wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 04:54 am BST

PDB ID	:	3TJD
Title	:	co-crystal structure of Jak2 with thienopyridine 19
Authors	:	Huang, X.
Deposited on	:	2011-08-24
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.11
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)	:	2.11

1   Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.
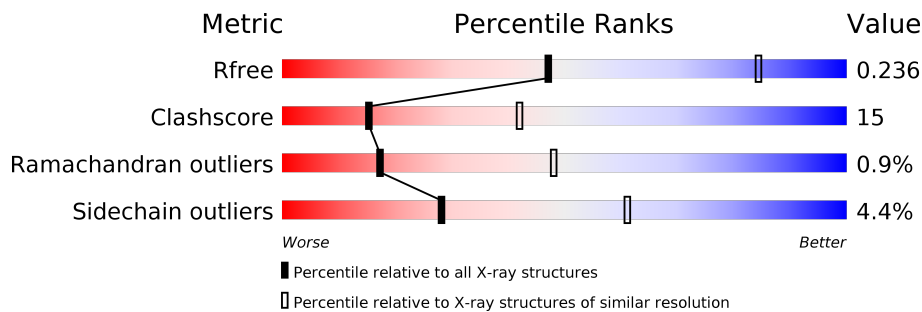
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	298	63% 29% · ·
1	B	298	71% 24% · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4886 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	286	Total 2373	C 1506	N 408	O 443	P 2	S 14	0	0	0
1	B	289	Total 2395	C 1519	N 411	O 449	P 2	S 14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	835	GLY	-	EXPRESSION TAG	UNP O60674
A	836	SER	-	EXPRESSION TAG	UNP O60674
B	835	GLY	-	EXPRESSION TAG	UNP O60674
B	836	SER	-	EXPRESSION TAG	UNP O60674

- Molecule 2 is 4-amino-2-[4-(tert-butylsulfamoyl)phenyl]-N-methylthieno[3,2-c]pyridine-7-carboxamide (three-letter code: 6TP) (formula: $C_{19}H_{22}N_4O_3S_2$).
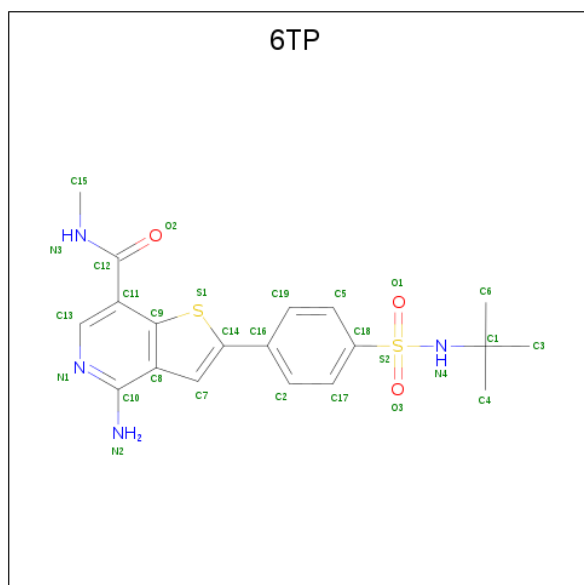
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 19	N 4	O 3	S 2	0	0
2	B	1	Total 28	C 19	N 4	O 3	S 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total 26	O 26	0	0
3	B	36	Total 36	O 36	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
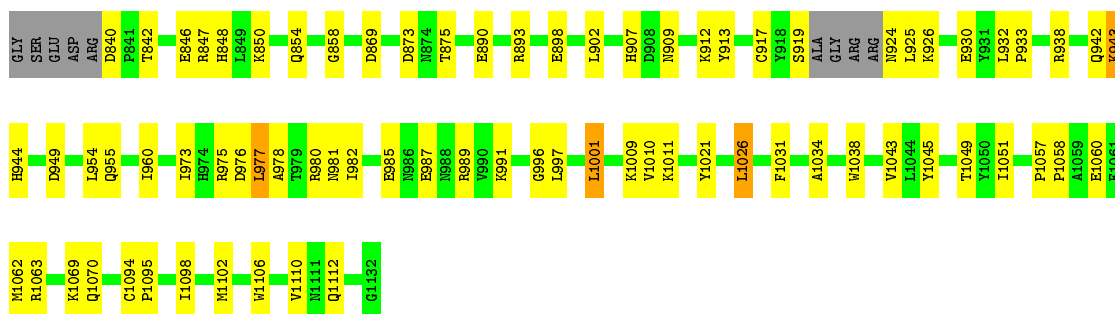
- Molecule 1: Tyrosine-protein kinase JAK2

Chain A:
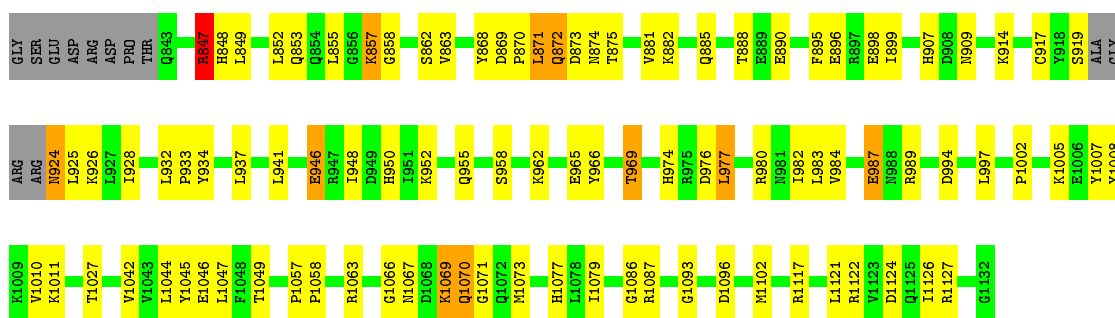
- Molecule 1: Tyrosine-protein kinase JAK2

Chain B:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	111.82Å 111.82Å 71.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 43.95 – 2.84	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.90) 94.9 (43.95-2.84)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.47 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.286 , 0.312 0.216 , 0.236	Depositor DCC
R_{free} test set	1014 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.1	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4886	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: 6TP, 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	0.60	2/2389 (0.1%)	0.75	3/3211 (0.1%)
1	B	0.57	0/2412	0.71	0/3244
All	All	0.58	2/4801 (0.0%)	0.73	3/6455 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	847	ARG	CZ-NH1	5.82	1.40	1.33
1	A	847	ARG	CZ-NH2	5.07	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	847	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	A	980	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	857	LYS	CD-CE-NZ	-5.02	100.16	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	847	ARG	Sidechain

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	2373	0	2343	81	0
1	B	2395	0	2362	63	0
2	A	28	0	22	4	0
2	B	28	0	22	2	0
3	A	26	0	0	2	0
3	B	36	0	0	7	0
All	All	4886	0	4749	143	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 15.

The worst 5 of 143 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:1069:LYS:HA	1:A:1069:LYS:HE3	1.20	1.17
1:A:1069:LYS:HA	1:A:1069:LYS:CE	1.85	1.04
1:A:977:LEU:HD21	1:A:982:ILE:HD11	1.49	0.95
1:B:890:GLU:HG2	1:B:893:ARG:HH22	1.41	0.86
1:B:854:GLN:HG3	3:B:27:HOH:O	1.76	0.84

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	280/298 (94%)	263 (94%)	14 (5%)	3 (1%)	14	42
1	B	283/298 (95%)	270 (95%)	11 (4%)	2 (1%)	22	54
All	All	563/596 (94%)	533 (95%)	25 (4%)	5 (1%)	17	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1070	GLN
1	B	987	GLU
1	B	1070	GLN
1	A	987	GLU
1	A	1071	GLY

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	260/269 (97%)	245 (94%)	15 (6%)	20	50
1	B	263/269 (98%)	255 (97%)	8 (3%)	41	75
All	All	523/538 (97%)	500 (96%)	23 (4%)	28	61

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1011	LYS
1	A	1096	ASP
1	B	1026	LEU
1	A	1069	LYS
1	A	1117	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	974	HIS
1	A	1067	ASN
1	B	924	ASN
1	A	955	GLN
1	B	955	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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	1.13	1 (6%)	19,22,24	0.75	0
1	PTR	A	1008	1	15,16,17	0.92	1 (6%)	19,22,24	0.77	0
1	PTR	A	1007	1	15,16,17	0.96	1 (6%)	19,22,24	0.83	0
1	PTR	B	1007	1	15,16,17	0.90	1 (6%)	19,22,24	0.78	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	B	1008	1	-	2/10/11/13	0/1/1/1
1	PTR	A	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	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	B	1008	PTR	P-OH	3.17	1.64	1.59
1	A	1007	PTR	P-OH	2.92	1.63	1.59
1	B	1007	PTR	P-OH	2.91	1.63	1.59
1	A	1008	PTR	P-OH	2.32	1.62	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1008	PTR	O-C-CA-CB
1	B	1008	PTR	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1008	PTR	1	0
1	A	1007	PTR	2	0

5.5   Carbohydrates ⓘ

There are no carbohydrates 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	6TP	A	1	-	24,30,30	2.83	9 (37%)	33,46,46	2.62	15 (45%)
2	6TP	B	1	-	24,30,30	3.17	11 (45%)	33,46,46	2.43	11 (33%)

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	6TP	A	1	-	-	5/22/22/22	0/3/3/3
2	6TP	B	1	-	-	6/22/22/22	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	6TP	S2-N4	10.66	1.77	1.61
2	A	1	6TP	S2-N4	9.88	1.76	1.61
2	A	1	6TP	C2-C16	4.65	1.49	1.39
2	B	1	6TP	C2-C16	4.55	1.49	1.39
2	A	1	6TP	C18-S2	-4.00	1.70	1.76

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	6TP	C5-C18-S2	-6.52	112.68	119.77
2	B	1	6TP	C5-C18-S2	-6.40	112.81	119.77
2	A	1	6TP	C17-C18-C5	5.53	128.17	120.44
2	B	1	6TP	C2-C17-C18	-5.42	113.83	119.45
2	B	1	6TP	C17-C18-C5	5.07	127.53	120.44

There are no chirality outliers.
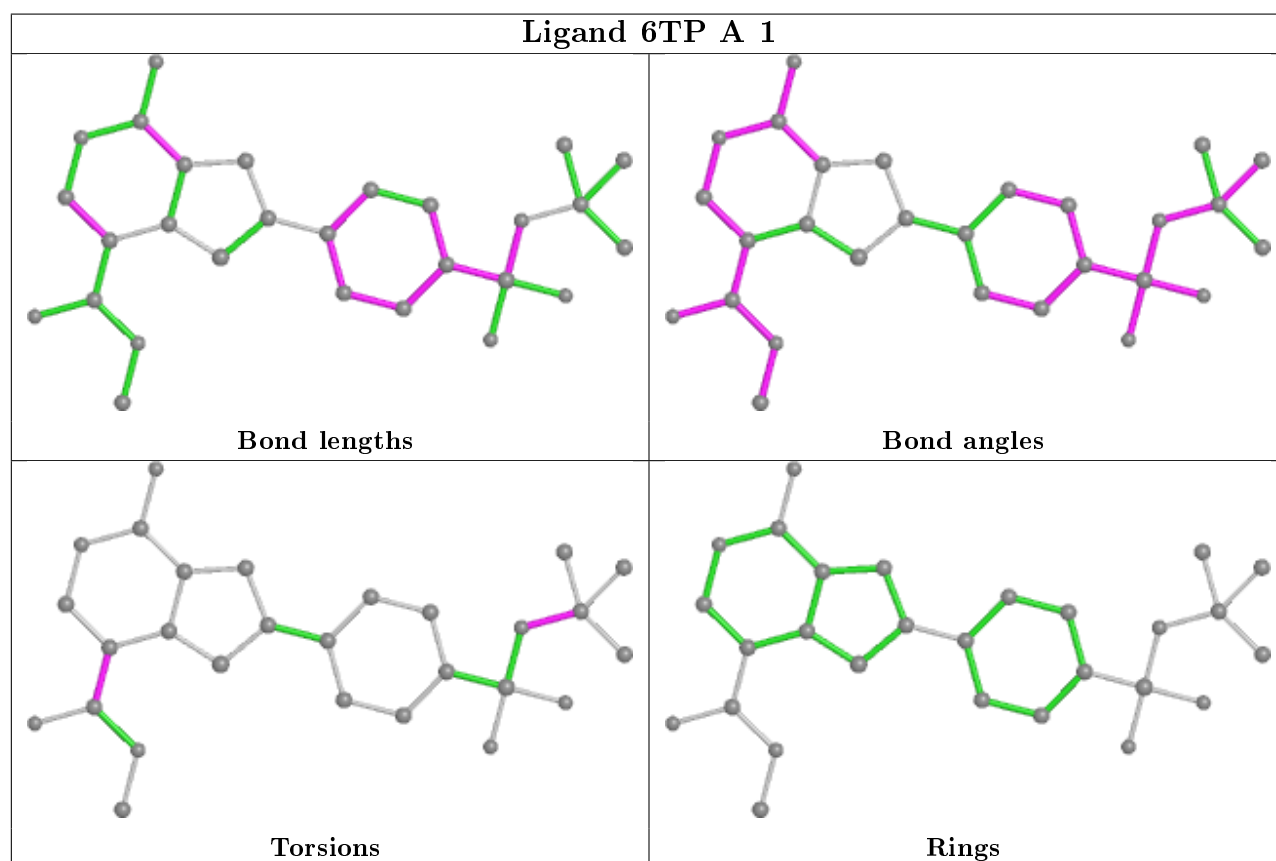
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	6TP	C13-C11-C12-O2
2	B	1	6TP	C13-C11-C12-O2
2	B	1	6TP	C13-C11-C12-N3
2	A	1	6TP	C9-C11-C12-O2
2	B	1	6TP	C9-C11-C12-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	6TP	4	0
2	B	1	6TP	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 6TP A 1

Bond lengths   Bond angles

Torsions   Rings

Ligand 6TP B 1

Bond lengths   Bond angles

Torsions   Rings
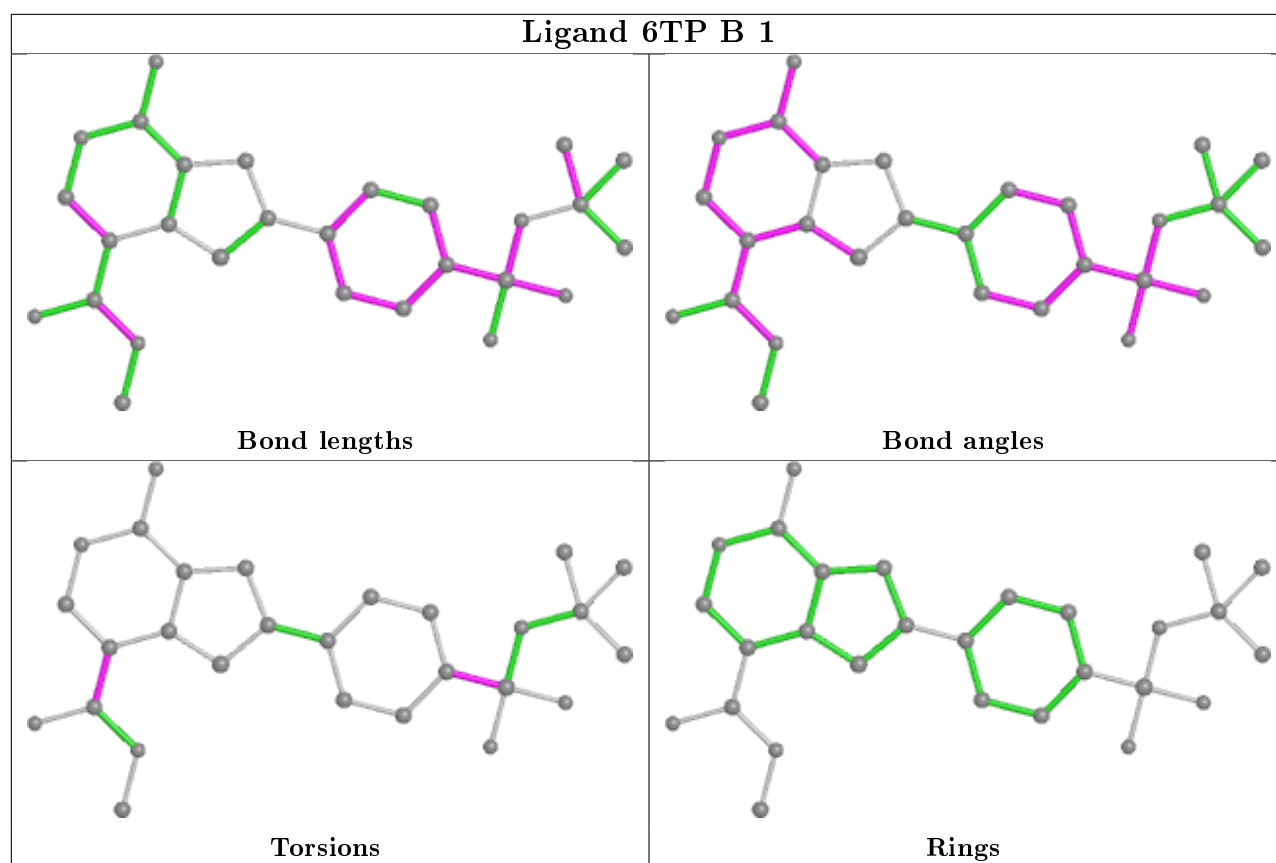
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.
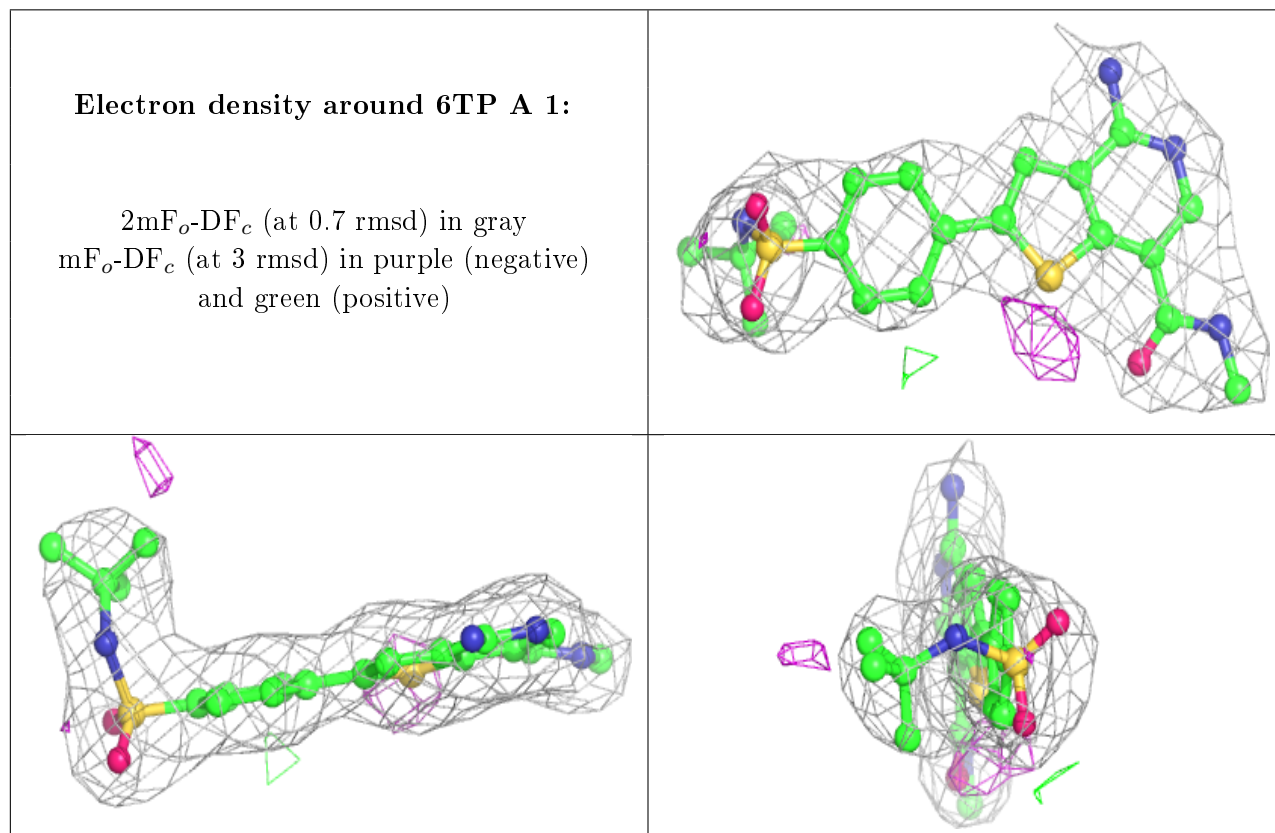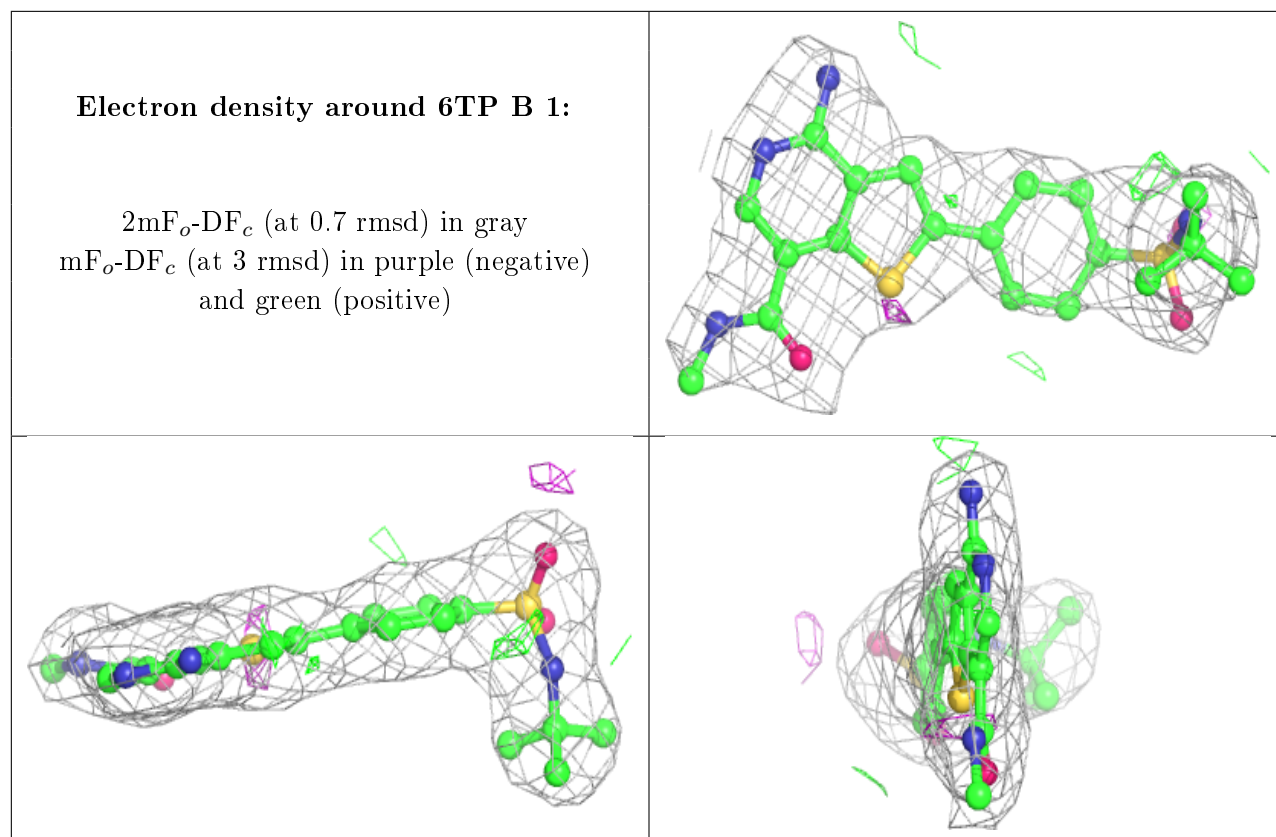
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 6TP A 1:

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

Electron density around 6TP B 1:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.