



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:41 PM UTC

PDB ID : 1HTT / pdb_00001htt
Title : HISTIDYL-TRNA SYNTHETASE
Authors : Arnez, J.G.; Harris, D.C.; Mitschler, A.; Rees, B.; Francklyn, C.S.; Moras, D.
Deposited on : 1996-03-09
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

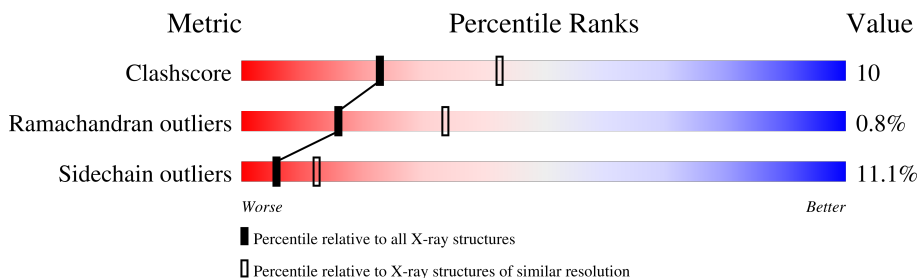
1 Overall quality at a glance

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	423	
1	B	423	
1	C	423	
1	D	423	

2 Entry composition [i](#)

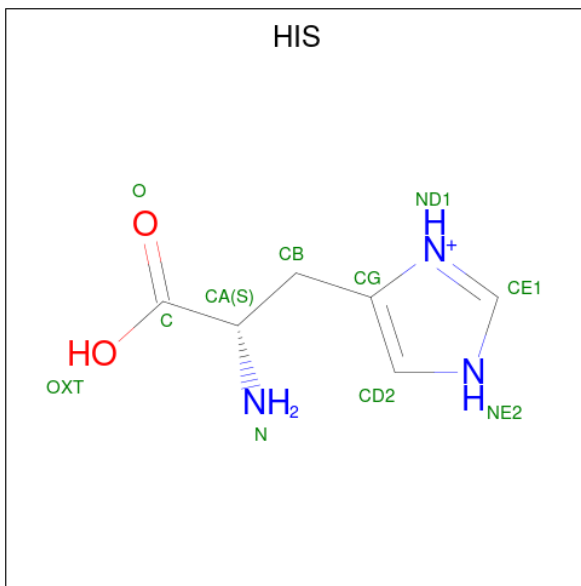
There are 4 unique types of molecules in this entry. The entry contains 11543 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HISTIDYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	Total 2848	C 1790	N 512	O 535	S 11	0	0	0
1	B	357	Total 2779	C 1748	N 499	O 521	S 11	0	0	0
1	C	366	Total 2848	C 1790	N 512	O 535	S 11	0	0	0
1	D	357	Total 2779	C 1748	N 499	O 521	S 11	0	0	0

- Molecule 2 is HISTIDINE (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



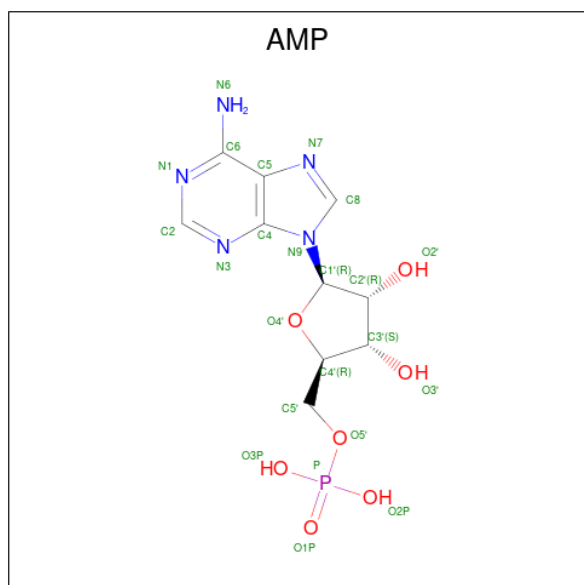
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 10	C 6	N 3	O 1	0	0
2	B	1	Total 10	C 6	N 3	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			10	6	3	1		
2	D	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	41	Total	O	0	0
			41	41		
4	C	38	Total	O	0	0
			38	38		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	29	Total	O	0	0
			29	29		

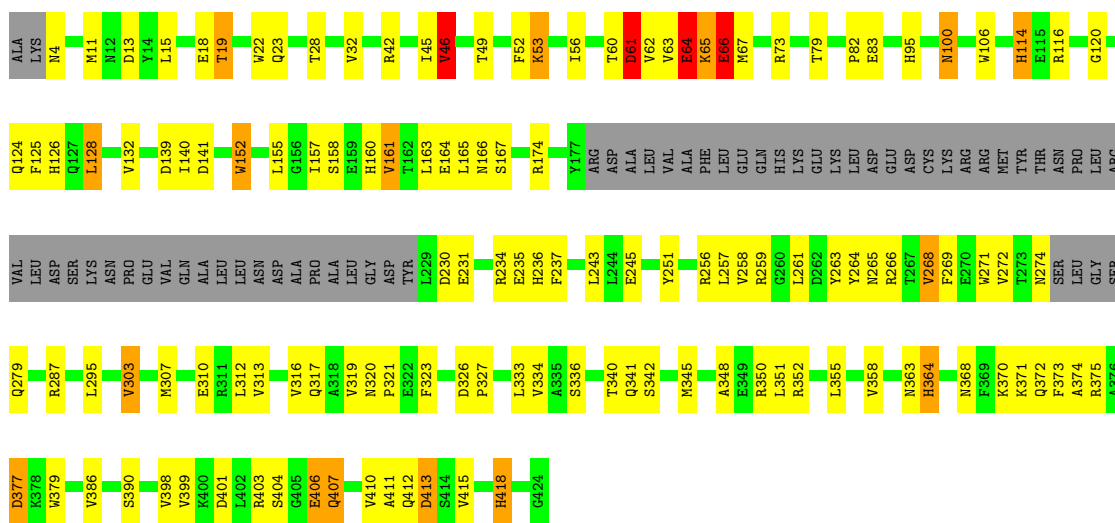
3 Residue-property plots

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.

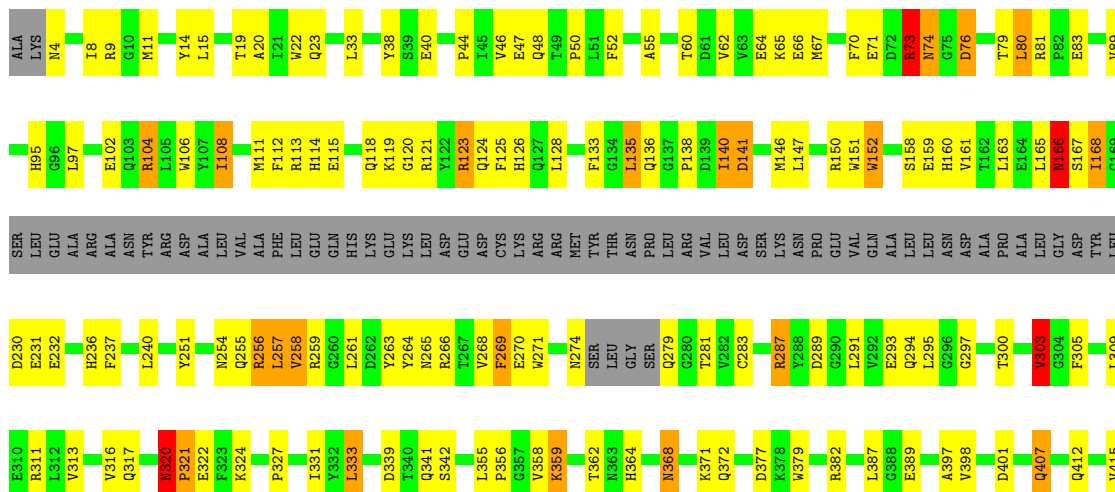
- Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain A:  55% 27% 13%



- Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain B:  49% 29% 5% 16%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.40Å 110.70Å 108.70Å 115.00° 97.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	69.9 (8.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.246 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11543	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: AMP

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	1.05	12/2899 (0.4%)	1.72	48/3920 (1.2%)
1	B	1.04	8/2829 (0.3%)	1.70	45/3825 (1.2%)
1	C	1.05	15/2899 (0.5%)	1.72	52/3920 (1.3%)
1	D	1.04	11/2829 (0.4%)	1.68	38/3825 (1.0%)
All	All	1.04	46/11456 (0.4%)	1.71	183/15490 (1.2%)

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	C	0	1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	VAL	CA-CB	8.43	1.64	1.54
1	C	56	ILE	CA-CB	7.71	1.64	1.54
1	A	364	HIS	CD2-NE2	-7.58	1.29	1.37
1	D	288	TYR	CA-CB	7.33	1.60	1.53
1	C	364	HIS	CD2-NE2	-7.25	1.29	1.37
1	D	95	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	160	HIS	CD2-NE2	-7.13	1.30	1.37
1	C	95	HIS	CD2-NE2	-6.98	1.30	1.37
1	D	364	HIS	CD2-NE2	-6.98	1.30	1.37
1	C	46	VAL	CA-CB	6.80	1.62	1.54
1	C	114	HIS	CD2-NE2	-6.79	1.30	1.37
1	B	95	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	236	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	95	HIS	CD2-NE2	-6.57	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	HIS	CD2-NE2	-6.55	1.30	1.37
1	B	364	HIS	CD2-NE2	-6.51	1.30	1.37
1	C	236	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.36	1.30	1.37
1	C	160	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	114	HIS	CD2-NE2	-6.20	1.31	1.37
1	D	236	HIS	CD2-NE2	-6.13	1.31	1.37
1	D	126	HIS	CD2-NE2	-6.00	1.31	1.37
1	D	160	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	364	HIS	CG-ND1	-5.81	1.31	1.38
1	B	236	HIS	CD2-NE2	-5.81	1.31	1.37
1	B	418	HIS	CD2-NE2	-5.80	1.31	1.37
1	C	126	HIS	CD2-NE2	-5.79	1.31	1.37
1	D	114	HIS	CD2-NE2	-5.78	1.31	1.37
1	C	418	HIS	CD2-NE2	-5.67	1.31	1.37
1	C	95	HIS	CG-ND1	-5.66	1.32	1.38
1	A	160	HIS	CG-ND1	-5.60	1.32	1.38
1	B	114	HIS	CD2-NE2	-5.54	1.31	1.37
1	D	418	HIS	CD2-NE2	-5.50	1.31	1.37
1	B	160	HIS	CD2-NE2	-5.50	1.31	1.37
1	C	160	HIS	CG-ND1	-5.48	1.32	1.38
1	D	160	HIS	CG-ND1	-5.46	1.32	1.38
1	D	95	HIS	CG-ND1	-5.43	1.32	1.38
1	D	364	HIS	CG-ND1	-5.41	1.32	1.38
1	B	95	HIS	CG-ND1	-5.33	1.32	1.38
1	A	95	HIS	CG-ND1	-5.31	1.32	1.38
1	C	126	HIS	CG-ND1	-5.28	1.32	1.38
1	C	114	HIS	CG-ND1	-5.28	1.32	1.38
1	C	392	VAL	CA-CB	5.24	1.61	1.54
1	A	418	HIS	CD2-NE2	-5.18	1.32	1.37
1	A	114	HIS	CG-ND1	-5.14	1.32	1.38
1	C	288	TYR	CA-CB	5.12	1.57	1.53

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CA-CB-CG	11.65	124.25	112.60
1	B	339	ASP	CA-CB-CG	11.14	123.74	112.60
1	C	166	ASN	CA-CB-CG	11.03	123.63	112.60
1	A	274	ASN	CA-CB-CG	10.14	122.74	112.60
1	B	95	HIS	CA-CB-CG	-9.83	103.97	113.80
1	D	254	ASN	CA-CB-CG	9.81	122.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ASN	CA-CB-CG	9.70	122.30	112.60
1	C	74	ASN	OD1-CG-ND2	-9.57	113.03	122.60
1	B	4	ASN	OD1-CG-ND2	-9.46	113.14	122.60
1	C	4	ASN	OD1-CG-ND2	-9.34	113.26	122.60
1	C	168	ILE	N-CA-CB	-9.23	100.00	112.28
1	C	95	HIS	CA-CB-CG	-8.92	104.88	113.80
1	D	368	ASN	CA-CB-CG	8.84	121.44	112.60
1	D	23	GLN	OE1-CD-NE2	-8.81	113.79	122.60
1	A	166	ASN	CA-CB-CG	8.68	121.28	112.60
1	D	166	ASN	CA-CB-CG	8.59	121.19	112.60
1	A	230	ASP	CA-CB-CG	8.13	120.73	112.60
1	A	139	ASP	CA-CB-CG	8.05	120.65	112.60
1	B	389	GLU	CB-CG-CD	7.91	126.05	112.60
1	D	74	ASN	CA-CB-CG	7.87	120.47	112.60
1	A	341	GLN	OE1-CD-NE2	-7.83	114.77	122.60
1	D	168	ILE	N-CA-CB	-7.71	102.12	112.22
1	B	166	ASN	CA-CB-CG	7.70	120.30	112.60
1	C	76	ASP	CA-CB-CG	7.69	120.29	112.60
1	B	73	ARG	CA-CB-CG	7.62	129.35	114.10
1	C	23	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	B	265	ASN	CA-CB-CG	7.59	120.19	112.60
1	C	339	ASP	CA-CB-CG	-7.58	105.02	112.60
1	D	230	ASP	CA-CB-CG	7.53	120.13	112.60
1	D	124	GLN	OE1-CD-NE2	-7.49	115.11	122.60
1	B	274	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	D	341	GLN	N-CA-C	7.39	119.33	111.28
1	C	152	TRP	CG-CD2-CE3	7.34	141.24	133.90
1	C	139	ASP	CA-CB-CG	7.32	119.92	112.60
1	D	152	TRP	CG-CD2-CE3	7.29	141.19	133.90
1	C	265	ASN	CA-CB-CG	7.28	119.88	112.60
1	C	136	GLN	CA-CB-CG	7.27	128.64	114.10
1	A	152	TRP	CB-CG-CD1	-7.19	116.12	126.90
1	C	100	ASN	CA-CB-CG	7.18	119.78	112.60
1	D	152	TRP	CB-CG-CD1	-7.11	116.23	126.90
1	A	323	PHE	N-CA-C	-7.10	98.93	109.15
1	C	152	TRP	CB-CG-CD1	-7.10	116.25	126.90
1	D	139	ASP	CA-CB-CG	7.08	119.69	112.60
1	C	232	GLU	CA-CB-CG	-7.05	100.00	114.10
1	A	377	ASP	CA-CB-CG	7.04	119.64	112.60
1	B	74	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	B	269	PHE	CA-CB-CG	6.92	120.72	113.80
1	A	125	PHE	CA-CB-CG	6.85	120.65	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	GLN	OE1-CD-NE2	-6.76	115.84	122.60
1	B	320	ASN	CA-CB-CG	6.72	119.32	112.60
1	C	323	PHE	N-CA-C	-6.71	99.48	109.15
1	B	230	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	152	TRP	CG-CD2-CE3	6.65	140.55	133.90
1	B	372	GLN	OE1-CD-NE2	-6.59	116.00	122.60
1	A	269	PHE	CA-CB-CG	6.56	120.36	113.80
1	B	141	ASP	CA-CB-CG	6.54	119.14	112.60
1	C	327	PRO	N-CA-C	-6.53	100.77	111.68
1	D	262	ASP	CA-CB-CG	6.51	119.11	112.60
1	D	321	PRO	CA-N-CD	-6.51	102.89	112.00
1	C	341	GLN	CB-CG-CD	6.50	123.66	112.60
1	A	274	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	C	341	GLN	N-CA-C	6.42	119.10	111.33
1	B	379	TRP	CG-CD2-CE3	6.40	140.30	133.90
1	B	387	LEU	CA-CB-CG	6.35	138.51	116.30
1	A	340	THR	CA-CB-OG1	-6.33	100.11	109.60
1	C	125	PHE	CA-CB-CG	6.33	120.13	113.80
1	B	152	TRP	CG-CD2-CE3	6.31	140.21	133.90
1	B	289	ASP	CA-CB-CG	6.27	118.87	112.60
1	D	303	VAL	CB-CA-C	-6.25	99.22	110.48
1	D	44	PRO	CA-N-CD	-6.25	103.25	112.00
1	D	407	GLN	CB-CG-CD	-6.23	102.01	112.60
1	D	23	GLN	CG-CD-NE2	6.22	125.73	116.40
1	D	269	PHE	CA-CB-CG	6.21	120.00	113.80
1	B	377	ASP	CA-CB-CG	6.20	118.80	112.60
1	C	168	ILE	CB-CA-C	6.20	119.73	111.85
1	C	387	LEU	CB-CA-C	-6.20	101.57	110.62
1	C	230	ASP	CA-CB-CG	6.17	118.77	112.60
1	D	320	ASN	CA-C-N	6.16	127.53	119.84
1	D	320	ASN	C-N-CA	6.16	127.53	119.84
1	A	66	GLU	N-CA-C	6.10	121.78	113.97
1	C	274	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	B	368	ASN	CA-CB-CG	6.10	118.70	112.60
1	A	320	ASN	CA-C-N	6.10	127.46	119.84
1	A	320	ASN	C-N-CA	6.10	127.46	119.84
1	D	320	ASN	CA-CB-CG	6.08	118.68	112.60
1	D	136	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	B	152	TRP	CB-CG-CD1	-6.06	117.81	126.90
1	C	74	ASN	CB-CG-ND2	6.05	125.48	116.40
1	D	152	TRP	CE2-CD2-CG	-6.03	99.97	107.20
1	C	110	PRO	CA-N-CD	-6.03	103.56	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	A	341	GLN	N-CA-C	6.00	117.82	111.28
1	B	83	GLU	CA-CB-CG	5.96	126.03	114.10
1	B	152	TRP	CE2-CD2-CG	-5.95	100.06	107.20
1	B	320	ASN	CA-C-N	5.95	127.27	119.84
1	B	320	ASN	C-N-CA	5.95	127.27	119.84
1	D	141	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	81	ARG	N-CA-C	5.90	116.83	109.57
1	D	50	PRO	CA-N-CD	-5.89	103.75	112.00
1	A	368	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	66	GLU	CA-CB-CG	-5.88	102.34	114.10
1	A	95	HIS	CA-CB-CG	-5.87	107.93	113.80
1	A	326	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	289	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	321	PRO	CA-N-CD	-5.81	103.86	112.00
1	B	124	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	327	PRO	N-CA-C	-5.72	102.12	111.68
1	A	271	TRP	CG-CD2-CE3	5.72	139.62	133.90
1	A	403	ARG	CA-CB-CG	5.72	125.54	114.10
1	B	341	GLN	N-CA-C	5.72	117.52	111.28
1	C	126	HIS	CA-CB-CG	-5.72	108.08	113.80
1	A	128	LEU	N-CA-C	-5.71	99.60	108.90
1	A	341	GLN	CB-CG-CD	5.70	122.29	112.60
1	D	287	ARG	CG-CD-NE	-5.68	99.50	112.00
1	A	64	GLU	CA-CB-CG	5.66	125.42	114.10
1	A	100	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	C	379	TRP	CE2-CD2-CG	-5.63	100.44	107.20
1	B	382	ARG	CA-CB-CG	-5.62	102.87	114.10
1	C	293	GLU	CB-CG-CD	-5.60	103.09	112.60
1	B	303	VAL	CB-CA-C	-5.59	100.41	110.48
1	A	407	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	A	106	TRP	CG-CD2-CE3	5.57	139.47	133.90
1	C	353	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	161	VAL	CB-CA-C	5.52	119.00	110.28
1	B	379	TRP	CB-CG-CD1	-5.52	118.63	126.90
1	D	300	THR	CA-CB-OG1	-5.51	101.34	109.60
1	C	129	GLY	O-C-N	5.50	127.68	123.23
1	C	127	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	D	389	GLU	CB-CG-CD	5.50	121.94	112.60
1	D	316	VAL	N-CA-C	-5.49	104.97	110.30
1	C	152	TRP	CE2-CD2-CG	-5.46	100.64	107.20
1	C	269	PHE	CA-CB-CG	5.46	119.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	TRP	CE2-CD2-CG	-5.45	100.67	107.20
1	D	319	VAL	CA-CB-CG2	-5.44	101.15	110.40
1	B	255	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	D	379	TRP	CE2-CD2-CG	-5.43	100.69	107.20
1	A	141	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	316	VAL	N-CA-C	-5.38	105.08	110.30
1	C	400	LYS	CA-CB-CG	5.36	124.81	114.10
1	A	231	GLU	N-CA-C	5.35	117.81	111.33
1	D	119	LYS	N-CA-C	5.35	122.20	110.80
1	B	379	TRP	CE2-CD2-CG	-5.35	100.78	107.20
1	C	136	GLN	N-CA-CB	-5.34	101.05	110.34
1	C	52	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	44	PRO	CA-N-CD	-5.33	104.54	112.00
1	D	22	TRP	CE2-CD2-CG	-5.32	100.82	107.20
1	D	379	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	D	95	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	265	ASN	O-C-N	-5.30	115.54	122.59
1	C	320	ASN	CA-C-N	5.30	126.46	119.84
1	C	320	ASN	C-N-CA	5.30	126.46	119.84
1	A	379	TRP	CE2-CD2-CG	-5.26	100.89	107.20
1	C	377	ASP	CA-CB-CG	-5.26	107.34	112.60
1	C	303	VAL	CB-CA-C	-5.25	101.72	111.18
1	A	326	ASP	N-CA-C	5.25	115.63	109.60
1	C	298	ARG	CG-CD-NE	-5.24	100.48	112.00
1	B	356	PRO	CA-N-CD	-5.23	104.67	112.00
1	C	339	ASP	N-CA-CB	-5.23	104.23	112.13
1	A	406	GLU	CB-CG-CD	5.19	121.42	112.60
1	C	255	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	22	TRP	CG-CD2-CE3	5.18	139.09	133.90
1	A	258	VAL	N-CA-C	-5.18	100.87	108.85
1	B	50	PRO	CA-N-CD	-5.18	104.74	112.00
1	A	164	GLU	CB-CG-CD	5.15	121.35	112.60
1	B	401	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	311	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	C	22	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	C	4	ASN	CB-CG-ND2	5.11	124.07	116.40
1	A	271	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	B	271	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	A	53	LYS	CA-CB-CG	5.10	124.31	114.10
1	C	379	TRP	CG-CD2-CE3	5.09	138.99	133.90
1	C	356	PRO	CA-N-CD	-5.08	104.88	112.00
1	B	294	GLN	OE1-CD-NE2	-5.08	117.52	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	GLU	CB-CG-CD	5.07	121.21	112.60
1	B	22	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	B	287	ARG	CG-CD-NE	-5.06	100.87	112.00
1	A	106	TRP	CB-CG-CD1	-5.04	119.33	126.90
1	C	106	TRP	CE2-CD2-CG	-5.04	101.16	107.20
1	D	104	ARG	CG-CD-NE	-5.03	100.94	112.00
1	A	13	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	341	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	A	407	GLN	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	68	TYR	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	2848	0	2809	56	0
1	B	2779	0	2747	83	0
1	C	2848	0	2809	58	0
1	D	2779	0	2747	60	0
2	A	10	0	6	0	0
2	B	10	0	6	0	0
2	C	10	0	6	0	0
2	D	10	0	6	0	0
3	A	23	0	12	0	0
3	B	23	0	12	3	0
3	C	23	0	12	0	0
3	D	23	0	12	0	0
4	A	49	0	0	1	0
4	B	41	0	0	1	0
4	C	38	0	0	2	0
4	D	29	0	0	0	0
All	All	11543	0	11184	235	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 (235) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HB3	1:A:65:LYS:HD3	1.61	0.82
1:B:20:ALA:HA	1:B:23:GLN:NE2	1.98	0.79
1:B:120:GLY:HA3	1:B:279:GLN:HG2	1.65	0.79
1:A:410:VAL:HG21	1:A:418:HIS:HD2	1.53	0.74
1:B:67:MET:SD	1:B:79:THR:HG21	2.26	0.74
1:A:46:VAL:HG22	1:B:11:MET:SD	2.28	0.73
1:A:19:THR:HG21	1:B:40:GLU:O	1.90	0.70
1:A:42:ARG:HB2	1:B:14:TYR:HB2	1.72	0.70
1:B:136:GLN:HA	1:B:287:ARG:NH2	2.07	0.69
1:C:168:ILE:HD11	1:C:258:VAL:HA	1.74	0.69
1:A:386:VAL:HB	1:A:398:VAL:HB	1.75	0.69
1:D:332:TYR:HE1	1:D:361:MET:HE2	1.57	0.69
1:A:287:ARG:HG2	1:A:303:VAL:HG13	1.75	0.68
1:C:345:MET:HB3	1:D:146:MET:HE1	1.74	0.68
1:D:265:ASN:HD22	1:D:266:ARG:HG3	1.55	0.68
1:B:331:ILE:HD11	1:B:423:LEU:HD11	1.75	0.67
1:A:259:ARG:HG3	1:A:268:VAL:HG22	1.76	0.67
1:A:152:TRP:CD1	1:A:161:VAL:HG11	2.31	0.66
1:A:313:VAL:HG12	1:A:317:GLN:HE21	1.61	0.65
1:A:350:ARG:HH22	1:A:413:ASP:HA	1.61	0.65
1:A:307:MET:SD	1:A:312:LEU:HD22	2.36	0.65
1:D:136:GLN:HA	1:D:287:ARG:NH2	2.11	0.65
1:C:400:LYS:HD2	1:C:407:GLN:HB3	1.79	0.64
1:C:42:ARG:HB2	1:D:14:TYR:HB2	1.79	0.64
1:B:46:VAL:HG22	1:B:80:LEU:HD12	1.81	0.62
1:C:120:GLY:HA3	1:C:279:GLN:HB2	1.82	0.61
1:A:334:VAL:HG21	1:A:373:PHE:CE1	2.35	0.61
1:B:163:LEU:HD23	1:B:251:TYR:HB3	1.82	0.61
1:C:412:GLN:O	1:C:415:VAL:HG22	2.01	0.61
1:D:293:GLU:HA	1:D:297:GLY:O	2.00	0.61
1:D:369:PHE:HE2	1:D:386:VAL:HG13	1.66	0.60
1:D:292:VAL:HG21	1:D:300:THR:HG22	1.82	0.60
1:B:108:ILE:HD11	1:B:309:LEU:HD11	1.83	0.60
1:D:30:LYS:HB2	1:D:30:LYS:NZ	2.17	0.59
1:D:266:ARG:HH21	1:D:287:ARG:HE	1.50	0.59
1:A:364:HIS:HD2	1:B:104:ARG:NH2	2.00	0.59
1:B:47:GLU:HB2	1:B:52:PHE:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:HB2	1:B:52:PHE:CE2	2.37	0.59
1:B:166:ASN:ND2	1:B:268:VAL:HG23	2.17	0.59
1:A:412:GLN:O	1:A:415:VAL:HG22	2.03	0.59
1:A:350:ARG:NH2	1:A:413:ASP:HA	2.17	0.59
1:C:58:GLU:HA	1:C:63:VAL:HG11	1.85	0.58
1:C:74:ASN:HD21	1:C:76:ASP:HB2	1.69	0.58
1:D:165:LEU:HD23	1:D:269:PHE:HB3	1.85	0.58
1:B:89:VAL:HG21	1:B:291:LEU:HD22	1.84	0.58
1:A:60:THR:O	1:A:64:GLU:HB2	2.03	0.58
1:B:20:ALA:HA	1:B:23:GLN:HE21	1.67	0.58
1:C:168:ILE:HD12	1:C:268:VAL:HG21	1.86	0.58
1:B:108:ILE:CD1	1:B:309:LEU:HD11	2.34	0.57
1:D:121:ARG:HH11	1:D:311:ARG:HH22	1.52	0.57
1:C:99:TYR:CD1	1:C:298:ARG:HG3	2.40	0.57
1:C:112:PHE:HZ	1:D:45:ILE:HD12	1.70	0.57
1:A:28:THR:O	1:A:32:VAL:HG23	2.04	0.57
1:C:401:ASP:HB3	1:C:406:GLU:HG2	1.86	0.56
1:C:359:LYS:HG2	1:D:34:GLY:O	2.06	0.56
1:B:412:GLN:O	1:B:415:VAL:HG22	2.06	0.56
1:D:38:TYR:CE1	1:D:104:ARG:HG2	2.41	0.56
1:C:310:GLU:HB2	4:C:627:HOH:O	2.05	0.55
1:B:254:ASN:HD21	1:B:256:ARG:NH2	2.04	0.55
1:B:266:ARG:HH21	1:B:287:ARG:HE	1.55	0.55
1:D:136:GLN:NE2	1:D:266:ARG:NH2	2.55	0.55
1:D:273:THR:HG21	1:D:315:LEU:HD22	1.88	0.55
1:B:166:ASN:HA	1:B:237:PHE:CZ	2.42	0.54
1:B:165:LEU:HD23	1:B:269:PHE:HB3	1.89	0.54
1:C:364:HIS:HD2	1:D:104:ARG:NH2	2.06	0.54
1:A:345:MET:HB3	1:B:146:MET:HE1	1.90	0.54
1:B:113:ARG:O	1:B:123:ARG:HA	2.08	0.53
1:C:14:TYR:HB2	1:D:42:ARG:HB2	1.89	0.53
1:B:136:GLN:HA	1:B:287:ARG:HH22	1.72	0.53
1:C:163:LEU:HG	1:C:165:LEU:HD12	1.89	0.53
1:D:30:LYS:HB2	1:D:30:LYS:HZ3	1.71	0.53
1:B:279:GLN:N	1:B:311:ARG:NE	2.57	0.53
1:A:313:VAL:O	1:A:317:GLN:HG3	2.09	0.53
1:B:254:ASN:OD1	1:B:256:ARG:HG3	2.09	0.52
1:C:367:GLY:HA3	1:C:375:ARG:HH12	1.74	0.52
1:A:264:TYR:HA	1:A:287:ARG:O	2.10	0.52
1:B:152:TRP:CD1	1:B:161:VAL:HG21	2.45	0.52
1:C:372:GLN:HA	1:C:375:ARG:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:HH12	1:A:412:GLN:HB3	1.74	0.51
1:B:70:PHE:HE1	1:B:80:LEU:HD13	1.74	0.51
1:B:283:CYS:SG	1:B:305:PHE:CD2	3.03	0.51
1:D:161:VAL:HG13	1:D:273:THR:HG22	1.91	0.51
1:A:49:THR:HG23	1:A:79:THR:OG1	2.10	0.51
1:B:333:LEU:HB3	1:B:362:THR:HA	1.91	0.51
1:B:259:ARG:NH1	1:B:264:TYR:OH	2.43	0.51
1:A:355:LEU:O	1:A:358:VAL:HG22	2.10	0.51
1:B:331:ILE:HD12	1:B:358:VAL:HG11	1.91	0.51
1:B:102:GLU:HA	1:B:133:PHE:O	2.11	0.50
1:D:51:LEU:HD22	1:D:86:ALA:HB1	1.94	0.50
1:A:120:GLY:HA3	1:A:279:GLN:HB2	1.93	0.50
1:D:311:ARG:HG2	1:D:311:ARG:HH11	1.76	0.50
1:A:401:ASP:HB3	1:A:406:GLU:HG2	1.94	0.50
1:B:397:ALA:HB3	1:B:415:VAL:HG11	1.93	0.50
1:B:60:THR:O	1:B:64:GLU:HB2	2.12	0.50
1:B:270:GLU:HG3	1:B:281:THR:HG23	1.93	0.50
1:C:56:ILE:HD11	1:C:62:VAL:HB	1.94	0.50
1:D:115:GLU:O	1:D:123:ARG:HD3	2.11	0.50
1:B:150:ARG:HD3	4:B:514:HOH:O	2.11	0.49
1:C:410:VAL:HG21	1:C:418:HIS:CD2	2.48	0.49
1:C:417:ALA:HA	1:C:420:ARG:NH1	2.28	0.49
1:C:47:GLU:HB2	1:C:52:PHE:CE2	2.48	0.49
1:D:256:ARG:NH1	1:D:257:LEU:HA	2.27	0.49
1:D:388:GLY:O	1:D:392:VAL:HG23	2.13	0.49
1:A:52:PHE:CE1	1:A:82:PRO:HD2	2.47	0.49
1:B:111:MET:HB2	1:B:125:PHE:CE1	2.48	0.48
1:C:150:ARG:NH1	1:C:153:ARG:HH22	2.11	0.48
1:B:121:ARG:HD2	3:B:451:AMP:C6	2.47	0.48
1:D:264:TYR:HA	1:D:287:ARG:O	2.13	0.48
1:A:167:SER:HA	1:A:266:ARG:O	2.14	0.48
1:B:115:GLU:O	1:B:123:ARG:HD3	2.13	0.48
1:A:132:VAL:HG11	1:A:140:ILE:HG12	1.95	0.48
1:D:19:THR:O	1:D:23:GLN:HG2	2.14	0.48
1:C:310:GLU:O	1:C:314:LEU:HD23	2.13	0.48
1:B:167:SER:HA	1:B:266:ARG:O	2.14	0.48
1:B:279:GLN:N	1:B:311:ARG:HE	2.13	0.47
1:C:62:VAL:HA	1:C:66:GLU:HB2	1.96	0.47
1:A:61:ASP:HB3	1:A:65:LYS:HE3	1.96	0.47
1:A:62:VAL:HA	1:A:66:GLU:HB2	1.97	0.47
1:A:371:LYS:HD3	1:A:375:ARG:HH21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:VAL:HG13	1:B:407:GLN:HE21	1.79	0.47
1:C:60:THR:O	1:C:64:GLU:HB2	2.14	0.47
1:B:254:ASN:HD21	1:B:256:ARG:HH21	1.62	0.47
1:D:111:MET:HB2	1:D:125:PHE:CZ	2.50	0.47
1:B:254:ASN:ND2	1:B:257:LEU:HB2	2.30	0.47
1:B:168:ILE:HG21	1:B:258:VAL:HG12	1.97	0.47
1:A:345:MET:SD	1:A:364:HIS:HE1	2.38	0.47
1:B:55:ALA:HB2	1:B:295:LEU:HD21	1.97	0.46
1:D:121:ARG:HH11	1:D:311:ARG:NH2	2.12	0.46
1:C:72:ASP:HB2	1:C:78:LEU:HD22	1.98	0.46
1:D:417:ALA:HA	1:D:420:ARG:HH11	1.80	0.46
1:D:136:GLN:NE2	1:D:266:ARG:HH22	2.14	0.46
1:D:397:ALA:HB3	1:D:415:VAL:HG21	1.97	0.46
1:B:320:ASN:O	1:B:322:GLU:N	2.48	0.46
1:B:293:GLU:HA	1:B:297:GLY:O	2.15	0.46
1:A:364:HIS:CD2	1:B:104:ARG:NH2	2.82	0.46
1:B:368:ASN:H	1:B:371:LYS:NZ	2.14	0.46
1:C:142:ALA:CB	1:C:243:LEU:HD22	2.45	0.46
1:C:313:VAL:O	1:C:317:GLN:HG3	2.16	0.46
1:D:128:LEU:HB2	1:D:309:LEU:HD11	1.98	0.46
1:A:363:ASN:OD1	1:A:372:GLN:HG2	2.16	0.45
1:A:374:ALA:HA	1:A:377:ASP:OD2	2.15	0.45
1:C:264:TYR:HA	1:C:287:ARG:O	2.16	0.45
1:B:283:CYS:SG	1:B:305:PHE:HD2	2.39	0.45
1:A:15:LEU:HD22	1:B:97:LEU:HD11	1.97	0.45
1:D:28:THR:O	1:D:32:VAL:HG23	2.16	0.45
1:C:387:LEU:HD23	1:C:392:VAL:HG12	1.99	0.45
1:C:46:VAL:HG22	1:C:80:LEU:HD12	1.99	0.45
1:D:340:THR:HG22	1:D:392:VAL:HG21	1.99	0.45
1:D:347:LEU:CD2	1:D:387:LEU:HD11	2.47	0.45
1:A:399:VAL:O	1:A:407:GLN:HA	2.17	0.45
1:B:138:PRO:HB3	1:B:240:LEU:HB2	1.98	0.45
1:D:265:ASN:ND2	1:D:266:ARG:HG3	2.28	0.45
1:D:266:ARG:HH21	1:D:287:ARG:NE	2.12	0.45
1:A:46:VAL:HG23	1:B:8:ILE:HG13	1.98	0.44
1:C:152:TRP:CD1	1:C:161:VAL:HG21	2.52	0.44
1:D:168:ILE:HD13	1:D:168:ILE:HA	1.78	0.44
1:A:56:ILE:HG22	1:A:60:THR:HG21	1.98	0.44
1:B:135:LEU:HD23	1:B:140:ILE:HG12	1.98	0.44
1:C:355:LEU:O	1:C:358:VAL:HG22	2.17	0.44
1:D:18:GLU:O	1:D:22:TRP:HD1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PHE:O	1:B:240:LEU:HB3	2.18	0.44
1:C:386:VAL:HB	1:C:398:VAL:HB	1.99	0.44
1:D:72:ASP:HB2	1:D:78:LEU:HD22	2.00	0.44
1:C:15:LEU:HD22	1:D:97:LEU:HD11	1.99	0.44
1:B:264:TYR:HA	1:B:287:ARG:O	2.17	0.44
1:C:110:PRO:HG2	1:D:45:ILE:HD11	1.98	0.44
1:A:398:VAL:HG11	1:A:407:GLN:OE1	2.18	0.43
1:B:9:ARG:HD2	1:B:9:ARG:HA	1.75	0.43
1:B:151:TRP:HZ3	1:B:305:PHE:HE2	1.66	0.43
1:B:263:TYR:CG	1:B:291:LEU:HD12	2.53	0.43
1:B:287:ARG:NH1	1:B:303:VAL:HG22	2.33	0.43
1:A:333:LEU:CD1	1:A:348:ALA:HB2	2.47	0.43
1:B:263:TYR:CB	1:B:291:LEU:HD12	2.49	0.43
1:C:5:ILE:HD13	1:D:51:LEU:HA	1.99	0.43
1:C:150:ARG:NH2	1:D:349:GLU:OE1	2.51	0.43
1:A:410:VAL:HG21	1:A:418:HIS:CD2	2.42	0.43
1:B:311:ARG:HH12	3:B:451:AMP:H2'	1.83	0.43
1:C:371:LYS:HB3	1:C:375:ARG:HH11	1.83	0.43
1:D:113:ARG:O	1:D:123:ARG:HA	2.18	0.43
1:D:259:ARG:HH11	1:D:264:TYR:HH	1.67	0.43
1:D:350:ARG:HD3	1:D:354:GLU:OE1	2.18	0.43
1:A:42:ARG:HD2	1:B:19:THR:HG22	2.00	0.43
1:B:355:LEU:HB3	1:B:358:VAL:HG21	2.01	0.43
1:D:167:SER:HA	1:D:266:ARG:O	2.18	0.43
1:A:62:VAL:O	1:A:67:MET:HG3	2.19	0.42
1:C:146:MET:HE2	1:C:247:ALA:HB2	2.00	0.42
1:D:279:GLN:N	1:D:311:ARG:HD2	2.34	0.42
1:D:320:ASN:O	1:D:322:GLU:N	2.51	0.42
1:D:307:MET:SD	1:D:312:LEU:HD22	2.58	0.42
1:A:114:HIS:CE1	1:B:73:ARG:HE	2.37	0.42
1:B:38:TYR:CE1	1:B:104:ARG:HG2	2.53	0.42
1:C:255:GLN:O	1:C:255:GLN:NE2	2.52	0.42
1:C:400:LYS:HB3	1:C:400:LYS:HZ2	1.84	0.42
1:B:102:GLU:OE2	1:B:135:LEU:HD11	2.19	0.42
1:C:259:ARG:NH1	1:C:264:TYR:OH	2.53	0.42
1:A:53:LYS:HD3	1:A:63:VAL:CG1	2.50	0.42
1:A:351:LEU:O	1:A:355:LEU:HD12	2.19	0.42
1:C:56:ILE:HD13	1:C:261:LEU:HD22	2.01	0.42
1:A:46:VAL:CG2	1:B:11:MET:SD	3.03	0.42
1:B:313:VAL:O	1:B:317:GLN:HG3	2.20	0.42
1:C:128:LEU:HD13	1:C:129:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASN:HB3	1:B:76:ASP:OD1	2.20	0.42
1:C:237:PHE:O	1:C:240:LEU:HB3	2.19	0.42
1:D:369:PHE:HE2	1:D:386:VAL:CG1	2.31	0.41
1:D:136:GLN:HA	1:D:287:ARG:HH22	1.82	0.41
1:A:163:LEU:HD23	1:A:251:TYR:HB3	2.02	0.41
1:C:22:TRP:CE2	1:C:313:VAL:HG21	2.56	0.41
1:C:32:VAL:HG13	1:C:150:ARG:HD2	2.01	0.41
1:C:287:ARG:NH1	1:C:303:VAL:HG22	2.35	0.41
1:B:33:LEU:HD13	1:B:106:TRP:CG	2.55	0.41
1:B:266:ARG:HH21	1:B:287:ARG:NE	2.18	0.41
1:A:352:ARG:HH11	1:A:352:ARG:HD2	1.70	0.41
1:B:62:VAL:HA	1:B:66:GLU:HB2	2.03	0.41
1:C:112:PHE:CZ	1:D:45:ILE:HD12	2.52	0.41
1:D:382:ARG:NH2	1:D:423:LEU:HD22	2.36	0.41
1:A:11:MET:HG2	1:A:124:GLN:HB2	2.03	0.41
1:A:165:LEU:HG	1:A:237:PHE:CE1	2.56	0.41
1:A:410:VAL:HG12	1:A:411:ALA:O	2.21	0.41
1:B:327:PRO:O	1:B:359:LYS:NZ	2.54	0.41
1:C:72:ASP:HB3	1:C:74:ASN:ND2	2.36	0.41
1:C:135:LEU:HA	1:C:135:LEU:HD23	1.89	0.41
1:D:279:GLN:N	1:D:311:ARG:NE	2.68	0.41
1:B:128:LEU:HB2	1:B:309:LEU:HD21	2.02	0.41
1:B:316:VAL:O	1:B:320:ASN:HB2	2.21	0.41
1:D:336:SER:O	1:D:388:GLY:HA2	2.21	0.41
1:A:152:TRP:CE3	1:A:157:ILE:HD11	2.56	0.40
1:C:167:SER:HA	1:C:266:ARG:O	2.21	0.40
1:A:310:GLU:HB2	4:A:594:HOH:O	2.21	0.40
1:B:20:ALA:HA	1:B:23:GLN:HE22	1.80	0.40
1:C:166:ASN:ND2	1:C:257:LEU:O	2.53	0.40
1:B:259:ARG:NH2	3:B:451:AMP:O1P	2.54	0.40
1:C:351:LEU:O	1:C:355:LEU:HD12	2.21	0.40
1:D:108:ILE:HD13	1:D:309:LEU:HD21	2.02	0.40
1:B:112:PHE:HA	1:B:123:ARG:O	2.22	0.40
1:C:292:VAL:HG23	4:C:600:HOH:O	2.22	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	360/423 (85%)	344 (96%)	14 (4%)	2 (1%)	21	42
1	B	351/423 (83%)	334 (95%)	13 (4%)	4 (1%)	11	25
1	C	360/423 (85%)	341 (95%)	17 (5%)	2 (1%)	21	42
1	D	351/423 (83%)	327 (93%)	20 (6%)	4 (1%)	11	25
All	All	1422/1692 (84%)	1346 (95%)	64 (4%)	12 (1%)	16	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	PRO
1	B	321	PRO
1	C	321	PRO
1	D	321	PRO
1	A	73	ARG
1	C	73	ARG
1	D	73	ARG
1	B	73	ARG
1	B	119	LYS
1	D	119	LYS
1	B	320	ASN
1	D	320	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/341 (85%)	255 (88%)	36 (12%)	4	9
1	B	285/341 (84%)	254 (89%)	31 (11%)	6	13
1	C	291/341 (85%)	263 (90%)	28 (10%)	8	17
1	D	285/341 (84%)	252 (88%)	33 (12%)	5	11
All	All	1152/1364 (84%)	1024 (89%)	128 (11%)	6	12

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	18	GLU
1	A	19	THR
1	A	23	GLN
1	A	45	ILE
1	A	46	VAL
1	A	61	ASP
1	A	64	GLU
1	A	65	LYS
1	A	66	GLU
1	A	83	GLU
1	A	100	ASN
1	A	116	ARG
1	A	128	LEU
1	A	155	LEU
1	A	158	SER
1	A	174	ARG
1	A	234	ARG
1	A	235	GLU
1	A	243	LEU
1	A	245	GLU
1	A	256	ARG
1	A	257	LEU
1	A	261	LEU
1	A	263	TYR
1	A	268	VAL
1	A	272	VAL
1	A	295	LEU
1	A	303	VAL
1	A	319	VAL
1	A	336	SER
1	A	342	SER
1	A	370	LYS

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Mol	Chain	Res	Type
1	A	390	SER
1	A	404	SER
1	A	413	ASP
1	B	15	LEU
1	B	48	GLN
1	B	65	LYS
1	B	71	GLU
1	B	76	ASP
1	B	80	LEU
1	B	104	ARG
1	B	108	ILE
1	B	118	GLN
1	B	123	ARG
1	B	135	LEU
1	B	140	ILE
1	B	141	ASP
1	B	147	LEU
1	B	158	SER
1	B	166	ASN
1	B	168	ILE
1	B	231	GLU
1	B	232	GLU
1	B	256	ARG
1	B	257	LEU
1	B	258	VAL
1	B	261	LEU
1	B	300	THR
1	B	303	VAL
1	B	320	ASN
1	B	324	LYS
1	B	333	LEU
1	B	342	SER
1	B	359	LYS
1	B	407	GLN
1	C	12	ASN
1	C	39	SER
1	C	56	ILE
1	C	60	THR
1	C	66	GLU
1	C	74	ASN
1	C	83	GLU
1	C	116	ARG

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Mol	Chain	Res	Type
1	C	128	LEU
1	C	165	LEU
1	C	166	ASN
1	C	168	ILE
1	C	171	LEU
1	C	240	LEU
1	C	242	LYS
1	C	243	LEU
1	C	244	LEU
1	C	257	LEU
1	C	263	TYR
1	C	287	ARG
1	C	295	LEU
1	C	300	THR
1	C	303	VAL
1	C	350	ARG
1	C	370	LYS
1	C	382	ARG
1	C	396	THR
1	C	400	LYS
1	D	4	ASN
1	D	15	LEU
1	D	23	GLN
1	D	30	LYS
1	D	51	LEU
1	D	61	ASP
1	D	76	ASP
1	D	78	LEU
1	D	83	GLU
1	D	104	ARG
1	D	108	ILE
1	D	118	GLN
1	D	123	ARG
1	D	161	VAL
1	D	164	GLU
1	D	166	ASN
1	D	231	GLU
1	D	232	GLU
1	D	256	ARG
1	D	268	VAL
1	D	279	GLN
1	D	300	THR

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Mol	Chain	Res	Type
1	D	303	VAL
1	D	311	ARG
1	D	319	VAL
1	D	320	ASN
1	D	324	LYS
1	D	342	SER
1	D	350	ARG
1	D	375	ARG
1	D	403	ARG
1	D	407	GLN
1	D	414	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	HIS
1	A	236	HIS
1	A	274	ASN
1	A	317	GLN
1	A	364	HIS
1	B	4	ASN
1	B	166	ASN
1	B	394	ASN
1	B	407	GLN
1	C	12	ASN
1	C	74	ASN
1	C	95	HIS
1	C	101	GLN
1	C	166	ASN
1	C	255	GLN
1	C	418	HIS
1	D	6	GLN
1	D	74	ASN
1	D	114	HIS
1	D	136	GLN
1	D	265	ASN
1	D	274	ASN

5.3.3 RNA

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](#)

8 ligands are modelled in this entry.

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
3	AMP	C	451	2	25,25,25	1.39	2 (8%)	37,38,38	1.04	0
2	HIS	D	450	3	9,10,11	1.36	1 (11%)	8,12,14	1.33	1 (12%)
2	HIS	B	450	3	9,10,11	1.40	1 (11%)	8,12,14	1.70	2 (25%)
3	AMP	D	451	2	25,25,25	1.26	1 (4%)	37,38,38	0.81	0
2	HIS	A	450	3	9,10,11	1.49	1 (11%)	8,12,14	1.16	0
2	HIS	C	450	3	9,10,11	1.46	2 (22%)	8,12,14	1.84	4 (50%)
3	AMP	B	451	2	25,25,25	1.29	1 (4%)	37,38,38	0.95	0
3	AMP	A	451	2	25,25,25	1.40	2 (8%)	37,38,38	0.79	0

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
3	AMP	C	451	2	-	0/10/26/26	0/3/3/3
2	HIS	D	450	3	-	0/5/6/8	0/1/1/1
2	HIS	B	450	3	-	0/5/6/8	0/1/1/1
3	AMP	D	451	2	-	3/10/26/26	0/3/3/3
2	HIS	A	450	3	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIS	C	450	3	-	1/5/6/8	0/1/1/1
3	AMP	B	451	2	-	0/10/26/26	0/3/3/3
3	AMP	A	451	2	-	0/10/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	451	AMP	P-O3P	5.72	1.76	1.54
3	A	451	AMP	P-O3P	5.52	1.75	1.54
3	B	451	AMP	P-O3P	5.26	1.74	1.54
3	D	451	AMP	P-O3P	4.86	1.72	1.54
2	B	450	HIS	CB-CG	2.71	1.57	1.49
2	A	450	HIS	CG-ND1	-2.67	1.31	1.38
2	D	450	HIS	CG-ND1	-2.48	1.32	1.38
3	A	451	AMP	P-O2P	-2.40	1.45	1.54
2	C	450	HIS	CB-CG	2.15	1.55	1.49
3	C	451	AMP	P-O2P	-2.08	1.47	1.54
2	C	450	HIS	CG-ND1	-2.04	1.33	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	HIS	CD2-NE2-CE1	2.93	112.59	107.36
2	C	450	HIS	CD2-NE2-CE1	2.81	112.38	107.36
2	C	450	HIS	CG-CD2-NE2	-2.50	102.69	106.54
2	D	450	HIS	CD2-NE2-CE1	2.29	111.45	107.36
2	B	450	HIS	CG-CD2-NE2	-2.27	103.06	106.54
2	C	450	HIS	CA-CB-CG	2.08	118.89	113.77
2	C	450	HIS	CB-CG-CD2	-2.05	125.15	129.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

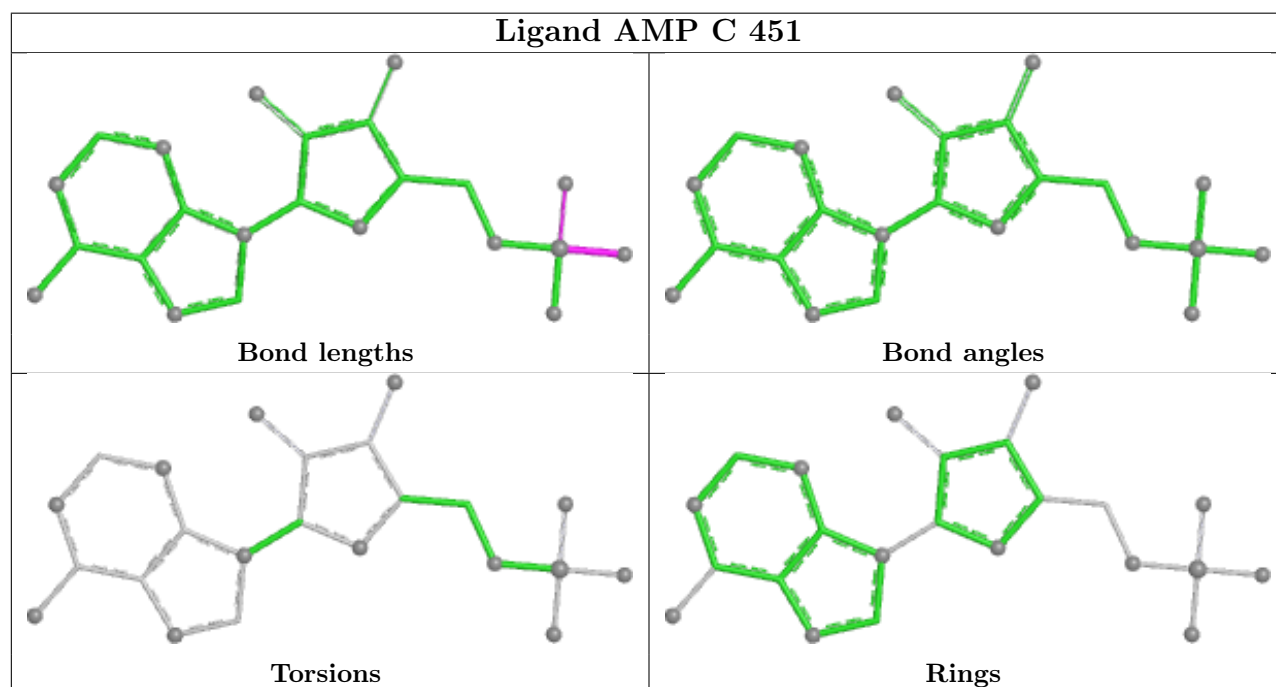
Mol	Chain	Res	Type	Atoms
2	C	450	HIS	O-C-CA-CB
3	D	451	AMP	C5'-O5'-P-O2P
3	D	451	AMP	C5'-O5'-P-O1P
3	D	451	AMP	C5'-O5'-P-O3P

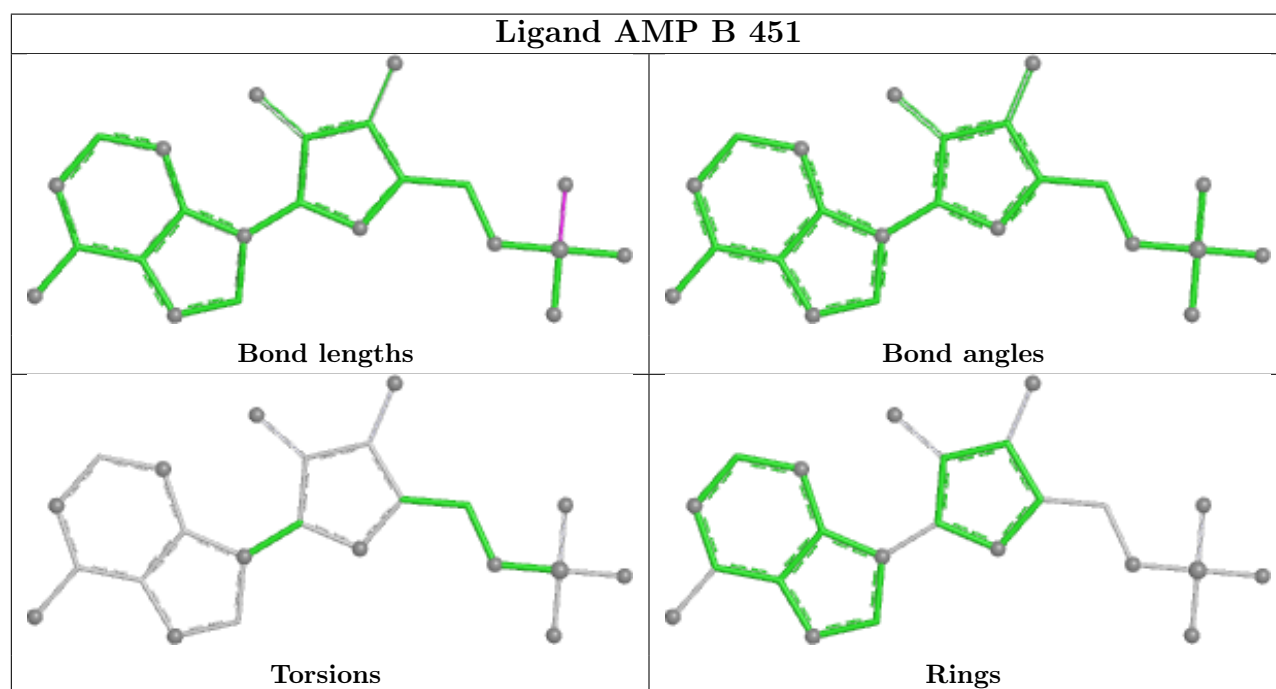
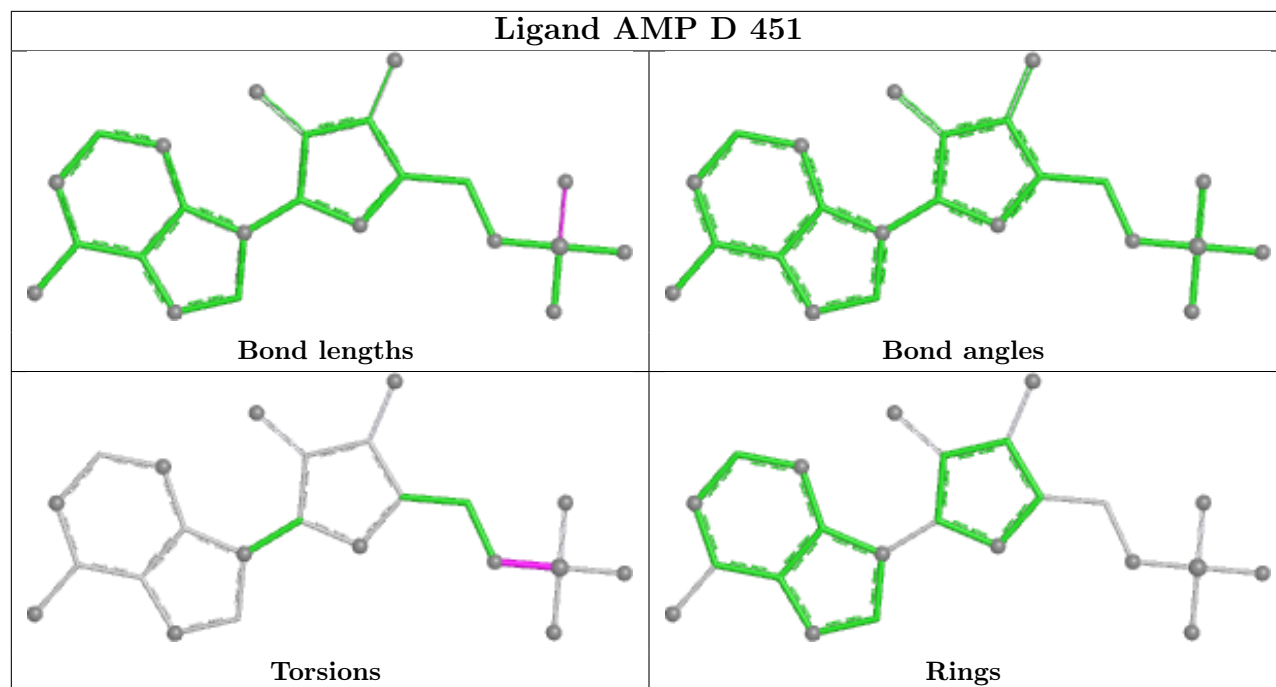
There are no ring outliers.

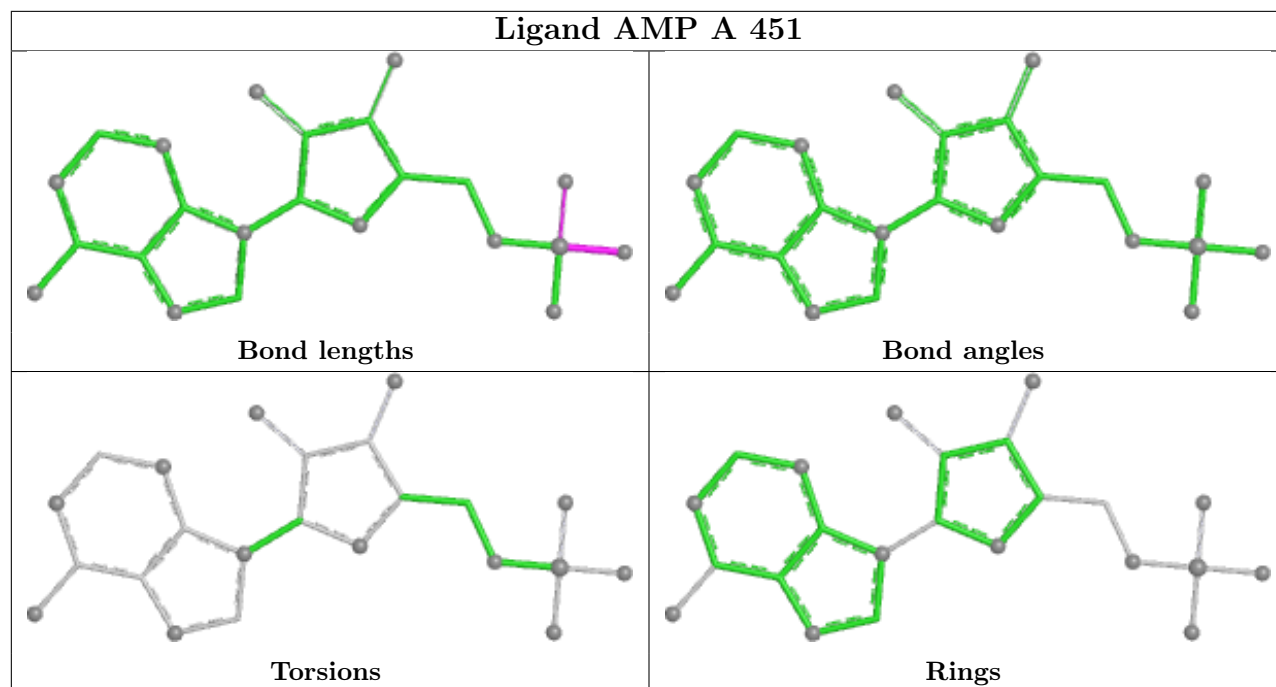
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	451	AMP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.