Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2025 – 12:08 PM JST

PDB ID	:	9LVG / pdb_00009lvg
Title	:	Crystal structure of the mouse RIP3 kinase domain in complexed with Robinetin
Authors	:	Xie, H.; Su, H.X.; Li, M.J.; Xu, Y.C.
Deposited on	:	2025-02-12
Resolution	:	2.03 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

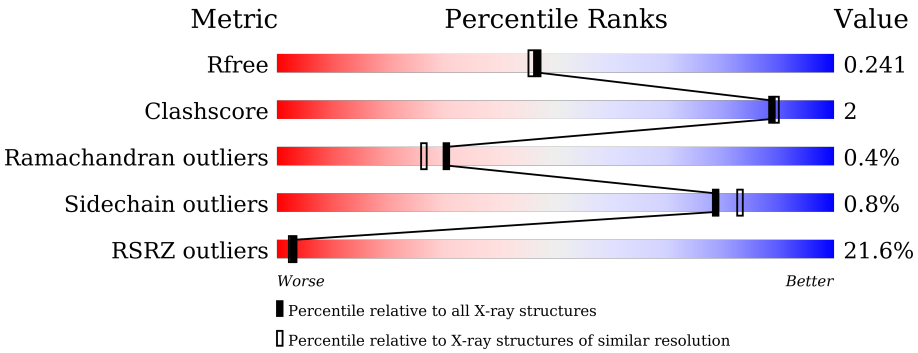
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.03 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}	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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	325	8% 78% · 18%
1	B	325	26% 72% 5% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4028 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 Receptor-interacting serine/threonine-protein kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2065	1335	352	370	8			
1	B	250	Total	C	N	O	S	0	0	0
			1820	1166	312	334	8			

There are 30 discrepancies between the modelled and reference sequences:

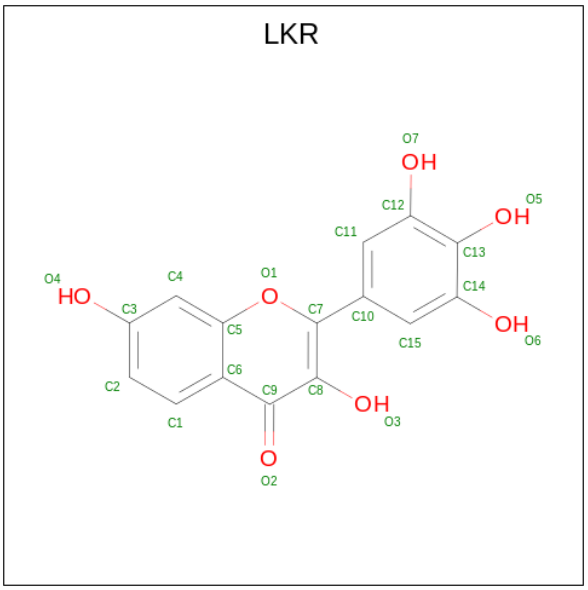
Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ALA	CYS	conflict	UNP Q9QZL0
A	136	ASP	ASN	conflict	UNP Q9QZL0
A	198	LYS	ASP	conflict	UNP Q9QZL0
A	314	LEU	-	expression tag	UNP Q9QZL0
A	315	GLU	-	expression tag	UNP Q9QZL0
A	316	HIS	-	expression tag	UNP Q9QZL0
A	317	HIS	-	expression tag	UNP Q9QZL0
A	318	HIS	-	expression tag	UNP Q9QZL0
A	319	HIS	-	expression tag	UNP Q9QZL0
A	320	HIS	-	expression tag	UNP Q9QZL0
A	321	HIS	-	expression tag	UNP Q9QZL0
A	322	HIS	-	expression tag	UNP Q9QZL0
A	323	HIS	-	expression tag	UNP Q9QZL0
A	324	HIS	-	expression tag	UNP Q9QZL0
A	325	HIS	-	expression tag	UNP Q9QZL0
B	111	ALA	CYS	conflict	UNP Q9QZL0
B	136	ASP	ASN	conflict	UNP Q9QZL0
B	198	LYS	ASP	conflict	UNP Q9QZL0
B	314	LEU	-	expression tag	UNP Q9QZL0
B	315	GLU	-	expression tag	UNP Q9QZL0
B	316	HIS	-	expression tag	UNP Q9QZL0
B	317	HIS	-	expression tag	UNP Q9QZL0
B	318	HIS	-	expression tag	UNP Q9QZL0
B	319	HIS	-	expression tag	UNP Q9QZL0
B	320	HIS	-	expression tag	UNP Q9QZL0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	321	HIS	-	expression tag	UNP Q9QZL0
B	322	HIS	-	expression tag	UNP Q9QZL0
B	323	HIS	-	expression tag	UNP Q9QZL0
B	324	HIS	-	expression tag	UNP Q9QZL0
B	325	HIS	-	expression tag	UNP Q9QZL0

- Molecule 2 is 3,7-bis(oxidanyl)-2-[3,4,5-tris(oxidanyl)phenyl]chromen-4-one (CCD ID: LKR) (formula: $C_{15}H_{10}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 22 15 7	0	0
2	B	1	Total C O 22 15 7	0	0

- Molecule 3 is water.

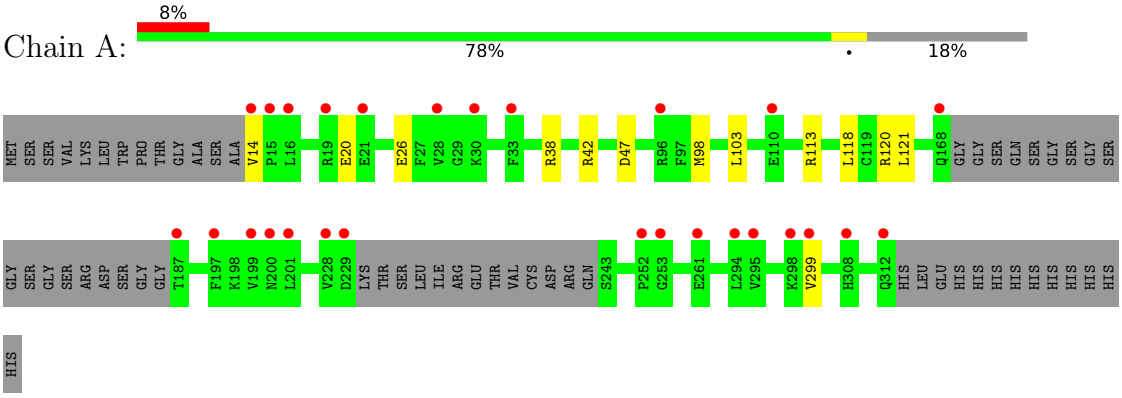
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	30	Total O 30 30	0	0

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.

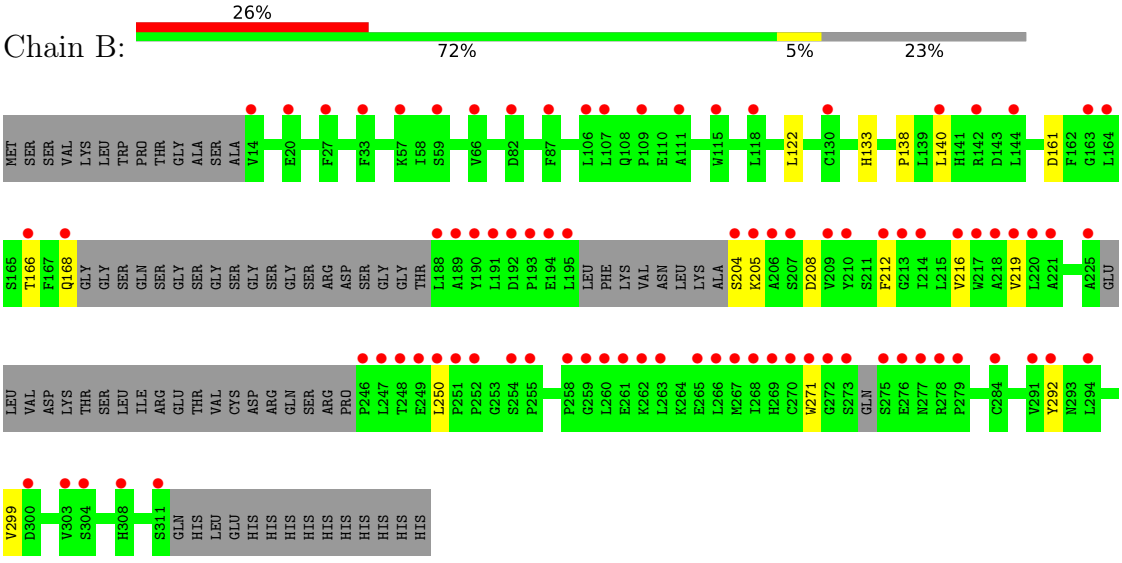
• Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain A:



• Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.94Å 51.35Å 106.19Å 90.00° 132.57° 90.00°	Depositor
Resolution (Å)	39.10 – 2.03 39.10 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.10-2.03) 97.5 (39.10-2.03)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.217 , 0.236 0.223 , 0.241	Depositor DCC
R_{free} test set	1958 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4028	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LKR

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	0.36	0/2115	0.44	0/2884
1	B	0.16	0/1859	0.36	0/2542
All	All	0.29	0/3974	0.40	0/5426

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

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	2065	0	2033	6	0
1	B	1820	0	1688	8	0
2	A	22	0	0	1	0
2	B	22	0	0	0	0
3	A	69	0	0	0	0
3	B	30	0	0	0	0
All	All	4028	0	3721	14	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 2.

All (14) 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:98:MET:N	2:A:401:LKR:O2	2.27	0.64
1:B:138:PRO:HG2	1:B:168:GLN:HB3	1.81	0.63
1:B:140:LEU:HD13	1:B:208:ASP:OD2	2.03	0.58
1:B:292:TYR:HE1	1:B:299:VAL:HG11	1.71	0.55
1:A:120:ARG:HD3	1:A:299:VAL:HG21	1.91	0.51
1:A:103:LEU:HD13	1:A:121:LEU:HD13	1.94	0.48
1:B:133:HIS:HB3	1:B:205:LYS:HE3	1.96	0.47
1:B:212:PHE:O	1:B:216:VAL:HG23	2.16	0.46
1:B:140:LEU:HB2	1:B:166:THR:O	2.17	0.45
1:B:271:TRP:CD1	1:B:271:TRP:C	2.96	0.44
1:A:38:ARG:NH1	1:A:47:ASP:OD2	2.53	0.42
1:A:113:ARG:HB3	1:A:118:LEU:HD11	2.01	0.42
1:A:20:GLU:O	1:A:42:ARG:HD2	2.20	0.41
1:B:122:LEU:HD21	1:B:219:VAL:HG11	2.02	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	262/325 (81%)	257 (98%)	5 (2%)	0	100 100
1	B	240/325 (74%)	226 (94%)	12 (5%)	2 (1%)	16 11
All	All	502/650 (77%)	483 (96%)	17 (3%)	2 (0%)	30 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	LEU
1	B	161	ASP

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	219/283 (77%)	217 (99%)	2 (1%)	75 80
1	B	178/283 (63%)	177 (99%)	1 (1%)	84 88
All	All	397/566 (70%)	394 (99%)	3 (1%)	79 83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	26	GLU
1	B	204	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	168	GLN
1	B	84	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides 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	LKR	B	401	-	24,24,24	0.57	0	36,36,36	0.74	2 (5%)
2	LKR	A	401	-	24,24,24	0.94	1 (4%)	36,36,36	0.97	2 (5%)

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	LKR	B	401	-	-	0/4/4/4	0/3/3/3
2	LKR	A	401	-	-	0/4/4/4	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	LKR	C6-C9	-2.15	1.44	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	LKR	O1-C7-C10	3.02	115.29	110.86
2	A	401	LKR	C10-C7-C8	-2.59	123.87	128.32
2	B	401	LKR	O1-C7-C10	2.11	113.95	110.86
2	B	401	LKR	C1-C6-C9	2.10	123.17	120.10

There are no chirality outliers.

There are no torsion outliers.

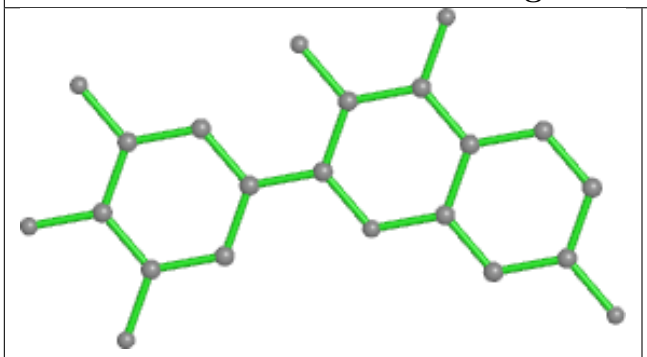
There are no ring outliers.

1 monomer is involved in 1 short contact:

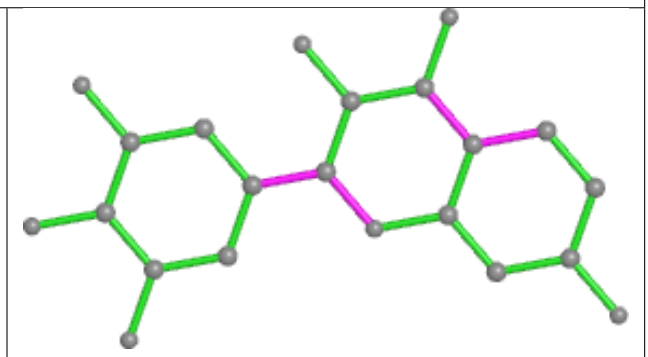
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	LKR	1	0

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 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.

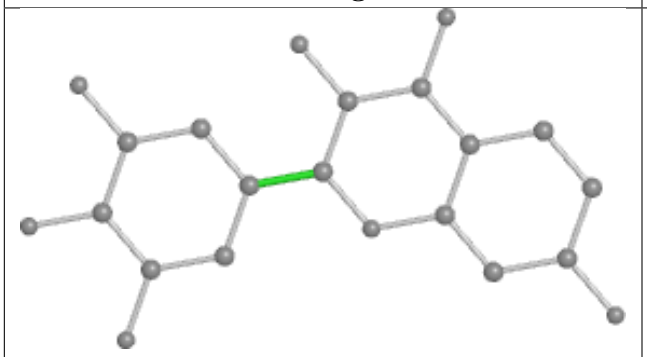
Ligand LKR B 401



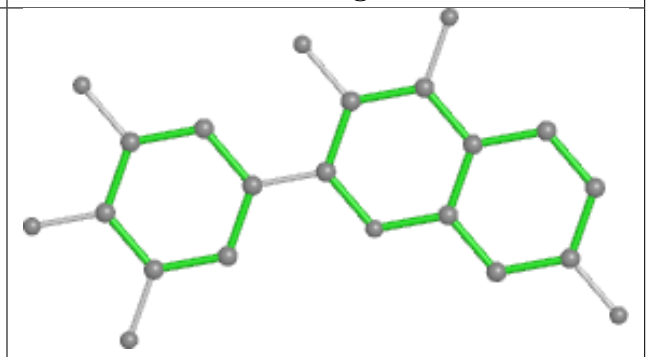
Bond lengths



Bond angles

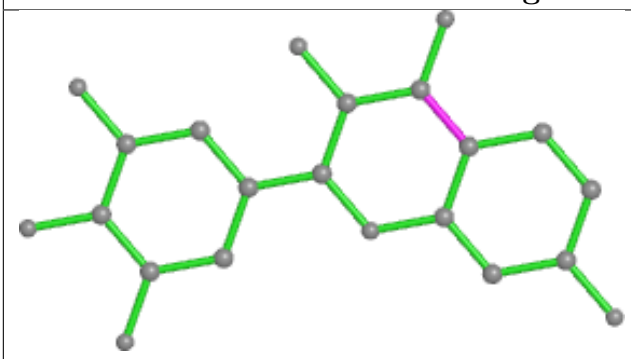


Torsions

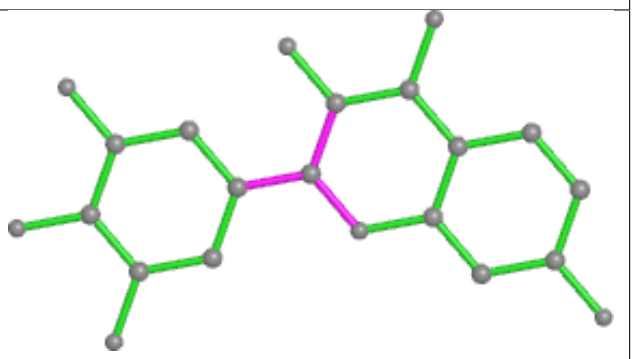


Rings

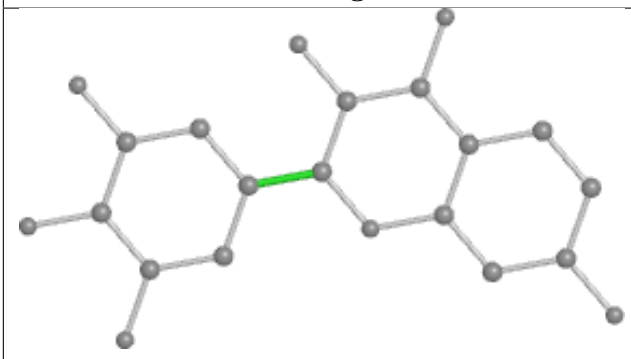
Ligand LKR A 401



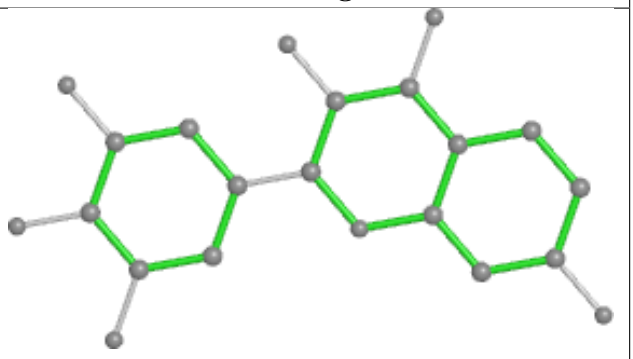
Bond lengths



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

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^{th} 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	268/325 (82%)	0.63	27 (10%) 14 13	30, 42, 64, 77	0
1	B	250/325 (76%)	1.57	85 (34%) 1 1	34, 61, 91, 108	0
All	All	518/650 (79%)	1.09	112 (21%) 3 2	30, 50, 80, 108	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	VAL	6.2
1	A	14	VAL	6.0
1	B	195	LEU	5.1
1	B	193	PRO	4.6
1	B	246	PRO	4.6
1	A	200	ASN	4.5
1	B	189	ALA	4.5
1	A	33	PHE	4.2
1	B	163	GLY	4.2
1	B	214	ILE	4.1
1	B	225	ALA	4.1
1	B	248	THR	4.0
1	A	197	PHE	3.9
1	B	217	TRP	3.7
1	B	277	ASN	3.6
1	B	266	LEU	3.6
1	B	270	CYS	3.6
1	B	247	LEU	3.5
1	B	275	SER	3.5
1	B	273	SER	3.5
1	B	269	HIS	3.5
1	B	190	TYR	3.5
1	B	272	GLY	3.5
1	A	187	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	111	ALA	3.4
1	A	21	GLU	3.4
1	B	249	GLU	3.4
1	B	250	LEU	3.4
1	B	164	LEU	3.3
1	B	210	TYR	3.3
1	B	220	LEU	3.3
1	A	201	LEU	3.2
1	B	188	LEU	3.2
1	B	109	PRO	3.2
1	B	255	PRO	3.1
1	A	96	ARG	3.1
1	B	191	LEU	3.1
1	B	219	VAL	3.1
1	B	259	GLY	3.0
1	A	312	GLN	3.0
1	B	213	GLY	3.0
1	B	221	ALA	3.0
1	B	265	GLU	3.0
1	B	271	TRP	2.9
1	B	192	ASP	2.9
1	A	15	PRO	2.9
1	A	228	VAL	2.9
1	B	206	ALA	2.9
1	B	251	PRO	2.8
1	B	262	LYS	2.8
1	B	82	ASP	2.7
1	B	254	SER	2.7
1	A	261	GLU	2.7
1	B	194	GLU	2.7
1	B	87	PHE	2.7
1	A	16	LEU	2.7
1	A	19	ARG	2.7
1	B	204	SER	2.6
1	B	260	LEU	2.6
1	A	294	LEU	2.6
1	B	308	HIS	2.6
1	B	144	LEU	2.6
1	B	209	VAL	2.6
1	A	252	PRO	2.6
1	B	166	THR	2.5
1	B	311	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	106	LEU	2.5
1	B	252	PRO	2.5
1	B	276	GLU	2.5
1	B	107	LEU	2.5
1	B	279	PRO	2.4
1	B	27	PHE	2.4
1	B	142	ARG	2.4
1	B	14	VAL	2.4
1	B	57	LYS	2.4
1	B	59	SER	2.4
1	B	212	PHE	2.4
1	B	218	ALA	2.4
1	B	284	CYS	2.4
1	B	66	VAL	2.4
1	B	303	VAL	2.4
1	A	308	HIS	2.3
1	B	267	MET	2.3
1	B	205	LYS	2.3
1	A	295	VAL	2.3
1	B	115	TRP	2.3
1	A	229	ASP	2.3
1	B	20	GLU	2.3
1	B	118	LEU	2.3
1	B	140	LEU	2.3
1	B	304	SER	2.2
1	B	216	VAL	2.2
1	B	33	PHE	2.2
1	A	110	GLU	2.2
1	B	292	TYR	2.2
1	B	263	LEU	2.1
1	B	268	ILE	2.1
1	B	258	PRO	2.1
1	A	299	VAL	2.1
1	A	30	LYS	2.1
1	B	168	GLN	2.1
1	B	207	SER	2.1
1	A	168	GLN	2.1
1	A	298	LYS	2.1
1	B	278	ARG	2.1
1	A	253	GLY	2.0
1	B	130	CYS	2.0
1	B	291	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	300	ASP	2.0
1	B	294	LEU	2.0
1	B	261	GLU	2.0
1	A	28	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

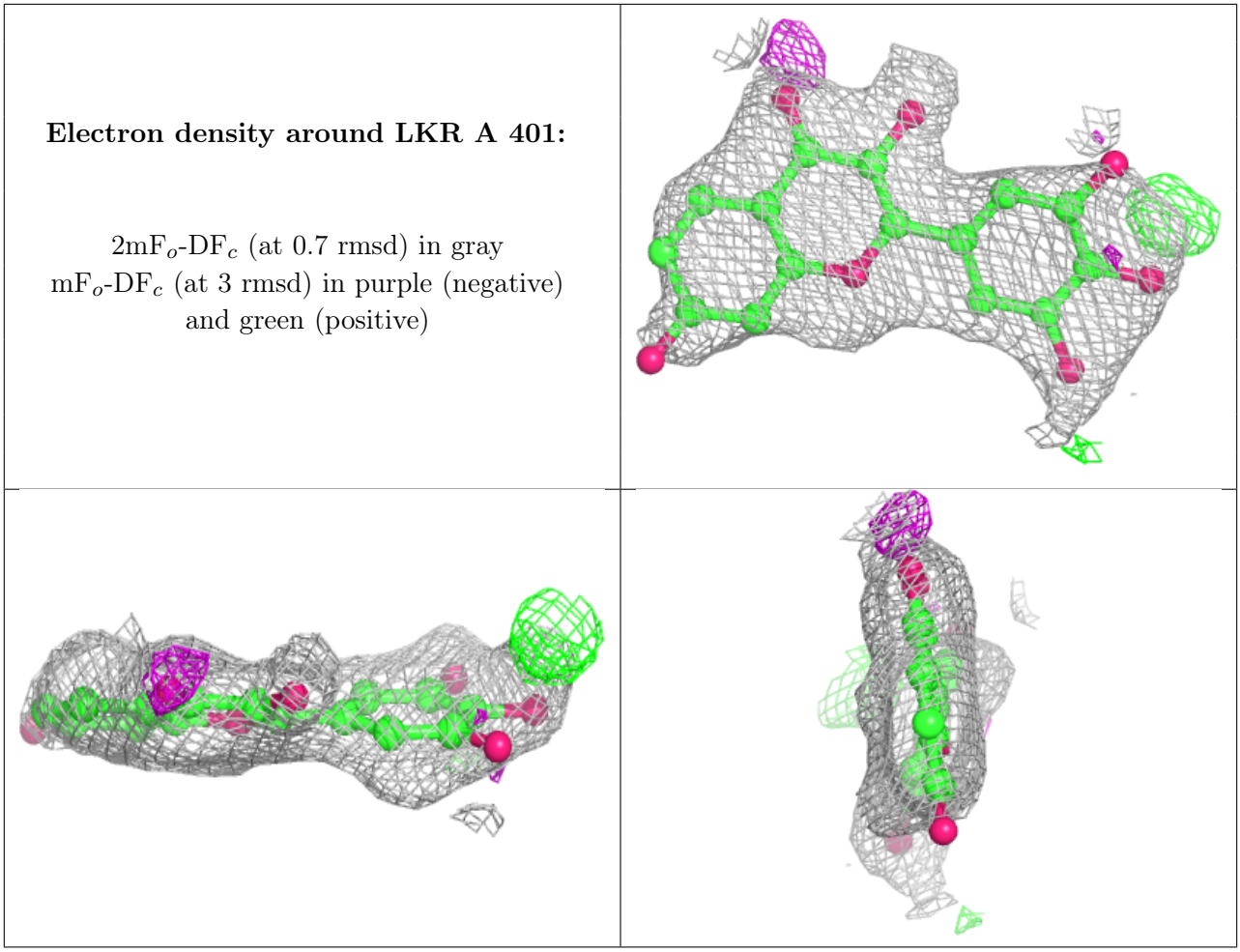
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	LKR	A	401	22/22	0.83	0.13	39,56,68,104	0
2	LKR	B	401	22/22	0.90	0.12	46,53,63,69	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.

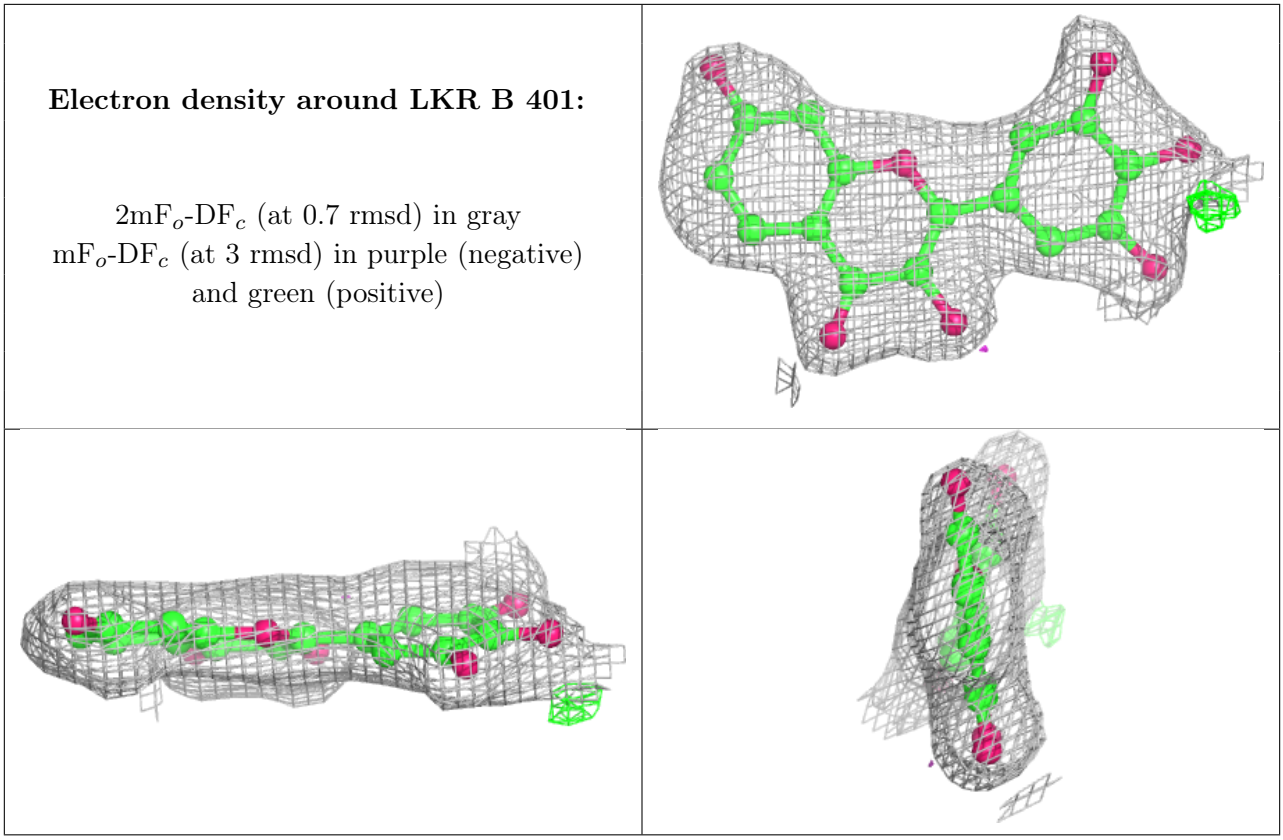
Electron density around LKR A 401:

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



Electron density around LKR B 401:

$2mF_o$-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.