



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:50 AM UTC

PDB ID : 1BWV / pdb_00001bwv
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

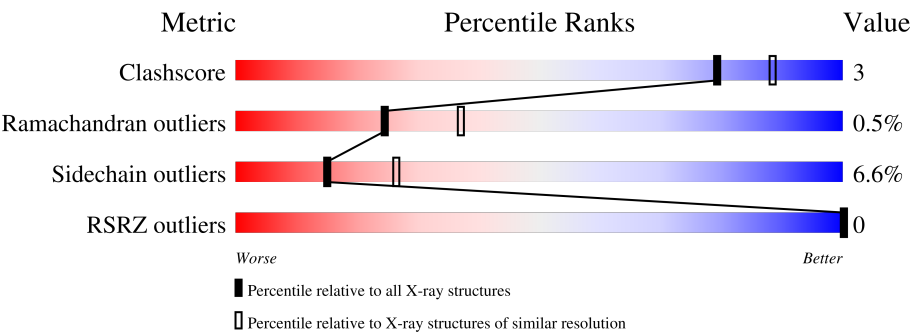
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	493	77% 16% . .
1	C	493	78% 16% . .
1	E	493	78% 16% . .
1	G	493	78% 16% . .
2	S	138	82% 16% ..
2	U	138	82% 15% .

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Mol	Chain	Length	Quality of chain
2	W	138	 83% 14% .
2	Y	138	 80% 17% ..

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			

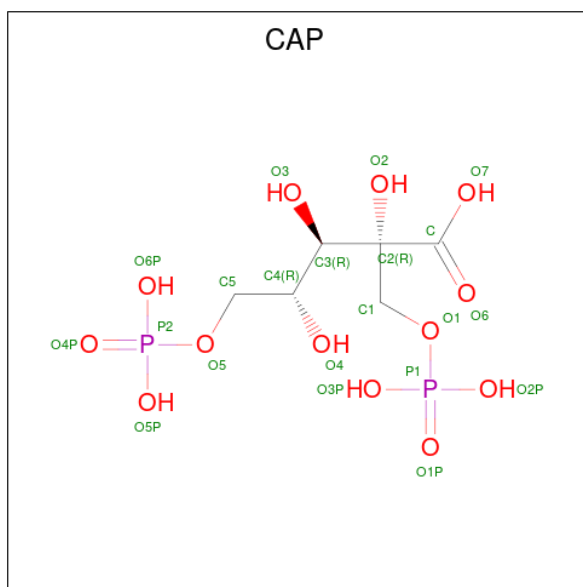
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

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

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



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

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

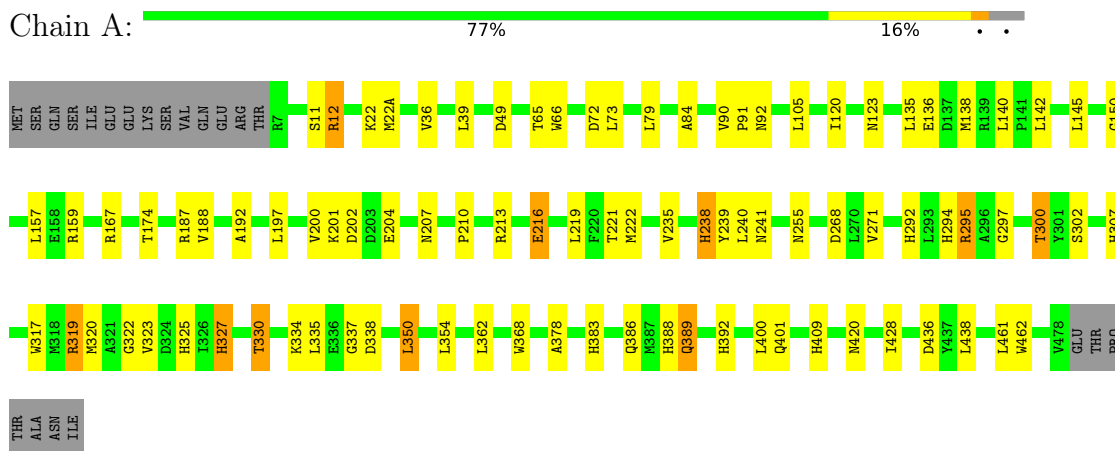
- Molecule 5 is water.

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		

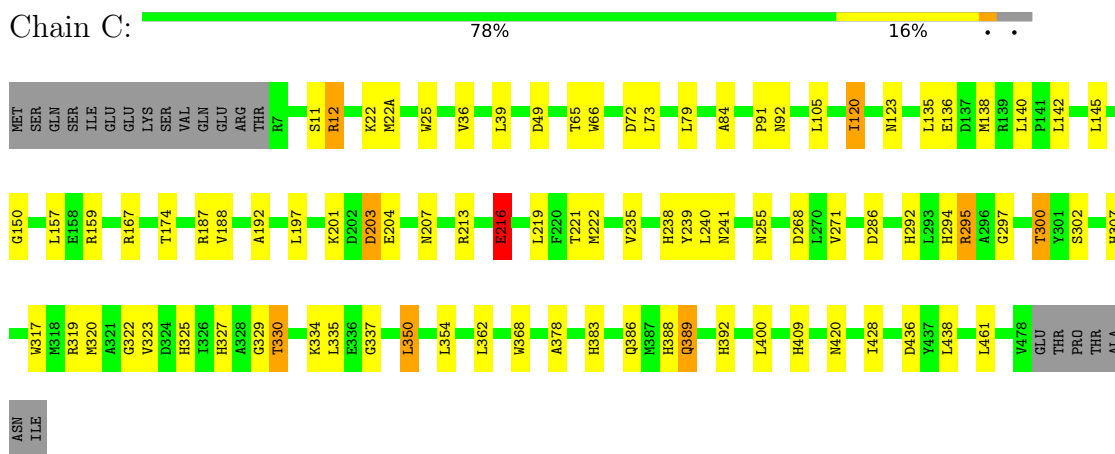
3 Residue-property plots [i](#)

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

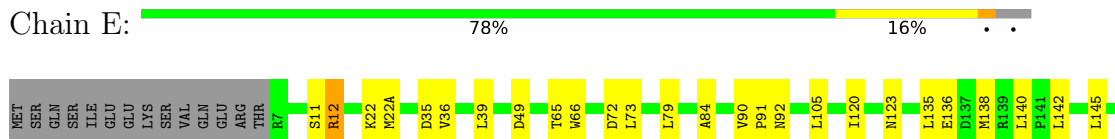
- Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE)

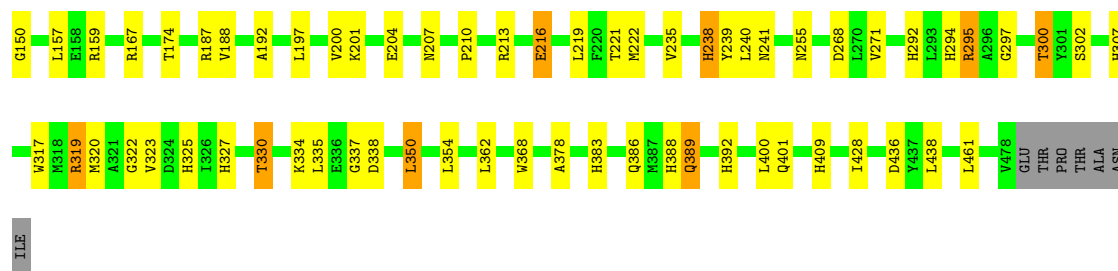


- Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE)

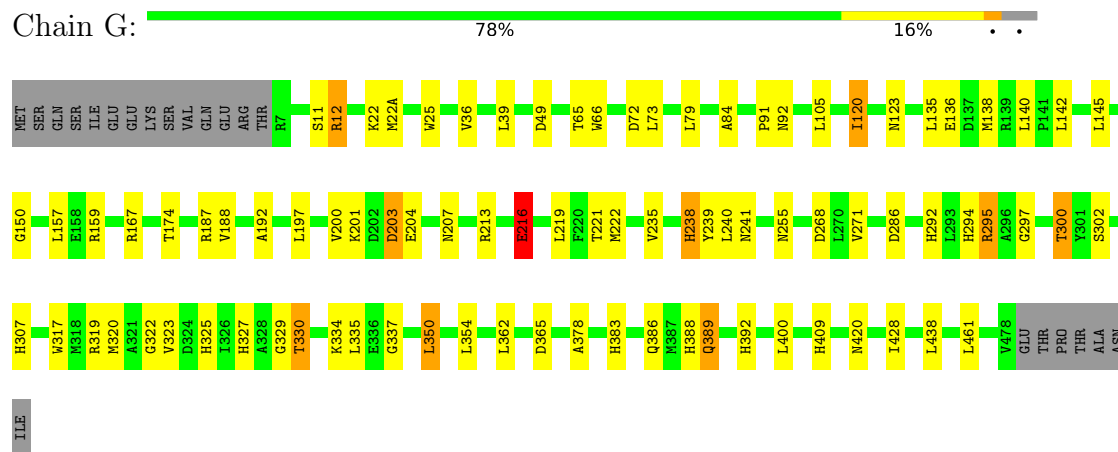


- Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE)

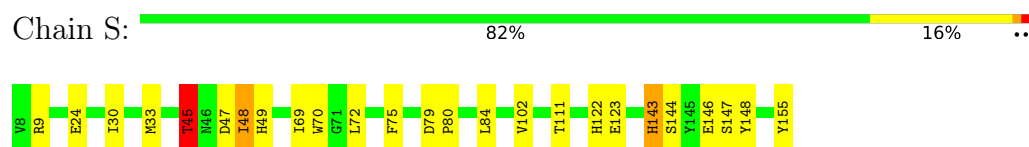




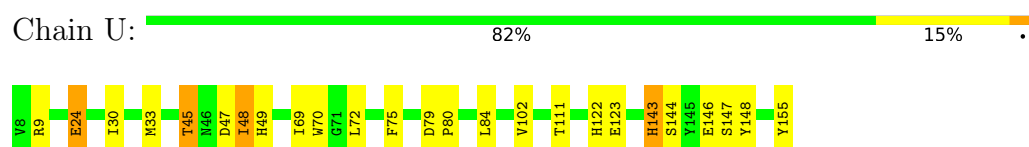
- Molecule 1: PROTEIN (RIBULOSE BIPHOSPHATE CARBOXYLASE)



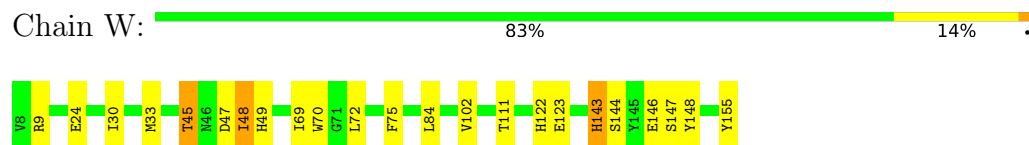
- Molecule 2: PROTEIN (RIBULOSE BIPHOSPHATE CARBOXYLASE)



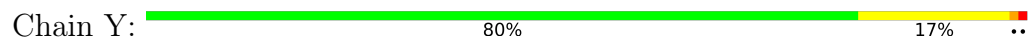
- Molecule 2: PROTEIN (RIBULOSE BIPHOSPHATE CARBOXYLASE)



- Molecule 2: PROTEIN (RIBULOSE BIPHOSPHATE CARBOXYLASE)



- Molecule 2: PROTEIN (RIBULOSE BIPHOSPHATE CARBOXYLASE)





4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	117.07Å 117.07Å 319.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.0 (20.00-2.40) 86.4 (20.00-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.163 , 0.197 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 3.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20038	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CAP, MG, 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	0.77	11/3777 (0.3%)	1.44	36/5116 (0.7%)
1	C	0.77	13/3777 (0.3%)	1.44	33/5116 (0.6%)
1	E	0.76	11/3777 (0.3%)	1.44	35/5116 (0.7%)
1	G	0.78	12/3777 (0.3%)	1.44	33/5116 (0.6%)
2	S	0.74	3/1172 (0.3%)	1.42	10/1583 (0.6%)
2	U	0.74	3/1172 (0.3%)	1.43	8/1583 (0.5%)
2	W	0.75	3/1172 (0.3%)	1.42	9/1583 (0.6%)
2	Y	0.74	3/1172 (0.3%)	1.42	10/1583 (0.6%)
All	All	0.76	59/19796 (0.3%)	1.44	174/26796 (0.6%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	204	GLU	CD-OE1	-10.90	1.04	1.25
1	A	204	GLU	CD-OE1	-8.49	1.09	1.25
1	C	204	GLU	CD-OE1	-7.67	1.10	1.25
1	E	204	GLU	CD-OE1	-7.42	1.11	1.25
1	A	292	HIS	CD2-NE2	-7.18	1.29	1.37
1	E	292	HIS	CD2-NE2	-7.14	1.29	1.37
1	C	388	HIS	CD2-NE2	-7.10	1.30	1.37
1	E	238	HIS	CD2-NE2	-7.08	1.30	1.37
1	G	292	HIS	CD2-NE2	-7.04	1.30	1.37
1	C	292	HIS	CD2-NE2	-7.01	1.30	1.37
1	C	238	HIS	CD2-NE2	-6.96	1.30	1.37
1	A	388	HIS	CD2-NE2	-6.96	1.30	1.37
1	G	238	HIS	CD2-NE2	-6.95	1.30	1.37
1	G	388	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	238	HIS	CD2-NE2	-6.89	1.30	1.37
1	E	325	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	325	HIS	CD2-NE2	-6.80	1.30	1.37
1	C	307	HIS	CD2-NE2	-6.77	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	388	HIS	CD2-NE2	-6.76	1.30	1.37
1	G	409	HIS	CD2-NE2	-6.67	1.30	1.37
1	C	409	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	307	HIS	CD2-NE2	-6.66	1.30	1.37
1	G	307	HIS	CD2-NE2	-6.64	1.30	1.37
1	E	409	HIS	CD2-NE2	-6.60	1.30	1.37
2	S	143	HIS	CD2-NE2	-6.59	1.30	1.37
1	G	325	HIS	CD2-NE2	-6.56	1.30	1.37
2	W	143	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	409	HIS	CD2-NE2	-6.48	1.30	1.37
2	Y	143	HIS	CD2-NE2	-6.48	1.30	1.37
2	U	143	HIS	CD2-NE2	-6.45	1.30	1.37
1	E	307	HIS	CD2-NE2	-6.45	1.30	1.37
2	W	49	HIS	CD2-NE2	-6.41	1.30	1.37
1	C	325	HIS	CD2-NE2	-6.40	1.30	1.37
2	Y	49	HIS	CD2-NE2	-6.37	1.30	1.37
2	U	49	HIS	CD2-NE2	-6.31	1.30	1.37
1	E	392	HIS	CD2-NE2	-6.31	1.30	1.37
2	S	49	HIS	CD2-NE2	-6.30	1.30	1.37
1	G	392	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	392	HIS	CD2-NE2	-6.30	1.30	1.37
2	U	122	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	392	HIS	CD2-NE2	-6.27	1.30	1.37
1	G	327	HIS	CD2-NE2	-6.23	1.30	1.37
1	C	327	HIS	CD2-NE2	-6.15	1.31	1.37
2	Y	122	HIS	CD2-NE2	-6.12	1.31	1.37
2	S	122	HIS	CD2-NE2	-6.10	1.31	1.37
2	W	122	HIS	CD2-NE2	-6.03	1.31	1.37
1	C	383	HIS	CD2-NE2	-5.89	1.31	1.37
1	E	383	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	383	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	327	HIS	CD2-NE2	-5.79	1.31	1.37
1	E	327	HIS	CD2-NE2	-5.78	1.31	1.37
1	G	383	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	294	HIS	CD2-NE2	-5.58	1.31	1.37
1	E	294	HIS	CD2-NE2	-5.53	1.31	1.37
1	G	294	HIS	CD2-NE2	-5.53	1.31	1.37
1	C	294	HIS	CD2-NE2	-5.43	1.31	1.37
1	C	203	ASP	CG-OD1	-5.07	1.15	1.25
1	G	327	HIS	CG-ND1	-5.03	1.32	1.38
1	C	327	HIS	CG-ND1	-5.02	1.32	1.38

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	HIS	CA-CB-CG	9.47	123.27	113.80
1	G	325	HIS	CA-CB-CG	9.40	123.20	113.80
1	E	325	HIS	CA-CB-CG	9.22	123.03	113.80
1	A	325	HIS	CA-CB-CG	9.21	123.01	113.80
1	A	292	HIS	CB-CG-CD2	-6.99	122.12	131.20
1	E	292	HIS	CB-CG-CD2	-6.96	122.15	131.20
2	U	9	ARG	N-CA-C	-6.96	97.07	108.41
2	Y	9	ARG	N-CA-C	-6.94	97.10	108.41
1	A	409	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	A	241	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	E	409	HIS	CB-CG-CD2	-6.74	122.44	131.20
1	G	409	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	E	241	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	G	292	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	C	409	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	C	292	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	12	ARG	CA-CB-CG	6.57	127.23	114.10
1	E	12	ARG	CA-CB-CG	6.56	127.22	114.10
1	C	241	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	G	12	ARG	CA-CB-CG	6.54	127.18	114.10
1	C	12	ARG	CA-CB-CG	6.54	127.17	114.10
1	G	241	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	G	207	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	72	ASP	CA-CB-CG	6.34	118.94	112.60
1	E	72	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	207	ASN	CA-CB-CG	6.33	118.93	112.60
1	C	72	ASP	CA-CB-CG	6.31	118.91	112.60
1	E	207	ASN	CA-CB-CG	6.28	118.88	112.60
2	W	123	GLU	CA-C-N	6.27	126.02	119.05
2	W	123	GLU	C-N-CA	6.27	126.02	119.05
1	A	207	ASN	CA-CB-CG	6.26	118.86	112.60
2	S	123	GLU	CA-C-N	6.26	125.99	119.05
2	S	123	GLU	C-N-CA	6.26	125.99	119.05
1	G	72	ASP	CA-CB-CG	6.23	118.83	112.60
2	U	123	GLU	CA-C-N	6.19	125.92	119.05
2	U	123	GLU	C-N-CA	6.19	125.92	119.05
2	Y	123	GLU	CA-C-N	6.17	125.90	119.05
2	Y	123	GLU	C-N-CA	6.17	125.90	119.05
1	A	268	ASP	CA-CB-CG	6.03	118.63	112.60
1	E	268	ASP	CA-CB-CG	6.01	118.61	112.60
2	S	9	ARG	N-CA-C	-6.01	98.61	108.41
2	W	9	ARG	N-CA-C	-6.01	98.61	108.41
1	G	268	ASP	CA-CB-CG	5.97	118.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	ASP	CA-CB-CG	5.93	118.53	112.60
1	G	330	THR	N-CA-C	-5.92	99.74	109.40
1	C	330	THR	N-CA-C	-5.92	99.76	109.40
1	A	292	HIS	CB-CG-ND1	5.77	131.35	122.70
1	E	235	VAL	N-CA-C	-5.74	101.31	108.89
2	W	49	HIS	CB-CG-CD2	-5.73	123.75	131.20
2	S	49	HIS	CB-CG-CD2	-5.72	123.77	131.20
1	E	292	HIS	CB-CG-ND1	5.71	131.26	122.70
1	A	235	VAL	N-CA-C	-5.70	101.37	108.89
2	U	49	HIS	CB-CG-CD2	-5.69	123.80	131.20
2	Y	49	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	G	388	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	84	ALA	N-CA-C	-5.65	100.78	109.76
1	C	235	VAL	N-CA-C	-5.65	101.44	108.89
1	C	84	ALA	N-CA-C	-5.64	100.79	109.76
1	E	92	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	E	84	ALA	N-CA-C	-5.63	100.81	109.76
1	G	235	VAL	N-CA-C	-5.63	101.46	108.89
1	E	330	THR	N-CA-C	-5.62	100.24	109.40
1	A	92	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	330	THR	N-CA-C	-5.61	100.26	109.40
1	G	292	HIS	CB-CG-ND1	5.61	131.11	122.70
1	G	84	ALA	N-CA-C	-5.60	100.86	109.76
1	C	216	GLU	CB-CA-C	-5.59	101.51	110.79
1	A	238	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	C	388	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	G	216	GLU	CB-CA-C	-5.57	101.55	110.79
1	A	388	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	E	388	HIS	CB-CG-CD2	-5.56	123.98	131.20
1	C	92	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	E	238	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	C	238	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	A	216	GLU	CB-CA-C	-5.52	101.63	110.79
1	C	292	HIS	CB-CG-ND1	5.51	130.97	122.70
1	E	216	GLU	CB-CA-C	-5.49	101.68	110.79
1	E	36	VAL	N-CA-C	-5.49	100.68	108.58
1	G	65	THR	CA-CB-OG1	-5.48	101.38	109.60
1	G	238	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	G	92	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	C	65	THR	CA-CB-OG1	-5.46	101.41	109.60
1	C	302	SER	N-CA-C	5.46	120.04	113.17
1	E	307	HIS	CB-CG-CD2	-5.45	124.12	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	E	49	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	307	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	A	36	VAL	N-CA-C	-5.42	100.77	108.58
1	G	307	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	C	307	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	A	49	ASP	CA-CB-CG	5.39	117.99	112.60
1	G	203	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	123	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	G	420	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	C	203	ASP	CA-CB-CG	5.36	117.96	112.60
1	G	302	SER	N-CA-C	5.36	119.92	113.17
2	S	148	TYR	N-CA-C	-5.34	106.81	113.38
2	U	148	TYR	N-CA-C	-5.32	106.84	113.38
1	C	350	LEU	N-CA-C	5.32	119.90	113.41
1	E	350	LEU	N-CA-C	5.32	119.90	113.41
1	A	338	ASP	CA-C-N	5.31	124.77	119.24
1	A	338	ASP	C-N-CA	5.31	124.77	119.24
1	C	49	ASP	CA-CB-CG	5.31	117.91	112.60
1	E	338	ASP	CA-C-N	5.31	124.76	119.24
1	E	338	ASP	C-N-CA	5.31	124.76	119.24
1	C	420	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	A	123	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	G	49	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	350	LEU	N-CA-C	5.29	119.86	113.41
1	G	350	LEU	N-CA-C	5.29	119.87	113.41
1	E	401	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	W	75	PHE	N-CA-C	5.28	119.64	111.56
2	W	148	TYR	N-CA-C	-5.26	106.91	113.38
1	G	120	ILE	N-CA-C	5.25	115.46	110.42
2	Y	148	TYR	N-CA-C	-5.24	106.93	113.38
2	S	75	PHE	N-CA-C	5.23	119.57	111.56
1	C	36	VAL	N-CA-C	-5.23	101.05	108.58
1	C	255	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	E	65	THR	CA-CB-OG1	-5.22	101.78	109.60
1	A	65	THR	CA-CB-OG1	-5.21	101.79	109.60
1	E	255	ASN	OD1-CG-ND2	-5.21	117.39	122.60
2	Y	75	PHE	N-CA-C	5.21	119.52	111.56
1	G	123	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	202	ASP	CA-C-N	-5.20	112.75	121.39
1	A	202	ASP	C-N-CA	-5.20	112.75	121.39
2	U	75	PHE	N-CA-C	5.19	119.51	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	302	SER	N-CA-C	5.19	119.71	113.17
2	U	70	TRP	CE2-CD2-CG	-5.19	100.97	107.20
2	W	143	HIS	CB-CG-CD2	-5.19	124.46	131.20
2	S	70	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	66	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	401	GLN	OE1-CD-NE2	-5.17	117.42	122.60
2	U	49	HIS	N-CA-C	-5.17	103.26	109.83
2	Y	49	HIS	N-CA-C	-5.17	103.26	109.83
1	G	123	ASN	CA-CB-CG	5.16	117.76	112.60
2	S	143	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	E	207	ASN	OD1-CG-ND2	-5.16	117.44	122.60
2	W	70	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	G	36	VAL	N-CA-C	-5.15	101.16	108.58
1	C	120	ILE	N-CA-C	5.15	115.36	110.42
2	Y	70	TRP	CE2-CD2-CG	-5.15	101.03	107.20
1	A	436	ASP	CA-CB-CG	5.14	117.74	112.60
1	E	436	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	302	SER	N-CA-C	5.13	119.64	113.17
1	A	319	ARG	N-CA-C	-5.12	105.78	111.36
2	W	49	HIS	N-CA-C	-5.10	103.35	109.83
1	C	123	ASN	CA-CB-CG	5.10	117.70	112.60
1	E	66	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	E	319	ARG	N-CA-C	-5.09	105.81	111.36
1	E	35	ASP	CA-CB-CG	5.08	117.68	112.60
1	G	25	TRP	CE2-CD2-CG	-5.08	101.11	107.20
2	S	49	HIS	N-CA-C	-5.07	103.39	109.83
1	A	420	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	G	66	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	E	368	TRP	CE2-CD2-CG	-5.04	101.14	107.20
1	C	392	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	G	286	ASP	CA-CB-CG	5.03	117.63	112.60
2	S	45	THR	CB-CA-C	-5.03	101.26	110.62
1	A	368	TRP	CE2-CD2-CG	-5.02	101.17	107.20
1	G	255	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	E	90	VAL	CA-C-N	5.02	126.11	119.84
1	E	90	VAL	C-N-CA	5.02	126.11	119.84
2	Y	143	HIS	CB-CG-CD2	-5.02	124.68	131.20
2	Y	45	THR	CB-CA-C	-5.01	101.29	110.62
1	G	365	ASP	N-CA-C	-5.01	102.28	110.20
1	G	392	HIS	CB-CG-CD2	-5.01	124.68	131.20
1	C	25	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	C	66	TRP	CE2-CD2-CG	-5.01	101.19	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	A	90	VAL	CA-C-N	5.00	126.10	119.84
1	A	90	VAL	C-N-CA	5.00	126.10	119.84
1	C	286	ASP	CA-CB-CG	5.00	117.60	112.60
1	C	436	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3709	0	3688	22	0
1	C	3709	0	3688	20	0
1	E	3709	0	3688	21	0
1	G	3709	0	3688	21	0
2	S	1143	0	1131	6	0
2	U	1143	0	1131	7	0
2	W	1143	0	1131	5	0
2	Y	1143	0	1131	7	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20038	0	19304	105	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 3.

All (105) 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:120:ILE:HG21	1:A:138:MET:HE2	1.83	0.61
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:C:120:ILE:HG21	1:C:138:MET:HE2	1.84	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:G:120:ILE:HG21	1:G:138:MET:HE2	1.84	0.59
1:E:120:ILE:HG21	1:E:138:MET:HE2	1.82	0.58
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
2:S:30:ILE:HA	2:S:33:MET:HE3	1.90	0.54
2:Y:30:ILE:HA	2:Y:33:MET:HE3	1.89	0.54
2:W:30:ILE:HA	2:W:33:MET:HE3	1.90	0.53
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
2:U:30:ILE:HA	2:U:33:MET:HE3	1.89	0.53
1:A:138:MET:HE1	1:A:317:TRP:HZ2	1.75	0.52
1:E:138:MET:HE1	1:E:317:TRP:HZ2	1.75	0.52
1:E:222:MET:HE3	1:E:240:LEU:HD11	1.92	0.51
1:G:222:MET:HE3	1:G:240:LEU:HD11	1.93	0.51
1:A:222:MET:HE3	1:A:240:LEU:HD11	1.92	0.51
1:C:330:THR:HG22	1:C:378:ALA:HB1	1.93	0.50
1:C:138:MET:HE1	1:C:317:TRP:HZ2	1.76	0.50
1:G:330:THR:HG22	1:G:378:ALA:HB1	1.93	0.50
1:C:222:MET:HE3	1:C:240:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:138:MET:HE1	1:G:317:TRP:HZ2	1.76	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:A:221:THR:HG22	1:A:222:MET:HE2	1.96	0.48
1:G:221:THR:HG22	1:G:222:MET:HE2	1.95	0.48
1:C:221:THR:HG22	1:C:222:MET:HE2	1.95	0.48
1:E:135:LEU:HD21	1:E:138:MET:CE	2.44	0.48
2:W:45:THR:HB	2:W:47:ASP:H	1.79	0.47
1:G:135:LEU:HD21	1:G:138:MET:CE	2.44	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:A:135:LEU:HD21	1:A:138:MET:CE	2.44	0.47
1:E:174:THR:HG23	1:E:188:VAL:HG11	1.97	0.47
2:Y:45:THR:HB	2:Y:47:ASP:H	1.79	0.47
1:E:221:THR:HG22	1:E:222:MET:HE2	1.96	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
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
2:U:143:HIS:HE1	2:U:147:SER:O	1.99	0.45
1:G:334:LYS:HG3	1:G:335:LEU:HD22	1.98	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:213:ARG:HB2	1:E:216:GLU:OE2	2.18	0.44
1:E:216:GLU:HG2	1:G:157:LEU:CD1	2.47	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
2:S:102:VAL:HG13	2:S:111:THR:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:150:GLY:C	1:G:322:GLY:HA2	2.44	0.43
1:C:150:GLY:C	1:C:322:GLY:HA2	2.44	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:150:GLY:C	1:E:322:GLY:HA2	2.45	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:150:GLY:C	1:A:322:GLY:HA2	2.45	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: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
2:Y:129:MET:HB2	2:Y:141:THR:HB	2.03	0.40
1:E:135:LEU:HD21	1:E:138:MET:HE3	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	30	43
1	C	469/493 (95%)	451 (96%)	16 (3%)	2 (0%)	30	43
1	E	469/493 (95%)	452 (96%)	15 (3%)	2 (0%)	30	43
1	G	469/493 (95%)	451 (96%)	16 (3%)	2 (0%)	30	43
2	S	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	18	28
2	U	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	18	28
2	W	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	18	28
2	Y	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	18	28
All	All	2420/2524 (96%)	2317 (96%)	91 (4%)	12 (0%)	24	37

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
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%)	356 (93%)	26 (7%)	14	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	382/402 (95%)	355 (93%)	27 (7%)	13	23
1	E	382/402 (95%)	356 (93%)	26 (7%)	14	25
1	G	382/402 (95%)	355 (93%)	27 (7%)	13	23
2	S	126/126 (100%)	119 (94%)	7 (6%)	19	33
2	U	126/126 (100%)	119 (94%)	7 (6%)	19	33
2	W	126/126 (100%)	119 (94%)	7 (6%)	19	33
2	Y	126/126 (100%)	119 (94%)	7 (6%)	19	33
All	All	2032/2112 (96%)	1898 (93%)	134 (7%)	15	26

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	22	LYS
1	A	22(A)	MET
1	A	73	LEU
1	A	79	LEU
1	A	91	PRO
1	A	105	LEU
1	A	142	LEU
1	A	145	LEU
1	A	187	ARG
1	A	210	PRO
1	A	219	LEU
1	A	239	TYR
1	A	271	VAL
1	A	295	ARG
1	A	300	THR
1	A	319	ARG
1	A	323	VAL
1	A	350	LEU
1	A	354	LEU
1	A	362	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

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Mol	Chain	Res	Type
2	S	48	ILE
2	S	69	ILE
2	S	72	LEU
2	S	84	LEU
2	S	144	SER
1	C	12	ARG
1	C	22	LYS
1	C	22(A)	MET
1	C	73	LEU
1	C	79	LEU
1	C	91	PRO
1	C	105	LEU
1	C	142	LEU
1	C	145	LEU
1	C	187	ARG
1	C	203	ASP
1	C	216	GLU
1	C	219	LEU
1	C	239	TYR
1	C	271	VAL
1	C	295	ARG
1	C	300	THR
1	C	319	ARG
1	C	323	VAL
1	C	350	LEU
1	C	354	LEU
1	C	362	LEU
1	C	389	GLN
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	72	LEU
2	U	84	LEU
2	U	144	SER
1	E	12	ARG
1	E	22	LYS
1	E	22(A)	MET

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Mol	Chain	Res	Type
1	E	73	LEU
1	E	79	LEU
1	E	91	PRO
1	E	105	LEU
1	E	142	LEU
1	E	145	LEU
1	E	187	ARG
1	E	210	PRO
1	E	219	LEU
1	E	239	TYR
1	E	271	VAL
1	E	295	ARG
1	E	300	THR
1	E	319	ARG
1	E	323	VAL
1	E	350	LEU
1	E	354	LEU
1	E	362	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	72	LEU
2	W	84	LEU
2	W	144	SER
1	G	12	ARG
1	G	22	LYS
1	G	22(A)	MET
1	G	73	LEU
1	G	79	LEU
1	G	91	PRO
1	G	105	LEU
1	G	142	LEU
1	G	145	LEU
1	G	187	ARG
1	G	203	ASP
1	G	216	GLU

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Mol	Chain	Res	Type
1	G	219	LEU
1	G	239	TYR
1	G	271	VAL
1	G	295	ARG
1	G	300	THR
1	G	319	ARG
1	G	323	VAL
1	G	350	LEU
1	G	354	LEU
1	G	362	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	72	LEU
2	Y	84	LEU
2	Y	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	92	ASN
1	A	123	ASN
1	A	241	ASN
1	A	298	ASN
1	A	468	ASN
2	S	118	ASN
2	S	143	HIS
1	C	92	ASN
1	C	123	ASN
1	C	241	ASN
1	C	434	ASN
2	U	118	ASN
2	U	143	HIS
1	E	10	ASN
1	E	92	ASN

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Mol	Chain	Res	Type
1	E	123	ASN
1	E	241	ASN
1	E	298	ASN
2	W	118	ASN
2	W	143	HIS
1	G	92	ASN
1	G	123	ASN
1	G	241	ASN
1	G	298	ASN
2	Y	88	ASN
2	Y	118	ASN
2	Y	143	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	A	201	1,3	10,11,12	0.84	0	6,12,14	1.92	3 (50%)
1	KCX	C	201	1,3	10,11,12	1.03	1 (10%)	6,12,14	1.97	2 (33%)
1	KCX	E	201	1,3	10,11,12	0.88	0	6,12,14	1.38	1 (16%)
1	KCX	G	201	1,3	10,11,12	0.92	0	6,12,14	1.66	2 (33%)

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	A	201	1,3	-	0/9/10/12	-
1	KCX	C	201	1,3	-	0/9/10/12	-
1	KCX	E	201	1,3	-	0/9/10/12	-
1	KCX	G	201	1,3	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	KCX	CX-NZ	-2.20	1.31	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	KCX	OQ1-CX-NZ	-3.92	118.97	124.92
1	G	201	KCX	OQ1-CX-NZ	-3.16	120.13	124.92
1	A	201	KCX	OQ1-CX-NZ	-3.13	120.16	124.92
1	C	201	KCX	CE-NZ-CX	2.50	126.22	121.98
1	G	201	KCX	CE-NZ-CX	2.20	125.71	121.98
1	A	201	KCX	CG-CD-CE	2.12	123.35	113.56
1	A	201	KCX	CD-CE-NZ	-2.07	106.40	112.20
1	E	201	KCX	OQ1-CX-NZ	-2.05	121.81	124.92

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CAP	G	491	3	18,20,20	1.46	1 (5%)	23,31,31	1.18	3 (13%)
4	CAP	A	491	3	18,20,20	1.05	0	23,31,31	1.43	4 (17%)
4	CAP	E	491	3	18,20,20	1.13	2 (11%)	23,31,31	1.40	3 (13%)
4	CAP	C	491	3	18,20,20	1.71	2 (11%)	23,31,31	1.12	2 (8%)

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	G	491	3	-	9/29/29/29	-
4	CAP	A	491	3	-	8/29/29/29	-
4	CAP	E	491	3	-	7/29/29/29	-
4	CAP	C	491	3	-	10/29/29/29	-

All (5) 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	C	491	CAP	C2-C	-2.77	1.50	1.53
4	E	491	CAP	O4-C4	-2.16	1.38	1.43
4	E	491	CAP	O7-C	-2.07	1.23	1.30

All (12) 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	-2.62	108.80	114.03
4	C	491	CAP	O5P-P2-O4P	2.38	120.10	110.83
4	G	491	CAP	O2-C2-C	-2.34	104.67	109.07
4	E	491	CAP	O5P-P2-O4P	2.33	119.93	110.83
4	G	491	CAP	O5P-P2-O4P	2.32	119.86	110.83
4	A	491	CAP	O5P-P2-O4P	2.30	119.79	110.83
4	E	491	CAP	O2P-P1-O1P	2.15	119.20	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	491	CAP	O2P-P1-O1P	2.12	119.08	110.83
4	G	491	CAP	O2P-P1-O1P	2.04	118.79	110.83
4	C	491	CAP	O2P-P1-O1P	2.04	118.77	110.83

There are no chirality outliers.

All (34) torsion outliers are listed below:

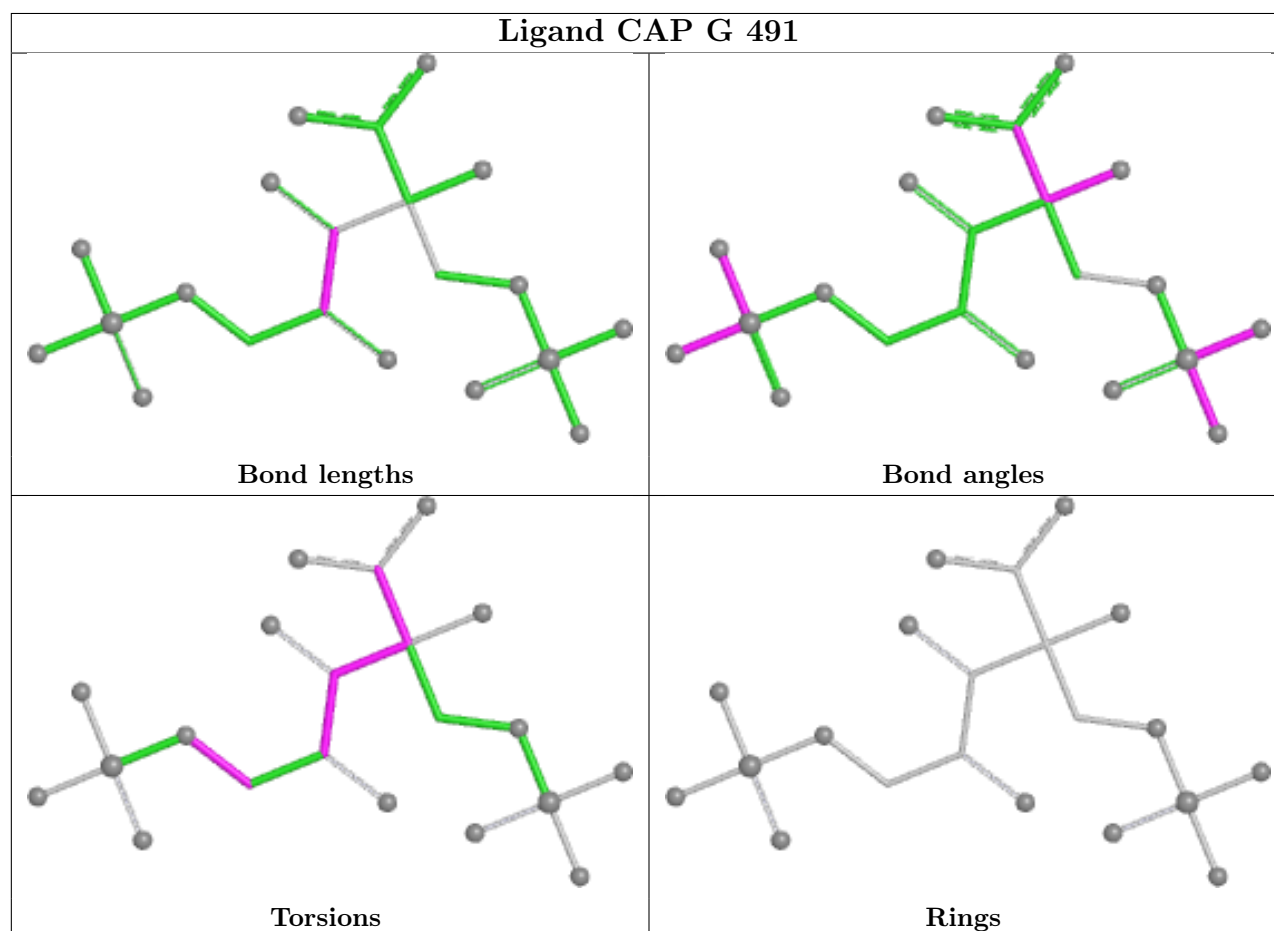
Mol	Chain	Res	Type	Atoms
4	A	491	CAP	O6-C-C2-C1
4	A	491	CAP	O6-C-C2-O2
4	A	491	CAP	O7-C-C2-O2
4	A	491	CAP	C2-C3-C4-O4
4	A	491	CAP	O3-C3-C4-O4
4	C	491	CAP	O6-C-C2-O2
4	C	491	CAP	O7-C-C2-O2
4	C	491	CAP	C2-C3-C4-O4
4	C	491	CAP	O3-C3-C4-O4
4	E	491	CAP	O6-C-C2-C1
4	E	491	CAP	O6-C-C2-O2
4	E	491	CAP	O7-C-C2-O2
4	E	491	CAP	C2-C3-C4-O4
4	E	491	CAP	O3-C3-C4-O4
4	G	491	CAP	O6-C-C2-O2
4	G	491	CAP	O7-C-C2-O2
4	G	491	CAP	C2-C3-C4-O4
4	G	491	CAP	O3-C3-C4-O4
4	A	491	CAP	O7-C-C2-C1
4	C	491	CAP	O6-C-C2-C1
4	G	491	CAP	O6-C-C2-C1
4	C	491	CAP	O7-C-C2-C1
4	E	491	CAP	O7-C-C2-C1
4	G	491	CAP	O7-C-C2-C1
4	C	491	CAP	O3-C3-C4-C5
4	A	491	CAP	O2-C2-C3-C4
4	C	491	CAP	C1-C2-C3-O3
4	C	491	CAP	O2-C2-C3-C4
4	E	491	CAP	O2-C2-C3-C4
4	G	491	CAP	O2-C2-C3-C4
4	G	491	CAP	O3-C3-C4-C5
4	A	491	CAP	C4-C5-O5-P2
4	C	491	CAP	C4-C5-O5-P2
4	G	491	CAP	C4-C5-O5-P2

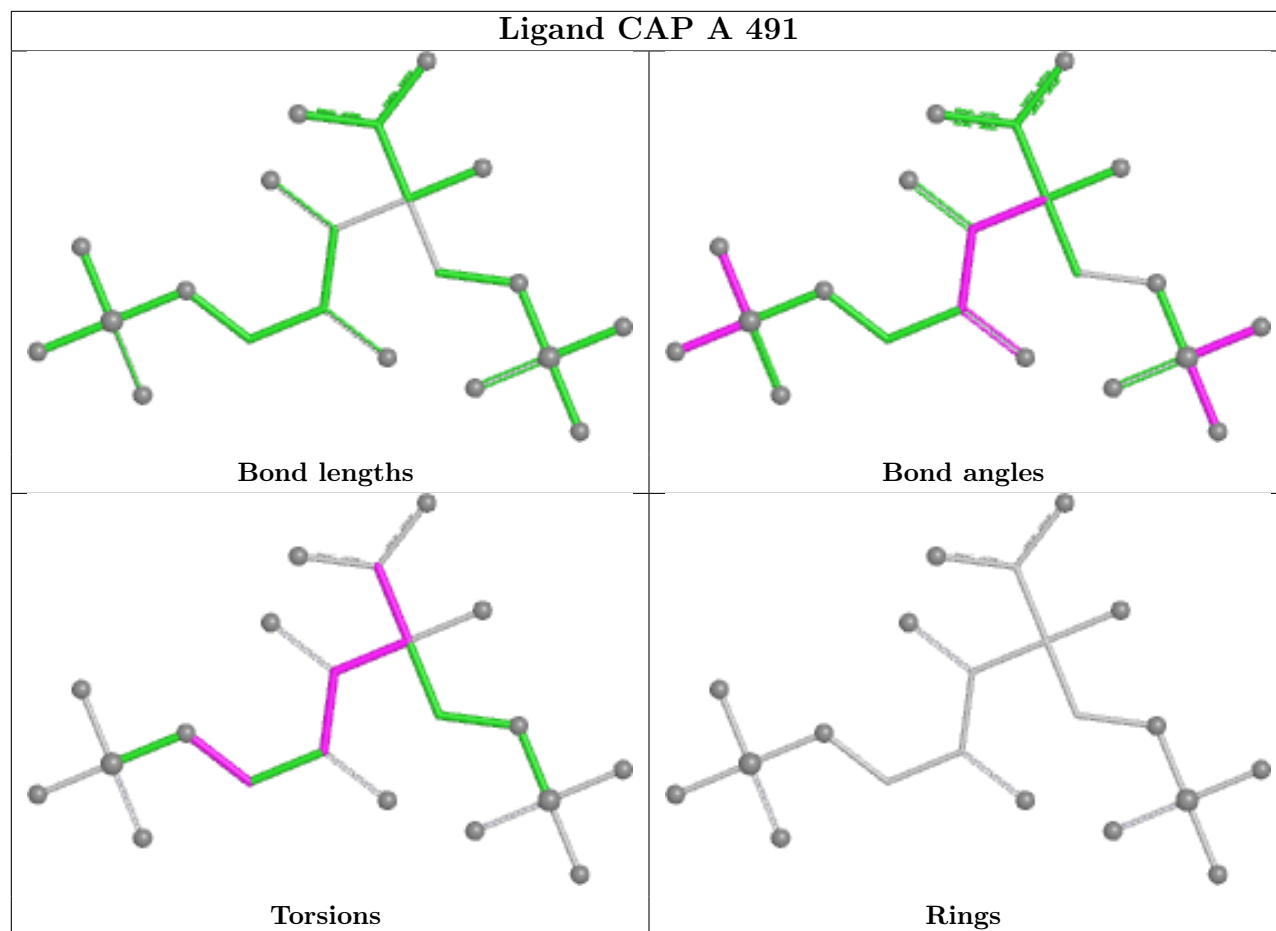
There are no ring outliers.

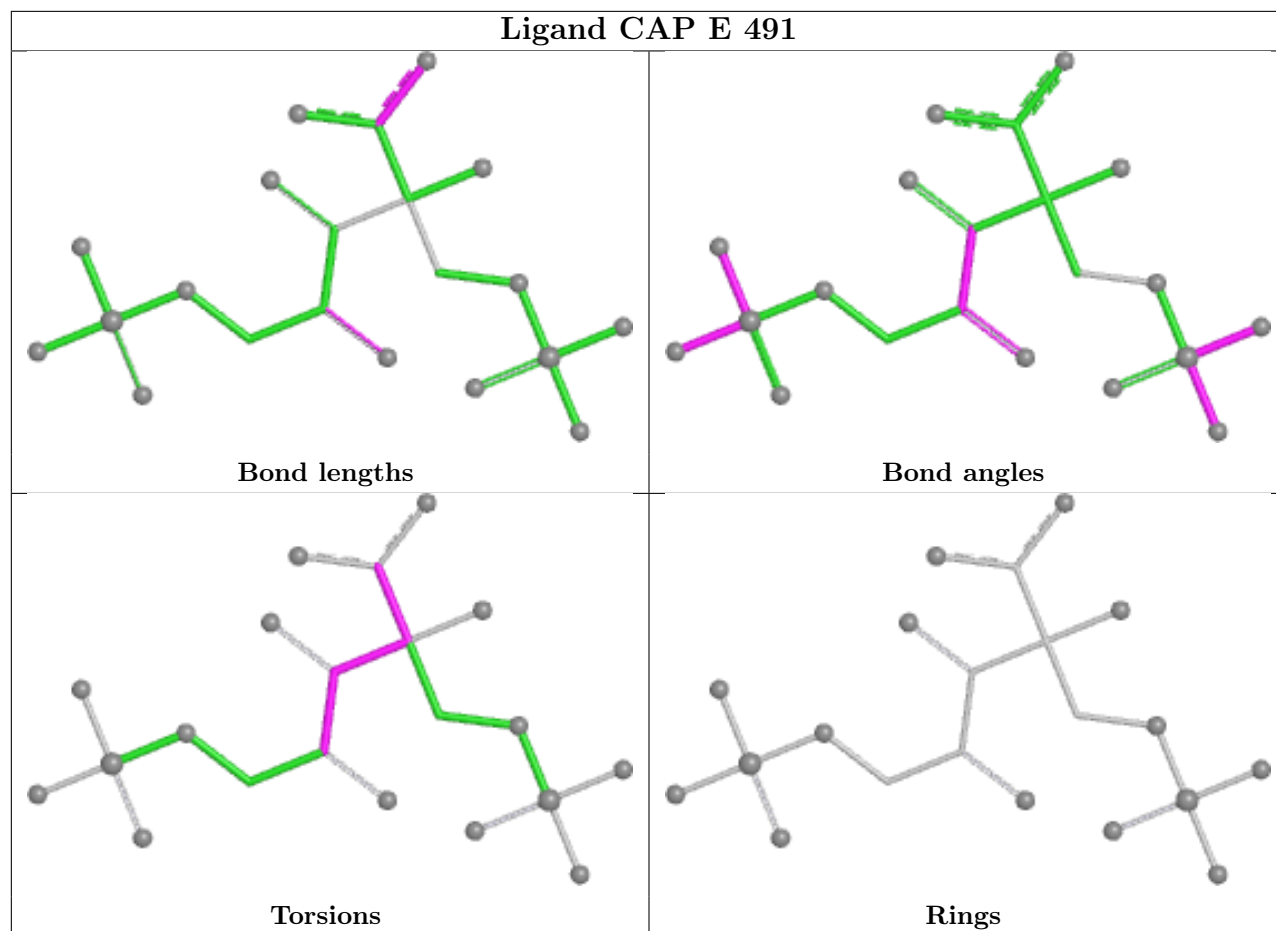
4 monomers are involved in 4 short contacts:

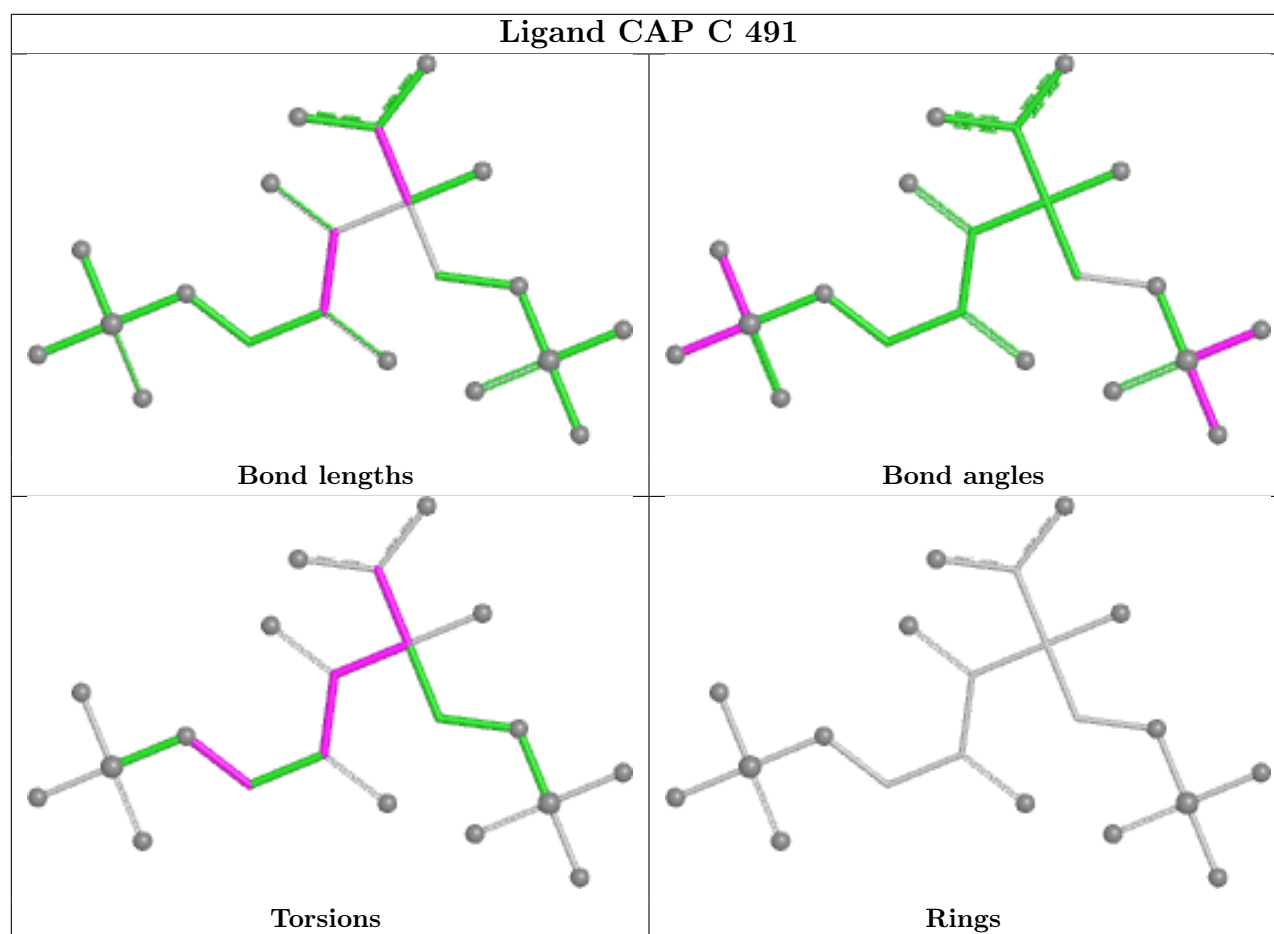
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	491	CAP	1	0
4	A	491	CAP	1	0
4	E	491	CAP	1	0
4	C	491	CAP	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	471/493 (95%)	-1.85	0 100 100	8, 18, 39, 83	0
1	C	471/493 (95%)	-1.85	0 100 100	7, 18, 42, 84	0
1	E	471/493 (95%)	-1.86	0 100 100	6, 18, 40, 84	0
1	G	471/493 (95%)	-1.84	0 100 100	7, 18, 42, 84	0
2	S	138/138 (100%)	-1.83	0 100 100	13, 24, 50, 64	0
2	U	138/138 (100%)	-1.82	0 100 100	10, 24, 48, 62	0
2	W	138/138 (100%)	-1.84	0 100 100	12, 24, 49, 64	0
2	Y	138/138 (100%)	-1.82	0 100 100	10, 24, 48, 62	0
All	All	2436/2524 (96%)	-1.85	0 100 100	6, 19, 44, 84	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	A	201	12/13	1.00	0.02	3,12,22,23	0
1	KCX	C	201	12/13	1.00	0.01	3,12,14,15	0
1	KCX	E	201	12/13	1.00	0.02	2,12,23,25	0
1	KCX	G	201	12/13	1.00	0.01	5,9,15,15	0

6.3 Carbohydrates [i](#)

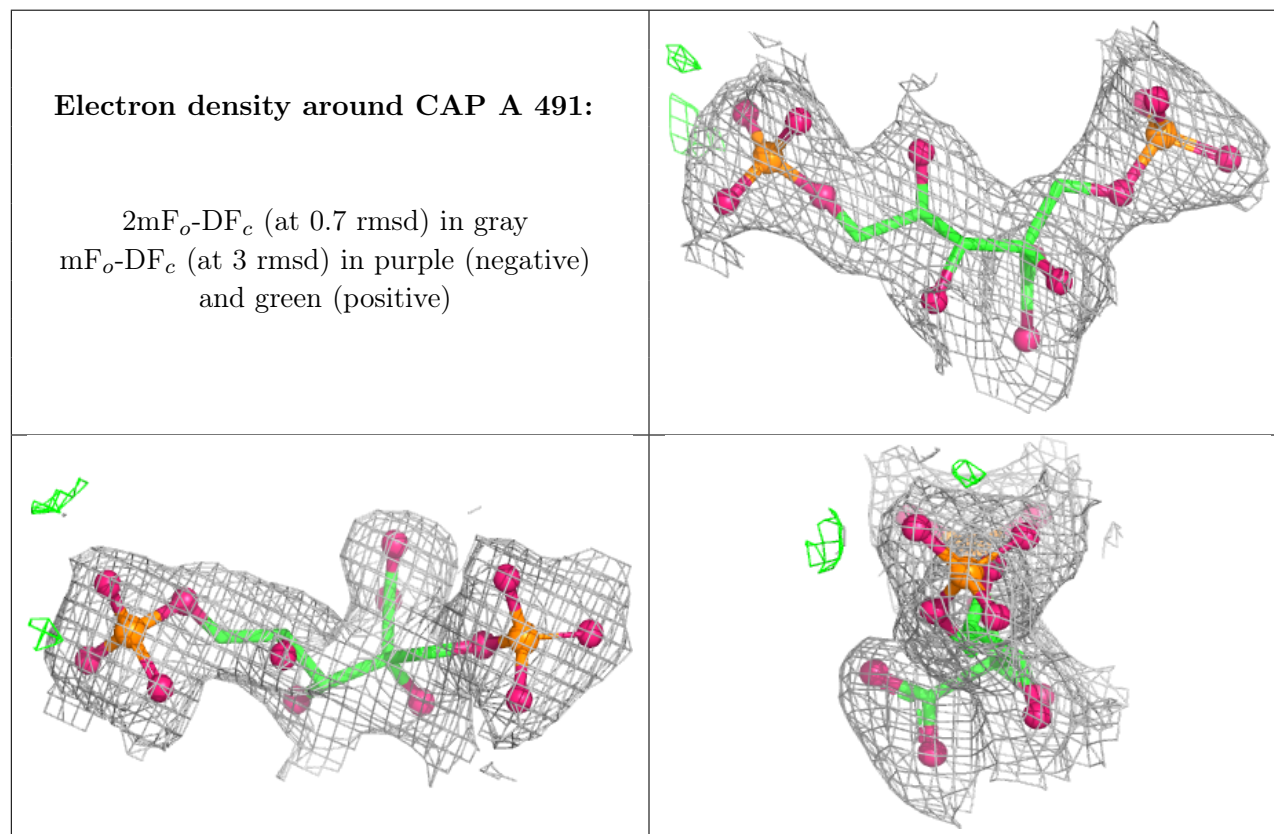
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

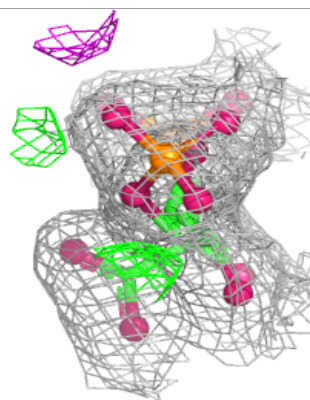
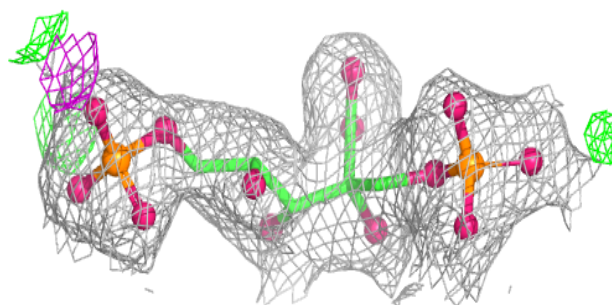
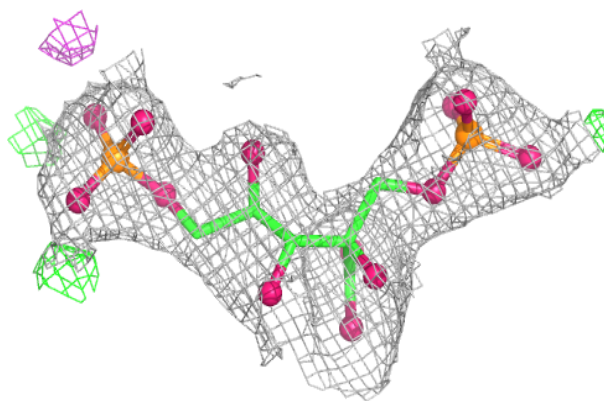
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	490	1/1	1.00	0.02	27,27,27,27	0
3	MG	C	490	1/1	1.00	0.03	29,29,29,29	0
3	MG	E	490	1/1	1.00	0.03	25,25,25,25	0
3	MG	G	490	1/1	1.00	0.03	29,29,29,29	0
4	CAP	A	491	21/21	1.00	0.01	2,22,27,29	0
4	CAP	C	491	21/21	1.00	0.02	12,21,27,27	0
4	CAP	E	491	21/21	1.00	0.01	3,20,26,31	0
4	CAP	G	491	21/21	1.00	0.02	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.

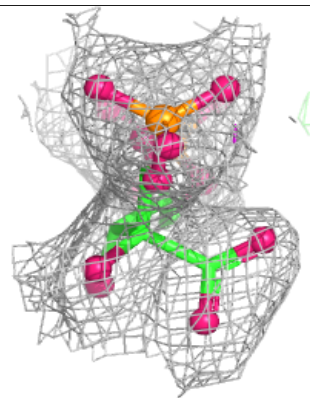
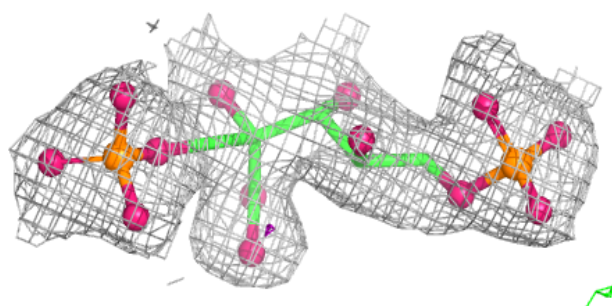
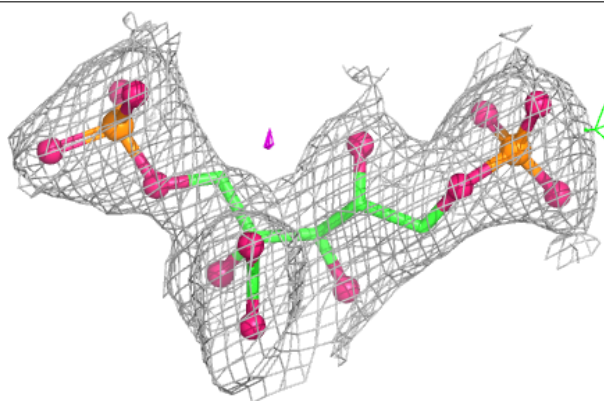


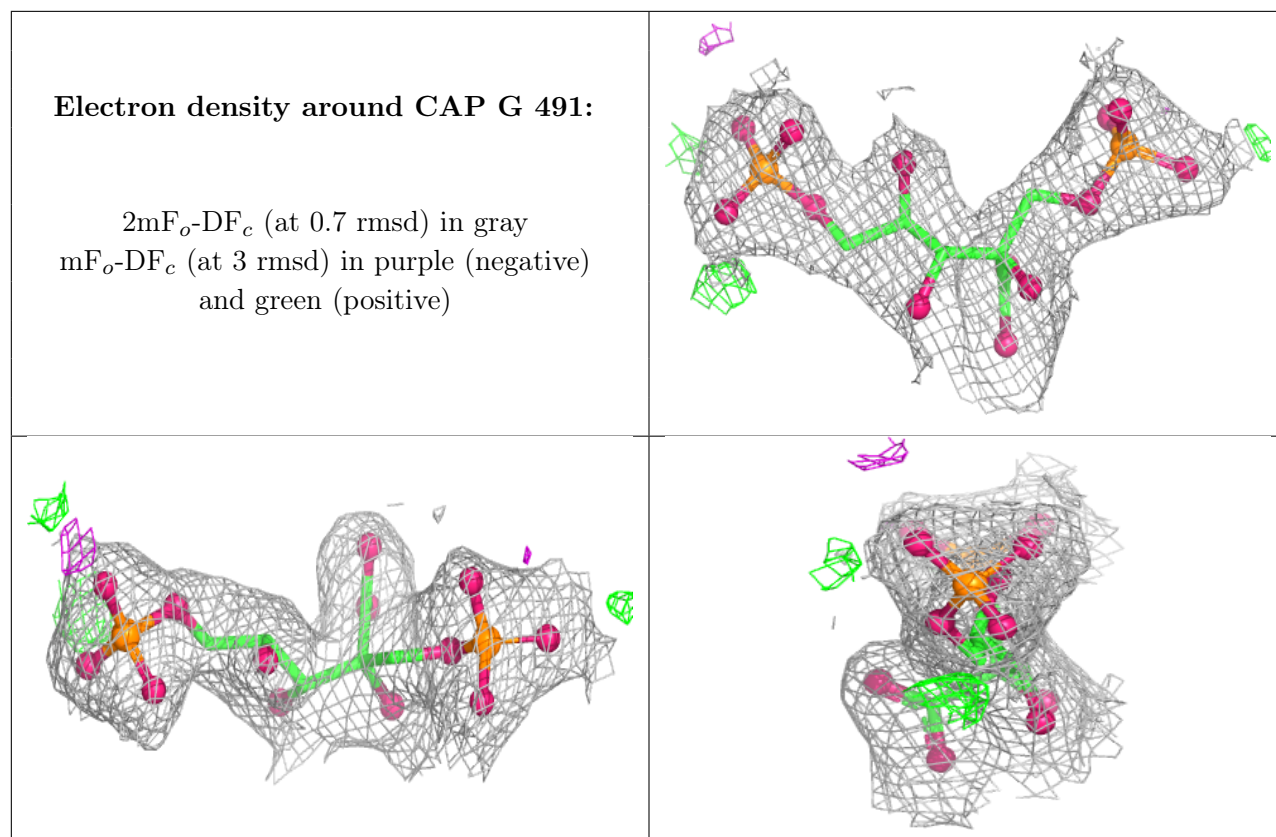
Electron density around CAP C 491:

$2mF_o-DF_c$ (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)





6.5 Other polymers ⓘ

There are no such residues in this entry.