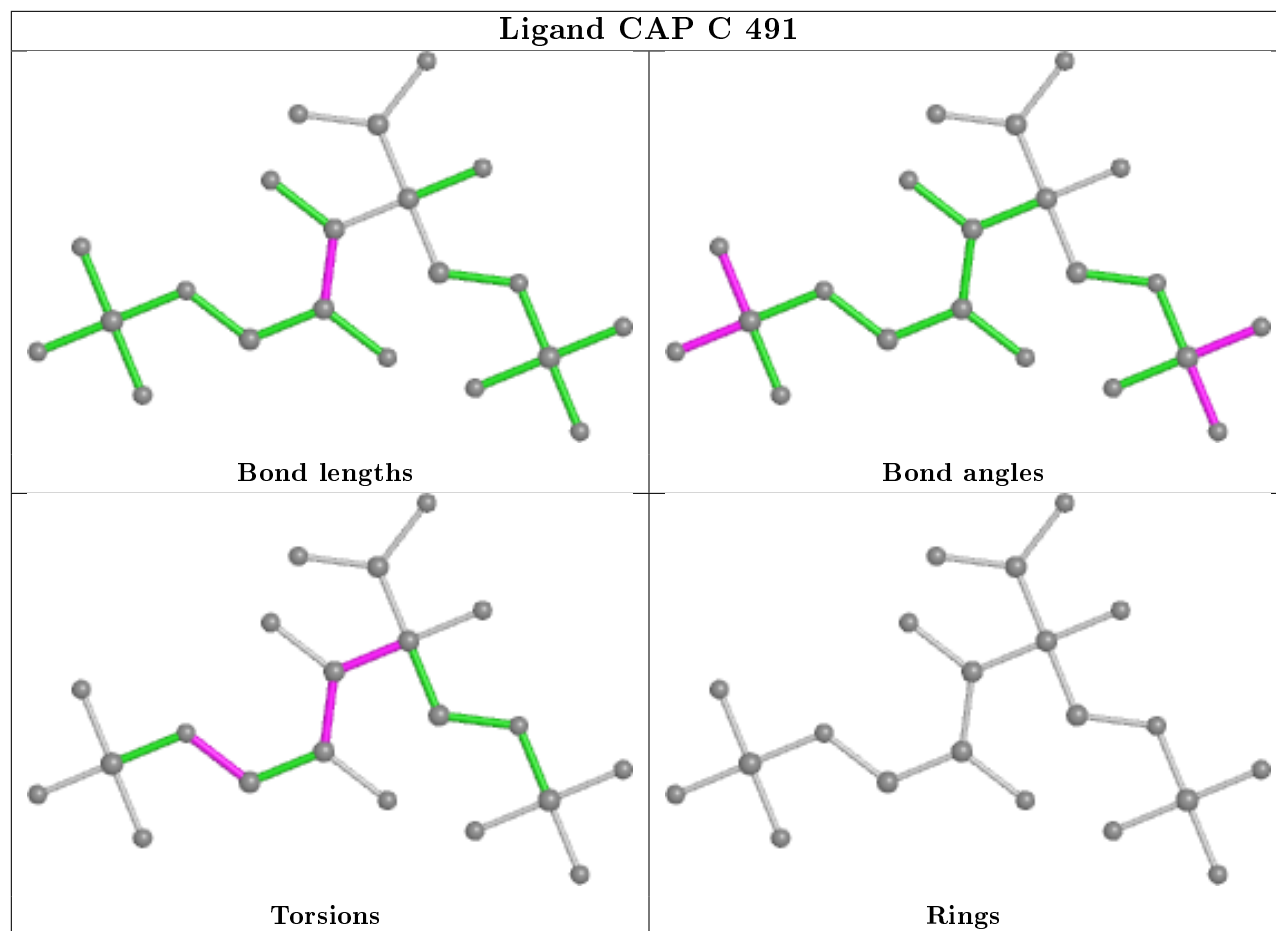
Mol	Chain	Res	Type	Atoms
4	C	491	CAP	O3-C3-C4-C5
4	G	491	CAP	O3-C3-C4-C5
4	C	491	CAP	C4-C5-O5-P2
4	A	491	CAP	C4-C5-O5-P2
4	G	491	CAP	C4-C5-O5-P2

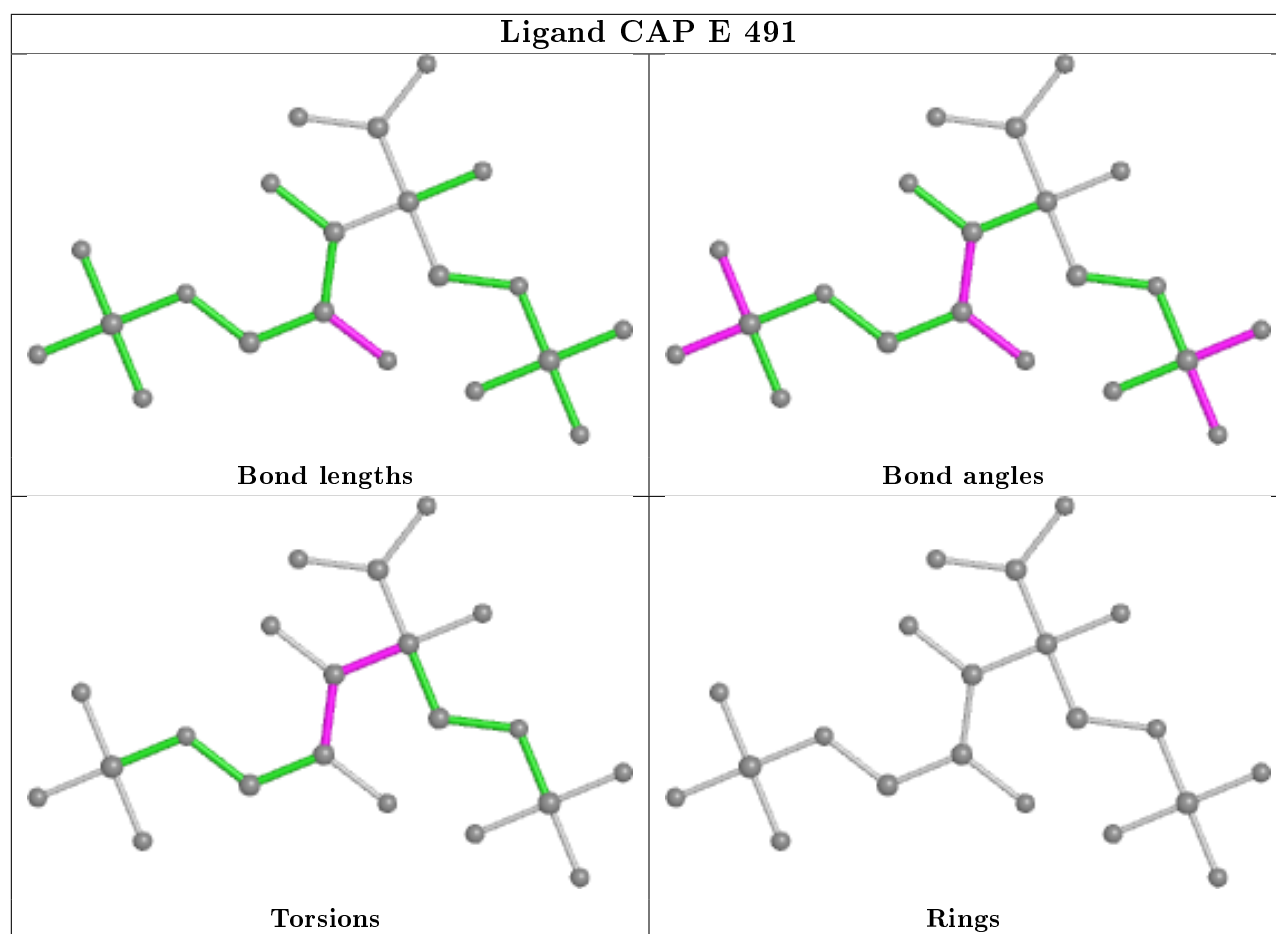
There are no ring outliers.

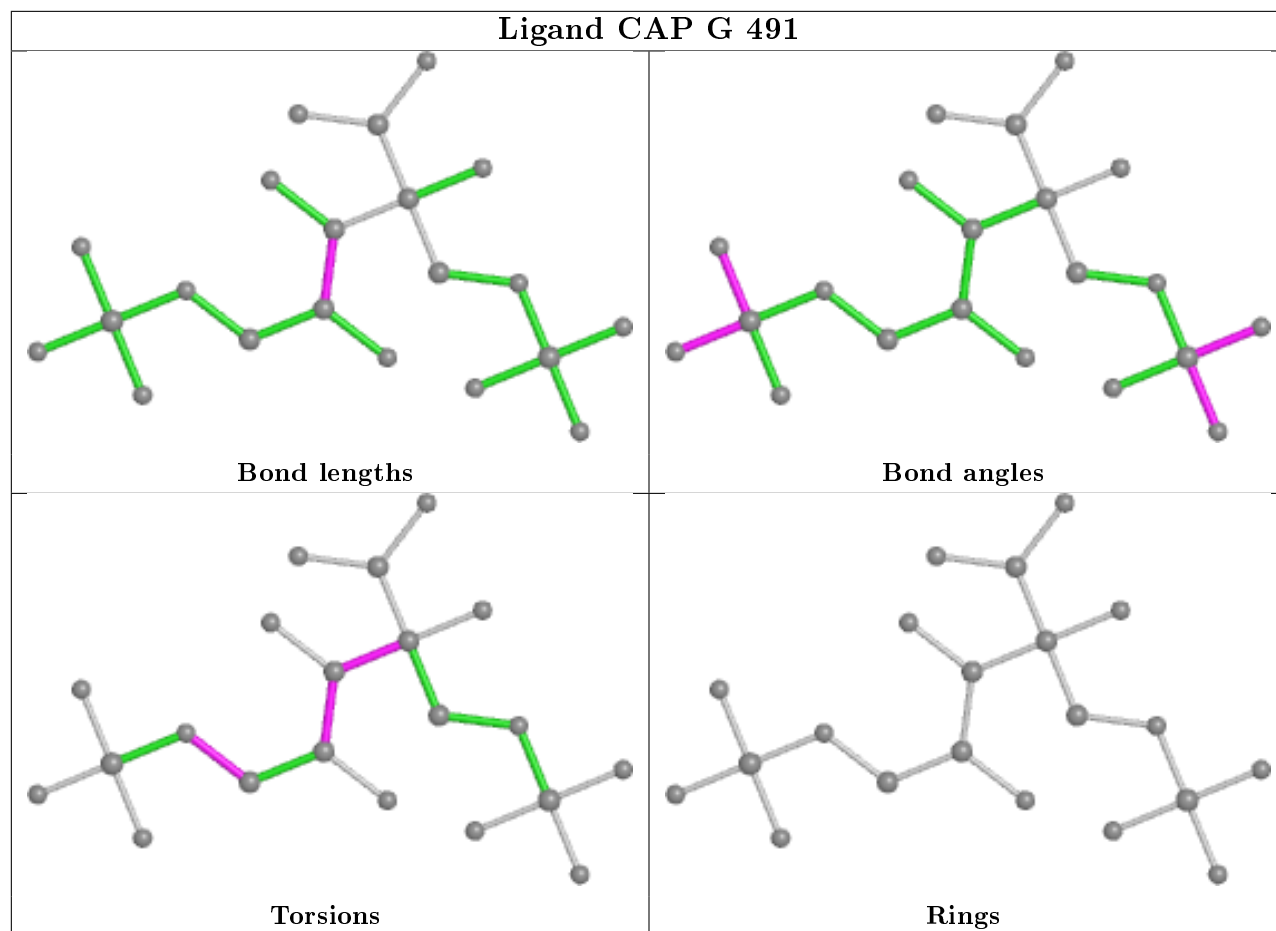
4 monomers are involved in 4 short contacts:

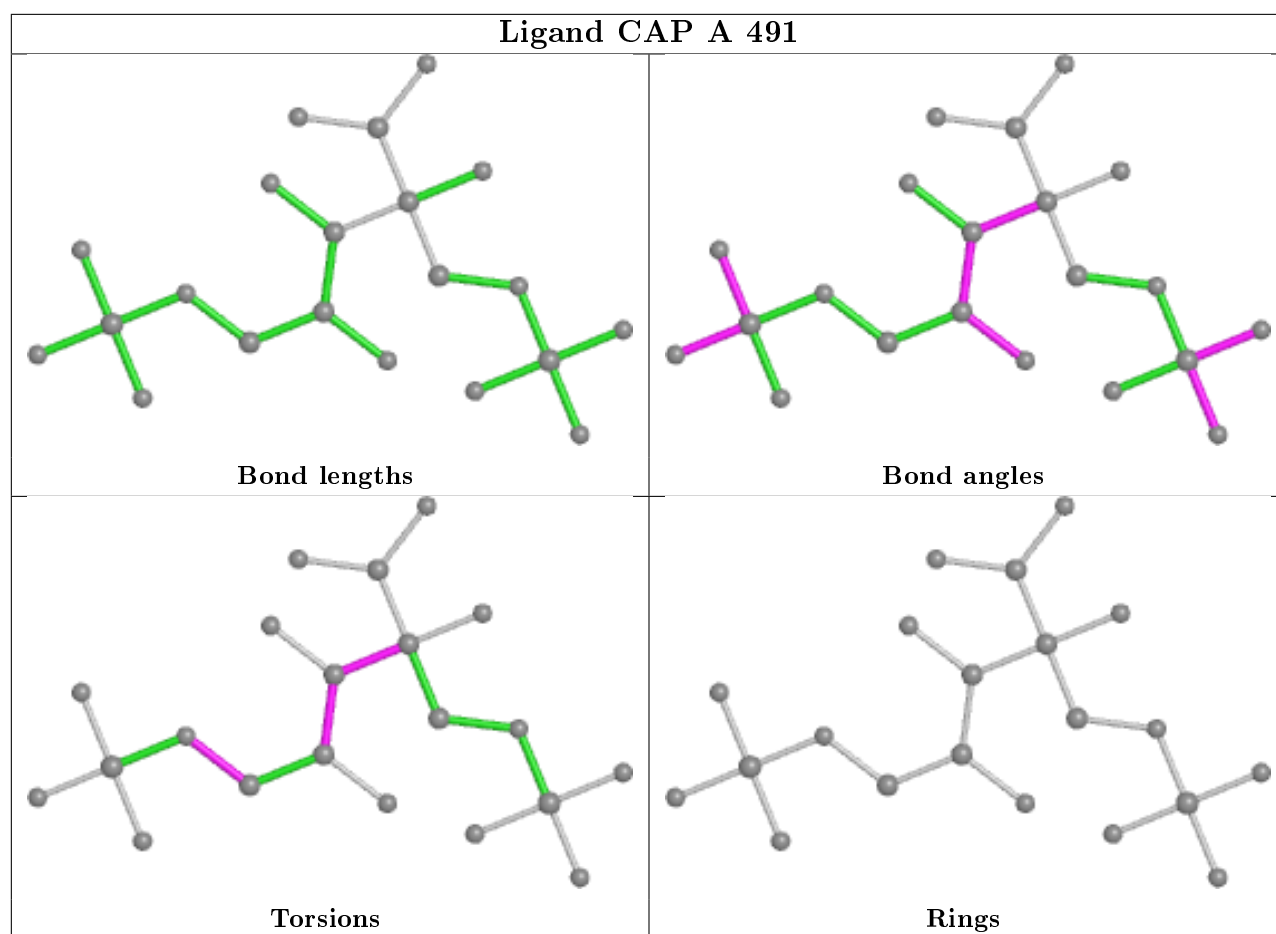
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	491	CAP	1	0
4	E	491	CAP	1	0
4	G	491	CAP	1	0
4	A	491	CAP	1	0

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









## 5.7 Other polymers [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	471/493 (95%)	-1.20	1 (0%) 95 94	8, 18, 39, 83	0
1	C	471/493 (95%)	-1.21	0 100 100	7, 18, 42, 84	0
1	E	471/493 (95%)	-1.21	1 (0%) 95 94	6, 18, 40, 84	0
1	G	471/493 (95%)	-1.20	0 100 100	7, 18, 42, 84	0
2	S	138/138 (100%)	-1.07	0 100 100	13, 24, 50, 64	0
2	U	138/138 (100%)	-1.08	0 100 100	10, 24, 48, 62	0
2	W	138/138 (100%)	-1.06	0 100 100	12, 24, 49, 64	0
2	Y	138/138 (100%)	-1.08	0 100 100	10, 24, 48, 62	0
All	All	2436/2524 (96%)	-1.18	2 (0%) 95 95	6, 19, 44, 84	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	10	ASN	4.3
1	A	10	ASN	3.9

### 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	KCX	C	201	12/13	0.98	0.07	3,12,14,15	0
1	KCX	A	201	12/13	0.98	0.08	3,12,22,23	0
1	KCX	G	201	12/13	0.98	0.07	5,9,15,15	0
1	KCX	E	201	12/13	0.98	0.07	2,12,23,25	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

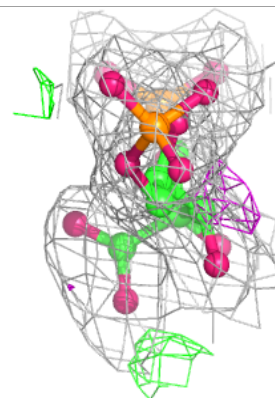
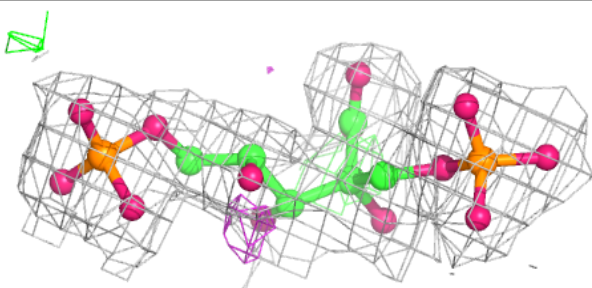
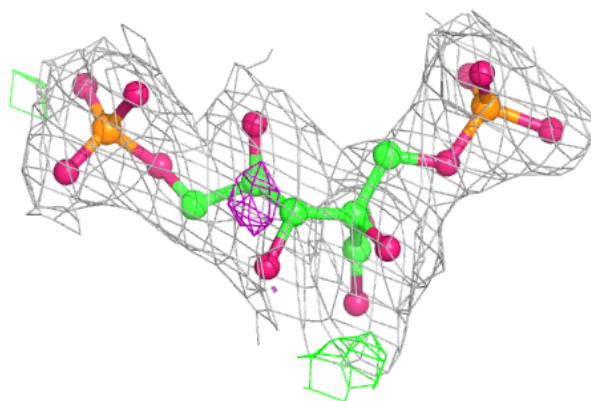
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	G	490	1/1	0.43	0.15	29,29,29,29	0
3	MG	C	490	1/1	0.47	0.15	29,29,29,29	0
3	MG	A	490	1/1	0.75	0.16	27,27,27,27	0
3	MG	E	490	1/1	0.87	0.20	25,25,25,25	0
4	CAP	A	491	21/21	0.98	0.08	2,22,27,29	0
4	CAP	C	491	21/21	0.98	0.09	12,21,27,27	0
4	CAP	E	491	21/21	0.98	0.09	3,20,26,31	0
4	CAP	G	491	21/21	0.98	0.09	11,20,27,27	0

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

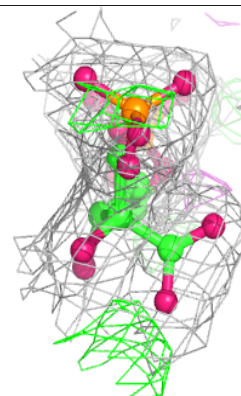
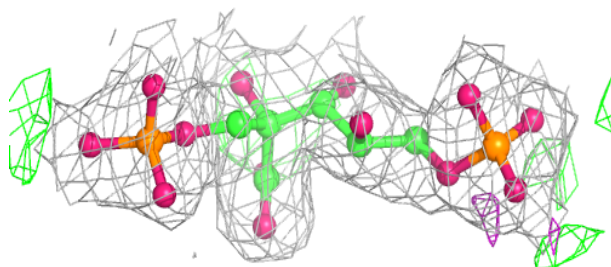
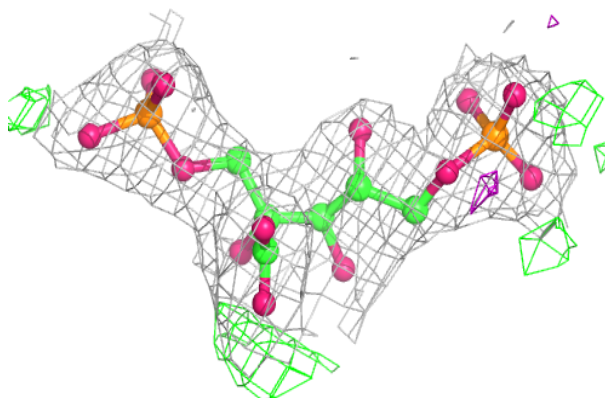


**Electron density around CAP A 491:**

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

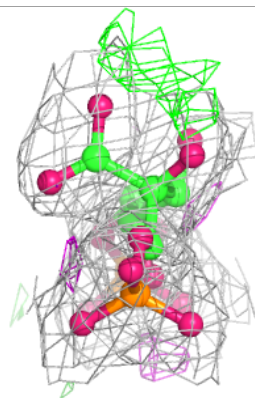
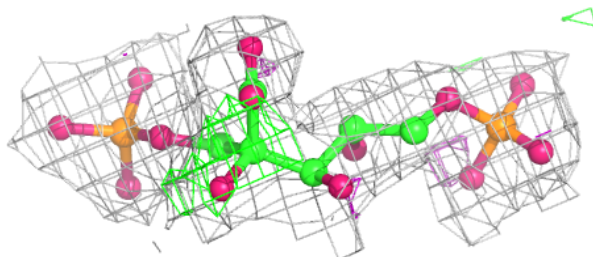
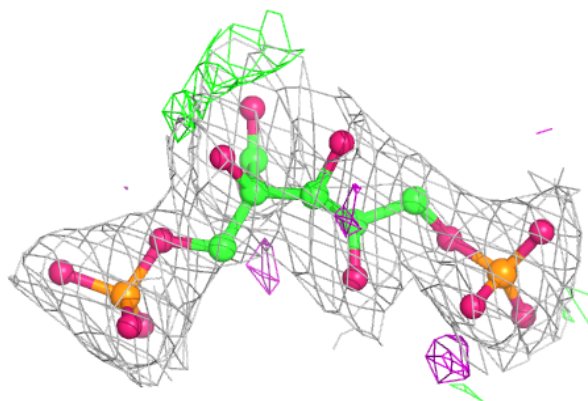
**Electron density around CAP C 491:**

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

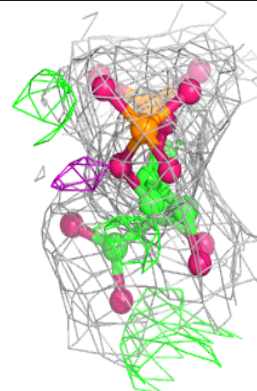
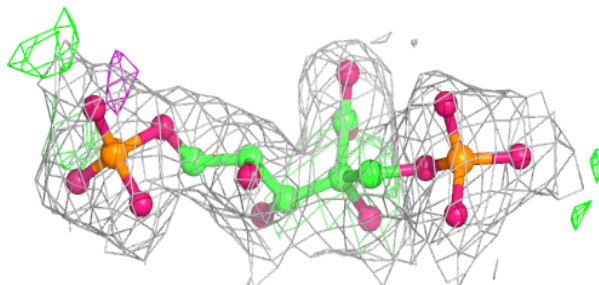
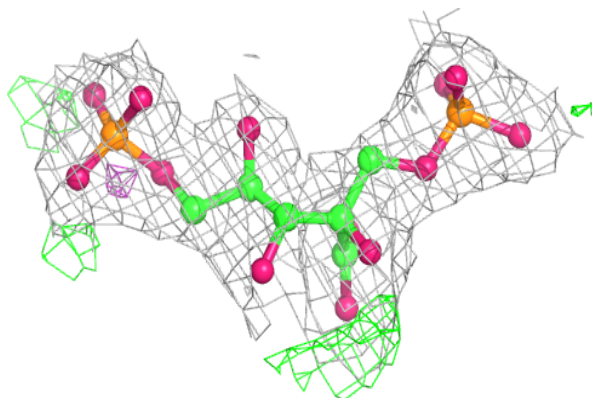


**Electron density around CAP E 491:**

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

**Electron density around CAP G 491:**

$2mF_o-DF_c$  (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.