Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 12:36 AM EDT

PDB ID	:	3TJC
Title	:	Co-crystal structure of jak2 with thienopyridine 8
Authors	:	Huang, X.
Deposited on	:	2011-08-24
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

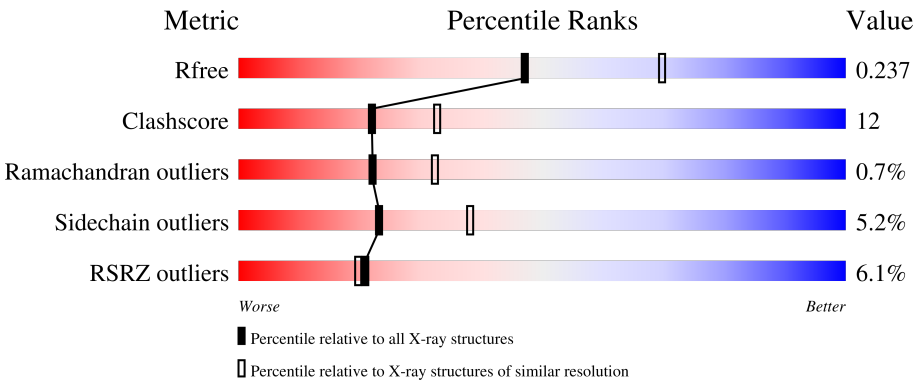
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	298	6% 74% 19%
1	B	298	5% 76% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5073 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.

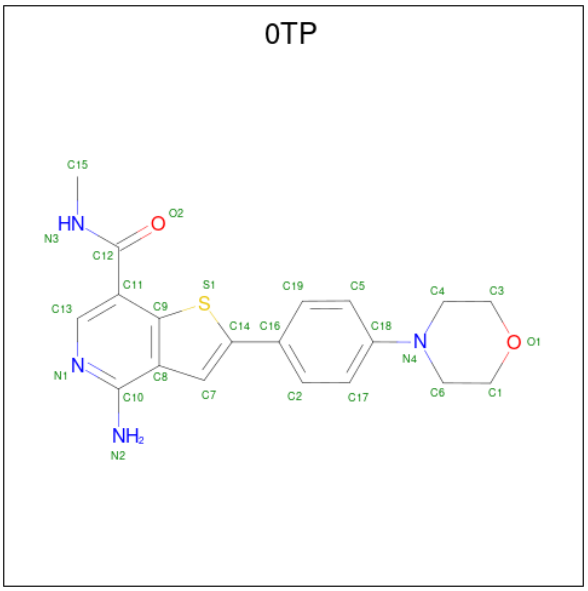
- Molecule 1 is a protein called Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	286	2373	1506	408	443	2	14	0	0	0
1	B	289	2395	1519	411	449	2	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-N-methyl-2-[4-(morpholin-4-yl)phenyl]thieno[3,2-c]pyridine-7-carboxamide (three-letter code: 0TP) (formula: $C_{19}H_{20}N_4O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	26	19	4	2	1	0	0
			Total	C	N	O	S		
2	B	1	26	19	4	2	1	0	0

- Molecule 3 is water.

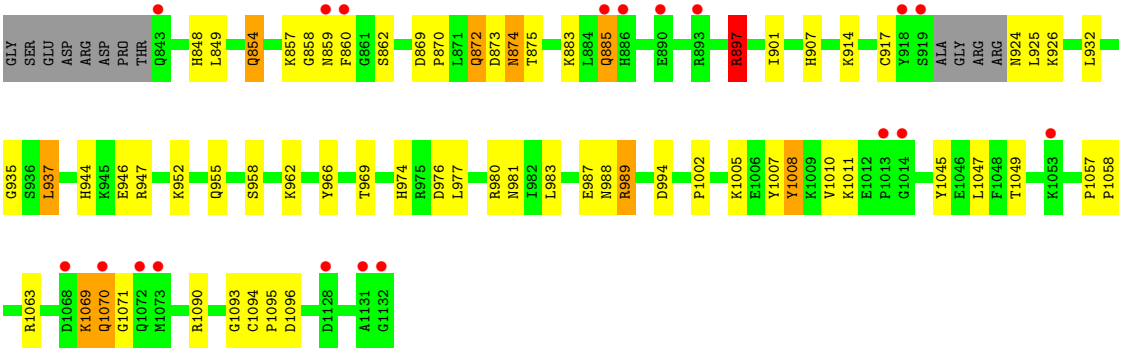
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	129	129	129	0	0
			Total	O		
3	B	124	124	124	0	0

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.

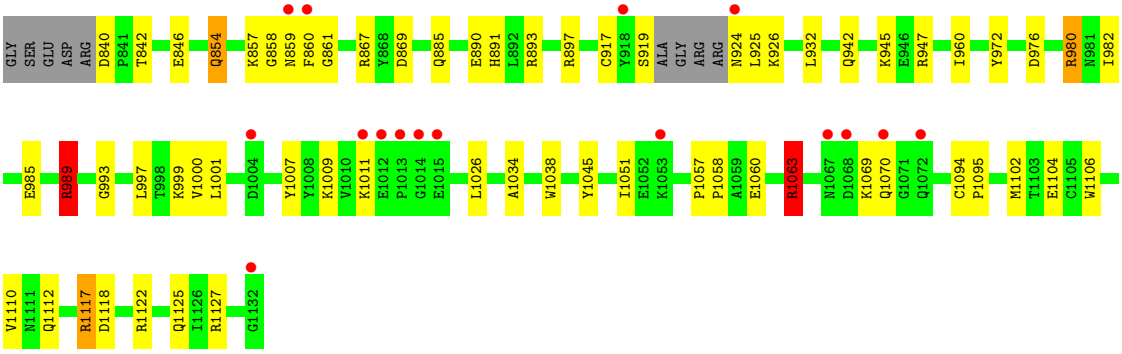
• Molecule 1: Tyrosine-protein kinase JAK2

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	112.47Å 112.47Å 70.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 28.95 – 2.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 93.6 (28.95-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.275 0.223 , 0.237	Depositor DCC
R_{free} test set	1859 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5073	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 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PTR, 0TP

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	0.59	0/2389	0.72	4/3211 (0.1%)
1	B	0.57	0/2412	0.82	8/3244 (0.2%)
All	All	0.58	0/4801	0.77	12/6455 (0.2%)

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	B	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1063	ARG	NE-CZ-NH2	-13.52	113.54	120.30
1	B	1063	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	B	1117	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	989	ARG	NE-CZ-NH1	-6.71	116.95	120.30
1	A	980	ARG	CG-CD-NE	-6.69	97.74	111.80
1	A	980	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	897	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	897	ARG	CG-CD-NE	6.16	124.73	111.80
1	B	980	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	B	980	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
1	B	980	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	993	GLY	N-CA-C	5.29	126.32	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1063	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	2344	68	1
1	B	2395	0	2362	48	1
2	A	26	0	20	4	0
2	B	26	0	20	5	0
3	A	129	0	0	6	0
3	B	124	0	0	7	1
All	All	5073	0	4746	113	2

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 12.

All (113) 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:857:LYS:NZ	1:A:885:GLN:HG2	1.57	1.20
1:A:952:LYS:HE3	1:A:955:GLN:NE2	1.65	1.09
1:A:885:GLN:OE1	1:A:885:GLN:HA	1.49	1.06
1:A:857:LYS:HZ2	1:A:885:GLN:HG2	1.07	1.05
1:B:1125:GLN:HG3	3:B:188:HOH:O	1.56	1.04
1:A:952:LYS:NZ	1:A:988:ASN:OD1	1.96	0.97
1:A:952:LYS:HE3	1:A:955:GLN:HE22	1.24	0.95
1:A:1008:PTR:HE1	1:A:1010:VAL:HB	1.53	0.90
1:A:1069:LYS:HA	1:A:1069:LYS:HE2	1.55	0.89
1:A:1069:LYS:HA	1:A:1069:LYS:CE	2.03	0.88
1:A:873:ASP:O	1:A:875:THR:HG23	1.74	0.87
1:A:857:LYS:NZ	1:A:885:GLN:CG	2.38	0.86
1:B:861:GLY:HA2	1:B:885:GLN:HG2	1.59	0.82
1:B:858:GLY:HA3	2:B:1:0TP:C1	2.12	0.79
1:B:917:CYS:HB3	1:B:926:LYS:HE3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:SER:O	1:A:962:LYS:HG3	1.85	0.76
3:A:112:HOH:O	1:B:1122:ARG:HD2	1.85	0.76
1:B:1060:GLU:OE1	1:B:1063:ARG:NH2	2.17	0.76
1:A:857:LYS:HZ1	1:A:885:GLN:HE21	1.35	0.74
1:A:1090:ARG:NH2	1:B:1104:GLU:OE1	2.21	0.74
1:A:966:TYR:O	1:A:969:THR:HG22	1.87	0.73
1:B:860:PHE:O	1:B:885:GLN:N	2.15	0.73
1:B:858:GLY:HA3	2:B:1:0TP:H1	1.74	0.69
1:B:985:GLU:OE1	1:B:989:ARG:NE	2.26	0.69
1:B:1118:ASP:OD2	3:B:271:HOH:O	2.11	0.68
1:A:944:HIS:CD2	1:A:947:ARG:HH11	2.12	0.67
1:B:890:GLU:HG2	1:B:893:ARG:HH22	1.58	0.67
1:B:932:LEU:O	2:B:1:0TP:H13	1.96	0.66
1:B:917:CYS:SG	1:B:926:LYS:HE3	2.37	0.65
1:A:872:GLN:CD	3:A:151:HOH:O	2.35	0.65
1:A:1069:LYS:CE	1:A:1069:LYS:CA	2.75	0.63
1:B:917:CYS:SG	1:B:926:LYS:NZ	2.69	0.63
1:B:917:CYS:CB	1:B:926:LYS:HE3	2.28	0.62
1:A:1069:LYS:HG3	1:A:1070:GLN:H	1.65	0.62
1:A:858:GLY:O	1:A:860:PHE:N	2.33	0.62
1:B:1045:TYR:HB2	1:B:1102:MET:HE3	1.82	0.62
1:A:857:LYS:NZ	1:A:885:GLN:HE21	1.96	0.61
1:A:854:GLN:HG3	3:A:399:HOH:O	2.01	0.61
1:B:854:GLN:NE2	3:B:307:HOH:O	2.33	0.60
1:A:857:LYS:NZ	1:A:885:GLN:NE2	2.50	0.59
1:B:919:SER:HG	1:B:924:ASN:N	2.00	0.59
1:A:932:LEU:O	2:A:1:0TP:H13	2.03	0.58
1:A:858:GLY:HA3	2:A:1:0TP:H4A	1.85	0.58
1:A:944:HIS:CD2	1:A:947:ARG:NH1	2.71	0.58
1:B:917:CYS:HB3	1:B:926:LYS:HB2	1.85	0.57
1:B:890:GLU:HG2	1:B:893:ARG:NH2	2.19	0.57
1:B:942:GLN:HG2	1:B:1051:ILE:HB	1.86	0.57
1:A:857:LYS:HZ1	1:A:885:GLN:CG	2.17	0.56
1:A:952:LYS:HE2	1:A:987:GLU:O	2.06	0.56
1:A:873:ASP:OD1	1:A:875:THR:OG1	2.15	0.55
1:B:1057:PRO:HB2	1:B:1058:PRO:HD3	1.87	0.55
1:B:917:CYS:SG	1:B:926:LYS:CE	2.94	0.55
1:A:857:LYS:HZ1	1:A:885:GLN:HG2	1.64	0.54
1:A:857:LYS:HZ1	1:A:885:GLN:NE2	2.02	0.53
1:A:1002:PRO:HG2	1:A:1005:LYS:HB2	1.90	0.53
1:A:869:ASP:OD2	1:A:872:GLN:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:ASP:O	1:A:874:ASN:C	2.48	0.52
1:B:840:ASP:OD1	1:B:842:THR:HG22	2.09	0.52
1:A:1069:LYS:CA	1:A:1069:LYS:HE3	2.38	0.52
1:A:989:ARG:NH1	3:A:233:HOH:O	2.42	0.52
1:A:952:LYS:CE	1:A:955:GLN:HE22	2.10	0.51
1:B:861:GLY:HA2	1:B:885:GLN:CG	2.38	0.51
1:A:854:GLN:CG	3:A:399:HOH:O	2.59	0.50
1:B:976:ASP:HB2	1:B:997:LEU:HD12	1.93	0.50
1:B:932:LEU:O	2:B:1:0TP:C13	2.60	0.50
1:A:974:HIS:HE1	1:A:994:ASP:O	1.95	0.50
1:A:1045:TYR:O	1:A:1049:THR:HG23	2.11	0.49
1:A:932:LEU:HD12	1:A:983:LEU:CD1	2.42	0.49
1:B:1038:TRP:CE3	1:B:1106:TRP:HA	2.47	0.49
1:A:917:CYS:HB3	1:A:926:LYS:HB2	1.95	0.48
1:A:1057:PRO:HB2	1:A:1058:PRO:HD3	1.95	0.48
1:A:907:HIS:HB2	1:A:966:TYR:CE2	2.49	0.48
1:B:999:LYS:NZ	3:B:157:HOH:O	2.32	0.47
1:A:897:ARG:O	1:A:901:ILE:HG12	2.15	0.47
1:B:867:ARG:HG2	1:B:869:ASP:HB2	1.95	0.47
1:A:1008:PTR:CE1	1:A:1010:VAL:HB	2.36	0.46
1:B:980:ARG:CD	3:B:31:HOH:O	2.64	0.46
1:B:960:ILE:CD1	1:B:982:ILE:HD13	2.46	0.45
1:A:848:HIS:CG	1:A:870:PRO:HA	2.51	0.45
1:B:860:PHE:CE2	1:B:891:HIS:CE1	3.04	0.45
1:B:960:ILE:HD13	1:B:982:ILE:HD13	1.97	0.45
1:B:846:GLU:CD	1:B:926:LYS:NZ	2.70	0.45
1:B:860:PHE:CD2	1:B:891:HIS:CE1	3.05	0.45
1:A:873:ASP:O	1:A:873:ASP:CG	2.55	0.45
1:A:974:HIS:CE1	1:A:994:ASP:O	2.69	0.45
1:A:872:GLN:HE21	1:A:872:GLN:HB3	1.56	0.44
1:A:974:HIS:HD2	1:A:976:ASP:H	1.66	0.44
1:A:1090:ARG:HH22	1:B:1104:GLU:CD	2.20	0.44
1:A:873:ASP:OD1	1:A:873:ASP:C	2.56	0.44
1:A:873:ASP:OD2	1:A:875:THR:HG21	2.17	0.43
1:A:1069:LYS:HA	1:A:1069:LYS:HE3	1.90	0.43
1:B:932:LEU:HD22	1:B:985:GLU:HA	2.00	0.43
1:A:1093:GLY:HA3	1:B:1112:GLN:O	2.18	0.43
1:B:854:GLN:HE21	1:B:854:GLN:HB3	1.52	0.43
1:B:1127:ARG:NH2	3:B:211:HOH:O	2.51	0.43
1:B:1034:ALA:CB	1:B:1110:VAL:HG13	2.48	0.42
1:A:1069:LYS:HG3	1:A:1070:GLN:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:GLY:CA	2:B:1:0TP:C1	2.90	0.42
1:B:1094:CYS:HA	1:B:1095:PRO:HD3	1.92	0.42
1:A:944:HIS:HD2	1:A:947:ARG:HD2	1.83	0.42
1:A:946:GLU:CD	1:A:946:GLU:H	2.23	0.41
1:A:914:LYS:HE3	3:A:4:HOH:O	2.19	0.41
1:B:1117:ARG:HG3	3:B:314:HOH:O	2.19	0.41
1:A:883:LYS:HB3	1:A:926:LYS:HG2	2.03	0.41
1:A:977:LEU:HD12	1:A:977:LEU:HA	1.90	0.41
1:A:873:ASP:CG	1:A:875:THR:HG23	2.41	0.41
1:A:849:LEU:HD23	1:A:849:LEU:HA	1.84	0.41
1:A:935:GLY:CA	2:A:1:0TP:H15B	2.50	0.41
1:B:972:TYR:CE2	1:B:1000:VAL:HG22	2.56	0.41
1:B:926:LYS:HE3	1:B:926:LYS:HB2	1.92	0.40
1:A:981:ASN:OD1	2:A:1:0TP:H3	2.20	0.40
1:A:937:LEU:HD13	1:A:1047:LEU:HD21	2.03	0.40
1:A:1094:CYS:HA	1:A:1095:PRO:HD3	1.95	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:NH2	1:B:989:ARG:NH1[3_755]	2.07	0.13
3:B:329:HOH:O	3:B:497:HOH:O[3_755]	2.14	0.06

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%)	266 (95%)	11 (4%)	3 (1%)	14 20
1	B	283/298 (95%)	275 (97%)	7 (2%)	1 (0%)	34 48
All	All	563/596 (94%)	541 (96%)	18 (3%)	4 (1%)	22 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	859	ASN
1	A	1070	GLN
1	A	1071	GLY
1	B	1070	GLN

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%)	246 (95%)	14 (5%)	22	36
1	B	263/269 (98%)	250 (95%)	13 (5%)	25	40
All	All	523/538 (97%)	496 (95%)	27 (5%)	23	38

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

Mol	Chain	Res	Type
1	A	854	GLN
1	A	862	SER
1	A	872	GLN
1	A	874	ASN
1	A	885	GLN
1	A	897	ARG
1	A	924	ASN
1	A	925	LEU
1	A	937	LEU
1	A	989	ARG
1	A	1011	LYS
1	A	1063	ARG
1	A	1069	LYS
1	A	1096	ASP
1	B	854	GLN
1	B	857	LYS
1	B	859	ASN
1	B	897	ARG
1	B	925	LEU

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Mol	Chain	Res	Type
1	B	945	LYS
1	B	947	ARG
1	B	989	ARG
1	B	1001	LEU
1	B	1009	LYS
1	B	1011	LYS
1	B	1026	LEU
1	B	1069	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	848	HIS
1	A	854	GLN
1	A	872	GLN
1	A	885	GLN
1	A	909	ASN
1	A	944	HIS
1	A	950	HIS
1	A	955	GLN
1	A	974	HIS
1	A	1077	HIS
1	A	1129	ASN
1	B	843	GLN
1	B	854	GLN
1	B	891	HIS
1	B	909	ASN
1	B	924	ASN
1	B	944	HIS
1	B	955	GLN
1	B	1129	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	A	1008	1	15,16,17	1.21	2 (13%)	17,22,24	0.58	0
1	PTR	A	1007	1	15,16,17	1.07	1 (6%)	17,22,24	0.67	0
1	PTR	B	1008	1	15,16,17	0.96	0	17,22,24	0.69	0
1	PTR	B	1007	1	15,16,17	1.00	1 (6%)	17,22,24	0.67	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	A	1008	1	-	1/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1008	1	-	2/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	1/10/11/13	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	CB-CA	2.88	1.59	1.53
1	A	1008	PTR	CE1-CD1	2.82	1.43	1.38
1	A	1008	PTR	CE2-CD2	2.18	1.42	1.38
1	B	1007	PTR	CB-CA	2.18	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1008	PTR	O-C-CA-CB
1	B	1008	PTR	CZ-OH-P-O1P
1	A	1008	PTR	CZ-OH-P-O2P
1	B	1007	PTR	CZ-OH-P-O1P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	0TP	B	1	-	24,29,29	2.71	11 (45%)	28,41,41	1.56	5 (17%)
2	0TP	A	1	-	24,29,29	3.21	9 (37%)	28,41,41	1.71	10 (35%)

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	0TP	B	1	-	-	5/14/22/22	0/4/4/4
2	0TP	A	1	-	-	6/14/22/22	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	0TP	C13-C11	10.68	1.46	1.37
2	B	1	0TP	C13-C11	7.96	1.43	1.37
2	A	1	0TP	C10-C8	4.85	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	0TP	C17-C18	4.73	1.48	1.39
2	A	1	0TP	C19-C16	4.29	1.47	1.39
2	A	1	0TP	C5-C18	4.26	1.47	1.39
2	B	1	0TP	C2-C16	4.26	1.47	1.39
2	B	1	0TP	C5-C18	4.06	1.47	1.39
2	B	1	0TP	C17-C18	4.05	1.46	1.39
2	A	1	0TP	C2-C16	3.95	1.47	1.39
2	B	1	0TP	C17-C2	3.54	1.44	1.38
2	B	1	0TP	C19-C16	3.33	1.46	1.39
2	B	1	0TP	C8-C9	2.78	1.44	1.41
2	A	1	0TP	C11-C12	-2.78	1.46	1.50
2	A	1	0TP	C14-S1	-2.61	1.68	1.72
2	B	1	0TP	C19-C5	2.54	1.42	1.38
2	B	1	0TP	C10-C8	2.28	1.47	1.45
2	B	1	0TP	C12-N3	2.26	1.36	1.33
2	A	1	0TP	C6-N4	2.17	1.50	1.46
2	B	1	0TP	C11-C12	-2.04	1.47	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	0TP	C17-C18-N4	-2.89	117.38	121.39
2	A	1	0TP	C13-N1-C10	2.85	121.39	118.64
2	A	1	0TP	C3-C4-N4	-2.72	104.77	109.93
2	A	1	0TP	C5-C18-N4	-2.56	117.83	121.39
2	A	1	0TP	C8-C10-N1	2.53	124.66	121.90
2	B	1	0TP	C1-C6-N4	-2.47	105.25	109.93
2	A	1	0TP	O1-C3-C4	-2.47	106.46	111.77
2	A	1	0TP	C4-N4-C18	2.24	124.21	118.11
2	B	1	0TP	C3-C4-N4	-2.23	105.70	109.93
2	A	1	0TP	C11-C9-S1	2.21	128.67	124.59
2	B	1	0TP	C6-N4-C4	2.19	116.48	111.57
2	A	1	0TP	C19-C16-C2	2.18	121.58	117.68
2	B	1	0TP	O2-C12-C11	2.15	124.48	121.73
2	A	1	0TP	O2-C12-C11	2.04	124.34	121.73
2	A	1	0TP	O1-C1-C6	-2.02	107.42	111.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	0TP	C9-C11-C12-O2

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Mol	Chain	Res	Type	Atoms
2	A	1	0TP	C9-C11-C12-N3
2	B	1	0TP	C9-C11-C12-O2
2	B	1	0TP	C9-C11-C12-N3
2	A	1	0TP	C13-C11-C12-O2
2	B	1	0TP	C13-C11-C12-O2
2	A	1	0TP	C13-C11-C12-N3
2	B	1	0TP	C13-C11-C12-N3
2	A	1	0TP	C11-C12-N3-C15
2	A	1	0TP	O2-C12-N3-C15
2	B	1	0TP	C5-C18-N4-C4

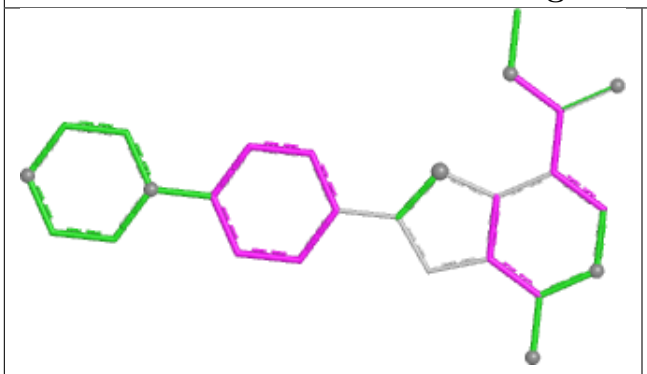
There are no ring outliers.

2 monomers are involved in 9 short contacts:

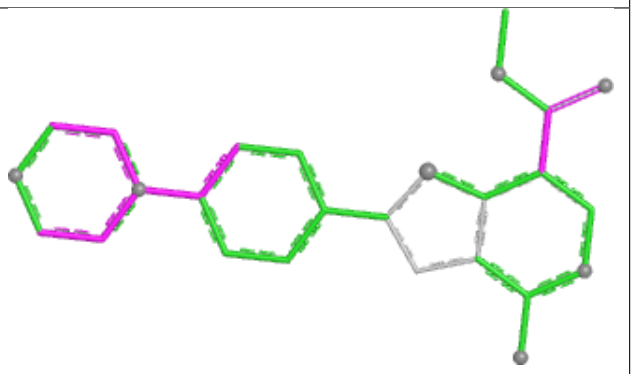
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	0TP	5	0
2	A	1	0TP	4	0

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.

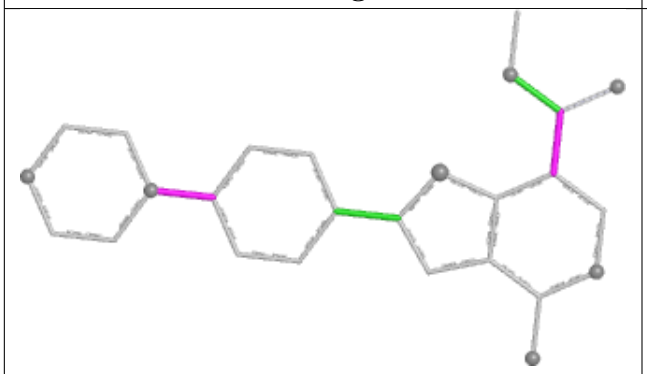
Ligand 0TP B 1



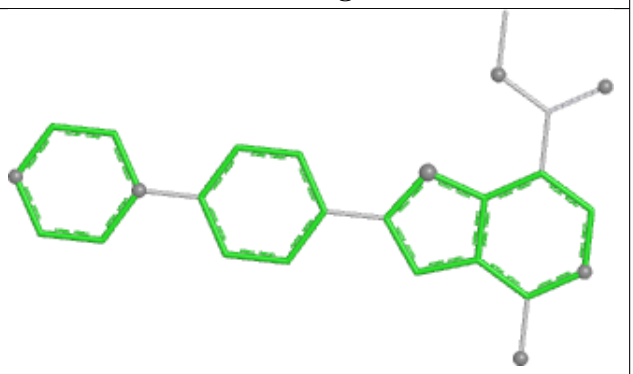
Bond lengths



Bond angles

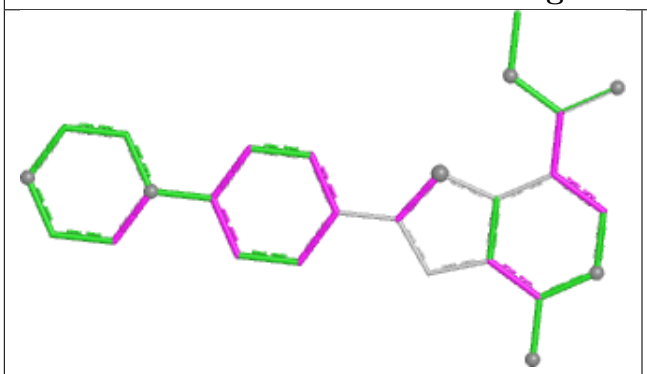


Torsions

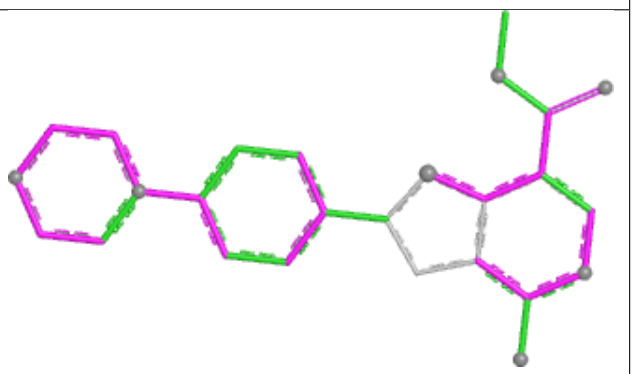


Rings

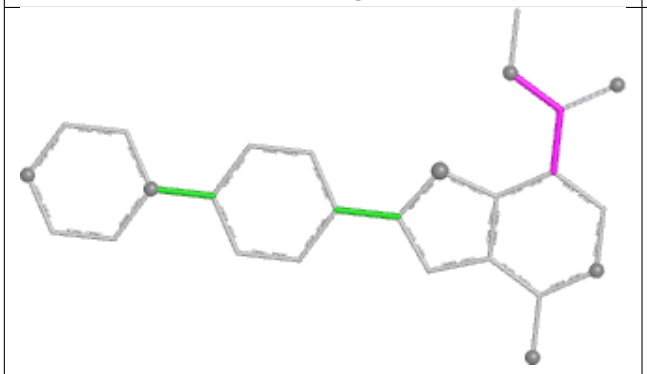
Ligand 0TP A 1



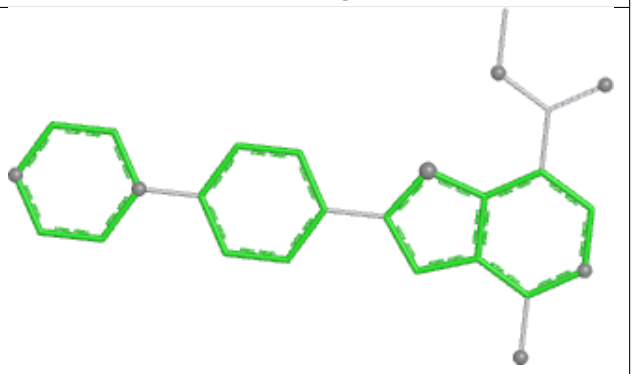
Bond lengths



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)

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	284/298 (95%)	0.14	19 (6%)	17	16	14, 30, 60, 79	0
1	B	287/298 (96%)	0.07	16 (5%)	24	23	17, 31, 58, 75	0
All	All	571/596 (95%)	0.10	35 (6%)	21	20	14, 30, 59, 79	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1013	PRO	7.5
1	A	1132	GLY	7.2
1	B	1068	ASP	6.0
1	A	859	ASN	5.0
1	B	1012	GLU	4.6
1	A	918	TYR	4.4
1	B	1070	GLN	4.4
1	B	1011	LYS	4.3
1	A	1131	ALA	3.9
1	A	1068	ASP	3.8
1	B	1053	LYS	3.7
1	A	1070	GLN	3.6
1	A	1014	GLY	3.6
1	A	1072	GLN	3.3
1	B	1014	GLY	3.3
1	B	1132	GLY	3.2
1	A	919	SER	3.2
1	B	918	TYR	3.1
1	B	1072	GLN	3.0
1	B	1015	GLU	2.9
1	A	860	PHE	2.9
1	B	1067	ASN	2.8
1	A	1053	LYS	2.7
1	A	1128	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	859	ASN	2.5
1	B	860	PHE	2.5
1	A	1073	MET	2.4
1	A	885	GLN	2.3
1	A	890	GLU	2.3
1	B	924	ASN	2.3
1	A	893	ARG	2.3
1	B	1004	ASP	2.2
1	A	843	GLN	2.2
1	A	886	HIS	2.2
1	A	1013	PRO	2.1

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	1007	16/17	0.82	0.17	47,49,55,56	0
1	PTR	B	1008	16/17	0.84	0.17	47,49,56,57	0
1	PTR	A	1008	16/17	0.85	0.15	38,46,54,55	0
1	PTR	A	1007	16/17	0.88	0.17	39,47,60,61	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

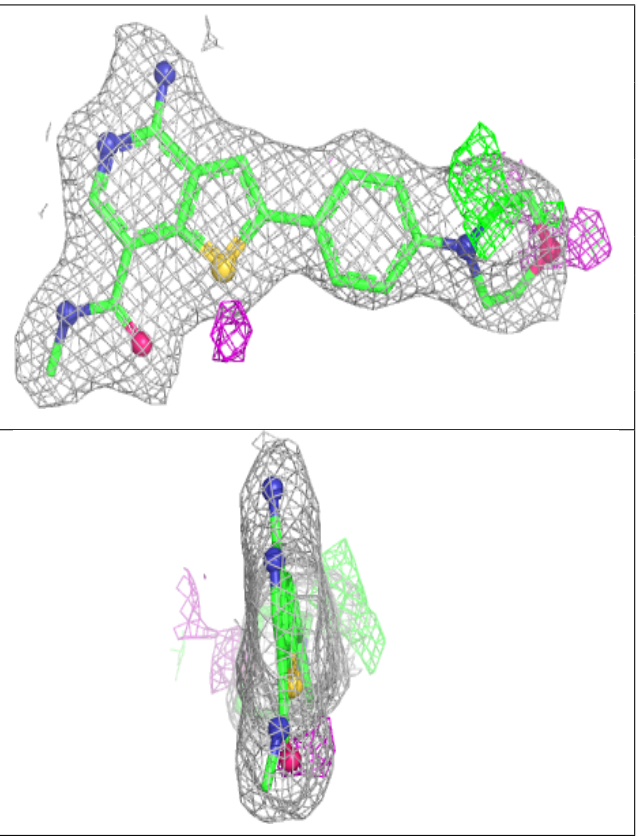
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	0TP	A	1	26/26	0.91	0.19	17,23,46,49	0
2	0TP	B	1	26/26	0.91	0.16	16,24,42,43	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.

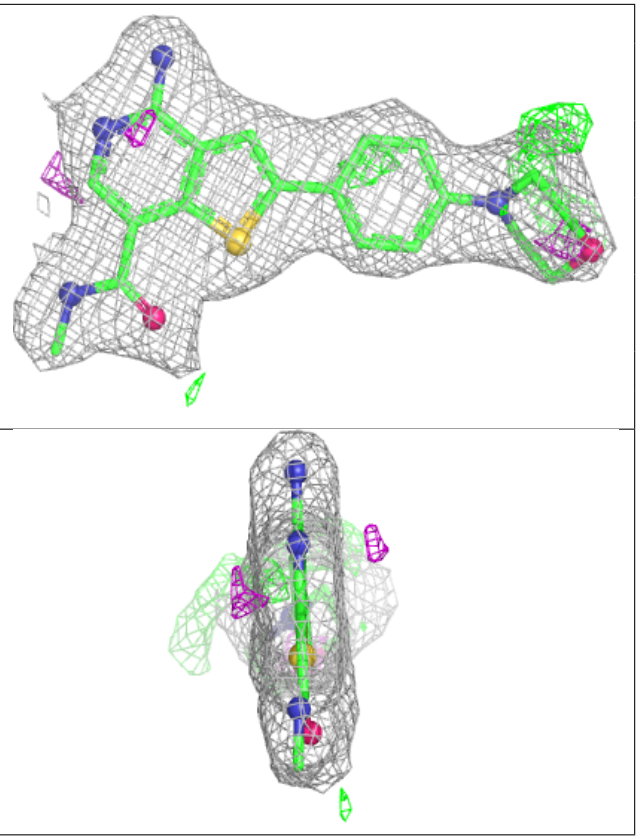
Electron density around 0TP A 1:

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



Electron density around 0TP 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)

There are no such residues in this entry.