



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:11 PM UTC

PDB ID : 6EJ4 / pdb_00006ej4
Title : DYRK1A in complex with XMD7-112
Authors : Rothweiler, U.
Deposited on : 2017-09-20
Resolution : 2.88 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

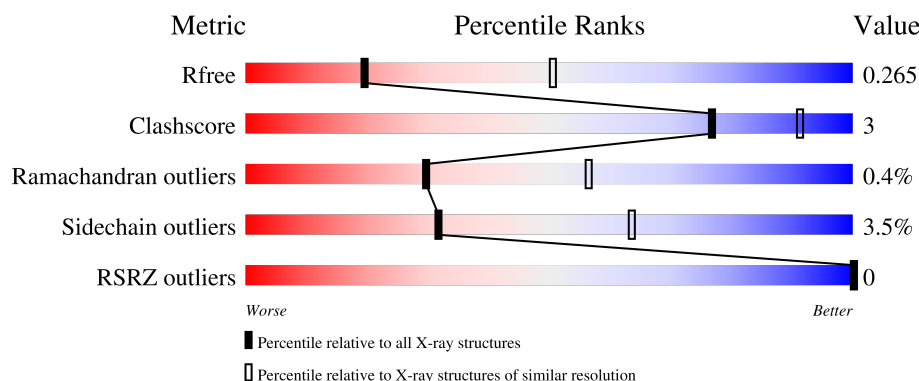
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	368	
1	B	368	
1	C	368	
1	D	368	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11022 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.

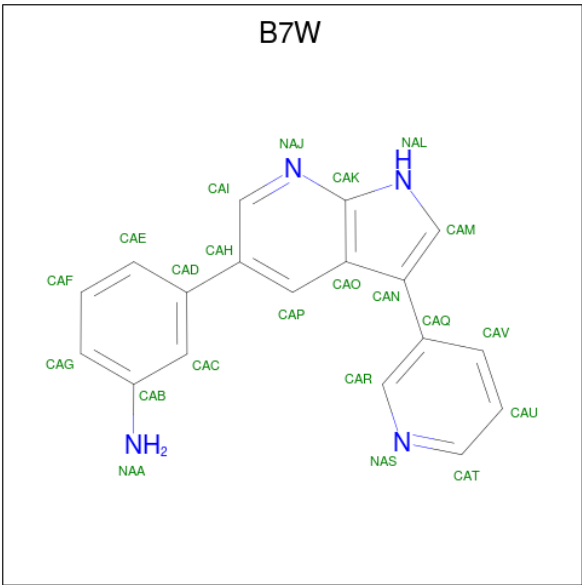
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	P	S	0	0	0
			2800	1802	479	501	1	17			
1	B	338	Total	C	N	O	P	S	0	0	0
			2739	1763	468	491	1	16			
1	C	332	Total	C	N	O	P	S	0	0	0
			2646	1697	448	483	1	17			
1	D	331	Total	C	N	O	P	S	0	0	0
			2693	1741	450	484	1	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	expression tag	UNP Q13627
A	124	ALA	-	expression tag	UNP Q13627
A	125	SER	-	expression tag	UNP Q13627
B	123	GLY	-	expression tag	UNP Q13627
B	124	ALA	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
C	123	GLY	-	expression tag	UNP Q13627
C	124	ALA	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
D	123	GLY	-	expression tag	UNP Q13627
D	124	ALA	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627

- Molecule 2 is 3-(3-pyridin-3-yl)-1 {H}-pyrrolo[2,3-b]pyridin-5-yl)aniline (CCD ID: B7W) (formula: C₁₈H₁₄N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			22	18	4		
2	B	1	Total	C	N	0	0
			22	18	4		
2	C	1	Total	C	N	0	0
			22	18	4		
2	D	1	Total	C	N	0	0
			22	18	4		

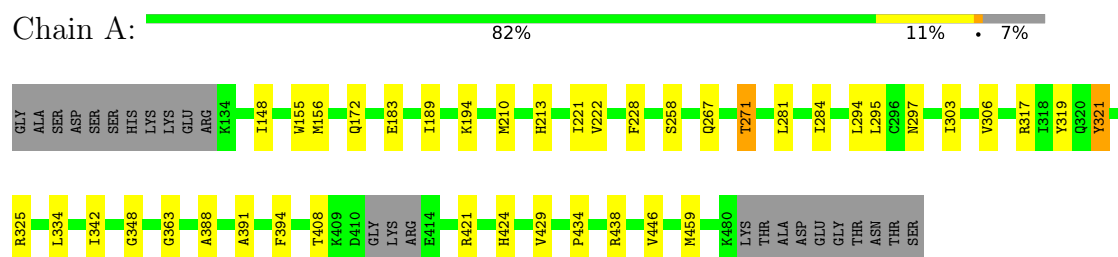
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	13	Total	O	0	0
			13	13		
3	C	14	Total	O	0	0
			14	14		
3	D	11	Total	O	0	0
			11	11		

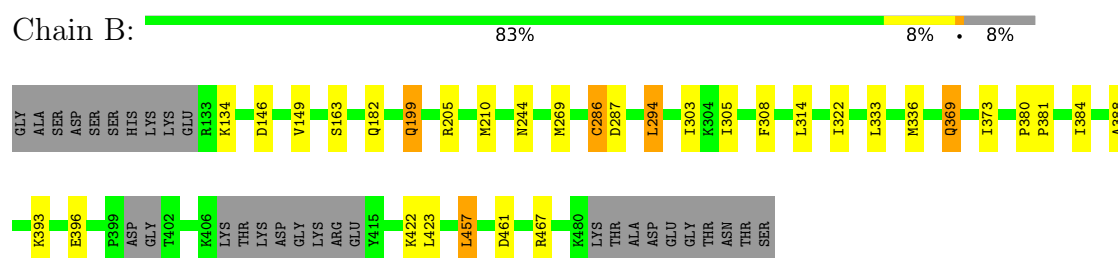
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

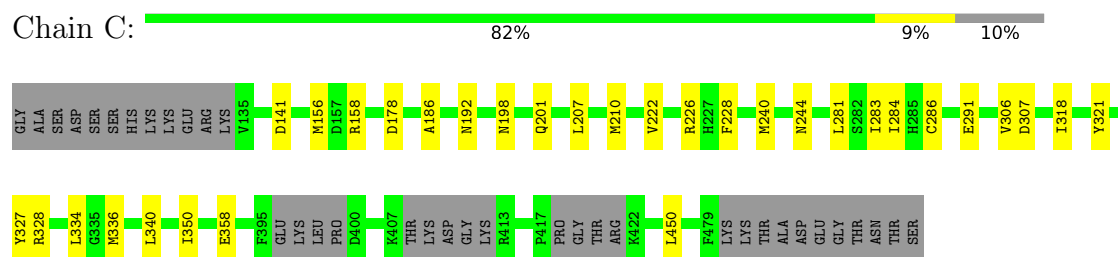
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



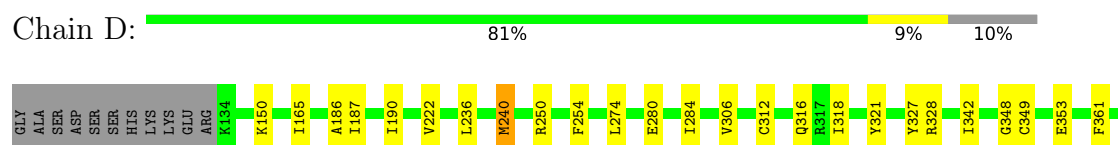
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

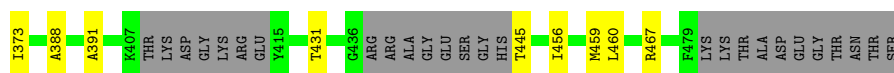


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.15Å 88.19Å 229.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.88 48.30 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.30-2.88) 98.9 (48.30-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.220 , 0.270 0.219 , 0.265	Depositor DCC
R_{free} test set	2020 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 18.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.190 for k,h,-l	Xtriage
Reported twinning fraction	0.737 for H, K, L 0.263 for K, H, -L	Depositor
Outliers	0 of 40868 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11022	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, B7W

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	0.65	0/2848	0.88	1/3842 (0.0%)
1	B	0.60	0/2785	0.81	0/3759
1	C	0.62	0/2688	0.86	1/3638 (0.0%)
1	D	0.60	0/2739	0.84	0/3699
All	All	0.62	0/11060	0.85	2/14938 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ARG	N-CA-C	7.36	124.02	114.75
1	A	363	GLY	N-CA-C	5.30	117.57	111.36

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	2800	0	2787	18	0
1	B	2739	0	2710	15	0
1	C	2646	0	2544	13	0
1	D	2693	0	2672	18	0
2	A	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	22	0	0	0	0
2	C	22	0	0	0	0
2	D	22	0	0	1	0
3	A	18	0	0	0	0
3	B	13	0	0	0	0
3	C	14	0	0	0	0
3	D	11	0	0	0	0
All	All	11022	0	10713	62	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 3.

All (62) 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:C:321:PTR:O3P	1:C:328:ARG:NH2	2.06	0.88
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.79	0.63
1:B:286:CYS:SG	1:B:322:ILE:HD11	2.38	0.63
1:D:186:ALA:HB2	1:D:240:MET:HE3	1.87	0.57
1:B:269:MET:HE3	1:B:303:ILE:HD12	1.88	0.55
1:C:207:LEU:HD23	1:C:210:MET:CE	2.36	0.55
1:D:321:PTR:P	1:D:328:ARG:HH12	2.30	0.55
1:C:334:LEU:HD22	1:C:336:MET:CG	2.38	0.54
1:A:321:PTR:O2P	1:A:325:ARG:NH1	2.41	0.54
1:A:284:ILE:HG21	1:A:342:ILE:HD11	1.90	0.53
1:C:222:VAL:HG21	1:C:306:VAL:HG13	1.89	0.53
1:B:269:MET:HE1	1:B:305:ILE:HG13	1.91	0.52
1:A:295:LEU:HD23	1:A:303:ILE:HG22	1.92	0.51
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.91	0.51
1:B:423:LEU:HD23	1:B:457:LEU:HD22	1.93	0.51
1:B:269:MET:HE1	1:B:305:ILE:CG1	2.42	0.49
1:B:336:MET:HE3	1:B:384:ILE:HG23	1.94	0.49
1:B:244:ASN:HB3	1:B:294:LEU:HD22	1.94	0.49
1:A:213:HIS:CE1	1:A:281:LEU:HD21	2.49	0.48
1:B:369:GLN:HE22	1:B:373:ILE:HD11	1.79	0.48
1:B:461:ASP:HB3	1:B:467:ARG:HG2	1.96	0.47
1:C:207:LEU:HD23	1:C:210:MET:HE3	1.96	0.47
1:C:156:MET:HE1	1:C:228:PHE:CD1	2.49	0.47
1:D:361:PHE:CE1	1:D:373:ILE:HA	2.49	0.46
1:B:210:MET:HE1	1:B:308:PHE:CE2	2.50	0.46
1:C:178:ASP:OD2	1:C:226:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG21	1:A:306:VAL:CG1	2.46	0.46
1:A:334:LEU:HB3	1:A:388:ALA:HB1	1.99	0.45
1:D:284:ILE:HG21	1:D:342:ILE:HD11	1.99	0.45
1:B:423:LEU:HD23	1:B:457:LEU:CD2	2.47	0.45
1:A:348:GLY:N	1:A:459:MET:HE2	2.31	0.45
1:D:327:TYR:OH	1:D:353:GLU:OE1	2.22	0.44
1:D:222:VAL:CG1	1:D:306:VAL:HG12	2.47	0.44
1:D:459:MET:O	1:D:467:ARG:HD2	2.18	0.44
1:C:186:ALA:HB2	1:C:240:MET:CE	2.48	0.44
1:A:210:MET:HE2	1:A:221:ILE:HG21	1.99	0.43
1:A:267:GLN:O	1:A:271:THR:HG23	2.17	0.43
1:D:222:VAL:HG11	1:D:306:VAL:HG12	1.99	0.43
1:D:240:MET:HE2	2:D:501:B7W:CAI	2.47	0.43
1:D:250:ARG:HG2	1:D:254:PHE:CZ	2.52	0.43
1:D:165:ILE:HD11	1:D:240:MET:HE1	2.00	0.43
1:A:429:VAL:O	1:A:446:VAL:HG22	2.17	0.43
1:B:149:VAL:O	1:B:149:VAL:HG23	2.18	0.43
1:A:348:GLY:CA	1:A:459:MET:HE2	2.49	0.43
1:A:317:ARG:NH1	1:D:280:GLU:OE1	2.52	0.43
1:C:192:ASN:HD21	1:D:321:PTR:CE1	2.31	0.42
1:D:190:ILE:HD13	1:D:236:LEU:HD13	2.01	0.42
1:A:156:MET:HE1	1:A:228:PHE:CE1	2.54	0.42
1:A:222:VAL:HG21	1:A:306:VAL:HG13	2.00	0.42
1:A:155:TRP:HB3	1:A:156:MET:HE2	2.01	0.42
1:C:284:ILE:HG22	1:C:340:LEU:HA	2.00	0.42
1:B:336:MET:HE1	1:B:388:ALA:HB2	2.01	0.42
1:B:199:GLN:HE21	1:B:199:GLN:HB3	1.72	0.41
1:B:380:PRO:HA	1:B:381:PRO:HD3	1.99	0.41
1:D:348:GLY:O	1:D:349:CYS:C	2.63	0.41
1:D:165:ILE:CD1	1:D:240:MET:HE1	2.50	0.41
1:A:172:GLN:O	1:A:189:ILE:N	2.52	0.41
1:A:424:HIS:CD2	1:A:429:VAL:HG22	2.56	0.40
1:D:456:ILE:HG22	1:D:460:LEU:HD12	2.03	0.40
1:C:327:TYR:CE1	1:C:350:ILE:HG22	2.56	0.40
1:C:244:ASN:ND2	1:C:291:GLU:OE1	2.54	0.40
1:C:281:LEU:C	1:C:283:ILE:HD12	2.46	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	339/368 (92%)	309 (91%)	29 (9%)	1 (0%)	36	62
1	B	331/368 (90%)	304 (92%)	25 (8%)	2 (1%)	21	48
1	C	323/368 (88%)	293 (91%)	29 (9%)	1 (0%)	36	62
1	D	324/368 (88%)	299 (92%)	24 (7%)	1 (0%)	36	62
All	All	1317/1472 (90%)	1205 (92%)	107 (8%)	5 (0%)	30	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	LYS
1	D	316	GLN
1	A	434	PRO
1	C	307	ASP
1	B	287	ASP

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	300/324 (93%)	288 (96%)	12 (4%)	28	60
1	B	292/324 (90%)	278 (95%)	14 (5%)	23	53
1	C	276/324 (85%)	269 (98%)	7 (2%)	42	72
1	D	290/324 (90%)	282 (97%)	8 (3%)	38	70
All	All	1158/1296 (89%)	1117 (96%)	41 (4%)	32	63

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ILE
1	A	183	GLU
1	A	194	LYS
1	A	258	SER
1	A	271	THR
1	A	294	LEU
1	A	297	ASN
1	A	319	TYR
1	A	394	PHE
1	A	408	THR
1	A	421	ARG
1	A	438	ARG
1	B	146	ASP
1	B	163	SER
1	B	182	GLN
1	B	199	GLN
1	B	205	ARG
1	B	286	CYS
1	B	294	LEU
1	B	314	LEU
1	B	333	LEU
1	B	369	GLN
1	B	393	LYS
1	B	396	GLU
1	B	422	LYS
1	B	457	LEU
1	C	141	ASP
1	C	198	ASN
1	C	201	GLN
1	C	286	CYS
1	C	318	ILE
1	C	358	GLU
1	C	450	LEU
1	D	150	LYS
1	D	187	ILE
1	D	240	MET
1	D	274	LEU
1	D	312	CYS
1	D	318	ILE
1	D	431	THR
1	D	445	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	198	ASN
1	A	201	GLN
1	A	404	ASN
1	A	425	ASN
1	B	182	GLN
1	B	199	GLN
1	B	268	GLN
1	B	297	ASN
1	B	369	GLN
1	C	137	ASN
1	C	182	GLN
1	C	192	ASN
1	C	211	ASN
1	C	232	ASN
1	D	192	ASN
1	D	201	GLN
1	D	268	GLN
1	D	316	GLN
1	D	469	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	C	321	1	15,16,17	0.85	0	17,22,24	1.04	0
1	PTR	B	321	1	15,16,17	0.83	0	17,22,24	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PTR	A	321	1	15,16,17	0.91	0	17,22,24	1.05	1 (5%)
1	PTR	D	321	1	15,16,17	0.76	0	17,22,24	0.93	0

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
1	PTR	C	321	1	-	2/10/11/13	0/1/1/1
1	PTR	B	321	1	-	0/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1
1	PTR	D	321	1	-	1/10/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	321	PTR	OH-P-O1P	-2.53	101.03	109.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	321	PTR	O-C-CA-CB
1	C	321	PTR	CZ-OH-P-O3P
1	D	321	PTR	CZ-OH-P-O2P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	321	PTR	1	0
1	A	321	PTR	1	0
1	D	321	PTR	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	B7W	D	501	-	25,25,25	3.10	11 (44%)	34,35,35	1.86	8 (23%)
2	B7W	C	501	-	25,25,25	3.09	10 (40%)	34,35,35	1.84	7 (20%)
2	B7W	B	501	-	25,25,25	3.12	11 (44%)	34,35,35	1.75	7 (20%)
2	B7W	A	501	-	25,25,25	3.26	11 (44%)	34,35,35	2.03	8 (23%)

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	B7W	D	501	-	-	0/8/8/8	0/4/4/4
2	B7W	C	501	-	-	0/8/8/8	0/4/4/4
2	B7W	B	501	-	-	0/8/8/8	0/4/4/4
2	B7W	A	501	-	-	0/8/8/8	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	B7W	CAQ-CAN	-10.43	1.34	1.49
2	B	501	B7W	CAQ-CAN	-9.73	1.35	1.49
2	C	501	B7W	CAQ-CAN	-9.69	1.35	1.49
2	D	501	B7W	CAQ-CAN	-9.67	1.35	1.49
2	A	501	B7W	CAO-CAK	-6.26	1.34	1.41
2	D	501	B7W	CAO-CAK	-5.97	1.35	1.41
2	A	501	B7W	CAO-CAN	-5.96	1.34	1.47
2	B	501	B7W	CAO-CAK	-5.90	1.35	1.41
2	B	501	B7W	CAO-CAN	-5.79	1.34	1.47
2	D	501	B7W	CAO-CAN	-5.68	1.34	1.47
2	C	501	B7W	CAO-CAN	-5.67	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	B7W	CAO-CAK	-5.66	1.35	1.41
2	A	501	B7W	CAM-CAN	-4.43	1.33	1.37
2	B	501	B7W	CAM-CAN	-3.96	1.33	1.37
2	C	501	B7W	CAM-CAN	-3.92	1.33	1.37
2	D	501	B7W	CAM-CAN	-3.90	1.33	1.37
2	B	501	B7W	CAH-CAD	-3.72	1.40	1.49
2	C	501	B7W	CAH-CAD	-3.63	1.40	1.49
2	C	501	B7W	CAR-NAS	3.51	1.41	1.34
2	A	501	B7W	CAH-CAD	-3.45	1.40	1.49
2	D	501	B7W	CAR-NAS	3.39	1.41	1.34
2	B	501	B7W	CAR-NAS	3.37	1.41	1.34
2	D	501	B7W	CAH-CAD	-3.35	1.41	1.49
2	A	501	B7W	CAR-NAS	3.28	1.41	1.34
2	A	501	B7W	CAI-NAJ	3.06	1.40	1.34
2	C	501	B7W	CAI-NAJ	3.04	1.40	1.34
2	B	501	B7W	CAI-NAJ	3.03	1.40	1.34
2	B	501	B7W	CAP-CAO	-2.99	1.35	1.39
2	A	501	B7W	CAP-CAO	-2.98	1.35	1.39
2	C	501	B7W	CAP-CAO	-2.96	1.35	1.39
2	D	501	B7W	CAP-CAO	-2.96	1.35	1.39
2	D	501	B7W	CAI-NAJ	2.93	1.40	1.34
2	A	501	B7W	CAT-NAS	2.61	1.41	1.33
2	D	501	B7W	CAT-NAS	2.57	1.41	1.33
2	D	501	B7W	CAM-NAL	-2.51	1.33	1.37
2	C	501	B7W	CAT-NAS	2.49	1.40	1.33
2	A	501	B7W	CAM-NAL	-2.48	1.33	1.37
2	C	501	B7W	CAM-NAL	-2.43	1.33	1.37
2	B	501	B7W	CAT-NAS	2.39	1.40	1.33
2	B	501	B7W	CAM-NAL	-2.32	1.33	1.37
2	B	501	B7W	CAK-NAL	-2.28	1.33	1.36
2	D	501	B7W	CAK-NAL	-2.11	1.33	1.36
2	A	501	B7W	CAK-NAL	-2.08	1.33	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	B7W	CAO-CAN-CAM	5.96	109.72	105.98
2	D	501	B7W	CAO-CAN-CAM	4.97	109.09	105.98
2	A	501	B7W	CAN-CAM-NAL	-4.95	107.26	110.46
2	C	501	B7W	CAO-CAN-CAM	4.94	109.08	105.98
2	B	501	B7W	CAO-CAN-CAM	4.50	108.81	105.98
2	A	501	B7W	CAO-CAK-NAJ	-4.44	120.93	126.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	B7W	CAP-CAO-CAK	4.43	120.91	117.64
2	D	501	B7W	CAO-CAK-NAJ	-4.38	121.00	126.31
2	C	501	B7W	CAO-CAK-NAJ	-4.33	121.06	126.31
2	D	501	B7W	CAN-CAM-NAL	-4.23	107.73	110.46
2	B	501	B7W	CAO-CAK-NAJ	-4.16	121.27	126.31
2	C	501	B7W	CAN-CAM-NAL	-4.12	107.80	110.46
2	B	501	B7W	CAN-CAM-NAL	-4.02	107.87	110.46
2	C	501	B7W	CAP-CAO-CAK	3.90	120.52	117.64
2	D	501	B7W	CAP-CAO-CAK	3.80	120.45	117.64
2	B	501	B7W	CAP-CAO-CAK	3.52	120.24	117.64
2	B	501	B7W	CAH-CAI-NAJ	-3.45	118.80	124.28
2	C	501	B7W	CAH-CAI-NAJ	-3.34	118.97	124.28
2	D	501	B7W	CAH-CAI-NAJ	-3.15	119.28	124.28
2	A	501	B7W	CAH-CAI-NAJ	-3.00	119.51	124.28
2	A	501	B7W	CAQ-CAR-NAS	-2.40	119.93	123.50
2	A	501	B7W	NAL-CAK-NAJ	2.24	130.32	126.69
2	D	501	B7W	CAQ-CAR-NAS	-2.24	120.17	123.50
2	C	501	B7W	NAL-CAK-NAJ	2.23	130.30	126.69
2	D	501	B7W	CAI-NAJ-CAK	2.19	120.48	116.19
2	B	501	B7W	CAI-NAJ-CAK	2.18	120.47	116.19
2	C	501	B7W	CAI-NAJ-CAK	2.12	120.34	116.19
2	D	501	B7W	NAL-CAK-NAJ	2.12	130.12	126.69
2	B	501	B7W	NAL-CAK-NAJ	2.07	130.04	126.69
2	A	501	B7W	CAI-NAJ-CAK	2.04	120.19	116.19

There are no chirality outliers.

There are no torsion outliers.

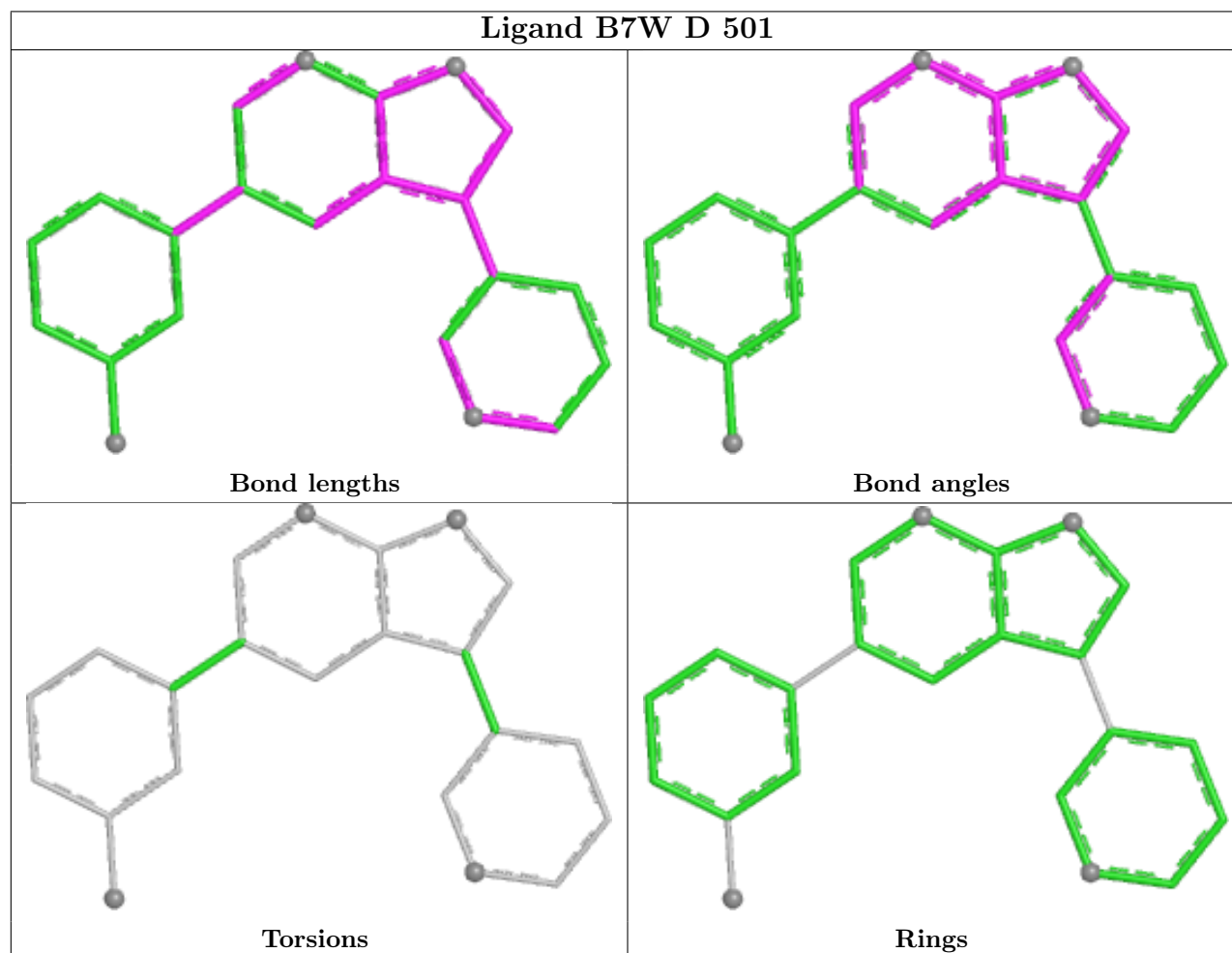
There are no ring outliers.

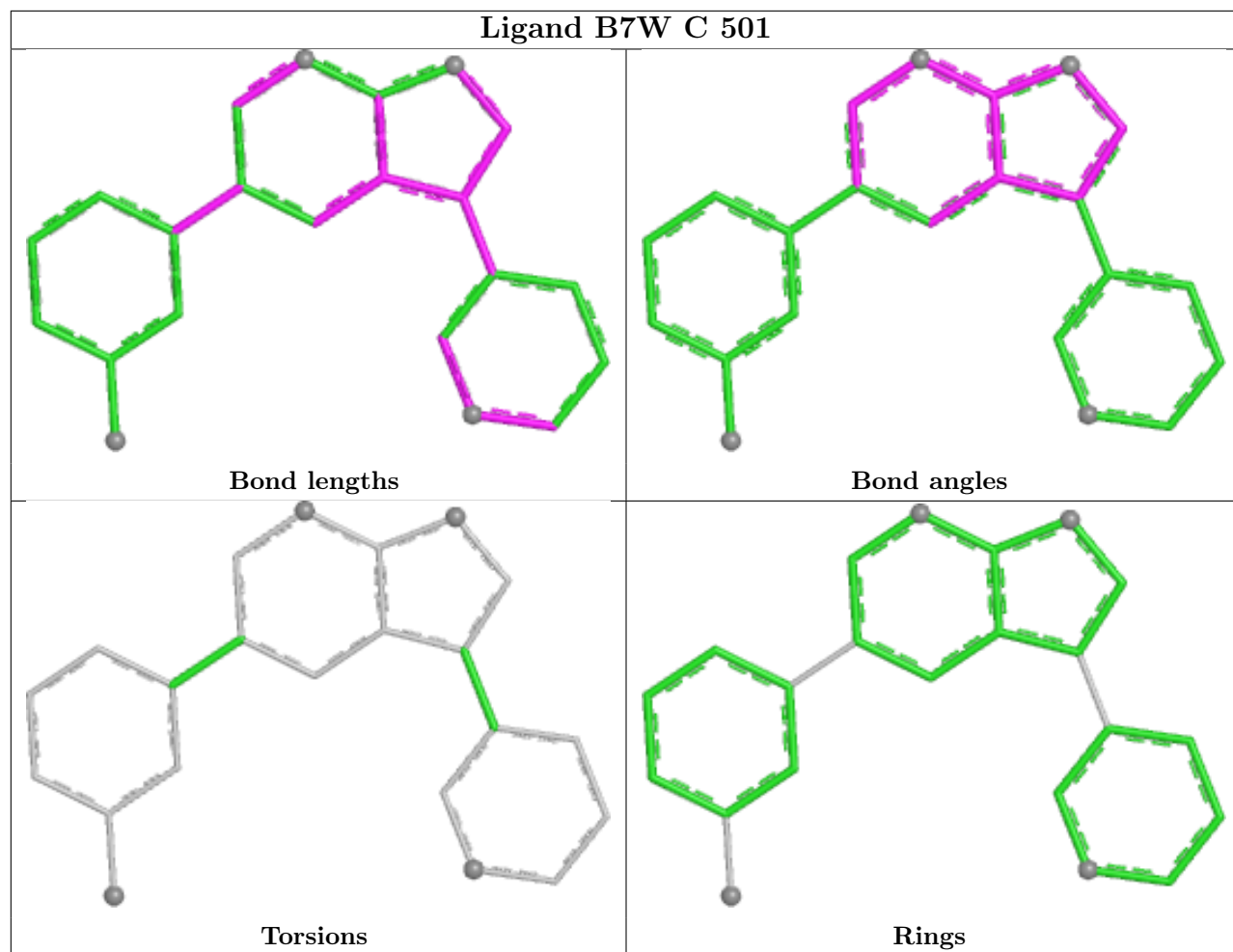
1 monomer is involved in 1 short contact:

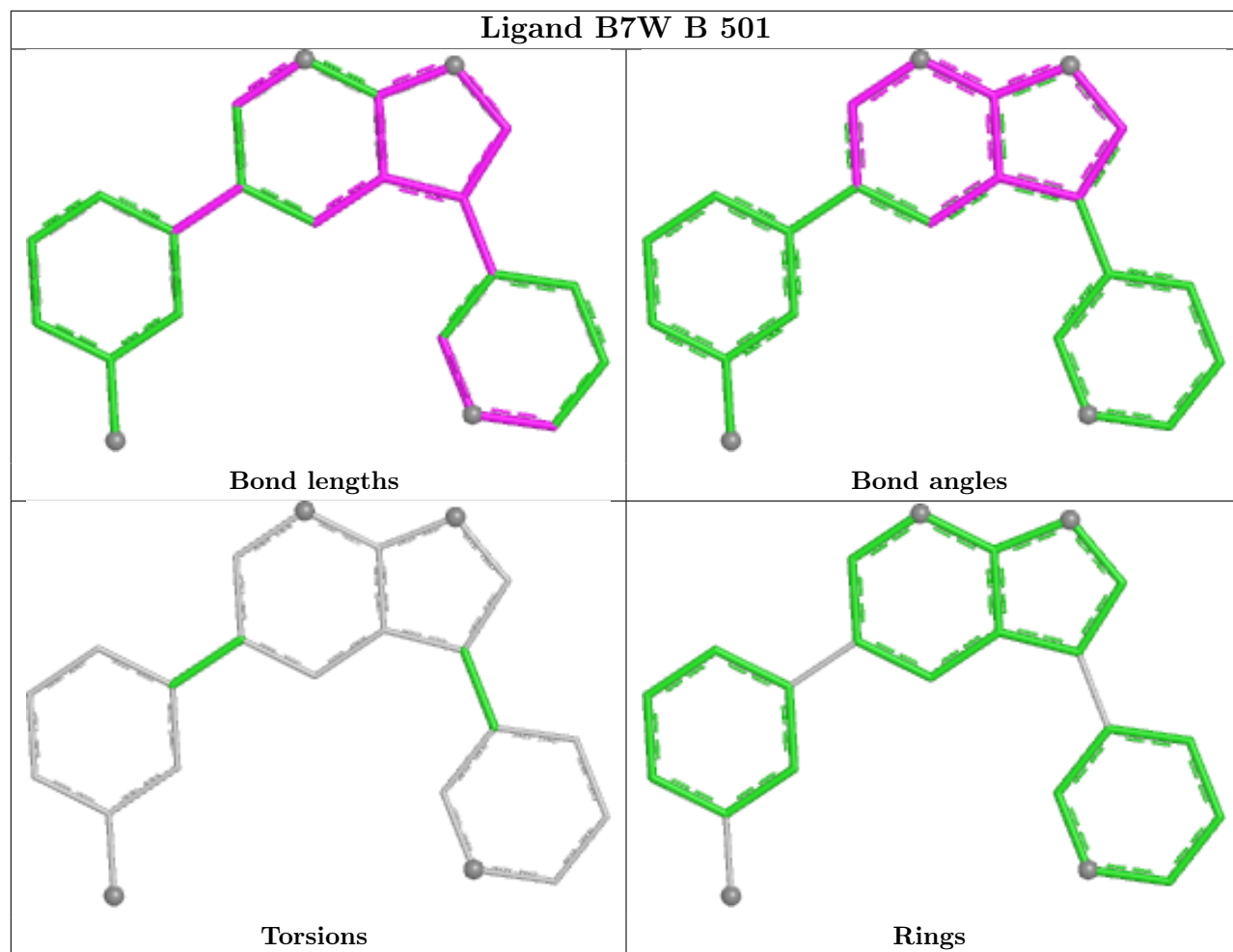
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	B7W	1	0

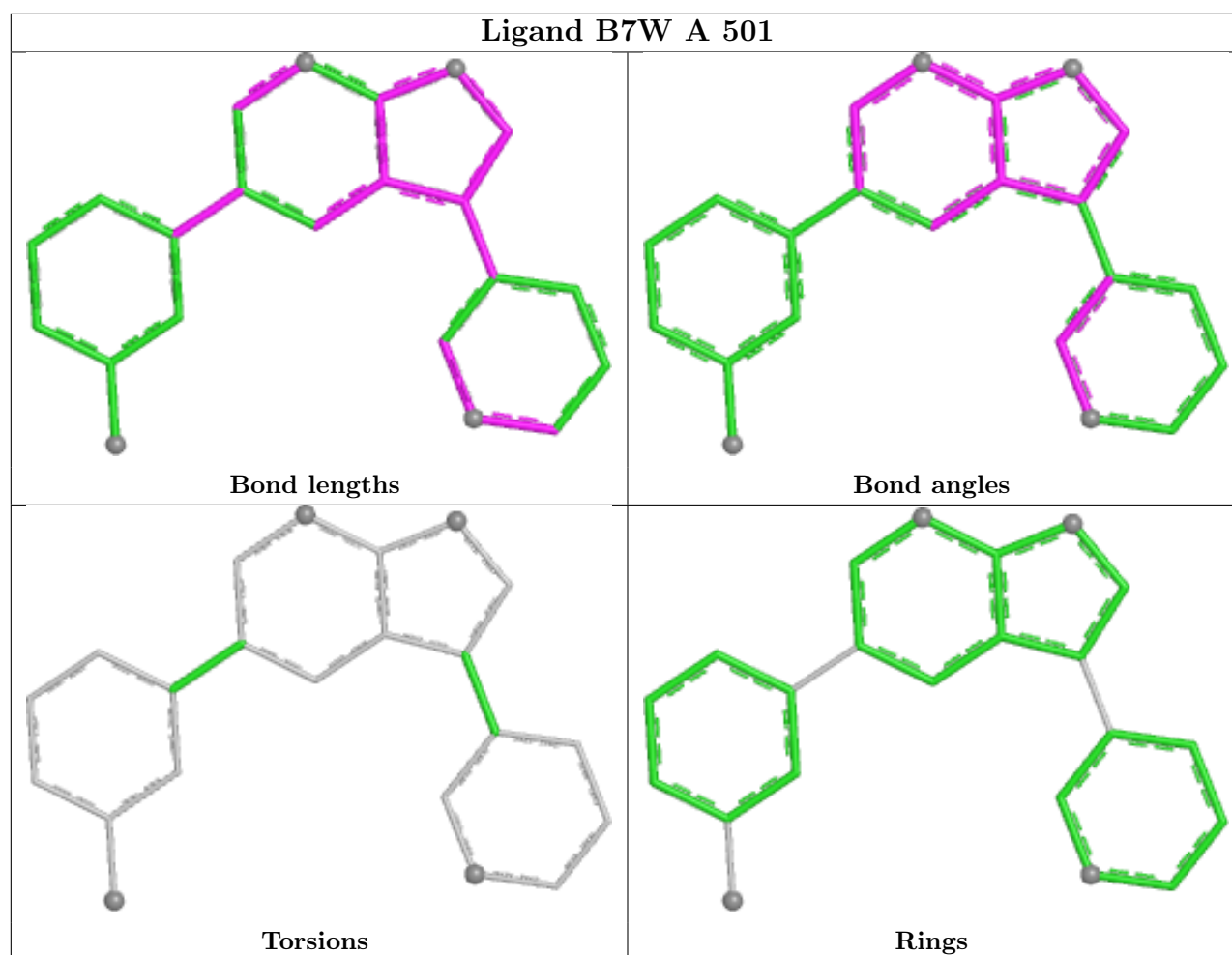
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	343/368 (93%)	-1.01	0 100 100	28, 44, 68, 86	0
1	B	337/368 (91%)	-0.55	0 100 100	42, 68, 108, 117	0
1	C	331/368 (89%)	-0.57	0 100 100	35, 63, 101, 106	0
1	D	330/368 (89%)	-0.76	0 100 100	33, 56, 80, 96	0
All	All	1341/1472 (91%)	-0.72	0 100 100	28, 56, 97, 117	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PTR	B	321	16/17	0.98	0.07	76,81,82,83	0
1	PTR	C	321	16/17	0.98	0.06	65,68,69,69	0
1	PTR	A	321	16/17	0.99	0.06	40,42,42,42	0
1	PTR	D	321	16/17	0.99	0.05	37,39,40,41	0

6.3 Carbohydrates [i](#)

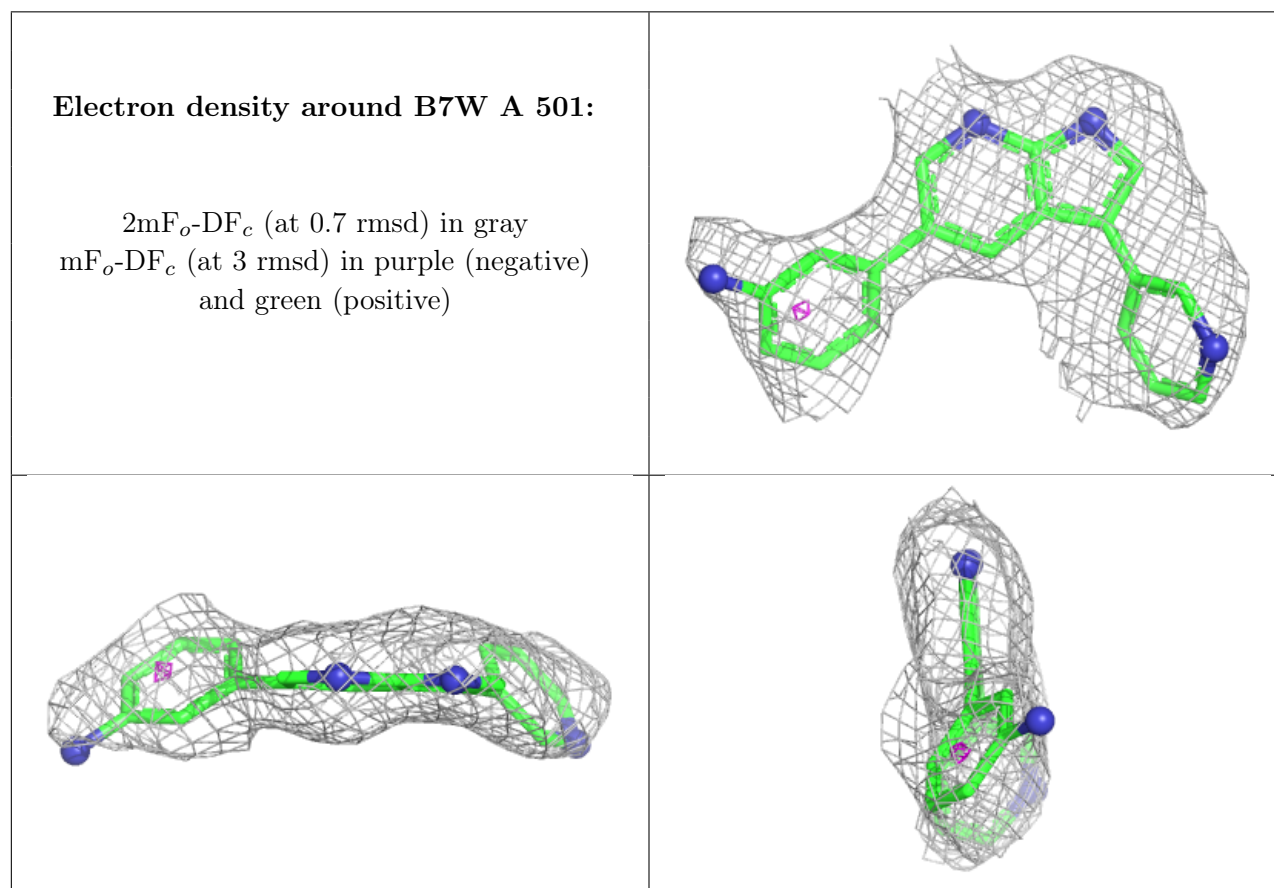
There are no oligosaccharides in this entry.

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.

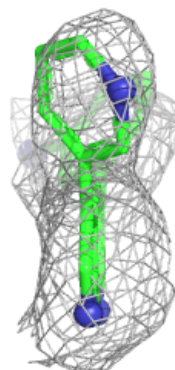
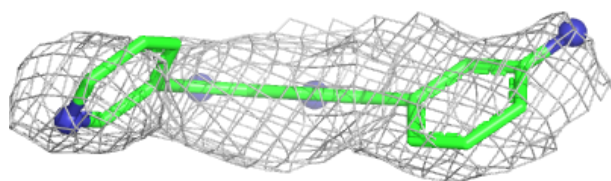
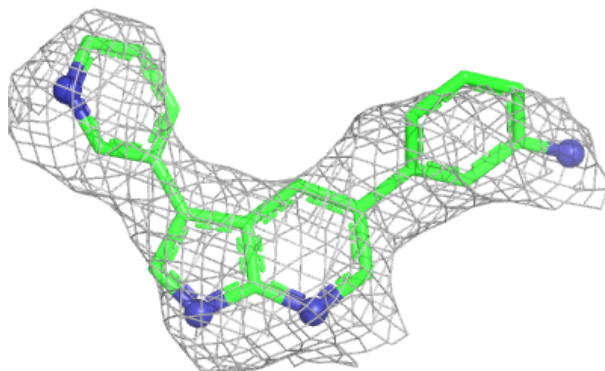
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B7W	A	501	22/22	0.98	0.07	53,55,62,63	0
2	B7W	B	501	22/22	0.98	0.07	56,57,60,60	0
2	B7W	D	501	22/22	0.98	0.07	46,48,52,55	0
2	B7W	C	501	22/22	0.99	0.06	51,53,55,56	0

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.

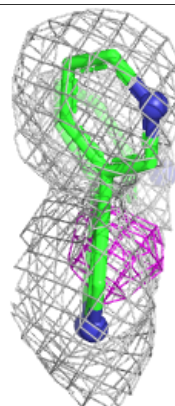
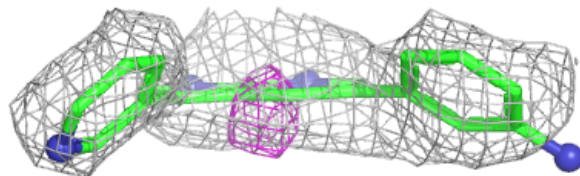
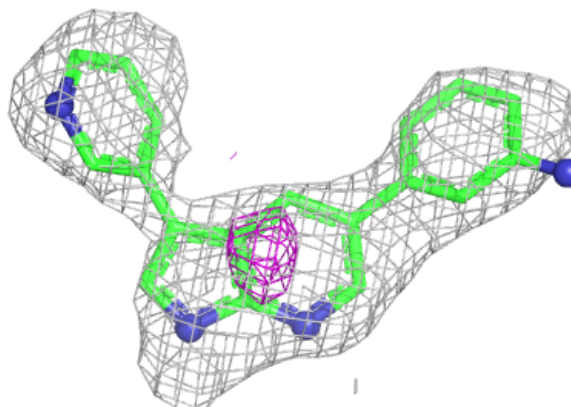


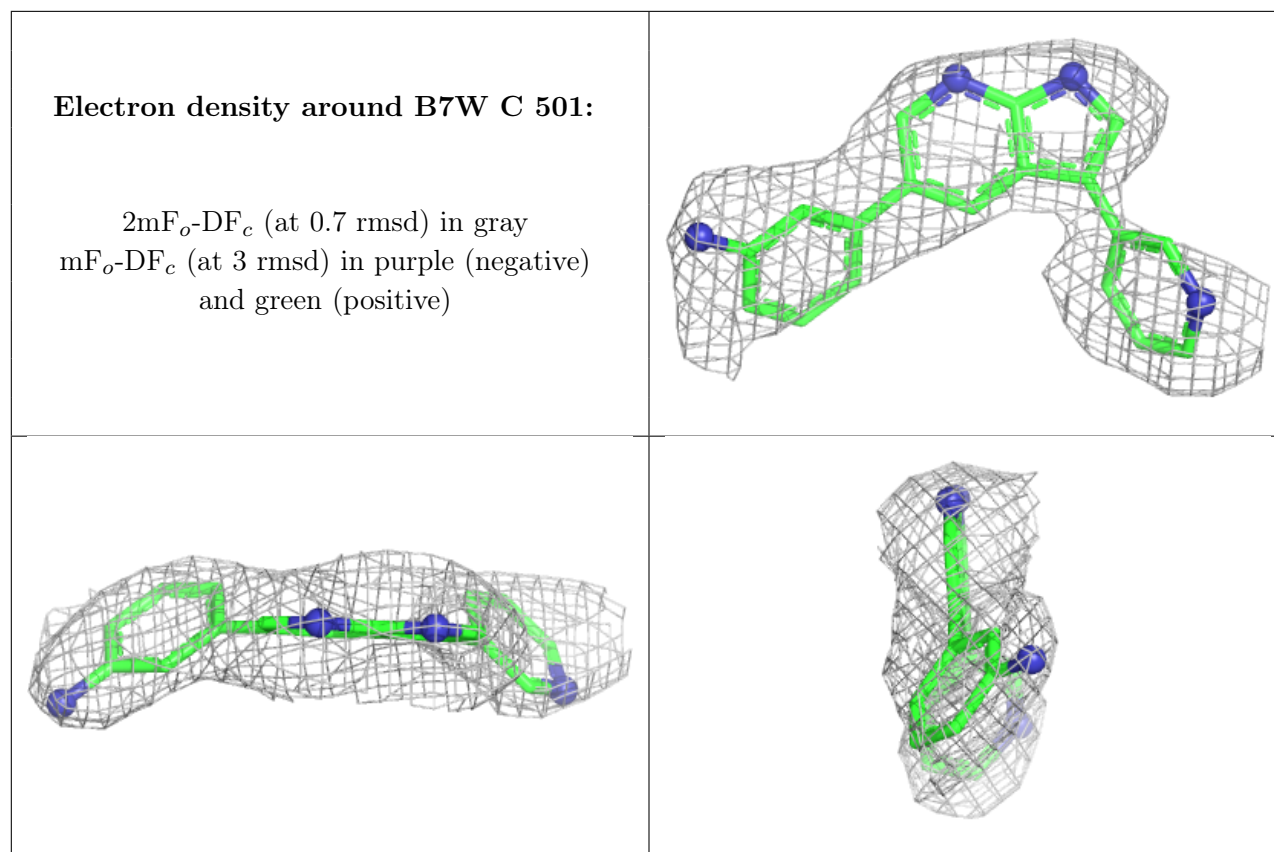
Electron density around B7W B 501:

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

**Electron density around B7W D 501:**

$2mF_o-DF_c$ (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.