



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:34 pm BST

PDB ID : 5T1T  
Title : Irak4 kinase - compound 1 co-structure  
Authors : Fischmann, T.O.  
Deposited on : 2016-08-22  
Resolution : 2.34 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	:	2.11
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

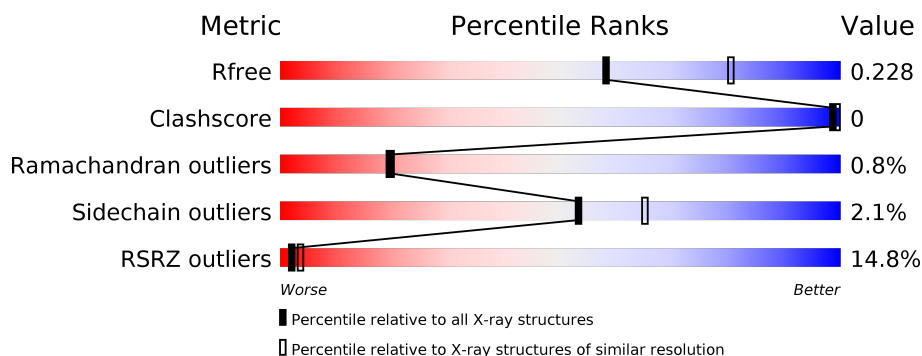
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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  $\geq 3$ , 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	301	<div> <div>13%</div> <div>93%</div> <div>5%</div> </div>
1	B	301	<div> <div>17%</div> <div>92%</div> <div>6%</div> </div>
1	C	301	<div> <div>10%</div> <div>91%</div> <div>• • •</div> </div>
1	D	301	<div> <div>16%</div> <div>92%</div> <div>• 5%</div> </div>

## 2 Entry composition [i](#)

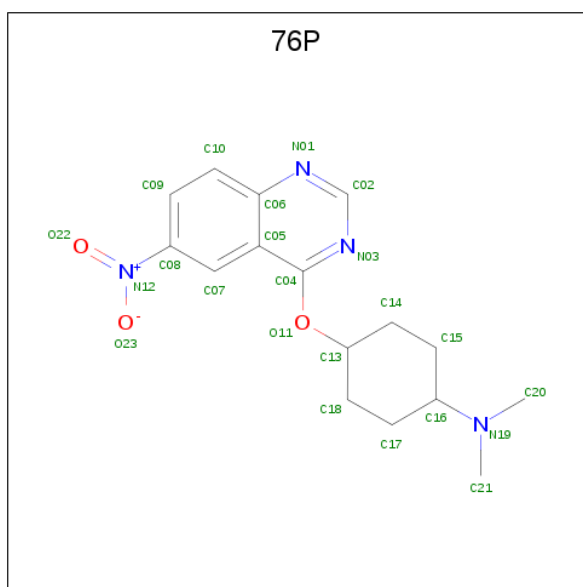
There are 3 unique types of molecules in this entry. The entry contains 9166 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	2
			2253	1411	380	445	3	14			
1	B	283	Total	C	N	O	P	S	0	0	2
			2221	1390	375	439	3	14			
1	C	289	Total	C	N	O	P	S	0	0	2
			2265	1418	382	448	3	14			
1	D	286	Total	C	N	O	P	S	0	0	1
			2254	1412	380	445	3	14			

- Molecule 2 is {N}, {N}-dimethyl-4-(6-nitroquinazolin-4-yl)oxy-cyclohexan-1-amine (three-letter code: 76P) (formula: C<sub>16</sub>H<sub>20</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	4	3		
2	B	1	Total	C	N	O	0	0
			23	16	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			23	16	4	3		
2	D	1	Total	C	N	O	0	0
			23	16	4	3		

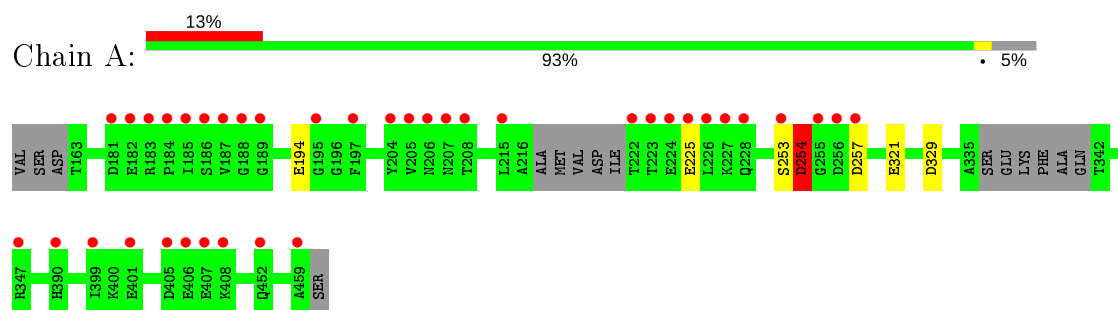
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	26	Total	O	0	0
			26	26		
3	C	17	Total	O	0	0
			17	17		
3	D	21	Total	O	0	0
			21	21		

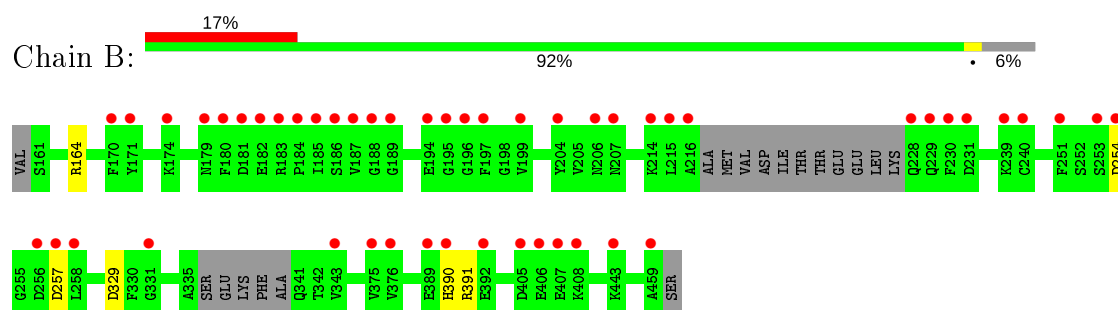
### 3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

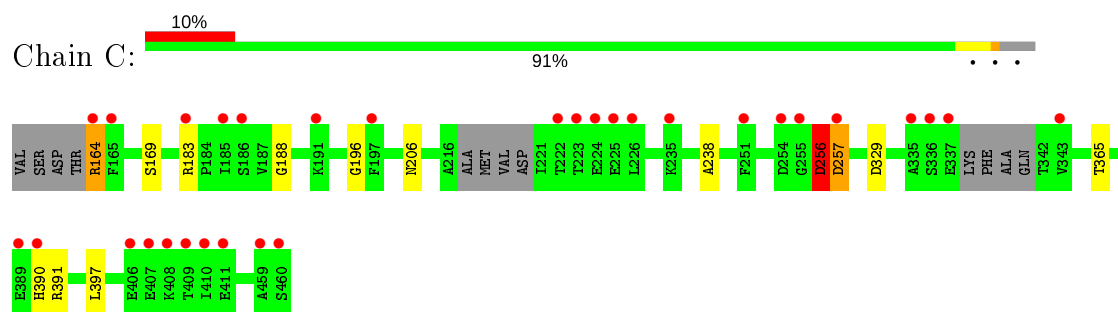
- Molecule 1: Interleukin-1 receptor-associated kinase 4



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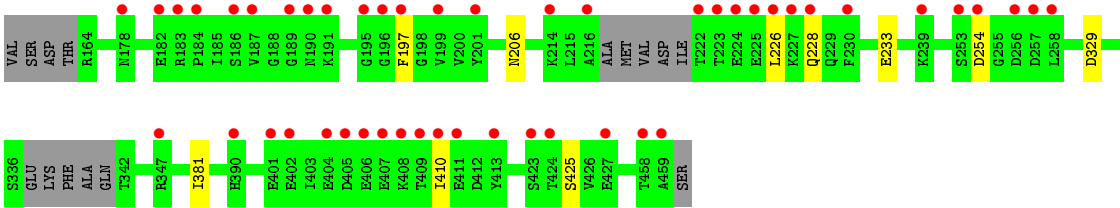


- Molecule 1: Interleukin-1 receptor-associated kinase 4



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.00 Å   139.56 Å   87.34 Å 90.00°   124.45°   90.00°	Depositor
Resolution (Å)	34.26 – 2.34 38.62 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.26-2.34) 99.6 (38.62-2.34)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.34 Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.206   ,   0.228 0.208   ,   0.228	Depositor DCC
$R_{free}$ test set	3047 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.66% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 76P, SEP

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	0.51	0/2257	0.60	0/3041
1	B	0.51	0/2224	0.62	0/2995
1	C	0.51	0/2269	0.62	0/3057
1	D	0.50	0/2258	0.61	0/3042
All	All	0.51	0/9008	0.61	0/12135

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	2253	0	2214	1	0
1	B	2221	0	2172	2	0
1	C	2265	0	2223	4	0
1	D	2254	0	2216	3	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
3	A	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	0	0	0
3	C	17	0	0	0	0
3	D	21	0	0	0	0
All	All	9166	0	8825	8	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 0.

All (8) 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:D:381:ILE:HG21	1:D:410:ILE:HD11	1.89	0.54
1:C:256:ASP:O	1:C:257:ASP:C	2.46	0.54
1:B:391:ARG:HA	1:C:390:HIS:O	2.14	0.48
1:D:197:PHE:CB	1:D:226:LEU:HD11	2.45	0.46
1:C:164:ARG:NH2	1:C:238:ALA:O	2.50	0.45
1:B:390:HIS:O	1:C:391:ARG:HA	2.17	0.45
1:D:197:PHE:HB3	1:D:226:LEU:HD11	2.00	0.43
1:A:254:ASP:N	1:A:254:ASP:OD1	2.52	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/301 (92%)	269 (97%)	8 (3%)	1 (0%)	34	38
1	B	274/301 (91%)	263 (96%)	10 (4%)	1 (0%)	34	38
1	C	281/301 (93%)	266 (95%)	10 (4%)	5 (2%)	8	5
1	D	278/301 (92%)	270 (97%)	6 (2%)	2 (1%)	22	22
All	All	1111/1204 (92%)	1068 (96%)	34 (3%)	9 (1%)	19	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	254	ASP
1	C	256	ASP
1	C	257	ASP
1	D	254	ASP
1	D	206	ASN
1	C	196	GLY
1	C	206	ASN
1	A	254	ASP
1	C	188	GLY

### 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	246/259 (95%)	239 (97%)	7 (3%)	43	53
1	B	242/259 (93%)	239 (99%)	3 (1%)	71	82
1	C	246/259 (95%)	239 (97%)	7 (3%)	43	53
1	D	246/259 (95%)	242 (98%)	4 (2%)	62	74
All	All	980/1036 (95%)	959 (98%)	21 (2%)	53	65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	225	GLU
1	A	253	SER
1	A	254	ASP
1	A	257	ASP
1	A	321	GLU
1	A	329	ASP
1	B	164	ARG
1	B	257	ASP
1	B	329	ASP
1	C	164	ARG

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Mol	Chain	Res	Type
1	C	169	SER
1	C	183	ARG
1	C	256	ASP
1	C	329	ASP
1	C	365	THR
1	C	397	LEU
1	D	228	GLN
1	D	233	GLU
1	D	329	ASP
1	D	425	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	346	1	8,9,10	0.79	0	8,12,14	1.97	2 (25%)
1	TPO	A	342	1	8,10,11	1.02	0	10,14,16	1.43	1 (10%)
1	TPO	A	345	1	8,10,11	0.95	0	10,14,16	1.23	1 (10%)
1	TPO	C	345	1	8,10,11	1.19	0	10,14,16	1.13	1 (10%)
1	SEP	D	346	1	8,9,10	0.95	0	8,12,14	1.95	2 (25%)
1	TPO	D	342	1	8,10,11	0.98	1 (12%)	10,14,16	1.46	1 (10%)
1	SEP	C	346	1	8,9,10	0.82	0	8,12,14	1.84	2 (25%)
1	SEP	B	346	1	8,9,10	0.85	0	8,12,14	1.89	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	B	342	1	8,10,11	1.01	1 (12%)	10,14,16	1.45	1 (10%)
1	TPO	C	342	1	8,10,11	1.11	1 (12%)	10,14,16	1.40	1 (10%)
1	TPO	B	345	1	8,10,11	1.08	0	10,14,16	1.20	0
1	TPO	D	345	1	8,10,11	0.99	0	10,14,16	1.21	1 (10%)

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	346	1	-	1/5/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	C	345	1	-	2/9/11/13	-
1	SEP	D	346	1	-	1/5/8/10	-
1	TPO	D	342	1	-	2/9/11/13	-
1	SEP	C	346	1	-	1/5/8/10	-
1	SEP	B	346	1	-	1/5/8/10	-
1	TPO	B	342	1	-	2/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	TPO	P-OG1	-2.30	1.55	1.59
1	D	342	TPO	P-OG1	-2.03	1.55	1.59
1	B	342	TPO	P-OG1	-2.01	1.55	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-CB-CA	4.17	112.20	108.14
1	D	346	SEP	OG-CB-CA	4.02	112.05	108.14
1	A	346	SEP	OG-CB-CA	3.90	111.94	108.14
1	C	346	SEP	OG-CB-CA	3.74	111.78	108.14
1	A	342	TPO	P-OG1-CB	-3.55	112.47	123.21
1	D	342	TPO	P-OG1-CB	-3.51	112.61	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	TPO	P-OG1-CB	-3.49	112.66	123.21
1	B	342	TPO	P-OG1-CB	-3.49	112.66	123.21
1	A	346	SEP	P-OG-CB	-3.39	108.97	118.30
1	D	346	SEP	P-OG-CB	-3.26	109.31	118.30
1	C	346	SEP	P-OG-CB	-3.09	109.79	118.30
1	B	346	SEP	P-OG-CB	-2.94	110.20	118.30
1	A	345	TPO	P-OG1-CB	-2.12	116.80	123.21
1	D	345	TPO	P-OG1-CB	-2.08	116.92	123.21
1	C	345	TPO	CG2-CB-CA	-2.04	109.14	113.16

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	C	345	TPO	N-CA-CB-OG1
1	D	342	TPO	CB-OG1-P-O1P
1	B	342	TPO	CB-OG1-P-O1P
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	CB-OG1-P-O1P
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	CB-OG1-P-O1P
1	D	342	TPO	CB-OG1-P-O3P
1	B	342	TPO	CB-OG1-P-O3P
1	C	342	TPO	CB-OG1-P-O2P
1	A	346	SEP	N-CA-CB-OG
1	D	346	SEP	N-CA-CB-OG
1	B	346	SEP	N-CA-CB-OG
1	C	346	SEP	CB-OG-P-O1P
1	A	342	TPO	CB-OG1-P-O2P
1	A	345	TPO	O-C-CA-CB
1	C	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	76P	B	9901	-	21,25,25	0.31	0	29,35,35	1.02	3 (10%)
2	76P	A	9901	-	21,25,25	0.32	0	29,35,35	1.09	3 (10%)
2	76P	D	9901	-	21,25,25	0.35	0	29,35,35	1.04	3 (10%)
2	76P	C	9901	-	21,25,25	0.35	0	29,35,35	1.12	3 (10%)

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	76P	B	9901	-	-	3/10/22/22	0/3/3/3
2	76P	A	9901	-	-	2/10/22/22	0/3/3/3
2	76P	D	9901	-	-	0/10/22/22	0/3/3/3
2	76P	C	9901	-	-	1/10/22/22	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9901	76P	C05-C04-N03	-3.48	121.44	124.37
2	A	9901	76P	C21-N19-C16	3.36	118.16	112.39
2	D	9901	76P	C05-C04-N03	-3.23	121.65	124.37
2	A	9901	76P	C05-C04-N03	-2.95	121.89	124.37
2	B	9901	76P	C21-N19-C16	2.86	117.31	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9901	76P	O11-C04-N03	2.45	123.00	118.89
2	D	9901	76P	C21-N19-C16	2.40	116.51	112.39
2	D	9901	76P	O11-C04-N03	2.35	122.84	118.89
2	B	9901	76P	C05-C04-N03	-2.30	122.43	124.37
2	C	9901	76P	C21-N19-C16	2.28	116.30	112.39
2	B	9901	76P	O11-C04-N03	2.17	122.52	118.89
2	A	9901	76P	O11-C04-N03	2.15	122.50	118.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

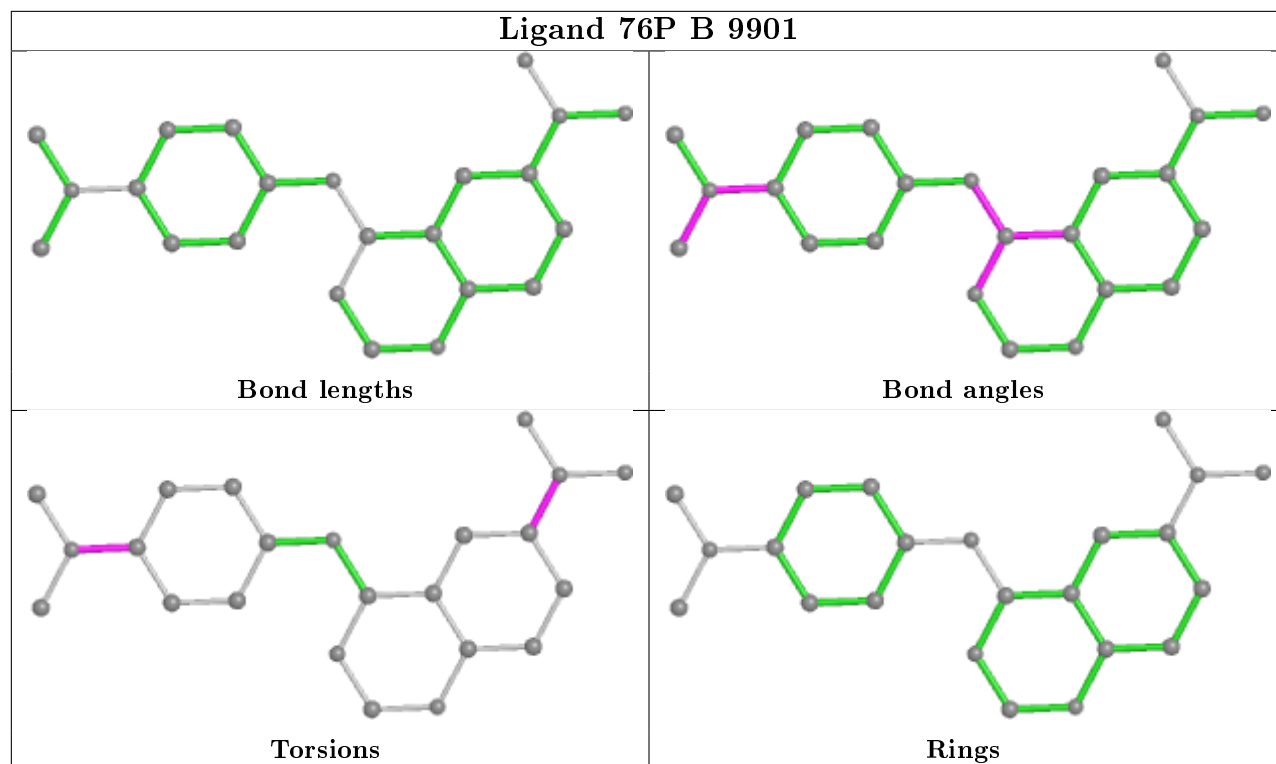
Mol	Chain	Res	Type	Atoms
2	B	9901	76P	C07-C08-N12-O22
2	A	9901	76P	C07-C08-N12-O22
2	B	9901	76P	C15-C16-N19-C20
2	A	9901	76P	C15-C16-N19-C20
2	C	9901	76P	C15-C16-N19-C20
2	B	9901	76P	C09-C08-N12-O22

There are no ring outliers.

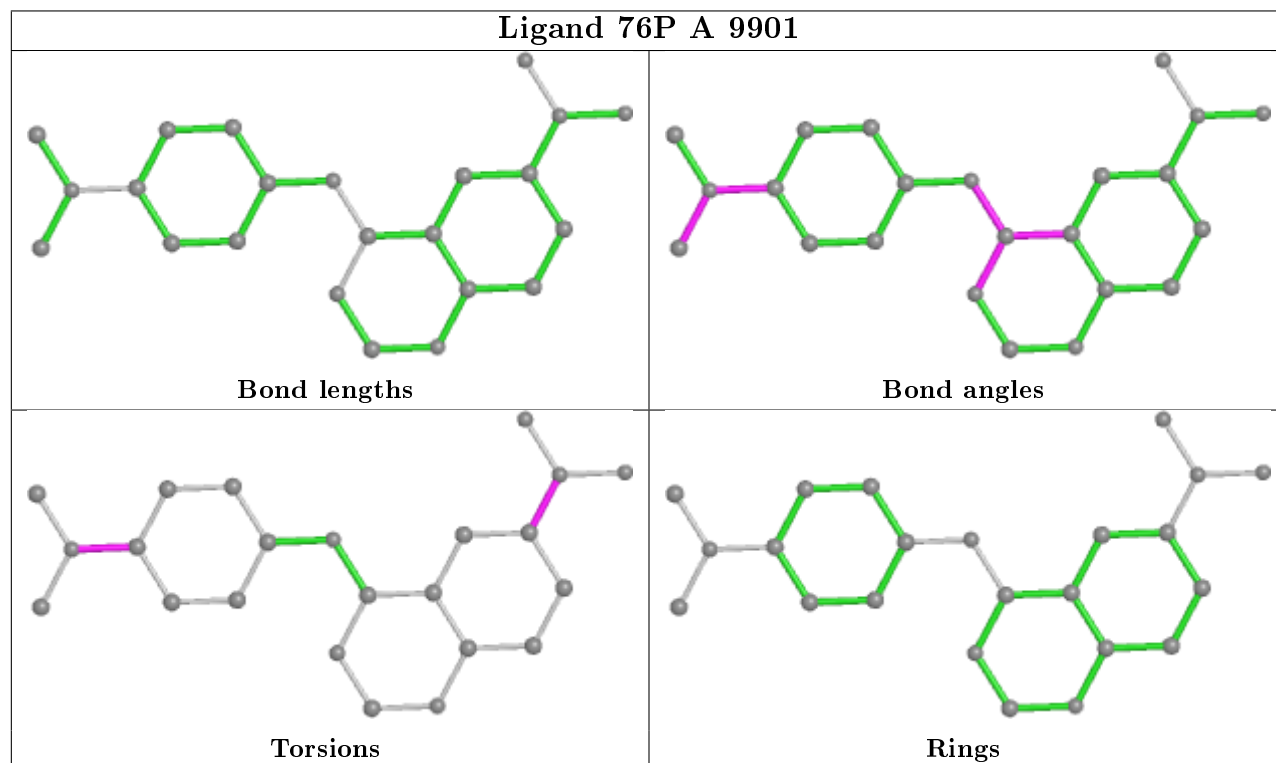
No monomer is involved in short contacts.

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

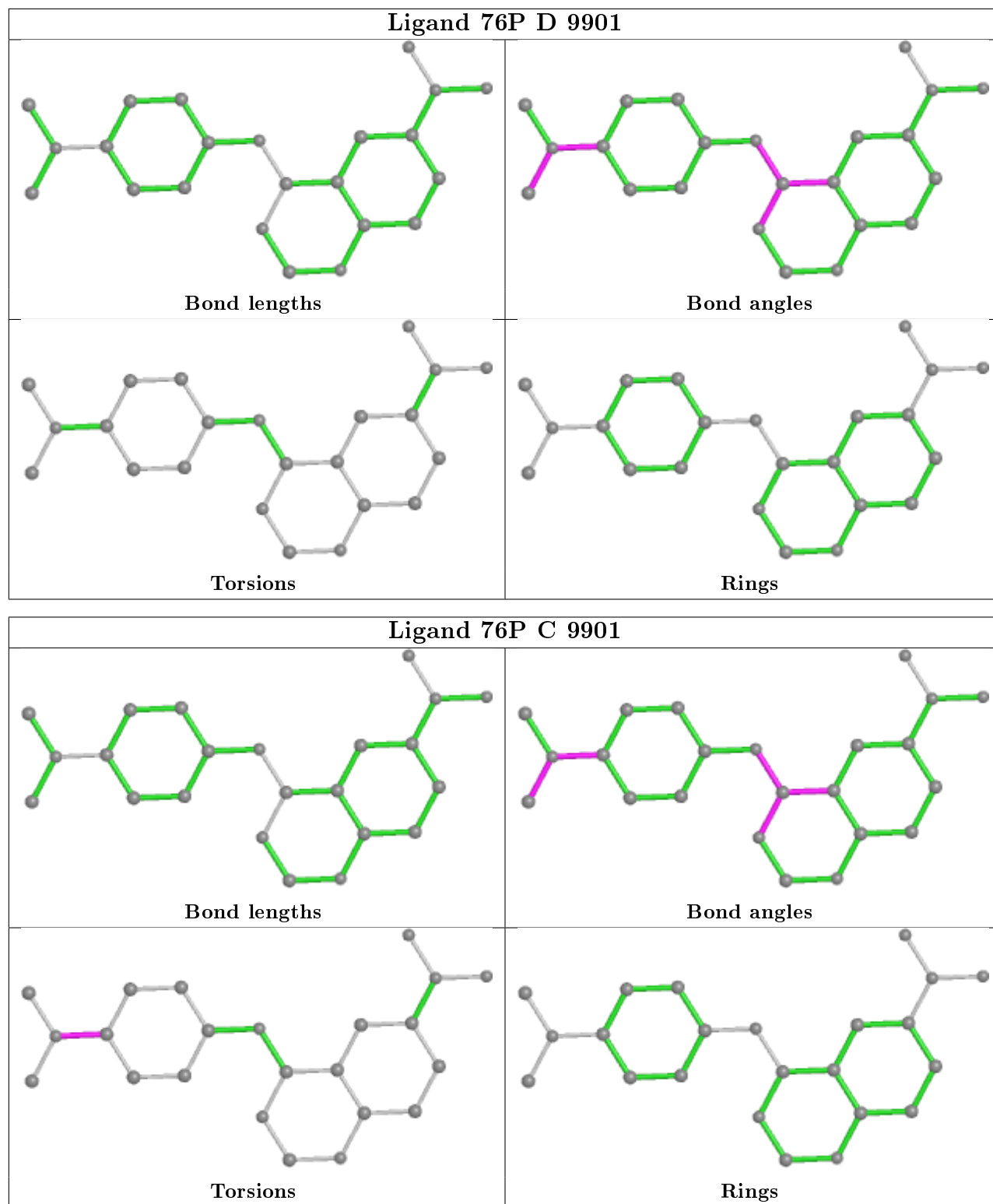
## Ligand 76P B 9901



## Ligand 76P A 9901







## 5.7 Other polymers [i](#)

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, 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	283/301 (94%)	0.86	38 (13%) <b>3</b> <b>5</b>	36, 58, 103, 122	0
1	B	280/301 (93%)	0.92	50 (17%) <b>1</b> <b>2</b>	34, 61, 101, 118	0
1	C	286/301 (95%)	0.62	31 (10%) <b>5</b> <b>9</b>	33, 56, 100, 118	0
1	D	283/301 (94%)	0.82	48 (16%) <b>1</b> <b>2</b>	36, 59, 108, 147	0
All	All	1132/1204 (94%)	0.80	167 (14%) <b>2</b> <b>3</b>	33, 58, 103, 147	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	PHE	11.7
1	A	188	GLY	11.1
1	A	187	VAL	10.3
1	B	187	VAL	9.7
1	C	460	SER	9.7
1	D	223	THR	9.6
1	D	226	LEU	8.1
1	A	223	THR	8.1
1	A	224	GLU	7.9
1	A	183	ARG	7.9
1	D	222	THR	6.9
1	A	256	ASP	6.7
1	A	222	THR	6.7
1	A	255	GLY	6.5
1	B	257	ASP	6.4
1	C	337	GLU	6.4
1	D	459	ALA	6.4
1	B	188	GLY	5.9
1	B	228	GLN	5.8
1	B	229	GLN	5.7
1	A	459	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	5.7
1	D	186	SER	5.7
1	B	258	LEU	5.6
1	D	227	LYS	5.5
1	D	224	GLU	5.3
1	B	197	PHE	5.2
1	C	459	ALA	5.2
1	A	407	GLU	5.0
1	D	184	PRO	5.0
1	A	226	LEU	5.0
1	D	409	THR	5.0
1	D	406	GLU	4.8
1	B	196	GLY	4.8
1	D	405	ASP	4.7
1	A	225	GLU	4.7
1	A	189	GLY	4.7
1	A	186	SER	4.6
1	D	216	ALA	4.6
1	B	406	GLU	4.5
1	B	407	GLU	4.4
1	B	183	ARG	4.4
1	A	197	PHE	4.4
1	A	206	ASN	4.3
1	B	459	ALA	4.3
1	B	214	LYS	4.3
1	B	256	ASP	4.3
1	A	207	ASN	4.2
1	D	187	VAL	4.2
1	D	183	ARG	4.2
1	C	336	SER	4.0
1	D	256	ASP	3.9
1	D	230	PHE	3.9
1	A	204	TYR	3.8
1	B	230	PHE	3.8
1	D	225	GLU	3.8
1	A	405	ASP	3.8
1	B	185	ILE	3.7
1	B	207	ASN	3.7
1	C	224	GLU	3.7
1	A	228	GLN	3.7
1	D	347	ARG	3.6
1	B	392	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	3.6
1	D	228	GLN	3.6
1	C	406	GLU	3.5
1	B	231	ASP	3.5
1	C	197	PHE	3.5
1	D	196	GLY	3.5
1	B	254	ASP	3.5
1	C	257	ASP	3.5
1	A	253	SER	3.4
1	B	204	TYR	3.4
1	C	407	GLU	3.4
1	D	195	GLY	3.3
1	A	406	GLU	3.3
1	B	189	GLY	3.2
1	C	409	THR	3.2
1	D	201	TYR	3.2
1	B	186	SER	3.1
1	C	186	SER	3.1
1	B	195	GLY	3.1
1	C	343	VAL	3.1
1	A	257	ASP	3.1
1	D	191	LYS	3.1
1	B	199	VAL	3.0
1	B	240	CYS	3.0
1	C	390	HIS	3.0
1	B	184	PRO	2.9
1	D	402	GLU	2.9
1	B	443	LYS	2.8
1	B	216	ALA	2.8
1	D	407	GLU	2.8
1	C	411	GLU	2.8
1	D	408	LYS	2.7
1	A	184	PRO	2.7
1	D	254	ASP	2.7
1	A	390	HIS	2.7
1	C	408	LYS	2.7
1	A	408	LYS	2.7
1	B	180	PHE	2.7
1	B	239	LYS	2.6
1	C	389	GLU	2.6
1	D	458	THR	2.6
1	B	408	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	206	ASN	2.6
1	D	182	GLU	2.5
1	D	401	GLU	2.5
1	B	389	GLU	2.5
1	B	170	PHE	2.5
1	C	185	ILE	2.5
1	C	335	ALA	2.5
1	B	390	HIS	2.5
1	B	253	SER	2.4
1	D	214	LYS	2.4
1	A	347	ARG	2.4
1	D	423	SER	2.4
1	D	390	HIS	2.4
1	D	411	GLU	2.4
1	D	410	ILE	2.4
1	C	164	ARG	2.4
1	B	251	PHE	2.3
1	A	181	ASP	2.3
1	B	179	ASN	2.3
1	B	171	TYR	2.3
1	B	181	ASP	2.3
1	C	254	ASP	2.3
1	C	165	PHE	2.3
1	D	190	ASN	2.3
1	A	227	LYS	2.3
1	A	399	ILE	2.3
1	C	222	THR	2.3
1	D	258	LEU	2.3
1	A	452	GLN	2.3
1	D	404	GLU	2.2
1	B	194	GLU	2.2
1	C	183	ARG	2.2
1	D	424	THR	2.2
1	B	182	GLU	2.2
1	A	205	VAL	2.2
1	A	208	THR	2.2
1	B	376	VAL	2.1
1	C	410	ILE	2.1
1	B	331	GLY	2.1
1	D	178	ASN	2.1
1	C	191	LYS	2.1
1	C	223	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	199	VAL	2.1
1	A	185	ILE	2.1
1	D	413	TYR	2.1
1	C	251	PHE	2.1
1	D	189	GLY	2.1
1	B	215	LEU	2.1
1	C	225	GLU	2.1
1	C	235	LYS	2.1
1	D	239	LYS	2.1
1	D	427	GLU	2.0
1	A	215	LEU	2.0
1	C	255	GLY	2.0
1	B	174	LYS	2.0
1	A	182	GLU	2.0
1	D	253	SER	2.0
1	B	375	VAL	2.0
1	A	401	GLU	2.0
1	C	226	LEU	2.0
1	B	405	ASP	2.0
1	D	257	ASP	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, 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	B	346	10/11	0.66	0.22	90,96,104,104	0
1	TPO	D	342	11/12	0.74	0.24	94,99,106,106	0
1	SEP	C	346	10/11	0.80	0.17	78,85,95,95	0
1	SEP	D	346	10/11	0.80	0.21	84,90,99,99	0
1	TPO	A	342	11/12	0.82	0.18	88,91,100,101	0
1	TPO	C	342	11/12	0.84	0.19	89,92,100,100	0
1	SEP	A	346	10/11	0.88	0.21	79,84,91,92	0
1	TPO	B	342	11/12	0.89	0.19	104,105,110,110	0
1	TPO	B	345	11/12	0.92	0.14	87,88,90,91	0
1	TPO	D	345	11/12	0.92	0.14	77,78,84,84	0
1	TPO	A	345	11/12	0.94	0.16	75,77,80,81	0
1	TPO	C	345	11/12	0.96	0.10	73,74,78,79	0

## 6.3 Carbohydrates [i](#)

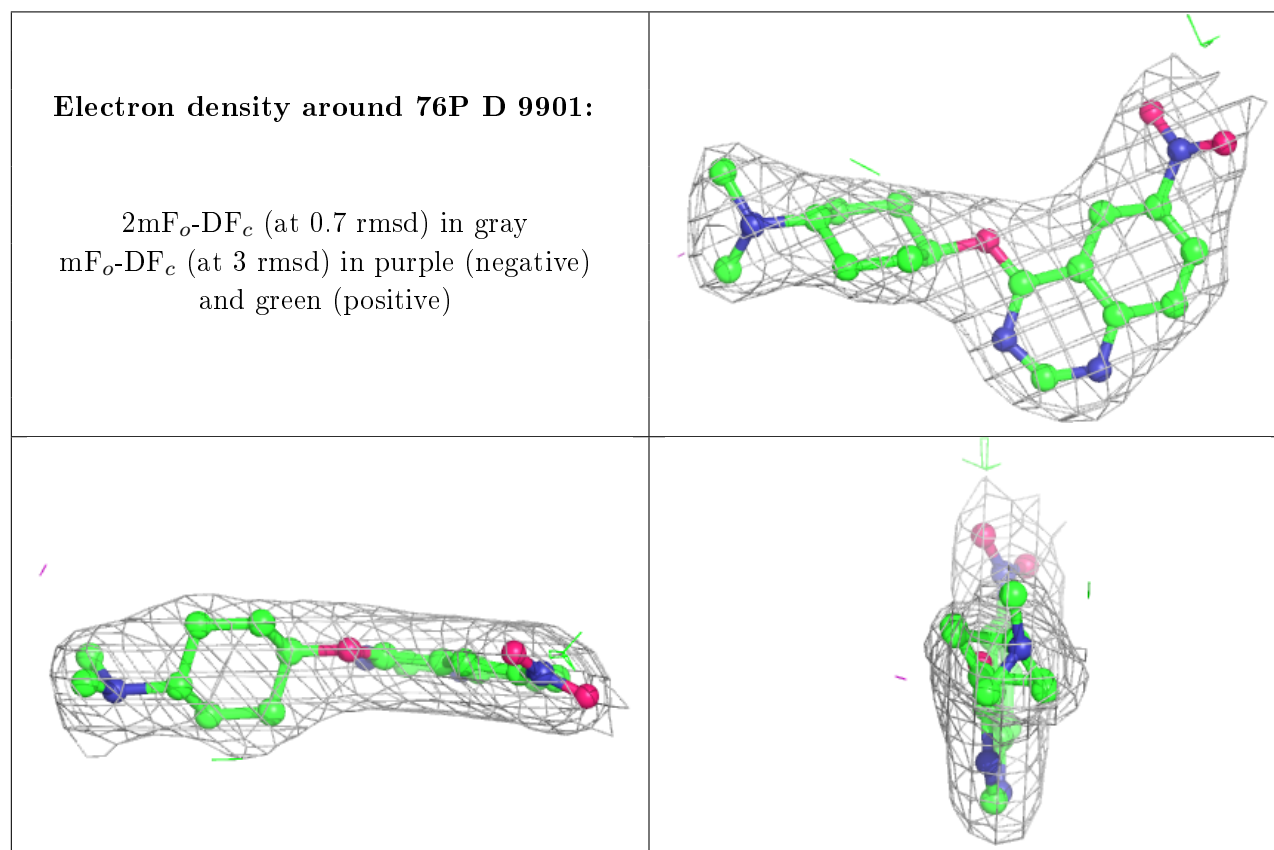
There are no carbohydrates in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
2	76P	D	9901	23/23	0.95	0.13	44,51,55,61	0
2	76P	A	9901	23/23	0.96	0.13	39,45,57,59	0
2	76P	B	9901	23/23	0.97	0.12	39,42,53,55	0
2	76P	C	9901	23/23	0.98	0.12	32,41,46,50	0

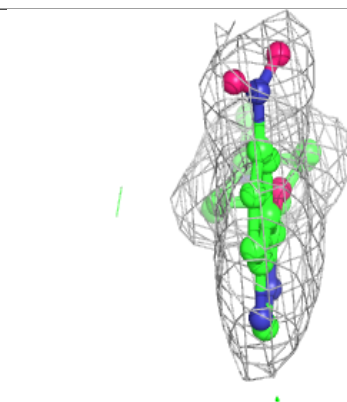
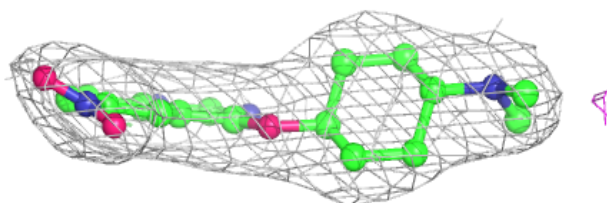
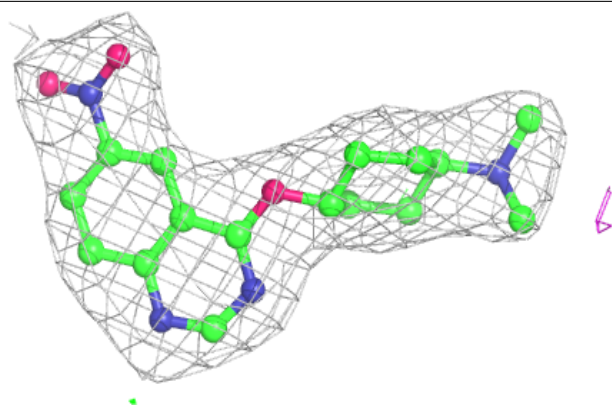
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



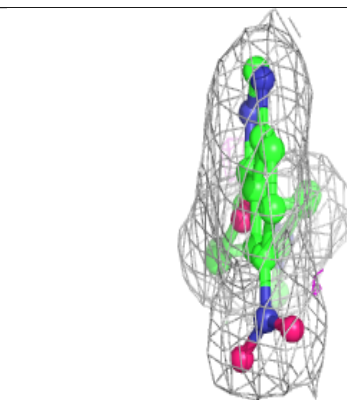
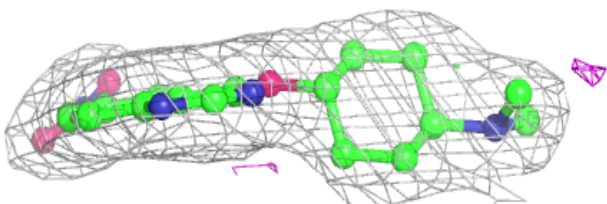
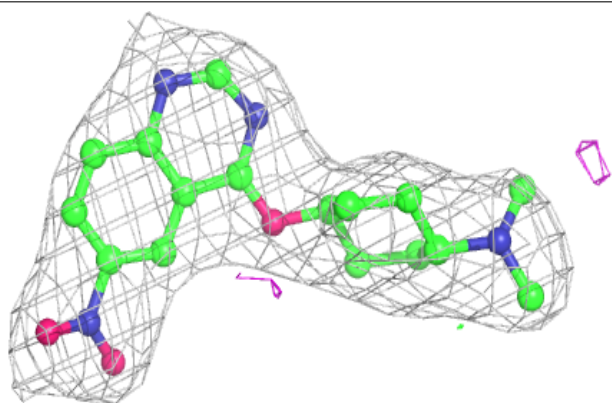


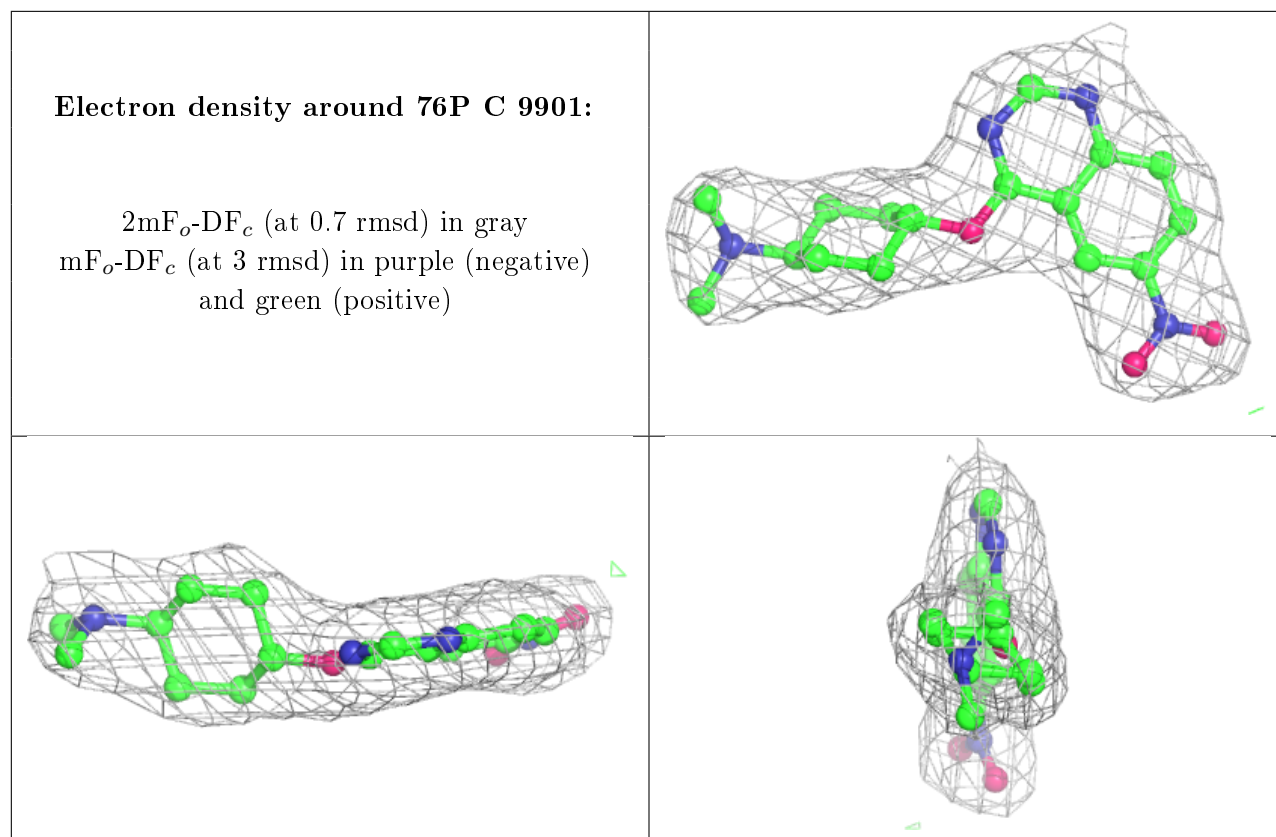
**Electron density around 76P A 9901:**

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

**Electron density around 76P B 9901:**

$2mF_o-DF_c$  (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.