



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:21 PM UTC

PDB ID : 5AT1 / pdb_00005at1
Title : STRUCTURAL CONSEQUENCES OF EFFECTOR BINDING TO THE T STATE OF ASPARTATE CARBAMOYLTRANSFERASE. CRYSTAL STRUCTURES OF THE UNLIGATED AND ATP-, AND CTP-COMPLEXED ENZYMES AT 2.6-ANGSTROMS RESOLUTION
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Deposited on : 1990-04-26
Resolution : 2.60 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

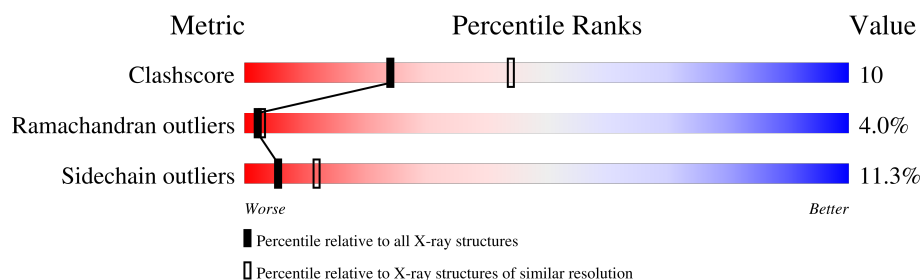
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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% 34% 9% •
1	C	310	55% 34% 10% •
2	B	153	45% 39% 11% • 5%
2	D	153	54% 31% 8% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7166 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 (T STATE), 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			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	conflict	UNP P0A786
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLU	GLN	conflict	UNP P0A786
A	196	GLU	GLN	conflict	UNP P0A786
C	60	GLN	GLU	conflict	UNP P0A786
C	147	GLN	GLU	conflict	UNP P0A786
C	149	GLU	GLN	conflict	UNP P0A786
C	196	GLU	GLN	conflict	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

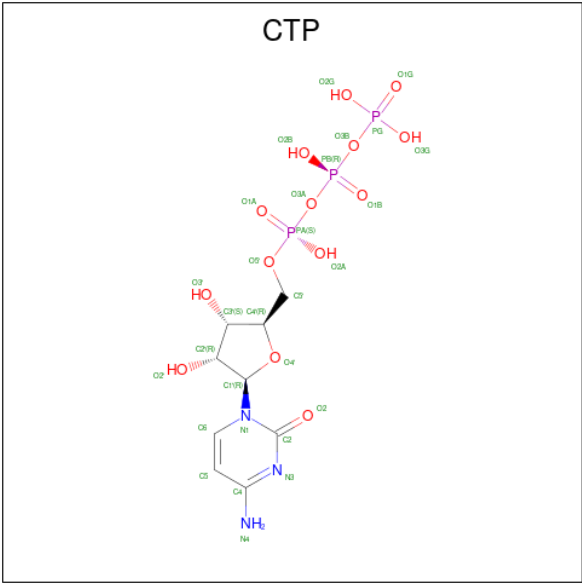
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	conflict	UNP P0A7F3
D	8	GLY	GLN	conflict	UNP P0A7F3

- 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).

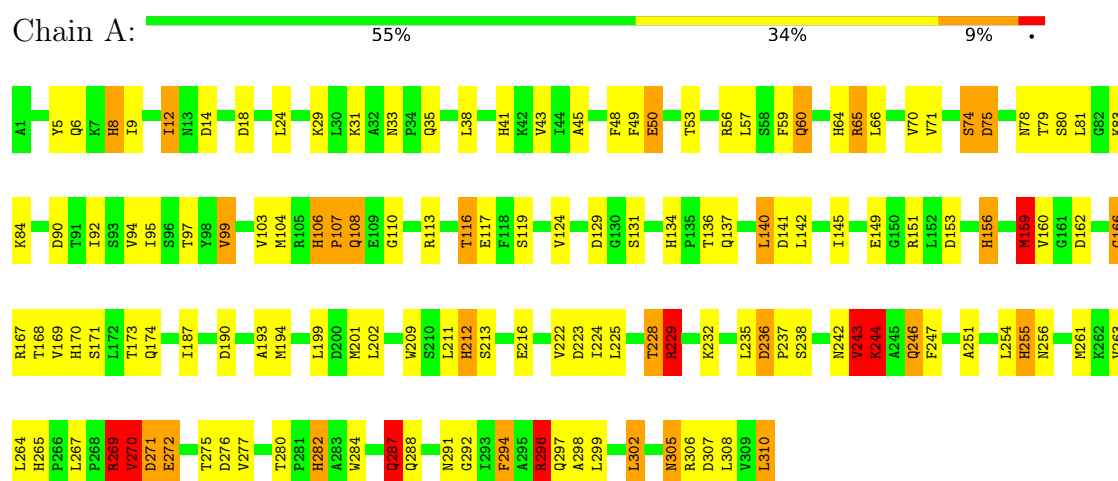


3 Residue-property plots

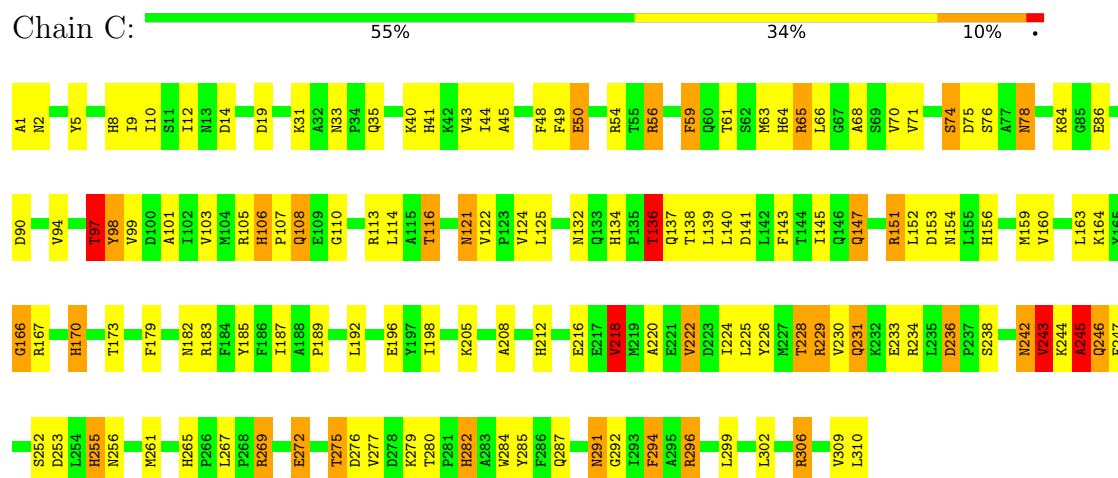
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

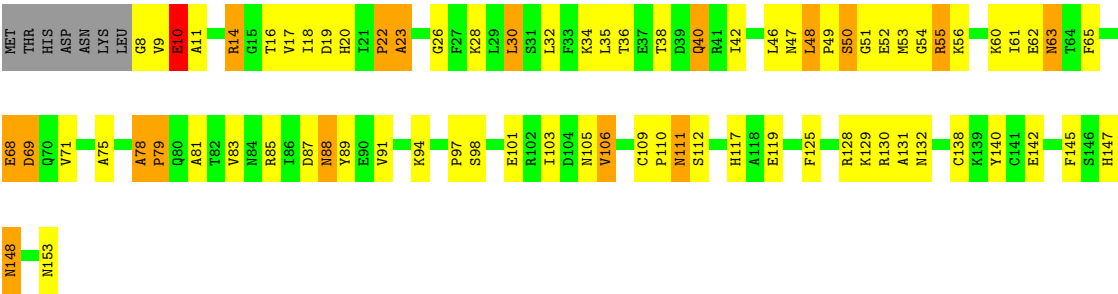


• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN

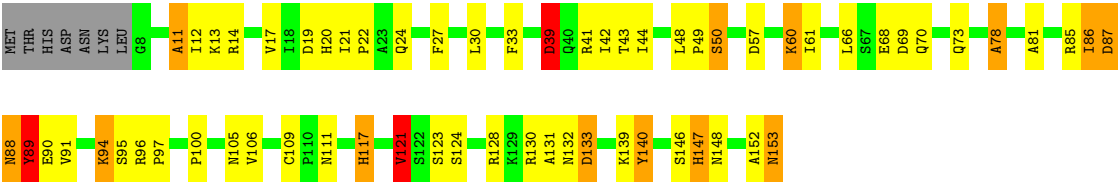


• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





● 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	122.00Å 122.00Å 142.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7166	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: CTP, ZN

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	1.12	14/2461 (0.6%)	2.02	82/3339 (2.5%)
1	C	1.20	12/2461 (0.5%)	2.06	83/3339 (2.5%)
2	B	0.97	4/1155 (0.3%)	1.90	29/1561 (1.9%)
2	D	0.98	5/1155 (0.4%)	1.96	37/1561 (2.4%)
All	All	1.10	35/7232 (0.5%)	2.00	231/9800 (2.4%)

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

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	156	HIS	CD2-NE2	-7.11	1.30	1.37
1	A	265	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	212	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	41	HIS	CD2-NE2	-6.97	1.30	1.37
1	C	282	HIS	CD2-NE2	-6.94	1.30	1.37
1	C	212	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	282	HIS	CD2-NE2	-6.80	1.30	1.37
2	D	60	LYS	CD-CE	-6.55	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	HIS	CD2-NE2	-6.54	1.30	1.37
2	D	20	HIS	CD2-NE2	-6.50	1.30	1.37
2	D	147	HIS	CD2-NE2	-6.48	1.30	1.37
1	C	106	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	170	HIS	CD2-NE2	-6.41	1.30	1.37
1	C	170	HIS	CD2-NE2	-6.36	1.30	1.37
1	C	134	HIS	CD2-NE2	-6.30	1.30	1.37
2	B	20	HIS	CD2-NE2	-6.27	1.30	1.37
1	C	64	HIS	CD2-NE2	-6.27	1.30	1.37
1	C	156	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.13	1.31	1.37
2	D	117	HIS	CD2-NE2	-6.10	1.31	1.37
2	D	117	HIS	CG-ND1	-6.05	1.31	1.38
1	A	8	HIS	CD2-NE2	-6.04	1.31	1.37
1	C	134	HIS	CG-ND1	-6.04	1.31	1.38
2	B	147	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	64	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	255	HIS	CD2-NE2	-5.78	1.31	1.37
1	C	212	HIS	CG-ND1	-5.46	1.32	1.38
1	A	265	HIS	CG-ND1	-5.45	1.32	1.38
1	A	8	HIS	CG-ND1	-5.39	1.32	1.38
1	A	212	HIS	CG-ND1	-5.34	1.32	1.38
2	B	117	HIS	CD2-NE2	-5.25	1.32	1.37
1	C	31	LYS	CA-CB	-5.15	1.45	1.53
2	B	103	ILE	CA-CB	5.03	1.59	1.53

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ASP	CA-CB-CG	12.72	125.32	112.60
2	D	153	ASN	CA-CB-CG	11.97	124.58	112.60
1	A	307	ASP	CA-CB-CG	9.76	122.36	112.60
1	C	269	ARG	NE-CZ-NH2	9.32	127.59	119.20
2	D	69	ASP	CA-CB-CG	9.28	121.88	112.60
1	C	136	THR	N-CA-CB	-9.25	95.94	110.28
1	C	255	HIS	CA-CB-CG	-9.21	104.58	113.80
1	A	272	GLU	N-CA-C	9.15	124.24	112.34
1	C	218	VAL	N-CA-CB	-9.10	100.53	112.36
2	D	117	HIS	N-CA-C	8.91	123.41	112.54
1	C	198	ILE	N-CA-C	-8.90	102.64	110.74
1	A	222	VAL	N-CA-CB	-8.55	101.21	110.53
1	A	276	ASP	CA-CB-CG	8.44	121.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ARG	CA-CB-CG	8.36	130.81	114.10
2	D	133	ASP	CA-CB-CG	8.33	120.93	112.60
1	A	129	ASP	CA-CB-CG	8.30	120.91	112.60
1	A	162	ASP	CA-CB-CG	8.30	120.90	112.60
1	A	291	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	C	236	ASP	CA-CB-CG	8.22	120.82	112.60
1	A	107	PRO	N-CA-C	8.19	124.55	113.98
1	A	269	ARG	NE-CZ-NH2	8.16	126.55	119.20
2	B	62	GLU	CA-CB-CG	8.03	130.15	114.10
1	A	294	PHE	CA-CB-CG	-8.02	105.78	113.80
1	C	97	THR	N-CA-CB	-8.00	98.20	110.44
1	C	71	VAL	O-C-N	-8.00	114.16	123.04
1	A	305	ASN	CA-CB-CG	-7.87	104.73	112.60
1	C	132	ASN	OD1-CG-ND2	-7.86	114.74	122.60
1	C	61	THR	N-CA-C	-7.86	102.02	111.69
1	C	147	GLN	OE1-CD-NE2	-7.81	114.79	122.60
1	C	54	ARG	NE-CZ-NH2	7.77	126.19	119.20
1	A	116	THR	CA-CB-OG1	-7.75	97.97	109.60
1	A	236	ASP	CA-CB-CG	7.66	120.26	112.60
1	C	54	ARG	NE-CZ-NH1	-7.63	113.87	121.50
1	A	307	ASP	N-CA-C	-7.58	96.17	108.52
2	D	89	TYR	N-CA-C	7.54	126.86	110.80
2	B	153	ASN	OD1-CG-ND2	-7.53	115.08	122.60
1	C	287	GLN	OE1-CD-NE2	-7.53	115.07	122.60
2	B	18	ILE	N-CA-C	-7.46	97.69	108.36
1	C	147	GLN	CG-CD-NE2	7.45	127.57	116.40
2	D	86	ILE	N-CA-C	-7.43	96.72	107.78
2	B	106	VAL	N-CA-CB	-7.42	99.13	111.98
1	A	106	HIS	CA-C-N	7.35	127.02	119.82
1	A	106	HIS	C-N-CA	7.35	127.02	119.82
2	B	34	LYS	N-CA-C	7.31	121.55	111.90
1	C	275	THR	CA-CB-OG1	-7.26	98.70	109.60
1	A	71	VAL	O-C-N	-7.21	115.29	123.00
1	C	166	GLY	CA-C-N	7.20	131.62	120.82
1	C	166	GLY	C-N-CA	7.20	131.62	120.82
2	D	152	ALA	O-C-N	7.19	129.75	122.12
2	D	148	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	C	302	LEU	N-CA-C	7.12	118.69	111.07
1	C	14	ASP	CA-CB-CG	7.07	119.67	112.60
2	B	52	GLU	N-CA-C	7.03	120.58	110.24
1	C	228	THR	CA-CB-OG1	-7.03	99.06	109.60
1	A	57	LEU	N-CA-C	-6.98	104.23	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	HIS	CA-CB-CG	6.95	120.75	113.80
1	C	56	ARG	CG-CD-NE	-6.92	96.77	112.00
1	C	10	ILE	CB-CA-C	6.85	117.88	111.30
2	D	152	ALA	CA-C-N	6.85	134.04	121.70
2	D	152	ALA	C-N-CA	6.85	134.04	121.70
1	C	220	ALA	N-CA-C	6.83	120.50	111.75
1	A	99	VAL	O-C-N	6.82	128.46	122.12
1	C	105	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	A	269	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	C	50	GLU	N-CA-C	-6.78	97.84	108.90
1	C	54	ARG	CB-CG-CD	-6.75	95.77	111.30
1	C	245	ALA	N-CA-C	-6.75	96.43	110.80
1	C	291	ASN	OD1-CG-ND2	-6.73	115.87	122.60
2	B	69	ASP	CA-CB-CG	6.71	119.31	112.60
1	C	136	THR	CB-CA-C	6.71	123.55	110.67
1	A	78	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	A	256	ASN	CA-CB-CG	6.63	119.23	112.60
1	C	256	ASN	CA-CB-CG	-6.62	105.97	112.60
2	D	109	CYS	CA-C-N	6.60	126.73	119.87
2	D	109	CYS	C-N-CA	6.60	126.73	119.87
2	B	40	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	C	116	THR	CA-CB-OG1	-6.54	99.80	109.60
1	C	56	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	C	139	LEU	CA-C-O	-6.49	114.00	120.82
2	D	57	ASP	CA-CB-CG	6.46	119.06	112.60
2	B	148	ASN	CA-CB-CG	6.43	119.03	112.60
2	B	117	HIS	CA-CB-CG	-6.42	107.38	113.80
1	A	33	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	C	49	PHE	CA-CB-CG	6.39	120.19	113.80
1	A	271	ASP	CA-CB-CG	6.39	118.99	112.60
1	C	243	VAL	N-CA-C	-6.36	96.12	109.34
1	C	276	ASP	CA-CB-CG	6.33	118.94	112.60
1	A	275	THR	CA-CB-OG1	-6.25	100.23	109.60
1	A	264	LEU	O-C-N	-6.24	115.92	123.10
1	C	121	ASN	CA-CB-CG	-6.22	106.38	112.60
2	D	33	PHE	CA-CB-CG	-6.20	107.60	113.80
1	C	269	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	A	244	LYS	N-CA-C	6.18	123.97	110.80
2	D	27	PHE	CA-CB-CG	-6.17	107.63	113.80
1	A	6	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	A	193	ALA	N-CA-C	6.15	118.47	110.53
1	A	167	ARG	CA-CB-CG	6.10	126.30	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	21	ILE	N-CA-C	-6.10	102.97	108.95
1	A	296	ARG	NE-CZ-NH2	6.09	124.69	119.20
1	A	43	VAL	CG1-CB-CG2	-6.09	97.41	110.80
1	A	244	LYS	CA-CB-CG	6.08	126.27	114.10
2	B	51	GLY	N-CA-C	-6.06	98.81	113.18
2	D	140	TYR	N-CA-C	6.06	120.44	111.04
1	C	113	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	C	116	THR	N-CA-CB	-6.01	100.33	110.49
1	C	242	ASN	CA-CB-CG	6.01	118.61	112.60
2	D	87	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	269	ARG	N-CA-C	-5.99	98.65	108.41
1	C	2	ASN	O-C-N	-5.97	114.84	121.53
1	C	231	GLN	OE1-CD-NE2	-5.97	116.63	122.60
2	D	88	ASN	N-CA-C	-5.94	98.14	110.80
2	D	132	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	A	190	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	280	THR	N-CA-C	-5.88	102.18	110.29
1	C	253	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	218	VAL	CB-CA-C	5.86	117.37	110.93
1	A	156	HIS	CA-CB-CG	5.85	119.65	113.80
1	C	291	ASN	CB-CG-ND2	5.84	125.16	116.40
2	B	19	ASP	CA-CB-CG	5.84	118.44	112.60
1	C	66	LEU	N-CA-C	-5.83	104.83	112.41
1	A	50	GLU	N-CA-C	-5.83	99.90	109.40
1	C	68	ALA	O-C-N	-5.83	116.15	122.79
1	C	33	ASN	CA-C-N	5.82	125.76	119.76
1	C	33	ASN	C-N-CA	5.82	125.76	119.76
1	A	92	ILE	N-CA-C	-5.81	105.07	110.53
2	B	119	GLU	N-CA-C	5.79	119.55	109.82
1	C	97	THR	CB-CA-C	5.76	120.37	110.01
1	A	18	ASP	CA-CB-CG	5.75	118.36	112.60
2	B	23	ALA	N-CA-C	-5.75	98.54	110.80
1	C	164	LYS	CB-CG-CD	-5.75	98.08	111.30
2	D	153	ASN	OD1-CG-ND2	-5.75	116.86	122.60
1	A	216	GLU	CA-CB-CG	5.74	125.58	114.10
1	A	255	HIS	CA-CB-CG	5.74	119.54	113.80
1	A	78	ASN	CB-CG-ND2	5.73	125.00	116.40
2	B	9	VAL	N-CA-C	-5.71	97.46	109.34
1	C	10	ILE	N-CA-CB	-5.70	102.29	111.82
2	B	35	LEU	CA-C-O	5.70	126.39	119.49
1	C	40	LYS	CA-CB-CG	5.70	125.50	114.10
1	A	287	GLN	OE1-CD-NE2	-5.70	116.90	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	A	156	HIS	N-CA-C	-5.68	98.08	108.02
2	B	148	ASN	CB-CA-C	-5.67	101.98	110.88
1	A	75	ASP	CA-CB-CG	5.66	118.26	112.60
2	B	54	GLY	N-CA-C	-5.66	99.78	113.18
2	D	48	LEU	N-CA-C	-5.65	102.28	110.08
1	A	117	GLU	CB-CG-CD	5.64	122.19	112.60
1	C	154	ASN	N-CA-C	5.64	119.36	111.74
2	B	79	PRO	N-CA-C	5.63	124.08	112.47
1	A	229	ARG	CA-CB-CG	5.63	125.37	114.10
1	C	182	ASN	CB-CG-ND2	5.62	124.84	116.40
1	A	194	MET	CA-C-N	5.59	125.60	119.90
1	A	194	MET	C-N-CA	5.59	125.60	119.90
2	D	130	ARG	O-C-N	5.58	128.55	122.64
1	A	166	GLY	CA-C-N	5.57	128.01	120.38
1	A	166	GLY	C-N-CA	5.57	128.01	120.38
1	C	243	VAL	O-C-N	-5.54	115.64	122.57
1	C	228	THR	CA-CB-CG2	5.53	119.90	110.50
1	A	251	ALA	N-CA-C	5.52	117.30	111.28
1	A	171	SER	CA-CB-OG	5.52	122.14	111.10
1	A	267	LEU	O-C-N	-5.52	114.98	121.32
2	B	105	ASN	N-CA-C	5.50	122.52	110.80
2	D	105	ASN	N-CA-C	5.49	122.50	110.80
1	A	159	MET	CA-CB-CG	-5.46	103.18	114.10
2	B	153	ASN	CB-CG-ND2	5.45	124.57	116.40
1	C	136	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	43	VAL	N-CA-C	-5.44	100.50	108.11
1	C	309	VAL	N-CA-C	-5.44	99.72	107.77
2	D	19	ASP	CA-CB-CG	5.43	118.03	112.60
2	D	106	VAL	N-CA-CB	-5.42	100.71	110.95
1	C	56	ARG	NE-CZ-NH2	5.41	124.07	119.20
2	D	78	ALA	CA-C-N	5.40	125.49	119.87
2	D	78	ALA	C-N-CA	5.40	125.49	119.87
2	D	153	ASN	N-CA-C	5.40	126.11	111.00
1	A	291	ASN	CB-CG-ND2	5.39	124.48	116.40
1	A	116	THR	CA-CB-CG2	5.37	119.63	110.50
1	A	65	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	B	132	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	C	103	VAL	N-CA-C	-5.35	100.04	107.80
1	C	196	GLU	N-CA-C	5.35	122.19	110.80
1	C	230	VAL	N-CA-C	-5.33	99.41	107.73
1	A	90	ASP	CA-CB-CG	5.33	117.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	LEU	CD1-CG-CD2	-5.33	99.08	110.80
2	D	11	ALA	N-CA-C	5.31	117.54	110.53
2	B	111	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	95	ILE	O-C-N	-5.30	116.52	121.87
2	B	78	ALA	CA-C-O	-5.29	112.92	120.16
1	A	60	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	C	122	VAL	CA-C-N	5.28	125.04	119.76
1	C	122	VAL	C-N-CA	5.28	125.04	119.76
2	D	57	ASP	N-CA-C	-5.28	101.50	109.85
1	A	288	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	C	182	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	56	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	C	284	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	A	14	ASP	CB-CA-C	-5.25	100.14	110.11
1	A	216	GLU	CB-CG-CD	5.25	121.52	112.60
1	C	113	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	C	222	VAL	O-C-N	5.22	128.46	123.14
1	C	275	THR	CA-CB-CG2	5.21	119.36	110.50
1	C	294	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	103	VAL	N-CA-C	-5.21	100.91	108.36
1	C	309	VAL	O-C-N	5.21	128.59	123.18
2	B	36	THR	N-CA-CB	-5.19	102.01	110.42
1	A	247	PHE	CA-CB-CG	5.17	118.97	113.80
1	C	138	THR	CA-CB-OG1	-5.17	101.84	109.60
2	B	88	ASN	N-CA-C	5.15	118.43	111.17
1	C	43	VAL	CG1-CB-CG2	-5.15	99.48	110.80
2	B	10	GLU	CA-CB-CG	5.14	124.39	114.10
2	D	39	ASP	O-C-N	5.13	128.89	122.63
2	D	146	SER	N-CA-C	-5.12	102.29	109.96
2	D	50	SER	CA-CB-OG	5.11	121.33	111.10
2	D	94	LYS	N-CA-C	-5.10	100.38	109.06
1	A	296	ARG	N-CA-C	5.08	116.82	111.28
1	C	137	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	D	121	VAL	N-CA-CB	-5.08	102.69	111.63
1	A	108	GLN	CB-CG-CD	-5.08	103.97	112.60
1	C	90	ASP	N-CA-C	5.07	116.80	111.28
1	A	228	THR	CA-CB-OG1	-5.06	102.00	109.60
1	A	8	HIS	CA-CB-CG	5.05	118.85	113.80
1	A	255	HIS	N-CA-C	5.04	117.67	111.82
1	A	65	ARG	CA-C-N	5.04	130.09	122.08
1	A	65	ARG	C-N-CA	5.04	130.09	122.08
2	B	75	ALA	N-CA-C	5.04	117.51	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	HIS	CA-C-N	5.04	125.32	119.47
1	C	134	HIS	C-N-CA	5.04	125.32	119.47
1	A	255	HIS	CB-CG-CD2	-5.04	124.65	131.20
2	D	85	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	A	131	SER	N-CA-C	-5.03	106.99	112.72
1	C	19	ASP	CA-C-O	-5.03	115.52	120.90
1	A	113	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	A	170	HIS	CA-C-O	-5.01	115.11	120.42

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	HIS	Sidechain
1	A	5	TYR	Sidechain
2	B	48	LEU	Peptide
2	B	89	TYR	Sidechain
1	C	226	TYR	Sidechain
1	C	255	HIS	Sidechain
1	C	294	PHE	Sidechain
1	C	98	TYR	Sidechain
2	D	89	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	45	0
1	C	2415	0	2422	44	0
2	B	1138	0	1154	31	0
2	D	1138	0	1154	26	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	29	0	12	7	0
4	D	29	0	11	7	0
All	All	7166	0	7175	143	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 (143) 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:D:12:ILE:O	4:D:155:CTP:N4	2.00	0.95
1:A:136:THR:HB	1:A:296:ARG:HH21	1.35	0.90
1:C:136:THR:HG23	1:C:296:ARG:HH21	1.44	0.81
1:C:280:THR:HG22	1:C:282:HIS:H	1.53	0.73
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.71	0.73
2:D:60:LYS:NZ	4:D:155:CTP:O2	2.23	0.71
1:C:292:GLY:O	1:C:296:ARG:HB2	1.91	0.70
1:A:106:HIS:HD2	1:A:108:GLN:H	1.36	0.70
2:D:94:LYS:NZ	4:D:155:CTP:O2A	2.20	0.70
1:A:136:THR:HB	1:A:296:ARG:NH2	2.06	0.70
2:B:94:LYS:HE3	4:B:155:CTP:O2A	1.92	0.69
2:B:94:LYS:CE	4:B:155:CTP:O2A	2.41	0.68
1:A:159:MET:HE1	1:A:173:THR:OG1	1.92	0.68
2:B:8:GLY:N	2:B:50:SER:HG	1.94	0.66
1:C:94:VAL:O	1:C:97:THR:HB	1.96	0.65
2:B:17:VAL:HG21	4:B:155:CTP:O2	1.97	0.65
1:A:8:HIS:HD2	1:A:124:VAL:H	1.45	0.65
1:C:136:THR:HG23	1:C:296:ARG:NH2	2.12	0.64
1:A:94:VAL:O	1:A:97:THR:HG22	1.98	0.63
2:D:42:ILE:HG12	2:D:61:ILE:HG23	1.78	0.63
1:A:160:VAL:O	1:A:228:THR:HG22	1.99	0.63
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.79	0.63
2:B:48:LEU:O	2:B:55:ARG:HA	1.98	0.62
2:B:38:THR:HG22	2:B:40:GLN:H	1.65	0.61
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.82	0.61
1:A:261:MET:O	1:A:282:HIS:HD2	1.84	0.60
1:C:1:ALA:HA	1:C:306:ARG:HD3	1.84	0.60
2:D:14:ARG:HG3	2:D:87:ASP:HA	1.83	0.60
1:C:9:ILE:HB	1:C:125:LEU:HD13	1.84	0.60
1:C:189:PRO:HG2	1:C:192:LEU:HD12	1.84	0.60
2:D:30:LEU:HD11	2:D:44:ILE:HD13	1.84	0.59
2:D:60:LYS:CE	4:D:155:CTP:O2	2.50	0.59
1:C:163:LEU:O	1:C:170:HIS:HE1	1.86	0.59
1:C:277:VAL:O	1:C:280:THR:HB	2.03	0.58
1:A:29:LYS:HD3	1:A:310:LEU:HB2	1.85	0.58
2:B:22:PRO:O	2:B:56:LYS:HA	2.03	0.58
1:A:270:VAL:HG13	1:A:271:ASP:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.19	0.58
1:C:151:ARG:HG3	1:C:153:ASP:O	2.03	0.57
1:A:159:MET:HE3	1:A:169:VAL:HB	1.86	0.57
1:A:229:ARG:NH1	1:A:270:VAL:HG11	2.20	0.56
2:B:71:VAL:HG13	2:B:83:VAL:HG21	1.86	0.56
1:A:254:LEU:HD11	1:A:277:VAL:HG13	1.87	0.55
1:A:187:ILE:HG13	1:A:212:HIS:HB2	1.89	0.55
1:C:50:GLU:HB2	1:C:107:PRO:HD3	1.88	0.55
1:C:145:ILE:HG23	1:C:224:ILE:HG13	1.89	0.54
1:C:261:MET:O	1:C:282:HIS:HD2	1.89	0.54
1:C:45:ALA:HB2	1:C:99:VAL:HG11	1.89	0.54
2:B:91:VAL:HG21	4:B:155:CTP:PA	2.48	0.53
2:D:81:ALA:O	2:D:97:PRO:HD3	2.09	0.52
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.92	0.52
4:D:155:CTP:H5'1	4:D:155:CTP:H6	1.74	0.52
2:D:133:ASP:HB2	2:D:147:HIS:CE1	2.45	0.52
1:A:209:TRP:HZ3	1:A:211:LEU:HG	1.75	0.52
1:C:152:LEU:HD23	1:C:179:PHE:CZ	2.44	0.52
2:B:14:ARG:HH21	2:B:63:ASN:HA	1.75	0.52
2:B:47:ASN:ND2	2:D:39:ASP:HA	2.25	0.51
1:C:48:PHE:O	1:C:74:SER:HA	2.10	0.50
1:A:142:LEU:HA	1:A:145:ILE:HD12	1.93	0.50
2:D:60:LYS:HE3	4:D:155:CTP:O2	2.12	0.50
2:D:124:SER:HB3	2:D:139:LYS:HB2	1.94	0.50
1:A:66:LEU:HG	1:A:297:GLN:HE21	1.77	0.49
1:A:145:ILE:HG23	1:A:224:ILE:HG13	1.94	0.49
2:B:71:VAL:HG22	2:B:83:VAL:HG11	1.95	0.49
2:D:14:ARG:HA	2:D:86:ILE:O	2.13	0.49
2:B:81:ALA:O	2:B:97:PRO:HD2	2.13	0.48
2:B:17:VAL:HG11	4:B:155:CTP:O3'	2.14	0.48
2:D:17:VAL:HG13	2:D:60:LYS:HG2	1.95	0.48
1:A:223:ASP:O	1:A:261:MET:HA	2.13	0.48
1:C:143:PHE:HD1	1:C:291:ASN:HB3	1.79	0.48
1:C:185:TYR:CD2	1:C:218:VAL:HG21	2.49	0.47
2:B:109:CYS:HA	2:B:125:PHE:HZ	1.80	0.47
1:C:189:PRO:CG	1:C:192:LEU:HD12	2.45	0.47
2:B:16:THR:OG1	2:B:65:PHE:HA	2.15	0.47
2:D:13:LYS:HD3	2:D:14:ARG:HB2	1.96	0.47
1:A:261:MET:O	1:A:282:HIS:CD2	2.65	0.47
1:C:160:VAL:HG22	1:C:187:ILE:HD13	1.96	0.47
2:D:111:ASN:O	2:D:117:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:HIS:HD2	1:C:108:GLN:H	1.63	0.46
1:A:140:LEU:HD22	1:A:292:GLY:HA2	1.96	0.46
1:C:75:ASP:OD2	1:C:78:ASN:HA	2.16	0.45
1:A:12:ILE:HD13	1:A:12:ILE:HA	1.75	0.45
1:A:31:LYS:HA	1:A:294:PHE:CE1	2.52	0.45
2:B:60:LYS:NZ	4:B:155:CTP:O2'	2.50	0.45
1:C:65:ARG:HH21	1:C:65:ARG:HD2	1.63	0.45
1:A:60:GLN:HG2	1:A:70:VAL:HG11	1.99	0.45
2:B:138:CYS:O	2:B:142:GLU:HA	2.17	0.45
2:D:11:ALA:HB1	4:D:155:CTP:C4	2.52	0.45
2:B:11:ALA:HB1	4:B:155:CTP:N4	2.31	0.45
1:A:9:ILE:HG12	1:A:299:LEU:HD11	1.99	0.44
2:D:66:LEU:HA	2:D:70:GLN:OE1	2.18	0.44
1:A:174:GLN:HA	1:A:201:MET:HE1	1.98	0.44
1:A:199:LEU:O	1:A:202:LEU:HB2	2.18	0.44
1:C:243:VAL:HG12	1:C:244:LYS:H	1.83	0.44
1:A:225:LEU:HD12	1:A:263:VAL:HG13	1.99	0.44
1:C:183:ARG:HG2	1:C:208:ALA:HB3	1.99	0.44
1:A:48:PHE:O	1:A:74:SER:HA	2.18	0.44
1:A:110:GLY:HA3	2:B:140:TYR:HB3	2.00	0.43
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.18	0.43
1:C:229:ARG:HA	1:C:272:GLU:OE2	2.18	0.43
1:A:38:LEU:HD21	1:A:308:LEU:HD11	1.99	0.43
2:B:55:ARG:HD3	2:B:55:ARG:H	1.83	0.43
1:C:245:ALA:O	1:C:246:GLN:HG2	2.18	0.43
2:D:133:ASP:HB2	2:D:147:HIS:HE1	1.83	0.43
1:A:174:GLN:HG2	1:A:201:MET:HE1	2.01	0.43
2:D:17:VAL:HG22	2:D:60:LYS:HG2	2.01	0.43
1:A:141:ASP:O	1:A:145:ILE:HG13	2.19	0.43
2:B:14:ARG:NH2	2:B:63:ASN:HA	2.34	0.43
1:C:97:THR:HG22	1:C:98:TYR:CD2	2.54	0.43
1:C:141:ASP:O	1:C:145:ILE:HG13	2.19	0.43
1:A:243:VAL:HG23	1:A:246:GLN:NE2	2.34	0.42
2:B:130:ARG:HH11	2:B:131:ALA:HB2	1.83	0.42
1:A:145:ILE:O	1:A:149:GLU:HG2	2.20	0.42
1:C:8:HIS:HD2	1:C:124:VAL:H	1.66	0.42
1:C:160:VAL:HG21	1:C:225:LEU:HD11	2.01	0.42
1:C:159:MET:HE3	1:C:173:THR:OG1	2.20	0.42
2:B:110:PRO:HD2	2:B:145:PHE:CD1	2.54	0.42
1:C:189:PRO:HD3	1:C:247:PHE:CD2	2.54	0.42
1:C:261:MET:O	1:C:282:HIS:CD2	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:O	1:A:302:LEU:HD12	2.19	0.42
1:C:44:ILE:HG23	1:C:101:ALA:HB3	2.02	0.42
2:B:68:GLU:H	2:B:68:GLU:CD	2.27	0.42
1:A:151:ARG:NH2	1:A:153:ASP:O	2.53	0.42
1:C:205:LYS:HE2	1:C:205:LYS:HB3	1.82	0.42
2:D:111:ASN:O	2:D:117:HIS:CE1	2.73	0.41
1:C:110:GLY:HA2	2:D:140:TYR:O	2.19	0.41
1:A:49:PHE:CE1	1:A:104:MET:HE3	2.55	0.41
2:B:109:CYS:SG	2:B:111:ASN:HB3	2.60	0.41
2:B:42:ILE:HG12	2:B:61:ILE:HG23	2.03	0.41
1:C:59:PHE:CE2	1:C:296:ARG:HG3	2.56	0.41
1:C:63:MET:SD	1:C:70:VAL:HG22	2.61	0.41
2:D:22:PRO:HD2	2:D:78:ALA:HB1	2.03	0.41
2:B:26:GLY:O	2:B:30:LEU:HD22	2.20	0.41
1:C:5:TYR:CE1	1:C:306:ARG:HG2	2.56	0.41
2:D:12:ILE:HD12	2:D:14:ARG:O	2.21	0.41
2:B:28:LYS:HE3	2:B:28:LYS:HB2	1.95	0.40
2:B:65:PHE:CD2	2:B:85:ARG:HG3	2.56	0.40
1:A:166:GLY:O	1:A:169:VAL:HG22	2.22	0.40
1:A:229:ARG:HH11	1:A:270:VAL:HG11	1.86	0.40
1:C:114:LEU:HD12	2:D:121:VAL:HG21	2.02	0.40
1:C:238:SER:O	1:C:242:ASN:HB3	2.21	0.40
1:C:246:GLN:HA	1:C:246:GLN:OE1	2.21	0.40
2:D:73:GLN:NE2	2:D:100:PRO:HG3	2.37	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%)	279 (91%)	20 (6%)	9 (3%)	3 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	308/310 (99%)	279 (91%)	20 (6%)	9 (3%)	3	6
2	B	144/153 (94%)	113 (78%)	21 (15%)	10 (7%)	1	1
2	D	144/153 (94%)	130 (90%)	6 (4%)	8 (6%)	1	1
All	All	904/926 (98%)	801 (89%)	67 (7%)	36 (4%)	2	3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
2	B	50	SER
2	D	49	PRO
2	D	89	TYR
2	D	131	ALA
1	A	83	LYS
1	A	243	VAL
1	A	270	VAL
2	B	10	GLU
2	B	22	PRO
2	B	53	MET
1	C	76	SER
2	D	88	ASN
1	A	75	ASP
1	A	80	SER
2	B	129	LYS
1	C	275	THR
2	D	50	SER
1	A	242	ASN
1	A	246	GLN
2	B	14	ARG
2	B	23	ALA
1	C	78	ASN
1	C	86	GLU
1	C	245	ALA
1	C	246	GLN
2	D	68	GLU
1	A	306	ARG
1	C	166	GLY
1	C	267	LEU
2	D	24	GLN
2	B	78	ALA
1	C	243	VAL

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Mol	Chain	Res	Type
2	B	49	PRO
2	B	79	PRO
2	D	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%)	231 (88%)	30 (12%)	5	11
1	C	261/261 (100%)	228 (87%)	33 (13%)	4	9
2	B	129/136 (95%)	114 (88%)	15 (12%)	5	11
2	D	129/136 (95%)	119 (92%)	10 (8%)	11	26
All	All	780/794 (98%)	692 (89%)	88 (11%)	5	12

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	24	LEU
1	A	35	GLN
1	A	53	THR
1	A	59	PHE
1	A	65	ARG
1	A	74	SER
1	A	79	THR
1	A	81	LEU
1	A	84	LYS
1	A	116	THR
1	A	119	SER
1	A	140	LEU
1	A	159	MET
1	A	213	SER
1	A	229	ARG
1	A	232	LYS
1	A	235	LEU

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Mol	Chain	Res	Type
1	A	236	ASP
1	A	237	PRO
1	A	238	SER
1	A	243	VAL
1	A	244	LYS
1	A	255	HIS
1	A	269	ARG
1	A	270	VAL
1	A	287	GLN
1	A	296	ARG
1	A	305	ASN
1	A	310	LEU
2	B	10	GLU
2	B	30	LEU
2	B	32	LEU
2	B	46	LEU
2	B	55	ARG
2	B	68	GLU
2	B	69	ASP
2	B	87	ASP
2	B	88	ASN
2	B	98	SER
2	B	101	GLU
2	B	106	VAL
2	B	112	SER
2	B	128	ARG
2	B	148	ASN
1	C	12	ILE
1	C	35	GLN
1	C	56	ARG
1	C	59	PHE
1	C	65	ARG
1	C	74	SER
1	C	84	LYS
1	C	97	THR
1	C	108	GLN
1	C	116	THR
1	C	121	ASN
1	C	136	THR
1	C	140	LEU
1	C	147	GLN
1	C	151	ARG

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Mol	Chain	Res	Type
1	C	216	GLU
1	C	218	VAL
1	C	222	VAL
1	C	228	THR
1	C	229	ARG
1	C	231	GLN
1	C	233	GLU
1	C	234	ARG
1	C	236	ASP
1	C	252	SER
1	C	269	ARG
1	C	272	GLU
1	C	279	LYS
1	C	285	TYR
1	C	296	ARG
1	C	299	LEU
1	C	306	ARG
1	C	310	LEU
2	D	39	ASP
2	D	41	ARG
2	D	43	THR
2	D	90	GLU
2	D	95	SER
2	D	96	ARG
2	D	121	VAL
2	D	123	SER
2	D	128	ARG
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	13	ASN
1	A	21	ASN
1	A	78	ASN
1	A	108	GLN
1	A	170	HIS
1	A	174	GLN
1	A	212	HIS
1	A	231	GLN
1	A	282	HIS

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Mol	Chain	Res	Type
1	A	287	GLN
1	A	297	GLN
2	B	20	HIS
2	B	40	GLN
2	B	47	ASN
2	B	105	ASN
2	B	117	HIS
2	B	147	HIS
1	C	6	GLN
1	C	8	HIS
1	C	13	ASN
1	C	60	GLN
1	C	106	HIS
1	C	108	GLN
1	C	156	HIS
1	C	170	HIS
1	C	174	GLN
1	C	231	GLN
1	C	282	HIS
1	C	291	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	155	-	29,30,30	3.74	14 (48%)	43,47,47	2.52	15 (34%)
4	CTP	B	155	-	29,30,30	3.46	14 (48%)	43,47,47	2.48	15 (34%)

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	155	-	-	8/22/38/38	0/2/2/2
4	CTP	B	155	-	-	0/22/38/38	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	155	CTP	O2-C2	-10.15	1.04	1.23
4	B	155	CTP	PB-O3A	10.05	1.70	1.59
4	D	155	CTP	PB-O3A	9.70	1.70	1.59
4	B	155	CTP	PB-O3B	8.90	1.69	1.59
4	D	155	CTP	PB-O3B	8.50	1.68	1.59
4	D	155	CTP	C3'-C4'	-5.69	1.38	1.53
4	B	155	CTP	O2-C2	5.59	1.34	1.23
4	B	155	CTP	C3'-C4'	-5.52	1.39	1.53
4	B	155	CTP	O3'-C3'	4.26	1.53	1.43
4	B	155	CTP	O4'-C4'	4.20	1.54	1.45
4	D	155	CTP	O4'-C4'	4.10	1.54	1.45
4	B	155	CTP	PA-O3A	-3.92	1.55	1.59
4	D	155	CTP	O3'-C3'	3.64	1.52	1.43
4	D	155	CTP	PA-O3A	-3.53	1.55	1.59
4	D	155	CTP	O5'-C5'	3.31	1.57	1.44
4	B	155	CTP	O5'-C5'	3.31	1.57	1.44
4	D	155	CTP	PG-O3G	-2.93	1.43	1.54
4	D	155	CTP	PA-O5'	-2.81	1.48	1.59
4	B	155	CTP	PA-O5'	-2.79	1.48	1.59
4	B	155	CTP	PG-O3G	-2.46	1.45	1.54
4	D	155	CTP	C6-N1	2.41	1.43	1.38
4	B	155	CTP	O4'-C1'	2.35	1.47	1.42
4	D	155	CTP	O4'-C1'	2.21	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	155	CTP	C4-N4	-2.11	1.28	1.33
4	D	155	CTP	PA-O1A	2.09	1.58	1.50
4	B	155	CTP	PA-O1A	2.03	1.57	1.50
4	B	155	CTP	C6-N1	2.03	1.42	1.38
4	B	155	CTP	PG-O1G	-2.02	1.44	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	155	CTP	C2'-C3'-C4'	8.25	118.55	102.61
4	B	155	CTP	C2'-C3'-C4'	6.58	115.32	102.61
4	D	155	CTP	C2'-C1'-N1	6.41	131.09	113.25
4	B	155	CTP	C2'-C1'-N1	5.28	127.96	113.25
4	B	155	CTP	C3'-C2'-C1'	-4.70	92.58	101.46
4	B	155	CTP	O4'-C1'-N1	-4.62	97.89	108.36
4	B	155	CTP	C5-C4-N4	4.47	128.46	120.63
4	B	155	CTP	C5-C6-N1	-4.24	114.94	121.84
4	D	155	CTP	C6-C5-C4	4.23	124.47	117.53
4	D	155	CTP	C5-C6-N1	-4.12	115.15	121.84
4	D	155	CTP	C5-C4-N4	4.11	127.82	120.63
4	B	155	CTP	C6-C5-C4	3.82	123.79	117.53
4	B	155	CTP	O4'-C4'-C3'	-3.43	98.34	105.15
4	D	155	CTP	O4'-C4'-C3'	-3.41	98.39	105.15
4	B	155	CTP	O3A-PA-O1A	-3.34	100.65	110.70
4	D	155	CTP	O3A-PA-O1A	-3.24	100.96	110.70
4	B	155	CTP	O2'-C2'-C1'	-3.23	98.99	110.10
4	D	155	CTP	O4'-C1'-N1	-3.07	101.40	108.36
4	D	155	CTP	C5-C4-N3	-3.06	116.17	121.32
4	D	155	CTP	O2'-C2'-C1'	-3.05	99.59	110.10
4	B	155	CTP	O3'-C3'-C4'	-2.94	102.64	111.08
4	D	155	CTP	C3'-C2'-C1'	-2.81	96.14	101.46
4	B	155	CTP	C5-C4-N3	-2.78	116.64	121.32
4	D	155	CTP	N1-C2-N3	2.51	123.16	118.80
4	B	155	CTP	O3A-PB-O1B	-2.38	103.55	110.70
4	D	155	CTP	O2B-PB-O3B	2.25	113.36	107.27
4	D	155	CTP	O3A-PB-O1B	-2.25	103.94	110.70
4	B	155	CTP	O2B-PB-O3B	2.19	113.20	107.27
4	D	155	CTP	O2-C2-N1	-2.05	114.88	118.90
4	B	155	CTP	O2B-PB-O3A	-2.04	101.77	107.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

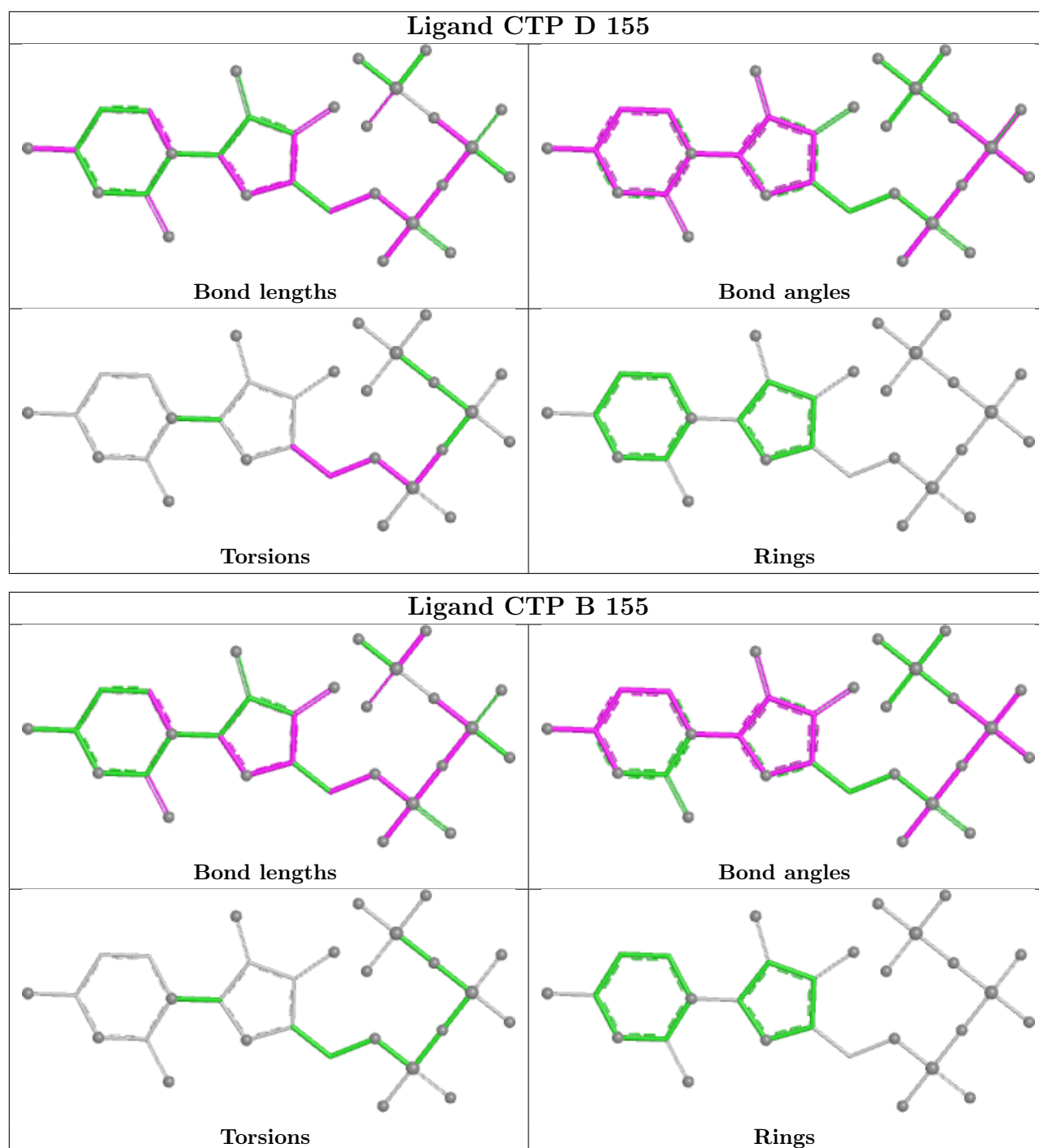
Mol	Chain	Res	Type	Atoms
4	D	155	CTP	C5'-O5'-PA-O1A
4	D	155	CTP	O4'-C4'-C5'-O5'
4	D	155	CTP	C5'-O5'-PA-O2A
4	D	155	CTP	C5'-O5'-PA-O3A
4	D	155	CTP	C3'-C4'-C5'-O5'
4	D	155	CTP	PB-O3A-PA-O1A
4	D	155	CTP	PB-O3A-PA-O2A
4	D	155	CTP	C4'-C5'-O5'-PA

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	155	CTP	7	0
4	B	155	CTP	7	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.