



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:41 AM UTC

PDB ID : 1RAH / pdb_00001rah
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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

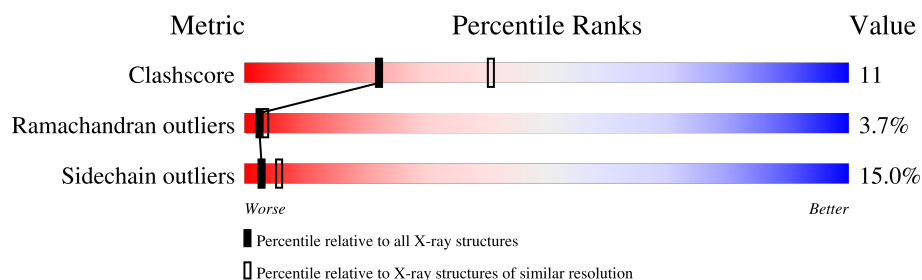
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



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

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

2 Entry composition

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

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

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

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

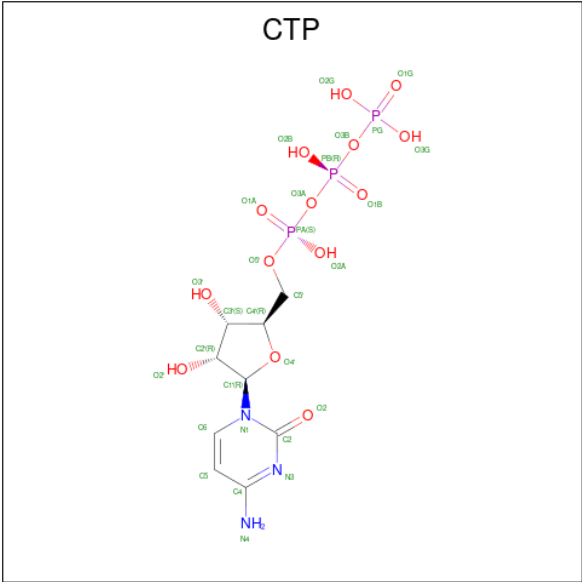
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

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

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

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

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



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

- Molecule 5 is water.

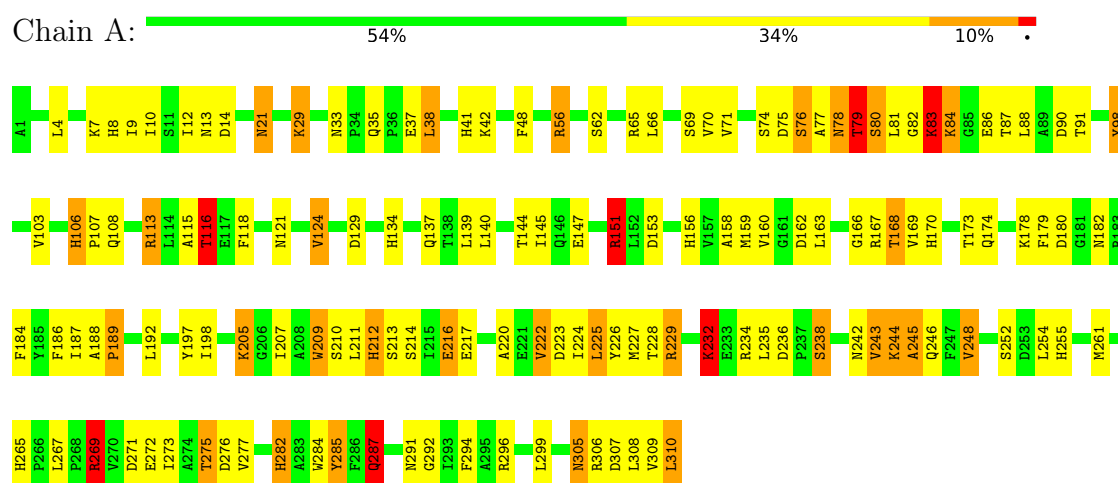
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	9	Total	O	0	0
			9	9		
5	C	44	Total	O	0	0
			44	44		
5	D	9	Total	O	0	0
			9	9		

3 Residue-property plots

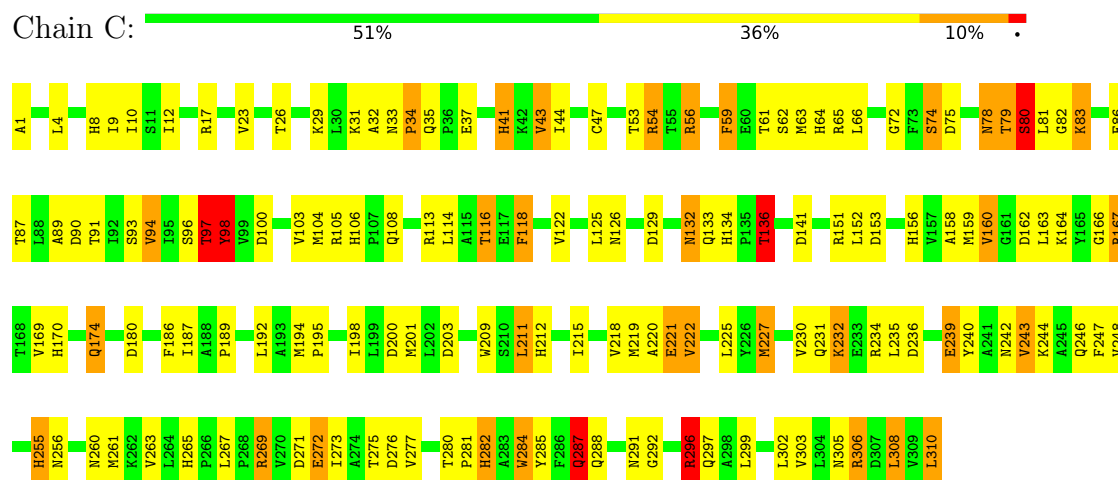
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Aspartate carbamoyltransferase catalytic chain

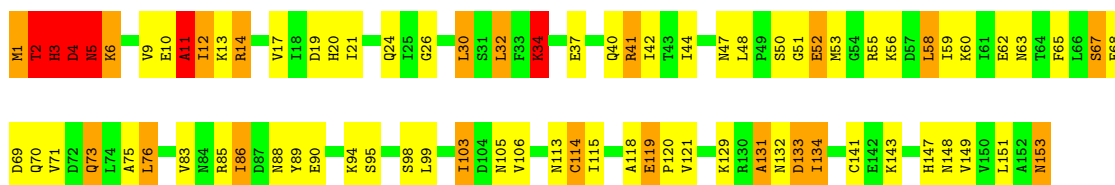


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

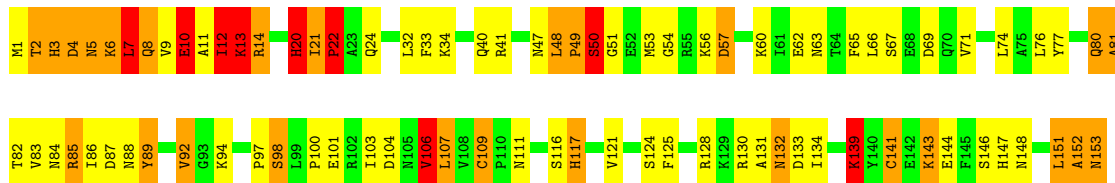


- Molecule 2: Aspartate carbamoyltransferase regulatory chain





• 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}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7375	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.28	19/2461 (0.8%)	2.12	100/3339 (3.0%)
1	C	1.34	18/2461 (0.7%)	2.21	131/3339 (3.9%)
2	B	1.17	5/1214 (0.4%)	2.20	50/1640 (3.0%)
2	D	1.28	8/1214 (0.7%)	2.20	59/1640 (3.6%)
All	All	1.29	50/7350 (0.7%)	2.18	340/9958 (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	2
All	All	0	8

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	VAL	CA-CB	12.50	1.67	1.54
2	D	141	CYS	CA-CB	-7.48	1.41	1.53
1	A	170	HIS	CD2-NE2	-6.97	1.30	1.37
1	A	56	ARG	CA-CB	-6.82	1.42	1.53
2	D	82	THR	CA-CB	6.81	1.63	1.53
1	C	8	HIS	CD2-NE2	-6.76	1.30	1.37
1	C	64	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.57	1.30	1.37
2	D	117	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	41	HIS	CD2-NE2	-6.52	1.30	1.37
1	C	41	HIS	CD2-NE2	-6.43	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	147	HIS	CG-ND1	-6.37	1.31	1.38
1	A	156	HIS	CD2-NE2	-6.32	1.30	1.37
2	B	2	THR	CA-CB	6.32	1.64	1.53
1	C	156	HIS	CD2-NE2	-6.31	1.30	1.37
1	C	8	HIS	CG-ND1	-6.30	1.31	1.38
1	C	212	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	170	HIS	CD2-NE2	-6.18	1.31	1.37
2	D	147	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	8	HIS	CG-ND1	-6.10	1.31	1.38
1	C	265	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	265	HIS	CD2-NE2	-6.01	1.31	1.37
2	B	147	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	134	HIS	CD2-NE2	-5.95	1.31	1.37
1	C	134	HIS	CG-ND1	-5.93	1.31	1.38
1	A	124	VAL	CA-CB	5.91	1.62	1.54
1	C	134	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	106	HIS	CG-ND1	-5.84	1.31	1.38
1	C	56	ARG	CA-CB	-5.81	1.44	1.53
1	C	34	PRO	CA-CB	-5.79	1.46	1.53
2	D	117	HIS	CG-ND1	-5.74	1.31	1.38
1	C	265	HIS	CG-ND1	-5.67	1.32	1.38
2	D	20	HIS	CD2-NE2	-5.64	1.31	1.37
1	C	156	HIS	CG-ND1	-5.64	1.32	1.38
1	A	69	SER	CA-CB	-5.63	1.44	1.53
1	C	108	GLN	CA-CB	-5.62	1.44	1.53
1	A	255	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	41	HIS	CG-ND1	-5.57	1.32	1.38
1	C	255	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	282	HIS	CD2-NE2	-5.52	1.31	1.37
1	C	106	HIS	CG-ND1	-5.50	1.32	1.38
1	C	106	HIS	CD2-NE2	-5.49	1.31	1.37
2	B	20	HIS	CD2-NE2	-5.45	1.31	1.37
2	B	3	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	212	HIS	CD2-NE2	-5.40	1.31	1.37
1	A	265	HIS	CG-ND1	-5.40	1.32	1.38
2	B	70	GLN	CA-CB	-5.23	1.45	1.53
1	A	134	HIS	CG-ND1	-5.15	1.32	1.38
1	A	33	ASN	CA-CB	5.11	1.60	1.53
1	A	212	HIS	CG-ND1	-5.05	1.32	1.38

All (340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	GLN	OE1-CD-NE2	-12.04	110.56	122.60
2	D	2	THR	N-CA-C	11.70	131.20	107.69
2	B	53	MET	N-CA-C	-11.38	100.11	114.56
2	D	3	HIS	CA-CB-CG	-11.21	102.59	113.80
1	C	33	ASN	OD1-CG-ND2	-10.78	111.82	122.60
2	D	5	ASN	CA-CB-CG	10.42	123.02	112.60
1	A	291	ASN	OD1-CG-ND2	-10.32	112.28	122.60
1	A	276	ASP	CA-CB-CG	10.21	122.81	112.60
1	A	21	ASN	OD1-CG-ND2	-10.19	112.41	122.60
2	B	133	ASP	N-CA-C	10.10	132.31	110.80
1	A	14	ASP	CA-CB-CG	10.00	122.60	112.60
1	C	75	ASP	CA-CB-CG	9.93	122.53	112.60
1	C	297	GLN	OE1-CD-NE2	-9.82	112.78	122.60
2	B	4	ASP	CA-CB-CG	9.71	122.31	112.60
2	D	141	CYS	CB-CA-C	-9.64	94.73	110.74
2	D	21	ILE	N-CA-C	-9.28	100.65	108.63
2	B	11	ALA	N-CA-C	9.13	130.24	110.80
1	C	141	ASP	CA-CB-CG	9.09	121.69	112.60
1	A	79	THR	N-CA-C	9.07	130.11	110.80
1	C	26	THR	CA-CB-OG1	-8.92	96.22	109.60
1	A	80	SER	N-CA-C	8.78	129.49	110.80
1	C	54	ARG	CA-CB-CG	8.77	131.64	114.10
1	C	97	THR	N-CA-CB	-8.75	95.03	110.42
2	B	75	ALA	CA-C-O	-8.64	111.39	120.55
2	D	147	HIS	ND1-CG-CD2	8.62	114.72	106.10
1	C	287	GLN	CG-CD-NE2	8.49	129.13	116.40
1	C	33	ASN	CA-C-N	8.48	128.54	119.89
1	C	33	ASN	C-N-CA	8.48	128.54	119.89
1	C	90	ASP	N-CA-C	8.39	121.48	111.33
2	B	52	GLU	N-CA-C	8.39	128.66	110.80
2	B	119	GLU	N-CA-C	8.38	121.62	108.55
1	C	93	SER	N-CA-C	-8.36	102.12	111.82
1	A	75	ASP	CA-CB-CG	8.36	120.96	112.60
2	B	75	ALA	N-CA-C	8.34	120.37	111.28
1	A	41	HIS	ND1-CG-CD2	8.31	114.41	106.10
1	C	275	THR	CA-CB-OG1	-8.27	97.20	109.60
2	B	67	SER	N-CA-C	8.18	121.15	108.96
1	A	84	LYS	N-CA-C	-8.14	93.46	110.80
1	A	134	HIS	ND1-CG-CD2	8.06	114.16	106.10
1	A	265	HIS	ND1-CG-CD2	7.95	114.05	106.10
1	C	80	SER	N-CA-C	7.95	127.73	110.80
1	C	305	ASN	N-CA-C	7.94	121.68	108.73
2	D	89	TYR	N-CA-C	7.92	127.67	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	HIS	ND1-CG-CD2	7.88	113.98	106.10
1	A	62	SER	CA-CB-OG	-7.86	95.38	111.10
1	A	182	ASN	OD1-CG-ND2	-7.84	114.76	122.60
1	C	66	LEU	N-CA-C	-7.76	102.00	112.94
2	B	5	ASN	CA-CB-CG	7.74	120.34	112.60
1	C	33	ASN	CB-CG-ND2	7.68	127.92	116.40
1	C	272	GLU	N-CA-C	7.67	122.31	112.34
1	C	129	ASP	CA-CB-CG	7.52	120.12	112.60
2	D	33	PHE	CA-CB-CG	-7.49	106.31	113.80
1	C	273	ILE	N-CA-C	-7.49	96.69	107.77
2	B	131	ALA	N-CA-C	7.46	126.70	110.80
2	D	141	CYS	CA-CB-SG	7.38	131.37	114.40
2	D	2	THR	CA-C-O	7.35	129.83	120.57
1	C	244	LYS	N-CA-C	-7.25	104.24	113.23
1	C	62	SER	CA-CB-OG	7.25	125.60	111.10
2	D	67	SER	N-CA-C	7.25	120.43	109.41
1	C	276	ASP	CA-CB-CG	7.25	119.85	112.60
2	B	21	ILE	N-CA-C	-7.24	102.40	108.63
1	C	63	MET	N-CA-C	-7.21	103.50	111.36
2	D	21	ILE	CA-C-N	7.20	128.84	119.84
2	D	21	ILE	C-N-CA	7.20	128.84	119.84
1	C	255	HIS	CB-CA-C	-7.17	98.94	110.84
1	C	269	ARG	N-CA-C	-7.13	97.98	109.96
2	D	133	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	42	LYS	CA-CB-CG	-7.12	99.87	114.10
1	A	69	SER	CA-CB-OG	-7.08	96.94	111.10
1	A	82	GLY	N-CA-C	-7.01	106.74	115.08
1	A	134	HIS	CB-CG-CD2	-6.99	122.11	131.20
1	A	33	ASN	OD1-CG-ND2	-6.98	115.62	122.60
2	B	134	ILE	N-CA-C	6.97	123.84	109.34
2	D	106	VAL	N-CA-CB	-6.93	103.31	111.83
1	C	100	ASP	CA-CB-CG	6.91	119.51	112.60
2	D	63	ASN	OD1-CG-ND2	-6.90	115.70	122.60
2	B	132	ASN	CA-C-N	6.90	134.72	121.54
2	B	132	ASN	C-N-CA	6.90	134.72	121.54
2	B	133	ASP	CA-CB-CG	6.90	119.50	112.60
2	B	47	ASN	CA-CB-CG	6.86	119.46	112.60
2	B	119	GLU	CA-C-N	6.84	128.39	119.84
2	B	119	GLU	C-N-CA	6.84	128.39	119.84
1	A	291	ASN	CB-CG-ND2	6.83	126.64	116.40
1	C	160	VAL	N-CA-CB	-6.80	102.02	111.41
1	A	116	THR	N-CA-CB	-6.79	99.41	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	109	CYS	CA-C-N	6.78	126.48	119.56
2	D	109	CYS	C-N-CA	6.78	126.48	119.56
1	C	78	ASN	N-CA-C	6.77	125.23	110.80
1	A	33	ASN	CA-CB-CG	6.77	119.37	112.60
1	A	42	LYS	CG-CD-CE	-6.75	95.77	111.30
2	D	88	ASN	N-CA-C	-6.75	95.75	107.49
1	A	232	LYS	N-CA-C	6.74	120.95	112.87
1	C	98	TYR	N-CA-C	6.73	124.12	114.16
1	C	232	LYS	N-CA-C	6.73	120.94	112.87
1	C	26	THR	CA-CB-CG2	6.73	121.94	110.50
2	B	149	VAL	CA-C-O	-6.72	113.72	120.85
1	A	269	ARG	CA-CB-CG	6.69	127.48	114.10
1	A	243	VAL	N-CA-C	6.68	123.23	109.34
1	C	134	HIS	ND1-CG-CD2	6.67	112.77	106.10
1	A	134	HIS	CA-CB-CG	6.67	120.47	113.80
1	C	72	GLY	CA-C-O	-6.66	114.96	121.75
1	A	129	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	162	ASP	CA-CB-CG	6.63	119.23	112.60
1	C	87	THR	O-C-N	-6.63	115.23	122.79
1	A	134	HIS	CG-CD2-NE2	-6.62	100.58	107.20
2	D	3	HIS	CA-C-N	6.59	134.12	121.54
2	D	3	HIS	C-N-CA	6.59	134.12	121.54
1	C	116	THR	N-CA-CB	-6.58	99.74	110.14
2	D	11	ALA	N-CA-C	-6.58	98.96	109.76
1	C	174	GLN	CA-CB-CG	-6.58	100.95	114.10
1	A	56	ARG	NE-CZ-NH2	-6.56	113.30	119.20
2	D	134	ILE	N-CA-CB	-6.55	103.20	111.46
1	A	265	HIS	CG-CD2-NE2	-6.54	100.67	107.20
1	A	116	THR	CA-CB-OG1	-6.50	99.84	109.60
1	A	255	HIS	CA-CB-CG	6.50	120.30	113.80
1	C	10	ILE	N-CA-C	-6.47	106.00	111.56
1	A	87	THR	N-CA-C	6.45	119.04	110.53
1	C	288	GLN	N-CA-C	-6.45	103.87	111.03
1	A	234	ARG	CA-CB-CG	6.44	126.97	114.10
1	C	32	ALA	CA-C-O	-6.44	113.66	120.55
2	D	50	SER	CA-CB-OG	-6.43	98.24	111.10
1	C	61	THR	N-CA-C	-6.40	104.38	111.36
1	A	76	SER	N-CA-C	-6.39	99.48	109.25
1	C	230	VAL	N-CA-C	-6.39	99.16	108.87
1	A	306	ARG	N-CA-C	6.38	118.24	111.28
1	A	77	ALA	N-CA-C	6.38	119.97	111.30
1	C	94	VAL	O-C-N	-6.35	113.64	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	22	PRO	N-CA-C	6.33	125.51	112.47
1	C	126	ASN	OD1-CG-ND2	-6.32	116.28	122.60
2	B	63	ASN	CB-CG-ND2	6.31	125.87	116.40
1	A	78	ASN	CA-C-N	6.30	133.57	121.54
1	A	78	ASN	C-N-CA	6.30	133.57	121.54
1	C	227	MET	O-C-N	-6.29	116.01	123.06
1	C	200	ASP	CA-CB-CG	6.25	118.85	112.60
2	B	63	ASN	OD1-CG-ND2	-6.24	116.36	122.60
2	D	94	LYS	N-CA-C	-6.24	99.54	109.59
1	C	291	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	C	74	SER	N-CA-C	-6.22	99.25	109.40
1	C	56	ARG	CG-CD-NE	-6.22	98.31	112.00
2	B	88	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	C	284	TRP	CB-CG-CD1	-6.22	117.58	126.90
1	A	197	TYR	CA-CB-CG	6.21	125.08	113.90
2	D	9	VAL	CA-C-O	6.21	128.19	121.36
1	C	23	VAL	N-CA-C	-6.21	104.29	110.62
2	D	92	VAL	N-CA-C	-6.20	104.28	113.39
2	D	128	ARG	CB-CG-CD	-6.19	97.07	111.30
1	A	168	THR	O-C-N	-6.17	115.71	122.07
2	D	6	LYS	N-CA-C	6.17	118.93	111.40
1	C	122	VAL	N-CA-C	-6.17	101.53	107.76
1	C	136	THR	N-CA-CB	-6.17	100.15	110.39
1	C	43	VAL	N-CA-C	-6.12	99.54	108.11
1	C	297	GLN	CG-CD-NE2	6.11	125.57	116.40
1	C	159	MET	CG-SD-CE	-6.10	87.48	100.90
2	B	5	ASN	O-C-N	-6.09	114.48	122.59
2	B	75	ALA	O-C-N	-6.09	115.66	122.12
1	A	224	ILE	N-CA-CB	-6.08	103.80	111.46
1	C	108	GLN	CB-CG-CD	-6.07	102.27	112.60
2	B	149	VAL	O-C-N	-6.07	115.58	121.83
1	C	106	HIS	ND1-CG-CD2	6.07	112.17	106.10
2	B	37	GLU	CA-CB-CG	-6.06	101.98	114.10
1	A	271	ASP	CA-CB-CG	6.05	118.66	112.60
2	B	103	ILE	CB-CA-C	-6.01	104.42	111.09
1	C	247	PHE	N-CA-C	-6.01	98.01	110.80
1	A	189	PRO	CA-C-O	-6.00	114.97	121.27
1	C	82	GLY	N-CA-C	-5.98	106.98	115.30
2	D	147	HIS	CG-CD2-NE2	-5.96	101.24	107.20
2	B	13	LYS	O-C-N	5.92	130.26	123.27
2	B	50	SER	O-C-N	5.92	129.62	122.75
1	C	222	VAL	CA-CB-CG1	5.92	120.46	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	HIS	ND1-CG-CD2	5.90	112.00	106.10
1	A	107	PRO	N-CA-CB	5.88	109.08	103.19
2	D	13	LYS	CA-C-O	-5.87	114.85	120.90
1	C	255	HIS	ND1-CG-CD2	5.85	111.95	106.10
1	C	134	HIS	CA-C-N	5.83	125.96	119.32
1	C	134	HIS	C-N-CA	5.83	125.96	119.32
1	C	106	HIS	CA-C-N	5.83	125.69	119.28
1	C	106	HIS	C-N-CA	5.83	125.69	119.28
1	C	162	ASP	N-CA-C	-5.83	98.24	108.20
1	A	41	HIS	CG-CD2-NE2	-5.82	101.38	107.20
1	C	284	TRP	CG-CD2-CE3	5.82	139.72	133.90
1	C	242	ASN	O-C-N	5.82	130.36	122.57
1	A	70	VAL	CA-C-O	-5.79	114.12	120.43
2	D	51	GLY	N-CA-C	-5.79	105.77	112.83
2	B	6	LYS	N-CA-C	5.79	120.46	113.17
1	C	103	VAL	N-CA-C	-5.75	100.13	108.36
2	B	3	HIS	CA-CB-CG	5.75	119.55	113.80
1	A	269	ARG	CG-CD-NE	-5.75	99.36	112.00
2	B	52	GLU	CA-C-O	5.74	128.71	120.51
1	A	245	ALA	N-CA-C	-5.73	98.59	110.80
2	D	117	HIS	N-CA-C	5.73	118.47	111.82
1	C	281	PRO	N-CA-C	5.73	121.38	113.98
1	C	275	THR	CA-CB-CG2	5.73	120.24	110.50
1	A	10	ILE	CB-CG1-CD1	-5.72	101.79	113.80
1	A	174	GLN	CA-CB-CG	-5.72	102.67	114.10
1	A	38	LEU	O-C-N	-5.71	116.07	122.12
1	A	118	PHE	O-C-N	-5.68	116.09	122.34
1	A	275	THR	CA-CB-OG1	-5.68	101.07	109.60
1	C	132	ASN	O-C-N	-5.65	115.08	122.59
1	C	8	HIS	CG-CD2-NE2	-5.65	101.55	107.20
2	D	12	ILE	CB-CG1-CD1	-5.65	101.94	113.80
1	A	305	ASN	CA-CB-CG	-5.64	106.96	112.60
1	C	47	CYS	O-C-N	-5.64	116.16	122.93
1	C	136	THR	CB-CA-C	5.63	122.08	110.31
2	D	144	GLU	CA-CB-CG	-5.63	102.84	114.10
1	A	74	SER	O-C-N	-5.61	114.99	122.74
1	A	174	GLN	OE1-CD-NE2	-5.61	116.99	122.60
2	B	121	VAL	N-CA-C	-5.60	100.22	108.85
2	B	13	LYS	CA-CB-CG	5.60	125.30	114.10
1	C	97	THR	CB-CA-C	5.60	121.13	110.27
1	C	221	GLU	N-CA-CB	-5.60	102.21	110.49
2	B	105	ASN	N-CA-C	5.59	122.71	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	TYR	N-CA-C	5.59	118.14	111.71
2	D	9	VAL	O-C-N	5.59	128.55	122.63
1	C	222	VAL	N-CA-CB	-5.58	101.94	110.86
1	A	216	GLU	CA-CB-CG	5.57	125.25	114.10
1	A	91	THR	N-CA-C	-5.57	105.13	111.14
2	D	40	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	269	ARG	NE-CZ-NH1	5.55	127.06	121.50
1	A	222	VAL	N-CA-C	5.55	117.57	108.97
1	C	220	ALA	N-CA-C	5.54	118.08	111.71
1	C	108	GLN	CA-CB-CG	-5.54	103.02	114.10
2	D	3	HIS	N-CA-C	-5.54	98.78	109.24
2	B	32	LEU	N-CA-C	5.53	117.31	111.28
1	A	198	ILE	N-CA-C	-5.52	105.14	110.72
1	C	167	ARG	CB-CG-CD	-5.51	98.62	111.30
2	B	106	VAL	N-CA-CB	-5.51	99.27	111.50
1	A	121	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	236	ASP	N-CA-C	-5.50	103.14	110.07
2	B	34	LYS	CA-CB-CG	5.50	125.09	114.10
2	D	152	ALA	CA-C-N	5.49	131.58	121.70
2	D	152	ALA	C-N-CA	5.49	131.58	121.70
2	D	83	VAL	N-CA-C	-5.47	102.00	109.55
1	A	287	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	C	282	HIS	CG-CD2-NE2	-5.46	101.74	107.20
1	C	105	ARG	CG-CD-NE	-5.45	100.00	112.00
2	D	69	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	79	THR	N-CA-CB	-5.45	101.28	110.49
1	C	239	GLU	N-CA-C	-5.44	104.89	112.45
1	C	160	VAL	O-C-N	-5.44	117.39	123.26
1	A	83	LYS	N-CA-C	5.44	122.38	110.80
1	A	115	ALA	CA-C-N	5.42	128.30	120.38
1	A	115	ALA	C-N-CA	5.42	128.30	120.38
1	C	104	MET	N-CA-C	5.42	118.27	109.06
1	A	224	ILE	O-C-N	-5.41	116.77	123.10
1	C	260	ASN	CA-CB-CG	5.40	118.00	112.60
2	B	56	LYS	CG-CD-CE	-5.40	98.88	111.30
1	C	236	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	306	ARG	CB-CA-C	-5.39	102.18	110.81
2	B	12	ILE	CA-C-N	-5.39	115.50	123.05
2	B	12	ILE	C-N-CA	-5.39	115.50	123.05
2	D	152	ALA	O-C-N	5.39	127.83	122.12
1	C	35	GLN	CA-C-N	5.39	126.43	120.45
1	C	35	GLN	C-N-CA	5.39	126.43	120.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	VAL	CA-C-N	5.39	131.02	122.94
1	C	263	VAL	C-N-CA	5.39	131.02	122.94
1	A	147	GLU	O-C-N	-5.38	115.65	122.27
2	B	73	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	C	134	HIS	CG-CD2-NE2	-5.37	101.83	107.20
2	D	5	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	C	242	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	246	GLN	N-CA-C	5.35	122.19	110.80
1	C	41	HIS	ND1-CG-CD2	5.35	111.45	106.10
1	A	248	VAL	N-CA-C	-5.33	100.68	108.99
2	B	65	PHE	N-CA-C	-5.32	99.61	108.34
1	C	209	TRP	CE2-CD2-CG	-5.32	100.82	107.20
2	B	70	GLN	CA-CB-CG	-5.31	103.47	114.10
1	A	37	GLU	CA-CB-CG	-5.30	103.50	114.10
1	A	116	THR	CA-CB-CG2	5.29	119.50	110.50
1	A	174	GLN	CG-CD-NE2	5.28	124.32	116.40
2	D	57	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	267	LEU	O-C-N	-5.27	115.26	121.32
1	C	56	ARG	CB-CG-CD	-5.27	99.19	111.30
1	A	220	ALA	N-CA-C	5.26	117.09	111.36
1	C	97	THR	OG1-CB-CG2	5.25	119.80	109.30
1	A	10	ILE	N-CA-C	5.24	116.52	112.12
1	C	158	ALA	CA-C-O	-5.24	114.98	120.80
1	C	255	HIS	CA-C-N	-5.24	114.13	122.66
1	C	255	HIS	C-N-CA	-5.24	114.13	122.66
1	A	103	VAL	N-CA-C	-5.23	100.88	108.36
2	D	148	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	C	180	ASP	N-CA-C	5.22	118.25	109.95
1	C	78	ASN	CA-CB-CG	5.21	117.81	112.60
2	D	94	LYS	CB-CG-CD	-5.21	99.32	111.30
2	D	98	SER	O-C-N	-5.21	117.11	123.10
1	C	53	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	225	LEU	O-C-N	-5.21	116.57	123.13
1	C	203	ASP	CB-CA-C	-5.21	102.71	110.88
2	D	148	ASN	N-CA-C	-5.20	105.69	111.36
1	A	209	TRP	CG-CD1-NE1	-5.19	103.45	110.20
1	C	136	THR	N-CA-C	-5.18	106.21	112.54
2	B	113	ASN	N-CA-C	-5.17	106.66	113.17
1	C	31	LYS	N-CA-C	-5.17	105.73	111.36
1	A	106	HIS	CA-C-N	5.17	125.85	120.12
1	A	106	HIS	C-N-CA	5.17	125.85	120.12
1	C	275	THR	N-CA-CB	-5.16	101.76	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	ILE	N-CA-CB	-5.16	100.56	110.78
2	D	139	LYS	CA-CB-CG	5.15	124.39	114.10
2	D	40	GLN	CB-CG-CD	5.15	121.35	112.60
1	A	83	LYS	CA-C-N	5.14	131.36	121.54
1	A	83	LYS	C-N-CA	5.14	131.36	121.54
1	A	151	ARG	CG-CD-NE	-5.14	100.69	112.00
1	C	222	VAL	CA-CB-CG2	-5.13	101.67	110.40
1	C	280	THR	CA-C-N	5.13	124.85	119.82
1	C	280	THR	C-N-CA	5.13	124.85	119.82
1	C	180	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	71	VAL	O-C-N	-5.12	117.49	122.97
2	D	51	GLY	CA-C-N	5.12	128.80	120.60
2	D	51	GLY	C-N-CA	5.12	128.80	120.60
1	A	144	THR	CA-CB-OG1	-5.12	101.92	109.60
2	D	7	LEU	N-CA-C	5.12	121.70	110.80
2	B	134	ILE	CB-CA-C	-5.11	102.91	111.29
1	C	96	SER	CA-C-O	5.10	125.67	119.05
1	A	98	TYR	N-CA-C	-5.09	107.13	113.55
1	C	209	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	A	178	LYS	CB-CG-CD	5.09	123.00	111.30
1	C	134	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	C	284	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	C	248	VAL	CG1-CB-CG2	-5.08	99.63	110.80
1	C	277	VAL	N-CA-C	-5.07	105.60	110.72
1	A	90	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	296	ARG	N-CA-CB	-5.07	102.72	110.07
2	B	113	ASN	CA-C-O	-5.07	113.42	119.35
1	A	229	ARG	O-C-N	-5.06	117.12	123.04
1	A	209	TRP	CE2-CD2-CG	-5.06	101.13	107.20
2	D	81	ALA	N-CA-C	-5.05	101.16	109.40
1	A	134	HIS	O-C-N	-5.04	117.51	121.19
1	A	145	ILE	CA-C-N	5.04	127.30	120.44
1	A	145	ILE	C-N-CA	5.04	127.30	120.44
2	D	84	ASN	CA-CB-CG	5.04	117.64	112.60
1	C	56	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	C	54	ARG	N-CA-C	-5.03	104.88	111.02
1	C	141	ASP	N-CA-C	-5.03	105.71	111.14
2	D	132	ASN	OD1-CG-ND2	-5.03	117.58	122.60
1	A	144	THR	CA-CB-CG2	5.02	119.03	110.50
1	C	212	HIS	N-CA-C	-5.02	101.75	109.52
1	C	97	THR	CA-CB-OG1	-5.01	102.09	109.60
2	D	82	THR	N-CA-C	-5.01	100.25	108.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	88	LEU	N-CA-C	-5.00	105.74	111.14
1	C	296	ARG	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	TYR	Sidechain
1	A	294	PHE	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
2	D	20	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	46	0
1	C	2415	0	2422	47	0
2	B	1196	0	1212	34	0
2	D	1196	0	1212	38	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	1	0
5	C	44	0	0	5	0
5	D	9	0	0	1	0
All	All	7375	0	7292	155	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 11.

All (155) 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	1.19	1.01
2:B:6:LYS:HB3	2:D:10:GLU:HG3	1.47	0.97
2:B:76:LEU:HD11	2:B:103:ILE:HD11	1.61	0.83
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.63	0.81
2:B:4:ASP:HA	2:B:10:GLU:HB2	1.65	0.77
2:B:114:CYS:HB2	2:B:141:CYS:HB3	1.67	0.76
1:A:106:HIS:HD2	1:A:108:GLN:H	1.33	0.74
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.70	0.74
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.69	0.73
1:A:83:LYS:HB3	1:A:86:GLU:HB3	1.70	0.72
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.71	0.71
2:B:2:THR:HG22	2:B:10:GLU:HB3	1.74	0.70
2:D:20:HIS:HB2	5:D:1008:HOH:O	1.94	0.67
2:D:116:SER:HA	2:D:121:VAL:HG11	1.75	0.66
1:C:29:LYS:HD3	1:C:310:LEU:HD22	1.77	0.65
1:C:292:GLY:O	1:C:296:ARG:HB2	1.96	0.65
1:A:151:ARG:HD2	1:A:153:ASP:O	1.97	0.65
1:C:113:ARG:O	1:C:116:THR:HB	1.98	0.64
2:D:65:PHE:HB3	2:D:85:ARG:HH22	1.61	0.64
1:C:94:VAL:O	1:C:97:THR:HB	1.98	0.64
2:B:12:ILE:HB	2:B:62:GLU:HG2	1.80	0.63
1:A:261:MET:O	1:A:282:HIS:HD2	1.81	0.63
2:B:6:LYS:HE2	2:D:41:ARG:HD2	1.81	0.63
2:D:14:ARG:HB3	2:D:87:ASP:HA	1.80	0.62
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.14	0.62
1:A:187:ILE:HG13	1:A:212:HIS:HB2	1.81	0.61
2:D:32:LEU:HD22	2:D:106:VAL:HG13	1.80	0.61
1:C:136:THR:HG23	1:C:296:ARG:NH1	2.03	0.61
2:B:41:ARG:HD3	2:D:48:LEU:HA	1.83	0.60
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.03	0.60
2:D:65:PHE:HB3	2:D:85:ARG:NH2	2.17	0.60
2:D:22:PRO:HG3	2:D:80:GLN:OE1	2.03	0.59
1:A:153:ASP:HB3	1:A:180:ASP:O	2.03	0.59
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.37	0.59
2:D:20:HIS:HA	2:D:56:LYS:HD2	1.85	0.58
2:B:48:LEU:O	2:B:55:ARG:HA	2.03	0.58
2:B:6:LYS:HZ2	2:D:12:ILE:HG12	1.69	0.58
2:D:81:ALA:O	2:D:97:PRO:HD2	2.03	0.57
1:C:235:LEU:HB3	1:C:239:GLU:HB3	1.86	0.57
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:HIS:HB2	5:C:322:HOH:O	2.04	0.57
1:A:159:MET:HE1	1:A:173:THR:OG1	2.05	0.56
2:B:11:ALA:HA	4:B:999:CTP:N3	2.20	0.56
1:A:159:MET:HE3	1:A:169:VAL:HB	1.88	0.55
2:B:41:ARG:NE	2:D:49:PRO:HD3	2.20	0.55
1:A:214:SER:O	1:A:217:GLU:HG2	2.06	0.55
1:C:163:LEU:HD13	1:C:194:MET:HE2	1.88	0.55
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.06	0.55
1:C:302:LEU:HD23	1:C:308:LEU:HD13	1.89	0.55
1:A:292:GLY:O	1:A:296:ARG:HG3	2.07	0.54
2:D:12:ILE:HG21	2:D:62:GLU:HB3	1.89	0.54
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.22	0.54
1:C:9:ILE:HG21	1:C:299:LEU:HD21	1.91	0.53
1:A:227:MET:HG3	1:A:273:ILE:HD11	1.91	0.53
1:A:29:LYS:HE2	1:A:310:LEU:HD23	1.91	0.52
1:A:38:LEU:HD23	1:A:66:LEU:HD22	1.91	0.52
1:C:97:THR:HG22	1:C:98:TYR:HD2	1.72	0.52
1:A:184:PHE:O	1:A:209:TRP:HA	2.11	0.51
1:C:231:GLN:HB2	1:C:234:ARG:HG2	1.91	0.51
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.92	0.51
1:A:287:GLN:NE2	1:A:287:GLN:H	2.09	0.51
1:A:160:VAL:HG22	1:A:187:ILE:HB	1.93	0.50
1:A:106:HIS:CD2	1:A:108:GLN:H	2.20	0.50
2:D:141:CYS:HB2	2:D:143:LYS:H	1.74	0.50
2:B:14:ARG:HA	2:B:86:ILE:O	2.12	0.50
1:C:261:MET:O	1:C:282:HIS:HD2	1.95	0.49
2:B:42:ILE:HA	2:B:60:LYS:O	2.13	0.49
2:B:4:ASP:HB2	2:D:8:GLN:C	2.38	0.48
1:C:86:GLU:HA	5:C:329:HOH:O	2.13	0.48
2:B:94:LYS:HE2	4:B:999:CTP:O2G	2.13	0.48
1:A:287:GLN:H	1:A:287:GLN:HE21	1.61	0.47
2:B:5:ASN:O	2:B:9:VAL:HA	2.13	0.47
1:C:83:LYS:HA	1:C:83:LYS:NZ	2.29	0.47
1:C:189:PRO:HG2	1:C:192:LEU:HD12	1.96	0.47
2:D:151:LEU:HA	2:D:151:LEU:HD13	1.71	0.47
1:C:227:MET:HE3	1:C:227:MET:HB3	1.75	0.47
2:D:124:SER:HB3	2:D:139:LYS:HG2	1.97	0.47
1:A:232:LYS:HA	1:A:235:LEU:HD12	1.97	0.47
1:A:29:LYS:HE2	1:A:310:LEU:CD2	2.45	0.47
1:C:174:GLN:HG2	1:C:201:MET:HE2	1.96	0.47
1:C:80:SER:O	1:C:83:LYS:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:O	1:A:261:MET:HA	2.15	0.46
2:B:4:ASP:HA	2:B:10:GLU:CB	2.41	0.46
1:C:59:PHE:CE2	1:C:136:THR:HG21	2.50	0.46
2:B:4:ASP:HA	2:B:10:GLU:H	1.80	0.46
1:C:186:PHE:HB2	1:C:211:LEU:HD12	1.97	0.46
1:C:1:ALA:HB2	1:C:306:ARG:NH2	2.31	0.46
2:D:10:GLU:O	2:D:60:LYS:HE2	2.16	0.46
2:B:1:MET:HA	2:D:7:LEU:HG	1.98	0.46
2:B:44:ILE:HG23	2:B:59:ILE:HG12	1.98	0.45
1:C:287:GLN:HE21	1:C:287:GLN:H	1.64	0.45
1:A:248:VAL:HG12	1:A:272:GLU:HA	1.99	0.45
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.80	0.45
1:C:287:GLN:NE2	1:C:287:GLN:H	2.14	0.45
1:A:261:MET:O	1:A:282:HIS:CD2	2.67	0.45
2:D:111:ASN:O	2:D:117:HIS:CE1	2.69	0.45
2:B:4:ASP:HA	2:B:10:GLU:N	2.32	0.45
1:C:160:VAL:HG22	1:C:187:ILE:HB	1.98	0.45
2:B:26:GLY:O	2:B:30:LEU:HD22	2.17	0.45
1:C:215:ILE:HG22	1:C:219:MET:HE2	1.99	0.45
1:A:113:ARG:O	1:A:116:THR:HB	2.17	0.44
1:C:59:PHE:CE1	1:C:296:ARG:HG3	2.52	0.44
1:C:41:HIS:HB2	5:C:320:HOH:O	2.16	0.44
1:A:205:LYS:HB3	1:A:207:ILE:HG13	1.99	0.44
2:D:12:ILE:HD11	2:D:60:LYS:HB3	1.98	0.44
1:A:21:ASN:HD21	1:A:179:PHE:HE1	1.65	0.44
1:A:163:LEU:HG	1:A:188:ALA:HB2	1.98	0.44
1:C:43:VAL:C	1:C:44:ILE:HG13	2.42	0.44
1:C:164:LYS:HA	1:C:195:PRO:HD3	2.00	0.44
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.17	0.44
1:A:137:GLN:HG2	1:A:168:THR:HG22	2.00	0.43
1:C:232:LYS:HA	1:C:240:TYR:CD2	2.53	0.43
2:D:1:MET:N	2:D:6:LYS:HE3	2.33	0.43
2:D:50:SER:O	2:D:54:GLY:N	2.51	0.43
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.81	0.43
1:A:4:LEU:O	1:A:7:LYS:HB2	2.19	0.43
2:B:41:ARG:HG2	2:D:47:ASN:O	2.19	0.43
1:C:194:MET:SD	1:C:198:ILE:HG21	2.58	0.43
2:B:24:GLN:HA	5:B:1003:HOH:O	2.16	0.43
1:A:254:LEU:HD11	1:A:277:VAL:HG13	2.00	0.43
1:A:238:SER:O	1:A:242:ASN:HB2	2.19	0.43
1:C:1:ALA:HA	1:C:306:ARG:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:GLY:O	1:C:169:VAL:HG22	2.18	0.43
2:D:13:LYS:O	2:D:86:ILE:HG22	2.18	0.43
2:B:71:VAL:HG13	2:B:83:VAL:HG21	2.01	0.42
1:A:232:LYS:HE3	1:A:232:LYS:H	1.84	0.42
2:B:1:MET:HB3	2:D:7:LEU:HG	2.01	0.42
1:C:136:THR:HG22	5:C:317:HOH:O	2.19	0.42
2:D:20:HIS:O	2:D:20:HIS:CG	2.73	0.42
1:C:17:ARG:NH1	5:C:341:HOH:O	2.52	0.42
1:A:158:ALA:HB2	1:A:222:VAL:HG21	2.02	0.42
2:B:41:ARG:CZ	2:D:49:PRO:HD3	2.49	0.42
1:C:261:MET:C	1:C:261:MET:SD	3.03	0.42
2:D:106:VAL:O	2:D:107:LEU:HG	2.20	0.42
1:A:166:GLY:O	1:A:169:VAL:HG22	2.19	0.42
2:D:77:TYR:CE1	2:D:151:LEU:HD11	2.55	0.42
2:D:152:ALA:O	2:D:153:ASN:HB2	2.20	0.42
2:B:1:MET:N	2:B:89:TYR:OH	2.52	0.41
1:A:189:PRO:HG2	1:A:192:LEU:HD12	2.01	0.41
2:B:3:HIS:ND1	2:B:3:HIS:N	2.69	0.41
1:A:163:LEU:CD1	1:A:186:PHE:HB3	2.50	0.41
1:A:244:LYS:HB3	1:A:245:ALA:H	1.75	0.41
2:D:10:GLU:H	2:D:10:GLU:CD	2.27	0.41
2:B:118:ALA:C	2:B:119:GLU:HG2	2.44	0.41
1:C:81:LEU:HD21	1:C:91:THR:HG21	2.01	0.41
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.81	0.41
2:D:71:VAL:HA	2:D:74:LEU:HD12	2.02	0.41
1:C:79:THR:O	1:C:81:LEU:N	2.53	0.41
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.99	0.41
2:B:19:ASP:OD1	2:B:58:LEU:HD12	2.19	0.41
1:C:272:GLU:H	1:C:272:GLU:CD	2.29	0.40
1:A:140:LEU:HD22	1:A:292:GLY:HA2	2.02	0.40
1:C:89:ALA:HB1	1:C:118:PHE:CE1	2.56	0.40
1:A:9:ILE:HG21	1:A:299:LEU:HD21	2.04	0.40
1:A:267:LEU:HD23	1:A:269:ARG:HB3	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%)	280 (91%)	22 (7%)	6 (2%)	6	11
1	C	308/310 (99%)	283 (92%)	22 (7%)	3 (1%)	12	24
2	B	151/153 (99%)	123 (82%)	15 (10%)	13 (9%)	0	0
2	D	151/153 (99%)	124 (82%)	15 (10%)	12 (8%)	1	0
All	All	918/926 (99%)	810 (88%)	74 (8%)	34 (4%)	2	3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	83	LYS
1	A	84	LYS
2	B	3	HIS
2	B	11	ALA
2	B	68	GLU
2	B	131	ALA
2	B	133	ASP
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	8	GLN
2	D	24	GLN
2	D	89	TYR
2	B	4	ASP
1	C	78	ASN
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	52	GLU
2	B	129	LYS
2	D	22	PRO
2	D	131	ALA
1	A	79	THR
1	A	243	VAL
1	A	244	LYS
2	B	14	ARG
2	B	51	GLY
2	B	120	PRO
2	D	53	MET
2	B	34	LYS

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%)	228 (87%)	33 (13%)	4	9
1	C	261/261 (100%)	226 (87%)	35 (13%)	4	8
2	B	136/137 (99%)	111 (82%)	25 (18%)	1	3
2	D	136/137 (99%)	110 (81%)	26 (19%)	1	3
All	All	794/796 (100%)	675 (85%)	119 (15%)	3	6

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	29	LYS
1	A	35	GLN
1	A	56	ARG
1	A	65	ARG
1	A	76	SER
1	A	78	ASN
1	A	79	THR
1	A	81	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	113	ARG
1	A	116	THR
1	A	124	VAL
1	A	151	ARG
1	A	167	ARG
1	A	205	LYS
1	A	210	SER
1	A	211	LEU
1	A	213	SER
1	A	216	GLU
1	A	225	LEU
1	A	228	THR
1	A	229	ARG
1	A	232	LYS
1	A	238	SER
1	A	252	SER
1	A	269	ARG
1	A	275	THR
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	32	LEU
2	B	34	LYS
2	B	40	GLN
2	B	41	ARG
2	B	58	LEU
2	B	67	SER
2	B	69	ASP
2	B	73	GLN
2	B	76	LEU
2	B	85	ARG
2	B	86	ILE
2	B	90	GLU
2	B	95	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	98	SER
2	B	99	LEU
2	B	114	CYS
2	B	143	LYS
2	B	148	ASN
2	B	151	LEU
2	B	153	ASN
1	C	4	LEU
1	C	12	ILE
1	C	34	PRO
1	C	37	GLU
1	C	54	ARG
1	C	56	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	114	LEU
1	C	125	LEU
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	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	303	VAL
1	C	308	LEU
1	C	310	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	3	HIS
2	D	4	ASP
2	D	7	LEU
2	D	10	GLU
2	D	12	ILE
2	D	13	LYS
2	D	14	ARG
2	D	34	LYS
2	D	48	LEU
2	D	49	PRO
2	D	50	SER
2	D	66	LEU
2	D	80	GLN
2	D	85	ARG
2	D	92	VAL
2	D	98	SER
2	D	100	PRO
2	D	101	GLU
2	D	104	ASP
2	D	106	VAL
2	D	130	ARG
2	D	139	LYS
2	D	143	LYS
2	D	146	SER
2	D	151	LEU
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	106	HIS
1	A	282	HIS
1	A	287	GLN
2	B	147	HIS
1	C	21	ASN
1	C	149	GLN
1	C	256	ASN
1	C	260	ASN
1	C	282	HIS
1	C	287	GLN
2	D	5	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	63	ASN
2	D	73	GLN
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	B	999	-	29,30,30	2.31	8 (27%)	43,47,47	1.39	6 (13%)
4	CTP	D	999	-	29,30,30	2.13	7 (24%)	43,47,47	1.18	4 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CTP	D	999	-	-	3/22/38/38	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	CTP	PB-O3B	6.08	1.66	1.59
4	B	999	CTP	PA-O3A	5.81	1.65	1.59
4	B	999	CTP	PB-O3A	5.67	1.65	1.59
4	D	999	CTP	PB-O3B	5.59	1.65	1.59
4	D	999	CTP	PB-O3A	5.54	1.65	1.59
4	D	999	CTP	PA-O3A	4.92	1.64	1.59
4	D	999	CTP	PG-O1G	2.82	1.59	1.50
4	B	999	CTP	C6-N1	-2.62	1.31	1.38
4	B	999	CTP	PG-O1G	2.49	1.58	1.50
4	B	999	CTP	PB-O1B	2.29	1.58	1.50
4	B	999	CTP	C2-N1	-2.23	1.35	1.40
4	B	999	CTP	C5-C4	-2.21	1.37	1.42
4	D	999	CTP	C5-C4	-2.21	1.37	1.42
4	D	999	CTP	PB-O1B	2.17	1.58	1.50
4	D	999	CTP	C6-N1	-2.14	1.33	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	CTP	O2-C2-N3	-4.76	114.83	122.33
4	D	999	CTP	O2-C2-N3	-4.07	115.92	122.33
4	B	999	CTP	N1-C2-N3	2.58	123.27	118.80
4	D	999	CTP	C6-N1-C2	-2.54	116.17	120.46
4	B	999	CTP	C6-N1-C2	-2.43	116.35	120.46
4	B	999	CTP	C4'-O4'-C1'	-2.28	104.42	109.47
4	B	999	CTP	C5'-C4'-C3'	-2.26	107.07	115.21
4	D	999	CTP	N1-C2-N3	2.15	122.53	118.80
4	B	999	CTP	O4'-C1'-N1	2.14	113.21	108.36
4	D	999	CTP	O4'-C1'-N1	2.08	113.07	108.36

There are no chirality outliers.

All (8) 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...

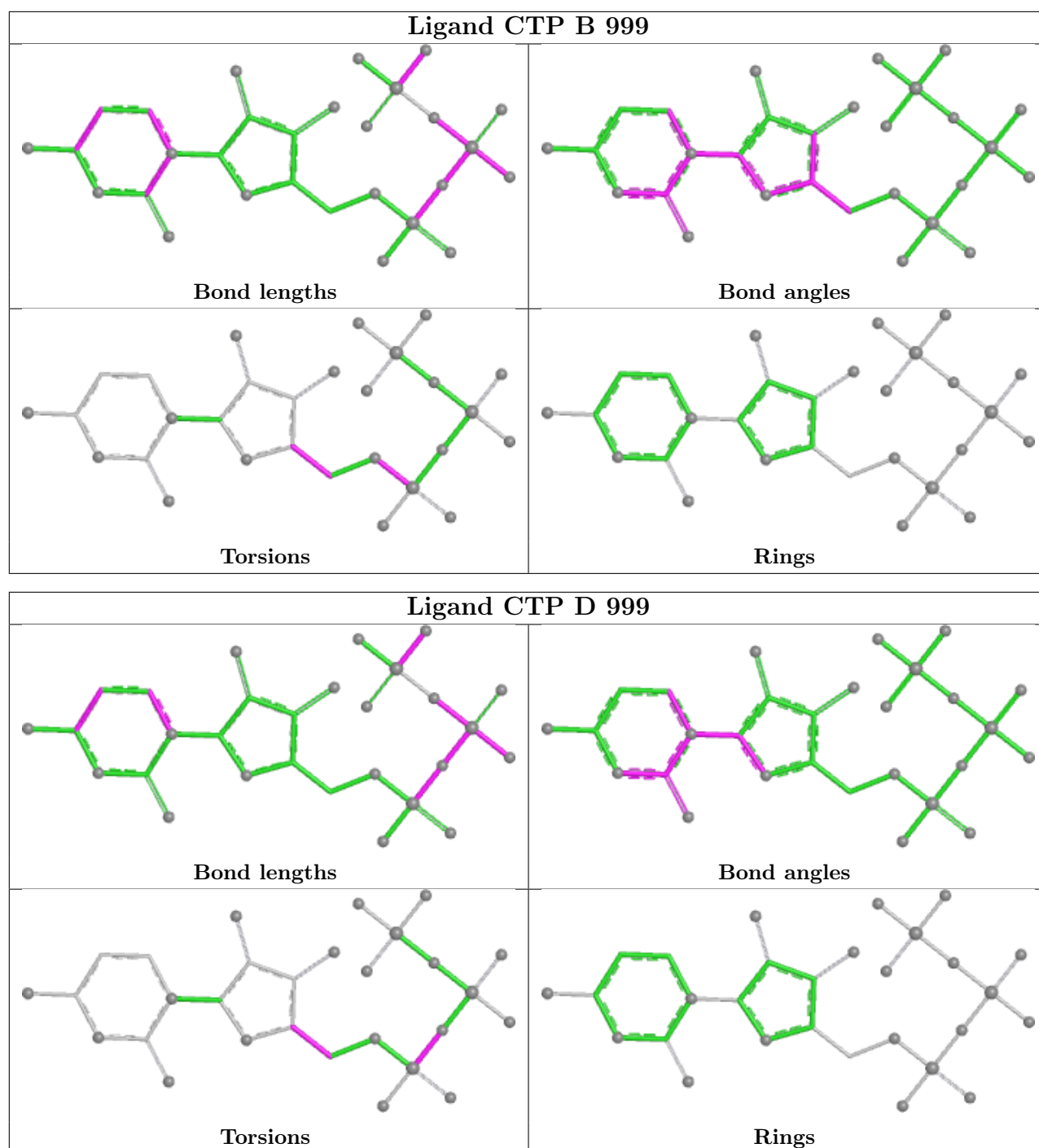
Mol	Chain	Res	Type	Atoms
4	B	999	CTP	C5'-O5'-PA-O2A
4	B	999	CTP	C5'-O5'-PA-O3A
4	B	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	O4'-C4'-C5'-O5'
4	D	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	PB-O3A-PA-O5'

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

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.