



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2021 – 10:05 AM EDT

PDB ID : 6W9E  
Title : Crystal Structure of Human CDK9/cyclinT1 in complex with MC180295  
Authors : Zhang, P.; Wu, J.  
Deposited on : 2020-03-22  
Resolution : 3.10 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](mailto: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.

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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 : 2.23.1  
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) : 2.23.1

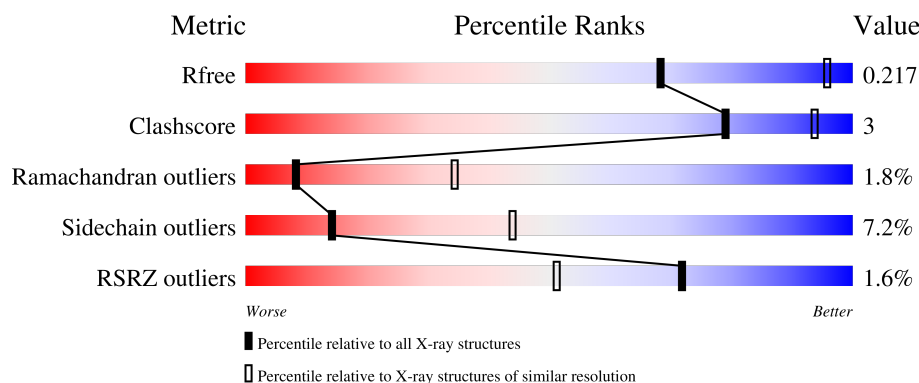
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

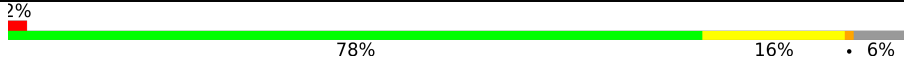

The reported resolution of this entry is 3.10 Å.

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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	330	
2	B	259	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4688 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 Cyclin-dependent kinase 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	P	S	0	0	0
			2494	1596	429	453	2	14			

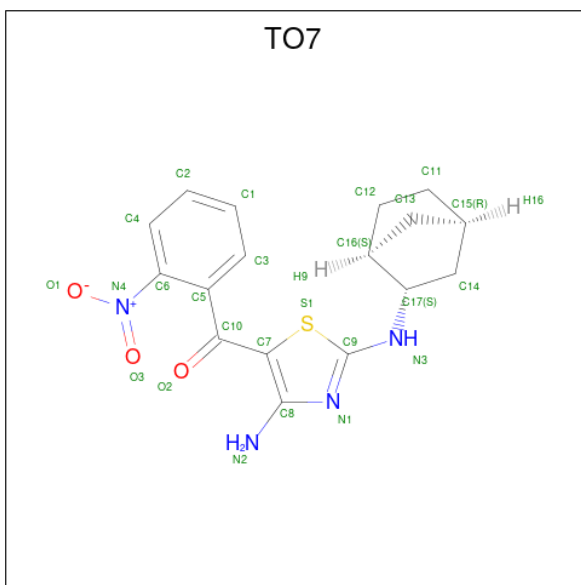
- Molecule 2 is a protein called Cyclin-T1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			2061	1318	360	374	9			

There are 3 discrepancies between the modelled and reference sequences:

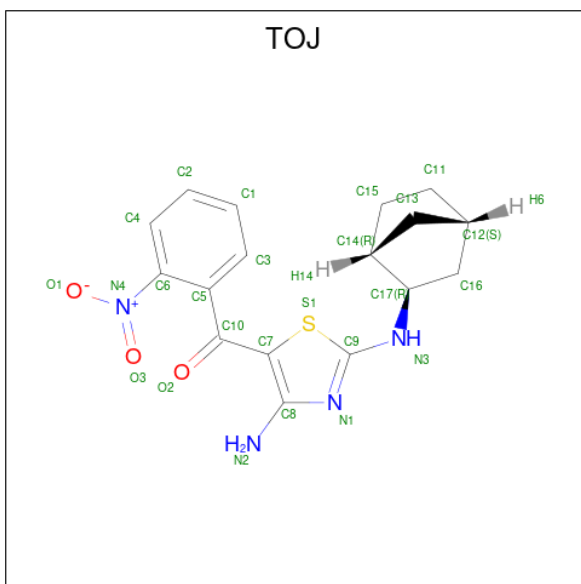
Chain	Residue	Modelled	Actual	Comment	Reference
B	77	ARG	GLN	engineered mutation	UNP O60563
B	96	GLY	GLU	engineered mutation	UNP O60563
B	241	LEU	PHE	engineered mutation	UNP O60563

- Molecule 3 is (4-amino-2-{{[(1S,2S,4R)-bicyclo[2.2.1]heptan-2-yl]amino}-1,3-thiazol-5-yl})(2-nitrophenyl)methanone (three-letter code: TO7) (formula: C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			25	17	4	3	1		
3	A	1	Total	C	N	O	S	0	1
			25	17	4	3	1		

- Molecule 4 is (4-amino-2-[(1R,2R,4S)-bicyclo[2.2.1]heptan-2-yl]amino}-1,3-thiazol-5-yl)(2-nitrophenyl)methanone (three-letter code: TOJ) (formula: C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			25	17	4	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			25	17	4	3	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

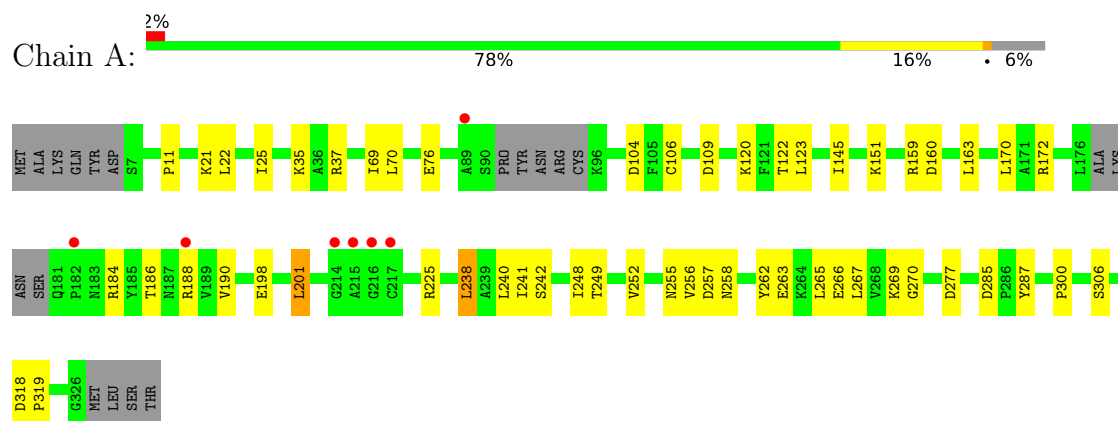
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	15	Total	O	0	0
			15	15		

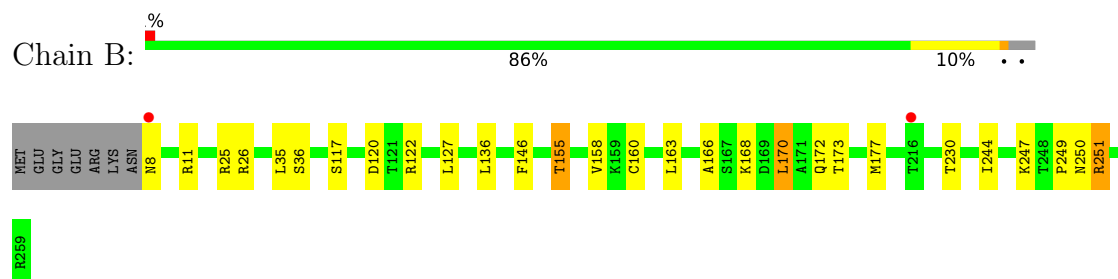
### 3 Residue-property plots [i](#)

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: Cyclin-dependent kinase 9



#### • Molecule 2: Cyclin-T1



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.34Å 173.34Å 97.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.67 – 3.10 28.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (86.67-3.10) 99.7 (28.89-3.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.172 , 0.221 0.172 , 0.217	Depositor DCC
$R_{free}$ test set	1014 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.8	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SEP, TO7, PO4, TPO, TOJ

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	0.54	0/2521	0.84	1/3404 (0.0%)
2	B	0.49	0/2114	0.78	0/2879
All	All	0.52	0/4635	0.81	1/6283 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	37	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	GLU	Peptide

### 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	2494	0	2511	14	0
2	B	2061	0	2049	8	0
3	A	50	0	0	2	0
4	A	50	0	0	3	0
5	B	5	0	0	0	0
6	A	13	0	0	0	0
6	B	15	0	0	0	0
All	All	4688	0	4560	26	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 (26) 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:248:ILE:HG22	1:A:256:VAL:HG21	1.78	0.65
3:A:401[A]:TO7:C10	3:A:401[A]:TO7:O3	2.48	0.61
1:A:21:LYS:O	1:A:22:LEU:HD23	2.00	0.60
4:A:404[D]:TOJ:C10	4:A:404[D]:TOJ:O3	2.52	0.57
1:A:69:ILE:HG23	1:A:145:ILE:HD13	1.88	0.55
2:B:166:ALA:HB1	2:B:170:LEU:HB3	1.90	0.54
1:A:257:ASP:HA	1:A:262:TYR:CD2	2.46	0.51
2:B:8:ASN:HB3	2:B:11:ARG:HB2	1.94	0.49
1:A:25:ILE:CG2	1:A:35:LYS:HB2	2.43	0.49
1:A:123:LEU:HD23	1:A:319:PRO:HD2	1.96	0.48
2:B:168:LYS:O	2:B:172:GLN:HG2	2.16	0.45
1:A:106:CYS:O	4:A:403[C]:TOJ:N3	2.49	0.45
2:B:155:THR:HA	2:B:158:VAL:HG12	1.98	0.45
1:A:285:ASP:OD1	1:A:287:TYR:HB2	2.17	0.45
1:A:198:GLU:HG2	1:A:300:PRO:HG3	1.99	0.44
4:A:404[D]:TOJ:C16	4:A:404[D]:TOJ:S1	3.06	0.43
1:A:238:LEU:HA	1:A:241:ILE:HD12	2.00	0.43
2:B:173:THR:O	2:B:177:MET:HG2	2.20	0.42
2:B:120:ASP:C	2:B:122:ARG:H	2.23	0.42
1:A:25:ILE:HG23	1:A:35:LYS:HB2	2.02	0.41
1:A:120:LYS:HA	1:A:225:ARG:HH22	1.84	0.41
1:A:248:ILE:CG2	1:A:256:VAL:HG21	2.49	0.41
3:A:402[B]:TO7:O3	3:A:402[B]:TO7:C10	2.69	0.41
2:B:247:LYS:O	2:B:249:PRO:HD3	2.20	0.41
2:B:251:ARG:HD3	2:B:251:ARG:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD23	1:A:238:LEU:HD11	2.04	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	303/330 (92%)	259 (86%)	36 (12%)	8 (3%)	5	26
2	B	250/259 (96%)	239 (96%)	9 (4%)	2 (1%)	19	54
All	All	553/589 (94%)	498 (90%)	45 (8%)	10 (2%)	8	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	LYS
1	A	190	VAL
1	A	258	ASN
1	A	266	GLU
1	A	267	LEU
2	B	146	PHE
1	A	201	LEU
2	B	250	ASN
1	A	270	GLY
1	A	255	ASN

### 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	267/290 (92%)	245 (92%)	22 (8%)	11	38
2	B	230/236 (98%)	216 (94%)	14 (6%)	18	49
All	All	497/526 (94%)	461 (93%)	36 (7%)	14	44

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	70	LEU
1	A	76	GLU
1	A	104	ASP
1	A	109	ASP
1	A	122	THR
1	A	151	LYS
1	A	159	ARG
1	A	160	ASP
1	A	163	LEU
1	A	170	LEU
1	A	172	ARG
1	A	184	ARG
1	A	188	ARG
1	A	238	LEU
1	A	240	LEU
1	A	242	SER
1	A	249	THR
1	A	252	VAL
1	A	265	LEU
1	A	277	ASP
1	A	318	ASP
2	B	25	ARG
2	B	26	ARG
2	B	35	LEU
2	B	36	SER
2	B	117	SER
2	B	127	LEU
2	B	136	LEU
2	B	155	THR
2	B	160	CYS
2	B	163	LEU
2	B	170	LEU

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Mol	Chain	Res	Type
2	B	230	THR
2	B	244	ILE
2	B	251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	258	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	SEP	A	306	1	8,9,10	1.14	0	8,12,14	5.02	4 (50%)
1	TPO	A	186	1	8,10,11	0.71	0	10,14,16	1.63	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	SEP	A	306	1	-	5/5/8/10	-
1	TPO	A	186	1	-	0/9/11/13	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	SEP	OG-CB-CA	12.69	120.50	108.14
1	A	306	SEP	P-OG-CB	3.60	128.20	118.30
1	A	306	SEP	OG-P-O1P	3.52	116.36	106.47
1	A	186	TPO	P-OG1-CB	-3.44	112.82	123.21
1	A	306	SEP	O3P-P-O2P	3.05	119.30	107.64
1	A	186	TPO	CG2-CB-CA	2.04	117.18	113.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	306	SEP	N-CA-CB-OG
1	A	306	SEP	CB-OG-P-O1P
1	A	306	SEP	CB-OG-P-O2P
1	A	306	SEP	CB-OG-P-O3P
1	A	306	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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
3	TO7	A	402[B]	-	21,28,28	2.59	3 (14%)	25,41,41	1.05	3 (12%)
4	TOJ	A	404[D]	-	21,28,28	2.56	3 (14%)	25,41,41	1.15	2 (8%)
5	PO4	B	301	-	4,4,4	0.96	0	6,6,6	0.67	0
4	TOJ	A	403[C]	-	21,28,28	2.57	3 (14%)	25,41,41	1.23	3 (12%)
3	TO7	A	401[A]	-	21,28,28	2.57	3 (14%)	25,41,41	1.02	3 (12%)

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
4	TOJ	A	403[C]	-	-	3/8/33/33	0/5/4/4
4	TOJ	A	404[D]	-	-	3/8/33/33	0/5/4/4
3	TO7	A	402[B]	-	-	1/8/33/33	0/5/4/4
3	TO7	A	401[A]	-	-	2/8/33/33	0/5/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[B]	TO7	O3-N4	10.28	1.40	1.22
4	A	403[C]	TOJ	O3-N4	10.15	1.40	1.22
4	A	404[D]	TOJ	O3-N4	9.86	1.39	1.22
3	A	401[A]	TO7	O3-N4	9.84	1.39	1.22
4	A	403[C]	TOJ	C8-N2	4.51	1.45	1.34
4	A	404[D]	TOJ	C8-N2	4.48	1.45	1.34
3	A	401[A]	TO7	C8-N2	4.35	1.45	1.34
3	A	402[B]	TO7	C8-N2	4.28	1.44	1.34
4	A	404[D]	TOJ	C6-N4	-3.90	1.38	1.45
3	A	401[A]	TO7	C6-N4	-3.85	1.38	1.45
4	A	403[C]	TOJ	C6-N4	-3.15	1.40	1.45
3	A	402[B]	TO7	C6-N4	-3.10	1.40	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403[C]	TOJ	C4-C6-N4	3.56	120.28	116.47
3	A	402[B]	TO7	C4-C6-N4	3.15	119.84	116.47
4	A	403[C]	TOJ	C16-C17-N3	2.70	118.65	112.67
4	A	404[D]	TOJ	C16-C17-N3	2.48	118.17	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404[D]	TOJ	C13-C14-C17	2.42	103.83	100.76
4	A	403[C]	TOJ	C6-C5-C10	-2.33	120.26	124.26
3	A	401[A]	TO7	C13-C16-C17	2.27	103.64	100.76
3	A	401[A]	TO7	O2-C10-C7	-2.22	114.60	118.58
3	A	401[A]	TO7	C4-C6-N4	2.17	118.79	116.47
3	A	402[B]	TO7	C13-C16-C17	2.15	103.49	100.76
3	A	402[B]	TO7	C6-C5-C10	-2.13	120.60	124.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403[C]	TOJ	C4-C6-N4-O3
4	A	403[C]	TOJ	C5-C6-N4-O3
4	A	403[C]	TOJ	C16-C17-N3-C9
4	A	404[D]	TOJ	C16-C17-N3-C9
3	A	401[A]	TO7	O2-C10-C5-C6
3	A	401[A]	TO7	C7-C10-C5-C6
4	A	404[D]	TOJ	C7-C10-C5-C6
4	A	404[D]	TOJ	O2-C10-C5-C6
3	A	402[B]	TO7	C4-C6-N4-O3

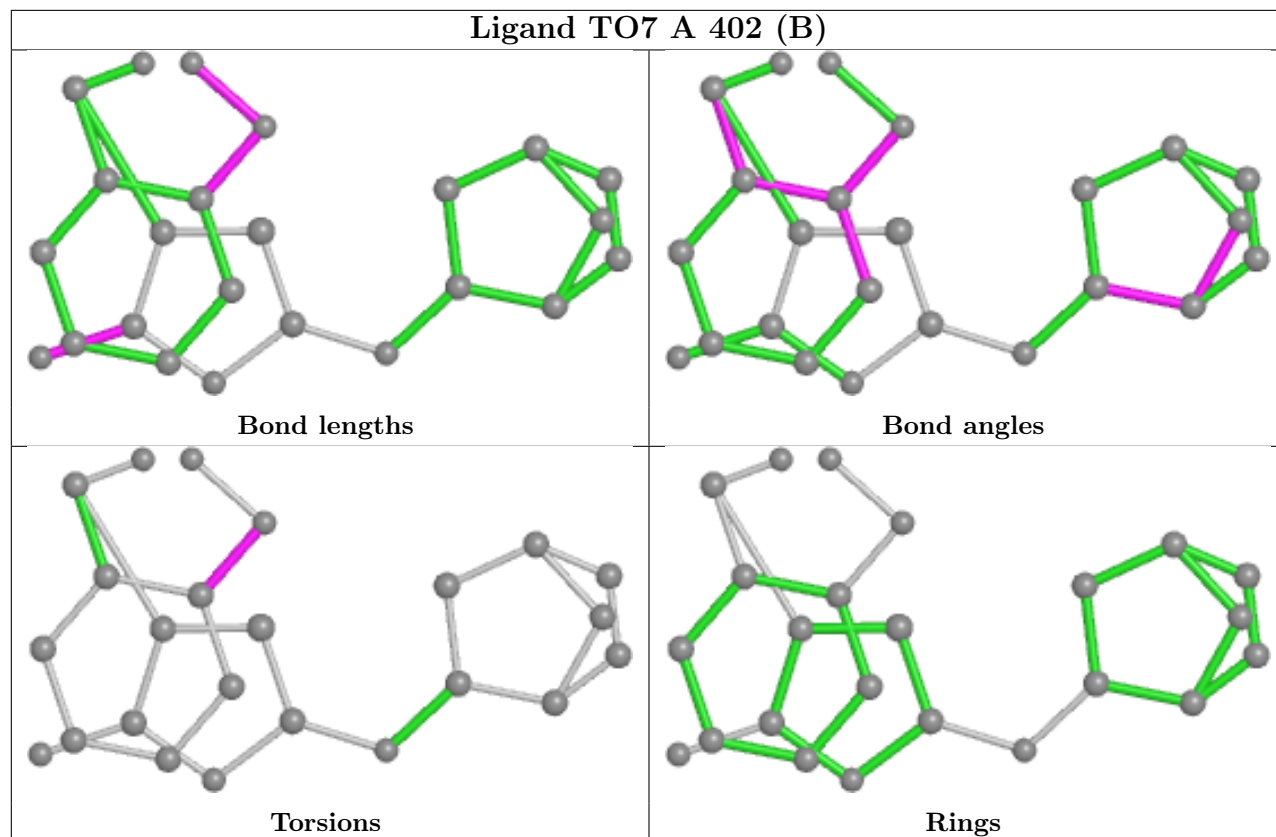
There are no ring outliers.

4 monomers are involved in 5 short contacts:

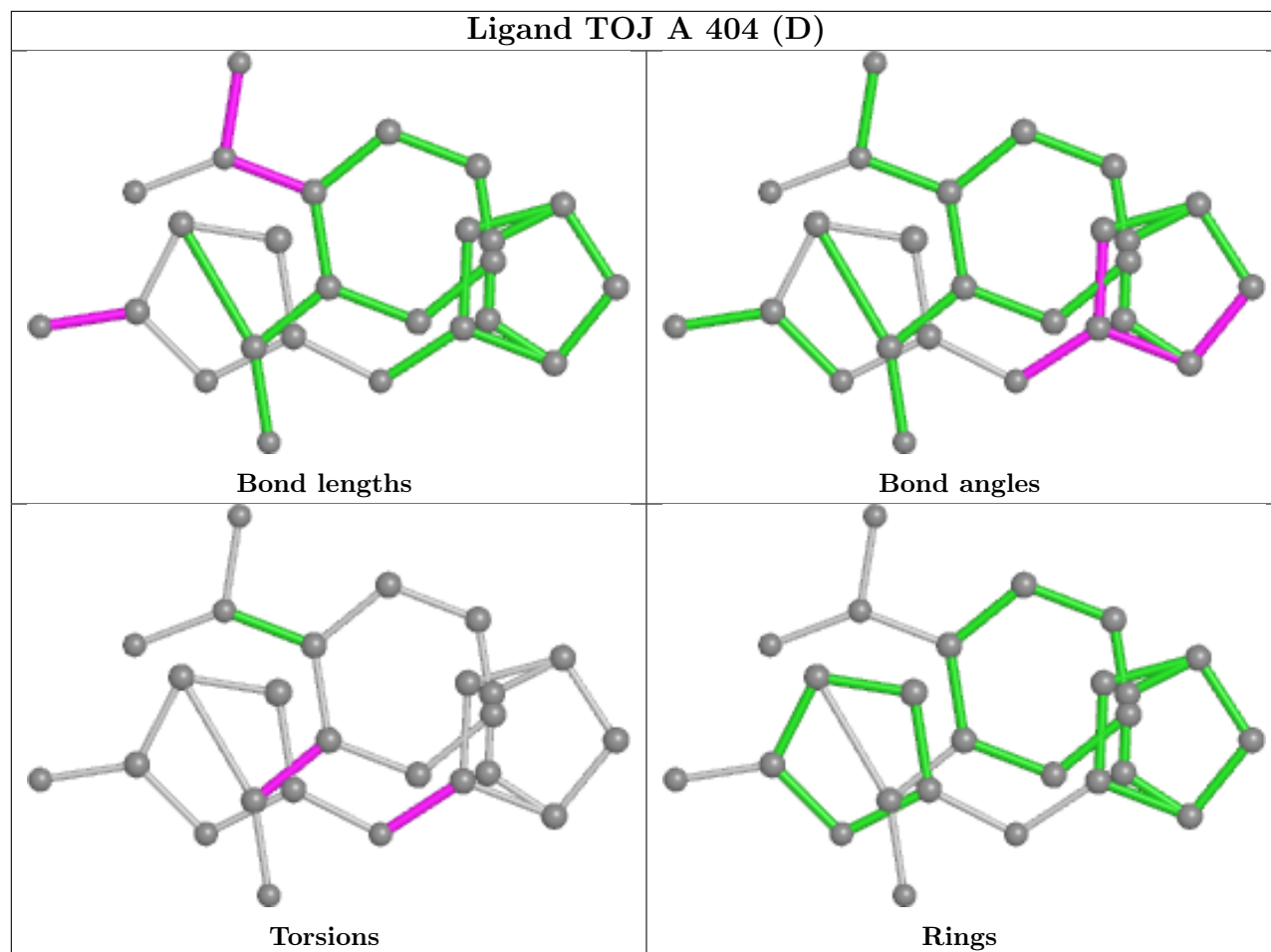
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402[B]	TO7	1	0
4	A	404[D]	TOJ	2	0
4	A	403[C]	TOJ	1	0
3	A	401[A]	TO7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

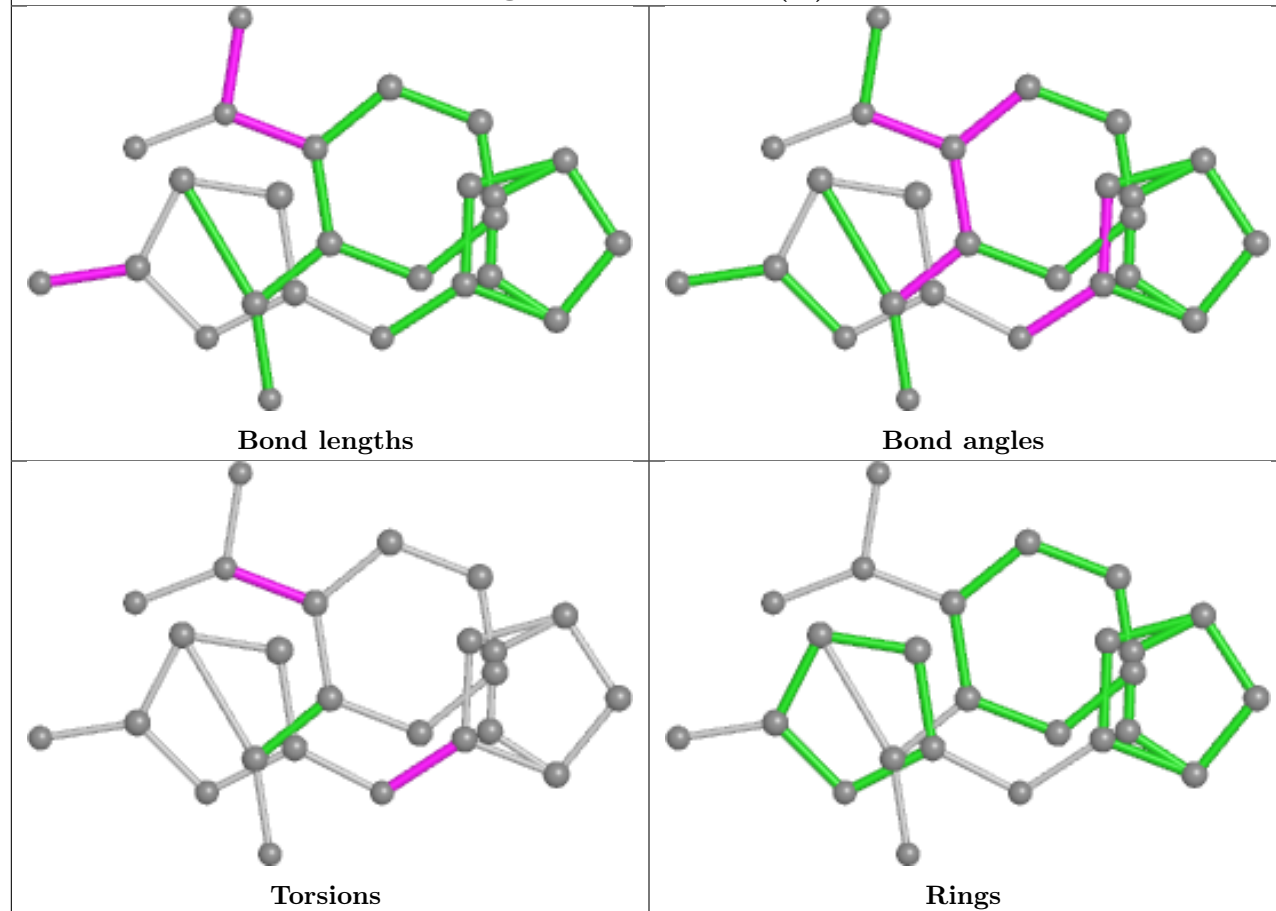
equivalents in the CSD to analyse the geometry.



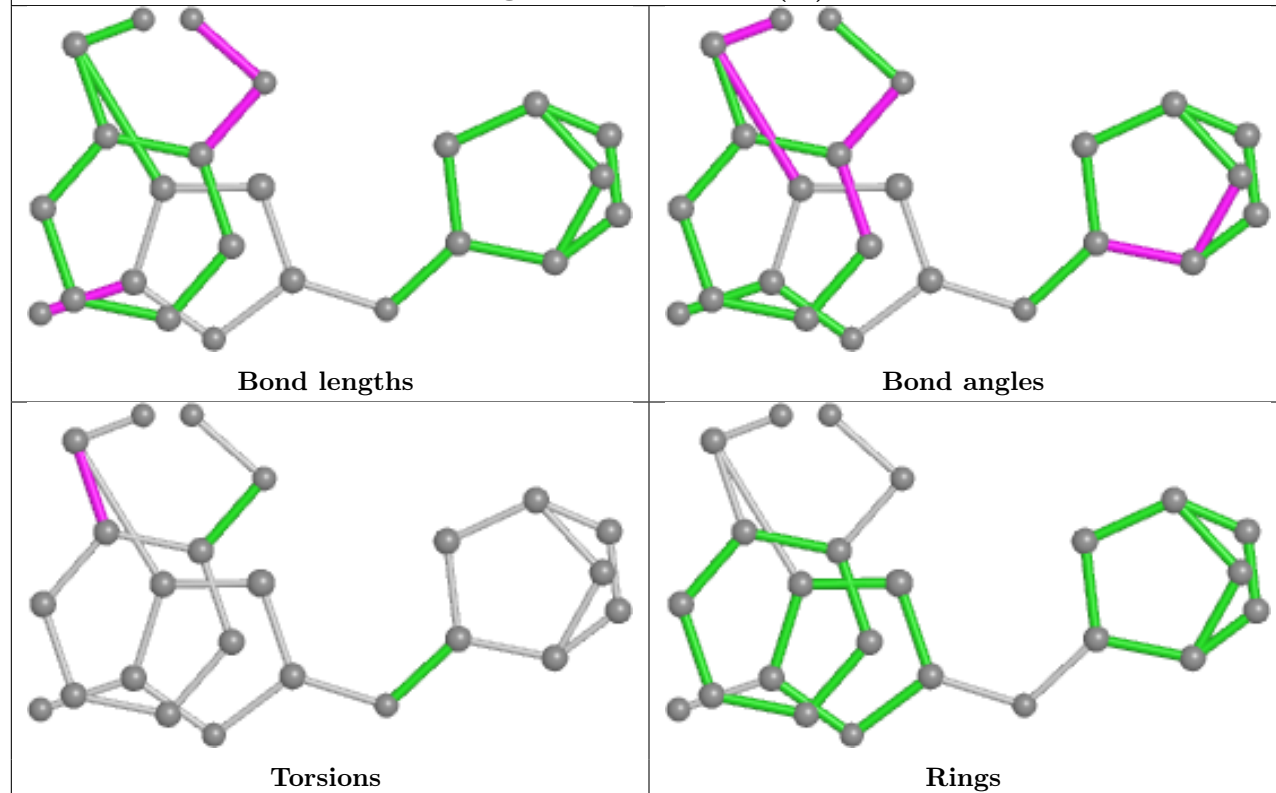




## Ligand TOJ A 403 (C)



## Ligand TO7 A 401 (A)



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	309/330 (93%)	-0.24	7 (2%) 60 39	67, 109, 167, 202	0
2	B	252/259 (97%)	-0.50	2 (0%) 86 72	68, 93, 153, 185	0
All	All	561/589 (95%)	-0.36	9 (1%) 72 51	67, 103, 164, 202	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	CYS	3.7
1	A	214	GLY	3.3
1	A	89	ALA	3.1
1	A	188	ARG	3.0
1	A	216	GLY	2.7
1	A	215	ALA	2.5
2	B	8	ASN	2.2
2	B	216	THR	2.2
1	A	182	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	A	306	10/11	0.97	0.15	81,102,107,109	0
1	TPO	A	186	11/12	0.98	0.14	92,99,115,115	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

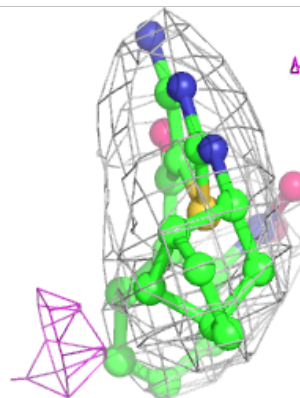
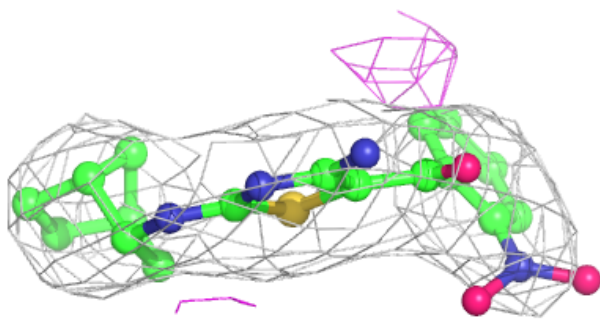
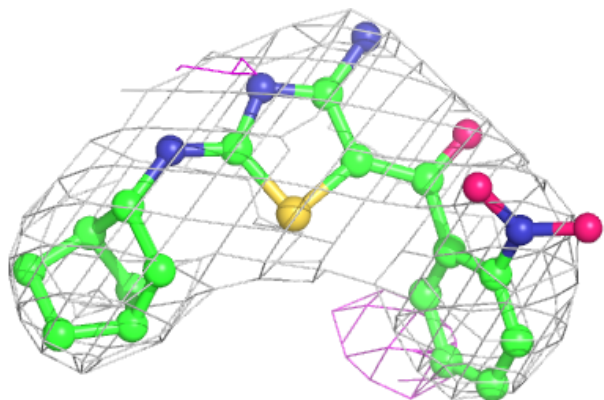
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	B	301	5/5	0.96	0.12	89,93,110,135	0
4	TOJ	A	403[C]	25/25	0.97	0.21	91,97,109,111	25
3	TO7	A	401[A]	25/25	0.98	0.21	85,88,103,108	25
4	TOJ	A	404[D]	25/25	0.98	0.21	91,95,108,113	25
3	TO7	A	402[B]	25/25	0.98	0.22	85,87,108,112	25

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.

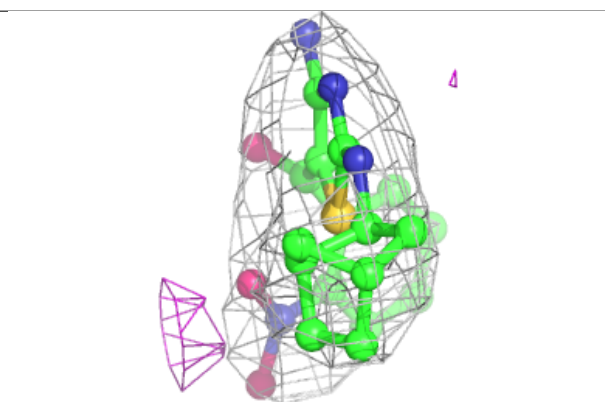
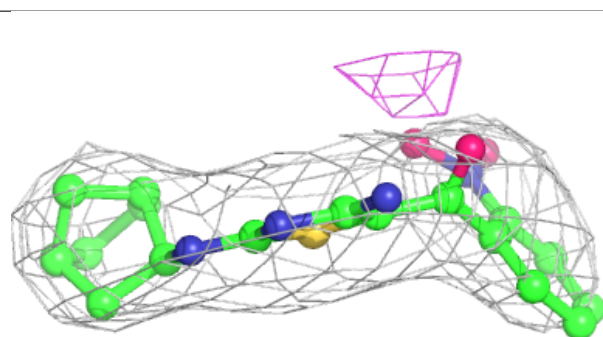
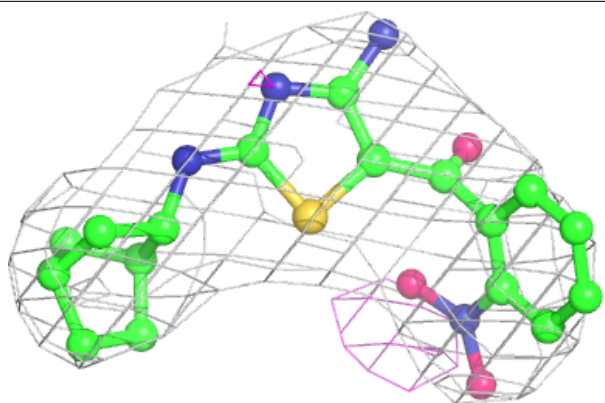
#### Electron density around TOJ A 403 (C):

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

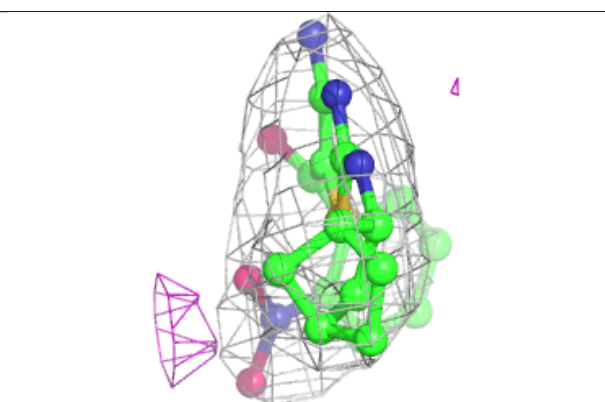
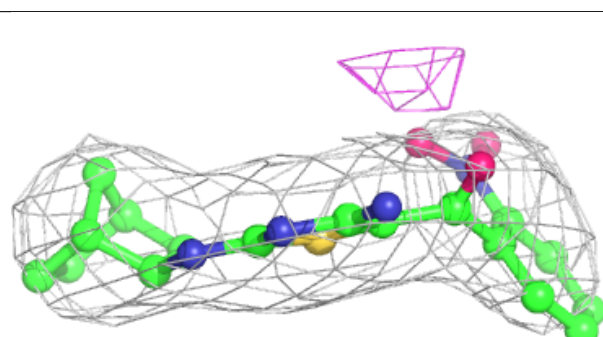
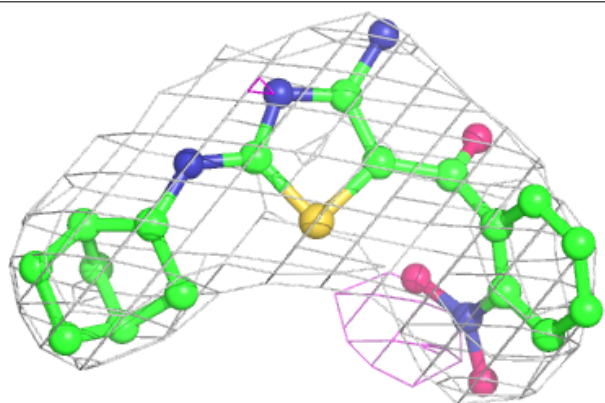


**Electron density around TO7 A 401 (A):**

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

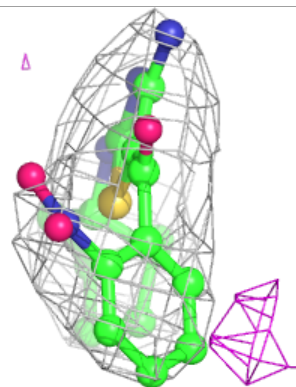
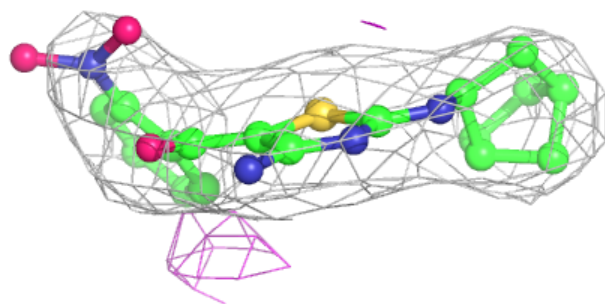
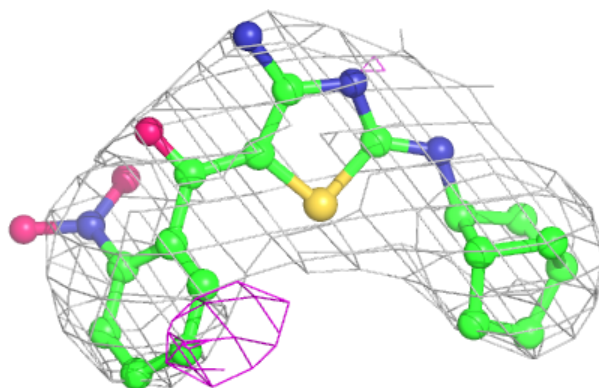
**Electron density around TOJ A 404 (D):**

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



**Electron density around TO7 A 402 (B):**

$2mF_o - DF_c$  (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.