



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:54 AM UTC

PDB ID : 1RAE / pdb_00001rae
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

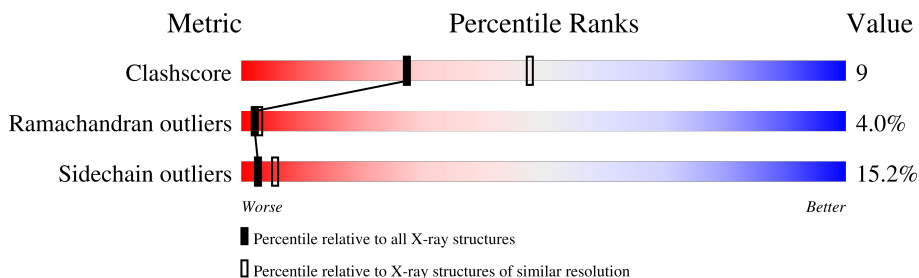
1 Overall quality at a glance

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	55% 32% 11% •
1	C	310	51% 37% 10% •
2	B	153	49% 28% 19% •
2	D	153	48% 33% 13% 6%

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			

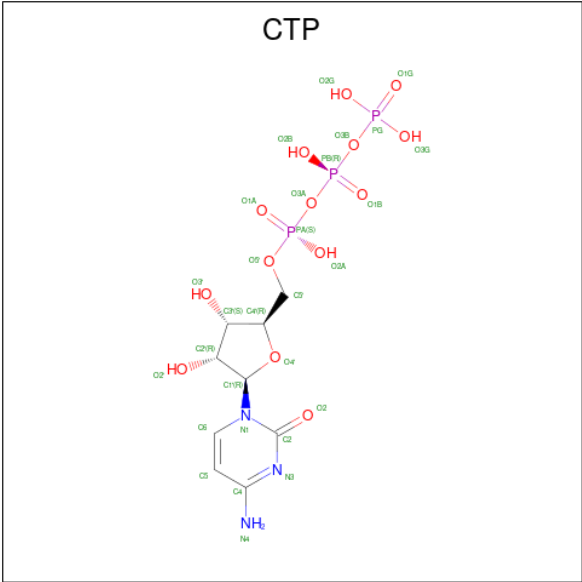
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

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.

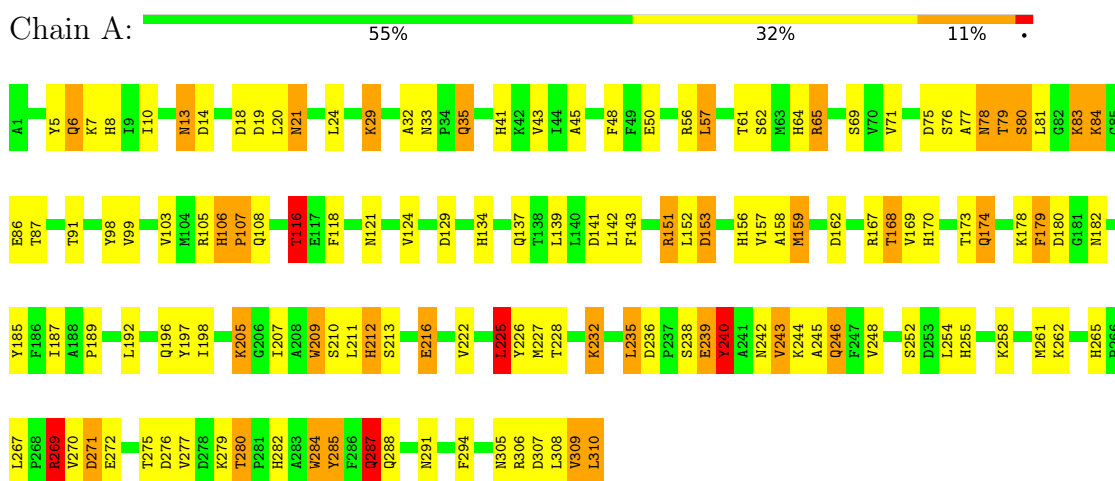
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	10	Total	O	0	0
			10	10		
5	C	44	Total	O	0	0
			44	44		
5	D	9	Total	O	0	0
			9	9		

3 Residue-property plots

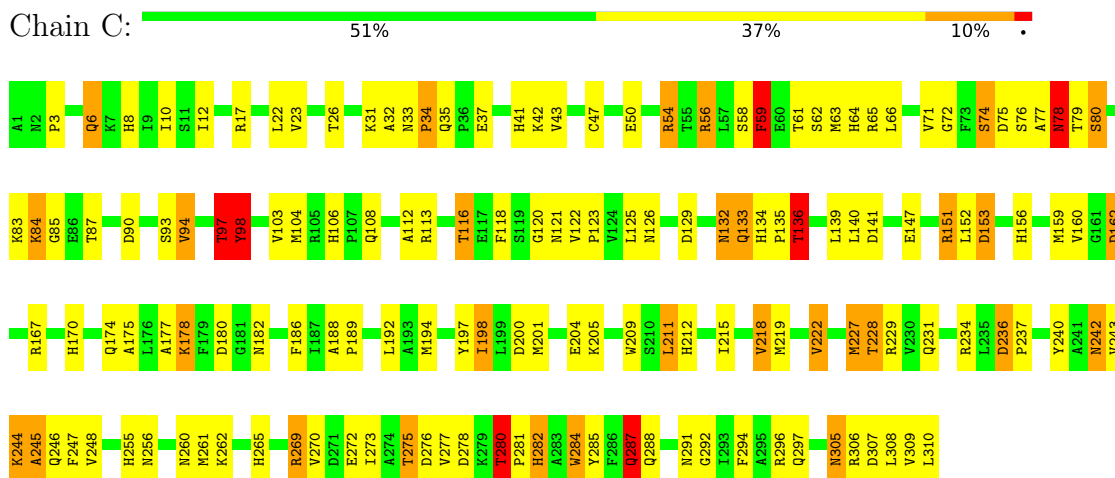
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

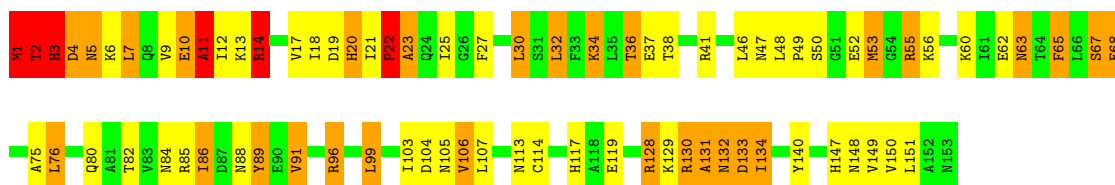


- Molecule 1: Aspartate carbamoyltransferase catalytic chain



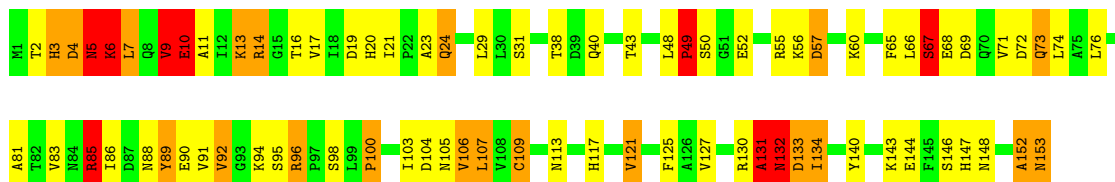
- Molecule 2: Aspartate carbamoyltransferase regulatory chain





• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D: 48% 33% 13% 6%



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}	0.189 , (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	1.28	17/2461 (0.7%)	2.15	103/3339 (3.1%)
1	C	1.38	25/2461 (1.0%)	2.24	132/3339 (4.0%)
2	B	1.20	5/1214 (0.4%)	2.18	57/1640 (3.5%)
2	D	1.20	5/1214 (0.4%)	2.20	52/1640 (3.2%)
All	All	1.29	52/7350 (0.7%)	2.19	344/9958 (3.5%)

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	A	0	6
1	C	0	2
2	B	0	2
2	D	0	2
All	All	0	12

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	HIS	CG-ND1	-7.22	1.30	1.38
1	A	106	HIS	CD2-NE2	-7.19	1.29	1.37
1	C	134	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	265	HIS	CD2-NE2	-7.14	1.29	1.37
2	B	147	HIS	CD2-NE2	-6.98	1.30	1.37
1	C	212	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	309	VAL	CA-CB	6.89	1.62	1.54
1	C	134	HIS	CG-ND1	-6.89	1.30	1.38
1	C	35	GLN	CA-CB	-6.81	1.45	1.53
1	A	8	HIS	CG-ND1	-6.68	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	156	HIS	CD2-NE2	-6.56	1.30	1.37
1	C	170	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	106	HIS	CG-ND1	-6.45	1.31	1.38
1	A	56	ARG	CA-CB	-6.19	1.43	1.53
1	A	134	HIS	CG-ND1	-6.12	1.31	1.38
1	A	212	HIS	CD2-NE2	-6.12	1.31	1.37
1	C	64	HIS	CD2-NE2	-6.12	1.31	1.37
1	C	41	HIS	CD2-NE2	-6.05	1.31	1.37
2	D	147	HIS	CD2-NE2	-5.99	1.31	1.37
1	C	56	ARG	CA-CB	-5.98	1.43	1.53
1	C	79	THR	CA-CB	5.96	1.60	1.53
1	C	8	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	134	HIS	CD2-NE2	-5.92	1.31	1.37
1	C	8	HIS	CG-ND1	-5.92	1.31	1.38
1	A	156	HIS	CD2-NE2	-5.91	1.31	1.37
1	C	34	PRO	CA-CB	-5.90	1.46	1.53
1	C	33	ASN	CA-CB	5.85	1.60	1.53
1	A	170	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	41	HIS	CD2-NE2	-5.75	1.31	1.37
1	C	265	HIS	CD2-NE2	-5.73	1.31	1.37
2	D	117	HIS	CD2-NE2	-5.72	1.31	1.37
1	C	156	HIS	CG-ND1	-5.70	1.31	1.38
2	B	20	HIS	CD2-NE2	-5.68	1.31	1.37
1	C	108	GLN	CA-CB	-5.68	1.44	1.53
2	B	2	THR	CA-CB	5.66	1.62	1.53
1	C	170	HIS	CG-ND1	-5.63	1.32	1.38
2	D	3	HIS	CD2-NE2	-5.60	1.31	1.37
1	C	112	ALA	CA-CB	-5.59	1.44	1.53
2	B	3	HIS	CD2-NE2	-5.56	1.31	1.37
2	B	117	HIS	CD2-NE2	-5.55	1.31	1.37
2	D	147	HIS	CG-ND1	-5.51	1.32	1.38
1	C	106	HIS	CD2-NE2	-5.47	1.31	1.37
1	C	12	ILE	CA-CB	5.42	1.61	1.54
1	C	94	VAL	CA-CB	-5.35	1.47	1.54
1	C	34	PRO	CA-C	-5.33	1.46	1.52
1	A	212	HIS	CG-ND1	-5.33	1.32	1.38
1	C	106	HIS	CG-ND1	-5.32	1.32	1.38
1	C	282	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	69	SER	CA-CB	-5.25	1.44	1.53
1	A	255	HIS	CD2-NE2	-5.20	1.32	1.37
1	A	64	HIS	CD2-NE2	-5.17	1.32	1.37
2	D	9	VAL	CA-CB	5.02	1.60	1.54

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	GLN	OE1-CD-NE2	-12.51	110.09	122.60
2	D	5	ASN	CA-CB-CG	11.42	124.02	112.60
1	C	287	GLN	CG-CD-NE2	11.12	133.08	116.40
2	D	5	ASN	OD1-CG-ND2	-11.09	111.51	122.60
1	C	122	VAL	N-CA-C	-10.82	95.65	107.77
1	A	276	ASP	CA-CB-CG	10.49	123.09	112.60
1	C	309	VAL	O-C-N	10.40	134.09	123.18
1	A	245	ALA	N-CA-C	-10.15	98.43	110.41
1	C	33	ASN	OD1-CG-ND2	-10.15	112.45	122.60
2	D	67	SER	N-CA-C	10.15	124.08	108.96
1	A	291	ASN	OD1-CG-ND2	-10.15	112.45	122.60
2	B	133	ASP	N-CA-C	9.96	132.02	110.80
2	D	9	VAL	N-CA-C	9.81	122.15	109.30
2	B	21	ILE	N-CA-C	-9.74	100.25	108.63
1	C	75	ASP	CA-CB-CG	9.53	122.13	112.60
1	A	21	ASN	OD1-CG-ND2	-9.51	113.09	122.60
1	C	247	PHE	N-CA-C	-9.40	96.66	109.54
2	D	3	HIS	N-CA-C	-9.35	90.89	110.80
1	C	80	SER	N-CA-C	9.28	130.56	110.80
1	C	33	ASN	CA-C-N	9.25	129.33	119.89
1	C	33	ASN	C-N-CA	9.25	129.33	119.89
1	C	200	ASP	CA-CB-CG	9.21	121.81	112.60
2	B	11	ALA	N-CA-C	9.20	130.38	110.80
2	D	106	VAL	N-CA-C	-9.12	95.45	108.58
2	D	106	VAL	N-CA-CB	-9.11	100.78	110.72
1	A	271	ASP	CA-CB-CG	9.09	121.69	112.60
1	A	6	GLN	CA-CB-CG	9.06	132.22	114.10
1	C	297	GLN	OE1-CD-NE2	-9.05	113.55	122.60
2	D	147	HIS	ND1-CG-CD2	9.01	115.11	106.10
2	B	5	ASN	CA-CB-CG	8.96	121.56	112.60
1	C	244	LYS	CA-C-O	-8.85	111.07	120.63
1	C	104	MET	CG-SD-CE	-8.79	81.56	100.90
2	D	2	THR	CA-C-O	8.64	129.47	120.40
1	C	174	GLN	CA-CB-CG	-8.64	96.82	114.10
1	A	162	ASP	CA-CB-CG	8.62	121.22	112.60
1	A	56	ARG	NE-CZ-NH2	-8.62	111.44	119.20
1	C	280	THR	N-CA-CB	-8.62	97.53	110.11
2	D	6	LYS	N-CA-C	8.60	122.33	111.24
1	C	218	VAL	N-CA-CB	-8.59	102.11	112.33
2	B	52	GLU	CA-C-O	8.56	130.22	120.98
1	C	97	THR	N-CA-CB	-8.42	95.65	110.39
2	D	40	GLN	OE1-CD-NE2	-8.26	114.34	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	ASN	N-CA-C	8.25	122.18	108.73
1	A	14	ASP	CA-CB-CG	8.21	120.81	112.60
1	A	33	ASN	OD1-CG-ND2	-8.20	114.40	122.60
1	C	90	ASP	N-CA-C	8.20	120.22	111.28
1	C	54	ARG	CA-CB-CG	8.19	130.48	114.10
1	C	141	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	18	ASP	CA-CB-CG	8.13	120.73	112.60
2	D	5	ASN	CB-CG-ND2	8.11	128.56	116.40
1	C	134	HIS	ND1-CG-CD2	8.02	114.12	106.10
1	A	129	ASP	CA-CB-CG	8.00	120.59	112.60
1	A	80	SER	N-CA-C	7.89	127.61	110.80
1	A	106	HIS	CA-C-N	7.82	128.00	119.87
1	A	106	HIS	C-N-CA	7.82	128.00	119.87
1	A	79	THR	N-CA-CB	-7.78	97.33	110.49
1	C	275	THR	CA-CB-OG1	-7.78	97.93	109.60
2	B	52	GLU	N-CA-C	7.77	121.60	108.23
2	D	132	ASN	N-CA-C	-7.71	94.39	110.80
2	B	32	LEU	N-CA-C	7.67	119.64	111.28
1	A	75	ASP	CA-CB-CG	7.67	120.27	112.60
1	C	129	ASP	CA-CB-CG	7.65	120.25	112.60
2	B	3	HIS	CA-CB-CG	7.61	121.41	113.80
1	A	84	LYS	N-CA-C	-7.58	94.67	110.80
1	C	87	THR	O-C-N	-7.55	113.52	122.81
2	B	63	ASN	N-CA-C	7.55	122.21	113.38
2	D	11	ALA	N-CA-C	-7.54	96.95	109.24
2	B	96	ARG	O-C-N	-7.50	116.91	121.71
1	C	228	THR	CA-CB-OG1	-7.50	98.35	109.60
1	A	269	ARG	NE-CZ-NH1	7.48	128.98	121.50
2	D	94	LYS	N-CA-C	-7.40	96.26	108.76
1	C	32	ALA	CA-C-O	-7.39	113.04	120.80
1	C	291	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	C	74	SER	N-CA-C	-7.33	97.27	109.07
1	A	265	HIS	ND1-CG-CD2	7.32	113.42	106.10
1	C	10	ILE	N-CA-C	-7.30	105.28	111.56
1	A	178	LYS	N-CA-C	-7.30	104.18	113.23
1	A	41	HIS	ND1-CG-CD2	7.29	113.39	106.10
1	C	8	HIS	ND1-CG-CD2	7.27	113.37	106.10
1	A	269	ARG	CA-CB-CG	7.18	128.47	114.10
1	A	6	GLN	N-CA-C	7.15	126.03	110.80
1	A	134	HIS	CA-CB-CG	7.15	120.95	113.80
1	C	106	HIS	ND1-CG-CD2	7.14	113.24	106.10
1	C	132	ASN	OD1-CG-ND2	-7.13	115.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	ASP	CA-CB-CG	-7.12	105.47	112.60
1	A	225	LEU	O-C-N	-7.11	114.59	123.05
2	B	130	ARG	N-CA-C	7.10	120.67	110.24
1	C	78	ASN	N-CA-C	7.04	125.80	110.80
1	C	104	MET	N-CA-CB	-7.02	99.06	110.71
1	A	258	LYS	CB-CG-CD	-6.95	95.31	111.30
1	C	33	ASN	CB-CG-ND2	6.95	126.82	116.40
1	A	134	HIS	ND1-CG-CD2	6.93	113.03	106.10
1	C	236	ASP	CA-CB-CG	6.90	119.50	112.60
1	C	37	GLU	CA-CB-CG	-6.87	100.36	114.10
1	A	222	VAL	N-CA-CB	-6.86	101.10	110.56
1	A	287	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	C	284	TRP	CG-CD2-CE3	6.81	140.71	133.90
1	C	43	VAL	N-CA-C	-6.80	98.33	108.12
1	C	269	ARG	NE-CZ-NH1	6.80	128.30	121.50
1	C	116	THR	N-CA-CB	-6.80	99.75	110.22
1	A	141	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	196	GLN	CB-CG-CD	6.77	124.11	112.60
1	A	71	VAL	O-C-N	-6.71	115.79	122.97
1	C	218	VAL	N-CA-C	6.70	120.24	113.47
1	A	240	TYR	N-CA-C	-6.70	103.67	110.97
1	C	180	ASP	N-CA-C	6.69	121.20	109.96
1	C	198	ILE	N-CA-C	-6.69	104.33	110.82
1	A	79	THR	N-CA-C	6.69	125.04	110.80
1	A	198	ILE	N-CA-C	-6.68	103.97	110.72
1	A	87	THR	N-CA-C	6.66	119.40	110.35
1	C	280	THR	O-C-N	-6.65	114.21	121.53
1	A	153	ASP	CA-CB-CG	6.62	119.22	112.60
1	C	61	THR	N-CA-C	-6.61	104.15	111.36
2	B	53	MET	N-CA-C	-6.61	96.72	110.80
1	C	288	GLN	N-CA-C	-6.56	103.75	111.03
2	D	106	VAL	CB-CA-C	6.54	119.02	110.91
1	A	307	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	243	VAL	N-CA-C	6.53	122.92	109.34
2	D	121	VAL	CA-CB-CG2	-6.53	99.30	110.40
2	B	47	ASN	CA-CB-CG	6.52	119.12	112.60
2	B	5	ASN	OD1-CG-ND2	-6.50	116.10	122.60
2	D	147	HIS	CG-CD2-NE2	-6.50	100.70	107.20
1	C	222	VAL	N-CA-CB	-6.49	100.47	110.86
1	C	56	ARG	CG-CD-NE	-6.47	97.76	112.00
1	C	47	CYS	O-C-N	-6.47	115.17	122.93
2	B	75	ALA	N-CA-C	6.46	119.14	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	89	TYR	N-CA-C	6.45	124.54	110.80
2	B	52	GLU	O-C-N	6.45	131.21	122.57
1	C	84	LYS	CA-CB-CG	-6.45	101.21	114.10
2	B	10	GLU	N-CA-C	6.43	120.11	110.14
1	C	58	SER	CB-CA-C	-6.40	100.83	110.88
1	A	116	THR	N-CA-CB	-6.37	99.72	110.49
2	B	23	ALA	N-CA-C	-6.37	97.23	110.80
1	A	61	THR	N-CA-C	-6.37	104.42	111.36
1	A	56	ARG	CG-CD-NE	-6.36	98.02	112.00
1	C	273	ILE	N-CA-C	-6.35	98.32	107.78
1	A	10	ILE	N-CA-CB	-6.34	104.44	111.41
1	C	59	PHE	N-CA-C	-6.34	104.06	110.97
1	C	26	THR	CA-CB-OG1	-6.33	100.11	109.60
1	C	162	ASP	N-CA-C	-6.32	97.39	108.20
1	A	182	ASN	OD1-CG-ND2	-6.31	116.29	122.60
2	B	67	SER	N-CA-C	6.31	116.77	107.88
1	A	197	TYR	CA-CB-CG	6.31	125.25	113.90
1	C	284	TRP	CB-CG-CD1	-6.30	117.45	126.90
2	B	131	ALA	N-CA-C	6.28	124.17	110.80
1	A	134	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	C	270	VAL	CA-C-N	-6.27	112.22	121.99
1	C	270	VAL	C-N-CA	-6.27	112.22	121.99
1	A	32	ALA	N-CA-C	6.25	117.76	111.07
1	C	98	TYR	N-CA-C	6.25	123.80	113.50
2	D	96	ARG	CA-C-N	6.24	126.45	119.90
2	D	96	ARG	C-N-CA	6.24	126.45	119.90
1	A	168	THR	O-C-N	-6.22	115.53	122.12
2	D	19	ASP	CA-CB-CG	6.22	118.82	112.60
2	B	67	SER	O-C-N	6.21	129.50	123.04
2	B	149	VAL	CA-C-O	-6.21	114.16	121.05
2	D	69	ASP	CA-CB-CG	6.21	118.81	112.60
2	B	133	ASP	O-C-N	6.20	130.83	122.59
2	D	133	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	116	THR	CA-CB-OG1	-6.18	100.32	109.60
1	A	118	PHE	N-CA-C	-6.17	106.72	114.56
2	B	119	GLU	N-CA-C	6.17	118.18	108.55
1	A	134	HIS	CG-CD2-NE2	-6.17	101.03	107.20
1	C	182	ASN	O-C-N	6.16	129.93	122.96
2	B	106	VAL	N-CA-CB	-6.13	97.89	111.50
1	C	244	LYS	O-C-N	-6.12	115.63	122.12
1	C	242	ASN	N-CA-C	-6.10	101.89	110.50
2	D	132	ASN	OD1-CG-ND2	-6.10	116.50	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	VAL	CA-CB-CG2	-6.10	100.03	110.40
1	C	280	THR	CB-CA-C	6.09	119.08	109.27
2	B	134	ILE	CB-CA-C	-6.04	101.39	111.29
2	D	146	SER	CA-C-O	-6.04	114.55	121.19
1	C	246	GLN	CA-C-O	6.04	129.14	120.51
2	B	134	ILE	N-CA-C	6.04	121.89	109.34
1	A	57	LEU	O-C-N	-6.01	115.75	122.12
2	B	1	MET	CA-CB-CG	6.01	126.11	114.10
1	C	133	GLN	CG-CD-NE2	6.00	125.40	116.40
1	C	93	SER	N-CA-C	-5.99	104.87	111.82
2	B	21	ILE	CA-C-N	5.96	127.29	119.84
2	B	21	ILE	C-N-CA	5.96	127.29	119.84
2	B	52	GLU	CA-C-N	5.95	132.90	121.54
2	B	52	GLU	C-N-CA	5.95	132.90	121.54
1	C	31	LYS	N-CA-C	-5.95	104.88	111.36
1	A	75	ASP	CA-C-N	-5.92	113.84	122.19
1	A	75	ASP	C-N-CA	-5.92	113.84	122.19
1	A	62	SER	CA-CB-OG	-5.89	99.31	111.10
2	D	131	ALA	O-C-N	5.89	130.42	122.59
1	A	29	LYS	CB-CG-CD	-5.89	97.76	111.30
2	B	132	ASN	CA-C-N	5.89	132.78	121.54
2	B	132	ASN	C-N-CA	5.89	132.78	121.54
1	C	160	VAL	N-CA-CB	-5.88	103.29	111.41
2	D	49	PRO	O-C-N	5.88	130.58	122.64
1	C	147	GLU	CA-C-O	-5.87	113.46	120.10
1	C	160	VAL	O-C-N	-5.87	116.92	123.26
1	C	151	ARG	CG-CD-NE	-5.87	99.09	112.00
1	C	108	GLN	CA-CB-CG	-5.84	102.41	114.10
1	C	136	THR	N-CA-CB	-5.83	101.32	110.30
1	C	276	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	288	GLN	CA-C-O	-5.81	114.72	120.70
2	D	134	ILE	N-CA-CB	-5.81	103.92	111.82
2	B	82	THR	O-C-N	-5.79	115.70	123.23
1	A	275	THR	N-CA-C	5.79	119.87	112.34
2	B	114	CYS	CA-C-O	5.77	127.54	121.19
1	A	236	ASP	N-CA-C	-5.76	102.78	109.93
1	C	222	VAL	CB-CA-C	5.75	119.09	110.98
2	D	10	GLU	N-CA-C	-5.72	98.62	110.80
1	C	275	THR	CA-CB-CG2	5.72	120.22	110.50
1	C	188	ALA	O-C-N	-5.71	117.83	121.88
1	A	179	PHE	O-C-N	-5.70	115.25	122.43
2	B	46	LEU	CD1-CG-CD2	-5.69	98.28	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	GLU	O-C-N	-5.69	118.07	121.71
1	A	275	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	216	GLU	CA-CB-CG	5.67	125.45	114.10
1	C	8	HIS	CG-CD2-NE2	-5.67	101.53	107.20
2	D	144	GLU	CA-CB-CG	-5.67	102.75	114.10
1	A	265	HIS	CG-CD2-NE2	-5.67	101.53	107.20
1	A	291	ASN	CB-CG-ND2	5.66	124.89	116.40
2	B	38	THR	N-CA-C	-5.66	100.70	109.24
1	A	246	GLN	N-CA-C	5.64	122.82	110.80
2	B	5	ASN	O-C-N	-5.63	115.11	122.59
1	C	177	ALA	N-CA-C	-5.62	106.38	113.18
2	D	38	THR	CA-CB-OG1	-5.61	101.18	109.60
2	D	90	GLU	O-C-N	5.60	129.42	123.42
1	A	307	ASP	N-CA-C	-5.57	99.94	109.24
2	B	18	ILE	N-CA-C	-5.57	99.22	107.51
1	A	19	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	242	ASN	CA-CB-CG	5.56	118.16	112.60
1	C	297	GLN	CG-CD-NE2	5.55	124.73	116.40
2	D	24	GLN	N-CA-C	5.55	122.63	110.80
2	B	13	LYS	O-C-N	5.54	129.65	123.05
1	C	269	ARG	N-CA-C	-5.54	100.21	109.24
1	C	306	ARG	CA-CB-CG	5.54	125.17	114.10
1	C	37	GLU	CB-CG-CD	5.53	122.00	112.60
1	C	222	VAL	CA-CB-CG2	-5.51	101.03	110.40
1	A	196	GLN	N-CA-C	-5.51	105.43	111.82
2	B	22	PRO	CA-N-CD	-5.50	104.30	112.00
1	C	282	HIS	ND1-CG-CD2	5.50	111.60	106.10
2	B	55	ARG	N-CA-C	-5.50	101.90	110.42
1	C	280	THR	CA-C-N	5.50	125.21	119.82
1	C	280	THR	C-N-CA	5.50	125.21	119.82
1	A	284	TRP	CG-CD2-CE3	5.49	139.39	133.90
2	B	105	ASN	N-CA-C	5.49	122.50	110.80
1	C	278	ASP	CA-C-O	-5.49	114.05	120.20
1	C	260	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	C	134	HIS	CG-CD2-NE2	-5.47	101.72	107.20
1	A	170	HIS	N-CA-C	-5.47	104.72	111.40
1	C	197	TYR	CA-CB-CG	5.47	123.75	113.90
1	C	309	VAL	CA-C-O	5.47	126.28	120.48
1	A	65	ARG	CB-CG-CD	5.46	123.87	111.30
1	C	222	VAL	CA-CB-CG1	5.46	119.69	110.40
2	D	152	ALA	N-CA-C	-5.46	99.97	110.56
2	D	81	ALA	N-CA-C	-5.45	99.80	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	8	HIS	ND1-CG-CD2	5.44	111.54	106.10
1	C	281	PRO	N-CA-C	5.43	120.98	113.98
1	A	105	ARG	N-CA-C	-5.42	99.60	108.76
1	A	243	VAL	CA-C-N	5.42	131.89	121.54
1	A	243	VAL	C-N-CA	5.42	131.89	121.54
2	D	107	LEU	N-CA-CB	5.42	119.65	110.49
1	C	72	GLY	CA-C-O	-5.41	116.12	121.48
1	C	78	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	A	279	LYS	CA-CB-CG	-5.41	103.29	114.10
2	D	109	CYS	CA-C-N	5.40	125.74	119.47
2	D	109	CYS	C-N-CA	5.40	125.74	119.47
2	D	52	GLU	N-CA-C	5.39	119.34	112.87
1	A	157	VAL	CA-C-O	-5.38	114.77	120.53
1	C	66	LEU	N-CA-C	-5.38	105.35	112.94
1	C	228	THR	CA-CB-CG2	5.38	119.64	110.50
2	B	128	ARG	N-CA-C	5.37	117.01	108.79
1	C	97	THR	OG1-CB-CG2	5.37	120.05	109.30
1	C	106	HIS	CG-CD2-NE2	-5.37	101.83	107.20
2	B	88	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	287	GLN	CG-CD-NE2	5.36	124.44	116.40
2	B	65	PHE	N-CA-C	-5.36	99.67	108.41
1	C	116	THR	OG1-CB-CG2	5.36	120.02	109.30
2	D	83	VAL	N-CA-C	-5.36	100.66	109.12
1	A	107	PRO	N-CA-C	5.36	120.62	114.03
1	C	103	VAL	O-C-N	-5.35	117.25	122.93
1	C	178	LYS	CA-CB-CG	-5.33	103.44	114.10
1	C	23	VAL	N-CA-C	-5.33	105.34	110.72
1	C	63	MET	N-CA-C	-5.32	105.14	111.69
2	B	34	LYS	CB-CG-CD	5.32	123.53	111.30
1	C	42	LYS	CG-CD-CE	-5.32	99.07	111.30
1	C	97	THR	CB-CA-C	5.31	121.01	110.17
1	A	65	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	C	56	ARG	CB-CG-CD	-5.29	99.13	111.30
2	D	148	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	21	ASN	CA-CB-CG	5.28	117.88	112.60
1	C	134	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	35	GLN	CA-CB-CG	-5.27	103.57	114.10
1	C	305	ASN	O-C-N	-5.26	117.22	123.22
2	D	57	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	282	HIS	CG-CD2-NE2	-5.25	101.95	107.20
2	B	84	ASN	CA-CB-CG	-5.25	107.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLN	N-CA-C	-5.25	105.48	111.14
1	C	54	ARG	CB-CA-C	-5.24	102.59	110.92
2	D	113	ASN	OD1-CG-ND2	-5.23	117.37	122.60
2	B	50	SER	N-CA-C	5.22	121.93	110.80
1	C	64	HIS	O-C-N	-5.21	116.60	122.12
1	A	285	TYR	N-CA-C	5.19	116.94	111.28
1	A	83	LYS	CA-C-N	5.19	131.45	121.54
1	A	83	LYS	C-N-CA	5.19	131.45	121.54
1	A	43	VAL	CG1-CB-CG2	-5.19	99.38	110.80
1	A	239	GLU	N-CA-C	-5.19	107.08	113.41
2	D	9	VAL	CB-CA-C	-5.18	103.52	111.71
1	C	136	THR	N-CA-C	-5.17	105.71	112.23
1	A	209	TRP	CE2-CD2-CG	-5.16	101.01	107.20
2	B	88	ASN	CA-CB-CG	5.15	117.75	112.60
2	D	127	VAL	N-CA-CB	-5.14	104.82	110.99
1	A	280	THR	CA-C-N	5.14	124.81	119.56
1	A	280	THR	C-N-CA	5.14	124.81	119.56
1	C	126	ASN	OD1-CG-ND2	-5.14	117.46	122.60
2	D	85	ARG	N-CA-C	-5.13	103.62	110.55
1	C	209	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	205	LYS	CA-CB-CG	5.11	124.33	114.10
2	D	2	THR	O-C-N	5.11	129.87	123.12
2	D	147	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	A	103	VAL	CA-C-O	-5.09	115.12	120.57
2	B	36	THR	N-CA-CB	-5.09	102.50	110.44
1	C	265	HIS	ND1-CG-CD2	5.09	111.19	106.10
1	A	222	VAL	CG1-CB-CG2	-5.08	99.62	110.80
1	A	265	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	C	120	GLY	CA-C-N	-5.08	115.56	122.87
1	C	120	GLY	C-N-CA	-5.08	115.56	122.87
2	B	19	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	7	LYS	CA-CB-CG	5.08	124.25	114.10
2	D	19	ASP	N-CA-CB	-5.08	103.44	111.05
1	C	71	VAL	CA-C-N	-5.06	114.45	121.23
1	C	71	VAL	C-N-CA	-5.06	114.45	121.23
1	C	156	HIS	CA-CB-CG	5.05	118.85	113.80
1	A	174	GLN	CB-CA-C	-5.05	102.73	110.81
2	D	73	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	B	149	VAL	O-C-N	-5.04	116.66	121.90
1	A	134	HIS	CA-C-N	5.04	125.07	119.32
1	A	134	HIS	C-N-CA	5.04	125.07	119.32
1	A	13	ASN	O-C-N	5.04	128.11	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ASP	N-CA-C	-5.04	100.83	109.24
2	D	105	ASN	CB-CA-C	-5.03	100.41	110.42
1	A	6	GLN	CA-C-O	5.02	127.69	120.51
1	C	162	ASP	CA-CB-CG	5.02	117.62	112.60
1	C	141	ASP	N-CA-C	-5.01	105.72	111.14
2	B	133	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	62	SER	CA-CB-OG	5.01	121.11	111.10
1	C	275	THR	N-CA-CB	-5.00	102.04	110.49

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	PHE	Sidechain
1	A	226	TYR	Sidechain
1	A	240	TYR	Sidechain
1	A	294	PHE	Sidechain
1	A	48	PHE	Sidechain
1	A	98	TYR	Sidechain
2	B	140	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	294	PHE	Sidechain
1	C	98	TYR	Sidechain
2	D	140	TYR	Sidechain
2	D	48	LEU	Peptide

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	45	0
1	C	2415	0	2422	37	0
2	B	1196	0	1212	31	0
2	D	1196	0	1212	26	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	29	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	29	0	12	0	0
5	A	30	0	0	0	0
5	B	10	0	0	0	0
5	C	44	0	0	1	0
5	D	9	0	0	0	0
All	All	7375	0	7292	132	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 (132) 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:4:ASP:HA	2:B:10:GLU:HB2	1.49	0.93
1:A:106:HIS:HD2	1:A:108:GLN:H	1.27	0.82
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.67	0.75
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.69	0.73
2:B:6:LYS:HB3	2:D:10:GLU:HG3	1.70	0.72
1:C:113:ARG:O	1:C:116:THR:HB	1.91	0.70
1:A:209:TRP:HZ3	1:A:211:LEU:HG	1.57	0.69
1:C:277:VAL:O	1:C:280:THR:HB	1.93	0.68
2:B:41:ARG:HH21	2:D:49:PRO:HB2	1.58	0.67
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.06	0.67
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.30	0.66
1:C:136:THR:HB	5:C:317:HOH:O	1.97	0.65
1:A:159:MET:HE1	1:A:173:THR:OG1	1.97	0.64
2:D:5:ASN:ND2	2:D:6:LYS:HD2	2.12	0.64
1:A:287:GLN:NE2	1:A:287:GLN:H	1.97	0.63
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.81	0.63
2:B:1:MET:HA	2:D:7:LEU:HD21	1.81	0.62
1:A:151:ARG:HD2	1:A:153:ASP:O	2.00	0.62
1:A:159:MET:HE3	1:A:169:VAL:HB	1.81	0.61
2:D:152:ALA:O	2:D:153:ASN:HB2	1.99	0.61
2:B:2:THR:HG22	2:B:11:ALA:HB3	1.81	0.61
2:B:76:LEU:HD12	2:B:103:ILE:HD11	1.81	0.61
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.82	0.60
2:B:14:ARG:NH1	2:B:63:ASN:HA	2.16	0.60
1:A:153:ASP:HB3	1:A:180:ASP:O	2.01	0.60
2:B:65:PHE:CE1	2:B:85:ARG:HG3	2.36	0.60
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.17	0.59
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:CG2	1:C:296:ARG:HD3	2.33	0.58
1:C:97:THR:HG22	1:C:98:TYR:HD2	1.66	0.57
2:B:5:ASN:OD1	2:B:7:LEU:HG	2.05	0.57
1:C:136:THR:HG23	1:C:296:ARG:HD3	1.85	0.57
2:B:76:LEU:HD12	2:B:103:ILE:CD1	2.35	0.56
2:B:6:LYS:HA	2:B:9:VAL:HG22	1.88	0.56
1:C:50:GLU:HA	1:C:76:SER:OG	2.05	0.56
1:C:242:ASN:O	1:C:244:LYS:N	2.39	0.56
2:B:48:LEU:O	2:B:55:ARG:HA	2.05	0.55
1:C:231:GLN:HB2	1:C:234:ARG:HG2	1.86	0.55
2:D:72:ASP:HB3	2:D:100:PRO:HB3	1.87	0.55
1:C:94:VAL:O	1:C:97:THR:HB	2.07	0.55
2:B:86:ILE:HG13	2:B:91:VAL:HA	1.89	0.55
2:D:65:PHE:HB3	2:D:85:ARG:NH2	2.22	0.55
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.89	0.55
2:B:6:LYS:CB	2:D:10:GLU:HG3	2.37	0.55
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.22	0.54
1:C:6:GLN:HG3	1:C:123:PRO:HG3	1.90	0.54
1:A:76:SER:O	1:A:78:ASN:HB2	2.08	0.54
1:C:215:ILE:HG22	1:C:219:MET:HE2	1.89	0.54
2:D:65:PHE:HB3	2:D:85:ARG:HH22	1.73	0.53
2:B:107:LEU:HD22	2:B:150:VAL:HG12	1.90	0.53
1:A:235:LEU:HG	1:A:239:GLU:HG3	1.91	0.53
1:A:232:LYS:HD3	1:A:240:TYR:HE2	1.74	0.52
2:B:14:ARG:HH11	2:B:14:ARG:HG2	1.74	0.52
2:B:129:LYS:HG2	2:B:132:ASN:OD1	2.09	0.52
2:D:20:HIS:O	2:D:20:HIS:ND1	2.44	0.52
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.11	0.51
2:D:29:LEU:HD13	2:D:74:LEU:HD22	1.91	0.51
1:A:5:TYR:CD1	1:A:306:ARG:HA	2.46	0.51
2:B:1:MET:N	2:B:89:TYR:OH	2.45	0.50
1:A:21:ASN:HD21	1:A:179:PHE:HE2	1.58	0.50
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.92	0.50
1:A:5:TYR:CZ	1:A:306:ARG:HG2	2.47	0.49
1:A:81:LEU:HD12	1:A:91:THR:HG23	1.93	0.49
1:C:240:TYR:O	1:C:245:ALA:HB2	2.12	0.49
1:C:261:MET:C	1:C:261:MET:SD	2.96	0.49
2:D:50:SER:HB3	2:D:56:LYS:HE3	1.94	0.49
1:A:142:LEU:HD22	1:A:152:LEU:HD13	1.94	0.49
1:A:261:MET:SD	1:A:262:LYS:N	2.86	0.48
1:A:243:VAL:O	1:A:246:GLN:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.96	0.48
1:C:280:THR:HG22	1:C:282:HIS:H	1.78	0.48
1:C:227:MET:HE3	1:C:227:MET:HB3	1.77	0.47
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.96	0.47
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.95	0.47
1:A:106:HIS:CD2	1:A:108:GLN:H	2.18	0.47
2:D:131:ALA:O	2:D:132:ASN:HB2	2.14	0.47
2:B:6:LYS:HE3	2:B:6:LYS:HB2	1.63	0.47
2:B:27:PHE:HA	2:B:30:LEU:HD23	1.97	0.47
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.81	0.46
1:A:232:LYS:HD3	1:A:240:TYR:CE2	2.49	0.46
1:A:248:VAL:HG12	1:A:272:GLU:HA	1.98	0.45
2:B:41:ARG:HE	2:D:49:PRO:HD2	1.82	0.45
1:A:205:LYS:HB2	1:A:207:ILE:HD12	1.98	0.45
2:B:11:ALA:HA	4:B:999:CTP:N3	2.30	0.45
1:C:292:GLY:O	1:C:296:ARG:HG3	2.16	0.45
1:C:59:PHE:CE2	1:C:136:THR:HG21	2.52	0.45
1:C:186:PHE:HB2	1:C:211:LEU:HD12	1.97	0.45
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.17	0.45
1:C:201:MET:HE3	1:C:201:MET:HB3	1.95	0.45
1:C:162:ASP:HA	1:C:192:LEU:HB3	1.99	0.45
2:D:130:ARG:HD2	2:D:130:ARG:HA	1.55	0.45
1:A:81:LEU:HD12	1:A:91:THR:OG1	2.16	0.44
2:B:14:ARG:HA	2:B:86:ILE:O	2.17	0.44
1:A:270:VAL:HG23	1:A:271:ASP:H	1.82	0.44
2:B:41:ARG:NE	2:D:49:PRO:HD2	2.33	0.44
1:A:209:TRP:CZ3	1:A:211:LEU:HG	2.44	0.44
2:B:5:ASN:O	2:B:9:VAL:HA	2.17	0.44
2:B:22:PRO:HB2	2:B:25:ILE:HD13	1.99	0.44
1:C:310:LEU:H	1:C:310:LEU:HG	1.68	0.44
1:A:108:GLN:HG2	2:B:113:ASN:OD1	2.18	0.43
1:A:29:LYS:HD2	1:A:310:LEU:HG	2.00	0.43
1:A:235:LEU:HG	1:A:239:GLU:CG	2.47	0.43
1:C:189:PRO:CG	1:C:192:LEU:HD12	2.47	0.43
1:C:3:PRO:HD2	1:C:22:LEU:CD2	2.49	0.43
1:C:175:ALA:O	1:C:178:LYS:HB2	2.17	0.43
2:D:14:ARG:HA	2:D:86:ILE:O	2.18	0.43
1:A:262:LYS:HG3	1:A:284:TRP:HB2	2.00	0.43
1:C:151:ARG:HD2	1:C:153:ASP:O	2.18	0.42
1:A:185:TYR:HD1	1:A:212:HIS:NE2	2.17	0.42
1:A:158:ALA:HB3	1:A:225:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:ILE:HB	2:B:62:GLU:HG2	2.02	0.42
1:A:267:LEU:HD23	1:A:269:ARG:HB3	2.01	0.42
1:C:194:MET:SD	1:C:198:ILE:HG21	2.59	0.42
1:C:135:PRO:O	1:C:139:LEU:HG	2.20	0.42
2:D:6:LYS:HB2	2:D:9:VAL:HG22	2.01	0.42
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.84	0.41
1:A:254:LEU:HD12	1:A:280:THR:HG21	2.02	0.41
2:B:99:LEU:HB2	2:B:130:ARG:HD3	2.02	0.41
1:A:261:MET:O	1:A:282:HIS:HD2	2.04	0.41
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.86	0.41
2:B:7:LEU:H	2:B:7:LEU:HD23	1.85	0.41
1:C:17:ARG:HH11	1:C:17:ARG:HD3	1.69	0.41
1:C:272:GLU:CD	1:C:272:GLU:H	2.29	0.41
2:D:13:LYS:O	2:D:86:ILE:HG22	2.20	0.41
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.98	0.40
1:C:261:MET:O	1:C:282:HIS:HD2	2.03	0.40
1:A:20:LEU:O	1:A:24:LEU:HD13	2.21	0.40
1:A:254:LEU:HD11	1:A:277:VAL:HG13	2.02	0.40
1:C:229:ARG:CZ	1:C:229:ARG:HB2	2.51	0.40
2:D:67:SER:HA	2:D:71:VAL:HG23	2.03	0.40
2:D:92:VAL:HG13	2:D:92:VAL:O	2.22	0.40
2:D:133:ASP:C	2:D:134:ILE:HG13	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/310 (99%)	281 (91%)	19 (6%)	8 (3%)	4	7
1	C	308/310 (99%)	284 (92%)	17 (6%)	7 (2%)	5	8
2	B	151/153 (99%)	121 (80%)	19 (13%)	11 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	151/153 (99%)	125 (83%)	15 (10%)	11 (7%)	1	1
All	All	918/926 (99%)	811 (88%)	70 (8%)	37 (4%)	2	3

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	80	SER
2	B	3	HIS
2	B	11	ALA
2	B	14	ARG
2	B	23	ALA
2	B	131	ALA
2	B	133	ASP
2	B	134	ILE
1	C	78	ASN
1	C	80	SER
1	C	243	VAL
2	D	4	ASP
2	D	5	ASN
2	D	7	LEU
2	D	24	GLN
2	D	89	TYR
2	D	107	LEU
2	D	132	ASN
1	A	84	LYS
2	B	4	ASP
1	C	245	ALA
1	A	83	LYS
1	A	116	THR
1	A	244	LYS
2	B	22	PRO
2	B	68	GLU
2	B	91	VAL
1	C	77	ALA
2	D	68	GLU
1	A	77	ALA
1	C	84	LYS
2	D	131	ALA
1	A	6	GLN
2	D	23	ALA
1	C	85	GLY

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Mol	Chain	Res	Type
2	D	91	VAL

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%)	232 (89%)	29 (11%)	6	12
1	C	261/261 (100%)	223 (85%)	38 (15%)	3	6
2	B	136/137 (99%)	111 (82%)	25 (18%)	1	3
2	D	136/137 (99%)	107 (79%)	29 (21%)	1	2
All	All	794/796 (100%)	673 (85%)	121 (15%)	3	5

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	GLN
1	A	57	LEU
1	A	65	ARG
1	A	78	ASN
1	A	86	GLU
1	A	116	THR
1	A	121	ASN
1	A	124	VAL
1	A	151	ARG
1	A	159	MET
1	A	167	ARG
1	A	174	GLN
1	A	210	SER
1	A	213	SER
1	A	216	GLU
1	A	225	LEU
1	A	227	MET
1	A	228	THR
1	A	232	LYS

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Mol	Chain	Res	Type
1	A	235	LEU
1	A	238	SER
1	A	252	SER
1	A	269	ARG
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	3	HIS
2	B	7	LEU
2	B	14	ARG
2	B	20	HIS
2	B	30	LEU
2	B	32	LEU
2	B	34	LYS
2	B	36	THR
2	B	37	GLU
2	B	49	PRO
2	B	53	MET
2	B	56	LYS
2	B	67	SER
2	B	68	GLU
2	B	76	LEU
2	B	80	GLN
2	B	86	ILE
2	B	96	ARG
2	B	99	LEU
2	B	106	VAL
2	B	128	ARG
2	B	148	ASN
2	B	151	LEU
1	C	6	GLN
1	C	34	PRO
1	C	54	ARG
1	C	56	ARG
1	C	59	PHE
1	C	65	ARG
1	C	74	SER
1	C	78	ASN

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Mol	Chain	Res	Type
1	C	83	LYS
1	C	97	THR
1	C	121	ASN
1	C	125	LEU
1	C	136	THR
1	C	140	LEU
1	C	152	LEU
1	C	153	ASP
1	C	159	MET
1	C	167	ARG
1	C	204	GLU
1	C	205	LYS
1	C	211	LEU
1	C	218	VAL
1	C	222	VAL
1	C	227	MET
1	C	228	THR
1	C	236	ASP
1	C	237	PRO
1	C	248	VAL
1	C	255	HIS
1	C	256	ASN
1	C	262	LYS
1	C	269	ARG
1	C	275	THR
1	C	280	THR
1	C	285	TYR
1	C	287	GLN
1	C	305	ASN
1	C	308	LEU
2	D	3	HIS
2	D	4	ASP
2	D	5	ASN
2	D	6	LYS
2	D	9	VAL
2	D	10	GLU
2	D	13	LYS
2	D	14	ARG
2	D	16	THR
2	D	31	SER
2	D	43	THR
2	D	49	PRO

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Mol	Chain	Res	Type
2	D	55	ARG
2	D	66	LEU
2	D	67	SER
2	D	73	GLN
2	D	85	ARG
2	D	88	ASN
2	D	92	VAL
2	D	95	SER
2	D	96	ARG
2	D	98	SER
2	D	100	PRO
2	D	104	ASP
2	D	106	VAL
2	D	121	VAL
2	D	132	ASN
2	D	143	LYS
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	21	ASN
1	A	35	GLN
1	A	106	HIS
1	A	242	ASN
1	A	282	HIS
1	A	287	GLN
1	A	297	GLN
2	B	5	ASN
2	B	80	GLN
1	C	33	ASN
1	C	149	GLN
1	C	260	ASN
1	C	282	HIS
1	C	287	GLN
2	D	5	ASN
2	D	24	GLN
2	D	40	GLN
2	D	63	ASN
2	D	117	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	2.33	9 (31%)	43,47,47	1.37	4 (9%)
4	CTP	D	999	-	29,30,30	2.27	8 (27%)	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	-	-	6/22/38/38	0/2/2/2
4	CTP	D	999	-	-	4/22/38/38	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	CTP	PB-O3B	6.83	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	PB-O3B	6.64	1.66	1.59
4	D	999	CTP	PB-O3A	5.65	1.65	1.59
4	B	999	CTP	PB-O3A	5.49	1.65	1.59
4	B	999	CTP	PA-O3A	5.32	1.65	1.59
4	D	999	CTP	PA-O3A	5.15	1.65	1.59
4	D	999	CTP	PG-O1G	2.65	1.58	1.50
4	D	999	CTP	C6-N1	-2.52	1.32	1.38
4	B	999	CTP	PG-O1G	2.51	1.58	1.50
4	B	999	CTP	C2-N3	-2.50	1.31	1.36
4	B	999	CTP	C2-N1	-2.40	1.35	1.40
4	D	999	CTP	C5-C4	-2.40	1.37	1.42
4	B	999	CTP	C6-N1	-2.37	1.32	1.38
4	D	999	CTP	PB-O1B	2.23	1.58	1.50
4	B	999	CTP	PB-O1B	2.20	1.58	1.50
4	D	999	CTP	PA-O1A	2.17	1.58	1.50
4	B	999	CTP	C5-C4	-2.16	1.37	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	CTP	O2-C2-N3	-4.79	114.78	122.33
4	D	999	CTP	O2-C2-N3	-4.02	115.99	122.33
4	B	999	CTP	N1-C2-N3	2.58	123.28	118.80
4	B	999	CTP	C6-N1-C2	-2.47	116.30	120.46
4	D	999	CTP	C6-N1-C2	-2.43	116.35	120.46
4	D	999	CTP	N1-C2-N3	2.25	122.70	118.80
4	D	999	CTP	O4'-C1'-N1	2.13	113.18	108.36
4	D	999	CTP	C3'-C2'-C1'	2.11	105.45	101.46
4	B	999	CTP	C5'-C4'-C3'	-2.04	107.87	115.21

There are no chirality outliers.

All (10) 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	B	999	CTP	PB-O3A-PA-O1A
4	B	999	CTP	C5'-O5'-PA-O3A

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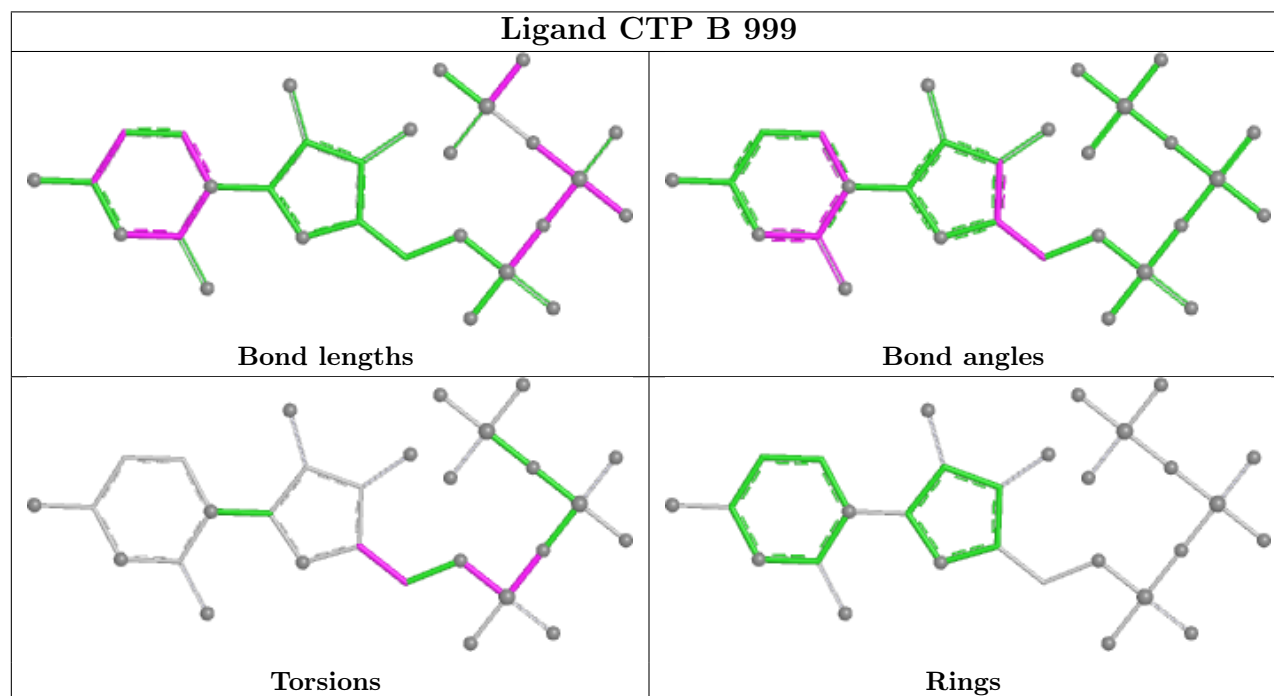
Mol	Chain	Res	Type	Atoms
4	D	999	CTP	PB-O3A-PA-O1A
4	D	999	CTP	C3'-C4'-C5'-O5'

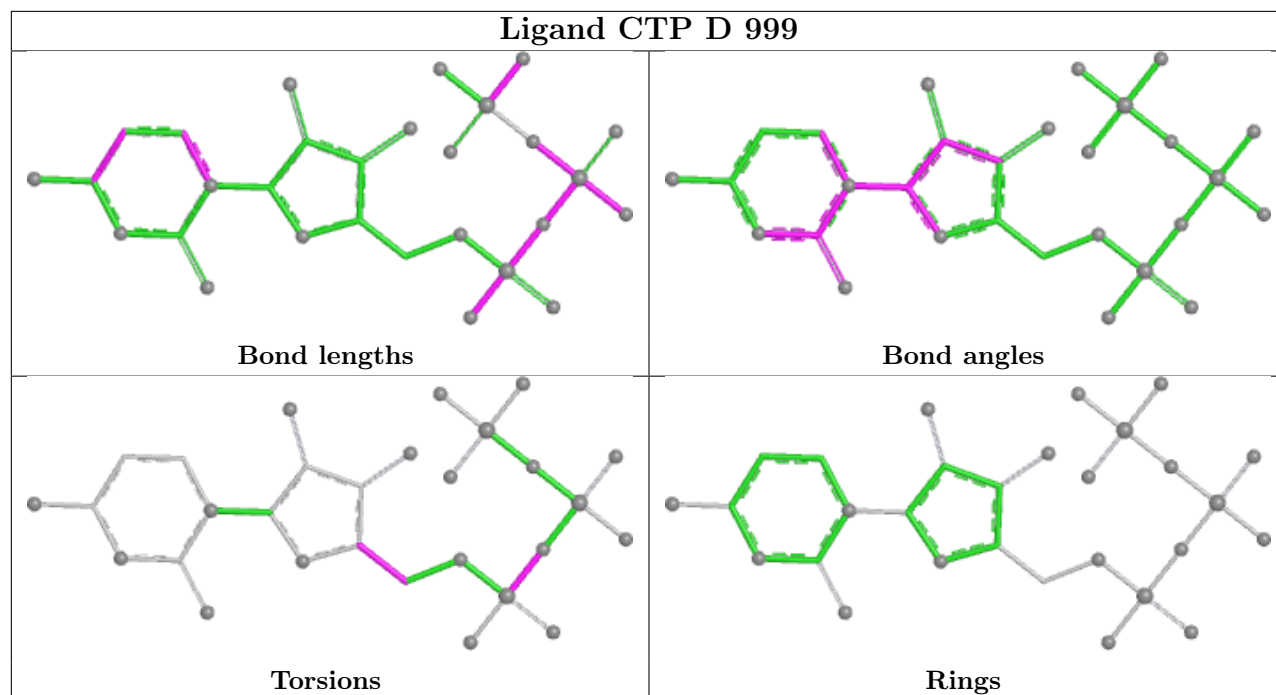
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	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.