



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:35 PM UTC

PDB ID : 1PVN / pdb_00001pvn
Title : The crystal structure of the complex between IMP dehydrogenase catalytic domain and a transition state analogue MZP
Authors : Gan, L.; Seyedsayamdost, M.; Shuto, S.; Matsuda, A.; Petsko, G.A.; Hedstrom, L.
Deposited on : 2003-06-27
Resolution : 2.00 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

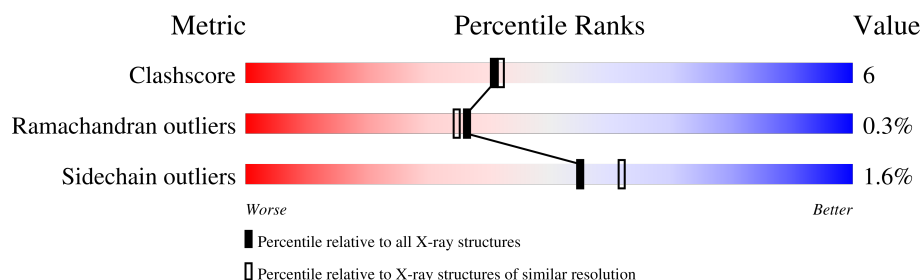
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	A	376	 83% 11% . .
1	B	376	 81% 14% . .
1	C	376	 83% 11% . .
1	D	376	 83% 12% . .

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
4	TRS	A	993	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12198 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.

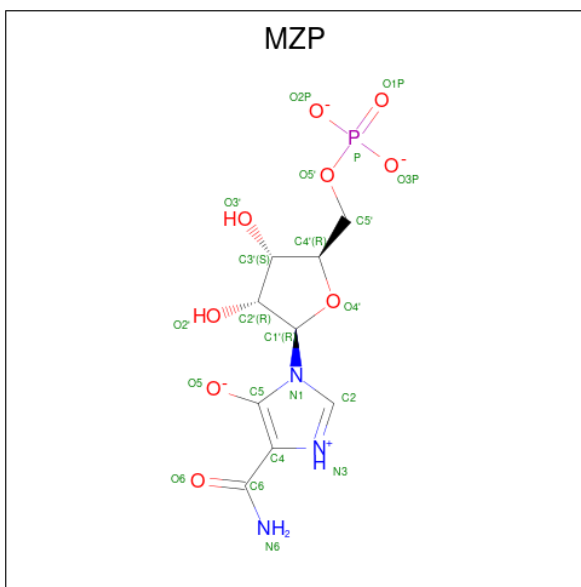
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2771	1757	473	526	15			
1	B	362	Total	C	N	O	S	0	0	0
			2771	1757	473	526	15			
1	C	362	Total	C	N	O	S	0	0	0
			2771	1757	473	526	15			
1	D	362	Total	C	N	O	S	0	0	0
			2771	1757	473	526	15			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

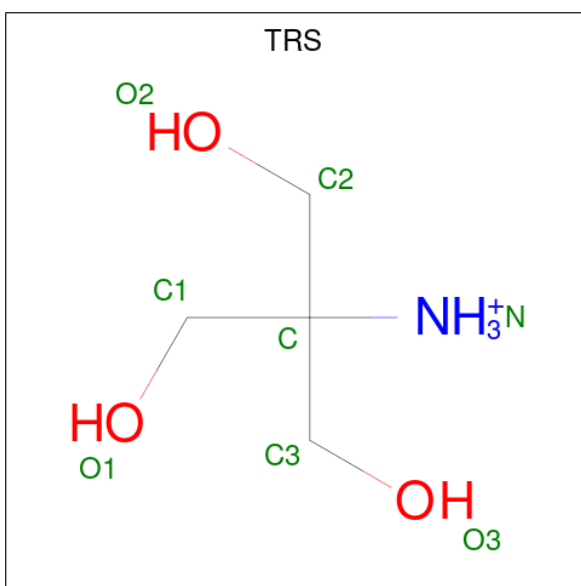
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	K	0	0
			3	3		
2	B	2	Total	K	0	0
			2	2		
2	C	2	Total	K	0	0
			2	2		
2	D	1	Total	K	0	0
			1	1		

- Molecule 3 is 4-CARBAMOYL-1-BETA-D-RIBOFURANOSYL-IMIDAZOLIUM-5-OLATE-5'-PHOSPHATE (CCD ID: MZP) (formula: C₉H₁₂N₃O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	9	3	9	1		
3	B	1	Total	C	N	O	P	0	0
			22	9	3	9	1		
3	C	1	Total	C	N	O	P	0	0
			22	9	3	9	1		
3	D	1	Total	C	N	O	P	0	0
			22	9	3	9	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	A	1	Total C N O 8 4 1 3	0	0
4	B	1	Total C N O 8 4 1 3	0	0
4	B	1	Total C N O 8 4 1 3	0	0
4	C	1	Total C N O 8 4 1 3	0	0
4	D	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is water.

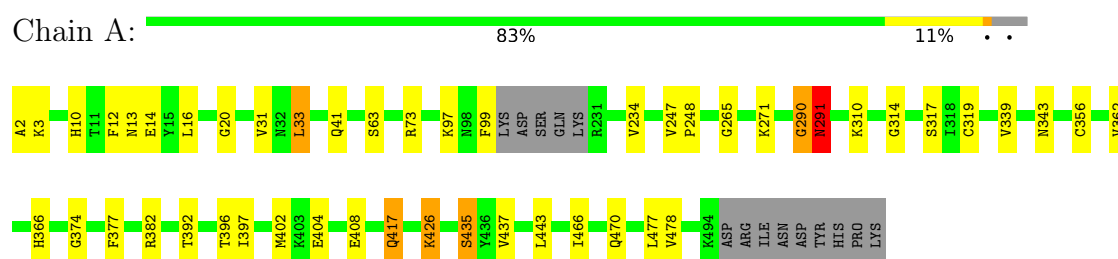
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	260	Total O 260 260	0	0
5	B	249	Total O 249 249	0	0
5	C	232	Total O 232 232	0	0
5	D	229	Total O 229 229	0	0

3 Residue-property plots [i](#)

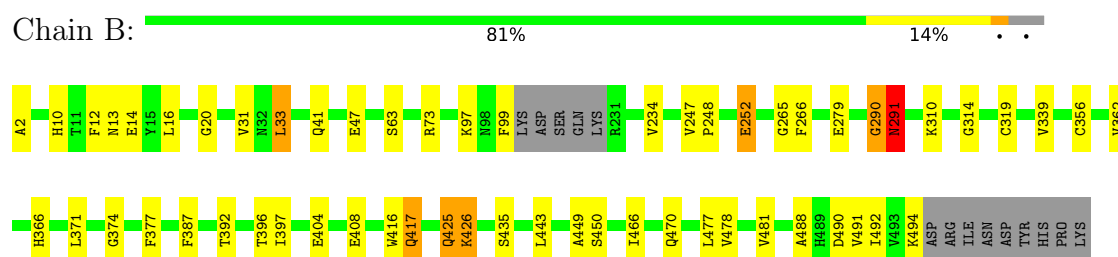
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 was not executed.

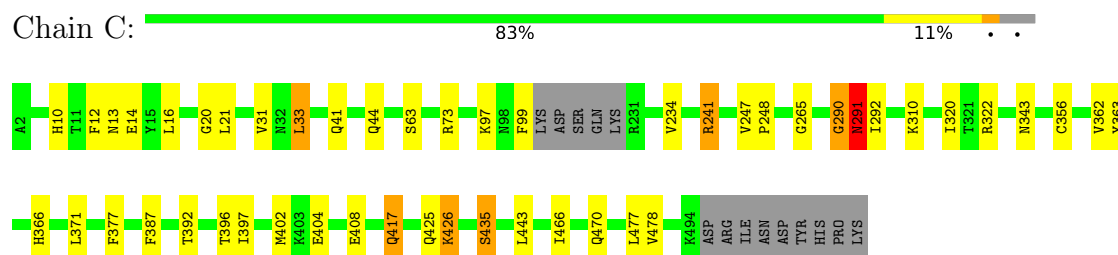
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



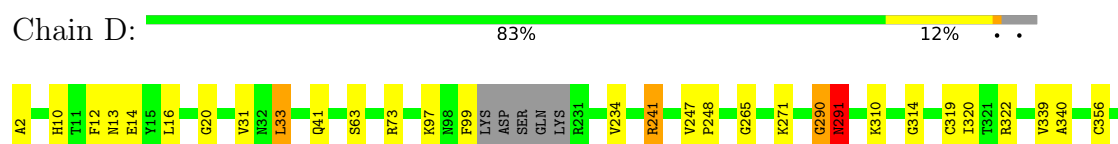
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.75Å 112.57Å 159.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 2.00	Depositor
% Data completeness (in resolution range)	97.4 (29.71-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.196 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12198	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: K, TRS, MZP

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	0.37	0/2820	0.91	7/3802 (0.2%)
1	B	0.38	0/2820	0.91	8/3802 (0.2%)
1	C	0.37	0/2820	0.90	9/3802 (0.2%)
1	D	0.38	0/2820	0.93	10/3802 (0.3%)
All	All	0.37	0/11280	0.91	34/15208 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	GLY	N-CA-C	10.98	127.60	111.24
1	C	290	GLY	N-CA-C	10.88	127.46	111.24
1	D	290	GLY	N-CA-C	10.81	127.35	111.24
1	B	290	GLY	N-CA-C	10.73	127.23	111.24
1	D	382	ARG	NE-CZ-NH2	8.37	126.73	119.20
1	D	382	ARG	NE-CZ-NH1	-8.36	113.14	121.50
1	D	291	ASN	N-CA-C	-6.59	96.77	110.80
1	B	291	ASN	N-CA-C	-6.58	96.78	110.80
1	C	291	ASN	N-CA-C	-6.56	96.83	110.80
1	A	291	ASN	N-CA-C	-6.50	96.96	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	SER	N-CA-C	6.44	116.56	108.45
1	C	435	SER	N-CA-C	6.29	116.38	108.45
1	D	20	GLY	N-CA-C	-6.22	105.33	112.79
1	C	63	SER	N-CA-C	6.21	119.37	108.56
1	B	63	SER	N-CA-C	6.20	119.35	108.56
1	A	435	SER	N-CA-C	6.18	116.24	108.45
1	C	20	GLY	N-CA-C	-6.17	105.39	112.79
1	B	20	GLY	N-CA-C	-6.14	105.43	112.79
1	A	63	SER	N-CA-C	6.13	119.23	108.56
1	D	435	SER	N-CA-C	6.13	116.18	108.45
1	D	63	SER	N-CA-C	6.11	119.19	108.56
1	A	20	GLY	N-CA-C	-6.06	105.51	112.79
1	C	477	LEU	N-CA-C	-5.44	103.21	110.55
1	B	477	LEU	N-CA-C	-5.37	103.30	110.55
1	C	387	PHE	N-CA-C	5.37	117.80	110.55
1	D	12	PHE	N-CA-C	5.31	122.11	110.80
1	D	382	ARG	CD-NE-CZ	5.24	131.74	124.40
1	C	12	PHE	N-CA-C	5.24	121.96	110.80
1	B	387	PHE	N-CA-C	5.22	117.60	110.55
1	A	477	LEU	N-CA-C	-5.19	103.54	110.55
1	C	292	ILE	N-CA-C	-5.19	101.60	108.96
1	D	477	LEU	N-CA-C	-5.18	103.56	110.55
1	B	12	PHE	N-CA-C	5.16	121.79	110.80
1	A	12	PHE	N-CA-C	5.10	121.66	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	241	ARG	Sidechain
1	D	241	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2771	0	2770	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2771	0	2770	42	0
1	C	2771	0	2770	36	0
1	D	2771	0	2770	37	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	22	0	12	1	0
3	B	22	0	12	1	0
3	C	22	0	12	1	0
3	D	22	0	12	1	0
4	A	16	0	24	6	0
4	B	16	0	24	4	0
4	C	8	0	12	4	0
4	D	8	0	12	2	0
5	A	260	0	0	5	0
5	B	249	0	0	4	0
5	C	232	0	0	3	0
5	D	229	0	0	5	0
All	All	12198	0	11200	145	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 6.

All (145) 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:D:241:ARG:HH21	1:D:425:GLN:HG2	1.31	0.93
1:D:408:GLU:H	3:D:974:MZP:HN3	1.18	0.90
1:B:408:GLU:H	3:B:972:MZP:HN3	1.20	0.90
1:C:408:GLU:H	3:C:973:MZP:HN3	1.20	0.88
1:D:417:GLN:HE21	1:D:417:GLN:H	1.21	0.88
1:A:408:GLU:H	3:A:971:MZP:HN3	1.18	0.88
1:C:417:GLN:HE21	1:C:417:GLN:H	1.23	0.87
1:A:417:GLN:HE21	1:A:417:GLN:H	1.23	0.86
1:B:417:GLN:H	1:B:417:GLN:HE21	1.23	0.86
1:A:402:MET:CE	1:B:492:ILE:HD12	2.12	0.79
1:A:402:MET:HE2	1:B:492:ILE:HD12	1.65	0.78
1:D:241:ARG:NH2	1:D:425:GLN:HG2	2.00	0.76
1:A:417:GLN:H	1:A:417:GLN:NE2	1.84	0.75
1:D:417:GLN:H	1:D:417:GLN:NE2	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLN:H	1:B:417:GLN:NE2	1.85	0.73
1:C:417:GLN:H	1:C:417:GLN:NE2	1.86	0.72
4:A:993:TRS:H22	5:A:1001:HOH:O	1.90	0.71
4:D:995:TRS:H21	5:D:998:HOH:O	1.90	0.70
4:B:994:TRS:H21	5:B:999:HOH:O	1.91	0.69
1:C:241:ARG:HH21	1:C:425:GLN:HG2	1.59	0.68
4:A:993:TRS:HO1	1:D:2:ALA:N	1.94	0.65
1:C:241:ARG:NH2	1:C:425:GLN:HG2	2.11	0.65
1:B:252:GLU:HG2	5:B:1155:HOH:O	1.97	0.65
1:C:402:MET:HE2	1:D:492:ILE:HD12	1.78	0.64
4:C:992:TRS:H11	5:C:997:HOH:O	1.98	0.63
1:A:339:VAL:HG12	4:A:993:TRS:O2	1.97	0.63
1:A:435:SER:HB2	1:B:492:ILE:O	2.02	0.58
1:B:2:ALA:N	4:C:992:TRS:HO3	2.01	0.58
1:C:291:ASN:HA	1:C:310:LYS:O	2.04	0.58
1:D:362:VAL:H	1:D:366:HIS:HD2	1.52	0.58
1:D:290:GLY:O	1:D:291:ASN:HB2	2.04	0.57
1:A:290:GLY:O	1:A:291:ASN:HB2	2.03	0.57
1:A:402:MET:HE1	1:B:492:ILE:HD12	1.85	0.57
1:B:362:VAL:H	1:B:366:HIS:HD2	1.52	0.57
1:B:290:GLY:O	1:B:291:ASN:HB2	2.05	0.57
1:A:97:LYS:HD3	1:A:234:VAL:HG12	1.86	0.57
1:B:449:ALA:HB3	4:B:991:TRS:H21	1.87	0.56
1:C:290:GLY:O	1:C:291:ASN:HB2	2.06	0.56
1:A:317:SER:O	1:B:488:ALA:HA	2.06	0.56
1:C:362:VAL:H	1:C:366:HIS:HD2	1.51	0.56
1:B:97:LYS:HD3	1:B:234:VAL:HG12	1.88	0.56
1:A:291:ASN:HA	1:A:310:LYS:O	2.06	0.55
1:C:97:LYS:HD3	1:C:234:VAL:HG12	1.87	0.55
1:A:362:VAL:H	1:A:366:HIS:HD2	1.54	0.54
1:D:417:GLN:HE21	1:D:417:GLN:N	1.99	0.54
1:B:247:VAL:HB	1:B:248:PRO:HD3	1.90	0.54
1:D:97:LYS:HD3	1:D:234:VAL:HG12	1.88	0.54
1:D:247:VAL:HB	1:D:248:PRO:HD3	1.90	0.54
1:D:291:ASN:HA	1:D:310:LYS:O	2.08	0.54
1:B:291:ASN:HA	1:B:310:LYS:O	2.08	0.54
1:C:320:ILE:HA	5:D:1220:HOH:O	2.08	0.54
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.90	0.53
1:C:247:VAL:HB	1:C:248:PRO:HD3	1.89	0.53
1:B:417:GLN:HE21	1:B:417:GLN:N	2.01	0.53
1:A:2:ALA:N	4:B:994:TRS:HO1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1042:HOH:O	1:D:320:ILE:HA	2.09	0.53
1:A:435:SER:HA	1:B:494:LYS:H	1.74	0.52
1:A:382:ARG:HD2	1:B:490:ASP:O	2.09	0.52
1:A:356:CYS:HB2	1:A:377:PHE:CE2	2.45	0.51
1:D:271:LYS:HE3	5:D:1123:HOH:O	2.10	0.51
1:D:339:VAL:HG12	4:D:995:TRS:O2	2.10	0.51
1:A:339:VAL:HG12	4:A:993:TRS:HO2	1.73	0.51
1:C:356:CYS:HB2	1:C:377:PHE:CE2	2.46	0.51
1:B:356:CYS:HB2	1:B:377:PHE:CE2	2.46	0.51
1:C:435:SER:HB2	1:D:492:ILE:O	2.10	0.51
1:A:3:LYS:HE2	5:A:1071:HOH:O	2.10	0.50
1:A:417:GLN:HE21	1:A:417:GLN:N	2.01	0.50
1:A:396:THR:C	1:A:397:ILE:HD12	2.36	0.50
1:C:343:ASN:ND2	4:C:992:TRS:H12	2.26	0.50
1:D:340:ALA:HB1	5:D:1086:HOH:O	2.12	0.50
1:A:10:HIS:HD2	1:A:14:GLU:OE1	1.95	0.50
1:B:47:GLU:HG3	5:B:1134:HOH:O	2.11	0.50
1:B:416:TRP:CZ2	1:B:425:GLN:HB3	2.48	0.49
1:C:417:GLN:HE21	1:C:417:GLN:N	2.02	0.49
1:A:466:ILE:O	1:A:470:GLN:HG3	2.13	0.49
1:C:396:THR:C	1:C:397:ILE:HD12	2.38	0.49
4:A:993:TRS:H21	5:A:1093:HOH:O	2.12	0.49
1:C:402:MET:CE	1:D:492:ILE:HD12	2.41	0.49
1:C:10:HIS:HD2	1:C:14:GLU:OE1	1.95	0.49
1:B:396:THR:C	1:B:397:ILE:HD12	2.37	0.48
1:C:466:ILE:O	1:C:470:GLN:HG3	2.14	0.48
1:D:396:THR:C	1:D:397:ILE:HD12	2.37	0.48
1:B:466:ILE:O	1:B:470:GLN:HG3	2.14	0.48
1:D:466:ILE:O	1:D:470:GLN:HG3	2.14	0.48
1:B:31:VAL:HG12	1:B:33:LEU:HD13	1.97	0.47
1:B:73:ARG:HH21	1:B:99:PHE:HE2	1.63	0.47
1:D:356:CYS:HB2	1:D:377:PHE:CE2	2.49	0.47
1:C:44:GLN:NE2	5:C:1006:HOH:O	2.31	0.47
1:C:73:ARG:HH21	1:C:99:PHE:HE2	1.63	0.47
1:D:73:ARG:HH21	1:D:99:PHE:HE2	1.63	0.47
1:A:73:ARG:HH21	1:A:99:PHE:HE2	1.63	0.47
1:D:10:HIS:HD2	1:D:14:GLU:OE1	1.98	0.47
1:A:392:THR:HB	1:A:404:GLU:HB2	1.97	0.46
1:B:10:HIS:HD2	1:B:14:GLU:OE1	1.98	0.46
1:C:443:LEU:C	1:C:443:LEU:HD23	2.40	0.46
1:D:241:ARG:NH2	1:D:425:GLN:CG	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:VAL:HG12	1:D:33:LEU:HD13	1.98	0.46
1:D:443:LEU:C	1:D:443:LEU:HD23	2.41	0.46
1:A:443:LEU:C	1:A:443:LEU:HD23	2.42	0.45
1:D:392:THR:HB	1:D:404:GLU:HB2	1.99	0.45
1:B:443:LEU:HD23	1:B:443:LEU:C	2.41	0.45
1:B:450:SER:OG	4:B:991:TRS:H22	2.16	0.45
1:B:392:THR:HB	1:B:404:GLU:HB2	1.99	0.45
1:C:31:VAL:HG12	1:C:33:LEU:HD13	1.97	0.45
1:B:13:ASN:ND2	1:B:366:HIS:CE1	2.86	0.44
1:C:343:ASN:HD22	4:C:992:TRS:H12	1.81	0.44
1:D:362:VAL:H	1:D:366:HIS:CD2	2.34	0.44
1:B:16:LEU:HG	1:B:478:VAL:HG21	1.98	0.44
1:C:392:THR:HB	1:C:404:GLU:HB2	2.00	0.44
1:D:10:HIS:HE1	5:D:1106:HOH:O	2.00	0.44
1:B:426:LYS:NZ	1:B:426:LYS:HB2	2.33	0.43
1:A:31:VAL:HG12	1:A:33:LEU:HD13	1.99	0.43
1:C:10:HIS:HE1	5:C:1178:HOH:O	2.01	0.43
1:C:362:VAL:H	1:C:366:HIS:CD2	2.34	0.43
1:B:362:VAL:H	1:B:366:HIS:CD2	2.35	0.43
1:A:13:ASN:ND2	1:A:366:HIS:CE1	2.87	0.43
1:C:426:LYS:HB2	1:C:426:LYS:NZ	2.34	0.43
1:B:266:PHE:CE1	1:C:21:LEU:HB2	2.55	0.42
1:A:426:LYS:HB2	1:A:426:LYS:NZ	2.34	0.42
1:D:13:ASN:ND2	1:D:366:HIS:CE1	2.87	0.42
1:A:314:GLY:HA2	1:A:319:CYS:SG	2.60	0.42
1:D:426:LYS:HB2	1:D:426:LYS:NZ	2.35	0.42
1:B:265:GLY:HA3	1:B:290:GLY:HA2	2.01	0.42
1:D:265:GLY:HA3	1:D:290:GLY:HA2	2.02	0.42
1:A:14:GLU:HG2	1:B:481:VAL:HG21	2.02	0.42
1:A:265:GLY:HA3	1:A:290:GLY:HA2	2.01	0.42
1:C:371:LEU:O	1:C:470:GLN:HG2	2.20	0.41
1:A:362:VAL:H	1:A:366:HIS:CD2	2.35	0.41
1:C:13:ASN:ND2	1:C:366:HIS:CE1	2.88	0.41
1:A:343:ASN:ND2	4:A:993:TRS:O2	2.53	0.41
1:B:314:GLY:HA2	1:B:319:CYS:SG	2.60	0.41
1:A:271:LYS:HE3	5:A:1222:HOH:O	2.19	0.41
1:C:265:GLY:HA3	1:C:290:GLY:HA2	2.03	0.41
1:A:16:LEU:HG	1:A:478:VAL:HG21	2.02	0.41
1:B:10:HIS:HE1	5:B:1085:HOH:O	2.03	0.41
1:D:16:LEU:HG	1:D:478:VAL:HG21	2.02	0.41
1:A:339:VAL:HG21	1:A:374:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LEU:O	1:B:470:GLN:HG2	2.20	0.41
1:C:16:LEU:HG	1:C:478:VAL:HG21	2.02	0.40
1:C:322:ARG:HD2	1:D:486:GLY:HA2	2.03	0.40
1:B:339:VAL:HG21	1:B:374:GLY:HA3	2.03	0.40
1:D:314:GLY:HA3	1:D:322:ARG:HG3	2.03	0.40
1:D:314:GLY:HA2	1:D:319:CYS:SG	2.61	0.40
1:A:437:VAL:HG12	1:B:491:VAL:HG12	2.02	0.40
1:C:363:TYR:O	1:C:366:HIS:HB2	2.21	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	358/376 (95%)	349 (98%)	8 (2%)	1 (0%)	36	35
1	B	358/376 (95%)	349 (98%)	8 (2%)	1 (0%)	36	35
1	C	358/376 (95%)	350 (98%)	7 (2%)	1 (0%)	36	35
1	D	358/376 (95%)	349 (98%)	8 (2%)	1 (0%)	36	35
All	All	1432/1504 (95%)	1397 (98%)	31 (2%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	B	291	ASN
1	C	291	ASN
1	D	291	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/308 (96%)	290 (99%)	4 (1%)	59	66
1	B	294/308 (96%)	287 (98%)	7 (2%)	43	47
1	C	294/308 (96%)	290 (99%)	4 (1%)	59	66
1	D	294/308 (96%)	290 (99%)	4 (1%)	59	66
All	All	1176/1232 (96%)	1157 (98%)	19 (2%)	55	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	41	GLN
1	A	417	GLN
1	A	426	LYS
1	B	33	LEU
1	B	41	GLN
1	B	252	GLU
1	B	279	GLU
1	B	417	GLN
1	B	425	GLN
1	B	426	LYS
1	C	33	LEU
1	C	41	GLN
1	C	417	GLN
1	C	426	LYS
1	D	33	LEU
1	D	41	GLN
1	D	417	GLN
1	D	426	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	13	ASN
1	A	41	GLN
1	A	94	HIS
1	A	331	GLN
1	A	343	ASN
1	A	366	HIS
1	A	417	GLN
1	A	425	GLN
1	A	446	ASN
1	B	10	HIS
1	B	13	ASN
1	B	41	GLN
1	B	49	ASN
1	B	331	GLN
1	B	366	HIS
1	B	417	GLN
1	B	425	GLN
1	C	10	HIS
1	C	13	ASN
1	C	41	GLN
1	C	98	ASN
1	C	331	GLN
1	C	366	HIS
1	C	417	GLN
1	C	425	GLN
1	C	446	ASN
1	D	10	HIS
1	D	13	ASN
1	D	41	GLN
1	D	98	ASN
1	D	331	GLN
1	D	366	HIS
1	D	417	GLN
1	D	425	GLN
1	D	446	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MZP	A	971	-	21,23,23	1.27	2 (9%)	29,35,35	1.19	3 (10%)
3	MZP	B	972	-	21,23,23	1.28	3 (14%)	29,35,35	1.18	3 (10%)
4	TRS	B	994	-	7,7,7	0.84	0	9,9,9	1.87	2 (22%)
4	TRS	D	995	-	7,7,7	0.88	0	9,9,9	1.91	2 (22%)
4	TRS	A	993	-	7,7,7	0.95	0	9,9,9	1.75	2 (22%)
3	MZP	D	974	-	21,23,23	1.32	3 (14%)	29,35,35	1.19	3 (10%)
4	TRS	A	996	-	7,7,7	0.88	0	9,9,9	1.98	2 (22%)
4	TRS	C	992	-	7,7,7	0.89	0	9,9,9	1.86	2 (22%)
4	TRS	B	991	-	7,7,7	0.83	0	9,9,9	1.91	2 (22%)
3	MZP	C	973	-	21,23,23	1.33	3 (14%)	29,35,35	1.19	3 (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
3	MZP	A	971	-	-	0/14/30/30	0/2/2/2
3	MZP	B	972	-	-	0/14/30/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	B	994	-	-	3/9/9/9	-
4	TRS	D	995	-	-	4/9/9/9	-
4	TRS	A	993	-	-	5/9/9/9	-
3	MZP	D	974	-	-	0/14/30/30	0/2/2/2
4	TRS	A	996	-	-	6/9/9/9	-
4	TRS	C	992	-	-	0/9/9/9	-
4	TRS	B	991	-	-	1/9/9/9	-
3	MZP	C	973	-	-	0/14/30/30	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	974	MZP	P-O5'	-2.29	1.53	1.60
3	A	971	MZP	P-O5'	-2.23	1.53	1.60
3	B	972	MZP	O5-C5	2.13	1.37	1.31
3	A	971	MZP	C6-N6	2.13	1.39	1.33
3	C	973	MZP	P-O5'	-2.13	1.53	1.60
3	B	972	MZP	C6-N6	2.11	1.39	1.33
3	C	973	MZP	C4-N3	-2.07	1.34	1.39
3	B	972	MZP	P-O5'	-2.04	1.53	1.60
3	D	974	MZP	C6-N6	2.03	1.39	1.33
3	C	973	MZP	O5-C5	2.01	1.37	1.31
3	D	974	MZP	O5-C5	2.01	1.37	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	996	TRS	C2-C-N	4.39	119.38	108.17
4	B	991	TRS	C2-C-N	4.36	119.28	108.17
4	D	995	TRS	C2-C-N	4.33	119.20	108.17
4	B	994	TRS	C2-C-N	4.32	119.18	108.17
4	A	993	TRS	C2-C-N	4.12	118.69	108.17
4	C	992	TRS	C2-C-N	4.09	118.61	108.17
3	D	974	MZP	C1'-N1-C2	3.64	137.08	126.73
3	A	971	MZP	C1'-N1-C2	3.63	137.04	126.73
3	B	972	MZP	C1'-N1-C2	3.63	137.03	126.73
3	C	973	MZP	C1'-N1-C2	3.56	136.85	126.73
3	C	973	MZP	C4-C6-N6	2.91	121.87	116.73
3	D	974	MZP	C4-C6-N6	2.87	121.79	116.73
3	A	971	MZP	C4-C6-N6	2.83	121.72	116.73
3	B	972	MZP	C4-C6-N6	2.81	121.68	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	973	MZP	O6-C6-N6	-2.56	117.15	122.89
3	A	971	MZP	O6-C6-N6	-2.49	117.30	122.89
3	D	974	MZP	O6-C6-N6	-2.48	117.34	122.89
3	B	972	MZP	O6-C6-N6	-2.47	117.36	122.89
4	A	996	TRS	C1-C-N	-2.39	102.07	108.17
4	B	991	TRS	C1-C-N	-2.24	102.46	108.17
4	A	993	TRS	C1-C-N	-2.18	102.62	108.17
4	C	992	TRS	C2-C-C1	-2.13	104.98	110.66
4	B	994	TRS	C1-C-N	-2.03	103.00	108.17
4	D	995	TRS	C1-C-N	-2.01	103.05	108.17

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	993	TRS	N-C-C2-O2
4	A	996	TRS	N-C-C1-O1
4	D	995	TRS	C3-C-C2-O2
4	A	993	TRS	C3-C-C2-O2
4	A	996	TRS	C1-C-C3-O3
4	D	995	TRS	C1-C-C2-O2
4	A	993	TRS	C1-C-C2-O2
4	A	996	TRS	N-C-C3-O3
4	B	994	TRS	N-C-C2-O2
4	D	995	TRS	N-C-C2-O2
4	A	993	TRS	C2-C-C3-O3
4	A	996	TRS	C1-C-C2-O2
4	A	996	TRS	C3-C-C2-O2
4	A	996	TRS	C2-C-C3-O3
4	A	993	TRS	C1-C-C3-O3
4	B	991	TRS	C3-C-C2-O2
4	B	994	TRS	C3-C-C2-O2
4	B	994	TRS	C1-C-C2-O2
4	D	995	TRS	N-C-C3-O3

There are no ring outliers.

9 monomers are involved in 20 short contacts:

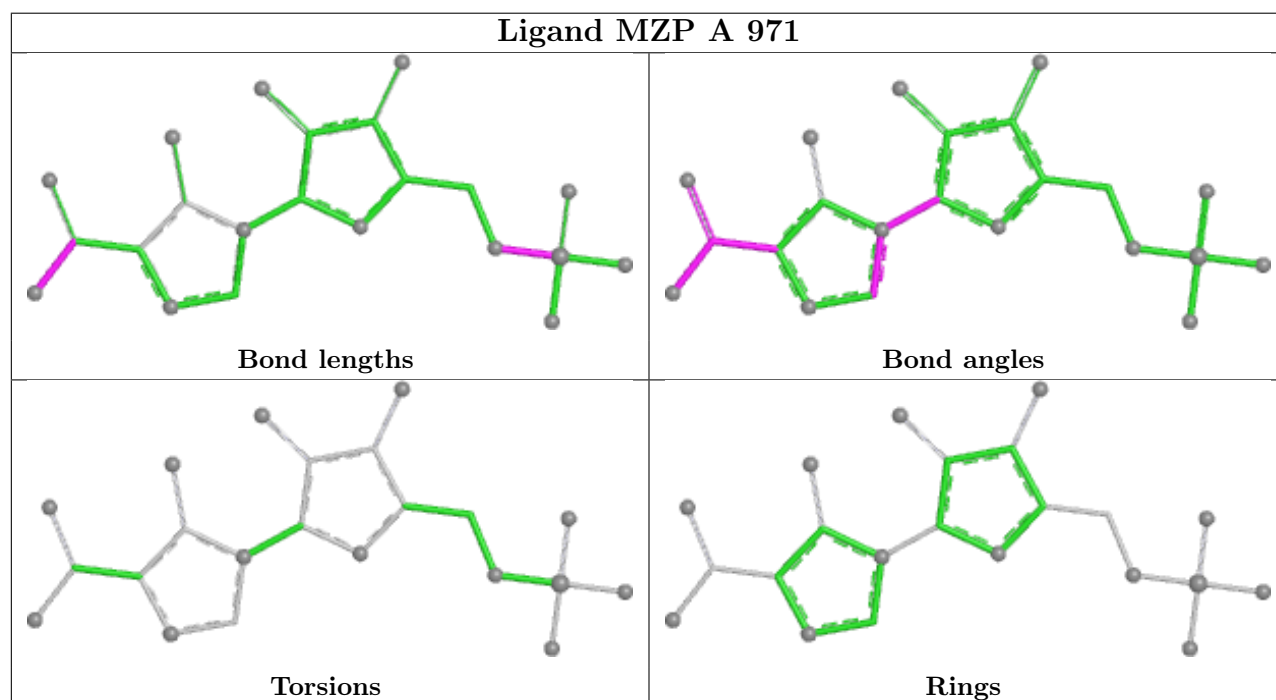
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	971	MZP	1	0
3	B	972	MZP	1	0

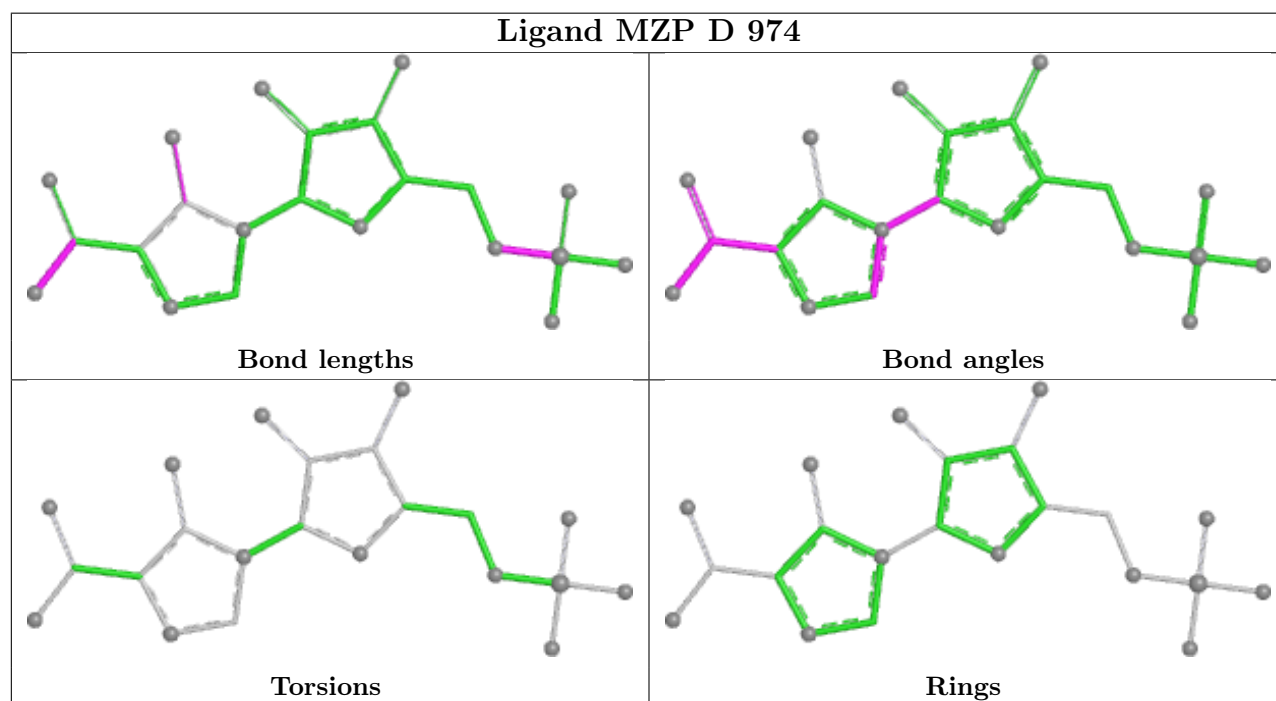
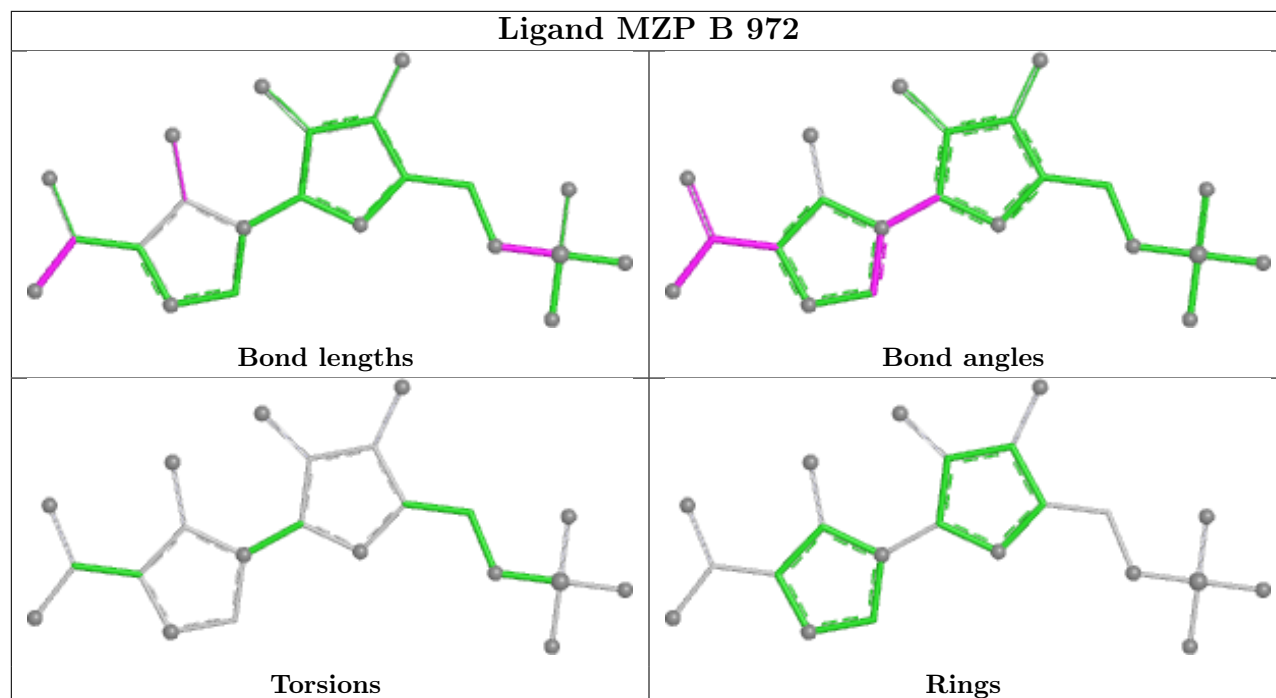
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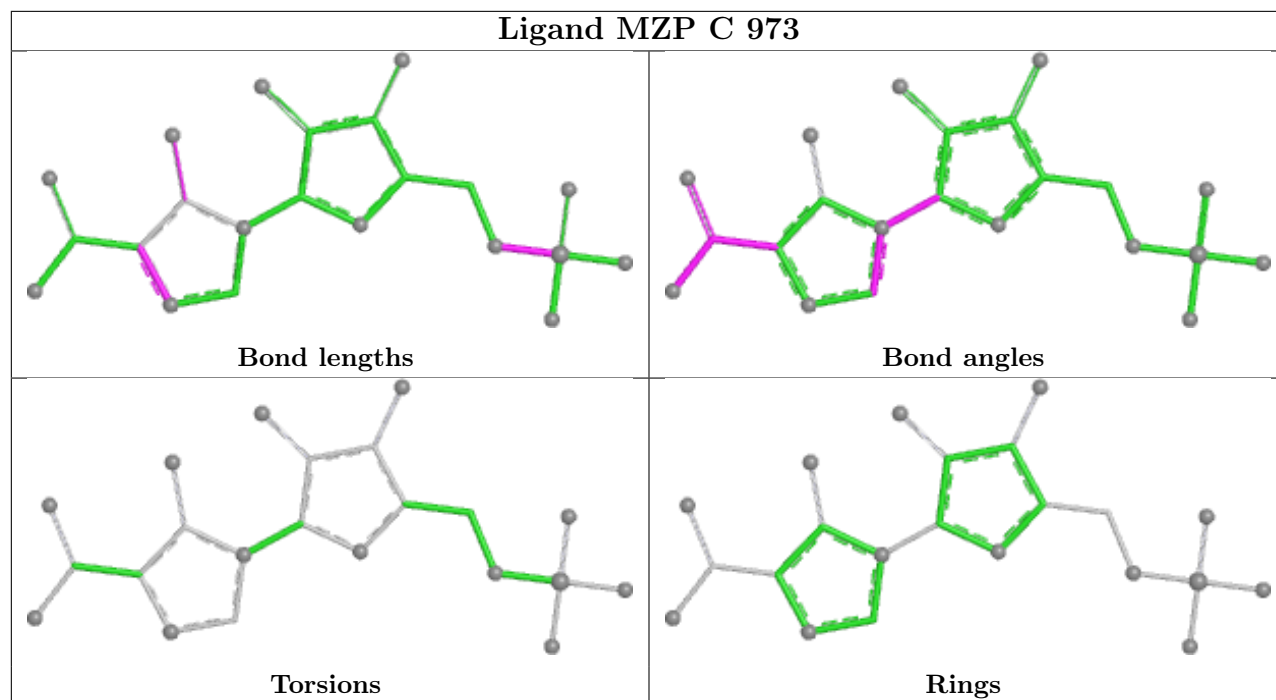
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	994	TRS	2	0
4	D	995	TRS	2	0
4	A	993	TRS	6	0
3	D	974	MZP	1	0
4	C	992	TRS	4	0
4	B	991	TRS	2	0
3	C	973	MZP	1	0

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.







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.