



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:40 AM UTC

PDB ID : 1RAA / pdb_00001raa
Title : CRYSTAL STRUCTURE OF CTP-LIGATED T STATE ASPARTATE
TRANSCARBAMOYLASE AT 2.5 ANGSTROMS RESOLUTION: IMPLI-
CATIONS FOR ATCASE MUTANTS AND THE MECHANISM OF NEGA-
TIVE COOPERATIVITY
Authors : Kosman, R.P.; Gouaux, J.E.; Lipscomb, W.N.
Deposited on : 1992-08-14
Resolution : 2.50 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)
Xtrriage (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

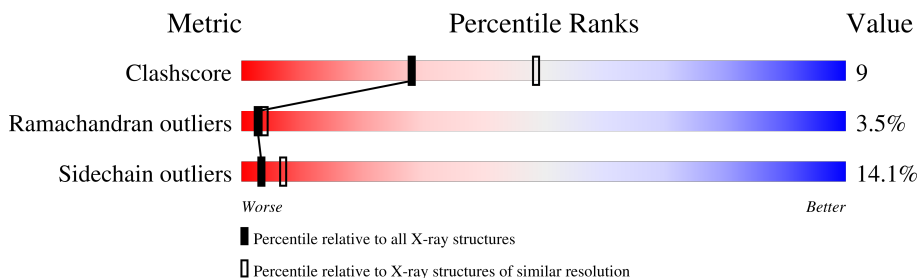
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	A	310	 58% 30% 10% .
1	C	310	 54% 33% 11% .
2	B	153	 50% 31% 16% .
2	D	153	 49% 30% 16% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7375 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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

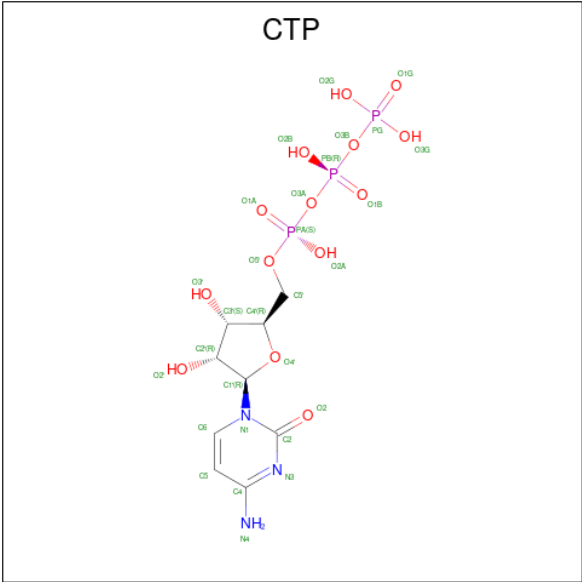
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1196	749	212	229	6			
2	D	153	Total	C	N	O	S	0	0	0
			1196	749	212	229	6			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 5 is water.

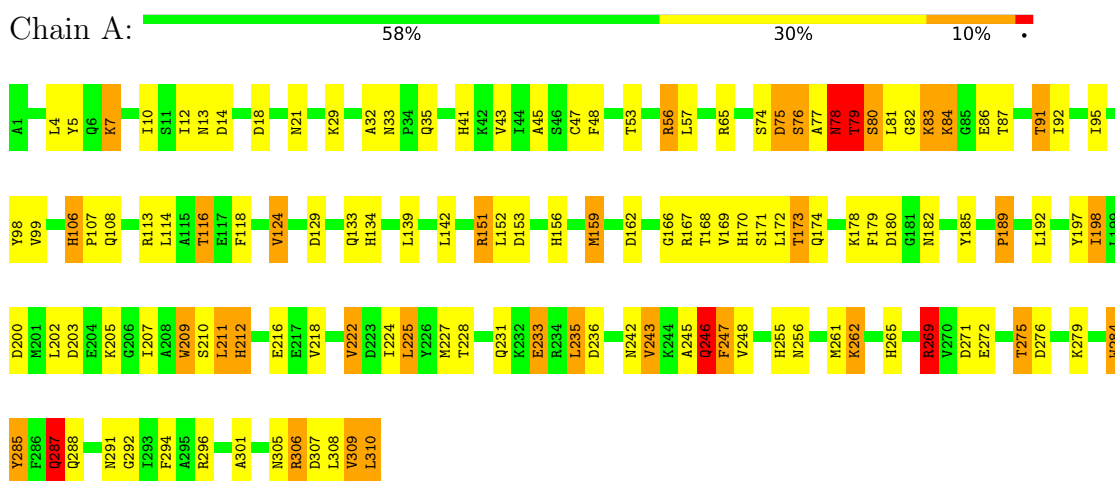
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	10	Total	O	0	0
			10	10		
5	C	43	Total	O	0	0
			43	43		
5	D	9	Total	O	0	0
			9	9		

3 Residue-property plots

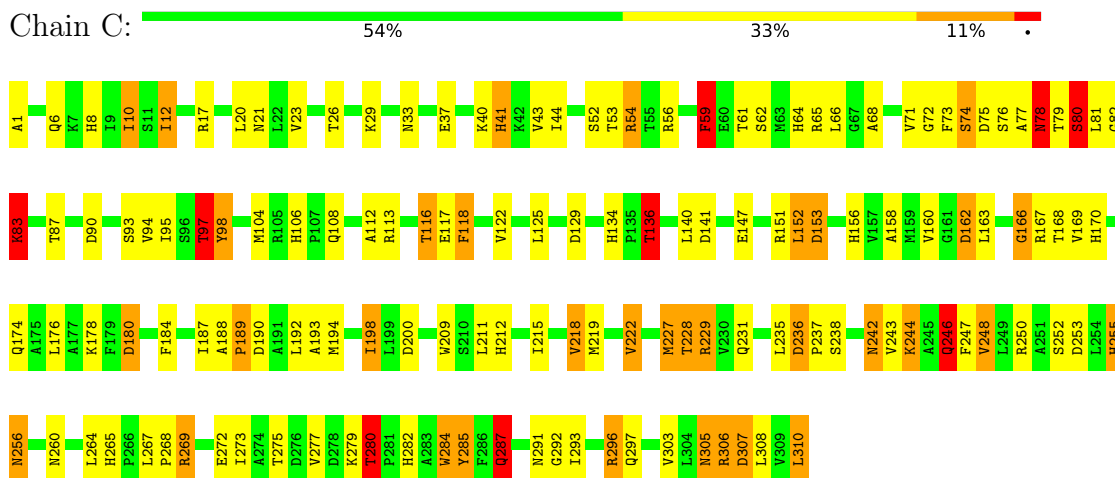
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

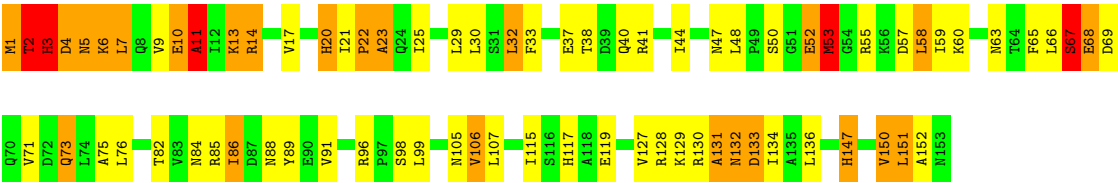


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

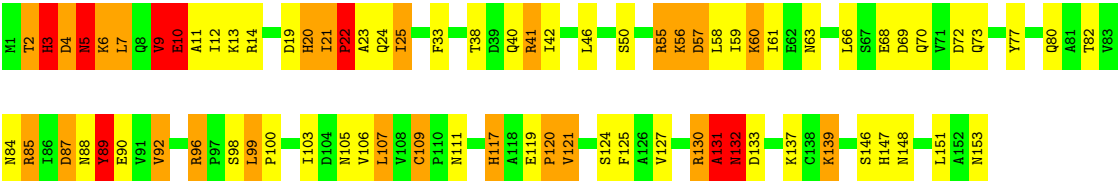


- Molecule 2: Aspartate carbamoyltransferase regulatory chain





• Molecule 2: Aspartate carbamoyltransferase regulatory chain



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.13Å 122.13Å 142.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7375	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CTP

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	1.32	18/2461 (0.7%)	2.16	98/3339 (2.9%)
1	C	1.36	19/2461 (0.8%)	2.25	141/3339 (4.2%)
2	B	1.18	4/1214 (0.3%)	2.21	57/1640 (3.5%)
2	D	1.23	8/1214 (0.7%)	2.27	71/1640 (4.3%)
All	All	1.30	49/7350 (0.7%)	2.22	367/9958 (3.7%)

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	A	0	3
1	C	0	1
2	B	0	1
2	D	0	1
All	All	0	6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	HIS	CD2-NE2	-7.43	1.29	1.37
1	A	265	HIS	CD2-NE2	-7.26	1.29	1.37
1	A	106	HIS	CG-ND1	-7.13	1.30	1.38
1	C	134	HIS	CD2-NE2	-7.09	1.30	1.37
2	D	82	THR	CA-CB	6.94	1.64	1.53
1	C	134	HIS	CG-ND1	-6.92	1.30	1.38
1	C	212	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	265	HIS	CG-ND1	-6.78	1.30	1.38
1	A	170	HIS	CD2-NE2	-6.77	1.30	1.37
1	C	41	HIS	CD2-NE2	-6.71	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	HIS	CG-ND1	-6.69	1.30	1.38
1	C	64	HIS	CD2-NE2	-6.64	1.30	1.37
1	C	265	HIS	CD2-NE2	-6.61	1.30	1.37
2	B	147	HIS	CD2-NE2	-6.58	1.30	1.37
2	D	147	HIS	CD2-NE2	-6.37	1.30	1.37
1	C	106	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	170	HIS	CD2-NE2	-6.21	1.31	1.37
2	D	147	HIS	CG-ND1	-6.21	1.31	1.38
1	C	282	HIS	CD2-NE2	-6.19	1.31	1.37
2	B	2	THR	CA-CB	6.17	1.63	1.53
1	A	156	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	41	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	56	ARG	CA-CB	-6.03	1.43	1.53
1	A	212	HIS	CD2-NE2	-5.89	1.31	1.37
1	C	8	HIS	CG-ND1	-5.88	1.31	1.38
2	D	20	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	124	VAL	CA-CB	5.80	1.62	1.54
2	D	120	PRO	CA-CB	-5.80	1.50	1.53
2	B	3	HIS	CD2-NE2	-5.76	1.31	1.37
1	C	156	HIS	CD2-NE2	-5.76	1.31	1.37
2	D	117	HIS	CD2-NE2	-5.68	1.31	1.37
1	A	243	VAL	CA-CB	5.67	1.62	1.54
1	C	282	HIS	CG-ND1	-5.63	1.32	1.38
1	C	56	ARG	CA-CB	-5.52	1.44	1.53
1	C	156	HIS	CG-ND1	-5.50	1.32	1.38
1	C	212	HIS	CG-ND1	-5.49	1.32	1.38
1	A	255	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	47	CYS	CA-CB	-5.37	1.45	1.52
2	D	20	HIS	CB-CG	5.37	1.57	1.50
1	C	112	ALA	CA-CB	-5.36	1.44	1.53
2	B	117	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	203	ASP	CA-C	-5.32	1.45	1.52
1	C	8	HIS	CD2-NE2	-5.30	1.32	1.37
2	D	9	VAL	CA-CB	5.29	1.60	1.54
1	A	134	HIS	CG-ND1	-5.29	1.32	1.38
1	C	147	GLU	CD-OE2	5.15	1.35	1.25
1	A	41	HIS	CG-ND1	-5.04	1.32	1.38
1	A	269	ARG	CZ-NH2	-5.02	1.26	1.33

All (367) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	HIS	CA-CB-CG	-14.13	99.67	113.80
1	C	33	ASN	OD1-CG-ND2	-12.44	110.16	122.60
1	C	287	GLN	OE1-CD-NE2	-11.88	110.72	122.60
2	D	3	HIS	CA-CB-CG	-11.19	102.61	113.80
1	A	14	ASP	CA-CB-CG	11.10	123.70	112.60
2	B	5	ASN	CA-CB-CG	11.04	123.64	112.60
1	A	245	ALA	N-CA-C	-10.98	97.26	110.44
2	B	11	ALA	N-CA-C	10.96	134.14	110.80
1	C	255	HIS	N-CA-C	10.78	124.11	111.71
1	C	287	GLN	CG-CD-NE2	10.36	131.94	116.40
1	A	271	ASP	CA-CB-CG	10.35	122.95	112.60
1	A	276	ASP	CA-CB-CG	10.30	122.90	112.60
1	A	106	HIS	CA-C-N	10.03	129.69	119.56
1	A	106	HIS	C-N-CA	10.03	129.69	119.56
2	D	73	GLN	OE1-CD-NE2	-10.00	112.60	122.60
1	C	280	THR	N-CA-CB	-9.87	96.16	109.78
1	C	33	ASN	CB-CG-ND2	9.85	131.18	116.40
1	C	297	GLN	OE1-CD-NE2	-9.69	112.91	122.60
2	B	50	SER	N-CA-C	9.66	123.53	109.14
1	C	174	GLN	CA-CB-CG	-9.54	95.02	114.10
1	A	107	PRO	N-CA-CB	9.50	112.63	103.51
2	D	9	VAL	O-C-N	9.40	132.26	122.67
1	C	90	ASP	N-CA-C	9.11	121.21	111.28
1	C	80	SER	N-CA-C	9.06	130.11	110.80
1	A	75	ASP	CA-CB-CG	9.00	121.60	112.60
1	A	80	SER	N-CA-C	8.96	129.89	110.80
2	D	2	THR	N-CA-C	8.85	123.56	107.99
2	B	20	HIS	CA-CB-CG	-8.84	104.96	113.80
2	B	88	ASN	CA-CB-CG	8.84	121.44	112.60
2	D	63	ASN	OD1-CG-ND2	-8.83	113.77	122.60
1	A	129	ASP	CA-CB-CG	8.80	121.40	112.60
1	C	134	HIS	ND1-CG-CD2	8.48	114.58	106.10
1	A	256	ASN	CA-CB-CG	8.45	121.05	112.60
1	C	75	ASP	CA-CB-CG	8.45	121.05	112.60
1	A	21	ASN	OD1-CG-ND2	-8.38	114.22	122.60
2	B	130	ARG	N-CA-C	8.31	122.46	110.24
1	C	296	ARG	NE-CZ-NH1	8.26	129.75	121.50
1	A	269	ARG	NE-CZ-NH1	8.23	129.73	121.50
1	C	236	ASP	CA-CB-CG	8.21	120.81	112.60
1	C	291	ASN	OD1-CG-ND2	-8.21	114.39	122.60
2	D	73	GLN	CG-CD-NE2	8.17	128.65	116.40
1	C	247	PHE	N-CA-C	-8.15	93.45	110.80
1	A	224	ILE	O-C-N	-8.11	114.66	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	147	HIS	ND1-CG-CD2	8.10	114.20	106.10
2	D	9	VAL	N-CA-CB	8.05	120.91	110.13
1	C	97	THR	N-CA-CB	-8.00	96.39	110.39
2	D	2	THR	CA-C-O	7.95	129.19	120.92
1	C	136	THR	N-CA-CB	-7.93	98.09	110.30
2	D	89	TYR	N-CA-C	7.89	127.60	110.80
1	A	162	ASP	CA-CB-CG	7.86	120.46	112.60
1	A	134	HIS	ND1-CG-CD2	7.84	113.94	106.10
1	A	265	HIS	ND1-CG-CD2	7.80	113.90	106.10
1	C	198	ILE	N-CA-C	-7.62	103.43	110.82
2	B	105	ASN	N-CA-C	7.61	127.00	110.80
1	C	284	TRP	CG-CD2-CE3	7.59	141.49	133.90
1	A	79	THR	N-CA-C	7.58	126.94	110.80
1	C	33	ASN	CA-C-N	7.51	127.47	120.03
1	C	33	ASN	C-N-CA	7.51	127.47	120.03
1	C	200	ASP	CA-CB-CG	7.50	120.10	112.60
1	A	287	GLN	OE1-CD-NE2	-7.49	115.11	122.60
1	C	54	ARG	CA-CB-CG	7.46	129.02	114.10
1	C	222	VAL	CA-CB-CG1	7.45	123.07	110.40
1	A	222	VAL	N-CA-CB	-7.37	100.39	110.56
1	A	134	HIS	CG-CD2-NE2	-7.37	99.83	107.20
2	B	133	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	291	ASN	OD1-CG-ND2	-7.29	115.31	122.60
2	D	5	ASN	CA-CB-CG	7.25	119.85	112.60
1	C	66	LEU	N-CA-C	-7.23	102.75	112.94
1	C	61	THR	N-CA-C	-7.21	103.35	111.07
1	C	106	HIS	ND1-CG-CD2	7.21	113.31	106.10
1	A	84	LYS	N-CA-C	-7.13	95.62	110.80
1	A	43	VAL	CG1-CB-CG2	-7.11	95.15	110.80
1	C	26	THR	CA-CB-OG1	-7.11	98.93	109.60
1	C	180	ASP	N-CA-C	7.08	121.85	109.96
1	C	87	THR	O-C-N	-7.04	114.51	122.75
1	A	107	PRO	CB-CA-C	-7.03	101.41	111.68
2	D	40	GLN	OE1-CD-NE2	-7.03	115.57	122.60
1	C	8	HIS	ND1-CG-CD2	7.02	113.12	106.10
2	B	67	SER	O-C-N	7.00	130.32	123.04
2	B	133	ASP	O-C-N	7.00	131.90	122.59
1	C	275	THR	CA-CB-OG1	-6.99	99.12	109.60
2	B	96	ARG	O-C-N	-6.95	114.83	121.57
1	A	41	HIS	ND1-CG-CD2	6.93	113.03	106.10
2	D	148	ASN	CB-CG-ND2	6.93	126.80	116.40
2	B	73	GLN	OE1-CD-NE2	-6.92	115.68	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	57	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	309	VAL	O-C-N	6.90	131.19	122.57
1	C	306	ARG	CB-CA-C	-6.87	100.00	110.92
2	D	107	LEU	N-CA-CB	6.86	122.08	110.49
1	A	78	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	134	HIS	CA-CB-CG	6.83	120.63	113.80
1	C	116	THR	N-CA-CB	-6.83	99.36	110.14
1	A	134	HIS	CB-CG-CD2	-6.81	122.34	131.20
2	D	133	ASP	CA-CB-CG	6.81	119.41	112.60
2	D	55	ARG	N-CA-C	-6.81	98.00	108.76
1	C	307	ASP	N-CA-C	-6.80	97.27	108.76
2	B	152	ALA	CA-C-N	6.79	133.91	121.70
2	B	152	ALA	C-N-CA	6.79	133.91	121.70
1	C	97	THR	OG1-CB-CG2	6.78	122.86	109.30
1	A	83	LYS	N-CA-C	6.77	125.22	110.80
2	B	10	GLU	CA-CB-CG	6.77	127.64	114.10
1	C	260	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	C	296	ARG	CB-CG-CD	6.76	126.84	111.30
1	C	162	ASP	N-CA-C	-6.76	96.64	108.20
2	D	117	HIS	N-CA-C	6.73	118.27	111.07
1	A	275	THR	CA-CB-OG1	-6.72	99.51	109.60
2	D	106	VAL	N-CA-CB	-6.71	103.35	111.00
2	B	106	VAL	N-CA-CB	-6.71	96.31	111.87
1	A	56	ARG	NE-CZ-NH2	-6.64	113.23	119.20
2	D	3	HIS	N-CA-C	-6.62	96.69	110.80
1	A	225	LEU	O-C-N	-6.58	115.22	123.05
1	A	198	ILE	N-CA-C	-6.55	104.10	110.72
1	A	95	ILE	O-C-N	-6.55	115.28	121.90
1	C	152	LEU	N-CA-C	-6.53	103.29	113.02
1	C	280	THR	O-C-N	-6.53	114.22	121.53
1	A	265	HIS	CG-CD2-NE2	-6.52	100.68	107.20
1	A	306	ARG	N-CA-C	6.51	118.46	111.36
1	C	222	VAL	N-CA-CB	-6.50	103.19	110.99
1	C	296	ARG	CD-NE-CZ	6.50	133.50	124.40
1	C	280	THR	CB-CA-C	6.49	121.20	109.45
1	C	74	SER	N-CA-C	-6.49	99.63	109.95
2	B	134	ILE	N-CA-C	6.48	122.83	109.34
1	A	287	GLN	CG-CD-NE2	6.47	126.11	116.40
2	D	69	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	236	ASP	N-CA-C	-6.46	101.40	110.31
2	B	10	GLU	N-CA-C	6.45	117.95	108.86
1	C	284	TRP	CB-CG-CD1	-6.42	117.27	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	55	ARG	O-C-N	-6.42	116.29	123.48
2	B	13	LYS	O-C-N	6.41	130.70	123.27
1	C	222	VAL	CA-CB-CG2	-6.39	99.53	110.40
1	C	93	SER	N-CA-C	-6.38	104.42	111.82
1	C	76	SER	N-CA-C	-6.37	102.60	111.52
2	B	10	GLU	N-CA-CB	-6.35	100.71	111.31
1	C	59	PHE	N-CA-C	-6.34	104.29	111.14
1	A	168	THR	O-C-N	-6.34	114.47	122.27
2	D	21	ILE	CA-C-N	6.33	127.75	119.84
2	D	21	ILE	C-N-CA	6.33	127.75	119.84
1	C	72	GLY	CA-C-O	-6.31	115.39	121.83
1	A	116	THR	CA-CB-OG1	-6.30	100.14	109.60
2	B	33	PHE	CA-CB-CG	-6.30	107.50	113.80
1	A	288	GLN	CA-C-O	-6.30	114.39	121.00
1	A	178	LYS	N-CA-C	-6.29	105.43	113.23
2	D	3	HIS	O-C-N	6.27	130.93	122.59
1	C	129	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	200	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	246	GLN	N-CA-C	6.24	124.09	110.80
2	D	9	VAL	CB-CA-C	-6.24	101.42	111.59
1	A	76	SER	N-CA-C	-6.23	99.04	109.07
2	D	131	ALA	O-C-N	6.21	130.85	122.59
1	C	246	GLN	CA-C-O	6.20	128.72	121.78
2	D	11	ALA	N-CA-C	-6.20	100.23	109.15
1	C	23	VAL	N-CA-C	-6.18	104.32	110.62
1	A	107	PRO	N-CA-C	6.17	121.58	113.86
2	B	119	GLU	N-CA-C	6.16	118.17	108.55
1	C	136	THR	CB-CA-C	6.16	122.95	110.38
1	C	106	HIS	O-C-N	-6.16	117.54	121.85
1	A	307	ASP	CA-CB-CG	6.13	118.73	112.60
2	B	73	GLN	N-CA-C	-6.13	105.06	112.54
2	D	109	CYS	CA-C-N	6.10	126.28	119.32
2	D	109	CYS	C-N-CA	6.10	126.28	119.32
1	C	141	ASP	CA-CB-CG	6.10	118.70	112.60
2	B	132	ASN	CA-C-N	6.10	133.19	121.54
2	B	132	ASN	C-N-CA	6.10	133.19	121.54
2	D	148	ASN	OD1-CG-ND2	-6.08	116.52	122.60
2	D	73	GLN	CB-CG-CD	6.07	122.92	112.60
1	A	307	ASP	N-CA-C	-6.07	99.11	109.24
1	C	78	ASN	OD1-CG-ND2	-6.05	116.55	122.60
2	D	22	PRO	N-CA-C	6.04	124.92	112.47
1	A	18	ASP	CA-CB-CG	6.04	118.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	63	ASN	CB-CG-ND2	6.03	125.45	116.40
1	A	116	THR	N-CA-CB	-6.01	100.33	110.49
1	C	269	ARG	N-CA-C	-6.00	99.46	109.24
2	D	19	ASP	N-CA-CB	-5.99	101.90	111.43
2	B	131	ALA	N-CA-C	5.99	123.55	110.80
1	C	74	SER	O-C-N	-5.99	115.61	123.16
2	D	84	ASN	OD1-CG-ND2	-5.99	116.61	122.60
2	B	47	ASN	CA-CB-CG	5.98	118.58	112.60
2	D	96	ARG	CA-C-N	5.97	126.17	119.90
2	D	96	ARG	C-N-CA	5.97	126.17	119.90
1	A	32	ALA	N-CA-C	5.97	117.87	111.36
1	C	52	SER	O-C-N	-5.97	118.01	123.50
1	A	53	THR	N-CA-CB	-5.96	101.11	110.06
1	A	203	ASP	CA-C-O	-5.94	113.64	120.24
1	C	56	ARG	CB-CG-CD	-5.94	97.63	111.30
2	D	80	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	C	192	LEU	CA-C-N	5.91	129.51	120.82
1	C	192	LEU	C-N-CA	5.91	129.51	120.82
2	B	5	ASN	O-C-N	-5.90	114.74	122.59
2	B	13	LYS	CA-CB-CG	5.90	125.89	114.10
2	D	3	HIS	CA-C-N	5.89	132.78	121.54
2	D	3	HIS	C-N-CA	5.89	132.78	121.54
2	D	147	HIS	CG-CD2-NE2	-5.88	101.32	107.20
1	C	134	HIS	CG-CD2-NE2	-5.87	101.33	107.20
2	B	52	GLU	N-CA-C	5.87	123.30	110.80
1	C	306	ARG	CA-CB-CG	5.87	125.83	114.10
2	B	10	GLU	CA-C-N	5.86	132.74	121.54
2	B	10	GLU	C-N-CA	5.86	132.74	121.54
1	C	168	THR	O-C-N	-5.86	115.47	122.15
1	C	296	ARG	CG-CD-NE	-5.86	99.10	112.00
1	C	98	TYR	N-CA-C	5.86	122.42	112.99
2	D	106	VAL	CA-C-O	-5.85	113.81	120.65
1	A	118	PHE	O-C-N	-5.84	115.49	122.27
1	C	68	ALA	O-C-N	-5.84	116.40	122.94
1	A	261	MET	N-CA-C	-5.84	101.64	110.28
1	A	10	ILE	CB-CG1-CD1	-5.83	101.56	113.80
1	A	247	PHE	CA-CB-CG	5.81	119.61	113.80
2	B	53	MET	N-CA-C	-5.80	98.44	110.80
1	C	170	HIS	N-CA-C	-5.80	105.04	111.36
2	D	90	GLU	CB-CG-CD	5.80	122.46	112.60
2	D	6	LYS	O-C-N	5.79	129.20	121.67
2	D	87	ASP	CA-CB-CG	5.79	118.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	33	PHE	CA-CB-CG	-5.78	108.02	113.80
1	C	291	ASN	CB-CG-ND2	5.77	125.05	116.40
1	A	285	TYR	N-CA-C	5.74	118.31	111.71
1	C	21	ASN	OD1-CG-ND2	-5.73	116.87	122.60
2	D	139	LYS	CB-CG-CD	-5.73	98.13	111.30
1	A	233	GLU	CA-CB-CG	5.72	125.55	114.10
1	A	279	LYS	CA-CB-CG	-5.72	102.67	114.10
1	C	43	VAL	N-CA-C	-5.71	99.89	108.12
1	C	95	ILE	O-C-N	-5.71	116.33	121.87
2	D	103	ILE	N-CA-C	-5.70	99.33	107.77
2	D	121	VAL	N-CA-CB	-5.70	101.95	112.43
1	C	97	THR	CA-CB-OG1	-5.69	101.06	109.60
2	D	105	ASN	CB-CA-C	-5.67	99.14	110.42
2	B	73	GLN	CB-CG-CD	5.66	122.22	112.60
1	C	178	LYS	CA-CB-CG	-5.66	102.79	114.10
1	A	78	ASN	CA-C-N	5.65	132.33	121.54
1	A	78	ASN	C-N-CA	5.65	132.33	121.54
2	D	121	VAL	CB-CA-C	5.64	119.26	111.19
2	D	146	SER	CA-C-O	-5.64	115.57	121.55
2	B	128	ARG	N-CA-C	5.64	117.41	108.79
1	A	182	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	C	188	ALA	CA-C-N	5.63	125.63	119.89
1	C	188	ALA	C-N-CA	5.63	125.63	119.89
2	B	75	ALA	N-CA-C	5.62	118.17	111.71
1	C	282	HIS	ND1-CG-CD2	5.62	111.72	106.10
2	B	105	ASN	CA-CB-CG	-5.61	106.99	112.60
1	C	250	ARG	CA-CB-CG	5.60	125.30	114.10
1	A	33	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	A	91	THR	N-CA-C	-5.60	105.08	111.07
2	B	134	ILE	CB-CA-C	-5.59	102.12	111.29
2	B	2	THR	N-CA-C	-5.58	98.92	110.80
1	A	134	HIS	O-C-N	-5.56	117.13	121.19
1	C	236	ASP	CA-C-N	5.56	125.03	119.24
1	C	236	ASP	C-N-CA	5.56	125.03	119.24
2	B	1	MET	CA-C-N	5.55	132.14	121.54
2	B	1	MET	C-N-CA	5.55	132.14	121.54
2	D	38	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	216	GLU	CA-CB-CG	5.54	125.18	114.10
1	C	282	HIS	CG-CD2-NE2	-5.54	101.66	107.20
1	C	134	HIS	CB-CG-CD2	-5.53	124.02	131.20
2	B	82	THR	O-C-N	-5.52	116.01	123.19
1	C	87	THR	N-CA-C	5.52	117.66	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23	ALA	N-CA-C	-5.52	99.04	110.80
1	C	158	ALA	CA-C-O	-5.51	114.68	120.80
1	A	133	GLN	CA-C-N	5.50	127.49	122.37
1	A	133	GLN	C-N-CA	5.50	127.49	122.37
1	C	78	ASN	N-CA-C	5.50	122.51	110.80
1	C	118	PHE	CA-CB-CG	-5.50	108.30	113.80
2	D	50	SER	N-CA-C	-5.49	97.28	107.71
1	C	106	HIS	CG-CD2-NE2	-5.47	101.73	107.20
1	C	265	HIS	ND1-CG-CD2	5.47	111.57	106.10
2	D	58	LEU	O-C-N	-5.47	117.19	123.42
1	A	74	SER	O-C-N	-5.47	116.60	123.27
1	C	140	LEU	CD1-CG-CD2	-5.46	98.79	110.80
1	A	7	LYS	CA-CB-CG	5.46	125.02	114.10
1	C	264	LEU	O-C-N	-5.45	116.30	123.16
1	A	106	HIS	ND1-CG-CD2	5.44	111.54	106.10
2	B	84	ASN	CA-CB-CG	-5.42	107.18	112.60
1	C	218	VAL	CA-CB-CG2	-5.42	101.18	110.40
1	C	267	LEU	O-C-N	-5.42	115.08	121.32
1	C	231	GLN	OE1-CD-NE2	-5.42	117.18	122.60
2	D	84	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	171	SER	CA-CB-OG	5.42	121.93	111.10
1	C	53	THR	N-CA-C	5.41	117.60	111.11
1	C	122	VAL	N-CA-C	-5.41	102.30	107.76
2	B	23	ALA	N-CA-CB	5.40	119.61	110.49
1	C	166	GLY	CA-C-N	5.39	128.04	120.28
1	C	166	GLY	C-N-CA	5.39	128.04	120.28
1	C	71	VAL	CB-CA-C	-5.38	103.15	110.90
2	D	153	ASN	CB-CG-ND2	5.38	124.48	116.40
1	C	167	ARG	N-CA-CB	-5.38	101.94	110.22
1	A	156	HIS	CA-CB-CG	5.37	119.17	113.80
2	B	127	VAL	CA-C-O	-5.37	114.67	121.48
1	C	117	GLU	CB-CG-CD	5.37	121.72	112.60
1	A	197	TYR	CA-CB-CG	5.35	123.53	113.90
2	D	107	LEU	CB-CA-C	-5.34	99.80	110.42
1	C	108	GLN	CA-CB-CG	-5.33	103.43	114.10
1	C	229	ARG	CA-CB-CG	5.33	124.77	114.10
1	C	12	ILE	CB-CG1-CD1	5.33	124.98	113.80
1	C	21	ASN	CB-CG-ND2	5.31	124.37	116.40
1	C	285	TYR	N-CA-C	5.29	117.96	111.82
1	C	104	MET	N-CA-C	5.28	117.78	108.75
1	A	179	PHE	O-C-N	-5.27	115.39	122.14
1	C	62	SER	CB-CA-C	-5.27	101.72	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	25	ILE	CA-C-N	5.27	125.95	119.99
2	D	25	ILE	C-N-CA	5.27	125.95	119.99
2	D	7	LEU	N-CA-C	-5.27	104.75	110.91
1	C	253	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	293	ILE	O-C-N	-5.26	116.77	121.87
1	A	301	ALA	N-CA-C	-5.25	105.47	111.14
2	D	56	LYS	N-CA-C	5.25	115.99	108.74
1	C	305	ASN	OD1-CG-ND2	-5.25	117.35	122.60
2	D	99	LEU	O-C-N	-5.25	117.08	121.38
2	B	133	ASP	N-CA-C	5.25	121.97	110.80
1	C	305	ASN	N-CA-C	5.24	116.94	108.41
1	A	170	HIS	N-CA-C	-5.23	105.49	111.14
2	D	121	VAL	CA-CB-CG2	-5.23	101.51	110.40
1	C	307	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	180	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	82	GLY	N-CA-C	-5.21	108.43	115.21
1	C	10	ILE	N-CA-CB	-5.21	104.76	111.90
1	A	53	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	83	LYS	CA-C-N	5.20	131.47	121.54
1	A	83	LYS	C-N-CA	5.20	131.47	121.54
1	C	296	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	C	8	HIS	CG-CD2-NE2	-5.20	102.00	107.20
1	A	242	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	284	TRP	CE2-CD2-CG	-5.16	101.00	107.20
1	C	83	LYS	N-CA-C	-5.16	103.22	110.50
1	C	244	LYS	CA-C-O	-5.15	113.58	119.60
1	C	136	THR	N-CA-C	-5.15	105.75	112.23
1	C	189	PRO	N-CA-CB	5.14	107.64	103.32
1	A	92	ILE	CA-C-O	-5.14	115.34	121.05
2	D	153	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	C	162	ASP	CA-CB-CG	5.14	117.74	112.60
2	B	4	ASP	CA-C-N	5.13	131.35	121.54
2	B	4	ASP	C-N-CA	5.13	131.35	121.54
1	C	26	THR	CA-CB-CG2	5.13	119.23	110.50
1	C	269	ARG	NE-CZ-NH1	5.13	126.63	121.50
2	B	133	ASP	CA-C-N	5.12	131.19	121.97
2	B	133	ASP	C-N-CA	5.12	131.19	121.97
1	A	265	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	A	189	PRO	CA-C-O	-5.12	115.76	121.23
1	C	184	PHE	N-CA-C	5.12	117.83	109.59
2	D	88	ASN	CB-CA-C	-5.11	105.09	111.43
1	A	116	THR	CA-CB-CG2	5.11	119.18	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	LEU	N-CA-C	5.10	116.84	111.28
1	A	235	LEU	N-CA-C	-5.10	101.66	109.41
1	A	209	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	A	173	THR	O-C-N	-5.09	116.34	122.15
1	C	273	ILE	N-CA-C	-5.09	100.24	107.77
1	C	193	ALA	N-CA-C	5.08	116.84	110.24
1	C	243	VAL	N-CA-CB	-5.08	102.85	111.23
2	B	52	GLU	CA-C-O	5.07	127.76	120.51
2	B	66	LEU	N-CA-C	-5.07	101.61	109.72
2	B	119	GLU	O-C-N	-5.07	118.47	121.71
2	D	60	LYS	N-CA-C	-5.06	100.16	108.41
1	C	80	SER	N-CA-CB	-5.06	101.94	110.49
1	A	173	THR	N-CA-C	-5.04	105.86	111.36
2	D	151	LEU	N-CA-C	5.04	118.69	112.54
2	B	150	VAL	O-C-N	5.04	126.96	121.87
1	A	275	THR	CA-CB-CG2	5.04	119.06	110.50
1	C	82	GLY	CA-C-O	5.04	124.59	119.10
1	A	82	GLY	CA-C-N	5.03	131.15	121.54
1	A	82	GLY	C-N-CA	5.03	131.15	121.54
1	C	71	VAL	O-C-N	-5.03	117.59	122.97
1	C	260	ASN	CA-CB-CG	5.03	117.63	112.60
1	C	209	TRP	CE2-CD2-CG	-5.03	101.17	107.20
2	D	70	GLN	OE1-CD-NE2	-5.03	117.58	122.60
1	C	279	LYS	CB-CG-CD	-5.02	99.76	111.30
1	C	306	ARG	N-CA-C	5.01	117.14	111.02
1	A	82	GLY	N-CA-C	-5.01	108.69	115.21
2	B	73	GLN	CG-CD-NE2	5.01	123.92	116.40
1	C	243	VAL	CB-CA-C	5.00	119.50	111.29
1	C	209	TRP	CB-CG-CD1	-5.00	119.40	126.90
2	D	80	GLN	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	294	PHE	Sidechain
1	A	48	PHE	Sidechain
1	A	98	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	118	PHE	Sidechain
2	D	3	HIS	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	38	0
1	C	2415	0	2422	35	0
2	B	1196	0	1212	32	0
2	D	1196	0	1212	29	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	29	0	12	1	0
4	D	29	0	12	1	0
5	A	31	0	0	0	0
5	B	10	0	0	0	0
5	C	43	0	0	1	0
5	D	9	0	0	2	0
All	All	7375	0	7292	129	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 9.

All (129) 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)
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.65	0.79
2:B:6:LYS:HA	2:B:9:VAL:HG22	1.63	0.79
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.67	0.76
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.00	0.74
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.24	0.73
1:A:159:MET:HE3	1:A:169:VAL:HB	1.70	0.73
1:A:106:HIS:HD2	1:A:108:GLN:H	1.36	0.72
1:C:277:VAL:O	1:C:280:THR:HB	1.91	0.70
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.74	0.69
2:B:14:ARG:HA	2:B:86:ILE:O	1.96	0.65
2:B:48:LEU:O	2:B:55:ARG:HA	1.97	0.64
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.62	0.64
2:B:6:LYS:HZ2	2:D:12:ILE:HG22	1.62	0.63
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.82	0.61
2:B:3:HIS:O	2:B:10:GLU:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.82	0.61
1:A:262:LYS:HE2	1:A:284:TRP:CE3	2.36	0.61
2:B:14:ARG:NH1	2:B:63:ASN:HA	2.16	0.61
2:D:85:ARG:HG3	2:D:92:VAL:HG12	1.83	0.60
1:A:248:VAL:HG12	1:A:272:GLU:HA	1.83	0.60
1:C:256:ASN:ND2	1:C:256:ASN:H	1.99	0.60
1:C:94:VAL:O	1:C:97:THR:HB	2.01	0.60
1:A:159:MET:HE1	1:A:173:THR:OG1	2.02	0.59
2:B:67:SER:HA	2:B:71:VAL:HG23	1.83	0.58
1:C:136:THR:HG23	1:C:296:ARG:HD3	1.85	0.58
1:C:113:ARG:O	1:C:116:THR:HB	2.03	0.58
2:B:21:ILE:HG22	2:B:25:ILE:HB	1.86	0.57
2:B:6:LYS:HE3	2:D:10:GLU:HB3	1.85	0.57
2:B:38:THR:HG22	2:B:40:GLN:H	1.69	0.57
2:D:124:SER:HB3	2:D:139:LYS:HD2	1.87	0.57
2:B:2:THR:HG22	2:B:11:ALA:HB3	1.87	0.57
2:B:86:ILE:HG13	2:B:91:VAL:HA	1.87	0.57
1:A:151:ARG:HD2	1:A:153:ASP:O	2.06	0.56
1:A:287:GLN:NE2	1:A:287:GLN:H	2.03	0.56
1:C:136:THR:HG23	1:C:296:ARG:HH11	1.69	0.56
1:C:246:GLN:HA	1:C:248:VAL:HG12	1.87	0.56
2:B:25:ILE:HG22	2:B:29:LEU:HG	1.88	0.55
2:D:25:ILE:HD13	2:D:77:TYR:O	2.07	0.55
2:B:65:PHE:CE1	2:B:85:ARG:HG3	2.42	0.55
2:D:5:ASN:HB3	2:D:6:LYS:HG2	1.88	0.54
1:C:292:GLY:O	1:C:296:ARG:HG2	2.06	0.54
1:C:97:THR:HG22	1:C:98:TYR:HD2	1.71	0.54
1:C:151:ARG:HD2	1:C:153:ASP:O	2.09	0.53
2:B:76:LEU:HD13	2:B:151:LEU:HD11	1.89	0.53
1:A:29:LYS:HD2	1:A:310:LEU:HG	1.91	0.53
2:B:14:ARG:HH11	2:B:14:ARG:HG2	1.74	0.53
2:D:42:ILE:HG12	2:D:61:ILE:HG23	1.91	0.52
1:A:198:ILE:O	1:A:202:LEU:HG	2.10	0.52
1:C:29:LYS:HD3	1:C:310:LEU:HB2	1.90	0.52
2:D:89:TYR:C	4:D:999:CTP:HN42	2.17	0.52
2:B:6:LYS:NZ	2:D:12:ILE:HG22	2.25	0.51
2:D:131:ALA:O	2:D:132:ASN:HB2	2.10	0.51
1:A:106:HIS:CD2	1:A:108:GLN:H	2.23	0.51
1:A:205:LYS:HB2	1:A:207:ILE:HD12	1.92	0.51
1:C:229:ARG:HD2	1:C:268:PRO:O	2.10	0.51
2:D:59:ILE:HG22	2:D:61:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:PHE:CD1	2:B:85:ARG:HG3	2.46	0.51
2:D:14:ARG:HG3	2:D:87:ASP:HA	1.93	0.51
2:B:21:ILE:HB	2:B:57:ASP:HB2	1.94	0.50
1:C:136:THR:HB	5:C:316:HOH:O	2.11	0.50
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.26	0.50
1:C:215:ILE:HG22	1:C:219:MET:HE2	1.94	0.49
1:C:40:LYS:O	1:C:41:HIS:HB2	2.12	0.49
1:A:185:TYR:HD1	1:A:212:HIS:NE2	2.10	0.49
2:D:56:LYS:HB3	5:D:1007:HOH:O	2.11	0.49
1:A:5:TYR:CZ	1:A:306:ARG:HG2	2.48	0.49
1:A:166:GLY:O	1:A:169:VAL:HG22	2.13	0.48
1:C:10:ILE:HD11	1:C:116:THR:OG1	2.13	0.48
1:C:163:LEU:HD13	1:C:194:MET:HE2	1.95	0.48
2:B:129:LYS:HG2	2:B:132:ASN:OD1	2.13	0.48
1:A:113:ARG:O	1:A:116:THR:HB	2.13	0.48
1:C:160:VAL:HG22	1:C:187:ILE:HB	1.95	0.48
2:B:7:LEU:H	2:B:7:LEU:HD23	1.79	0.47
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.15	0.47
2:B:136:LEU:HD12	2:B:147:HIS:HA	1.96	0.47
1:C:189:PRO:HB3	1:C:244:LYS:HD3	1.96	0.47
1:A:227:MET:HE3	1:A:227:MET:HB3	1.81	0.47
1:A:292:GLY:O	1:A:296:ARG:HG3	2.14	0.47
2:B:11:ALA:HA	4:B:999:CTP:N3	2.29	0.47
1:C:1:ALA:HA	1:C:306:ARG:O	2.15	0.47
2:D:6:LYS:HB2	2:D:9:VAL:HG22	1.96	0.47
2:B:4:ASP:HA	2:B:10:GLU:HB3	1.97	0.46
1:C:80:SER:O	1:C:83:LYS:HB2	2.15	0.46
1:A:185:TYR:HD1	1:A:212:HIS:HE2	1.62	0.46
1:A:287:GLN:H	1:A:287:GLN:HE21	1.62	0.46
1:C:73:PHE:CE2	1:C:81:LEU:HD21	2.52	0.45
1:C:59:PHE:CE2	1:C:136:THR:HG21	2.51	0.45
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.99	0.45
1:C:162:ASP:H	1:C:228:THR:HG22	1.81	0.45
1:A:189:PRO:CG	1:A:192:LEU:HD12	2.48	0.44
1:C:305:ASN:ND2	1:C:307:ASP:O	2.50	0.44
1:A:209:TRP:HZ3	1:A:211:LEU:HD11	1.81	0.44
1:A:5:TYR:CD1	1:A:306:ARG:HA	2.52	0.44
1:C:227:MET:HE3	1:C:227:MET:HB3	1.77	0.44
1:A:246:GLN:C	1:A:247:PHE:HD1	2.26	0.44
1:A:76:SER:O	1:A:78:ASN:HB2	2.18	0.44
2:B:44:ILE:HG23	2:B:59:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LEU:HD22	2:B:150:VAL:HG12	2.01	0.43
1:C:305:ASN:HD22	1:C:308:LEU:HD12	1.84	0.43
2:B:48:LEU:HD23	2:D:41:ARG:HD3	1.99	0.43
2:D:99:LEU:HG	2:D:127:VAL:HG11	2.00	0.43
2:D:22:PRO:HB2	2:D:25:ILE:HD12	2.01	0.43
1:A:81:LEU:HD12	1:A:91:THR:OG1	2.19	0.42
1:A:142:LEU:HD22	1:A:152:LEU:HD13	1.99	0.42
2:D:20:HIS:HB2	5:D:1008:HOH:O	2.18	0.42
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.34	0.42
2:D:5:ASN:HB3	2:D:6:LYS:HE3	2.01	0.42
2:B:22:PRO:HA	2:B:53:MET:SD	2.60	0.42
2:D:119:GLU:HB3	2:D:120:PRO:CD	2.49	0.42
1:C:20:LEU:HD23	1:C:20:LEU:HA	1.86	0.42
2:D:3:HIS:O	2:D:5:ASN:N	2.53	0.42
1:C:176:LEU:HA	1:C:176:LEU:HD23	1.88	0.41
1:A:185:TYR:CD1	1:A:218:VAL:HG11	2.54	0.41
1:C:166:GLY:O	1:C:169:VAL:HG22	2.20	0.41
2:B:41:ARG:HA	2:D:46:LEU:O	2.21	0.41
1:A:81:LEU:HD12	1:A:91:THR:HG23	2.02	0.41
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.92	0.41
2:D:13:LYS:HB3	2:D:13:LYS:HE2	1.88	0.41
2:D:72:ASP:HB3	2:D:100:PRO:HB3	2.02	0.41
2:B:22:PRO:HB2	2:B:25:ILE:HG13	2.02	0.41
2:D:6:LYS:HB2	2:D:9:VAL:HG13	2.03	0.41
1:A:4:LEU:HD23	1:A:7:LYS:HD2	2.03	0.41
1:A:308:LEU:HG	1:A:310:LEU:CD2	2.45	0.41
2:D:111:ASN:O	2:D:117:HIS:CE1	2.74	0.41
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.82	0.41
1:C:238:SER:O	1:C:242:ASN:HB2	2.20	0.40
2:D:130:ARG:HD3	2:D:130:ARG:HA	1.75	0.40
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.85	0.40
1:A:189:PRO:HG2	1:A:192:LEU:HD12	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	A	308/310 (99%)	283 (92%)	19 (6%)	6 (2%)	6	11
1	C	308/310 (99%)	285 (92%)	19 (6%)	4 (1%)	9	18
2	B	151/153 (99%)	121 (80%)	19 (13%)	11 (7%)	1	1
2	D	151/153 (99%)	123 (82%)	17 (11%)	11 (7%)	1	1
All	All	918/926 (99%)	812 (88%)	74 (8%)	32 (4%)	3	4

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	83	LYS
2	B	3	HIS
2	B	23	ALA
2	B	53	MET
2	B	131	ALA
2	B	133	ASP
1	C	77	ALA
1	C	78	ASN
1	C	80	SER
1	C	242	ASN
2	D	4	ASP
2	D	10	GLU
2	D	89	TYR
2	D	107	LEU
1	A	79	THR
1	A	84	LYS
2	B	11	ALA
2	B	14	ARG
2	D	132	ASN
1	A	246	GLN
2	B	2	THR
2	D	23	ALA
2	D	131	ALA
2	B	5	ASN
2	B	68	GLU
2	D	22	PRO
2	B	52	GLU

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Mol	Chain	Res	Type
2	D	5	ASN
2	D	24	GLN
1	A	77	ALA
2	D	68	GLU

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	261/261 (100%)	227 (87%)	34 (13%)	4	8
1	C	261/261 (100%)	222 (85%)	39 (15%)	3	6
2	B	136/137 (99%)	115 (85%)	21 (15%)	2	5
2	D	136/137 (99%)	118 (87%)	18 (13%)	4	8
All	All	794/796 (100%)	682 (86%)	112 (14%)	3	7

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	13	ASN
1	A	35	GLN
1	A	56	ARG
1	A	57	LEU
1	A	65	ARG
1	A	75	ASP
1	A	78	ASN
1	A	79	THR
1	A	86	GLU
1	A	87	THR
1	A	114	LEU
1	A	124	VAL
1	A	151	ARG
1	A	159	MET
1	A	167	ARG
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	210	SER
1	A	211	LEU
1	A	222	VAL
1	A	225	LEU
1	A	228	THR
1	A	231	GLN
1	A	233	GLU
1	A	235	LEU
1	A	243	VAL
1	A	262	LYS
1	A	269	ARG
1	A	275	THR
1	A	285	TYR
1	A	287	GLN
1	A	305	ASN
1	A	309	VAL
1	A	310	LEU
2	B	1	MET
2	B	2	THR
2	B	6	LYS
2	B	7	LEU
2	B	13	LYS
2	B	20	HIS
2	B	22	PRO
2	B	30	LEU
2	B	32	LEU
2	B	37	GLU
2	B	58	LEU
2	B	67	SER
2	B	68	GLU
2	B	69	ASP
2	B	73	GLN
2	B	86	ILE
2	B	98	SER
2	B	99	LEU
2	B	106	VAL
2	B	115	ILE
2	B	151	LEU
1	C	6	GLN
1	C	12	ILE
1	C	17	ARG
1	C	37	GLU

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Mol	Chain	Res	Type
1	C	44	ILE
1	C	54	ARG
1	C	59	PHE
1	C	65	ARG
1	C	74	SER
1	C	78	ASN
1	C	79	THR
1	C	83	LYS
1	C	97	THR
1	C	125	LEU
1	C	136	THR
1	C	152	LEU
1	C	153	ASP
1	C	180	ASP
1	C	190	ASP
1	C	211	LEU
1	C	218	VAL
1	C	222	VAL
1	C	227	MET
1	C	228	THR
1	C	235	LEU
1	C	236	ASP
1	C	237	PRO
1	C	246	GLN
1	C	248	VAL
1	C	252	SER
1	C	255	HIS
1	C	256	ASN
1	C	269	ARG
1	C	272	GLU
1	C	280	THR
1	C	285	TYR
1	C	287	GLN
1	C	303	VAL
1	C	310	LEU
2	D	2	THR
2	D	3	HIS
2	D	4	ASP
2	D	7	LEU
2	D	9	VAL
2	D	10	GLU
2	D	41	ARG

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Mol	Chain	Res	Type
2	D	55	ARG
2	D	60	LYS
2	D	66	LEU
2	D	85	ARG
2	D	92	VAL
2	D	96	ARG
2	D	98	SER
2	D	121	VAL
2	D	130	ARG
2	D	132	ASN
2	D	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	106	HIS
1	A	149	GLN
1	A	196	GLN
1	A	282	HIS
1	A	287	GLN
2	B	70	GLN
1	C	149	GLN
1	C	256	ASN
1	C	260	ASN
1	C	282	HIS
1	C	287	GLN
1	C	305	ASN
2	D	5	ASN
2	D	24	GLN
2	D	148	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	CTP	B	999	-	29,30,30	2.28	8 (27%)	43,47,47	1.39	6 (13%)
4	CTP	D	999	-	29,30,30	2.20	10 (34%)	43,47,47	1.23	5 (11%)

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	CTP	B	999	-	-	5/22/38/38	0/2/2/2
4	CTP	D	999	-	-	3/22/38/38	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	CTP	PB-O3B	6.93	1.67	1.59
4	D	999	CTP	PB-O3B	6.04	1.66	1.59
4	B	999	CTP	PA-O3A	5.32	1.65	1.59
4	B	999	CTP	PB-O3A	5.28	1.65	1.59
4	D	999	CTP	PB-O3A	5.21	1.65	1.59
4	D	999	CTP	PA-O3A	4.91	1.64	1.59
4	D	999	CTP	PG-O1G	2.64	1.58	1.50
4	B	999	CTP	PG-O1G	2.53	1.58	1.50
4	B	999	CTP	C6-N1	-2.47	1.32	1.38
4	D	999	CTP	C6-N1	-2.42	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	C5-C4	-2.42	1.37	1.42
4	D	999	CTP	PB-O1B	2.26	1.58	1.50
4	B	999	CTP	C2-N1	-2.25	1.35	1.40
4	D	999	CTP	C2-N1	-2.15	1.35	1.40
4	B	999	CTP	PB-O1B	2.14	1.58	1.50
4	B	999	CTP	C5-C4	-2.07	1.38	1.42
4	D	999	CTP	C2-N3	-2.00	1.32	1.36
4	D	999	CTP	C4-N3	-2.00	1.30	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	CTP	O2-C2-N3	-4.82	114.73	122.33
4	D	999	CTP	O2-C2-N3	-4.37	115.45	122.33
4	B	999	CTP	N1-C2-N3	3.33	124.58	118.80
4	B	999	CTP	C6-N1-C2	-2.80	115.74	120.46
4	D	999	CTP	N1-C2-N3	2.75	123.57	118.80
4	D	999	CTP	C6-N1-C2	-2.66	115.97	120.46
4	B	999	CTP	O4'-C1'-N1	2.24	113.43	108.36
4	D	999	CTP	O4'-C1'-N1	2.10	113.11	108.36
4	B	999	CTP	C5'-C4'-C3'	-2.05	107.82	115.21
4	B	999	CTP	O2A-PA-O3A	2.03	112.75	107.27
4	D	999	CTP	O2'-C2'-C1'	-2.02	103.13	110.10

There are no chirality outliers.

All (8) torsion outliers are listed below:

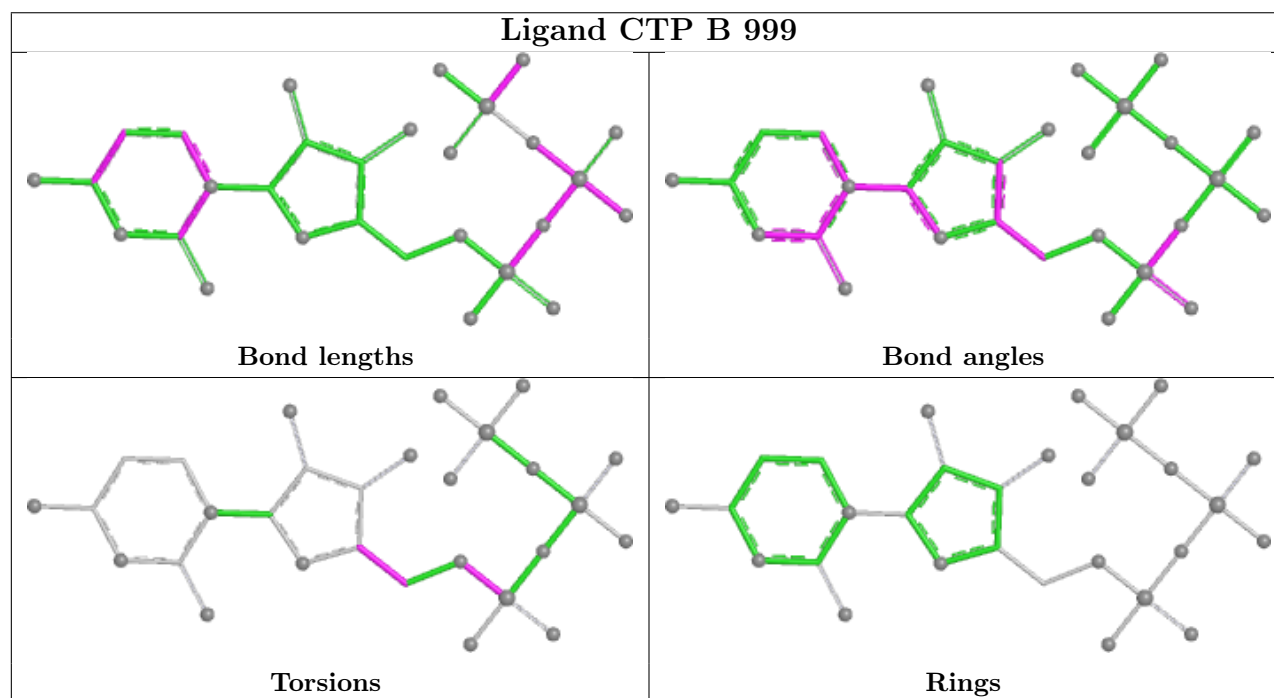
Mol	Chain	Res	Type	Atoms
4	B	999	CTP	O4'-C4'-C5'-O5'
4	B	999	CTP	C5'-O5'-PA-O1A
4	B	999	CTP	C5'-O5'-PA-O2A
4	B	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	O4'-C4'-C5'-O5'
4	D	999	CTP	PB-O3A-PA-O5'
4	D	999	CTP	C3'-C4'-C5'-O5'
4	B	999	CTP	C5'-O5'-PA-O3A

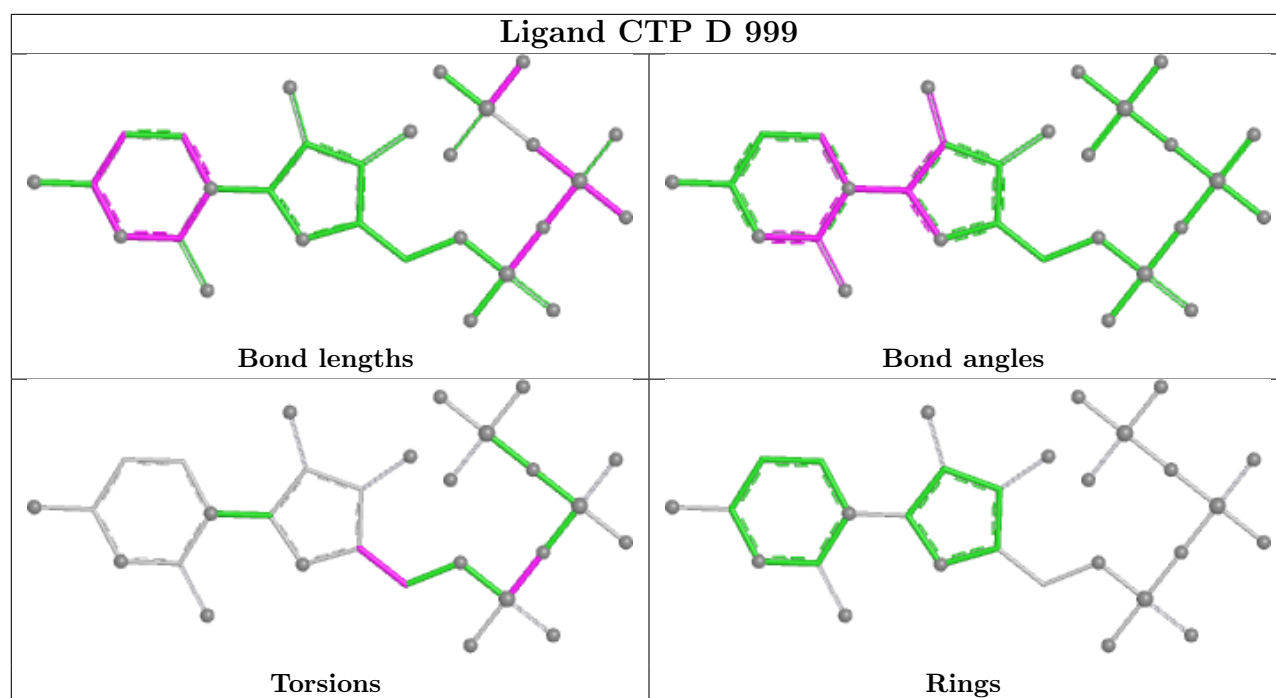
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	CTP	1	0
4	D	999	CTP	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.