



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:38 AM UTC

PDB ID : 1RAB / pdb_00001rab
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

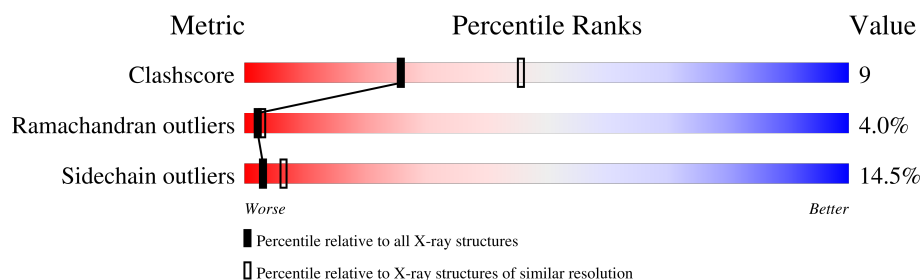
1 Overall quality at a glance

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	56% 31% 12% .
1	C	310	52% 35% 13% .
2	B	153	44% 36% 15% 5%
2	D	153	41% 42% 13% 5%

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			

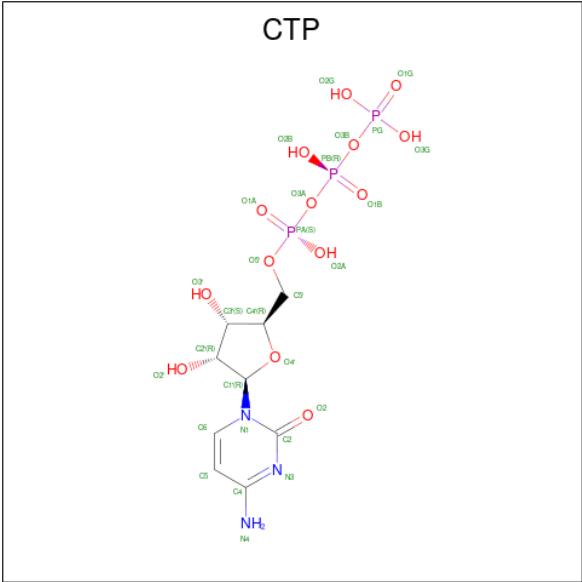
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

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.

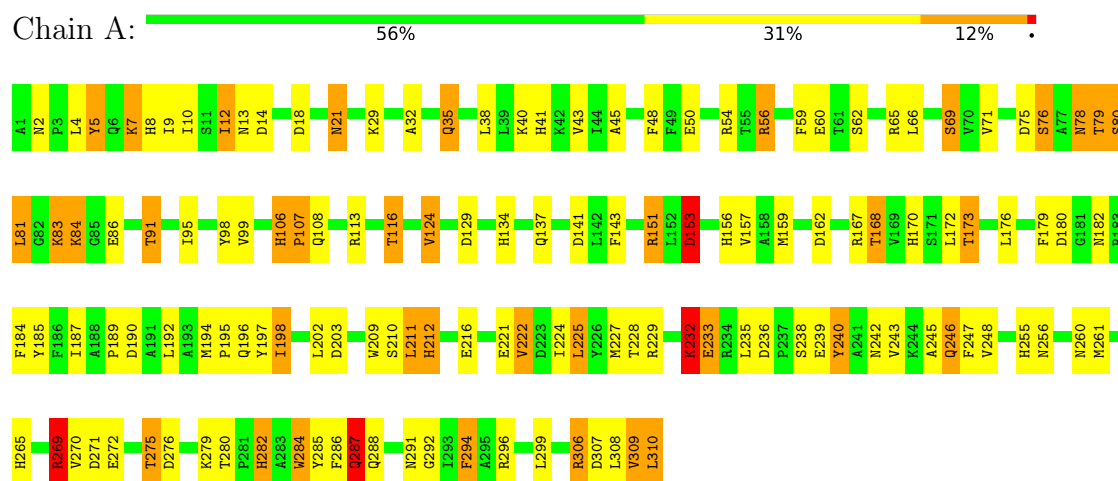
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	11	Total	O	0	0
			11	11		
5	C	43	Total	O	0	0
			43	43		
5	D	9	Total	O	0	0
			9	9		

3 Residue-property plots [i](#)

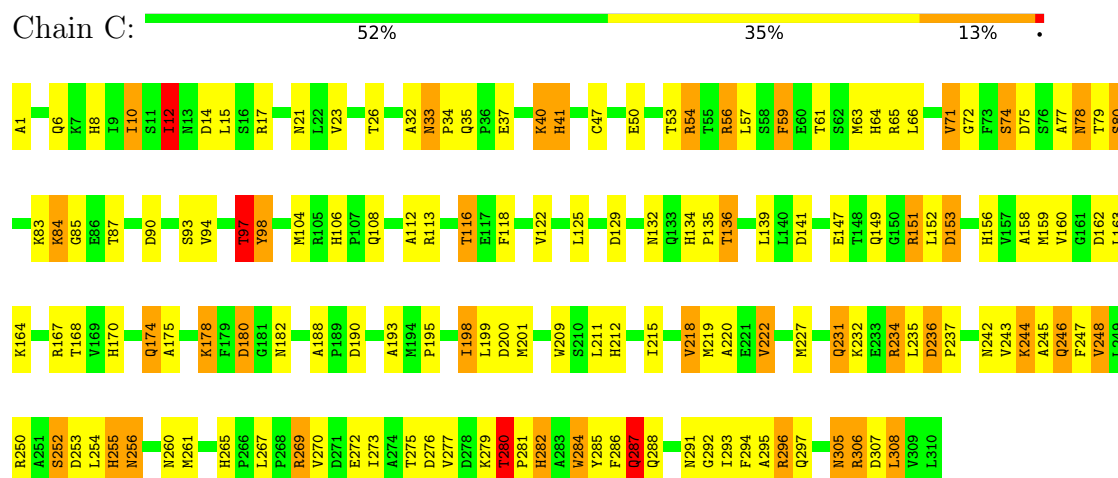
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

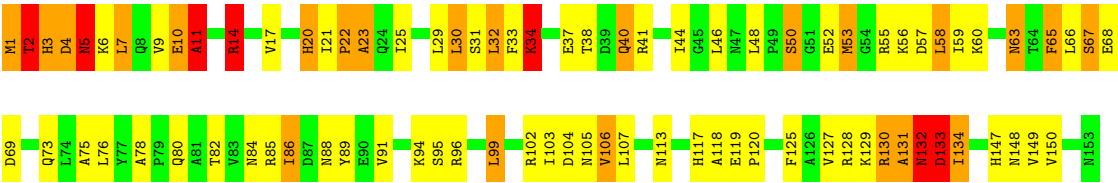


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

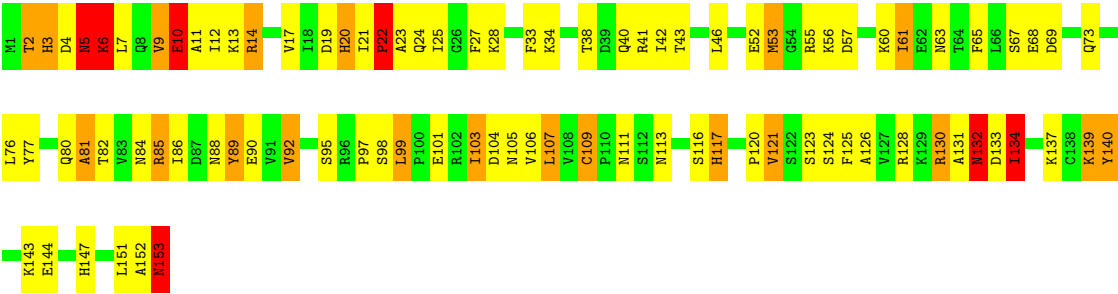


- Molecule 2: Aspartate carbamoyltransferase regulatory chain





• 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}	0.190 , (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	1.32	17/2461 (0.7%)	2.17	95/3339 (2.8%)
1	C	1.38	23/2461 (0.9%)	2.27	138/3339 (4.1%)
2	B	1.17	5/1214 (0.4%)	2.15	53/1640 (3.2%)
2	D	1.23	9/1214 (0.7%)	2.24	71/1640 (4.3%)
All	All	1.30	54/7350 (0.7%)	2.21	357/9958 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	C	0	3
2	B	0	3
2	D	0	1
All	All	0	14

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	VAL	CA-CB	9.15	1.64	1.54
1	C	212	HIS	CD2-NE2	-7.40	1.29	1.37
1	C	134	HIS	CD2-NE2	-7.32	1.29	1.37
1	A	56	ARG	CA-CB	-7.23	1.42	1.53
1	C	56	ARG	CA-CB	-7.20	1.42	1.53
1	A	106	HIS	CD2-NE2	-7.08	1.30	1.37
2	B	2	THR	CA-CB	7.05	1.65	1.53
1	A	265	HIS	CD2-NE2	-7.01	1.30	1.37
1	C	170	HIS	CD2-NE2	-6.74	1.30	1.37
1	C	106	HIS	CD2-NE2	-6.74	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	82	THR	CA-CB	6.69	1.62	1.53
1	A	170	HIS	CD2-NE2	-6.69	1.30	1.37
2	D	147	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	265	HIS	CG-ND1	-6.63	1.30	1.38
1	C	41	HIS	CD2-NE2	-6.63	1.30	1.37
1	C	134	HIS	CG-ND1	-6.53	1.31	1.38
1	C	156	HIS	CD2-NE2	-6.49	1.30	1.37
2	B	147	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	41	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.10	1.31	1.37
1	C	64	HIS	CD2-NE2	-6.09	1.31	1.37
2	B	3	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	124	VAL	CA-CB	5.93	1.62	1.54
1	C	8	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	8	HIS	CG-ND1	-5.92	1.31	1.38
1	C	282	HIS	CD2-NE2	-5.89	1.31	1.37
1	C	35	GLN	CA-CB	-5.89	1.45	1.53
1	A	156	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	134	HIS	CG-ND1	-5.76	1.31	1.38
2	D	120	PRO	CA-CB	-5.76	1.49	1.53
1	C	170	HIS	CG-ND1	-5.75	1.31	1.38
2	D	147	HIS	CG-ND1	-5.71	1.31	1.38
1	C	106	HIS	CG-ND1	-5.69	1.31	1.38
1	C	265	HIS	CG-ND1	-5.66	1.32	1.38
2	D	117	HIS	CD2-NE2	-5.64	1.31	1.37
1	C	8	HIS	CG-ND1	-5.58	1.32	1.38
2	D	20	HIS	CD2-NE2	-5.54	1.31	1.37
1	C	112	ALA	CA-CB	-5.53	1.44	1.53
1	A	212	HIS	CD2-NE2	-5.47	1.31	1.37
1	C	147	GLU	CD-OE1	5.47	1.35	1.25
1	A	59	PHE	CA-C	-5.44	1.46	1.52
1	A	282	HIS	CD2-NE2	-5.41	1.31	1.37
2	D	117	HIS	CG-ND1	-5.36	1.32	1.38
1	A	8	HIS	CD2-NE2	-5.36	1.31	1.37
1	C	212	HIS	CG-ND1	-5.36	1.32	1.38
1	C	282	HIS	CG-ND1	-5.33	1.32	1.38
1	C	156	HIS	CG-ND1	-5.31	1.32	1.38
1	A	106	HIS	CG-ND1	-5.30	1.32	1.38
2	B	20	HIS	CD2-NE2	-5.28	1.32	1.37
1	C	149	GLN	CD-NE2	-5.23	1.22	1.33
2	B	117	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	255	HIS	CD2-NE2	-5.04	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	HIS	CD2-NE2	-5.02	1.32	1.37
2	D	28	LYS	CA-CB	-5.01	1.45	1.53

All (357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	HIS	CA-CB-CG	-15.18	98.62	113.80
1	C	287	GLN	OE1-CD-NE2	-13.81	108.79	122.60
1	C	33	ASN	OD1-CG-ND2	-12.38	110.22	122.60
1	A	14	ASP	CA-CB-CG	12.22	124.83	112.60
2	B	133	ASP	N-CA-C	11.85	136.04	110.80
2	D	3	HIS	CA-CB-CG	-11.74	102.06	113.80
1	C	287	GLN	CG-CD-NE2	11.25	133.27	116.40
1	A	153	ASP	CA-CB-CG	11.07	123.67	112.60
1	C	33	ASN	CB-CG-ND2	10.93	132.79	116.40
1	A	276	ASP	CA-CB-CG	10.70	123.30	112.60
1	C	297	GLN	OE1-CD-NE2	-10.44	112.16	122.60
1	A	80	SER	N-CA-C	10.05	132.21	110.80
2	B	11	ALA	N-CA-C	9.78	131.64	110.80
1	C	280	THR	N-CA-CB	-9.47	96.43	109.88
1	C	247	PHE	N-CA-C	-9.38	96.69	109.54
2	D	9	VAL	O-C-N	9.33	132.78	122.61
2	D	2	THR	CA-C-O	9.32	131.83	121.39
1	A	21	ASN	OD1-CG-ND2	-9.17	113.43	122.60
1	A	306	ARG	N-CA-C	9.09	120.79	111.07
1	A	91	THR	N-CA-C	-9.06	101.37	111.07
2	D	147	HIS	ND1-CG-CD2	9.03	115.13	106.10
1	A	245	ALA	N-CA-C	-8.93	99.75	111.71
1	C	255	HIS	N-CA-C	8.90	120.98	111.28
1	A	307	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	35	GLN	CA-C-N	8.80	128.44	119.82
1	A	35	GLN	C-N-CA	8.80	128.44	119.82
1	C	134	HIS	ND1-CG-CD2	8.80	114.90	106.10
1	A	75	ASP	CA-CB-CG	8.71	121.31	112.60
1	A	256	ASN	CA-CB-CG	8.60	121.20	112.60
1	C	129	ASP	CA-CB-CG	8.59	121.19	112.60
1	A	271	ASP	CA-CB-CG	8.55	121.15	112.60
1	A	84	LYS	N-CA-C	-8.49	92.73	110.80
1	C	90	ASP	N-CA-C	8.43	121.40	111.71
2	D	67	SER	N-CA-C	8.40	122.18	109.41
1	A	134	HIS	ND1-CG-CD2	8.34	114.44	106.10
1	C	122	VAL	N-CA-C	-8.26	99.42	107.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASP	CA-CB-CG	8.25	120.85	112.60
1	C	97	THR	N-CA-CB	-8.18	96.08	110.39
2	B	67	SER	N-CA-C	8.17	120.53	108.60
1	C	75	ASP	CA-CB-CG	8.17	120.77	112.60
1	C	26	THR	CA-CB-OG1	-8.04	97.53	109.60
2	B	88	ASN	CA-CB-CG	8.04	120.64	112.60
1	C	141	ASP	CA-CB-CG	7.90	120.50	112.60
1	C	222	VAL	N-CA-CB	-7.89	101.53	110.99
1	C	33	ASN	CA-C-N	7.84	127.89	119.89
1	C	33	ASN	C-N-CA	7.84	127.89	119.89
1	C	280	THR	CB-CA-C	7.84	120.92	109.09
1	A	269	ARG	NE-CZ-NH1	7.80	129.30	121.50
1	C	87	THR	O-C-N	-7.74	113.97	122.79
1	A	224	ILE	O-C-N	-7.72	115.08	123.18
1	C	59	PHE	N-CA-C	-7.70	102.82	111.14
1	C	106	HIS	ND1-CG-CD2	7.68	113.78	106.10
1	C	280	THR	CA-C-N	7.65	127.36	119.56
1	C	280	THR	C-N-CA	7.65	127.36	119.56
1	A	129	ASP	CA-CB-CG	7.64	120.24	112.60
1	C	8	HIS	ND1-CG-CD2	7.61	113.71	106.10
1	C	72	GLY	CA-C-O	-7.61	114.07	121.83
2	D	69	ASP	CA-CB-CG	7.55	120.16	112.60
1	A	141	ASP	CA-CB-CG	7.54	120.14	112.60
1	C	10	ILE	CA-C-O	-7.54	113.21	120.30
1	A	29	LYS	CB-CG-CD	-7.52	94.01	111.30
2	D	89	TYR	N-CA-C	7.46	126.70	110.80
1	A	307	ASP	N-CA-C	-7.45	96.12	108.34
1	A	41	HIS	ND1-CG-CD2	7.45	113.55	106.10
2	B	20	HIS	CA-CB-CG	-7.42	106.38	113.80
2	B	80	GLN	N-CA-C	-7.42	95.03	108.02
1	C	106	HIS	O-C-N	-7.41	116.67	121.85
2	D	117	HIS	N-CA-C	7.39	119.34	111.28
1	C	218	VAL	N-CA-CB	-7.39	103.54	112.33
2	D	9	VAL	N-CA-CB	7.37	121.63	110.13
1	C	170	HIS	N-CA-C	-7.36	103.34	111.36
1	C	198	ILE	N-CA-C	-7.35	103.69	110.82
2	D	11	ALA	N-CA-C	-7.31	98.06	109.25
2	D	3	HIS	N-CA-C	-7.30	98.52	109.83
1	A	265	HIS	ND1-CG-CD2	7.27	113.37	106.10
2	D	92	VAL	N-CA-C	-7.25	105.58	111.81
1	A	107	PRO	N-CA-CB	7.19	110.17	103.41
1	C	167	ARG	CB-CG-CD	-7.15	94.85	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	VAL	N-CA-CB	-7.06	95.48	111.87
1	C	116	THR	N-CA-CB	-7.04	99.02	110.14
1	C	291	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	A	76	SER	N-CA-C	-6.96	97.86	109.07
1	C	61	THR	N-CA-C	-6.95	103.78	111.36
2	B	134	ILE	N-CA-C	6.95	123.79	109.34
2	D	40	GLN	OE1-CD-NE2	-6.92	115.68	122.60
2	D	84	ASN	CA-CB-CG	6.92	119.52	112.60
1	C	236	ASP	CA-CB-CG	6.91	119.51	112.60
1	C	260	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	168	THR	O-C-N	-6.89	114.15	122.22
1	C	244	LYS	CA-C-O	-6.89	113.58	120.82
1	C	174	GLN	CA-CB-CG	-6.88	100.35	114.10
1	A	247	PHE	N-CA-C	-6.87	102.20	110.44
2	D	55	ARG	N-CA-C	-6.87	98.88	109.52
2	B	96	ARG	O-C-N	-6.85	115.91	121.80
1	A	198	ILE	N-CA-C	-6.83	103.82	110.72
2	D	57	ASP	CA-CB-CG	6.82	119.42	112.60
2	D	147	HIS	CG-CD2-NE2	-6.82	100.38	107.20
2	D	113	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	C	54	ARG	CA-CB-CG	6.80	127.70	114.10
1	A	236	ASP	N-CA-C	-6.79	100.94	110.31
2	D	9	VAL	CB-CA-C	-6.78	100.95	111.26
1	A	134	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	C	66	LEU	N-CA-C	-6.76	104.16	112.88
1	C	78	ASN	N-CA-C	6.76	125.19	110.80
2	D	132	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	106	HIS	CA-C-N	6.73	126.87	119.87
1	A	106	HIS	C-N-CA	6.73	126.87	119.87
1	C	74	SER	N-CA-C	-6.71	99.28	109.95
1	C	269	ARG	N-CA-C	-6.70	98.78	109.76
1	C	178	LYS	CA-CB-CG	-6.68	100.73	114.10
1	C	288	GLN	N-CA-C	-6.66	103.95	111.14
1	C	168	THR	O-C-N	-6.65	114.57	122.15
1	C	236	ASP	CB-CA-C	6.62	119.09	109.09
2	D	80	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	A	287	GLN	CG-CD-NE2	6.59	126.29	116.40
2	B	131	ALA	N-CA-C	6.57	124.80	110.80
1	C	56	ARG	CG-CD-NE	-6.57	97.55	112.00
1	C	269	ARG	NE-CZ-NH1	6.57	128.06	121.50
2	D	143	LYS	CA-CB-CG	-6.54	101.02	114.10
1	A	43	VAL	CG1-CB-CG2	-6.52	96.47	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ASP	CA-C-O	-6.49	113.67	120.55
1	C	134	HIS	CG-CD2-NE2	-6.49	100.71	107.20
1	C	279	LYS	CB-CG-CD	-6.48	96.41	111.30
2	D	9	VAL	CA-C-O	6.47	128.16	121.23
1	C	307	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	62	SER	CA-CB-OG	-6.45	98.21	111.10
2	D	6	LYS	O-C-N	6.44	130.63	122.19
2	B	23	ALA	N-CA-C	-6.44	97.08	110.80
2	B	105	ASN	N-CA-C	6.42	124.47	110.80
1	C	180	ASP	N-CA-C	6.40	120.72	109.96
1	C	162	ASP	N-CA-C	-6.39	97.28	108.20
2	D	73	GLN	OE1-CD-NE2	-6.37	116.23	122.60
2	B	5	ASN	CA-CB-CG	6.36	118.96	112.60
1	C	97	THR	CA-CB-OG1	-6.36	100.06	109.60
2	B	53	MET	N-CA-C	-6.32	97.33	110.80
1	C	222	VAL	CA-CB-CG1	6.29	121.09	110.40
1	C	296	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	A	134	HIS	CG-CD2-NE2	-6.28	100.92	107.20
2	D	99	LEU	O-C-N	-6.28	116.23	121.38
1	C	193	ALA	N-CA-C	6.27	118.39	110.24
1	A	18	ASP	CA-CB-CG	6.26	118.86	112.60
2	D	109	CYS	CA-C-N	6.26	126.73	119.47
2	D	109	CYS	C-N-CA	6.26	126.73	119.47
2	D	63	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	A	294	PHE	CA-CB-CG	-6.22	107.58	113.80
1	C	273	ILE	N-CA-C	-6.20	98.59	107.77
1	C	32	ALA	CA-C-O	-6.20	114.51	120.90
1	C	23	VAL	N-CA-C	-6.19	104.31	110.62
1	C	93	SER	N-CA-C	-6.16	104.68	111.82
1	C	26	THR	CA-CB-CG2	6.15	120.96	110.50
1	C	134	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	C	151	ARG	CG-CD-NE	-6.15	98.47	112.00
2	D	105	ASN	CB-CA-C	-6.15	98.19	110.42
2	D	92	VAL	CA-CB-CG2	-6.14	99.96	110.40
1	A	182	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	C	305	ASN	O-C-N	-6.12	116.05	123.27
1	A	265	HIS	CG-CD2-NE2	-6.11	101.09	107.20
1	A	107	PRO	N-CA-C	6.09	121.52	114.03
1	C	56	ARG	CB-CG-CD	-6.09	97.30	111.30
2	D	53	MET	N-CA-C	6.08	118.53	108.49
2	B	4	ASP	CA-C-N	6.08	133.16	121.54
2	B	4	ASP	C-N-CA	6.08	133.16	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	VAL	O-C-N	-6.08	116.30	123.04
2	D	84	ASN	OD1-CG-ND2	-6.07	116.53	122.60
2	D	144	GLU	CA-CB-CG	-6.07	101.96	114.10
1	C	32	ALA	O-C-N	-6.05	115.50	122.03
1	C	284	TRP	CB-CG-CD1	-6.04	117.83	126.90
1	C	56	ARG	NE-CZ-NH2	-6.03	113.77	119.20
2	D	3	HIS	CA-C-N	6.03	133.06	121.54
2	D	3	HIS	C-N-CA	6.03	133.06	121.54
1	A	239	GLU	O-C-N	6.01	129.44	122.17
1	A	8	HIS	ND1-CG-CD2	6.01	112.11	106.10
1	C	222	VAL	CA-CB-CG2	-6.01	100.19	110.40
2	B	5	ASN	O-C-N	-6.00	114.60	122.59
2	B	34	LYS	CA-CB-CG	-6.00	102.09	114.10
1	C	218	VAL	N-CA-C	6.00	119.53	113.47
1	C	118	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	95	ILE	O-C-N	-5.97	115.84	121.87
1	C	218	VAL	CA-CB-CG2	-5.94	100.30	110.40
1	C	269	ARG	CA-C-N	-5.92	117.17	122.97
1	C	269	ARG	C-N-CA	-5.92	117.17	122.97
1	A	196	GLN	CA-C-O	-5.92	114.28	120.55
1	C	236	ASP	N-CA-CB	-5.91	101.48	109.88
2	D	22	PRO	N-CA-C	5.91	124.65	112.47
1	C	8	HIS	CG-CD2-NE2	-5.91	101.29	107.20
1	C	71	VAL	CA-C-N	-5.90	112.72	121.22
1	C	71	VAL	C-N-CA	-5.90	112.72	121.22
2	B	80	GLN	OE1-CD-NE2	-5.90	116.70	122.60
2	D	88	ASN	OD1-CG-ND2	-5.90	116.70	122.60
2	D	103	ILE	N-CA-C	-5.89	99.05	107.77
1	A	225	LEU	O-C-N	-5.89	115.71	123.13
1	C	284	TRP	CG-CD2-CE3	5.89	139.79	133.90
2	D	106	VAL	CA-C-O	-5.88	114.18	120.59
1	A	275	THR	CA-CB-OG1	-5.88	100.78	109.60
2	B	119	GLU	CA-C-N	5.87	127.18	119.84
2	B	119	GLU	C-N-CA	5.87	127.18	119.84
1	C	80	SER	N-CA-C	5.87	123.30	110.80
2	D	5	ASN	CA-CB-CG	5.87	118.47	112.60
2	B	33	PHE	CA-CB-CG	-5.86	107.94	113.80
2	D	90	GLU	CB-CG-CD	5.85	122.55	112.60
1	C	106	HIS	CA-C-O	-5.85	113.94	119.91
1	C	235	LEU	N-CA-C	-5.85	100.88	109.18
1	A	7	LYS	CA-CB-CG	5.84	125.78	114.10
1	C	200	ASP	CA-CB-CG	5.84	118.44	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ASN	OD1-CG-ND2	-5.83	116.77	122.60
2	B	117	HIS	CA-CB-CG	-5.83	107.97	113.80
2	D	107	LEU	N-CA-CB	5.83	120.35	110.49
1	A	222	VAL	N-CA-C	5.83	116.98	108.53
1	C	270	VAL	CA-C-N	-5.83	112.90	121.99
1	C	270	VAL	C-N-CA	-5.83	112.90	121.99
2	B	67	SER	O-C-N	5.82	129.37	123.26
1	A	116	THR	CA-CB-OG1	-5.79	100.91	109.60
1	A	256	ASN	N-CA-CB	-5.79	102.02	110.47
1	A	286	PHE	CA-CB-CG	-5.75	108.05	113.80
1	C	160	VAL	N-CA-CB	-5.75	103.48	111.41
1	C	132	ASN	OD1-CG-ND2	-5.75	116.86	122.60
1	C	293	ILE	CB-CA-C	-5.74	104.39	112.14
1	A	182	ASN	CB-CG-ND2	5.74	125.01	116.40
2	B	75	ALA	N-CA-C	5.73	118.30	111.71
1	A	287	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	C	97	THR	OG1-CB-CG2	5.73	120.76	109.30
1	C	252	SER	CA-CB-OG	5.73	122.56	111.10
1	A	245	ALA	CA-C-N	5.71	132.45	121.54
1	A	245	ALA	C-N-CA	5.71	132.45	121.54
1	A	69	SER	CA-CB-OG	-5.69	99.73	111.10
1	C	98	TYR	N-CA-C	5.67	122.86	113.50
1	C	63	MET	N-CA-C	-5.67	105.18	111.36
1	A	240	TYR	N-CA-C	-5.66	104.11	111.02
1	C	162	ASP	CA-CB-CG	5.66	118.26	112.60
2	B	65	PHE	N-CA-C	-5.64	97.97	108.02
2	B	128	ARG	N-CA-C	5.64	117.37	108.96
1	C	295	ALA	O-C-N	-5.63	116.15	122.12
2	B	66	LEU	N-CA-C	-5.62	100.54	109.76
1	C	276	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	232	LYS	N-CA-C	5.62	118.94	111.75
2	D	55	ARG	O-C-N	-5.62	115.84	123.15
1	A	54	ARG	N-CA-C	5.60	117.46	111.36
2	B	104	ASP	CA-CB-CG	-5.59	107.01	112.60
1	C	267	LEU	O-C-N	-5.58	114.91	121.32
1	C	40	LYS	CB-CG-CD	-5.58	98.47	111.30
2	D	153	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	C	287	GLN	CB-CG-CD	5.56	122.05	112.60
1	A	233	GLU	CA-CB-CG	5.56	125.21	114.10
1	C	83	LYS	N-CA-C	-5.55	101.42	110.20
2	B	134	ILE	CB-CA-C	-5.55	102.19	111.29
1	C	246	GLN	OE1-CD-NE2	-5.54	117.06	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	HIS	CA-CB-CG	5.54	119.34	113.80
1	C	158	ALA	CA-C-O	-5.53	114.66	120.80
1	A	216	GLU	CA-CB-CG	5.53	125.16	114.10
2	D	92	VAL	CA-CB-CG1	5.51	119.77	110.40
1	C	306	ARG	N-CA-C	5.50	119.25	112.54
2	D	19	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	173	THR	O-C-N	-5.49	115.09	122.23
1	C	281	PRO	N-CA-C	5.48	120.96	113.84
1	C	282	HIS	ND1-CG-CD2	5.47	111.58	106.10
2	B	125	PHE	O-C-N	-5.47	116.91	123.31
1	A	10	ILE	CB-CG1-CD1	-5.46	102.33	113.80
1	A	84	LYS	N-CA-CB	5.46	119.71	110.49
1	C	35	GLN	CA-C-N	5.45	125.93	120.04
1	C	35	GLN	C-N-CA	5.45	125.93	120.04
2	B	32	LEU	N-CA-C	5.44	117.21	111.28
1	A	56	ARG	CA-CB-CG	-5.43	103.23	114.10
1	A	83	LYS	CA-C-N	5.43	131.92	121.54
1	A	83	LYS	C-N-CA	5.43	131.92	121.54
1	C	23	VAL	CG1-CB-CG2	-5.42	98.88	110.80
1	A	10	ILE	N-CA-CB	-5.42	102.78	111.82
1	C	297	GLN	CG-CD-NE2	5.41	124.52	116.40
1	C	253	ASP	CA-CB-CG	5.41	118.01	112.60
2	D	132	ASN	N-CA-C	-5.41	99.28	110.80
1	C	10	ILE	N-CA-C	-5.41	107.52	111.90
1	C	280	THR	O-C-N	-5.41	114.67	121.21
2	D	106	VAL	N-CA-CB	-5.39	104.91	111.21
2	B	52	GLU	CA-C-O	5.38	128.20	120.51
1	A	116	THR	N-CA-CB	-5.38	101.40	110.49
2	B	63	ASN	CB-CG-ND2	5.37	124.46	116.40
1	A	78	ASN	OD1-CG-ND2	-5.36	117.25	122.60
1	C	284	TRP	CE2-CD2-CG	-5.35	100.78	107.20
2	B	4	ASP	N-CA-C	-5.35	99.40	110.80
1	A	309	VAL	O-C-N	5.35	129.18	122.66
1	A	60	GLU	CA-CB-CG	-5.35	103.41	114.10
2	D	21	ILE	CA-C-N	5.34	126.52	119.84
2	D	21	ILE	C-N-CA	5.34	126.52	119.84
1	C	293	ILE	O-C-N	-5.34	116.69	121.87
2	D	133	ASP	CA-CB-CG	5.34	117.94	112.60
2	D	134	ILE	CA-CB-CG1	-5.33	101.33	110.40
1	C	57	LEU	O-C-N	-5.33	116.47	122.12
1	C	136	THR	OG1-CB-CG2	-5.33	98.64	109.30
2	D	38	THR	CA-CB-OG1	-5.32	101.63	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TYR	CA-CB-CG	5.30	123.44	113.90
1	A	221	GLU	CA-CB-CG	5.30	124.70	114.10
2	B	118	ALA	N-CA-C	5.30	119.46	113.15
1	C	87	THR	N-CA-C	5.29	117.52	110.53
1	A	288	GLN	CA-C-O	-5.29	115.27	120.82
1	C	108	GLN	CA-CB-CG	-5.28	103.54	114.10
1	C	12	ILE	CB-CG1-CD1	5.25	124.83	113.80
2	D	151	LEU	N-CA-C	5.25	118.95	112.54
1	C	97	THR	CB-CA-C	5.25	120.89	110.17
1	A	291	ASN	OD1-CG-ND2	-5.25	117.35	122.60
2	D	81	ALA	O-C-N	-5.25	117.05	123.30
2	B	10	GLU	CA-C-N	5.24	131.55	121.54
2	B	10	GLU	C-N-CA	5.24	131.55	121.54
2	B	130	ARG	CA-C-N	5.24	131.54	121.54
2	B	130	ARG	C-N-CA	5.24	131.54	121.54
2	B	82	THR	O-C-N	-5.23	116.39	123.19
1	A	32	ALA	N-CA-C	5.23	116.98	111.28
2	D	120	PRO	CA-C-O	5.22	125.17	121.31
2	B	132	ASN	N-CA-C	-5.22	106.06	112.90
2	B	96	ARG	N-CA-C	-5.22	101.08	109.58
1	C	250	ARG	CA-CB-CG	5.21	124.53	114.10
2	B	10	GLU	N-CA-CB	-5.21	103.14	111.43
1	C	222	VAL	CB-CA-C	5.21	117.93	110.84
1	A	280	THR	CA-C-N	5.20	124.81	119.56
1	A	280	THR	C-N-CA	5.20	124.81	119.56
1	A	203	ASP	CA-C-O	-5.19	114.92	120.42
2	D	73	GLN	CB-CG-CD	5.19	121.42	112.60
1	C	106	HIS	CG-CD2-NE2	-5.19	102.01	107.20
2	D	2	THR	N-CA-C	5.18	117.63	107.57
2	D	33	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	284	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	236	ASP	CB-CA-C	5.16	115.85	108.68
1	C	14	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	56	ARG	CB-CG-CD	-5.14	99.48	111.30
1	A	106	HIS	ND1-CG-CD2	5.14	111.24	106.10
1	A	157	VAL	CA-C-O	-5.14	115.03	120.53
1	C	291	ASN	CB-CG-ND2	5.13	124.10	116.40
1	A	78	ASN	N-CA-C	5.13	114.81	108.19
2	D	126	ALA	N-CA-C	-5.12	101.35	109.96
2	D	143	LYS	CB-CG-CD	5.12	123.08	111.30
2	D	121	VAL	N-CA-CB	-5.12	103.87	112.47
2	B	78	ALA	CA-C-N	5.12	124.62	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	ALA	C-N-CA	5.12	124.62	119.19
1	C	182	ASN	O-C-N	5.12	128.74	122.96
2	D	139	LYS	CB-CG-CD	-5.11	99.54	111.30
2	D	9	VAL	CA-C-N	5.10	131.28	121.54
2	D	9	VAL	C-N-CA	5.10	131.28	121.54
1	C	78	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	C	280	THR	N-CA-C	-5.10	103.72	110.40
1	C	21	ASN	OD1-CG-ND2	-5.09	117.51	122.60
2	B	40	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	D	43	THR	N-CA-C	-5.08	99.83	108.26
2	B	132	ASN	CA-C-N	5.08	131.24	121.54
2	B	132	ASN	C-N-CA	5.08	131.24	121.54
1	C	53	THR	N-CA-C	5.08	117.20	111.11
1	A	265	HIS	CB-CG-CD2	-5.07	124.60	131.20
1	C	231	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	C	50	GLU	N-CA-C	-5.06	100.64	108.90
2	D	56	LYS	N-CA-C	5.06	115.72	108.74
1	C	74	SER	O-C-N	-5.04	116.81	123.16
1	A	260	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	C	220	ALA	N-CA-C	5.03	118.19	111.75
2	D	27	PHE	CA-CB-CG	-5.03	108.77	113.80
2	B	127	VAL	CA-C-O	-5.03	115.09	121.48
2	D	14	ARG	CA-CB-CG	5.03	124.15	114.10
2	B	149	VAL	CA-C-O	-5.01	115.54	120.85
2	B	130	ARG	N-CA-C	5.01	117.69	110.28
2	D	113	ASN	CA-CB-CG	5.01	117.61	112.60
2	B	95	SER	CA-CB-OG	5.00	121.11	111.10

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	PHE	Sidechain
1	A	185	TYR	Sidechain
1	A	240	TYR	Sidechain
1	A	294	PHE	Sidechain
1	A	48	PHE	Sidechain
1	A	5	TYR	Sidechain
1	A	98	TYR	Sidechain
2	B	132	ASN	Peptide
2	B	133	ASP	Mainchain
2	B	89	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	255	HIS	Sidechain
1	C	286	PHE	Sidechain
1	C	294	PHE	Sidechain
2	D	140	TYR	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	40	0
1	C	2415	0	2422	35	0
2	B	1196	0	1212	38	0
2	D	1196	0	1212	32	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	29	0	12	1	0
4	D	29	0	12	0	0
5	A	30	0	0	0	0
5	B	11	0	0	0	0
5	C	43	0	0	1	0
5	D	9	0	0	1	0
All	All	7375	0	7292	138	0

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

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HA	2:D:7:LEU:HD21	1.46	0.97
1:A:308:LEU:HG	1:A:310:LEU:HD22	1.57	0.86
2:B:6:LYS:HB3	2:D:10:GLU:HG3	1.58	0.85
2:B:6:LYS:HA	2:B:9:VAL:HG22	1.64	0.79
1:A:106:HIS:HD2	1:A:108:GLN:H	1.31	0.79
2:D:6:LYS:HB2	2:D:9:VAL:HG22	1.65	0.77
1:C:136:THR:HG21	1:C:296:ARG:HD3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:VAL:O	1:C:280:THR:HB	1.92	0.70
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.70	0.70
2:B:2:THR:HG22	2:B:11:ALA:HB3	1.74	0.69
1:A:153:ASP:HB2	1:A:180:ASP:O	1.95	0.66
1:C:136:THR:HB	5:C:316:HOH:O	1.95	0.66
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.31	0.65
2:D:22:PRO:HG2	2:D:25:ILE:HD12	1.79	0.65
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.79	0.65
1:A:248:VAL:HG12	1:A:272:GLU:HA	1.80	0.64
1:C:113:ARG:O	1:C:116:THR:HB	2.01	0.60
1:A:232:LYS:HZ1	1:A:270:VAL:HG21	1.68	0.59
2:D:5:ASN:HD22	2:D:6:LYS:HE2	1.68	0.59
1:C:292:GLY:O	1:C:296:ARG:HG3	2.03	0.59
2:B:129:LYS:HG2	2:B:132:ASN:OD1	2.03	0.58
2:B:11:ALA:HA	4:B:999:CTP:N3	2.18	0.58
2:B:48:LEU:O	2:B:55:ARG:HA	2.03	0.58
1:C:174:GLN:HG2	1:C:201:MET:HE2	1.87	0.57
2:B:38:THR:HG22	2:B:40:GLN:H	1.69	0.57
2:D:116:SER:HA	2:D:121:VAL:HG11	1.84	0.57
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.87	0.57
1:A:194:MET:SD	1:A:195:PRO:HD2	2.44	0.57
2:B:3:HIS:O	2:B:10:GLU:HB3	2.04	0.56
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.86	0.56
1:A:232:LYS:NZ	1:A:270:VAL:HG21	2.20	0.56
2:D:99:LEU:HD21	2:D:134:ILE:HG12	1.88	0.56
1:A:261:MET:O	1:A:282:HIS:HD2	1.89	0.55
1:C:136:THR:CG2	1:C:296:ARG:HD3	2.37	0.55
1:A:151:ARG:HD2	1:A:153:ASP:O	2.07	0.54
2:B:21:ILE:HG22	2:B:25:ILE:HB	1.89	0.54
2:B:3:HIS:HB2	2:B:10:GLU:OE1	2.08	0.54
1:C:1:ALA:HA	1:C:306:ARG:O	2.08	0.54
2:B:14:ARG:NH1	2:B:63:ASN:HA	2.22	0.54
1:C:256:ASN:ND2	1:C:256:ASN:H	2.04	0.54
2:B:14:ARG:HH11	2:B:14:ARG:HG2	1.73	0.53
2:D:6:LYS:O	2:D:9:VAL:HG13	2.08	0.53
1:A:292:GLY:O	1:A:296:ARG:HG3	2.09	0.53
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.90	0.53
2:B:50:SER:HB2	2:B:56:LYS:HG2	1.90	0.52
1:A:113:ARG:O	1:A:116:THR:HB	2.09	0.52
2:B:65:PHE:CE1	2:B:85:ARG:HG3	2.45	0.52
1:A:287:GLN:HE21	1:A:287:GLN:H	1.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:HG22	1:C:296:ARG:HH11	1.73	0.52
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.25	0.51
1:A:5:TYR:CD1	1:A:306:ARG:HA	2.45	0.51
1:A:9:ILE:HG21	1:A:299:LEU:HD21	1.93	0.51
1:A:287:GLN:H	1:A:287:GLN:NE2	2.08	0.50
1:A:198:ILE:O	1:A:202:LEU:HG	2.11	0.50
2:D:81:ALA:O	2:D:97:PRO:HD2	2.11	0.50
2:D:20:HIS:HB2	5:D:1008:HOH:O	2.11	0.49
1:C:234:ARG:HA	1:C:234:ARG:HE	1.77	0.49
1:A:151:ARG:HG3	1:A:153:ASP:H	1.77	0.49
1:C:151:ARG:HD2	1:C:153:ASP:O	2.13	0.49
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.78	0.48
1:C:261:MET:O	1:C:282:HIS:HD2	1.96	0.48
1:A:21:ASN:HD21	1:A:179:PHE:HE1	1.62	0.48
1:A:159:MET:HE1	1:A:173:THR:OG1	2.13	0.48
2:B:21:ILE:HB	2:B:57:ASP:HB2	1.94	0.48
2:B:25:ILE:HG22	2:B:29:LEU:HG	1.96	0.48
2:D:6:LYS:CB	2:D:9:VAL:HG22	2.40	0.48
1:C:94:VAL:O	1:C:97:THR:HB	2.13	0.47
2:B:6:LYS:HD2	2:D:10:GLU:HB3	1.95	0.47
2:D:14:ARG:HG3	2:D:65:PHE:HZ	1.78	0.47
2:D:124:SER:HB2	2:D:139:LYS:HD2	1.97	0.47
2:D:13:LYS:O	2:D:86:ILE:HG22	2.14	0.47
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.96	0.47
1:A:38:LEU:HD23	1:A:66:LEU:HD22	1.96	0.47
2:D:14:ARG:HA	2:D:86:ILE:O	2.14	0.47
1:C:164:LYS:HA	1:C:195:PRO:HD3	1.97	0.47
1:A:2:ASN:ND2	1:A:5:TYR:HB2	2.30	0.47
2:D:25:ILE:HD13	2:D:77:TYR:O	2.16	0.47
1:C:10:ILE:HD11	1:C:116:THR:OG1	2.15	0.46
2:D:65:PHE:HB3	2:D:85:ARG:HH22	1.79	0.46
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.98	0.46
1:C:227:MET:HB3	1:C:227:MET:HE3	1.82	0.46
2:B:14:ARG:HA	2:B:86:ILE:O	2.15	0.46
1:A:187:ILE:HG13	1:A:212:HIS:HB2	1.98	0.46
1:A:243:VAL:HG23	1:A:246:GLN:HG3	1.98	0.46
1:A:227:MET:HE3	1:A:227:MET:HB3	1.83	0.45
2:B:7:LEU:H	2:B:7:LEU:HD23	1.80	0.45
1:C:242:ASN:O	1:C:244:LYS:N	2.48	0.45
2:D:130:ARG:HD3	2:D:130:ARG:HA	1.65	0.45
1:C:135:PRO:O	1:C:139:LEU:HG	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LEU:HD22	2:B:150:VAL:HG12	1.99	0.44
1:C:40:LYS:O	1:C:41:HIS:HB2	2.18	0.44
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.17	0.44
1:C:199:LEU:HD13	1:C:209:TRP:CH2	2.53	0.44
2:B:41:ARG:HA	2:D:46:LEU:O	2.18	0.44
2:D:121:VAL:HG21	2:D:140:TYR:CZ	2.53	0.44
2:D:65:PHE:HB3	2:D:85:ARG:NH2	2.33	0.43
1:C:254:LEU:HD22	1:C:261:MET:HE1	2.01	0.43
1:A:81:LEU:CD1	1:A:91:THR:HG23	2.49	0.43
2:B:65:PHE:CD1	2:B:85:ARG:HG3	2.53	0.43
2:D:17:VAL:HG22	2:D:60:LYS:HG2	2.00	0.43
2:B:6:LYS:NZ	2:D:12:ILE:HG22	2.34	0.43
2:D:152:ALA:O	2:D:153:ASN:HB2	2.18	0.43
1:A:184:PHE:O	1:A:209:TRP:HA	2.19	0.43
2:B:30:LEU:HD21	2:B:44:ILE:HD13	2.01	0.43
1:C:12:ILE:HD13	1:C:15:LEU:HD12	2.01	0.43
1:C:136:THR:CG2	1:C:296:ARG:HH11	2.31	0.43
1:A:176:LEU:HA	1:A:176:LEU:HD23	1.80	0.42
1:A:248:VAL:CG1	1:A:272:GLU:HA	2.49	0.42
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.85	0.42
2:D:14:ARG:HG3	2:D:65:PHE:CZ	2.53	0.42
2:B:84:ASN:OD1	2:B:94:LYS:HG2	2.19	0.42
1:A:209:TRP:HZ3	1:A:211:LEU:HD11	1.83	0.42
1:C:17:ARG:HH11	1:C:17:ARG:HD3	1.72	0.42
1:C:47:CYS:O	1:C:104:MET:HA	2.19	0.42
1:C:215:ILE:HG22	1:C:219:MET:HE2	2.00	0.42
2:B:14:ARG:HA	2:B:86:ILE:HG22	2.02	0.42
1:A:4:LEU:O	1:A:7:LYS:HB2	2.19	0.42
2:B:2:THR:HG23	2:B:3:HIS:N	2.35	0.42
2:B:5:ASN:OD1	2:B:7:LEU:HG	2.20	0.42
2:B:46:LEU:HD23	2:D:42:ILE:HD12	2.02	0.42
2:B:76:LEU:HD22	2:B:103:ILE:CD1	2.50	0.42
2:B:31:SER:O	2:B:34:LYS:HG3	2.20	0.42
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.35	0.42
2:D:42:ILE:HG12	2:D:61:ILE:HG23	2.02	0.42
1:A:12:ILE:HD13	1:A:12:ILE:HA	1.96	0.42
1:C:308:LEU:HD13	1:C:308:LEU:HA	1.88	0.42
1:C:175:ALA:O	1:C:178:LYS:HB2	2.20	0.41
1:C:136:THR:HG22	1:C:296:ARG:NH1	2.35	0.41
1:C:163:LEU:HG	1:C:188:ALA:HB2	2.02	0.41
2:B:14:ARG:HH11	2:B:14:ARG:CG	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LEU:HB2	2:B:130:ARG:HD3	2.03	0.41
1:C:246:GLN:HA	1:C:248:VAL:HG12	2.03	0.41
1:A:108:GLN:HG2	2:B:113:ASN:OD1	2.21	0.41
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.82	0.41
1:A:232:LYS:HD3	1:A:232:LYS:H	1.85	0.40
2:B:44:ILE:HG23	2:B:59:ILE:HG12	2.04	0.40
2:D:10:GLU:H	2:D:10:GLU:CD	2.28	0.40
2:D:111:ASN:O	2:D:117:HIS:CE1	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/310 (99%)	283 (92%)	20 (6%)	5 (2%)	7	14
1	C	308/310 (99%)	285 (92%)	16 (5%)	7 (2%)	5	8
2	B	151/153 (99%)	119 (79%)	18 (12%)	14 (9%)	0	0
2	D	151/153 (99%)	128 (85%)	12 (8%)	11 (7%)	1	1
All	All	918/926 (99%)	815 (89%)	66 (7%)	37 (4%)	2	3

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	83	LYS
1	A	84	LYS
2	B	5	ASN
2	B	11	ALA
2	B	14	ARG
2	B	131	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	133	ASP
2	B	134	ILE
1	C	77	ALA
1	C	78	ASN
1	C	80	SER
2	D	4	ASP
2	D	10	GLU
2	D	89	TYR
2	D	107	LEU
2	D	131	ALA
2	D	132	ASN
1	A	79	THR
2	B	2	THR
2	B	22	PRO
2	B	53	MET
1	C	85	GLY
1	C	243	VAL
1	C	245	ALA
2	B	23	ALA
2	B	68	GLU
1	C	84	LYS
2	D	5	ASN
2	D	23	ALA
2	D	22	PRO
2	D	68	GLU
2	B	34	LYS
1	A	190	ASP
2	D	24	GLN
2	B	120	PRO
2	B	91	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	261/261 (100%)	227 (87%)	34 (13%)	4 8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	261/261 (100%)	222 (85%)	39 (15%)	3	6
2	B	136/137 (99%)	116 (85%)	20 (15%)	3	6
2	D	136/137 (99%)	114 (84%)	22 (16%)	2	4
All	All	794/796 (100%)	679 (86%)	115 (14%)	3	6

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	13	ASN
1	A	35	GLN
1	A	40	LYS
1	A	56	ARG
1	A	65	ARG
1	A	69	SER
1	A	76	SER
1	A	78	ASN
1	A	79	THR
1	A	81	LEU
1	A	86	GLU
1	A	124	VAL
1	A	151	ARG
1	A	153	ASP
1	A	167	ARG
1	A	210	SER
1	A	211	LEU
1	A	222	VAL
1	A	225	LEU
1	A	228	THR
1	A	229	ARG
1	A	232	LYS
1	A	233	GLU
1	A	235	LEU
1	A	238	SER
1	A	246	GLN
1	A	269	ARG
1	A	275	THR
1	A	279	LYS
1	A	285	TYR
1	A	287	GLN
1	A	309	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	310	LEU
2	B	1	MET
2	B	4	ASP
2	B	7	LEU
2	B	14	ARG
2	B	20	HIS
2	B	22	PRO
2	B	30	LEU
2	B	32	LEU
2	B	34	LYS
2	B	37	GLU
2	B	50	SER
2	B	58	LEU
2	B	67	SER
2	B	69	ASP
2	B	73	GLN
2	B	86	ILE
2	B	99	LEU
2	B	102	ARG
2	B	106	VAL
2	B	148	ASN
1	C	6	GLN
1	C	12	ILE
1	C	33	ASN
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	71	VAL
1	C	74	SER
1	C	79	THR
1	C	84	LYS
1	C	97	THR
1	C	125	LEU
1	C	152	LEU
1	C	153	ASP
1	C	159	MET
1	C	180	ASP
1	C	190	ASP
1	C	211	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	218	VAL
1	C	222	VAL
1	C	231	GLN
1	C	232	LYS
1	C	234	ARG
1	C	236	ASP
1	C	237	PRO
1	C	248	VAL
1	C	252	SER
1	C	256	ASN
1	C	269	ARG
1	C	272	GLU
1	C	275	THR
1	C	280	THR
1	C	285	TYR
1	C	287	GLN
1	C	305	ASN
1	C	308	LEU
2	D	2	THR
2	D	3	HIS
2	D	6	LYS
2	D	10	GLU
2	D	34	LYS
2	D	41	ARG
2	D	52	GLU
2	D	53	MET
2	D	61	ILE
2	D	85	ARG
2	D	92	VAL
2	D	95	SER
2	D	98	SER
2	D	101	GLU
2	D	104	ASP
2	D	123	SER
2	D	128	ARG
2	D	130	ARG
2	D	132	ASN
2	D	134	ILE
2	D	137	LYS
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	106	HIS
1	A	132	ASN
1	A	154	ASN
1	A	174	GLN
1	A	231	GLN
1	A	282	HIS
1	A	287	GLN
1	A	297	GLN
2	B	70	GLN
2	B	80	GLN
1	C	146	GLN
1	C	149	GLN
1	C	246	GLN
1	C	256	ASN
1	C	260	ASN
1	C	282	HIS
1	C	287	GLN
1	C	297	GLN
2	D	5	ASN
2	D	24	GLN
2	D	105	ASN
2	D	132	ASN
2	D	148	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	2.20	9 (31%)	43,47,47	1.20	4 (9%)
4	CTP	B	999	-	29,30,30	2.11	9 (31%)	43,47,47	1.42	7 (16%)

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

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	999	CTP	PB-O3B	6.28	1.66	1.59
4	B	999	CTP	PB-O3B	6.05	1.66	1.59
4	D	999	CTP	PB-O3A	5.52	1.65	1.59
4	D	999	CTP	PA-O3A	4.93	1.64	1.59
4	B	999	CTP	PB-O3A	4.77	1.64	1.59
4	B	999	CTP	PA-O3A	4.64	1.64	1.59
4	D	999	CTP	PG-O1G	2.59	1.58	1.50
4	B	999	CTP	C6-N1	-2.58	1.31	1.38
4	B	999	CTP	PG-O1G	2.53	1.58	1.50
4	D	999	CTP	C6-N1	-2.33	1.32	1.38
4	D	999	CTP	C5-C4	-2.30	1.37	1.42
4	B	999	CTP	C2-N1	-2.24	1.35	1.40
4	D	999	CTP	C2-N1	-2.22	1.35	1.40
4	B	999	CTP	C2-N3	-2.09	1.32	1.36
4	B	999	CTP	PB-O1B	2.09	1.58	1.50
4	B	999	CTP	C5-C4	-2.04	1.38	1.42
4	D	999	CTP	PB-O1B	2.03	1.57	1.50
4	D	999	CTP	PA-O1A	2.00	1.57	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	CTP	O2-C2-N3	-4.80	114.76	122.33
4	D	999	CTP	O2-C2-N3	-4.15	115.78	122.33
4	B	999	CTP	N1-C2-N3	2.83	123.72	118.80
4	B	999	CTP	O4'-C1'-N1	2.55	114.14	108.36
4	D	999	CTP	N1-C2-N3	2.46	123.07	118.80
4	B	999	CTP	C6-N1-C2	-2.44	116.34	120.46
4	D	999	CTP	C6-N1-C2	-2.36	116.47	120.46
4	B	999	CTP	C5'-C4'-C3'	-2.21	107.26	115.21
4	B	999	CTP	C2'-C1'-N1	-2.04	107.57	113.25
4	D	999	CTP	O4'-C1'-N1	2.03	112.96	108.36
4	B	999	CTP	C4'-O4'-C1'	-2.02	105.01	109.47

There are no chirality outliers.

All (9) 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
4	B	999	CTP	C5'-O5'-PA-O2A
4	B	999	CTP	C5'-O5'-PA-O3A
4	D	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	O4'-C4'-C5'-O5'
4	B	999	CTP	C3'-C4'-C5'-O5'
4	D	999	CTP	PB-O3A-PA-O5'
4	D	999	CTP	PA-O3A-PB-O1B

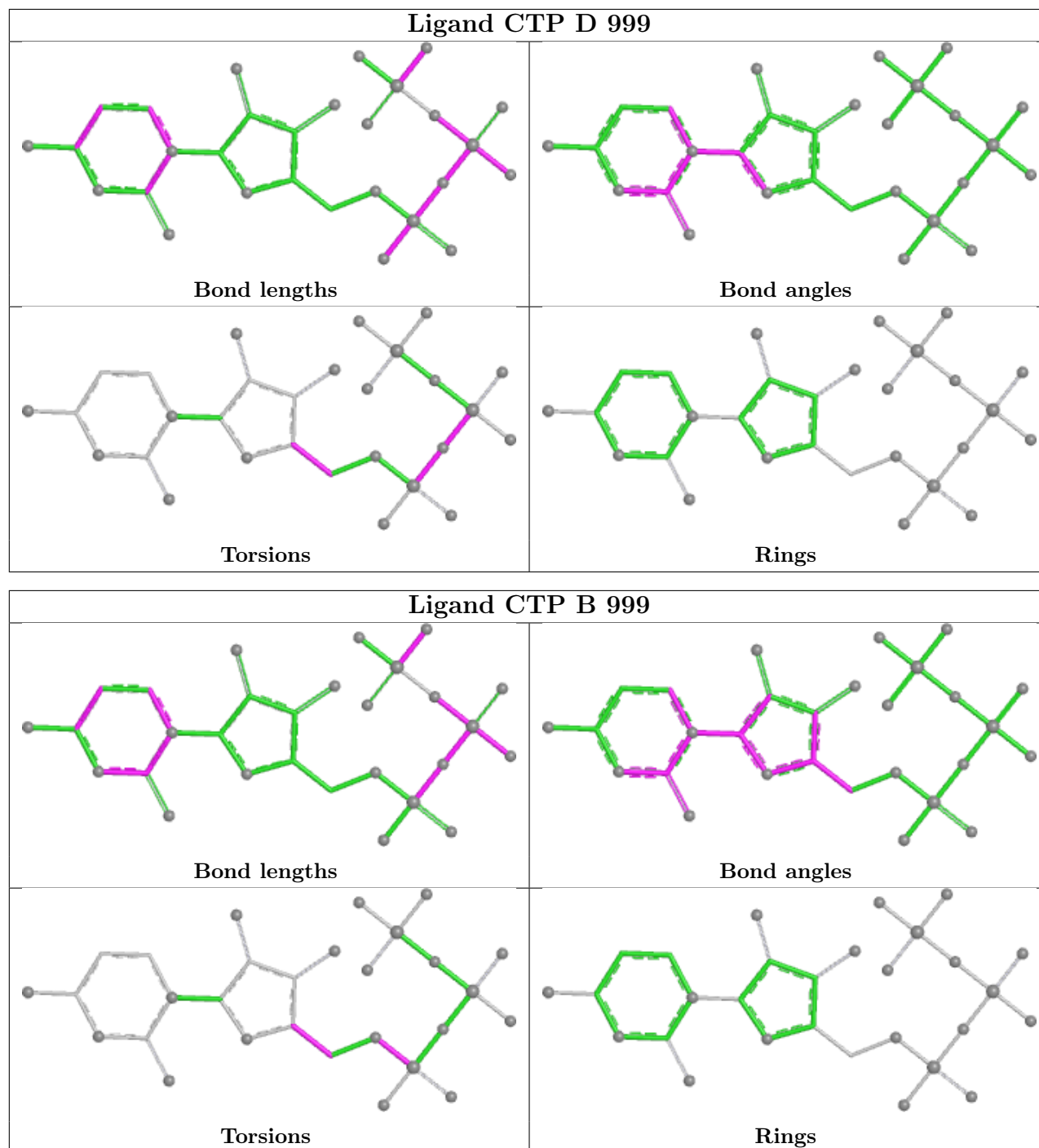
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.