



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:56 PM GMT

PDB ID : 1RAG  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

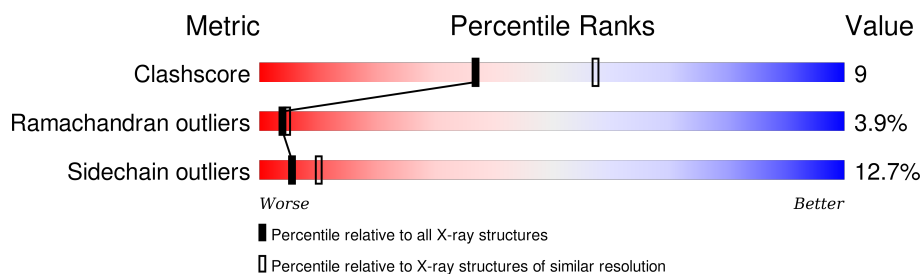
# 1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>).



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.

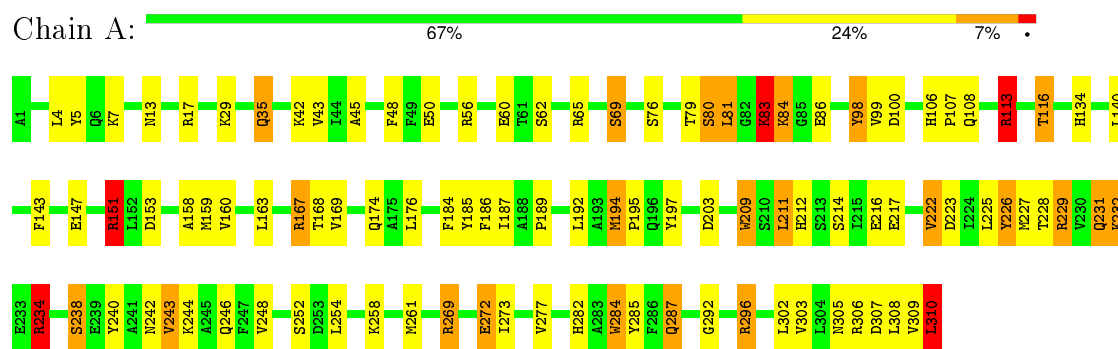
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	9	Total O 9 9	0	0
5	C	43	Total O 43 43	0	0
5	D	10	Total O 10 10	0	0

### 3 Residue-property plots [i](#)

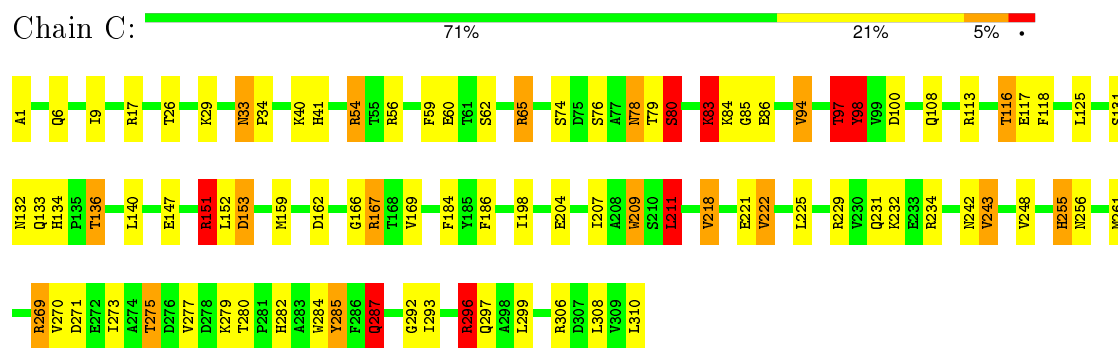
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

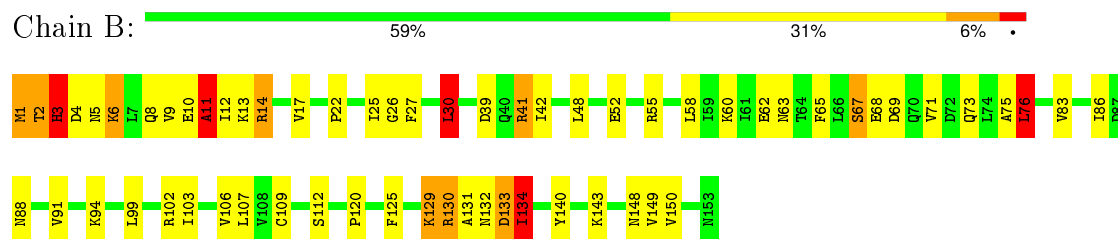
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



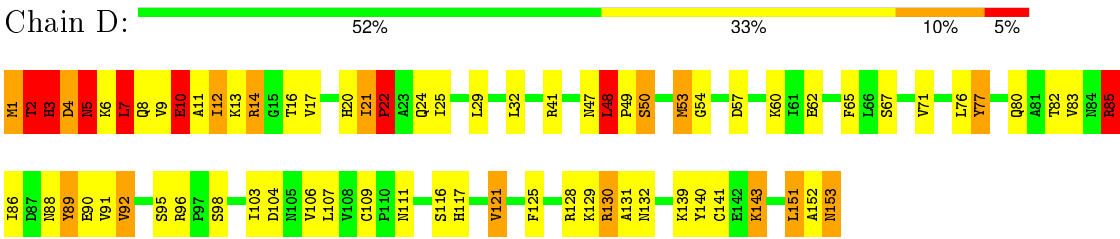
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



- 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 will therefore be incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	0.98	3/2461 (0.1%)	1.78	56/3339 (1.7%)
1	C	0.99	2/2461 (0.1%)	1.84	57/3339 (1.7%)
2	B	0.92	0/1214	1.73	22/1640 (1.3%)
2	D	0.94	0/1214	1.81	23/1640 (1.4%)
All	All	0.97	5/7350 (0.1%)	1.80	158/9958 (1.6%)

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	4
1	C	0	2
2	D	0	3
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLU	CD-OE2	8.82	1.35	1.25
1	C	147	GLU	CD-OE2	8.45	1.34	1.25
1	A	60	GLU	CD-OE2	6.75	1.33	1.25
1	A	69	SER	CA-CB	-6.32	1.43	1.52
1	C	60	GLU	CD-OE2	5.24	1.31	1.25

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	ARG	NE-CZ-NH1	15.26	127.93	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	ARG	NE-CZ-NH1	13.69	127.14	120.30
1	C	269	ARG	NE-CZ-NH2	-13.50	113.55	120.30
1	A	269	ARG	NE-CZ-NH1	13.23	126.91	120.30
2	D	2	THR	CA-C-N	-13.17	88.22	117.20
1	A	56	ARG	NE-CZ-NH2	-12.42	114.09	120.30
1	A	229	ARG	NE-CZ-NH1	11.12	125.86	120.30
2	D	2	THR	N-CA-C	10.62	139.67	111.00
1	C	209	TRP	CD1-CG-CD2	9.74	114.09	106.30
1	A	209	TRP	CD1-CG-CD2	9.48	113.88	106.30
1	A	234	ARG	NE-CZ-NH1	9.21	124.90	120.30
2	D	128	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	C	54	ARG	CA-CB-CG	8.96	133.12	113.40
1	C	56	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	56	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	C	97	THR	N-CA-CB	-8.56	94.03	110.30
1	C	296	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	43	VAL	CG1-CB-CG2	-8.46	97.36	110.90
1	C	209	TRP	CE2-CD2-CG	-8.24	100.71	107.30
1	A	310	LEU	CA-CB-CG	8.18	134.12	115.30
1	A	65	ARG	NE-CZ-NH1	7.99	124.29	120.30
2	B	133	ASP	CA-C-N	-7.95	99.71	117.20
2	D	9	VAL	CA-C-N	-7.79	100.05	117.20
2	B	133	ASP	N-CA-C	7.59	131.50	111.00
1	A	284	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	167	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	209	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	C	284	TRP	CD1-CG-CD2	7.48	112.28	106.30
2	D	3	HIS	CA-CB-CG	-7.48	100.88	113.60
2	D	14	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	C	284	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	A	284	TRP	CD1-CG-CD2	7.29	112.13	106.30
1	A	17	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	56	ARG	NE-CZ-NH1	7.19	123.90	120.30
2	B	52	GLU	CA-C-N	-7.18	101.41	117.20
1	C	159	MET	CG-SD-CE	-7.16	88.75	100.20
1	C	159	MET	CA-CB-CG	-7.08	101.26	113.30
2	B	11	ALA	N-CA-C	7.06	130.07	111.00
1	A	229	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	C	284	TRP	CB-CG-CD1	-6.93	117.99	127.00
1	A	79	THR	N-CA-C	6.86	129.53	111.00
2	D	128	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	B	13	LYS	CA-CB-CG	6.84	128.44	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ASP	CB-CG-OD1	6.82	124.44	118.30
1	C	80	SER	N-CA-C	6.74	129.19	111.00
1	C	56	ARG	CG-CD-NE	-6.69	97.76	111.80
1	A	269	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	248	VAL	CG1-CB-CG2	-6.67	100.23	110.90
1	C	284	TRP	CG-CD2-CE3	6.67	139.90	133.90
1	A	306	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	113	ARG	NE-CZ-NH1	6.61	123.61	120.30
2	B	106	VAL	N-CA-CB	-6.61	96.96	111.50
1	C	285	TYR	CB-CG-CD1	-6.59	117.05	121.00
2	D	89	TYR	N-CA-C	6.56	128.71	111.00
1	A	211	LEU	CB-CG-CD1	-6.56	99.85	111.00
1	C	140	LEU	CA-CB-CG	6.44	130.12	115.30
2	D	3	HIS	CA-C-N	-6.44	103.04	117.20
2	B	13	LYS	CB-CG-CD	-6.43	94.88	111.60
1	C	54	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	80	SER	N-CA-C	6.37	128.20	111.00
1	A	306	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	98	TYR	CB-CG-CD2	-6.25	117.25	121.00
2	B	52	GLU	N-CA-C	6.25	127.88	111.00
1	C	54	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	C	33	ASN	CB-CG-ND2	6.24	131.69	116.70
1	C	209	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	A	159	MET	CA-CB-CG	-6.21	102.73	113.30
1	A	209	TRP	CG-CD1-NE1	-6.21	103.89	110.10
1	C	151	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	B	41	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	197	TYR	CA-CB-CG	6.12	125.03	113.40
1	C	218	VAL	CA-CB-CG2	-6.11	101.74	110.90
1	A	296	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	269	ARG	CA-CB-CG	6.07	126.75	113.40
1	C	151	ARG	CG-CD-NE	-6.07	99.06	111.80
2	B	140	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	C	116	THR	N-CA-CB	-6.04	98.82	110.30
1	A	203	ASP	CB-CG-OD2	-6.00	112.90	118.30
2	B	76	LEU	CB-CA-C	-5.91	98.97	110.20
2	D	121	VAL	CA-CB-CG2	-5.85	102.13	110.90
1	A	258	LYS	CB-CG-CD	-5.83	96.45	111.60
1	C	269	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	174	GLN	CA-CB-CG	-5.79	100.67	113.40
1	C	60	GLU	OE1-CD-OE2	-5.79	116.36	123.30
1	C	242	ASN	CA-C-N	-5.76	104.52	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	B	130	ARG	CA-CB-CG	5.75	126.04	113.40
2	D	77	TYR	CB-CG-CD1	-5.74	117.55	121.00
1	C	65	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	116	THR	CA-CB-CG2	5.72	120.41	112.40
2	D	22	PRO	N-CA-C	5.72	126.98	112.10
1	A	84	LYS	CA-C-N	-5.71	104.78	116.20
2	D	2	THR	O-C-N	5.71	131.83	122.70
2	D	41	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	D	92	VAL	CA-CB-CG2	-5.69	102.36	110.90
1	A	98	TYR	CB-CG-CD2	-5.69	117.59	121.00
2	D	2	THR	CA-C-O	5.68	132.03	120.10
1	A	60	GLU	CA-CB-CG	-5.68	100.91	113.40
1	A	113	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	5	TYR	CB-CG-CD1	-5.66	117.60	121.00
2	B	3	HIS	CA-CB-CG	5.63	123.17	113.60
1	C	125	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	226	TYR	CB-CG-CD2	-5.60	117.64	121.00
2	B	13	LYS	O-C-N	5.60	131.67	122.70
2	B	13	LYS	CA-C-N	-5.60	104.88	117.20
1	A	84	LYS	N-CA-C	-5.59	95.92	111.00
1	A	229	ARG	CA-C-N	5.59	129.49	117.20
1	C	287	GLN	CG-CD-NE2	5.58	130.10	116.70
1	A	83	LYS	N-CA-C	5.57	126.05	111.00
1	A	296	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	83	LYS	CA-C-N	-5.56	104.97	117.20
1	C	273	ILE	N-CA-C	-5.54	96.04	111.00
1	C	78	ASN	N-CA-C	5.53	125.93	111.00
2	D	21	ILE	N-CA-C	-5.51	96.11	111.00
1	C	108	GLN	CA-CB-CG	-5.45	101.41	113.40
2	D	48	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	79	THR	CA-C-N	-5.38	105.36	117.20
2	B	6	LYS	CA-CB-CG	5.36	125.20	113.40
1	C	211	LEU	CA-CB-CG	5.33	127.55	115.30
2	D	130	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	116	THR	N-CA-CB	-5.30	100.23	110.30
2	B	6	LYS	CB-CG-CD	-5.30	97.82	111.60
1	C	162	ASP	N-CA-C	-5.30	96.69	111.00
1	C	84	LYS	CA-CB-CG	5.29	125.05	113.40
2	B	75	ALA	CA-C-N	5.29	128.84	117.20
1	C	26	THR	CA-CB-CG2	5.28	119.80	112.40
1	A	168	THR	O-C-N	-5.27	114.27	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	167	ARG	CB-CG-CD	-5.25	97.94	111.60
1	A	151	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	284	TRP	CB-CG-CD1	-5.25	120.18	127.00
2	B	133	ASP	O-C-N	5.24	131.08	122.70
1	C	204	GLU	CA-CB-CG	5.24	124.92	113.40
2	D	11	ALA	N-CA-C	-5.21	96.92	111.00
1	C	17	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	117	GLU	CA-CB-CG	-5.15	102.07	113.40
1	A	69	SER	CA-CB-OG	-5.13	97.34	111.20
2	B	134	ILE	CB-CA-C	-5.12	101.37	111.60
1	A	303	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	C	296	ARG	N-CA-CB	-5.11	101.41	110.60
1	C	62	SER	CB-CA-C	-5.10	100.41	110.10
2	B	149	VAL	CA-C-N	5.07	128.36	117.20
2	D	85	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	62	SER	CA-CB-OG	-5.07	97.52	111.20
1	A	84	LYS	N-CA-CB	5.07	119.72	110.60
2	B	30	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	275	THR	CA-CB-OG1	-5.05	98.39	109.00
1	A	234	ARG	CA-C-N	-5.05	106.09	117.20
2	D	85	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	269	ARG	CG-CD-NE	-5.04	101.21	111.80
1	C	222	VAL	N-CA-CB	-5.04	100.41	111.50
1	C	94	VAL	O-C-N	-5.04	114.64	122.70
1	A	56	ARG	CG-CD-NE	-5.04	101.23	111.80
1	C	255	HIS	CB-CA-C	-5.03	100.33	110.40
1	C	56	ARG	CB-CG-CD	-5.03	98.52	111.60
1	C	284	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	A	194	MET	CG-SD-CE	-5.01	92.18	100.20
2	D	83	VAL	CA-CB-CG2	-5.00	103.40	110.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	PHE	Sidechain
1	A	226	TYR	Sidechain
1	A	48	PHE	Sidechain
1	A	98	TYR	Sidechain
1	C	118	PHE	Sidechain
1	C	98	TYR	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	D	2	THR	Mainchain,Peptide
2	D	3	HIS	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	38	0
1	C	2415	0	2422	32	0
2	B	1196	0	1212	34	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	2	0
4	D	29	0	12	0	0
5	A	31	0	0	0	0
5	B	9	0	0	0	0
5	C	43	0	0	3	0
5	D	10	0	0	1	0
All	All	7375	0	7292	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (137) 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)
1:C:136:THR:HG23	1:C:296:ARG:HH11	1.23	1.04
2:B:4:ASP:HA	2:B:10:GLU:HB2	1.45	0.97
1:A:29:LYS:HD2	1:A:310:LEU:HD23	1.60	0.83
2:B:6:LYS:HD3	2:D:10:GLU:HG3	1.65	0.77
1:C:231:GLN:HB2	1:C:234:ARG:HG2	1.67	0.76
1:A:106:HIS:HD2	1:A:108:GLN:H	1.32	0.76
1:A:151:ARG:HD2	1:A:153:ASP:O	1.87	0.74
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.00	0.72
1:A:83:LYS:HB3	1:A:86:GLU:HB3	1.73	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.72	0.69
2:D:82:THR:HG22	2:D:96:ARG:HE	1.59	0.68
2:D:48:LEU:HD13	2:D:49:PRO:HD2	1.76	0.67
2:D:67:SER:HA	2:D:71:VAL:HG23	1.76	0.66
1:C:292:GLY:O	1:C:296:ARG:HB2	1.95	0.65
2:D:20:HIS:HE1	2:D:53:MET:SD	2.20	0.64
2:B:6:LYS:HA	2:B:9:VAL:HG22	1.78	0.64
1:C:229:ARG:HH12	1:C:270:VAL:HG23	1.63	0.62
2:D:5:ASN:HD22	2:D:6:LYS:HG2	1.64	0.62
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.80	0.62
2:B:76:LEU:HD21	2:B:103:ILE:CD1	2.29	0.62
2:D:12:ILE:HG21	2:D:62:GLU:HB3	1.82	0.62
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.81	0.61
1:A:189:PRO:HG2	1:A:192:LEU:HD12	1.82	0.61
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.83	0.60
1:C:255:HIS:HB2	5:C:321:HOH:O	2.00	0.60
2:D:22:PRO:HG2	2:D:25:ILE:HG13	1.83	0.60
1:C:94:VAL:O	1:C:97:THR:HB	2.02	0.59
1:C:113:ARG:O	1:C:116:THR:HB	2.02	0.59
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.38	0.59
1:C:280:THR:HG22	1:C:282:HIS:H	1.68	0.58
2:B:99:LEU:HD21	2:B:134:ILE:HD12	1.84	0.58
2:B:11:ALA:HA	4:B:999:CTP:N3	2.18	0.58
1:C:29:LYS:HD2	1:C:310:LEU:HD22	1.86	0.58
2:B:14:ARG:HH11	2:B:65:PHE:HE2	1.52	0.57
1:A:214:SER:O	1:A:217:GLU:HG2	2.05	0.57
2:B:76:LEU:HD21	2:B:103:ILE:HD11	1.87	0.57
1:A:106:HIS:HD2	1:A:108:GLN:N	2.02	0.57
2:B:41:ARG:HG2	2:D:47:ASN:O	2.04	0.56
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.87	0.56
1:C:80:SER:O	1:C:83:LYS:HB2	2.06	0.56
2:B:76:LEU:HD22	2:B:76:LEU:H	1.71	0.56
2:B:107:LEU:HD22	2:B:150:VAL:HG12	1.88	0.56
2:B:48:LEU:O	2:B:55:ARG:HA	2.07	0.55
1:A:231:GLN:HE21	1:A:234:ARG:NH1	2.04	0.55
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.89	0.55
1:A:229:ARG:HH22	1:A:232:LYS:NZ	2.05	0.55
2:B:14:ARG:HA	2:B:86:ILE:O	2.07	0.54
1:A:292:GLY:O	1:A:296:ARG:HG3	2.08	0.54
1:C:287:GLN:H	1:C:287:GLN:HE21	1.56	0.54
1:A:184:PHE:O	1:A:209:TRP:HA	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:PHE:HB3	2:D:85:ARG:NH2	2.23	0.53
1:A:227:MET:HG3	1:A:273:ILE:HD11	1.90	0.52
1:A:261:MET:O	1:A:282:HIS:HD2	1.91	0.52
2:D:109:CYS:SG	2:D:111:ASN:HB3	2.50	0.52
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.91	0.52
2:B:41:ARG:NE	2:D:49:PRO:HD3	2.25	0.51
1:A:185:TYR:HD1	1:A:212:HIS:NE2	2.08	0.51
2:B:27:PHE:HA	2:B:30:LEU:HD23	1.93	0.51
2:D:152:ALA:O	2:D:153:ASN:HB2	2.10	0.50
2:D:13:LYS:NZ	2:D:13:LYS:HB3	2.26	0.50
2:D:65:PHE:HB3	2:D:85:ARG:HH22	1.77	0.50
1:C:9:ILE:HG21	1:C:299:LEU:HD21	1.94	0.50
2:B:76:LEU:HD21	2:B:103:ILE:HD13	1.95	0.49
2:D:116:SER:HA	2:D:121:VAL:HG11	1.94	0.49
1:C:261:MET:C	1:C:261:MET:SD	2.90	0.49
1:C:86:GLU:HA	5:C:328:HOH:O	2.13	0.49
2:D:20:HIS:CE1	2:D:53:MET:SD	3.04	0.48
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.78	0.48
2:B:26:GLY:O	2:B:30:LEU:HD22	2.12	0.48
1:C:97:THR:HG22	1:C:98:TYR:HD2	1.78	0.48
2:B:2:THR:HG22	2:B:11:ALA:HB3	1.96	0.47
1:A:113:ARG:O	1:A:116:THR:HB	2.14	0.47
1:A:189:PRO:CG	1:A:192:LEU:HD12	2.44	0.47
1:C:83:LYS:NZ	1:C:83:LYS:HA	2.29	0.47
2:D:50:SER:O	2:D:54:GLY:N	2.47	0.47
1:C:293:ILE:O	1:C:297:GLN:HG3	2.15	0.47
1:A:163:LEU:HA	1:A:169:VAL:HG21	1.97	0.47
2:B:129:LYS:O	2:B:134:ILE:HD13	2.15	0.46
2:D:22:PRO:HG2	2:D:25:ILE:CG1	2.45	0.46
1:C:40:LYS:O	1:C:41:HIS:HB2	2.16	0.46
2:D:1:MET:N	2:D:6:LYS:HG3	2.29	0.46
1:A:231:GLN:HE21	1:A:234:ARG:HH11	1.63	0.46
1:C:1:ALA:HA	1:C:306:ARG:O	2.16	0.46
2:D:32:LEU:HD22	2:D:106:VAL:HG13	1.97	0.46
1:A:231:GLN:HB3	1:A:234:ARG:HD3	1.97	0.45
2:B:1:MET:HB2	2:D:7:LEU:HG	1.99	0.45
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.32	0.45
2:D:77:TYR:CE1	2:D:151:LEU:HD11	2.51	0.45
1:A:287:GLN:H	1:A:287:GLN:HE21	1.64	0.45
1:A:194:MET:SD	1:A:195:PRO:HD2	2.57	0.45
1:A:4:LEU:HD23	1:A:7:LYS:HD3	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:CD1	1:A:186:PHE:HB3	2.47	0.45
1:A:160:VAL:HG22	1:A:187:ILE:HB	1.99	0.45
2:B:22:PRO:HB2	2:B:25:ILE:HG12	1.99	0.45
1:A:302:LEU:HD23	1:A:308:LEU:HD23	1.98	0.45
2:D:141:CYS:SG	2:D:143:LYS:HB2	2.57	0.44
2:B:86:ILE:HD11	2:B:91:VAL:HG22	2.00	0.44
2:D:111:ASN:O	2:D:117:HIS:HE1	2.00	0.44
2:B:109:CYS:HA	2:B:125:PHE:HZ	1.82	0.44
2:B:71:VAL:HG13	2:B:83:VAL:HG21	2.00	0.44
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.17	0.44
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.85	0.44
1:A:243:VAL:O	1:A:246:GLN:HA	2.18	0.44
2:D:111:ASN:O	2:D:117:HIS:CE1	2.71	0.43
1:C:136:THR:HG22	5:C:316:HOH:O	2.18	0.43
1:C:1:ALA:HB2	1:C:306:ARG:NH2	2.33	0.43
1:C:207:ILE:HG21	1:C:207:ILE:HD13	1.84	0.43
2:B:129:LYS:HD3	2:B:132:ASN:OD1	2.18	0.43
1:C:166:GLY:O	1:C:169:VAL:HG22	2.17	0.43
2:D:20:HIS:CD2	2:D:20:HIS:O	2.71	0.43
2:B:4:ASP:HA	2:B:10:GLU:CB	2.32	0.43
1:A:254:LEU:HD11	1:A:277:VAL:HG13	2.00	0.43
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.87	0.43
2:D:85:ARG:O	2:D:86:ILE:HG13	2.19	0.43
2:B:6:LYS:HB3	2:D:10:GLU:HG3	2.01	0.42
2:D:14:ARG:HA	2:D:86:ILE:O	2.20	0.42
2:D:121:VAL:HG21	2:D:140:TYR:CZ	2.54	0.42
1:A:35:GLN:OE1	1:A:310:LEU:HD12	2.20	0.42
1:A:238:SER:O	1:A:242:ASN:HB2	2.20	0.42
1:C:186:PHE:HB2	1:C:211:LEU:HD12	2.00	0.42
1:C:229:ARG:NH1	1:C:270:VAL:HG23	2.34	0.41
2:B:12:ILE:HB	2:B:62:GLU:HG2	2.01	0.41
2:B:42:ILE:HA	2:B:60:LYS:O	2.21	0.41
2:B:94:LYS:HE2	4:B:999:CTP:O2G	2.21	0.41
1:A:223:ASP:O	1:A:261:MET:HA	2.21	0.41
1:C:277:VAL:O	1:C:280:THR:HB	2.20	0.41
2:B:67:SER:HA	2:B:71:VAL:HG23	2.01	0.41
2:D:20:HIS:HB2	5:D:1009:HOH:O	2.21	0.41
2:D:21:ILE:HG22	2:D:25:ILE:HB	2.02	0.41
1:C:151:ARG:HD2	1:C:153:ASP:O	2.20	0.41
1:A:158:ALA:HB2	1:A:222:VAL:HG21	2.03	0.41
1:A:140:LEU:HD22	1:A:292:GLY:HA2	2.03	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:ILE:HG22	2:D:29:LEU:HG	2.03	0.40
2:B:41:ARG:HD3	2:D:48:LEU:HA	2.02	0.40
1:C:184:PHE:O	1:C:209:TRP:HA	2.21	0.40
1:A:248:VAL:HG12	1:A:272:GLU:HA	2.04	0.40
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.85	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%)	278 (90%)	24 (8%)	6 (2%)	10	16
1	C	308/310 (99%)	287 (93%)	15 (5%)	6 (2%)	10	16
2	B	151/153 (99%)	125 (83%)	15 (10%)	11 (7%)	1	1
2	D	151/153 (99%)	126 (83%)	12 (8%)	13 (9%)	1	1
All	All	918/926 (99%)	816 (89%)	66 (7%)	36 (4%)	4	5

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	83	LYS
2	B	3	HIS
2	B	8	GLN
2	B	131	ALA
2	B	134	ILE
1	C	80	SER
1	C	243	VAL
2	D	4	ASP
2	D	5	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	7	LEU
2	D	53	MET
2	D	89	TYR
1	A	84	LYS
2	B	11	ALA
2	B	133	ASP
1	C	78	ASN
1	C	85	GLY
2	D	8	GLN
2	D	10	GLU
2	D	107	LEU
2	D	132	ASN
2	B	14	ARG
2	B	68	GLU
2	D	22	PRO
2	D	24	GLN
1	A	244	LYS
2	B	129	LYS
1	C	275	THR
2	D	131	ALA
1	A	231	GLN
2	B	63	ASN
1	C	76	SER
2	D	91	VAL
1	A	243	VAL
2	B	120	PRO

### 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%)	233 (89%)	28 (11%)	8	15
1	C	261/261 (100%)	229 (88%)	32 (12%)	6	11
2	B	136/137 (99%)	120 (88%)	16 (12%)	6	12
2	D	136/137 (99%)	111 (82%)	25 (18%)	2	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	794/796 (100%)	693 (87%)	101 (13%)	<b>5</b> <b>10</b>

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	GLN
1	A	42	LYS
1	A	69	SER
1	A	76	SER
1	A	81	LEU
1	A	113	ARG
1	A	134	HIS
1	A	151	ARG
1	A	167	ARG
1	A	211	LEU
1	A	216	GLU
1	A	222	VAL
1	A	225	LEU
1	A	228	THR
1	A	232	LYS
1	A	234	ARG
1	A	238	SER
1	A	240	TYR
1	A	252	SER
1	A	269	ARG
1	A	272	GLU
1	A	285	TYR
1	A	287	GLN
1	A	305	ASN
1	A	307	ASP
1	A	309	VAL
1	A	310	LEU
2	B	1	MET
2	B	2	THR
2	B	3	HIS
2	B	5	ASN
2	B	30	LEU
2	B	39	ASP
2	B	67	SER
2	B	69	ASP
2	B	73	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	76	LEU
2	B	88	ASN
2	B	102	ARG
2	B	112	SER
2	B	130	ARG
2	B	143	LYS
2	B	148	ASN
1	C	6	GLN
1	C	33	ASN
1	C	34	PRO
1	C	54	ARG
1	C	59	PHE
1	C	65	ARG
1	C	74	SER
1	C	79	THR
1	C	83	LYS
1	C	97	THR
1	C	131	SER
1	C	134	HIS
1	C	136	THR
1	C	151	ARG
1	C	152	LEU
1	C	153	ASP
1	C	167	ARG
1	C	211	LEU
1	C	218	VAL
1	C	221	GLU
1	C	222	VAL
1	C	225	LEU
1	C	232	LYS
1	C	243	VAL
1	C	256	ASN
1	C	269	ARG
1	C	271	ASP
1	C	279	LYS
1	C	285	TYR
1	C	287	GLN
1	C	296	ARG
1	C	308	LEU
2	D	1	MET
2	D	2	THR
2	D	3	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	4	ASP
2	D	5	ASN
2	D	7	LEU
2	D	10	GLU
2	D	12	ILE
2	D	16	THR
2	D	48	LEU
2	D	50	SER
2	D	80	GLN
2	D	85	ARG
2	D	88	ASN
2	D	90	GLU
2	D	92	VAL
2	D	95	SER
2	D	98	SER
2	D	104	ASP
2	D	129	LYS
2	D	130	ARG
2	D	139	LYS
2	D	143	LYS
2	D	151	LEU
2	D	153	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	146	GLN
1	A	282	HIS
1	A	287	GLN
1	C	21	ASN
1	C	255	HIS
1	C	282	HIS
1	C	287	GLN
1	C	297	GLN
2	D	5	ASN
2	D	20	HIS
2	D	117	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	CTP	B	999	-	21,30,30	1.28	1 (4%)	31,47,47	2.39	8 (25%)
4	CTP	D	999	-	21,30,30	1.26	2 (9%)	31,47,47	2.05	7 (22%)

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	-	-	0/18/38/38	0/2/2/2
4	CTP	D	999	-	-	0/18/38/38	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	CTP	C6-N1	-2.87	1.31	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	C6-N1	-2.33	1.32	1.35
4	D	999	CTP	PG-O1G	2.43	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	CTP	PB-O3A-PA	-7.84	110.70	132.73
4	D	999	CTP	PB-O3A-PA	-6.57	114.28	132.73
4	D	999	CTP	PB-O3B-PG	-5.81	113.19	132.67
4	B	999	CTP	PB-O3B-PG	-5.10	115.57	132.67
4	B	999	CTP	C4'-O4'-C1'	-4.62	104.64	109.72
4	B	999	CTP	C6-N1-C2	-3.62	115.42	121.28
4	D	999	CTP	C6-N1-C2	-2.97	116.47	121.28
4	B	999	CTP	C5-C4-N3	-2.29	118.92	121.80
4	D	999	CTP	C5-C4-N3	-2.23	118.98	121.80
4	D	999	CTP	O4'-C1'-N1	2.12	112.55	108.08
4	B	999	CTP	O4'-C1'-N1	2.16	112.64	108.08
4	D	999	CTP	O3A-PA-O5'	2.70	110.10	102.94
4	B	999	CTP	C2-N3-C4	3.12	120.01	115.61
4	B	999	CTP	O3A-PA-O5'	3.58	112.44	102.94
4	D	999	CTP	C2-N3-C4	4.05	121.33	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	CTP	2	0

## 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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.