



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 02:26 AM UTC

PDB ID : 1QK4 / pdb_00001qk4
Title : TOXOPLASMA GONDII HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE IMP COMPLEX
Authors : Heroux, A.; White, E.L.; Ross, L.J.; Borhani, D.W.
Deposited on : 1999-07-09
Resolution : 1.90 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)	:	2.0
EDS	:	FAILED
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

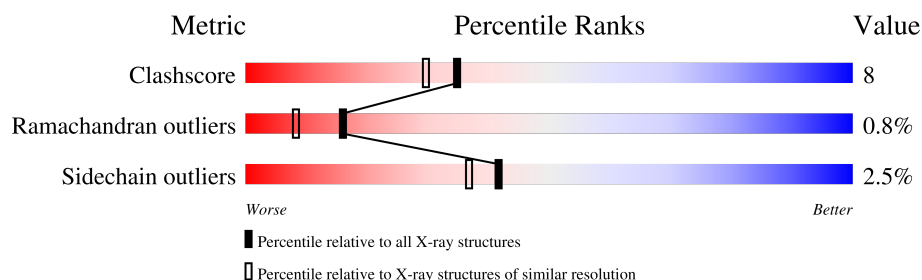
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	233	
1	B	233	
1	C	233	
1	D	233	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7683 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

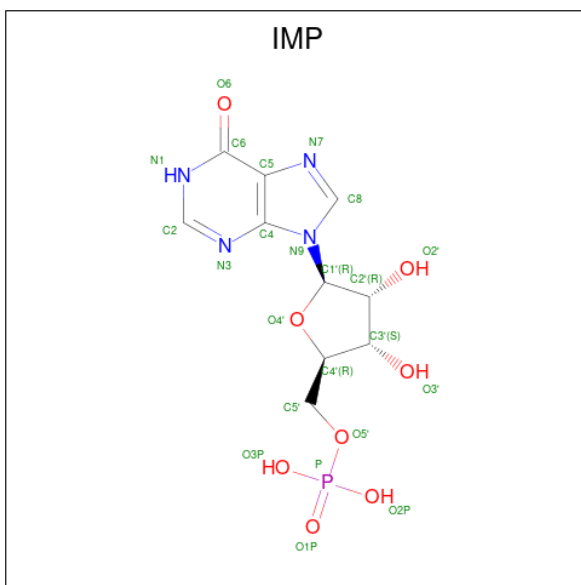
- Molecule 1 is a protein called HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1815	1173	301	333	8			
1	B	224	Total	C	N	O	S	0	2	0
			1807	1168	300	330	9			
1	C	213	Total	C	N	O	S	0	5	0
			1725	1117	282	319	7			
1	D	219	Total	C	N	O	S	0	3	0
			1759	1144	286	320	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0A	GLY	-	cloning artifact	UNP Q26997
A	0B	SER	-	cloning artifact	UNP Q26997
A	0C	HIS	-	cloning artifact	UNP Q26997
B	0A	GLY	-	cloning artifact	UNP Q26997
B	0B	SER	-	cloning artifact	UNP Q26997
B	0C	HIS	-	cloning artifact	UNP Q26997
C	0A	GLY	-	cloning artifact	UNP Q26997
C	0B	SER	-	cloning artifact	UNP Q26997
C	0C	HIS	-	cloning artifact	UNP Q26997
D	0A	GLY	-	cloning artifact	UNP Q26997
D	0B	SER	-	cloning artifact	UNP Q26997
D	0C	HIS	-	cloning artifact	UNP Q26997

- Molecule 2 is INOSINIC ACID (CCD ID: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	105	Total	O	0	0
			105	105		
3	C	135	Total	O	0	0
			135	135		
3	D	121	Total	O	0	0
			121	121		

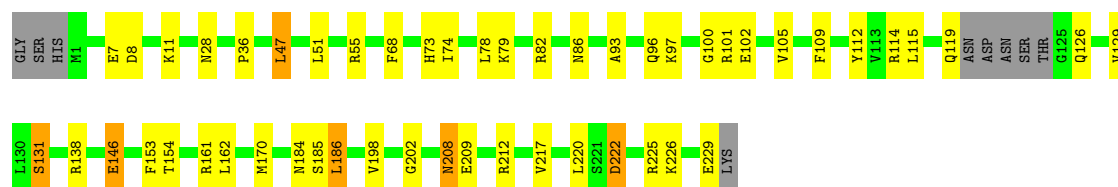
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

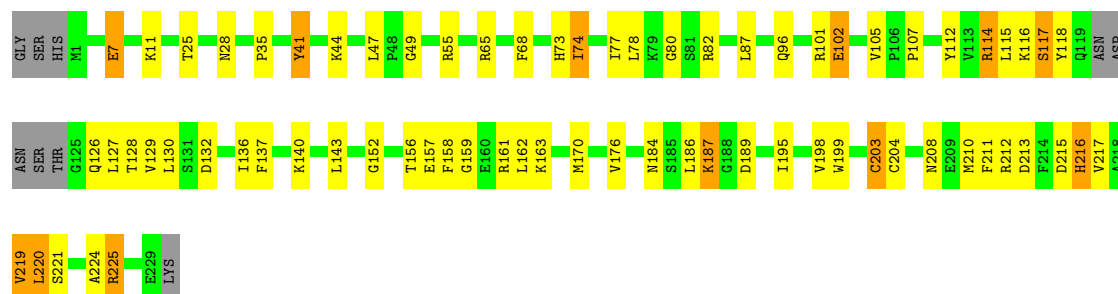
• Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE

Chain A: 



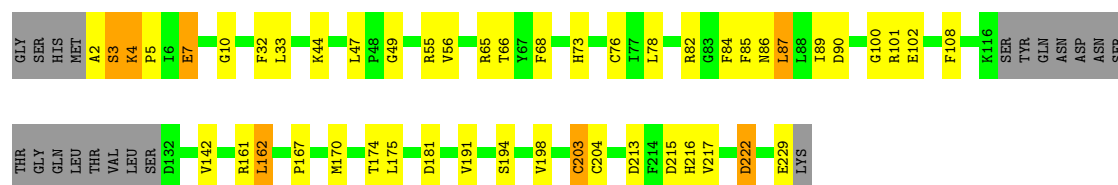
• Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE

Chain B: 



• Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE

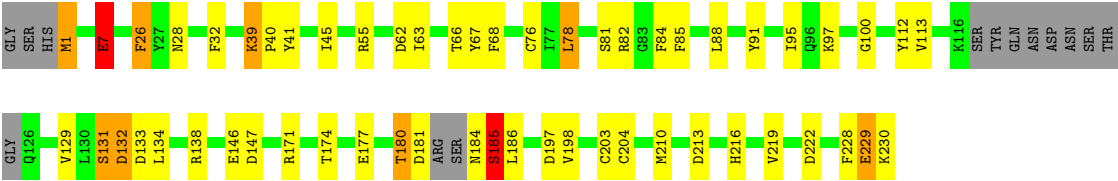
Chain C: 



• Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE

Chain D: 





4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.54Å 102.44Å 108.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.50 – 1.90	Depositor
% Data completeness (in resolution range)	99.6 (12.50-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.238	Depositor
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.396	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7683	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	0/1858	1.71	27/2505 (1.1%)
1	B	0.86	0/1860	1.81	40/2510 (1.6%)
1	C	0.95	0/1792	1.77	35/2422 (1.4%)
1	D	0.90	0/1818	1.76	30/2453 (1.2%)
All	All	0.91	0/7328	1.76	132/9890 (1.3%)

There are no bond length outliers.

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	LYS	N-CA-C	15.13	130.06	110.39
1	B	65	ARG	CD-NE-CZ	12.46	141.84	124.40
1	D	78	LEU	O-C-N	-11.65	109.80	122.96
1	B	78	LEU	O-C-N	-11.42	109.83	122.85
1	B	212	ARG	NE-CZ-NH2	10.81	128.93	119.20
1	D	82	ARG	CD-NE-CZ	10.69	139.37	124.40
1	D	131	SER	N-CA-C	9.76	123.37	110.88
1	D	185	SER	N-CA-C	9.61	131.26	110.80
1	B	65	ARG	NE-CZ-NH1	9.43	130.93	121.50
1	D	138	ARG	CD-NE-CZ	9.12	137.18	124.40
1	B	55	ARG	CD-NE-CZ	9.11	137.15	124.40
1	B	225	ARG	CD-NE-CZ	8.97	136.96	124.40
1	C	73	HIS	CA-CB-CG	-8.79	105.01	113.80
1	D	185	SER	CA-C-O	8.34	132.44	120.51
1	C	3	SER	CA-C-O	8.24	132.29	120.51
1	A	138	ARG	NE-CZ-NH2	8.14	126.52	119.20
1	B	213	ASP	CA-CB-CG	-7.97	104.63	112.60
1	C	229	GLU	CA-C-O	-7.86	107.43	120.80
1	B	77	ILE	O-C-N	7.81	132.46	122.77
1	D	113	VAL	CA-C-O	-7.70	113.82	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	ASP	CA-CB-CG	7.64	120.24	112.60
1	C	222	ASP	CA-CB-CG	-7.63	104.97	112.60
1	C	101	ARG	CA-C-N	7.48	131.33	120.71
1	C	101	ARG	C-N-CA	7.48	131.33	120.71
1	A	86	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	C	102	GLU	N-CA-C	7.45	121.03	110.23
1	B	73	HIS	CA-CB-CG	-7.40	106.40	113.80
1	A	114	ARG	NH1-CZ-NH2	7.35	128.86	119.30
1	D	55	ARG	CG-CD-NE	-7.27	96.01	112.00
1	C	86	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	A	78	LEU	O-C-N	-7.18	114.84	122.96
1	A	73	HIS	CA-CB-CG	-7.17	106.63	113.80
1	A	212	ARG	NE-CZ-NH2	7.12	125.61	119.20
1	C	3	SER	O-C-N	-7.11	113.14	122.59
1	B	35	PRO	CA-C-O	7.06	125.98	120.90
1	D	147	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	105	VAL	CA-C-N	7.04	124.80	119.66
1	B	105	VAL	C-N-CA	7.04	124.80	119.66
1	C	3	SER	CA-C-N	6.89	159.85	121.41
1	C	3	SER	C-N-CA	6.89	159.85	121.41
1	D	28	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	D	131	SER	N-CA-CB	-6.79	101.46	111.51
1	C	4	LYS	N-CA-CB	-6.76	98.87	110.10
1	C	102	GLU	CA-C-O	6.67	128.53	121.19
1	C	161	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	B	68	PHE	CA-CB-CG	-6.57	107.23	113.80
1	A	198	VAL	CA-C-O	-6.55	114.79	121.67
1	D	26[A]	PHE	CA-CB-CG	6.55	120.35	113.80
1	D	26[B]	PHE	CA-CB-CG	6.55	120.35	113.80
1	D	198	VAL	CA-C-O	-6.34	115.36	121.63
1	B	55	ARG	CG-CD-NE	-6.32	98.10	112.00
1	A	93	ALA	O-C-N	6.27	129.30	122.15
1	A	222	ASP	CA-CB-CG	-6.25	106.35	112.60
1	B	55	ARG	NE-CZ-NH2	-6.24	113.58	119.20
1	D	222	ASP	CA-CB-CG	-6.24	106.36	112.60
1	B	186	LEU	CA-C-O	-6.24	113.64	120.81
1	A	146	GLU	CB-CG-CD	6.22	123.18	112.60
1	B	132	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	25	THR	CA-C-O	-6.17	113.86	120.46
1	C	198	VAL	CA-C-O	-6.12	115.57	121.63
1	D	7	GLU	CB-CG-CD	6.10	122.97	112.60
1	A	138	ARG	NE-CZ-NH1	-6.09	115.41	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	GLU	N-CA-C	6.09	119.53	110.52
1	B	176	VAL	O-C-N	6.06	129.48	123.00
1	B	80	GLY	N-CA-C	6.04	120.20	112.83
1	D	68	PHE	CA-CB-CG	-6.03	107.77	113.80
1	C	100	GLY	CA-C-N	6.02	131.20	122.16
1	C	100	GLY	C-N-CA	6.02	131.20	122.16
1	D	216	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	55	ARG	CG-CD-NE	-6.00	98.81	112.00
1	B	55	ARG	NH1-CZ-NH2	5.96	127.05	119.30
1	D	213	ASP	CA-CB-CG	-5.80	106.80	112.60
1	D	229	GLU	CA-C-O	-5.80	114.77	121.15
1	C	90	ASP	CA-C-O	5.80	126.91	120.82
1	B	216	HIS	CA-CB-CG	-5.79	108.01	113.80
1	C	181[A]	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	181[B]	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	213	ASP	CA-CB-CG	-5.71	106.89	112.60
1	C	86	ASN	CB-CG-ND2	5.70	124.95	116.40
1	A	109	PHE	CA-CB-CG	-5.67	108.12	113.80
1	B	74	ILE	CA-C-O	5.62	126.43	120.48
1	A	96	GLN	OE1-CD-NE2	-5.61	117.00	122.60
1	A	74	ILE	CB-CA-C	5.60	119.17	110.83
1	C	194	SER	O-C-N	-5.57	116.88	123.22
1	A	154	THR	CA-C-O	-5.56	114.95	120.90
1	B	219	VAL	CA-C-O	5.54	127.26	120.84
1	D	41	TYR	N-CA-C	5.46	120.82	113.72
1	A	47	LEU	CB-CA-C	-5.43	103.51	111.01
1	B	101	ARG	N-CA-CB	-5.42	101.75	110.69
1	C	142	VAL	CA-C-N	-5.42	115.36	123.00
1	C	142	VAL	C-N-CA	-5.42	115.36	123.00
1	A	202	GLY	CA-C-O	-5.40	118.50	122.23
1	C	84	PHE	CA-CB-CG	5.39	119.19	113.80
1	C	10	GLY	N-CA-C	-5.38	107.89	115.32
1	D	185	SER	O-C-N	-5.38	115.43	122.59
1	A	79	LYS	CA-C-N	5.36	125.93	119.98
1	A	79	LYS	C-N-CA	5.36	125.93	119.98
1	D	180	THR	CA-C-O	-5.36	114.56	120.24
1	D	129	VAL	N-CA-C	5.36	116.00	109.30
1	B	41	TYR	N-CA-C	5.30	119.90	113.38
1	B	137	PHE	CA-CB-CG	-5.30	108.50	113.80
1	B	195	ILE	CA-C-O	-5.29	116.27	121.67
1	D	81	SER	CA-C-N	-5.29	113.19	120.28
1	D	81	SER	C-N-CA	-5.29	113.19	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ARG	NH1-CZ-NH2	-5.22	112.52	119.30
1	A	186	LEU	CA-C-O	-5.21	115.32	121.16
1	B	189	ASP	CA-CB-CG	-5.21	107.39	112.60
1	C	55	ARG	CG-CD-NE	-5.20	100.55	112.00
1	D	230	LYS	CA-C-O	-5.19	111.98	120.80
1	D	84	PHE	N-CA-CB	-5.17	102.57	110.07
1	B	80	GLY	CA-C-O	-5.17	115.73	120.80
1	A	68	PHE	CA-CB-CG	-5.17	108.64	113.80
1	C	44	LYS	CA-C-N	-5.16	116.10	123.11
1	C	44	LYS	C-N-CA	-5.16	116.10	123.11
1	B	203	CYS	CA-C-O	-5.14	115.88	121.84
1	C	203	CYS	CB-CA-C	-5.11	104.47	111.73
1	A	51	LEU	N-CA-C	-5.10	105.80	111.36
1	B	212	ARG	NH1-CZ-NH2	-5.10	112.67	119.30
1	C	68	PHE	CA-CB-CG	-5.09	108.71	113.80
1	B	198	VAL	CA-C-O	-5.09	116.33	121.67
1	D	229	GLU	CB-CA-C	-5.07	101.53	109.70
1	B	208	ASN	CB-CA-C	-5.07	105.07	111.86
1	C	32	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	114	ARG	CA-C-N	-5.07	115.58	122.93
1	B	114	ARG	C-N-CA	-5.07	115.58	122.93
1	B	87	LEU	CB-CA-C	-5.06	102.94	110.88
1	A	114	ARG	NE-CZ-NH1	-5.04	116.45	121.50
1	A	208	ASN	CA-CB-CG	-5.03	107.57	112.60
1	A	131	SER	O-C-N	5.03	128.54	123.26
1	B	28	ASN	CA-C-O	-5.03	114.96	120.69
1	C	101	ARG	N-CA-CB	5.03	117.35	110.57
1	A	114	ARG	NE-CZ-NH2	-5.02	114.68	119.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1815	0	1802	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1807	0	1789	45	0
1	C	1725	0	1690	18	0
1	D	1759	0	1726	30	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
3	A	124	0	0	2	0
3	B	105	0	0	2	0
3	C	135	0	0	0	0
3	D	121	0	0	2	0
All	All	7683	0	7051	107	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 8.

All (107) 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:C:49:GLY:H	1:C:216:HIS:HD2	1.07	0.98
1:B:156[A]:THR:HG21	1:B:184:ASN:HD21	1.25	0.97
1:B:49:GLY:H	1:B:216:HIS:HD2	1.16	0.91
1:D:184:ASN:O	1:D:185:SER:HB2	1.72	0.90
1:B:220:LEU:HD23	1:B:225:ARG:HG2	1.55	0.86
1:B:156[A]:THR:HG21	1:B:184:ASN:ND2	1.90	0.86
1:C:49:GLY:H	1:C:216:HIS:CD2	1.93	0.83
1:C:7:GLU:CD	1:C:7:GLU:H	1.90	0.79
1:D:210[A]:MET:HG3	1:D:228:PHE:CD2	2.18	0.79
1:B:49:GLY:H	1:B:216:HIS:CD2	2.01	0.78
1:B:156[A]:THR:CG2	1:B:184:ASN:HD21	1.97	0.78
1:C:162[B]:LEU:HD23	1:C:170:MET:HE3	1.66	0.77
1:D:180:THR:HG22	1:D:197:ASP:CG	2.12	0.75
1:B:199:TRP:HD1	1:B:220:LEU:HD11	1.50	0.73
1:A:184:ASN:O	1:A:185:SER:HB2	1.91	0.70
1:B:127:LEU:HD23	1:B:161:ARG:HH22	1.58	0.69
1:A:100:GLY:H	1:D:100:GLY:H	1.39	0.68
1:A:162:LEU:HD23	1:A:170:MET:HE3	1.79	0.65
1:D:131:SER:HB2	1:D:134:LEU:HD21	1.78	0.65
1:A:131:SER:HA	1:B:130:LEU:HD21	1.80	0.64
1:B:114:ARG:HB3	1:B:130:LEU:HB3	1.81	0.63
1:B:118:TYR:HB2	1:B:126:GLN:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PRO:HG2	1:B:102:GLU:HB2	1.81	0.62
1:B:152:GLY:O	1:B:156[A]:THR:HG23	1.99	0.62
1:D:26[A]:PHE:CE2	1:D:219:VAL:HG21	2.36	0.61
1:C:203:CYS:O	1:C:204:CYS:HB2	1.99	0.60
1:B:158:PHE:HD1	1:B:161:ARG:HH21	1.48	0.59
1:B:115:LEU:HD22	1:B:127:LEU:HD21	1.84	0.59
1:C:76:CYS:HB2	1:C:85:PHE:CD1	2.39	0.58
1:B:117:SER:HA	1:B:127:LEU:HD12	1.85	0.58
1:B:136:ILE:O	1:B:140:LYS:HD2	2.05	0.57
1:B:161:ARG:HD3	3:B:2065:HOH:O	2.04	0.56
1:A:28:ASN:HB3	3:A:2020:HOH:O	2.06	0.55
1:B:115:LEU:CD2	1:B:129:VAL:HG22	2.37	0.55
1:A:7:GLU:H	1:A:7:GLU:CD	2.16	0.54
1:D:177:GLU:HG3	3:D:2098:HOH:O	2.08	0.54
1:D:76:CYS:HB2	1:D:85:PHE:CD1	2.43	0.54
1:B:102:GLU:HB3	3:B:2050:HOH:O	2.06	0.54
1:A:184:ASN:O	1:A:185:SER:CB	2.57	0.53
1:B:74:ILE:HD12	1:B:143:LEU:HD23	1.90	0.52
1:C:82:ARG:HG3	1:D:112:TYR:OH	2.10	0.52
1:D:63:ILE:HD12	1:D:88:LEU:HD11	1.90	0.52
1:C:49:GLY:N	1:C:216:HIS:HD2	1.90	0.52
1:C:56:VAL:HG11	1:C:87:LEU:HB3	1.92	0.52
1:D:180:THR:O	1:D:181:ASP:C	2.53	0.51
1:B:41:TYR:HB3	1:B:224:ALA:HB2	1.93	0.50
1:A:97:LYS:NZ	1:B:215:ASP:OD1	2.38	0.50
1:A:131:SER:CA	1:B:130:LEU:HD21	2.41	0.50
1:B:199:TRP:O	1:B:220:LEU:HD13	2.12	0.50
1:B:11:LYS:O	1:B:187:LYS:HE3	2.12	0.49
1:B:115:LEU:HD22	1:B:127:LEU:CD2	2.42	0.49
1:D:32:PHE:CD2	1:D:45[B]:ILE:HD12	2.48	0.49
1:A:105:VAL:HG13	3:A:2040:HOH:O	2.13	0.48
1:A:82:ARG:HG3	1:B:112:TYR:OH	2.12	0.48
1:C:162[A]:LEU:HD12	1:C:167:PRO:HG3	1.95	0.48
1:A:119:GLN:NE2	1:A:153:PHE:HB2	2.29	0.48
1:A:208:ASN:O	1:A:209:GLU:HB2	2.14	0.48
1:D:180:THR:HG22	1:D:197:ASP:OD2	2.12	0.48
1:D:186:LEU:C	1:D:186:LEU:HD23	2.39	0.47
1:B:47:LEU:HB2	1:B:217:VAL:HB	1.95	0.47
1:D:203:CYS:O	1:D:204:CYS:HB2	2.14	0.47
1:D:131:SER:O	1:D:132:ASP:C	2.57	0.47
1:B:96:GLN:OE1	1:B:107:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:HE21	1:A:153:PHE:HB2	1.81	0.45
1:A:8:ASP:HA	1:A:11:LYS:HD2	1.98	0.45
1:B:44:LYS:HB2	1:B:219:VAL:HG22	1.98	0.45
1:C:78:LEU:HD11	1:D:78:LEU:HD11	1.99	0.45
1:D:67:TYR:OH	1:D:171:ARG:HD2	2.17	0.45
1:B:115:LEU:HD23	1:B:129:VAL:HG22	1.99	0.45
1:B:219:VAL:O	1:B:220:LEU:C	2.60	0.45
1:D:7:GLU:CD	1:D:7:GLU:H	2.23	0.45
1:D:1:MET:HA	1:D:1:MET:HE3	1.99	0.44
1:A:112:TYR:OH	1:B:82:ARG:HG3	2.18	0.44
1:D:210[B]:MET:HE3	1:D:228:PHE:CE2	2.52	0.44
1:B:220:LEU:HD23	1:B:225:ARG:CG	2.37	0.44
1:D:76:CYS:HB2	1:D:85:PHE:CG	2.53	0.44
1:B:127:LEU:HD23	1:B:161:ARG:NH2	2.28	0.44
1:A:115:LEU:CD2	1:A:129:VAL:HG22	2.48	0.44
1:A:225:ARG:O	1:A:229:GLU:N	2.51	0.43
1:B:210:MET:HG3	1:B:211:PHE:CD2	2.52	0.43
1:C:89:ILE:HB	1:C:108:PHE:CZ	2.53	0.43
1:C:47:LEU:HB2	1:C:217:VAL:HB	2.00	0.43
1:A:161:ARG:HG3	1:A:161:ARG:HH11	1.83	0.43
1:D:180:THR:HG21	3:D:2077:HOH:O	2.19	0.43
1:A:36:PRO:CG	1:B:102:GLU:HB2	2.47	0.43
1:C:215:ASP:OD1	1:D:97:LYS:NZ	2.47	0.42
1:B:7:GLU:H	1:B:7:GLU:HG3	1.41	0.42
1:C:2:ALA:HA	1:C:66:THR:O	2.19	0.42
1:A:222:ASP:O	1:A:226:LYS:HG3	2.20	0.42
1:C:4:LYS:HA	1:C:5:PRO:HD3	1.88	0.42
1:A:220:LEU:HD21	1:A:225:ARG:HG2	2.02	0.42
1:B:116:LYS:HB2	1:B:128:THR:HB	2.01	0.42
1:D:1:MET:HB3	1:D:66:THR:O	2.19	0.42
1:C:174:THR:O	1:C:191:VAL:HA	2.21	0.41
1:A:47:LEU:HB2	1:A:217:VAL:HB	2.03	0.41
1:B:199:TRP:CD1	1:B:220:LEU:HD11	2.41	0.41
1:B:203:CYS:O	1:B:204[A]:CYS:HB2	2.21	0.41
1:D:91:TYR:O	1:D:95:ILE:HG13	2.21	0.41
1:B:159:GLY:O	1:B:163:LYS:HG3	2.21	0.41
1:D:146:GLU:O	1:D:174:THR:HA	2.21	0.41
1:A:186:LEU:C	1:A:186:LEU:HD23	2.45	0.41
1:D:39:LYS:HB2	1:D:40:PRO:HD3	2.03	0.41
1:A:100:GLY:H	1:D:100:GLY:N	2.14	0.40
1:A:100:GLY:N	1:D:100:GLY:H	2.13	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HG23	1:B:161:ARG:NH1	2.37	0.40
1:B:162:LEU:HD23	1:B:170:MET:HE3	2.03	0.40
1:C:76:CYS:HB2	1:C:85:PHE:CG	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/233 (94%)	212 (96%)	7 (3%)	1 (0%)	24	16
1	B	222/233 (95%)	213 (96%)	7 (3%)	2 (1%)	14	6
1	C	214/233 (92%)	211 (99%)	2 (1%)	1 (0%)	24	16
1	D	216/233 (93%)	210 (97%)	3 (1%)	3 (1%)	9	3
All	All	872/932 (94%)	846 (97%)	19 (2%)	7 (1%)	16	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	LEU
1	B	221	SER
1	C	3	SER
1	D	132	ASP
1	D	133	ASP
1	D	185	SER
1	A	101	ARG

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/207 (96%)	196 (98%)	3 (2%)	57	56
1	B	198/207 (96%)	194 (98%)	4 (2%)	48	46
1	C	190/207 (92%)	182 (96%)	8 (4%)	26	19
1	D	191/207 (92%)	186 (97%)	5 (3%)	40	35
All	All	778/828 (94%)	758 (97%)	20 (3%)	42	35

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLU
1	A	126	GLN
1	A	146	GLU
1	B	7	GLU
1	B	117	SER
1	B	157	GLU
1	B	187	LYS
1	C	7	GLU
1	C	33	LEU
1	C	65	ARG
1	C	87	LEU
1	C	162[A]	LEU
1	C	162[B]	LEU
1	C	175	LEU
1	C	222	ASP
1	D	1	MET
1	D	7	GLU
1	D	39	LYS
1	D	185	SER
1	D	229	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	B	216	HIS
1	C	24	ASN

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Mol	Chain	Res	Type
1	C	184	ASN
1	C	216	HIS
1	D	86	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	IMP	C	300	-	25,25,25	0.92	2 (8%)	37,38,38	1.31	4 (10%)
2	IMP	A	300	-	25,25,25	0.84	1 (4%)	37,38,38	1.11	2 (5%)
2	IMP	D	300	-	25,25,25	0.81	0	37,38,38	1.22	5 (13%)
2	IMP	B	300	-	25,25,25	1.02	2 (8%)	37,38,38	1.23	3 (8%)

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	IMP	C	300	-	-	0/10/26/26	0/3/3/3
2	IMP	A	300	-	-	3/10/26/26	0/3/3/3
2	IMP	D	300	-	-	5/10/26/26	0/3/3/3
2	IMP	B	300	-	-	2/10/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	IMP	C2-N1	3.20	1.41	1.35
2	C	300	IMP	C2-N1	2.37	1.39	1.35
2	A	300	IMP	C2-N3	2.25	1.34	1.30
2	B	300	IMP	C2-N3	2.22	1.34	1.30
2	C	300	IMP	P-O2P	-2.07	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	IMP	O3P-P-O5'	-3.09	98.62	106.67
2	D	300	IMP	O2'-C2'-C1'	2.90	120.08	110.10
2	B	300	IMP	O3'-C3'-C2'	2.70	120.48	111.82
2	D	300	IMP	C2'-C1'-N9	-2.70	105.73	113.25
2	C	300	IMP	O2'-C2'-C1'	2.59	119.03	110.10
2	C	300	IMP	O5'-P-O1P	-2.58	99.47	106.44
2	D	300	IMP	C5'-C4'-C3'	-2.42	106.49	115.21
2	C	300	IMP	C2'-C3'-C4'	2.35	107.16	102.61
2	B	300	IMP	C5'-C4'-C3'	-2.21	107.25	115.21
2	D	300	IMP	O4'-C4'-C5'	2.13	116.16	109.33
2	A	300	IMP	O4'-C4'-C5'	-2.10	102.62	109.33
2	A	300	IMP	O5'-P-O1P	2.08	112.06	106.44
2	C	300	IMP	O4'-C1'-C2'	2.02	110.93	106.62
2	D	300	IMP	O2P-P-O5'	2.01	111.91	106.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	IMP	C5'-O5'-P-O2P
2	A	300	IMP	C5'-O5'-P-O3P
2	B	300	IMP	O4'-C4'-C5'-O5'
2	D	300	IMP	C5'-O5'-P-O2P
2	D	300	IMP	C5'-O5'-P-O3P

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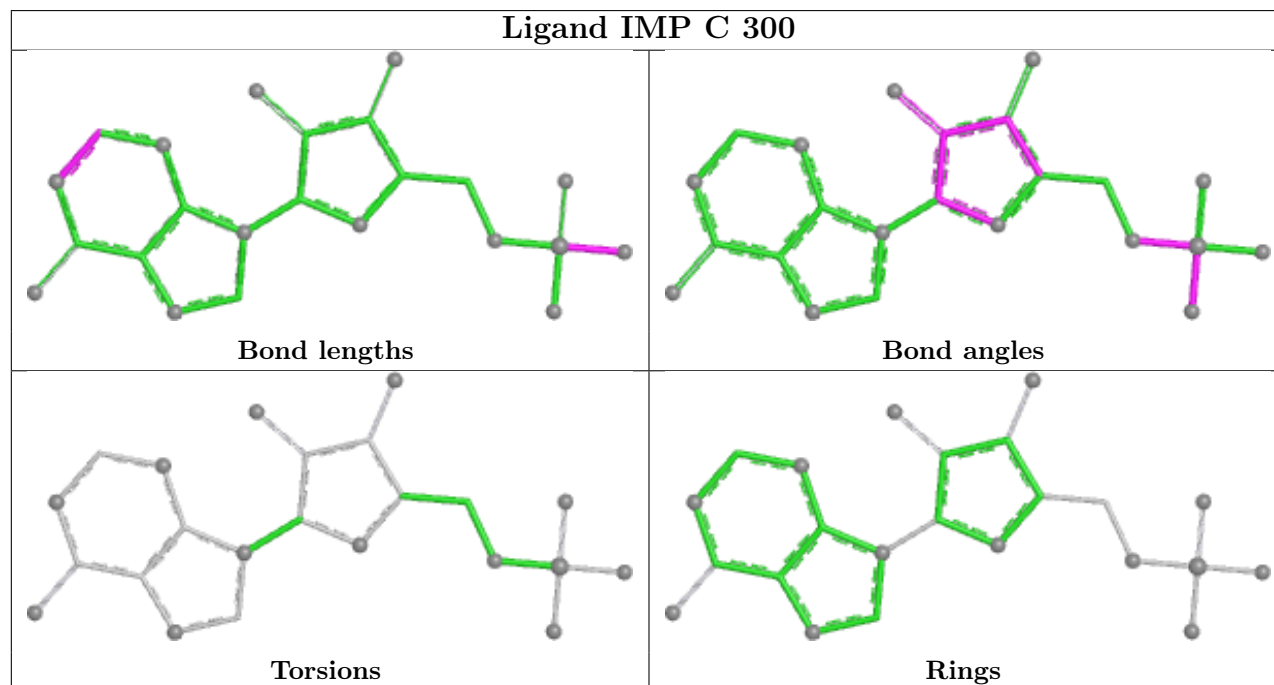
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Mol	Chain	Res	Type	Atoms
2	D	300	IMP	O4'-C4'-C5'-O5'
2	B	300	IMP	C3'-C4'-C5'-O5'
2	D	300	IMP	C3'-C4'-C5'-O5'
2	A	300	IMP	C5'-O5'-P-O1P
2	D	300	IMP	C5'-O5'-P-O1P

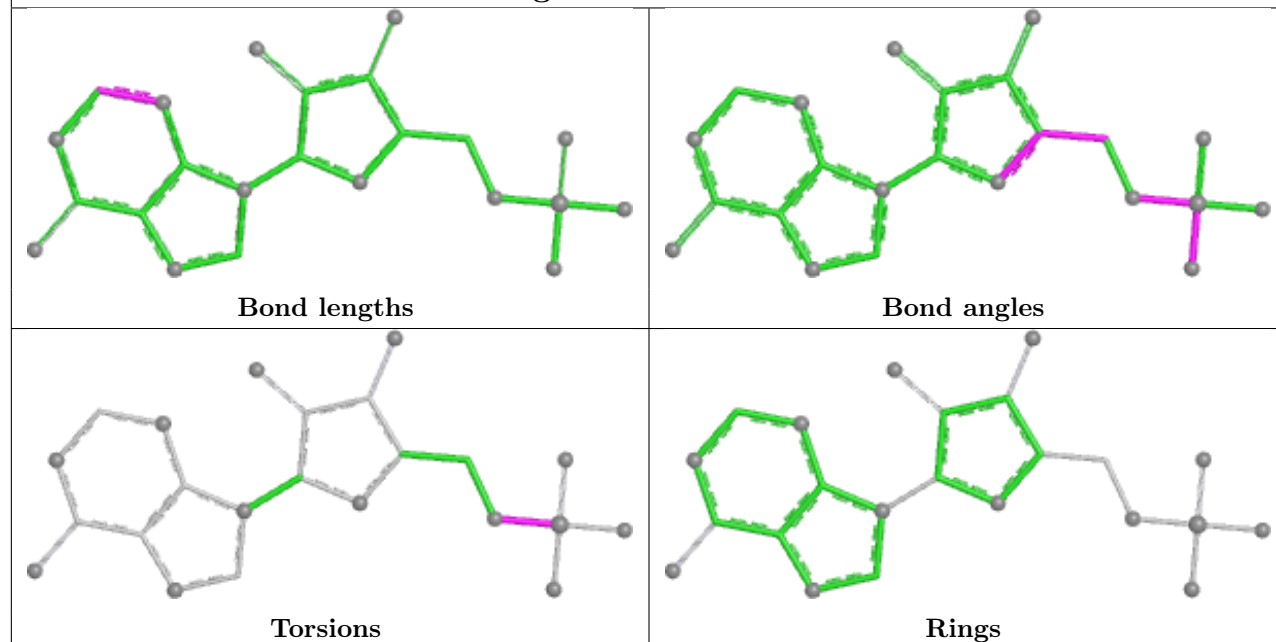
There are no ring outliers.

No monomer is involved in short contacts.

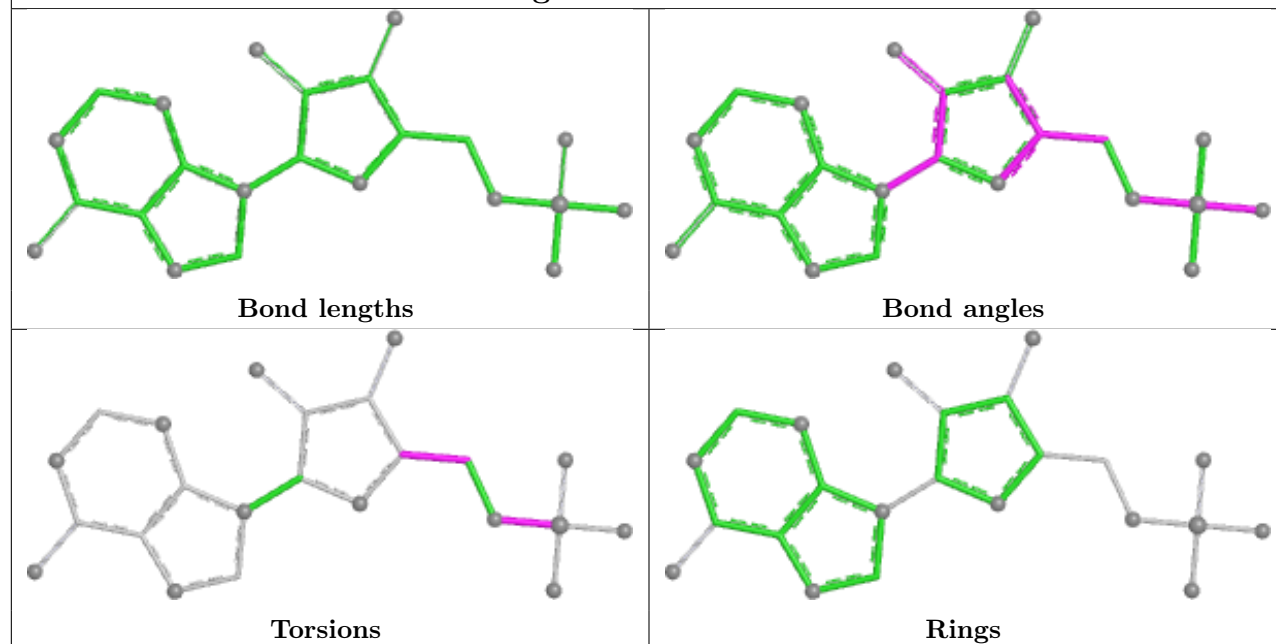
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

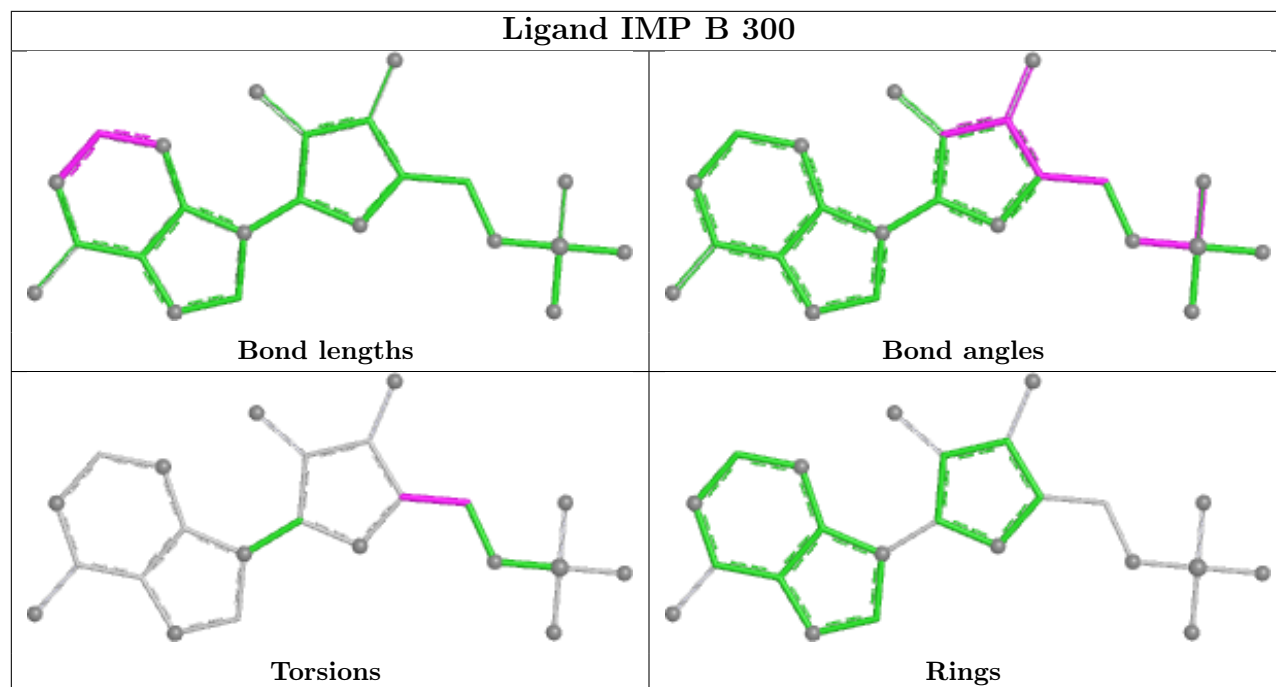


Ligand IMP A 300



Ligand IMP D 300





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.