



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 09:31 AM EST

PDB ID : 1BMK
Title : THE COMPLEX STRUCTURE OF THE MAP KINASE P38/SB218655
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Deposited on : 1998-07-23
Resolution : 2.40 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.36

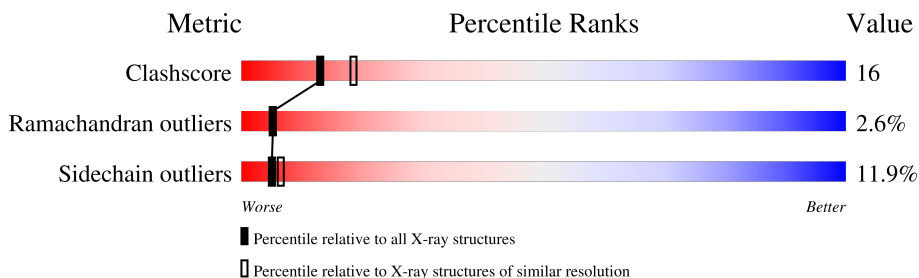
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	379	 60% 27% . . 7%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 2950 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.

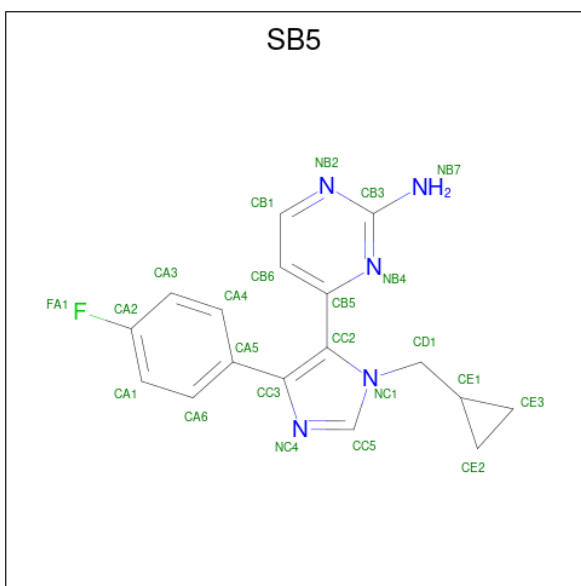
- Molecule 1 is a protein called PROTEIN (MAP KINASE P38).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2833	1812	485	523	13	50	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	HIS	LEU	conflict	UNP Q16539
A	263	ALA	THR	conflict	UNP Q16539

- Molecule 2 is 4-(FLUOROPHENYL)-1-CYCLOPROPYLMETHYL-5-(2-AMINO-4-PYRIDINYL)IMIDAZOLE (three-letter code: SB5) (formula: C₁₇H₁₆FN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
2	A	1	23	17	1	5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	94	Total O 94 94	0	0

4 Data and refinement statistics

Xtrriage (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	45.58Å 85.22Å 123.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2950	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: SB5

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	0.41	0/2900	0.65	2/3938 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ARG	N-CA-C	-5.38	96.46	111.00
1	A	167	LEU	CA-CB-CG	5.09	127.00	115.30

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	2833	0	2815	92	0
2	A	23	0	16	3	0
3	A	94	0	0	4	0
All	All	2950	0	2831	92	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 16.

All (92) 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:179:MET:HE1	1:A:189:ARG:HD2	1.46	0.95
1:A:36:GLY:HA3	1:A:53:LYS:HD2	1.57	0.83
1:A:179:MET:CE	1:A:189:ARG:HD2	2.09	0.82
1:A:32:SER:HB2	1:A:37:SER:HA	1.66	0.76
1:A:80:HIS:HD2	1:A:82:ASN:H	1.35	0.72
1:A:33:GLY:HA3	1:A:35:TYR:CE2	2.27	0.70
1:A:113:LEU:O	1:A:117:VAL:HG23	1.91	0.70
1:A:148:HIS:O	1:A:149:ARG:HB2	1.94	0.68
1:A:117:VAL:HG13	1:A:216:LEU:HD23	1.78	0.64
1:A:60:GLN:HE21	1:A:64:HIS:CD2	2.14	0.64
1:A:119:CYS:O	1:A:120:GLN:HB2	1.97	0.63
1:A:17:ILE:O	1:A:54:LYS:HE2	1.97	0.63
1:A:80:HIS:CD2	1:A:82:ASN:H	2.16	0.63
1:A:332:LEU:HB3	1:A:336:GLU:HB3	1.81	0.63
1:A:155:ASN:O	1:A:167:LEU:HD22	1.98	0.62
1:A:30:VAL:CG1	1:A:38:VAL:HG12	2.29	0.62
1:A:282:VAL:O	1:A:286:GLU:HG3	2.00	0.61
1:A:122:LEU:HA	3:A:520:HOH:O	2.01	0.61
1:A:179:MET:HE3	1:A:186:ARG:HG3	1.82	0.61
1:A:122:LEU:HD23	3:A:520:HOH:O	2.01	0.60
1:A:62:ILE:HG12	1:A:334:ILE:HG12	1.84	0.60
1:A:189:ARG:CG	1:A:189:ARG:HH11	2.15	0.58
1:A:10:ARG:HG3	1:A:19:GLU:HG3	1.85	0.58
1:A:114:ASN:C	1:A:116:ILE:H	2.07	0.58
1:A:267:LYS:HE3	1:A:270:PHE:CE1	2.39	0.57
1:A:157:ALA:HB2	1:A:167:LEU:HD11	1.85	0.57
1:A:200:TYR:HB2	1:A:204:VAL:HG11	1.86	0.56
1:A:171:LEU:N	1:A:171:LEU:HD23	2.21	0.55
1:A:149:ARG:NH2	1:A:171:LEU:HB3	2.21	0.55
1:A:184:ALA:HA	1:A:187:TRP:CE3	2.41	0.54
1:A:99:PHE:O	1:A:338:LYS:HE3	2.07	0.54
1:A:144:ALA:HB2	1:A:320:ALA:HB3	1.89	0.54
1:A:119:CYS:O	1:A:120:GLN:CB	2.56	0.53
1:A:117:VAL:HG22	1:A:216:LEU:CD2	2.39	0.53
1:A:117:VAL:HG22	1:A:216:LEU:HD21	1.92	0.51
1:A:38:VAL:HB	2:A:800:SB5:HC31	1.91	0.51
1:A:155:ASN:ND2	1:A:168:ASP:OD1	2.43	0.51
1:A:75:LEU:HB3	1:A:86:LEU:HG	1.91	0.51
1:A:190:ALA:HB3	1:A:193:ILE:HG22	1.93	0.51
1:A:30:VAL:HG12	1:A:38:VAL:HG12	1.92	0.50
1:A:5:ARG:NH1	1:A:92:PRO:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:MET:HE1	1:A:189:ARG:CD	2.33	0.50
1:A:57:ARG:HD3	1:A:60:GLN:OE1	2.12	0.50
1:A:200:TYR:HB2	1:A:204:VAL:CG1	2.41	0.50
1:A:62:ILE:HG12	1:A:334:ILE:CG1	2.41	0.49
1:A:332:LEU:HB3	1:A:336:GLU:CB	2.42	0.49
1:A:147:ILE:HG22	1:A:149:ARG:HG3	1.94	0.49
1:A:57:ARG:HB3	1:A:60:GLN:HB3	1.95	0.48
1:A:11:GLN:OE1	1:A:13:LEU:HD21	2.12	0.48
1:A:171:LEU:HD13	3:A:528:HOH:O	2.14	0.48
1:A:43:ASP:OD2	1:A:46:THR:HG23	2.14	0.47
1:A:109:MET:HG2	2:A:800:SB5:HCB1	1.96	0.47
1:A:223:PHE:CE2	1:A:235:ILE:HA	2.50	0.47
1:A:12:GLU:O	1:A:13:LEU:HD23	2.15	0.46
1:A:80:HIS:CD2	1:A:82:ASN:HB2	2.51	0.46
1:A:111:ALA:HB1	1:A:115:ASN:HB2	1.98	0.46
1:A:122:LEU:HD22	1:A:126:HIS:HB3	1.98	0.46
1:A:117:VAL:CG1	1:A:216:LEU:HD23	2.45	0.45
1:A:69:TYR:CE1	1:A:340:LEU:HB3	2.52	0.45
1:A:80:HIS:HD2	1:A:82:ASN:N	2.10	0.45
1:A:160:GLU:H	1:A:160:GLU:CD	2.19	0.45
1:A:5:ARG:HB3	1:A:6:PRO:HD2	1.99	0.45
1:A:66:LYS:HD2	1:A:337:TRP:CZ2	2.51	0.44
1:A:179:MET:CE	1:A:186:ARG:HG3	2.48	0.44
1:A:31:GLY:O	1:A:32:SER:HB3	2.16	0.44
1:A:113:LEU:HD12	1:A:113:LEU:HA	1.84	0.44
1:A:127:VAL:O	1:A:131:ILE:HG12	2.17	0.44
1:A:323:TYR:CD2	1:A:325:GLN:HG2	2.53	0.44
1:A:16:THR:HB	1:A:18:TRP:HE1	1.83	0.43
1:A:35:TYR:OH	2:A:800:SB5:HCC5	2.18	0.43
1:A:242:PRO:HB3	1:A:246:LEU:HD13	2.00	0.43
1:A:30:VAL:HG13	1:A:30:VAL:O	2.17	0.43
1:A:353:LEU:HB3	1:A:354:ASP:H	1.66	0.43
1:A:189:ARG:CG	1:A:189:ARG:NH1	2.73	0.43
1:A:112:ASP:OD2	1:A:114:ASN:HB2	2.19	0.43
1:A:189:ARG:NH1	1:A:189:ARG:HG2	2.33	0.43
1:A:267:LYS:HB3	1:A:267:LYS:HE2	1.78	0.43
1:A:114:ASN:C	1:A:116:ILE:N	2.72	0.43
1:A:27:LEU:HD12	1:A:41:ALA:HB2	2.01	0.42
1:A:122:LEU:HD22	1:A:126:HIS:CB	2.48	0.42
1:A:61:SER:HA	1:A:334:ILE:HD11	2.02	0.42
1:A:244:ALA:O	1:A:248:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HA	1:A:40:ALA:O	2.19	0.41
1:A:67:ARG:HG2	3:A:603:HOH:O	2.20	0.41
1:A:170:GLY:O	1:A:171:LEU:C	2.59	0.41
1:A:171:LEU:HD23	1:A:171:LEU:H	1.86	0.41
1:A:5:ARG:CB	1:A:6:PRO:HD2	2.51	0.41
1:A:317:GLU:N	1:A:318:PRO:CD	2.84	0.41
1:A:88:ASP:HA	1:A:348:PHE:CE2	2.56	0.40
1:A:122:LEU:HD12	1:A:216:LEU:HD22	2.03	0.40
1:A:159:ASN:C	1:A:159:ASN:OD1	2.60	0.40
1:A:215:GLU:HG3	1:A:220:ARG:O	2.20	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	349/379 (92%)	326 (93%)	14 (4%)	9 (3%)	5 5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	172	ALA
1	A	56	SER
1	A	118	LYS
1	A	32	SER
1	A	171	LEU
1	A	115	ASN
1	A	11	GLN
1	A	116	ILE

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	310/335 (92%)	273 (88%)	37 (12%)	5 6

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	11	GLN
1	A	32	SER
1	A	37	SER
1	A	39	CYS
1	A	45	LYS
1	A	61	SER
1	A	62	ILE
1	A	63	ILE
1	A	74	LEU
1	A	75	LEU
1	A	86	LEU
1	A	109	MET
1	A	116	ILE
1	A	121	LYS
1	A	122	LEU
1	A	123	THR
1	A	160	GLU
1	A	167	LEU
1	A	171	LEU
1	A	173	ARG
1	A	175	THR
1	A	189	ARG
1	A	195	LEU
1	A	198	MET
1	A	246	LEU
1	A	249	LYS
1	A	262	LEU
1	A	267	LYS
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	310	GLN
1	A	330	ARG
1	A	331	ASP
1	A	333	LEU
1	A	336	GLU
1	A	340	LEU
1	A	353	LEU

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

Mol	Chain	Res	Type
1	A	60	GLN
1	A	80	HIS
1	A	100	ASN
1	A	155	ASN
1	A	196	ASN
1	A	257	ASN
1	A	272	ASN
1	A	312	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	SB5	A	800	-	20,26,26	2.12	7 (35%)	22,37,37	1.29	2 (9%)

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	SB5	A	800	-	-	0/3/14/14	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	SB5	CD1-NC1	5.04	1.53	1.48
2	A	800	SB5	CB6-CB1	4.41	1.42	1.36
2	A	800	SB5	CA1-CA2	2.76	1.42	1.37
2	A	800	SB5	CA6-CA1	2.62	1.42	1.36
2	A	800	SB5	CA3-CA2	2.52	1.42	1.37
2	A	800	SB5	CB6-CB5	2.42	1.46	1.41
2	A	800	SB5	CA4-CA3	2.19	1.41	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	SB5	CB1-CB6-CB5	-3.84	116.03	119.31
2	A	800	SB5	CB6-CB1-NB2	-2.10	121.74	123.81

There are no chirality outliers.

There are no torsion outliers.

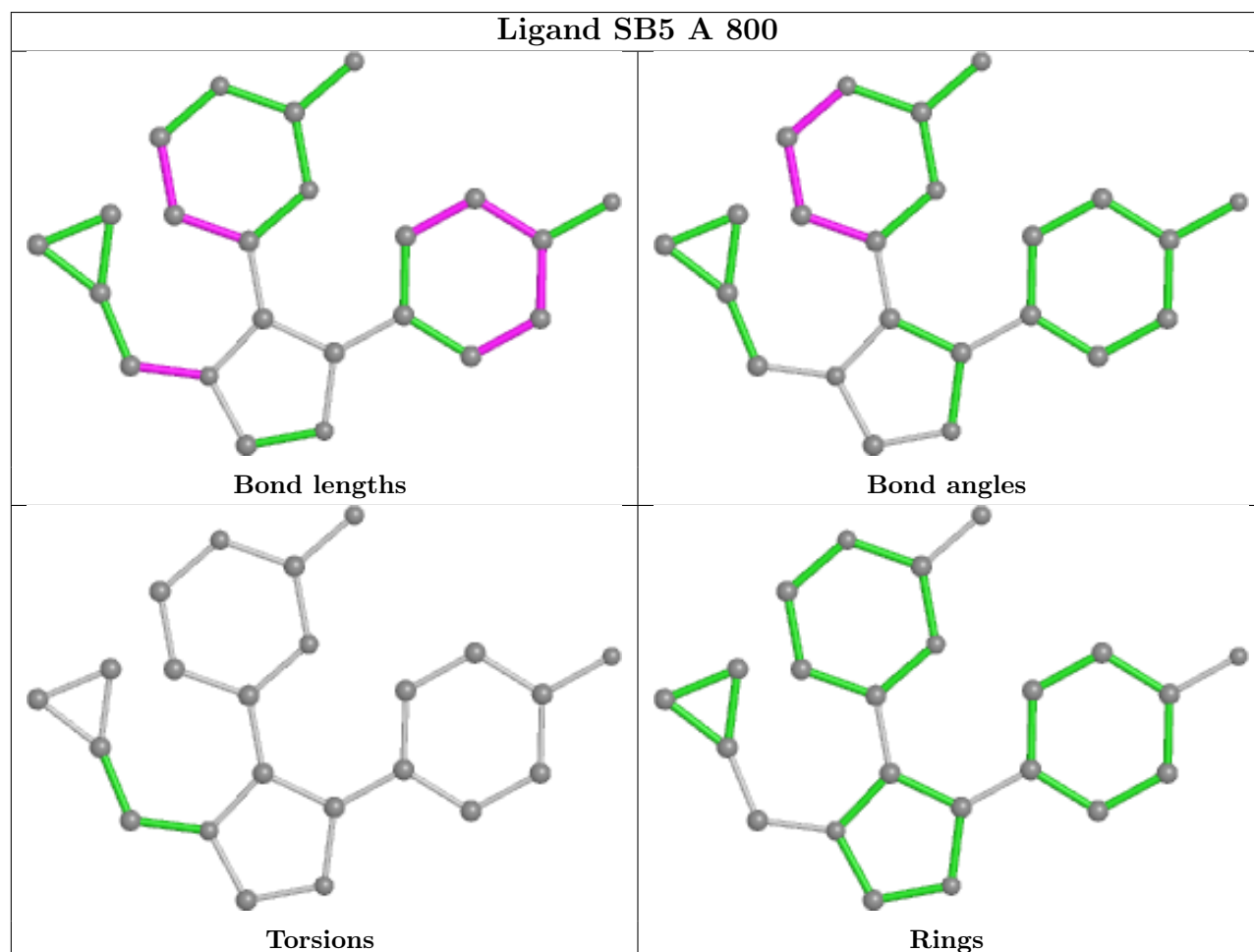
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	SB5	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 [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.