



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:56 am BST

PDB ID : 1GPH
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

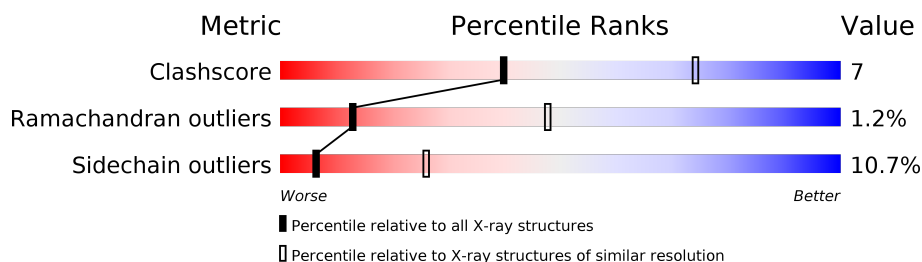
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 on 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	70% 25% . .
1	2	465	72% 23% . .
1	3	465	73% 22% 5% .
1	4	465	69% 25% 5% .

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.

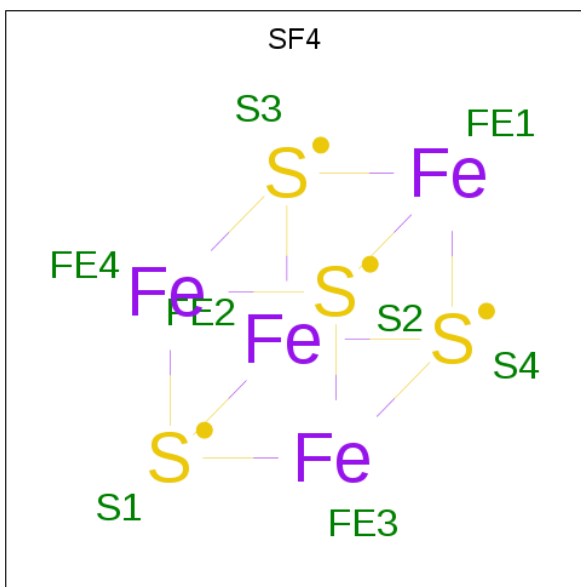
- Molecule 1 is a protein called GLUTAMINE PHOSPHORIBOSYL-PYROPHOSPHATE AMIDOTRANSFERASE.

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:

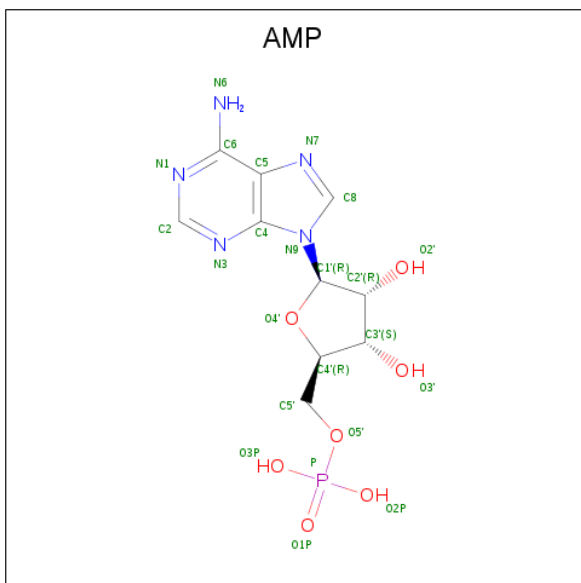
Chain	Residue	Modelled	Actual	Comment	Reference
1	402	ASP	GLY	CONFLICT	UNP P00497
2	402	ASP	GLY	CONFLICT	UNP P00497
3	402	ASP	GLY	CONFLICT	UNP P00497
4	402	ASP	GLY	CONFLICT	UNP P00497

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: 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 (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



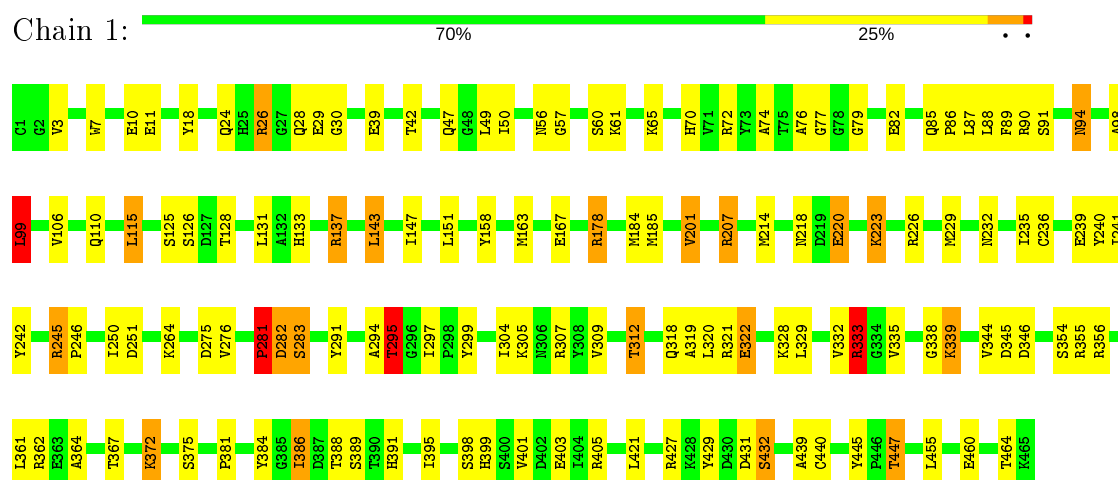
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	1	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4	1	Total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

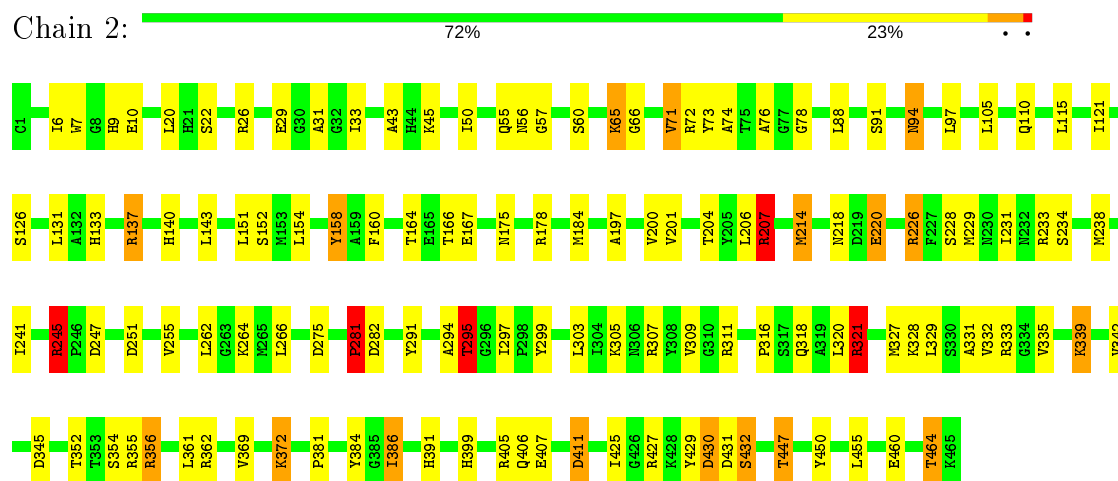
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



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L361	K264	T109	C1
K372	M265	Q110	G2
F383	L266	K112	V3
Y384	A267		W7
I386	A271	L115	E11
H391	V272	Q118	I15
I395	D275	I121	L20
S398	P282	S126	R26
R405	S283	L131	G27
D411	Y291	R137	Q38
L416	A294	S138	A31
R427	T295	L143	E39
S432	G296	Q146	K40
T447	L297	L154	L41
E448	E300	E165	T42
I449	L303	T166	L49
T463	L304	E167	I50
V464	K306	M168	V53
K465	V307	I169	M56
	V309	R178	G57
	T312	V190	S60
	Q318	V201	K63
	A319	L206	G64
	R321	R207	K65
	E322	M214	G69
	V325	E220	H70
	R326	R233	V71
	K328	C236	R72
	L329	E239	A76
	S330	R245	G77
	V332	P246	Y81
	R333	D247	Q85
	G334	S248	P86
	V335	I249	L87
	K339	J250	L88
	V344	D251	S91
	S347	M254	Q92
	R355	V255	N93
	K356		N94
	T357		L105
			A102

Chain 4:  69% 25% 5%

S330	N232	Q110	G1
A331	R233	E116	G2
V332	E239	M117	V3
R333	Y240	Q118	F4
K339	I241	I121	G5
R340	Y242	F122	I6
D345	R245	T128	M7
D346	I250	L131	E11
T352	D251	R137	A12
T353	K260	S138	P13
S354	K264	L143	Q14
R355	Q268	K144	S22
R356	D275	I145	R26
R362	P281	A159	E29
K372	D282	I162	E39
I373	S283	K167	K40
I378	G290	V170	L41
Y384	Y291	M175	Q55
G385	A292	G176	I56
I386	E293	L177	G57
T390	A294	R178	S60
R391	L394	P179	K65
E392	G296	L180	G66
E393	I297	I182	H70
L394	P298	V189	R72
I395	Y299	V190	V73
A396	L303	V191	T75
S397	I304	V200	A76
S398	K305	L206	G77
V401	V309	R207	G78
R405	G310	E210	E82
Q406	R311	M214	L87
F415	T312	I218	L88
L422	P316	D220	F89
D431	S317	R226	A90
S432	Q318	V228	S91
L438	A319	E230	I92
A439	L320	K244	I93
C440	R321	I244	M94
T447	E322	M218	A98
E460	V325	D219	I99
T464	R326	E220	A100
G465	K327	R226	H101
	K328	V228	L105

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	158.80 Å 75.70 Å 94.10 Å 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: AMP, SF4

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	0.86	1/3597 (0.0%)	1.63	51/4857 (1.1%)
1	2	0.82	0/3597	1.58	47/4857 (1.0%)
1	3	0.84	1/3597 (0.0%)	1.59	42/4857 (0.9%)
1	4	0.82	0/3597	1.60	45/4857 (0.9%)
All	All	0.83	2/14388 (0.0%)	1.60	185/19428 (1.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	190	VAL	CA-CB	5.40	1.66	1.54
1	1	375	SER	CA-CB	-5.08	1.45	1.52

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	26	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	1	281	PRO	CA-C-N	-12.07	90.65	117.20
1	3	207	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	3	207	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	2	427	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	2	362	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	2	26	ARG	NE-CZ-NH2	-11.05	114.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	178	ARG	NE-CZ-NH2	-10.81	114.89	120.30
1	2	26	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	3	72	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	1	26	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	4	281	PRO	CA-C-N	-10.04	95.10	117.20
1	4	137	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	2	405	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	3	26	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	1	207	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	1	427	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	2	207	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	4	26	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	2	207	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	4	321	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	4	321	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	1	245	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	4	178	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	3	333	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	3	281	PRO	CA-C-N	-8.95	97.52	117.20
1	1	26	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	1	356	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	3	355	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	1	281	PRO	O-C-N	8.69	136.60	122.70
1	3	245	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	3	26	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	2	356	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	3	214	MET	CA-CB-CG	8.48	127.72	113.30
1	4	245	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	3	245	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	3	427	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	2	405	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	4	405	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	1	295	THR	N-CA-CB	-8.26	94.61	110.30
1	1	429	TYR	CB-CG-CD1	-8.06	116.16	121.00
1	1	427	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	4	207	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	1	178	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	1	207	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	1	355	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	1	245	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	1	362	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	1	7	TRP	CD1-CG-CD2	7.89	112.61	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	321	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	2	356	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	3	405	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	2	281	PRO	CA-C-N	-7.60	100.47	117.20
1	4	233	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	4	207	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	3	7	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	2	321	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	4	405	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	3	295	THR	N-CA-CB	-7.32	96.39	110.30
1	3	7	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	1	445	TYR	CB-CG-CD1	-7.30	116.62	121.00
1	2	214	MET	CA-CB-CG	7.27	125.66	113.30
1	3	72	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	4	355	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	1	333	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	3	137	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	1	245	ARG	CB-CG-CD	-7.15	93.01	111.60
1	2	178	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	1	356	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	4	281	PRO	O-C-N	6.99	133.88	122.70
1	1	214	MET	CA-CB-CG	6.93	125.08	113.30
1	2	72	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	1	299	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	4	245	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	1	7	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	4	299	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	2	7	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	1	345	ASP	CB-CG-OD1	6.77	124.39	118.30
1	4	214	MET	CA-CB-CG	6.76	124.78	113.30
1	3	81	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	2	430	ASP	CA-C-N	-6.72	102.42	117.20
1	3	427	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	2	245	ARG	CB-CG-CD	-6.64	94.33	111.60
1	2	57	GLY	N-CA-C	-6.64	96.50	113.10
1	4	7	TRP	CD1-CG-CD2	6.61	111.58	106.30
1	2	362	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	4	311	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	1	158	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	4	90	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	4	72	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	1	99	LEU	CA-CB-CG	6.42	130.05	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	355	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	4	340	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	2	137	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	4	57	GLY	N-CA-C	-6.32	97.29	113.10
1	1	283	SER	CA-CB-OG	6.31	128.23	111.20
1	2	110	GLN	CA-CB-CG	6.29	127.25	113.40
1	3	126	SER	N-CA-CB	-6.29	101.06	110.50
1	4	283	SER	CA-CB-OG	6.28	128.17	111.20
1	2	7	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	2	427	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	2	73	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	4	362	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	3	118	GLN	CA-CB-CG	6.21	127.07	113.40
1	2	137	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	4	110	GLN	CA-CB-CG	6.19	127.01	113.40
1	4	7	TRP	CE2-CD2-CG	-6.14	102.39	107.30
1	1	178	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	2	345	ASP	CB-CG-OD1	6.11	123.80	118.30
1	3	395	ILE	CA-CB-CG2	-6.10	98.70	110.90
1	1	362	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	1	110	GLN	CA-CB-CG	6.04	126.68	113.40
1	3	307	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	2	450	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	3	233	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	1	281	PRO	C-N-CA	5.99	136.67	121.70
1	3	321	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	2	233	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	1	163	MET	CA-CB-CG	-5.97	103.15	113.30
1	2	281	PRO	O-C-N	5.97	132.26	122.70
1	3	326	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	1	76	ALA	N-CA-C	-5.96	94.90	111.00
1	4	90	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	3	76	ALA	N-CA-C	-5.88	95.12	111.00
1	2	45	LYS	CA-CB-CG	5.86	126.30	113.40
1	2	178	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	2	126	SER	N-CA-CB	-5.83	101.75	110.50
1	3	281	PRO	O-C-N	5.81	131.99	122.70
1	4	105	LEU	CB-CG-CD1	-5.80	101.15	111.00
1	4	82	GLU	CB-CA-C	-5.79	98.83	110.40
1	3	178	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	1	137	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	1	184	MET	CA-CB-CG	-5.75	103.52	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	118	GLN	OE1-CD-NE2	-5.71	108.76	121.90
1	1	401	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	4	245	ARG	CB-CG-CD	-5.70	96.79	111.60
1	3	283	SER	CA-CB-OG	5.66	126.48	111.20
1	3	220	GLU	CA-CB-CG	5.65	125.83	113.40
1	1	185	MET	CG-SD-CE	-5.63	91.20	100.20
1	3	57	GLY	N-CA-C	-5.62	99.06	113.10
1	1	110	GLN	N-CA-CB	-5.61	100.50	110.60
1	3	56	ASN	CA-C-N	-5.61	104.98	116.20
1	4	333	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	2	307	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	4	329	LEU	CA-CB-CG	5.54	128.05	115.30
1	1	405	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	1	440	CYS	CA-CB-SG	5.54	123.97	114.00
1	1	90	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	3	329	LEU	CA-CB-CG	5.50	127.96	115.30
1	1	57	GLY	N-CA-C	-5.50	99.36	113.10
1	1	137	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	2	429	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	2	311	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	2	311	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	4	226	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	4	295	THR	N-CA-CB	-5.43	99.97	110.30
1	3	307	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	2	406	GLN	CA-CB-CG	-5.40	101.52	113.40
1	2	76	ALA	N-CA-C	-5.36	96.54	111.00
1	3	190	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	2	295	THR	N-CA-CB	-5.33	100.18	110.30
1	2	299	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	1	106	VAL	CA-CB-CG2	-5.31	102.94	110.90
1	1	345	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	3	282	ASP	CA-C-O	-5.26	109.06	120.10
1	1	276	VAL	CA-CB-CG2	-5.26	103.02	110.90
1	2	71	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	1	126	SER	N-CA-CB	-5.25	102.63	110.50
1	2	158	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	1	42	THR	N-CA-CB	-5.23	100.37	110.30
1	4	281	PRO	C-N-CA	5.19	134.67	121.70
1	1	201	VAL	N-CA-CB	-5.16	100.15	111.50
1	4	264	LYS	CA-CB-CG	-5.15	102.06	113.40
1	2	140	HIS	CA-C-N	-5.15	105.86	117.20
1	4	76	ALA	N-CA-C	-5.15	97.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	55	GLN	C-N-CA	5.15	134.57	121.70
1	4	386	ILE	CB-CA-C	-5.14	101.31	111.60
1	3	118	GLN	CG-CD-NE2	5.14	129.03	116.70
1	3	405	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	1	7	TRP	CG-CD1-NE1	-5.12	104.97	110.10
1	3	395	ILE	CA-CB-CG1	5.12	120.72	111.00
1	4	340	ARG	N-CA-C	-5.09	97.25	111.00
1	4	333	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	2	255	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	4	137	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	47	0
1	3	3539	76	3524	56	0
1	4	3539	76	3524	63	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	207	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 (207) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:4:138:SER:HB3	1:4:146:GLN:HG2	1.89	0.55
1:4:78:GLY:HA3	1:4:464:THR:OG1	2.06	0.55
1:1:386:ILE:H	1:1:386:ILE:HD13	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
1:1:295: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:CD2	1:2:391:HIS:H	2.29	0.50
1:4:391:HIS:CD2	1:4:391:HIS:H	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
1:2:381:PRO:HB3	1:2:455:LEU:HD21	1.95	0.49
1:2:9:HIS:O	1:2:65:LYS:HA	2.13	0.49
1:1:29:GLU:HG2	1:1:74:ALA:HB3	1.94	0.48
1:2:197:ALA:O	1:2:201:VAL:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:384:TYR:HH	1:3:447:THR:HB	1.77	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
1:3:383: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
1:3:344:VAL:HA	1:3:372:LYS:O	2.14	0.47
1:3:91:SER:OG	1:3:94:ASN:HB3	2.14	0.47
1:2:245:ARG:HD3	1:2:247:ASP:OD1	2.15	0.47
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
1:4:303: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
1:1:338:GLY:HA2	1:1:367:THR:HG23	1.96	0.46
1:1:99:LEU:HB2	1:1:128:THR:CG2	2.45	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
1:4:218: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
1:4:5:GLY:O	1:4:190:VAL:HA	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:1:307:ARG:HH11	1.70	0.43
1:3:11:GLU:O	1:3:15:ILE:HG12	2.19	0.43
1:3:178:ARG:HD3	1:3:178:ARG:HA	1.61	0.43
1:4:178:ARG:HA	1:4:178:ARG:HD3	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
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
1:3:105:LEU:HD13	1:3:154:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:4:242:TYR:HB2	1:4:346:ASP:OD2	2.20	0.42
1:4:39:GLU:HB3	1:4:40:LYS:HG2	2.02	0.42
1:1:82:GLU:CD	1:1:82:GLU:H	2.23	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
1:3:31:ALA:HB2	1:3:50:ILE:HD13	2.01	0.42
1:3:7:TRP:CZ2	1:3:65:LYS:HE3	2.55	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:HA	1:1:226:ARG:HD3	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:H	1:1:391:HIS:CD2	2.37	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
1:3:236:CYS:HB3	1:3:239:GLU:CG	2.51	0.41
1:3:395:ILE:HG21	1:3:395:ILE:HD13	1.93	0.41
1:1:178:ARG:HA	1:1:178:ARG:HD3	1.62	0.40
1:2:137:ARG:HH22	1:4:137:ARG:NH2	2.19	0.40
1:3:281:PRO:HD2	1:3:329:LEU:HD11	2.03	0.40
1:3:20:LEU:HD11	1:3:69:GLY:HA3	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
1:2:321:ARG:NH1	1:2:327:MET:SD	2.92	0.40
1:2:97:LEU:CD1	1:2:164:THR:HG22	2.51	0.40
1:3:267:ALA:O	1:3:271:ALA:HB2	2.22	0.40
1:4:395:ILE:HG21	1:4:395:ILE:HD13	1.93	0.40
1:4:394:LEU:HB2	1:4:397:SER:OG	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	9	39
1	2	463/465 (100%)	433 (94%)	23 (5%)	7 (2%)	10	42
1	3	463/465 (100%)	437 (94%)	23 (5%)	3 (1%)	25	64
1	4	463/465 (100%)	434 (94%)	24 (5%)	5 (1%)	14	50
All	All	1852/1860 (100%)	1740 (94%)	89 (5%)	23 (1%)	13	48

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
1	1	282	ASP
1	1	432	SER
1	3	56	ASN
1	4	432	SER
1	1	464	THR

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Mol	Chain	Res	Type
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%)	339 (89%)	43 (11%)	6	24
1	2	382/382 (100%)	343 (90%)	39 (10%)	7	28
1	3	382/382 (100%)	340 (89%)	42 (11%)	6	25
1	4	382/382 (100%)	343 (90%)	39 (10%)	7	28
All	All	1528/1528 (100%)	1365 (89%)	163 (11%)	6	26

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	GLU
1	1	11	GLU
1	1	26	ARG
1	1	28	GLN
1	1	39	GLU
1	1	49	LEU
1	1	60	SER
1	1	65	LYS
1	1	88	LEU
1	1	99	LEU

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Mol	Chain	Res	Type
1	1	115	LEU
1	1	125	SER
1	1	131	LEU
1	1	143	LEU
1	1	167	GLU
1	1	201	VAL
1	1	207	ARG
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	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	333	ARG
1	1	339	LYS
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	432	SER
1	1	447	THR
1	1	460	GLU
1	2	10	GLU
1	2	60	SER
1	2	65	LYS
1	2	88	LEU
1	2	115	LEU
1	2	121	ILE
1	2	131	LEU
1	2	143	LEU
1	2	152	SER

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Mol	Chain	Res	Type
1	2	166	THR
1	2	167	GLU
1	2	184	MET
1	2	204	THR
1	2	207	ARG
1	2	214	MET
1	2	220	GLU
1	2	226	ARG
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	333	ARG
1	2	339	LYS
1	2	342	VAL
1	2	354	SER
1	2	361	LEU
1	2	372	LYS
1	2	386	ILE
1	2	399	HIS
1	2	407	GLU
1	2	411	ASP
1	2	430	ASP
1	2	432	SER
1	2	447	THR
1	2	460	GLU
1	3	11	GLU
1	3	28	GLN
1	3	39	GLU
1	3	40	LYS
1	3	49	LEU
1	3	60	SER
1	3	65	LYS
1	3	71	VAL
1	3	88	LEU
1	3	109	THR
1	3	115	LEU
1	3	131	LEU

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Mol	Chain	Res	Type
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	207	ARG
1	3	220	GLU
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	333	ARG
1	3	339	LYS
1	3	361	LEU
1	3	372	LYS
1	3	386	ILE
1	3	398	SER
1	3	411	ASP
1	3	416	LEU
1	3	432	SER
1	3	456	PRO
1	3	460	GLU
1	4	22	SER
1	4	39	GLU
1	4	60	SER
1	4	65	LYS
1	4	75	THR
1	4	87	LEU
1	4	88	LEU
1	4	131	LEU
1	4	143	LEU
1	4	162	ILE
1	4	167	GLU
1	4	177	LEU

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Mol	Chain	Res	Type
1	4	181	SER
1	4	190	VAL
1	4	207	ARG
1	4	214	MET
1	4	220	GLU
1	4	229	MET
1	4	245	ARG
1	4	251	ASP
1	4	268	GLN
1	4	281	PRO
1	4	295	THR
1	4	309	VAL
1	4	312	THR
1	4	318	GLN
1	4	320	LEU
1	4	321	ARG
1	4	322	GLU
1	4	333	ARG
1	4	339	LYS
1	4	354	SER
1	4	372	LYS
1	4	386	ILE
1	4	393	GLU
1	4	398	SER
1	4	432	SER
1	4	447	THR
1	4	460	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	391	HIS
1	2	55	GLN
1	2	391	HIS
1	3	391	HIS
1	4	55	GLN
1	4	315	GLN
1	4	380	HIS
1	4	391	HIS

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 carbohydrates 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	0.00	-	-		
3	AMP	2	467	-	22,25,25	1.35	4 (18%)	25,38,38	1.59	4 (16%)
2	SF4	2	466	1	0,12,12	0.00	-	-		
2	SF4	1	466	1	0,12,12	0.00	-	-		
2	SF4	3	466	1	0,12,12	0.00	-	-		
3	AMP	1	467	-	22,25,25	1.29	2 (9%)	25,38,38	2.11	7 (28%)
3	AMP	4	467	-	22,25,25	0.99	1 (4%)	25,38,38	1.39	2 (8%)
3	AMP	2	468	-	22,25,25	1.64	3 (13%)	25,38,38	1.51	5 (20%)
3	AMP	3	467	-	22,25,25	1.30	3 (13%)	25,38,38	1.61	7 (28%)
3	AMP	4	468	-	22,25,25	1.15	3 (13%)	25,38,38	1.35	5 (20%)
3	AMP	1	468	-	22,25,25	1.16	2 (9%)	25,38,38	1.23	3 (12%)
3	AMP	3	468	-	22,25,25	1.13	2 (9%)	25,38,38	1.54	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	4	466	1	-	-	0/6/5/5
2	SF4	2	466	1	-	-	0/6/5/5
3	AMP	2	467	-	-	0/6/26/26	0/3/3/3
2	SF4	1	466	1	-	-	0/6/5/5
3	AMP	3	467	-	-	0/6/26/26	0/3/3/3
3	AMP	1	467	-	-	2/6/26/26	0/3/3/3
3	AMP	4	467	-	-	1/6/26/26	0/3/3/3
3	AMP	2	468	-	-	1/6/26/26	0/3/3/3
2	SF4	3	466	1	-	-	0/6/5/5
3	AMP	4	468	-	-	3/6/26/26	0/3/3/3
3	AMP	1	468	-	-	3/6/26/26	0/3/3/3
3	AMP	3	468	-	-	3/6/26/26	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	468	AMP	C2'-C1'	-4.75	1.46	1.53
3	2	468	AMP	C8-N7	-3.18	1.29	1.34
3	2	467	AMP	C2'-C1'	-3.09	1.49	1.53
3	2	467	AMP	C8-N7	-3.03	1.29	1.34
3	4	468	AMP	C2'-C1'	-3.02	1.49	1.53
3	1	467	AMP	C8-N7	-2.99	1.29	1.34
3	3	467	AMP	C2'-C1'	-2.93	1.49	1.53
3	3	468	AMP	C2'-C1'	-2.50	1.50	1.53
3	1	467	AMP	O3'-C3'	2.40	1.48	1.43
3	4	467	AMP	C8-N7	-2.31	1.30	1.34
3	1	468	AMP	P-O3P	-2.30	1.46	1.54
3	3	468	AMP	C8-N7	-2.28	1.30	1.34
3	3	467	AMP	O4'-C4'	-2.24	1.40	1.45
3	3	467	AMP	O3'-C3'	2.21	1.48	1.43
3	2	467	AMP	O4'-C4'	-2.19	1.40	1.45
3	2	468	AMP	C3'-C4'	-2.19	1.47	1.53
3	4	468	AMP	C8-N7	-2.18	1.30	1.34
3	1	468	AMP	C8-N7	-2.17	1.30	1.34
3	4	468	AMP	P-O3P	-2.07	1.46	1.54
3	2	467	AMP	P-O3P	-2.00	1.47	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	467	AMP	C3'-C2'-C1'	5.86	109.80	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	467	AMP	P-O5'-C5'	4.31	130.17	118.30
3	3	468	AMP	C3'-C2'-C1'	4.09	107.13	100.98
3	2	467	AMP	C3'-C2'-C1'	3.70	106.54	100.98
3	2	468	AMP	O3'-C3'-C4'	-3.63	100.56	111.05
3	4	467	AMP	P-O5'-C5'	3.35	127.53	118.30
3	4	467	AMP	C3'-C2'-C1'	3.32	105.97	100.98
3	1	467	AMP	C5'-C4'-C3'	3.27	127.42	115.18
3	3	467	AMP	C3'-C2'-C1'	3.16	105.74	100.98
3	3	468	AMP	C5-C6-N6	3.09	125.05	120.35
3	2	468	AMP	C5-C6-N6	3.00	124.91	120.35
3	1	467	AMP	O3'-C3'-C2'	-2.93	102.36	111.82
3	3	468	AMP	O4'-C1'-C2'	-2.70	102.98	106.93
3	3	467	AMP	C5-C6-N6	2.67	124.42	120.35
3	2	467	AMP	P-O5'-C5'	2.64	125.57	118.30
3	1	467	AMP	O4'-C4'-C3'	2.61	110.27	105.11
3	2	468	AMP	O2'-C2'-C1'	-2.58	101.34	110.85
3	1	468	AMP	C5-C6-N6	2.53	124.19	120.35
3	3	467	AMP	P-O5'-C5'	2.52	125.25	118.30
3	3	467	AMP	C1'-N9-C4	-2.50	122.25	126.64
3	2	468	AMP	C3'-C2'-C1'	2.48	104.71	100.98
3	3	467	AMP	C5'-C4'-C3'	2.43	124.27	115.18
3	1	467	AMP	O2'-C2'-C1'	-2.28	102.44	110.85
3	4	468	AMP	O3P-P-O5'	-2.27	100.70	106.73
3	1	467	AMP	O3'-C3'-C4'	2.21	117.44	111.05
3	2	467	AMP	O3P-P-O5'	-2.19	100.91	106.73
3	4	468	AMP	C5-C6-N6	2.17	123.66	120.35
3	2	467	AMP	O3'-C3'-C2'	-2.17	104.80	111.82
3	3	467	AMP	O3'-C3'-C4'	2.16	117.28	111.05
3	4	468	AMP	C1'-N9-C4	-2.16	122.85	126.64
3	2	468	AMP	O3P-P-O2P	2.13	115.77	107.64
3	1	468	AMP	P-O5'-C5'	2.12	124.14	118.30
3	3	468	AMP	N3-C2-N1	2.12	131.99	128.68
3	4	468	AMP	O3'-C3'-C4'	-2.10	104.99	111.05
3	4	468	AMP	C3'-C2'-C1'	2.07	104.10	100.98
3	1	468	AMP	O3P-P-O2P	2.06	115.49	107.64
3	3	467	AMP	C2'-C3'-C4'	-2.04	98.68	102.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1	467	AMP	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
3	1	467	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	3	468	AMP	C5'-O5'-P-O2P
3	3	468	AMP	C5'-O5'-P-O3P
3	4	468	AMP	C5'-O5'-P-O1P
3	1	468	AMP	C5'-O5'-P-O1P
3	3	468	AMP	C5'-O5'-P-O1P
3	1	468	AMP	C4'-C5'-O5'-P
3	1	468	AMP	C5'-O5'-P-O3P
3	2	468	AMP	C4'-C5'-O5'-P

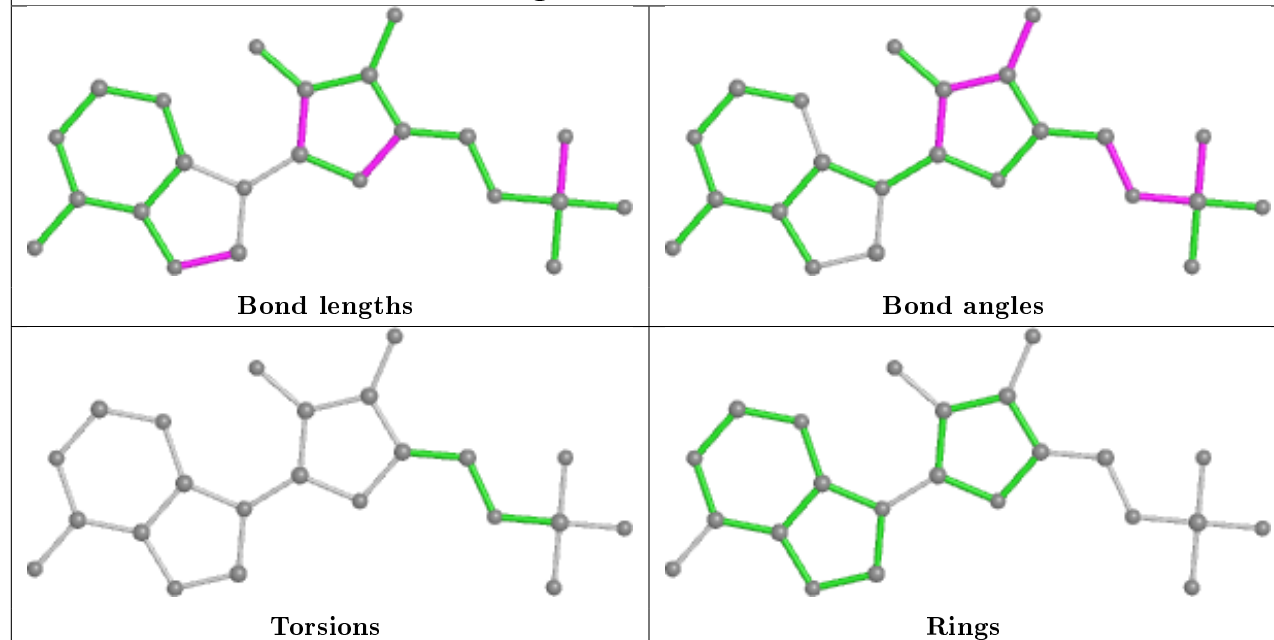
There are no ring outliers.

4 monomers are involved in 6 short contacts:

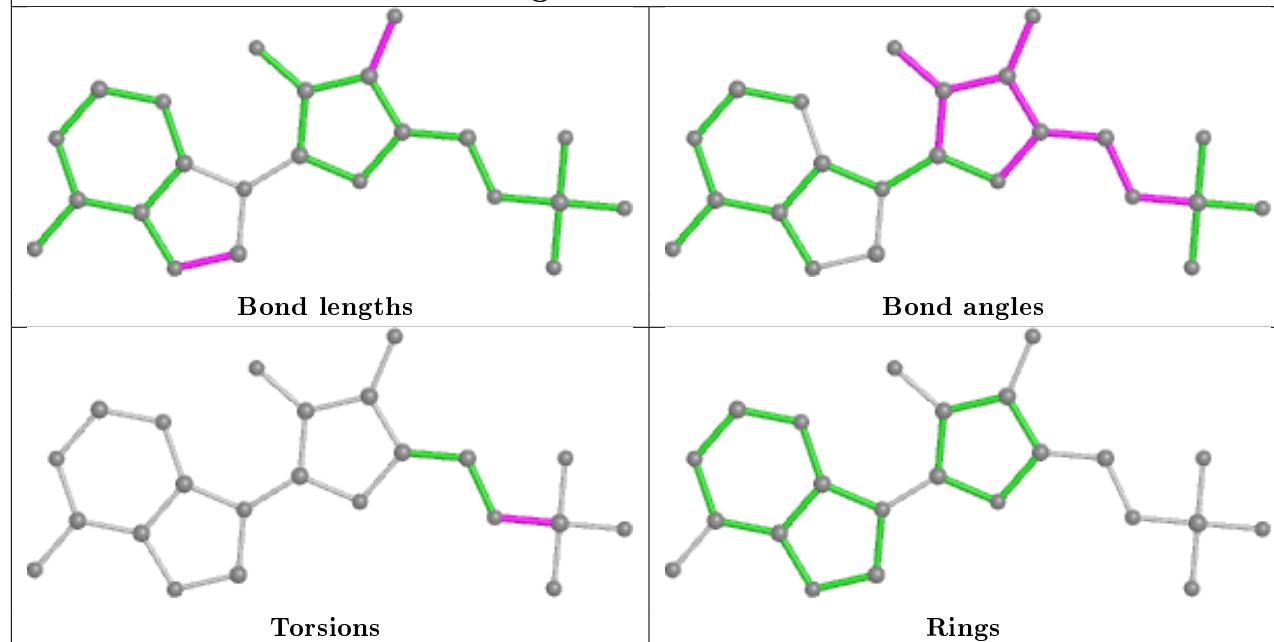
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	466	SF4	2	0
3	3	467	AMP	1	0
3	4	468	AMP	1	0
3	1	468	AMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

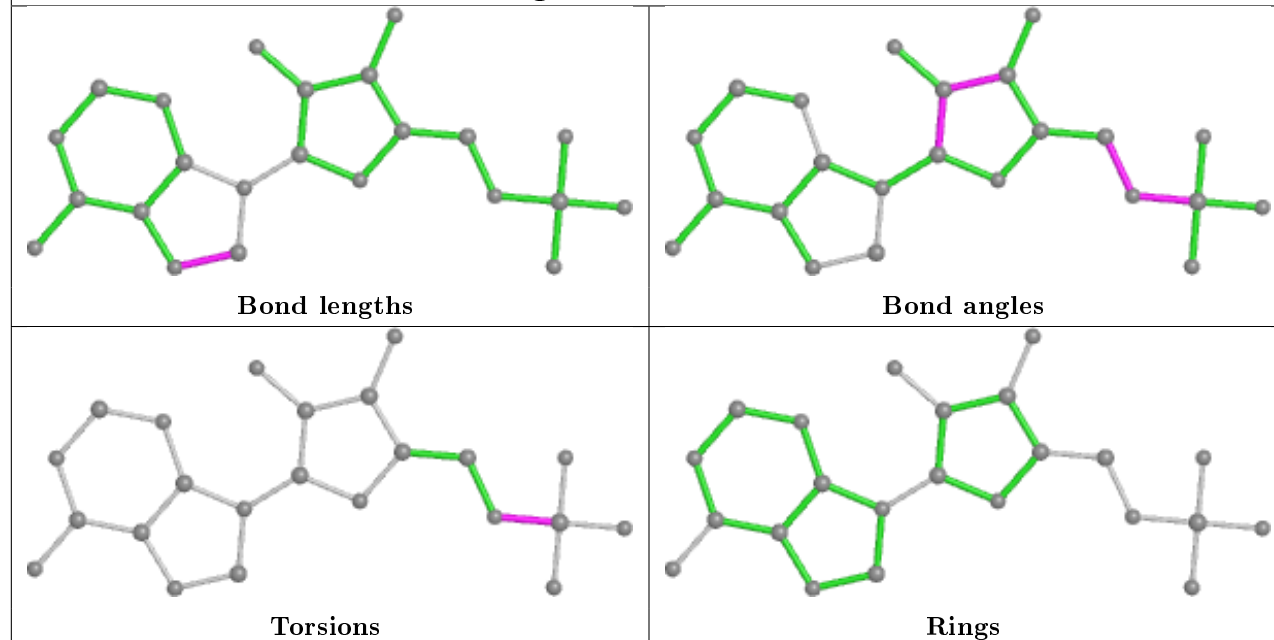
Ligand AMP 2 467



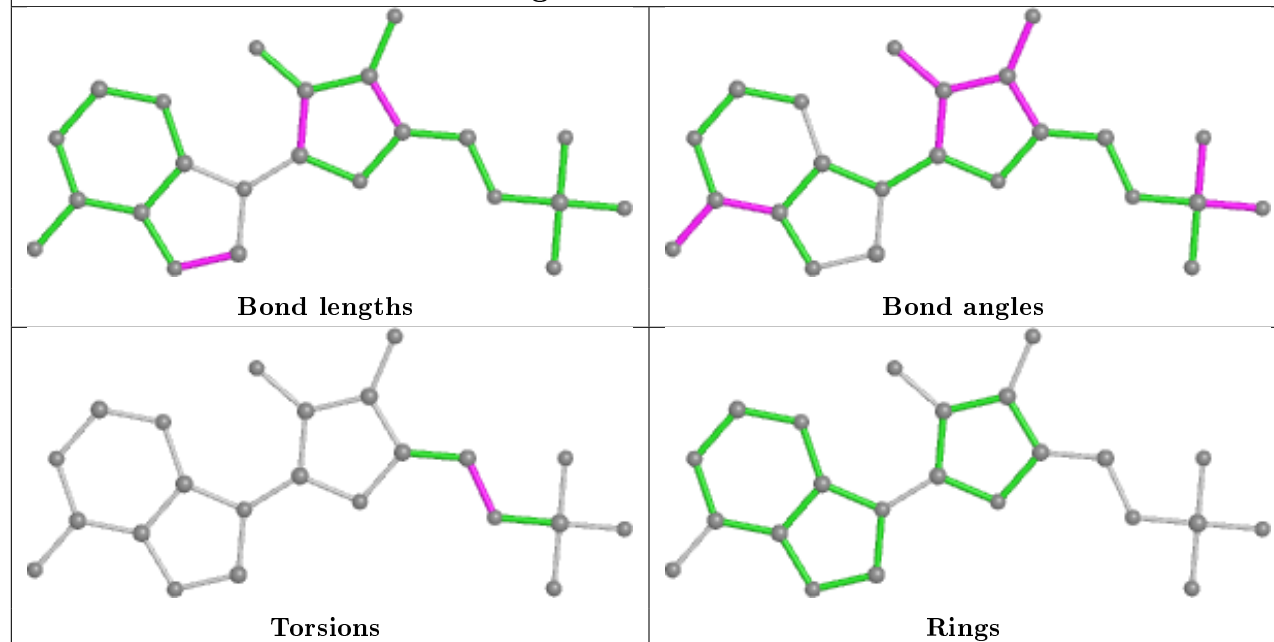
Ligand AMP 1 467



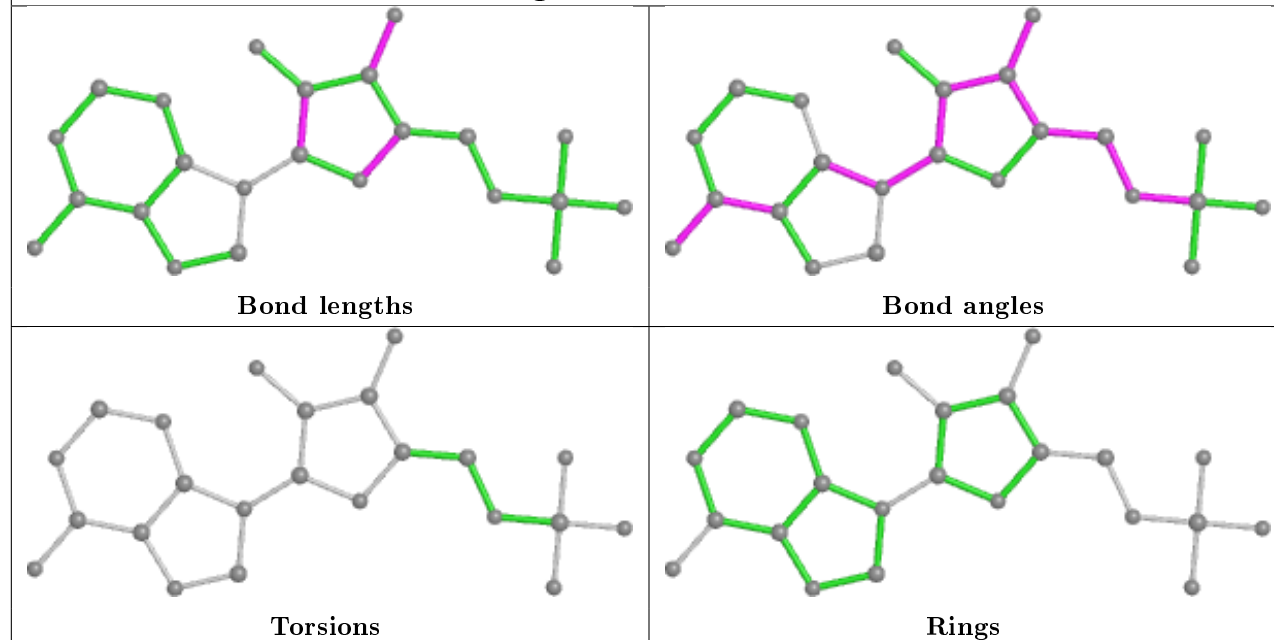
Ligand AMP 4 467



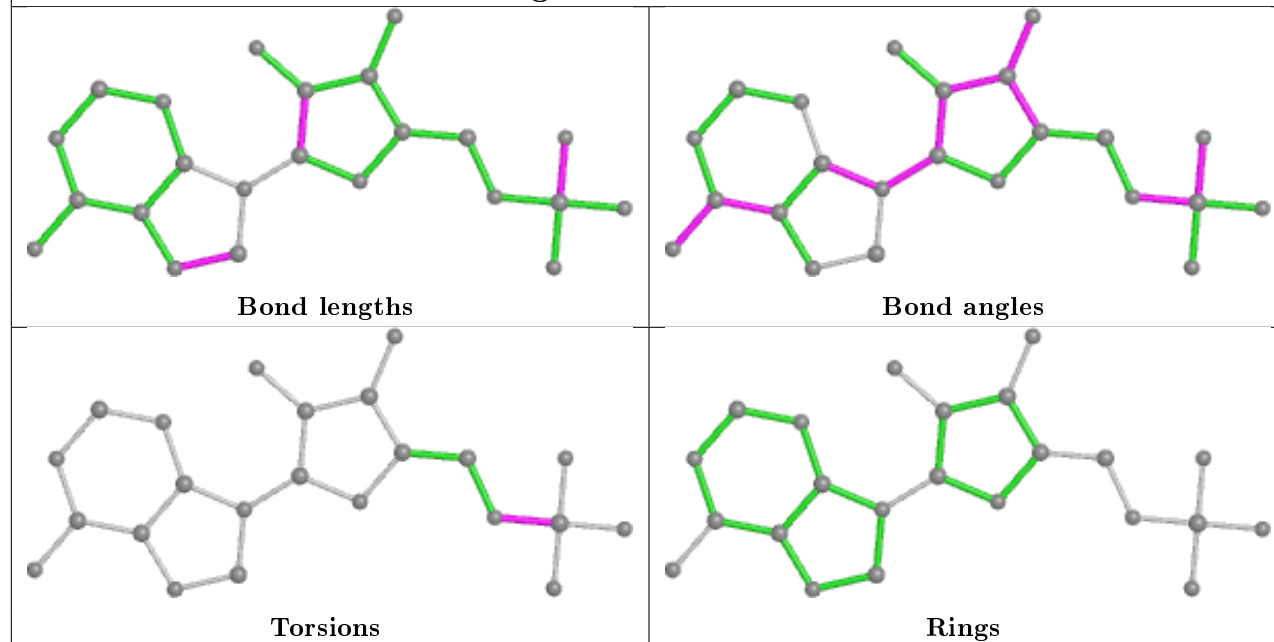
Ligand AMP 2 468

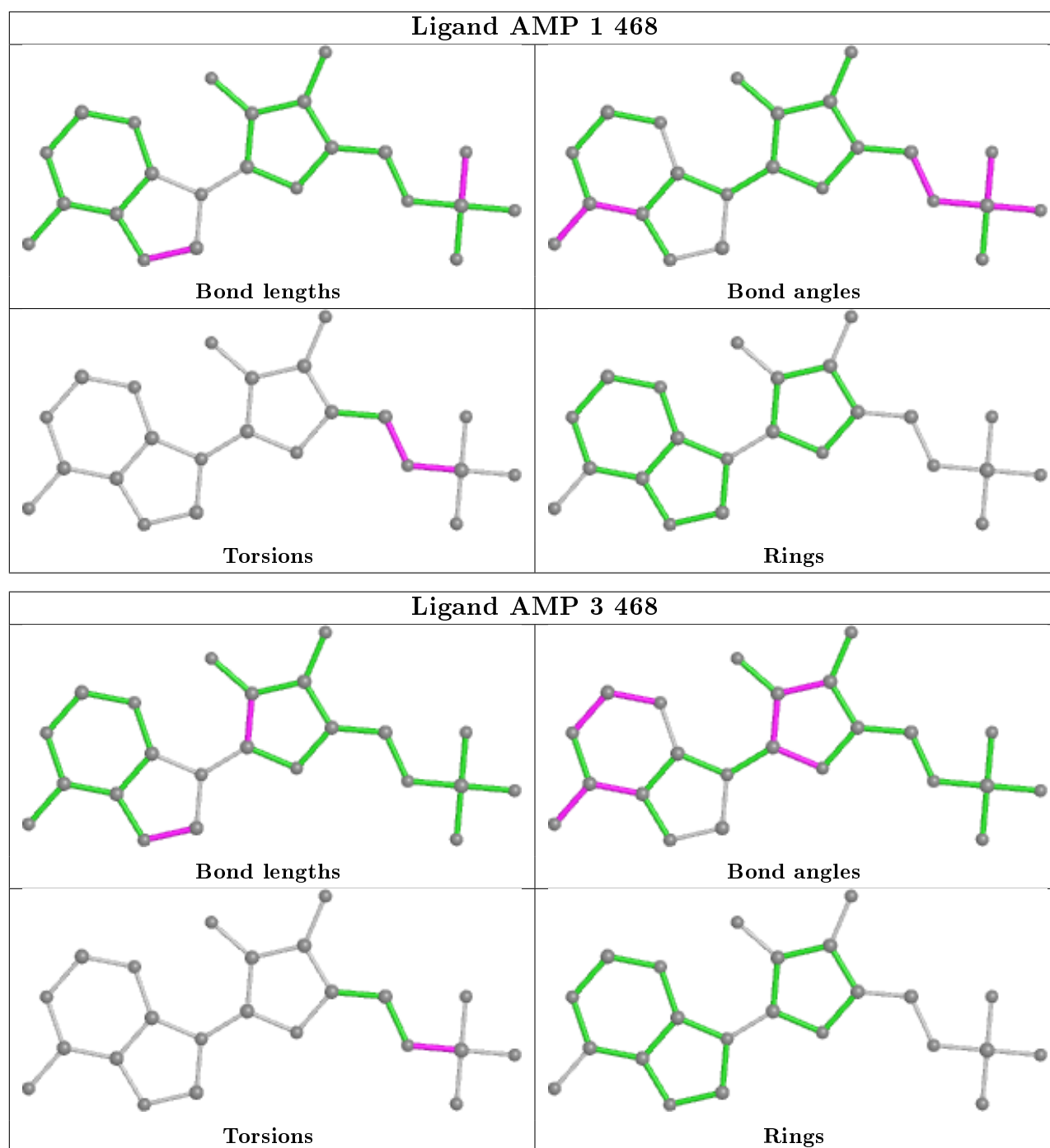


Ligand AMP 3 467



Ligand AMP 4 468





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.