WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2023 – 10:08 AM JST

PDB ID	:	6AAJ
Title	:	Crystal structure of JAK2 in complex with peficitinib
Authors	:	Amano, Y.; Tateishi, Y.
Deposited on	:	2018-07-18
Resolution	:	2.37 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.37 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		5
Ramachandran outliers		0.9%
Sidechain outliers		7.5%
RSRZ outliers		5.1%

Worse — *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
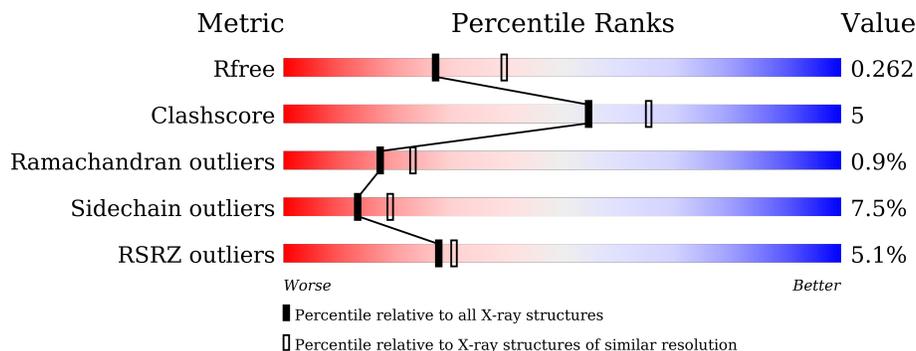
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	299	7% / 81% 13% · 5%
1	B	299	2% / 74% 15% · 8%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4665 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 Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	P	S	0	0	0
			2322	1472	397	437	2	14			
1	B	274	Total	C	N	O	P	S	0	0	0
			2253	1433	385	419	2	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	943	ALA	LYS	engineered mutation	UNP O60674
A	945	ALA	LYS	engineered mutation	UNP O60674
B	943	ALA	LYS	engineered mutation	UNP O60674
B	945	ALA	LYS	engineered mutation	UNP O60674

- Molecule 2 is 4-[[(1S,3R)-5-oxidanyl-2-adamantyl]amino]-1H-pyrrolo[2,3-b]pyridine-5-carbox amide (three-letter code: 9T6) (formula: $C_{18}H_{22}N_4O_2$).
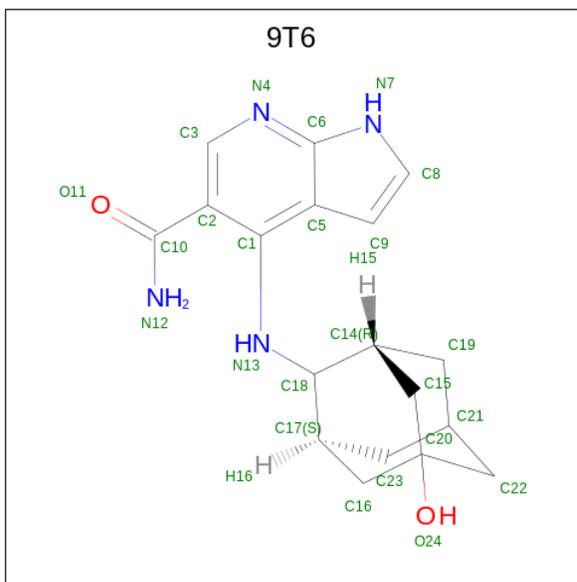
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 24	C 18	N 4	O 2	0	0
2	B	1	Total 24	C 18	N 4	O 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	20	Total 20	O 20	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Tyrosine-protein kinase JAK2
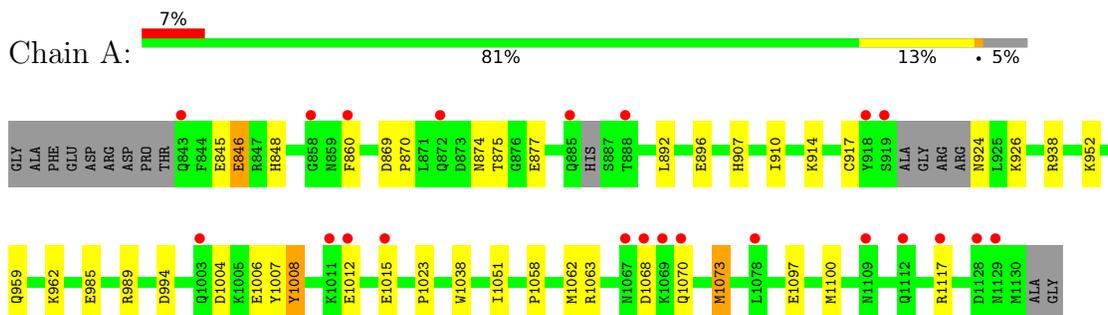
- Molecule 1: Tyrosine-protein kinase JAK2
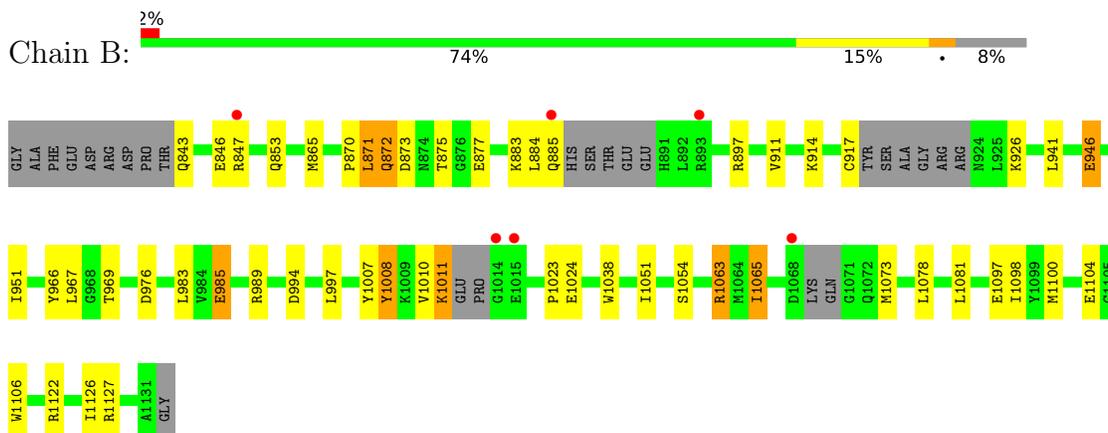
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	43.15Å 126.66Å 132.91Å 90.00° 96.49° 90.00°	Depositor
Resolution (Å)	19.24 – 2.37 19.24 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.24-2.37) 99.8 (19.24-2.37)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.208 , 0.262 0.208 , 0.262	Depositor DCC
R_{free} test set	1386 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4665	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 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 9T6, PTR

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	0.39	0/2335	0.62	0/3144
1	B	0.42	0/2263	0.64	0/3044
All	All	0.41	0/4598	0.63	0/6188

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 (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	2322	0	2265	12	0
1	B	2253	0	2209	32	0
2	A	24	0	0	2	0
2	B	24	0	0	1	0
3	A	22	0	0	0	0
3	B	20	0	0	0	0
All	All	4665	0	4474	47	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 5.

All (47) 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:871:LEU:H	1:B:871:LEU:HD13	1.26	0.96
1:B:1051:ILE:HG22	1:B:1051:ILE:O	1.87	0.74
1:B:871:LEU:H	1:B:871:LEU:CD1	2.03	0.71
1:B:1008:PTR:HE1	1:B:1010:VAL:HG12	1.79	0.63
1:B:1065:ILE:HD11	1:B:1078:LEU:HA	1.79	0.63
1:A:917:CYS:HB3	1:A:926:LYS:HB2	1.86	0.58
1:B:1097:GLU:HA	1:B:1100:MET:HE2	1.89	0.55
1:B:883:LYS:HB3	1:B:926:LYS:HG2	1.90	0.54
1:A:907:HIS:HB3	1:A:910:ILE:HG13	1.91	0.53
2:A:1201:9T6:C18	2:A:1201:9T6:C9	2.87	0.53
1:B:941:LEU:HD23	1:B:1051:ILE:HD13	1.91	0.52
1:B:871:LEU:HD13	1:B:871:LEU:N	2.09	0.52
1:B:941:LEU:HD23	1:B:1051:ILE:CD1	2.40	0.51
1:B:976:ASP:HB2	1:B:997:LEU:HD12	1.92	0.51
1:B:1098:ILE:HD11	1:B:1126:ILE:HG21	1.92	0.50
1:B:1051:ILE:O	1:B:1051:ILE:CG2	2.57	0.49
1:B:1063:ARG:HH11	1:B:1063:ARG:HG3	1.76	0.49
1:A:959:GLN:OE1	1:A:989:ARG:HA	2.12	0.49
1:B:853:GLN:HG2	1:B:865:MET:HE3	1.96	0.47
1:B:877:GLU:OE2	1:B:914:LYS:NZ	2.47	0.47
2:B:1201:9T6:C18	2:B:1201:9T6:C9	2.93	0.46
1:B:951:ILE:HG23	1:B:1127:ARG:HE	1.81	0.46
1:A:1023:PRO:HD3	1:A:1038:TRP:CZ3	2.51	0.46
1:B:871:LEU:CD1	1:B:871:LEU:N	2.75	0.46
1:B:1038:TRP:CE3	1:B:1106:TRP:HA	2.49	0.46
1:B:911:VAL:CG2	1:B:983:LEU:HD12	2.45	0.46
1:B:966:TYR:O	1:B:969:THR:HB	2.17	0.45
1:B:911:VAL:HG21	1:B:983:LEU:HD12	1.97	0.45
1:A:1070:GLN:O	1:A:1073:MET:HB2	2.17	0.44
1:B:985:GLU:HG2	1:B:989:ARG:HB3	2.00	0.44
1:B:1063:ARG:HH11	1:B:1063:ARG:CG	2.30	0.44
1:B:1065:ILE:HD12	1:B:1081:LEU:HD22	2.00	0.44
1:B:884:LEU:HD23	1:B:884:LEU:HA	1.85	0.43
1:B:946:GLU:CD	1:B:946:GLU:H	2.21	0.43
1:B:1023:PRO:HD2	1:B:1024:GLU:OE1	2.18	0.43
1:A:877:GLU:OE2	1:A:914:LYS:HE2	2.19	0.43
1:A:1058:PRO:O	1:A:1062:MET:HG2	2.18	0.43
1:A:848:HIS:CG	1:A:870:PRO:HA	2.55	0.42
1:A:1008:PTR:C	1:A:1008:PTR:HD1	2.50	0.42
1:A:846:GLU:HG2	1:A:917:CYS:SG	2.59	0.42
2:A:1201:9T6:O11	2:A:1201:9T6:N13	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:LEU:O	1:B:872:GLN:C	2.59	0.41
1:B:1104:GLU:OE1	1:B:1122:ARG:NH2	2.42	0.41
1:A:869:ASP:OD1	1:A:875:THR:O	2.38	0.41
1:A:1063:ARG:HH11	1:A:1063:ARG:HG3	1.86	0.41
1:B:1008:PTR:HD1	1:B:1008:PTR:C	2.51	0.41
1:B:1011:LYS:HE2	1:B:1011:LYS:H	1.86	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	275/299 (92%)	265 (96%)	9 (3%)	1 (0%)	34	46
1	B	262/299 (88%)	250 (95%)	8 (3%)	4 (2%)	10	12
All	All	537/598 (90%)	515 (96%)	17 (3%)	5 (1%)	17	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	873	ASP
1	A	994	ASP
1	B	872	GLN
1	B	994	ASP
1	B	870	PRO

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	251/267 (94%)	230 (92%)	21 (8%)	11	15
1	B	244/267 (91%)	228 (93%)	16 (7%)	16	24
All	All	495/534 (93%)	458 (92%)	37 (8%)	13	19

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	845	GLU
1	A	846	GLU
1	A	860	PHE
1	A	874	ASN
1	A	892	LEU
1	A	896	GLU
1	A	924	ASN
1	A	938	ARG
1	A	952	LYS
1	A	962	LYS
1	A	985	GLU
1	A	1004	ASP
1	A	1006	GLU
1	A	1012	GLU
1	A	1015	GLU
1	A	1051	ILE
1	A	1068	ASP
1	A	1073	MET
1	A	1097	GLU
1	A	1100	MET
1	A	1117	ARG
1	B	843	GLN
1	B	846	GLU
1	B	847	ARG
1	B	871	LEU
1	B	875	THR
1	B	885	GLN
1	B	897	ARG
1	B	917	CYS
1	B	946	GLU
1	B	967	LEU
1	B	985	GLU
1	B	1011	LYS

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Mol	Chain	Res	Type
1	B	1054	SER
1	B	1063	ARG
1	B	1065	ILE
1	B	1073	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	848	HIS
1	A	859	ASN
1	A	874	ASN
1	A	950	HIS
1	A	1072	GLN
1	B	906	GLN
1	B	1072	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	B	1008	1	15,16,17	0.81	1 (6%)	19,22,24	1.18	2 (10%)
1	PTR	A	1007	1	15,16,17	1.01	1 (6%)	19,22,24	0.83	1 (5%)
1	PTR	A	1008	1	15,16,17	0.83	1 (6%)	19,22,24	1.20	2 (10%)
1	PTR	B	1007	1	15,16,17	0.90	1 (6%)	19,22,24	1.33	3 (15%)

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	B	1008	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1008	1	-	1/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1007	PTR	P-OH	3.39	1.64	1.59
1	A	1008	PTR	P-OH	2.54	1.63	1.59
1	B	1007	PTR	P-OH	2.50	1.63	1.59
1	B	1008	PTR	P-OH	2.02	1.62	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1007	PTR	O3P-P-OH	-2.38	97.79	105.24
1	B	1008	PTR	OH-P-O1P	-2.20	101.01	109.31
1	B	1008	PTR	O3P-P-O2P	2.12	115.72	107.64
1	B	1007	PTR	OH-CZ-CE2	-2.10	112.99	119.23
1	B	1007	PTR	OH-CZ-CE1	2.08	125.42	119.23
1	A	1008	PTR	OH-CZ-CE2	2.07	125.40	119.23
1	A	1007	PTR	OH-P-O1P	-2.03	101.67	109.31
1	A	1008	PTR	O3P-P-O2P	2.01	115.34	107.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1008	PTR	CZ-OH-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1008	PTR	2	0
1	A	1008	PTR	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	9T6	B	1201	-	26,28,28	1.21	2 (7%)	30,44,44	1.89	7 (23%)
2	9T6	A	1201	-	26,28,28	1.23	1 (3%)	30,44,44	1.94	9 (30%)

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	9T6	B	1201	-	-	2/8/39/39	0/6/5/5
2	9T6	A	1201	-	-	2/8/39/39	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	9T6	C2-C10	-3.84	1.44	1.50
2	B	1201	9T6	C2-C10	-3.60	1.45	1.50
2	B	1201	9T6	C10-N12	2.11	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	9T6	C20-C16-C17	-5.89	106.98	109.95
2	A	1201	9T6	C2-C10-N12	-5.17	110.35	118.29
2	A	1201	9T6	C20-C16-C17	-4.17	107.85	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1201	9T6	C2-C10-N12	-4.08	112.02	118.29
2	A	1201	9T6	O11-C10-N12	3.62	127.73	122.58
2	A	1201	9T6	C23-C17-C18	2.80	114.94	109.56
2	A	1201	9T6	C17-C18-N13	-2.75	106.49	112.00
2	A	1201	9T6	C2-C1-C5	-2.67	115.44	120.29
2	B	1201	9T6	C3-N4-C6	-2.51	114.18	116.69
2	B	1201	9T6	C2-C1-C5	-2.44	115.87	120.29
2	A	1201	9T6	C3-N4-C6	-2.42	114.27	116.69
2	B	1201	9T6	C23-C21-C22	-2.36	103.73	109.07
2	B	1201	9T6	O11-C10-N12	2.23	125.75	122.58
2	A	1201	9T6	O24-C20-C16	-2.17	103.45	109.28
2	A	1201	9T6	C2-C3-N4	-2.12	122.26	125.14
2	B	1201	9T6	C16-C20-C22	2.02	113.11	109.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	9T6	C2-C1-N13-C18
2	A	1201	9T6	C5-C1-N13-C18
2	B	1201	9T6	C5-C1-N13-C18
2	A	1201	9T6	C2-C1-N13-C18

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	9T6	1	0
2	A	1201	9T6	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 9T6 B 1201

Bond lengths

Bond angles

Torsions

Rings

Ligand 9T6 A 1201

Bond lengths

Bond angles

Torsions

Rings
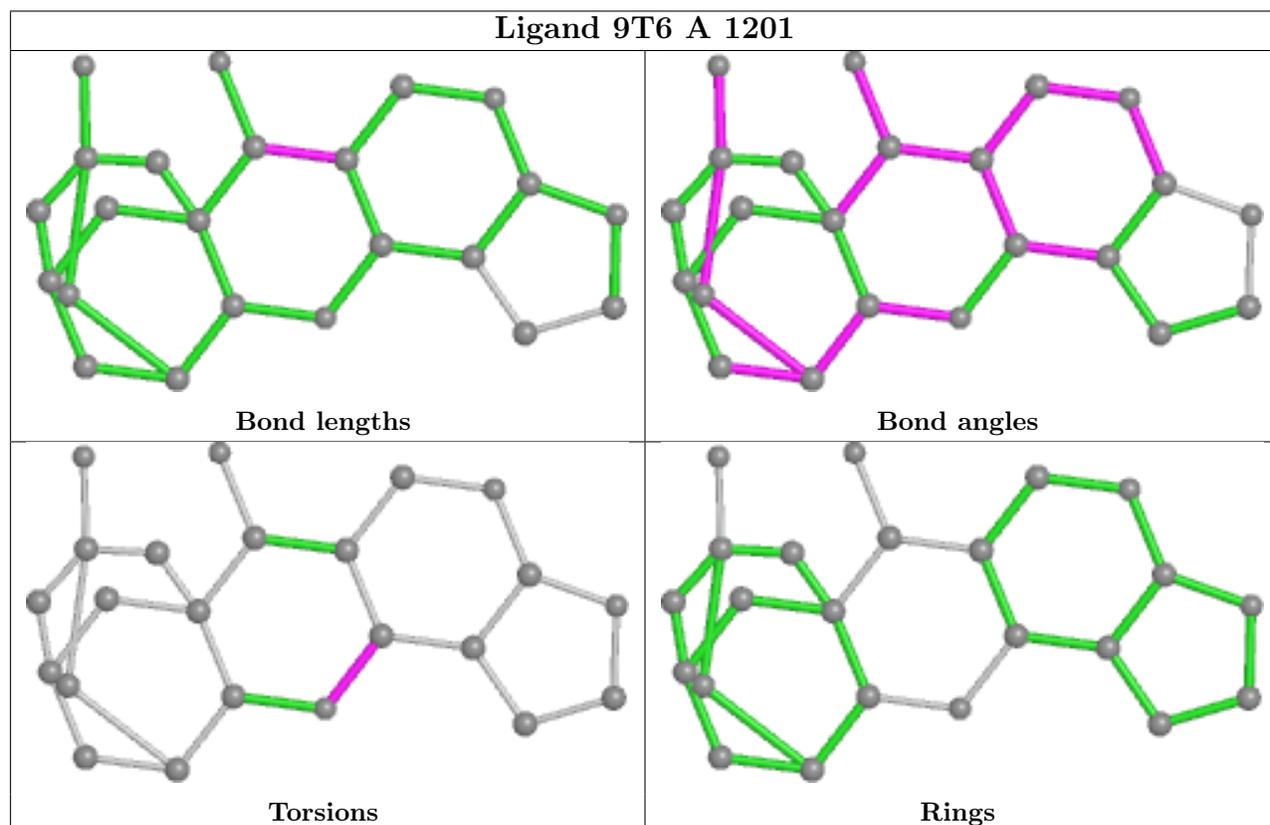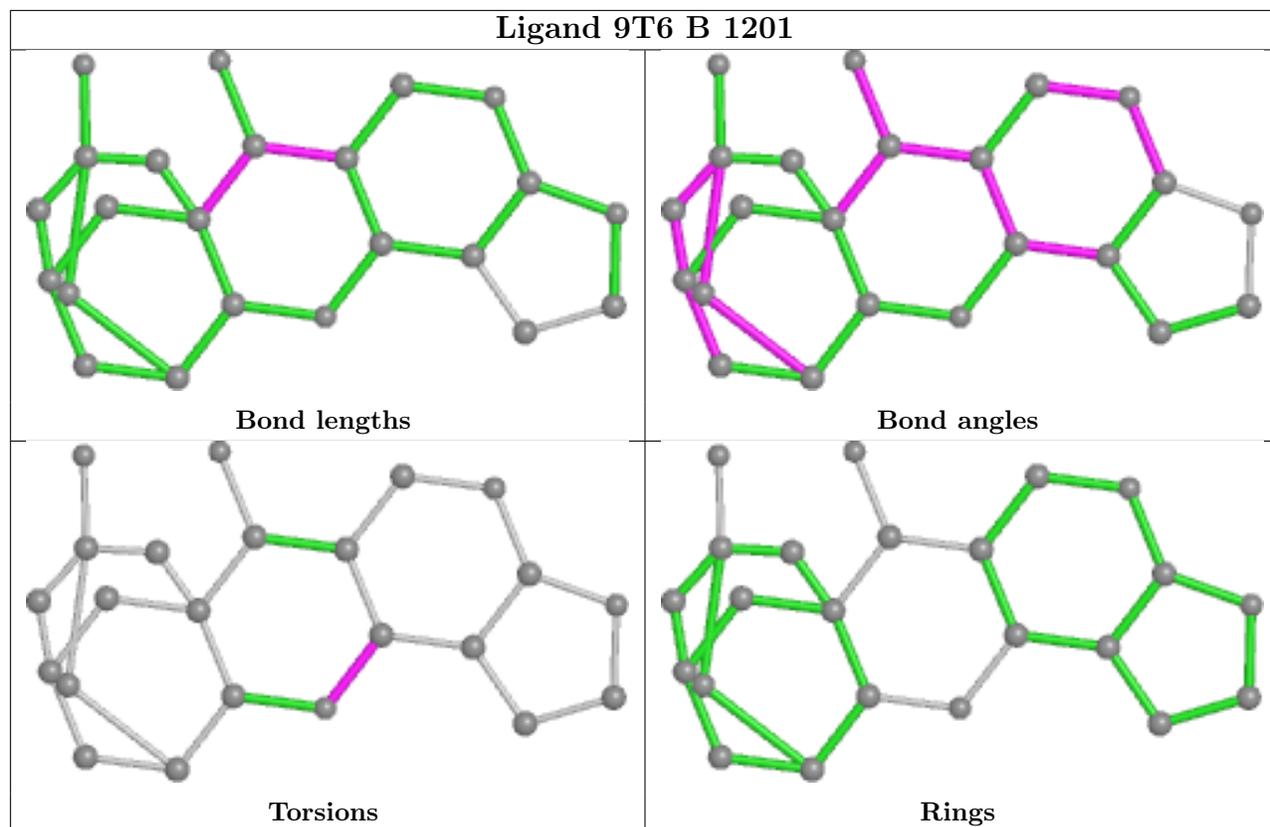
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	281/299 (93%)	0.25	22 (7%)	13	14	37, 58, 102, 139	1 (0%)
1	B	272/299 (90%)	0.09	6 (2%)	62	63	33, 51, 93, 107	0
All	All	553/598 (92%)	0.17	28 (5%)	28	30	33, 55, 98, 139	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1012	GLU	4.6
1	A	1070	GLN	4.1
1	A	918	TYR	3.8
1	A	1068	ASP	3.7
1	A	872	GLN	3.6
1	A	1067	ASN	3.4
1	A	1011	LYS	3.2
1	B	885	GLN	3.2
1	B	1068	ASP	3.2
1	B	847	ARG	3.1
1	A	1128	ASP	3.0
1	A	843	GLN	3.0
1	A	1117	ARG	2.9
1	A	885	GLN	2.8
1	A	1078	LEU	2.8
1	A	1015	GLU	2.8
1	A	888	THR	2.6
1	A	1112	GLN	2.6
1	A	1129	ASN	2.5
1	B	1014	GLY	2.4
1	A	919	SER	2.4
1	B	1015	GLU	2.4
1	A	1069	LYS	2.2
1	A	1003	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	893	ARG	2.1
1	A	860	PHE	2.1
1	A	858	GLY	2.1
1	A	1109	ASN	2.0

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

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	A	1007	16/17	0.79	0.23	69,102,125,126	0
1	PTR	B	1007	16/17	0.88	0.14	59,73,84,84	0
1	PTR	B	1008	16/17	0.89	0.14	55,66,81,90	0
1	PTR	A	1008	16/17	0.93	0.13	60,69,98,100	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	9T6	A	1201	24/24	0.92	0.15	45,57,65,68	0
2	9T6	B	1201	24/24	0.94	0.13	45,54,63,75	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 9T6 A 1201:

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

Electron density around 9T6 B 1201:

$2mF_o$-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 ⓘ

There are no such residues in this entry.