



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 06:34 PM EDT

PDB ID : 6HK6
Title : Human RIOK2 bound to inhibitor
Authors : Wang, J.; Krojer, T.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.; Knapp, S.; Elkins, J.M.
Deposited on : 2018-09-05
Resolution : 2.35 Å(reported)

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

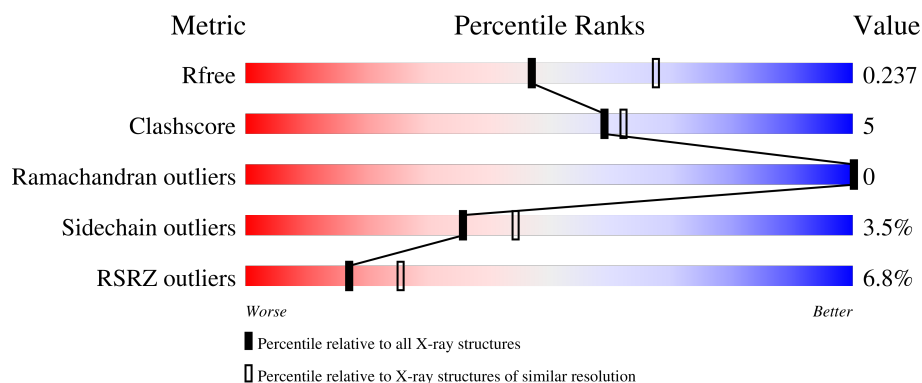
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 $\leq 5\%$. 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	<div> <div> <div>0%</div> <div>75%</div> <div>12%</div> <div>12%</div> </div> </div>
1	B	330	<div> <div> <div>0%</div> <div>75%</div> <div>11%</div> <div>12%</div> </div> </div>
1	C	330	<div> <div> <div>2%</div> <div>76%</div> <div>11%</div> <div>12%</div> </div> </div>
1	D	330	<div> <div> <div>6%</div> <div>77%</div> <div>11%</div> <div>12%</div> </div> </div>
1	E	330	<div> <div> <div>8%</div> <div>78%</div> <div>8%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	330	<div> <div>6%</div> <div>78%</div> <div>9%</div> <div>12%</div> </div>
1	G	330	<div> <div>17%</div> <div>73%</div> <div>9%</div> <div>18%</div> </div>
1	H	330	<div> <div>5%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>
1	I	330	<div> <div>3%</div> <div>78%</div> <div>8%</div> <div>13%</div> </div>
1	J	330	<div> <div>11%</div> <div>75%</div> <div>11%</div> <div>12%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23349 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 Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2336	1496	400	426	14			
1	B	290	Total	C	N	O	S	0	0	0
			2323	1487	397	425	14			
1	C	290	Total	C	N	O	S	0	0	0
			2314	1482	395	423	14			
1	D	290	Total	C	N	O	S	0	0	0
			2272	1457	383	418	14			
1	E	289	Total	C	N	O	S	0	0	0
			2262	1457	379	412	14			
1	F	289	Total	C	N	O	S	0	0	0
			2268	1456	378	419	15			
1	G	271	Total	C	N	O	S	0	0	0
			2141	1380	351	396	14			
1	H	282	Total	C	N	O	S	0	0	0
			2241	1438	374	416	13			
1	I	288	Total	C	N	O	S	0	0	0
			2288	1470	384	420	14			
1	J	290	Total	C	N	O	S	0	0	0
			2236	1438	369	415	14			

There are 20 discrepancies between the modelled and reference sequences:

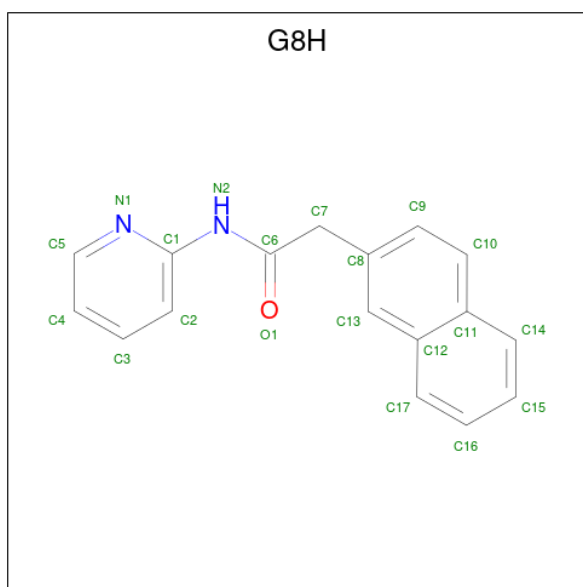
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9BVS4
A	144	TYR	HIS	conflict	UNP Q9BVS4
B	0	SER	-	expression tag	UNP Q9BVS4
B	144	TYR	HIS	conflict	UNP Q9BVS4
C	0	SER	-	expression tag	UNP Q9BVS4
C	144	TYR	HIS	conflict	UNP Q9BVS4
D	0	SER	-	expression tag	UNP Q9BVS4
D	144	TYR	HIS	conflict	UNP Q9BVS4
E	0	SER	-	expression tag	UNP Q9BVS4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	144	TYR	HIS	conflict	UNP Q9BVS4
F	0	SER	-	expression tag	UNP Q9BVS4
F	144	TYR	HIS	conflict	UNP Q9BVS4
G	0	SER	-	expression tag	UNP Q9BVS4
G	144	TYR	HIS	conflict	UNP Q9BVS4
H	0	SER	-	expression tag	UNP Q9BVS4
H	144	TYR	HIS	conflict	UNP Q9BVS4
I	0	SER	-	expression tag	UNP Q9BVS4
I	144	TYR	HIS	conflict	UNP Q9BVS4
J	0	SER	-	expression tag	UNP Q9BVS4
J	144	TYR	HIS	conflict	UNP Q9BVS4

- Molecule 2 is 2-naphthalen-2-yl- {N}-pyridin-2-yl-ethanamide (three-letter code: G8H) (formula: C₁₇H₁₄N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	17	2	1		
2	B	1	Total	C	N	O	0	0
			20	17	2	1		
2	C	1	Total	C	N	O	0	0
			20	17	2	1		
2	D	1	Total	C	N	O	0	0
			20	17	2	1		
2	E	1	Total	C	N	O	0	0
			20	17	2	1		

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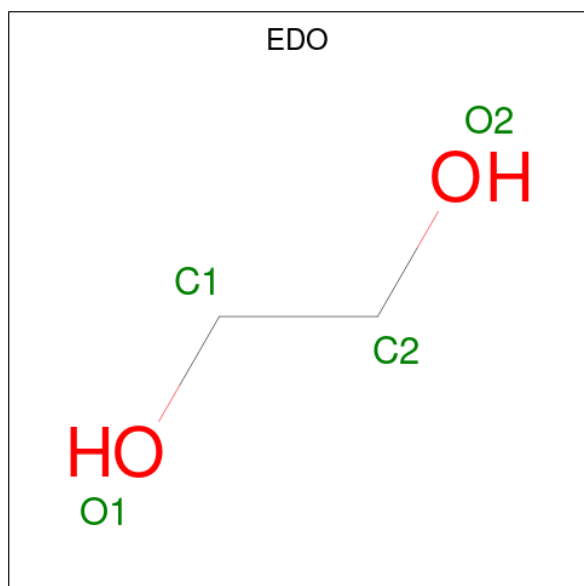
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			20	17	2	1		
2	G	1	Total	C	N	O	0	0
			20	17	2	1		
2	H	1	Total	C	N	O	0	0
			20	17	2	1		
2	I	1	Total	C	N	O	0	0
			20	17	2	1		
2	J	1	Total	C	N	O	0	0
			20	17	2	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



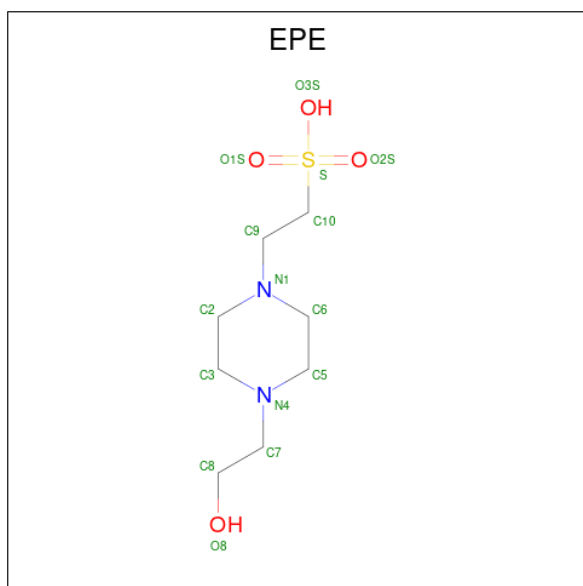
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

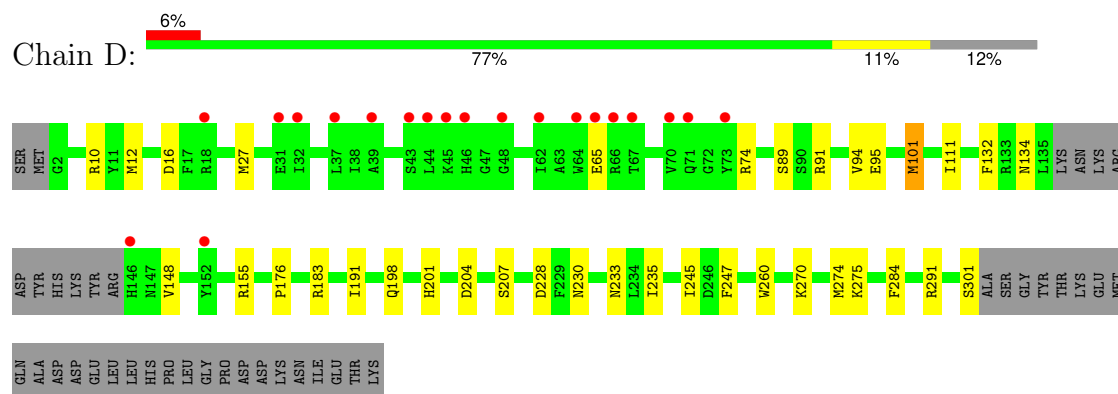
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total 79	O 79	0	0
6	B	59	Total 59	O 59	0	0
6	C	55	Total 55	O 55	0	0
6	D	17	Total 17	O 17	0	0
6	E	26	Total 26	O 26	0	0
6	F	44	Total 44	O 44	0	0
6	G	3	Total 3	O 3	0	0
6	H	51	Total 51	O 51	0	0
6	I	35	Total 35	O 35	0	0
6	J	7	Total 7	O 7	0	0

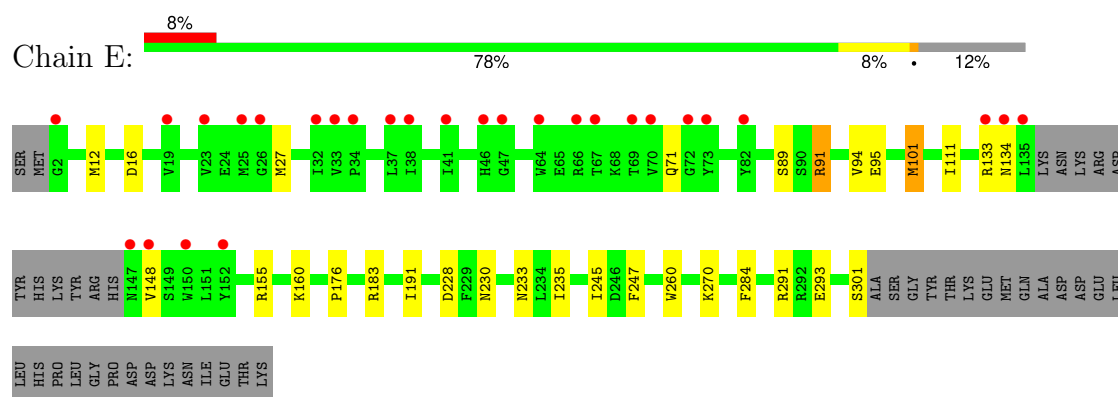
- Molecule 1: Serine/threonine-protein kinase RIO2



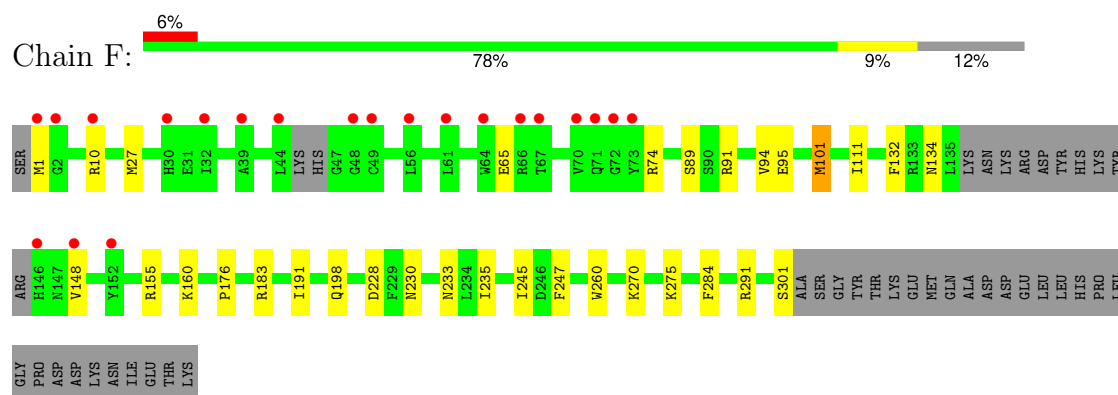
- Molecule 1: Serine/threonine-protein kinase RIO2



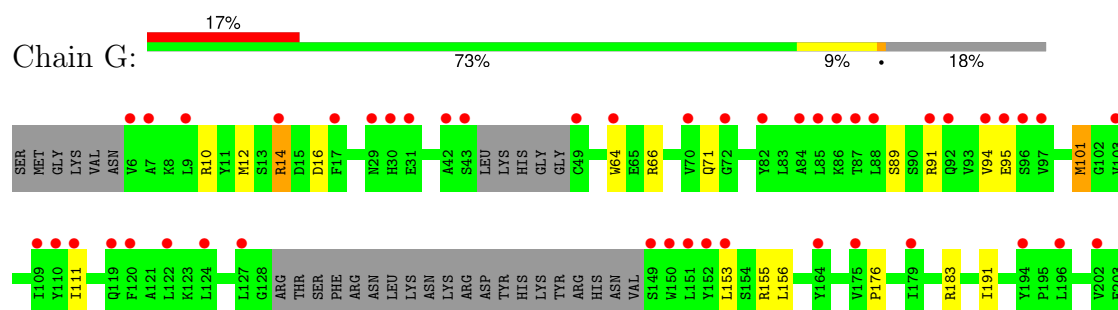
- Molecule 1: Serine/threonine-protein kinase RIO2

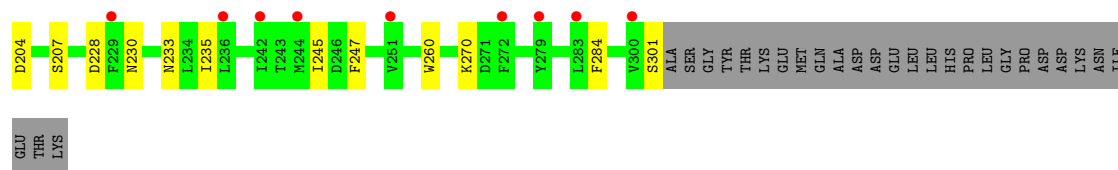


- Molecule 1: Serine/threonine-protein kinase RIO2

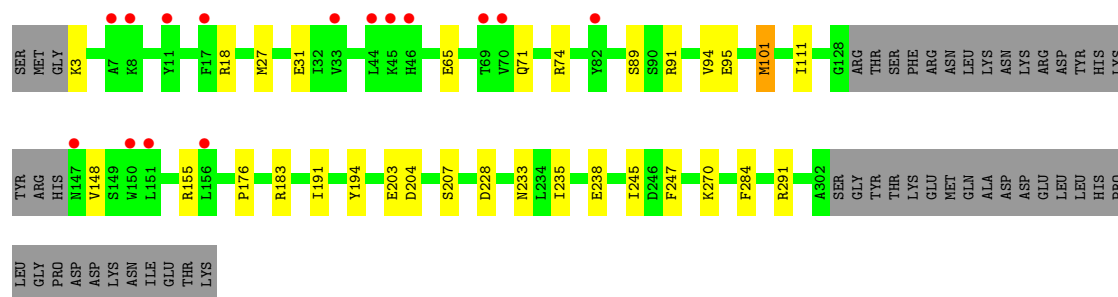
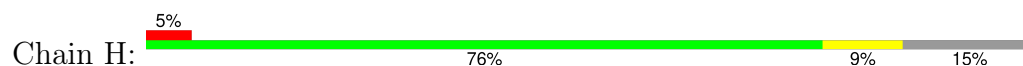


- Molecule 1: Serine/threonine-protein kinase RIO2

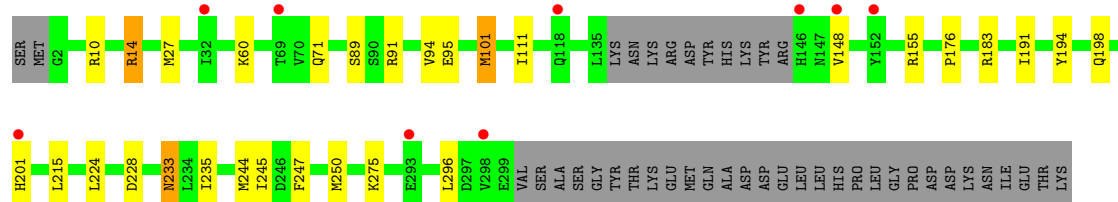
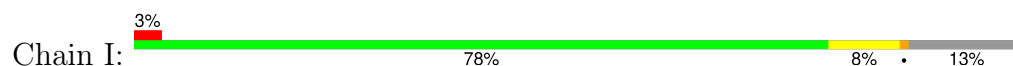




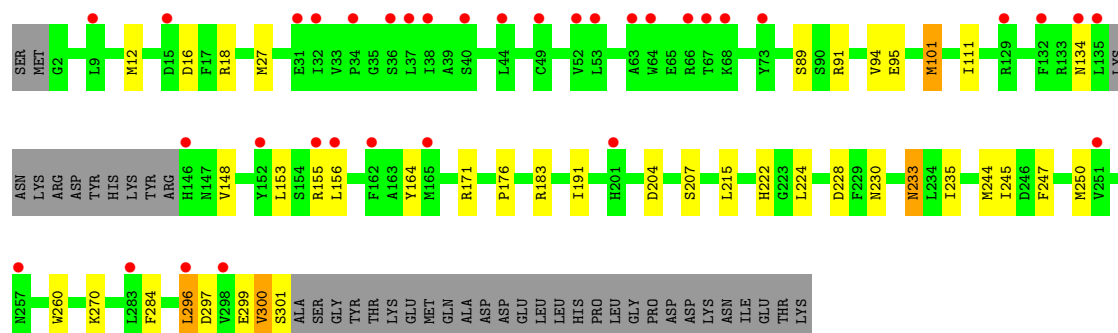
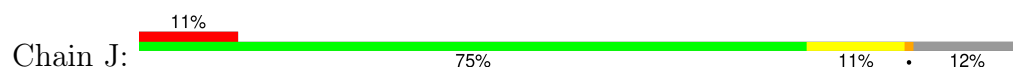
- Molecule 1: Serine/threonine-protein kinase RIO2



- Molecule 1: Serine/threonine-protein kinase RIO2



- Molecule 1: Serine/threonine-protein kinase RIO2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.01Å 92.86Å 237.65Å 90.00° 99.10° 90.00°	Depositor
Resolution (Å)	78.34 – 2.35 78.22 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (78.34-2.35) 99.7 (78.22-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.215 , 0.235 0.217 , 0.237	Depositor DCC
R_{free} test set	8217 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23349	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G8H, EDO, EPE, CL

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	0.70	0/2388	0.82	0/3225
1	B	0.66	0/2375	0.80	0/3210
1	C	0.67	0/2365	0.81	1/3197 (0.0%)
1	D	0.65	0/2322	0.78	0/3147
1	E	0.65	0/2313	0.77	0/3134
1	F	0.66	0/2317	0.77	0/3137
1	G	0.64	0/2188	0.78	0/2963
1	H	0.68	0/2290	0.80	2/3100 (0.1%)
1	I	0.68	0/2339	0.82	1/3164 (0.0%)
1	J	0.67	0/2286	0.80	3/3105 (0.1%)
All	All	0.67	0/23183	0.80	7/31382 (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	J	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	171	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	H	194	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	H	194	TYR	CB-CG-CD1	5.33	124.19	121.00
1	I	233	ASN	CB-CA-C	-5.25	99.89	110.40
1	J	233	ASN	CB-CA-C	-5.23	99.94	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	300	VAL	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	2336	0	2276	33	0
1	B	2323	0	2266	30	0
1	C	2314	0	2247	27	0
1	D	2272	0	2167	26	0
1	E	2262	0	2166	21	0
1	F	2268	0	2175	22	0
1	G	2141	0	2046	21	0
1	H	2241	0	2153	18	0
1	I	2288	0	2200	23	0
1	J	2236	0	2106	31	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	1	0
2	E	20	0	0	0	0
2	F	20	0	0	1	0
2	G	20	0	0	0	0
2	H	20	0	0	1	0
2	I	20	0	0	1	0
2	J	20	0	0	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	0	18	0	0
4	B	12	0	18	0	0
4	F	4	0	6	0	0
5	B	15	0	18	1	0
5	D	15	0	18	0	0
5	E	15	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	15	0	18	0	0
6	A	79	0	0	3	0
6	B	59	0	0	1	0
6	C	55	0	0	0	0
6	D	17	0	0	0	0
6	E	26	0	0	0	0
6	F	44	0	0	0	0
6	G	3	0	0	0	0
6	H	51	0	0	0	0
6	I	35	0	0	0	0
6	J	7	0	0	0	0
All	All	23349	0	21916	209	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 5.

The worst 5 of 209 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:J:296:LEU:O	1:J:300:VAL:HG22	1.52	1.08
1:D:301:SER:HA	1:E:134:ASN:HB3	1.51	0.92
1:J:297:ASP:O	1:J:301:SER:HA	1.70	0.91
1:C:301:SER:HA	1:F:134:ASN:HB3	1.57	0.85
1:J:222:HIS:HB3	1:J:296:LEU:HD12	1.62	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	286/330 (87%)	279 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	286/330 (87%)	281 (98%)	5 (2%)	0	100	100
1	C	286/330 (87%)	280 (98%)	6 (2%)	0	100	100
1	D	286/330 (87%)	279 (98%)	7 (2%)	0	100	100
1	E	285/330 (86%)	281 (99%)	4 (1%)	0	100	100
1	F	283/330 (86%)	279 (99%)	4 (1%)	0	100	100
1	G	265/330 (80%)	262 (99%)	3 (1%)	0	100	100
1	H	278/330 (84%)	272 (98%)	6 (2%)	0	100	100
1	I	284/330 (86%)	276 (97%)	8 (3%)	0	100	100
1	J	286/330 (87%)	278 (97%)	8 (3%)	0	100	100
All	All	2825/3300 (86%)	2767 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	247/294 (84%)	237 (96%)	10 (4%)	31	39
1	B	248/294 (84%)	238 (96%)	10 (4%)	31	39
1	C	244/294 (83%)	232 (95%)	12 (5%)	25	29
1	D	234/294 (80%)	227 (97%)	7 (3%)	41	50
1	E	232/294 (79%)	225 (97%)	7 (3%)	41	50
1	F	236/294 (80%)	229 (97%)	7 (3%)	41	50
1	G	221/294 (75%)	214 (97%)	7 (3%)	39	47
1	H	233/294 (79%)	224 (96%)	9 (4%)	32	40
1	I	237/294 (81%)	229 (97%)	8 (3%)	37	46
1	J	228/294 (78%)	222 (97%)	6 (3%)	46	56
All	All	2360/2940 (80%)	2277 (96%)	83 (4%)	36	44

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	95	GLU
1	I	71	GLN
1	G	247	PHE
1	H	95	GLU
1	I	201	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	200	HIS
1	I	71	GLN
1	I	198	GLN
1	H	119	GLN
1	C	71	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 for Mogul analysis.

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	G8H	H	401	-	22,22,22	0.50	0	29,29,29	0.33	0
4	EDO	B	403	-	3,3,3	0.10	0	2,2,2	0.08	0
2	G8H	J	600	-	22,22,22	0.47	0	29,29,29	0.32	0
2	G8H	G	600	-	22,22,22	0.46	0	29,29,29	0.33	0
2	G8H	I	600	-	22,22,22	0.48	0	29,29,29	0.30	0
5	EPE	E	402	-	15,15,15	1.87	1 (6%)	19,20,20	1.39	2 (10%)
4	EDO	A	405	-	3,3,3	0.15	0	2,2,2	0.16	0
5	EPE	H	402	-	15,15,15	1.90	1 (6%)	19,20,20	1.26	1 (5%)
4	EDO	A	404	-	3,3,3	0.09	0	2,2,2	0.06	0
5	EPE	D	402	-	15,15,15	2.02	1 (6%)	19,20,20	1.33	2 (10%)
4	EDO	B	405	-	3,3,3	0.10	0	2,2,2	0.11	0
2	G8H	A	401	-	22,22,22	0.49	0	29,29,29	0.35	0
5	EPE	B	402	-	15,15,15	1.95	1 (6%)	19,20,20	1.37	2 (10%)
2	G8H	B	401	-	22,22,22	0.47	0	29,29,29	0.32	0
2	G8H	F	401	-	22,22,22	0.47	0	29,29,29	0.33	0
4	EDO	B	404	-	3,3,3	0.11	0	2,2,2	0.08	0
4	EDO	F	402	-	3,3,3	0.11	0	2,2,2	0.13	0
2	G8H	C	401	-	22,22,22	0.45	0	29,29,29	0.29	0
2	G8H	E	401	-	22,22,22	0.49	0	29,29,29	0.32	0
2	G8H	D	401	-	22,22,22	0.48	0	29,29,29	0.29	0
4	EDO	A	406	-	3,3,3	0.12	0	2,2,2	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G8H	H	401	-	-	0/8/8/8	0/3/3/3
4	EDO	B	403	-	-	1/1/1/1	-
2	G8H	J	600	-	-	0/8/8/8	0/3/3/3
2	G8H	G	600	-	-	0/8/8/8	0/3/3/3
2	G8H	I	600	-	-	0/8/8/8	0/3/3/3
5	EPE	E	402	-	-	4/9/19/19	0/1/1/1
4	EDO	A	405	-	-	1/1/1/1	-
5	EPE	H	402	-	-	4/9/19/19	0/1/1/1
4	EDO	A	404	-	-	1/1/1/1	-
5	EPE	D	402	-	-	4/9/19/19	0/1/1/1
4	EDO	B	405	-	-	1/1/1/1	-
2	G8H	A	401	-	-	0/8/8/8	0/3/3/3
5	EPE	B	402	-	-	4/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G8H	B	401	-	-	0/8/8/8	0/3/3/3
2	G8H	F	401	-	-	0/8/8/8	0/3/3/3
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	F	402	-	-	1/1/1/1	-
2	G8H	C	401	-	-	0/8/8/8	0/3/3/3
2	G8H	E	401	-	-	0/8/8/8	0/3/3/3
2	G8H	D	401	-	-	0/8/8/8	0/3/3/3
4	EDO	A	406	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	402	EPE	C10-S	-7.45	1.67	1.77
5	B	402	EPE	C10-S	-6.98	1.67	1.77
5	H	402	EPE	C10-S	-6.78	1.68	1.77
5	E	402	EPE	C10-S	-6.69	1.68	1.77

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	402	EPE	O2S-S-C10	3.69	112.30	106.73
5	B	402	EPE	O1S-S-C10	3.50	112.01	106.73
5	H	402	EPE	O3S-S-C10	3.01	111.89	106.00
5	D	402	EPE	O1S-S-C10	2.81	110.97	106.73
5	D	402	EPE	C6-N1-C2	2.44	114.10	108.84

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	402	EPE	C9-C10-S-O1S
5	E	402	EPE	C9-C10-S-O3S
5	H	402	EPE	C9-C10-S-O1S
5	H	402	EPE	C9-C10-S-O2S
5	B	402	EPE	N4-C7-C8-O8

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401	G8H	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	600	G8H	1	0
5	E	402	EPE	2	0
5	B	402	EPE	1	0
2	F	401	G8H	1	0
2	D	401	G8H	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	290/330 (87%)	0.36	2 (0%) 87 92	23, 36, 66, 106	0
1	B	290/330 (87%)	0.29	4 (1%) 75 83	27, 41, 73, 99	0
1	C	290/330 (87%)	0.39	6 (2%) 63 74	29, 45, 95, 139	0
1	D	290/330 (87%)	0.57	20 (6%) 16 24	40, 57, 119, 152	0
1	E	289/330 (87%)	0.57	28 (9%) 7 12	34, 56, 126, 155	0
1	F	289/330 (87%)	0.48	21 (7%) 15 22	34, 51, 112, 140	0
1	G	271/330 (82%)	1.28	55 (20%) 1 1	56, 85, 117, 128	0
1	H	282/330 (85%)	0.45	15 (5%) 26 38	25, 42, 99, 124	0
1	I	288/330 (87%)	0.38	9 (3%) 49 61	34, 51, 84, 106	0
1	J	290/330 (87%)	0.84	35 (12%) 4 7	54, 76, 117, 142	0
All	All	2869/3300 (86%)	0.56	195 (6%) 17 25	23, 54, 110, 155	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	6	VAL	9.8
1	D	44	LEU	7.7
1	E	64	TRP	7.4
1	E	34	PRO	6.6
1	E	73	TYR	6.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	EPE	B	402	15/15	0.80	0.21	76,88,97,97	0
5	EPE	E	402	15/15	0.80	0.22	83,105,112,112	0
3	CL	C	402	1/1	0.82	0.15	69,69,69,69	0
4	EDO	A	405	4/4	0.82	0.17	59,60,60,60	0
5	EPE	D	402	15/15	0.83	0.29	101,111,122,122	0
3	CL	H	403	1/1	0.84	0.12	67,67,67,67	0
5	EPE	H	402	15/15	0.86	0.16	79,97,108,109	0
3	CL	A	403	1/1	0.89	0.10	78,78,78,78	0
4	EDO	B	405	4/4	0.90	0.19	51,52,53,54	0
2	G8H	G	600	20/20	0.91	0.27	65,95,114,114	0
4	EDO	B	403	4/4	0.91	0.17	53,55,56,57	0
4	EDO	A	404	4/4	0.91	0.21	52,52,52,52	0
4	EDO	F	402	4/4	0.91	0.20	64,65,66,67	0
4	EDO	A	406	4/4	0.93	0.16	42,45,47,51	0
3	CL	A	402	1/1	0.94	0.13	43,43,43,43	0
2	G8H	E	401	20/20	0.96	0.16	39,49,56,56	0
2	G8H	F	401	20/20	0.96	0.13	41,43,46,48	0
2	G8H	A	401	20/20	0.96	0.15	27,30,37,37	0
4	EDO	B	404	4/4	0.96	0.14	47,49,49,50	0
2	G8H	D	401	20/20	0.96	0.18	36,47,59,59	0
2	G8H	J	600	20/20	0.97	0.15	53,62,70,71	0
2	G8H	B	401	20/20	0.97	0.15	26,30,36,36	0
2	G8H	C	401	20/20	0.97	0.15	24,33,44,45	0
2	G8H	I	600	20/20	0.97	0.17	35,40,43,44	0
2	G8H	H	401	20/20	0.98	0.15	20,29,37,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.