



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:22 PM UTC

PDB ID : 1YOL / pdb_00001yol
Title : Crystal structure of Src kinase domain in complex with CGP77675
Authors : Breitenlechner, C.B.; Kairies, N.A.; Honold, K.; Scheiblich, S.; Koll, H.; Greiter, E.; Koch, S.; Schaefer, W.; Huber, R.; Engh, R.A.
Deposited on : 2005-01-27
Resolution : 2.30 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

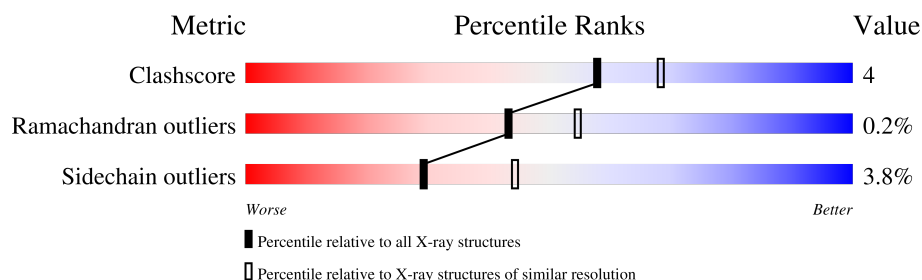
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	283	
1	B	283	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4411 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.

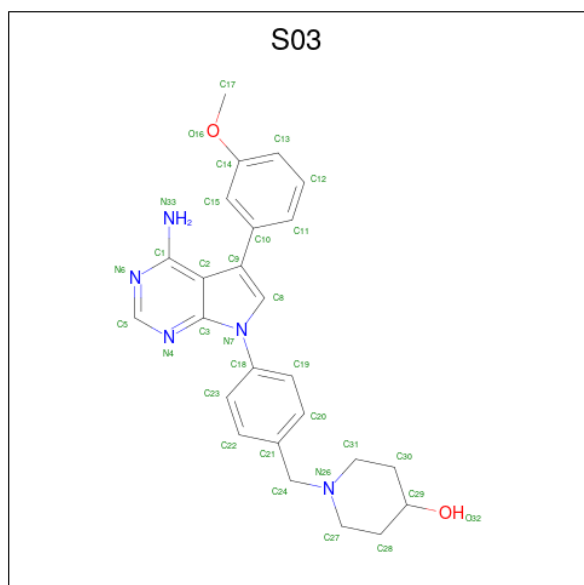
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2053	1313	344	381	15			
1	B	253	Total	C	N	O	S	0	0	0
			2038	1304	342	377	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	ASN	SER	engineered mutation	UNP P12931
A	369	SER	ALA	engineered mutation	UNP P12931
B	344	ASN	SER	engineered mutation	UNP P12931
B	369	SER	ALA	engineered mutation	UNP P12931

- Molecule 2 is 1-{4-[4-AMINO-5-(3-METHOXYPHENYL)-7H-PYRROLO[2,3-D]PYRIMIDI N-7-YL]BENZYL}PIPERIDIN-4-OL (CCD ID: S03) (formula: C₂₅H₂₇N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	25	5	2		
2	B	1	Total	C	N	O	0	0
			32	25	5	2		

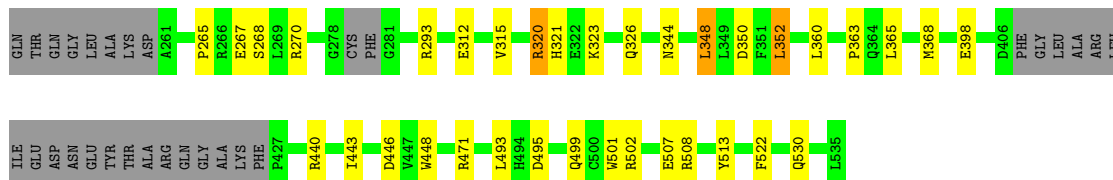
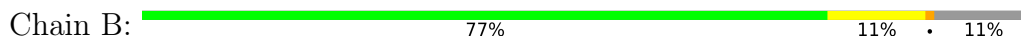
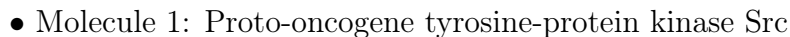
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	127	Total	O	0	0
			127	127		

i

Note EDS was not executed.

- Chain A: 82% 7% • 10%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.53Å 62.95Å 72.79Å 100.38° 89.16° 89.99°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	97.1 (20.00-2.30)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.193 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4411	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: S03

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	0.73	0/2101	0.86	1/2844 (0.0%)
1	B	0.73	0/2086	0.82	0/2824
All	All	0.73	0/4187	0.84	1/5668 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	GLN	N-CA-C	-5.07	105.22	111.40

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	2053	0	2035	14	0
1	B	2038	0	2027	21	0
2	A	32	0	27	3	0
2	B	32	0	27	2	0
3	A	129	0	0	1	0
3	B	127	0	0	3	0
All	All	4411	0	4116	37	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 4.

All (37) 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:365:LEU:HD23	1:A:368:MET:CE	2.15	0.77
1:A:365:LEU:HA	1:A:368:MET:HE2	1.68	0.74
1:A:297:LYS:HB2	2:A:601:S03:H173	1.70	0.72
1:B:350:ASP:OD2	2:B:602:S03:H311	1.98	0.64
1:A:365:LEU:HD23	1:A:368:MET:HE1	1.83	0.60
1:A:365:LEU:HD23	1:A:368:MET:HE2	1.84	0.58
1:B:507:GLU:HG2	3:B:632:HOH:O	2.05	0.56
2:B:602:S03:C29	3:B:723:HOH:O	2.56	0.54
1:A:321:HIS:CD2	1:A:323:LYS:H	2.26	0.53
1:A:285:MET:HG2	1:A:342:TYR:CE1	2.46	0.50
1:B:326:GLN:NE2	3:B:646:HOH:O	2.46	0.48
1:B:365:LEU:HA	1:B:368:MET:HE3	1.95	0.48
1:A:265:PRO:O	1:A:268:SER:OG	2.31	0.48
1:A:368:MET:HE3	1:A:457:LEU:HD22	1.95	0.48
1:B:344:ASN:HD21	1:B:398:GLU:HG2	1.79	0.47
1:B:265:PRO:O	1:B:268:SER:OG	2.30	0.47
1:A:491:GLU:HG2	3:A:646:HOH:O	2.13	0.47
2:A:601:S03:C15	2:A:601:S03:H332	2.28	0.47
1:B:344:ASN:HD21	1:B:398:GLU:CD	2.23	0.46
1:A:325:VAL:HG21	1:A:395:LEU:HD12	1.97	0.46
1:B:348:LEU:HD22	1:B:352:LEU:HD22	1.97	0.46
1:B:312:GLU:O	1:B:315:VAL:HG22	2.16	0.46
1:B:320:ARG:HD3	1:B:326:GLN:NE2	2.31	0.46
1:B:448:TRP:CE3	1:B:501:TRP:HA	2.51	0.45
1:B:495:ASP:OD2	1:B:499:GLN:NE2	2.50	0.45
1:B:499:GLN:O	1:B:502:ARG:HG3	2.16	0.45
1:A:453:LEU:HD12	1:A:453:LEU:O	2.16	0.45
1:B:360:LEU:HD22	1:B:368:MET:HE1	1.99	0.45
1:B:363:PRO:HA	1:B:522:PHE:CE2	2.53	0.44
1:B:443:ILE:O	1:B:446:ASP:HB2	2.18	0.43
1:B:499:GLN:HG2	1:B:502:ARG:HH21	1.84	0.43
1:B:513:TYR:CD1	1:B:513:TYR:C	2.97	0.43
1:B:344:ASN:HD21	1:B:398:GLU:CG	2.32	0.41
1:A:297:LYS:CB	2:A:601:S03:H173	2.44	0.41
1:A:304:MET:HE2	1:A:308:ALA:HB1	2.02	0.41
1:B:321:HIS:CD2	1:B:323:LYS:H	2.39	0.41
1:B:499:GLN:O	1:B:508:ARG:HG3	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	250/283 (88%)	243 (97%)	6 (2%)	1 (0%)	30	38
1	B	247/283 (87%)	241 (98%)	6 (2%)	0	100	100
All	All	497/566 (88%)	484 (97%)	12 (2%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	GLY

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	221/244 (91%)	214 (97%)	7 (3%)	34	51
1	B	221/244 (91%)	211 (96%)	10 (4%)	24	37
All	All	442/488 (91%)	425 (96%)	17 (4%)	29	44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	MET
1	A	333	GLU

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Mol	Chain	Res	Type
1	A	348	LEU
1	A	352	LEU
1	A	398	GLU
1	A	453	LEU
1	A	493	LEU
1	B	267	GLU
1	B	270	ARG
1	B	293	ARG
1	B	320	ARG
1	B	348	LEU
1	B	352	LEU
1	B	440	ARG
1	B	471	ARG
1	B	493	LEU
1	B	530	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	A	321	HIS
1	A	326	GLN
1	A	399	ASN
1	A	476	GLN
1	B	289	ASN
1	B	326	GLN
1	B	344	ASN
1	B	399	ASN
1	B	499	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	S03	B	602	-	36,36,36	1.61	6 (16%)	46,51,51	2.62	21 (45%)
2	S03	A	601	-	36,36,36	1.61	7 (19%)	46,51,51	3.09	22 (47%)

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	S03	B	602	-	-	7/14/24/24	0/5/5/5
2	S03	A	601	-	-	4/14/24/24	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	S03	C3-N4	5.51	1.44	1.34
2	B	602	S03	C3-N4	5.06	1.43	1.34
2	B	602	S03	C18-N7	-4.66	1.33	1.43
2	B	602	S03	C3-N7	-3.51	1.34	1.39
2	A	601	S03	C18-N7	-3.48	1.36	1.43
2	A	601	S03	C8-C9	3.01	1.40	1.37
2	A	601	S03	C2-C9	-2.86	1.39	1.46
2	A	601	S03	C3-N7	-2.77	1.35	1.39
2	B	602	S03	C2-C9	-2.70	1.39	1.46
2	A	601	S03	C2-C3	-2.62	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	S03	C2-C3	-2.38	1.37	1.40
2	B	602	S03	C8-C9	2.21	1.39	1.37
2	A	601	S03	C20-C19	2.14	1.42	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	S03	C1-C2-C3	7.12	121.08	115.74
2	A	601	S03	C27-C28-C29	7.11	119.05	111.14
2	A	601	S03	C2-C3-N4	-6.97	119.58	126.97
2	A	601	S03	C2-C9-C8	6.94	110.10	106.03
2	B	602	S03	C2-C9-C8	6.63	109.92	106.03
2	B	602	S03	C1-C2-C3	6.37	120.51	115.74
2	B	602	S03	C2-C3-N4	-5.50	121.13	126.97
2	A	601	S03	C19-C18-N7	5.02	126.36	119.89
2	A	601	S03	C21-C24-N26	4.92	123.22	113.15
2	B	602	S03	C27-C28-C29	4.70	116.37	111.14
2	A	601	S03	C24-C21-C20	4.54	129.12	120.75
2	A	601	S03	C24-N26-C27	4.17	120.03	111.07
2	A	601	S03	N4-C3-N7	4.09	131.00	125.55
2	B	602	S03	C24-C21-C22	4.06	128.22	120.75
2	A	601	S03	C24-N26-C31	4.04	119.75	111.07
2	B	602	S03	C23-C18-N7	4.02	125.08	119.89
2	A	601	S03	C31-C30-C29	3.94	115.52	111.14
2	A	601	S03	N4-C5-N6	-3.87	122.72	128.58
2	B	602	S03	C24-C21-C20	-3.73	113.87	120.75
2	B	602	S03	C31-N26-C27	3.62	116.65	108.84
2	B	602	S03	N4-C5-N6	-3.44	123.37	128.58
2	B	602	S03	N4-C3-N7	3.32	129.97	125.55
2	B	602	S03	C21-C24-N26	3.23	119.76	113.15
2	A	601	S03	C24-C21-C22	-3.15	114.95	120.75
2	B	602	S03	C31-C30-C29	3.11	114.60	111.14
2	B	602	S03	C18-N7-C8	-2.98	120.66	124.78
2	A	601	S03	C15-C10-C9	-2.96	116.89	120.74
2	B	602	S03	C24-N26-C31	2.91	117.33	111.07
2	A	601	S03	C23-C18-C19	-2.90	113.65	119.18
2	A	601	S03	C22-C23-C18	2.82	123.87	120.30
2	A	601	S03	C31-N26-C27	2.67	114.58	108.84
2	B	602	S03	C17-O16-C14	2.61	123.11	117.50
2	B	602	S03	C24-N26-C27	2.48	116.40	111.07
2	A	601	S03	C20-C19-C18	2.45	123.40	120.30
2	B	602	S03	C10-C9-C8	-2.44	119.62	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	S03	C5-N6-C1	2.44	122.73	118.73
2	A	601	S03	C11-C10-C9	2.37	123.96	120.98
2	A	601	S03	C17-O16-C14	2.28	122.40	117.50
2	B	602	S03	C30-C31-N26	-2.17	107.56	111.08
2	A	601	S03	C5-N4-C3	2.11	117.00	111.83
2	A	601	S03	C5-N6-C1	2.08	122.16	118.73
2	B	602	S03	C23-C18-C19	-2.08	115.21	119.18
2	B	602	S03	C22-C23-C18	2.03	122.87	120.30

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	S03	C21-C24-N26-C31
2	B	602	S03	C21-C24-N26-C27
2	A	601	S03	C13-C14-O16-C17
2	A	601	S03	C15-C14-O16-C17
2	B	602	S03	C21-C24-N26-C31
2	A	601	S03	C21-C24-N26-C27
2	B	602	S03	C22-C21-C24-N26
2	B	602	S03	C11-C10-C9-C8
2	B	602	S03	C20-C21-C24-N26
2	B	602	S03	C15-C10-C9-C8
2	B	602	S03	C15-C10-C9-C2

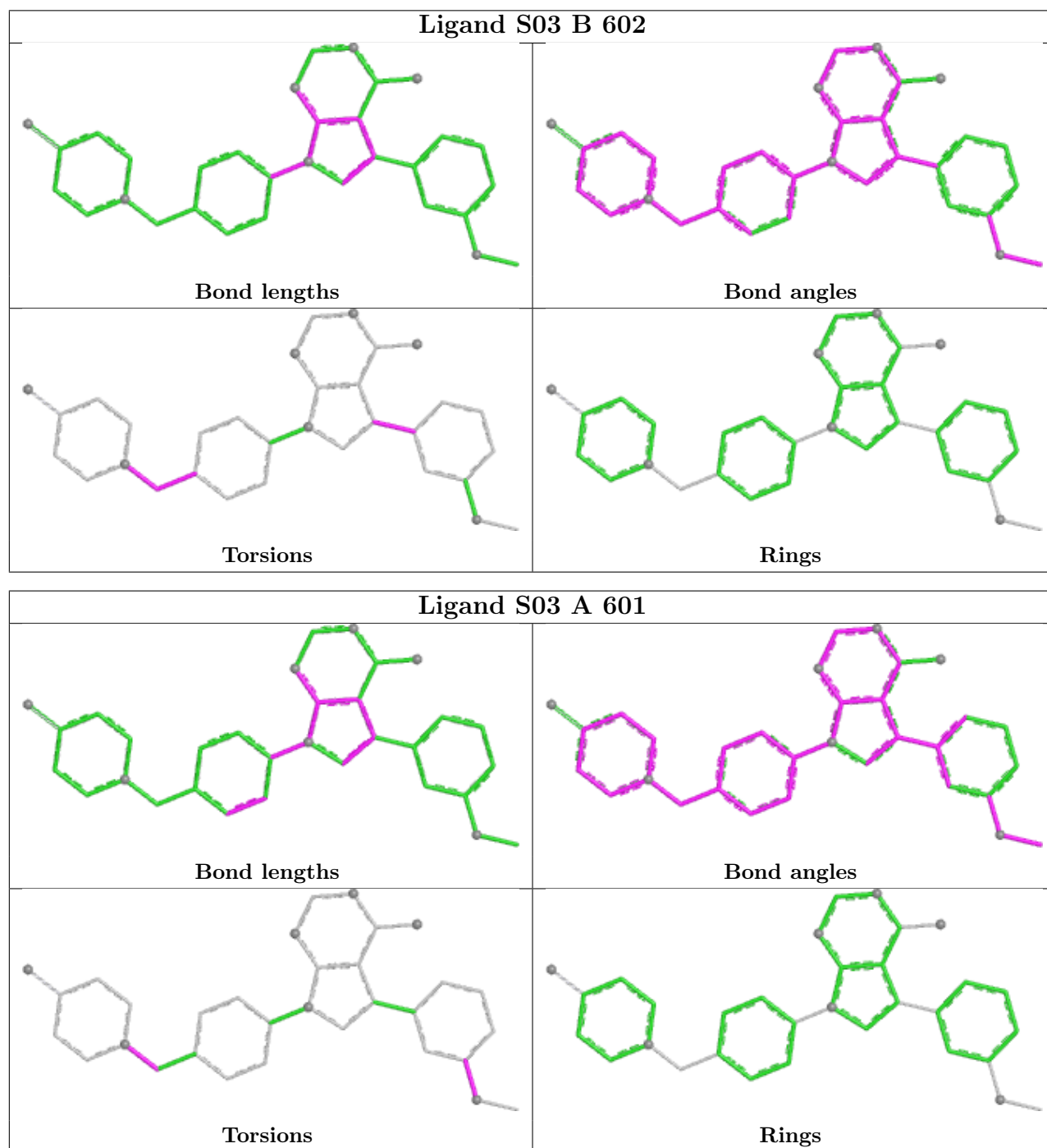
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	S03	2	0
2	A	601	S03	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.