



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:17 am BST

PDB ID : 5T1S
Title : Irak4 kinase - compound 1 co-structure
Authors : Fischmann, T.O.
Deposited on : 2016-08-22
Resolution : 2.30 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 ⓘ symbol.

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

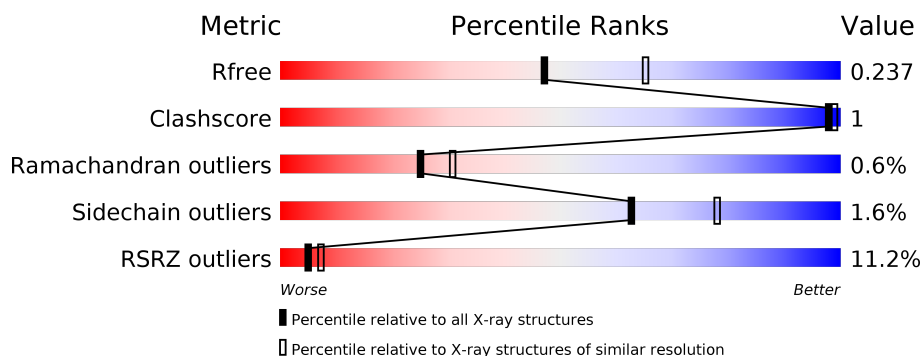
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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>8%</div> <div>91%</div> <div>6%</div> </div>
1	B	301	<div> <div>13%</div> <div>92%</div> <div>5%</div> </div>
1	C	301	<div> <div>14%</div> <div>93%</div> <div>5%</div> </div>
1	D	301	<div> <div>8%</div> <div>91%</div> <div>6%</div> </div>

2 Entry composition [i](#)

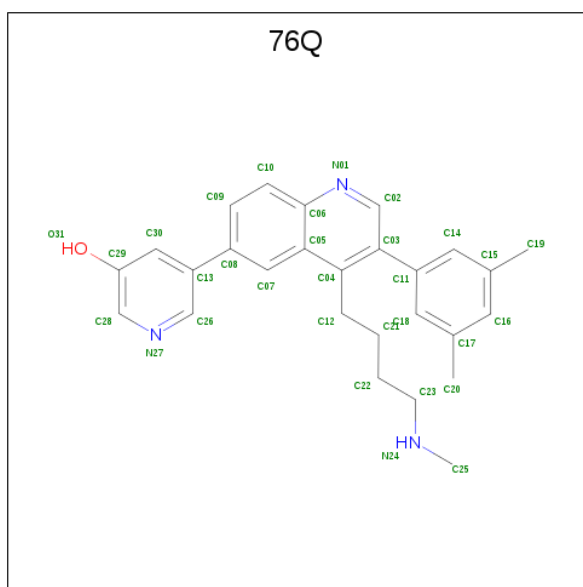
There are 3 unique types of molecules in this entry. The entry contains 9178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	283	Total	C	N	O	P	S	0	0	3
			2227	1395	375	440	3	14			
1	B	285	Total	C	N	O	P	S	0	0	2
			2233	1398	377	441	3	14			
1	C	287	Total	C	N	O	P	S	0	0	1
			2249	1410	376	446	3	14			
1	D	284	Total	C	N	O	P	S	0	0	0
			2236	1403	377	439	3	14			

- Molecule 2 is 5-[3-(3,5-dimethylphenyl)-4-[4-(methylamino)butyl]quinolin-6-yl]pyridin-3-ol (three-letter code: 76Q) (formula: C₂₇H₂₉N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	27	3	1		
2	B	1	Total	C	N	O	0	0
			31	27	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			31	27	3	1		
2	D	1	Total	C	N	O	0	0
			31	27	3	1		

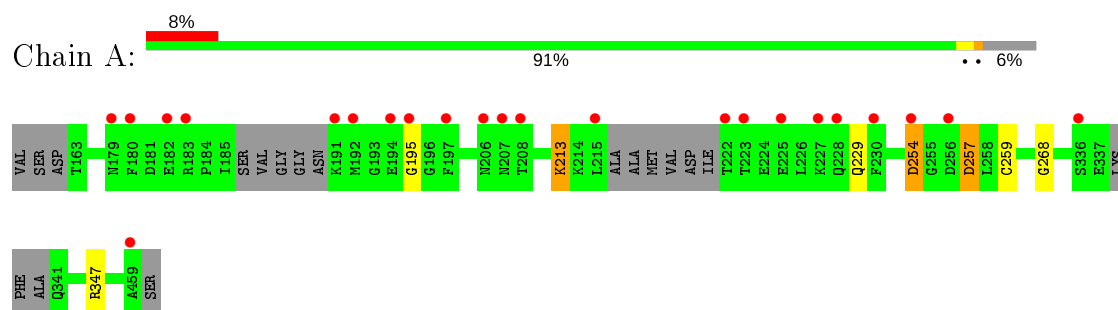
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	24	Total	O	0	0
			24	24		
3	C	31	Total	O	0	0
			31	31		
3	D	31	Total	O	0	0
			31	31		

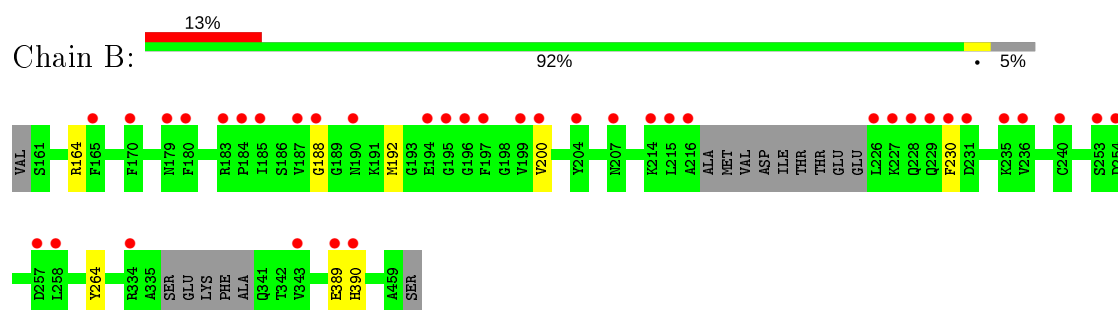
3 Residue-property plots [i](#)

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.

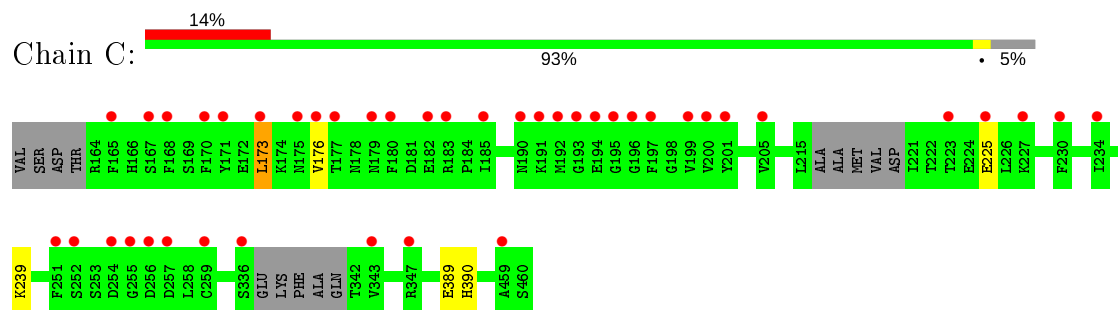
- Molecule 1: Interleukin-1 receptor-associated kinase 4



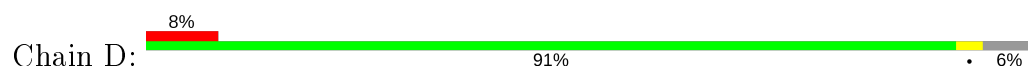
- Molecule 1: Interleukin-1 receptor-associated kinase 4

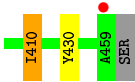
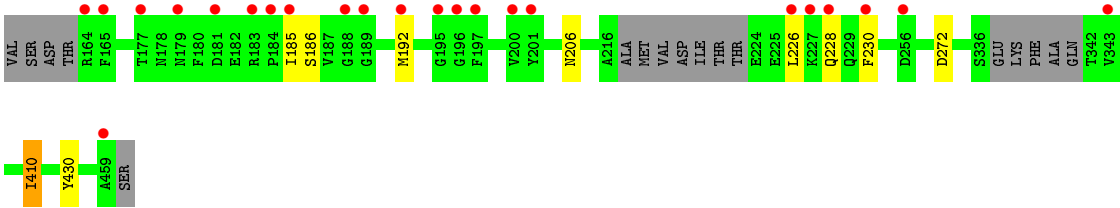


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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, α , β , γ	144.34Å 139.30Å 88.09Å 90.00° 125.05° 90.00°	Depositor
Resolution (Å)	37.20 – 2.30 37.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.20-2.30) 97.7 (37.20-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.207 , 0.223 0.217 , 0.237	Depositor DCC
R_{free} test set	3138 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.109 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9178	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 76Q, 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	0.49	0/2229	0.62	0/3000
1	B	0.49	0/2236	0.62	0/3010
1	C	0.50	0/2253	0.62	0/3036
1	D	0.50	0/2240	0.64	0/3017
All	All	0.49	0/8958	0.62	0/12063

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	2227	0	2180	2	0
1	B	2233	0	2186	4	0
1	C	2249	0	2205	2	0
1	D	2236	0	2201	4	0
2	A	31	0	0	1	0
2	B	31	0	0	0	0
2	C	31	0	0	0	0
2	D	31	0	0	3	0
3	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	0	0	0
3	C	31	0	0	0	0
3	D	31	0	0	0	0
All	All	9178	0	8772	12	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 1.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:MET:HB2	1:B:200:VAL:HG23	1.75	0.66
1:D:192:MET:HB3	2:D:9901:76Q:C14	2.40	0.52
1:D:410:ILE:HD12	1:D:410:ILE:H	1.74	0.51
1:B:192:MET:HE2	1:B:264:TYR:HE1	1.76	0.51
1:B:390:HIS:O	1:C:390:HIS:O	2.32	0.47
1:B:192:MET:CE	1:B:264:TYR:HE1	2.30	0.45
1:D:272:ASP:OD2	2:D:9901:76Q:C23	2.65	0.44
1:A:213:LYS:O	1:A:259:CYS:HA	2.17	0.44
1:A:268:GLY:HA2	2:A:9901:76Q:C18	2.50	0.42
1:D:410:ILE:HG12	1:D:430:TYR:CD2	2.55	0.41
1:C:173:LEU:HD12	1:C:176:VAL:HB	2.02	0.41
2:D:9901:76Q:C21	2:D:9901:76Q:C14	2.98	0.41

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	272/301 (90%)	258 (95%)	11 (4%)	3 (1%)	14	15
1	B	276/301 (92%)	262 (95%)	12 (4%)	2 (1%)	22	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	279/301 (93%)	267 (96%)	12 (4%)	0	100	100
1	D	276/301 (92%)	262 (95%)	12 (4%)	2 (1%)	22	26
All	All	1103/1204 (92%)	1049 (95%)	47 (4%)	7 (1%)	25	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	186	SER
1	A	254	ASP
1	D	185	ILE
1	A	257	ASP
1	B	230	PHE
1	A	195	GLY
1	B	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	243/259 (94%)	238 (98%)	5 (2%)	53	70
1	B	243/259 (94%)	241 (99%)	2 (1%)	81	91
1	C	245/259 (95%)	241 (98%)	4 (2%)	62	78
1	D	243/259 (94%)	238 (98%)	5 (2%)	53	70
All	All	974/1036 (94%)	958 (98%)	16 (2%)	62	78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	LYS
1	A	229	GLN
1	A	254	ASP
1	A	257	ASP
1	A	347	ARG

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Mol	Chain	Res	Type
1	B	164	ARG
1	B	389	GLU
1	C	173	LEU
1	C	225	GLU
1	C	239	LYS
1	C	389	GLU
1	D	206	ASN
1	D	226	LEU
1	D	228	GLN
1	D	230	PHE
1	D	410	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN

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	TPO	D	342	1	8,10,11	0.99	1 (12%)	10,14,16	1.32	1 (10%)
1	SEP	B	346	1	8,9,10	1.03	1 (12%)	8,12,14	1.76	2 (25%)
1	SEP	C	346	1	8,9,10	0.86	0	8,12,14	1.65	2 (25%)
1	TPO	A	342	1	8,10,11	0.96	0	10,14,16	1.36	1 (10%)
1	SEP	A	346	1	8,9,10	0.92	0	8,12,14	1.69	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	C	342	1	8,10,11	1.04	0	10,14,16	1.36	1 (10%)
1	TPO	C	345	1	8,10,11	1.24	0	10,14,16	1.10	0
1	TPO	A	345	1	8,10,11	1.04	0	10,14,16	1.25	2 (20%)
1	TPO	B	342	1	8,10,11	0.98	0	10,14,16	1.35	1 (10%)
1	TPO	B	345	1	8,10,11	1.11	0	10,14,16	1.17	1 (10%)
1	TPO	D	345	1	8,10,11	0.97	0	10,14,16	1.23	1 (10%)
1	SEP	D	346	1	8,9,10	1.00	0	8,12,14	1.69	2 (25%)

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	TPO	D	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-
1	SEP	C	346	1	-	0/5/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	C	342	1	-	2/9/11/13	-
1	TPO	C	345	1	-	4/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	346	SEP	P-O1P	2.22	1.57	1.50
1	D	342	TPO	P-OG1	-2.11	1.55	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	SEP	P-OG-CB	-3.63	108.29	118.30
1	B	346	SEP	P-OG-CB	-3.46	108.77	118.30
1	C	342	TPO	P-OG1-CB	-3.34	113.12	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TPO	P-OG1-CB	-3.33	113.16	123.21
1	B	342	TPO	P-OG1-CB	-3.25	113.40	123.21
1	D	342	TPO	P-OG1-CB	-3.23	113.45	123.21
1	D	346	SEP	OG-CB-CA	3.22	111.28	108.14
1	D	346	SEP	P-OG-CB	-3.21	109.47	118.30
1	C	346	SEP	P-OG-CB	-3.19	109.52	118.30
1	B	346	SEP	OG-CB-CA	3.00	111.06	108.14
1	C	346	SEP	OG-CB-CA	2.95	111.02	108.14
1	A	345	TPO	O3P-P-OG1	2.32	116.39	105.99
1	A	346	SEP	OG-CB-CA	2.30	110.39	108.14
1	A	345	TPO	P-OG1-CB	-2.26	116.38	123.21
1	D	345	TPO	O3P-P-OG1	2.10	115.40	105.99
1	B	345	TPO	O3P-P-OG1	2.06	115.20	105.99

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	342	TPO	O-C-CA-CB
1	A	342	TPO	O-C-CA-CB
1	C	342	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	A	345	TPO	N-CA-CB-OG1
1	B	342	TPO	O-C-CA-CB
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	C	342	TPO	C-CA-CB-CG2
1	C	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O3P
1	B	345	TPO	CB-OG1-P-O3P
1	C	345	TPO	O-C-CA-CB
1	A	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	76Q	D	9901	-	33,34,34	1.66	1 (3%)	45,47,47	0.94	3 (6%)
2	76Q	C	9901	-	33,34,34	1.36	1 (3%)	45,47,47	0.85	2 (4%)
2	76Q	B	9901	-	33,34,34	0.97	1 (3%)	45,47,47	0.89	2 (4%)
2	76Q	A	9901	-	33,34,34	1.40	1 (3%)	45,47,47	0.92	3 (6%)

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	76Q	D	9901	-	-	4/14/14/14	0/4/4/4
2	76Q	C	9901	-	-	3/14/14/14	0/4/4/4
2	76Q	B	9901	-	-	3/14/14/14	0/4/4/4
2	76Q	A	9901	-	-	4/14/14/14	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9901	76Q	C03-C04	8.72	1.55	1.41
2	A	9901	76Q	C03-C04	7.40	1.53	1.41
2	C	9901	76Q	C03-C04	7.04	1.53	1.41
2	B	9901	76Q	C03-C04	4.96	1.49	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9901	76Q	C03-C04-C05	-3.69	116.20	119.39
2	A	9901	76Q	C03-C04-C05	-3.53	116.33	119.39
2	D	9901	76Q	C03-C04-C05	-3.22	116.60	119.39
2	B	9901	76Q	C03-C04-C05	-2.99	116.80	119.39
2	A	9901	76Q	C03-C02-N01	2.74	128.77	124.52
2	D	9901	76Q	C03-C02-N01	2.69	128.68	124.52
2	B	9901	76Q	C03-C02-N01	2.56	128.48	124.52
2	D	9901	76Q	C11-C03-C04	2.53	126.56	122.94
2	C	9901	76Q	C03-C02-N01	2.46	128.32	124.52
2	A	9901	76Q	C11-C03-C04	2.27	126.19	122.94

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	9901	76Q	C03-C04-C12-C21
2	D	9901	76Q	C05-C04-C12-C21
2	C	9901	76Q	C05-C04-C12-C21
2	B	9901	76Q	C05-C04-C12-C21
2	A	9901	76Q	C03-C04-C12-C21
2	A	9901	76Q	C05-C04-C12-C21
2	C	9901	76Q	C21-C22-C23-N24
2	A	9901	76Q	C04-C12-C21-C22
2	D	9901	76Q	C04-C12-C21-C22
2	C	9901	76Q	C03-C04-C12-C21
2	B	9901	76Q	C03-C04-C12-C21
2	A	9901	76Q	C12-C21-C22-C23
2	B	9901	76Q	C12-C21-C22-C23
2	D	9901	76Q	C12-C21-C22-C23

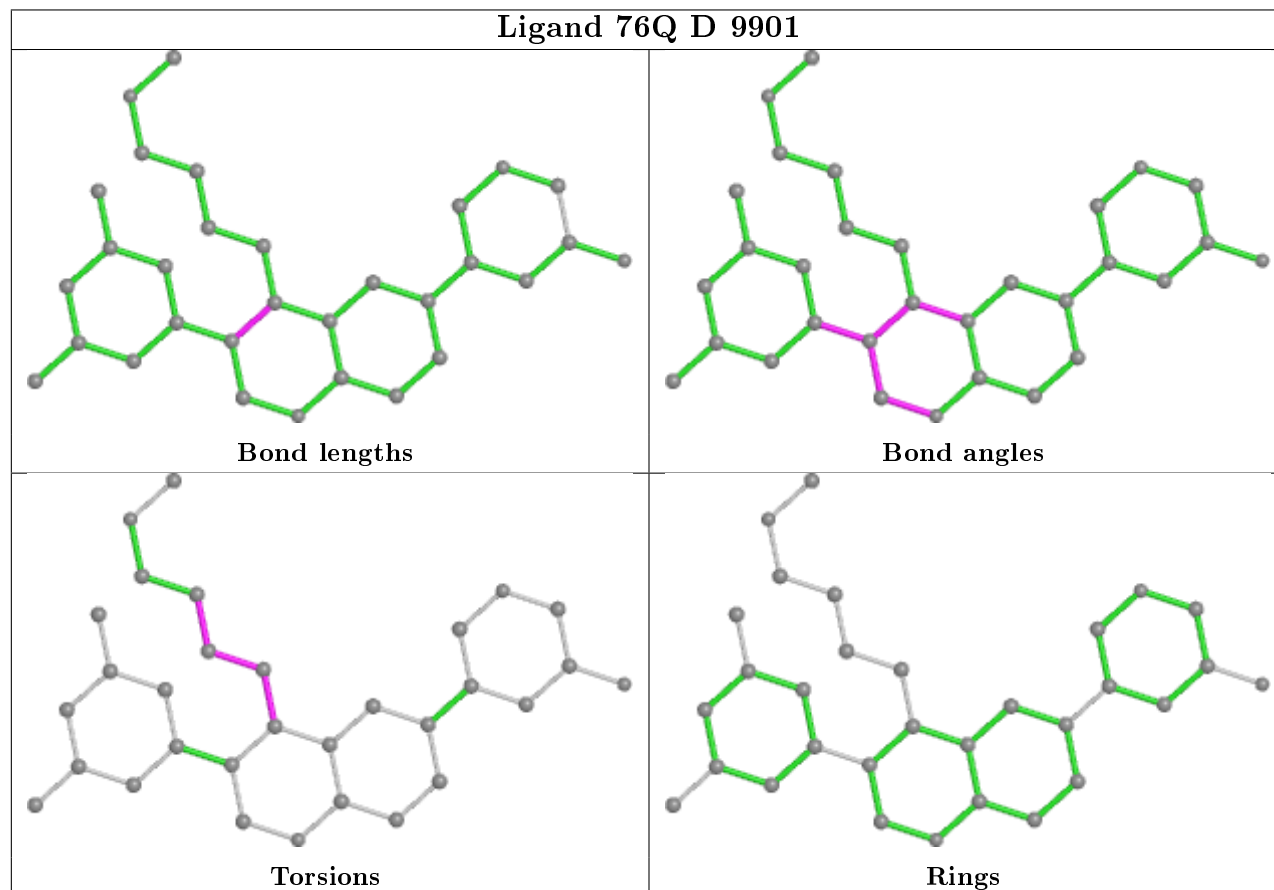
There are no ring outliers.

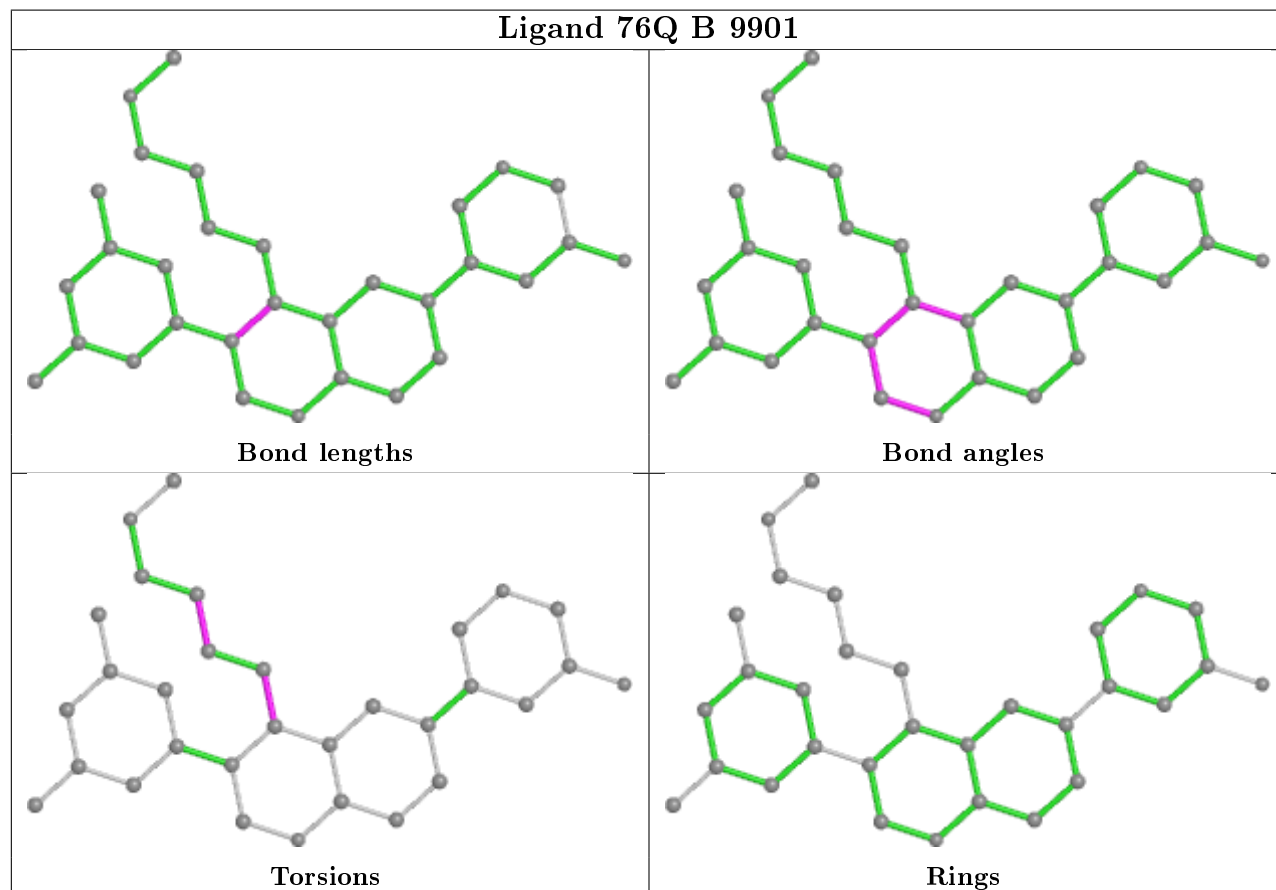
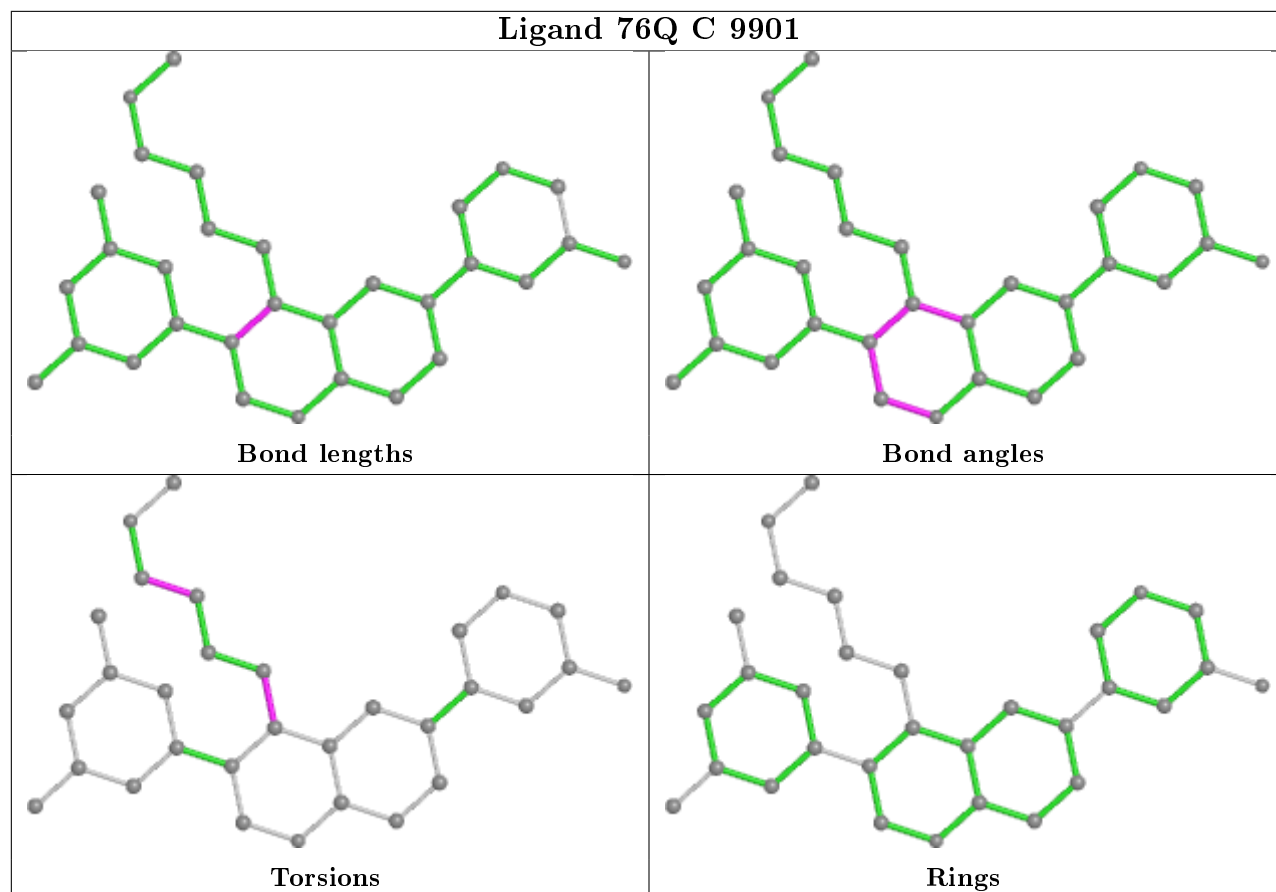
2 monomers are involved in 4 short contacts:

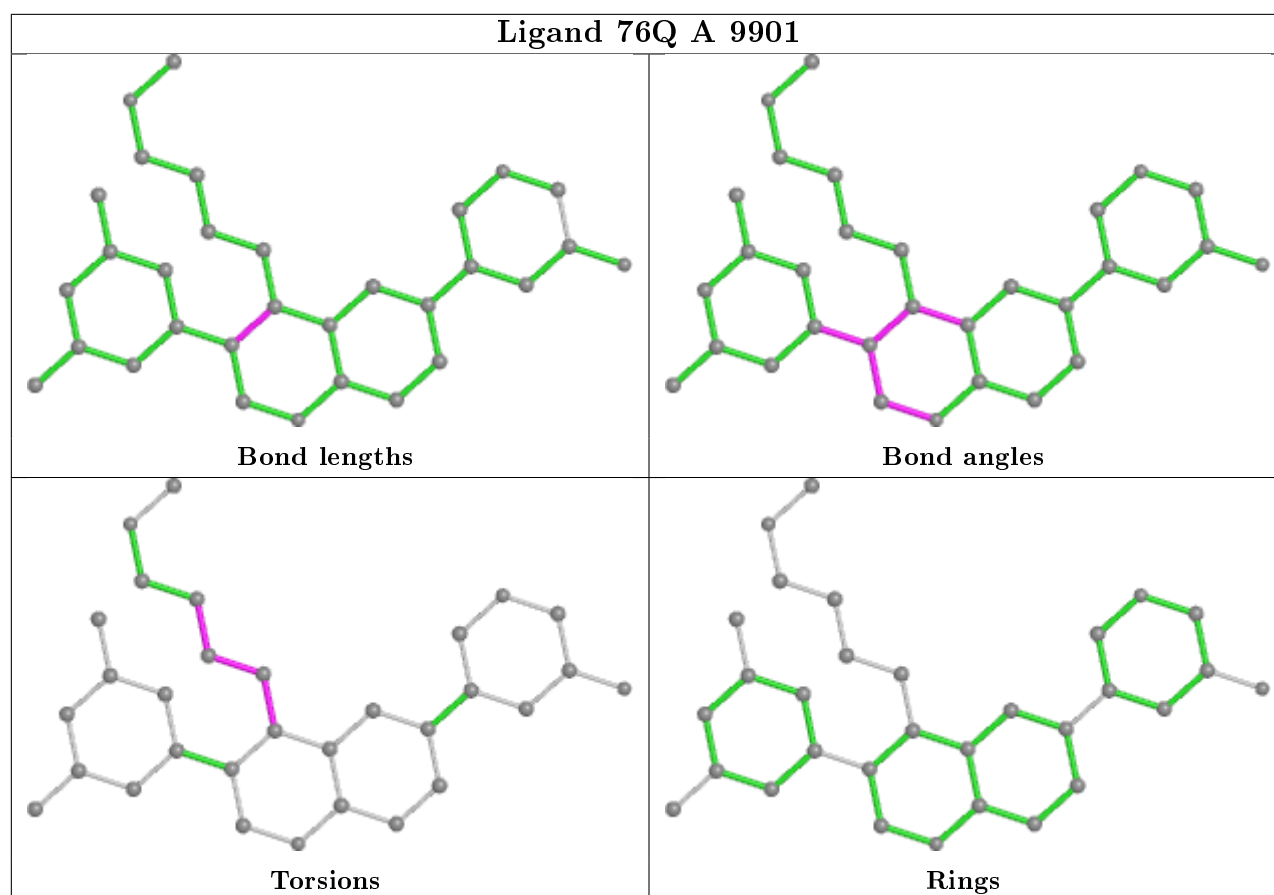
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	9901	76Q	3	0
2	A	9901	76Q	1	0

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.







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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	280/301 (93%)	0.46	23 (8%) 11 15	34, 58, 122, 149	0
1	B	282/301 (93%)	0.76	38 (13%) 3 4	34, 61, 136, 156	0
1	C	284/301 (94%)	0.68	42 (14%) 2 3	29, 58, 124, 150	0
1	D	281/301 (93%)	0.52	23 (8%) 11 15	31, 55, 114, 141	0
All	All	1127/1204 (93%)	0.61	126 (11%) 5 7	29, 58, 124, 156	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	GLY	13.7
1	D	197	PHE	11.0
1	C	197	PHE	10.1
1	B	187	VAL	9.3
1	D	183	ARG	7.9
1	B	197	PHE	7.5
1	C	192	MET	7.5
1	C	196	GLY	7.5
1	B	216	ALA	7.5
1	B	195	GLY	6.5
1	A	197	PHE	6.3
1	B	204	TYR	6.1
1	C	255	GLY	6.1
1	D	184	PRO	5.9
1	D	227	LYS	5.8
1	B	230	PHE	5.8
1	B	227	LYS	5.7
1	B	188	GLY	5.7
1	B	194	GLU	5.5
1	A	207	ASN	5.5
1	B	196	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	228	GLN	5.1
1	B	257	ASP	5.1
1	D	188	GLY	4.9
1	B	215	LEU	4.9
1	B	229	GLN	4.8
1	D	185	ILE	4.7
1	A	256	ASP	4.5
1	B	180	PHE	4.5
1	C	194	GLU	4.4
1	D	196	GLY	4.3
1	B	253	SER	4.3
1	B	228	GLN	4.1
1	B	185	ILE	3.9
1	B	343	VAL	3.9
1	A	192	MET	3.9
1	A	215	LEU	3.9
1	B	179	ASN	3.8
1	B	258	LEU	3.8
1	A	222	THR	3.7
1	B	236	VAL	3.7
1	D	189	GLY	3.5
1	C	257	ASP	3.4
1	D	230	PHE	3.4
1	B	183	ARG	3.4
1	A	194	GLU	3.3
1	D	459	ALA	3.3
1	C	190	ASN	3.3
1	A	183	ARG	3.3
1	C	182	GLU	3.2
1	C	183	ARG	3.2
1	D	200	VAL	3.2
1	A	182	GLU	3.2
1	B	390	HIS	3.1
1	C	251	PHE	3.1
1	B	235	LYS	3.1
1	A	336	SER	3.1
1	A	227	LYS	3.1
1	A	206	ASN	3.0
1	D	192	MET	3.0
1	D	226	LEU	3.0
1	D	164	ARG	3.0
1	B	199	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	170	PHE	3.0
1	B	165	PHE	2.9
1	C	191	LYS	2.9
1	B	190	ASN	2.9
1	A	230	PHE	2.9
1	A	191	LYS	2.8
1	B	389	GLU	2.8
1	B	226	LEU	2.8
1	A	225	GLU	2.8
1	C	185	ILE	2.8
1	C	195	GLY	2.7
1	D	181	ASP	2.7
1	C	336	SER	2.6
1	C	227	LYS	2.6
1	B	184	PRO	2.6
1	C	225	GLU	2.6
1	B	231	ASP	2.5
1	D	195	GLY	2.5
1	C	173	LEU	2.5
1	B	240	CYS	2.5
1	D	165	PHE	2.5
1	C	256	ASP	2.5
1	B	170	PHE	2.4
1	A	208	THR	2.4
1	A	179	ASN	2.4
1	C	201	TYR	2.4
1	C	199	VAL	2.4
1	D	177	THR	2.4
1	D	201	TYR	2.4
1	D	256	ASP	2.4
1	C	168	PHE	2.4
1	A	223	THR	2.4
1	C	180	PHE	2.4
1	C	171	TYR	2.3
1	B	207	ASN	2.3
1	C	177	THR	2.3
1	C	165	PHE	2.3
1	B	334	ARG	2.3
1	C	252	SER	2.3
1	B	254	ASP	2.2
1	A	228	GLN	2.2
1	C	234	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	230	PHE	2.2
1	C	223	THR	2.2
1	B	214	LYS	2.2
1	C	167	SER	2.2
1	A	195	GLY	2.2
1	C	176	VAL	2.1
1	A	180	PHE	2.1
1	C	254	ASP	2.1
1	C	179	ASN	2.1
1	C	200	VAL	2.1
1	C	343	VAL	2.1
1	C	459	ALA	2.1
1	A	254	ASP	2.1
1	C	205	VAL	2.1
1	C	347	ARG	2.1
1	D	179	ASN	2.1
1	D	343	VAL	2.1
1	B	200	VAL	2.1
1	C	175	ASN	2.0
1	A	459	ALA	2.0
1	C	259	CYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	C	346	10/11	0.71	0.15	79,86,95,95	0
1	SEP	B	346	10/11	0.79	0.14	87,91,97,97	0
1	TPO	D	342	11/12	0.83	0.13	83,86,94,94	0
1	SEP	A	346	10/11	0.85	0.11	78,82,89,89	0
1	SEP	D	346	10/11	0.85	0.11	75,82,91,91	0
1	TPO	A	342	11/12	0.90	0.15	88,89,96,96	0
1	TPO	B	342	11/12	0.91	0.14	93,95,95,95	0
1	TPO	C	342	11/12	0.91	0.13	89,90,95,95	0
1	TPO	B	345	11/12	0.92	0.12	85,87,88,89	0
1	TPO	A	345	11/12	0.93	0.14	74,76,79,80	0
1	TPO	D	345	11/12	0.94	0.12	70,74,75,76	0
1	TPO	C	345	11/12	0.95	0.11	71,72,76,78	0

6.3 Carbohydrates [i](#)

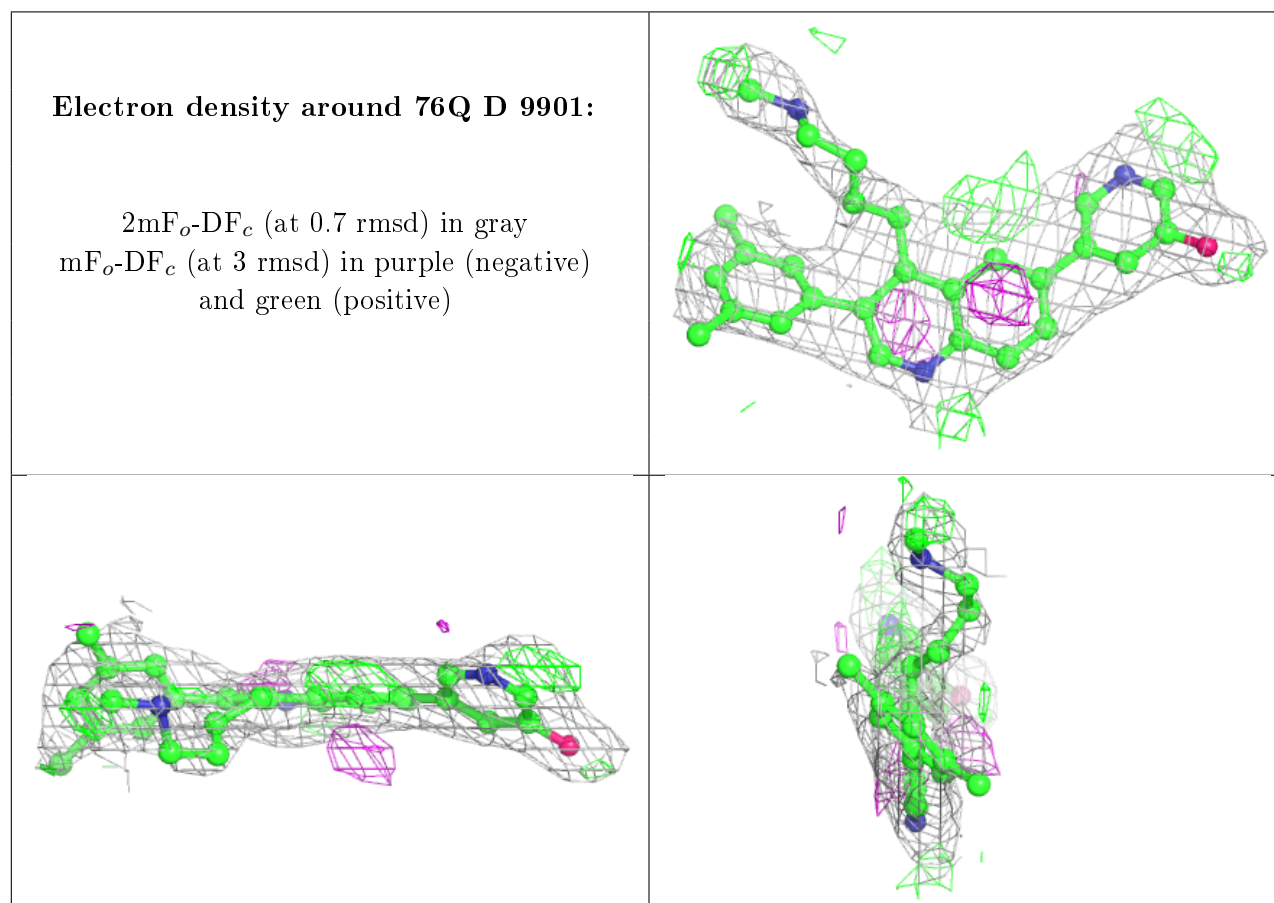
There are no carbohydrates in this entry.

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, 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.

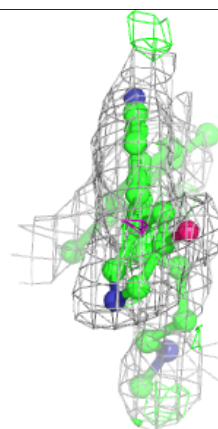
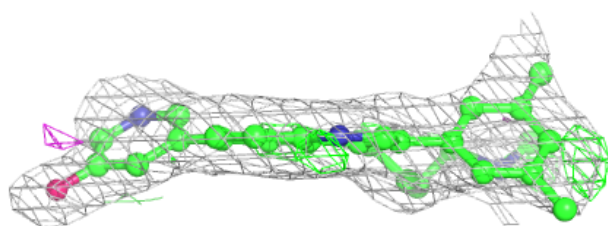
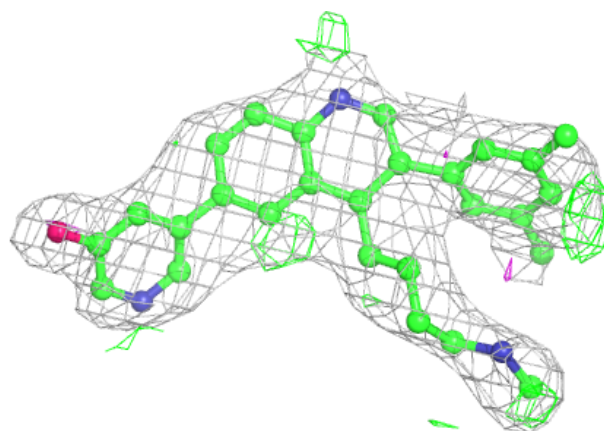
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	76Q	D	9901	31/31	0.79	0.25	66,73,78,78	0
2	76Q	C	9901	31/31	0.84	0.19	58,69,74,75	0
2	76Q	A	9901	31/31	0.87	0.24	61,71,77,78	0
2	76Q	B	9901	31/31	0.91	0.23	58,67,75,80	0

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.

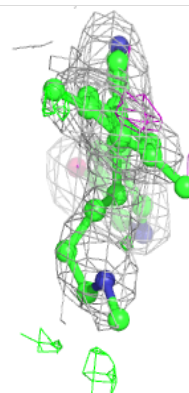
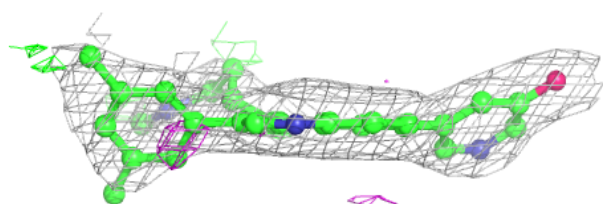
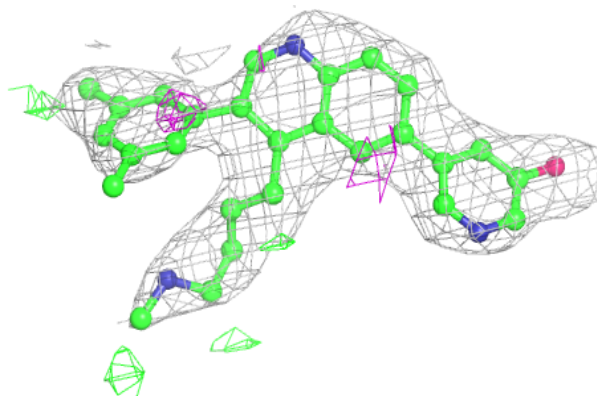


Electron density around 76Q C 9901:

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

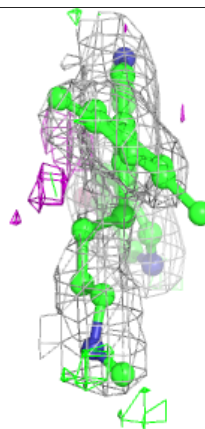
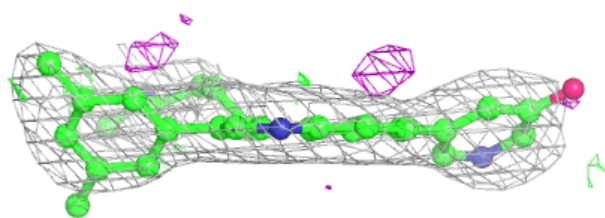
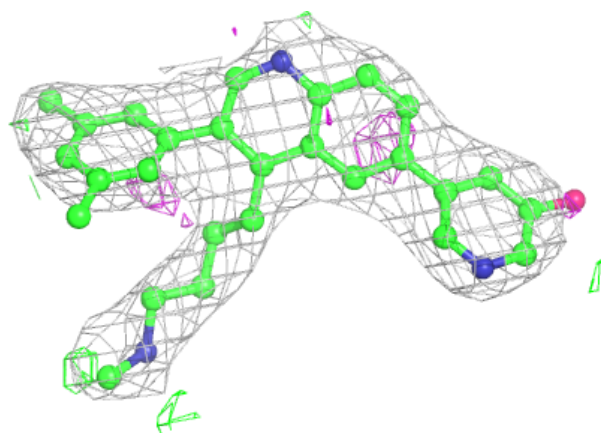
**Electron density around 76Q A 9901:**

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



Electron density around 76Q 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 ⓘ

There are no such residues in this entry.