



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:23 AM UTC

PDB ID : 1GPH / pdb_00001gph
Title : STRUCTURE OF THE ALLOSTERIC REGULATORY ENZYME OF
PURINE BIOSYNTHESIS
Authors : Smith, J.L.
Deposited on : 1994-04-20
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

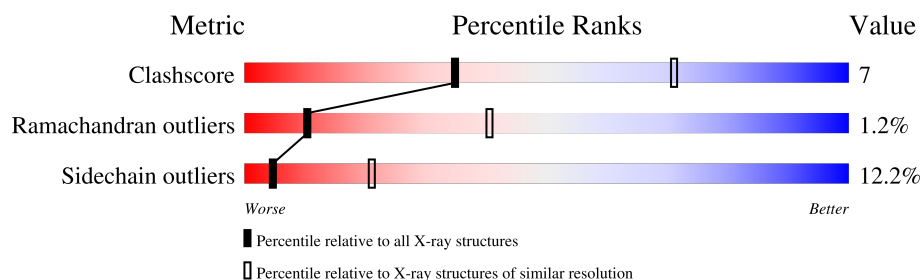
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	1	465	
1	2	465	
1	3	465	
1	4	465	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	1	466	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14676 atoms, of which 304 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.

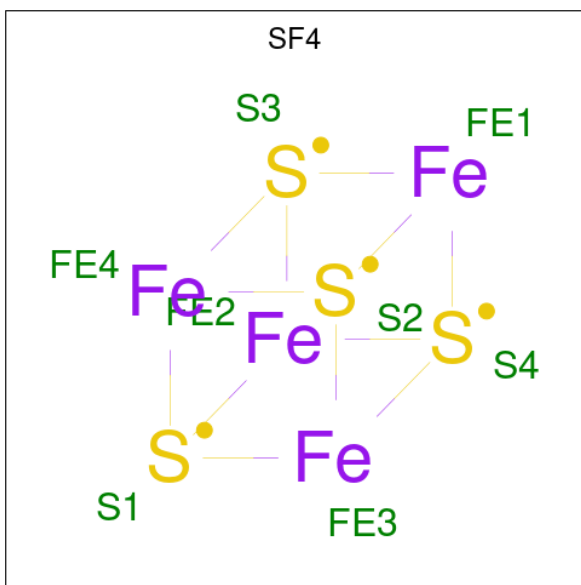
- Molecule 1 is a protein called GLUTAMINE PHOSPHORIBOSYL-PYROPHOSPHATE AMIDOTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1	465	Total	C	H	N	O	S	0	0	0
			3615	2212	76	620	687	20			
1	2	465	Total	C	H	N	O	S	0	0	0
			3615	2212	76	620	687	20			
1	3	465	Total	C	H	N	O	S	0	0	0
			3615	2212	76	620	687	20			
1	4	465	Total	C	H	N	O	S	0	0	0
			3615	2212	76	620	687	20			

There are 4 discrepancies between the modelled and reference sequences:

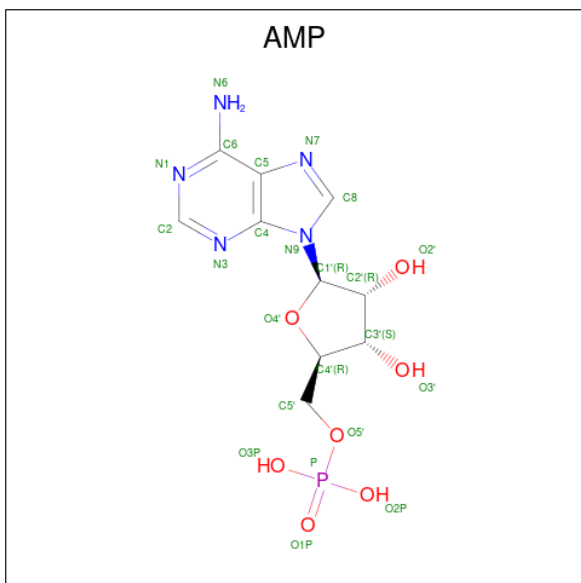
Chain	Residue	Modelled	Actual	Comment	Reference
1	402	ASP	GLY	conflict	UNP P00497
2	402	ASP	GLY	conflict	UNP P00497
3	402	ASP	GLY	conflict	UNP P00497
4	402	ASP	GLY	conflict	UNP P00497

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1	1	Total	Fe	S	0	0
			8	4	4		
2	2	1	Total	Fe	S	0	0
			8	4	4		
2	3	1	Total	Fe	S	0	0
			8	4	4		
2	4	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



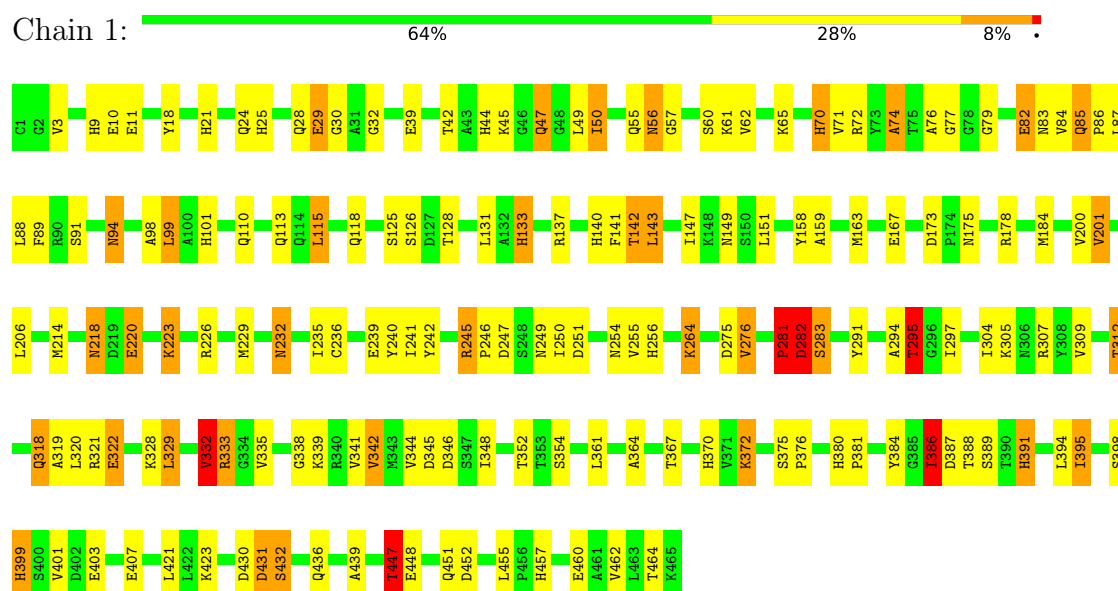
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	1	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

3 Residue-property plots

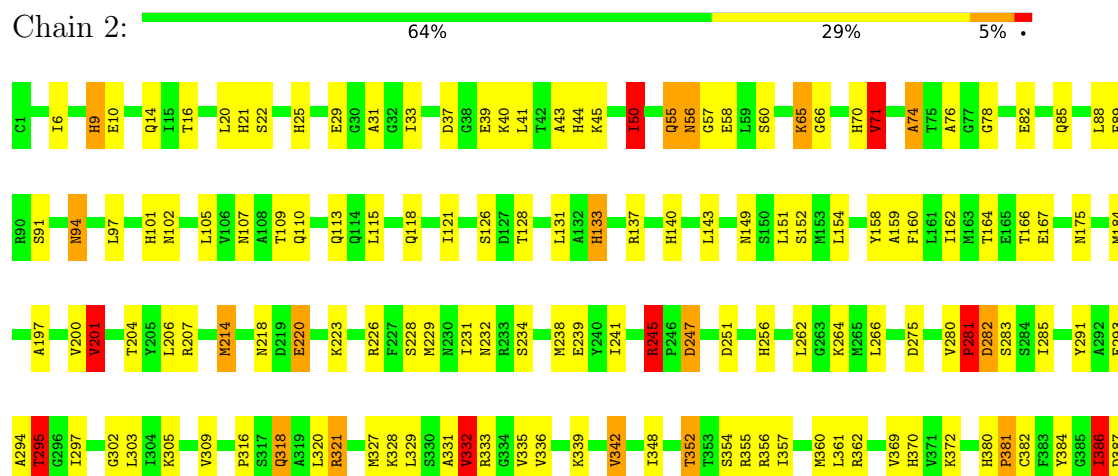
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



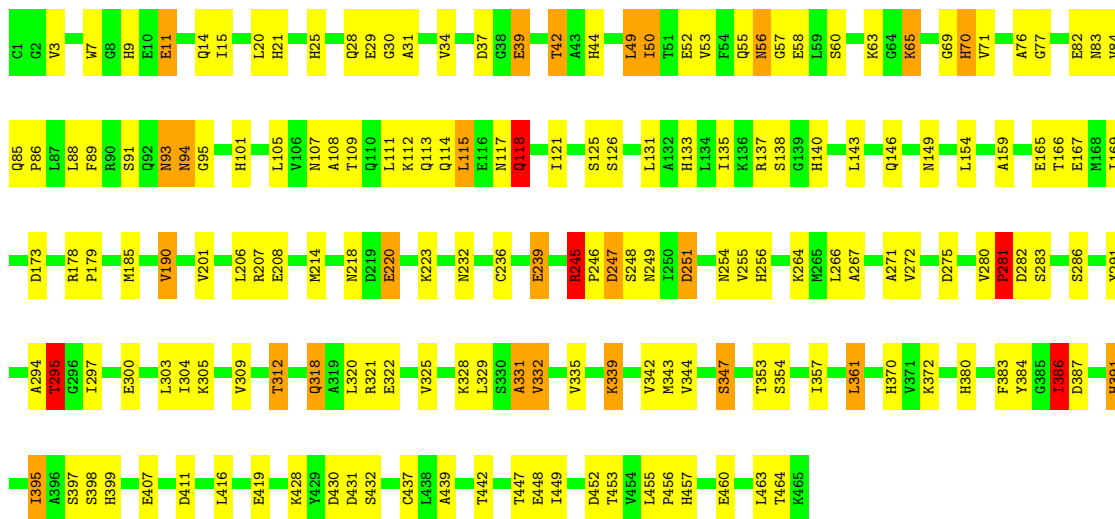
- Molecule 1: GLUTAMINE PHOSPHORIBOSYL-PYROPHOSPHATE AMIDOTRANSFERASE





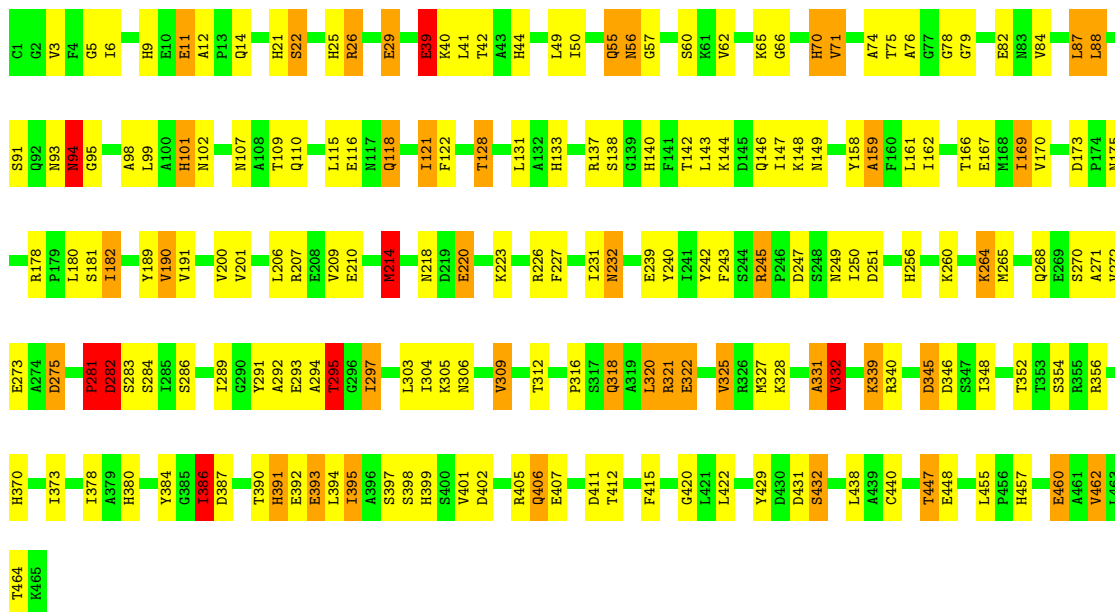
• Molecule 1: GLUTAMINE PHOSPHORIBOSYL-PYROPHOSPHATE AMIDOTRANSFERASE

Chain 3: 63% 31% 5% •



• Molecule 1: GLUTAMINE PHOSPHORIBOSYL-PYROPHOSPHATE AMIDOTRANSFERASE

Chain 4: 59% 30% 9% •



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	158.80Å 75.70Å 94.10Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14676	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: SF4, 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	1	1.13	32/3597 (0.9%)	1.97	118/4857 (2.4%)
1	2	1.09	28/3597 (0.8%)	1.92	105/4857 (2.2%)
1	3	1.08	26/3597 (0.7%)	1.95	112/4857 (2.3%)
1	4	1.08	28/3597 (0.8%)	1.93	115/4857 (2.4%)
All	All	1.10	114/14388 (0.8%)	1.95	450/19428 (2.3%)

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	1	0	1

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	370	HIS	CD2-NE2	-7.73	1.29	1.37
1	1	25	HIS	CD2-NE2	-7.68	1.29	1.37
1	4	332	VAL	CA-CB	7.57	1.62	1.53
1	3	70	HIS	CD2-NE2	-7.51	1.29	1.37
1	2	25	HIS	CD2-NE2	-7.29	1.29	1.37
1	4	70	HIS	CD2-NE2	-7.06	1.30	1.37
1	2	256	HIS	CD2-NE2	-7.04	1.30	1.37
1	1	70	HIS	CD2-NE2	-7.04	1.30	1.37
1	3	256	HIS	CD2-NE2	-6.92	1.30	1.37
1	2	380	HIS	CD2-NE2	-6.87	1.30	1.37
1	2	70	HIS	CD2-NE2	-6.77	1.30	1.37
1	3	44	HIS	CD2-NE2	-6.73	1.30	1.37
1	1	380	HIS	CD2-NE2	-6.72	1.30	1.37
1	3	25	HIS	CD2-NE2	-6.72	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	370	HIS	CD2-NE2	-6.72	1.30	1.37
1	2	25	HIS	CG-ND1	-6.71	1.30	1.38
1	2	342	VAL	CA-CB	6.66	1.62	1.54
1	2	399	HIS	CD2-NE2	-6.63	1.30	1.37
1	1	342	VAL	CA-CB	6.52	1.62	1.54
1	3	190	VAL	CA-CB	6.51	1.66	1.55
1	2	391	HIS	CD2-NE2	-6.50	1.30	1.37
1	1	332	VAL	CA-CB	6.45	1.61	1.53
1	1	25	HIS	CG-ND1	-6.41	1.31	1.38
1	3	380	HIS	CD2-NE2	-6.40	1.30	1.37
1	1	9	HIS	CD2-NE2	-6.39	1.30	1.37
1	2	332	VAL	CA-CB	6.37	1.61	1.53
1	3	101	HIS	CD2-NE2	-6.34	1.30	1.37
1	3	391	HIS	CG-ND1	-6.27	1.31	1.38
1	4	133	HIS	CD2-NE2	-6.26	1.30	1.37
1	4	391	HIS	CD2-NE2	-6.24	1.30	1.37
1	1	101	HIS	CD2-NE2	-6.23	1.30	1.37
1	3	70	HIS	CG-ND1	-6.21	1.31	1.38
1	3	399	HIS	CD2-NE2	-6.19	1.31	1.37
1	1	399	HIS	CD2-NE2	-6.18	1.31	1.37
1	3	133	HIS	CD2-NE2	-6.18	1.31	1.37
1	2	457	HIS	CD2-NE2	-6.15	1.31	1.37
1	1	391	HIS	CD2-NE2	-6.04	1.31	1.37
1	2	391	HIS	CG-ND1	-6.04	1.31	1.38
1	4	133	HIS	CG-ND1	-6.04	1.31	1.38
1	2	21	HIS	CD2-NE2	-6.03	1.31	1.37
1	2	101	HIS	CD2-NE2	-6.03	1.31	1.37
1	3	140	HIS	CD2-NE2	-6.03	1.31	1.37
1	1	386	ILE	CA-CB	6.02	1.61	1.54
1	1	21	HIS	CD2-NE2	-6.01	1.31	1.37
1	1	256	HIS	CD2-NE2	-5.98	1.31	1.37
1	3	399	HIS	CG-ND1	-5.98	1.31	1.38
1	4	256	HIS	CD2-NE2	-5.96	1.31	1.37
1	1	370	HIS	CD2-NE2	-5.96	1.31	1.37
1	2	457	HIS	CG-ND1	-5.89	1.31	1.38
1	1	457	HIS	CD2-NE2	-5.88	1.31	1.37
1	2	133	HIS	CG-ND1	-5.88	1.31	1.38
1	3	391	HIS	CD2-NE2	-5.86	1.31	1.37
1	3	44	HIS	CG-ND1	-5.86	1.31	1.38
1	3	457	HIS	CD2-NE2	-5.82	1.31	1.37
1	4	44	HIS	CD2-NE2	-5.82	1.31	1.37
1	1	21	HIS	CG-ND1	-5.81	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	21	HIS	CG-ND1	-5.81	1.31	1.38
1	1	375	SER	CA-CB	-5.80	1.45	1.54
1	4	21	HIS	CD2-NE2	-5.79	1.31	1.37
1	1	256	HIS	CG-ND1	-5.77	1.31	1.38
1	2	44	HIS	CD2-NE2	-5.75	1.31	1.37
1	1	44	HIS	CD2-NE2	-5.74	1.31	1.37
1	3	457	HIS	CG-ND1	-5.74	1.31	1.38
1	3	9	HIS	CD2-NE2	-5.73	1.31	1.37
1	4	457	HIS	CD2-NE2	-5.72	1.31	1.37
1	2	44	HIS	CG-ND1	-5.70	1.31	1.38
1	4	25	HIS	CD2-NE2	-5.67	1.31	1.37
1	4	380	HIS	CD2-NE2	-5.67	1.31	1.37
1	1	380	HIS	CG-ND1	-5.66	1.32	1.38
1	4	9	HIS	CD2-NE2	-5.65	1.31	1.37
1	4	399	HIS	CD2-NE2	-5.65	1.31	1.37
1	3	140	HIS	CG-ND1	-5.65	1.32	1.38
1	1	70	HIS	CG-ND1	-5.60	1.32	1.38
1	2	101	HIS	CG-ND1	-5.59	1.32	1.38
1	4	386	ILE	CA-CB	5.58	1.61	1.54
1	3	101	HIS	CG-ND1	-5.57	1.32	1.38
1	3	133	HIS	CG-ND1	-5.54	1.32	1.38
1	4	140	HIS	CD2-NE2	-5.52	1.31	1.37
1	1	370	HIS	CG-ND1	-5.51	1.32	1.38
1	1	133	HIS	CG-ND1	-5.50	1.32	1.38
1	1	133	HIS	CD2-NE2	-5.50	1.31	1.37
1	2	9	HIS	CD2-NE2	-5.48	1.31	1.37
1	4	44	HIS	CG-ND1	-5.47	1.32	1.38
1	1	391	HIS	CG-ND1	-5.44	1.32	1.38
1	2	140	HIS	CD2-NE2	-5.44	1.31	1.37
1	4	304	ILE	CA-CB	5.44	1.61	1.54
1	2	380	HIS	CG-ND1	-5.43	1.32	1.38
1	1	9	HIS	CG-ND1	-5.39	1.32	1.38
1	1	399	HIS	CG-ND1	-5.39	1.32	1.38
1	1	281	PRO	CA-CB	-5.38	1.46	1.53
1	3	21	HIS	CD2-NE2	-5.36	1.31	1.37
1	4	21	HIS	CG-ND1	-5.35	1.32	1.38
1	4	101	HIS	CG-ND1	-5.35	1.32	1.38
1	4	399	HIS	CG-ND1	-5.33	1.32	1.38
1	1	101	HIS	CG-ND1	-5.31	1.32	1.38
1	1	457	HIS	CG-ND1	-5.31	1.32	1.38
1	2	133	HIS	CD2-NE2	-5.30	1.32	1.37
1	3	25	HIS	CG-ND1	-5.26	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	70	HIS	CG-ND1	-5.24	1.32	1.38
1	4	101	HIS	CD2-NE2	-5.22	1.32	1.37
1	4	380	HIS	CG-ND1	-5.21	1.32	1.38
1	4	391	HIS	CG-ND1	-5.20	1.32	1.38
1	3	9	HIS	CG-ND1	-5.20	1.32	1.38
1	4	62	VAL	CA-CB	5.19	1.60	1.53
1	2	256	HIS	CG-ND1	-5.19	1.32	1.38
1	4	256	HIS	CG-ND1	-5.19	1.32	1.38
1	1	140	HIS	CD2-NE2	-5.17	1.32	1.37
1	4	25	HIS	CG-ND1	-5.16	1.32	1.38
1	2	370	HIS	CG-ND1	-5.16	1.32	1.38
1	3	332	VAL	CA-CB	5.11	1.60	1.53
1	2	281	PRO	CA-CB	-5.11	1.46	1.53
1	1	44	HIS	CG-ND1	-5.03	1.32	1.38
1	2	140	HIS	CG-ND1	-5.02	1.32	1.38
1	4	169	ILE	CA-CB	5.01	1.60	1.54

All (450) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	118	GLN	OE1-CD-NE2	-13.84	108.76	122.60
1	3	57	GLY	N-CA-C	-13.57	99.06	113.58
1	2	430	ASP	CA-CB-CG	10.91	123.51	112.60
1	1	281	PRO	O-C-N	10.34	136.60	122.64
1	1	295	THR	N-CA-CB	-10.19	94.61	110.30
1	3	295	THR	N-CA-CB	-9.62	96.39	110.53
1	4	118	GLN	OE1-CD-NE2	-9.50	113.10	122.60
1	2	247	ASP	CA-CB-CG	9.14	121.74	112.60
1	1	387	ASP	CA-CB-CG	8.98	121.58	112.60
1	2	56	ASN	CA-CB-CG	-8.83	103.77	112.60
1	4	70	HIS	ND1-CG-CD2	8.72	114.82	106.10
1	2	21	HIS	ND1-CG-CD2	8.70	114.80	106.10
1	1	452	ASP	CA-CB-CG	8.66	121.26	112.60
1	1	283	SER	CA-CB-OG	8.56	128.23	111.10
1	1	430	ASP	CA-CB-CG	8.56	121.16	112.60
1	4	283	SER	CA-CB-OG	8.53	128.17	111.10
1	3	118	GLN	CG-CD-NE2	8.42	129.03	116.40
1	1	21	HIS	ND1-CG-CD2	8.41	114.51	106.10
1	4	281	PRO	O-C-N	8.33	133.88	122.64
1	2	76	ALA	N-CA-C	-8.31	96.54	109.25
1	4	386	ILE	CB-CA-C	-8.19	101.31	112.04
1	3	247	ASP	CA-CB-CG	8.05	120.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	282	ASP	CA-C-O	-8.01	109.06	120.51
1	4	387	ASP	CA-CB-CG	7.99	120.59	112.60
1	3	439	ALA	N-CA-C	7.97	120.68	111.11
1	1	245	ARG	CB-CG-CD	-7.95	93.01	111.30
1	3	281	PRO	O-C-N	7.94	131.99	123.10
1	3	380	HIS	ND1-CG-CD2	7.93	114.03	106.10
1	1	281	PRO	CA-C-N	7.92	136.67	121.54
1	1	281	PRO	C-N-CA	7.92	136.67	121.54
1	3	457	HIS	ND1-CG-CD2	7.91	114.01	106.10
1	3	107	ASN	OD1-CG-ND2	-7.89	114.71	122.60
1	2	391	HIS	ND1-CG-CD2	7.82	113.92	106.10
1	2	399	HIS	ND1-CG-CD2	7.81	113.91	106.10
1	1	76	ALA	N-CA-C	-7.75	94.90	108.23
1	1	386	ILE	CB-CA-C	-7.73	101.98	111.88
1	2	280	VAL	N-CA-C	-7.72	98.93	107.73
1	1	431	ASP	CA-CB-CG	7.72	120.32	112.60
1	1	232	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	3	283	SER	CA-CB-OG	7.69	126.48	111.10
1	3	76	ALA	N-CA-C	-7.62	95.12	108.23
1	1	25	HIS	ND1-CG-CD2	7.58	113.68	106.10
1	4	457	HIS	ND1-CG-CD2	7.55	113.65	106.10
1	3	140	HIS	ND1-CG-CD2	7.54	113.64	106.10
1	4	399	HIS	ND1-CG-CD2	7.52	113.62	106.10
1	2	457	HIS	ND1-CG-CD2	7.51	113.61	106.10
1	2	387	ASP	CA-CB-CG	7.51	120.11	112.60
1	3	391	HIS	ND1-CG-CD2	7.50	113.60	106.10
1	1	391	HIS	ND1-CG-CD2	7.49	113.59	106.10
1	1	247	ASP	CA-CB-CG	7.48	120.08	112.60
1	3	133	HIS	ND1-CG-CD2	7.47	113.57	106.10
1	3	256	HIS	ND1-CG-CD2	7.46	113.56	106.10
1	3	342	VAL	N-CA-C	-7.45	97.73	108.17
1	2	239	GLU	N-CA-C	-7.45	103.09	111.14
1	1	399	HIS	ND1-CG-CD2	7.40	113.50	106.10
1	3	101	HIS	CA-CB-CG	7.38	121.18	113.80
1	2	245	ARG	CB-CG-CD	-7.38	94.33	111.30
1	3	251	ASP	CA-CB-CG	-7.35	105.25	112.60
1	2	118	GLN	OE1-CD-NE2	-7.35	115.25	122.60
1	1	370	HIS	ND1-CG-CD2	7.35	113.45	106.10
1	1	352	THR	N-CA-C	7.34	119.98	111.02
1	1	380	HIS	ND1-CG-CD2	7.34	113.44	106.10
1	2	140	HIS	ND1-CG-CD2	7.31	113.41	106.10
1	3	387	ASP	CA-CB-CG	7.29	119.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	70	HIS	ND1-CG-CD2	7.28	113.38	106.10
1	2	370	HIS	ND1-CG-CD2	7.25	113.35	106.10
1	2	402	ASP	CA-CB-CG	-7.24	105.36	112.60
1	2	431	ASP	CA-CB-CG	7.24	119.83	112.60
1	2	85	GLN	CA-C-O	-7.18	114.69	121.08
1	3	30	GLY	CA-C-O	-7.17	114.61	121.49
1	2	70	HIS	CA-CB-CG	7.14	120.94	113.80
1	3	399	HIS	ND1-CG-CD2	7.14	113.24	106.10
1	4	380	HIS	ND1-CG-CD2	7.13	113.23	106.10
1	3	232	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	2	281	PRO	O-C-N	7.12	132.26	122.64
1	4	273	GLU	N-CA-C	-7.11	97.62	109.07
1	1	201	VAL	N-CA-CB	-7.10	100.15	112.08
1	1	149	ASN	CA-CB-CG	-7.08	105.52	112.60
1	1	140	HIS	ND1-CG-CD2	7.07	113.17	106.10
1	3	21	HIS	ND1-CG-CD2	7.07	113.17	106.10
1	2	71	VAL	N-CA-C	-7.07	97.94	108.12
1	3	14	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	1	255	VAL	CA-C-O	-7.06	113.73	121.29
1	2	57	GLY	N-CA-C	-7.04	96.50	113.18
1	4	76	ALA	N-CA-C	-7.03	97.09	108.41
1	2	140	HIS	CA-CB-CG	-7.03	106.77	113.80
1	1	457	HIS	ND1-CG-CD2	7.02	113.12	106.10
1	3	149	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	1	401	VAL	CA-C-O	-6.99	113.09	120.57
1	2	439	ALA	N-CA-C	6.97	119.53	111.02
1	2	201	VAL	N-CA-CB	-6.96	102.74	112.35
1	3	419	GLU	N-CA-C	-6.95	103.64	111.14
1	4	391	HIS	ND1-CG-CD2	6.95	113.05	106.10
1	3	395	ILE	CA-CB-CG2	-6.94	98.70	110.50
1	4	256	HIS	ND1-CG-CD2	6.94	113.04	106.10
1	2	380	HIS	ND1-CG-CD2	6.93	113.03	106.10
1	1	282	ASP	CA-C-O	-6.92	110.61	120.51
1	3	9	HIS	ND1-CG-CD2	6.89	112.99	106.10
1	4	21	HIS	ND1-CG-CD2	6.88	112.98	106.10
1	1	380	HIS	CA-C-N	6.88	126.84	120.03
1	1	380	HIS	C-N-CA	6.88	126.84	120.03
1	3	218	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	4	281	PRO	CA-C-N	6.87	134.67	121.54
1	4	281	PRO	C-N-CA	6.87	134.67	121.54
1	2	462	VAL	O-C-N	6.87	129.68	122.67
1	4	9	HIS	ND1-CG-CD2	6.85	112.95	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	282	ASP	CA-C-O	-6.83	110.74	120.51
1	1	118	GLN	OE1-CD-NE2	-6.82	115.78	122.60
1	4	55	GLN	CA-C-N	6.82	134.57	121.54
1	4	55	GLN	C-N-CA	6.82	134.57	121.54
1	4	386	ILE	N-CA-CB	6.82	118.99	110.47
1	3	214	MET	CA-CB-CG	6.81	127.72	114.10
1	1	295	THR	N-CA-C	6.81	120.81	112.23
1	1	173	ASP	CA-C-N	6.81	126.49	119.82
1	1	173	ASP	C-N-CA	6.81	126.49	119.82
1	2	25	HIS	ND1-CG-CD2	6.81	112.91	106.10
1	2	70	HIS	ND1-CG-CD2	6.80	112.90	106.10
1	3	114	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	3	256	HIS	CG-CD2-NE2	-6.77	100.43	107.20
1	3	50	ILE	CB-CA-C	-6.77	103.31	111.97
1	1	9	HIS	ND1-CG-CD2	6.75	112.85	106.10
1	2	102	ASN	CA-CB-CG	6.74	119.34	112.60
1	4	247	ASP	CA-CB-CG	6.74	119.34	112.60
1	4	370	HIS	ND1-CG-CD2	6.74	112.83	106.10
1	3	83	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	1	44	HIS	ND1-CG-CD2	6.71	112.81	106.10
1	4	295	THR	N-CA-CB	-6.71	99.97	110.44
1	4	57	GLY	N-CA-C	-6.71	97.29	113.18
1	3	353	THR	N-CA-C	6.70	119.15	111.11
1	2	14	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	2	355	ARG	N-CA-C	-6.69	103.92	111.14
1	3	95	GLY	N-CA-C	6.68	118.86	112.04
1	3	280	VAL	N-CA-C	-6.67	100.61	107.89
1	1	142	THR	CA-CB-OG1	-6.67	99.59	109.60
1	3	70	HIS	ND1-CG-CD2	6.65	112.75	106.10
1	1	84	VAL	N-CA-C	-6.65	100.17	109.21
1	2	282	ASP	CA-C-O	-6.63	111.02	120.51
1	2	101	HIS	ND1-CG-CD2	6.63	112.73	106.10
1	1	386	ILE	N-CA-CB	6.63	117.87	110.51
1	4	402	ASP	CA-CB-CG	-6.62	105.97	112.60
1	2	21	HIS	CG-CD2-NE2	-6.62	100.58	107.20
1	3	58	GLU	N-CA-C	6.61	120.56	112.23
1	3	295	THR	CB-CA-C	6.60	121.31	109.29
1	2	110	GLN	CA-CB-CG	6.57	127.25	114.10
1	2	9	HIS	ND1-CG-CD2	6.56	112.66	106.10
1	2	295	THR	N-CA-CB	-6.55	100.18	110.46
1	3	430	ASP	CA-CB-CG	6.54	119.14	112.60
1	3	386	ILE	CB-CA-C	-6.50	103.36	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	118	GLN	CA-CB-CG	6.49	127.07	114.10
1	3	397	SER	N-CA-C	-6.47	103.73	111.69
1	3	29	GLU	CB-CG-CD	6.46	123.59	112.60
1	4	110	GLN	CA-CB-CG	6.45	127.01	114.10
1	2	55	GLN	CA-C-N	6.45	133.86	121.54
1	2	55	GLN	C-N-CA	6.45	133.86	121.54
1	1	110	GLN	N-CA-CB	-6.45	100.50	109.91
1	4	44	HIS	ND1-CG-CD2	6.45	112.55	106.10
1	2	16	THR	CA-C-O	-6.44	113.59	120.42
1	3	140	HIS	CA-CB-CG	-6.44	107.36	113.80
1	4	133	HIS	ND1-CG-CD2	6.42	112.52	106.10
1	1	376	PRO	O-C-N	-6.41	113.90	121.46
1	2	149	ASN	CA-CB-CG	-6.40	106.20	112.60
1	1	332	VAL	CA-C-O	6.38	128.57	120.97
1	2	201	VAL	CB-CA-C	6.38	117.84	110.88
1	4	25	HIS	ND1-CG-CD2	6.38	112.48	106.10
1	1	158	TYR	N-CA-C	6.37	118.44	107.93
1	2	110	GLN	N-CA-C	-6.37	104.26	111.14
1	1	113	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	3	370	HIS	ND1-CG-CD2	6.35	112.45	106.10
1	1	395	ILE	CB-CG1-CD1	-6.34	100.48	113.80
1	1	345	ASP	CA-CB-CG	6.34	118.94	112.60
1	4	159	ALA	N-CA-C	-6.33	97.95	108.34
1	2	283	SER	N-CA-C	6.32	118.17	111.28
1	3	220	GLU	CB-CG-CD	6.32	123.34	112.60
1	4	245	ARG	CB-CG-CD	-6.31	96.79	111.30
1	3	25	HIS	ND1-CG-CD2	6.30	112.40	106.10
1	2	406	GLN	CA-CB-CG	-6.29	101.52	114.10
1	1	110	GLN	CA-CB-CG	6.29	126.68	114.10
1	2	381	PRO	N-CA-C	6.28	121.37	111.38
1	1	85	GLN	OE1-CD-NE2	-6.28	116.32	122.60
1	1	133	HIS	ND1-CG-CD2	6.28	112.38	106.10
1	4	348	ILE	N-CA-C	-6.27	99.34	108.11
1	2	386	ILE	CB-CA-C	-6.26	103.68	112.14
1	1	50	ILE	N-CA-CB	6.26	117.46	110.51
1	3	101	HIS	ND1-CG-CD2	6.23	112.33	106.10
1	4	393	GLU	N-CA-C	6.22	118.81	110.35
1	1	370	HIS	CG-CD2-NE2	-6.19	101.01	107.20
1	4	109	THR	CA-C-N	6.19	128.49	120.44
1	4	109	THR	C-N-CA	6.19	128.49	120.44
1	1	55	GLN	CA-C-N	6.18	133.34	121.54
1	1	55	GLN	C-N-CA	6.18	133.34	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	50	ILE	CB-CA-C	-6.17	103.99	111.88
1	3	179	PRO	N-CA-C	6.16	120.93	111.57
1	4	56	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	4	29	GLU	CB-CG-CD	6.12	123.00	112.60
1	1	159	ALA	N-CA-C	-6.11	98.56	108.52
1	2	45	LYS	CA-CB-CG	6.10	126.30	114.10
1	3	44	HIS	ND1-CG-CD2	6.08	112.19	106.10
1	3	431	ASP	CA-CB-CG	6.08	118.68	112.60
1	4	331	ALA	CA-C-O	-6.08	114.93	121.56
1	4	26	ARG	NE-CZ-NH1	6.07	127.57	121.50
1	3	395	ILE	CA-CB-CG1	6.07	120.72	110.40
1	3	52	GLU	N-CA-C	-6.07	104.59	111.14
1	2	399	HIS	CB-CG-CD2	-6.07	123.32	131.20
1	4	340	ARG	N-CA-C	-6.07	97.25	107.99
1	4	70	HIS	CG-CD2-NE2	-6.06	101.14	107.20
1	2	380	HIS	CA-C-N	6.06	125.97	119.85
1	2	380	HIS	C-N-CA	6.06	125.97	119.85
1	4	140	HIS	ND1-CG-CD2	6.06	112.16	106.10
1	1	42	THR	N-CA-CB	-6.04	100.37	111.37
1	1	254	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	4	55	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	4	173	ASP	CA-C-N	6.02	125.72	119.82
1	4	173	ASP	C-N-CA	6.02	125.72	119.82
1	4	264	LYS	CA-CB-CG	-6.02	102.06	114.10
1	3	55	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	3	166	THR	N-CA-C	6.00	121.52	113.72
1	2	318	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	3	133	HIS	CG-CD2-NE2	-5.99	101.22	107.20
1	4	297	ILE	N-CA-C	-5.98	103.49	108.63
1	4	118	GLN	N-CA-C	-5.97	106.04	113.15
1	1	101	HIS	ND1-CG-CD2	5.96	112.06	106.10
1	3	126	SER	N-CA-CB	-5.96	101.06	110.06
1	3	380	HIS	CG-CD2-NE2	-5.96	101.24	107.20
1	3	380	HIS	CA-C-N	5.95	125.92	120.03
1	3	380	HIS	C-N-CA	5.95	125.92	120.03
1	2	430	ASP	O-C-N	5.94	130.44	122.96
1	4	380	HIS	CA-C-N	5.93	125.69	119.76
1	4	380	HIS	C-N-CA	5.93	125.69	119.76
1	1	232	ASN	CB-CG-ND2	5.93	125.30	116.40
1	4	84	VAL	N-CA-C	-5.93	101.06	108.89
1	4	166	THR	N-CA-CB	-5.93	103.16	110.98
1	2	370	HIS	CB-CG-CD2	-5.92	123.50	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	118	GLN	CG-CD-NE2	5.91	125.27	116.40
1	3	452	ASP	CA-CB-CG	5.91	118.51	112.60
1	3	159	ALA	N-CA-C	-5.89	97.71	108.02
1	3	140	HIS	CG-CD2-NE2	-5.89	101.31	107.20
1	4	95	GLY	N-CA-C	5.89	118.04	112.04
1	4	275	ASP	CA-CB-CG	5.88	118.48	112.60
1	2	397	SER	N-CA-C	-5.86	104.97	111.36
1	3	220	GLU	CA-CB-CG	5.86	125.83	114.10
1	3	125	SER	CA-C-O	5.84	127.02	119.95
1	1	57	GLY	N-CA-C	-5.83	99.36	113.18
1	3	457	HIS	CG-CD2-NE2	-5.83	101.37	107.20
1	4	82	GLU	CB-CA-C	-5.83	98.83	110.42
1	2	281	PRO	CA-C-N	5.82	132.66	121.54
1	2	281	PRO	C-N-CA	5.82	132.66	121.54
1	3	380	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	2	128	THR	N-CA-CB	-5.82	101.33	110.06
1	4	306	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	1	256	HIS	ND1-CG-CD2	5.80	111.90	106.10
1	2	58	GLU	N-CA-C	5.79	117.26	111.07
1	2	214	MET	CA-CB-CG	5.78	125.66	114.10
1	4	272	VAL	N-CA-C	-5.77	99.98	108.23
1	3	56	ASN	CA-CB-CG	-5.77	106.83	112.60
1	4	325	VAL	N-CA-C	5.76	116.71	108.93
1	3	318	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	4	56	ASN	CA-CB-CG	-5.76	106.84	112.60
1	1	55	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	4	283	SER	N-CA-C	5.74	117.22	110.97
1	1	83	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	2	133	HIS	ND1-CG-CD2	5.73	111.83	106.10
1	4	429	TYR	N-CA-C	-5.72	98.96	108.34
1	2	126	SER	CA-CB-OG	5.71	122.51	111.10
1	3	239	GLU	CA-C-N	5.71	130.24	120.71
1	3	239	GLU	C-N-CA	5.71	130.24	120.71
1	1	200	VAL	N-CA-CB	-5.71	102.78	110.54
1	2	44	HIS	ND1-CG-CD2	5.70	111.80	106.10
1	1	348	ILE	N-CA-C	-5.69	99.55	107.80
1	4	380	HIS	CA-CB-CG	-5.68	108.12	113.80
1	2	232	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	2	391	HIS	CG-CD2-NE2	-5.68	101.52	107.20
1	2	462	VAL	N-CA-C	5.66	117.01	109.37
1	2	40	LYS	O-C-N	5.65	129.81	123.48
1	3	93	ASN	CA-CB-CG	5.65	118.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	399	HIS	CG-CD2-NE2	-5.64	101.56	107.20
1	1	391	HIS	CG-CD2-NE2	-5.64	101.56	107.20
1	3	84	VAL	N-CA-C	-5.63	102.26	109.30
1	4	158	TYR	N-CA-C	5.63	117.56	108.32
1	2	50	ILE	CB-CA-C	-5.63	104.54	112.14
1	2	85	GLN	O-C-N	-5.63	117.09	121.14
1	3	331	ALA	O-C-N	-5.62	116.44	122.85
1	1	175	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	2	126	SER	N-CA-CB	-5.62	101.75	110.29
1	2	336	VAL	N-CA-C	5.61	120.12	113.22
1	4	149	ASN	CA-CB-CG	-5.61	106.99	112.60
1	3	399	HIS	CA-CB-CG	-5.61	108.19	113.80
1	4	231	ILE	N-CA-C	5.61	117.42	108.89
1	2	256	HIS	ND1-CG-CD2	5.61	111.71	106.10
1	3	25	HIS	CG-CD2-NE2	-5.61	101.59	107.20
1	1	56	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	1	399	HIS	CG-CD2-NE2	-5.60	101.60	107.20
1	3	37	ASP	CA-CB-CG	5.59	118.19	112.60
1	3	55	GLN	CA-C-N	5.59	132.22	121.54
1	3	55	GLN	C-N-CA	5.59	132.22	121.54
1	2	109	THR	CA-CB-OG1	-5.58	101.22	109.60
1	2	37	ASP	CA-CB-CG	5.57	118.17	112.60
1	3	370	HIS	CG-CD2-NE2	-5.56	101.64	107.20
1	4	249	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	1	32	GLY	O-C-N	-5.54	119.06	123.27
1	2	370	HIS	CG-CD2-NE2	-5.54	101.67	107.20
1	4	460	GLU	N-CA-C	5.53	117.83	110.53
1	4	406	GLN	CA-CB-CG	-5.51	103.07	114.10
1	4	209	VAL	N-CA-C	-5.51	99.94	107.99
1	3	21	HIS	O-C-N	-5.51	116.28	122.12
1	2	382	CYS	N-CA-C	-5.51	100.72	109.76
1	3	283	SER	N-CA-C	5.50	118.20	111.82
1	4	102	ASN	N-CA-C	-5.50	99.31	108.34
1	4	411	ASP	N-CA-C	-5.50	105.36	111.36
1	1	214	MET	CA-CB-CG	5.49	125.08	114.10
1	2	352	THR	N-CA-C	5.49	117.12	111.03
1	1	436	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	3	442	THR	N-CA-C	5.49	120.10	113.41
1	1	163	MET	CA-CB-CG	-5.48	103.15	114.10
1	3	9	HIS	CG-CD2-NE2	-5.47	101.73	107.20
1	3	89	PHE	N-CA-C	-5.47	100.48	109.40
1	4	49	LEU	N-CA-C	5.47	117.75	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	47	GLN	CA-CB-CG	-5.45	103.19	114.10
1	1	44	HIS	CG-CD2-NE2	-5.45	101.75	107.20
1	2	455	LEU	CA-C-N	5.45	126.65	119.84
1	2	455	LEU	C-N-CA	5.45	126.65	119.84
1	4	166	THR	N-CA-C	5.45	122.29	114.39
1	1	29	GLU	N-CA-C	5.45	119.62	112.92
1	1	21	HIS	CG-CD2-NE2	-5.44	101.76	107.20
1	2	399	HIS	CG-CD2-NE2	-5.44	101.76	107.20
1	4	128	THR	CA-CB-OG1	-5.44	101.44	109.60
1	1	101	HIS	CA-CB-CG	5.44	119.24	113.80
1	1	45	LYS	CB-CG-CD	-5.43	98.80	111.30
1	4	182	ILE	CB-CA-C	-5.43	102.53	110.62
1	3	245	ARG	CA-CB-CG	-5.43	103.25	114.10
1	2	394	LEU	O-C-N	-5.42	115.77	122.82
1	3	21	HIS	CG-CD2-NE2	-5.42	101.78	107.20
1	3	370	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	2	332	VAL	CA-C-N	5.42	127.80	120.38
1	2	332	VAL	C-N-CA	5.42	127.80	120.38
1	3	50	ILE	N-CA-CB	5.41	116.88	110.55
1	1	126	SER	CA-CB-OG	5.40	121.90	111.10
1	2	285	ILE	N-CA-C	-5.40	105.35	110.42
1	3	347	SER	CA-CB-OG	5.39	121.89	111.10
1	4	169	ILE	N-CA-C	-5.39	100.57	108.11
1	4	110	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	4	318	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	1	62	VAL	N-CA-C	-5.38	99.34	107.73
1	2	437	CYS	N-CA-C	-5.37	100.54	109.46
1	4	214	MET	CA-CB-CG	5.34	124.78	114.10
1	1	74	ALA	N-CA-C	-5.34	99.24	108.69
1	2	89	PHE	N-CA-C	-5.34	100.32	109.24
1	4	109	THR	CA-C-O	5.33	126.61	120.90
1	4	462	VAL	CA-C-N	5.33	127.74	120.54
1	4	462	VAL	C-N-CA	5.33	127.74	120.54
1	1	140	HIS	N-CA-C	5.33	117.42	110.43
1	4	71	VAL	CA-C-O	-5.33	114.83	120.48
1	1	9	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	2	348	ILE	N-CA-C	-5.32	100.66	108.11
1	4	161	LEU	N-CA-C	-5.32	100.51	109.07
1	2	74	ALA	N-CA-C	-5.31	98.91	108.48
1	4	462	VAL	O-C-N	5.31	128.46	122.67
1	1	318	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	4	101	HIS	ND1-CG-CD2	5.30	111.40	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	455	LEU	CA-C-N	5.30	124.75	119.24
1	4	455	LEU	C-N-CA	5.30	124.75	119.24
1	2	395	ILE	CA-CB-CG2	-5.30	101.50	110.50
1	4	271	ALA	N-CA-C	-5.29	102.63	110.46
1	1	184	MET	CA-CB-CG	-5.29	103.52	114.10
1	1	376	PRO	CB-CA-C	5.29	117.37	110.92
1	1	380	HIS	CG-CD2-NE2	-5.29	101.91	107.20
1	3	34	VAL	N-CA-C	-5.28	100.52	108.12
1	1	394	LEU	O-C-N	-5.28	117.06	123.13
1	4	281	PRO	CA-C-O	5.28	130.20	120.60
1	3	173	ASP	CA-CB-CG	5.27	117.87	112.60
1	1	42	THR	N-CA-C	-5.27	101.17	109.50
1	2	380	HIS	CB-CG-CD2	-5.27	124.34	131.20
1	4	232	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	3	42	THR	N-CA-CB	-5.26	102.08	111.08
1	3	399	HIS	CG-CD2-NE2	-5.26	101.94	107.20
1	3	437	CYS	N-CA-C	-5.25	100.17	108.73
1	4	243	PHE	N-CA-C	5.25	118.15	111.69
1	2	107	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	3	42	THR	N-CA-C	-5.25	101.32	109.72
1	4	286	SER	N-CA-C	5.25	117.41	111.11
1	1	264	LYS	CA-CB-CG	-5.24	103.62	114.10
1	3	286	SER	N-CA-C	5.23	117.39	111.11
1	1	175	ASN	N-CA-C	-5.23	107.28	113.97
1	2	113	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	2	457	HIS	CG-CD2-NE2	-5.23	101.97	107.20
1	4	55	GLN	CA-C-O	5.22	126.00	120.10
1	2	390	THR	N-CA-C	-5.22	100.19	109.06
1	1	341	VAL	CA-C-N	-5.21	116.73	123.19
1	1	341	VAL	C-N-CA	-5.21	116.73	123.19
1	4	370	HIS	CG-CD2-NE2	-5.21	102.00	107.20
1	2	386	ILE	N-CA-CB	5.20	117.61	110.54
1	4	107	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	3	117	ASN	CA-C-O	-5.19	115.37	120.82
1	4	25	HIS	CG-CD2-NE2	-5.19	102.01	107.20
1	2	395	ILE	CA-CB-CG1	5.19	119.22	110.40
1	4	71	VAL	N-CA-C	-5.19	100.91	108.17
1	4	457	HIS	CG-CD2-NE2	-5.19	102.01	107.20
1	1	56	ASN	CA-CB-CG	-5.19	107.41	112.60
1	1	118	GLN	N-CA-C	-5.18	106.81	112.72
1	2	140	HIS	CG-CD2-NE2	-5.18	102.02	107.20
1	3	256	HIS	CB-CG-CD2	-5.17	124.48	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	412	THR	O-C-N	-5.17	117.27	123.27
1	1	42	THR	CB-CA-C	5.17	120.18	109.38
1	1	249	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	4	39	GLU	N-CA-C	-5.16	105.81	112.68
1	1	451	GLN	N-CA-C	-5.16	106.25	112.54
1	1	70	HIS	CG-CD2-NE2	-5.16	102.05	107.20
1	2	9	HIS	CG-CD2-NE2	-5.15	102.05	107.20
1	2	159	ALA	N-CA-C	-5.15	98.85	108.02
1	3	343	MET	N-CA-C	-5.13	100.16	108.52
1	3	391	HIS	CG-CD2-NE2	-5.12	102.08	107.20
1	4	395	ILE	CB-CG1-CD1	-5.12	103.04	113.80
1	4	42	THR	CA-CB-OG1	-5.12	101.92	109.60
1	2	293	GLU	CB-CA-C	-5.12	102.85	110.88
1	4	462	VAL	N-CA-C	5.11	115.69	109.30
1	1	133	HIS	CG-CD2-NE2	-5.11	102.09	107.20
1	1	447	THR	CA-CB-OG1	-5.11	101.94	109.60
1	1	462	VAL	O-C-N	5.10	128.74	122.72
1	3	135	ILE	CA-C-O	-5.10	115.77	121.17
1	1	342	VAL	N-CA-C	-5.09	101.04	108.17
1	1	141	PHE	CA-CB-CG	-5.09	108.71	113.80
1	1	42	THR	O-C-N	-5.09	116.98	123.24
1	2	56	ASN	CA-C-O	5.09	127.79	120.51
1	3	207	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	1	142	THR	CA-CB-CG2	5.08	119.14	110.50
1	1	447	THR	CA-CB-CG2	5.08	119.13	110.50
1	2	362	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	1	276	VAL	N-CA-CB	-5.07	103.14	111.45
1	3	428	LYS	N-CA-CB	-5.07	104.67	110.35
1	4	322	GLU	CA-CB-CG	5.06	124.22	114.10
1	1	462	VAL	CA-C-N	5.06	127.02	120.44
1	1	462	VAL	C-N-CA	5.06	127.02	120.44
1	3	245	ARG	CA-C-N	5.05	125.33	119.47
1	3	245	ARG	C-N-CA	5.05	125.33	119.47
1	1	218	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	2	332	VAL	CA-C-O	5.05	126.56	120.66
1	1	9	HIS	CG-CD2-NE2	-5.04	102.16	107.20
1	2	149	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	4	94	ASN	O-C-N	-5.04	115.88	122.59
1	4	345	ASP	CA-CB-CG	5.04	117.64	112.60
1	4	391	HIS	CG-CD2-NE2	-5.04	102.16	107.20
1	1	451	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	1	149	ASN	OD1-CG-ND2	-5.03	117.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	284	SER	N-CA-C	5.03	118.25	112.57
1	4	380	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	3	281	PRO	CA-C-O	5.02	126.75	121.03
1	4	227	PHE	CA-CB-CG	5.02	118.82	113.80
1	3	149	ASN	CA-CB-CG	-5.01	107.58	112.60
1	4	82	GLU	CA-CB-CG	5.01	124.13	114.10
1	1	423	LYS	CA-C-N	5.00	125.50	119.94
1	1	423	LYS	C-N-CA	5.00	125.50	119.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	18	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	1	3539	76	3524	52	0
1	2	3539	76	3524	50	0
1	3	3539	76	3524	57	0
1	4	3539	76	3524	66	0
2	1	8	0	0	2	0
2	2	8	0	0	0	0
2	3	8	0	0	0	0
2	4	8	0	0	0	0
3	1	46	0	24	2	0
3	2	46	0	24	0	0
3	3	46	0	24	1	0
3	4	46	0	24	1	0
All	All	14372	304	14192	214	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 7.

All (214) 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)
1:4:275:ASP:HB2	1:4:339:LYS:HG3	1.61	0.82
1:4:41:LEU:HD12	1:4:88:LEU:HD21	1.63	0.81
1:4:316:PRO:HG2	1:4:321:ARG:HD3	1.68	0.75
1:3:264:LYS:HG2	1:3:294:ALA:HB2	1.69	0.74
1:1:291:TYR:O	1:1:295:THR:HB	1.92	0.68
1:3:384:TYR:OH	1:3:447:THR:HB	1.94	0.67
1:4:309:VAL:HG21	1:4:328:LYS:HG3	1.77	0.67
1:4:384:TYR:OH	1:4:447:THR:HB	1.94	0.67
1:4:321:ARG:HD2	1:4:327:MET:SD	2.36	0.66
1:2:332:VAL:HG22	1:2:335:VAL:HB	1.79	0.65
1:3:320:LEU:HG	1:3:325:VAL:HG21	1.79	0.64
1:4:175:ASN:HA	1:4:232:ASN:O	1.97	0.64
1:2:275:ASP:HB2	1:2:339:LYS:HG3	1.80	0.63
1:2:386:ILE:HD13	1:2:386:ILE:H	1.63	0.63
1:2:29:GLU:HG2	1:2:74:ALA:HB3	1.80	0.63
1:1:264:LYS:HG2	1:1:294:ALA:HB2	1.80	0.62
1:4:386:ILE:HD13	1:4:386:ILE:H	1.64	0.61
1:3:386:ILE:HD13	1:3:386:ILE:H	1.65	0.61
1:4:295:THR:HG23	1:4:297:ILE:H	1.66	0.60
1:2:206:LEU:HG	1:2:207:ARG:HG2	1.84	0.59
1:2:316:PRO:HG2	1:2:321:ARG:HD3	1.84	0.59
1:1:133:HIS:CE1	1:3:121:ILE:HD11	2.38	0.59
1:4:3:VAL:HG12	1:4:70:HIS:HD2	1.68	0.58
1:3:309:VAL:HG21	1:3:328:LYS:HG3	1.86	0.58
1:4:378:ILE:HG23	1:4:440:CYS:HB2	1.84	0.58
1:2:264:LYS:HG2	1:2:294:ALA:HB2	1.85	0.58
1:4:118:GLN:OE1	1:4:137:ARG:HD3	2.04	0.57
1:4:282:ASP:HB2	3:4:468:AMP:O3P	2.04	0.57
1:1:384:TYR:OH	1:1:447:THR:HB	2.05	0.57
1:4:99:LEU:HB2	1:4:128:THR:HG23	1.85	0.57
1:2:309:VAL:HG21	1:2:328:LYS:HG3	1.86	0.57
1:1:137:ARG:HH22	1:3:137:ARG:NH2	2.02	0.56
1:1:275:ASP:HB2	1:1:339:LYS:HG3	1.86	0.56
1:3:275:ASP:HB2	1:3:339:LYS:HG3	1.87	0.56
1:4:29:GLU:HG2	1:4:74:ALA:HB3	1.87	0.56
1:4:144:LYS:O	1:4:148:LYS:HB2	2.06	0.56
1:2:133:HIS:CE1	1:4:121:ILE:HD11	2.41	0.56
1:1:61:LYS:HB3	1:3:463:LEU:HD11	1.87	0.55
1:3:245:ARG:HD2	1:3:247:ASP:OD1	2.05	0.55
1:2:309:VAL:HG21	1:2:328:LYS:HE2	1.89	0.55
1:4:352:THR:HG22	1:4:356:ARG:HH11	1.71	0.55
1:1:24:GLN:OE1	1:1:50:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:78:GLY:HA3	1:4:464:THR:OG1	2.06	0.55
1:4:138:SER:HB3	1:4:146:GLN:HG2	1.89	0.55
1:1:386:ILE:HD13	1:1:386:ILE:H	1.71	0.55
1:3:3:VAL:HG12	1:3:70:HIS:HD2	1.72	0.54
1:1:399:HIS:HB3	1:1:403:GLU:HB2	1.88	0.54
1:3:138:SER:HB3	1:3:146:GLN:HG2	1.88	0.54
1:3:118:GLN:OE1	1:3:137:ARG:HD3	2.08	0.54
1:3:300:GLU:HB3	1:3:335:VAL:HG11	1.89	0.54
1:1:282:ASP:HB2	3:1:468:AMP:O3P	2.09	0.53
1:1:137:ARG:HH22	1:3:137:ARG:HH22	1.58	0.52
1:3:303:LEU:HD23	1:3:331:ALA:HA	1.91	0.52
1:4:170:VAL:HG21	1:4:191:VAL:HG21	1.92	0.52
1:2:357:ILE:HA	1:2:360:MET:HE2	1.90	0.52
1:1:295:THR:HG22	1:1:297:ILE:H	1.74	0.51
1:4:260:LYS:HE3	1:4:289:ILE:HG22	1.92	0.51
1:2:105:LEU:HD13	1:2:154:LEU:HD22	1.90	0.51
1:4:101:HIS:HA	1:4:159:ALA:O	2.11	0.51
1:4:264:LYS:HG2	1:4:294:ALA:HB2	1.92	0.51
1:2:91:SER:OG	1:2:94:ASN:HB3	2.11	0.51
1:2:22:SER:HB3	1:2:200:VAL:HG11	1.92	0.51
1:1:309:VAL:HG21	1:1:328:LYS:HG3	1.93	0.51
1:3:42:THR:HG21	1:3:63:LYS:H	1.75	0.50
1:1:89:PHE:CE1	1:3:121:ILE:HD12	2.46	0.50
1:2:391:HIS:H	1:2:391:HIS:CD2	2.29	0.50
1:4:391:HIS:H	1:4:391:HIS:CD2	2.30	0.50
1:3:291:TYR:O	1:3:295:THR:HB	2.11	0.50
1:4:93:ASN:O	1:4:94:ASN:HB2	2.12	0.50
1:1:439:ALA:HB3	2:1:466:SF4:S2	2.51	0.50
1:1:147:ILE:O	1:1:151:LEU:HG	2.12	0.50
1:2:20:LEU:HD22	1:2:71:VAL:HG23	1.93	0.50
1:1:3:VAL:HG12	1:1:70:HIS:HD2	1.76	0.50
1:1:30:GLY:HA2	1:1:47:GLN:HA	1.93	0.50
1:2:262:LEU:HD21	1:2:425:ILE:HG13	1.94	0.49
1:3:275:ASP:CB	1:3:339:LYS:HG3	2.41	0.49
1:4:91:SER:OG	1:4:94:ASN:HB3	2.13	0.49
1:1:236:CYS:HB3	1:1:239:GLU:HG2	1.93	0.49
1:4:147:ILE:HG22	1:4:214:MET:HE1	1.93	0.49
1:2:9:HIS:O	1:2:65:LYS:HA	2.13	0.49
1:2:381:PRO:HB3	1:2:455:LEU:HD21	1.95	0.49
1:3:384:TYR:HH	1:3:447:THR:HB	1.77	0.49
1:1:29:GLU:HG2	1:1:74:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:197:ALA:O	1:2:201:VAL:HB	2.13	0.48
1:2:291:TYR:O	1:2:295:THR:HB	2.12	0.48
1:4:11:GLU:HG3	1:4:14:GLN:NE2	2.29	0.48
1:1:332:VAL:HG22	1:1:335:VAL:HB	1.95	0.48
1:3:449:ILE:HG23	1:3:453:THR:HG21	1.96	0.48
1:4:320:LEU:HG	1:4:325:VAL:HG21	1.96	0.47
1:1:72:ARG:HH22	1:1:79:GLY:HA3	1.79	0.47
1:4:180:LEU:HD22	1:4:191:VAL:HG12	1.96	0.47
1:4:422:LEU:HD21	1:4:438:LEU:HD21	1.97	0.47
1:3:85:GLN:HB3	1:3:86:PRO:HA	1.96	0.47
1:3:312:THR:HG21	1:4:55:GLN:NE2	2.29	0.47
1:1:82:GLU:CD	1:1:82:GLU:H	2.23	0.47
1:3:383:PHE:CE1	1:3:455:LEU:HG	2.50	0.47
1:4:22:SER:HB3	1:4:200:VAL:HG21	1.96	0.47
1:2:218:ASN:OD1	1:2:220:GLU:HB3	2.15	0.47
1:3:91:SER:OG	1:3:94:ASN:HB3	2.14	0.47
1:3:344:VAL:HA	1:3:372:LYS:O	2.14	0.47
1:2:245:ARG:HD3	1:2:247:ASP:OD1	2.15	0.47
1:3:15:ILE:HD12	1:3:185:MET:HE1	1.97	0.46
1:1:283:SER:HA	3:1:468:AMP:H4'	1.96	0.46
1:3:77:GLY:O	1:3:464:THR:HG21	2.15	0.46
1:3:248:SER:O	1:3:255:VAL:HG23	2.15	0.46
1:4:265:MET:HE2	1:4:420:GLY:HA2	1.96	0.46
1:4:303:LEU:HD23	1:4:331:ALA:HA	1.97	0.46
1:3:249:ASN:HA	1:3:254:ASN:HA	1.97	0.46
1:3:357:ILE:O	1:3:361:LEU:HB2	2.15	0.46
1:1:99:LEU:HB2	1:1:128:THR:CG2	2.45	0.46
1:1:338:GLY:HA2	1:1:367:THR:HG23	1.96	0.46
1:3:93:ASN:O	1:3:94:ASN:HB2	2.15	0.46
1:4:390:THR:HG23	1:4:392:GLU:O	2.15	0.46
1:1:85:GLN:HB3	1:1:86:PRO:HA	1.98	0.46
1:2:175:ASN:HB3	1:2:234:SER:OG	2.16	0.46
1:4:289:ILE:O	1:4:293:GLU:HG3	2.16	0.46
1:2:369:VAL:O	1:2:411:ASP:HB2	2.16	0.46
1:4:5:GLY:O	1:4:190:VAL:HA	2.16	0.46
1:4:218:ASN:OD1	1:4:220:GLU:HB3	2.16	0.46
1:4:240:TYR:CE1	1:4:250:ILE:HB	2.50	0.46
1:3:312:THR:HG21	1:4:55:GLN:HE22	1.80	0.46
1:1:388:THR:HB	2:1:466:SF4:S1	2.55	0.46
1:1:241:ILE:HD11	1:1:421:LEU:HD11	1.98	0.45
1:3:266:LEU:HD21	1:3:372:LYS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:218:ASN:OD1	1:1:220:GLU:HB3	2.16	0.45
1:2:384:TYR:OH	1:2:447:THR:HB	2.17	0.45
1:2:281:PRO:HB2	1:2:305:LYS:HB2	1.99	0.45
1:1:304:ILE:O	1:1:329:LEU:HA	2.17	0.45
1:2:151:LEU:HA	1:2:154:LEU:HD12	1.98	0.45
1:3:236:CYS:HB3	1:3:239:GLU:HG2	1.99	0.45
1:1:305:LYS:HE3	1:1:328:LYS:HD3	1.99	0.44
1:1:143:LEU:HD13	1:1:147:ILE:HD11	1.99	0.44
1:4:6:ILE:HA	1:4:189:TYR:O	2.18	0.44
1:3:281:PRO:HB2	1:3:305:LYS:HB2	1.98	0.44
1:4:206:LEU:HG	1:4:207:ARG:HG2	1.99	0.44
1:4:275:ASP:CB	1:4:339:LYS:HG3	2.39	0.44
1:1:281:PRO:HB2	1:1:305:LYS:HB2	1.99	0.44
1:2:50:ILE:HD11	1:2:71:VAL:CG2	2.47	0.44
1:2:31:ALA:HB1	1:2:50:ILE:HD13	1.99	0.44
1:4:345:ASP:O	1:4:373:ILE:HA	2.18	0.44
1:1:223:LYS:NZ	1:1:223:LYS:HB3	2.33	0.44
1:1:395:ILE:HG21	1:1:395:ILE:HD13	1.72	0.44
1:2:226:ARG:HG3	1:2:228:SER:O	2.18	0.44
1:2:295:THR:HG23	1:2:297:ILE:HG13	1.99	0.44
1:1:87:LEU:O	1:1:98:ALA:HA	2.18	0.43
1:1:333:ARG:HA	1:1:364:ALA:HB1	2.00	0.43
1:3:49:LEU:O	1:3:53:VAL:HG23	2.18	0.43
1:1:312:THR:HG21	1:2:55:GLN:HE22	1.83	0.43
1:3:304:ILE:O	1:3:329:LEU:HA	2.18	0.43
1:1:91:SER:OG	1:1:94:ASN:HB3	2.19	0.43
1:1:307:ARG:HH11	1:1:307:ARG:HD3	1.70	0.43
1:3:11:GLU:O	1:3:15:ILE:HG12	2.19	0.43
1:3:178:ARG:HA	1:3:178:ARG:HD3	1.61	0.43
1:4:178:ARG:HD3	1:4:178:ARG:HA	1.68	0.43
1:4:182:ILE:HD12	1:4:207:ARG:HG3	2.00	0.43
1:1:275:ASP:CB	1:1:339:LYS:HG3	2.49	0.43
1:2:352:THR:HG22	1:2:356:ARG:HH11	1.83	0.43
1:2:33:ILE:O	1:2:43:ALA:HA	2.19	0.43
1:4:292:ALA:O	1:4:295:THR:HG22	2.17	0.43
1:3:39:GLU:O	1:3:165:GLU:HG2	2.19	0.42
1:1:381:PRO:HB3	1:1:455:LEU:HD21	2.01	0.42
1:2:238:MET:HA	1:2:241:ILE:HB	2.01	0.42
1:2:295:THR:HG23	1:2:297:ILE:H	1.83	0.42
1:3:391:HIS:CD2	1:3:391:HIS:H	2.36	0.42
1:4:210:GLU:HB3	1:4:226:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:242:TYR:HB2	1:1:346:ASP:OD2	2.19	0.42
1:2:281:PRO:HD2	1:2:329:LEU:HD11	2.01	0.42
1:2:302:GLY:C	1:2:332:VAL:HG13	2.44	0.42
1:3:105:LEU:HD13	1:3:154:LEU:HD22	2.01	0.42
1:3:295:THR:HG23	1:3:297:ILE:HG13	2.01	0.42
1:4:291:TYR:O	1:4:295:THR:HB	2.19	0.42
1:4:405:ARG:NH2	1:4:406:GLN:HG3	2.33	0.42
1:2:78:GLY:HA3	1:2:464:THR:OG1	2.20	0.42
1:3:247:ASP:HB2	1:4:332:VAL:HB	2.02	0.42
1:4:39:GLU:HB3	1:4:40:LYS:HG2	2.02	0.42
1:4:242:TYR:HB2	1:4:346:ASP:OD2	2.20	0.42
1:2:266:LEU:HD21	1:2:372:LYS:HB3	2.02	0.42
1:2:303:LEU:HD23	1:2:331:ALA:HA	2.02	0.42
1:3:7:TRP:CZ2	1:3:65:LYS:HE3	2.55	0.42
1:3:31:ALA:HB2	1:3:50:ILE:HD13	2.01	0.42
1:4:116:GLU:HG3	1:4:122:PHE:HE1	1.85	0.42
1:4:26:ARG:NH2	1:4:239:GLU:OE1	2.53	0.41
1:1:226:ARG:HD3	1:1:226:ARG:HA	1.91	0.41
1:3:108:ALA:O	1:3:112:LYS:HG3	2.20	0.41
1:1:115:LEU:HD12	1:1:137:ARG:HD2	2.02	0.41
1:1:391:HIS:CD2	1:1:391:HIS:H	2.37	0.41
1:4:79:GLY:C	1:4:462:VAL:HB	2.46	0.41
1:4:401:VAL:HG22	1:4:415:PHE:CE2	2.56	0.41
1:3:309:VAL:HG21	1:3:328:LYS:HE2	2.03	0.41
1:1:240:TYR:CZ	1:1:250:ILE:HB	2.55	0.41
1:4:6:ILE:HG23	1:4:12:ALA:HB1	2.03	0.41
1:1:344:VAL:HA	1:1:372:LYS:O	2.21	0.41
1:2:429:TYR:HB2	1:2:434:CYS:C	2.45	0.41
1:3:236:CYS:HB3	1:3:239:GLU:CG	2.51	0.41
1:3:395:ILE:HD13	1:3:395:ILE:HG21	1.93	0.41
1:1:178:ARG:HD3	1:1:178:ARG:HA	1.62	0.40
1:2:137:ARG:HH22	1:4:137:ARG:NH2	2.19	0.40
1:3:20:LEU:HD11	1:3:69:GLY:HA3	2.03	0.40
1:3:281:PRO:HD2	1:3:329:LEU:HD11	2.03	0.40
1:4:87:LEU:O	1:4:98:ALA:HA	2.21	0.40
1:2:158:TYR:HB2	1:2:160:PHE:CE2	2.56	0.40
1:3:347:SER:OG	3:3:467:AMP:H8	2.04	0.40
1:4:6:ILE:O	1:4:66:GLY:HA2	2.21	0.40
1:2:31:ALA:CB	1:2:50:ILE:HD13	2.51	0.40
1:2:97:LEU:CD1	1:2:164:THR:HG22	2.51	0.40
1:2:321:ARG:NH1	1:2:327:MET:SD	2.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:267:ALA:O	1:3:271:ALA:HB2	2.22	0.40
1:4:394:LEU:HB2	1:4:397:SER:OG	2.21	0.40
1:4:395:ILE:HG21	1:4:395:ILE:HD13	1.93	0.40
1:2:6:ILE:O	1:2:66:GLY:HA2	2.21	0.40
1:3:111:LEU:O	1:3:115:LEU:HB2	2.20	0.40
1:1:319:ALA:O	1:1:322:GLU:HG2	2.22	0.40
1:2:384:TYR:HH	1:2:447:THR:HB	1.87	0.40
1:4:281:PRO:HB2	1:4:305:LYS:HB2	2.03	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	1	463/465 (100%)	436 (94%)	19 (4%)	8 (2%)	7	32
1	2	463/465 (100%)	433 (94%)	23 (5%)	7 (2%)	8	35
1	3	463/465 (100%)	437 (94%)	23 (5%)	3 (1%)	21	56
1	4	463/465 (100%)	434 (94%)	24 (5%)	5 (1%)	11	43
All	All	1852/1860 (100%)	1740 (94%)	89 (5%)	23 (1%)	10	40

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	56	ASN
1	2	282	ASP
1	2	431	ASP
1	3	94	ASN
1	4	56	ASN
1	4	94	ASN
1	1	94	ASN

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Mol	Chain	Res	Type
1	1	282	ASP
1	1	432	SER
1	3	56	ASN
1	4	432	SER
1	1	464	THR
1	2	94	ASN
1	4	431	ASP
1	1	431	ASP
1	2	432	SER
1	2	464	THR
1	3	118	GLN
1	4	282	ASP
1	2	56	ASN
1	2	281	PRO
1	1	77	GLY
1	1	281	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	382/382 (100%)	332 (87%)	50 (13%)	4	19
1	2	382/382 (100%)	338 (88%)	44 (12%)	5	24
1	3	382/382 (100%)	337 (88%)	45 (12%)	5	22
1	4	382/382 (100%)	335 (88%)	47 (12%)	4	21
All	All	1528/1528 (100%)	1342 (88%)	186 (12%)	5	21

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	GLU
1	1	11	GLU
1	1	28	GLN
1	1	39	GLU
1	1	49	LEU

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Mol	Chain	Res	Type
1	1	60	SER
1	1	65	LYS
1	1	71	VAL
1	1	82	GLU
1	1	88	LEU
1	1	99	LEU
1	1	115	LEU
1	1	125	SER
1	1	131	LEU
1	1	142	THR
1	1	143	LEU
1	1	167	GLU
1	1	201	VAL
1	1	206	LEU
1	1	220	GLU
1	1	223	LYS
1	1	229	MET
1	1	232	ASN
1	1	235	ILE
1	1	245	ARG
1	1	246	PRO
1	1	251	ASP
1	1	276	VAL
1	1	281	PRO
1	1	295	THR
1	1	312	THR
1	1	318	GLN
1	1	320	LEU
1	1	321	ARG
1	1	322	GLU
1	1	329	LEU
1	1	332	VAL
1	1	333	ARG
1	1	342	VAL
1	1	354	SER
1	1	361	LEU
1	1	372	LYS
1	1	386	ILE
1	1	389	SER
1	1	398	SER
1	1	407	GLU
1	1	432	SER

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Mol	Chain	Res	Type
1	1	447	THR
1	1	448	GLU
1	1	460	GLU
1	2	10	GLU
1	2	39	GLU
1	2	41	LEU
1	2	50	ILE
1	2	60	SER
1	2	65	LYS
1	2	71	VAL
1	2	82	GLU
1	2	88	LEU
1	2	115	LEU
1	2	121	ILE
1	2	131	LEU
1	2	143	LEU
1	2	152	SER
1	2	162	ILE
1	2	166	THR
1	2	167	GLU
1	2	184	MET
1	2	201	VAL
1	2	204	THR
1	2	214	MET
1	2	220	GLU
1	2	223	LYS
1	2	229	MET
1	2	231	ILE
1	2	245	ARG
1	2	251	ASP
1	2	295	THR
1	2	318	GLN
1	2	320	LEU
1	2	321	ARG
1	2	332	VAL
1	2	333	ARG
1	2	342	VAL
1	2	354	SER
1	2	361	LEU
1	2	386	ILE
1	2	407	GLU
1	2	411	ASP

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Mol	Chain	Res	Type
1	2	430	ASP
1	2	432	SER
1	2	447	THR
1	2	448	GLU
1	2	460	GLU
1	3	11	GLU
1	3	28	GLN
1	3	39	GLU
1	3	49	LEU
1	3	60	SER
1	3	65	LYS
1	3	71	VAL
1	3	82	GLU
1	3	88	LEU
1	3	109	THR
1	3	113	GLN
1	3	115	LEU
1	3	131	LEU
1	3	143	LEU
1	3	167	GLU
1	3	169	ILE
1	3	190	VAL
1	3	201	VAL
1	3	206	LEU
1	3	208	GLU
1	3	220	GLU
1	3	223	LYS
1	3	245	ARG
1	3	246	PRO
1	3	251	ASP
1	3	272	VAL
1	3	281	PRO
1	3	295	THR
1	3	312	THR
1	3	318	GLN
1	3	321	ARG
1	3	322	GLU
1	3	332	VAL
1	3	339	LYS
1	3	354	SER
1	3	361	LEU
1	3	386	ILE

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Mol	Chain	Res	Type
1	3	398	SER
1	3	407	GLU
1	3	411	ASP
1	3	416	LEU
1	3	432	SER
1	3	448	GLU
1	3	456	PRO
1	3	460	GLU
1	4	11	GLU
1	4	22	SER
1	4	39	GLU
1	4	50	ILE
1	4	60	SER
1	4	65	LYS
1	4	71	VAL
1	4	75	THR
1	4	87	LEU
1	4	88	LEU
1	4	115	LEU
1	4	121	ILE
1	4	131	LEU
1	4	142	THR
1	4	143	LEU
1	4	162	ILE
1	4	167	GLU
1	4	169	ILE
1	4	181	SER
1	4	190	VAL
1	4	201	VAL
1	4	214	MET
1	4	220	GLU
1	4	223	LYS
1	4	245	ARG
1	4	251	ASP
1	4	268	GLN
1	4	270	SER
1	4	281	PRO
1	4	295	THR
1	4	309	VAL
1	4	312	THR
1	4	318	GLN
1	4	320	LEU

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Mol	Chain	Res	Type
1	4	321	ARG
1	4	322	GLU
1	4	332	VAL
1	4	339	LYS
1	4	354	SER
1	4	386	ILE
1	4	393	GLU
1	4	398	SER
1	4	407	GLU
1	4	432	SER
1	4	447	THR
1	4	448	GLU
1	4	460	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	44	HIS
1	1	110	GLN
1	1	113	GLN
1	1	123	GLN
1	1	149	ASN
1	1	175	ASN
1	1	268	GLN
1	1	391	HIS
1	1	436	GLN
1	2	55	GLN
1	2	104	ASN
1	2	110	GLN
1	2	149	ASN
1	2	380	HIS
1	2	391	HIS
1	2	433	ASN
1	2	436	GLN
1	3	55	GLN
1	3	123	GLN
1	4	55	GLN
1	4	104	ASN
1	4	110	GLN
1	4	123	GLN
1	4	315	GLN
1	4	380	HIS

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Mol	Chain	Res	Type
1	4	391	HIS
1	4	433	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
2	SF4	4	466	1	0,12,12	-	-	-		
3	AMP	4	467	-	25,25,25	0.79	0	37,38,38	0.93	1 (2%)
3	AMP	1	467	-	25,25,25	1.00	2 (8%)	37,38,38	1.48	7 (18%)
2	SF4	1	466	1	0,12,12	-	-	-		
3	AMP	4	468	-	25,25,25	0.89	1 (4%)	37,38,38	1.08	3 (8%)
2	SF4	2	466	1	0,12,12	-	-	-		
2	SF4	3	466	1	0,12,12	-	-	-		
3	AMP	1	468	-	25,25,25	1.04	1 (4%)	37,38,38	0.96	1 (2%)
3	AMP	3	467	-	25,25,25	1.02	3 (12%)	37,38,38	1.12	4 (10%)
3	AMP	3	468	-	25,25,25	0.90	0	37,38,38	1.12	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	2	468	-	25,25,25	1.24	2 (8%)	37,38,38	1.25	4 (10%)
3	AMP	2	467	-	25,25,25	0.97	2 (8%)	37,38,38	1.26	4 (10%)

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
2	SF4	4	466	1	-	-	0/6/5/5
3	AMP	4	467	-	-	3/10/26/26	0/3/3/3
3	AMP	1	467	-	-	3/10/26/26	0/3/3/3
2	SF4	1	466	1	-	-	0/6/5/5
3	AMP	4	468	-	-	3/10/26/26	0/3/3/3
3	AMP	3	467	-	-	1/10/26/26	0/3/3/3
3	AMP	1	468	-	-	4/10/26/26	0/3/3/3
2	SF4	2	466	1	-	-	0/6/5/5
2	SF4	3	466	1	-	-	0/6/5/5
3	AMP	3	468	-	-	4/10/26/26	0/3/3/3
3	AMP	2	468	-	-	2/10/26/26	0/3/3/3
3	AMP	2	467	-	-	1/10/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	468	AMP	P-O3P	-2.37	1.46	1.54
3	1	467	AMP	O3'-C3'	2.29	1.48	1.43
3	3	467	AMP	O4'-C4'	-2.25	1.40	1.45
3	2	468	AMP	C3'-C4'	-2.21	1.47	1.53
3	2	468	AMP	C2'-C1'	-2.21	1.46	1.53
3	2	467	AMP	O4'-C4'	-2.20	1.40	1.45
3	4	468	AMP	P-O3P	-2.14	1.46	1.54
3	3	467	AMP	O3'-C3'	2.11	1.48	1.43
3	2	467	AMP	P-O3P	-2.06	1.47	1.54
3	1	467	AMP	P-O3P	-2.03	1.47	1.54
3	3	467	AMP	P-O3P	-2.02	1.47	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	467	AMP	C3'-C2'-C1'	4.41	109.80	101.46
3	2	468	AMP	O3'-C3'-C4'	-3.66	100.56	111.08
3	1	467	AMP	C5'-C4'-C3'	3.39	127.42	115.21
3	2	468	AMP	O4'-C1'-N9	3.15	114.13	108.09
3	3	468	AMP	C3'-C2'-C1'	3.00	107.13	101.46
3	1	467	AMP	O3'-C3'-C2'	-2.95	102.36	111.82
3	2	467	AMP	O4'-C1'-N9	2.71	113.29	108.09
3	2	467	AMP	C3'-C2'-C1'	2.68	106.54	101.46
3	1	467	AMP	O4'-C4'-C3'	2.58	110.27	105.15
3	2	468	AMP	O2'-C2'-C1'	-2.55	101.34	110.10
3	3	467	AMP	C5'-C4'-C3'	2.52	124.27	115.21
3	1	467	AMP	O4'-C1'-N9	2.42	112.74	108.09
3	4	467	AMP	C3'-C2'-C1'	2.38	105.97	101.46
3	4	468	AMP	C4'-O4'-C1'	-2.38	104.21	109.47
3	4	468	AMP	O3P-P-O5'	-2.29	100.70	106.67
3	3	467	AMP	C3'-C2'-C1'	2.26	105.74	101.46
3	3	468	AMP	N3-C2-N1	2.25	131.99	128.58
3	1	467	AMP	O2'-C2'-C1'	-2.23	102.44	110.10
3	1	467	AMP	O3'-C3'-C4'	2.21	117.44	111.08
3	2	467	AMP	O3P-P-O5'	-2.21	100.91	106.67
3	2	467	AMP	O3'-C3'-C2'	-2.19	104.80	111.82
3	3	467	AMP	O3'-C3'-C4'	2.16	117.28	111.08
3	2	468	AMP	O3P-P-O2P	2.12	115.77	107.80
3	4	468	AMP	O3'-C3'-C4'	-2.12	104.99	111.08
3	3	468	AMP	C4-N9-C8	-2.10	103.53	105.74
3	1	468	AMP	O3P-P-O2P	2.05	115.49	107.80
3	3	467	AMP	C2'-C3'-C4'	-2.03	98.68	102.61

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1	467	AMP	C5'-O5'-P-O2P
3	1	467	AMP	C5'-O5'-P-O3P
3	3	468	AMP	C5'-O5'-P-O2P
3	3	468	AMP	C5'-O5'-P-O3P
3	4	467	AMP	C5'-O5'-P-O2P
3	4	468	AMP	C5'-O5'-P-O2P
3	4	468	AMP	C5'-O5'-P-O3P
3	4	467	AMP	C2'-C1'-N9-C4
3	1	468	AMP	C5'-O5'-P-O1P
3	3	468	AMP	C5'-O5'-P-O1P
3	4	468	AMP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
3	2	467	AMP	C2'-C1'-N9-C4
3	1	467	AMP	C2'-C1'-N9-C4
3	3	467	AMP	C2'-C1'-N9-C4
3	3	468	AMP	C2'-C1'-N9-C4
3	1	468	AMP	C4'-C5'-O5'-P
3	1	468	AMP	C5'-O5'-P-O3P
3	2	468	AMP	C4'-C5'-O5'-P
3	1	468	AMP	C2'-C1'-N9-C8
3	2	468	AMP	C2'-C1'-N9-C8
3	4	467	AMP	C2'-C1'-N9-C8

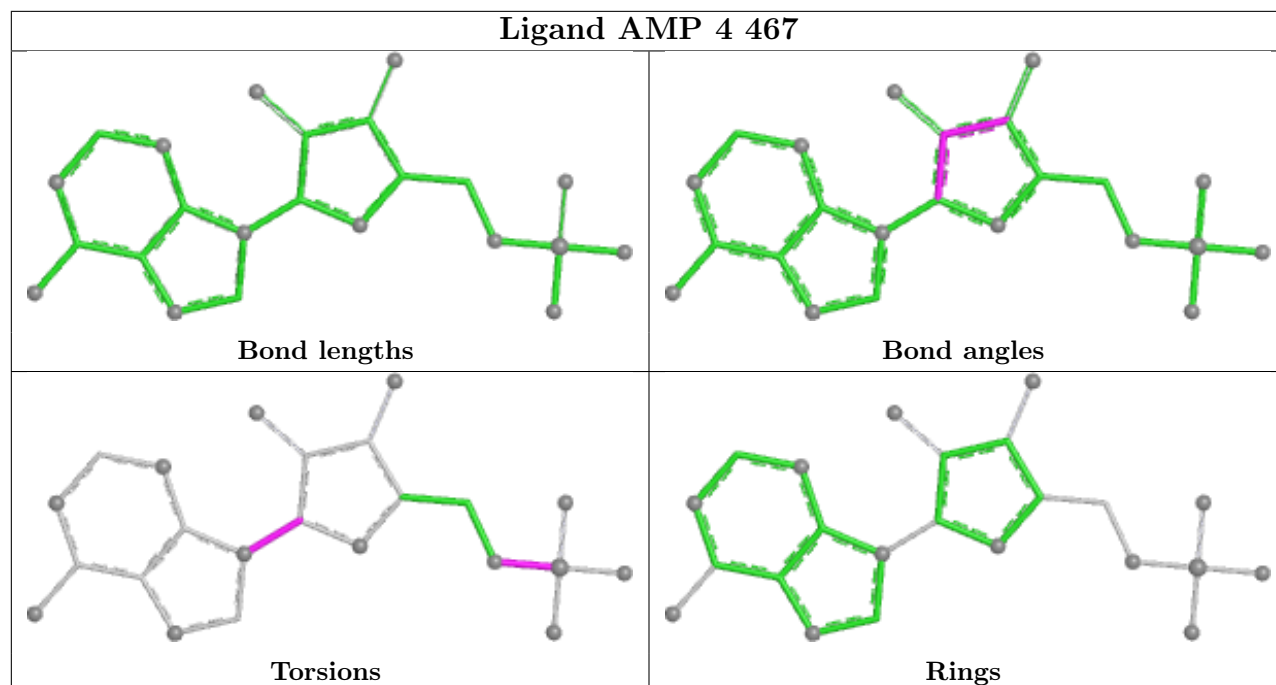
There are no ring outliers.

4 monomers are involved in 6 short contacts:

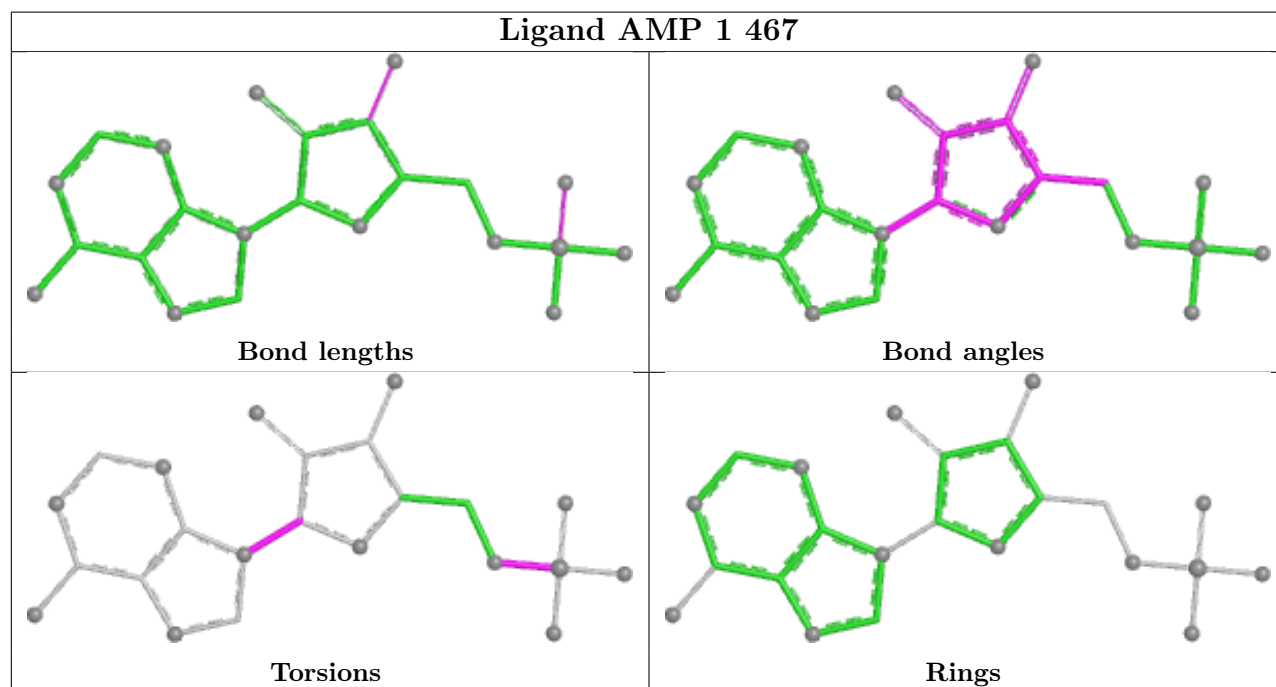
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	466	SF4	2	0
3	4	468	AMP	1	0
3	1	468	AMP	2	0
3	3	467	AMP	1	0

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.

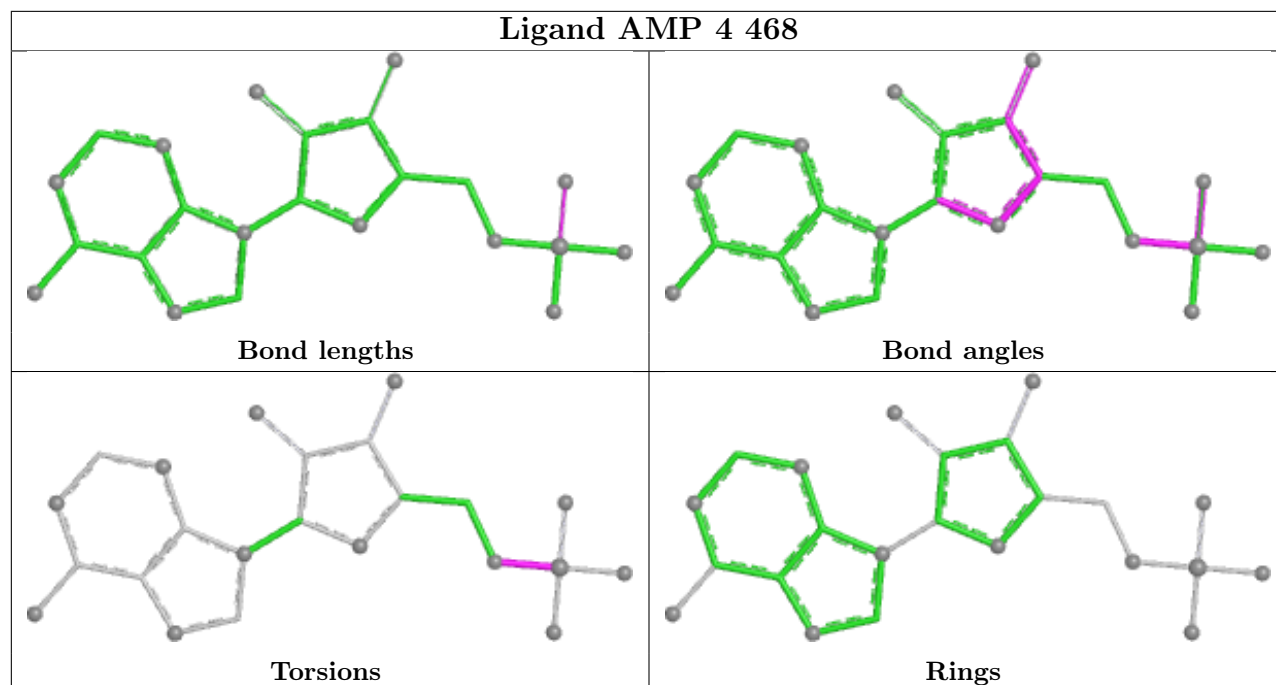
Ligand AMP 4 467



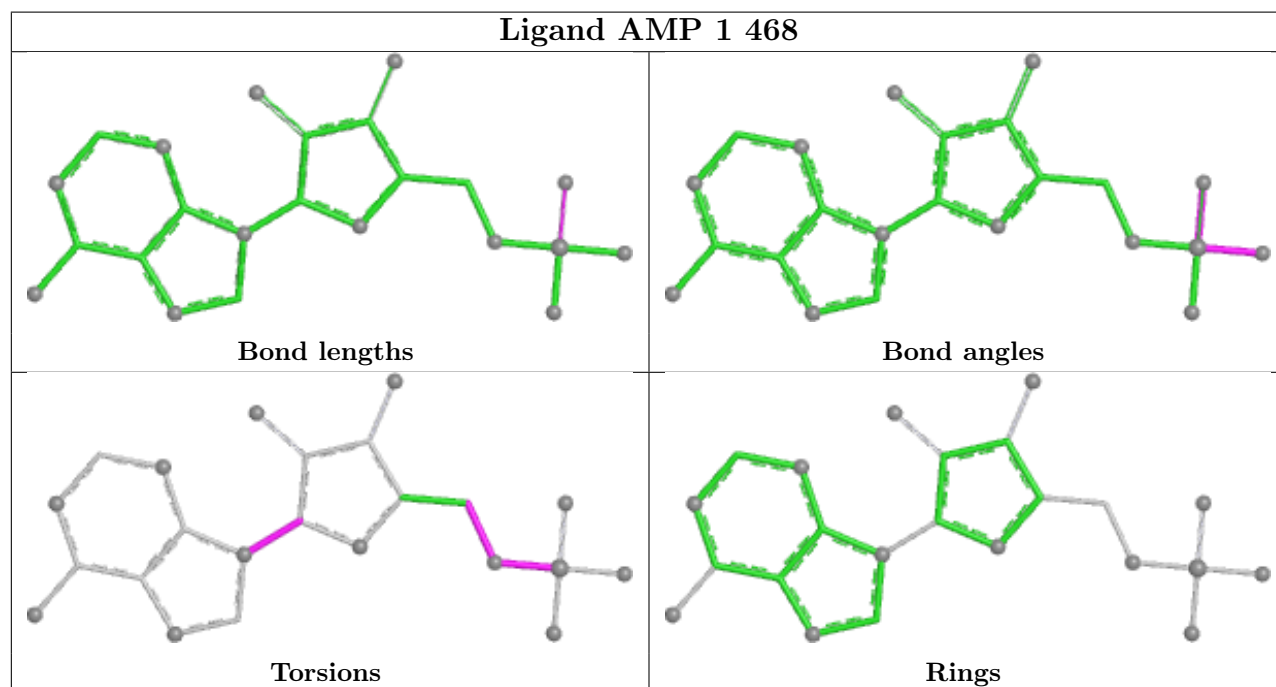
Ligand AMP 1 467



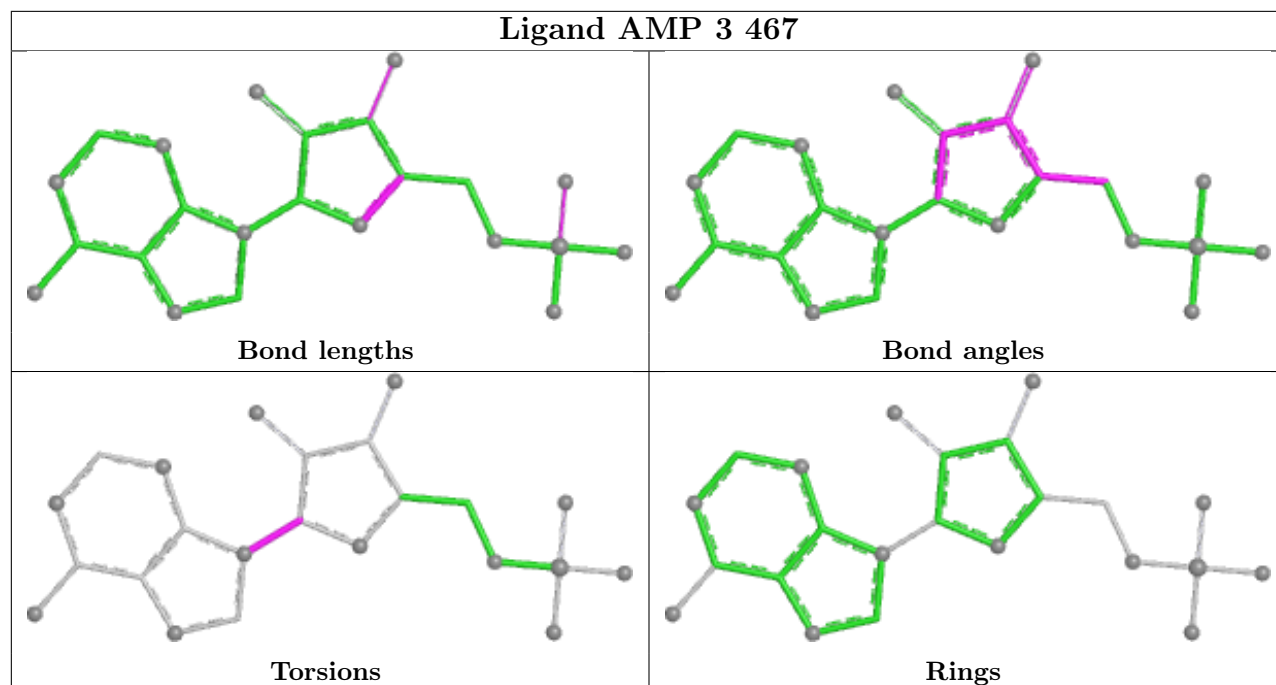
Ligand AMP 4 468



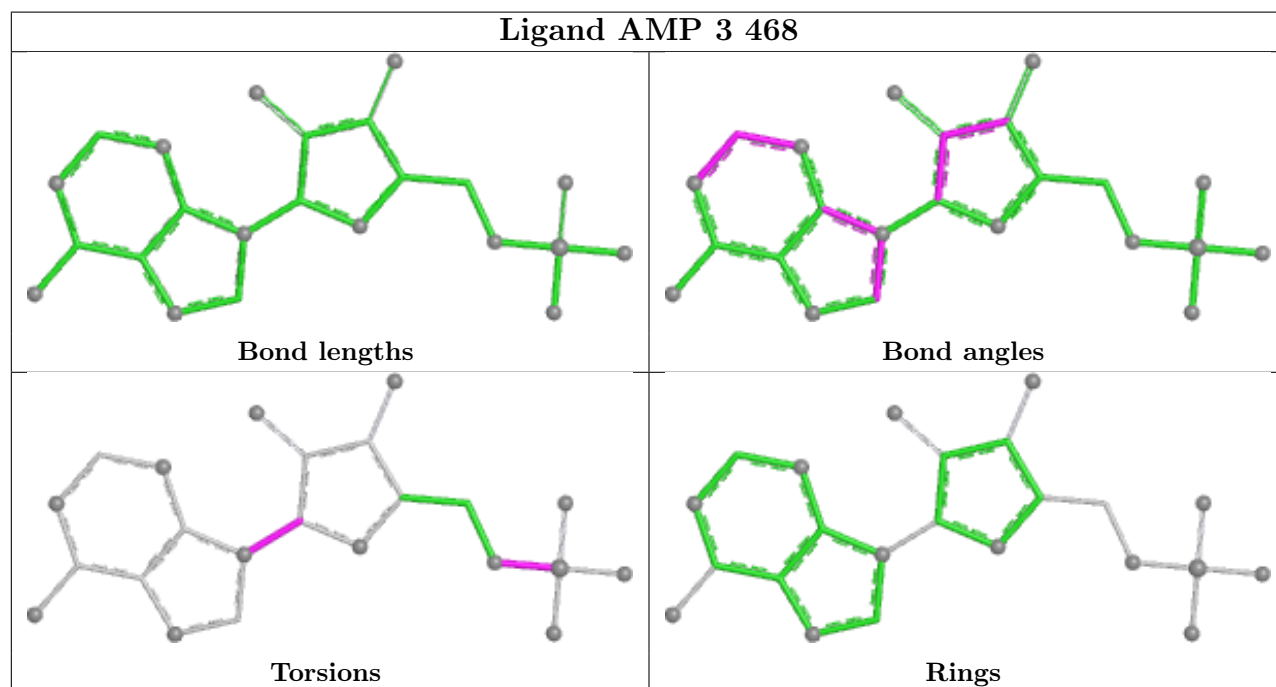
Ligand AMP 1 468

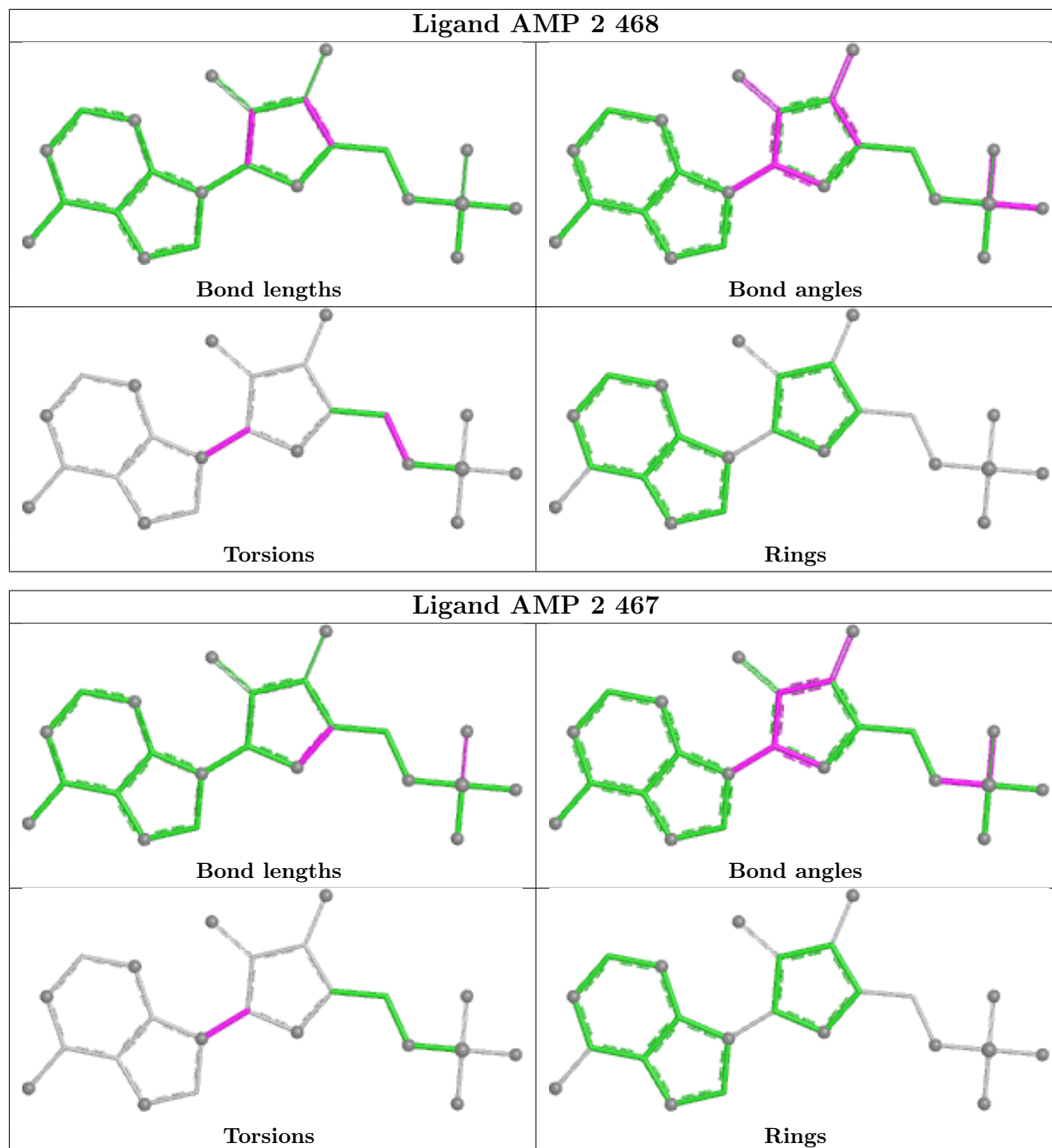


Ligand AMP 3 467



Ligand AMP 3 468





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.