



# wwPDB X-ray Structure Validation Summary Report

Jun 12, 2014 – 11:40 PM EDT

PDB ID : 4D0M  
Title : Phosphatidylinositol 4-kinase III beta in a complex with Rab11a-GTP-gamma-S and the Rab-binding domain of FIP3  
Authors : Burke, J.E.; Inglis, A.J.; Perisic, O.; Masson, G.R.; McLaughlin, S.H.; Rutaganira, F.; Shokat, K.M.; Williams, R.L.  
Deposited on : 2014-04-27  
Resolution : 6.00 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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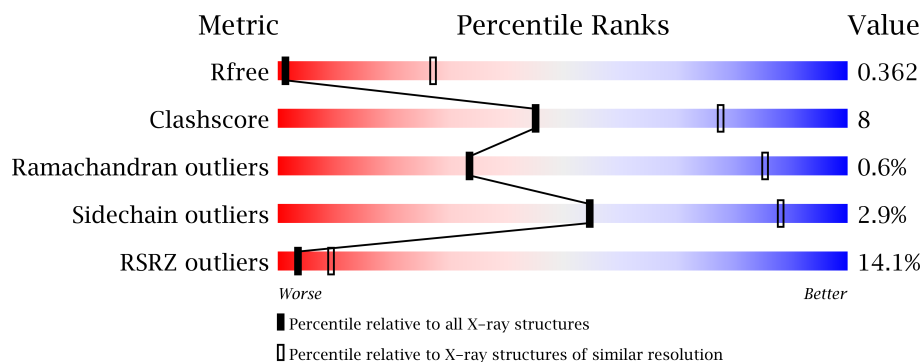
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 6.00 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))
$R_{free}$	66092	1089 (8.20-3.50)
Clashscore	79885	1024 (8.20-3.52)
Ramachandran outliers	78287	1283 (8.50-3.50)
Sidechain outliers	78261	1259 (8.50-3.50)
RSRZ outliers	66119	1088 (8.20-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	566	
1	C	566	
1	G	566	
1	I	566	
1	M	566	
1	O	566	
1	Q	566	
1	S	566	
1	W	566	
1	Y	566	
1	c	566	
1	g	566	
2	B	219	
2	D	219	

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Mol	Chain	Length	Quality of chain
2	H	219	
2	J	219	
2	N	219	
2	P	219	
2	R	219	
2	T	219	
2	X	219	
2	Z	219	
2	d	219	
2	h	219	
3	E	48	
3	F	48	
3	K	48	
3	L	48	
3	U	48	
3	V	48	
3	a	48	
3	b	48	
3	e	48	
3	f	48	
3	i	48	
3	j	48	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 65970 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHATIDYLINOSITOL 4-KINASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	C	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	G	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	I	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	M	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	O	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Q	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	S	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	W	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Y	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	c	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	g	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			

- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	D	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	J	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	N	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	P	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	R	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	T	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	X	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	Z	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	d	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	h	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
D	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
H	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
J	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
N	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
P	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
R	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
T	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
X	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
Z	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
d	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
h	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491

- Molecule 3 is a protein called RAB11 FAMILY-INTERACTING PROTEIN 3.

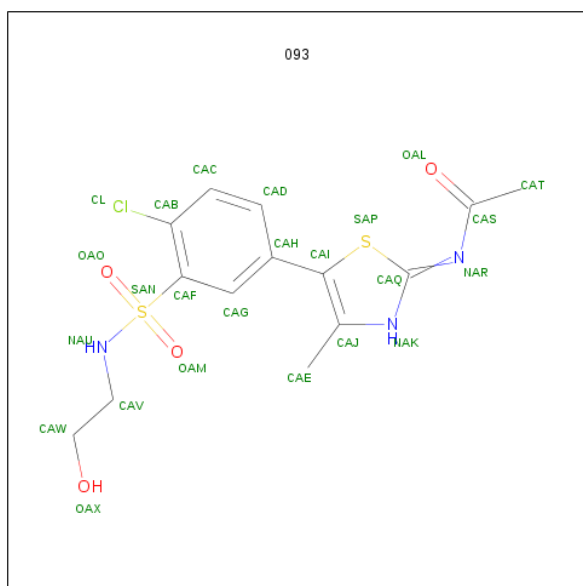
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			

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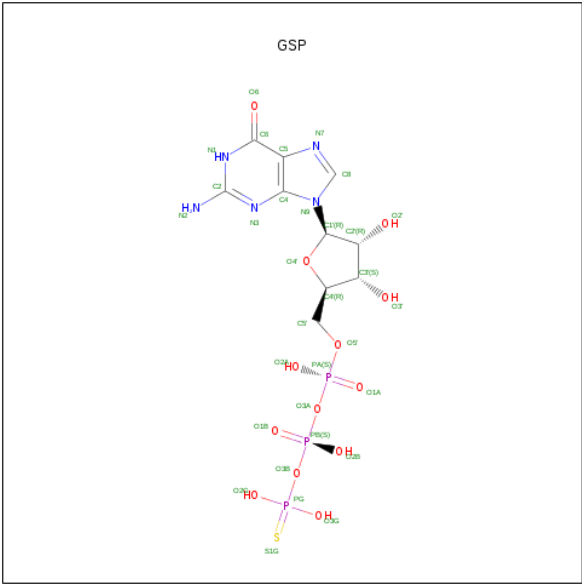
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	K	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	L	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	U	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	V	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	a	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	b	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	e	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	f	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	i	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	j	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			

- Molecule 4 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)-PHENYLTHIAZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C<sub>14</sub>H<sub>16</sub>ClN<sub>3</sub>O<sub>4</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	C	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	G	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	I	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	M	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	O	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	Q	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	S	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	W	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	Y	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	c	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	g	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	D	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	H	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	J	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	N	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	P	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	R	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	T	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	X	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	Z	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	d	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
5	h	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total 1	Mg 1	0	0
6	J	1	Total 1	Mg 1	0	0
6	D	1	Total 1	Mg 1	0	0
6	H	1	Total 1	Mg 1	0	0
6	B	1	Total 1	Mg 1	0	0
6	h	1	Total 1	Mg 1	0	0
6	Z	1	Total 1	Mg 1	0	0
6	T	1	Total 1	Mg 1	0	0

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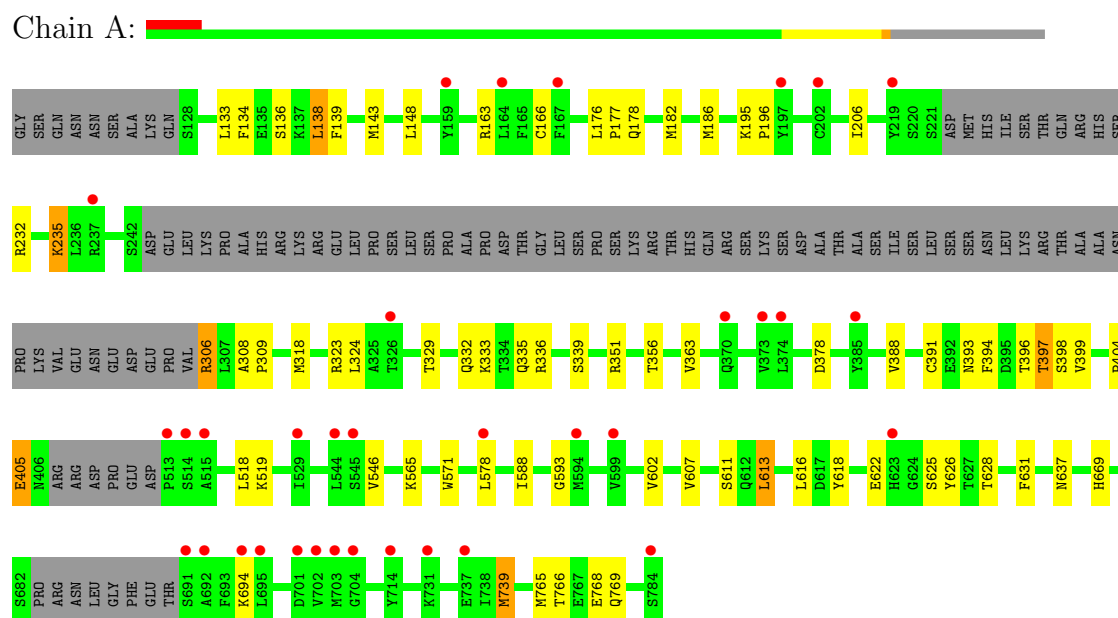
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	1	Total 1	Mg 1	0	0
6	X	1	Total 1	Mg 1	0	0
6	d	1	Total 1	Mg 1	0	0
6	R	1	Total 1	Mg 1	0	0

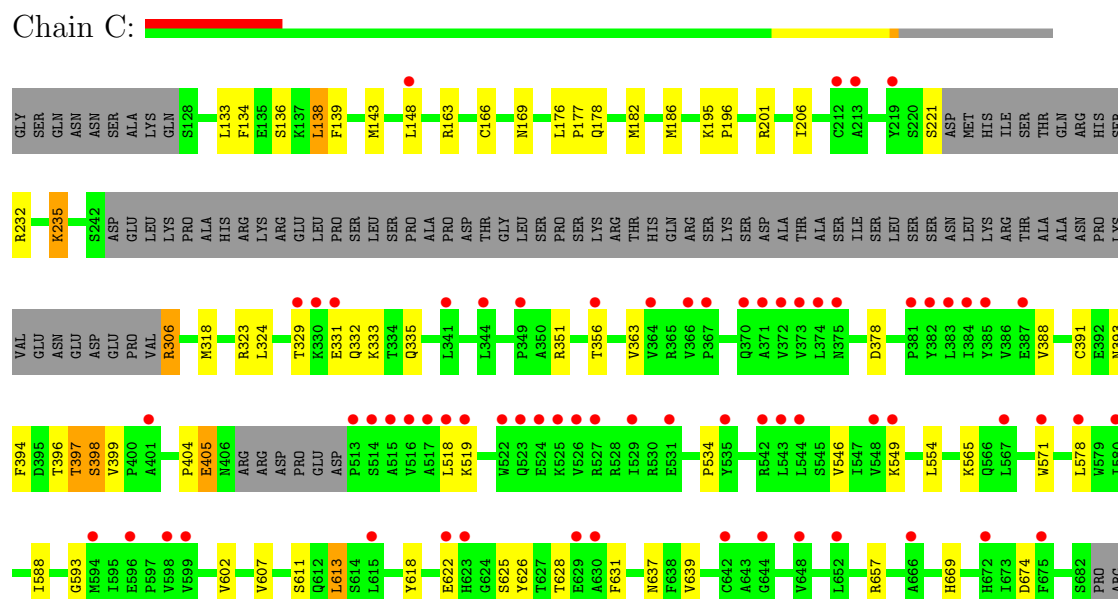
### 3 Residue-property plots

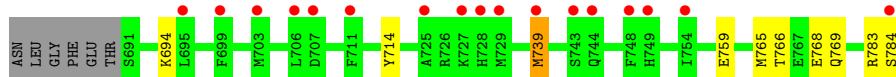
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PHOSPHATIDYLINOSITOL 4-KINASE BETA



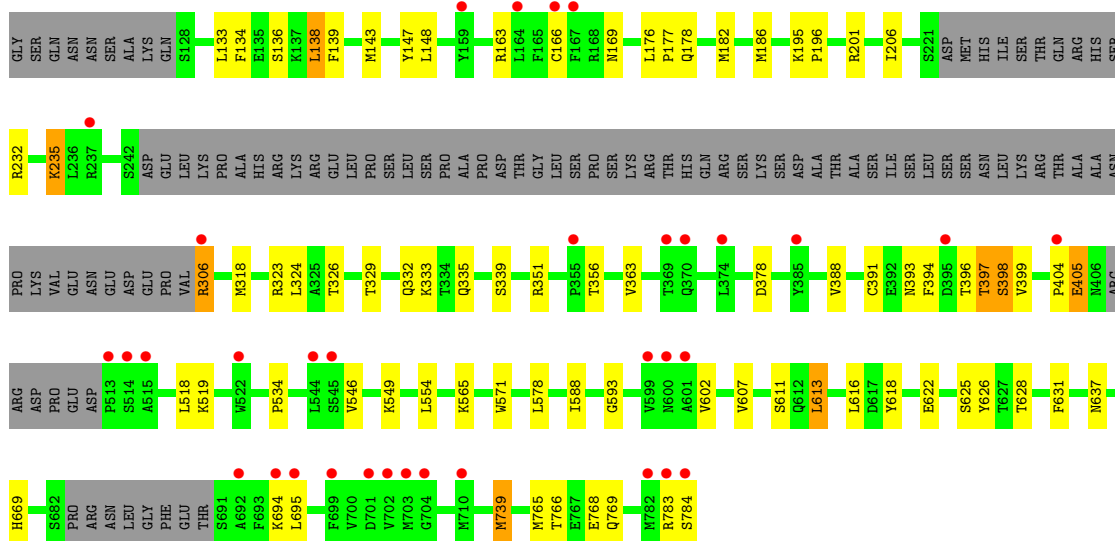
#### • Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA





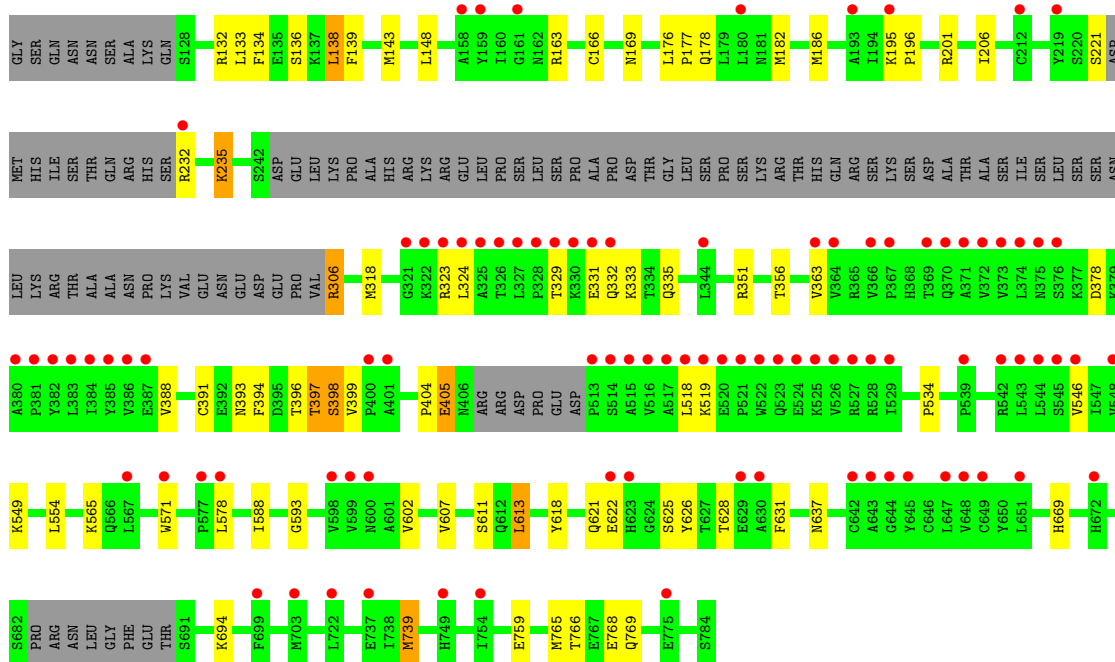
## ● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain G:



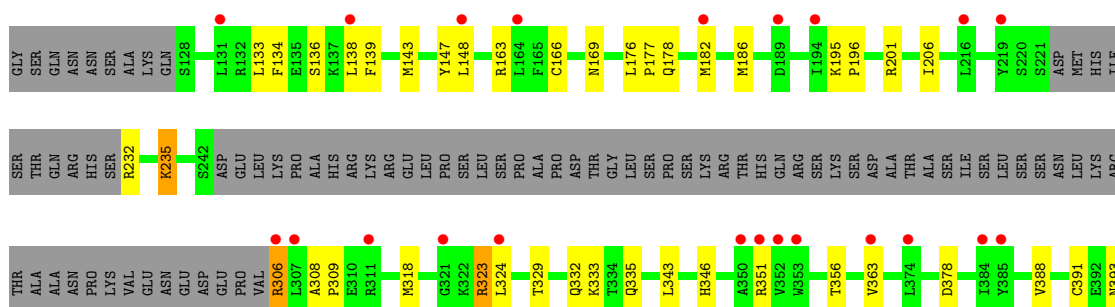
## ● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

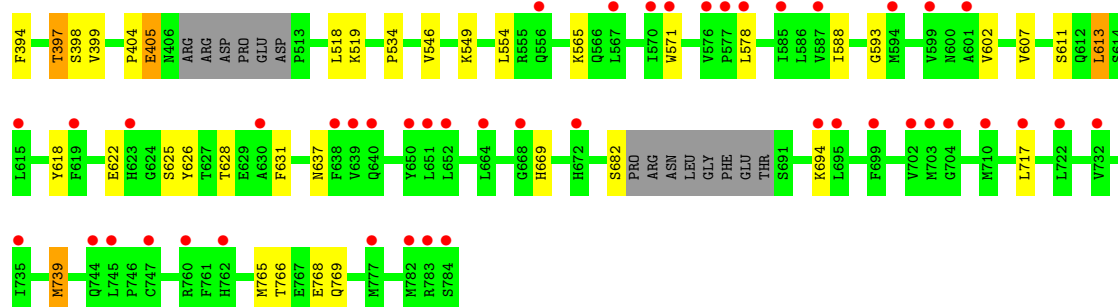
Chain I:



## ● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

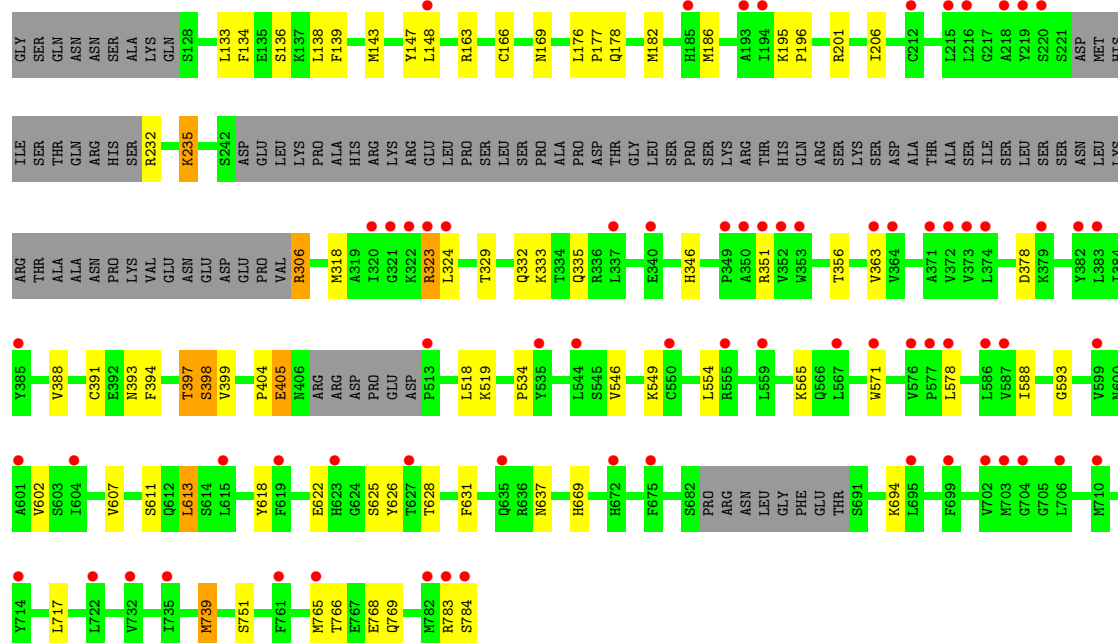
Chain M:





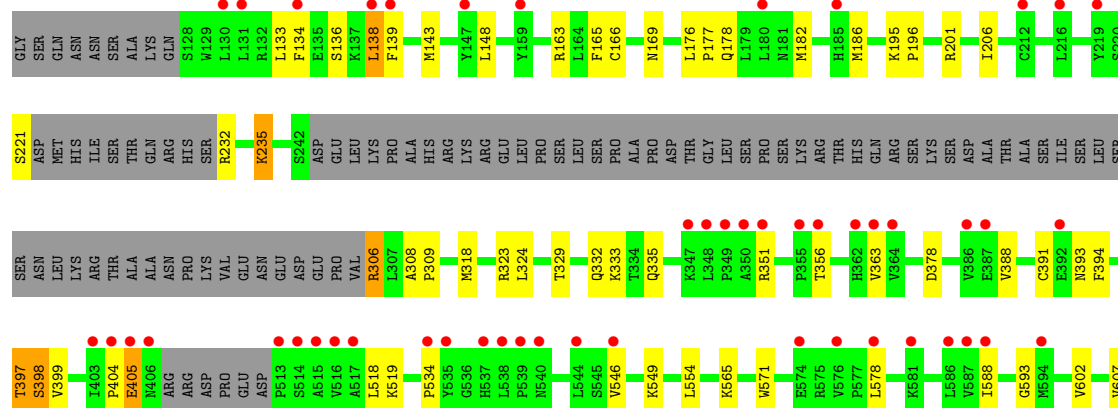
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

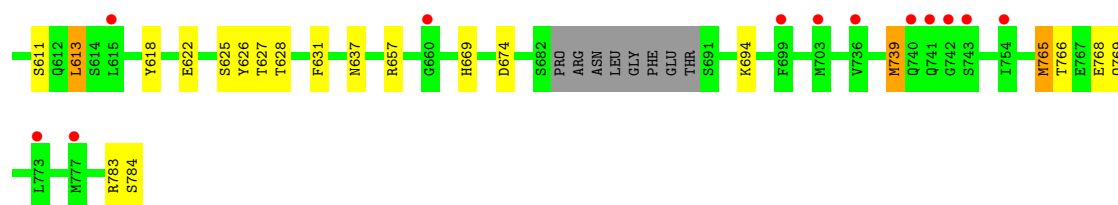
Chain S:



• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

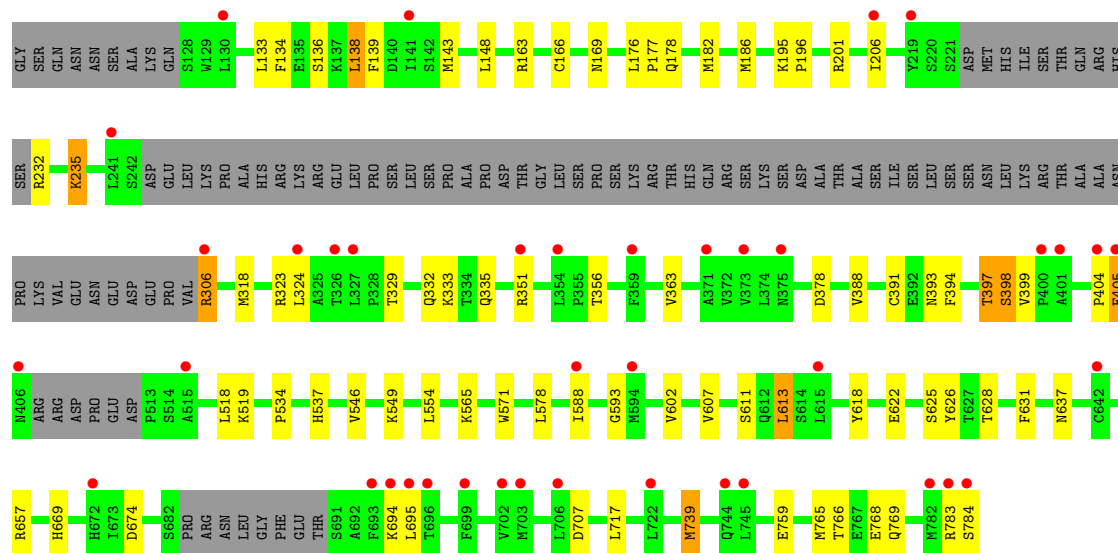
Chain W:





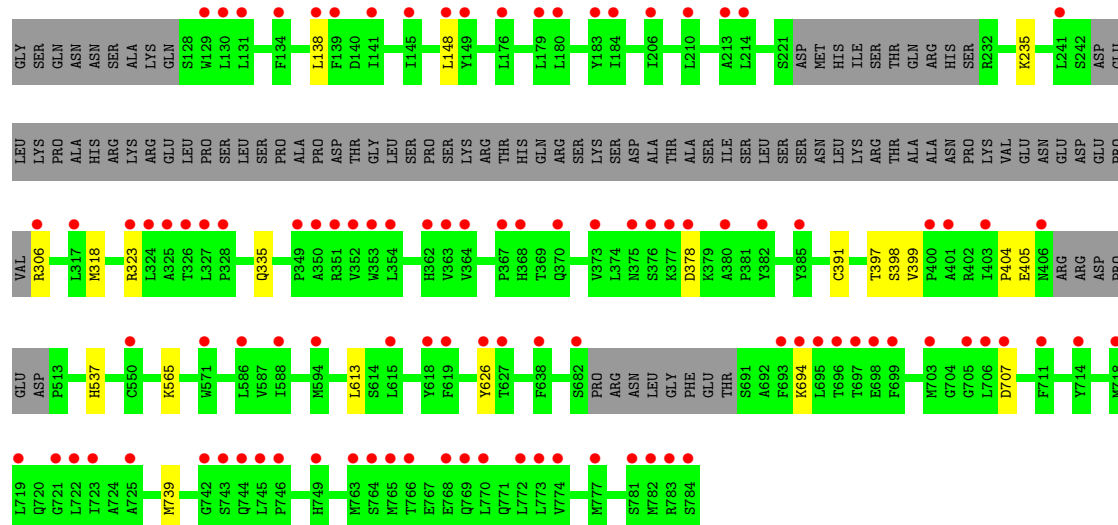
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain Y:



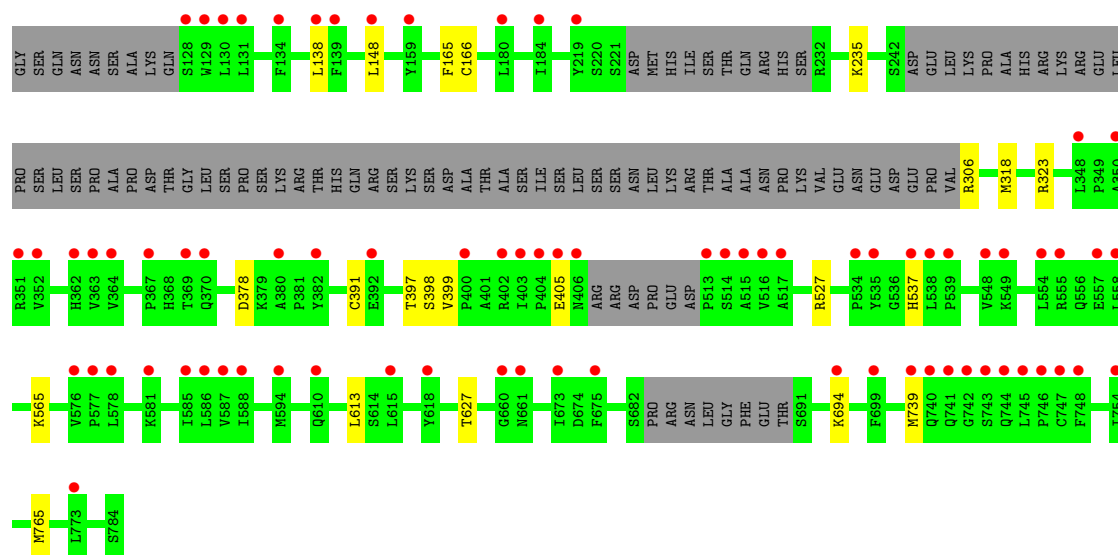
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain c:



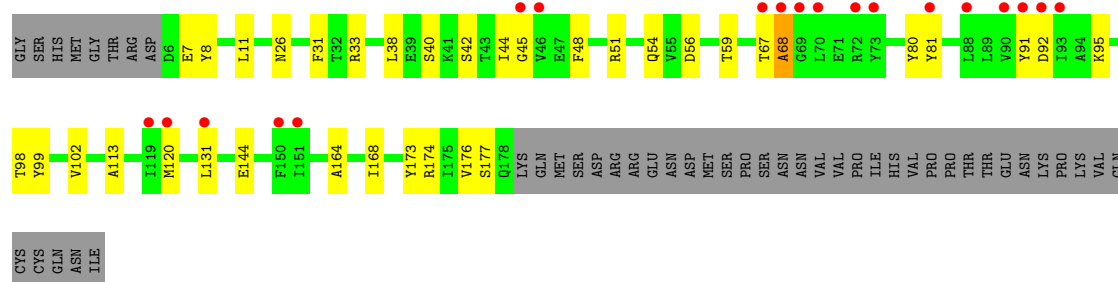
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain g:



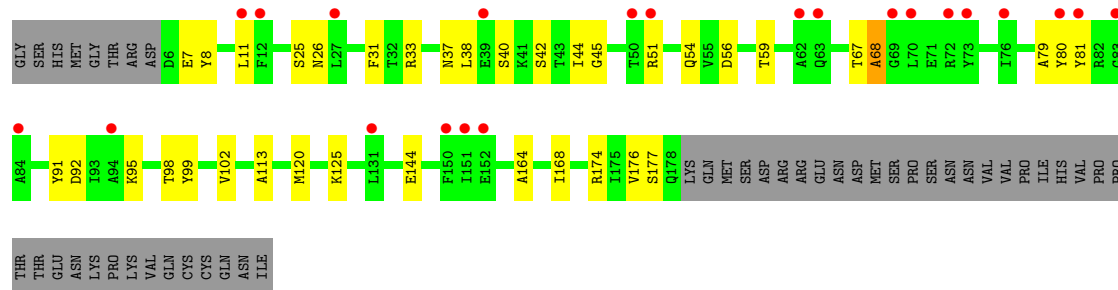
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain B:



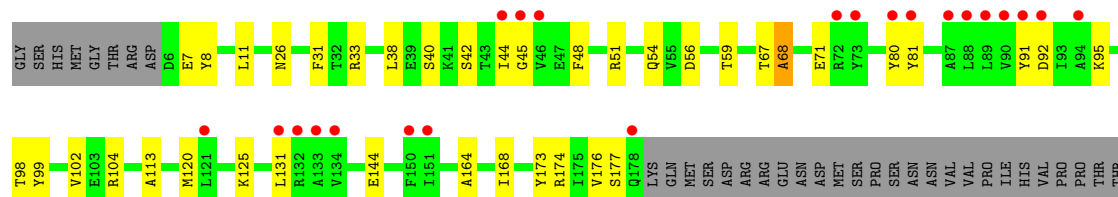
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain D:



• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain H:



GLU  
ASN  
LYS  
PRO  
LYS  
VAL  
GLN  
CYS  
CYS  
ASN  
ILE

• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain J:

GLY SER HIS MET GLY THR ARG ASP D6 E7 Y8 L11 F12 F13 D19 N26 L27 F31 T32 R33 L38 E39 I44 G45 R51 Q54 V55 D56 G57 R58 T59 T67 A68 G69 L70 E71 R72 A79 Y80 Y81 Y91 D92 K95 T98 Y99

• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain N:

GLY SER HIS MET THR ARG ASP D6 E7 Y8 L11 F12 K13 V14 V15 L16 L17 N26 F31 T32 R33 L38 E39 S40 K41 S42 T43 I44 G45 V46 E47 F48 A49 T50 R51 Q54 V55 D56 T59 A62 Q63 I64 T67 G69 G70 L70 L71 E71 R72 R73 R74

GLU ASN MET MET PRO PRO SER ASN ASN VAL VAL PRO ILE HIS VAL PRO THR THR GLU ASN LYS PRO LYS VAL GLN CYS CYS GLN ILE

• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain P:

GLY SER HIS MET THR ARG ASP D6 E7 Y8 L11 F12 L16 L17 N26 F31 T32 R33 N37 L38 E39 S40 K41 S42 G45 V46 E47 F48 A49 T50 R51 Q54 V55 D56 T59 A62 Q63 T67 A68 G69 E71 R72 Y73 R74 A75 T77

ARG ARG ASN ASP MET SER PRO SER ASN VAL VAL PRO ILE HIS VAL PRO PRO LYS LYS VAL GLN CYS CYS ASN GLN ASN ILE

• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain R:

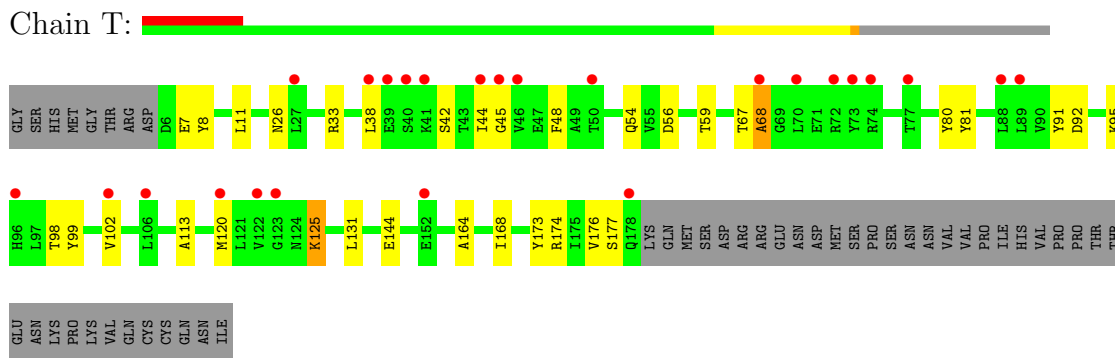
GLY SER HIS MET THR ARG ASP D6 E7 Y8 L11 N26 L27 R33 L38 E39 K41 I44 G45 V46 E47 F48 A49 T50 Q54 V55 D56 T59 T67 A68 R72 Y80 Y81 L89 Y90 D92 I93 A94 H96 L97 T98 Y99 E100 E101 V102

I103 R104 W105 L106 L109 R110 A113 I119 M120 L121 V122 G123 N124 K125 L131 E144 L148 S149 F150 I151 T152 S154 A155 A164 F165 I168 R174 I175 V176 S177 Q178 LYS GLN MET SER ASP ARG GLU ASN ASP MET SER PRO SER ASN VAL PRO

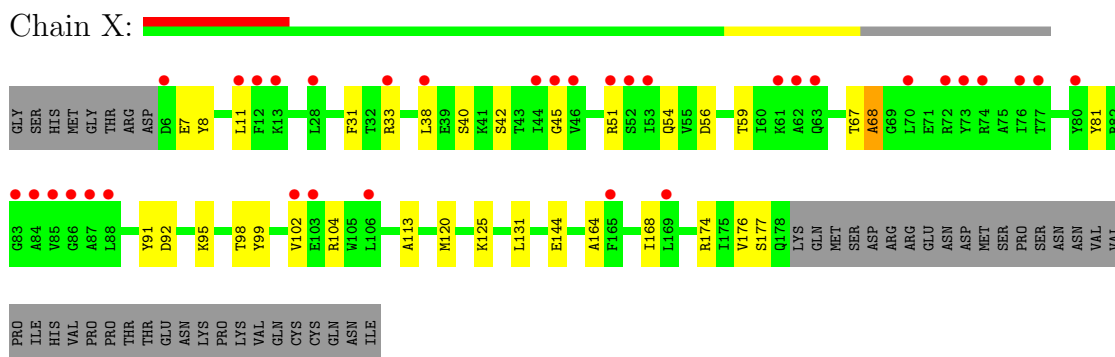
ILE HIS VAL PRO THR THR GLU ASN LYS LYS VAL GLN CYS CYS GLN ASN ILE



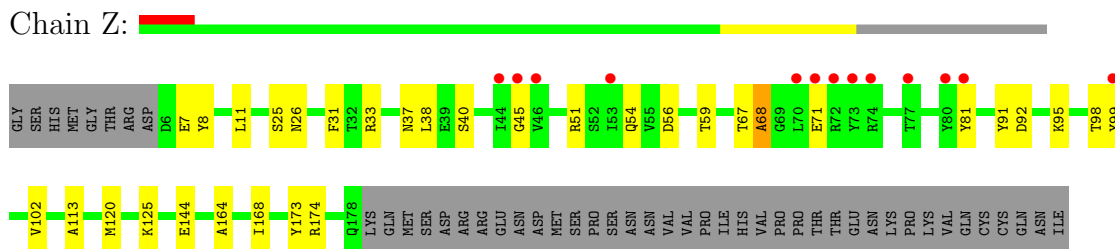
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



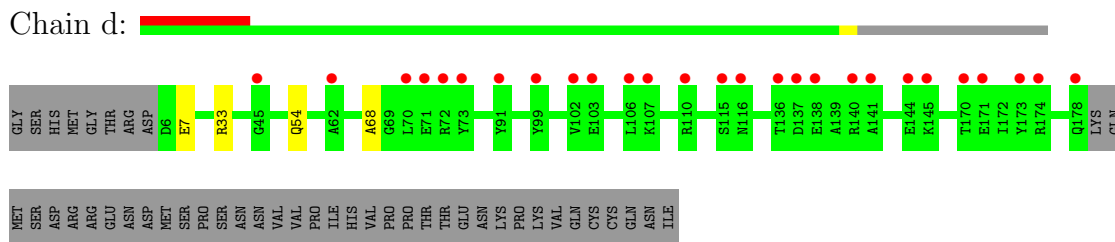
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



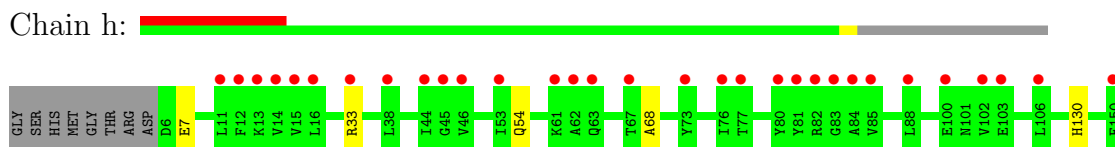
- Molecule 2: RAS-RELATED PROTEIN RAB-11A

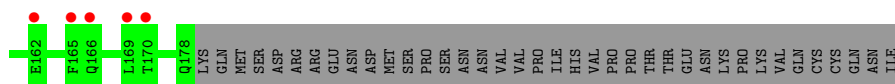


- Molecule 2: RAS-RELATED PROTEIN RAB-11A



- Molecule 2: RAS-RELATED PROTEIN RAB-11A





• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain E:



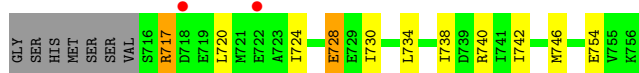
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain F:



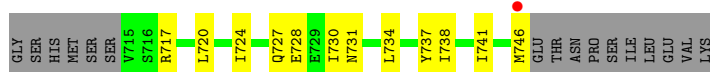
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain K:



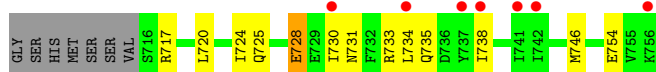
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain L:



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain U:



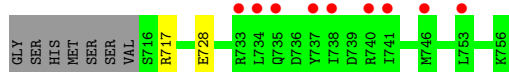
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain V:



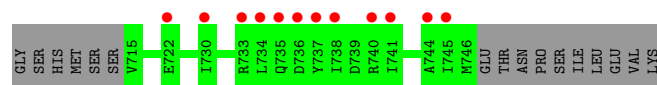
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain a:



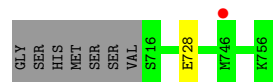
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain b: 



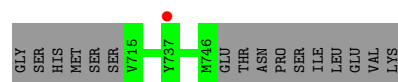
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain e: 



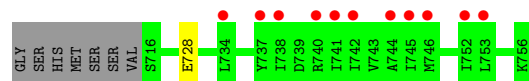
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain f: 



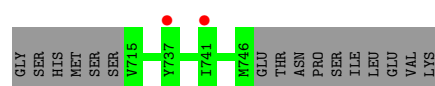
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain i: 



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain j: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.50Å 134.47Å 294.33Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	294.32 – 6.00 49.88 – 6.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (294.32-6.00) 93.0 (49.88-6.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 6.15Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.253 , 0.359 0.259 , 0.362	Depositor DCC
$R_{free}$ test set	1925 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	248.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 258.8	EDS
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 37330 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	65970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, MG, 093

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	0.59	0/3866	0.72	0/5219
1	C	0.56	0/3866	0.70	0/5219
1	G	0.59	0/3866	0.72	0/5219
1	I	0.56	0/3866	0.69	1/5219 (0.0%)
1	M	0.59	0/3866	0.71	1/5219 (0.0%)
1	O	0.59	0/3866	0.71	0/5219
1	Q	0.57	0/3866	0.70	0/5219
1	S	0.57	0/3866	0.70	0/5219
1	W	0.58	0/3866	0.70	1/5219 (0.0%)
1	Y	0.59	0/3866	0.70	0/5219
1	c	0.60	0/3866	0.71	0/5219
1	g	0.59	0/3866	0.70	2/5219 (0.0%)
2	B	0.64	0/1399	0.76	0/1892
2	D	0.61	0/1399	0.75	0/1892
2	H	0.63	0/1399	0.74	0/1892
2	J	0.63	0/1399	0.75	0/1892
2	N	0.58	0/1399	0.73	0/1892
2	P	0.59	0/1399	0.73	0/1892
2	R	0.59	0/1399	0.72	0/1892
2	T	0.58	0/1399	0.73	0/1892
2	X	0.58	0/1399	0.72	0/1892
2	Z	0.58	0/1399	0.73	0/1892
2	d	0.58	0/1399	0.73	0/1892
2	h	0.59	0/1399	0.72	0/1892
3	E	0.94	1/316 (0.3%)	0.98	1/429 (0.2%)
3	F	0.83	0/238	0.87	0/323
3	K	0.94	1/316 (0.3%)	0.97	1/429 (0.2%)
3	L	0.84	0/238	0.89	0/323
3	U	0.83	0/316	0.82	0/429
3	V	0.90	0/238	0.89	0/323
3	a	0.94	1/316 (0.3%)	0.96	1/429 (0.2%)
3	b	0.86	0/238	0.88	0/323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	e	0.85	0/316	0.86	0/429
3	f	0.88	0/238	0.89	0/323
3	i	0.85	0/316	0.81	0/429
3	j	0.88	0/238	0.87	0/323
All	All	0.60	3/66504 (0.0%)	0.72	8/89844 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
1	I	0	1
1	M	0	1
1	O	0	1
1	Q	0	1
1	S	0	1
1	W	0	1
1	Y	0	1
1	c	0	1
1	g	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	717	ARG	CD-NE	5.41	1.55	1.46
3	E	717	ARG	CD-NE	5.12	1.55	1.46
3	K	717	ARG	CD-NE	5.07	1.55	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	717	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	a	717	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	E	717	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	g	527	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	I	132	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	398	SER	Peptide
1	G	398	SER	Peptide
1	I	398	SER	Peptide
1	M	398	SER	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3788	0	3838	55	8
1	C	3788	0	3839	100	2
1	G	3788	0	3839	70	9
1	I	3788	0	3839	80	2
1	M	3788	0	3839	56	12
1	O	3788	0	3839	56	17
1	Q	3788	0	3839	62	4
1	S	3788	0	3839	65	12
1	W	3788	0	3838	56	4
1	Y	3788	0	3839	57	12
1	c	3788	0	3839	0	6
1	g	3788	0	3839	0	13
2	B	1377	0	1370	44	9
2	D	1377	0	1370	43	4
2	H	1377	0	1370	39	3
2	J	1377	0	1370	34	4
2	N	1377	0	1370	26	0
2	P	1377	0	1371	29	0
2	R	1377	0	1370	29	0
2	T	1377	0	1370	28	0
2	X	1377	0	1370	23	0
2	Z	1377	0	1371	24	0
2	d	1377	0	1370	0	0
2	h	1377	0	1370	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	314	0	298	89	0
3	F	237	0	222	78	0
3	K	314	0	298	52	0
3	L	237	0	222	35	0
3	U	314	0	298	23	0
3	V	237	0	222	47	0
3	a	314	0	298	0	0
3	b	237	0	222	0	0
3	e	314	0	298	0	0
3	f	237	0	222	0	0
3	i	314	0	298	0	0
3	j	237	0	222	0	0
4	A	24	0	16	0	0
4	C	24	0	16	0	0
4	G	24	0	16	0	0
4	I	24	0	16	0	0
4	M	24	0	16	0	0
4	O	24	0	16	0	0
4	Q	24	0	16	0	0
4	S	24	0	16	0	0
4	W	24	0	16	0	0
4	Y	24	0	16	0	0
4	c	24	0	16	0	0
4	g	24	0	16	0	0
5	B	32	0	12	6	0
5	D	32	0	12	11	0
5	H	32	0	12	7	0
5	J	32	0	12	4	0
5	N	32	0	12	6	0
5	P	32	0	12	7	0
5	R	32	0	12	5	0
5	T	32	0	12	5	0
5	X	32	0	12	6	0
5	Z	32	0	12	6	0
5	d	32	0	12	0	0
5	h	32	0	12	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	N	1	0	0	0	0
6	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	1	0	0	0	0
6	T	1	0	0	0	0
6	X	1	0	0	0	0
6	Z	1	0	0	1	0
6	d	1	0	0	0	0
6	h	1	0	0	0	0
All	All	65970	0	65964	993	61

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 993 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:44:ILE:HD11	3:K:734:LEU:CD2	1.30	1.59
2:J:44:ILE:CD1	3:K:734:LEU:HD22	1.30	1.59
2:D:44:ILE:HD11	3:E:734:LEU:CD2	1.41	1.50
1:C:138:LEU:HG	1:S:769:GLN:CG	1.41	1.48
2:D:44:ILE:CD1	3:E:734:LEU:HD22	1.44	1.47

The worst 5 of 61 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:174:ARG:NH2	1:M:166:CYS:O[2_545]	0.72	1.48
2:D:174:ARG:NH2	1:O:166:CYS:O[2_556]	0.76	1.44
2:B:174:ARG:NH2	1:g:166:CYS:O[2_656]	0.78	1.42
1:I:396:THR:OG1	1:M:627:THR:OG1[2_545]	0.85	1.35
1:C:396:THR:OG1	1:O:627:THR:OG1[2_556]	1.08	1.12

## 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	460/566 (81%)	442 (96%)	16 (4%)	2 (0%)	43 90

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	30	84
1	G	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	30	84
1	I	460/566 (81%)	440 (96%)	17 (4%)	3 (1%)	30	84
1	M	460/566 (81%)	441 (96%)	16 (4%)	3 (1%)	30	84
1	O	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	30	84
1	Q	460/566 (81%)	439 (95%)	19 (4%)	2 (0%)	43	90
1	S	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	30	84
1	W	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	30	84
1	Y	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	30	84
1	c	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	43	90
1	g	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	43	90
2	B	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	D	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	H	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	J	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	N	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	P	171/219 (78%)	162 (95%)	8 (5%)	1 (1%)	33	85
2	R	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	T	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	19	77
2	X	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	Z	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	19	77
2	d	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
2	h	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	33	85
3	E	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	F	30/48 (62%)	30 (100%)	0	0	100	100
3	K	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	L	30/48 (62%)	30 (100%)	0	0	100	100
3	U	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	V	30/48 (62%)	30 (100%)	0	0	100	100
3	a	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	b	30/48 (62%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	e	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	f	30/48 (62%)	30 (100%)	0	0	100	100
3	i	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	j	30/48 (62%)	30 (100%)	0	0	100	100
All	All	7986/9996 (80%)	7645 (96%)	295 (4%)	46 (1%)	33	85

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	GLU
2	B	68	ALA
1	C	405	GLU
2	D	68	ALA
1	G	405	GLU

### 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	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	C	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	G	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	I	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	M	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	O	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	Q	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	S	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	W	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	Y	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	c	422/508 (83%)	408 (97%)	14 (3%)	50	87
1	g	422/508 (83%)	409 (97%)	13 (3%)	52	88
2	B	147/191 (77%)	144 (98%)	3 (2%)	68	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	H	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	J	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	N	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	P	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	R	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	T	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	X	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	Z	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	d	147/191 (77%)	144 (98%)	3 (2%)	68	92
2	h	147/191 (77%)	144 (98%)	3 (2%)	68	92
3	E	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	F	21/45 (47%)	21 (100%)	0	100	100
3	K	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	L	21/45 (47%)	21 (100%)	0	100	100
3	U	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	V	21/45 (47%)	21 (100%)	0	100	100
3	a	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	b	21/45 (47%)	21 (100%)	0	100	100
3	e	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	f	21/45 (47%)	21 (100%)	0	100	100
3	i	31/45 (69%)	30 (97%)	1 (3%)	51	87
3	j	21/45 (47%)	21 (100%)	0	100	100
All	All	7140/8928 (80%)	6931 (97%)	209 (3%)	55	88

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	378	ASP
1	Q	694	LYS
1	g	148	LEU
1	O	565	LYS
1	Q	235	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	540	ASN
1	S	540	ASN
1	g	606	GLN
1	O	606	GLN
1	Q	606	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	$\# Z  > 2$
4	093	A	2002	-	25,25,25	4.21	9 (36%)	33,36,36	4.60	17 (51%)
5	GSP	B	2000	6	34,34,34	1.54	7 (20%)	52,54,54	4.94	13 (25%)
4	093	C	2002	-	25,25,25	4.23	9 (36%)	33,36,36	4.57	17 (51%)
5	GSP	D	2000	6	34,34,34	1.62	8 (23%)	52,54,54	3.98	16 (30%)
4	093	G	2002	1	25,25,25	4.21	9 (36%)	33,36,36	4.59	17 (51%)
5	GSP	H	2000	6	34,34,34	1.42	7 (20%)	52,54,54	4.39	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	093	I	2002	-	25,25,25	4.23	9 (36%)	33,36,36	4.57	17 (51%)
5	GSP	J	2000	6	34,34,34	1.68	8 (23%)	52,54,54	4.34	15 (28%)
4	093	M	2002	-	25,25,25	4.22	9 (36%)	33,36,36	4.60	17 (51%)
5	GSP	N	2000	6	34,34,34	1.50	7 (20%)	52,54,54	4.20	17 (32%)
4	093	O	2002	1	25,25,25	4.23	9 (36%)	33,36,36	4.62	17 (51%)
5	GSP	P	2000	6	34,34,34	1.49	8 (23%)	52,54,54	3.96	15 (28%)
4	093	Q	2002	1	25,25,25	4.22	9 (36%)	33,36,36	4.59	17 (51%)
5	GSP	R	2000	6	34,34,34	1.43	7 (20%)	52,54,54	3.34	13 (25%)
4	093	S	2002	1	25,25,25	4.22	9 (36%)	33,36,36	4.62	17 (51%)
5	GSP	T	2000	6	34,34,34	1.34	7 (20%)	52,54,54	4.00	15 (28%)
4	093	W	2002	1	25,25,25	4.22	9 (36%)	33,36,36	4.62	17 (51%)
5	GSP	X	2000	6	34,34,34	1.51	9 (26%)	52,54,54	3.76	15 (28%)
4	093	Y	2002	1	25,25,25	4.22	9 (36%)	33,36,36	4.60	17 (51%)
5	GSP	Z	2000	6	34,34,34	1.52	8 (23%)	52,54,54	4.02	16 (30%)
4	093	c	2002	1	25,25,25	4.23	9 (36%)	33,36,36	4.64	17 (51%)
5	GSP	d	2000	6	34,34,34	1.53	8 (23%)	52,54,54	4.60	14 (26%)
4	093	g	2002	1	25,25,25	4.23	9 (36%)	33,36,36	4.59	17 (51%)
5	GSP	h	2000	6	34,34,34	1.57	10 (29%)	52,54,54	4.01	15 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	093	A	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	B	2000	6	-	0/21/38/38	0/3/3/3
4	093	C	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	D	2000	6	-	0/21/38/38	0/3/3/3
4	093	G	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	H	2000	6	-	0/21/38/38	0/3/3/3
4	093	I	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	J	2000	6	-	0/21/38/38	0/3/3/3
4	093	M	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	N	2000	6	-	0/21/38/38	0/3/3/3
4	093	O	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	P	2000	6	-	0/21/38/38	0/3/3/3
4	093	Q	2002	1	-	0/17/19/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GSP	R	2000	6	-	0/21/38/38	0/3/3/3
4	093	S	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	T	2000	6	-	0/21/38/38	0/3/3/3
4	093	W	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	X	2000	6	-	0/21/38/38	0/3/3/3
4	093	Y	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	Z	2000	6	-	0/21/38/38	0/3/3/3
4	093	c	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	d	2000	6	-	0/21/38/38	0/3/3/3
4	093	g	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	h	2000	6	-	0/21/38/38	0/3/3/3

The worst 5 of 202 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2002	093	CAI-SAP	-15.42	1.55	1.75
4	Y	2002	093	CAI-SAP	-15.37	1.55	1.75
4	O	2002	093	CAI-SAP	-15.34	1.55	1.75
4	g	2002	093	CAI-SAP	-15.34	1.55	1.75
4	c	2002	093	CAI-SAP	-15.33	1.55	1.75

The worst 5 of 381 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2000	GSP	C6-C5-N7	22.61	137.18	134.14
5	h	2000	GSP	C6-C5-N7	22.16	137.12	134.14
5	B	2000	GSP	O3B-PG-S1G	-22.11	104.72	114.53
5	d	2000	GSP	C6-C5-N7	21.28	137.01	134.14
5	d	2000	GSP	O3B-PG-S1G	-21.17	105.14	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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	470/566 (83%)	0.72	34 (7%) 15 21	95, 212, 331, 500	0
1	C	470/566 (83%)	1.09	85 (18%) 2 6	126, 300, 456, 500	0
1	G	470/566 (83%)	0.77	34 (7%) 15 21	98, 214, 342, 500	0
1	I	470/566 (83%)	1.24	95 (20%) 2 5	124, 306, 474, 500	0
1	M	470/566 (83%)	0.79	42 (8%) 10 18	95, 217, 341, 500	0
1	O	470/566 (83%)	0.76	40 (8%) 11 18	102, 208, 335, 500	0
1	Q	470/566 (83%)	0.99	67 (14%) 3 9	102, 247, 364, 498	0
1	S	470/566 (83%)	1.05	71 (15%) 3 8	114, 251, 389, 500	0
1	W	470/566 (83%)	0.86	62 (13%) 4 10	99, 253, 387, 500	0
1	Y	470/566 (83%)	0.76	40 (8%) 11 18	115, 250, 365, 474	0
1	c	470/566 (83%)	1.28	104 (22%) 1 5	119, 305, 478, 500	0
1	g	470/566 (83%)	0.99	77 (16%) 2 7	126, 268, 416, 500	0
2	B	173/219 (78%)	0.75	19 (10%) 6 13	94, 201, 375, 493	0
2	D	173/219 (78%)	0.87	22 (12%) 4 11	95, 220, 341, 488	0
2	H	173/219 (78%)	0.90	22 (12%) 4 11	94, 207, 382, 499	0
2	J	173/219 (78%)	0.84	12 (6%) 17 23	92, 198, 338, 500	0
2	N	173/219 (78%)	1.40	43 (24%) 1 5	137, 282, 424, 496	0
2	P	173/219 (78%)	1.30	48 (27%) 1 4	132, 277, 432, 496	0
2	R	173/219 (78%)	1.10	39 (22%) 1 5	139, 269, 415, 496	0
2	T	173/219 (78%)	0.81	25 (14%) 3 9	136, 266, 407, 493	0
2	X	173/219 (78%)	0.95	34 (19%) 2 6	146, 282, 453, 500	0
2	Z	173/219 (78%)	0.70	13 (7%) 14 21	165, 262, 362, 494	0
2	d	173/219 (78%)	0.83	27 (15%) 3 8	146, 308, 447, 500	0
2	h	173/219 (78%)	1.10	36 (20%) 1 5	158, 294, 440, 500	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	E	41/48 (85%)	0.71	2 (4%) 28 30	153, 251, 365, 489	0
3	F	32/48 (66%)	0.25	1 (3%) 47 41	169, 285, 399, 466	0
3	K	41/48 (85%)	0.78	2 (4%) 28 30	131, 240, 410, 465	0
3	L	32/48 (66%)	0.50	1 (3%) 47 41	170, 263, 384, 436	0
3	U	41/48 (85%)	0.92	7 (17%) 2 7	175, 284, 408, 494	0
3	V	32/48 (66%)	0.59	1 (3%) 47 41	170, 260, 403, 435	0
3	a	41/48 (85%)	1.17	9 (21%) 1 5	195, 318, 423, 476	0
3	b	32/48 (66%)	1.59	12 (37%) 1 3	213, 309, 428, 479	0
3	e	41/48 (85%)	0.61	1 (2%) 56 47	175, 255, 384, 478	0
3	f	32/48 (66%)	0.38	1 (3%) 47 41	194, 288, 337, 363	0
3	i	41/48 (85%)	1.20	11 (26%) 1 5	202, 325, 441, 500	0
3	j	32/48 (66%)	0.66	2 (6%) 19 25	194, 282, 404, 462	0
All	All	8154/9996 (81%)	0.94	1141 (13%) 3 9	92, 255, 416, 500	0

The worst 5 of 1141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	523	GLN	12.4
1	C	517	ALA	11.4
1	c	695	LEU	10.4
1	I	522	TRP	9.9
1	g	405	GLU	9.3

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	d	2001	1/1	0.25	1.96	167,167,167,167	0
6	MG	D	2001	1/1	0.21	-0.33	64,64,64,64	0
5	GSP	Z	2000	32/32	0.22	-0.41	176,212,274,298	0
5	GSP	P	2000	32/32	0.24	-0.43	111,168,247,275	0
5	GSP	X	2000	32/32	0.24	-0.53	134,226,322,330	0
5	GSP	d	2000	32/32	0.17	-0.54	174,212,349,391	0
5	GSP	H	2000	32/32	0.25	-0.56	141,183,247,282	0
5	GSP	N	2000	32/32	0.23	-0.61	97,151,255,301	0
5	GSP	h	2000	32/32	0.22	-0.66	123,249,350,363	0
5	GSP	J	2000	32/32	0.26	-0.67	94,165,285,323	0
5	GSP	T	2000	32/32	0.26	-0.72	123,205,238,264	0
5	GSP	B	2000	32/32	0.22	-0.73	141,197,232,249	0
6	MG	B	2001	1/1	0.21	-0.78	159,159,159,159	0
5	GSP	D	2000	32/32	0.25	-0.81	110,193,250,272	0
6	MG	J	2001	1/1	0.16	-1.00	142,142,142,142	0
5	GSP	R	2000	32/32	0.21	-1.03	108,197,262,274	0
6	MG	T	2001	1/1	0.14	-1.17	127,127,127,127	0
6	MG	R	2001	1/1	0.13	-1.17	106,106,106,106	0
6	MG	H	2001	1/1	0.14	-1.19	139,139,139,139	0
6	MG	N	2001	1/1	0.11	-1.20	240,240,240,240	0
6	MG	P	2001	1/1	0.12	-1.21	244,244,244,244	0
6	MG	Z	2001	1/1	0.13	-1.43	178,178,178,178	0
6	MG	h	2001	1/1	0.09	-1.85	190,190,190,190	0
6	MG	X	2001	1/1	0.10	-2.01	255,255,255,255	0
4	093	I	2002	24/24	-	-	60,76,105,130	24
4	093	S	2002	24/24	-	-	60,76,105,130	24
4	093	Q	2002	24/24	-	-	60,76,105,130	24
4	093	W	2002	24/24	-	-	60,76,105,130	24
4	093	G	2002	24/24	-	-	60,76,105,130	24
4	093	Y	2002	24/24	-	-	60,76,105,130	24
4	093	g	2002	24/24	-	-	60,76,105,130	24
4	093	O	2002	24/24	-	-	60,76,105,130	24
4	093	A	2002	24/24	-	-	60,76,105,130	24
4	093	c	2002	24/24	-	-	60,76,105,130	24
4	093	M	2002	24/24	-	-	60,76,105,130	24
4	093	C	2002	24/24	-	-	60,76,105,130	24

## 6.5 Other polymers ⓘ

There are no such residues in this entry.