



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:56 pm BST

PDB ID : 2G01
Title : Pyrazoloquinolones as Novel, Selective JNK1 inhibitors
Authors : Abad-Zapatero, C.
Deposited on : 2006-02-10
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

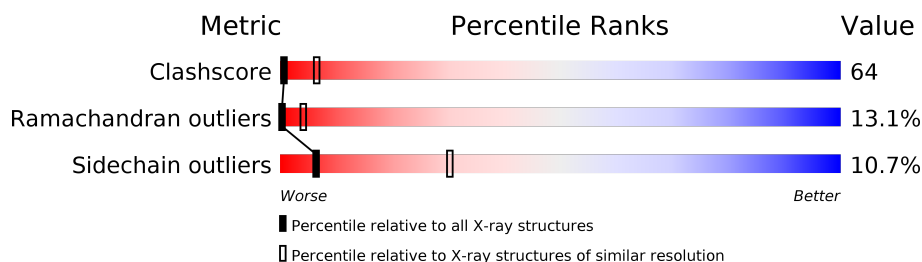
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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	A	370	
1	B	370	
2	F	11	
2	G	11	

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
3	SO4	A	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5918 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 Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	1
			2858	1834	482	520	22			
1	B	357	Total	C	N	O	S	0	0	1
			2858	1832	482	522	22			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	THR	ENGINEERED MUTATION	UNP P45983
A	185	GLU	TYR	ENGINEERED MUTATION	UNP P45983
A	365	HIS	-	EXPRESSION TAG	UNP P45983
A	366	HIS	-	EXPRESSION TAG	UNP P45983
A	367	HIS	-	EXPRESSION TAG	UNP P45983
A	368	HIS	-	EXPRESSION TAG	UNP P45983
A	369	HIS	-	EXPRESSION TAG	UNP P45983
A	370	HIS	-	EXPRESSION TAG	UNP P45983
B	183	GLU	THR	ENGINEERED MUTATION	UNP P45983
B	185	GLU	TYR	ENGINEERED MUTATION	UNP P45983
B	365	HIS	-	EXPRESSION TAG	UNP P45983
B	366	HIS	-	EXPRESSION TAG	UNP P45983
B	367	HIS	-	EXPRESSION TAG	UNP P45983
B	368	HIS	-	EXPRESSION TAG	UNP P45983
B	369	HIS	-	EXPRESSION TAG	UNP P45983
B	370	HIS	-	EXPRESSION TAG	UNP P45983

- Molecule 2 is a protein called C-jun-amino-terminal kinase-interacting protein 1.

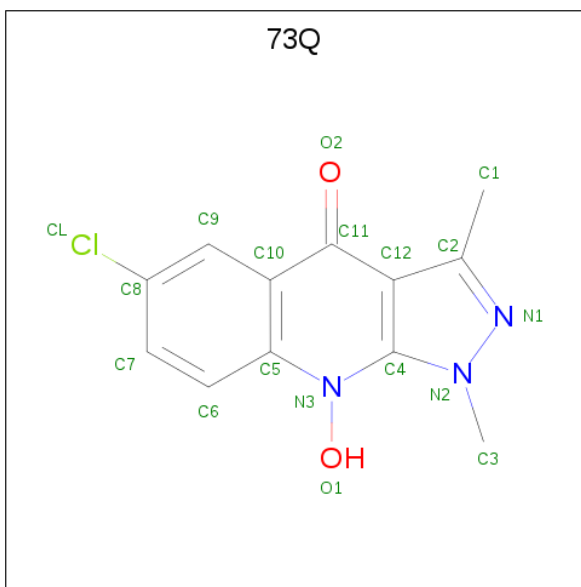
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	1
			73	46	15	12			
2	G	10	Total	C	N	O	0	0	1
			73	46	15	12			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

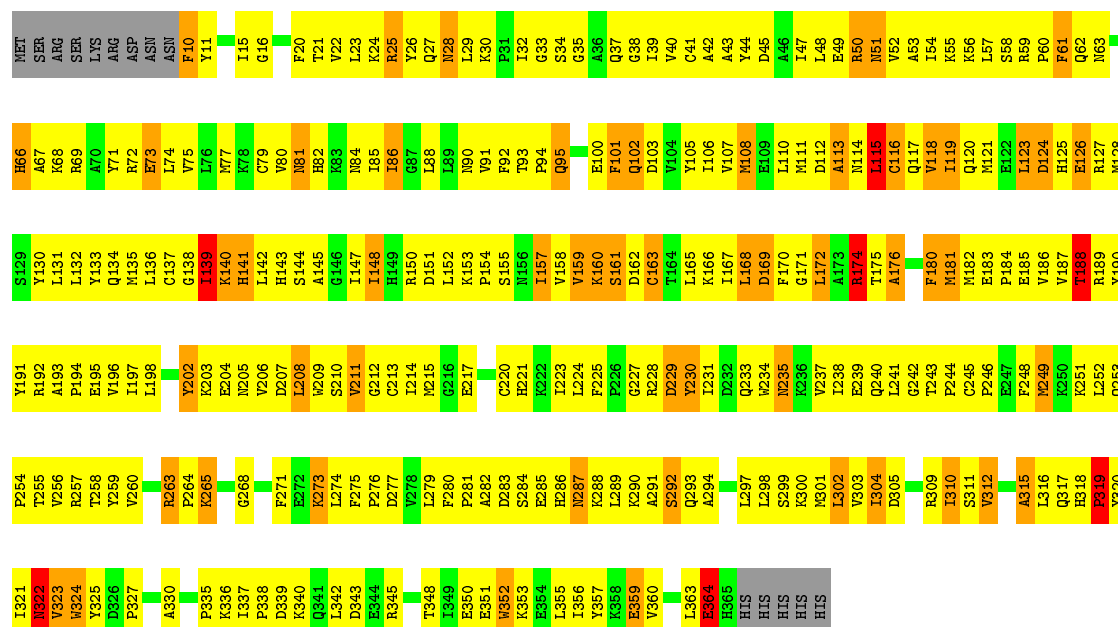
- Molecule 4 is 6-CHLORO-9-HYDROXY-1,3-DIMETHYL-1,9-DIHYDRO-4H-PYRAZOLO[3,4-B]QUINOLIN-4-ONE (three-letter code: 73Q) (formula: C₁₂H₁₀ClN₃O₂).



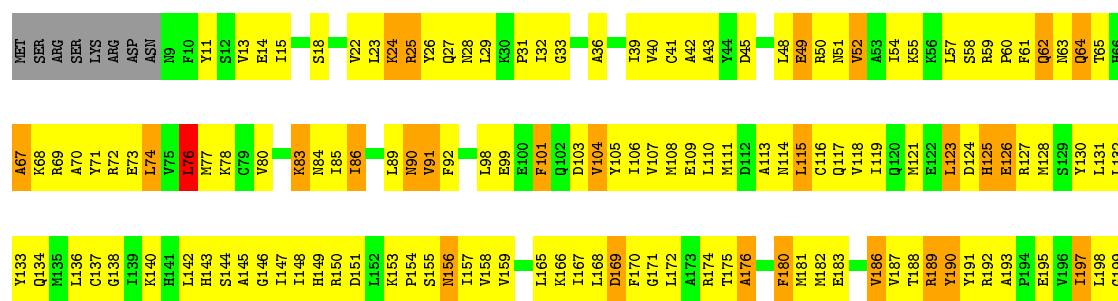
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			18	12	1	3	2		
4	B	1	Total	C	Cl	N	O	0	0
			18	12	1	3	2		

Note EDS was not executed.

- Chain A:  21% 58% 15% . .



- Chain B:  29% 54% 13% . .



- Molecule 2: C-jun-amino-terminal kinase-interacting protein 1



- Molecule 2: C-jun-amino-terminal kinase-interacting protein 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.62Å 150.62Å 119.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 3.50	Depositor
% Data completeness (in resolution range)	77.9 (19.89-3.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.283 , 0.354	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5918	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 73Q, SO4

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	0.39	0/2923	0.67	0/3956
1	B	0.41	0/2923	0.69	0/3959
2	F	0.62	0/74	0.87	0/100
2	G	0.58	0/74	0.75	0/100
All	All	0.41	0/5994	0.68	0/8115

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2858	0	2867	423	0
1	B	2858	0	2851	333	0
2	F	73	0	82	7	0
2	G	73	0	82	6	0
3	A	10	0	0	3	0
3	B	10	0	0	1	0
4	A	18	0	10	5	0
4	B	18	0	10	4	0
All	All	5918	0	5902	761	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 64.

The worst 5 of 761 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD23	1:A:118:VAL:HG13	1.24	1.12
1:B:304:ILE:HD12	1:B:304:ILE:H	1.08	1.10
1:A:59:ARG:HH21	1:A:66:HIS:HB3	1.14	1.07
1:A:263:ARG:HA	1:A:263:ARG:HH11	1.16	1.06
1:A:115:LEU:HD12	1:A:157:ILE:HG21	1.40	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	354/370 (96%)	213 (60%)	92 (26%)	49 (14%)	0	3
1	B	355/370 (96%)	229 (64%)	81 (23%)	45 (13%)	0	4
2	F	8/11 (73%)	6 (75%)	1 (12%)	1 (12%)	0	5
2	G	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
All	All	725/762 (95%)	454 (63%)	176 (24%)	95 (13%)	0	4

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	50	ARG
1	A	60	PRO
1	A	123	LEU
1	A	126	GLU

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	315/334 (94%)	274 (87%)	41 (13%)	4	21
1	B	314/334 (94%)	288 (92%)	26 (8%)	11	40
2	F	9/11 (82%)	7 (78%)	2 (22%)	1	5
2	G	9/11 (82%)	9 (100%)	0	100	100
All	All	647/690 (94%)	578 (89%)	69 (11%)	6	30

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ILE
1	A	352	TRP
1	B	286	HIS
1	A	312	VAL
1	A	322	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	561	ASN
1	B	28	ASN
1	B	141	HIS
1	A	317	GLN
1	A	322	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	73Q	B	1001	-	15,20,20	1.98	4 (26%)	14,31,31	2.35	5 (35%)
3	SO4	B	701	-	4,4,4	0.61	0	6,6,6	0.11	0
3	SO4	A	501	-	4,4,4	0.63	0	6,6,6	0.08	0
3	SO4	A	601	-	4,4,4	0.45	0	6,6,6	0.10	0
4	73Q	A	901	-	15,20,20	2.28	5 (33%)	14,31,31	2.46	6 (42%)
3	SO4	B	801	-	4,4,4	0.51	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	73Q	A	901	-	-	-	0/3/3/3
4	73Q	B	1001	-	-	-	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	73Q	C10-C5	5.64	1.45	1.41
4	B	1001	73Q	C10-C5	4.27	1.44	1.41
4	A	901	73Q	C7-C8	3.41	1.44	1.38
4	B	1001	73Q	C7-C8	3.12	1.43	1.38
4	A	901	73Q	O2-C11	2.66	1.28	1.23

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	1001	73Q	C2-N1-N2	5.44	109.03	104.35
4	A	901	73Q	C2-N1-N2	5.30	108.91	104.35
4	A	901	73Q	C6-C5-C10	-3.86	114.94	120.01
4	B	1001	73Q	C6-C5-C10	-3.65	115.21	120.01
4	A	901	73Q	C7-C8-C9	-3.25	118.14	121.99

There are no chirality outliers.

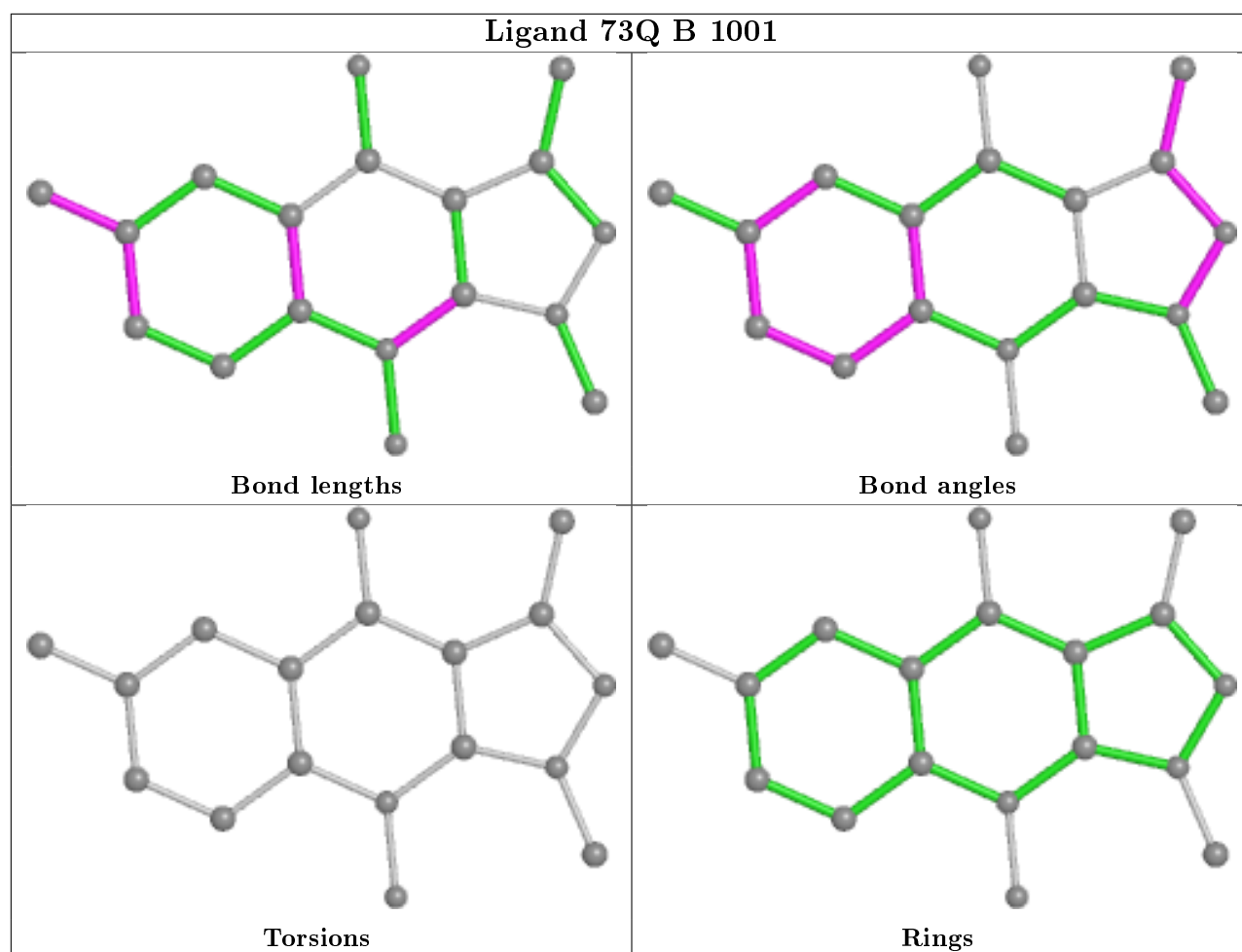
There are no torsion outliers.

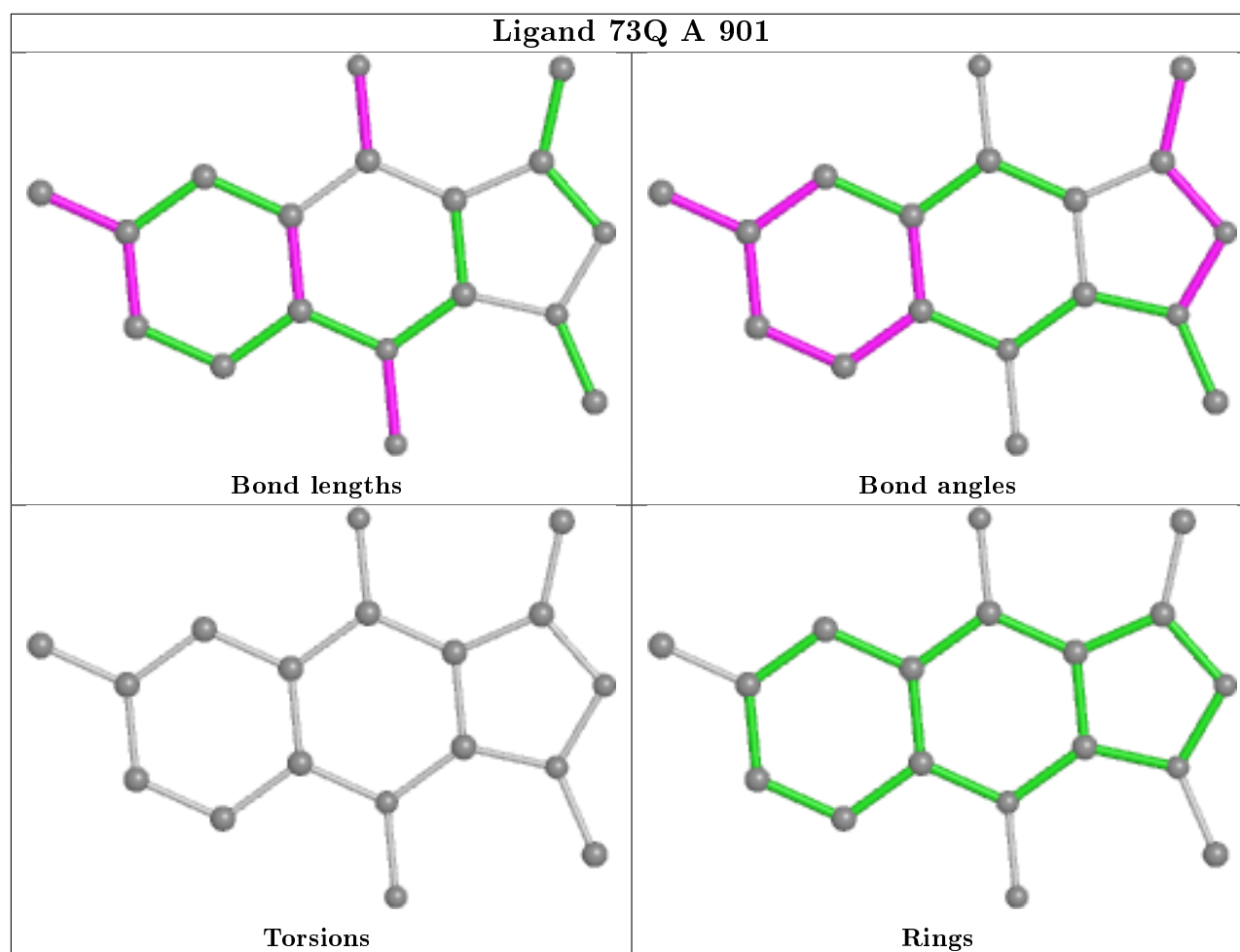
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	73Q	4	0
3	B	701	SO4	1	0
3	A	501	SO4	3	0
4	A	901	73Q	5	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.