



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 1RAG / pdb_00001rag
Title : CRYSTAL STRUCTURE OF CTP-LIGATED T STATE ASPARTATE
TRANSCARBAMOYLASE AT 2.5 ANGSTROMS RESOLUTION: IMPLI-
CATIONS FOR ATCASE MUTANTS AND THE MECHANISM OF NEGA-
TIVE COOPERATIVITY
Authors : Kosman, R.P.; Gouaux, J.E.; Lipscomb, W.N.
Deposited on : 1992-08-14
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

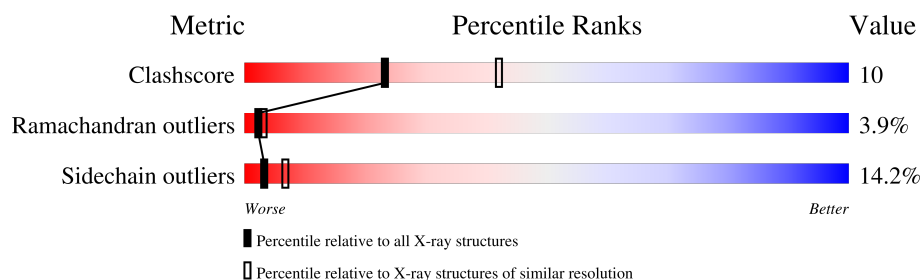
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	55% 33% 9% .
1	C	310	54% 34% 9% .
2	B	153	49% 34% 14% .
2	D	153	44% 35% 14% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7375 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

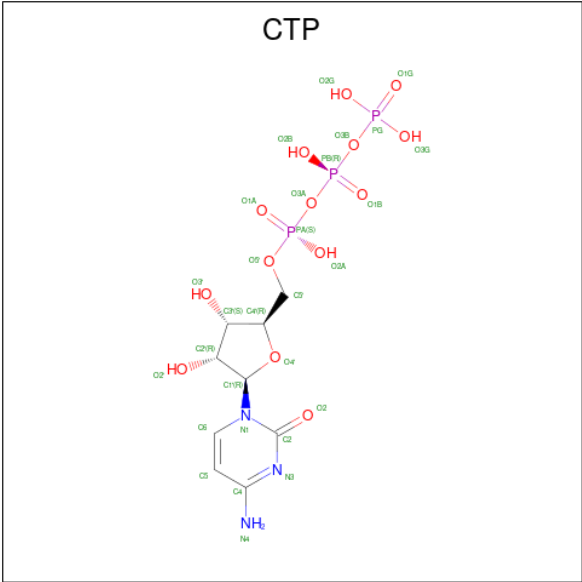
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1196	749	212	229	6			
2	D	153	Total	C	N	O	S	0	0	0
			1196	749	212	229	6			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: C₉H₁₆N₃O₁₄P₃).



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

- Molecule 5 is water.

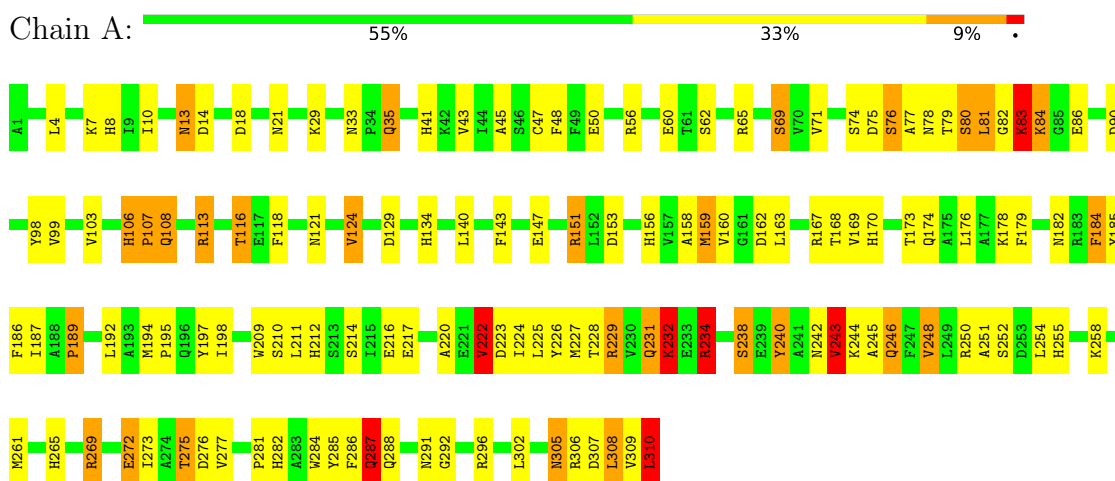
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	9	Total	O	0	0
			9	9		
5	C	43	Total	O	0	0
			43	43		
5	D	10	Total	O	0	0
			10	10		

3 Residue-property plots [i](#)

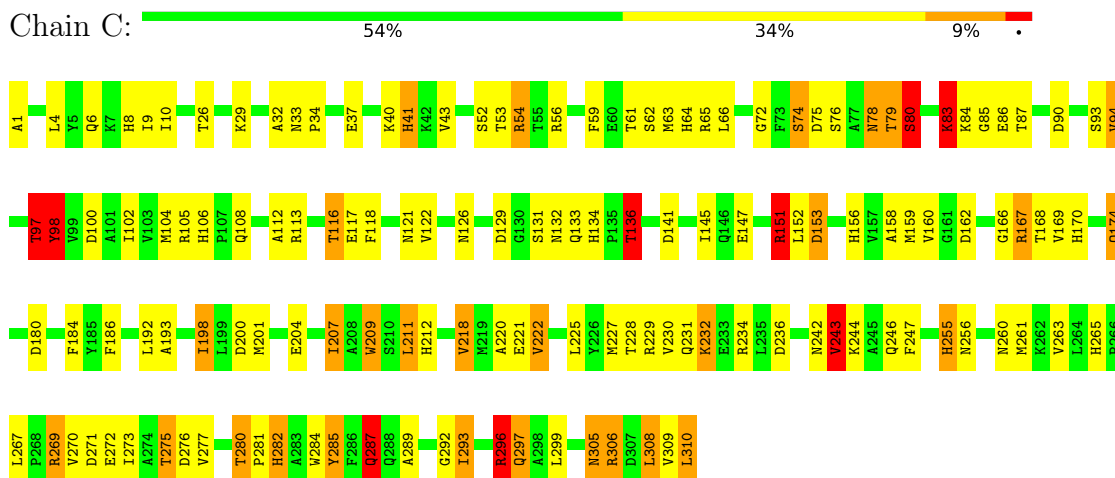
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

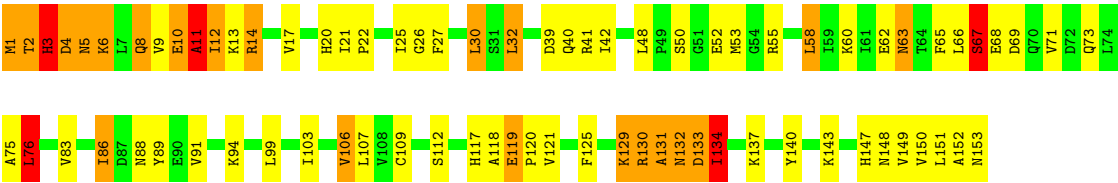


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

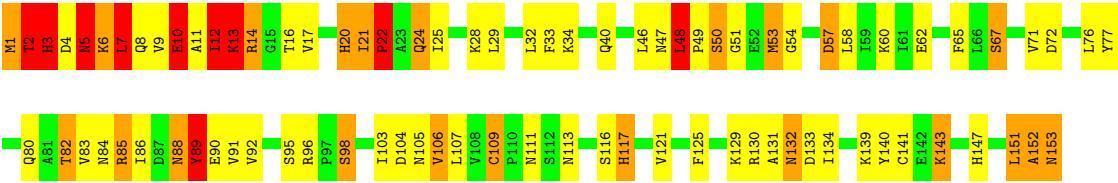


- Molecule 2: Aspartate carbamoyltransferase regulatory chain





• Molecule 2: Aspartate carbamoyltransferase regulatory chain



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.13Å 122.13Å 142.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7375	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

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	1.29	19/2461 (0.8%)	2.10	96/3339 (2.9%)
1	C	1.34	23/2461 (0.9%)	2.23	136/3339 (4.1%)
2	B	1.19	4/1214 (0.3%)	2.17	52/1640 (3.2%)
2	D	1.25	8/1214 (0.7%)	2.24	58/1640 (3.5%)
All	All	1.28	54/7350 (0.7%)	2.18	342/9958 (3.4%)

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 (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	VAL	CA-CB	9.28	1.65	1.54
1	A	124	VAL	CA-CB	7.63	1.63	1.54
1	C	64	HIS	CD2-NE2	-6.97	1.30	1.37
1	C	265	HIS	CG-ND1	-6.80	1.30	1.38
2	D	147	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	41	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	156	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	47	CYS	CA-CB	-6.42	1.44	1.52
1	C	170	HIS	CD2-NE2	-6.39	1.30	1.37
2	D	147	HIS	CG-ND1	-6.39	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	106	HIS	CG-ND1	-6.28	1.31	1.38
1	C	41	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	265	HIS	CG-ND1	-6.24	1.31	1.38
2	D	20	HIS	CD2-NE2	-6.21	1.31	1.37
2	B	147	HIS	CD2-NE2	-6.20	1.31	1.37
1	C	134	HIS	CD2-NE2	-6.18	1.31	1.37
1	C	212	HIS	CD2-NE2	-6.12	1.31	1.37
2	B	3	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	69	SER	CA-CB	-6.05	1.43	1.53
1	C	265	HIS	CD2-NE2	-5.98	1.31	1.37
1	C	156	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	134	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	265	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	56	ARG	CA-CB	-5.90	1.43	1.53
1	C	8	HIS	CG-ND1	-5.86	1.31	1.38
1	C	8	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	41	HIS	CG-ND1	-5.69	1.31	1.38
2	B	117	HIS	CD2-NE2	-5.68	1.31	1.37
1	C	255	HIS	CD2-NE2	-5.64	1.31	1.37
2	D	117	HIS	CD2-NE2	-5.60	1.31	1.37
1	C	56	ARG	CA-CB	-5.58	1.44	1.53
1	C	79	THR	CA-CB	5.56	1.59	1.52
1	C	106	HIS	CG-ND1	-5.55	1.32	1.38
1	C	134	HIS	CG-ND1	-5.53	1.32	1.38
1	C	106	HIS	CD2-NE2	-5.52	1.31	1.37
2	D	82	THR	CA-CB	5.52	1.63	1.53
1	A	255	HIS	CD2-NE2	-5.51	1.31	1.37
1	A	33	ASN	CA-CB	5.51	1.59	1.53
1	A	184	PHE	CA-CB	-5.50	1.45	1.53
2	D	2	THR	CA-CB	5.41	1.59	1.52
1	A	234	ARG	CA-CB	5.38	1.60	1.52
2	B	20	HIS	CD2-NE2	-5.37	1.31	1.37
1	C	170	HIS	CG-ND1	-5.34	1.32	1.38
1	C	64	HIS	CG-ND1	-5.30	1.32	1.38
1	C	108	GLN	CA-CB	-5.30	1.45	1.53
1	C	43	VAL	CA-C	-5.27	1.46	1.52
1	A	147	GLU	CD-OE2	5.27	1.35	1.25
1	C	282	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	134	HIS	CG-ND1	-5.16	1.32	1.38
1	C	112	ALA	CA-CB	-5.16	1.44	1.53
1	C	147	GLU	CD-OE2	5.05	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	117	HIS	CG-ND1	-5.04	1.32	1.38

All (342) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	THR	N-CA-C	18.28	139.67	108.23
2	B	53	MET	N-CA-C	-13.02	98.34	114.75
2	D	3	HIS	CA-CB-CG	-12.92	100.88	113.80
1	C	33	ASN	OD1-CG-ND2	-11.60	111.00	122.60
2	D	21	ILE	N-CA-C	-11.53	96.11	107.76
1	C	287	GLN	OE1-CD-NE2	-11.18	111.42	122.60
2	D	2	THR	CA-C-O	10.23	132.03	120.98
1	C	33	ASN	CB-CG-ND2	10.19	131.69	116.40
1	A	245	ALA	N-CA-C	-9.73	98.67	111.71
1	A	14	ASP	CA-CB-CG	9.72	122.32	112.60
2	B	133	ASP	N-CA-C	9.72	131.50	110.80
1	A	291	ASN	OD1-CG-ND2	-9.63	112.97	122.60
1	C	54	ARG	CA-CB-CG	9.51	133.12	114.10
2	B	3	HIS	CA-CB-CG	9.37	123.17	113.80
1	C	97	THR	N-CA-CB	-9.31	94.03	110.42
1	C	287	GLN	CG-CD-NE2	9.13	130.10	116.40
2	D	20	HIS	CA-C-N	-9.05	116.07	122.59
2	D	20	HIS	C-N-CA	-9.05	116.07	122.59
2	B	11	ALA	N-CA-C	9.05	130.07	110.80
1	A	276	ASP	CA-CB-CG	9.02	121.62	112.60
1	C	232	LYS	N-CA-C	8.94	123.60	112.87
1	A	21	ASN	OD1-CG-ND2	-8.91	113.69	122.60
2	D	147	HIS	ND1-CG-CD2	8.86	114.96	106.10
1	A	79	THR	N-CA-C	8.79	129.53	110.80
1	C	80	SER	N-CA-C	8.63	129.19	110.80
2	B	4	ASP	CA-CB-CG	8.57	121.17	112.60
1	C	33	ASN	CA-C-N	8.55	128.62	119.90
1	C	33	ASN	C-N-CA	8.55	128.62	119.90
2	B	119	GLU	N-CA-C	8.53	121.86	108.55
1	C	90	ASP	N-CA-C	8.51	121.49	111.71
1	A	75	ASP	CA-CB-CG	8.42	121.02	112.60
2	D	89	TYR	N-CA-C	8.41	128.71	110.80
1	C	75	ASP	CA-CB-CG	8.40	121.00	112.60
1	A	41	HIS	ND1-CG-CD2	8.33	114.43	106.10
1	C	247	PHE	N-CA-C	-8.30	98.17	109.54
1	A	129	ASP	CA-CB-CG	8.26	120.86	112.60
1	A	80	SER	N-CA-C	8.17	128.20	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	HIS	ND1-CG-CD2	8.06	114.16	106.10
2	B	52	GLU	N-CA-C	8.02	127.88	110.80
2	D	67	SER	N-CA-C	7.98	120.12	108.86
1	C	122	VAL	N-CA-C	-7.94	99.74	107.76
1	C	220	ALA	N-CA-C	7.86	120.84	111.33
1	C	54	ARG	N-CA-C	-7.84	102.68	111.07
2	D	11	ALA	N-CA-C	-7.83	96.92	109.76
2	D	33	PHE	CA-CB-CG	-7.80	106.00	113.80
1	C	129	ASP	CA-CB-CG	7.71	120.31	112.60
2	D	152	ALA	N-CA-C	-7.68	102.50	111.03
1	C	141	ASP	CA-CB-CG	7.68	120.28	112.60
2	D	40	GLN	OE1-CD-NE2	-7.67	114.93	122.60
1	C	83	LYS	N-CA-C	-7.62	97.64	109.76
2	B	67	SER	N-CA-C	7.54	119.62	108.60
1	C	297	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	C	275	THR	CA-CB-OG1	-7.47	98.39	109.60
1	A	182	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	265	HIS	ND1-CG-CD2	7.42	113.52	106.10
1	C	116	THR	N-CA-CB	-7.40	98.82	110.22
1	C	272	GLU	N-CA-C	7.38	121.72	112.87
2	D	5	ASN	CA-CB-CG	7.37	119.97	112.60
2	B	5	ASN	CA-CB-CG	7.36	119.96	112.60
1	C	222	VAL	N-CA-CB	-7.36	100.41	110.56
1	A	232	LYS	N-CA-C	7.29	121.82	112.34
1	C	134	HIS	ND1-CG-CD2	7.28	113.38	106.10
1	A	116	THR	CA-CB-OG1	-7.22	98.77	109.60
2	B	13	LYS	CA-CB-CG	7.17	128.44	114.10
1	C	26	THR	CA-CB-OG1	-7.16	98.85	109.60
1	A	83	LYS	N-CA-C	7.16	126.05	110.80
1	A	21	ASN	CA-CB-CG	7.15	119.75	112.60
2	B	13	LYS	CB-CG-CD	-7.14	94.88	111.30
1	C	100	ASP	CA-CB-CG	7.13	119.73	112.60
2	B	13	LYS	O-C-N	7.12	131.67	123.27
1	C	78	ASN	N-CA-C	7.10	125.93	110.80
2	D	22	PRO	N-CA-C	7.04	126.98	112.47
1	A	162	ASP	CA-CB-CG	6.99	119.59	112.60
2	D	6	LYS	N-CA-C	6.99	122.10	112.04
1	A	84	LYS	N-CA-C	-6.99	95.92	110.80
2	B	106	VAL	N-CA-CB	-6.98	96.96	111.76
1	C	244	LYS	N-CA-C	-6.96	104.26	112.89
1	C	61	THR	N-CA-C	-6.95	103.78	111.36
1	C	200	ASP	CA-CB-CG	6.95	119.55	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	168	THR	O-C-N	-6.91	114.27	122.15
2	D	2	THR	O-C-N	6.91	131.83	122.57
1	A	287	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	C	10	ILE	N-CA-C	-6.89	105.63	111.56
1	A	69	SER	CA-CB-OG	-6.88	97.34	111.10
2	B	50	SER	O-C-N	6.87	130.34	122.99
1	A	306	ARG	N-CA-C	6.85	119.59	111.71
1	C	141	ASP	N-CA-C	-6.84	103.75	111.14
1	A	33	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	178	LYS	N-CA-C	-6.82	105.24	113.97
1	C	43	VAL	N-CA-C	-6.81	98.31	108.12
1	A	62	SER	CA-CB-OG	-6.79	97.52	111.10
1	A	287	GLN	CG-CD-NE2	6.79	126.58	116.40
1	C	106	HIS	ND1-CG-CD2	6.75	112.85	106.10
2	B	32	LEU	N-CA-C	6.74	119.48	111.33
1	C	305	ASN	N-CA-C	6.72	119.47	108.52
1	A	174	GLN	CA-CB-CG	-6.71	100.67	114.10
1	A	134	HIS	CB-CG-CD2	-6.68	122.52	131.20
2	D	9	VAL	O-C-N	6.68	129.48	122.67
1	A	13	ASN	CA-CB-CG	-6.67	105.93	112.60
1	C	273	ILE	N-CA-C	-6.67	96.04	107.24
1	C	230	VAL	N-CA-C	-6.64	100.18	109.21
2	D	134	ILE	N-CA-CB	-6.62	103.03	111.64
1	A	60	GLU	CA-CB-CG	-6.59	100.91	114.10
1	C	260	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	C	93	SER	N-CA-C	-6.56	104.21	111.82
1	C	255	HIS	CB-CA-C	-6.55	100.33	110.81
1	C	8	HIS	ND1-CG-CD2	6.52	112.62	106.10
1	A	275	THR	CA-CB-OG1	-6.50	99.84	109.60
1	A	78	ASN	CA-C-N	6.49	133.93	121.54
1	A	78	ASN	C-N-CA	6.49	133.93	121.54
1	A	243	VAL	N-CA-C	6.48	122.82	109.34
1	A	189	PRO	CA-C-O	-6.48	114.47	121.27
1	C	56	ARG	CG-CD-NE	-6.47	97.76	112.00
2	B	140	TYR	CA-C-O	-6.46	114.02	120.80
1	C	98	TYR	N-CA-C	6.46	124.16	113.50
1	A	258	LYS	CB-CG-CD	-6.46	96.45	111.30
2	B	133	ASP	CA-CB-CG	6.44	119.04	112.60
1	C	296	ARG	NE-CZ-NH1	6.43	127.93	121.50
1	C	159	MET	CA-CB-CG	-6.42	101.26	114.10
1	A	121	ASN	CA-CB-CG	6.41	119.01	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	ASN	CA-C-N	6.40	133.76	121.54
2	B	132	ASN	C-N-CA	6.40	133.76	121.54
1	C	162	ASP	N-CA-C	-6.38	96.69	107.99
2	B	133	ASP	O-C-N	6.38	131.08	122.59
2	B	119	GLU	CA-C-N	6.38	127.81	119.84
2	B	119	GLU	C-N-CA	6.38	127.81	119.84
2	B	52	GLU	CA-C-O	6.37	129.62	120.51
1	C	108	GLN	CA-CB-CG	-6.35	101.41	114.10
2	D	147	HIS	CG-CD2-NE2	-6.34	100.86	107.20
1	A	76	SER	N-CA-C	-6.34	99.68	109.76
1	A	269	ARG	CA-CB-CG	6.32	126.75	114.10
1	C	83	LYS	O-C-N	6.31	130.42	123.04
2	D	82	THR	N-CA-C	-6.29	98.64	108.90
1	C	269	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	A	286	PHE	CA-CB-CG	-6.27	107.53	113.80
1	C	62	SER	CB-CA-C	-6.25	100.41	110.79
1	C	255	HIS	N-CA-C	6.25	118.61	111.11
1	A	134	HIS	CG-CD2-NE2	-6.24	100.96	107.20
1	C	193	ALA	N-CA-C	6.24	118.83	110.35
2	B	149	VAL	CA-C-O	-6.21	114.27	120.85
1	C	168	THR	O-C-N	-6.20	115.08	122.15
1	A	90	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	197	TYR	CA-CB-CG	6.18	125.03	113.90
2	B	131	ALA	N-CA-C	6.17	123.94	110.80
1	A	41	HIS	CG-CD2-NE2	-6.14	101.06	107.20
2	D	88	ASN	N-CA-C	-6.13	97.73	110.80
2	B	134	ILE	N-CA-C	6.12	122.08	109.34
1	A	71	VAL	O-C-N	-6.12	116.60	123.03
1	A	246	GLN	N-CA-C	6.12	123.83	110.80
1	A	43	VAL	CG1-CB-CG2	-6.11	97.36	110.80
1	C	87	THR	O-C-N	-6.11	115.60	122.75
1	A	220	ALA	N-CA-C	6.09	117.59	111.07
2	B	12	ILE	CA-C-N	-6.09	114.52	123.05
2	B	12	ILE	C-N-CA	-6.09	114.52	123.05
1	C	236	ASP	CA-CB-CG	6.08	118.68	112.60
2	D	57	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	116	THR	N-CA-CB	-6.07	100.23	110.49
2	B	63	ASN	OD1-CG-ND2	-6.06	116.54	122.60
2	B	134	ILE	CB-CA-C	-6.05	101.37	111.29
2	B	75	ALA	N-CA-C	6.05	119.92	112.54
1	C	97	THR	OG1-CB-CG2	6.03	121.37	109.30
1	C	117	GLU	CA-CB-CG	-6.01	102.07	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	HIS	ND1-CG-CD2	6.01	112.11	106.10
1	C	284	TRP	CG-CD2-CE3	6.00	139.90	133.90
1	A	83	LYS	CA-C-N	5.99	132.97	121.54
1	A	83	LYS	C-N-CA	5.99	132.97	121.54
1	C	66	LEU	N-CA-C	-5.97	104.52	112.94
2	B	130	ARG	CA-CB-CG	5.97	126.04	114.10
1	C	296	ARG	N-CA-CB	-5.97	101.41	110.07
1	A	229	ARG	O-C-N	-5.96	115.08	123.01
1	C	97	THR	CB-CA-C	5.96	121.84	110.27
1	A	134	HIS	CA-CB-CG	5.94	119.74	113.80
1	C	284	TRP	CB-CG-CD1	-5.94	117.99	126.90
1	C	72	GLY	CA-C-O	-5.94	115.77	121.83
2	B	63	ASN	CB-CG-ND2	5.92	125.27	116.40
1	C	198	ILE	N-CA-C	-5.92	105.08	110.82
1	C	180	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	179	PHE	O-C-N	-5.91	114.87	122.20
1	C	52	SER	O-C-N	-5.91	116.72	123.40
1	C	309	VAL	CB-CA-C	-5.91	104.17	111.08
1	C	160	VAL	N-CA-CB	-5.89	103.28	111.41
1	A	198	ILE	N-CA-C	-5.89	104.78	110.72
1	C	151	ARG	CG-CD-NE	-5.88	99.06	112.00
2	D	40	GLN	CB-CG-CD	5.88	122.60	112.60
2	D	13	LYS	CA-C-O	-5.87	114.63	120.80
2	D	133	ASP	CA-CB-CG	5.87	118.47	112.60
2	B	6	LYS	CB-CG-CD	-5.86	97.82	111.30
1	C	134	HIS	CB-CG-CD2	-5.86	123.58	131.20
2	D	72	ASP	CA-CB-CG	-5.84	106.76	112.60
1	A	18	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	291	ASN	CB-CG-ND2	5.83	125.15	116.40
1	C	121	ASN	CA-C-N	-5.83	118.39	122.59
1	C	121	ASN	C-N-CA	-5.83	118.39	122.59
1	A	116	THR	CA-CB-CG2	5.83	120.41	110.50
1	C	174	GLN	CA-CB-CG	-5.83	102.45	114.10
1	C	280	THR	O-C-N	-5.81	115.02	121.53
1	C	167	ARG	CB-CG-CD	-5.81	97.94	111.30
2	D	12	ILE	CB-CG1-CD1	-5.80	101.61	113.80
1	C	242	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	106	HIS	CA-C-N	5.79	125.90	119.87
1	A	106	HIS	C-N-CA	5.79	125.90	119.87
1	A	255	HIS	CA-CB-CG	5.77	119.57	113.80
2	D	3	HIS	CA-C-N	5.77	132.56	121.54
2	D	3	HIS	C-N-CA	5.77	132.56	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	ASN	O-C-N	5.76	130.31	122.48
1	A	224	ILE	O-C-N	-5.75	117.14	123.18
2	B	121	VAL	N-CA-C	-5.72	100.05	108.85
1	A	174	GLN	CG-CD-NE2	5.68	124.93	116.40
1	C	134	HIS	CG-CD2-NE2	-5.68	101.52	107.20
1	A	159	MET	CA-CB-CG	-5.68	102.73	114.10
1	C	105	ARG	N-CA-C	-5.68	100.63	109.72
1	A	56	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	C	116	THR	OG1-CB-CG2	5.67	120.63	109.30
2	D	106	VAL	N-CA-CB	-5.65	104.88	111.83
1	C	269	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	C	255	HIS	ND1-CG-CD2	5.64	111.74	106.10
1	A	107	PRO	N-CA-CB	5.62	108.70	103.41
2	D	105	ASN	N-CA-C	5.62	122.77	110.80
1	A	281	PRO	N-CA-C	5.61	121.13	113.84
1	C	287	GLN	N-CA-C	-5.59	105.95	112.89
1	C	94	VAL	O-C-N	-5.59	114.64	121.90
2	D	117	HIS	CA-CB-CG	-5.58	108.22	113.80
1	A	82	GLY	CA-C-N	5.58	132.19	121.54
1	A	82	GLY	C-N-CA	5.58	132.19	121.54
1	C	280	THR	CA-C-N	5.57	125.28	119.82
1	C	280	THR	C-N-CA	5.57	125.28	119.82
1	A	10	ILE	N-CA-C	5.57	116.41	111.90
1	C	56	ARG	CB-CG-CD	-5.56	98.52	111.30
1	C	280	THR	N-CA-CB	-5.56	102.11	109.78
2	D	84	ASN	OD1-CG-ND2	-5.56	117.04	122.60
2	B	6	LYS	CA-CB-CG	5.55	125.20	114.10
2	B	21	ILE	N-CA-C	-5.55	103.86	108.63
2	D	7	LEU	N-CA-C	5.54	122.60	110.80
1	C	263	VAL	CA-C-N	5.53	131.50	122.81
1	C	263	VAL	C-N-CA	5.53	131.50	122.81
1	A	74	SER	O-C-N	-5.53	115.36	122.94
1	C	106	HIS	O-C-N	-5.53	117.98	121.85
1	C	136	THR	N-CA-C	-5.53	105.79	112.54
1	C	159	MET	CG-SD-CE	-5.52	88.75	100.90
2	D	152	ALA	CA-C-O	-5.52	115.21	120.90
1	A	222	VAL	N-CA-C	5.52	117.28	108.89
2	D	51	GLY	N-CA-C	-5.50	106.03	113.24
2	D	9	VAL	CA-C-O	5.49	127.50	121.13
1	C	158	ALA	CA-C-O	-5.49	114.45	120.43
2	B	152	ALA	CA-C-N	5.47	131.55	121.70
2	B	152	ALA	C-N-CA	5.47	131.55	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	LYS	CA-CB-CG	5.47	125.05	114.10
1	A	265	HIS	CG-CD2-NE2	-5.47	101.73	107.20
1	C	26	THR	CA-CB-CG2	5.47	119.80	110.50
2	D	109	CYS	CA-C-N	5.46	125.80	119.47
2	D	109	CYS	C-N-CA	5.46	125.80	119.47
1	A	84	LYS	N-CA-CB	5.46	119.72	110.49
1	A	245	ALA	CA-C-N	5.46	131.97	121.54
1	A	245	ALA	C-N-CA	5.46	131.97	121.54
1	A	82	GLY	N-CA-C	-5.45	108.33	115.47
1	C	104	MET	N-CA-C	5.44	118.31	109.06
1	C	267	LEU	O-C-N	-5.43	115.08	121.32
1	A	103	VAL	N-CA-C	-5.42	100.61	108.36
2	D	28	LYS	CB-CG-CD	-5.42	98.84	111.30
1	C	162	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	269	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	C	192	LEU	CA-C-N	5.41	128.92	120.75
1	C	192	LEU	C-N-CA	5.41	128.92	120.75
1	C	204	GLU	CA-CB-CG	5.41	124.92	114.10
1	C	209	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	A	84	LYS	CA-C-O	5.41	128.24	120.51
1	C	53	THR	N-CA-C	5.41	116.86	111.07
2	B	5	ASN	O-C-N	-5.39	115.42	122.59
1	C	293	ILE	O-C-N	-5.39	116.64	121.87
2	D	48	LEU	CA-C-N	5.38	125.64	119.83
2	D	48	LEU	C-N-CA	5.38	125.64	119.83
2	B	133	ASP	CA-C-N	5.38	131.65	121.97
2	B	133	ASP	C-N-CA	5.38	131.65	121.97
2	D	105	ASN	CA-CB-CG	-5.37	107.23	112.60
1	C	108	GLN	CB-CG-CD	-5.36	103.50	112.60
2	B	66	LEU	N-CA-C	-5.35	100.52	109.24
1	A	251	ALA	O-C-N	-5.33	116.47	122.12
2	B	153	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	C	255	HIS	CA-CB-CG	-5.32	108.48	113.80
1	C	126	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	C	102	ILE	O-C-N	-5.32	116.88	123.10
2	D	106	VAL	CA-C-O	-5.31	113.79	120.86
2	B	40	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	C	282	HIS	CG-CD2-NE2	-5.31	101.89	107.20
1	C	281	PRO	N-CA-C	5.30	120.81	113.98
1	C	63	MET	N-CA-C	-5.29	105.59	111.36
2	B	76	LEU	CB-CA-C	-5.28	98.97	109.99
1	A	8	HIS	ND1-CG-CD2	5.27	111.37	106.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	C	145	ILE	N-CA-C	-5.26	105.41	110.72
1	C	289	ALA	N-CA-C	5.26	117.69	111.33
2	D	2	THR	N-CA-CB	-5.26	102.61	110.24
1	C	74	SER	N-CA-C	-5.26	99.88	108.76
1	C	269	ARG	CD-NE-CZ	5.25	131.75	124.40
1	C	207	ILE	CB-CG1-CD1	-5.25	102.78	113.80
1	A	305	ASN	CA-CB-CG	-5.24	107.36	112.60
1	C	160	VAL	O-C-N	-5.22	117.62	123.26
1	A	240	TYR	N-CA-C	-5.20	104.67	111.02
1	A	250	ARG	CB-CG-CD	5.20	123.27	111.30
1	A	248	VAL	N-CA-C	-5.20	101.14	109.20
1	C	308	LEU	CA-C-N	5.20	129.08	121.80
1	C	308	LEU	C-N-CA	5.20	129.08	121.80
1	C	180	ASP	N-CA-C	5.20	118.53	110.17
1	C	285	TYR	N-CA-C	5.18	117.83	111.82
1	A	10	ILE	CB-CG1-CD1	-5.18	102.92	113.80
2	B	10	GLU	N-CA-C	5.17	117.72	109.81
2	D	14	ARG	O-C-N	-5.17	116.96	123.27
2	D	113	ASN	OD1-CG-ND2	-5.16	117.44	122.60
2	D	5	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	A	103	VAL	CA-C-O	-5.14	115.06	120.57
1	A	77	ALA	N-CA-C	5.14	121.75	110.80
1	C	102	ILE	CB-CG1-CD1	-5.14	103.02	113.80
1	C	242	ASN	N-CA-CB	5.13	117.99	109.88
1	A	224	ILE	N-CA-CB	-5.13	104.28	111.25
2	B	3	HIS	CB-CG-CD2	-5.12	124.54	131.20
2	B	89	TYR	N-CA-C	5.12	119.38	113.38
2	B	137	LYS	CB-CA-C	-5.12	100.86	109.72
1	A	118	PHE	O-C-N	-5.11	116.34	122.27
1	C	218	VAL	CA-CB-CG2	-5.09	101.74	110.40
1	C	222	VAL	CB-CA-C	5.09	118.19	111.21
1	A	310	LEU	CA-CB-CG	5.09	134.12	116.30
2	D	132	ASN	OD1-CG-ND2	-5.08	117.53	122.60
2	B	8	GLN	N-CA-C	-5.07	99.99	110.80
1	C	275	THR	N-CA-CB	-5.07	101.93	110.49
2	D	58	LEU	O-C-N	-5.06	117.65	123.42
2	D	83	VAL	N-CA-C	-5.06	101.12	108.97
1	C	275	THR	CA-CB-CG2	5.05	119.09	110.50
2	D	3	HIS	CA-C-O	5.05	127.74	120.51
1	C	306	ARG	CB-CA-C	-5.05	102.73	110.81
1	C	32	ALA	CA-C-O	-5.04	115.16	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	98	SER	O-C-N	-5.04	117.31	123.10
1	A	84	LYS	CA-CB-CG	-5.03	104.04	114.10
1	A	288	GLN	N-CA-C	-5.03	105.69	111.07
2	D	2	THR	CA-C-N	5.03	131.15	121.54
2	D	2	THR	C-N-CA	5.03	131.15	121.54
2	D	21	ILE	CA-C-N	5.02	126.12	119.84
2	D	21	ILE	C-N-CA	5.02	126.12	119.84
2	B	67	SER	O-C-N	5.02	128.53	123.26
1	C	156	HIS	CA-CB-CG	5.02	118.82	113.80
1	C	243	VAL	N-CA-CB	-5.01	102.97	111.23
1	C	296	ARG	CB-CA-C	5.00	118.81	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
2	D	2	THR	Peptide,Mainchain
2	D	3	HIS	Sidechain

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	45	0
1	C	2415	0	2422	35	0
2	B	1196	0	1212	35	0
2	D	1196	0	1212	41	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	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	150	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 (150) 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:A:106:HIS:HD2	1:A:108:GLN:H	1.32	0.76
1:C:231:GLN:HB2	1:C:234:ARG:HG2	1.67	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
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:A:159:MET:HE3	1:A:169:VAL:HB	1.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:11:ALA:HA	4:B:999:CTP:N3	2.18	0.58
2:B:99:LEU:HD21	2:B:134:ILE:HD12	1.84	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
1:A:292:GLY:O	1:A:296:ARG:HG3	2.08	0.54
2:B:14:ARG:HA	2:B:86:ILE:O	2.07	0.54
1:C:261:MET:C	1:C:261:MET:SD	2.90	0.54
1:C:287:GLN:HE21	1:C:287:GLN:H	1.56	0.54
1:A:159:MET:HE1	1:A:173:THR:OG1	2.08	0.53
1:A:184:PHE:O	1:A:209:TRP:HA	2.08	0.53
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
1:C:174:GLN:HG2	1:C:201:MET:HE2	1.93	0.51
1:A:185:TYR:HD1	1:A:212:HIS:NE2	2.08	0.51
2:B:41:ARG:NE	2:D:49:PRO:HD3	2.25	0.51
2:B:27:PHE:HA	2:B:30:LEU:HD23	1.93	0.51
2:D:13:LYS:HB3	2:D:13:LYS:NZ	2.26	0.50
2:D:152:ALA:O	2:D:153:ASN:HB2	2.10	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:113:ARG:O	1:A:116:THR:HB	2.14	0.47
2:B:2:THR:HG22	2:B:11:ALA:HB3	1.96	0.47
1:A:189:PRO:CG	1:A:192:LEU:HD12	2.44	0.47
1:C:83:LYS:HA	1:C:83:LYS:NZ	2.29	0.47
1:A:163:LEU:HB3	1:A:194:MET:HE2	1.94	0.47
2:D:50:SER:O	2:D:54:GLY:N	2.47	0.47
1:A:163:LEU:HA	1:A:169:VAL:HG21	1.97	0.47
1:C:293:ILE:O	1:C:297:GLN:HG3	2.15	0.47
2:B:129:LYS:O	2:B:134:ILE:HD13	2.15	0.46
1:C:40:LYS:O	1:C:41:HIS:HB2	2.16	0.46
2:D:22:PRO:HG2	2:D:25:ILE:CG1	2.45	0.46
1:A:231:GLN:HE21	1:A:234:ARG:HH11	1.63	0.46
2:D:1:MET:N	2:D:6:LYS:HG3	2.29	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
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.32	0.45
2:B:1:MET:HB2	2:D:7:LEU:HG	1.99	0.45
2:D:77:TYR:CE1	2:D:151:LEU:HD11	2.51	0.45
1:A:287:GLN:HE21	1:A:287:GLN:H	1.64	0.45
1:A:4:LEU:HD23	1:A:7:LYS:HD3	1.97	0.45
1:A:194:MET:SD	1:A:195:PRO:HD2	2.57	0.45
1:A:160:VAL:HG22	1:A:187:ILE:HB	1.99	0.45
1:A:163:LEU:CD1	1:A:186:PHE:HB3	2.47	0.45
1:A:302:LEU:HD23	1:A:308:LEU:HD23	1.98	0.45
2:B:22:PRO:HB2	2:B:25:ILE:HG12	1.99	0.45
2:D:141:CYS:SG	2:D:143:LYS:HB2	2.57	0.44
1:A:272:GLU:H	1:A:272:GLU:CD	2.25	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
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.85	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:227:MET:HE3	1:A:227:MET:HB3	1.74	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:1:ALA:HB2	1:C:306:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:HG22	5:C:316:HOH:O	2.18	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:O	2:D:20:HIS:CD2	2.71	0.43
1:A:240:TYR:C	1:A:240:TYR:CD1	2.97	0.43
1:A:254:LEU:HD11	1:A:277:VAL:HG13	2.00	0.43
2:B:4:ASP:HA	2:B:10:GLU:CB	2.32	0.43
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.87	0.43
1:C:227:MET:HB3	1:C:227:MET:HE3	1.80	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:A:261:MET:C	1:A:261:MET:SD	3.02	0.42
2:B:118:ALA:C	2:B:119:GLU:HG2	2.44	0.42
1:C:186:PHE:HB2	1:C:211:LEU:HD12	2.00	0.42
2:D:1:MET:H2	2:D:6:LYS:HG3	1.85	0.41
2:B:12:ILE:HB	2:B:62:GLU:HG2	2.01	0.41
1:C:229:ARG:NH1	1:C:270:VAL:HG23	2.34	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
2:B:67:SER:HA	2:B:71:VAL:HG23	2.01	0.41
1:C:277:VAL:O	1:C:280:THR:HB	2.20	0.41
2:D:20:HIS:HB2	5:D:1009:HOH:O	2.21	0.41
1:C:151:ARG:HD2	1:C:153:ASP:O	2.20	0.41
2:D:21:ILE:HG22	2:D:25:ILE:HB	2.02	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
2:D:89:TYR:C	4:D:999:CTP:HN42	2.29	0.41
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:201:MET:HE3	1:C:201:MET:HB3	1.94	0.40
1:C:184:PHE:O	1:C:209:TRP:HA	2.21	0.40
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.85	0.40
1:A:248:VAL:HG12	1:A:272:GLU:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/310 (99%)	278 (90%)	24 (8%)	6 (2%)	6	11
1	C	308/310 (99%)	287 (93%)	15 (5%)	6 (2%)	6	11
2	B	151/153 (99%)	125 (83%)	15 (10%)	11 (7%)	1	1
2	D	151/153 (99%)	126 (83%)	12 (8%)	13 (9%)	0	0
All	All	918/926 (99%)	816 (89%)	66 (7%)	36 (4%)	2	3

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	231 (88%)	30 (12%)	5	11
1	C	261/261 (100%)	226 (87%)	35 (13%)	4	8
2	B	136/137 (99%)	116 (85%)	20 (15%)	3	6
2	D	136/137 (99%)	108 (79%)	28 (21%)	1	2
All	All	794/796 (100%)	681 (86%)	113 (14%)	3	7

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	GLN
1	A	65	ARG
1	A	69	SER
1	A	76	SER
1	A	81	LEU
1	A	113	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	VAL
1	A	151	ARG
1	A	167	ARG
1	A	210	SER
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	252	SER
1	A	269	ARG
1	A	272	GLU
1	A	275	THR
1	A	285	TYR
1	A	287	GLN
1	A	305	ASN
1	A	307	ASP
1	A	308	LEU
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	32	LEU
2	B	39	ASP
2	B	58	LEU
2	B	67	SER
2	B	69	ASP
2	B	73	GLN
2	B	76	LEU
2	B	86	ILE
2	B	88	ASN
2	B	106	VAL
2	B	112	SER
2	B	130	ARG
2	B	143	LYS
2	B	148	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	151	LEU
1	C	4	LEU
1	C	6	GLN
1	C	34	PRO
1	C	37	GLU
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	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	228	THR
1	C	232	LYS
1	C	243	VAL
1	C	246	GLN
1	C	256	ASN
1	C	269	ARG
1	C	271	ASP
1	C	285	TYR
1	C	287	GLN
1	C	296	ARG
1	C	305	ASN
1	C	308	LEU
1	C	310	LEU
2	D	1	MET
2	D	2	THR
2	D	3	HIS
2	D	5	ASN
2	D	7	LEU
2	D	10	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	12	ILE
2	D	13	LYS
2	D	16	THR
2	D	24	GLN
2	D	34	LYS
2	D	46	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	106	HIS
1	A	146	GLN
1	A	154	ASN
1	A	196	GLN
1	A	260	ASN
1	A	282	HIS
1	A	287	GLN
2	B	147	HIS
1	C	21	ASN
1	C	149	GLN
1	C	282	HIS
1	C	287	GLN
1	C	297	GLN
2	D	5	ASN
2	D	20	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	24	GLN
2	D	63	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CTP	D	999	-	29,30,30	2.29	9 (31%)	43,47,47	1.15	4 (9%)
4	CTP	B	999	-	29,30,30	2.23	7 (24%)	43,47,47	1.46	5 (11%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CTP	B	999	-	-	5/22/38/38	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	CTP	PB-O3B	6.38	1.66	1.59
4	D	999	CTP	PB-O3A	6.17	1.66	1.59
4	D	999	CTP	PB-O3B	6.01	1.66	1.59
4	D	999	CTP	PA-O3A	5.45	1.65	1.59
4	B	999	CTP	PB-O3A	5.42	1.65	1.59
4	B	999	CTP	PA-O3A	5.16	1.65	1.59
4	D	999	CTP	PG-O1G	2.79	1.59	1.50
4	B	999	CTP	C6-N1	-2.66	1.31	1.38
4	D	999	CTP	C5-C4	-2.36	1.37	1.42
4	D	999	CTP	C6-N1	-2.33	1.32	1.38
4	B	999	CTP	PG-O1G	2.30	1.57	1.50
4	B	999	CTP	PB-O1B	2.18	1.58	1.50
4	D	999	CTP	C2-N1	-2.15	1.35	1.40
4	D	999	CTP	PB-O1B	2.12	1.58	1.50
4	B	999	CTP	C5-C4	-2.10	1.38	1.42
4	D	999	CTP	PA-O1A	2.06	1.57	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	CTP	O2-C2-N3	-5.06	114.35	122.33
4	D	999	CTP	O2-C2-N3	-3.87	116.22	122.33
4	B	999	CTP	N1-C2-N3	3.13	124.23	118.80
4	B	999	CTP	C6-N1-C2	-2.99	115.42	120.46
4	D	999	CTP	C6-N1-C2	-2.36	116.47	120.46
4	B	999	CTP	C4'-O4'-C1'	-2.19	104.64	109.47
4	B	999	CTP	C5'-C4'-C3'	-2.15	107.49	115.21
4	D	999	CTP	N1-C2-N3	2.10	122.44	118.80
4	D	999	CTP	C3'-C2'-C1'	2.01	105.26	101.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

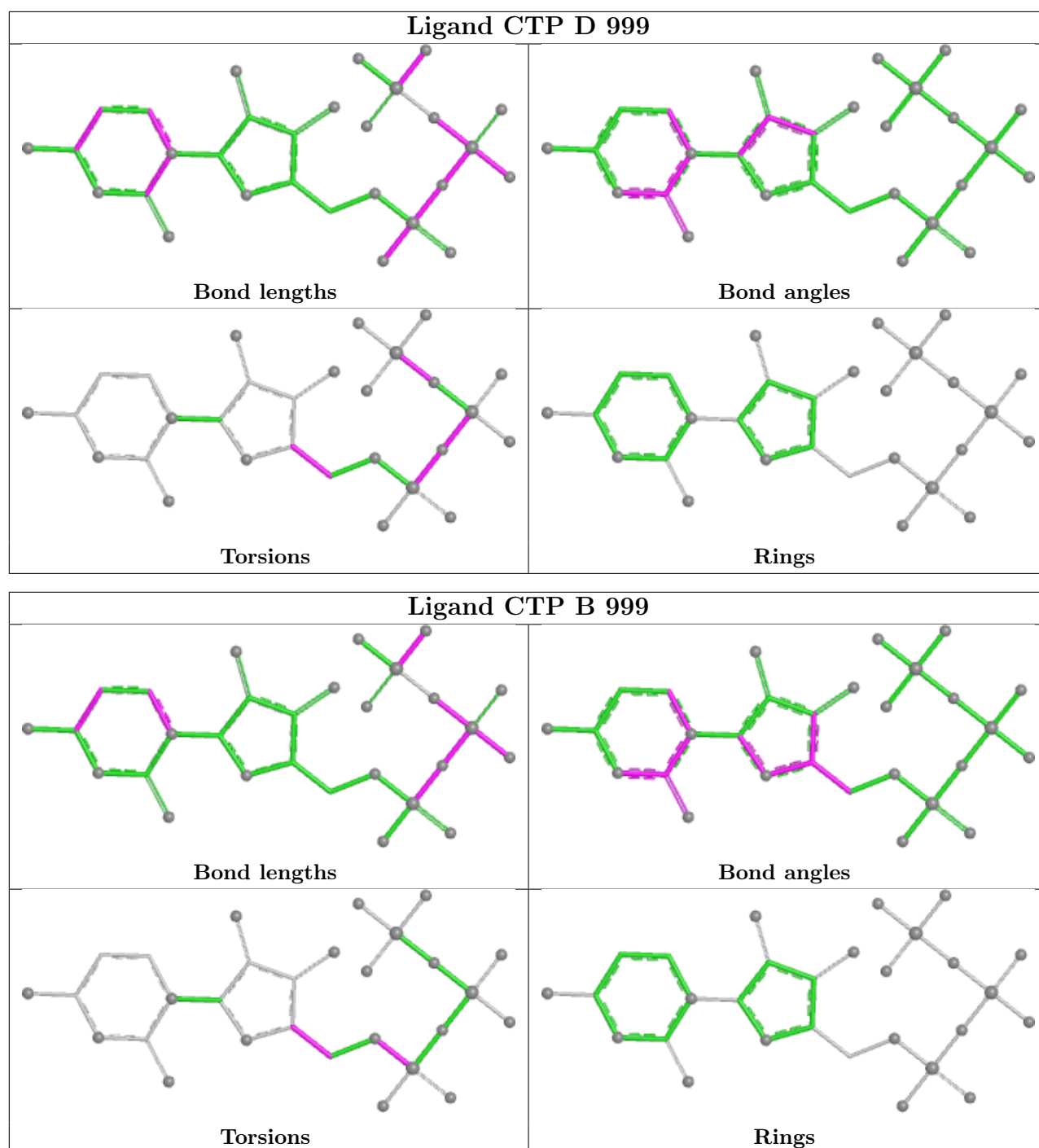
Mol	Chain	Res	Type	Atoms
4	B	999	CTP	C5'-O5'-PA-O2A
4	B	999	CTP	C5'-O5'-PA-O3A
4	D	999	CTP	PB-O3B-PG-O2G
4	B	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	O4'-C4'-C5'-O5'
4	D	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	PB-O3A-PA-O5'
4	D	999	CTP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	999	CTP	1	0
4	B	999	CTP	2	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.