



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:08 AM UTC

PDB ID : 1RAF / pdb_00001raf
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

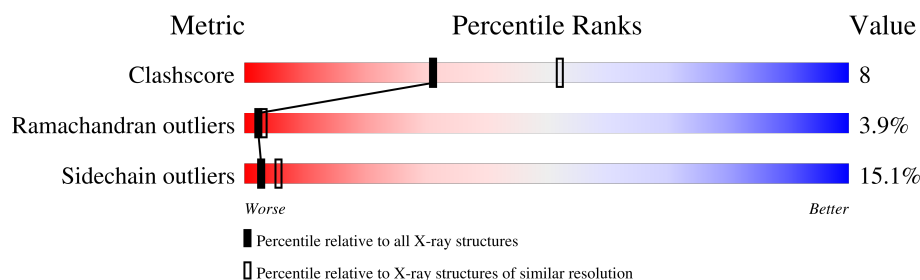
1 Overall quality at a glance

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	
1	C	310	
2	B	153	
2	D	153	

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			

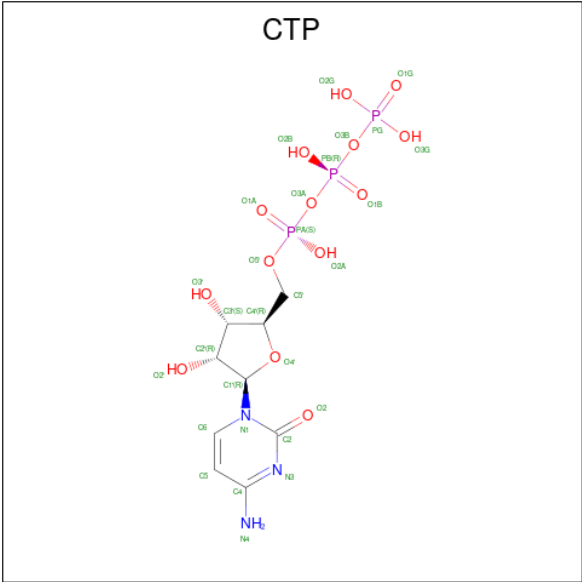
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

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.

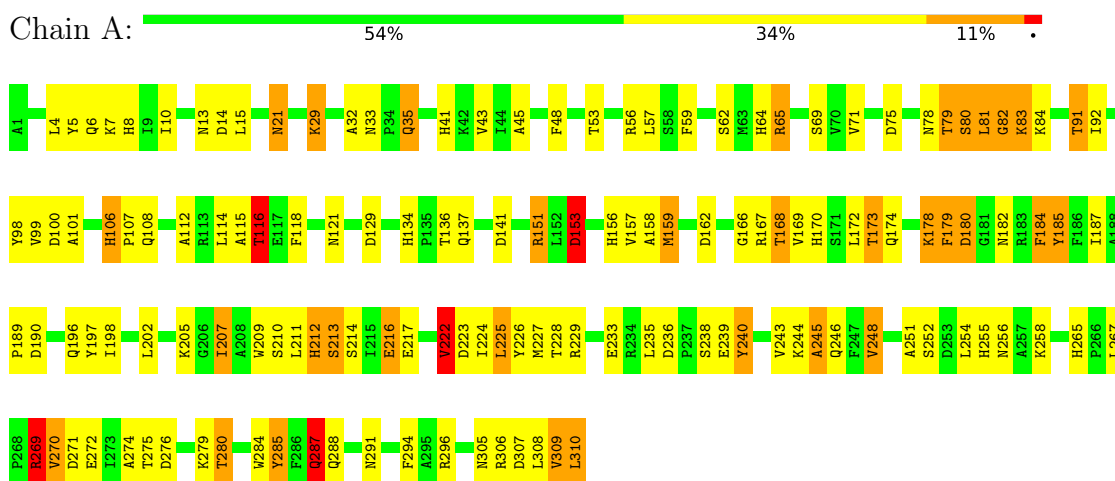
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total	O	0	0
			29	29		
5	B	11	Total	O	0	0
			11	11		
5	C	44	Total	O	0	0
			44	44		
5	D	9	Total	O	0	0
			9	9		

3 Residue-property plots

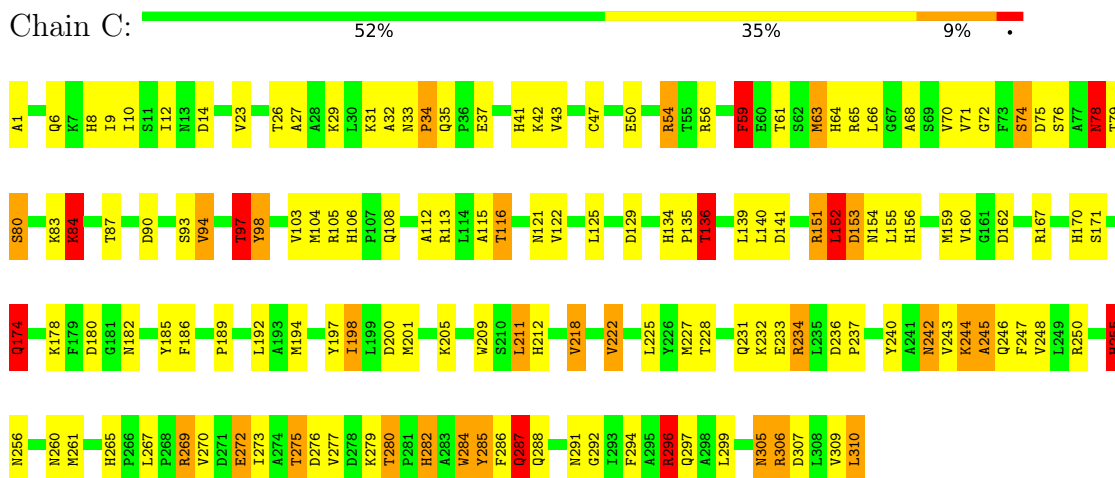
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

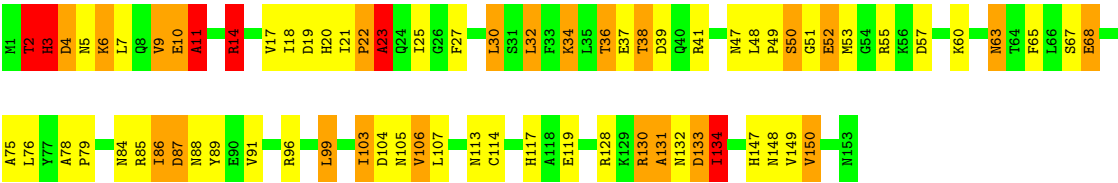


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

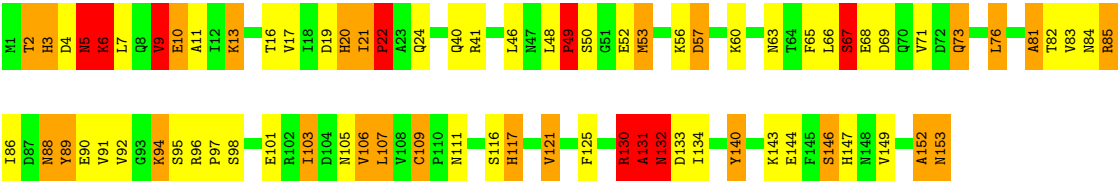


- Molecule 2: Aspartate carbamoyltransferase regulatory chain





• Molecule 2: Aspartate carbamoyltransferase regulatory chain



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}	0.188 , (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 [i](#)

5.1 Standard geometry [i](#)

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	1.27	15/2461 (0.6%)	2.12	107/3339 (3.2%)
1	C	1.35	24/2461 (1.0%)	2.21	125/3339 (3.7%)
2	B	1.16	4/1214 (0.3%)	2.16	57/1640 (3.5%)
2	D	1.18	7/1214 (0.6%)	2.19	58/1640 (3.5%)
All	All	1.27	50/7350 (0.7%)	2.17	347/9958 (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	7
1	C	0	5
2	B	0	1
2	D	0	2
All	All	0	15

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	HIS	CD2-NE2	-7.68	1.29	1.37
1	C	134	HIS	CD2-NE2	-7.10	1.30	1.37
1	C	134	HIS	CG-ND1	-7.00	1.30	1.38
1	A	265	HIS	CG-ND1	-6.91	1.30	1.38
1	C	56	ARG	CA-CB	-6.83	1.42	1.53
1	C	212	HIS	CD2-NE2	-6.79	1.30	1.37
1	C	34	PRO	CA-CB	-6.68	1.45	1.53
1	A	156	HIS	CD2-NE2	-6.44	1.30	1.37
2	B	147	HIS	CD2-NE2	-6.41	1.30	1.37
1	C	8	HIS	CG-ND1	-6.35	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	8	HIS	CG-ND1	-6.30	1.31	1.38
1	C	8	HIS	CD2-NE2	-6.29	1.30	1.37
2	D	147	HIS	CD2-NE2	-6.20	1.31	1.37
1	C	64	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	212	HIS	CG-ND1	-6.06	1.31	1.38
1	A	309	VAL	CA-CB	6.04	1.60	1.53
1	A	170	HIS	CD2-NE2	-6.00	1.31	1.37
2	D	3	HIS	CD2-NE2	-5.96	1.31	1.37
1	C	170	HIS	CG-ND1	-5.96	1.31	1.38
1	A	134	HIS	CD2-NE2	-5.95	1.31	1.37
1	C	282	HIS	CD2-NE2	-5.92	1.31	1.37
1	C	170	HIS	CD2-NE2	-5.87	1.31	1.37
1	C	106	HIS	CG-ND1	-5.85	1.31	1.38
1	A	41	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	212	HIS	CD2-NE2	-5.74	1.31	1.37
1	C	35	GLN	CA-CB	-5.73	1.46	1.53
1	C	156	HIS	CD2-NE2	-5.70	1.31	1.37
1	C	41	HIS	CD2-NE2	-5.69	1.31	1.37
2	D	117	HIS	CD2-NE2	-5.63	1.31	1.37
1	C	106	HIS	CD2-NE2	-5.60	1.31	1.37
2	B	117	HIS	CD2-NE2	-5.59	1.31	1.37
1	C	265	HIS	CD2-NE2	-5.55	1.31	1.37
2	D	82	THR	CA-CB	5.50	1.60	1.53
2	D	147	HIS	CG-ND1	-5.50	1.32	1.38
1	A	56	ARG	CA-CB	-5.46	1.44	1.53
1	C	112	ALA	CA-CB	-5.39	1.44	1.53
2	D	20	HIS	CD2-NE2	-5.32	1.31	1.37
1	A	134	HIS	CG-ND1	-5.30	1.32	1.38
1	C	156	HIS	CG-ND1	-5.24	1.32	1.38
2	B	20	HIS	CD2-NE2	-5.18	1.32	1.37
1	C	94	VAL	CA-CB	-5.18	1.47	1.54
1	A	255	HIS	CD2-NE2	-5.17	1.32	1.37
2	B	2	THR	CA-CB	5.15	1.62	1.53
1	C	108	GLN	CA-CB	-5.14	1.45	1.53
2	D	5	ASN	CA-CB	5.11	1.62	1.53
1	A	64	HIS	CD2-NE2	-5.09	1.32	1.37
1	C	12	ILE	CA-CB	5.03	1.61	1.54
1	C	282	HIS	CG-ND1	-5.03	1.32	1.38
1	C	34	PRO	CA-C	-5.01	1.47	1.52

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	ASN	CA-CB-CG	14.50	127.10	112.60
1	C	287	GLN	OE1-CD-NE2	-13.39	109.21	122.60
2	D	5	ASN	CA-CB-CG	11.50	124.10	112.60
1	A	271	ASP	CA-CB-CG	11.10	123.70	112.60
1	C	33	ASN	OD1-CG-ND2	-11.09	111.51	122.60
1	C	75	ASP	CA-CB-CG	10.55	123.15	112.60
2	B	11	ALA	N-CA-C	10.47	133.11	110.80
1	C	122	VAL	N-CA-C	-10.42	97.24	107.76
1	A	276	ASP	CA-CB-CG	10.28	122.88	112.60
1	C	287	GLN	CG-CD-NE2	10.00	131.40	116.40
1	C	97	THR	N-CA-CB	-9.84	95.39	110.44
2	D	67	SER	N-CA-C	9.78	123.53	108.96
1	C	218	VAL	N-CA-CB	-9.76	100.71	112.33
1	C	33	ASN	CA-C-N	9.60	129.68	119.89
1	C	33	ASN	C-N-CA	9.60	129.68	119.89
2	D	88	ASN	OD1-CG-ND2	-9.54	113.06	122.60
2	B	53	MET	N-CA-C	-9.50	100.20	114.64
1	A	14	ASP	CA-CB-CG	9.27	121.87	112.60
1	C	297	GLN	OE1-CD-NE2	-9.23	113.37	122.60
1	C	247	PHE	N-CA-C	-9.10	97.07	109.54
1	A	75	ASP	CA-CB-CG	8.98	121.58	112.60
2	B	67	SER	N-CA-C	8.84	122.51	109.07
2	D	147	HIS	ND1-CG-CD2	8.83	114.93	106.10
2	D	88	ASN	N-CA-C	-8.63	92.47	107.49
1	C	275	THR	CA-CB-OG1	-8.62	96.67	109.60
1	A	153	ASP	CA-CB-CG	8.60	121.19	112.60
2	D	5	ASN	OD1-CG-ND2	-8.52	114.08	122.60
2	D	94	LYS	N-CA-C	-8.47	95.87	109.76
2	D	40	GLN	OE1-CD-NE2	-8.42	114.18	122.60
2	B	133	ASP	N-CA-C	8.39	128.66	110.80
2	D	2	THR	CA-C-O	8.27	129.00	120.24
1	A	222	VAL	N-CA-CB	-8.26	97.65	110.86
2	B	21	ILE	N-CA-C	-8.19	101.59	108.63
2	D	9	VAL	N-CA-C	8.10	126.19	109.34
2	D	3	HIS	N-CA-C	-8.06	93.63	110.80
1	C	129	ASP	CA-CB-CG	7.99	120.59	112.60
1	C	78	ASN	N-CA-C	7.97	127.78	110.80
2	B	39	ASP	N-CA-C	-7.88	104.11	112.93
1	A	287	GLN	OE1-CD-NE2	-7.87	114.73	122.60
1	C	54	ARG	CA-CB-CG	7.86	129.82	114.10
1	A	129	ASP	CA-CB-CG	7.84	120.44	112.60
2	D	89	TYR	N-CA-C	7.79	127.38	110.80
1	C	8	HIS	ND1-CG-CD2	7.77	113.87	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	52	GLU	N-CA-C	7.74	127.29	110.80
1	C	87	THR	O-C-N	-7.70	114.01	122.79
1	A	291	ASN	OD1-CG-ND2	-7.69	114.91	122.60
1	A	79	THR	N-CA-CB	-7.62	97.61	110.49
1	C	280	THR	N-CA-CB	-7.59	99.79	110.04
1	C	200	ASP	CA-CB-CG	7.56	120.16	112.60
1	C	305	ASN	N-CA-C	7.55	121.03	108.73
1	C	134	HIS	ND1-CG-CD2	7.54	113.64	106.10
1	A	265	HIS	ND1-CG-CD2	7.47	113.57	106.10
1	A	134	HIS	ND1-CG-CD2	7.43	113.53	106.10
1	C	33	ASN	CB-CG-ND2	7.42	127.53	116.40
1	A	224	ILE	O-C-N	-7.40	115.41	123.18
1	C	198	ILE	N-CA-C	-7.39	103.65	110.82
1	C	80	SER	N-CA-C	7.38	126.51	110.80
1	C	90	ASP	N-CA-C	7.37	119.32	111.28
1	C	244	LYS	CA-C-O	-7.37	111.95	120.20
1	A	162	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	35	GLN	CA-CB-CG	-7.29	99.52	114.10
2	D	6	LYS	N-CA-C	7.29	122.53	112.04
1	C	309	VAL	O-C-N	7.25	130.79	123.18
2	D	132	ASN	N-CA-C	-7.23	95.40	110.80
1	C	160	VAL	N-CA-CB	-7.23	101.43	111.41
1	A	21	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	A	41	HIS	ND1-CG-CD2	7.15	113.25	106.10
1	C	141	ASP	CA-CB-CG	7.15	119.75	112.60
2	D	121	VAL	CA-CB-CG2	-7.11	98.32	110.40
1	C	74	SER	N-CA-C	-7.08	98.19	109.59
1	C	174	GLN	CA-CB-CG	-7.07	99.96	114.10
1	A	258	LYS	CB-CG-CD	-7.06	95.07	111.30
1	A	106	HIS	CA-C-N	7.04	127.19	119.87
1	A	106	HIS	C-N-CA	7.04	127.19	119.87
1	C	10	ILE	N-CA-C	-6.98	105.04	111.67
1	A	84	LYS	N-CA-C	-6.94	96.01	110.80
1	A	35	GLN	CA-C-N	6.90	126.59	119.82
1	A	35	GLN	C-N-CA	6.90	126.59	119.82
1	C	136	THR	N-CA-CB	-6.85	99.23	110.40
1	C	116	THR	N-CA-CB	-6.81	99.38	110.14
1	A	32	ALA	N-CA-C	6.78	118.32	111.07
1	C	276	ASP	CA-CB-CG	6.77	119.37	112.60
2	B	52	GLU	CA-C-O	6.77	130.19	120.51
1	A	80	SER	N-CA-C	6.75	125.19	110.80
1	A	134	HIS	CB-CG-CD2	-6.74	122.44	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	VAL	N-CA-CB	-6.74	101.27	110.56
1	A	269	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	A	134	HIS	CA-CB-CG	6.71	120.52	113.80
1	C	42	LYS	O-C-N	-6.71	115.54	123.06
1	C	296	ARG	NE-CZ-NH1	6.71	128.22	121.50
2	D	106	VAL	N-CA-C	-6.71	97.50	107.51
2	B	18	ILE	N-CA-C	-6.69	98.22	107.99
1	C	66	LEU	N-CA-C	-6.69	104.25	112.88
1	A	33	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	A	225	LEU	O-C-N	-6.64	115.15	123.05
2	D	50	SER	N-CA-C	-6.64	96.65	110.80
1	A	189	PRO	CA-C-O	-6.63	114.13	121.23
1	A	275	THR	CA-CB-OG1	-6.63	99.65	109.60
2	B	19	ASP	CA-CB-CG	6.62	119.22	112.60
1	C	180	ASP	N-CA-C	6.62	120.62	109.76
2	D	81	ALA	N-CA-C	-6.60	97.84	109.06
1	A	222	VAL	CB-CA-C	6.56	120.23	110.98
1	C	97	THR	CB-CA-C	6.56	121.82	110.01
1	C	269	ARG	NE-CZ-NH2	-6.56	113.30	119.20
1	C	106	HIS	ND1-CG-CD2	6.52	112.62	106.10
1	A	294	PHE	CA-CB-CG	-6.51	107.29	113.80
1	C	246	GLN	N-CA-C	6.50	118.83	110.65
2	D	69	ASP	CA-CB-CG	6.48	119.08	112.60
2	D	88	ASN	CB-CG-ND2	6.47	126.11	116.40
1	A	134	HIS	CG-CD2-NE2	-6.46	100.74	107.20
1	C	14	ASP	CA-CB-CG	6.44	119.04	112.60
1	C	32	ALA	CA-C-O	-6.44	114.04	120.80
2	D	133	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	168	THR	O-C-N	-6.40	115.33	122.12
1	A	255	HIS	CA-CB-CG	6.40	120.20	113.80
2	B	105	ASN	N-CA-C	6.39	124.42	110.80
1	C	136	THR	N-CA-C	-6.39	104.97	112.89
1	A	10	ILE	N-CA-CB	-6.35	103.20	111.90
1	A	116	THR	N-CA-CB	-6.35	99.76	110.49
2	D	22	PRO	N-CA-C	6.32	125.50	112.47
1	A	62	SER	CA-CB-OG	-6.32	98.45	111.10
1	C	288	GLN	OE1-CD-NE2	-6.32	116.28	122.60
2	D	147	HIS	CG-CD2-NE2	-6.30	100.89	107.20
1	C	103	VAL	N-CA-C	-6.30	99.35	108.36
2	D	57	ASP	CA-CB-CG	6.30	118.90	112.60
2	D	6	LYS	O-C-N	6.30	130.80	122.30
2	B	106	VAL	N-CA-CB	-6.29	98.42	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	146	SER	CA-C-O	-6.29	114.12	121.16
1	C	233	GLU	CA-CB-CG	6.28	126.67	114.10
2	D	103	ILE	N-CA-C	-6.28	98.48	107.77
1	A	279	LYS	CA-CB-CG	-6.25	101.59	114.10
1	A	179	PHE	O-C-N	-6.24	114.46	122.20
1	A	6	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	A	307	ASP	CA-CB-CG	6.24	118.84	112.60
2	B	63	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	C	108	GLN	CA-CB-CG	-6.22	101.66	114.10
1	C	222	VAL	CA-CB-CG2	-6.21	99.84	110.40
1	A	256	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	C	218	VAL	N-CA-C	6.17	119.70	113.47
2	B	148	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	196	GLN	CB-CG-CD	6.17	123.08	112.60
1	C	236	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	23	VAL	CB-CA-C	-6.13	103.87	112.14
2	D	21	ILE	CA-C-N	6.12	127.48	119.84
2	D	21	ILE	C-N-CA	6.12	127.48	119.84
1	A	69	SER	CA-CB-OG	-6.11	98.89	111.10
2	B	63	ASN	CB-CG-ND2	6.10	125.55	116.40
1	C	182	ASN	O-C-N	6.10	129.85	122.96
1	C	270	VAL	CA-C-N	-6.10	112.48	121.99
1	C	270	VAL	C-N-CA	-6.10	112.48	121.99
1	C	61	THR	N-CA-C	-6.09	104.72	111.36
2	B	103	ILE	CB-CA-C	-6.07	104.36	111.09
2	B	10	GLU	N-CA-C	6.07	119.39	110.59
1	C	288	GLN	N-CA-C	-6.05	104.61	111.14
2	D	131	ALA	O-C-N	6.04	130.62	122.59
1	C	136	THR	CB-CA-C	6.02	122.57	109.99
2	B	52	GLU	CA-C-N	6.00	132.38	121.41
2	B	52	GLU	C-N-CA	6.00	132.38	121.41
1	C	59	PHE	N-CA-C	-5.99	104.44	110.97
2	D	106	VAL	N-CA-CB	-5.99	103.92	111.41
1	C	244	LYS	O-C-N	-5.98	115.38	122.20
2	D	10	GLU	N-CA-C	-5.98	98.11	108.52
2	D	149	VAL	N-CA-C	-5.98	104.68	110.72
1	C	26	THR	CA-CB-OG1	-5.97	100.65	109.60
1	A	101	ALA	O-C-N	-5.96	116.59	123.33
2	B	134	ILE	N-CA-C	5.95	121.70	109.34
1	A	173	THR	N-CA-C	-5.94	104.72	111.14
1	C	280	THR	CB-CA-C	5.94	118.03	109.11
2	B	131	ALA	N-CA-C	5.93	123.44	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	VAL	N-CA-C	5.92	121.66	109.34
2	B	32	LEU	N-CA-C	5.92	118.50	111.33
1	A	116	THR	CA-CB-OG1	-5.91	100.73	109.60
2	D	152	ALA	N-CA-C	-5.91	98.21	110.80
1	C	8	HIS	O-C-N	-5.90	116.50	123.22
2	D	3	HIS	CA-C-N	5.89	132.79	121.54
2	D	3	HIS	C-N-CA	5.89	132.79	121.54
2	D	9	VAL	CB-CA-C	-5.88	101.65	111.29
1	A	141	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	178	LYS	CA-CB-CG	-5.86	102.38	114.10
1	A	307	ASP	N-CA-C	-5.86	99.10	109.06
1	C	307	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	43	VAL	N-CA-C	-5.85	99.92	108.11
2	B	114	CYS	CA-C-O	5.85	127.62	121.19
1	C	56	ARG	CB-CG-CD	-5.85	97.85	111.30
1	A	10	ILE	N-CA-C	5.84	117.03	112.12
1	A	236	ASP	N-CA-C	-5.84	102.72	110.07
2	D	130	ARG	O-C-N	5.84	130.02	122.43
1	A	287	GLN	CG-CD-NE2	5.83	125.15	116.40
2	B	38	THR	N-CA-C	-5.83	100.48	109.52
1	C	284	TRP	CB-CG-CD1	-5.82	118.17	126.90
2	B	57	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	222	VAL	CA-CB-CG1	5.81	120.28	110.40
2	D	11	ALA	N-CA-C	-5.79	99.08	108.52
1	A	240	TYR	N-CA-C	-5.79	103.96	111.02
1	C	63	MET	N-CA-C	-5.78	104.58	111.69
1	C	152	LEU	O-C-N	-5.78	115.20	122.19
2	D	63	ASN	OD1-CG-ND2	-5.77	116.83	122.60
2	D	83	VAL	N-CA-C	-5.77	101.58	109.55
1	C	273	ILE	N-CA-C	-5.77	99.23	107.77
2	D	105	ASN	CB-CA-C	-5.77	98.94	110.42
1	A	81	LEU	O-C-N	5.76	129.79	123.22
1	A	225	LEU	CD1-CG-CD2	-5.75	98.16	110.80
1	C	93	SER	N-CA-C	-5.73	105.18	111.82
1	C	280	THR	O-C-N	-5.72	114.37	121.64
1	A	265	HIS	CG-CD2-NE2	-5.71	101.48	107.20
1	C	156	HIS	CA-CB-CG	5.69	119.49	113.80
1	C	134	HIS	CA-C-N	5.69	125.81	119.32
1	C	134	HIS	C-N-CA	5.69	125.81	119.32
2	B	117	HIS	CA-CB-CG	-5.69	108.11	113.80
1	A	216	GLU	CA-CB-CG	5.69	125.48	114.10
2	B	52	GLU	O-C-N	5.69	130.16	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TYR	CA-CB-CG	5.68	124.13	113.90
1	C	269	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	A	8	HIS	ND1-CG-CD2	5.68	111.78	106.10
2	B	75	ALA	N-CA-C	5.67	119.01	111.75
2	B	68	GLU	CA-CB-CG	-5.66	102.77	114.10
1	C	269	ARG	N-CA-C	-5.66	100.06	109.46
1	A	65	ARG	CB-CG-CD	5.66	124.31	111.30
1	A	182	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	157	VAL	N-CA-CB	-5.65	104.35	111.46
2	B	104	ASP	CA-CB-CG	-5.63	106.97	112.60
1	C	134	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	A	100	ASP	CA-CB-CG	5.62	118.22	112.60
2	D	73	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	A	29	LYS	CB-CG-CD	-5.62	98.38	111.30
1	A	239	GLU	O-C-N	5.62	130.53	122.28
1	C	27	ALA	CA-C-N	5.61	127.73	120.44
1	C	27	ALA	C-N-CA	5.61	127.73	120.44
1	C	275	THR	CA-CB-CG2	5.60	120.02	110.50
1	C	37	GLU	CB-CG-CD	5.59	122.11	112.60
1	C	267	LEU	O-C-N	-5.59	114.89	121.32
1	C	275	THR	OG1-CB-CG2	5.58	120.46	109.30
1	A	79	THR	N-CA-C	5.58	122.68	110.80
2	B	134	ILE	CB-CA-C	-5.57	102.16	111.29
1	C	151	ARG	CG-CD-NE	-5.57	99.75	112.00
2	D	3	HIS	O-C-N	5.57	130.00	122.59
2	D	106	VAL	CA-C-O	-5.57	114.28	120.74
1	A	71	VAL	O-C-N	-5.57	117.05	123.00
1	C	218	VAL	CA-CB-CG2	-5.56	100.95	110.40
1	C	284	TRP	CG-CD2-CE3	5.56	139.46	133.90
2	B	3	HIS	CA-CB-CG	5.55	119.35	113.80
1	A	53	THR	N-CA-C	5.55	117.01	111.07
1	A	223	ASP	N-CA-C	-5.54	105.56	112.93
2	D	134	ILE	N-CA-CB	-5.54	104.44	111.64
1	C	209	TRP	CE2-CD2-CG	-5.53	100.56	107.20
1	C	285	TYR	N-CA-C	5.53	117.31	111.28
1	C	160	VAL	O-C-N	-5.52	117.30	123.26
1	A	196	GLN	N-CA-C	-5.51	105.42	111.82
2	B	34	LYS	CA-CB-CG	5.51	125.13	114.10
1	A	10	ILE	CB-CG1-CD1	-5.51	102.23	113.80
1	C	71	VAL	O-C-N	-5.50	117.08	122.97
1	A	274	ALA	O-C-N	-5.50	116.38	122.86
1	C	279	LYS	CA-CB-CG	-5.49	103.12	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	52	GLU	N-CA-C	5.49	119.46	112.87
2	B	10	GLU	CA-C-N	5.49	132.02	121.54
2	B	10	GLU	C-N-CA	5.49	132.02	121.54
1	C	305	ASN	O-C-N	-5.48	116.97	123.22
1	A	196	GLN	CA-C-O	-5.46	113.69	119.97
2	D	147	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	C	306	ARG	CA-CB-CG	5.45	125.01	114.10
1	C	265	HIS	ND1-CG-CD2	5.45	111.55	106.10
2	D	19	ASP	N-CA-CB	-5.45	102.37	111.20
1	C	260	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	41	HIS	CG-CD2-NE2	-5.43	101.77	107.20
1	C	282	HIS	ND1-CG-CD2	5.42	111.52	106.10
2	D	109	CYS	CA-C-N	5.42	125.76	119.47
2	D	109	CYS	C-N-CA	5.42	125.76	119.47
2	B	119	GLU	N-CA-C	5.42	117.00	108.55
1	C	31	LYS	N-CA-C	-5.41	105.46	111.36
2	B	133	ASP	CA-CB-CG	5.41	118.01	112.60
2	B	119	GLU	O-C-N	-5.40	118.25	121.71
1	C	72	GLY	CA-C-O	-5.40	115.26	121.47
1	C	105	ARG	O-C-N	-5.39	116.36	123.16
2	D	117	HIS	N-CA-C	5.39	117.24	111.36
1	A	91	THR	N-CA-C	-5.39	105.32	111.14
1	A	224	ILE	N-CA-CB	-5.39	103.92	111.25
1	C	115	ALA	CA-C-N	5.37	128.23	120.38
1	C	115	ALA	C-N-CA	5.37	128.23	120.38
2	B	133	ASP	O-C-N	5.37	129.73	122.59
2	D	90	GLU	O-C-N	5.35	129.14	123.42
1	A	178	LYS	N-CA-C	-5.35	106.60	113.23
1	C	84	LYS	N-CA-C	-5.34	99.43	110.80
1	A	270	VAL	CA-C-O	-5.33	114.11	120.78
1	C	162	ASP	N-CA-C	-5.33	99.09	108.20
2	B	78	ALA	O-C-N	-5.33	117.30	121.19
1	A	275	THR	N-CA-C	5.32	119.25	112.34
1	C	265	HIS	CG-CD2-NE2	-5.31	101.89	107.20
1	C	209	TRP	CG-CD1-NE1	-5.31	103.30	110.20
1	C	307	ASP	N-CA-C	-5.31	99.79	108.76
2	B	23	ALA	N-CA-CB	5.30	119.44	110.49
1	C	106	HIS	CA-C-O	-5.30	114.51	119.91
1	C	56	ARG	CG-CD-NE	-5.29	100.36	112.00
1	A	245	ALA	N-CA-C	-5.28	99.55	110.80
2	B	132	ASN	CA-C-N	5.28	131.63	121.54
2	B	132	ASN	C-N-CA	5.28	131.63	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH2	-5.27	114.45	119.20
1	C	78	ASN	OD1-CG-ND2	-5.27	117.33	122.60
2	B	84	ASN	CA-CB-CG	-5.26	107.34	112.60
1	A	118	PHE	O-C-N	-5.26	116.52	122.10
1	C	8	HIS	CG-CD2-NE2	-5.25	101.95	107.20
2	B	36	THR	N-CA-C	5.24	119.38	112.89
2	D	107	LEU	N-CA-CB	5.23	119.34	110.49
1	A	82	GLY	N-CA-C	-5.23	100.79	113.18
1	A	107	PRO	N-CA-C	5.22	120.46	114.03
1	C	242	ASN	N-CA-C	-5.22	103.14	110.50
1	C	54	ARG	CB-CA-C	-5.21	102.64	110.92
2	D	73	GLN	CG-CD-NE2	5.21	124.21	116.40
1	A	269	ARG	CA-CB-CG	5.20	124.51	114.10
1	C	296	ARG	CB-CG-CD	5.20	123.25	111.30
1	C	197	TYR	CA-CB-CG	5.19	123.24	113.90
1	A	92	ILE	CA-C-O	-5.18	115.74	121.29
1	A	213	SER	N-CA-CB	-5.18	103.70	110.59
1	A	81	LEU	CA-C-O	5.17	126.38	120.54
1	C	250	ARG	CA-CB-CG	5.15	124.41	114.10
1	A	251	ALA	CA-C-N	5.14	127.42	120.38
1	A	251	ALA	C-N-CA	5.14	127.42	120.38
1	C	291	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	248	VAL	N-CA-C	-5.13	101.24	109.20
1	A	116	THR	CA-CB-CG2	5.12	119.21	110.50
1	C	154	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	153	ASP	CB-CA-C	-5.11	99.31	109.79
1	A	280	THR	CA-C-N	5.11	124.72	119.56
1	A	280	THR	C-N-CA	5.11	124.72	119.56
2	B	149	VAL	O-C-N	-5.10	116.58	121.83
1	A	288	GLN	CA-C-O	-5.10	115.45	120.70
2	B	150	VAL	CA-C-O	5.09	125.97	120.47
2	D	49	PRO	O-C-N	5.09	129.52	122.64
1	A	6	GLN	N-CA-C	5.09	118.78	112.47
2	B	23	ALA	N-CA-C	-5.09	99.96	110.80
2	D	144	GLU	CA-CB-CG	-5.09	103.92	114.10
2	B	130	ARG	N-CA-C	5.09	117.68	110.10
2	D	121	VAL	CA-CB-CG1	5.08	119.04	110.40
1	A	285	TYR	N-CA-C	5.08	117.55	111.71
1	C	162	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	53	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	43	VAL	CG1-CB-CG2	-5.05	99.68	110.80
1	A	180	ASP	CA-CB-CG	5.05	117.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	ASN	CA-CB-CG	5.05	117.65	112.60
2	B	14	ARG	CA-CB-CG	5.05	124.20	114.10
1	A	190	ASP	N-CA-C	5.04	118.92	112.87
1	A	233	GLU	CA-CB-CG	5.04	124.19	114.10
2	B	21	ILE	CA-C-N	5.04	126.14	119.84
2	B	21	ILE	C-N-CA	5.04	126.14	119.84
2	B	88	ASN	OD1-CG-ND2	-5.04	117.56	122.60
2	B	6	LYS	CA-C-N	5.01	127.93	120.31
2	B	6	LYS	C-N-CA	5.01	127.93	120.31
1	C	68	ALA	O-C-N	-5.01	117.45	123.06

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	PHE	Sidechain
1	A	185	TYR	Sidechain
1	A	226	TYR	Sidechain
1	A	240	TYR	Sidechain
1	A	48	PHE	Sidechain
1	A	59	PHE	Sidechain
1	A	98	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	185	TYR	Sidechain
1	C	255	HIS	Sidechain
1	C	286	PHE	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	36	0
1	C	2415	0	2422	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1196	0	1212	23	0
2	D	1196	0	1212	28	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	0	0
5	A	29	0	0	0	0
5	B	11	0	0	0	0
5	C	44	0	0	2	0
5	D	9	0	0	1	0
All	All	7375	0	7292	119	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 8.

All (119) 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	1.56	0.87
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.58	0.86
1:A:81:LEU:HD13	1:A:91:THR:HG23	1.57	0.84
1:A:205:LYS:HB2	1:A:207:ILE:HD12	1.58	0.84
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.61	0.83
1:A:29:LYS:HD3	1:A:310:LEU:HG	1.62	0.81
2:D:6:LYS:HB2	2:D:9:VAL:HG13	1.63	0.80
1:A:106:HIS:HD2	1:A:108:GLN:H	1.31	0.78
2:D:5:ASN:ND2	2:D:6:LYS:HD2	2.00	0.76
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.03	0.71
1:A:153:ASP:HB3	1:A:180:ASP:O	1.91	0.71
1:C:186:PHE:HB2	1:C:211:LEU:HD12	1.74	0.69
2:B:76:LEU:HD12	2:B:103:ILE:HD11	1.76	0.68
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.74	0.68
2:B:6:LYS:HE2	2:D:41:ARG:HD2	1.78	0.66
1:A:159:MET:HE1	1:A:173:THR:OG1	1.97	0.65
1:C:292:GLY:O	1:C:296:ARG:HG3	1.96	0.65
1:C:113:ARG:O	1:C:116:THR:HB	1.98	0.64
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.31	0.64
2:D:6:LYS:HG3	2:D:9:VAL:HG22	1.79	0.62
2:D:20:HIS:HA	2:D:56:LYS:HD2	1.83	0.61
1:C:97:THR:HG22	1:C:98:TYR:HD2	1.65	0.61
1:C:284:TRP:HA	1:C:287:GLN:HE21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ALA:HB2	1:A:222:VAL:HG21	1.82	0.60
1:C:136:THR:HG23	1:C:296:ARG:HD3	1.83	0.60
2:D:152:ALA:O	2:D:153:ASN:HB2	2.00	0.60
1:A:151:ARG:HD2	1:A:153:ASP:O	2.02	0.59
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.18	0.59
2:B:14:ARG:NH1	2:B:63:ASN:HA	2.18	0.58
1:C:280:THR:HG22	1:C:282:HIS:H	1.69	0.57
1:A:15:LEU:O	1:A:178:LYS:HE2	2.04	0.57
2:B:22:PRO:HB2	2:B:25:ILE:HD13	1.85	0.57
1:C:174:GLN:HG3	1:C:201:MET:HE2	1.87	0.57
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.85	0.57
1:C:242:ASN:O	1:C:244:LYS:N	2.38	0.56
1:C:9:ILE:HG21	1:C:299:LEU:HD21	1.88	0.56
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.21	0.56
2:B:6:LYS:HA	2:B:9:VAL:HG22	1.88	0.56
1:C:94:VAL:O	1:C:97:THR:HB	2.06	0.56
1:A:287:GLN:NE2	1:A:287:GLN:H	2.04	0.55
1:A:159:MET:HE3	1:A:169:VAL:HB	1.88	0.55
2:D:67:SER:HA	2:D:71:VAL:HG23	1.89	0.55
1:C:277:VAL:O	1:C:280:THR:HB	2.07	0.55
1:A:214:SER:O	1:A:217:GLU:HB2	2.07	0.55
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.89	0.54
1:C:136:THR:HB	5:C:317:HOH:O	2.07	0.54
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.90	0.54
1:A:4:LEU:HD23	1:A:7:LYS:HD3	1.89	0.54
2:B:76:LEU:HD12	2:B:103:ILE:CD1	2.37	0.53
2:B:86:ILE:HG13	2:B:91:VAL:HA	1.90	0.53
1:A:254:LEU:HD12	1:A:280:THR:HG21	1.91	0.52
1:C:50:GLU:HA	1:C:76:SER:OG	2.09	0.52
1:A:136:THR:HB	1:A:296:ARG:HH11	1.75	0.52
1:A:21:ASN:HD21	1:A:179:PHE:HE1	1.57	0.52
1:C:231:GLN:HB2	1:C:234:ARG:HG3	1.92	0.52
1:C:136:THR:CG2	1:C:296:ARG:HD3	2.39	0.51
1:A:267:LEU:CD2	1:A:269:ARG:HG3	2.41	0.51
2:D:20:HIS:O	2:D:20:HIS:ND1	2.44	0.51
2:B:107:LEU:HD22	2:B:150:VAL:HG12	1.94	0.50
1:C:136:THR:HG23	1:C:296:ARG:HH11	1.72	0.50
2:B:11:ALA:HA	4:B:999:CTP:N3	2.28	0.49
2:D:121:VAL:HG21	2:D:140:TYR:CZ	2.48	0.49
2:B:48:LEU:O	2:B:55:ARG:HA	2.13	0.48
1:A:187:ILE:HG13	1:A:212:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:PHE:CE1	2:B:85:ARG:HG3	2.48	0.48
1:C:272:GLU:H	1:C:272:GLU:CD	2.21	0.48
2:D:131:ALA:O	2:D:132:ASN:HB2	2.14	0.47
1:A:248:VAL:HG12	1:A:272:GLU:HA	1.96	0.47
1:A:287:GLN:H	1:A:287:GLN:HE21	1.60	0.47
2:D:65:PHE:HB3	2:D:85:ARG:HH22	1.80	0.47
2:B:27:PHE:HA	2:B:30:LEU:HD23	1.97	0.46
2:D:5:ASN:HD22	2:D:6:LYS:H	1.63	0.46
1:A:5:TYR:CZ	1:A:306:ARG:HG2	2.51	0.46
1:A:108:GLN:HG2	2:B:113:ASN:OD1	2.15	0.46
1:C:227:MET:HE3	1:C:227:MET:HB3	1.73	0.46
2:D:111:ASN:O	2:D:117:HIS:HE1	1.99	0.46
1:C:135:PRO:O	1:C:139:LEU:HG	2.16	0.46
2:B:41:ARG:HE	2:D:49:PRO:HD2	1.80	0.46
2:D:13:LYS:O	2:D:86:ILE:HG22	2.16	0.45
2:D:53:MET:HB3	5:D:1007:HOH:O	2.16	0.45
1:A:198:ILE:O	1:A:202:LEU:HG	2.16	0.45
2:D:81:ALA:O	2:D:97:PRO:HD2	2.16	0.45
1:C:59:PHE:CE2	1:C:136:THR:HG21	2.52	0.45
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.99	0.44
2:B:6:LYS:HB3	2:D:10:GLU:HG3	2.00	0.44
1:A:112:ALA:O	1:A:115:ALA:HB3	2.17	0.44
2:B:23:ALA:O	2:B:25:ILE:HD12	2.18	0.44
1:C:261:MET:C	1:C:261:MET:SD	3.01	0.43
1:C:1:ALA:HA	1:C:306:ARG:O	2.18	0.43
1:A:5:TYR:CD1	1:A:306:ARG:HA	2.54	0.43
1:A:82:GLY:O	1:A:83:LYS:HB3	2.18	0.43
2:B:14:ARG:HB2	2:B:87:ASP:HA	1.99	0.43
1:C:47:CYS:O	1:C:104:MET:HA	2.18	0.43
1:C:232:LYS:HA	1:C:240:TYR:CD2	2.53	0.42
2:B:14:ARG:HA	2:B:86:ILE:O	2.18	0.42
1:C:189:PRO:HG2	1:C:192:LEU:HB2	2.02	0.42
1:C:63:MET:SD	1:C:70:VAL:HG22	2.60	0.42
2:B:6:LYS:HE2	2:D:41:ARG:CD	2.48	0.41
1:C:83:LYS:O	1:C:84:LYS:HB2	2.20	0.41
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.85	0.41
2:D:130:ARG:HD3	2:D:130:ARG:HA	1.59	0.41
2:B:99:LEU:HD23	2:B:130:ARG:HH11	1.84	0.41
2:D:116:SER:HA	2:D:121:VAL:HG11	2.03	0.41
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.88	0.41
1:A:227:MET:HE3	1:A:227:MET:HB3	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ARG:NH1	2:B:65:PHE:CE2	2.89	0.41
1:C:194:MET:SD	1:C:198:ILE:HG21	2.61	0.41
1:C:261:MET:O	1:C:282:HIS:HD2	2.04	0.41
1:A:166:GLY:O	1:A:169:VAL:HG22	2.21	0.41
1:C:29:LYS:HE2	1:C:310:LEU:HD13	2.03	0.41
1:C:240:TYR:O	1:C:245:ALA:HB2	2.21	0.41
2:D:92:VAL:O	2:D:92:VAL:HG13	2.21	0.41
2:D:111:ASN:O	2:D:117:HIS:CE1	2.73	0.41
1:C:152:LEU:HA	1:C:155:LEU:HD11	2.03	0.40
1:A:185:TYR:HD1	1:A:212:HIS:NE2	2.19	0.40
1:A:184:PHE:O	1:A:209:TRP:HA	2.20	0.40
1:A:4:LEU:HA	1:A:7:LYS:HD3	2.04	0.40
1:C:153:ASP:HB3	5:C:341:HOH:O	2.21	0.40
2:D:84:ASN:OD1	2:D:94:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/310 (99%)	288 (94%)	13 (4%)	7 (2%)	5	8
1	C	308/310 (99%)	283 (92%)	19 (6%)	6 (2%)	6	11
2	B	151/153 (99%)	120 (80%)	19 (13%)	12 (8%)	1	0
2	D	151/153 (99%)	124 (82%)	16 (11%)	11 (7%)	1	1
All	All	918/926 (99%)	815 (89%)	67 (7%)	36 (4%)	2	3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER

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Mol	Chain	Res	Type
1	A	245	ALA
1	A	270	VAL
2	B	3	HIS
2	B	11	ALA
2	B	14	ARG
2	B	23	ALA
2	B	52	GLU
2	B	68	GLU
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	7	LEU
2	D	22	PRO
2	D	89	TYR
2	D	107	LEU
2	D	132	ASN
1	A	79	THR
2	B	51	GLY
2	B	131	ALA
1	C	255	HIS
2	D	5	ASN
2	D	24	GLN
1	A	83	LYS
1	A	116	THR
1	A	246	GLN
1	C	84	LYS
2	D	68	GLU
2	D	131	ALA
2	B	50	SER
1	C	245	ALA
2	B	2	THR
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%)	229 (88%)	32 (12%)	4	10
1	C	261/261 (100%)	222 (85%)	39 (15%)	3	6
2	B	136/137 (99%)	114 (84%)	22 (16%)	2	4
2	D	136/137 (99%)	109 (80%)	27 (20%)	1	2
All	All	794/796 (100%)	674 (85%)	120 (15%)	3	5

All (120) 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	114	LEU
1	A	116	THR
1	A	121	ASN
1	A	151	ARG
1	A	153	ASP
1	A	159	MET
1	A	167	ARG
1	A	174	GLN
1	A	207	ILE
1	A	210	SER
1	A	211	LEU
1	A	213	SER
1	A	216	GLU
1	A	222	VAL
1	A	225	LEU
1	A	228	THR
1	A	229	ARG
1	A	235	LEU
1	A	238	SER
1	A	244	LYS
1	A	252	SER
1	A	269	ARG
1	A	285	TYR
1	A	287	GLN
1	A	305	ASN
1	A	309	VAL

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Mol	Chain	Res	Type
1	A	310	LEU
2	B	2	THR
2	B	3	HIS
2	B	4	ASP
2	B	7	LEU
2	B	9	VAL
2	B	22	PRO
2	B	30	LEU
2	B	32	LEU
2	B	34	LYS
2	B	36	THR
2	B	37	GLU
2	B	38	THR
2	B	49	PRO
2	B	50	SER
2	B	79	PRO
2	B	86	ILE
2	B	87	ASP
2	B	96	ARG
2	B	99	LEU
2	B	106	VAL
2	B	128	ARG
2	B	134	ILE
1	C	6	GLN
1	C	34	PRO
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	97	THR
1	C	121	ASN
1	C	125	LEU
1	C	136	THR
1	C	140	LEU
1	C	151	ARG
1	C	152	LEU
1	C	153	ASP
1	C	159	MET
1	C	167	ARG
1	C	171	SER

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Mol	Chain	Res	Type
1	C	174	GLN
1	C	205	LYS
1	C	211	LEU
1	C	218	VAL
1	C	222	VAL
1	C	225	LEU
1	C	228	THR
1	C	234	ARG
1	C	237	PRO
1	C	248	VAL
1	C	255	HIS
1	C	256	ASN
1	C	269	ARG
1	C	272	GLU
1	C	275	THR
1	C	285	TYR
1	C	287	GLN
1	C	296	ARG
1	C	305	ASN
1	C	310	LEU
2	D	2	THR
2	D	3	HIS
2	D	5	ASN
2	D	6	LYS
2	D	9	VAL
2	D	13	LYS
2	D	16	THR
2	D	22	PRO
2	D	46	LEU
2	D	49	PRO
2	D	53	MET
2	D	66	LEU
2	D	67	SER
2	D	73	GLN
2	D	76	LEU
2	D	85	ARG
2	D	88	ASN
2	D	95	SER
2	D	96	ARG
2	D	98	SER
2	D	101	GLU
2	D	106	VAL

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Mol	Chain	Res	Type
2	D	130	ARG
2	D	132	ASN
2	D	143	LYS
2	D	146	SER
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	21	ASN
1	A	106	HIS
1	A	174	GLN
1	A	196	GLN
1	A	242	ASN
1	A	282	HIS
1	A	287	GLN
1	A	297	GLN
2	B	147	HIS
2	B	148	ASN
1	C	33	ASN
1	C	121	ASN
1	C	149	GLN
1	C	196	GLN
1	C	260	ASN
1	C	287	GLN
1	C	305	ASN
2	D	5	ASN
2	D	73	GLN
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 [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	D	999	-	29,30,30	2.25	8 (27%)	43,47,47	1.19	4 (9%)
4	CTP	B	999	-	29,30,30	2.23	9 (31%)	43,47,47	1.42	4 (9%)

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	D	999	-	-	3/22/38/38	0/2/2/2
4	CTP	B	999	-	-	7/22/38/38	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	PB-O3B	6.62	1.66	1.59
4	B	999	CTP	PB-O3B	6.48	1.66	1.59
4	D	999	CTP	PB-O3A	5.66	1.65	1.59
4	D	999	CTP	PA-O3A	5.19	1.65	1.59
4	B	999	CTP	PA-O3A	5.08	1.65	1.59
4	B	999	CTP	PB-O3A	5.04	1.64	1.59
4	D	999	CTP	PG-O1G	2.77	1.59	1.50
4	B	999	CTP	PG-O1G	2.48	1.58	1.50
4	B	999	CTP	C6-N1	-2.45	1.32	1.38
4	B	999	CTP	C2-N3	-2.43	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	C5-C4	-2.39	1.37	1.42
4	B	999	CTP	PB-O1B	2.26	1.58	1.50
4	B	999	CTP	C2-N1	-2.26	1.35	1.40
4	D	999	CTP	PB-O1B	2.17	1.58	1.50
4	D	999	CTP	C6-N1	-2.13	1.33	1.38
4	D	999	CTP	PA-O1A	2.11	1.58	1.50
4	B	999	CTP	C5-C4	-2.06	1.38	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	CTP	O2-C2-N3	-5.26	114.04	122.33
4	D	999	CTP	O2-C2-N3	-4.12	115.83	122.33
4	B	999	CTP	N1-C2-N3	3.11	124.20	118.80
4	B	999	CTP	C6-N1-C2	-2.83	115.68	120.46
4	D	999	CTP	C6-N1-C2	-2.57	116.12	120.46
4	B	999	CTP	O2A-PA-O3A	2.23	113.29	107.27
4	D	999	CTP	C3'-C2'-C1'	2.17	105.58	101.46
4	D	999	CTP	N1-C2-N3	2.10	122.45	118.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

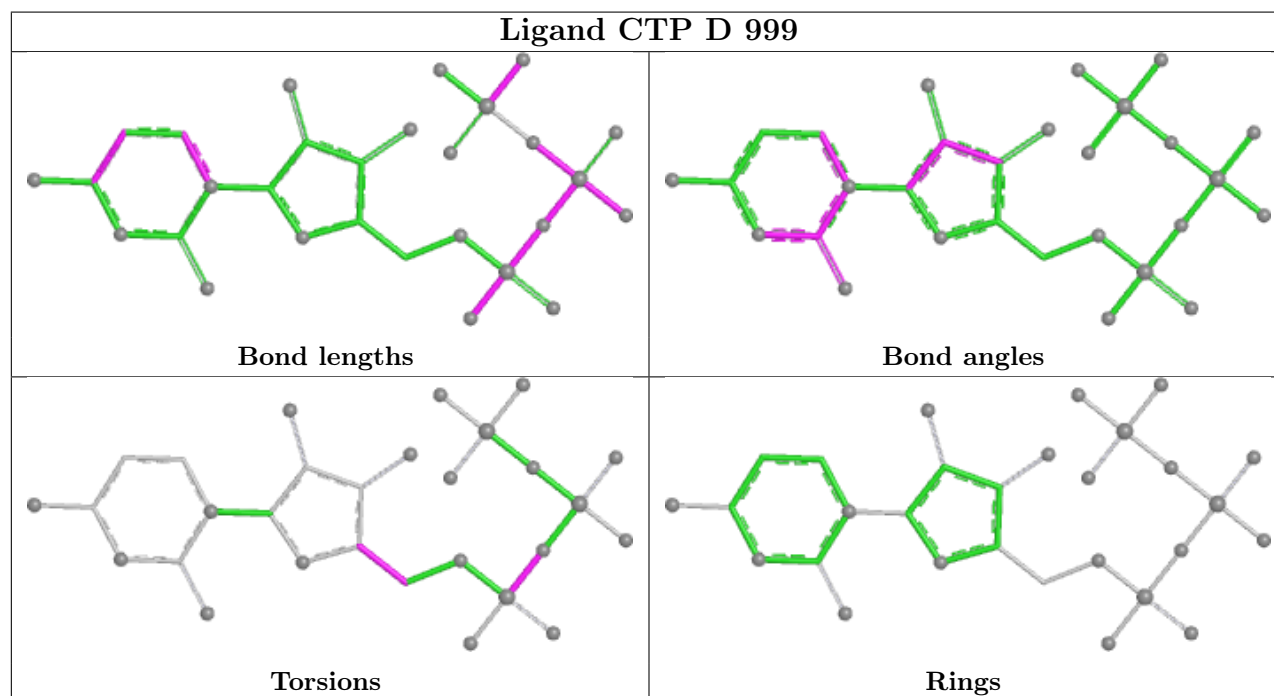
Mol	Chain	Res	Type	Atoms
4	B	999	CTP	O4'-C4'-C5'-O5'
4	B	999	CTP	C5'-O5'-PA-O1A
4	B	999	CTP	C5'-O5'-PA-O2A
4	D	999	CTP	O4'-C4'-C5'-O5'
4	B	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	C3'-C4'-C5'-O5'
4	B	999	CTP	PB-O3A-PA-O1A
4	D	999	CTP	PB-O3A-PA-O5'
4	B	999	CTP	C5'-O5'-PA-O3A
4	B	999	CTP	PB-O3A-PA-O2A

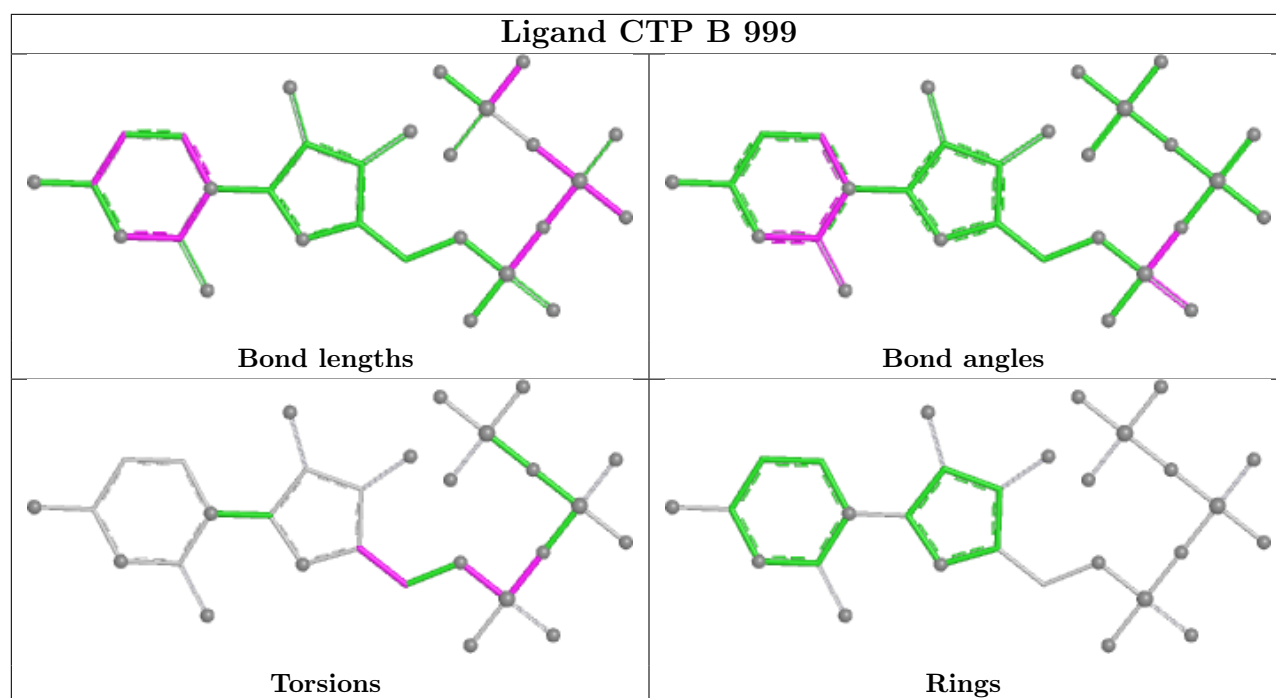
There are no ring outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.