



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:35 PM UTC

PDB ID : 2FL2 / pdb_00002fl2
Title : crystal structure of KSP in complex with inhibitor 19
Authors : Yan, Y.
Deposited on : 2006-01-05
Resolution : 2.50 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

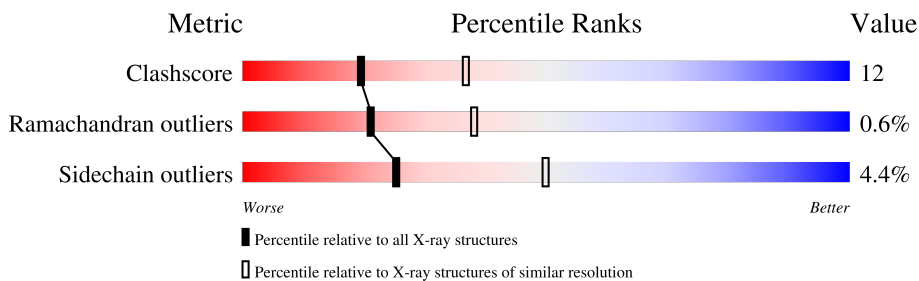
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	367	
1	B	367	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5425 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 Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			
1	B	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

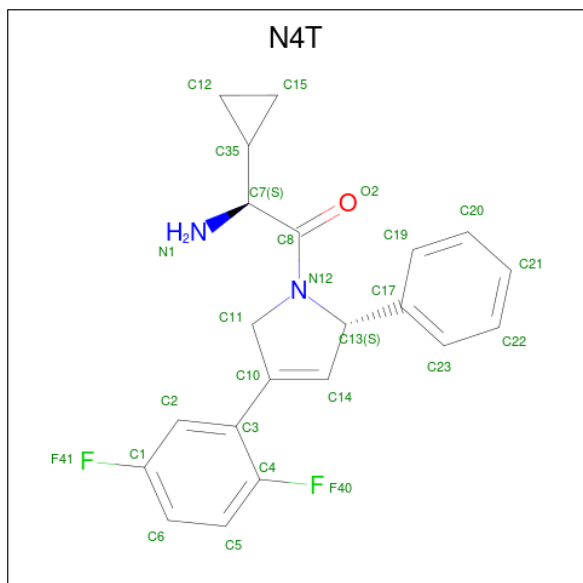
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is (1S)-1-CYCLOPROPYL-2-[(2S)-4-(2,5-DIFLUOROPHENYL)-2-PHENYL-L-2,5-DIHYDRO-1H-PYRROL-1-YL]-2-OXOETHANAMINE (CCD ID: N4T) (formula: C₂₁H₂₀F₂N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	21	2	2	1		
4	B	1	Total	C	F	N	O	0	0
			26	21	2	2	1		

- Molecule 5 is water.

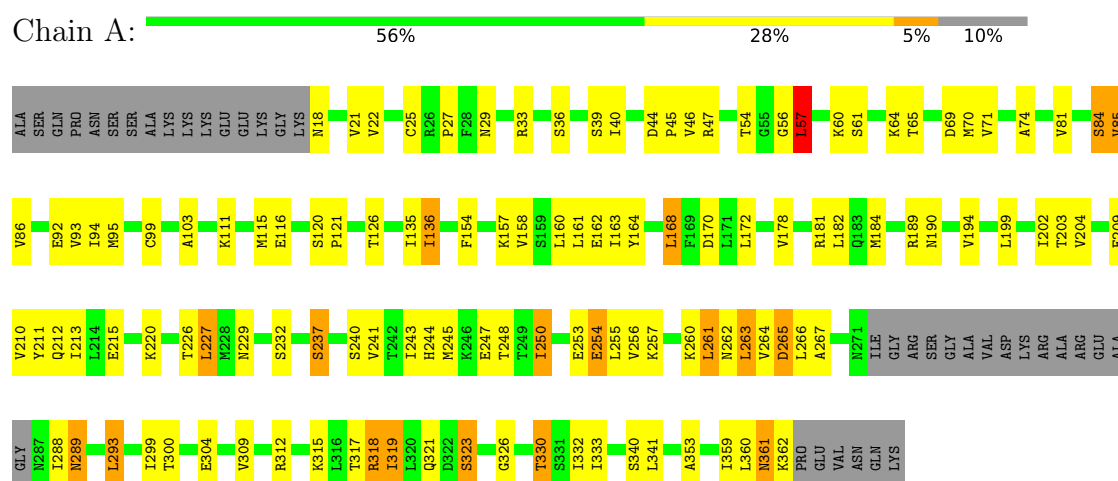
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	64	Total	O	0	0
			64	64		

3 Residue-property plots [i](#)

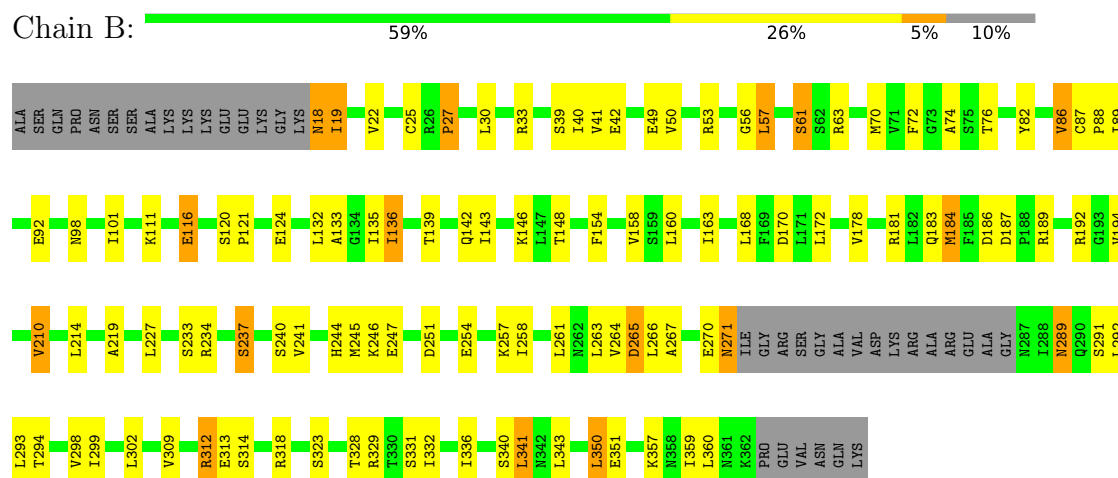
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Kinesin-like protein KIF11



• Molecule 1: Kinesin-like protein KIF11



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	68.80Å 79.50Å 159.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	53.0 (50.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: MG, ADP, N4T

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	1.19	29/2632 (1.1%)	1.03	9/3559 (0.3%)
1	B	1.20	30/2632 (1.1%)	1.02	7/3559 (0.2%)
All	All	1.20	59/5264 (1.1%)	1.03	16/7118 (0.2%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	ILE	CA-C	13.77	1.67	1.52
1	B	116	GLU	CA-C	-12.41	1.41	1.52
1	B	120	SER	CA-C	-12.38	1.39	1.52
1	A	120	SER	CA-C	-8.96	1.42	1.53
1	A	265	ASP	CA-C	8.93	1.63	1.53
1	A	267	ALA	CA-C	-8.66	1.41	1.53
1	B	186	ASP	CA-C	-8.62	1.41	1.52
1	A	25	CYS	CA-C	-8.39	1.42	1.52
1	A	237	SER	CA-C	-8.22	1.42	1.52
1	A	261	LEU	CA-C	8.03	1.61	1.52
1	B	136	ILE	CA-C	7.80	1.61	1.52
1	B	183	GLN	CA-C	-7.38	1.43	1.52
1	A	69	ASP	CA-C	7.34	1.62	1.52
1	B	142	GLN	CA-C	-7.28	1.42	1.52
1	A	184	MET	CA-C	7.13	1.61	1.52
1	B	292	LEU	CA-C	7.08	1.61	1.52
1	B	42	GLU	CA-C	-6.76	1.44	1.52
1	A	232	SER	CA-C	6.60	1.61	1.52
1	A	84	SER	CA-C	-6.53	1.44	1.52
1	A	288	ILE	CA-C	-6.35	1.44	1.52
1	B	267	ALA	CA-C	-6.33	1.44	1.52
1	B	313	GLU	CA-C	6.29	1.61	1.52
1	A	323	SER	CA-C	6.21	1.61	1.52
1	B	258	ILE	CA-C	-6.18	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	VAL	CA-C	-6.17	1.45	1.52
1	B	39	SER	CA-C	-6.03	1.44	1.52
1	A	319	ILE	CA-C	5.99	1.60	1.52
1	A	202	ILE	CA-C	-5.96	1.45	1.52
1	A	309	VAL	CA-C	5.93	1.57	1.53
1	B	148	THR	CA-C	5.92	1.60	1.52
1	B	265	ASP	CA-C	5.88	1.60	1.53
1	B	170	ASP	CA-C	-5.88	1.45	1.52
1	B	233	SER	CA-C	-5.87	1.44	1.52
1	B	178	VAL	CA-C	5.80	1.60	1.52
1	A	103	ALA	CA-C	5.77	1.59	1.52
1	B	332	ILE	CA-C	-5.77	1.45	1.52
1	B	132	LEU	CA-C	5.74	1.60	1.52
1	A	250	ILE	CA-C	5.64	1.60	1.52
1	A	194	VAL	CA-C	-5.64	1.46	1.52
1	A	190	ASN	CA-C	5.54	1.60	1.52
1	A	99	CYS	CA-C	-5.54	1.46	1.52
1	A	263	LEU	CA-C	-5.54	1.45	1.53
1	B	323	SER	CA-C	5.50	1.60	1.52
1	B	49	GLU	CA-C	-5.47	1.46	1.52
1	B	19	ILE	CA-C	5.47	1.58	1.52
1	A	164	TYR	CA-C	-5.47	1.46	1.52
1	B	312	ARG	CA-C	-5.43	1.45	1.52
1	B	184	MET	CA-C	5.40	1.59	1.52
1	B	27	PRO	CA-C	5.38	1.58	1.52
1	B	247	GLU	CA-C	-5.36	1.45	1.52
1	A	39	SER	CA-C	-5.34	1.45	1.52
1	A	229	ASN	CA-C	-5.33	1.45	1.52
1	B	133	ALA	CA-C	5.29	1.59	1.52
1	A	121	PRO	CA-C	-5.19	1.46	1.52
1	A	227	LEU	CA-C	5.17	1.59	1.52
1	B	237	SER	CA-C	-5.15	1.46	1.52
1	A	220	LYS	CA-C	5.15	1.59	1.52
1	B	219	ALA	CA-C	-5.13	1.46	1.52
1	B	41	VAL	CA-C	5.12	1.59	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	VAL	N-CA-C	9.89	119.83	110.53
1	A	86	VAL	N-CA-C	7.74	118.54	110.72
1	B	264	VAL	N-CA-C	7.45	118.87	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	VAL	N-CA-C	7.32	118.41	107.80
1	B	61	SER	N-CA-C	6.40	117.94	108.60
1	A	135	ILE	N-CA-C	6.30	116.47	110.42
1	A	44	ASP	CA-C-N	5.63	125.10	119.24
1	A	44	ASP	C-N-CA	5.63	125.10	119.24
1	A	126	THR	N-CA-C	-5.27	101.94	110.32
1	A	318	ARG	N-CA-C	-5.23	105.26	111.69
1	B	187	ASP	CA-C-N	5.16	125.20	119.32
1	B	187	ASP	C-N-CA	5.16	125.20	119.32
1	B	121	PRO	N-CA-C	5.11	119.26	111.34
1	B	227	LEU	N-CA-C	5.03	117.87	111.69
1	A	211	TYR	N-CA-C	5.02	117.13	111.11
1	A	85	VAL	N-CA-C	5.00	116.10	111.45

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	2594	0	2618	65	0
1	B	2594	0	2618	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	26	0	17	4	0
4	B	26	0	17	2	0
5	A	65	0	0	3	0
5	B	64	0	0	7	0
All	All	5425	0	5294	123	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 12.

All (123) 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:299:ILE:HG23	1:A:359:ILE:HD11	1.32	1.11
1:B:40:ILE:HD13	1:B:340:SER:HA	1.33	1.09
1:B:18:ASN:HB2	1:B:360:LEU:HD12	1.45	0.99
1:A:116:GLU:HB3	4:A:604:N4T:H14	1.48	0.95
1:A:56:GLY:O	1:A:57:LEU:HB2	1.71	0.88
1:A:21:VAL:HG22	1:A:332:ILE:HB	1.57	0.87
1:A:92:GLU:HA	1:A:95:MET:HE3	1.60	0.83
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.63	0.80
1:A:323:SER:O	1:A:330:THR:HG21	1.89	0.72
1:A:54:THR:HG21	1:A:64:LYS:HD3	1.70	0.72
1:B:124:GLU:OE1	5:B:607:HOH:O	2.08	0.71
1:B:341:LEU:O	1:B:341:LEU:HG	1.95	0.66
1:A:326:GLY:O	1:A:361:ASN:HB2	1.96	0.65
1:A:18:ASN:HB2	1:A:360:LEU:HD12	1.78	0.65
1:B:116:GLU:HB3	4:B:605:N4T:H14	1.79	0.65
1:B:40:ILE:CD1	1:B:340:SER:HA	2.20	0.64
1:A:40:ILE:HD13	1:A:340:SER:HA	1.79	0.63
1:B:92:GLU:OE2	1:B:329:ARG:HD2	1.99	0.63
1:A:361:ASN:O	1:A:362:LYS:HB2	1.99	0.62
1:B:312:ARG:HA	1:B:318:ARG:HG3	1.82	0.61
1:B:351:GLU:HA	5:B:638:HOH:O	2.02	0.60
1:A:70:MET:HE1	1:A:84:SER:HB3	1.84	0.59
1:A:178:VAL:HG23	1:A:227:LEU:HD23	1.84	0.59
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.85	0.59
1:B:237:SER:OG	1:B:265:ASP:HB3	2.03	0.58
1:B:139:THR:O	1:B:143:ILE:HG13	2.03	0.58
1:B:160:LEU:HB3	1:B:172:LEU:HG	1.85	0.57
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.69	0.56
1:A:45:PRO:HA	1:A:71:VAL:HG23	1.86	0.56
1:A:312:ARG:HA	1:A:318:ARG:HG2	1.87	0.56
1:A:312:ARG:HA	1:A:318:ARG:CG	2.37	0.55
1:B:63:ARG:HD2	5:B:615:HOH:O	2.05	0.55
1:B:111:LYS:HE3	1:B:266:LEU:O	2.07	0.55
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.90	0.54
1:A:22:VAL:HG12	1:A:70:MET:HB2	1.89	0.54
1:A:115:MET:CE	1:A:263:LEU:HB3	2.37	0.54
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.89	0.54
1:A:245:MET:HE3	1:A:257:LYS:HB2	1.90	0.53
1:A:57:LEU:HB3	1:A:60:LYS:O	2.08	0.53
1:A:315:LYS:O	1:A:319:ILE:HG13	2.08	0.53
1:B:19:ILE:HD12	1:B:359:ILE:HB	1.91	0.52
1:A:81:VAL:O	1:A:85:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD12	1:B:57:LEU:H	1.74	0.51
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.41	0.51
1:A:317:THR:O	1:A:321:GLN:HB3	2.12	0.51
1:B:146:LYS:HE3	5:B:618:HOH:O	2.11	0.50
1:B:184:MET:HE3	1:B:318:ARG:HH21	1.76	0.50
1:A:300:THR:O	1:A:304:GLU:HG3	2.12	0.50
1:B:18:ASN:HD22	1:B:360:LEU:HD11	1.77	0.50
1:A:27:PRO:HB3	1:A:74:ALA:HB1	1.93	0.49
1:A:116:GLU:HB3	4:A:604:N4T:C14	2.32	0.49
1:A:158:VAL:HA	1:A:240:SER:O	2.13	0.49
1:B:163:ILE:HG12	1:B:168:LEU:HD23	1.94	0.49
1:B:251:ASP:HB2	5:B:665:HOH:O	2.13	0.48
1:A:181:ARG:HD2	5:A:661:HOH:O	2.12	0.48
1:A:241:VAL:O	1:A:241:VAL:HG13	2.14	0.48
1:B:312:ARG:HA	1:B:318:ARG:CG	2.42	0.48
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.95	0.48
1:B:86:VAL:HG21	1:B:135:ILE:HG12	1.96	0.48
1:A:209:GLU:O	1:A:213:ILE:HG13	2.14	0.48
1:A:94:ILE:O	1:A:245:MET:HE1	2.14	0.47
1:A:93:VAL:HG21	1:A:261:LEU:HB2	1.96	0.47
1:A:57:LEU:CB	1:A:60:LYS:O	2.63	0.47
1:A:341:LEU:HD12	1:A:341:LEU:H	1.79	0.47
1:B:89:ILE:HD12	1:B:101:ILE:HD11	1.95	0.47
1:B:241:VAL:HG13	1:B:261:LEU:HB3	1.97	0.47
1:B:270:GLU:O	1:B:271:ASN:HB3	2.14	0.46
1:B:291:SER:HA	1:B:314:SER:HB2	1.97	0.46
1:B:210:VAL:O	1:B:214:LEU:HG	2.16	0.46
1:B:82:TYR:CD2	1:B:86:VAL:HB	2.51	0.46
1:A:181:ARG:HB2	5:A:624:HOH:O	2.14	0.46
1:B:57:LEU:O	1:B:61:SER:HB3	2.17	0.46
1:A:247:GLU:O	1:A:254:GLU:HA	2.16	0.45
1:B:158:VAL:HA	1:B:240:SER:O	2.16	0.45
1:A:22:VAL:HG22	1:A:333:ILE:HG12	1.99	0.45
1:B:289:ASN:HD22	1:B:289:ASN:C	2.25	0.45
1:A:18:ASN:CB	1:A:360:LEU:HD12	2.45	0.45
1:B:189:ARG:HD3	5:B:622:HOH:O	2.17	0.45
1:B:136:ILE:HG12	1:B:263:LEU:CD1	2.46	0.45
1:B:246:LYS:HD3	1:B:254:GLU:OE2	2.17	0.45
1:B:92:GLU:CD	1:B:329:ARG:HD2	2.42	0.44
1:B:184:MET:CG	1:B:194:VAL:HG21	2.47	0.44
1:B:336:ILE:HG21	1:B:350:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HG11	1:A:353:ALA:HB1	1.98	0.44
1:A:22:VAL:CG1	1:A:70:MET:HB2	2.47	0.44
1:A:154:PHE:HA	1:A:244:HIS:O	2.16	0.44
1:B:245:MET:HE3	1:B:257:LYS:HB2	1.99	0.44
1:A:162:GLU:HG2	1:A:237:SER:HA	1.98	0.44
1:B:30:LEU:HD23	1:B:33:ARG:HD3	2.00	0.44
1:A:111:LYS:HE3	1:A:266:LEU:O	2.17	0.44
1:A:245:MET:O	1:A:256:VAL:HA	2.16	0.43
1:A:163:ILE:HD11	1:A:319:ILE:HD12	2.00	0.43
1:A:29:ASN:O	1:A:33:ARG:HG2	2.19	0.43
1:A:243:ILE:HG22	1:A:245:MET:HG3	2.00	0.43
1:B:294:THR:O	1:B:298:VAL:HG23	2.18	0.43
1:A:136:ILE:HG12	1:A:263:LEU:CD1	2.49	0.43
1:A:157:LYS:HE2	1:A:203:THR:OG1	2.18	0.43
1:A:289:ASN:O	1:A:293:LEU:HB2	2.19	0.43
1:B:298:VAL:HG13	1:B:309:VAL:CG1	2.49	0.43
1:A:247:GLU:HB3	1:A:255:LEU:HB2	2.01	0.42
1:B:18:ASN:HD22	1:B:360:LEU:CD1	2.32	0.42
1:A:160:LEU:HB3	1:A:172:LEU:HG	2.02	0.42
1:B:53:ARG:HB2	1:B:63:ARG:NH1	2.34	0.42
1:A:212:GLN:HB2	5:A:643:HOH:O	2.19	0.42
1:A:257:LYS:HB2	1:A:257:LYS:HE3	1.92	0.42
1:B:154:PHE:HA	1:B:244:HIS:O	2.19	0.42
1:B:25:CYS:O	1:B:74:ALA:HA	2.19	0.42
1:B:192:ARG:NH1	1:B:192:ARG:HB3	2.35	0.42
1:A:163:ILE:HG12	1:A:168:LEU:HD12	2.02	0.41
1:A:116:GLU:CB	4:A:604:N4T:H14	2.34	0.41
1:A:215:GLU:HG2	4:A:604:N4T:C12	2.50	0.41
1:A:265:ASP:C	1:A:265:ASP:OD1	2.63	0.41
1:B:116:GLU:HB3	4:B:605:N4T:C14	2.49	0.41
1:A:46:VAL:HG13	1:A:47:ARG:HG3	2.03	0.41
1:A:204:VAL:HG22	1:A:213:ILE:CD1	2.50	0.41
1:B:351:GLU:CD	5:B:638:HOH:O	2.63	0.41
1:A:248:THR:HA	1:A:253:GLU:O	2.21	0.41
1:B:98:ASN:C	1:B:328:THR:HG23	2.46	0.41
1:B:50:VAL:O	1:B:50:VAL:HG13	2.22	0.40
1:A:57:LEU:O	1:A:61:SER:HB3	2.21	0.40
1:B:27:PRO:HB3	1:B:74:ALA:HB1	2.02	0.40
1:A:45:PRO:HA	1:A:71:VAL:CG2	2.51	0.40
1:B:72:PHE:HB3	1:B:76:THR:HG21	2.02	0.40

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	326/367 (89%)	314 (96%)	9 (3%)	3 (1%)	14	27
1	B	326/367 (89%)	317 (97%)	8 (2%)	1 (0%)	36	55
All	All	652/734 (89%)	631 (97%)	17 (3%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	189	ARG
1	A	36	SER
1	B	56	GLY

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	293/321 (91%)	281 (96%)	12 (4%)	27	53
1	B	293/321 (91%)	279 (95%)	14 (5%)	23	46
All	All	586/642 (91%)	560 (96%)	26 (4%)	25	50

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	65	THR

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Mol	Chain	Res	Type
1	A	161	LEU
1	A	168	LEU
1	A	199	LEU
1	A	226	THR
1	A	250	ILE
1	A	254	GLU
1	A	289	ASN
1	A	293	LEU
1	A	330	THR
1	A	361	ASN
1	B	18	ASN
1	B	57	LEU
1	B	181	ARG
1	B	210	VAL
1	B	234	ARG
1	B	271	ASN
1	B	289	ASN
1	B	293	LEU
1	B	302	LEU
1	B	331	SER
1	B	341	LEU
1	B	343	LEU
1	B	350	LEU
1	B	357	LYS

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	141	HIS
1	A	229	ASN
1	A	244	HIS
1	A	262	ASN
1	A	289	ASN
1	A	361	ASN
1	B	18	ASN
1	B	141	HIS
1	B	173	ASN
1	B	262	ASN
1	B	289	ASN
1	B	290	GLN
1	B	354	HIS
1	B	358	ASN

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Mol	Chain	Res	Type
1	B	361	ASN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
4	N4T	B	605	-	28,29,29	3.39	10 (35%)	31,42,42	2.50	12 (38%)
3	ADP	B	600	2	28,29,29	1.60	7 (25%)	43,45,45	2.02	9 (20%)
3	ADP	A	601	2	28,29,29	1.64	8 (28%)	43,45,45	1.97	8 (18%)
4	N4T	A	604	-	28,29,29	3.39	10 (35%)	31,42,42	2.33	9 (29%)

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	N4T	B	605	-	-	4/20/34/34	0/4/4/4
3	ADP	B	600	2	-	7/16/32/32	0/3/3/3
3	ADP	A	601	2	-	8/16/32/32	0/3/3/3
4	N4T	A	604	-	-	3/20/34/34	0/4/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	N4T	C13-C14	-11.32	1.40	1.50
4	A	604	N4T	C13-C14	-11.07	1.41	1.50
4	A	604	N4T	C35-C7	-9.88	1.36	1.53
4	B	605	N4T	C35-C7	-8.71	1.38	1.53
4	B	605	N4T	C23-C17	4.87	1.46	1.39
4	A	604	N4T	C19-C17	4.39	1.46	1.39
4	B	605	N4T	C3-C4	4.36	1.44	1.38
4	B	605	N4T	C19-C17	4.19	1.45	1.39
3	A	601	ADP	C5-N7	-4.07	1.31	1.39
3	B	600	ADP	C5-N7	-3.93	1.31	1.39
4	A	604	N4T	C23-C17	3.75	1.45	1.39
4	B	605	N4T	C11-C10	3.49	1.55	1.50
4	A	604	N4T	C3-C4	3.30	1.43	1.38
4	A	604	N4T	C17-C13	-3.26	1.49	1.52
4	A	604	N4T	C11-C10	3.11	1.55	1.50
3	B	600	ADP	C4-N3	3.00	1.40	1.34
4	B	605	N4T	C14-C10	2.90	1.39	1.34
3	A	601	ADP	C5-C4	2.63	1.43	1.39
3	A	601	ADP	C5'-C4'	2.61	1.59	1.51
4	A	604	N4T	C20-C19	2.59	1.43	1.38
3	A	601	ADP	C1'-N9	2.52	1.53	1.46
4	B	605	N4T	C21-C20	2.50	1.43	1.38
3	B	600	ADP	C2-N3	2.44	1.38	1.33
4	A	604	N4T	C6-C1	2.43	1.41	1.37
3	B	600	ADP	C5-C4	2.43	1.43	1.39
3	A	601	ADP	C4-N3	2.39	1.38	1.34
4	B	605	N4T	C20-C19	2.35	1.42	1.38
3	B	600	ADP	C5'-C4'	2.18	1.58	1.51
3	A	601	ADP	C4-N9	-2.18	1.33	1.37
3	A	601	ADP	C2-N3	2.17	1.37	1.33
4	A	604	N4T	C21-C20	2.17	1.43	1.38
3	B	600	ADP	C2-N1	2.17	1.37	1.33
3	A	601	ADP	O4'-C1'	2.07	1.46	1.42
4	B	605	N4T	C6-C1	2.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	ADP	C1'-N9	2.04	1.52	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605	N4T	C17-C13-N12	7.24	121.91	112.37
3	B	600	ADP	N3-C2-N1	-7.06	117.89	128.58
3	A	601	ADP	N3-C2-N1	-6.55	118.67	128.58
4	A	604	N4T	C17-C13-N12	6.17	120.51	112.37
4	B	605	N4T	C35-C7-C8	6.12	117.98	110.33
3	A	601	ADP	C5-C4-N3	-5.31	119.40	126.72
4	A	604	N4T	C17-C13-C14	5.24	126.39	112.98
3	B	600	ADP	C5-C4-N3	-5.01	119.81	126.72
4	A	604	N4T	O2-C8-C7	-4.65	111.20	119.95
4	A	604	N4T	C35-C7-C8	4.51	115.97	110.33
4	B	605	N4T	C17-C13-C14	4.48	124.47	112.98
3	A	601	ADP	C2-N3-C4	4.42	122.62	111.83
3	B	600	ADP	C2-N3-C4	4.35	122.45	111.83
3	B	600	ADP	N3-C4-N9	4.29	134.47	127.17
3	A	601	ADP	N3-C4-N9	4.16	134.24	127.17
4	B	605	N4T	O2-C8-C7	-3.75	112.88	119.95
3	B	600	ADP	C5-N7-C8	3.30	108.64	103.45
3	A	601	ADP	C5-N7-C8	3.19	108.47	103.45
4	A	604	N4T	C23-C17-C13	-2.85	116.21	120.64
3	B	600	ADP	N9-C8-N7	-2.84	109.91	113.94
4	B	605	N4T	C6-C5-C4	-2.69	115.73	119.04
3	A	601	ADP	N9-C8-N7	-2.67	110.14	113.94
4	B	605	N4T	C22-C21-C20	2.67	123.52	119.87
4	A	604	N4T	F41-C1-C2	-2.60	114.59	118.28
3	A	601	ADP	C4-C5-N7	-2.57	107.64	110.58
4	A	604	N4T	O2-C8-N12	2.53	125.92	121.38
4	B	605	N4T	C20-C19-C17	-2.42	117.75	120.65
4	B	605	N4T	C5-C4-C3	2.34	125.59	123.07
4	B	605	N4T	C8-C7-N1	2.33	114.01	110.09
3	B	600	ADP	C4-C5-N7	-2.32	107.93	110.58
3	B	600	ADP	C2-N1-C6	2.30	122.50	118.73
4	B	605	N4T	C23-C17-C13	-2.29	117.08	120.64
4	B	605	N4T	C7-C8-N12	2.24	124.13	118.65
4	A	604	N4T	C19-C17-C13	2.17	124.01	120.64
3	B	600	ADP	C2'-C3'-C4'	2.10	106.67	102.61
4	B	605	N4T	F40-C4-C5	-2.09	113.79	118.65
3	A	601	ADP	C2'-C3'-C4'	2.08	106.62	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	N4T	C3-C10-C14	2.02	130.85	126.89

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	PA-O3A-PB-O3B
3	A	601	ADP	C5'-O5'-PA-O1A
3	A	601	ADP	C5'-O5'-PA-O2A
3	A	601	ADP	C5'-O5'-PA-O3A
3	B	600	ADP	PA-O3A-PB-O2B
3	B	600	ADP	C5'-O5'-PA-O1A
3	B	600	ADP	C5'-O5'-PA-O2A
3	B	600	ADP	C5'-O5'-PA-O3A
4	A	604	N4T	C15-C35-C7-N1
4	A	604	N4T	C12-C35-C7-N1
4	B	605	N4T	C15-C35-C7-N1
4	B	605	N4T	C12-C35-C7-N1
3	A	601	ADP	C3'-C4'-C5'-O5'
3	B	600	ADP	O4'-C4'-C5'-O5'
3	B	600	ADP	C3'-C4'-C5'-O5'
3	A	601	ADP	O4'-C4'-C5'-O5'
4	B	605	N4T	O2-C8-N12-C13
3	B	600	ADP	PA-O3A-PB-O3B
3	A	601	ADP	PA-O3A-PB-O1B
3	A	601	ADP	PA-O3A-PB-O2B
4	A	604	N4T	N12-C13-C17-C19
4	B	605	N4T	N12-C13-C17-C19

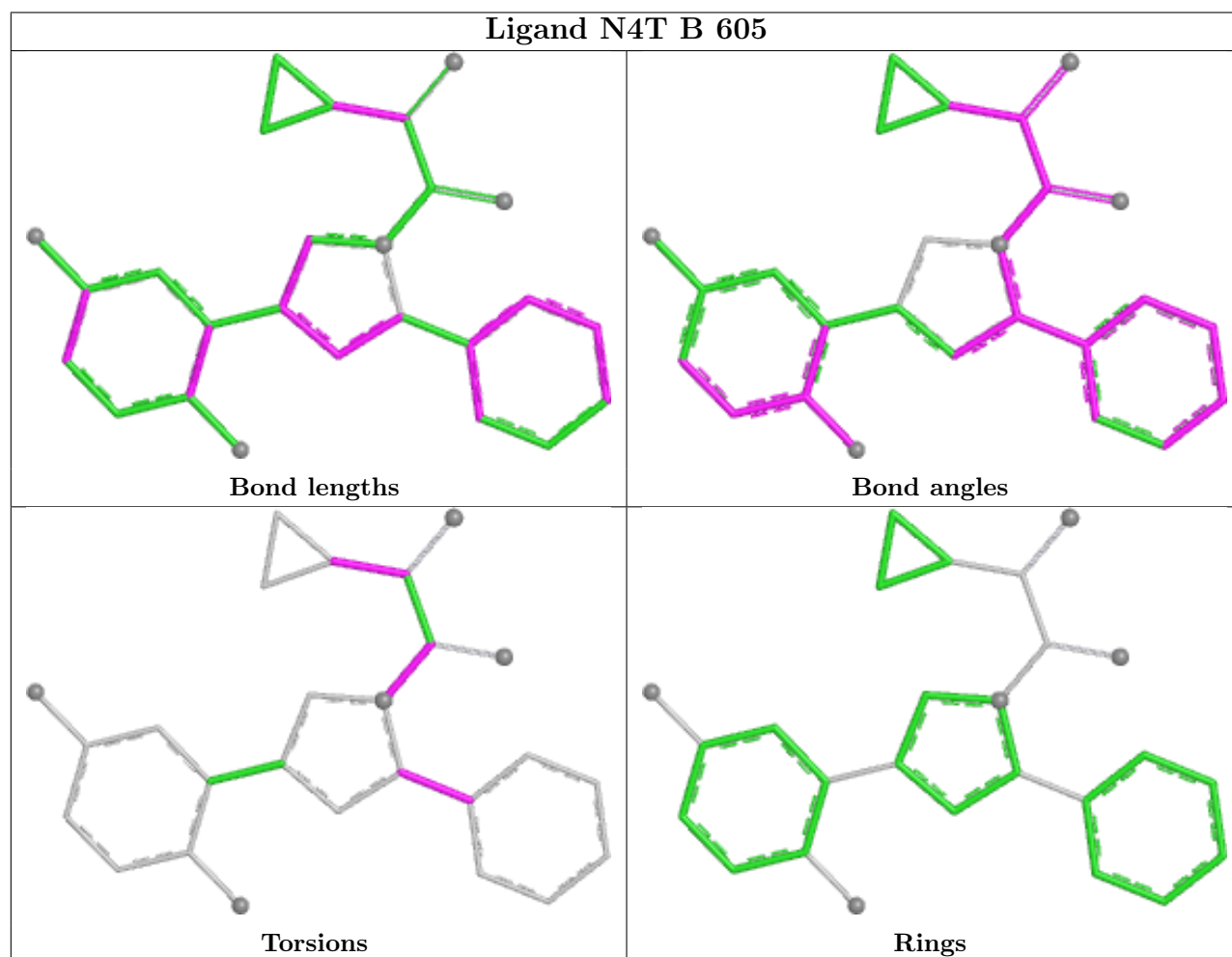
There are no ring outliers.

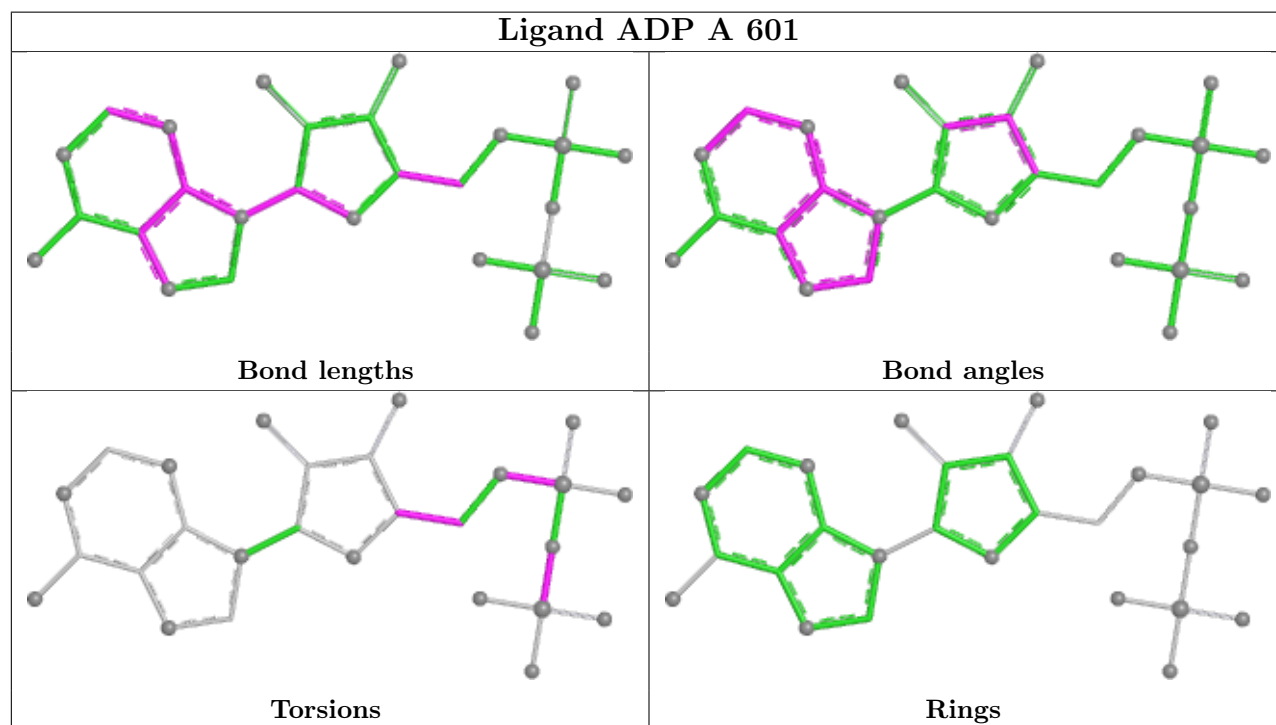
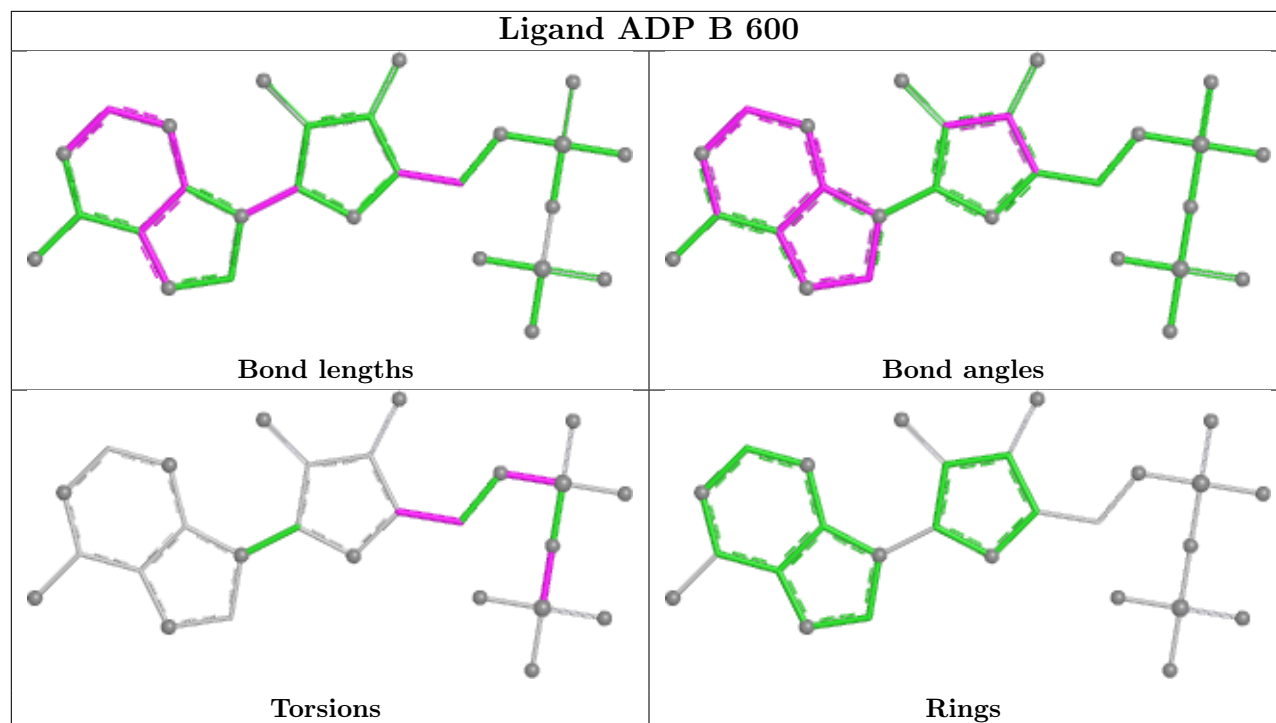
2 monomers are involved in 6 short contacts:

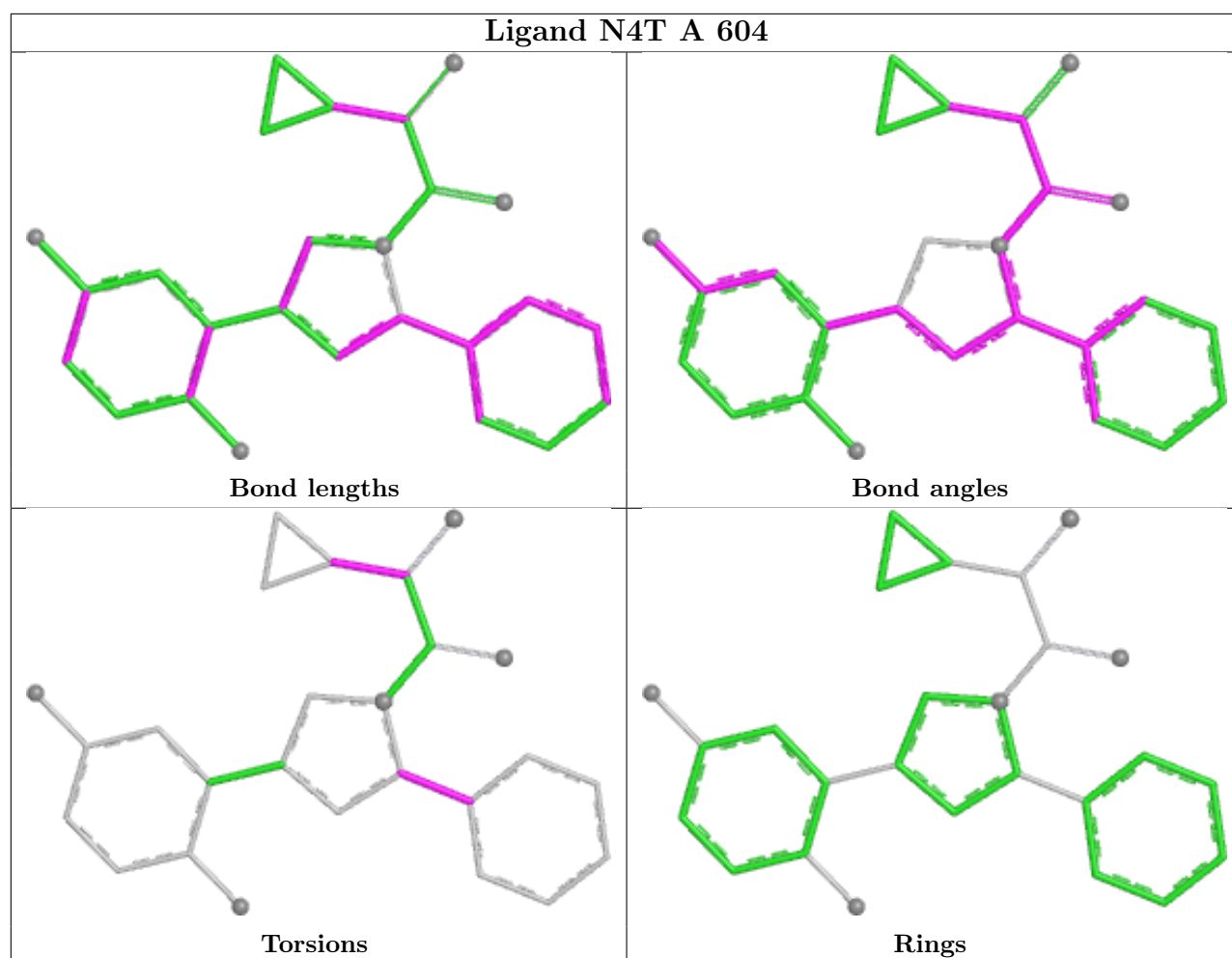
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	N4T	2	0
4	A	604	N4T	4	0

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.