



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:52 PM UTC

PDB ID : 9R9G / pdb_00009r9g
Title : IRAK4 in complex with inhibitor
Authors : Xue, Y.; Terstiege, I.; Aagaard, A.
Deposited on : 2025-05-20
Resolution : 1.88 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

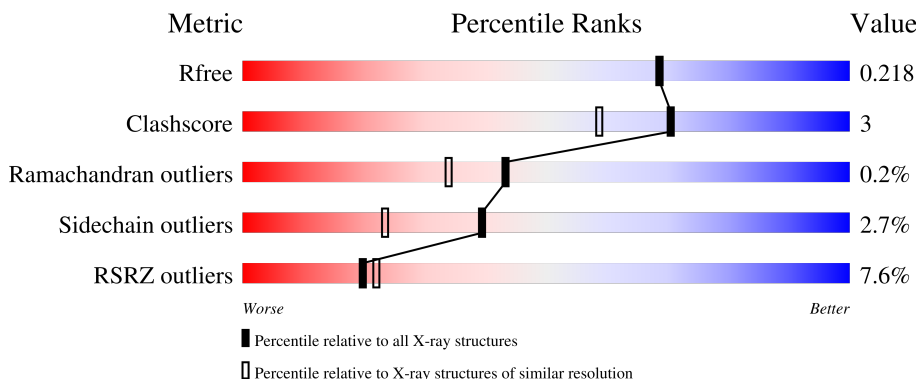
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	308	8% 84% 7% 7%
1	B	308	7% 85% 7% 7%
1	C	308	6% 84% 8% 7%
1	D	308	6% 85% 7% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10098 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.

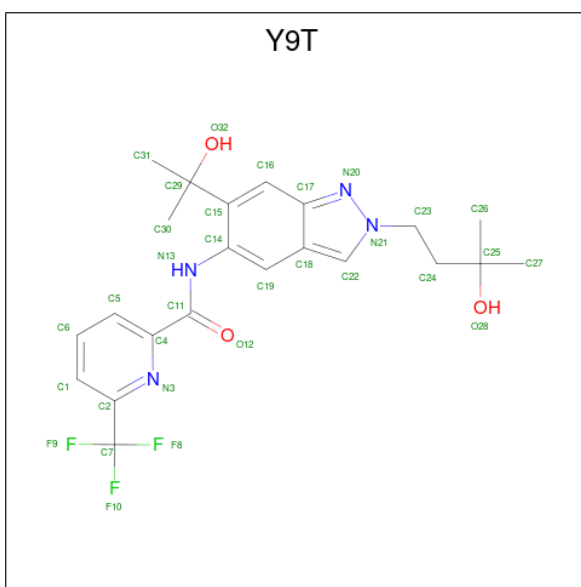
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	0
			2260	1417	381	446	2	14			
1	B	286	Total	C	N	O	P	S	0	0	0
			2260	1417	381	446	2	14			
1	C	286	Total	C	N	O	P	S	0	0	0
			2261	1419	381	445	2	14			
1	D	286	Total	C	N	O	P	S	0	0	0
			2260	1418	380	446	2	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3
C	153	GLY	-	expression tag	UNP Q9NWZ3
D	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is N-[2-(3-hydroxy-3-methylbutyl)-6-(2-hydroxypropan-2-yl)-2H-indazol-5-yl]-6-(trifluoromethyl)pyridine-2-carboxamide (CCD ID: Y9T) (formula: C₂₂H₂₅F₃N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 32	C 22	F 3	N 4	O 3	0	0
2	B	1	Total 32	C 22	F 3	N 4	O 3	0	0
2	C	1	Total 32	C 22	F 3	N 4	O 3	0	0
2	D	1	Total 32	C 22	F 3	N 4	O 3	0	0

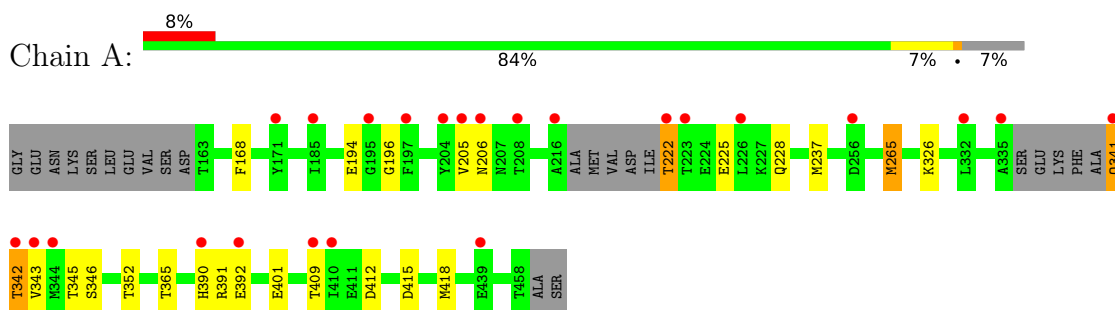
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total	O	0	0
			196	196		
3	B	206	Total	O	0	0
			206	206		
3	C	255	Total	O	0	0
			255	255		
3	D	272	Total	O	0	0
			272	272		

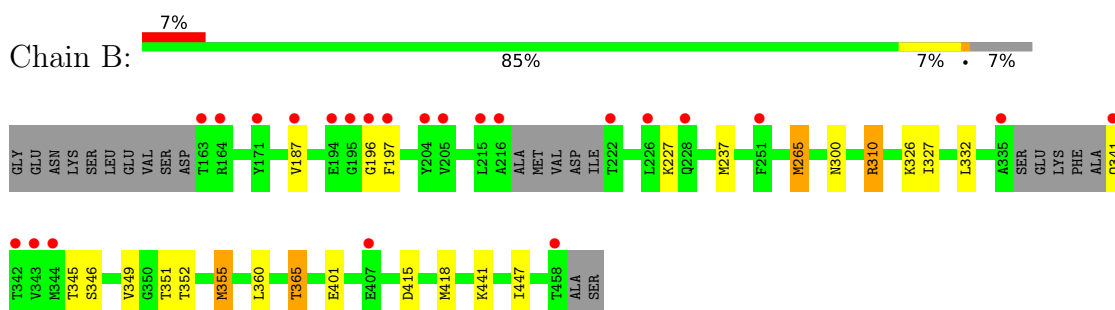
3 Residue-property plots [i](#)

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.

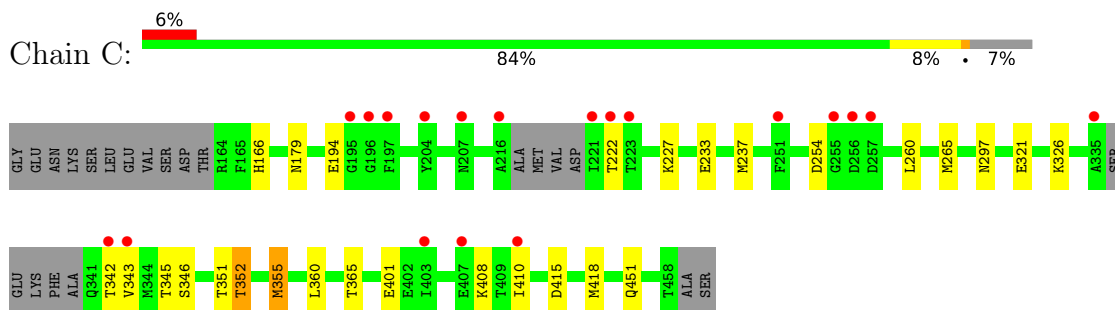
- Molecule 1: Interleukin-1 receptor-associated kinase 4



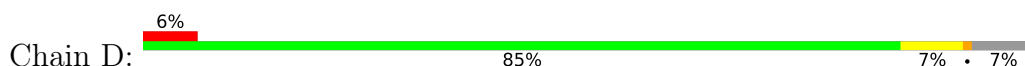
- Molecule 1: Interleukin-1 receptor-associated kinase 4

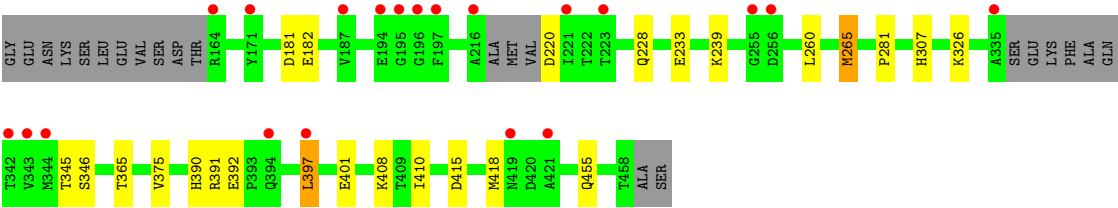


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.37Å 141.44Å 88.13Å 90.00° 124.80° 90.00°	Depositor
Resolution (Å)	27.50 – 1.88 27.50 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.50-1.88) 99.5 (27.50-1.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.88Å)	Xtriage
Refinement program	BUSTER 2.11.8 (10-JUL-2024)	Depositor
R, R_{free}	0.203 , 0.228 0.197 , 0.218	Depositor DCC
R_{free} test set	5854 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10098	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.84% 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: TPO, SEP, Y9T

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	0.68	1/2275 (0.0%)	1.03	3/3065 (0.1%)
1	B	0.74	3/2275 (0.1%)	1.03	1/3065 (0.0%)
1	C	0.73	1/2276 (0.0%)	1.02	4/3066 (0.1%)
1	D	0.71	1/2275 (0.0%)	0.99	1/3065 (0.0%)
All	All	0.72	6/9101 (0.1%)	1.01	9/12261 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	MET	SD-CE	-11.39	1.51	1.79
1	C	355	MET	SD-CE	-10.80	1.52	1.79
1	B	265	MET	SD-CE	-10.21	1.54	1.79
1	D	265	MET	SD-CE	-9.25	1.56	1.79
1	A	265	MET	SD-CE	-9.17	1.56	1.79
1	B	327	ILE	CG1-CD1	-5.40	1.30	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	GLN	CA-C-N	7.48	135.16	121.70
1	A	341	GLN	C-N-CA	7.48	135.16	121.70
1	C	342	THR	CA-C-N	6.80	133.80	122.57
1	C	342	THR	C-N-CA	6.80	133.80	122.57
1	A	206	ASN	CA-CB-CG	6.25	118.85	112.60
1	C	343	VAL	N-CA-CB	-5.79	102.74	112.47
1	C	254	ASP	CA-CB-CG	5.69	118.29	112.60
1	D	181	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	310	ARG	CD-NE-CZ	5.50	132.09	124.40

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	2260	0	2224	15	0
1	B	2260	0	2224	22	0
1	C	2261	0	2228	18	0
1	D	2260	0	2224	12	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	196	0	0	0	0
3	B	206	0	0	0	0
3	C	255	0	0	4	0
3	D	272	0	0	0	0
All	All	10098	0	8900	61	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 (61) 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:265:MET:HE1	1:A:326:LYS:HG3	1.31	1.09
1:A:265:MET:CE	1:A:326:LYS:HG3	1.91	1.00
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.42	0.99
1:B:341:GLN:HG2	1:B:441:LYS:NZ	1.90	0.86
1:C:352:THR:HA	1:C:355:MET:HE2	1.59	0.85
1:B:265:MET:CE	1:B:326:LYS:HG3	2.08	0.83
1:B:352:THR:HA	1:B:355:MET:HE2	1.60	0.82
1:B:310:ARG:HD3	1:B:332:LEU:O	1.84	0.76
1:B:341:GLN:HG2	1:B:441:LYS:HZ2	1.49	0.74
1:A:222:THR:HB	1:A:225:GLU:HB2	1.68	0.74
1:A:390:HIS:O	1:D:391:ARG:HA	1.87	0.74
1:A:391:ARG:HA	1:D:390:HIS:O	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ASN:ND2	1:C:451:GLN:HE21	1.87	0.71
1:B:341:GLN:HA	1:B:365:THR:HB	1.75	0.67
1:C:297:ASN:HD22	1:C:451:GLN:HE21	1.43	0.67
1:C:352:THR:CA	1:C:355:MET:HE2	2.26	0.66
1:A:265:MET:HE1	1:A:326:LYS:CG	2.18	0.66
1:C:352:THR:HA	1:C:355:MET:CE	2.25	0.65
1:B:352:THR:HA	1:B:355:MET:CE	2.26	0.65
1:B:352:THR:CA	1:B:355:MET:HE2	2.26	0.64
1:A:341:GLN:HA	1:A:342:THR:HB	1.77	0.64
1:A:342:THR:HG23	1:A:343:VAL:HG23	1.79	0.63
1:B:341:GLN:HG2	1:B:441:LYS:HZ1	1.64	0.61
1:D:375:VAL:HG22	1:D:397:LEU:HD13	1.85	0.58
1:B:355:MET:HE3	1:B:360:LEU:CD2	2.35	0.57
1:B:332:LEU:HD22	1:B:349:VAL:HG21	1.87	0.57
1:D:233:GLU:HG2	1:D:260:LEU:HD13	1.86	0.56
1:C:233:GLU:HG2	1:C:260:LEU:HD13	1.88	0.55
1:C:355:MET:HE3	1:C:360:LEU:CD2	2.37	0.55
1:B:355:MET:HE3	1:B:360:LEU:HD21	1.88	0.55
1:B:265:MET:HE1	1:B:326:LYS:CG	2.28	0.55
1:A:237:MET:HA	1:A:237:MET:HE2	1.90	0.54
1:C:179:ASN:HB3	3:C:780:HOH:O	2.07	0.54
1:D:239:LYS:HD3	1:D:307:HIS:HE1	1.72	0.54
1:B:352:THR:N	1:B:355:MET:HE2	2.24	0.53
1:C:352:THR:N	1:C:355:MET:HE2	2.23	0.53
1:B:310:ARG:CD	1:B:332:LEU:O	2.57	0.53
1:A:390:HIS:O	1:D:390:HIS:O	2.27	0.52
1:A:168:PHE:HE1	1:A:205:VAL:HG11	1.76	0.51
1:C:355:MET:HE3	1:C:360:LEU:HD21	1.92	0.50
1:A:390:HIS:HB3	1:D:392:GLU:H	1.78	0.48
1:D:265:MET:CE	1:D:326:LYS:HD2	2.44	0.48
1:C:166:HIS:CE1	3:C:619:HOH:O	2.68	0.47
1:A:409:THR:HG23	1:A:412:ASP:H	1.81	0.46
1:C:237:MET:HE2	1:C:237:MET:HA	1.98	0.46
1:B:237:MET:HA	1:B:237:MET:HE2	1.98	0.45
1:B:351:THR:O	1:B:355:MET:HG3	2.17	0.45
1:D:265:MET:HE1	1:D:326:LYS:HD2	2.00	0.43
1:C:415:ASP:HB3	1:C:418:MET:HE2	2.01	0.43
1:A:392:GLU:H	1:D:390:HIS:HB3	1.84	0.43
1:C:352:THR:HG22	3:C:782:HOH:O	2.18	0.43
1:C:351:THR:O	1:C:355:MET:HG3	2.18	0.43
1:C:166:HIS:HE1	3:C:619:HOH:O	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLY:HA2	1:B:197:PHE:HA	1.76	0.42
1:B:415:ASP:HB3	1:B:418:MET:HE2	2.02	0.42
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.02	0.41
1:A:415:ASP:HB3	1:A:418:MET:HE2	2.02	0.41
1:D:415:ASP:HB3	1:D:418:MET:HE2	2.03	0.41
1:C:265:MET:SD	1:C:326:LYS:HG3	2.61	0.40
1:B:355:MET:HE3	1:B:360:LEU:HD23	2.04	0.40
1:C:321:GLU:HG2	1:D:281:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/308 (90%)	267 (96%)	9 (3%)	2 (1%)	18	7
1	B	278/308 (90%)	268 (96%)	10 (4%)	0	100	100
1	C	278/308 (90%)	273 (98%)	5 (2%)	0	100	100
1	D	278/308 (90%)	269 (97%)	9 (3%)	0	100	100
All	All	1112/1232 (90%)	1077 (97%)	33 (3%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLY
1	A	342	THR

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	248/266 (93%)	242 (98%)	6 (2%)	43	27
1	B	248/266 (93%)	244 (98%)	4 (2%)	55	43
1	C	248/266 (93%)	240 (97%)	8 (3%)	34	17
1	D	248/266 (93%)	239 (96%)	9 (4%)	31	14
All	All	992/1064 (93%)	965 (97%)	27 (3%)	39	23

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	222	THR
1	A	228	GLN
1	A	352	THR
1	A	365	THR
1	A	401	GLU
1	B	187	VAL
1	B	227	LYS
1	B	365	THR
1	B	401	GLU
1	C	194	GLU
1	C	222	THR
1	C	227	LYS
1	C	352	THR
1	C	365	THR
1	C	401	GLU
1	C	408	LYS
1	C	410	ILE
1	D	182	GLU
1	D	220	ASP
1	D	228	GLN
1	D	365	THR
1	D	397	LEU
1	D	401	GLU
1	D	408	LYS
1	D	410	ILE
1	D	455	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	341	GLN
1	A	394	GLN
1	A	435	GLN
1	A	452	GLN
1	B	166	HIS
1	B	206	ASN
1	B	207	ASN
1	B	390	HIS
1	B	435	GLN
1	B	452	GLN
1	C	206	ASN
1	C	241	GLN
1	C	297	ASN
1	C	394	GLN
1	C	435	GLN
1	D	166	HIS
1	D	232	GLN
1	D	307	HIS
1	D	394	GLN
1	D	435	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	TPO	A	345	1	8,10,11	1.14	0	10,14,16	1.30	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	D	345	1	8,10,11	1.37	2 (25%)	10,14,16	1.49	2 (20%)
1	SEP	A	346	1	8,9,10	0.78	0	7,12,14	1.50	2 (28%)
1	SEP	C	346	1	8,9,10	0.85	0	7,12,14	1.55	1 (14%)
1	TPO	C	345	1	8,10,11	1.25	0	10,14,16	1.27	1 (10%)
1	SEP	B	346	1	8,9,10	0.87	0	7,12,14	1.41	1 (14%)
1	SEP	D	346	1	8,9,10	0.81	0	7,12,14	1.54	2 (28%)
1	TPO	B	345	1	8,10,11	1.16	1 (12%)	10,14,16	1.28	2 (20%)

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	TPO	A	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	SEP	C	346	1	-	0/6/8/10	-
1	TPO	C	345	1	-	4/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	D	346	1	-	0/6/8/10	-
1	TPO	B	345	1	-	5/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	TPO	P-OG1	-2.64	1.54	1.59
1	D	345	TPO	CB-CA	2.36	1.58	1.53
1	B	345	TPO	P-OG1	-2.11	1.55	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	TPO	O3P-P-OG1	3.27	118.59	105.85
1	C	346	SEP	OG-CB-CA	3.08	111.14	108.14
1	A	346	SEP	OG-CB-CA	2.94	111.00	108.14
1	D	346	SEP	OG-CB-CA	2.87	110.94	108.14
1	B	346	SEP	OG-CB-CA	2.84	110.91	108.14
1	A	345	TPO	O2P-P-OG1	2.80	116.74	105.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	TPO	O3P-P-OG1	2.73	116.49	105.85
1	C	345	TPO	O2P-P-OG1	2.64	116.12	105.85
1	D	345	TPO	P-OG1-CB	-2.35	116.93	123.33
1	B	345	TPO	P-OG1-CB	-2.25	117.22	123.33
1	D	346	SEP	O3P-P-OG	2.25	112.53	106.67
1	A	346	SEP	O3P-P-OG	2.11	112.18	106.67
1	A	345	TPO	P-OG1-CB	-2.09	117.66	123.33

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O1P
1	D	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	CB-OG1-P-O2P
1	B	345	TPO	CB-OG1-P-O3P
1	A	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CG2-CB-OG1-P
1	D	345	TPO	CG2-CB-OG1-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	Y9T	A	501	-	32,34,34	1.16	3 (9%)	44,53,53	1.64	6 (13%)
2	Y9T	C	501	-	32,34,34	1.01	3 (9%)	44,53,53	1.54	7 (15%)
2	Y9T	D	501	-	32,34,34	1.08	3 (9%)	44,53,53	1.61	7 (15%)
2	Y9T	B	501	-	32,34,34	1.07	3 (9%)	44,53,53	1.56	5 (11%)

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	Y9T	A	501	-	-	3/26/26/26	0/3/3/3
2	Y9T	C	501	-	-	0/26/26/26	0/3/3/3
2	Y9T	D	501	-	-	0/26/26/26	0/3/3/3
2	Y9T	B	501	-	-	0/26/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	Y9T	C29-C15	-3.39	1.51	1.54
2	A	501	Y9T	C16-C17	-3.00	1.37	1.40
2	B	501	Y9T	C16-C17	-2.98	1.37	1.40
2	A	501	Y9T	C29-C15	-2.88	1.51	1.54
2	C	501	Y9T	C16-C17	-2.48	1.37	1.40
2	A	501	Y9T	C22-N21	2.41	1.37	1.35
2	D	501	Y9T	C16-C17	-2.41	1.37	1.40
2	B	501	Y9T	C22-N21	2.23	1.37	1.35
2	C	501	Y9T	C22-N21	2.23	1.37	1.35
2	D	501	Y9T	C22-N21	2.22	1.37	1.35
2	B	501	Y9T	C29-C15	-2.18	1.52	1.54
2	C	501	Y9T	C29-C15	-2.12	1.52	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	Y9T	C14-C19-C18	-6.19	110.66	120.31
2	B	501	Y9T	C14-C19-C18	-5.73	111.38	120.31
2	D	501	Y9T	C14-C19-C18	-5.62	111.56	120.31
2	C	501	Y9T	C14-C19-C18	-5.57	111.63	120.31
2	D	501	Y9T	C15-C16-C17	-4.12	114.83	119.85
2	A	501	Y9T	C15-C16-C17	-3.77	115.25	119.85
2	B	501	Y9T	C15-C16-C17	-3.68	115.36	119.85
2	C	501	Y9T	C15-C16-C17	-3.51	115.57	119.85
2	A	501	Y9T	C19-C14-C15	3.34	124.22	120.07
2	D	501	Y9T	C16-C15-C14	3.33	122.97	118.80
2	B	501	Y9T	C16-C15-C14	3.32	122.97	118.80
2	C	501	Y9T	C16-C15-C14	3.15	122.76	118.80
2	A	501	Y9T	C16-C15-C14	2.91	122.45	118.80
2	B	501	Y9T	C15-C14-N13	-2.73	117.52	120.42
2	D	501	Y9T	C19-C14-C15	2.64	123.35	120.07
2	C	501	Y9T	C15-C14-N13	-2.58	117.68	120.42
2	A	501	Y9T	C15-C14-N13	-2.56	117.70	120.42
2	B	501	Y9T	C19-C14-C15	2.54	123.22	120.07
2	C	501	Y9T	C19-C14-C15	2.51	123.19	120.07
2	A	501	Y9T	F8-C7-C2	2.41	116.67	112.43
2	C	501	Y9T	F8-C7-C2	2.38	116.62	112.43
2	D	501	Y9T	C4-N3-C2	-2.31	115.74	118.78
2	C	501	Y9T	C31-C29-C30	-2.30	107.72	110.53
2	D	501	Y9T	C30-C29-C15	2.03	114.83	111.52
2	D	501	Y9T	C31-C29-C30	-2.02	108.07	110.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

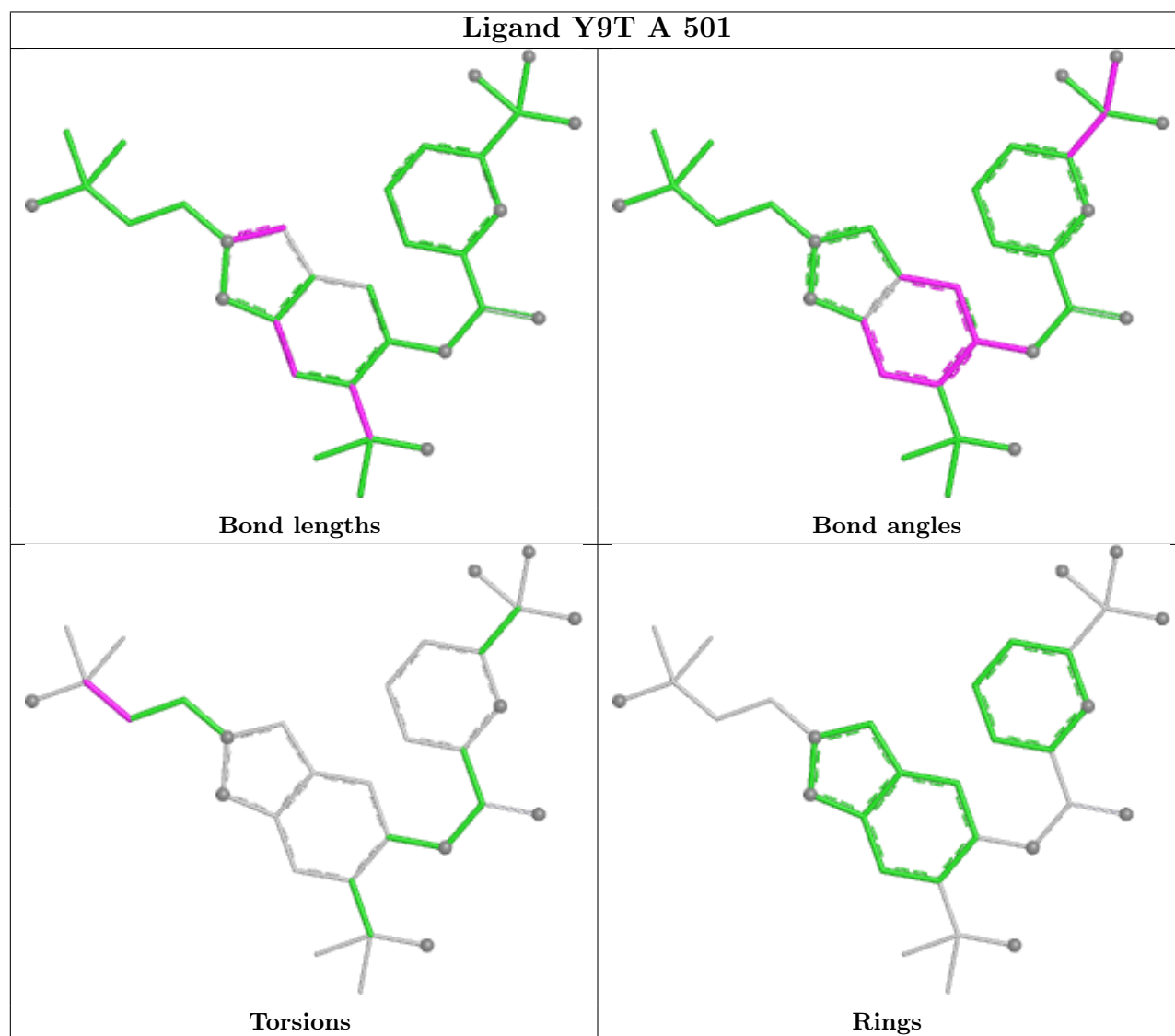
Mol	Chain	Res	Type	Atoms
2	A	501	Y9T	C23-C24-C25-C26
2	A	501	Y9T	C23-C24-C25-O28
2	A	501	Y9T	C23-C24-C25-C27

There are no ring outliers.

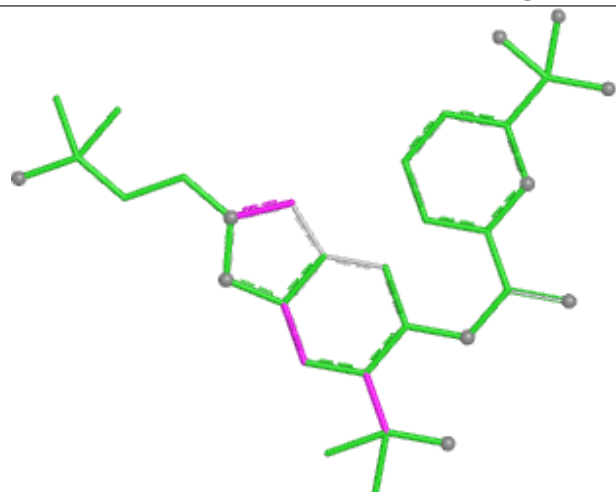
No monomer is involved in short contacts.

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

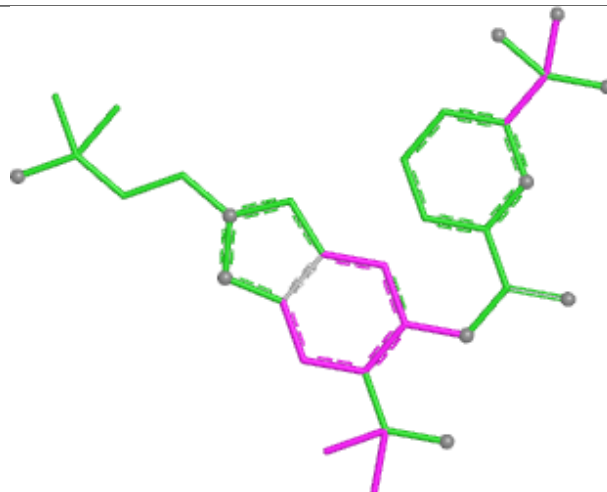
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



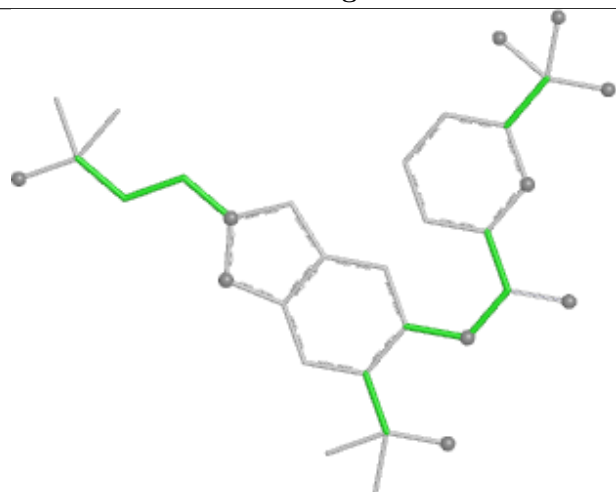
Ligand Y9T C 501



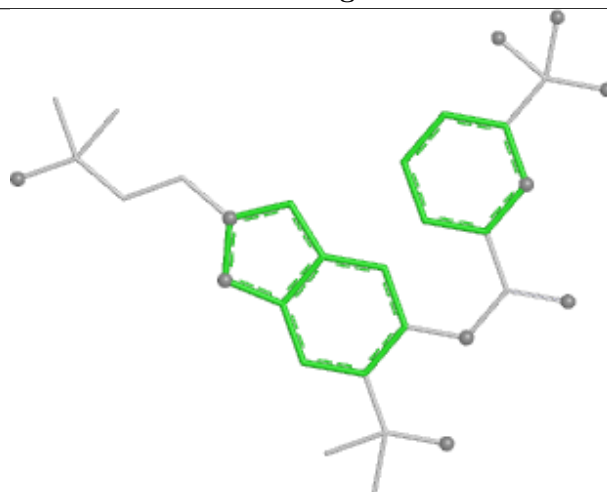
Bond lengths



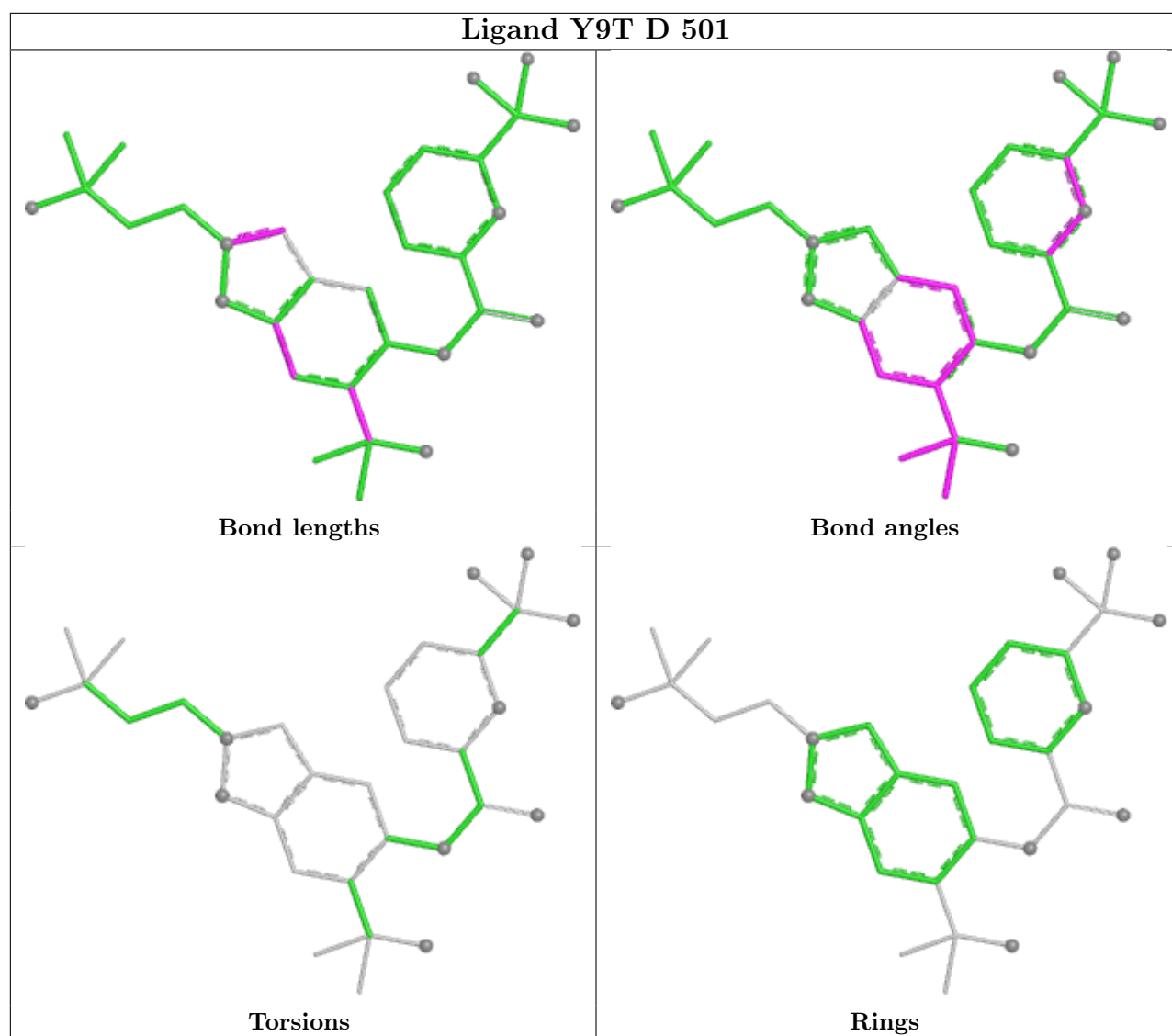
Bond angles

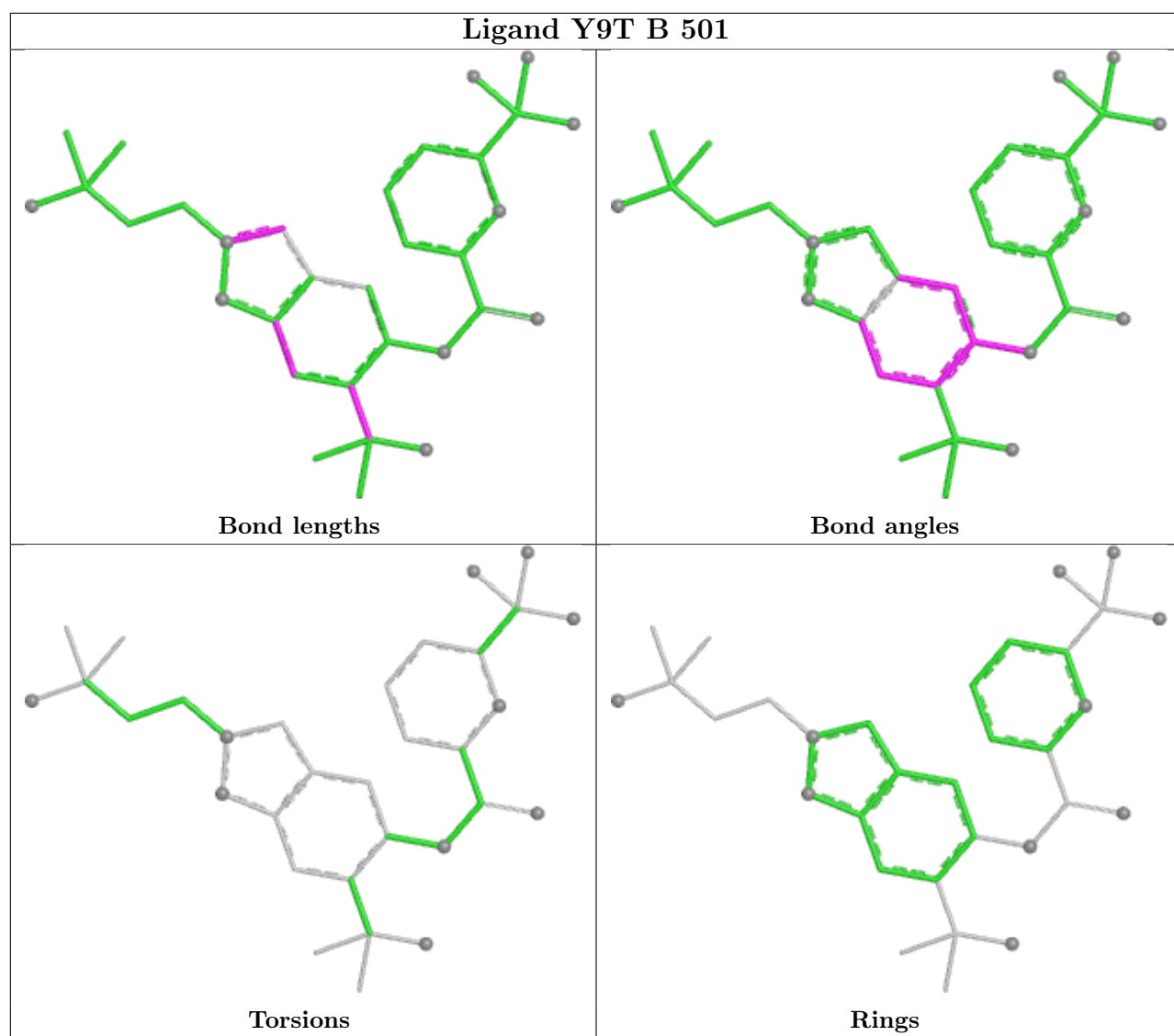


Torsions



Rings





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	284/308 (92%)	0.46	24 (8%) 16 18	23, 43, 73, 94	0
1	B	284/308 (92%)	0.50	23 (8%) 18 20	23, 43, 75, 101	0
1	C	284/308 (92%)	0.35	19 (6%) 24 26	22, 37, 64, 83	0
1	D	284/308 (92%)	0.33	20 (7%) 22 25	24, 37, 67, 86	0
All	All	1136/1232 (92%)	0.41	86 (7%) 20 22	22, 39, 73, 101	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	GLY	5.0
1	C	255	GLY	4.8
1	B	216	ALA	4.7
1	A	216	ALA	4.7
1	C	197	PHE	4.1
1	B	335	ALA	4.1
1	A	341	GLN	4.1
1	B	197	PHE	4.1
1	D	255	GLY	4.0
1	D	195	GLY	4.0
1	A	204	TYR	3.8
1	C	216	ALA	3.7
1	A	335	ALA	3.7
1	D	342	THR	3.6
1	C	221	ILE	3.6
1	B	196	GLY	3.5
1	D	221	ILE	3.4
1	A	343	VAL	3.4
1	B	205	VAL	3.4
1	A	344	MET	3.4
1	B	342	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	204	TYR	3.3
1	C	204	TYR	3.3
1	D	343	VAL	3.2
1	D	197	PHE	3.2
1	D	335	ALA	3.2
1	B	187	VAL	3.1
1	B	163	THR	3.1
1	D	171	TYR	3.1
1	B	341	GLN	3.1
1	B	344	MET	3.1
1	C	195	GLY	3.1
1	A	205	VAL	3.1
1	C	257	ASP	3.1
1	A	197	PHE	3.1
1	B	164	ARG	3.0
1	B	343	VAL	3.0
1	D	397	LEU	2.9
1	A	226	LEU	2.9
1	B	194	GLU	2.9
1	D	216	ALA	2.9
1	B	228	GLN	2.9
1	C	342	THR	2.8
1	C	410	ILE	2.8
1	B	222	THR	2.8
1	B	226	LEU	2.7
1	C	256	ASP	2.7
1	A	256	ASP	2.6
1	C	335	ALA	2.6
1	D	164	ARG	2.6
1	A	185	ILE	2.6
1	D	196	GLY	2.6
1	C	207	ASN	2.6
1	B	251	PHE	2.6
1	D	256	ASP	2.6
1	D	419	ASN	2.6
1	A	342	THR	2.6
1	C	223	THR	2.5
1	D	394	GLN	2.5
1	A	195	GLY	2.5
1	D	421	ALA	2.5
1	B	215	LEU	2.3
1	A	208	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	206	ASN	2.3
1	A	390	HIS	2.3
1	D	344	MET	2.3
1	B	195	GLY	2.3
1	B	458	THR	2.3
1	C	407	GLU	2.3
1	D	223	THR	2.3
1	C	403	ILE	2.3
1	A	392	GLU	2.2
1	D	194	GLU	2.2
1	A	410	ILE	2.2
1	A	223	THR	2.2
1	A	409	THR	2.2
1	A	332	LEU	2.2
1	C	343	VAL	2.2
1	C	251	PHE	2.2
1	A	171	TYR	2.1
1	B	171	TYR	2.1
1	A	439	GLU	2.1
1	A	222	THR	2.0
1	C	222	THR	2.0
1	B	407	GLU	2.0
1	D	187	VAL	2.0

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	SEP	B	346	10/11	0.72	0.11	63,68,101,106	0
1	SEP	A	346	10/11	0.74	0.12	65,71,105,107	0
1	SEP	C	346	10/11	0.81	0.13	54,59,91,92	0
1	SEP	D	346	10/11	0.86	0.09	57,62,94,94	0
1	TPO	B	345	11/12	0.92	0.10	56,62,67,73	0
1	TPO	A	345	11/12	0.92	0.09	60,65,69,70	0
1	TPO	C	345	11/12	0.95	0.08	49,53,56,57	0
1	TPO	D	345	11/12	0.96	0.07	51,56,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

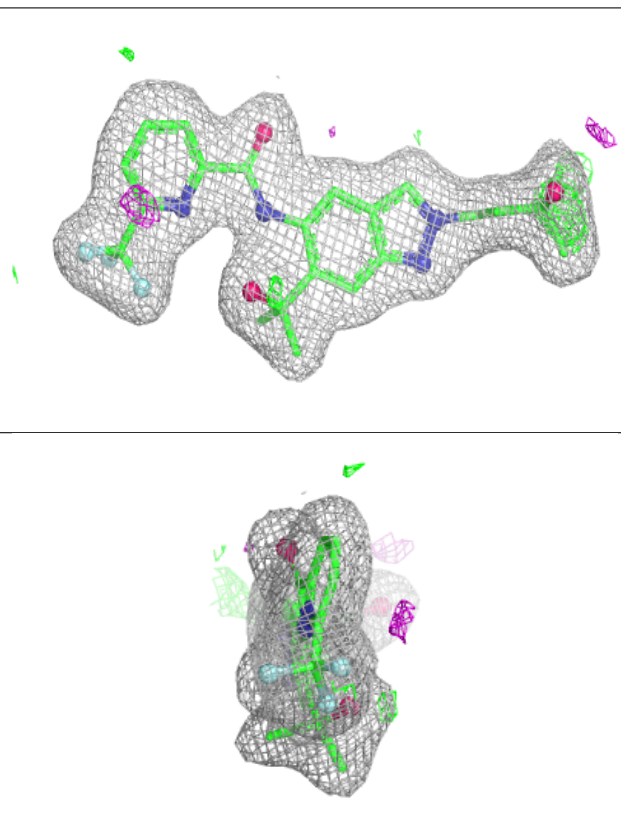
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	Y9T	B	501	32/32	0.94	0.07	31,33,39,40	0
2	Y9T	C	501	32/32	0.95	0.06	24,26,31,33	0
2	Y9T	D	501	32/32	0.95	0.06	24,27,33,34	0
2	Y9T	A	501	32/32	0.96	0.06	29,31,36,37	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.

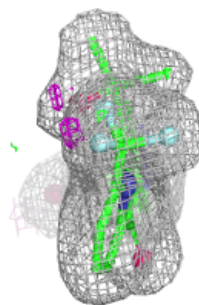
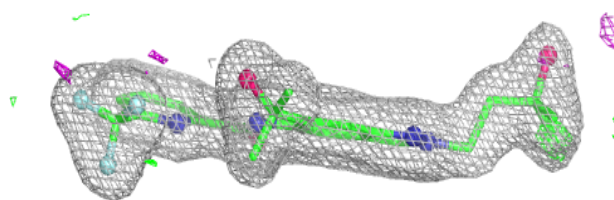
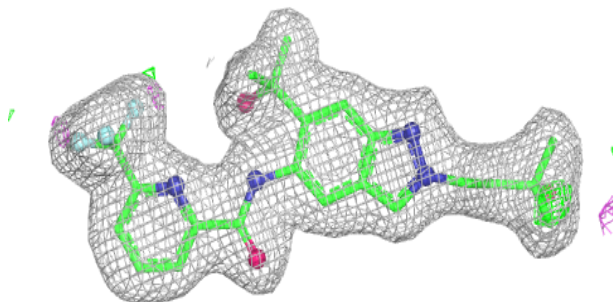
Electron density around Y9T B 501:

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

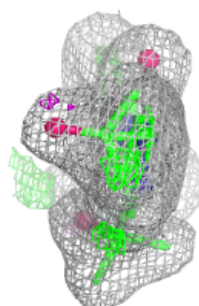
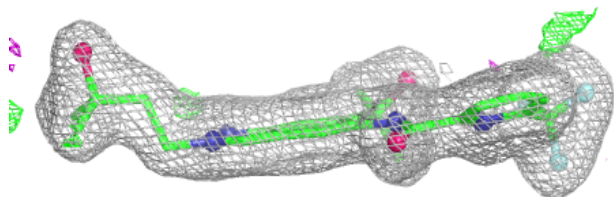
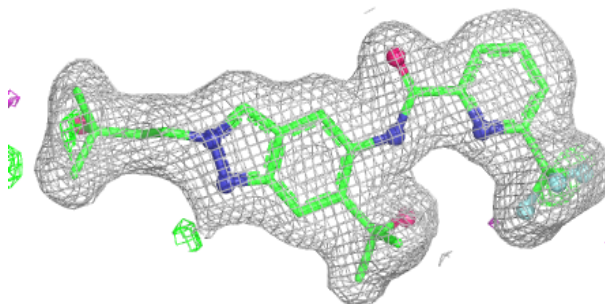


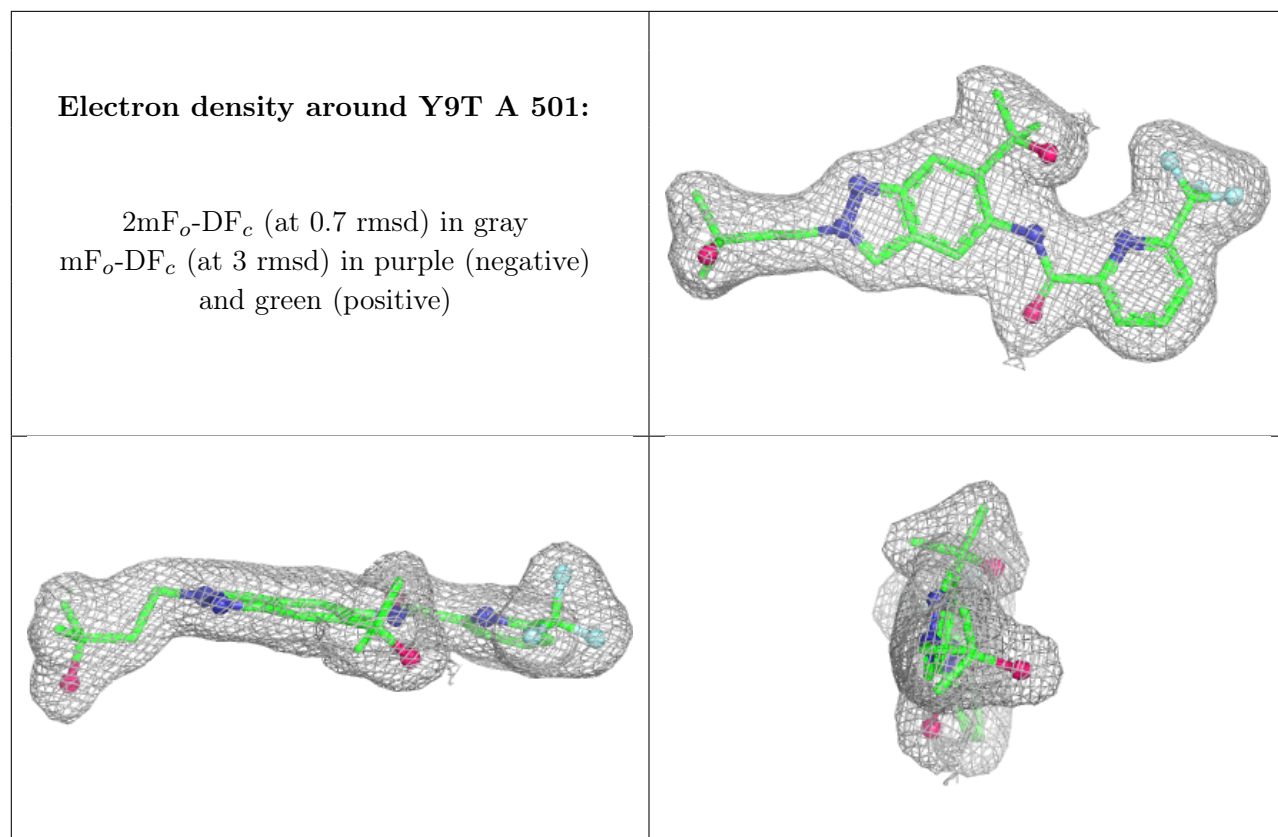
Electron density around Y9T C 501:

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

**Electron density around Y9T 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.