



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 11:54 PM UTC

PDB ID : 8S1B / pdb_00008s1b
Title : c-KIT kinase domain in complex with IDRX-42 via soaking
Authors : Teuber, A.; Mueller, M.P.; Rauh, D.
Deposited on : 2024-02-15
Resolution : 2.00 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

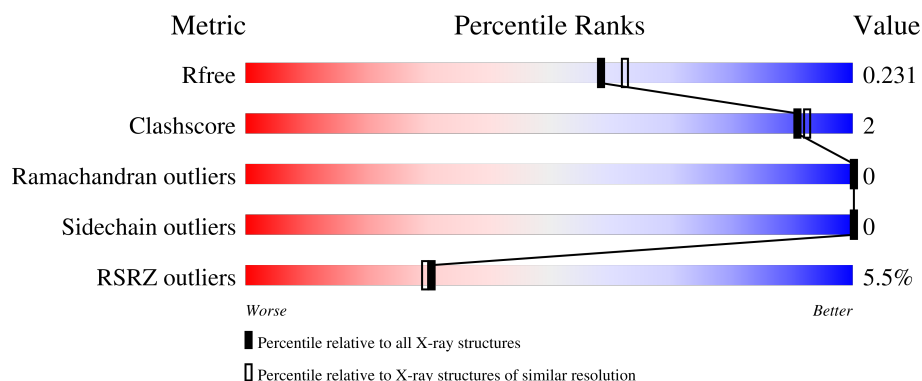
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	4% 77% 7% 15%
1	B	327	5% 86% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4664 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 Mast/stem cell growth factor receptor Kit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	2	0
			2157	1391	358	390	18			
1	B	285	Total	C	N	O	S	0	7	0
			2244	1448	371	406	19			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	GLY	-	expression tag	UNP P10721
A	549	SER	-	expression tag	UNP P10721
A	550	MET	-	expression tag	UNP P10721
A	563	SER	ILE	engineered mutation	UNP P10721
A	569	SER	VAL	engineered mutation	UNP P10721
A	609	GLN	TYR	engineered mutation	UNP P10721
A	631	SER	LEU	engineered mutation	UNP P10721
A	651	GLU	MET	engineered mutation	UNP P10721
A	662	HIS	ILE	engineered mutation	UNP P10721
A	688	GLU	-	linker	UNP P10721
A	689	PHE	-	linker	UNP P10721
A	690	VAL	-	linker	UNP P10721
A	691	PRO	-	linker	UNP P10721
A	752	TYR	-	linker	UNP P10721
A	753	LYS	-	linker	UNP P10721
A	754	VAL	-	linker	UNP P10721
A	755	ALA	-	linker	UNP P10721
A	756	PRO	-	linker	UNP P10721
A	757	GLU	-	linker	UNP P10721
A	758	ASP	-	linker	UNP P10721
A	759	LEU	-	linker	UNP P10721
A	760	TYR	-	linker	UNP P10721
A	761	LYS	-	linker	UNP P10721
A	762	ASP	-	linker	UNP P10721
A	763	PHE	-	linker	UNP P10721

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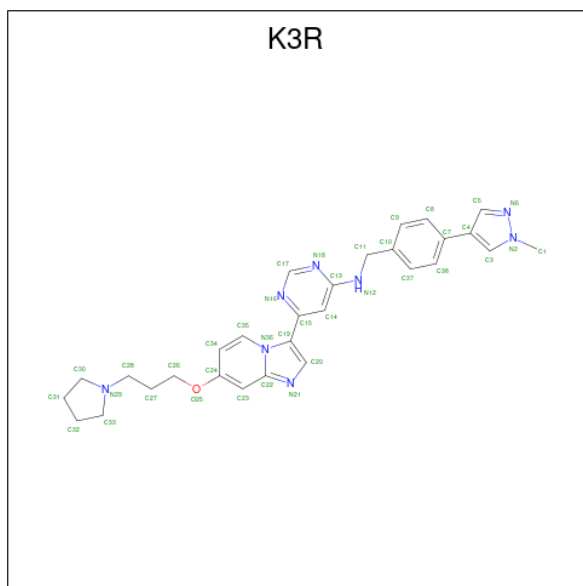
Chain	Residue	Modelled	Actual	Comment	Reference
A	764	LEU	-	linker	UNP P10721
A	765	THR	-	linker	UNP P10721
A	768	HIS	ASP	engineered mutation	UNP P10721
A	804	ASN	ARG	engineered mutation	UNP P10721
A	825	ASP	VAL	engineered mutation	UNP P10721
A	844	SER	CYS	engineered mutation	UNP P10721
A	890	SER	LEU	engineered mutation	UNP P10721
A	894	TYR	HIS	engineered mutation	UNP P10721
A	912	ASP	LEU	engineered mutation	UNP P10721
A	923	ASP	LEU	engineered mutation	UNP P10721
B	548	GLY	-	expression tag	UNP P10721
B	549	SER	-	expression tag	UNP P10721
B	550	MET	-	expression tag	UNP P10721
B	563	SER	ILE	engineered mutation	UNP P10721
B	569	SER	VAL	engineered mutation	UNP P10721
B	609	GLN	TYR	engineered mutation	UNP P10721
B	631	SER	LEU	engineered mutation	UNP P10721
B	651	GLU	MET	engineered mutation	UNP P10721
B	662	HIS	ILE	engineered mutation	UNP P10721
B	688	GLU	-	linker	UNP P10721
B	689	PHE	-	linker	UNP P10721
B	690	VAL	-	linker	UNP P10721
B	691	PRO	-	linker	UNP P10721
B	692	TYR	-	linker	UNP P10721
B	693	LYS	-	linker	UNP P10721
B	754	VAL	-	linker	UNP P10721
B	755	ALA	-	linker	UNP P10721
B	756	PRO	-	linker	UNP P10721
B	757	GLU	-	linker	UNP P10721
B	758	ASP	-	linker	UNP P10721
B	759	LEU	-	linker	UNP P10721
B	760	TYR	-	linker	UNP P10721
B	761	LYS	-	linker	UNP P10721
B	762	ASP	-	linker	UNP P10721
B	763	PHE	-	linker	UNP P10721
B	764	LEU	-	linker	UNP P10721
B	765	THR	-	linker	UNP P10721
B	768	HIS	ASP	engineered mutation	UNP P10721
B	804	ASN	ARG	engineered mutation	UNP P10721
B	825	ASP	VAL	engineered mutation	UNP P10721
B	844	SER	CYS	engineered mutation	UNP P10721
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Chain	Residue	Modelled	Actual	Comment	Reference
B	894	TYR	HIS	engineered mutation	UNP P10721
B	912	ASP	LEU	engineered mutation	UNP P10721
B	923	ASP	LEU	engineered mutation	UNP P10721

- Molecule 2 is {N}-[[4-(1-methylpyrazol-4-yl)phenyl]methyl]-6-[7-(3-pyrrolidin-1-ylpropoxy)imidazo[1,2-a]pyridin-3-yl]pyrimidin-4-amine (CCD ID: K3R) (formula: C₂₉H₃₂N₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	29	8	1		
2	B	1	Total	C	N	O	0	0
			38	29	8	1		
2	B	1	Total	C	N	O	0	0
			38	29	8	1		
2	B	1	Total	C	N	O	0	0
			38	29	8	1		

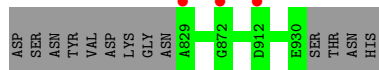
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	59	Total 59	O 59	0	0

- Molecule 1: Mast/stem cell growth factor receptor Kit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.74Å 59.29Å 192.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.12 – 2.00 48.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.12-2.00) 99.2 (48.12-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.231 0.203 , 0.231	Depositor DCC
R_{free} test set	2300 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4664	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, K3R

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	0.08	0/2218	0.24	0/3008
1	B	0.08	0/2321	0.26	0/3147
All	All	0.08	0/4539	0.25	0/6155

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

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	2157	0	2087	13	0
1	B	2244	0	2172	2	0
2	A	38	0	0	0	0
2	B	114	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	50	0	0	0	0
4	B	59	0	0	0	0
All	All	4664	0	4259	15	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 2.

All (15) 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:611:LEU:HD23	1:B:618:MET:HE3	1.90	0.54
1:A:630:HIS:NE2	1:A:632:THR:OG1	2.42	0.52
1:A:770:LEU:HB3	1:A:928:ILE:HD11	1.92	0.51
1:A:677:ASP:OD2	1:A:680:ASN:ND2	2.45	0.49
1:A:860:TRP:CD1	1:A:892:PRO:HG3	2.49	0.48
1:A:908:ASP:OD2	1:A:913:LYS:HD2	2.15	0.47
1:B:809[B]:CYS:SG	1:B:810:ASP:N	2.87	0.46
1:A:809[A]:CYS:SG	1:A:810:ASP:N	2.89	0.45
1:A:610:GLY:HA2	1:A:613:LYS:O	2.17	0.45
1:A:801:THR:OG1	1:A:802:HIS:N	2.51	0.44
1:A:859:LEU:HB3	1:A:903:MET:HE2	1.99	0.44
1:A:902:ILE:HD11	1:A:923:ASP:OD2	2.18	0.43
1:A:774:TYR:CE1	1:A:921:VAL:HG23	2.53	0.42
1:A:690:VAL:O	1:A:765:THR:HA	2.21	0.41
1:A:902:ILE:HD13	1:A:902:ILE:HA	1.90	0.41

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	271/327 (83%)	266 (98%)	5 (2%)	0	100	100
1	B	286/327 (88%)	282 (99%)	4 (1%)	0	100	100
All	All	557/654 (85%)	548 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	228/285 (80%)	228 (100%)	0	100	100
1	B	237/285 (83%)	237 (100%)	0	100	100
All	All	465/570 (82%)	465 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	787	ASN
1	B	587	ASN
1	B	680	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
2	K3R	B	1003	-	43,43,43	2.34	15 (34%)	52,59,59	2.36	19 (36%)
2	K3R	A	1001	-	43,43,43	2.12	13 (30%)	52,59,59	2.29	19 (36%)
2	K3R	B	1002	-	43,43,43	2.55	22 (51%)	52,59,59	2.47	21 (40%)
2	K3R	B	1001	-	43,43,43	2.15	13 (30%)	52,59,59	2.32	19 (36%)

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	K3R	B	1003	-	-	4/20/27/27	0/6/6/6
2	K3R	A	1001	-	-	4/20/27/27	0/6/6/6
2	K3R	B	1002	-	-	4/20/27/27	0/6/6/6
2	K3R	B	1001	-	-	2/20/27/27	0/6/6/6

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	K3R	C3-N2	6.27	1.41	1.34
2	B	1003	K3R	C3-N2	6.01	1.40	1.34
2	B	1002	K3R	C13-N12	5.32	1.44	1.36
2	B	1001	K3R	C1-N2	5.25	1.52	1.46
2	A	1001	K3R	C13-N12	5.18	1.43	1.36
2	B	1003	K3R	C13-N12	5.13	1.43	1.36
2	B	1003	K3R	C19-N36	4.94	1.45	1.39
2	B	1001	K3R	C13-N12	4.80	1.43	1.36
2	B	1001	K3R	C3-N2	4.77	1.39	1.34
2	A	1001	K3R	C3-N2	4.69	1.39	1.34
2	B	1002	K3R	C19-N36	4.69	1.44	1.39
2	B	1001	K3R	C22-N21	4.42	1.39	1.33
2	B	1002	K3R	C22-N21	4.09	1.39	1.33
2	B	1002	K3R	C20-C19	3.95	1.41	1.37
2	A	1001	K3R	C19-N36	3.90	1.43	1.39
2	B	1002	K3R	C11-C10	3.80	1.59	1.51
2	A	1001	K3R	C20-C19	3.73	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	K3R	C20-C19	3.70	1.40	1.37
2	B	1001	K3R	C20-C19	3.70	1.40	1.37
2	A	1001	K3R	C22-N21	3.65	1.38	1.33
2	B	1002	K3R	C15-C19	3.58	1.54	1.47
2	B	1002	K3R	C5-N6	3.52	1.38	1.32
2	B	1003	K3R	C22-N21	3.47	1.38	1.33
2	B	1001	K3R	C5-N6	3.39	1.37	1.32
2	B	1002	K3R	C1-N2	3.34	1.50	1.46
2	B	1003	K3R	C5-N6	3.20	1.37	1.32
2	A	1001	K3R	C5-N6	3.17	1.37	1.32
2	B	1003	K3R	C1-N2	3.03	1.49	1.46
2	B	1003	K3R	C15-C19	2.78	1.52	1.47
2	B	1002	K3R	C38-C37	2.76	1.43	1.38
2	B	1002	K3R	N2-N6	2.65	1.38	1.35
2	A	1001	K3R	N2-N6	2.61	1.38	1.35
2	A	1001	K3R	C15-C19	2.59	1.52	1.47
2	B	1003	K3R	C11-C10	2.51	1.57	1.51
2	B	1003	K3R	N2-N6	2.45	1.38	1.35
2	B	1002	K3R	C14-C13	2.44	1.45	1.39
2	B	1002	K3R	C7-C4	2.37	1.53	1.48
2	B	1001	K3R	C19-N36	2.35	1.42	1.39
2	B	1003	K3R	C35-C34	2.31	1.40	1.35
2	A	1001	K3R	C13-N18	2.28	1.38	1.34
2	A	1001	K3R	C11-C10	2.25	1.56	1.51
2	B	1001	K3R	C35-C34	2.21	1.40	1.35
2	B	1001	K3R	C13-N18	2.20	1.38	1.34
2	B	1002	K3R	C37-C10	2.18	1.43	1.38
2	B	1003	K3R	C9-C8	2.18	1.42	1.38
2	A	1001	K3R	C35-C34	2.13	1.40	1.35
2	B	1003	K3R	C22-N36	2.12	1.42	1.39
2	B	1002	K3R	C23-C22	2.11	1.46	1.41
2	B	1002	K3R	C5-C4	2.10	1.45	1.40
2	B	1001	K3R	C15-N16	2.10	1.38	1.34
2	B	1001	K3R	C30-N29	2.10	1.51	1.47
2	B	1002	K3R	C22-N36	2.09	1.42	1.39
2	A	1001	K3R	C38-C37	2.08	1.42	1.38
2	B	1002	K3R	C13-N18	2.08	1.37	1.34
2	B	1001	K3R	C11-C10	2.07	1.56	1.51
2	A	1001	K3R	C17-N18	2.07	1.37	1.33
2	B	1002	K3R	C38-C7	2.06	1.42	1.39
2	B	1003	K3R	C17-N18	2.05	1.37	1.33
2	B	1002	K3R	C9-C8	2.04	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	K3R	C3-C4	2.04	1.42	1.38
2	B	1002	K3R	C20-N21	2.02	1.41	1.37
2	B	1001	K3R	C9-C8	2.01	1.42	1.38
2	B	1003	K3R	C17-N16	2.00	1.37	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	K3R	C1-N2-N6	6.83	125.51	120.03
2	A	1001	K3R	C1-N2-N6	6.37	125.14	120.03
2	B	1002	K3R	C19-N36-C22	5.57	109.63	106.91
2	B	1002	K3R	C1-N2-N6	5.55	124.48	120.03
2	B	1003	K3R	C1-N2-N6	5.35	124.32	120.03
2	B	1003	K3R	C33-N29-C30	5.31	110.31	104.04
2	B	1003	K3R	C28-N29-C33	-5.18	100.98	113.25
2	B	1001	K3R	C3-N2-N6	-4.98	109.25	112.08
2	B	1003	K3R	C35-N36-C22	-4.91	116.92	121.97
2	B	1002	K3R	C35-N36-C22	-4.71	117.12	121.97
2	A	1001	K3R	C33-N29-C30	4.66	109.54	104.04
2	B	1002	K3R	C33-N29-C30	4.63	109.50	104.04
2	A	1001	K3R	C35-N36-C22	-4.61	117.22	121.97
2	B	1002	K3R	C17-N16-C15	4.37	118.27	115.81
2	B	1002	K3R	N36-C22-N21	-4.36	107.70	111.02
2	B	1002	K3R	C14-C15-N16	-4.32	118.09	123.27
2	A	1001	K3R	C19-N36-C22	4.29	109.00	106.91
2	B	1001	K3R	C28-N29-C33	-4.19	103.33	113.25
2	B	1001	K3R	C19-N36-C22	4.15	108.93	106.91
2	B	1003	K3R	C14-C15-N16	-4.11	118.33	123.27
2	B	1001	K3R	C35-N36-C22	-4.09	117.76	121.97
2	B	1002	K3R	C3-N2-N6	-3.99	109.81	112.08
2	B	1002	K3R	C28-N29-C33	-3.98	103.82	113.25
2	A	1001	K3R	C14-C15-N16	-3.96	118.51	123.27
2	B	1003	K3R	C35-N36-C19	3.86	134.56	130.52
2	B	1003	K3R	C3-N2-N6	-3.82	109.91	112.08
2	A	1001	K3R	C28-N29-C33	-3.71	104.44	113.25
2	A	1001	K3R	N36-C22-N21	-3.71	108.19	111.02
2	B	1001	K3R	C14-C15-N16	-3.68	118.86	123.27
2	B	1003	K3R	C14-C13-N18	-3.67	118.11	122.92
2	B	1001	K3R	N36-C22-N21	-3.67	108.22	111.02
2	A	1001	K3R	C14-C13-N18	-3.53	118.29	122.92
2	B	1002	K3R	C14-C13-N18	-3.48	118.35	122.92
2	B	1002	K3R	C20-N21-C22	3.43	107.40	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	K3R	C14-C13-N18	-3.41	118.45	122.92
2	B	1001	K3R	C33-N29-C30	3.38	108.03	104.04
2	A	1001	K3R	C3-N2-N6	-3.34	110.19	112.08
2	B	1003	K3R	C19-N36-C22	3.30	108.52	106.91
2	A	1001	K3R	C1-N2-C3	-3.25	124.68	127.94
2	B	1003	K3R	N36-C22-N21	-3.21	108.58	111.02
2	B	1002	K3R	C38-C7-C8	-3.19	114.51	118.57
2	B	1001	K3R	C17-N16-C15	3.13	117.57	115.81
2	A	1001	K3R	C35-N36-C19	3.10	133.77	130.52
2	A	1001	K3R	C20-N21-C22	3.04	107.14	105.11
2	A	1001	K3R	C17-N16-C15	3.00	117.50	115.81
2	B	1003	K3R	C20-N21-C22	2.99	107.11	105.11
2	B	1003	K3R	C38-C7-C8	-2.91	114.87	118.57
2	B	1003	K3R	C34-C24-C23	-2.87	117.93	121.54
2	B	1001	K3R	C38-C7-C8	-2.82	114.98	118.57
2	B	1001	K3R	C20-N21-C22	2.79	106.97	105.11
2	B	1001	K3R	C4-C3-N2	2.78	110.40	108.10
2	A	1001	K3R	C38-C7-C8	-2.69	115.14	118.57
2	B	1001	K3R	C1-N2-C3	-2.69	125.24	127.94
2	B	1003	K3R	C5-N6-N2	2.67	105.88	104.41
2	B	1003	K3R	C32-C33-N29	2.66	107.04	103.90
2	B	1001	K3R	C35-N36-C19	2.66	133.30	130.52
2	B	1001	K3R	C5-N6-N2	2.64	105.86	104.41
2	B	1002	K3R	C35-N36-C19	2.61	133.25	130.52
2	B	1001	K3R	C34-C35-N36	2.61	123.19	119.88
2	B	1002	K3R	C34-C24-C23	-2.58	118.29	121.54
2	B	1002	K3R	C5-N6-N2	2.58	105.83	104.41
2	B	1002	K3R	C9-C10-C37	-2.56	114.42	118.23
2	A	1001	K3R	C34-C24-C23	-2.56	118.32	121.54
2	B	1002	K3R	C38-C7-C4	2.51	124.68	121.16
2	B	1001	K3R	C34-C24-C23	-2.49	118.40	121.54
2	B	1002	K3R	C34-C35-N36	2.43	122.97	119.88
2	B	1002	K3R	C14-C13-N12	2.36	124.61	120.79
2	B	1003	K3R	C17-N16-C15	2.34	117.13	115.81
2	B	1003	K3R	C9-C10-C37	-2.23	114.92	118.23
2	B	1002	K3R	C1-N2-C3	-2.23	125.70	127.94
2	B	1003	K3R	C1-N2-C3	-2.16	125.77	127.94
2	B	1002	K3R	C9-C8-C7	2.15	123.10	120.80
2	B	1001	K3R	C9-C10-C37	-2.15	115.04	118.23
2	A	1001	K3R	C9-C10-C37	-2.14	115.05	118.23
2	A	1001	K3R	C5-N6-N2	2.11	105.57	104.41
2	A	1001	K3R	C38-C7-C4	2.04	124.02	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	K3R	C28-N29-C30	-2.03	108.42	113.25
2	A	1001	K3R	C34-C35-N36	2.01	122.43	119.88

There are no chirality outliers.

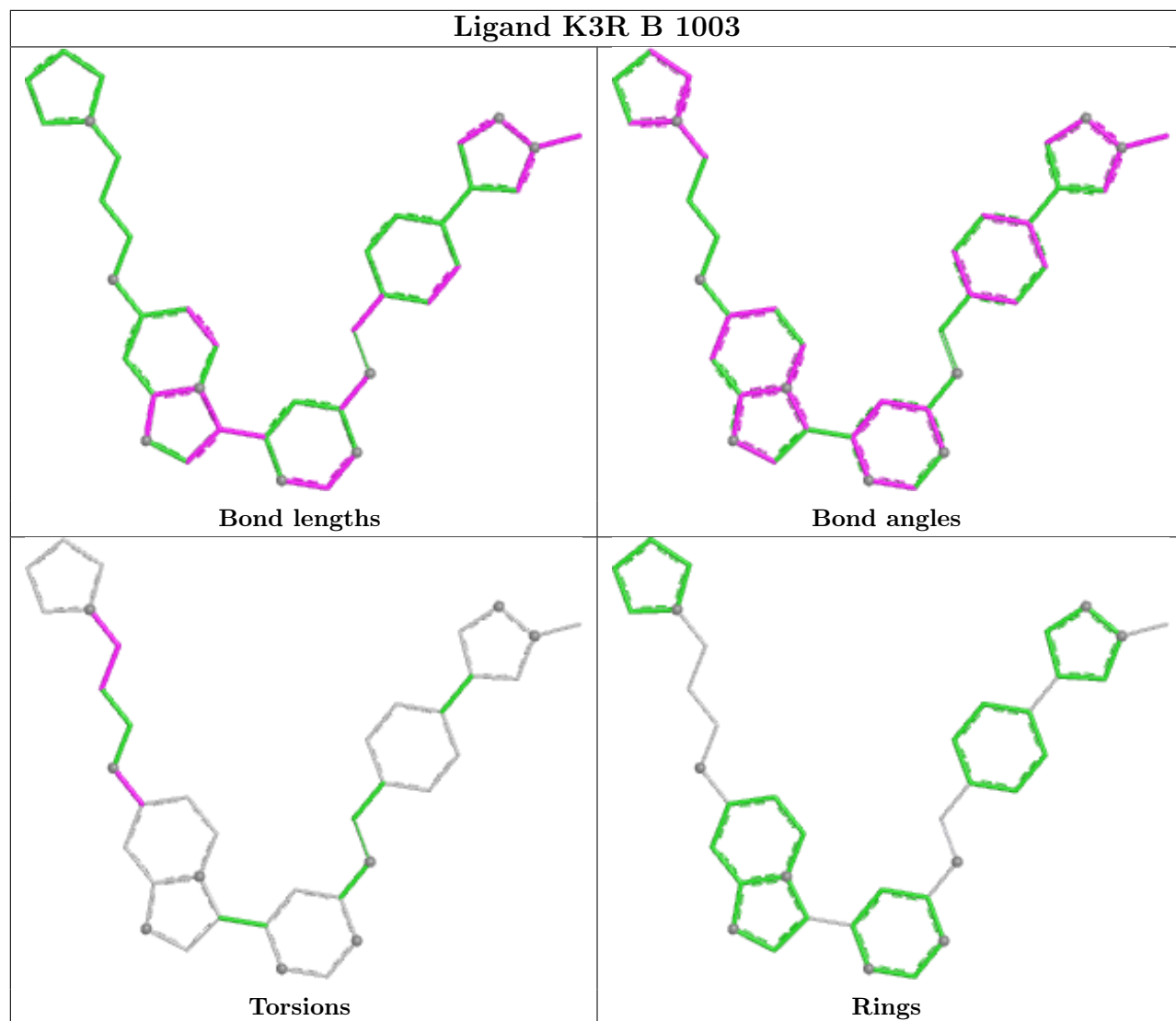
All (14) torsion outliers are listed below:

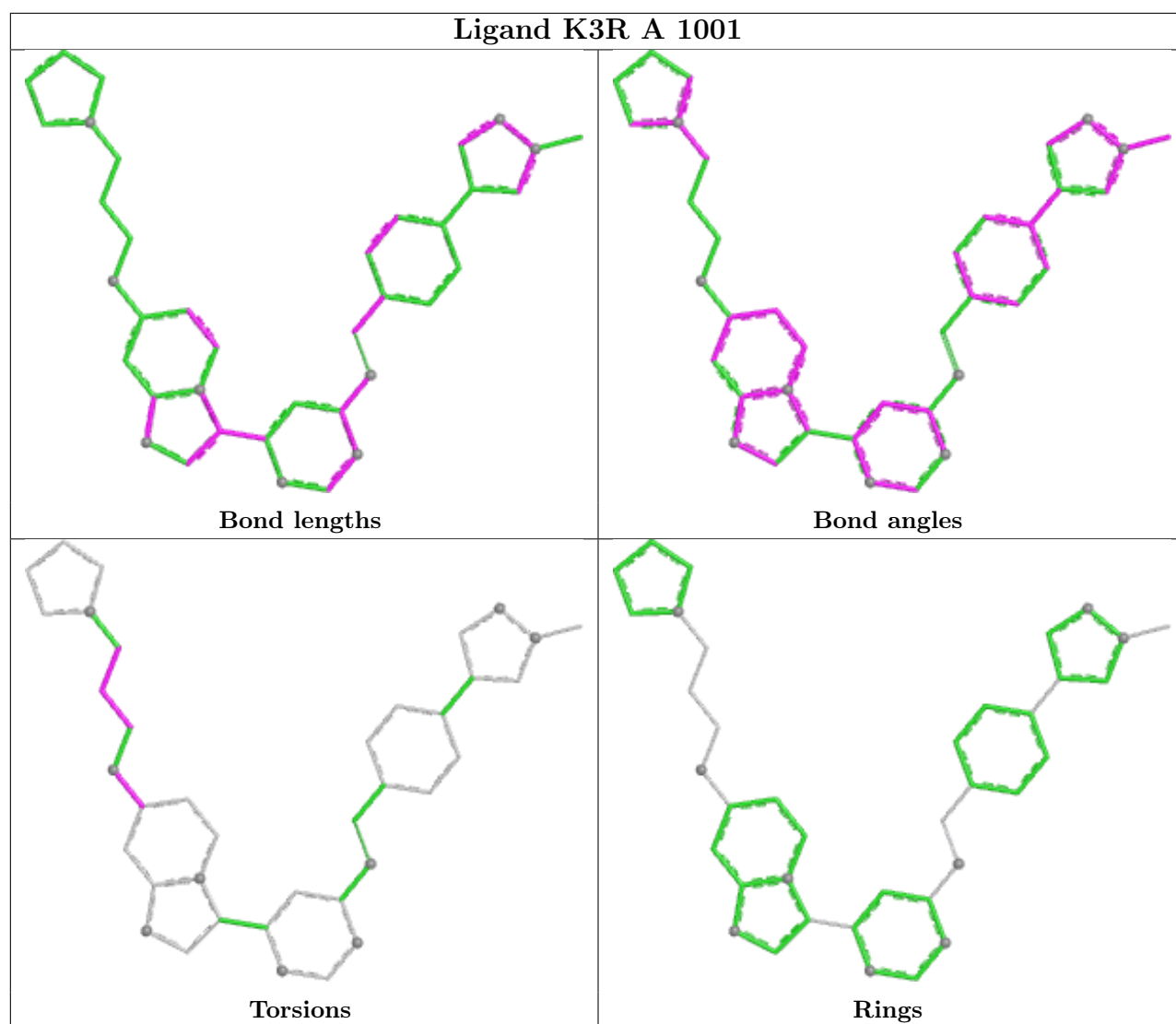
Mol	Chain	Res	Type	Atoms
2	A	1001	K3R	C26-C27-C28-N29
2	B	1002	K3R	C23-C24-O25-C26
2	B	1002	K3R	C26-C27-C28-N29
2	B	1003	K3R	C27-C28-N29-C33
2	A	1001	K3R	O25-C26-C27-C28
2	B	1001	K3R	O25-C26-C27-C28
2	B	1003	K3R	C26-C27-C28-N29
2	B	1002	K3R	O25-C26-C27-C28
2	B	1001	K3R	C26-C27-C28-N29
2	A	1001	K3R	C23-C24-O25-C26
2	A	1001	K3R	C34-C24-O25-C26
2	B	1003	K3R	C34-C24-O25-C26
2	B	1002	K3R	C27-C28-N29-C30
2	B	1003	K3R	C27-C28-N29-C30

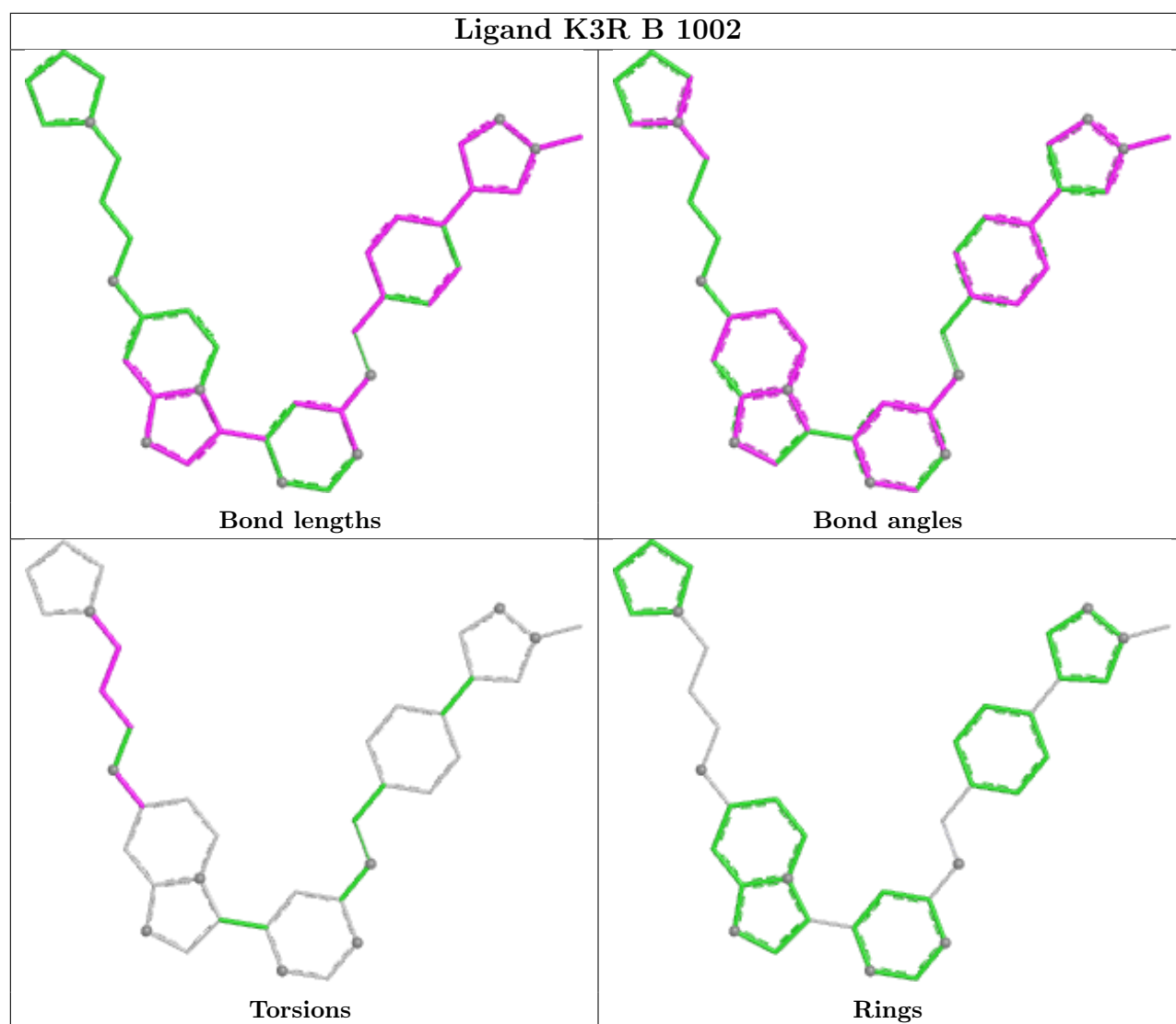
There are no ring outliers.

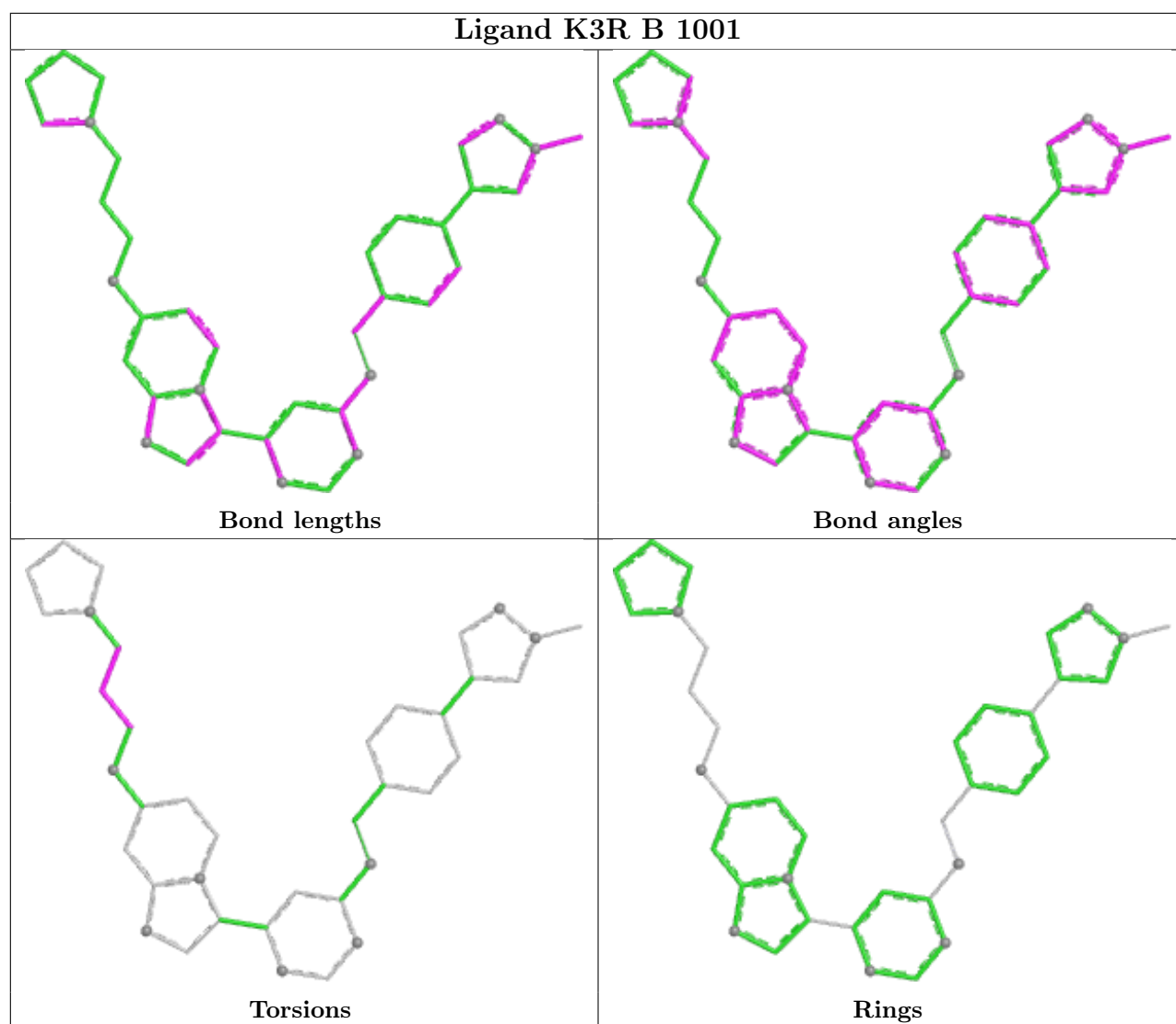
No monomer is involved in short contacts.

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/327 (84%)	0.49	14 (5%) 33 32	35, 59, 94, 125	2 (0%)
1	B	285/327 (87%)	0.38	17 (5%) 27 26	25, 52, 79, 121	7 (2%)
All	All	562/654 (85%)	0.44	31 (5%) 30 29	25, 55, 90, 125	9 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	601	GLY	4.3
1	B	763	PHE	3.5
1	A	597	ALA	3.5
1	B	646	TYR	3.1
1	B	614	SER	2.9
1	B	693	LYS	2.9
1	A	565	GLY	2.9
1	B	599	ALA	2.6
1	B	829	ALA	2.6
1	B	613	LYS	2.6
1	A	811	PHE	2.5
1	B	612	ILE	2.5
1	B	630	HIS	2.4
1	A	789	ILE	2.3
1	B	570	TYR	2.3
1	B	608	ALA	2.3
1	B	565	GLY	2.3
1	B	912	ASP	2.3
1	B	615	ASP	2.3
1	A	900	TYR	2.3
1	A	763	PHE	2.2
1	A	810	ASP	2.2
1	B	616	ALA	2.2
1	A	570	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	630	HIS	2.2
1	B	688	GLU	2.2
1	A	829	ALA	2.1
1	B	872	GLY	2.1
1	A	615	ASP	2.1
1	A	687	ASP	2.1
1	A	618	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

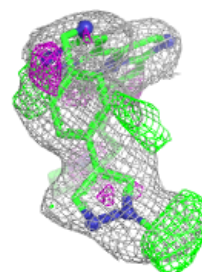
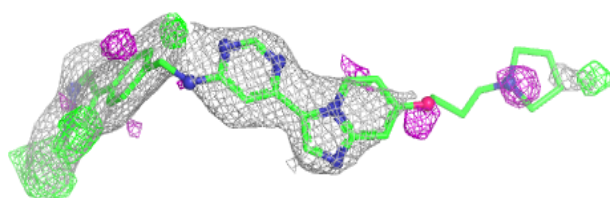
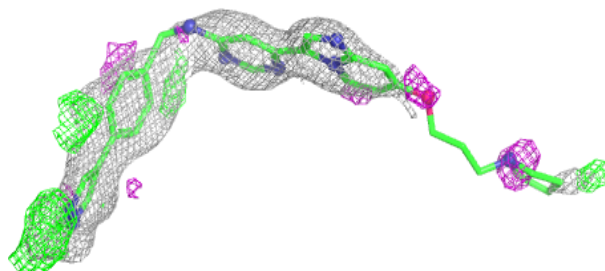
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K3R	B	1002	38/38	0.63	0.19	60,75,113,115	0
3	CL	B	1004	1/1	0.77	0.12	98,98,98,98	0
2	K3R	B	1003	38/38	0.79	0.14	55,82,130,133	0
3	CL	A	1002	1/1	0.87	0.10	82,82,82,82	0
2	K3R	A	1001	38/38	0.87	0.13	48,57,88,92	0
2	K3R	B	1001	38/38	0.92	0.11	34,44,69,74	0

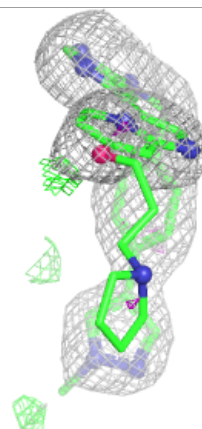
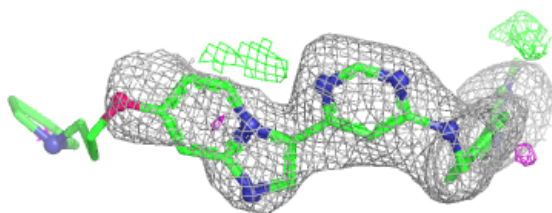
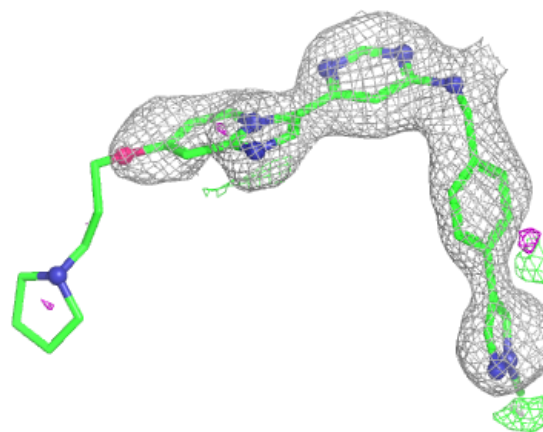
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around K3R B 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

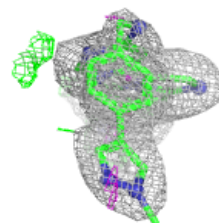
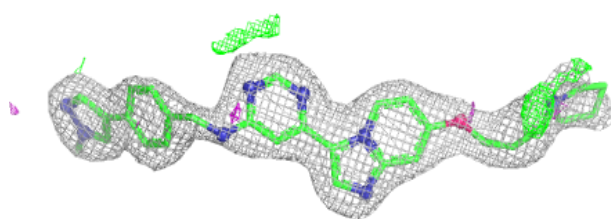
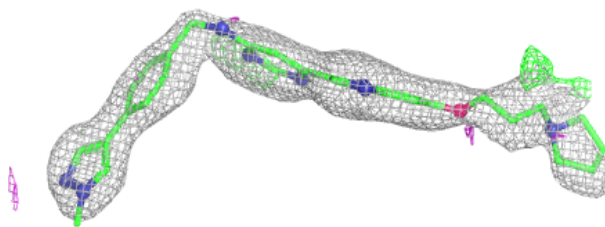
**Electron density around K3R B 1003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

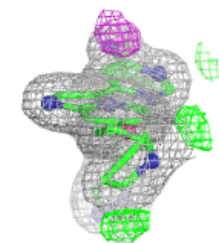
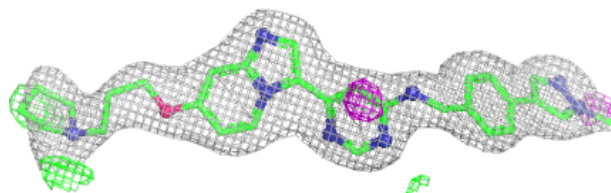
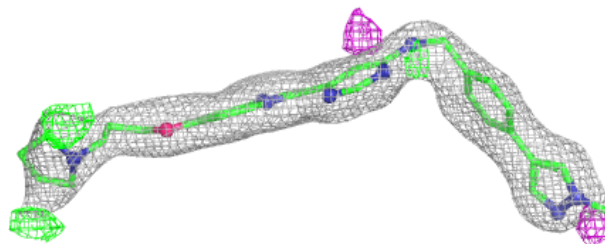


Electron density around K3R A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around K3R B 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.