



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:32 AM UTC

PDB ID : 1RLC / pdb_00001rlc
Title : CRYSTAL STRUCTURE OF THE UNACTIVATED RIBULOSE 1, 5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE COMPLEXED WITH A TRANSITION STATE ANALOG, 2-CARBOXY-D-ARABINITOL 1,5-BISPHOSPHATE
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Deposited on : 1993-08-04
Resolution : 2.70 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

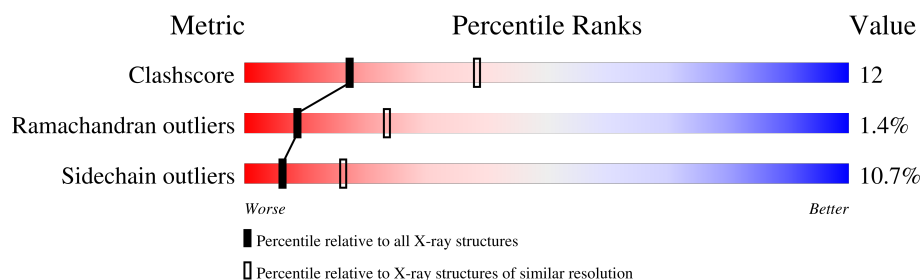
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	477	
2	S	123	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CAP	L	490	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4505 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.

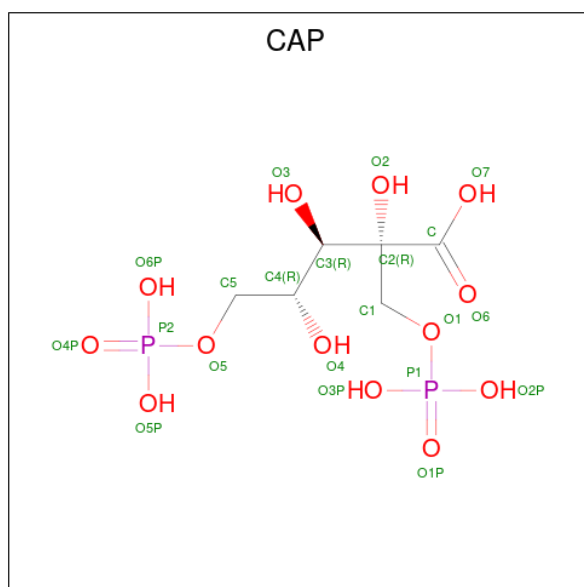
- Molecule 1 is a protein called RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	441	Total	C	N	O	S	0	0	0
			3455	2194	612	633	16			

- Molecule 2 is a protein called RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1029	672	163	188	6			

- Molecule 3 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$).



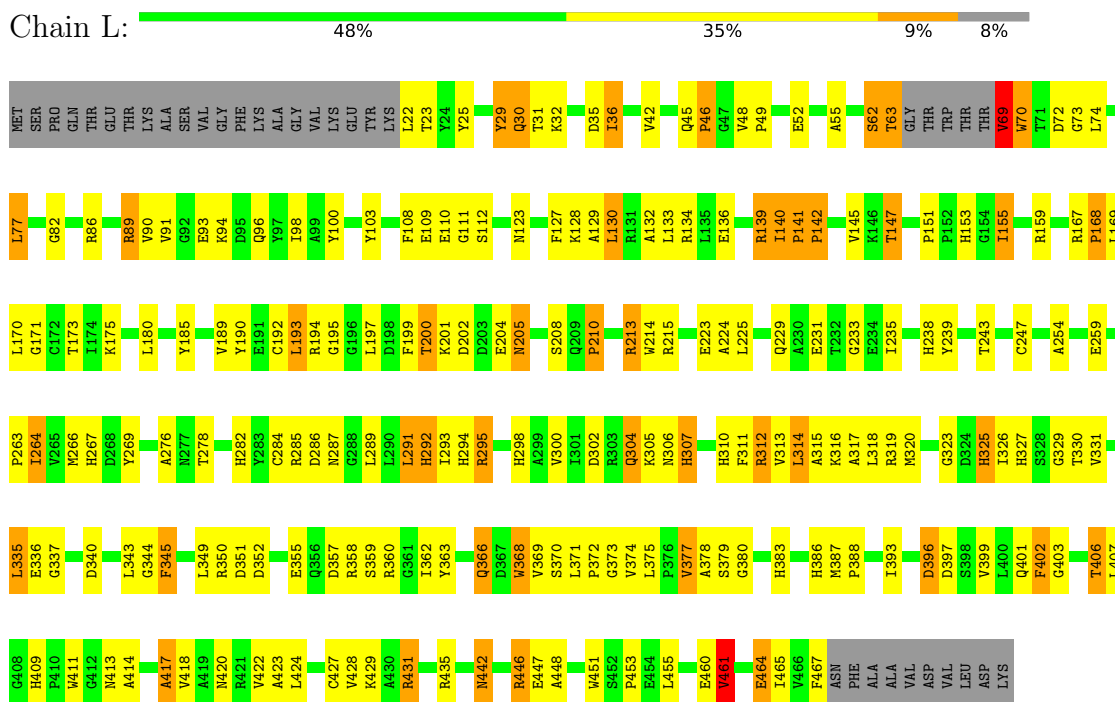
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	O	P	0	0
			21	6	13	2		

3 Residue-property plots

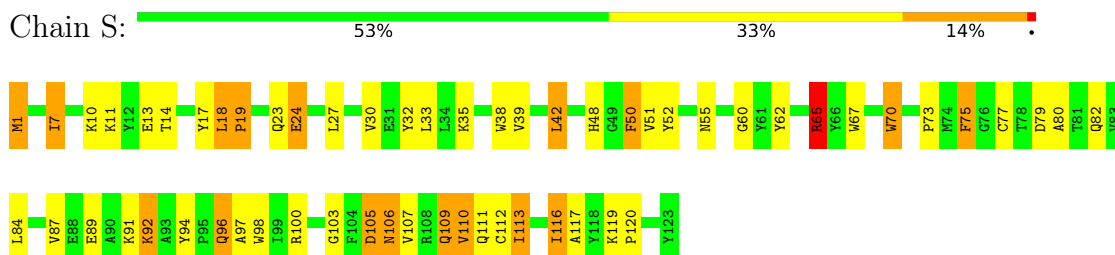
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

- Molecule 1: RIBULOSE 1,5 BISPSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



- Molecule 2: RIBULOSE 1,5 BISPSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.00Å 149.00Å 136.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4505	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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: CAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	1.36	28/3538 (0.8%)	2.12	120/4796 (2.5%)
2	S	1.11	1/1062 (0.1%)	2.00	34/1442 (2.4%)
All	All	1.30	29/4600 (0.6%)	2.09	154/6238 (2.5%)

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	L	0	1
2	S	0	1
All	All	0	2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	238	HIS	CD2-NE2	-8.38	1.28	1.37
1	L	267	HIS	CG-ND1	-7.35	1.30	1.38
1	L	383	HIS	CD2-NE2	-7.32	1.29	1.37
1	L	282	HIS	CD2-NE2	-7.05	1.30	1.37
1	L	153	HIS	CD2-NE2	-6.98	1.30	1.37
1	L	210	PRO	CA-CB	-6.73	1.44	1.53
1	L	69	VAL	CA-CB	6.71	1.63	1.54
1	L	294	HIS	CD2-NE2	-6.67	1.30	1.37
1	L	287	ASN	CA-CB	-6.65	1.43	1.53
1	L	292	HIS	CA-CB	-6.46	1.43	1.53
1	L	153	HIS	CG-ND1	-6.42	1.31	1.38
1	L	267	HIS	CD2-NE2	-6.41	1.30	1.37
1	L	386	HIS	CG-ND1	-6.35	1.31	1.38
1	L	140	ILE	CA-CB	6.35	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	386	HIS	CD2-NE2	-6.34	1.30	1.37
1	L	298	HIS	CG-ND1	-6.28	1.31	1.38
1	L	325	HIS	CD2-NE2	-6.27	1.30	1.37
1	L	292	HIS	CA-C	-6.21	1.45	1.52
1	L	141	PRO	CA-CB	-6.21	1.48	1.53
1	L	292	HIS	CD2-NE2	-6.08	1.31	1.37
1	L	409	HIS	CD2-NE2	-5.92	1.31	1.37
1	L	307	HIS	CD2-NE2	-5.92	1.31	1.37
1	L	276	ALA	CA-CB	-5.68	1.44	1.53
1	L	208	SER	CA-CB	-5.48	1.44	1.53
2	S	48	HIS	CD2-NE2	-5.42	1.31	1.37
1	L	282	HIS	CG-ND1	-5.39	1.32	1.38
1	L	397	ASP	CA-C	-5.36	1.47	1.53
1	L	49	PRO	CA-CB	-5.34	1.49	1.54
1	L	229	GLN	CD-NE2	-5.29	1.22	1.33

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	112	SER	CA-CB-OG	11.55	134.20	111.10
1	L	215	ARG	NE-CZ-NH2	-11.48	108.86	119.20
1	L	70	TRP	N-CA-C	10.80	133.80	110.80
1	L	214	TRP	N-CA-C	9.97	121.74	111.07
1	L	140	ILE	CA-C-O	9.20	126.24	119.25
1	L	141	PRO	O-C-N	-8.93	117.20	121.31
2	S	65	ARG	CB-CG-CD	-8.74	91.20	111.30
2	S	98	TRP	N-CA-C	-8.62	95.19	109.07
2	S	96	GLN	N-CA-C	-8.45	102.52	113.17
1	L	351	ASP	N-CA-C	8.41	123.71	110.17
1	L	155	ILE	N-CA-C	8.39	119.17	110.36
1	L	370	SER	N-CA-C	8.22	123.00	113.38
2	S	67	TRP	CG-CD2-CE3	8.21	142.10	133.90
1	L	63	THR	N-CA-C	8.06	118.61	108.45
1	L	345	PHE	CA-CB-CG	7.69	121.49	113.80
1	L	291	LEU	O-C-N	-7.66	114.25	123.29
2	S	18	LEU	N-CA-C	-7.64	100.12	110.36
1	L	317	ALA	O-C-N	-7.61	112.91	122.27
1	L	278	THR	N-CA-C	-7.56	102.98	111.14
2	S	52	TYR	O-C-N	-7.46	114.19	122.92
1	L	310	HIS	CA-CB-CG	-7.45	106.35	113.80
1	L	325	HIS	CA-CB-CG	7.38	121.18	113.80
1	L	311	PHE	CA-C-O	-7.26	113.13	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	48	VAL	CA-C-N	7.17	124.82	119.66
1	L	48	VAL	C-N-CA	7.17	124.82	119.66
2	S	109	GLN	CA-CB-CG	7.12	128.34	114.10
1	L	298	HIS	CA-CB-CG	7.11	120.91	113.80
1	L	233	GLY	N-CA-C	-7.07	105.30	115.27
1	L	215	ARG	NE-CZ-NH1	7.03	128.53	121.50
2	S	111	GLN	N-CA-C	-7.03	99.14	110.32
1	L	287	ASN	CB-CG-ND2	6.97	126.86	116.40
1	L	397	ASP	O-C-N	6.92	130.37	122.55
1	L	383	HIS	CB-CG-CD2	-6.84	122.31	131.20
1	L	435	ARG	CB-CG-CD	-6.78	95.70	111.30
1	L	442	ASN	OD1-CG-ND2	-6.78	115.83	122.60
1	L	401	GLN	CA-CB-CG	6.76	127.62	114.10
1	L	294	HIS	CB-CG-CD2	-6.73	122.45	131.20
1	L	292	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	L	264	ILE	CB-CG1-CD1	-6.60	99.93	113.80
1	L	180	LEU	N-CA-CB	-6.60	100.66	110.17
2	S	77	CYS	N-CA-C	-6.57	99.81	110.20
1	L	461	VAL	CB-CA-C	-6.56	103.28	112.14
1	L	200	THR	CA-C-O	-6.51	113.83	121.44
1	L	205	ASN	CA-CB-CG	6.50	119.10	112.60
2	S	105	ASP	CA-CB-CG	6.50	119.09	112.60
1	L	323	GLY	O-C-N	-6.46	117.75	123.76
1	L	89	ARG	N-CA-C	-6.39	98.99	109.40
1	L	35	ASP	CA-CB-CG	6.36	118.96	112.60
1	L	447	GLU	CA-CB-CG	6.34	126.78	114.10
1	L	49	PRO	CA-C-O	-6.33	115.73	120.73
1	L	373	GLY	O-C-N	6.31	130.78	123.21
1	L	69	VAL	N-CA-C	6.30	122.44	109.34
1	L	409	HIS	CB-CG-CD2	-6.29	123.02	131.20
2	S	7	ILE	CB-CA-C	-6.26	102.23	111.19
2	S	109	GLN	OE1-CD-NE2	-6.25	116.35	122.60
2	S	50	PHE	CA-CB-CG	6.18	119.98	113.80
1	L	352	ASP	CA-CB-CG	6.18	118.78	112.60
1	L	73	GLY	N-CA-C	-6.17	104.88	115.61
1	L	123	ASN	OD1-CG-ND2	-6.13	116.47	122.60
2	S	70	TRP	N-CA-C	-6.12	98.76	108.73
1	L	215	ARG	CA-CB-CG	6.09	126.27	114.10
1	L	340	ASP	CA-C-O	-6.08	113.97	120.42
1	L	406	THR	O-C-N	6.08	128.59	122.03
1	L	355	GLU	O-C-N	6.07	129.82	122.96
1	L	130	LEU	N-CA-C	-6.06	100.74	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	193	LEU	O-C-N	-6.01	115.75	122.12
1	L	29	TYR	N-CA-C	6.01	119.06	110.10
1	L	287	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	L	269	TYR	CA-C-O	-5.93	113.40	120.10
2	S	110	VAL	CB-CA-C	-5.92	103.09	111.38
1	L	269	TYR	CA-CB-CG	5.91	124.53	113.90
1	L	402	PHE	O-C-N	-5.90	116.34	123.13
1	L	318	LEU	O-C-N	-5.85	115.48	122.15
1	L	269	TYR	N-CA-C	5.81	118.39	111.71
1	L	325	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	L	123	ASN	CB-CG-ND2	5.80	125.10	116.40
1	L	409	HIS	CA-C-N	5.79	125.33	119.19
1	L	409	HIS	C-N-CA	5.79	125.33	119.19
1	L	69	VAL	O-C-N	-5.78	115.34	122.57
1	L	312	ARG	CA-C-O	-5.77	112.25	120.51
2	S	75	PHE	CA-CB-CG	-5.75	108.05	113.80
2	S	67	TRP	CB-CG-CD1	-5.74	118.29	126.90
1	L	295	ARG	CB-CG-CD	-5.74	98.11	111.30
1	L	69	VAL	CA-C-O	-5.70	113.65	120.78
1	L	417	ALA	N-CA-C	-5.66	104.49	111.40
1	L	314	LEU	O-C-N	-5.64	115.62	122.22
1	L	171	GLY	O-C-N	-5.62	116.85	123.09
1	L	294	HIS	CB-CG-ND1	5.62	131.13	122.70
1	L	213	ARG	CB-CG-CD	5.61	124.20	111.30
2	S	111	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	L	435	ARG	NE-CZ-NH2	5.58	124.22	119.20
2	S	14	THR	N-CA-C	5.55	118.52	110.42
1	L	292	HIS	N-CA-C	-5.54	100.15	109.07
2	S	13	GLU	CB-CG-CD	5.53	122.01	112.60
1	L	91	VAL	O-C-N	5.50	128.34	122.45
1	L	111	GLY	CA-C-O	-5.50	111.00	120.57
1	L	320	MET	CG-SD-CE	5.50	113.00	100.90
2	S	109	GLN	N-CA-CB	-5.50	103.78	112.08
1	L	294	HIS	CA-C-O	5.49	126.29	120.36
1	L	35	ASP	CA-C-N	-5.49	115.98	123.12
1	L	35	ASP	C-N-CA	-5.49	115.98	123.12
1	L	96	GLN	OE1-CD-NE2	-5.49	117.11	122.60
2	S	30	VAL	CA-CB-CG1	-5.48	101.08	110.40
2	S	48	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	L	366	GLN	CA-C-O	5.46	126.03	120.24
1	L	360	ARG	N-CA-C	-5.46	107.18	112.97
1	L	286	ASP	CA-CB-CG	5.45	118.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	368	TRP	CG-CD2-CE3	5.45	139.35	133.90
1	L	302	ASP	CA-CB-CG	5.44	118.04	112.60
2	S	24	GLU	N-CA-C	-5.44	105.44	111.36
1	L	413	ASN	N-CA-C	5.41	119.94	113.23
1	L	259	GLU	O-C-N	-5.40	116.40	122.12
1	L	313	VAL	CB-CA-C	-5.37	104.81	112.22
2	S	79	ASP	CA-C-O	5.37	126.28	120.32
1	L	223	GLU	CB-CG-CD	5.33	121.66	112.60
1	L	278	THR	CA-C-O	-5.32	115.22	120.70
1	L	82	GLY	O-C-N	-5.31	117.37	122.84
1	L	300	VAL	N-CA-C	-5.29	105.23	110.62
1	L	420	ASN	O-C-N	-5.27	116.05	122.22
1	L	243	THR	O-C-N	5.26	129.31	122.89
1	L	318	LEU	CA-C-O	-5.24	114.87	120.42
2	S	18	LEU	CA-C-N	5.21	126.36	119.84
2	S	18	LEU	C-N-CA	5.21	126.36	119.84
1	L	330	THR	CA-CB-CG2	5.21	119.35	110.50
1	L	370	SER	N-CA-CB	-5.20	104.82	112.78
1	L	180	LEU	O-C-N	-5.19	116.74	122.86
2	S	113	ILE	N-CA-C	-5.17	101.02	108.42
2	S	82	GLN	OE1-CD-NE2	-5.17	117.43	122.60
2	S	111	GLN	O-C-N	-5.17	117.27	123.06
1	L	263	PRO	N-CA-C	5.16	121.24	114.27
1	L	168	PRO	CB-CA-C	5.16	117.84	111.23
1	L	396	ASP	N-CA-C	5.14	117.79	111.82
1	L	139	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	L	431	ARG	N-CA-CB	-5.14	102.01	110.14
1	L	62	SER	N-CA-C	5.13	121.73	110.80
1	L	396	ASP	CA-C-N	-5.13	115.18	122.41
1	L	396	ASP	C-N-CA	-5.13	115.18	122.41
1	L	30	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	L	285	ARG	NE-CZ-NH1	5.12	126.61	121.50
2	S	111	GLN	CA-CB-CG	5.12	124.33	114.10
1	L	153	HIS	CB-CG-CD2	-5.11	124.56	131.20
2	S	23	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	L	36	ILE	N-CA-C	-5.09	100.42	107.80
1	L	147	THR	O-C-N	-5.09	114.86	122.39
1	L	401	GLN	N-CA-CB	-5.08	101.87	110.46
1	L	193	LEU	CA-C-O	-5.07	115.15	120.63
1	L	109	GLU	CB-CG-CD	5.06	121.20	112.60
1	L	343	LEU	O-C-N	-5.05	115.66	122.43
1	L	254	ALA	N-CA-C	-5.05	105.67	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	103	TYR	CA-C-N	5.03	125.03	119.90
1	L	103	TYR	C-N-CA	5.03	125.03	119.90
2	S	70	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	L	264	ILE	N-CA-CB	-5.02	103.12	111.36
2	S	55	ASN	N-CA-C	5.01	119.55	113.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	45	GLN	Peptide
2	S	65	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3455	0	3394	90	0
2	S	1029	0	994	25	0
3	L	21	0	9	1	0
All	All	4505	0	4397	110	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 12.

All (110) 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:L:315:ALA:HB1	1:L:349:LEU:HD21	1.51	0.89
1:L:335:LEU:HD23	1:L:337:GLY:H	1.47	0.79
1:L:127:PHE:CE2	1:L:129:ALA:HB3	2.22	0.74
1:L:388:PRO:HG3	1:L:427:CYS:SG	2.31	0.70
1:L:195:GLY:HA3	1:L:417:ALA:HB3	1.74	0.70
1:L:316:LYS:NZ	1:L:366:GLN:HE21	1.92	0.67
1:L:170:LEU:HD21	1:L:424:LEU:HD22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:10:LYS:HB3	2:S:50:PHE:CE1	2.35	0.61
1:L:402:PHE:HB2	1:L:406:THR:HG23	1.82	0.61
1:L:326:ILE:O	1:L:377:VAL:HG23	2.02	0.60
1:L:151:PRO:HD2	1:L:372:PRO:HD2	1.83	0.59
1:L:173:THR:HB	1:L:403:GLY:HA2	1.84	0.59
1:L:319:ARG:HG3	1:L:374:VAL:HG23	1.85	0.59
1:L:387:MET:HE3	1:L:424:LEU:HB2	1.85	0.59
1:L:291:LEU:HG	1:L:293:ILE:HD11	1.85	0.58
2:S:51:VAL:HG13	2:S:62:TYR:HB3	1.85	0.58
2:S:33:LEU:HD12	2:S:38:TRP:HE3	1.68	0.58
1:L:235:ILE:HD11	2:S:51:VAL:HG21	1.87	0.57
1:L:140:ILE:H	1:L:366:GLN:HE22	1.52	0.56
1:L:446:ARG:HG3	1:L:467:PHE:CE2	2.40	0.56
1:L:428:VAL:HG13	1:L:431:ARG:HH21	1.69	0.56
1:L:86:ARG:HB3	1:L:100:TYR:CD1	2.41	0.56
1:L:134:ARG:HD3	1:L:136:GLU:OE2	2.06	0.56
1:L:127:PHE:HD2	1:L:130:LEU:HG	1.73	0.54
1:L:190:TYR:HB2	1:L:224:ALA:HB1	1.89	0.54
2:S:97:ALA:O	2:S:120:PRO:HD3	2.06	0.54
1:L:133:LEU:O	1:L:307:HIS:HA	2.08	0.54
2:S:87:VAL:O	2:S:91:LYS:HG3	2.08	0.53
1:L:446:ARG:HG3	1:L:467:PHE:CZ	2.44	0.53
1:L:142:PRO:HB3	1:L:369:VAL:HG11	1.91	0.53
2:S:10:LYS:HB3	2:S:50:PHE:CZ	2.44	0.52
2:S:89:GLU:O	2:S:92:LYS:HG3	2.10	0.52
1:L:411:TRP:HH2	1:L:453:PRO:HB2	1.75	0.51
1:L:429:LYS:HD3	2:S:18:LEU:HD13	1.93	0.51
1:L:319:ARG:NH1	1:L:368:TRP:CD1	2.78	0.51
2:S:33:LEU:HD12	2:S:38:TRP:HB2	1.93	0.51
1:L:284:CYS:HB3	1:L:289:LEU:O	2.12	0.50
1:L:36:ILE:HD12	1:L:108:PHE:CE2	2.46	0.50
1:L:312:ARG:HB3	1:L:345:PHE:HB3	1.93	0.50
1:L:169:LEU:O	1:L:399:VAL:HA	2.12	0.50
1:L:194:ARG:HD2	1:L:231:GLU:OE2	2.11	0.50
2:S:11:LYS:HG3	2:S:17:TYR:CE1	2.48	0.49
1:L:25:TYR:HB2	1:L:55:ALA:HB2	1.94	0.49
1:L:29:TYR:OH	1:L:32:LYS:HE2	2.13	0.49
1:L:316:LYS:HZ1	1:L:366:GLN:HE21	1.56	0.49
1:L:451:TRP:HH2	2:S:18:LEU:HD23	1.78	0.48
2:S:94:TYR:HB3	2:S:97:ALA:HB2	1.94	0.48
1:L:428:VAL:HG13	1:L:431:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:168:PRO:HD2	1:L:424:LEU:HD11	1.97	0.47
1:L:110:GLU:HB3	1:L:147:THR:HB	1.96	0.47
1:L:295:ARG:HG2	1:L:327:HIS:HB2	1.97	0.47
2:S:42:LEU:HB3	2:S:70:TRP:HB3	1.97	0.47
1:L:414:ALA:O	1:L:418:VAL:HG23	2.15	0.47
1:L:199:PHE:HB3	1:L:239:TYR:CE1	2.50	0.46
1:L:292:HIS:HA	1:L:325:HIS:HB2	1.97	0.46
1:L:36:ILE:HD12	1:L:108:PHE:CD2	2.50	0.46
1:L:319:ARG:HG3	1:L:374:VAL:CG2	2.45	0.46
1:L:357:ASP:OD1	1:L:359:SER:HB3	2.15	0.46
1:L:170:LEU:CD2	1:L:424:LEU:HD22	2.45	0.46
2:S:38:TRP:CD2	2:S:112:CYS:SG	3.09	0.46
2:S:33:LEU:HD11	2:S:103:GLY:HA3	1.97	0.45
1:L:139:ARG:HH21	1:L:141:PRO:HB3	1.81	0.45
1:L:167:ARG:HG3	1:L:168:PRO:O	2.16	0.45
1:L:304:GLN:OE1	1:L:304:GLN:HA	2.17	0.45
2:S:73:PRO:HB2	2:S:75:PHE:CE2	2.52	0.45
1:L:201:LYS:HG2	1:L:202:ASP:O	2.17	0.45
1:L:344:GLY:HA2	1:L:362:ILE:HD11	1.98	0.45
2:S:60:GLY:O	2:S:65:ARG:NH2	2.50	0.45
1:L:136:GLU:O	1:L:312:ARG:NH1	2.51	0.44
1:L:169:LEU:HD12	1:L:375:LEU:HD21	1.98	0.44
2:S:106:ASN:OD1	2:S:107:VAL:HG13	2.17	0.44
1:L:422:VAL:HG23	1:L:455:LEU:HD22	1.99	0.44
1:L:140:ILE:HA	1:L:141:PRO:HD2	1.84	0.44
1:L:442:ASN:O	1:L:446:ARG:HB2	2.18	0.44
1:L:29:TYR:CE2	1:L:31:THR:HG22	2.53	0.43
1:L:175:LYS:HB2	1:L:407:LEU:HD12	2.00	0.43
1:L:159:ARG:NH2	1:L:396:ASP:O	2.52	0.43
1:L:169:LEU:HB2	1:L:399:VAL:HG22	2.00	0.43
2:S:27:LEU:HG	2:S:84:LEU:HD22	2.00	0.43
1:L:331:VAL:HG21	1:L:393:ILE:HD13	2.01	0.43
1:L:72:ASP:HB3	1:L:77:LEU:N	2.33	0.43
1:L:461:VAL:O	1:L:464:GLU:HB2	2.18	0.42
1:L:155:ILE:HG23	1:L:375:LEU:HD13	2.00	0.42
1:L:329:GLY:O	1:L:378:ALA:HA	2.18	0.42
1:L:239:TYR:CE2	1:L:292:HIS:CE1	3.08	0.42
1:L:358:ARG:HD3	1:L:363:TYR:HA	1.99	0.42
1:L:155:ILE:HG12	1:L:375:LEU:HD13	2.01	0.42
1:L:140:ILE:HG22	1:L:145:VAL:HG23	2.00	0.42
1:L:293:ILE:HD12	1:L:293:ILE:HG23	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:319:ARG:HH12	1:L:368:TRP:CD1	2.38	0.42
1:L:132:ALA:HB1	1:L:306:ASN:O	2.19	0.42
1:L:411:TRP:CE2	2:S:1:MET:HA	2.55	0.41
1:L:414:ALA:O	1:L:417:ALA:HB3	2.19	0.41
1:L:379:SER:OG	3:L:490:CAP:H12	2.20	0.41
2:S:116:ILE:HG13	2:S:117:ALA:N	2.34	0.41
1:L:185:TYR:O	1:L:189:VAL:HG23	2.21	0.41
2:S:39:VAL:O	2:S:103:GLY:HA2	2.19	0.41
1:L:42:VAL:HG23	1:L:130:LEU:HD13	2.03	0.41
1:L:86:ARG:HB3	1:L:100:TYR:HD1	1.84	0.41
1:L:448:ALA:HA	1:L:451:TRP:CE2	2.56	0.41
1:L:90:VAL:HG22	1:L:98:ILE:HG12	2.02	0.41
1:L:130:LEU:HD12	1:L:133:LEU:HD22	2.02	0.41
1:L:140:ILE:HG22	1:L:145:VAL:CG2	2.50	0.41
1:L:264:ILE:HD13	1:L:264:ILE:HG21	1.75	0.41
1:L:411:TRP:CD2	2:S:1:MET:HA	2.56	0.41
1:L:193:LEU:HG	1:L:200:THR:HG23	2.02	0.40
1:L:387:MET:HE2	1:L:423:ALA:HB3	2.02	0.40
1:L:168:PRO:HG3	1:L:396:ASP:HA	2.03	0.40
1:L:331:VAL:HG11	1:L:393:ILE:HG21	2.02	0.40
2:S:32:TYR:HA	2:S:35:LYS:HD3	2.03	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	L	439/477 (92%)	399 (91%)	34 (8%)	6 (1%)	9	23
2	S	121/123 (98%)	110 (91%)	9 (7%)	2 (2%)	7	19
All	All	560/600 (93%)	509 (91%)	43 (8%)	8 (1%)	9	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	46	PRO
1	L	69	VAL
1	L	94	LYS
1	L	380	GLY
1	L	62	SER
1	L	204	GLU
2	S	80	ALA
2	S	19	PRO

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	L	357/386 (92%)	322 (90%)	35 (10%)	7	19
2	S	110/110 (100%)	95 (86%)	15 (14%)	3	9
All	All	467/496 (94%)	417 (89%)	50 (11%)	6	16

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	22	LEU
1	L	23	THR
1	L	30	GLN
1	L	46	PRO
1	L	52	GLU
1	L	63	THR
1	L	69	VAL
1	L	70	TRP
1	L	74	LEU
1	L	77	LEU
1	L	89	ARG
1	L	93	GLU
1	L	128	LYS
1	L	142	PRO
1	L	192	CYS

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Mol	Chain	Res	Type
1	L	197	LEU
1	L	205	ASN
1	L	210	PRO
1	L	213	ARG
1	L	225	LEU
1	L	247	CYS
1	L	266	MET
1	L	304	GLN
1	L	305	LYS
1	L	314	LEU
1	L	335	LEU
1	L	336	GLU
1	L	350	ARG
1	L	371	LEU
1	L	377	VAL
1	L	446	ARG
1	L	460	GLU
1	L	461	VAL
1	L	464	GLU
1	L	465	ILE
2	S	1	MET
2	S	7	ILE
2	S	19	PRO
2	S	24	GLU
2	S	42	LEU
2	S	92	LYS
2	S	96	GLN
2	S	100	ARG
2	S	105	ASP
2	S	106	ASN
2	S	109	GLN
2	S	110	VAL
2	S	113	ILE
2	S	116	ILE
2	S	119	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	149	GLN
1	L	207	ASN
1	L	277	ASN

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Mol	Chain	Res	Type
1	L	366	GLN
1	L	401	GLN
1	L	420	ASN
2	S	36	ASN
2	S	55	ASN
2	S	109	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	CAP	L	490	-	18,20,20	2.25	5 (27%)	23,31,31	4.54	18 (78%)

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
3	CAP	L	490	-	-	14/29/29/29	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	490	CAP	C4-C3	5.48	1.59	1.54
3	L	490	CAP	P1-O1P	5.39	1.67	1.50
3	L	490	CAP	P2-O6P	2.71	1.64	1.54
3	L	490	CAP	O5-C5	2.59	1.54	1.44
3	L	490	CAP	C5-C4	2.21	1.54	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	490	CAP	O6-C-C2	10.47	141.81	122.32
3	L	490	CAP	C2-C3-C4	9.87	133.72	114.03
3	L	490	CAP	O2-C2-C1	5.94	122.81	108.72
3	L	490	CAP	C5-C4-C3	-5.51	100.93	111.96
3	L	490	CAP	O5P-P2-O5	5.12	120.02	106.67
3	L	490	CAP	O7-C-C2	-4.90	105.84	114.06
3	L	490	CAP	O3P-P1-O1	4.68	118.88	106.67
3	L	490	CAP	O2P-P1-O1P	-4.62	92.83	110.83
3	L	490	CAP	O5-P2-O4P	4.34	118.17	106.44
3	L	490	CAP	O7-C-O6	-3.60	112.35	123.86
3	L	490	CAP	O4-C4-C5	3.59	117.89	109.99
3	L	490	CAP	O2P-P1-O1	3.48	115.75	106.67
3	L	490	CAP	O3-C3-C4	-3.13	102.42	109.13
3	L	490	CAP	O1-P1-O1P	-3.13	97.99	106.44
3	L	490	CAP	O6P-P2-O5P	-3.10	96.18	107.80
3	L	490	CAP	O4-C4-C3	2.76	114.29	108.78
3	L	490	CAP	O2-C2-C	-2.36	104.64	109.07
3	L	490	CAP	O3P-P1-O2P	2.18	115.98	107.80

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	490	CAP	O1-C1-C2-C
3	L	490	CAP	O1-C1-C2-O2
3	L	490	CAP	C1-C2-C3-O3
3	L	490	CAP	C-C2-C3-O3
3	L	490	CAP	O2-C2-C3-C4

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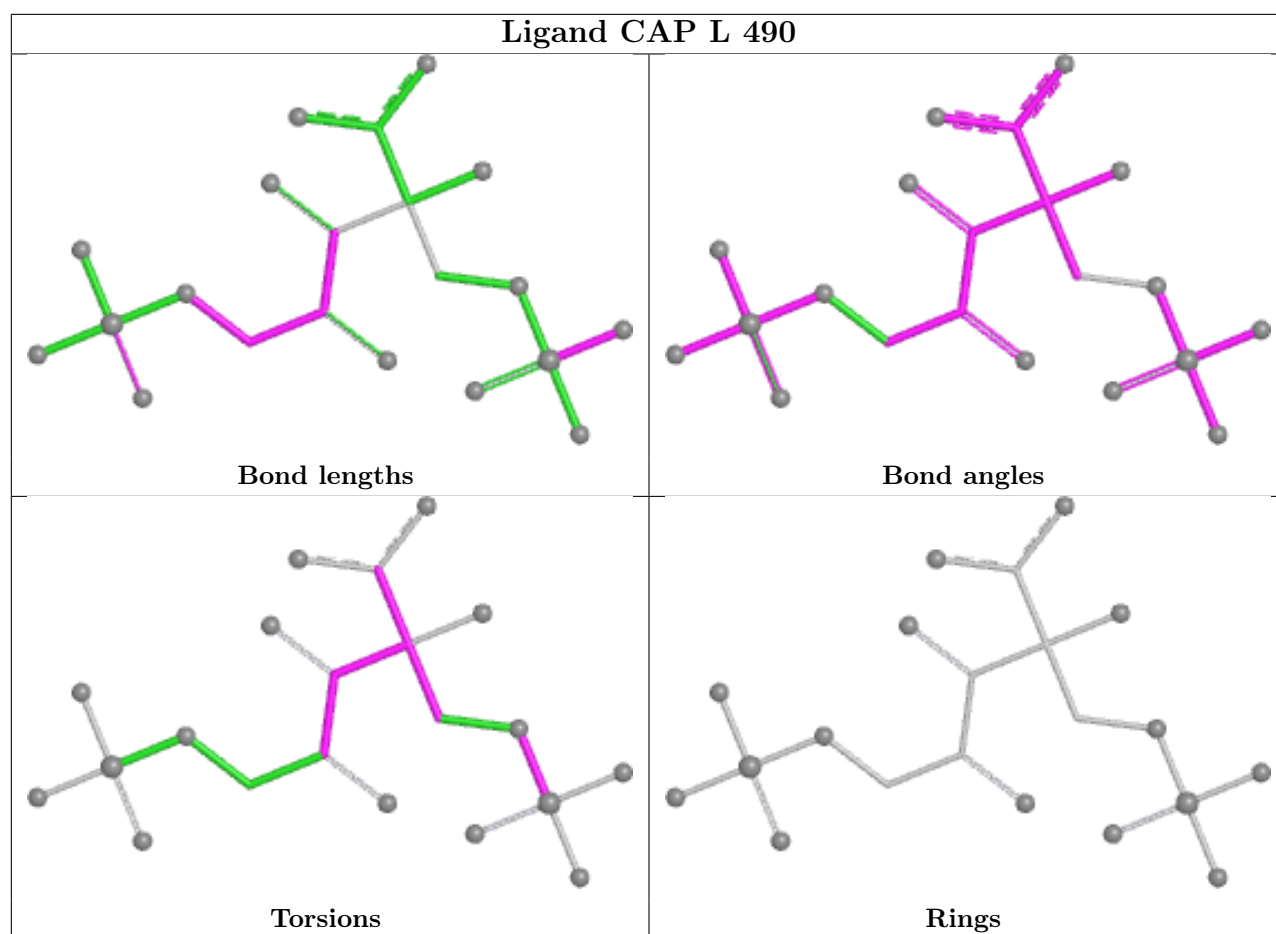
Mol	Chain	Res	Type	Atoms
3	L	490	CAP	O2-C2-C3-O3
3	L	490	CAP	O6-C-C2-C3
3	L	490	CAP	O7-C-C2-C3
3	L	490	CAP	O6-C-C2-O2
3	L	490	CAP	O7-C-C2-O2
3	L	490	CAP	C2-C3-C4-O4
3	L	490	CAP	O3-C3-C4-O4
3	L	490	CAP	C1-O1-P1-O2P
3	L	490	CAP	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	490	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.