Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 04:26 PM EST

PDB ID	:	1RAD
Title	:	CRYSTAL STRUCTURE OF CTP-LIGATED T STATE ASPARTATE TRANSCARBAMOYLASE AT 2.5 ANGSTROMS RESOLUTION: IMPLICATIONS FOR ATCASE MUTANTS AND THE MECHANISM OF NEGATIVE 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:

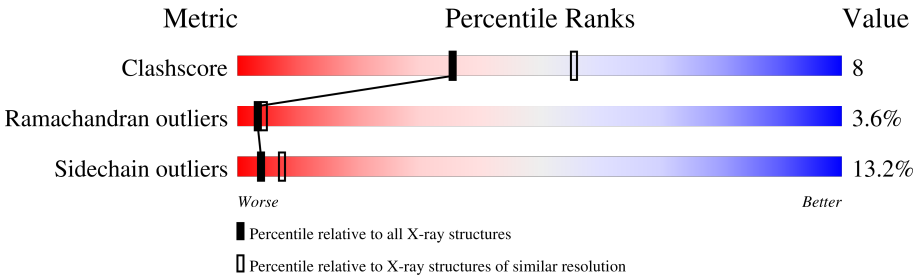
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	67% 26% 5% ·
1	C	310	69% 23% 6% ·
2	B	153	56% 29% 10% ·
2	D	153	61% 27% 8% 5%

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			

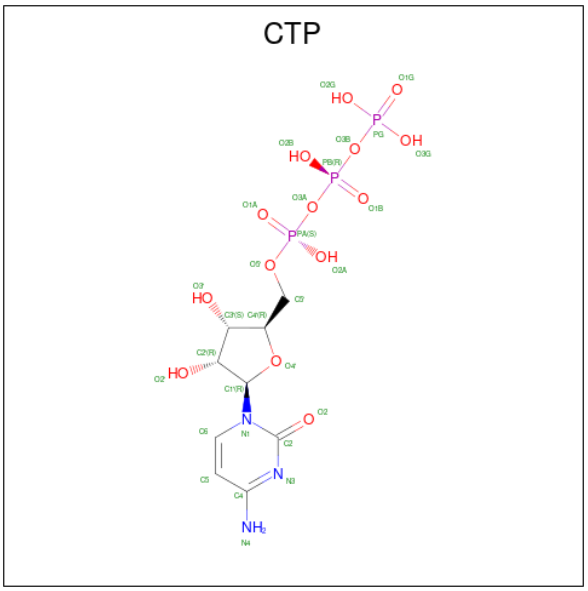
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

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: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 29 9 3 14 3	0	0
4	D	1	Total C N O P 29 9 3 14 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	44	Total O 44 44	0	0
5	D	9	Total O 9 9	0	0

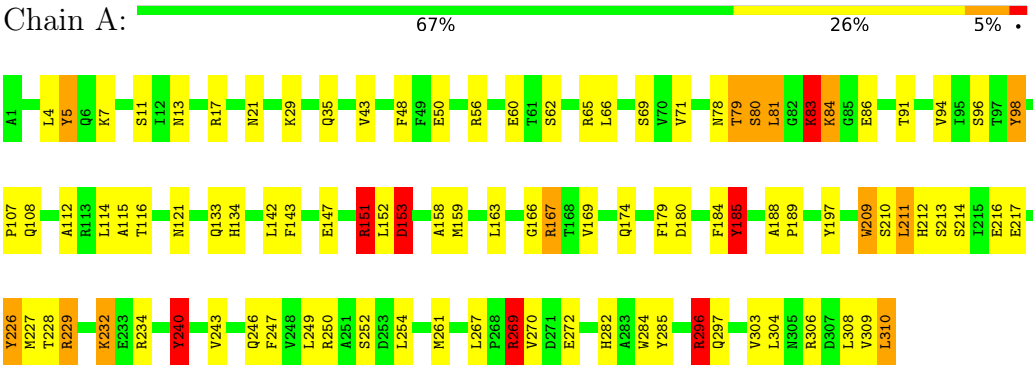
3 Residue-property plots (i)

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.

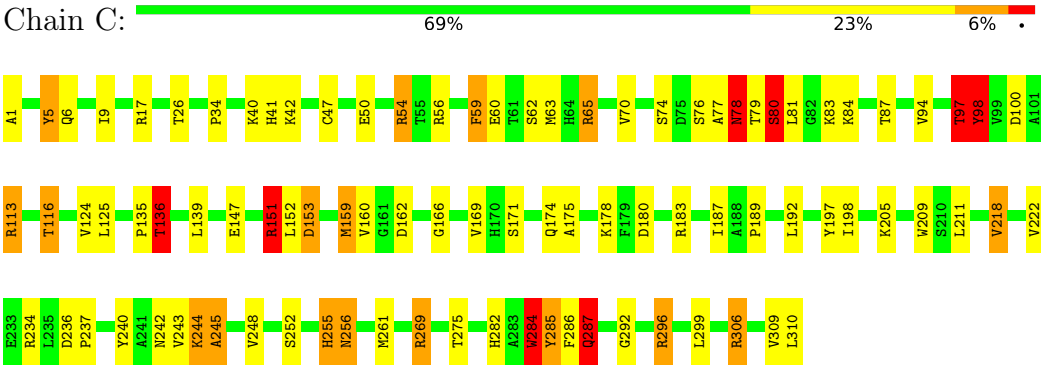
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A:



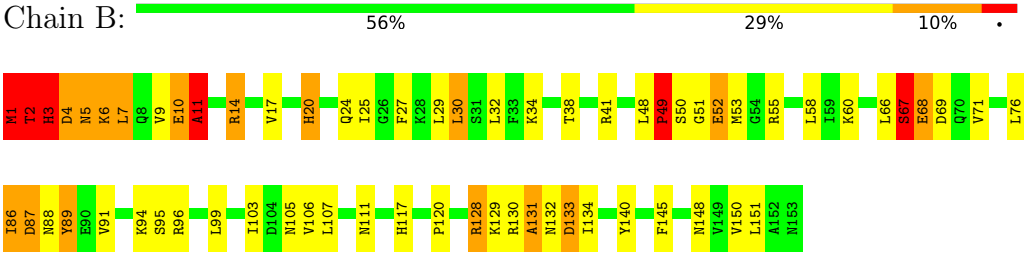
• Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain C:



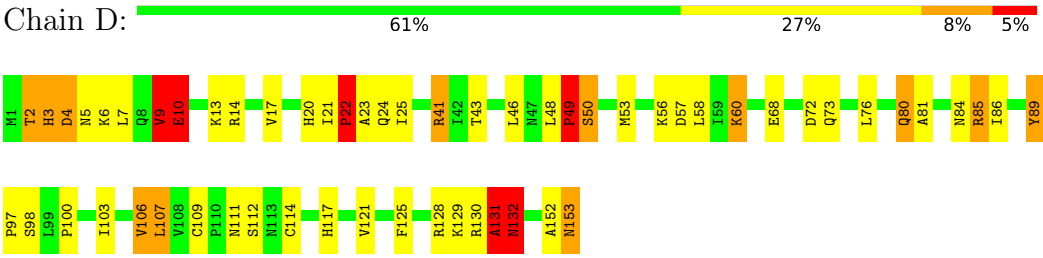
• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B:



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:


61%
27%
8%
5%
M1 T2 H3 D4 N5 K6 L7 Q8 V9 E10 K13 R14 V17 H20 T21 P22 A23 Q24 I25 R41 I42 T43 L46 N47 L48 P49 S50 M53 K56 D57 L58 I59 K60 E68 D72 Q73 L76 Q80 A81 N84 R85 I86 Y89 V92 R96
P97 S98 L99 P100 I103 V106 L107 V108 C109 P110 N111 S112 N113 C114 H117 V121 F125 R128 K129 R130 A131 N132 A152 N153

4 Data and refinement statistics (i)

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%)	1.76	45/3339 (1.3%)
1	C	1.01	2/2461 (0.1%)	1.84	60/3339 (1.8%)
2	B	0.91	0/1214	1.77	27/1640 (1.6%)
2	D	0.89	0/1214	1.77	22/1640 (1.3%)
All	All	0.96	4/7350 (0.1%)	1.79	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	7
1	C	0	3
2	B	0	2
2	D	0	1
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	GLU	CD-OE2	7.52	1.33	1.25
1	A	60	GLU	CD-OE2	7.27	1.33	1.25
1	A	147	GLU	CD-OE2	6.99	1.33	1.25
1	C	60	GLU	CD-OE2	5.07	1.31	1.25

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	296	ARG	NE-CZ-NH1	18.04	129.32	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	ARG	NE-CZ-NH1	14.61	127.61	120.30
1	A	65	ARG	NE-CZ-NH1	12.23	126.42	120.30
1	A	56	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	56	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	C	56	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	C	296	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	C	269	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	C	269	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	269	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	43	VAL	CG1-CB-CG2	-9.85	95.14	110.90
1	C	183	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	209	TRP	CD1-CG-CD2	9.50	113.90	106.30
1	C	65	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	5	TYR	CB-CG-CD1	-9.29	115.43	121.00
2	D	2	THR	CA-C-N	-8.91	97.59	117.20
1	C	284	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	C	209	TRP	CD1-CG-CD2	8.52	113.11	106.30
2	B	52	GLU	CA-C-N	-8.48	98.54	117.20
1	C	285	TYR	CB-CG-CD1	-8.25	116.05	121.00
2	B	1	MET	CA-CB-CG	8.18	127.21	113.30
1	C	54	ARG	CA-CB-CG	8.08	131.17	113.40
1	C	113	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	C	284	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	80	SER	N-CA-C	7.68	131.75	111.00
1	C	284	TRP	CB-CG-CD1	-7.64	117.06	127.00
1	C	287	GLN	CG-CD-NE2	7.64	135.04	116.70
2	D	128	ARG	NE-CZ-NH2	-7.46	116.57	120.30
2	B	66	LEU	CA-CB-CG	7.42	132.37	115.30
1	C	97	THR	N-CA-CB	-7.35	96.33	110.30
1	C	244	LYS	CA-C-N	7.33	133.34	117.20
2	D	3	HIS	N-CA-C	-7.31	91.25	111.00
1	C	296	ARG	CA-CB-CG	7.29	129.44	113.40
1	C	209	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	C	56	ARG	CB-CG-CD	-7.18	92.92	111.60
1	A	209	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	C	174	GLN	CA-CB-CG	-7.02	97.95	113.40
1	A	83	LYS	CA-CB-CG	6.97	128.74	113.40
2	B	133	ASP	N-CA-C	6.96	129.78	111.00
1	C	284	TRP	CG-CD2-CE3	6.96	140.16	133.90
2	B	11	ALA	N-CA-C	6.87	129.55	111.00
1	A	17	ARG	NE-CZ-NH1	6.83	123.72	120.30
2	B	80	GLN	CA-CB-CG	-6.83	98.36	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	TRP	CG-CD1-NE1	-6.77	103.33	110.10
1	C	234	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	81	LEU	CA-C-N	-6.73	102.75	116.20
1	C	80	SER	N-CA-C	6.70	129.09	111.00
1	C	98	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	A	303	VAL	CG1-CB-CG2	-6.65	100.26	110.90
2	B	30	LEU	CA-CB-CG	6.65	130.59	115.30
1	C	306	ARG	CA-CB-CG	6.54	127.79	113.40
1	A	234	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	B	128	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	227	MET	CG-SD-CE	-6.48	89.84	100.20
1	A	284	TRP	CE2-CD2-CG	-6.44	102.14	107.30
1	A	284	TRP	CD1-CG-CD2	6.42	111.43	106.30
1	C	296	ARG	CG-CD-NE	-6.41	98.35	111.80
1	A	151	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	167	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	C	287	GLN	OE1-CD-NE2	-6.36	107.28	121.90
2	D	121	VAL	CA-CB-CG2	-6.34	101.39	110.90
1	C	296	ARG	CD-NE-CZ	6.32	132.45	123.60
1	A	296	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	B	53	MET	N-CA-C	-6.29	94.01	111.00
2	D	130	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	159	MET	CA-CB-CG	6.25	123.93	113.30
2	D	96	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	183	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	209	TRP	CG-CD1-NE1	-6.10	104.00	110.10
2	B	106	VAL	N-CA-CB	-6.10	98.09	111.50
1	A	229	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	250	ARG	NE-CZ-NH1	6.07	123.34	120.30
2	B	52	GLU	N-CA-C	6.05	127.33	111.00
1	C	78	ASN	N-CA-C	5.99	127.17	111.00
1	A	226	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	116	THR	N-CA-CB	-5.98	98.93	110.30
1	C	6	GLN	CA-CB-CG	-5.95	100.32	113.40
1	A	189	PRO	CA-C-N	5.92	130.22	117.20
1	C	136	THR	N-CA-CB	-5.92	99.06	110.30
1	A	69	SER	CA-CB-OG	-5.90	95.27	111.20
1	C	284	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	A	185	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	C	218	VAL	CA-CB-CG2	-5.85	102.12	110.90
2	D	49	PRO	CA-C-N	-5.84	104.36	117.20
2	B	58	LEU	CA-CB-CG	5.81	128.67	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	10	GLU	N-CA-C	-5.79	95.36	111.00
1	C	248	VAL	CG1-CB-CG2	-5.76	101.68	110.90
2	D	106	VAL	N-CA-CB	-5.75	98.85	111.50
2	D	22	PRO	N-CA-C	5.73	127.00	112.10
2	B	128	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	D	130	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	C	151	ARG	CG-CD-NE	-5.71	99.82	111.80
1	C	125	LEU	CA-CB-CG	5.70	128.42	115.30
1	C	222	VAL	N-CA-CB	-5.67	99.03	111.50
2	D	132	ASN	N-CA-C	-5.67	95.70	111.00
1	C	56	ARG	CG-CD-NE	-5.64	99.95	111.80
2	B	68	GLU	CA-CB-CG	-5.60	101.08	113.40
1	C	56	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	D	50	SER	N-CA-C	-5.59	95.91	111.00
2	B	133	ASP	CA-C-N	-5.58	104.92	117.20
1	C	275	THR	N-CA-CB	-5.57	99.72	110.30
1	A	197	TYR	CA-CB-CG	5.57	123.98	113.40
1	A	71	VAL	CA-C-N	5.51	127.21	116.20
1	A	84	LYS	N-CA-C	-5.47	96.23	111.00
1	A	79	THR	CA-C-N	-5.44	105.22	117.20
1	A	94	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	C	252	SER	CA-CB-OG	5.39	125.76	111.20
1	A	17	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	B	52	GLU	CA-C-O	5.37	131.37	120.10
2	B	128	ARG	CB-CG-CD	-5.35	97.69	111.60
2	D	89	TYR	N-CA-C	5.35	125.44	111.00
2	B	3	HIS	CA-CB-CG	5.34	122.68	113.60
2	D	25	ILE	CG1-CB-CG2	-5.34	99.66	111.40
2	D	53	MET	CA-CB-CG	5.33	122.36	113.30
1	A	227	MET	N-CA-CB	-5.32	101.02	110.60
1	C	87	THR	O-C-N	-5.30	114.22	122.70
1	C	60	GLU	OE1-CD-OE2	-5.29	116.95	123.30
2	D	107	LEU	CB-CA-C	-5.27	100.18	110.20
1	C	116	THR	N-CA-CB	-5.25	100.33	110.30
2	B	5	ASN	CA-C-N	5.24	128.74	117.20
1	C	222	VAL	CA-CB-CG2	-5.22	103.06	110.90
1	C	81	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	224	ILE	O-C-N	-5.22	114.35	122.70
1	C	5	TYR	CB-CG-CD2	-5.21	117.88	121.00
2	D	107	LEU	N-CA-CB	5.21	120.81	110.40
1	C	159	MET	CG-SD-CE	-5.20	91.88	100.20
1	A	284	TRP	CG-CD2-CE3	5.17	138.56	133.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	153	ASP	CB-CA-C	-5.16	100.08	110.40
2	B	131	ALA	N-CA-C	5.16	124.94	111.00
1	C	113	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	153	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	98	TYR	CB-CA-C	-5.14	100.12	110.40
1	C	124	VAL	CG1-CB-CG2	-5.12	102.70	110.90
1	C	296	ARG	CB-CG-CD	5.12	124.91	111.60
1	C	26	THR	CA-CB-CG2	5.12	119.56	112.40
2	B	5	ASN	CA-CB-CG	5.12	124.65	113.40
1	A	246	GLN	N-CA-C	5.10	124.77	111.00
1	C	100	ASP	CB-CG-OD1	5.08	122.88	118.30
2	D	92	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	C	222	VAL	CA-CB-CG1	5.08	118.52	110.90
2	B	89	TYR	CB-CG-CD1	-5.08	117.95	121.00
2	B	20	HIS	CA-C-N	-5.07	106.04	117.20
2	B	96	ARG	NE-CZ-NH2	-5.07	117.76	120.30
2	B	67	SER	CA-C-N	-5.07	106.05	117.20
1	C	65	ARG	CA-CB-CG	-5.04	102.31	113.40
2	D	23	ALA	N-CA-CB	5.03	117.14	110.10
1	A	62	SER	CA-CB-OG	-5.02	97.64	111.20
1	C	309	VAL	CA-C-N	-5.02	106.15	117.20
2	B	5	ASN	O-C-N	-5.02	114.67	122.70
2	B	10	GLU	CA-C-N	-5.01	106.17	117.20
2	D	131	ALA	CA-C-N	-5.01	106.17	117.20
1	C	197	TYR	CA-CB-CG	5.01	122.92	113.40
2	D	9	VAL	CA-C-N	-5.00	106.19	117.20

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	PHE	Sidechain
1	A	185	TYR	Sidechain
1	A	226	TYR	Sidechain
1	A	240	TYR	Sidechain
1	A	296	ARG	Sidechain
1	A	48	PHE	Sidechain
1	A	98	TYR	Sidechain
2	B	140	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	286	PHE	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	5	TYR	Sidechain
1	C	98	TYR	Sidechain
2	D	48	LEU	Peptide

5.2 Too-close contacts (i)

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	34	0
1	C	2415	0	2422	36	0
2	B	1196	0	1212	29	0
2	D	1196	0	1212	24	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	31	0	0	0	0
5	B	9	0	0	0	0
5	C	44	0	0	1	0
5	D	9	0	0	1	0
All	All	7375	0	7292	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (118) 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:A:308:LEU:HG	1:A:310:LEU:HD22	1.54	0.90
2:B:1:MET:HA	2:D:7:LEU:HD21	1.58	0.84
2:B:4:ASP:HA	2:B:10:GLU:HB2	1.62	0.82
2:B:6:LYS:HB3	2:D:10:GLU:HG3	1.63	0.81
1:A:106:HIS:HD2	1:A:108:GLN:H	1.34	0.76
1:C:136:THR:CG2	1:C:296:ARG:HH11	1.99	0.75
2:B:6:LYS:HA	2:B:9:VAL:HG22	1.66	0.75
2:D:6:LYS:HB2	2:D:9:VAL:HG22	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:SER:HB2	2:D:56:LYS:HG2	1.72	0.70
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.73	0.70
1:C:292:GLY:O	1:C:296:ARG:HG2	1.95	0.66
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.78	0.66
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.29	0.66
2:B:99:LEU:HD23	2:B:130:ARG:HD2	1.77	0.65
2:B:41:ARG:HE	2:D:49:PRO:HD2	1.63	0.64
1:C:94:VAL:O	1:C:97:THR:HB	1.97	0.63
1:A:153:ASP:HB3	1:A:180:ASP:O	1.99	0.63
1:A:151:ARG:HD2	1:A:153:ASP:O	1.99	0.62
1:C:113:ARG:O	1:C:116:THR:HB	2.00	0.62
1:A:158:ALA:HB2	1:A:222:VAL:HG21	1.83	0.61
1:C:97:THR:HG22	1:C:98:TYR:HD2	1.66	0.60
2:D:17:VAL:HG22	2:D:60:LYS:HG3	1.84	0.59
1:A:232:LYS:HB3	1:A:240:TYR:CE2	2.37	0.59
2:B:107:LEU:HD22	2:B:150:VAL:HG12	1.83	0.59
1:A:29:LYS:HD2	1:A:310:LEU:HG	1.85	0.59
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.83	0.59
1:A:11:SER:HA	1:A:133:GLN:HG2	1.86	0.57
1:C:136:THR:HG23	1:C:296:ARG:HH11	1.67	0.57
1:A:267:LEU:CD2	1:A:269:ARG:HG3	2.35	0.56
2:D:20:HIS:HB2	5:D:1008:HOH:O	2.04	0.56
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.20	0.56
2:B:25:ILE:HG22	2:B:29:LEU:HG	1.87	0.56
1:C:242:ASN:O	1:C:244:LYS:N	2.39	0.55
2:B:48:LEU:O	2:B:55:ARG:HA	2.05	0.55
2:B:86:ILE:HG13	2:B:91:VAL:HA	1.87	0.55
2:B:48:LEU:HD23	2:D:41:ARG:HD3	1.88	0.55
1:A:81:LEU:HD12	1:A:91:THR:HG23	1.88	0.55
2:D:152:ALA:O	2:D:153:ASN:HB2	2.08	0.54
1:C:240:TYR:O	1:C:245:ALA:HB2	2.07	0.54
1:A:232:LYS:HB3	1:A:240:TYR:HE2	1.71	0.53
2:B:11:ALA:HA	4:B:999:CTP:N3	2.24	0.53
1:C:256:ASN:ND2	1:C:256:ASN:H	2.06	0.53
2:D:13:LYS:O	2:D:86:ILE:HG22	2.07	0.53
2:B:27:PHE:HA	2:B:30:LEU:HD23	1.90	0.52
2:B:129:LYS:HG2	2:B:132:ASN:OD1	2.10	0.52
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.92	0.52
1:A:166:GLY:O	1:A:169:VAL:HG22	2.11	0.50
1:C:151:ARG:HD2	1:C:153:ASP:O	2.11	0.50
1:A:142:LEU:HD22	1:A:152:LEU:HD13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:ALA:O	2:D:97:PRO:HD2	2.11	0.50
1:C:166:GLY:O	1:C:169:VAL:HG22	2.12	0.49
1:A:81:LEU:CD1	1:A:91:THR:HG23	2.42	0.49
1:C:261:MET:O	1:C:282:HIS:HD2	1.96	0.49
1:A:232:LYS:H	1:A:232:LYS:HE2	1.77	0.48
1:A:163:LEU:HG	1:A:188:ALA:HB2	1.96	0.48
1:A:4:LEU:HD23	1:A:7:LYS:HD2	1.96	0.47
2:B:2:THR:HG22	2:B:11:ALA:HB3	1.96	0.47
1:C:175:ALA:O	1:C:178:LYS:HB2	2.14	0.47
1:A:11:SER:HA	1:A:133:GLN:CG	2.44	0.47
2:B:67:SER:HA	2:B:71:VAL:HG23	1.97	0.47
1:C:229:ARG:CZ	1:C:229:ARG:HB2	2.44	0.47
1:A:101:ALA:HB2	1:A:304:LEU:HD21	1.97	0.47
2:B:14:ARG:HA	2:B:86:ILE:HG22	1.97	0.47
2:D:58:LEU:HD21	2:D:60:LYS:HD3	1.97	0.47
1:A:5:TYR:CD1	1:A:306:ARG:HA	2.51	0.46
1:C:232:LYS:HA	1:C:240:TYR:CD2	2.50	0.46
2:B:1:MET:HB2	2:D:7:LEU:HD11	1.98	0.46
1:A:209:TRP:HZ3	1:A:211:LEU:HG	1.81	0.45
1:A:184:PHE:O	1:A:209:TRP:HA	2.16	0.45
1:C:189:PRO:HG2	1:C:192:LEU:HB2	1.99	0.45
1:A:249:LEU:HD11	1:A:254:LEU:HD21	1.99	0.45
1:A:185:TYR:HD1	1:A:212:HIS:NE2	2.15	0.45
1:A:229:ARG:HH22	1:A:232:LYS:HE3	1.82	0.44
2:B:7:LEU:O	2:B:49:PRO:HD2	2.16	0.44
2:B:6:LYS:HB2	2:B:6:LYS:NZ	2.33	0.44
1:C:1:ALA:HA	1:C:306:ARG:O	2.18	0.44
1:C:9:ILE:HG21	1:C:299:LEU:HD21	1.99	0.44
2:D:131:ALA:O	2:D:132:ASN:HB2	2.16	0.44
1:C:50:GLU:HA	1:C:76:SER:OG	2.18	0.44
1:C:59:PHE:CE2	1:C:136:THR:HG21	2.53	0.44
1:C:153:ASP:HB3	5:C:341:HOH:O	2.16	0.44
1:A:66:LEU:HD21	1:A:297:GLN:HE21	1.83	0.43
1:A:214:SER:O	1:A:217:GLU:HB2	2.17	0.43
1:C:63:MET:SD	1:C:70:VAL:HG22	2.58	0.43
1:C:47:CYS:O	1:C:104:MET:HA	2.17	0.43
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.83	0.43
1:C:136:THR:HG23	1:C:296:ARG:NH1	2.32	0.42
2:B:103:ILE:HD13	2:B:103:ILE:HG21	1.86	0.42
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.87	0.42
2:B:14:ARG:HG3	2:B:87:ASP:OD1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:LEU:HD13	2:B:151:LEU:HD11	2.01	0.42
2:D:22:PRO:HG3	2:D:80:GLN:NE2	2.35	0.42
2:B:76:LEU:HD12	2:B:103:ILE:CD1	2.49	0.42
2:D:111:ASN:HB3	2:D:114:CYS:HB2	2.02	0.42
2:D:111:ASN:O	2:D:117:HIS:CE1	2.73	0.42
1:A:261:MET:O	1:A:282:HIS:HD2	2.03	0.41
1:A:102:ILE:HD13	1:A:102:ILE:HG21	1.88	0.41
2:B:84:ASN:OD1	2:B:94:LYS:HG2	2.19	0.41
2:B:111:ASN:O	2:B:117:HIS:HE1	2.03	0.41
1:A:112:ALA:O	1:A:115:ALA:HB3	2.20	0.41
1:C:80:SER:O	1:C:83:LYS:HB2	2.20	0.41
2:D:85:ARG:HH11	2:D:85:ARG:HB3	1.86	0.41
1:C:136:THR:HG23	1:C:296:ARG:HD3	2.02	0.41
2:D:85:ARG:HG3	2:D:92:VAL:HG12	2.02	0.41
1:C:160:VAL:HG22	1:C:187:ILE:HB	2.03	0.41
1:A:243:VAL:HB	1:A:247:PHE:HE1	1.86	0.41
1:C:40:LYS:O	1:C:41:HIS:HB2	2.21	0.41
1:A:21:ASN:HD21	1:A:179:PHE:HE2	1.68	0.40
2:B:76:LEU:HD23	2:B:76:LEU:HA	1.80	0.40
1:C:135:PRO:O	1:C:139:LEU:HG	2.20	0.40
2:D:14:ARG:HA	2:D:86:ILE:O	2.20	0.40
1:C:284:TRP:HA	1:C:287:GLN:HE21	1.85	0.40
1:C:42:LYS:HA	1:C:42:LYS:HD3	1.93	0.40
1:C:102:ILE:HD13	1:C:102:ILE:HG21	1.81	0.40
1:C:162:ASP:HA	1:C:192:LEU:HB3	2.03	0.40
1:A:5:TYR:CZ	1:A:306:ARG:HG2	2.57	0.40
2:B:111:ASN:HB2	2:B:145:PHE:HZ	1.86	0.40
2:D:111:ASN:O	2:D:117:HIS:HE1	2.04	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%)	284 (92%)	19 (6%)	5 (2%)	9 17
1	C	308/310 (99%)	284 (92%)	17 (6%)	7 (2%)	6 10
2	B	151/153 (99%)	122 (81%)	17 (11%)	12 (8%)	1 1
2	D	151/153 (99%)	125 (83%)	17 (11%)	9 (6%)	1 1
All	All	918/926 (99%)	815 (89%)	70 (8%)	33 (4%)	3 4

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	83	LYS
1	A	84	LYS
1	A	270	VAL
2	B	3	HIS
2	B	11	ALA
2	B	51	GLY
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	22	PRO
2	D	107	LEU
2	D	132	ASN
2	B	14	ARG
2	B	68	GLU
1	C	77	ALA
1	C	255	HIS
2	D	5	ASN
2	D	24	GLN
2	D	89	TYR
1	A	79	THR
2	B	105	ASN
1	C	245	ALA
2	B	49	PRO
1	C	84	LYS
2	D	68	GLU
2	D	131	ALA
2	B	2	THR
2	B	120	PRO

5.3.2 Protein sidechains (i)

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%)	231 (88%)	30 (12%)	5 11
2	B	136/137 (99%)	113 (83%)	23 (17%)	2 3
2	D	136/137 (99%)	113 (83%)	23 (17%)	2 3
All	All	794/796 (100%)	689 (87%)	105 (13%)	4 7

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	GLN
1	A	78	ASN
1	A	83	LYS
1	A	86	GLU
1	A	96	SER
1	A	114	LEU
1	A	121	ASN
1	A	134	HIS
1	A	151	ARG
1	A	153	ASP
1	A	167	ARG
1	A	174	GLN
1	A	210	SER
1	A	211	LEU
1	A	213	SER
1	A	216	GLU
1	A	222	VAL
1	A	225	LEU
1	A	228	THR
1	A	232	LYS
1	A	240	TYR
1	A	252	SER
1	A	269	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	272	GLU
1	A	285	TYR
1	A	296	ARG
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	5	ASN
2	B	6	LYS
2	B	7	LEU
2	B	20	HIS
2	B	24	GLN
2	B	32	LEU
2	B	34	LYS
2	B	38	THR
2	B	49	PRO
2	B	50	SER
2	B	52	GLU
2	B	67	SER
2	B	69	ASP
2	B	86	ILE
2	B	87	ASP
2	B	88	ASN
2	B	95	SER
2	B	128	ARG
2	B	148	ASN
1	C	17	ARG
1	C	34	PRO
1	C	54	ARG
1	C	59	PHE
1	C	62	SER
1	C	65	ARG
1	C	74	SER
1	C	78	ASN
1	C	79	THR
1	C	97	THR
1	C	136	THR
1	C	151	ARG
1	C	152	LEU
1	C	153	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	159	MET
1	C	171	SER
1	C	180	ASP
1	C	205	LYS
1	C	211	LEU
1	C	218	VAL
1	C	229	ARG
1	C	236	ASP
1	C	237	PRO
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	310	LEU
2	D	2	THR
2	D	3	HIS
2	D	4	ASP
2	D	9	VAL
2	D	10	GLU
2	D	41	ARG
2	D	43	THR
2	D	46	LEU
2	D	49	PRO
2	D	60	LYS
2	D	72	ASP
2	D	73	GLN
2	D	80	GLN
2	D	84	ASN
2	D	85	ARG
2	D	92	VAL
2	D	98	SER
2	D	100	PRO
2	D	106	VAL
2	D	112	SER
2	D	129	LYS
2	D	132	ASN
2	D	153	ASN

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	106	HIS
1	A	282	HIS
1	A	297	GLN
2	B	147	HIS
2	B	148	ASN
1	C	78	ASN
1	C	256	ASN
1	C	282	HIS
1	C	287	GLN
2	D	5	ASN
2	D	117	HIS

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 monosaccharides 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	-	26,30,30	1.33	5 (19%)	39,47,47	1.86	6 (15%)
4	CTP	B	999	-	26,30,30	1.37	6 (23%)	39,47,47	1.83	6 (15%)

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	-	-	5/22/38/38	0/2/2/2
4	CTP	B	999	-	-	5/22/38/38	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	PG-O1G	2.51	1.58	1.50
4	B	999	CTP	PG-O1G	2.50	1.58	1.50
4	B	999	CTP	C6-N1	-2.43	1.32	1.38
4	B	999	CTP	C2-N1	-2.41	1.34	1.40
4	D	999	CTP	C5-C4	-2.30	1.37	1.42
4	B	999	CTP	PB-O1B	2.25	1.58	1.50
4	D	999	CTP	C6-N1	-2.20	1.32	1.38
4	D	999	CTP	PB-O1B	2.10	1.58	1.50
4	B	999	CTP	C5-C4	-2.06	1.38	1.42
4	D	999	CTP	PA-O1A	2.06	1.58	1.50
4	B	999	CTP	C2-N3	-2.01	1.32	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	999	CTP	PB-O3A-PA	-6.66	109.98	132.83
4	B	999	CTP	PB-O3A-PA	-6.46	110.67	132.83
4	D	999	CTP	PB-O3B-PG	-5.76	113.07	132.83
4	B	999	CTP	PB-O3B-PG	-4.53	117.30	132.83
4	D	999	CTP	O2-C2-N3	-4.47	115.06	122.33
4	B	999	CTP	O2-C2-N3	-4.37	115.22	122.33
4	B	999	CTP	N1-C2-N3	2.99	124.26	118.81
4	B	999	CTP	C6-N1-C2	-2.63	115.94	120.49
4	D	999	CTP	N1-C2-N3	2.20	122.81	118.81
4	D	999	CTP	C6-N1-C2	-2.13	116.80	120.49
4	B	999	CTP	O4'-C1'-N1	2.12	113.21	108.36
4	D	999	CTP	O4'-C1'-N1	2.02	112.98	108.36

There are no chirality outliers.

All (10) 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
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	PB-O3A-PA-O5'
4	D	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	PA-O3A-PB-O1B
4	D	999	CTP	C5'-O5'-PA-O3A

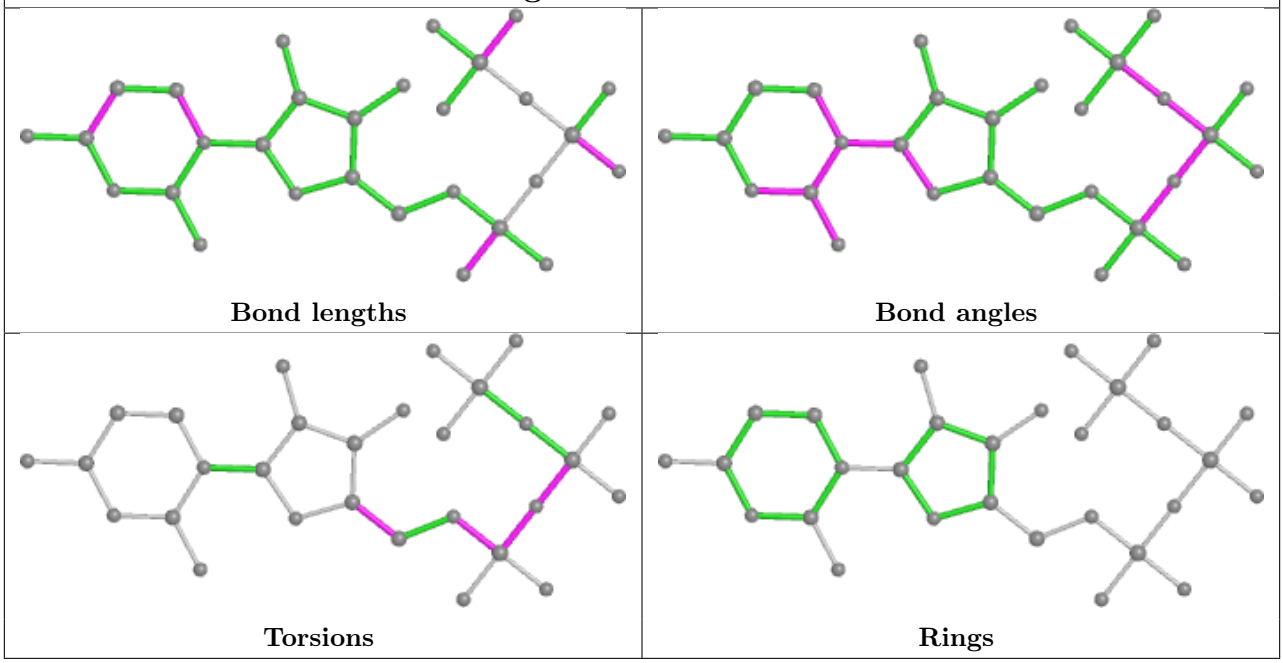
There are no ring outliers.

1 monomer is involved in 1 short contact:

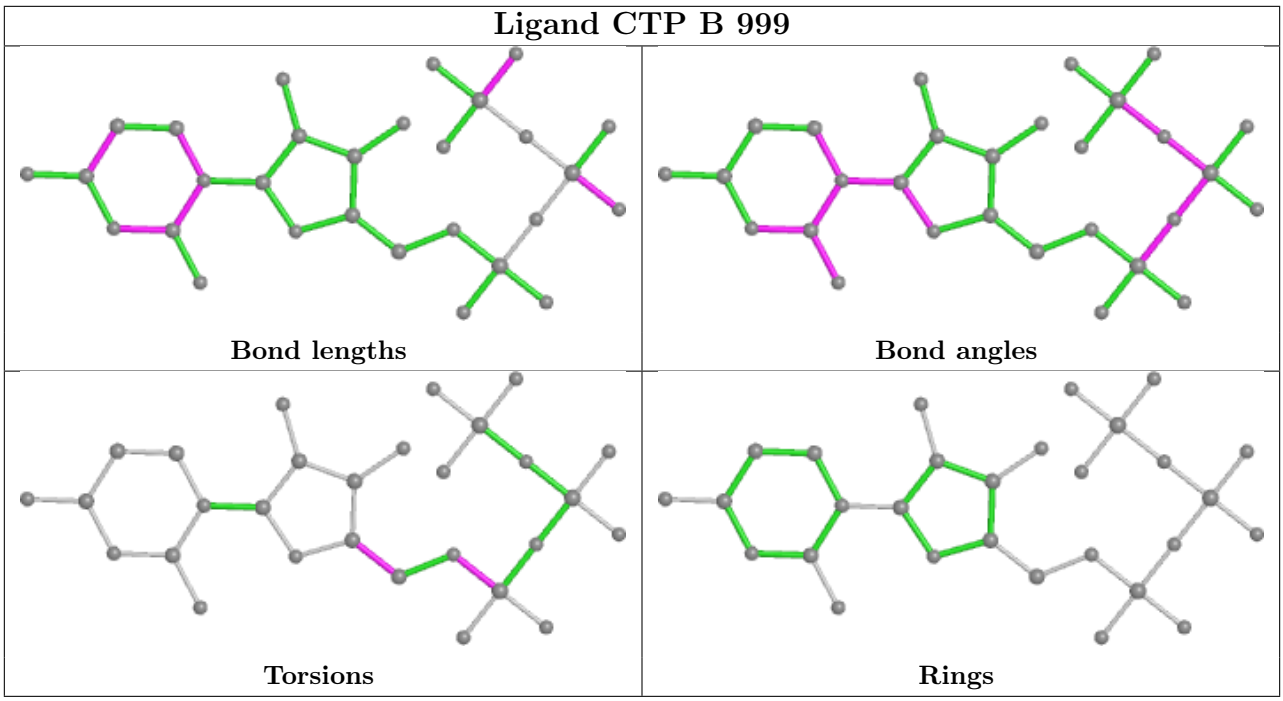
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	CTP	1	0

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 then 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.

Ligand CTP D 999



Ligand CTP B 999



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.