



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 PM UTC

PDB ID : 1J91 / pdb_00001j91
Title : Crystal structure of Z. mays CK2 kinase alpha subunit in complex with the ATP-competitive inhibitor 4,5,6,7-tetrabromobenzotriazole
Authors : Battistutta, R.; De Moliner, E.; Sarno, S.; Zanotti, G.; Pinna, L.A.
Deposited on : 2001-05-23
Resolution : 2.22 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

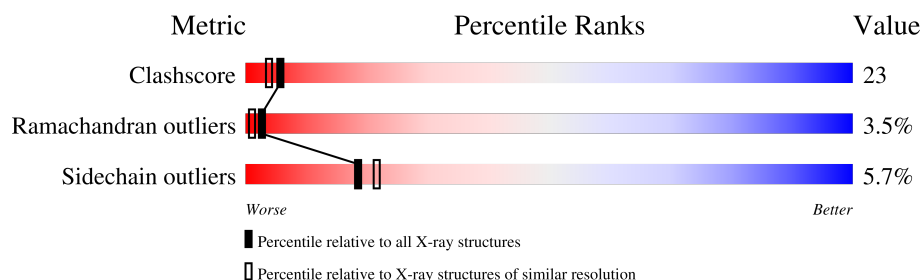
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)

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	332	 65% 26% 5% . .
1	B	332	 70% 21% 6% . .

2 Entry composition [i](#)

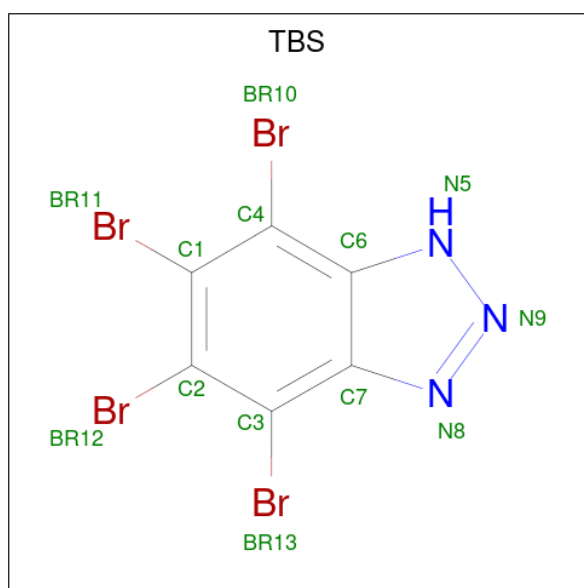
There are 3 unique types of molecules in this entry. The entry contains 5707 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CASEIN KINASE II, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2727	1757	470	489	11			
1	B	327	Total	C	N	O	S	0	0	0
			2727	1757	470	489	11			

- Molecule 2 is 4,5,6,7-TETRABROMOBENZOTRIAZOLE (CCD ID: TBS) (formula: $C_6HBr_4N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	0	0
			13	4	6	3		
2	B	1	Total	Br	C	N	0	0
			13	4	6	3		

- Molecule 3 is water.

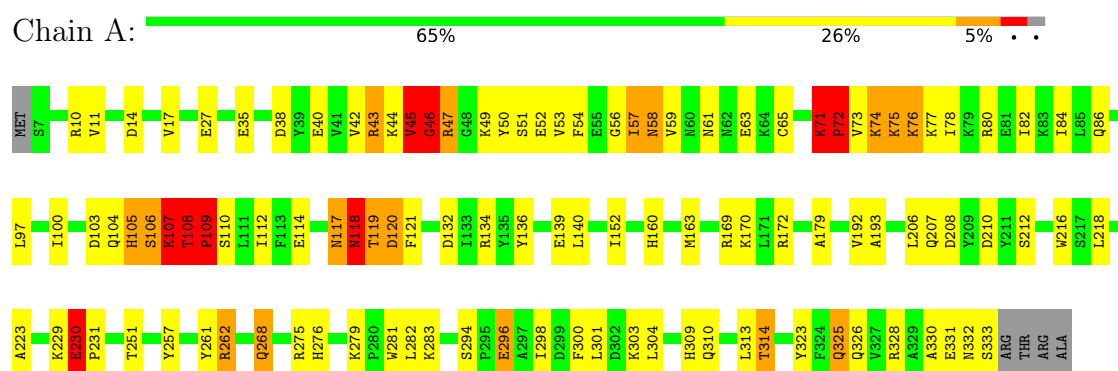
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0
3	B	109	Total 109	O 109	0	0

3 Residue-property plots

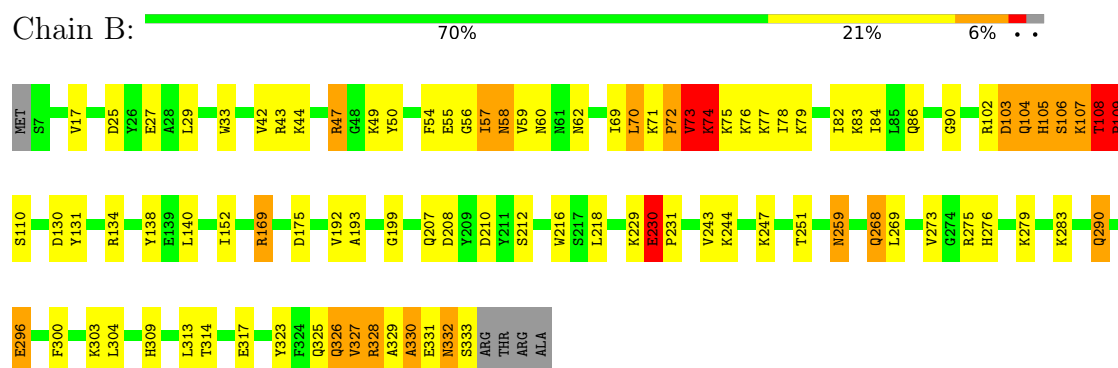
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: CASEIN KINASE II, ALPHA CHAIN



• Molecule 1: CASEIN KINASE II, ALPHA CHAIN



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	48.26 Å 55.94 Å 60.30 Å 89.77° 102.51° 99.27°	Depositor
Resolution (Å)	19.92 – 2.22	Depositor
% Data completeness (in resolution range)	89.0 (19.92-2.22)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.205 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5707	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: TBS

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	0.53	1/2795 (0.0%)	1.06	24/3778 (0.6%)
1	B	0.46	0/2795	0.97	13/3778 (0.3%)
All	All	0.49	1/5590 (0.0%)	1.02	37/7556 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	THR	CA-C	7.38	1.62	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	VAL	N-CA-C	-11.97	101.48	113.10
1	A	230	GLU	CA-C-N	-9.21	108.33	119.84
1	A	230	GLU	C-N-CA	-9.21	108.33	119.84
1	A	108	THR	CA-C-N	9.18	131.31	119.84
1	A	108	THR	C-N-CA	9.18	131.31	119.84
1	A	108	THR	N-CA-C	9.15	130.02	109.81
1	B	230	GLU	CA-C-N	-8.78	108.87	119.84
1	B	230	GLU	C-N-CA	-8.78	108.87	119.84
1	A	118	ASN	N-CA-CB	-8.67	98.51	110.38
1	B	109	PRO	N-CA-C	8.60	130.19	112.47
1	A	314	THR	N-CA-C	-8.35	99.76	110.53
1	A	109	PRO	N-CA-C	8.09	129.14	112.47
1	A	118	ASN	N-CA-C	8.04	120.30	110.41
1	B	108	THR	CA-C-N	7.92	129.74	119.84
1	B	108	THR	C-N-CA	7.92	129.74	119.84
1	A	117	ASN	CA-C-N	7.85	135.82	121.06
1	A	117	ASN	C-N-CA	7.85	135.82	121.06
1	A	51	SER	N-CA-C	7.42	119.42	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLY	N-CA-C	7.16	130.16	113.18
1	A	75	LYS	N-CA-C	6.96	125.63	110.80
1	B	207	GLN	N-CA-C	6.28	120.14	112.23
1	B	55	GLU	N-CA-C	-6.26	99.45	109.96
1	A	207	GLN	N-CA-C	6.21	120.05	112.23
1	A	105	HIS	N-CA-C	6.17	121.01	111.56
1	A	107	LYS	N-CA-C	6.16	123.92	110.80
1	A	47	ARG	N-CA-C	6.08	123.76	110.80
1	B	314	THR	N-CA-C	-5.96	102.84	110.53
1	B	71	LYS	N-CA-C	-5.62	101.87	110.07
1	B	74	LYS	N-CA-C	5.49	122.50	110.80
1	B	73	VAL	CA-CB-CG2	-5.44	101.14	110.40
1	A	49	LYS	N-CA-C	-5.35	99.41	110.80
1	A	106	SER	N-CA-C	5.26	122.01	110.80
1	A	117	ASN	N-CA-C	5.25	119.50	107.48
1	B	210	ASP	N-CA-C	5.18	114.87	108.19
1	A	210	ASP	N-CA-C	5.13	114.80	108.19
1	B	103	ASP	N-CA-C	-5.12	103.38	110.35
1	A	114	GLU	N-CA-C	-5.06	103.46	110.35

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	2727	0	2712	129	2
1	B	2727	0	2712	126	1
2	A	13	0	1	2	0
2	B	13	0	1	0	0
3	A	118	0	0	23	0
3	B	109	0	0	21	0
All	All	5707	0	5426	254	3

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 23.

All (254) 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:B:50:TYR:CD2	1:B:73:VAL:HG21	1.80	1.16
1:B:107:LYS:O	1:B:107:LYS:HD3	1.47	1.15
1:A:108:THR:HB	1:A:109:PRO:CD	1.74	1.14
1:A:108:THR:HB	1:A:109:PRO:HD2	1.10	1.08
1:A:119:THR:O	1:A:119:THR:HG22	1.57	1.04
1:A:117:ASN:HB2	3:A:452:HOH:O	1.54	1.04
1:A:46:GLY:HA3	1:A:53:VAL:H	1.23	1.02
1:B:50:TYR:CE2	1:B:73:VAL:HG21	1.95	1.02
1:A:46:GLY:HA2	1:A:53:VAL:HB	1.42	1.01
1:B:78:ILE:CD1	1:B:108:THR:HG21	1.91	1.01
1:B:78:ILE:HD13	1:B:108:THR:CB	1.90	1.00
1:A:279:LYS:HG3	1:A:283:LYS:HD2	1.45	0.99
1:B:107:LYS:O	1:B:107:LYS:CD	2.10	0.99
1:A:71:LYS:HB3	1:A:72:PRO:HD2	1.45	0.99
1:B:78:ILE:HD13	1:B:108:THR:CG2	1.94	0.97
1:A:50:TYR:HB3	1:A:73:VAL:HG21	1.48	0.95
1:B:74:LYS:O	1:B:78:ILE:HD12	1.66	0.95
1:B:230:GLU:HB2	1:B:231:PRO:HD3	1.49	0.95
1:A:52:GLU:CD	1:A:71:LYS:HE2	1.94	0.93
1:B:78:ILE:HD13	1:B:108:THR:HG21	1.46	0.91
1:A:301:LEU:HD12	3:A:430:HOH:O	1.70	0.91
1:A:46:GLY:N	1:A:53:VAL:O	2.05	0.90
1:B:74:LYS:CG	1:B:75:LYS:H	1.85	0.89
1:B:138:TYR:OH	1:B:328:ARG:HG3	1.73	0.88
1:A:46:GLY:O	1:A:47:ARG:HG3	1.74	0.88
1:A:230:GLU:HB2	1:A:231:PRO:HD3	1.54	0.88
1:A:119:THR:O	1:A:120:ASP:O	1.91	0.87
1:B:70:LEU:O	1:B:109:PRO:HG3	1.74	0.87
1:A:118:ASN:OD1	1:A:118:ASN:N	2.08	0.86
1:B:50:TYR:CD2	1:B:73:VAL:CG2	2.57	0.86
1:B:104:GLN:O	1:B:105:HIS:HB3	1.75	0.85
1:A:119:THR:O	1:A:119:THR:CG2	2.25	0.84
1:B:108:THR:H	1:B:109:PRO:HD2	1.41	0.84
1:A:108:THR:CB	1:A:109:PRO:CD	2.56	0.83
1:A:71:LYS:HB3	1:A:72:PRO:CD	2.09	0.83
1:A:46:GLY:HA3	1:A:53:VAL:N	1.93	0.82
1:B:58:ASN:ND2	1:B:60:ASN:H	1.77	0.81
1:B:27:GLU:CD	1:B:76:LYS:NZ	2.40	0.79
1:A:40:GLU:HB2	1:A:57:ILE:HD11	1.65	0.78
1:B:78:ILE:HD13	1:B:108:THR:OG1	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLY:CA	1:A:53:VAL:H	1.96	0.78
1:B:74:LYS:HG3	1:B:75:LYS:H	1.49	0.77
1:B:58:ASN:C	1:B:58:ASN:HD22	1.92	0.76
1:A:325:GLN:HA	1:A:328:ARG:NH1	2.01	0.76
1:A:304:LEU:HB2	3:A:430:HOH:O	1.85	0.76
1:A:119:THR:O	1:A:120:ASP:C	2.26	0.75
1:A:172:ARG:NH2	3:A:425:HOH:O	2.20	0.74
1:B:230:GLU:CD	1:B:230:GLU:H	1.96	0.73
1:B:107:LYS:HD3	1:B:107:LYS:C	2.13	0.73
1:A:17:VAL:HG23	3:A:375:HOH:O	1.88	0.73
1:B:70:LEU:HD23	1:B:108:THR:CG2	2.18	0.73
1:A:71:LYS:O	1:A:73:VAL:N	2.22	0.73
1:A:323:TYR:HE1	3:A:421:HOH:O	1.70	0.73
1:B:131:TYR:HE2	3:B:357:HOH:O	1.72	0.72
1:B:74:LYS:CG	1:B:75:LYS:N	2.52	0.72
1:B:70:LEU:HB2	1:B:109:PRO:HA	1.70	0.72
1:A:11:VAL:HG11	1:A:314:THR:HG21	1.71	0.72
1:B:329:ALA:HB1	3:B:390:HOH:O	1.89	0.71
1:B:17:VAL:HG21	3:B:429:HOH:O	1.90	0.71
1:A:230:GLU:CD	1:A:230:GLU:H	2.00	0.70
1:B:251:THR:HB	3:B:362:HOH:O	1.90	0.70
1:B:27:GLU:CD	1:B:76:LYS:HZ2	1.99	0.69
1:A:58:ASN:C	1:A:58:ASN:HD22	2.00	0.69
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.28	0.69
1:A:78:ILE:HD13	1:A:109:PRO:HG2	1.76	0.67
1:B:230:GLU:HB2	1:B:231:PRO:CD	2.20	0.67
1:B:107:LYS:CD	1:B:107:LYS:C	2.66	0.67
1:B:251:THR:HG21	1:B:275:ARG:HA	1.74	0.67
1:B:251:THR:CG2	1:B:276:HIS:H	2.08	0.66
1:B:29:LEU:HD22	1:B:83:LYS:HD3	1.78	0.66
1:A:108:THR:CG2	3:A:363:HOH:O	2.44	0.65
1:B:58:ASN:HD21	1:B:60:ASN:HB2	1.60	0.65
1:A:46:GLY:CA	1:A:53:VAL:O	2.45	0.65
1:B:27:GLU:CD	1:B:76:LYS:HZ1	2.05	0.65
1:A:46:GLY:HA2	1:A:53:VAL:CB	2.21	0.65
1:B:72:PRO:O	1:B:74:LYS:N	2.30	0.65
1:A:43:ARG:HB2	1:A:43:ARG:HH11	1.61	0.64
1:B:273:VAL:HG12	3:B:362:HOH:O	1.96	0.64
1:B:230:GLU:CB	1:B:231:PRO:HD3	2.25	0.63
1:B:251:THR:HG22	1:B:276:HIS:H	1.63	0.63
1:B:50:TYR:CE2	1:B:73:VAL:CG2	2.77	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LYS:HG3	1:B:283:LYS:HD2	1.80	0.63
1:A:170:LYS:HD3	3:A:425:HOH:O	1.99	0.62
1:B:103:ASP:O	1:B:105:HIS:N	2.31	0.62
1:B:108:THR:HG22	1:B:109:PRO:N	2.11	0.62
1:B:332:ASN:HA	3:B:405:HOH:O	1.99	0.61
1:B:70:LEU:HD23	1:B:108:THR:HG23	1.81	0.61
1:A:326:GLN:O	3:A:426:HOH:O	2.16	0.61
1:B:58:ASN:HD22	1:B:60:ASN:H	1.49	0.61
1:B:140:LEU:HD23	1:B:218:LEU:HD13	1.83	0.61
1:B:42:VAL:HG23	1:B:56:GLY:HA2	1.83	0.60
1:B:78:ILE:CG1	1:B:108:THR:HG21	2.32	0.60
1:B:325:GLN:HG2	3:B:438:HOH:O	2.01	0.60
1:A:282:LEU:HD12	1:A:282:LEU:H	1.67	0.59
1:A:296:GLU:CD	1:A:296:GLU:H	2.08	0.59
1:B:130:ASP:O	1:B:134:ARG:HG3	2.02	0.59
1:B:107:LYS:O	1:B:107:LYS:HD2	1.97	0.59
1:B:108:THR:HB	1:B:109:PRO:HD3	1.84	0.59
1:A:107:LYS:HD2	1:A:107:LYS:N	2.19	0.58
1:A:52:GLU:OE1	1:A:71:LYS:HE2	2.04	0.58
1:A:230:GLU:CB	1:A:231:PRO:HD3	2.28	0.58
1:A:27:GLU:OE1	1:A:76:LYS:HE3	2.04	0.58
1:B:108:THR:CB	1:B:109:PRO:HD3	2.34	0.58
1:A:230:GLU:HB2	1:A:231:PRO:CD	2.26	0.57
1:B:70:LEU:O	1:B:109:PRO:CG	2.51	0.57
1:A:52:GLU:CD	1:A:71:LYS:CE	2.72	0.57
1:A:325:GLN:HA	1:A:328:ARG:HH12	1.65	0.57
1:B:27:GLU:OE1	1:B:76:LYS:NZ	2.31	0.57
1:A:52:GLU:CG	1:A:71:LYS:HE2	2.34	0.57
1:B:47:ARG:HD2	1:B:47:ARG:O	2.04	0.57
1:B:259:ASN:C	1:B:259:ASN:HD22	2.12	0.57
1:B:82:ILE:O	1:B:86:GLN:HG3	2.05	0.57
1:B:243:VAL:HG12	1:B:247:LYS:HE3	1.87	0.56
1:A:46:GLY:HA3	1:A:53:VAL:O	2.06	0.56
1:A:212:SER:OG	1:A:309:HIS:HB2	2.06	0.56
1:A:107:LYS:HD2	1:A:107:LYS:H	1.71	0.55
1:B:72:PRO:O	1:B:73:VAL:C	2.48	0.55
1:B:102:ARG:HH11	1:B:107:LYS:HA	1.72	0.55
1:A:11:VAL:CG1	1:A:314:THR:HG21	2.36	0.55
1:B:58:ASN:ND2	1:B:58:ASN:C	2.60	0.55
1:A:47:ARG:NH2	1:A:160:HIS:CE1	2.75	0.55
1:A:97:LEU:HD21	1:A:100:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:O	1:B:73:VAL:CG1	2.55	0.55
1:B:84:ILE:HG23	1:B:152:ILE:HD13	1.89	0.54
1:A:57:ILE:HD13	1:A:57:ILE:H	1.71	0.54
1:A:40:GLU:HB2	1:A:57:ILE:CD1	2.34	0.54
1:B:74:LYS:HG2	1:B:75:LYS:H	1.68	0.54
1:A:303:LYS:HB3	1:A:313:LEU:HG	1.88	0.54
1:B:58:ASN:HD22	1:B:59:VAL:N	2.05	0.54
1:B:74:LYS:HE3	1:B:76:LYS:HG2	1.90	0.54
1:B:230:GLU:CB	1:B:231:PRO:CD	2.86	0.54
1:B:108:THR:H	1:B:109:PRO:CD	2.16	0.54
1:A:42:VAL:HG23	1:A:56:GLY:HA2	1.91	0.53
1:B:33:TRP:HH2	1:B:107:LYS:O	1.91	0.53
1:B:108:THR:N	1:B:109:PRO:CD	2.71	0.53
1:B:303:LYS:HB3	1:B:313:LEU:HG	1.91	0.53
1:A:301:LEU:HA	3:A:430:HOH:O	2.08	0.53
1:A:50:TYR:CB	1:A:73:VAL:HG21	2.31	0.53
1:A:261:TYR:C	1:A:262:ARG:HD2	2.33	0.53
1:B:73:VAL:HG11	1:B:77:LYS:NZ	2.23	0.53
1:B:58:ASN:ND2	1:B:60:ASN:N	2.54	0.53
1:B:296:GLU:CD	1:B:296:GLU:H	2.16	0.53
1:A:117:ASN:HA	1:A:118:ASN:OD1	2.09	0.52
1:A:82:ILE:O	1:A:86:GLN:HG3	2.09	0.52
1:B:73:VAL:O	1:B:73:VAL:HG12	2.09	0.52
1:B:75:LYS:HE2	1:B:79:LYS:NZ	2.24	0.52
1:A:65:CYS:HB2	3:A:440:HOH:O	2.09	0.52
1:B:108:THR:N	1:B:109:PRO:HD2	2.16	0.52
1:A:331:GLU:HG3	3:B:405:HOH:O	2.10	0.52
1:A:140:LEU:HD23	1:A:218:LEU:HD13	1.92	0.51
1:A:300:PHE:CZ	1:A:304:LEU:HD11	2.45	0.51
1:A:251:THR:HG21	1:A:275:ARG:HA	1.92	0.51
1:B:57:ILE:HD13	1:B:57:ILE:H	1.76	0.51
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.45	0.51
1:A:52:GLU:HB3	1:A:54:PHE:CE2	2.46	0.51
1:A:139:GLU:HG2	3:A:408:HOH:O	2.11	0.51
1:A:71:LYS:CB	1:A:72:PRO:HD2	2.30	0.51
1:A:47:ARG:NE	2:A:338:TBS:BR13	2.99	0.50
1:B:54:PHE:CE2	1:B:69:ILE:HD12	2.47	0.50
1:A:57:ILE:HD13	1:A:57:ILE:N	2.27	0.50
1:A:74:LYS:HG2	3:A:449:HOH:O	2.12	0.50
1:A:106:SER:O	1:A:108:THR:N	2.39	0.50
1:A:136:TYR:OH	1:A:169:ARG:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LYS:CG	1:A:283:LYS:HD2	2.31	0.50
1:A:14:ASP:HA	3:A:375:HOH:O	2.12	0.50
1:A:103:ASP:OD1	1:A:104:GLN:N	2.45	0.50
1:A:328:ARG:NH1	3:A:432:HOH:O	2.44	0.50
1:A:251:THR:CG2	1:A:276:HIS:H	2.25	0.49
1:A:35:GLU:HB2	1:A:38:ASP:OD2	2.12	0.49
1:A:328:ARG:NH1	3:A:400:HOH:O	2.46	0.49
1:A:27:GLU:CD	1:A:76:LYS:HE3	2.38	0.48
1:B:49:LYS:HD3	3:B:400:HOH:O	2.12	0.48
1:B:333:SER:HB3	3:B:390:HOH:O	2.12	0.48
1:B:78:ILE:HG12	1:B:108:THR:HG21	1.95	0.48
1:B:230:GLU:CD	1:B:230:GLU:N	2.69	0.48
1:A:47:ARG:H	1:A:52:GLU:HA	1.79	0.48
1:A:71:LYS:CB	1:A:72:PRO:CD	2.83	0.48
1:A:281:TRP:HB3	1:A:298:ILE:HD12	1.96	0.48
1:B:108:THR:CB	1:B:109:PRO:CD	2.91	0.48
1:B:199:GLY:HA2	1:B:216:TRP:CD1	2.48	0.48
1:B:244:LYS:HE3	3:B:386:HOH:O	2.14	0.47
1:B:325:GLN:HG3	1:B:326:GLN:NE2	2.29	0.47
1:B:300:PHE:CZ	1:B:304:LEU:HD11	2.50	0.47
1:A:230:GLU:CD	1:A:230:GLU:N	2.71	0.47
1:A:58:ASN:C	1:A:58:ASN:ND2	2.72	0.47
1:A:160:HIS:O	1:A:163:MET:HE2	2.14	0.47
1:A:10:ARG:NH2	1:A:310:GLN:O	2.46	0.47
1:A:75:LYS:O	1:A:76:LYS:C	2.57	0.47
1:A:77:LYS:HB3	3:A:441:HOH:O	2.14	0.46
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.80	0.46
1:A:118:ASN:HB3	1:A:163:MET:SD	2.56	0.46
1:B:74:LYS:HG2	1:B:75:LYS:N	2.27	0.46
1:A:229:LYS:O	1:A:230:GLU:C	2.58	0.46
1:B:43:ARG:HG2	1:B:44:LYS:N	2.30	0.46
1:A:230:GLU:CB	1:A:231:PRO:CD	2.89	0.45
1:B:212:SER:OG	1:B:309:HIS:HB2	2.16	0.45
1:A:80:ARG:HD3	1:A:179:ALA:O	2.16	0.45
1:A:105:HIS:C	1:A:106:SER:OG	2.60	0.45
1:B:47:ARG:NH1	3:B:391:HOH:O	2.49	0.45
1:B:229:LYS:O	1:B:230:GLU:C	2.59	0.45
1:A:84:ILE:HG23	1:A:152:ILE:HD13	1.98	0.45
1:A:206:LEU:C	1:A:206:LEU:HD23	2.42	0.45
1:B:332:ASN:ND2	3:B:401:HOH:O	2.44	0.45
1:B:33:TRP:CH2	1:B:102:ARG:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:HG22	1:B:109:PRO:CD	2.47	0.44
1:A:72:PRO:HA	3:A:449:HOH:O	2.17	0.44
1:B:331:GLU:HA	3:B:383:HOH:O	2.16	0.44
1:A:294:SER:HB2	1:A:296:GLU:OE2	2.18	0.44
1:B:90:GLY:HA3	3:B:427:HOH:O	2.18	0.44
1:B:268:GLN:HG3	1:B:269:LEU:N	2.33	0.44
3:A:426:HOH:O	1:B:169:ARG:NH1	2.50	0.43
1:A:206:LEU:HD13	1:A:257:TYR:OH	2.18	0.43
1:B:268:GLN:HE21	1:B:268:GLN:HB2	1.48	0.43
1:A:46:GLY:CA	1:A:53:VAL:N	2.69	0.43
1:A:251:THR:HG22	1:A:276:HIS:O	2.19	0.43
1:A:132:ASP:OD1	1:A:169:ARG:NH2	2.49	0.43
1:B:102:ARG:HB2	1:B:106:SER:O	2.18	0.43
1:B:251:THR:HG22	1:B:276:HIS:O	2.19	0.43
1:A:46:GLY:HA3	1:A:53:VAL:CA	2.49	0.42
1:B:33:TRP:CZ3	1:B:102:ARG:HD3	2.54	0.42
1:B:208:ASP:OD1	1:B:208:ASP:N	2.44	0.42
1:A:120:ASP:O	1:A:121:PHE:C	2.62	0.42
1:A:208:ASP:OD1	1:A:208:ASP:N	2.42	0.42
1:A:192:VAL:O	1:A:193:ALA:HB3	2.19	0.42
1:B:325:GLN:HB2	3:B:371:HOH:O	2.18	0.42
1:A:112:ILE:HG23	3:A:440:HOH:O	2.18	0.42
1:A:50:TYR:HD2	1:A:73:VAL:HG22	1.84	0.42
1:A:65:CYS:CB	3:A:440:HOH:O	2.67	0.42
1:B:78:ILE:HG21	1:B:108:THR:OG1	2.20	0.42
1:B:259:ASN:C	1:B:259:ASN:ND2	2.77	0.42
1:B:332:ASN:CA	3:B:405:HOH:O	2.64	0.42
1:B:247:LYS:NZ	3:B:386:HOH:O	2.45	0.42
1:A:44:LYS:HB2	1:A:54:PHE:CE1	2.55	0.42
1:A:223:ALA:HB2	1:A:301:LEU:HD11	2.02	0.41
1:B:290:GLN:HE21	1:B:290:GLN:HB3	1.55	0.41
1:A:170:LYS:CD	3:A:425:HOH:O	2.65	0.41
1:A:332:ASN:O	1:A:333:SER:HB3	2.20	0.41
1:A:330:ALA:HB2	1:B:169:ARG:HH11	1.85	0.41
1:A:331:GLU:CG	3:B:405:HOH:O	2.67	0.41
1:B:58:ASN:O	1:B:62:ASN:N	2.51	0.41
1:A:72:PRO:C	3:A:449:HOH:O	2.63	0.41
1:A:43:ARG:HB2	1:A:43:ARG:NH1	2.33	0.41
1:A:45:VAL:O	1:A:45:VAL:HG23	2.20	0.41
1:A:47:ARG:CZ	2:A:338:TBS:BR13	3.24	0.41
1:B:57:ILE:HD13	1:B:57:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:VAL:O	1:B:328:ARG:C	2.64	0.41
1:B:330:ALA:C	3:B:383:HOH:O	2.63	0.41
1:A:251:THR:HG22	1:A:276:HIS:H	1.85	0.40
1:B:169:ARG:NH1	3:B:357:HOH:O	2.42	0.40
1:A:61:ASN:OD1	1:A:63:GLU:HB2	2.21	0.40
1:A:216:TRP:CD1	1:A:216:TRP:C	3.00	0.40
1:A:268:GLN:HE21	1:A:268:GLN:HB2	1.51	0.40
1:B:108:THR:HG23	1:B:108:THR:O	2.20	0.40
1:B:192:VAL:O	1:B:193:ALA:HB3	2.20	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:NZ	1:A:314:THR:N[1_455]	1.82	0.38
1:B:105:HIS:NE2	1:B:317:GLU:OE1[1_655]	1.94	0.26
1:A:10:ARG:NH1	1:A:107:LYS:CE[1_655]	1.97	0.23

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	325/332 (98%)	296 (91%)	19 (6%)	10 (3%)	3	1
1	B	325/332 (98%)	295 (91%)	17 (5%)	13 (4%)	2	1
All	All	650/664 (98%)	591 (91%)	36 (6%)	23 (4%)	3	1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	LYS
1	A	72	PRO

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Mol	Chain	Res	Type
1	A	74	LYS
1	A	107	LYS
1	A	108	THR
1	A	120	ASP
1	A	230	GLU
1	B	73	VAL
1	B	74	LYS
1	B	105	HIS
1	B	109	PRO
1	B	230	GLU
1	B	328	ARG
1	A	46	GLY
1	B	104	GLN
1	B	110	SER
1	B	327	VAL
1	A	59	VAL
1	A	109	PRO
1	B	108	THR
1	B	175	ASP
1	B	332	ASN
1	B	330	ALA

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	296/300 (99%)	280 (95%)	16 (5%)	20	23
1	B	296/300 (99%)	278 (94%)	18 (6%)	17	19
All	All	592/600 (99%)	558 (94%)	34 (6%)	18	21

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	45	VAL

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Mol	Chain	Res	Type
1	A	57	ILE
1	A	58	ASN
1	A	71	LYS
1	A	72	PRO
1	A	76	LYS
1	A	109	PRO
1	A	110	SER
1	A	118	ASN
1	A	119	THR
1	A	230	GLU
1	A	262	ARG
1	A	268	GLN
1	A	296	GLU
1	A	325	GLN
1	B	25	ASP
1	B	47	ARG
1	B	57	ILE
1	B	58	ASN
1	B	70	LEU
1	B	72	PRO
1	B	73	VAL
1	B	106	SER
1	B	107	LYS
1	B	108	THR
1	B	109	PRO
1	B	169	ARG
1	B	230	GLU
1	B	259	ASN
1	B	268	GLN
1	B	290	GLN
1	B	296	GLU
1	B	326	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	160	HIS
1	A	268	GLN
1	A	291	HIS
1	A	310	GLN
1	A	325	GLN

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Mol	Chain	Res	Type
1	A	332	ASN
1	B	58	ASN
1	B	160	HIS
1	B	259	ASN
1	B	268	GLN
1	B	290	GLN
1	B	291	HIS
1	B	310	GLN
1	B	326	GLN

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](#)

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	TBS	A	338	-	13,14,14	1.90	4 (30%)	15,21,21	0.99	2 (13%)
2	TBS	B	338	-	13,14,14	1.90	5 (38%)	15,21,21	1.09	1 (6%)

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	TBS	A	338	-	-	-	0/2/2/2
2	TBS	B	338	-	-	-	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	338	TBS	C6-N5	3.39	1.38	1.36
2	B	338	TBS	N8-N9	-2.95	1.24	1.31
2	B	338	TBS	C2-C1	2.90	1.46	1.39
2	A	338	TBS	N8-N9	-2.73	1.24	1.31
2	A	338	TBS	C2-C1	2.50	1.45	1.39
2	B	338	TBS	C4-C1	2.21	1.45	1.39
2	A	338	TBS	N5-N9	2.09	1.42	1.34
2	B	338	TBS	C3-C2	2.08	1.44	1.39
2	B	338	TBS	N5-N9	2.01	1.42	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	TBS	C6-C7-C3	2.56	122.13	118.60
2	A	338	TBS	C6-C7-C3	2.25	121.70	118.60
2	A	338	TBS	C6-N5-N9	-2.07	106.23	110.01

There are no chirality outliers.

There are no torsion outliers.

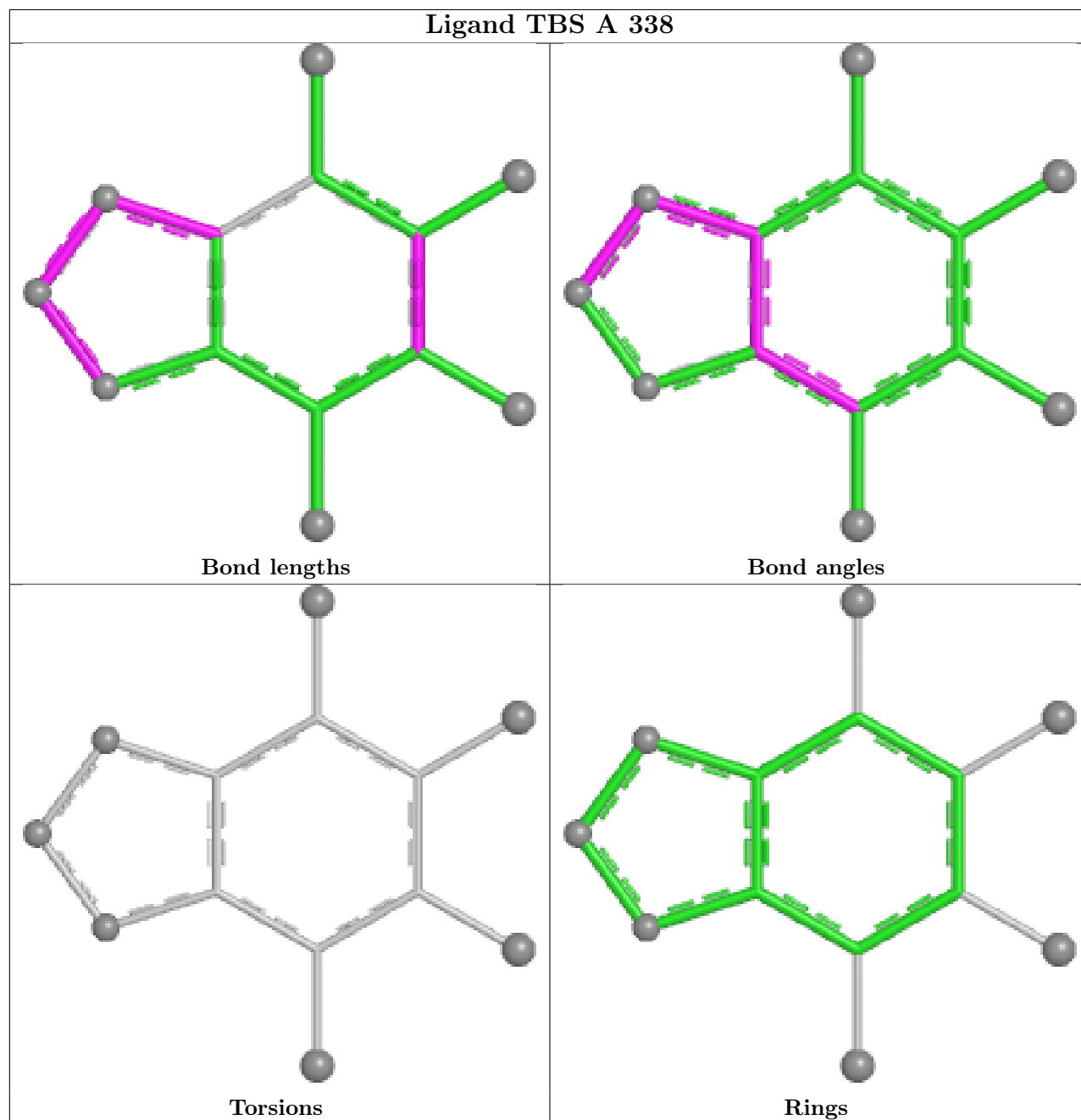
There are no ring outliers.

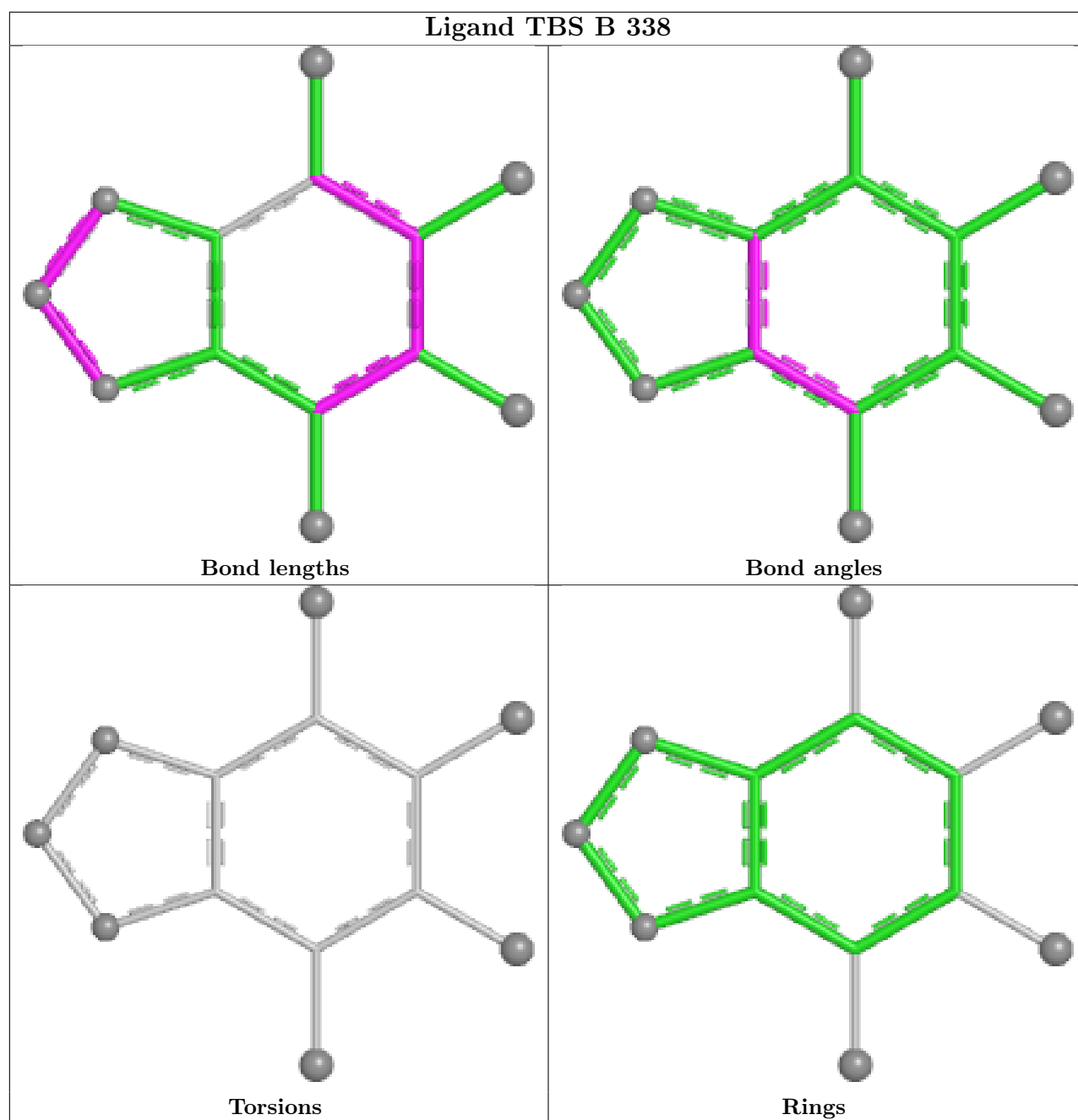
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	338	TBS	2	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.