



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:05 am BST

PDB ID : 1RAC
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

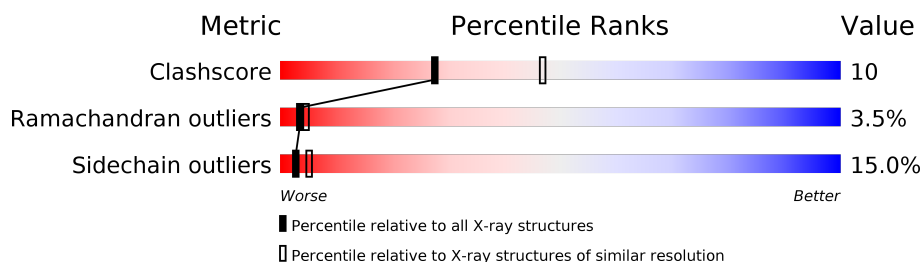
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 on 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 [i](#)

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			

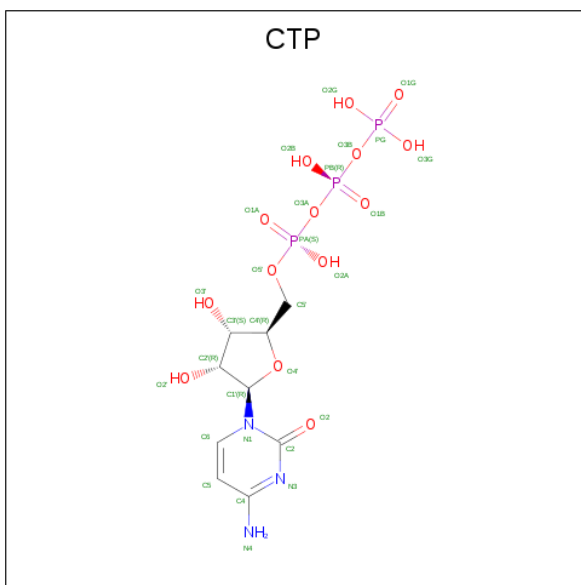
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

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 (three-letter code: 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 (three-letter code: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



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

- Molecule 5 is water.

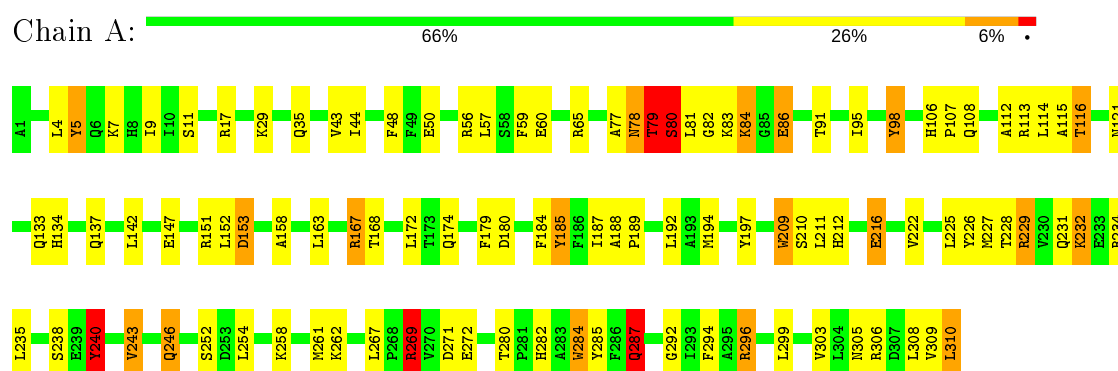
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	30	Total O 30 30	0	0
5	B	10	Total O 10 10	0	0
5	C	44	Total O 44 44	0	0
5	D	9	Total O 9 9	0	0

3 Residue-property plots

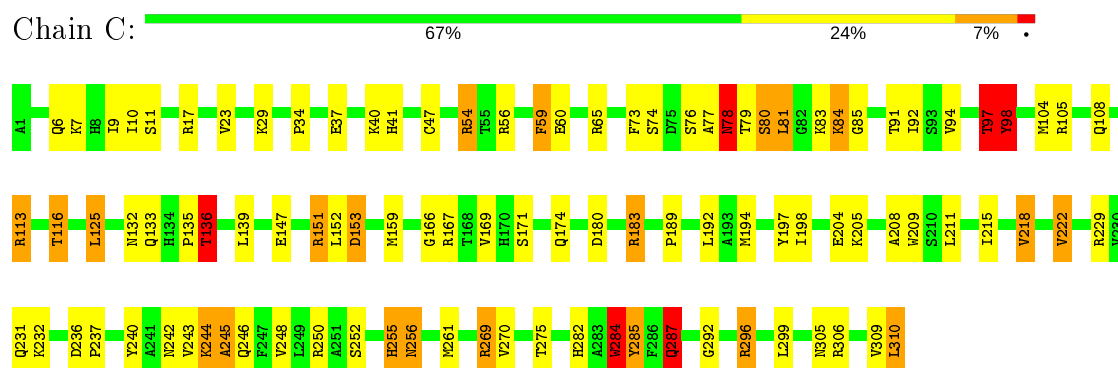
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

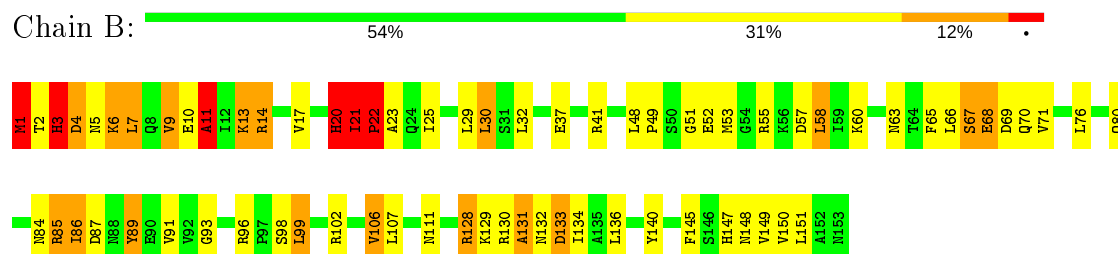
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



- Molecule 1: Aspartate carbamoyltransferase catalytic chain

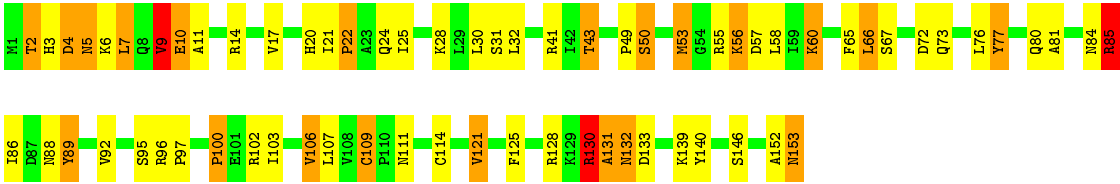


- Molecule 2: Aspartate carbamoyltransferase regulatory chain



- Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D: 56% 29% 14% .



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	0.97	2/2461 (0.1%)	1.77	45/3339 (1.3%)
1	C	1.02	2/2461 (0.1%)	1.90	58/3339 (1.7%)
2	B	0.90	0/1214	1.75	25/1640 (1.5%)
2	D	0.90	0/1214	1.78	26/1640 (1.6%)
All	All	0.96	4/7350 (0.1%)	1.81	154/9958 (1.5%)

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	5
1	C	0	1
2	B	0	3
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLU	CD-OE2	8.24	1.34	1.25
1	C	147	GLU	CD-OE1	8.16	1.34	1.25
1	A	60	GLU	CD-OE2	7.13	1.33	1.25
1	C	11	SER	CA-CB	-5.49	1.44	1.52

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	ARG	NE-CZ-NH1	20.40	130.50	120.30
1	A	269	ARG	NE-CZ-NH1	16.35	128.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	C	56	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	C	296	ARG	NE-CZ-NH2	-12.89	113.85	120.30
1	A	56	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	C	269	ARG	NE-CZ-NH2	-11.93	114.34	120.30
1	A	43	VAL	CG1-CB-CG2	-10.64	93.87	110.90
1	C	113	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	209	TRP	CD1-CG-CD2	9.60	113.98	106.30
1	A	5	TYR	CB-CG-CD1	-9.22	115.47	121.00
2	D	121	VAL	CA-CB-CG2	-9.16	97.16	110.90
1	C	287	GLN	CG-CD-NE2	8.78	137.77	116.70
2	D	2	THR	CA-C-N	-8.72	98.02	117.20
1	A	185	TYR	CB-CG-CD2	-8.61	115.83	121.00
1	A	65	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	C	209	TRP	CD1-CG-CD2	8.48	113.09	106.30
2	B	52	GLU	CA-C-N	-8.40	98.72	117.20
1	C	250	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	174	GLN	CA-CB-CG	-8.09	95.60	113.40
1	C	97	THR	N-CA-CB	-8.06	94.98	110.30
1	C	113	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	227	MET	CG-SD-CE	-7.96	87.46	100.20
1	C	284	TRP	CD1-CG-CD2	7.92	112.63	106.30
1	C	183	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	C	125	LEU	CA-CB-CG	7.91	133.48	115.30
1	A	80	SER	N-CA-C	7.90	132.34	111.00
1	C	54	ARG	CA-CB-CG	7.89	130.76	113.40
1	C	244	LYS	CA-C-N	7.75	134.26	117.20
1	A	284	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	C	65	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	B	11	ALA	N-CA-C	7.64	131.63	111.00
2	B	80	GLN	CA-CB-CG	-7.64	96.59	113.40
1	C	296	ARG	CD-NE-CZ	7.64	134.29	123.60
1	C	284	TRP	CB-CG-CD1	-7.60	117.12	127.00
1	A	56	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	209	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	C	56	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	C	105	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	C	296	ARG	CA-CB-CG	7.39	129.66	113.40
1	C	80	SER	N-CA-C	7.38	130.93	111.00
1	C	284	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	209	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	A	284	TRP	CD1-CG-CD2	7.13	112.00	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	D	96	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	D	50	SER	N-CA-C	-7.01	92.07	111.00
1	A	167	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	D	3	HIS	N-CA-C	-6.95	92.24	111.00
1	A	167	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	C	285	TYR	CB-CG-CD1	-6.92	116.85	121.00
2	D	130	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	C	284	TRP	CG-CD2-CE3	6.87	140.08	133.90
2	D	102	ARG	NE-CZ-NH1	6.83	123.71	120.30
2	B	1	MET	CA-CB-CG	6.71	124.72	113.30
2	B	106	VAL	N-CA-CB	-6.71	96.73	111.50
1	C	56	ARG	CB-CG-CD	-6.69	94.21	111.60
2	D	121	VAL	CA-CB-CG1	6.61	120.81	110.90
1	C	309	VAL	O-C-N	6.60	133.26	122.70
2	D	128	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	209	TRP	CG-CD1-NE1	-6.50	103.60	110.10
1	A	57	LEU	CB-CG-CD1	-6.48	99.99	111.00
1	C	309	VAL	CA-C-N	-6.46	102.98	117.20
2	B	30	LEU	CA-CB-CG	6.43	130.10	115.30
1	C	23	VAL	CG1-CB-CG2	-6.39	100.67	110.90
2	D	66	LEU	CA-CB-CG	6.33	129.85	115.30
2	D	139	LYS	CA-CB-CG	6.32	127.31	113.40
2	B	66	LEU	CA-CB-CG	6.25	129.67	115.30
1	A	79	THR	CA-C-N	-6.24	103.47	117.20
1	C	287	GLN	OE1-CD-NE2	-6.21	107.62	121.90
2	B	128	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	269	ARG	CA-CB-CG	6.16	126.96	113.40
2	B	133	ASP	N-CA-C	6.12	127.53	111.00
1	C	306	ARG	CA-CB-CG	6.07	126.75	113.40
1	C	147	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	C	183	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	C	56	ARG	CG-CD-NE	-5.98	99.24	111.80
2	D	106	VAL	N-CA-CB	-5.97	98.36	111.50
1	C	296	ARG	CG-CD-NE	-5.96	99.29	111.80
2	B	20	HIS	CA-CB-CG	-5.95	103.48	113.60
1	A	296	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	D	30	LEU	CB-CG-CD1	-5.89	100.98	111.00
2	D	96	ARG	NE-CZ-NH1	5.89	123.24	120.30
2	B	131	ALA	N-CA-C	5.88	126.87	111.00
1	C	222	VAL	CA-CB-CG2	-5.87	102.10	110.90
1	C	116	THR	N-CA-CB	-5.85	99.19	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	37	GLU	CA-CB-CG	-5.80	100.64	113.40
1	C	209	TRP	CG-CD1-NE1	-5.79	104.31	110.10
1	A	269	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	C	222	VAL	CA-CB-CG1	5.72	119.48	110.90
2	D	109	CYS	CA-CB-SG	-5.71	103.72	114.00
1	A	197	TYR	CA-CB-CG	5.70	124.23	113.40
2	B	58	LEU	CA-CB-CG	5.69	128.40	115.30
1	C	136	THR	N-CA-CB	-5.69	99.50	110.30
2	B	133	ASP	CA-C-N	-5.68	104.70	117.20
2	B	3	HIS	CA-C-N	5.68	129.69	117.20
1	A	17	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	60	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	A	116	THR	N-CA-CB	-5.63	99.59	110.30
1	A	227	MET	N-CA-CB	-5.63	100.47	110.60
2	D	32	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	98	TYR	CB-CG-CD2	-5.61	117.64	121.00
2	D	89	TYR	N-CA-C	5.59	126.09	111.00
1	A	284	TRP	CG-CD2-CE3	5.58	138.93	133.90
1	C	218	VAL	CA-CB-CG2	-5.58	102.53	110.90
1	A	284	TRP	CB-CG-CD1	-5.52	119.82	127.00
2	B	149	VAL	CA-C-N	5.50	129.31	117.20
2	B	13	LYS	CA-C-N	-5.47	105.17	117.20
1	C	284	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	287	GLN	CG-CD-NE2	5.38	129.60	116.70
1	C	6	GLN	CA-CB-CG	-5.35	101.63	113.40
1	C	108	GLN	CA-CB-CG	-5.34	101.65	113.40
2	D	140	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	A	185	TYR	CB-CG-CD1	5.31	124.19	121.00
1	C	250	ARG	CA-CB-CG	5.31	125.08	113.40
2	B	13	LYS	CA-CB-CG	5.30	125.07	113.40
1	A	98	TYR	CA-CB-CG	5.30	123.46	113.40
1	C	197	TYR	CA-CB-CG	5.30	123.46	113.40
2	D	9	VAL	CA-C-N	-5.29	105.56	117.20
2	B	21	ILE	N-CA-C	-5.28	96.74	111.00
2	B	3	HIS	CA-CB-CG	5.28	122.57	113.60
1	A	303	VAL	CG1-CB-CG2	-5.26	102.49	110.90
2	B	20	HIS	CA-C-N	-5.24	105.67	117.20
2	D	131	ALA	CA-C-N	-5.24	105.67	117.20
2	D	9	VAL	CB-CA-C	-5.24	101.45	111.40
2	D	85	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	78	ASN	C-N-CA	5.20	134.71	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	PHE	O-C-N	-5.20	114.38	122.70
2	D	53	MET	CG-SD-CE	5.20	108.52	100.20
2	D	77	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	A	44	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	A	86	GLU	N-CA-CB	-5.17	101.30	110.60
1	C	248	VAL	CG1-CB-CG2	-5.16	102.64	110.90
1	A	80	SER	CA-C-N	5.16	128.54	117.20
1	A	95	ILE	CA-C-N	5.16	128.54	117.20
2	B	13	LYS	O-C-N	5.13	130.91	122.70
2	B	52	GLU	O-C-N	5.13	130.90	122.70
2	B	53	MET	N-CA-C	-5.10	97.24	111.00
2	D	11	ALA	N-CA-C	-5.08	97.29	111.00
1	A	116	THR	CA-CB-CG2	5.07	119.50	112.40
1	C	54	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	98	TYR	CB-CG-CD2	-5.06	117.96	121.00
2	B	85	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	B	70	GLN	CA-CB-CG	-5.06	102.27	113.40
2	D	55	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	C	246	GLN	CA-C-N	-5.04	106.12	117.20
1	C	296	ARG	CB-CG-CD	5.03	124.68	111.60
1	A	216	GLU	CA-CB-CG	5.02	124.45	113.40
1	A	246	GLN	N-CA-C	5.02	124.56	111.00
1	A	83	LYS	C-N-CA	5.01	134.22	121.70
1	C	81	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	84	LYS	N-CA-CB	5.00	119.61	110.60
1	C	78	ASN	N-CA-C	5.00	124.51	111.00

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
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	32	0
2	B	1196	0	1212	41	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	145	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 (145) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:287:GLN:HE21	1.52	0.58
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.38	0.58
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: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
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:232:LYS:HB3	1:A:240:TYR:CE2	2.47	0.49
1:A:5:TYR:CZ	1:A:306:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:ASP:HB3	2:D:100:PRO:HB3	1.95	0.49
2:D:20:HIS:O	2:D:20:HIS:ND1	2.46	0.49
2:B:41:ARG:HE	2:D:49:PRO:HD3	1.76	0.49
1:C:256:ASN:H	1:C:256:ASN:ND2	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:HG2	2:B:14:ARG:HH11	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
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
2:B:6:LYS:HZ3	2:D:43:THR:HG21	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HG	1:A:188:ALA:HB2	2.00	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
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
2:D:53:MET:HE2	2:D:53:MET:HB3	1.87	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:HA	1:C:198:ILE:HD13	1.91	0.42
2:B:136:LEU:HD12	2:B:147:HIS:HA	2.02	0.42
2:B:111:ASN:HB2	2:B:145:PHE:HZ	1.85	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
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:84:ASN:HA	2:B:93:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:172:LEU:HD12	1.85	0.40
1:C:40:LYS:O	1:C:41:HIS:HB2	2.21	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 [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%)	283 (92%)	20 (6%)	5 (2%)	9	17
1	C	308/310 (99%)	281 (91%)	18 (6%)	9 (3%)	4	6
2	B	151/153 (99%)	119 (79%)	22 (15%)	10 (7%)	1	1
2	D	151/153 (99%)	122 (81%)	21 (14%)	8 (5%)	2	2
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

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Mol	Chain	Res	Type
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%)	232 (89%)	29 (11%)	6	11
1	C	261/261 (100%)	220 (84%)	41 (16%)	2	4
2	B	136/137 (99%)	111 (82%)	25 (18%)	1	2
2	D	136/137 (99%)	112 (82%)	24 (18%)	2	3
All	All	794/796 (100%)	675 (85%)	119 (15%)	3	5

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	59	PHE
1	A	80	SER
1	A	114	LEU
1	A	121	ASN
1	A	134	HIS
1	A	153	ASP
1	A	167	ARG
1	A	174	GLN
1	A	194	MET
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	271	ASP
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	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

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Mol	Chain	Res	Type
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	7	LYS
1	C	17	ARG
1	C	34	PRO
1	C	54	ARG
1	C	59	PHE
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	125	LEU
1	C	136	THR
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	180	ASP
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	231	GLN
1	C	232	LYS

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Mol	Chain	Res	Type
1	C	236	ASP
1	C	237	PRO
1	C	252	SER
1	C	255	HIS
1	C	256	ASN
1	C	269	ARG
1	C	284	TRP
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	31	SER
2	D	41	ARG
2	D	43	THR
2	D	56	LYS
2	D	60	LYS
2	D	66	LEU
2	D	67	SER
2	D	73	GLN
2	D	84	ASN
2	D	85	ARG
2	D	88	ASN
2	D	95	SER
2	D	100	PRO
2	D	106	VAL
2	D	121	VAL
2	D	130	ARG
2	D	132	ASN
2	D	146	SER
2	D	153	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	231	GLN
1	A	282	HIS

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Mol	Chain	Res	Type
1	A	287	GLN
2	B	117	HIS
1	C	33	ASN
1	C	246	GLN
1	C	256	ASN
1	C	282	HIS
1	C	287	GLN
2	D	113	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	23,30,30	1.61	6 (26%)	30,47,47	2.05	5 (16%)
4	CTP	B	999	-	23,30,30	1.56	5 (21%)	30,47,47	2.00	5 (16%)

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	-	-	4/20/38/38	0/2/2/2
4	CTP	B	999	-	-	5/20/38/38	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	CTP	C2-N3	-3.34	1.31	1.38
4	D	999	CTP	C6-N1	-3.12	1.32	1.35
4	B	999	CTP	C6-N1	-3.02	1.32	1.35
4	D	999	CTP	C2-N3	-2.94	1.32	1.38
4	B	999	CTP	C4-N3	-2.84	1.31	1.35
4	D	999	CTP	C2'-C1'	-2.80	1.49	1.53
4	D	999	CTP	C4-N3	-2.66	1.31	1.35
4	D	999	CTP	PG-O1G	2.59	1.58	1.50
4	B	999	CTP	PG-O1G	2.40	1.58	1.50
4	D	999	CTP	PB-O1B	2.16	1.58	1.50
4	B	999	CTP	PB-O1B	2.15	1.58	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	999	CTP	PB-O3A-PA	-7.00	108.81	132.83
4	B	999	CTP	PB-O3A-PA	-6.54	110.38	132.83
4	D	999	CTP	PB-O3B-PG	-5.17	115.09	132.83
4	B	999	CTP	PB-O3B-PG	-4.80	116.35	132.83
4	D	999	CTP	C2-N3-C4	4.13	120.53	116.34
4	B	999	CTP	C2-N3-C4	3.88	120.27	116.34
4	B	999	CTP	C6-N1-C2	-3.36	115.86	121.20
4	D	999	CTP	C6-N1-C2	-2.91	116.58	121.20
4	D	999	CTP	C3'-C2'-C1'	2.53	104.78	100.98
4	B	999	CTP	C5'-C4'-C3'	-2.14	107.16	115.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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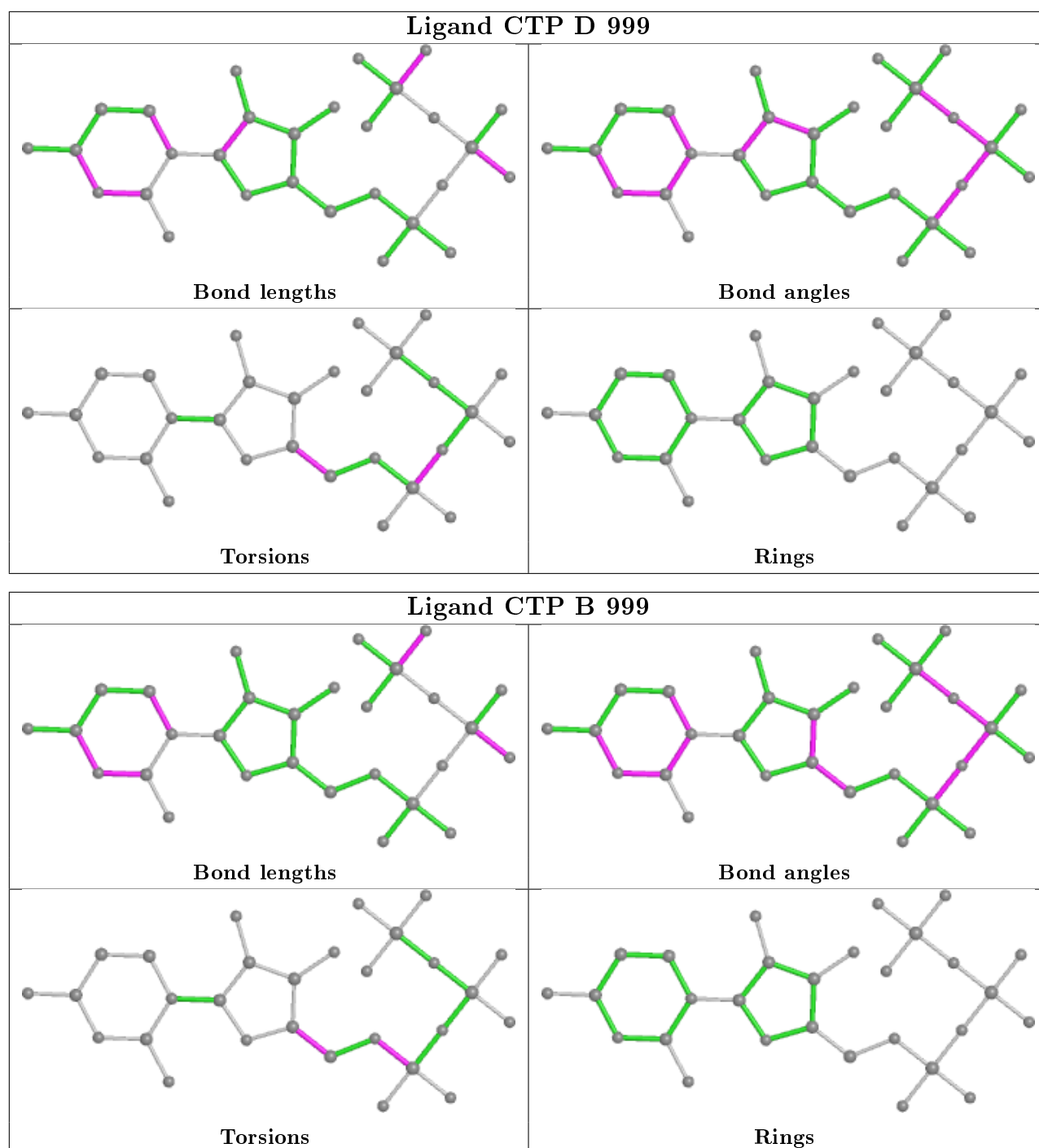
Mol	Chain	Res	Type	Atoms
4	B	999	CTP	C5'-O5'-PA-O2A
4	B	999	CTP	C5'-O5'-PA-O3A
4	D	999	CTP	O4'-C4'-C5'-O5'
4	D	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	PB-O3A-PA-O5'
4	D	999	CTP	PB-O3A-PA-O1A

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.