



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:07 AM UTC

PDB ID : 1RAC / pdb_00001rac
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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

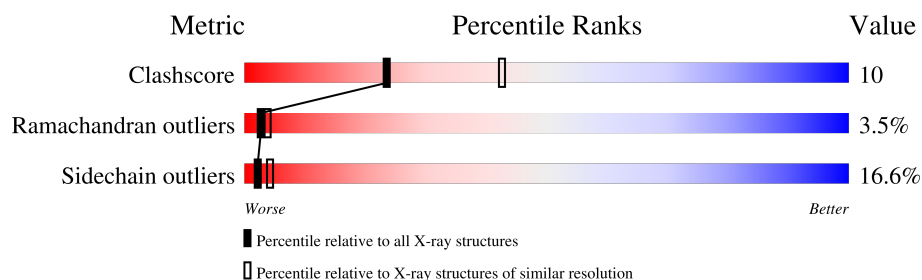
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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			

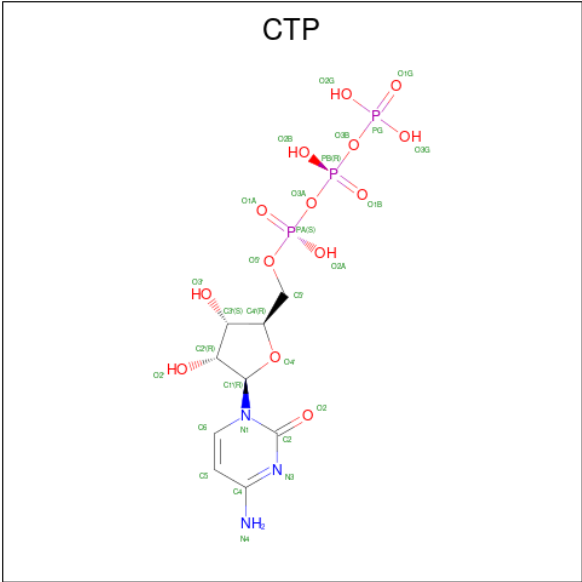
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

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.

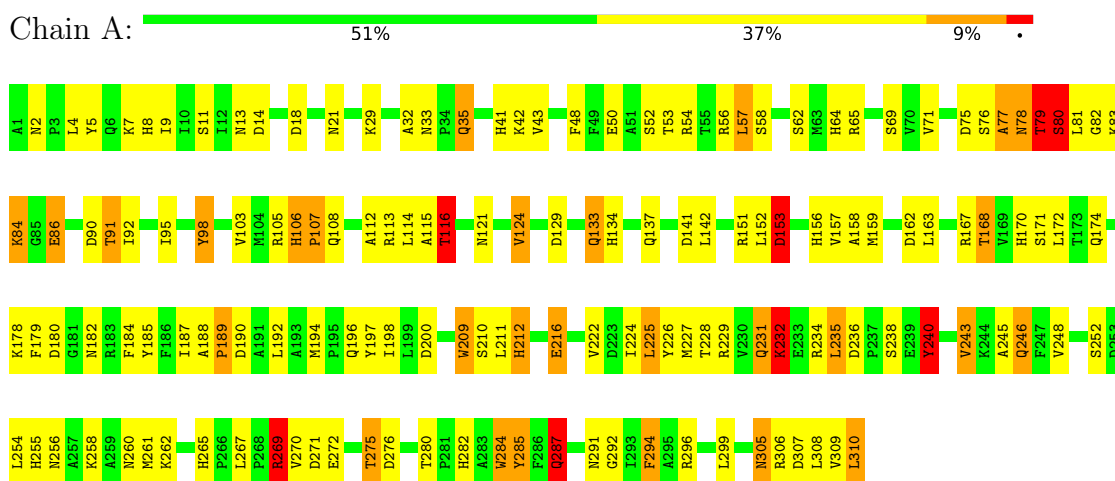
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	10	Total	O	0	0
			10	10		
5	C	44	Total	O	0	0
			44	44		
5	D	9	Total	O	0	0
			9	9		

3 Residue-property plots

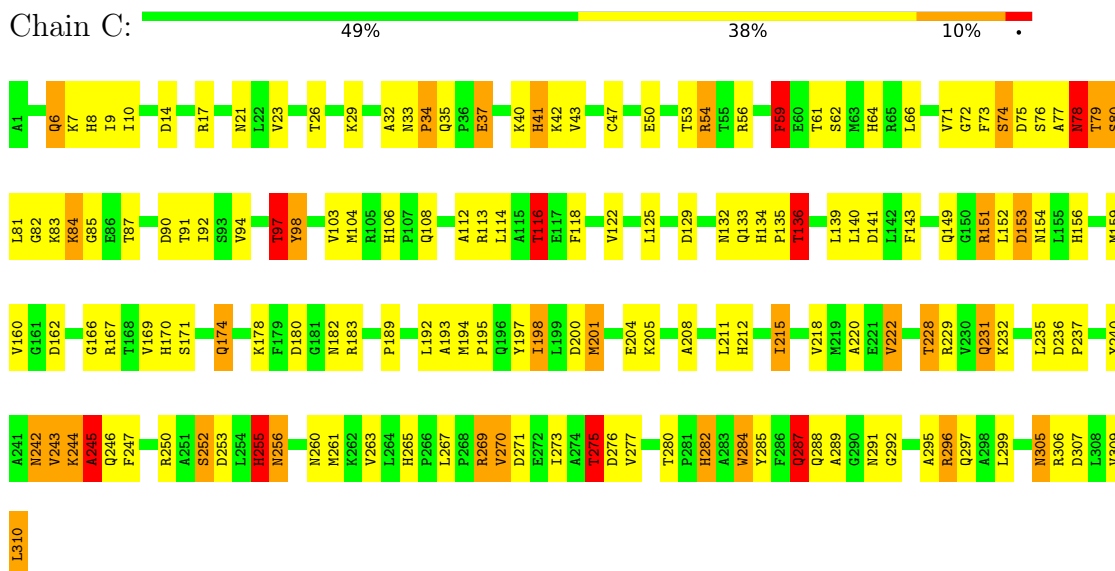
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

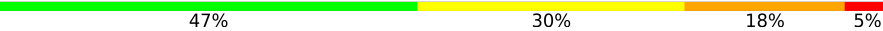
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

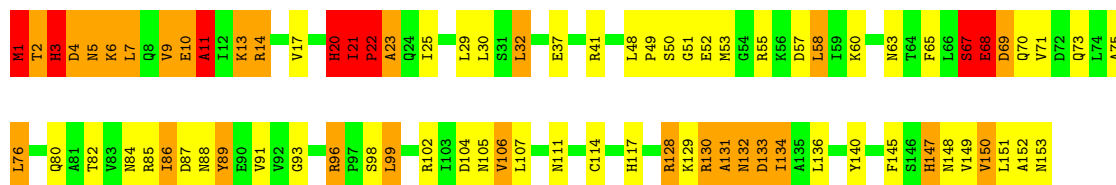


- Molecule 1: Aspartate carbamoyltransferase catalytic chain



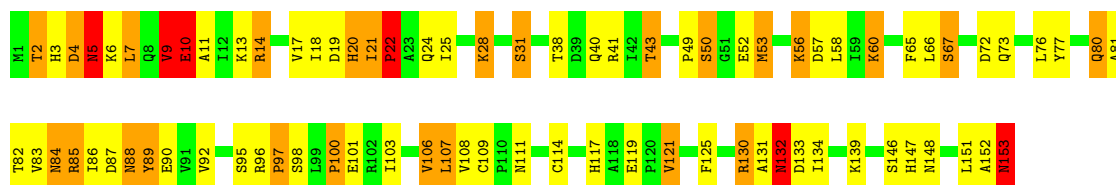
- Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B:  47% 30% 18% 5%



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:  47% 33% 16% 4%



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 (i)

5.1 Standard geometry (i)

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

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	1.30	18/2461 (0.7%)	2.16	113/3339 (3.4%)
1	C	1.37	24/2461 (1.0%)	2.27	144/3339 (4.3%)
2	B	1.20	4/1214 (0.3%)	2.19	57/1640 (3.5%)
2	D	1.17	6/1214 (0.5%)	2.19	55/1640 (3.4%)
All	All	1.29	52/7350 (0.7%)	2.21	369/9958 (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	5
1	C	0	1
2	B	0	3
All	All	0	9

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	THR	CA-CB	7.94	1.62	1.52
1	C	134	HIS	CD2-NE2	-7.30	1.29	1.37
2	B	147	HIS	CD2-NE2	-7.23	1.29	1.37
1	A	106	HIS	CD2-NE2	-7.19	1.29	1.37
1	A	124	VAL	CA-CB	7.18	1.64	1.54
1	A	265	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	106	HIS	CG-ND1	-6.99	1.30	1.38
1	C	212	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	265	HIS	CG-ND1	-6.77	1.30	1.38
1	A	212	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	156	HIS	CD2-NE2	-6.60	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	ARG	CA-CB	-6.55	1.43	1.53
2	D	82	THR	CA-CB	6.50	1.62	1.53
1	A	134	HIS	CD2-NE2	-6.41	1.30	1.37
1	C	134	HIS	CG-ND1	-6.37	1.31	1.38
2	D	147	HIS	CD2-NE2	-6.28	1.30	1.37
1	C	8	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	41	HIS	CD2-NE2	-6.08	1.31	1.37
2	D	147	HIS	CG-ND1	-6.05	1.31	1.38
1	C	8	HIS	CG-ND1	-6.05	1.31	1.38
1	C	156	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	170	HIS	CD2-NE2	-5.97	1.31	1.37
1	C	64	HIS	CD2-NE2	-5.84	1.31	1.37
1	C	34	PRO	CA-CB	-5.84	1.46	1.53
1	C	106	HIS	CD2-NE2	-5.83	1.31	1.37
2	B	3	HIS	CD2-NE2	-5.81	1.31	1.37
2	B	20	HIS	CD2-NE2	-5.78	1.31	1.37
1	C	41	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	255	HIS	CD2-NE2	-5.70	1.31	1.37
1	C	56	ARG	CA-CB	-5.70	1.44	1.53
1	C	170	HIS	CD2-NE2	-5.65	1.31	1.37
1	C	215	ILE	CA-CB	5.61	1.61	1.54
1	C	112	ALA	CA-CB	-5.55	1.44	1.53
1	C	156	HIS	CG-ND1	-5.54	1.32	1.38
1	A	64	HIS	CD2-NE2	-5.50	1.31	1.37
1	C	265	HIS	CD2-NE2	-5.49	1.31	1.37
1	C	282	HIS	CD2-NE2	-5.40	1.31	1.37
2	B	117	HIS	CD2-NE2	-5.40	1.31	1.37
1	A	8	HIS	CG-ND1	-5.33	1.32	1.38
1	A	212	HIS	CG-ND1	-5.33	1.32	1.38
1	C	35	GLN	CA-CB	-5.32	1.47	1.53
1	C	170	HIS	CG-ND1	-5.31	1.32	1.38
2	D	117	HIS	CD2-NE2	-5.26	1.32	1.37
1	C	108	GLN	CA-CB	-5.26	1.45	1.53
2	D	20	HIS	CD2-NE2	-5.26	1.32	1.37
1	A	270	VAL	CA-CB	5.25	1.60	1.54
1	A	134	HIS	CG-ND1	-5.20	1.32	1.38
1	C	265	HIS	CG-ND1	-5.20	1.32	1.38
1	A	41	HIS	CG-ND1	-5.19	1.32	1.38
2	D	3	HIS	CD2-NE2	-5.10	1.32	1.37
1	C	143	PHE	CA-CB	-5.10	1.45	1.53
1	C	149	GLN	CD-NE2	-5.06	1.22	1.33

All (369) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	GLN	OE1-CD-NE2	-14.98	107.62	122.60
1	C	287	GLN	CG-CD-NE2	14.24	137.77	116.40
2	B	21	ILE	N-CA-C	-13.82	96.74	108.63
2	D	50	SER	N-CA-C	-11.68	92.07	108.54
2	D	106	VAL	N-CA-CB	-11.34	98.36	110.72
2	B	5	ASN	CA-CB-CG	11.24	123.84	112.60
1	C	33	ASN	OD1-CG-ND2	-10.96	111.64	122.60
1	C	247	PHE	N-CA-C	-10.77	97.52	110.44
1	A	14	ASP	CA-CB-CG	10.39	122.99	112.60
2	B	20	HIS	CA-CB-CG	-10.32	103.48	113.80
2	D	40	GLN	OE1-CD-NE2	-10.26	112.34	122.60
1	A	80	SER	N-CA-C	10.11	132.34	110.80
1	A	287	GLN	OE1-CD-NE2	-9.93	112.67	122.60
2	B	11	ALA	N-CA-C	9.78	131.63	110.80
1	C	97	THR	N-CA-CB	-9.53	94.98	110.42
1	C	297	GLN	OE1-CD-NE2	-9.49	113.11	122.60
1	C	236	ASP	CA-CB-CG	9.47	122.07	112.60
1	C	80	SER	N-CA-C	9.45	130.93	110.80
1	C	174	GLN	CA-CB-CG	-9.25	95.60	114.10
1	A	276	ASP	CA-CB-CG	9.22	121.82	112.60
1	A	291	ASN	OD1-CG-ND2	-9.20	113.40	122.60
2	D	147	HIS	ND1-CG-CD2	9.15	115.25	106.10
1	A	153	ASP	CA-CB-CG	9.03	121.63	112.60
1	C	296	ARG	NE-CZ-NH1	9.00	130.50	121.50
1	A	129	ASP	CA-CB-CG	8.96	121.56	112.60
1	A	75	ASP	CA-CB-CG	8.93	121.53	112.60
2	D	2	THR	CA-C-O	8.89	129.98	120.46
1	A	287	GLN	CG-CD-NE2	8.80	129.60	116.40
1	A	190	ASP	CA-CB-CG	8.79	121.39	112.60
2	B	3	HIS	CA-CB-CG	8.77	122.57	113.80
2	B	80	GLN	CA-CB-CG	-8.75	96.59	114.10
2	D	3	HIS	N-CA-C	-8.71	92.24	110.80
1	A	271	ASP	CA-CB-CG	8.63	121.23	112.60
1	C	61	THR	N-CA-C	-8.60	101.85	111.14
1	C	33	ASN	CA-C-N	8.49	128.56	119.90
1	C	33	ASN	C-N-CA	8.49	128.56	119.90
1	C	244	LYS	CA-C-O	-8.49	110.21	119.97
1	C	90	ASP	N-CA-C	8.38	121.35	111.71
1	C	54	ARG	CA-CB-CG	8.33	130.76	114.10
1	C	134	HIS	ND1-CG-CD2	8.24	114.34	106.10
2	D	5	ASN	CA-CB-CG	8.21	120.81	112.60
1	C	78	ASN	OD1-CG-ND2	-8.10	114.50	122.60
1	A	134	HIS	ND1-CG-CD2	8.08	114.18	106.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	ASN	N-CA-C	8.03	121.92	108.20
1	C	141	ASP	CA-CB-CG	7.88	120.48	112.60
2	B	133	ASP	N-CA-C	7.86	127.53	110.80
1	C	33	ASN	CB-CG-ND2	7.83	128.15	116.40
1	C	309	VAL	O-C-N	7.79	133.26	122.97
2	D	121	VAL	CA-CB-CG2	-7.79	97.16	110.40
1	C	296	ARG	CA-CB-CG	7.78	129.66	114.10
1	A	43	VAL	CG1-CB-CG2	-7.70	93.87	110.80
1	C	75	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	134	HIS	CA-CB-CG	7.65	121.45	113.80
2	D	148	ASN	CB-CG-ND2	7.59	127.79	116.40
1	C	280	THR	CA-C-N	7.57	127.28	119.56
1	C	280	THR	C-N-CA	7.57	127.28	119.56
2	B	131	ALA	N-CA-C	7.55	126.87	110.80
1	A	265	HIS	ND1-CG-CD2	7.54	113.64	106.10
2	D	148	ASN	OD1-CG-ND2	-7.50	115.10	122.60
1	C	56	ARG	CB-CG-CD	-7.43	94.21	111.30
1	A	162	ASP	CA-CB-CG	7.39	119.99	112.60
2	B	10	GLU	N-CA-C	7.35	121.06	109.81
2	D	11	ALA	N-CA-C	-7.34	97.29	108.96
1	A	106	HIS	CA-C-N	7.25	126.89	119.56
1	A	106	HIS	C-N-CA	7.25	126.89	119.56
2	B	69	ASP	CA-CB-CG	7.21	119.81	112.60
2	D	89	TYR	N-CA-C	7.18	126.09	110.80
1	C	116	THR	N-CA-CB	-7.17	99.19	110.22
2	D	67	SER	N-CA-C	7.15	118.60	108.74
1	C	269	ARG	CA-C-N	-7.14	115.97	122.97
1	C	269	ARG	C-N-CA	-7.14	115.97	122.97
1	C	198	ILE	N-CA-C	-7.14	103.89	110.82
1	C	66	LEU	N-CA-C	-7.10	102.96	113.61
2	B	106	VAL	N-CA-CB	-7.09	96.73	111.76
1	A	134	HIS	CB-CG-CD2	-7.07	122.00	131.20
1	C	296	ARG	CD-NE-CZ	7.07	134.29	124.40
2	B	96	ARG	O-C-N	-7.05	116.05	121.55
1	C	23	VAL	N-CA-C	-7.04	103.61	110.72
1	C	8	HIS	ND1-CG-CD2	7.02	113.12	106.10
1	C	136	THR	N-CA-CB	-7.01	99.50	110.30
1	A	21	ASN	CA-CB-CG	7.00	119.60	112.60
2	B	133	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	18	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	269	ARG	NE-CZ-NH1	6.97	128.47	121.50
2	D	106	VAL	CB-CA-C	6.97	119.56	110.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	SER	N-CA-C	6.95	117.69	107.88
1	C	59	PHE	N-CA-C	-6.95	103.64	111.14
1	C	106	HIS	ND1-CG-CD2	6.93	113.03	106.10
1	A	95	ILE	O-C-N	-6.90	114.90	121.87
1	A	116	THR	CA-CB-OG1	-6.90	99.25	109.60
1	A	78	ASN	CA-C-N	6.90	134.71	121.54
1	A	78	ASN	C-N-CA	6.90	134.71	121.54
2	B	52	GLU	CA-C-O	6.81	130.25	120.51
1	A	92	ILE	CA-C-O	-6.80	114.02	121.29
1	A	245	ALA	N-CA-C	-6.77	101.38	111.81
2	D	106	VAL	N-CA-C	-6.76	98.84	108.58
2	D	21	ILE	CA-C-N	6.75	128.28	119.84
2	D	21	ILE	C-N-CA	6.75	128.28	119.84
2	D	147	HIS	CG-CD2-NE2	-6.74	100.46	107.20
1	C	37	GLU	CA-CB-CG	-6.73	100.64	114.10
1	A	41	HIS	ND1-CG-CD2	6.70	112.80	106.10
1	A	21	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	C	122	VAL	N-CA-C	-6.66	100.31	107.77
2	B	32	LEU	N-CA-C	6.64	118.52	111.28
1	A	83	LYS	CA-C-N	6.64	134.22	121.54
1	A	83	LYS	C-N-CA	6.64	134.22	121.54
2	B	149	VAL	CA-C-O	-6.63	114.14	121.17
1	C	72	GLY	CA-C-O	-6.63	115.07	121.83
1	C	276	ASP	CA-CB-CG	6.61	119.21	112.60
1	C	53	THR	N-CA-C	6.61	118.14	111.07
2	D	84	ASN	CA-CB-CG	6.61	119.21	112.60
2	D	139	LYS	CA-CB-CG	6.60	127.31	114.10
1	C	129	ASP	CA-CB-CG	6.57	119.17	112.60
1	C	275	THR	CA-CB-OG1	-6.57	99.74	109.60
2	B	73	GLN	N-CA-C	-6.57	104.53	112.54
2	B	88	ASN	CA-CB-CG	6.55	119.15	112.60
2	B	52	GLU	CA-C-N	6.55	134.04	121.54
2	B	52	GLU	C-N-CA	6.55	134.04	121.54
1	C	284	TRP	CB-CG-CD1	-6.52	117.12	126.90
1	A	305	ASN	CA-CB-CG	-6.51	106.08	112.60
1	A	134	HIS	CG-CD2-NE2	-6.49	100.71	107.20
1	C	180	ASP	N-CA-C	6.48	120.61	110.17
2	B	13	LYS	O-C-N	6.48	130.91	123.27
1	A	246	GLN	N-CA-C	6.46	124.56	110.80
1	A	116	THR	N-CA-CB	-6.45	99.59	110.49
1	C	78	ASN	N-CA-C	6.44	124.51	110.80
1	A	269	ARG	CA-CB-CG	6.43	126.96	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	156	HIS	CA-CB-CG	6.42	120.22	113.80
1	C	193	ALA	N-CA-C	6.42	118.58	110.24
2	D	80	GLN	CB-CG-CD	6.42	123.51	112.60
1	C	269	ARG	N-CA-C	-6.40	98.84	109.46
1	A	225	LEU	O-C-N	-6.37	115.03	122.87
1	C	136	THR	CB-CA-C	6.37	123.37	110.38
2	D	19	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	190	ASP	N-CA-C	6.37	120.62	112.34
2	B	53	MET	N-CA-C	-6.37	97.24	110.80
1	A	265	HIS	CG-CD2-NE2	-6.36	100.84	107.20
1	C	306	ARG	CA-CB-CG	6.33	126.75	114.10
2	B	132	ASN	N-CA-C	-6.31	105.74	113.50
1	A	133	GLN	CA-C-N	6.31	128.24	122.37
1	A	133	GLN	C-N-CA	6.31	128.24	122.37
1	A	179	PHE	O-C-N	-6.31	114.38	122.20
2	D	96	ARG	CA-C-N	6.29	127.71	119.84
2	D	96	ARG	C-N-CA	6.29	127.71	119.84
2	B	104	ASP	CA-CB-CG	-6.27	106.33	112.60
1	C	21	ASN	CA-CB-CG	-6.26	106.34	112.60
2	B	52	GLU	O-C-N	6.25	130.90	122.59
1	C	162	ASP	N-CA-C	-6.24	97.53	108.20
1	C	6	GLN	CA-CB-CG	-6.23	101.63	114.10
1	A	182	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	C	108	GLN	CA-CB-CG	-6.22	101.65	114.10
1	A	84	LYS	N-CA-C	-6.19	97.62	110.80
1	C	284	TRP	CG-CD2-CE3	6.18	140.08	133.90
1	C	160	VAL	N-CA-CB	-6.17	102.89	111.41
1	C	26	THR	CA-CB-OG1	-6.16	100.36	109.60
2	D	134	ILE	N-CA-CB	-6.16	103.64	111.64
1	C	134	HIS	CA-C-N	6.15	126.05	119.28
1	C	134	HIS	C-N-CA	6.15	126.05	119.28
1	A	189	PRO	CA-C-O	-6.15	114.02	121.03
1	C	271	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	91	THR	N-CA-C	-6.14	104.50	111.14
2	D	87	ASP	CA-CB-CG	6.14	118.74	112.60
2	B	88	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	C	252	SER	CA-CB-OG	6.13	123.36	111.10
1	A	168	THR	O-C-N	-6.13	115.16	122.15
2	D	121	VAL	CA-CB-CG1	6.12	120.81	110.40
1	A	227	MET	CG-SD-CE	-6.11	87.46	100.90
2	D	9	VAL	CB-CA-C	-6.10	101.45	111.51
1	A	52	SER	CB-CA-C	-6.08	103.46	111.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	90	GLU	CB-CG-CD	6.04	122.88	112.60
2	B	76	LEU	N-CA-C	6.04	118.83	111.82
1	A	33	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	C	222	VAL	N-CA-CB	-6.03	101.21	110.86
1	A	227	MET	N-CA-CB	-6.03	100.47	110.23
1	A	32	ALA	N-CA-C	6.02	117.64	111.14
2	D	83	VAL	N-CA-C	-6.00	99.65	109.12
1	C	134	HIS	CB-CG-CD2	-5.99	123.41	131.20
2	D	10	GLU	N-CA-C	-5.98	98.06	110.80
1	C	74	SER	N-CA-C	-5.97	99.97	109.59
2	B	67	SER	O-C-N	5.97	129.25	123.04
2	B	75	ALA	N-CA-C	5.95	117.77	111.28
1	C	97	THR	CB-CA-C	5.95	121.42	110.11
1	C	288	GLN	N-CA-C	-5.95	104.42	111.03
1	C	246	GLN	N-CA-C	5.95	118.09	109.71
1	C	56	ARG	NE-CZ-NH2	-5.94	113.85	119.20
1	C	296	ARG	NE-CZ-NH2	-5.94	113.85	119.20
2	D	31	SER	N-CA-C	-5.93	104.45	111.03
2	B	70	GLN	CA-CB-CG	-5.92	102.27	114.10
1	C	103	VAL	O-C-N	-5.91	116.47	123.03
1	C	307	ASP	N-CA-C	-5.91	100.17	109.50
1	C	78	ASN	CB-CG-ND2	5.90	125.25	116.40
1	C	291	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	107	PRO	N-CA-C	5.89	121.23	113.86
1	C	246	GLN	CA-C-O	5.88	130.39	122.51
1	C	180	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	265	HIS	ND1-CG-CD2	5.86	111.96	106.10
1	C	289	ALA	N-CA-C	5.85	118.41	111.33
2	B	52	GLU	N-CA-C	5.85	123.25	110.80
1	C	87	THR	O-C-N	-5.85	115.62	122.81
2	B	149	VAL	O-C-N	-5.84	116.18	121.91
1	C	215	ILE	CB-CG1-CD1	5.84	126.07	113.80
1	C	267	LEU	O-C-N	-5.83	114.61	121.32
1	C	296	ARG	CB-CG-CD	5.82	124.68	111.30
1	A	275	THR	CA-CB-OG1	-5.81	100.88	109.60
1	C	154	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	C	215	ILE	CB-CA-C	-5.81	104.30	112.14
1	A	231	GLN	N-CA-C	5.80	118.22	108.23
1	C	56	ARG	CG-CD-NE	-5.80	99.24	112.00
1	C	50	GLU	N-CA-C	-5.79	99.97	109.40
1	C	178	LYS	CA-CB-CG	-5.79	102.53	114.10
1	C	296	ARG	CG-CD-NE	-5.78	99.29	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	151	LEU	N-CA-C	5.78	120.06	113.19
1	C	134	HIS	CG-CD2-NE2	-5.77	101.43	107.20
1	A	76	SER	N-CA-C	-5.75	101.18	110.32
1	A	197	TYR	CA-CB-CG	5.74	124.23	113.90
2	B	152	ALA	CA-C-N	5.73	132.01	121.70
2	B	152	ALA	C-N-CA	5.73	132.01	121.70
1	A	171	SER	CA-CB-OG	5.72	122.55	111.10
2	B	2	THR	O-C-N	5.72	130.20	122.59
1	C	32	ALA	CA-C-O	-5.71	114.44	120.55
1	C	260	ASN	OD1-CG-ND2	-5.70	116.90	122.60
2	B	130	ARG	N-CA-C	5.70	118.10	110.35
1	C	220	ALA	N-CA-C	5.70	119.05	111.75
2	D	9	VAL	O-C-N	5.69	128.84	122.75
2	B	128	ARG	N-CA-C	5.69	116.90	108.60
2	B	105	ASN	N-CA-C	5.67	122.89	110.80
2	B	134	ILE	CB-CA-C	-5.67	101.98	111.29
1	A	198	ILE	N-CA-C	-5.67	104.99	110.72
2	D	38	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	307	ASP	N-CA-C	-5.66	99.43	109.06
1	C	103	VAL	N-CA-C	-5.65	100.28	108.36
2	B	23	ALA	N-CA-C	-5.64	98.78	110.80
1	A	86	GLU	CB-CA-C	5.64	119.64	110.22
1	C	106	HIS	CG-CD2-NE2	-5.64	101.56	107.20
2	B	153	ASN	OD1-CG-ND2	-5.63	116.97	122.60
2	B	50	SER	N-CA-C	5.63	122.79	110.80
1	C	297	GLN	CG-CD-NE2	5.62	124.83	116.40
1	C	200	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	235	LEU	N-CA-C	-5.62	100.17	108.99
1	A	62	SER	CA-CB-OG	-5.61	99.88	111.10
1	C	277	VAL	N-CA-C	-5.60	105.06	110.72
2	D	108	VAL	N-CA-C	-5.59	100.18	108.45
1	C	82	GLY	N-CA-C	-5.58	106.83	114.64
1	C	244	LYS	O-C-N	-5.58	115.41	122.27
1	C	253	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	222	VAL	CB-CA-C	5.58	118.84	110.98
2	B	82	THR	O-C-N	-5.57	115.99	123.23
1	C	231	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	C	160	VAL	O-C-N	-5.56	117.25	123.26
1	A	103	VAL	CA-C-O	-5.55	114.63	120.57
1	C	162	ASP	CA-CB-CG	5.53	118.13	112.60
2	D	18	ILE	N-CA-C	-5.53	100.45	108.36
2	B	134	ILE	N-CA-C	5.52	120.83	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	HIS	CA-C-O	-5.52	112.61	120.51
1	A	194	MET	CA-C-O	-5.52	114.67	120.02
1	A	307	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	282	HIS	ND1-CG-CD2	5.50	111.60	106.10
1	A	56	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	C	201	MET	CA-C-O	-5.50	114.73	120.55
1	C	250	ARG	CA-CB-CG	5.49	125.08	114.10
2	B	13	LYS	CA-CB-CG	5.48	125.07	114.10
2	D	19	ASP	N-CA-CB	-5.48	102.72	111.43
2	D	107	LEU	N-CA-CB	5.48	119.75	110.49
1	A	232	LYS	N-CA-C	5.46	119.04	112.38
1	C	116	THR	OG1-CB-CG2	5.46	120.21	109.30
1	A	291	ASN	CB-CG-ND2	5.46	124.58	116.40
1	C	287	GLN	CB-CG-CD	5.44	121.85	112.60
1	A	71	VAL	O-C-N	-5.43	117.19	123.00
1	A	285	TYR	N-CA-C	5.43	117.19	111.28
2	D	117	HIS	N-CA-C	5.42	117.27	111.36
1	C	228	THR	CA-CB-OG1	-5.41	101.48	109.60
2	D	148	ASN	CA-CB-CG	5.41	118.01	112.60
1	C	269	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	A	33	ASN	CA-CB-CG	5.40	118.00	112.60
1	C	269	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	A	77	ALA	N-CA-C	5.40	122.30	110.80
1	C	280	THR	O-C-N	-5.40	115.49	121.53
1	A	84	LYS	N-CA-CB	5.39	119.61	110.49
1	A	79	THR	N-CA-C	5.38	122.25	110.80
1	A	79	THR	N-CA-CB	-5.37	101.41	110.49
1	C	273	ILE	N-CA-C	-5.37	99.82	107.77
2	D	88	ASN	N-CA-C	-5.37	99.36	110.80
1	C	14	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	78	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	C	242	ASN	N-CA-C	-5.36	103.81	110.41
1	C	295	ALA	O-C-N	-5.36	116.44	122.12
1	A	196	GLN	CA-C-O	-5.36	114.74	120.42
1	C	8	HIS	CG-CD2-NE2	-5.36	101.84	107.20
1	A	8	HIS	ND1-CG-CD2	5.35	111.45	106.10
1	C	222	VAL	CA-CB-CG1	5.34	119.48	110.40
2	D	40	GLN	CG-CD-NE2	5.34	124.41	116.40
1	A	157	VAL	CA-C-O	-5.33	114.82	120.53
1	A	56	ARG	CB-CG-CD	-5.33	99.05	111.30
2	B	68	GLU	CB-CG-CD	5.33	121.65	112.60
2	D	119	GLU	CA-C-N	5.33	126.50	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	119	GLU	C-N-CA	5.33	126.50	119.84
1	A	53	THR	CA-CB-OG1	-5.32	101.62	109.60
1	A	98	TYR	CA-CB-CG	5.31	123.46	113.90
1	C	197	TYR	CA-CB-CG	5.31	123.46	113.90
1	C	42	LYS	O-C-N	-5.31	116.74	123.01
2	B	1	MET	CA-CB-CG	5.31	124.72	114.10
2	D	153	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	A	116	THR	CA-CB-CG2	5.29	119.50	110.50
1	C	243	VAL	N-CA-CB	-5.29	102.50	111.23
2	D	28	LYS	N-CA-CB	-5.28	102.35	110.01
1	A	86	GLU	N-CA-CB	-5.28	101.30	110.17
2	B	73	GLN	OE1-CD-NE2	-5.28	117.32	122.60
2	D	132	ASN	N-CA-C	-5.28	99.56	110.80
1	A	141	ASP	CA-CB-CG	5.26	117.86	112.60
2	D	14	ARG	O-C-N	-5.23	117.19	123.31
1	C	235	LEU	N-CA-C	-5.23	101.49	108.34
1	A	90	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	236	ASP	N-CA-C	-5.22	103.49	110.07
2	B	150	VAL	CA-C-O	5.22	126.15	120.57
1	A	69	SER	CA-CB-OG	-5.21	100.68	111.10
1	C	282	HIS	CG-CD2-NE2	-5.20	102.00	107.20
1	A	260	ASN	N-CA-C	5.20	119.26	113.02
1	A	294	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	35	GLN	CA-C-N	5.18	125.26	119.87
1	A	35	GLN	C-N-CA	5.18	125.26	119.87
1	C	270	VAL	O-C-N	-5.18	117.91	121.85
1	C	118	PHE	CA-CB-CG	-5.18	108.62	113.80
1	C	263	VAL	CA-C-N	5.18	130.94	122.81
1	C	263	VAL	C-N-CA	5.18	130.94	122.81
1	A	216	GLU	CA-CB-CG	5.17	124.45	114.10
1	A	58	SER	CA-CB-OG	5.17	121.44	111.10
1	A	178	LYS	N-CA-C	-5.17	106.82	113.23
1	C	97	THR	OG1-CB-CG2	5.17	119.63	109.30
2	D	121	VAL	CB-CA-C	5.17	118.78	110.82
1	C	245	ALA	O-C-N	-5.16	115.72	122.59
1	A	57	LEU	N-CA-C	5.15	117.63	111.71
2	D	52	GLU	N-CA-C	5.15	118.83	112.54
1	A	134	HIS	O-C-N	-5.14	117.44	121.19
1	C	136	THR	N-CA-C	-5.14	105.75	112.23
1	C	195	PRO	N-CA-C	5.14	119.39	111.21
1	C	106	HIS	O-C-N	-5.14	118.25	121.85
1	A	200	ASP	N-CA-C	-5.11	105.60	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	VAL	CB-CA-C	-5.11	103.55	110.90
1	A	248	VAL	N-CA-C	-5.10	102.04	109.29
2	D	22	PRO	N-CA-C	5.10	122.98	112.47
2	B	114	CYS	CA-C-O	5.10	126.80	121.19
1	C	182	ASN	O-C-N	5.10	128.88	122.86
1	A	224	ILE	O-C-N	-5.10	117.14	123.10
1	A	2	ASN	N-CA-C	-5.09	102.86	110.20
1	C	255	HIS	CA-CB-CG	5.09	118.89	113.80
1	C	54	ARG	N-CA-C	-5.09	105.42	110.97
1	C	296	ARG	O-C-N	-5.09	116.35	122.15
2	B	132	ASN	CA-C-N	5.09	131.25	121.54
2	B	132	ASN	C-N-CA	5.09	131.25	121.54
1	C	34	PRO	N-CA-C	5.08	119.18	111.15
1	A	209	TRP	CG-CD1-NE1	-5.08	103.60	110.20
1	A	105	ARG	N-CA-C	-5.07	100.19	108.76
1	C	43	VAL	N-CA-C	-5.07	101.18	108.48
2	B	133	ASP	O-C-N	5.07	129.33	122.59
2	D	3	HIS	CA-CB-CG	-5.06	108.74	113.80
1	A	224	ILE	N-CA-CB	-5.05	105.09	111.46
1	A	42	LYS	O-C-N	-5.05	117.31	123.16
1	A	256	ASN	CA-CB-CG	5.05	117.65	112.60
2	B	10	GLU	CA-C-N	5.04	131.18	121.54
2	B	10	GLU	C-N-CA	5.04	131.18	121.54
1	A	98	TYR	CB-CA-C	-5.04	101.24	109.56
1	A	284	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	A	54	ARG	N-CA-C	5.04	116.77	111.28
1	A	284	TRP	CG-CD2-CE3	5.03	138.93	133.90
2	D	84	ASN	OD1-CG-ND2	-5.03	117.57	122.60
2	D	9	VAL	N-CA-CB	5.02	118.22	110.14
1	A	240	TYR	N-CA-C	-5.01	105.50	110.97
1	C	270	VAL	N-CA-CB	-5.00	106.61	111.57
1	C	275	THR	CA-CB-CG2	5.00	119.00	110.50

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	140	TYR	Sidechain
2	B	20	HIS	Sidechain
2	B	89	TYR	Sidechain
1	C	98	TYR	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	44	0
1	C	2415	0	2422	35	0
2	B	1196	0	1212	42	0
2	D	1196	0	1212	39	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	30	0	0	0	0
5	B	10	0	0	0	0
5	C	44	0	0	2	0
5	D	9	0	0	1	0
All	All	7375	0	7292	149	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 10.

All (149) 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:6:LYS:HB3	2:D:10:GLU:HG3	1.46	0.95
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.56	0.87
1:A:106:HIS:HD2	1:A:108:GLN:H	1.24	0.83
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.71	0.72
2:B:4:ASP:HA	2:B:10:GLU:HB2	1.73	0.71
2:D:50:SER:HB2	2:D:56:LYS:HG2	1.72	0.70
1:A:151:ARG:HD2	1:A:153:ASP:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ARG:HH21	2:D:49:PRO:HD2	1.59	0.67
2:B:1:MET:HA	2:D:7:LEU:HD21	1.76	0.67
1:C:136:THR:HG23	1:C:296:ARG:HH11	1.59	0.67
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.07	0.67
1:C:292:GLY:O	1:C:296:ARG:HG2	1.95	0.66
2:B:14:ARG:HA	2:B:86:ILE:O	1.96	0.65
2:D:17:VAL:HG22	2:D:60:LYS:HG3	1.78	0.65
2:B:14:ARG:NH1	2:B:63:ASN:HA	2.11	0.65
1:A:153:ASP:HB3	1:A:180:ASP:O	1.97	0.65
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.80	0.64
2:B:6:LYS:HA	2:B:9:VAL:HG22	1.81	0.62
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.84	0.59
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.84	0.59
1:C:240:TYR:O	1:C:245:ALA:HB2	2.02	0.59
1:A:142:LEU:HD22	1:A:152:LEU:HD13	1.84	0.58
2:D:58:LEU:HD21	2:D:60:LYS:HD3	1.85	0.58
1:A:287:GLN:HE21	1:A:287:GLN:H	1.52	0.58
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.38	0.58
2:D:20:HIS:NE2	2:D:53:MET:HE2	2.18	0.57
1:A:232:LYS:HB3	1:A:240:TYR:HE2	1.70	0.57
1:A:81:LEU:HD12	1:A:91:THR:HG23	1.84	0.57
2:B:48:LEU:O	2:B:55:ARG:HA	2.05	0.56
2:D:25:ILE:HD13	2:D:77:TYR:O	2.06	0.56
1:C:113:ARG:O	1:C:116:THR:HB	2.05	0.56
2:B:129:LYS:HG2	2:B:132:ASN:OD1	2.07	0.55
2:B:6:LYS:HB2	2:B:6:LYS:NZ	2.22	0.55
1:C:174:GLN:HG2	1:C:201:MET:HE2	1.87	0.55
1:A:82:GLY:O	1:A:86:GLU:HB3	2.06	0.55
1:A:5:TYR:CD1	1:A:306:ARG:HA	2.42	0.55
2:B:65:PHE:CE1	2:B:85:ARG:HG3	2.43	0.54
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.89	0.54
2:B:4:ASP:HB2	2:D:7:LEU:O	2.09	0.53
2:B:11:ALA:HA	4:B:999:CTP:N3	2.23	0.53
1:C:183:ARG:HG2	1:C:208:ALA:HB3	1.91	0.53
2:B:3:HIS:O	2:B:10:GLU:HB2	2.08	0.53
1:C:242:ASN:O	1:C:244:LYS:N	2.42	0.53
1:A:11:SER:HA	1:A:133:GLN:HG2	1.92	0.52
2:D:20:HIS:HE1	2:D:80:GLN:OE1	1.92	0.52
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.92	0.52
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.75	0.52
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:PHE:CE2	1:C:136:THR:HG21	2.45	0.51
1:A:292:GLY:O	1:A:296:ARG:HG3	2.10	0.51
2:D:65:PHE:HB3	2:D:85:ARG:HH22	1.77	0.50
2:D:14:ARG:HG2	2:D:65:PHE:HZ	1.76	0.50
1:C:94:VAL:O	1:C:97:THR:HB	2.12	0.49
1:A:5:TYR:CZ	1:A:306:ARG:HG2	2.47	0.49
1:A:232:LYS:HB3	1:A:240:TYR:CE2	2.47	0.49
2:B:67:SER:HA	2:B:71:VAL:HG23	1.94	0.49
1:C:151:ARG:HD2	1:C:153:ASP:O	2.12	0.49
1:A:262:LYS:HE2	1:A:284:TRP:CE3	2.48	0.49
2:D:20:HIS:O	2:D:20:HIS:ND1	2.46	0.49
2:D:72:ASP:HB3	2:D:100:PRO:HB3	1.95	0.49
2:B:41:ARG:HE	2:D:49:PRO:HD3	1.76	0.49
1:C:256:ASN:ND2	1:C:256:ASN:H	2.10	0.49
2:D:20:HIS:HB2	5:D:1008:HOH:O	2.13	0.49
2:B:6:LYS:CB	2:D:10:GLU:HG3	2.30	0.49
1:C:229:ARG:HH12	1:C:270:VAL:CG2	2.25	0.49
1:C:29:LYS:HD3	1:C:310:LEU:HB2	1.96	0.48
1:A:185:TYR:HD1	1:A:212:HIS:NE2	2.11	0.48
1:A:243:VAL:O	1:A:246:GLN:HA	2.13	0.48
2:B:1:MET:HB2	2:D:7:LEU:HD11	1.96	0.48
2:B:41:ARG:HE	2:D:49:PRO:CD	2.27	0.48
1:A:4:LEU:HD23	1:A:7:LYS:HD2	1.96	0.48
2:B:5:ASN:O	2:B:9:VAL:HA	2.13	0.48
1:C:153:ASP:HB3	5:C:341:HOH:O	2.14	0.47
1:A:158:ALA:HB2	1:A:222:VAL:HG21	1.97	0.47
1:A:261:MET:O	1:A:282:HIS:HD2	1.97	0.47
1:A:189:PRO:HG2	1:A:192:LEU:HD12	1.97	0.47
2:B:21:ILE:HB	2:B:57:ASP:HB2	1.96	0.47
2:D:14:ARG:HA	2:D:86:ILE:O	2.15	0.47
1:A:112:ALA:O	1:A:115:ALA:HB3	2.15	0.47
1:A:287:GLN:HE21	1:A:287:GLN:N	2.13	0.46
2:B:76:LEU:HD13	2:B:151:LEU:HD11	1.98	0.46
1:A:78:ASN:HB3	1:A:79:THR:H	1.60	0.46
2:D:81:ALA:O	2:D:97:PRO:HD2	2.16	0.46
2:B:14:ARG:HH11	2:B:14:ARG:HG2	1.81	0.45
1:C:261:MET:O	1:C:282:HIS:HD2	1.99	0.45
1:A:11:SER:HA	1:A:133:GLN:CG	2.46	0.45
2:B:7:LEU:H	2:B:7:LEU:HD23	1.82	0.45
2:B:41:ARG:NH2	2:D:49:PRO:HD2	2.27	0.45
1:A:184:PHE:O	1:A:209:TRP:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:PRO:HG2	1:C:192:LEU:HD12	1.98	0.45
2:D:92:VAL:O	2:D:92:VAL:HG13	2.16	0.45
1:A:261:MET:SD	1:A:262:LYS:N	2.90	0.45
2:D:130:ARG:N	2:D:133:ASP:O	2.50	0.45
1:C:135:PRO:O	1:C:139:LEU:HG	2.17	0.45
2:B:13:LYS:HB3	2:B:89:TYR:CZ	2.52	0.44
1:A:106:HIS:CD2	1:A:108:GLN:H	2.16	0.44
1:C:73:PHE:CE2	1:C:81:LEU:HD21	2.52	0.44
1:A:81:LEU:HD12	1:A:91:THR:CG2	2.48	0.44
1:A:163:LEU:HG	1:A:188:ALA:HB2	2.00	0.44
2:B:6:LYS:HZ3	2:D:43:THR:HG21	1.83	0.44
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.18	0.44
2:D:65:PHE:HB3	2:D:85:ARG:NH2	2.33	0.44
2:D:85:ARG:O	2:D:86:ILE:HG13	2.18	0.44
1:A:267:LEU:HD23	1:A:269:ARG:HB3	2.00	0.44
1:C:166:GLY:O	1:C:169:VAL:HG22	2.17	0.44
2:B:20:HIS:HE1	2:B:51:GLY:HA3	1.82	0.43
2:D:14:ARG:HG2	2:D:65:PHE:CZ	2.53	0.43
1:C:136:THR:HB	5:C:317:HOH:O	2.17	0.43
2:B:5:ASN:O	2:B:9:VAL:HG13	2.17	0.43
2:B:21:ILE:HG22	2:B:25:ILE:HB	2.00	0.43
1:C:261:MET:C	1:C:261:MET:SD	3.02	0.43
2:B:86:ILE:HG13	2:B:91:VAL:HA	2.00	0.43
1:A:29:LYS:HD2	1:A:310:LEU:HG	2.01	0.43
1:C:10:ILE:HD11	1:C:116:THR:OG1	2.18	0.43
2:B:107:LEU:HD22	2:B:150:VAL:HG12	2.01	0.42
1:A:113:ARG:O	1:A:116:THR:HB	2.19	0.42
2:D:25:ILE:O	2:D:28:LYS:HB3	2.19	0.42
2:D:58:LEU:CD2	2:D:60:LYS:HD3	2.49	0.42
2:D:111:ASN:HB3	2:D:114:CYS:HB2	2.01	0.42
1:A:254:LEU:HD12	1:A:280:THR:HG21	2.01	0.42
1:C:189:PRO:HD2	1:C:192:LEU:HB2	2.02	0.42
1:A:137:GLN:HG2	1:A:168:THR:HG22	2.01	0.42
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.91	0.42
2:B:111:ASN:HB2	2:B:145:PHE:HZ	1.85	0.42
2:B:136:LEU:HD12	2:B:147:HIS:HA	2.02	0.42
1:C:287:GLN:HE21	1:C:287:GLN:H	1.67	0.42
2:D:5:ASN:HB2	2:D:6:LYS:HG2	2.02	0.42
2:D:6:LYS:HB2	2:D:9:VAL:HG13	2.02	0.42
1:A:229:ARG:HH22	1:A:232:LYS:HE2	1.85	0.42
2:D:22:PRO:HB2	2:D:25:ILE:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:HD12	1:C:91:THR:HG21	2.01	0.41
2:D:152:ALA:O	2:D:153:ASN:HB2	2.19	0.41
1:C:9:ILE:HG21	1:C:299:LEU:HD21	2.02	0.41
2:B:22:PRO:HB2	2:B:25:ILE:HG12	2.03	0.41
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.35	0.41
1:A:235:LEU:HA	1:A:235:LEU:HD12	1.81	0.41
2:B:25:ILE:HG22	2:B:29:LEU:HG	2.03	0.41
1:C:47:CYS:O	1:C:104:MET:HA	2.20	0.41
1:A:187:ILE:HG13	1:A:212:HIS:HB2	2.02	0.41
2:B:6:LYS:HB2	2:B:6:LYS:HZ3	1.85	0.41
2:B:84:ASN:HA	2:B:93:GLY:O	2.21	0.41
1:C:194:MET:SD	1:C:198:ILE:HG21	2.60	0.41
1:A:189:PRO:CG	1:A:192:LEU:HD12	2.51	0.40
2:B:99:LEU:HD23	2:B:130:ARG:HD2	2.02	0.40
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.85	0.40
1:C:40:LYS:O	1:C:41:HIS:HB2	2.21	0.40
1:C:114:LEU:C	1:C:114:LEU:HD23	2.46	0.40
1:A:9:ILE:HG21	1:A:299:LEU:HD21	2.04	0.40
2:B:1:MET:CB	2:D:7:LEU:HD11	2.52	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%)	20 (6%)	5 (2%)	7	14
1	C	308/310 (99%)	281 (91%)	18 (6%)	9 (3%)	3	5
2	B	151/153 (99%)	119 (79%)	22 (15%)	10 (7%)	1	1
2	D	151/153 (99%)	122 (81%)	21 (14%)	8 (5%)	1	1
All	All	918/926 (99%)	805 (88%)	81 (9%)	32 (4%)	3	4

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ALA
1	A	80	SER
1	A	84	LYS
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	89	TYR
2	D	107	LEU
2	D	131	ALA
2	D	132	ASN
2	B	3	HIS
2	B	11	ALA
2	B	22	PRO
1	C	77	ALA
1	C	255	HIS
2	D	24	GLN
1	A	79	THR
2	B	14	ARG
1	C	245	ALA
2	D	5	ASN
2	B	23	ALA
2	B	68	GLU
1	C	275	THR
2	D	22	PRO
1	C	84	LYS
1	C	85	GLY
2	B	9	VAL
1	A	243	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%)	216 (83%)	45 (17%)	2	4
2	B	136/137 (99%)	110 (81%)	26 (19%)	1	3
2	D	136/137 (99%)	107 (79%)	29 (21%)	1	2
All	All	794/796 (100%)	662 (83%)	132 (17%)	2	4

All (132) 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	80	SER
1	A	114	LEU
1	A	116	THR
1	A	121	ASN
1	A	124	VAL
1	A	153	ASP
1	A	159	MET
1	A	167	ARG
1	A	174	GLN
1	A	210	SER
1	A	211	LEU
1	A	216	GLU
1	A	225	LEU
1	A	228	THR
1	A	231	GLN
1	A	232	LYS
1	A	234	ARG
1	A	238	SER
1	A	240	TYR
1	A	252	SER
1	A	258	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2	THR
2	B	3	HIS
2	B	4	ASP
2	B	6	LYS
2	B	7	LEU
2	B	20	HIS
2	B	21	ILE
2	B	22	PRO
2	B	30	LEU
2	B	32	LEU
2	B	37	GLU
2	B	49	PRO
2	B	58	LEU
2	B	67	SER
2	B	68	GLU
2	B	69	ASP
2	B	86	ILE
2	B	87	ASP
2	B	96	ARG
2	B	98	SER
2	B	99	LEU
2	B	102	ARG
2	B	106	VAL
2	B	128	ARG
2	B	148	ASN
1	C	6	GLN
1	C	7	LYS
1	C	17	ARG
1	C	34	PRO
1	C	37	GLU
1	C	54	ARG
1	C	59	PHE
1	C	62	SER
1	C	74	SER
1	C	76	SER
1	C	78	ASN
1	C	79	THR
1	C	83	LYS
1	C	84	LYS
1	C	92	ILE
1	C	97	THR
1	C	116	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	C	204	GLU
1	C	205	LYS
1	C	211	LEU
1	C	215	ILE
1	C	218	VAL
1	C	222	VAL
1	C	228	THR
1	C	231	GLN
1	C	232	LYS
1	C	237	PRO
1	C	252	SER
1	C	255	HIS
1	C	256	ASN
1	C	269	ARG
1	C	275	THR
1	C	285	TYR
1	C	287	GLN
1	C	305	ASN
1	C	310	LEU
2	D	2	THR
2	D	4	ASP
2	D	7	LEU
2	D	9	VAL
2	D	10	GLU
2	D	13	LYS
2	D	31	SER
2	D	41	ARG
2	D	43	THR
2	D	53	MET
2	D	56	LYS
2	D	60	LYS
2	D	66	LEU
2	D	67	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	73	GLN
2	D	84	ASN
2	D	85	ARG
2	D	88	ASN
2	D	95	SER
2	D	97	PRO
2	D	98	SER
2	D	100	PRO
2	D	101	GLU
2	D	106	VAL
2	D	121	VAL
2	D	130	ARG
2	D	132	ASN
2	D	146	SER
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	108	GLN
1	A	154	ASN
1	A	174	GLN
1	A	196	GLN
1	A	282	HIS
1	A	287	GLN
2	B	70	GLN
2	B	117	HIS
1	C	21	ASN
1	C	33	ASN
1	C	149	GLN
1	C	196	GLN
1	C	256	ASN
1	C	282	HIS
1	C	287	GLN
2	D	24	GLN
2	D	40	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2.32	9 (31%)	43,47,47	1.39	5 (11%)
4	CTP	D	999	-	29,30,30	2.23	10 (34%)	43,47,47	1.19	3 (6%)

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	-	-	4/22/38/38	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	CTP	PB-O3B	6.55	1.66	1.59
4	D	999	CTP	PB-O3B	6.37	1.66	1.59
4	B	999	CTP	PB-O3A	5.74	1.65	1.59
4	B	999	CTP	PA-O3A	5.47	1.65	1.59
4	D	999	CTP	PB-O3A	5.32	1.65	1.59
4	D	999	CTP	PA-O3A	4.83	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	PG-O1G	2.71	1.58	1.50
4	D	999	CTP	C6-N1	-2.56	1.32	1.38
4	B	999	CTP	PG-O1G	2.51	1.58	1.50
4	B	999	CTP	C6-N1	-2.51	1.32	1.38
4	B	999	CTP	C2-N1	-2.48	1.34	1.40
4	B	999	CTP	C2-N3	-2.41	1.31	1.36
4	D	999	CTP	C5-C4	-2.33	1.37	1.42
4	D	999	CTP	PB-O1B	2.24	1.58	1.50
4	D	999	CTP	C2-N1	-2.24	1.35	1.40
4	B	999	CTP	PB-O1B	2.23	1.58	1.50
4	B	999	CTP	C5-C4	-2.13	1.38	1.42
4	D	999	CTP	PA-O1A	2.04	1.57	1.50
4	D	999	CTP	C2-N3	-2.02	1.32	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	CTP	O2-C2-N3	-4.97	114.50	122.33
4	D	999	CTP	O2-C2-N3	-4.32	115.52	122.33
4	B	999	CTP	N1-C2-N3	2.90	123.84	118.80
4	B	999	CTP	C6-N1-C2	-2.72	115.86	120.46
4	D	999	CTP	N1-C2-N3	2.39	122.95	118.80
4	B	999	CTP	O4'-C1'-N1	2.36	113.71	108.36
4	D	999	CTP	C6-N1-C2	-2.30	116.58	120.46
4	B	999	CTP	C5'-C4'-C3'	-2.24	107.16	115.21

There are no chirality outliers.

All (9) torsion outliers are listed below:

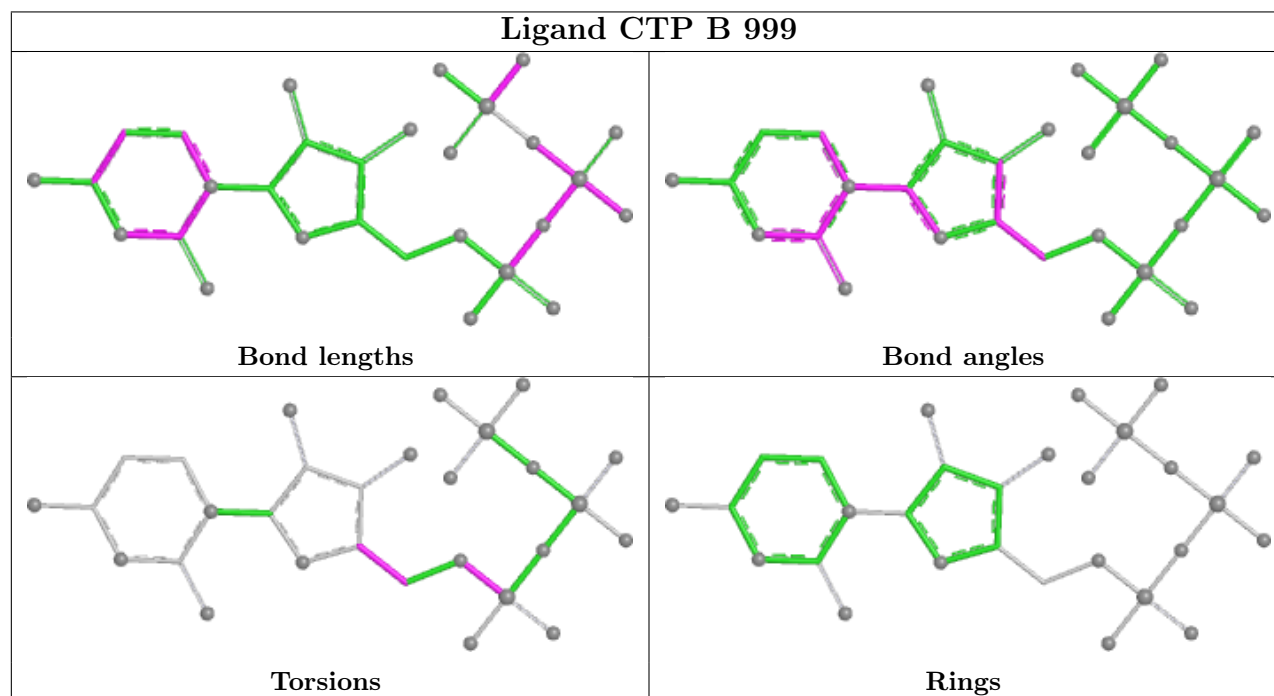
Mol	Chain	Res	Type	Atoms
4	B	999	CTP	O4'-C4'-C5'-O5'
4	B	999	CTP	C5'-O5'-PA-O1A
4	B	999	CTP	C5'-O5'-PA-O2A
4	B	999	CTP	C5'-O5'-PA-O3A
4	B	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	O4'-C4'-C5'-O5'
4	D	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	PB-O3A-PA-O5'
4	D	999	CTP	PB-O3A-PA-O1A

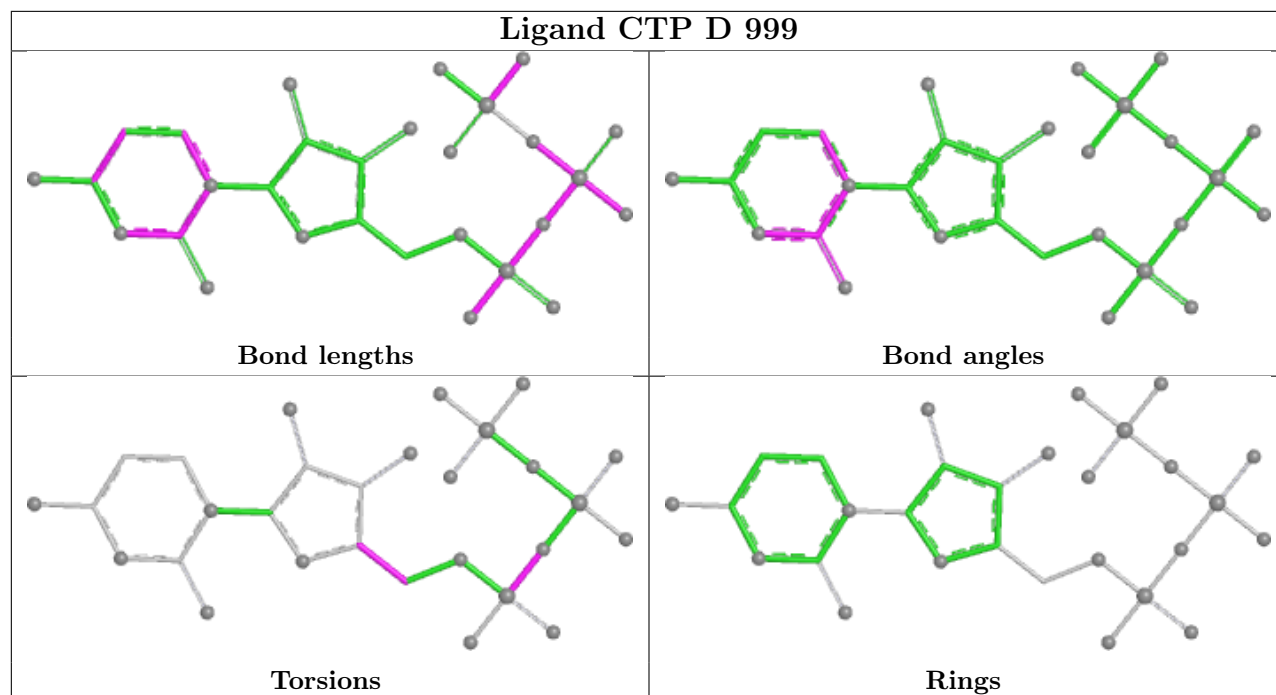
There are no ring outliers.

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.