



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:46 PM GMT

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 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

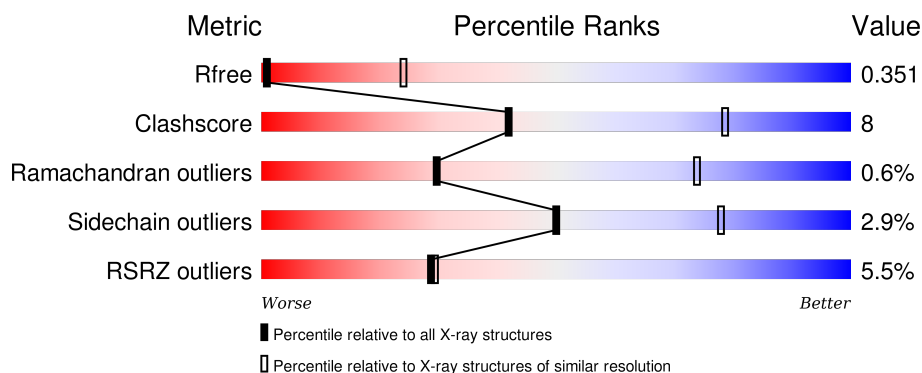
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

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. 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	566	<div> <div>70%</div> <div>11%</div> <div>•</div> <div>17%</div> </div>
1	C	566	<div>9%</div> <div>69%</div> <div>13%</div> <div>•</div> <div>17%</div>
1	G	566	<div>2%</div> <div>69%</div> <div>13%</div> <div>•</div> <div>17%</div>
1	I	566	<div>11%</div> <div>69%</div> <div>12%</div> <div>•</div> <div>17%</div>
1	M	566	<div>2%</div> <div>69%</div> <div>12%</div> <div>•</div> <div>17%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	a	48	 81% 15%
3	b	48	 67% 33%
3	e	48	 83% 15%
3	f	48	 67% 33%
3	i	48	 83% 15%
3	j	48	 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GSP	D	2000	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 65970 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 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			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
A	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
A	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
A	507	ARG	LYS	CONFLICT	UNP Q9UBF8
C	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
C	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
C	507	ARG	LYS	CONFLICT	UNP Q9UBF8
G	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
G	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
G	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
G	507	ARG	LYS	CONFLICT	UNP Q9UBF8
I	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
I	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
I	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
I	507	ARG	LYS	CONFLICT	UNP Q9UBF8
M	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
M	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
M	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
M	507	ARG	LYS	CONFLICT	UNP Q9UBF8
O	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
O	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
O	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
O	507	ARG	LYS	CONFLICT	UNP Q9UBF8
Q	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
Q	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
Q	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
Q	507	ARG	LYS	CONFLICT	UNP Q9UBF8
S	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
S	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
S	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
S	507	ARG	LYS	CONFLICT	UNP Q9UBF8
W	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
W	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
W	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
W	507	ARG	LYS	CONFLICT	UNP Q9UBF8
Y	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
Y	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
Y	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
Y	507	ARG	LYS	CONFLICT	UNP Q9UBF8
c	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
c	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
c	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8
c	507	ARG	LYS	CONFLICT	UNP Q9UBF8
g	119	GLY	-	EXPRESSION TAG	UNP Q9UBF8
g	120	SER	-	EXPRESSION TAG	UNP Q9UBF8
g	294	ALA	SER	ENGINEERED MUTATION	UNP Q9UBF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	507	ARG	LYS	CONFLICT	UNP Q9UBF8

- 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			
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 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP P62491
B	-1	SER	-	EXPRESSION TAG	UNP P62491
B	0	HIS	-	EXPRESSION TAG	UNP P62491
B	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
D	-2	GLY	-	EXPRESSION TAG	UNP P62491
D	-1	SER	-	EXPRESSION TAG	UNP P62491
D	0	HIS	-	EXPRESSION TAG	UNP P62491
D	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
H	-2	GLY	-	EXPRESSION TAG	UNP P62491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	SER	-	EXPRESSION TAG	UNP P62491
H	0	HIS	-	EXPRESSION TAG	UNP P62491
H	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
J	-2	GLY	-	EXPRESSION TAG	UNP P62491
J	-1	SER	-	EXPRESSION TAG	UNP P62491
J	0	HIS	-	EXPRESSION TAG	UNP P62491
J	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
N	-2	GLY	-	EXPRESSION TAG	UNP P62491
N	-1	SER	-	EXPRESSION TAG	UNP P62491
N	0	HIS	-	EXPRESSION TAG	UNP P62491
N	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
P	-2	GLY	-	EXPRESSION TAG	UNP P62491
P	-1	SER	-	EXPRESSION TAG	UNP P62491
P	0	HIS	-	EXPRESSION TAG	UNP P62491
P	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
R	-2	GLY	-	EXPRESSION TAG	UNP P62491
R	-1	SER	-	EXPRESSION TAG	UNP P62491
R	0	HIS	-	EXPRESSION TAG	UNP P62491
R	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
T	-2	GLY	-	EXPRESSION TAG	UNP P62491
T	-1	SER	-	EXPRESSION TAG	UNP P62491
T	0	HIS	-	EXPRESSION TAG	UNP P62491
T	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
X	-2	GLY	-	EXPRESSION TAG	UNP P62491
X	-1	SER	-	EXPRESSION TAG	UNP P62491
X	0	HIS	-	EXPRESSION TAG	UNP P62491
X	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
Z	-2	GLY	-	EXPRESSION TAG	UNP P62491
Z	-1	SER	-	EXPRESSION TAG	UNP P62491
Z	0	HIS	-	EXPRESSION TAG	UNP P62491
Z	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
d	-2	GLY	-	EXPRESSION TAG	UNP P62491
d	-1	SER	-	EXPRESSION TAG	UNP P62491
d	0	HIS	-	EXPRESSION TAG	UNP P62491
d	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
h	-2	GLY	-	EXPRESSION TAG	UNP P62491
h	-1	SER	-	EXPRESSION TAG	UNP P62491
h	0	HIS	-	EXPRESSION TAG	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			
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			

There are 48 discrepancies between the modelled and reference sequences:

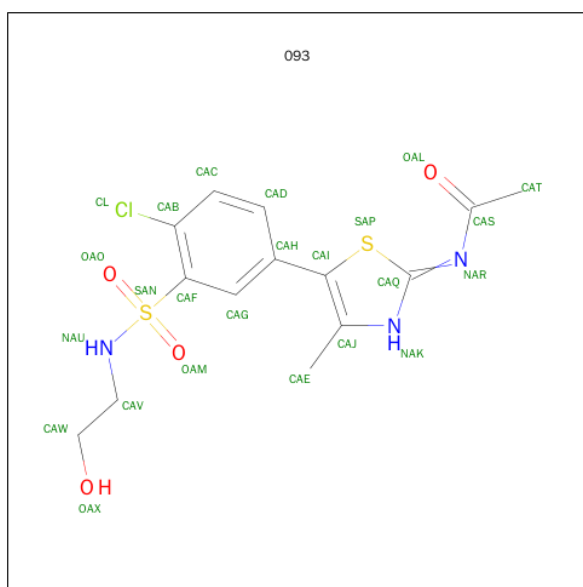
Chain	Residue	Modelled	Actual	Comment	Reference
E	709	GLY	-	EXPRESSION TAG	UNP O75154
E	710	SER	-	EXPRESSION TAG	UNP O75154
E	711	HIS	-	EXPRESSION TAG	UNP O75154
E	712	MET	-	EXPRESSION TAG	UNP O75154
F	709	GLY	-	EXPRESSION TAG	UNP O75154
F	710	SER	-	EXPRESSION TAG	UNP O75154
F	711	HIS	-	EXPRESSION TAG	UNP O75154
F	712	MET	-	EXPRESSION TAG	UNP O75154
K	709	GLY	-	EXPRESSION TAG	UNP O75154
K	710	SER	-	EXPRESSION TAG	UNP O75154
K	711	HIS	-	EXPRESSION TAG	UNP O75154
K	712	MET	-	EXPRESSION TAG	UNP O75154
L	709	GLY	-	EXPRESSION TAG	UNP O75154
L	710	SER	-	EXPRESSION TAG	UNP O75154
L	711	HIS	-	EXPRESSION TAG	UNP O75154
L	712	MET	-	EXPRESSION TAG	UNP O75154

Continued on next page...

Continued from previous page...

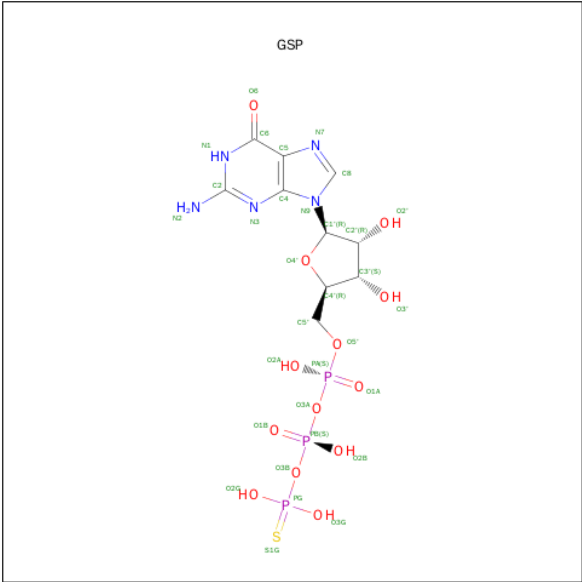
Chain	Residue	Modelled	Actual	Comment	Reference
U	709	GLY	-	EXPRESSION TAG	UNP O75154
U	710	SER	-	EXPRESSION TAG	UNP O75154
U	711	HIS	-	EXPRESSION TAG	UNP O75154
U	712	MET	-	EXPRESSION TAG	UNP O75154
V	709	GLY	-	EXPRESSION TAG	UNP O75154
V	710	SER	-	EXPRESSION TAG	UNP O75154
V	711	HIS	-	EXPRESSION TAG	UNP O75154
V	712	MET	-	EXPRESSION TAG	UNP O75154
a	709	GLY	-	EXPRESSION TAG	UNP O75154
a	710	SER	-	EXPRESSION TAG	UNP O75154
a	711	HIS	-	EXPRESSION TAG	UNP O75154
a	712	MET	-	EXPRESSION TAG	UNP O75154
b	709	GLY	-	EXPRESSION TAG	UNP O75154
b	710	SER	-	EXPRESSION TAG	UNP O75154
b	711	HIS	-	EXPRESSION TAG	UNP O75154
b	712	MET	-	EXPRESSION TAG	UNP O75154
e	709	GLY	-	EXPRESSION TAG	UNP O75154
e	710	SER	-	EXPRESSION TAG	UNP O75154
e	711	HIS	-	EXPRESSION TAG	UNP O75154
e	712	MET	-	EXPRESSION TAG	UNP O75154
f	709	GLY	-	EXPRESSION TAG	UNP O75154
f	710	SER	-	EXPRESSION TAG	UNP O75154
f	711	HIS	-	EXPRESSION TAG	UNP O75154
f	712	MET	-	EXPRESSION TAG	UNP O75154
i	709	GLY	-	EXPRESSION TAG	UNP O75154
i	710	SER	-	EXPRESSION TAG	UNP O75154
i	711	HIS	-	EXPRESSION TAG	UNP O75154
i	712	MET	-	EXPRESSION TAG	UNP O75154
j	709	GLY	-	EXPRESSION TAG	UNP O75154
j	710	SER	-	EXPRESSION TAG	UNP O75154
j	711	HIS	-	EXPRESSION TAG	UNP O75154
j	712	MET	-	EXPRESSION TAG	UNP O75154

- Molecule 4 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).



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

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



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

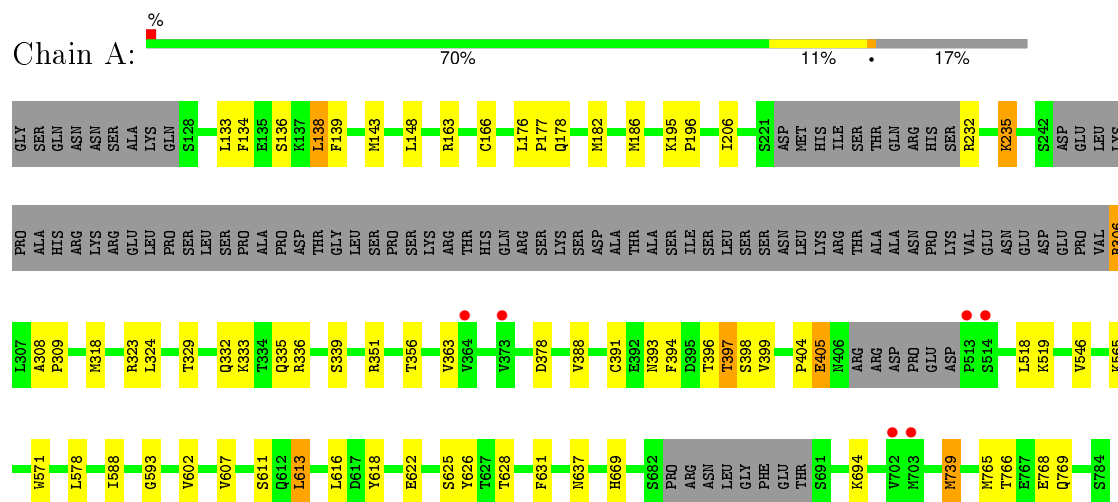
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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
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

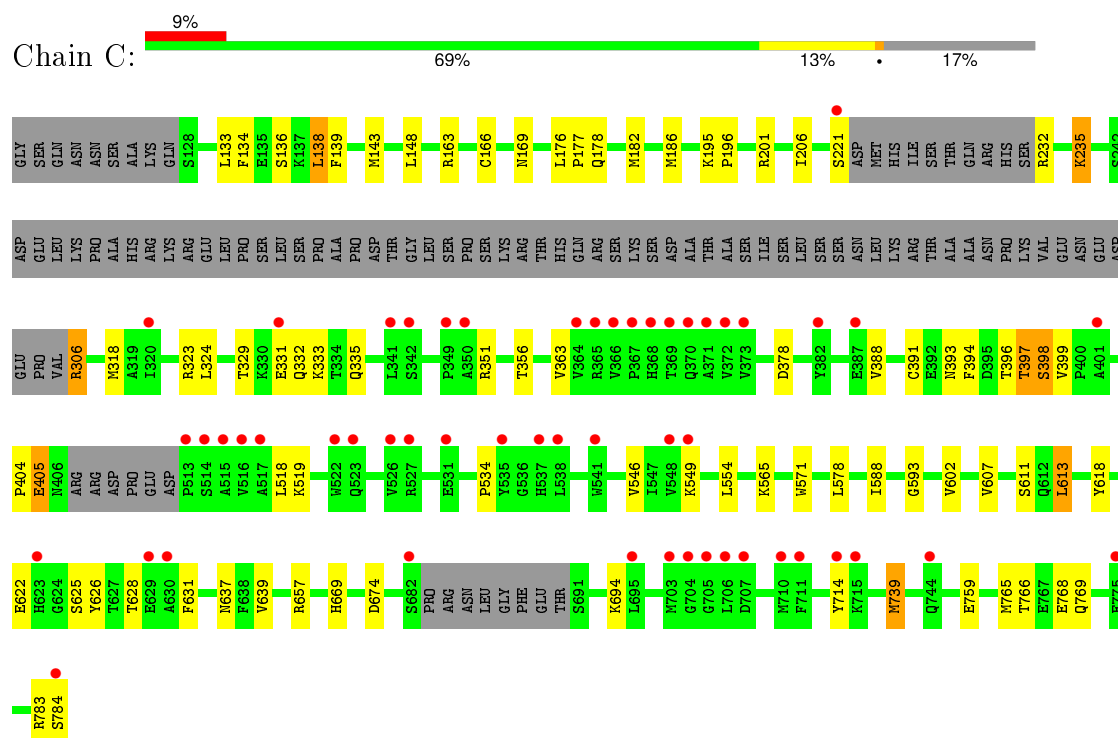
3 Residue-property plots

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.

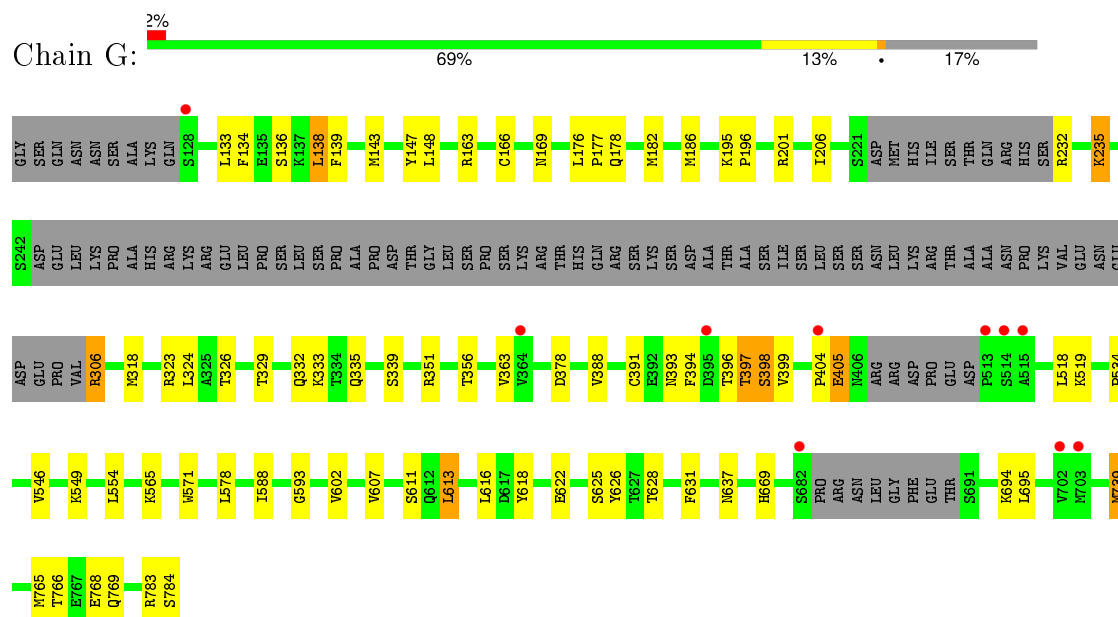
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



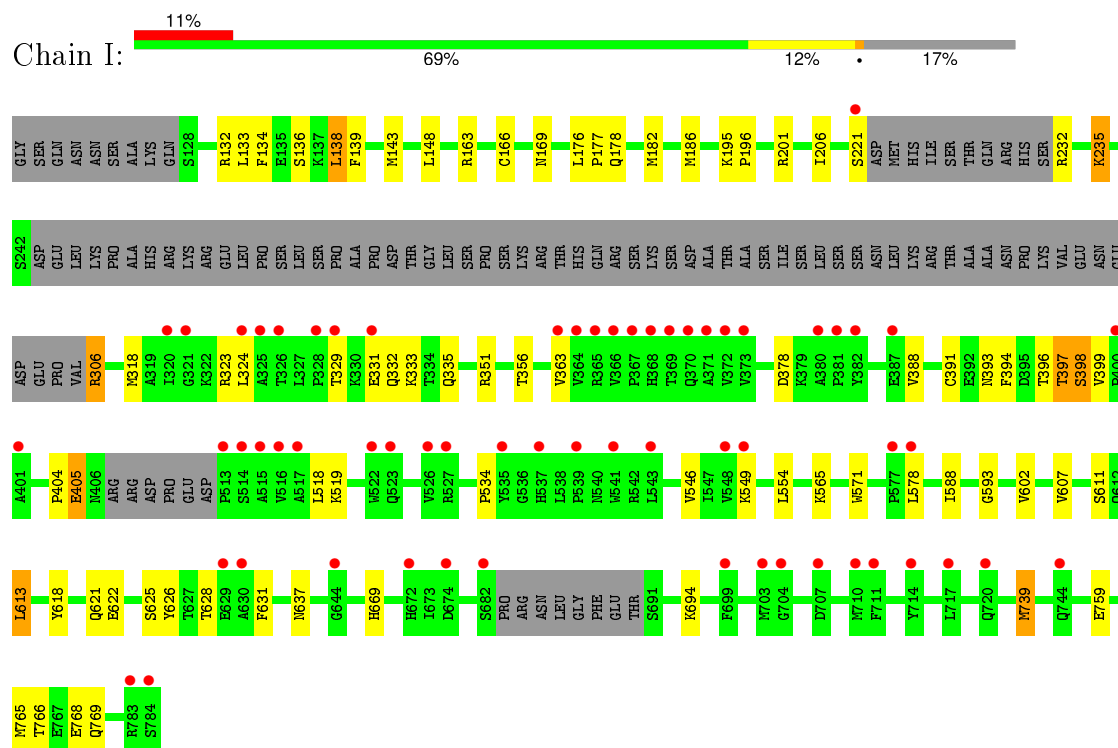
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



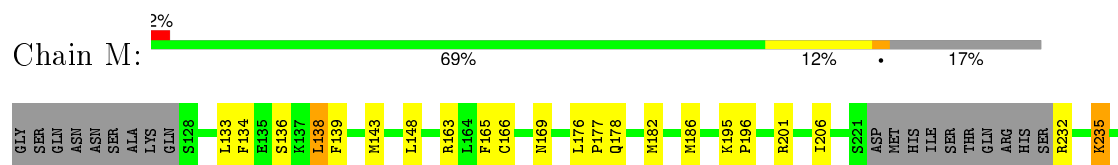
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

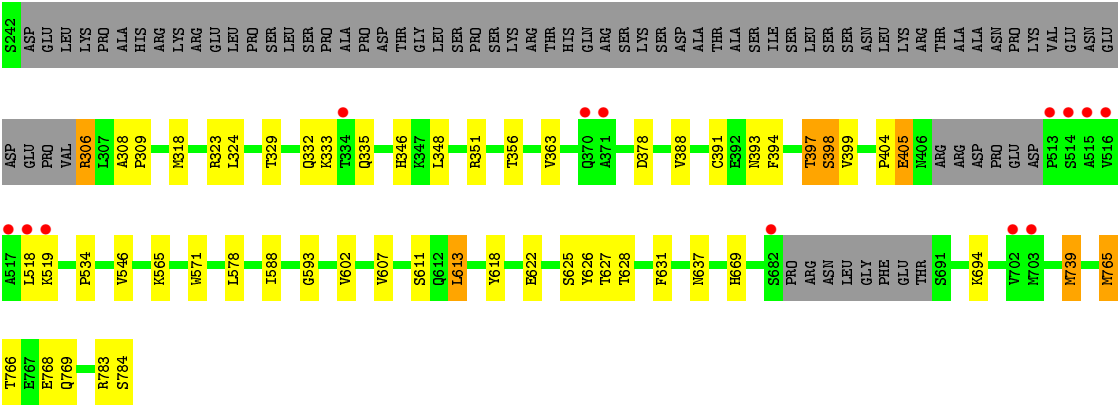


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

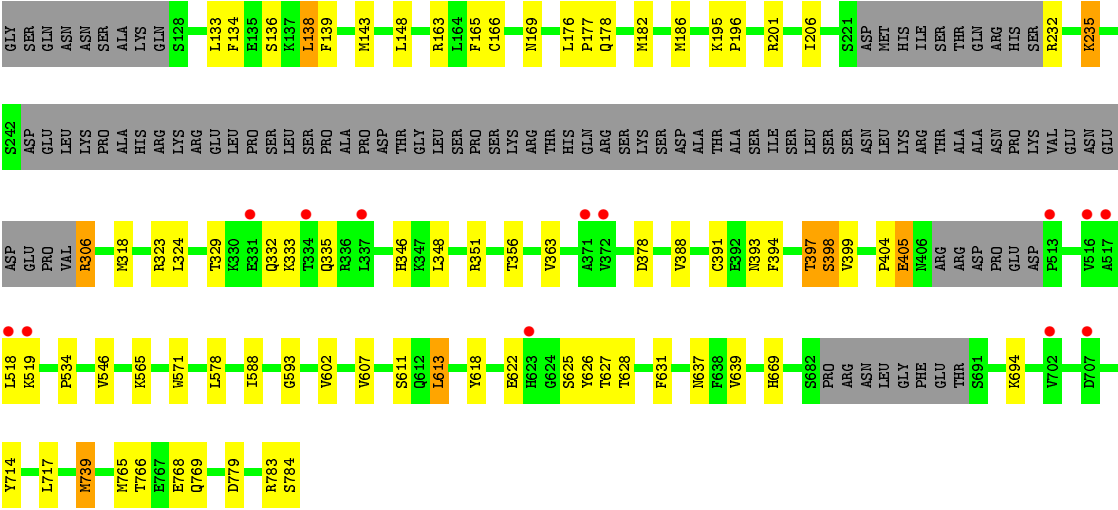


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

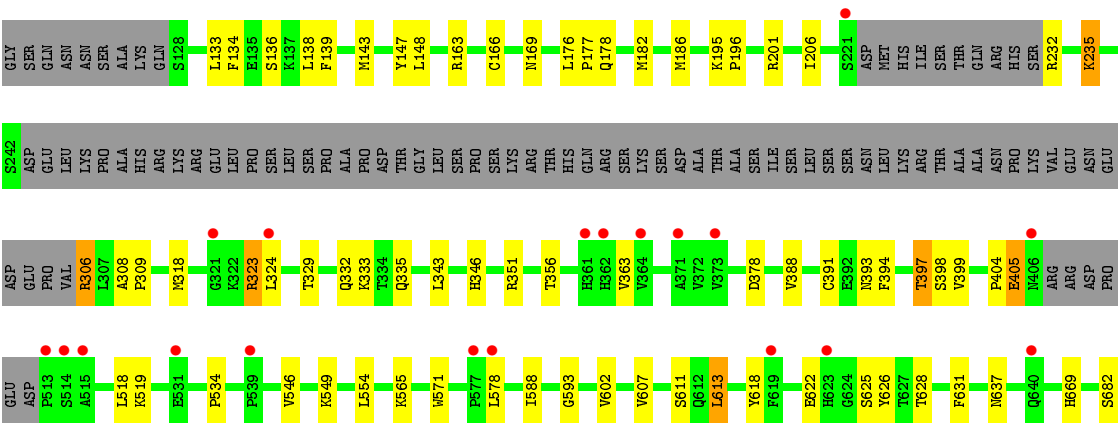


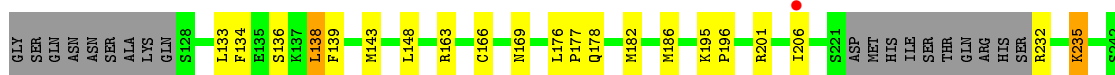


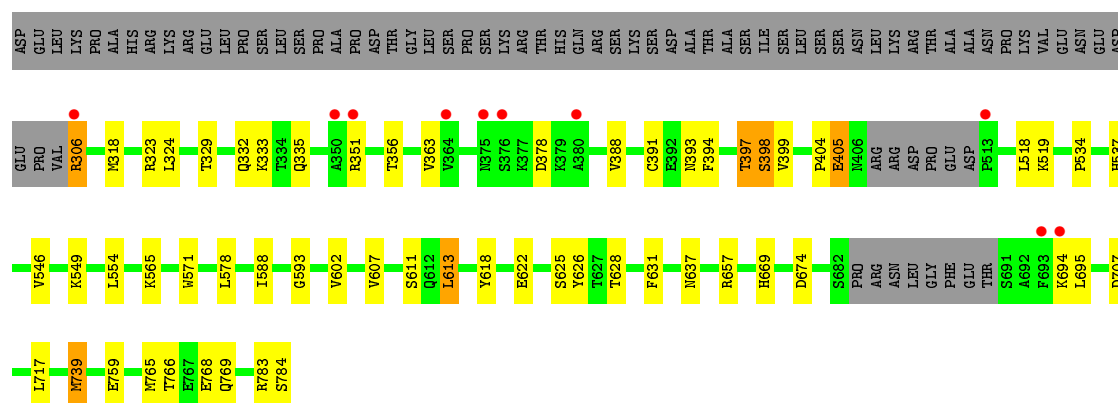
● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



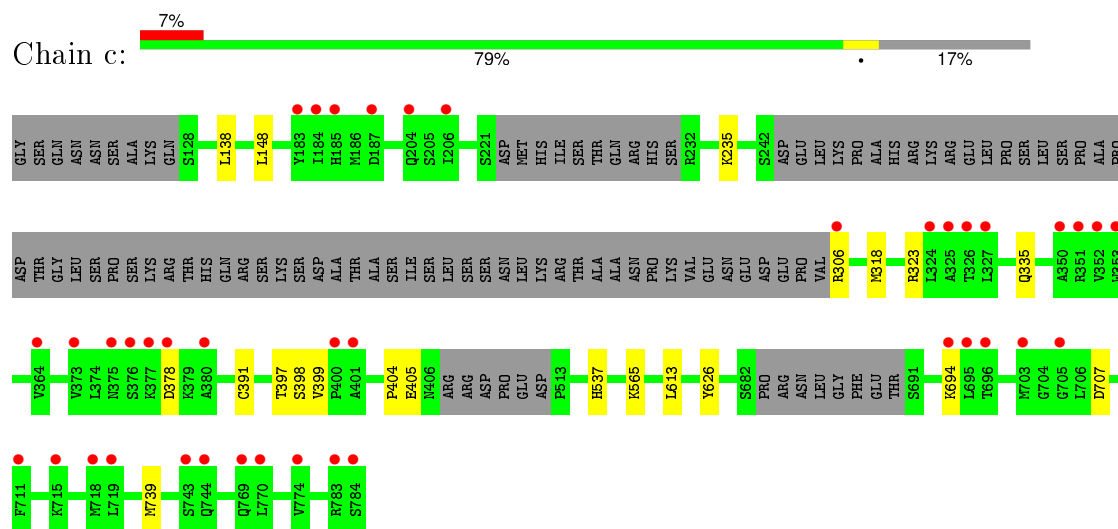
● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



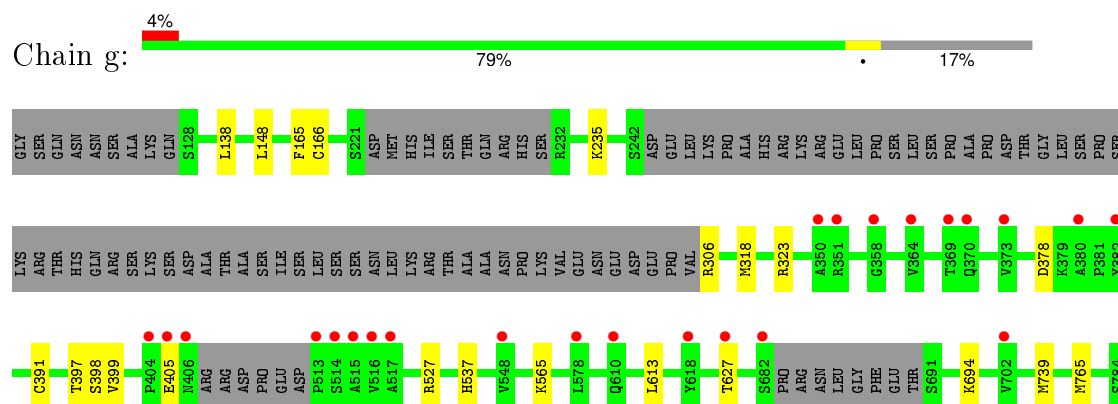




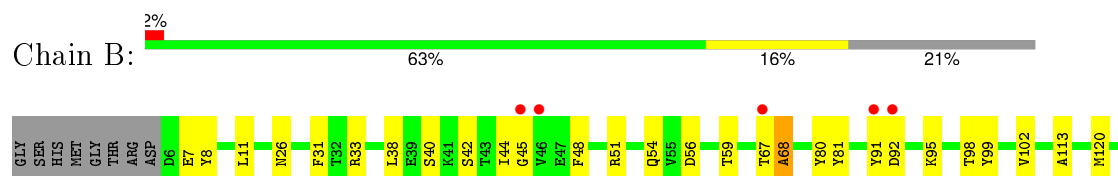
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

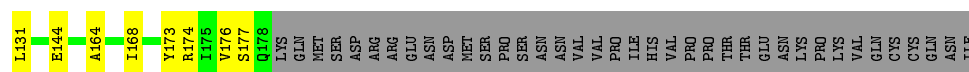


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

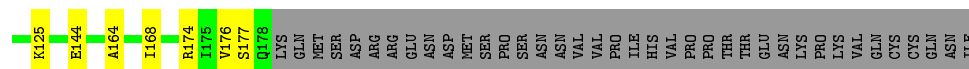
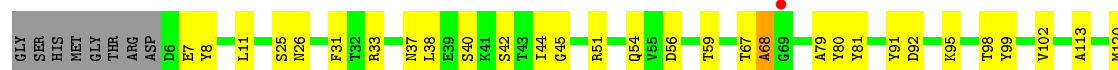


• Molecule 2: RAS-RELATED PROTEIN RAB-11A

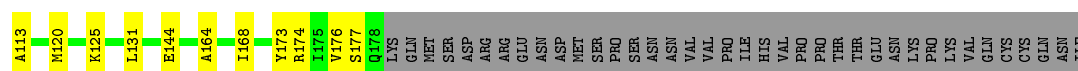
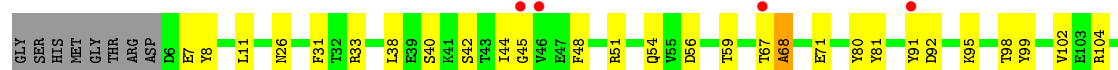




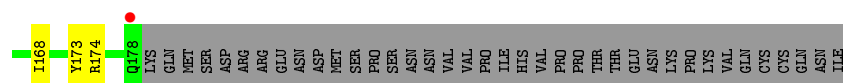
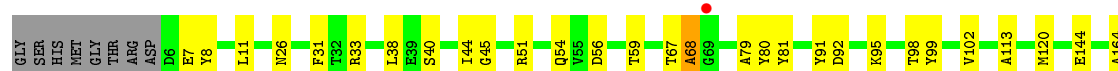
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



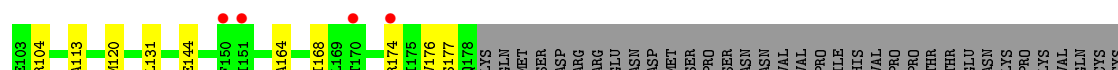
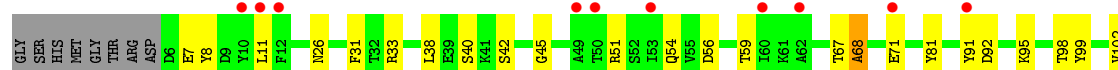
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



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

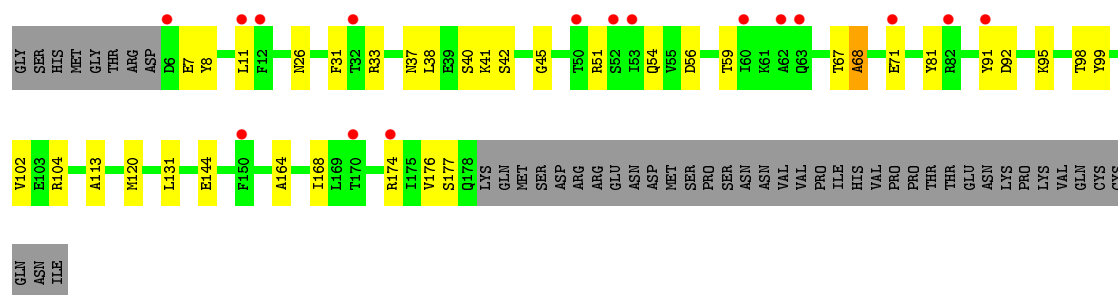


• Molecule 2: RAS-RELATED PROTEIN RAB-11A

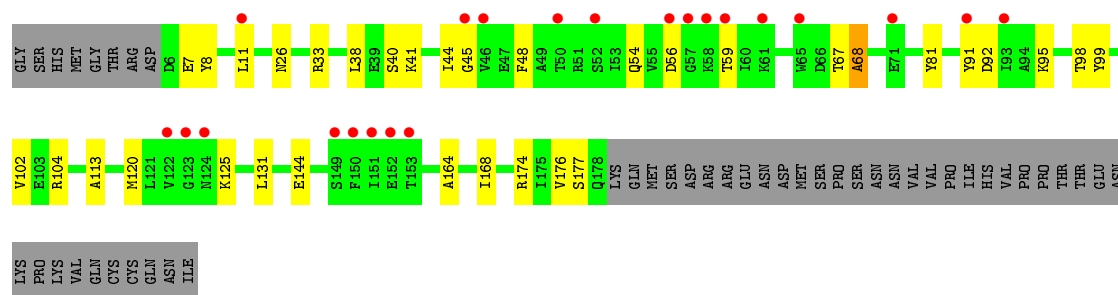


• Molecule 2: RAS-RELATED PROTEIN RAB-11A

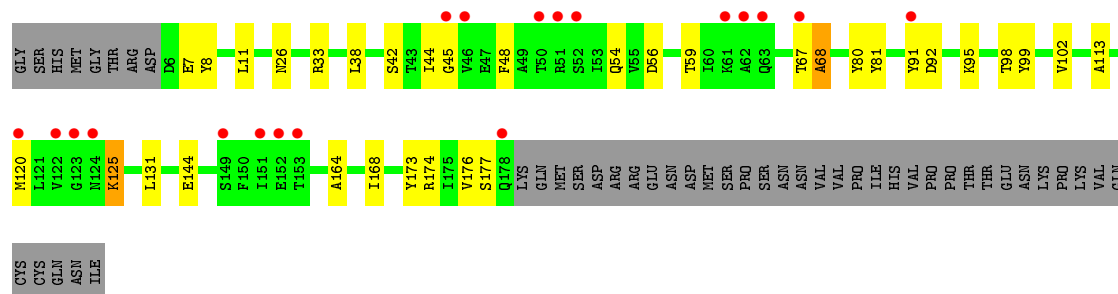




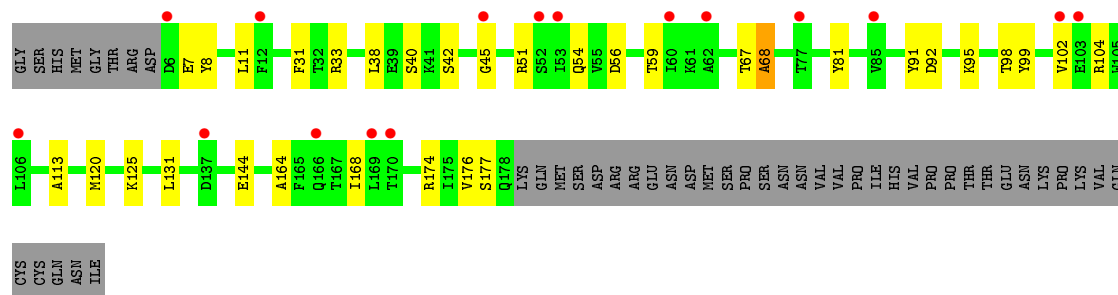
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



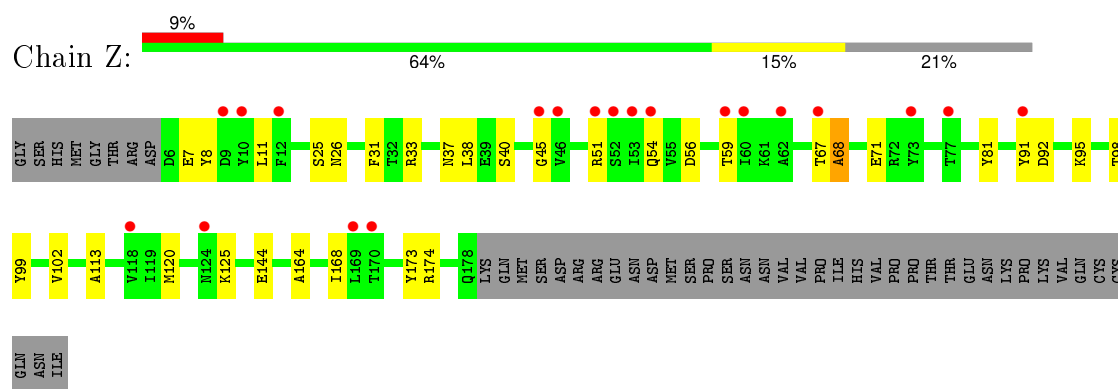
● Molecule 2: RAS-RELATED PROTEIN RAB-11A



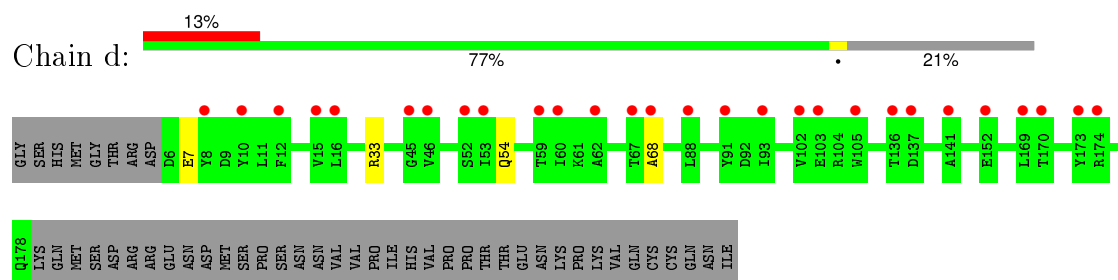
- Molecule 2: RAS-RELATED PROTEIN RAB-11A



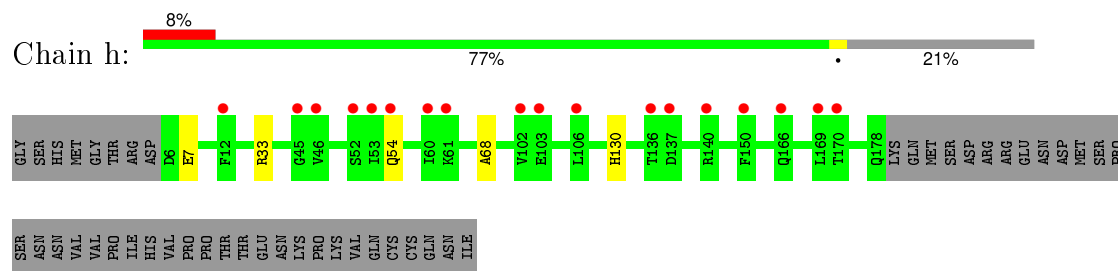
● Molecule 2: RAS-RELATED PROTEIN RAB-11A



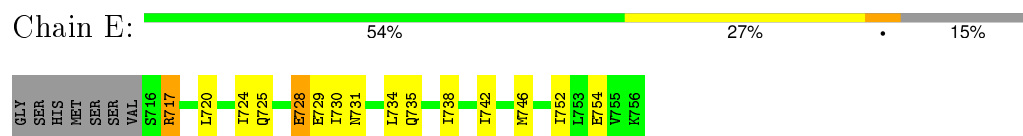
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



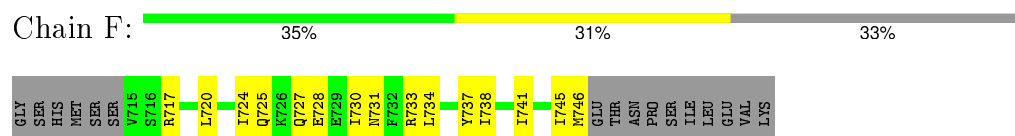
● Molecule 2: RAS-RELATED PROTEIN RAB-11A



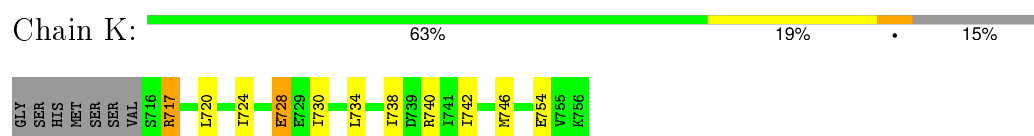
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

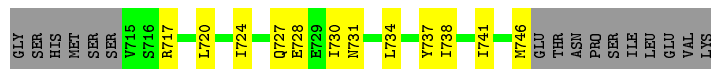


- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



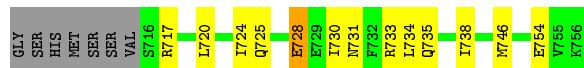
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain L: 



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain U: 




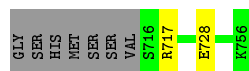
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain V: 



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain a: 




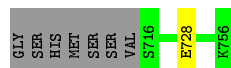
- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 94.5 (49.88-6.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 6.15Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.253 , 0.359 0.252 , 0.351	Depositor DCC
R_{free} test set	2048 reflections (5.78%)	DCC
Wilson B-factor (Å ²)	248.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 207.4	EDS
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 37330 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	65970	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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
3	E	314	0	298	89	0
3	F	237	0	222	78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	R	1	0	0	0	0
6	T	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 8.

The worst 5 of 993 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)
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	Interatomic distance (Å)	Clash overlap (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:S:346:HIS:O	1:Y:626:TYR:CE1[2_656]	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%)	39	80
1	C	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	26	71
1	G	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	26	71
1	I	460/566 (81%)	440 (96%)	17 (4%)	3 (1%)	26	71
1	M	460/566 (81%)	441 (96%)	16 (4%)	3 (1%)	26	71
1	O	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	26	71
1	Q	460/566 (81%)	439 (95%)	19 (4%)	2 (0%)	39	80
1	S	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	26	71
1	W	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	26	71
1	Y	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	26	71
1	c	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	39	80
1	g	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	39	80
2	B	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	D	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	H	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	J	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	N	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	P	171/219 (78%)	162 (95%)	8 (5%)	1 (1%)	30	74
2	R	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	T	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	16	61
2	X	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	Z	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	16	61
2	d	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
2	h	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	30	74
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

Continued on next page...

Continued from previous page...

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%)	30	74

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%)	45	76
1	C	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	G	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	I	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	M	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	O	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	Q	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	S	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	W	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	Y	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	c	422/508 (83%)	408 (97%)	14 (3%)	45	76
1	g	422/508 (83%)	409 (97%)	13 (3%)	47	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	D	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	H	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	J	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	N	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	P	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	R	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	T	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	X	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	Z	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	d	147/191 (77%)	144 (98%)	3 (2%)	63	85
2	h	147/191 (77%)	144 (98%)	3 (2%)	63	85
3	E	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	F	21/45 (47%)	21 (100%)	0	100	100
3	K	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	L	21/45 (47%)	21 (100%)	0	100	100
3	U	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	V	21/45 (47%)	21 (100%)	0	100	100
3	a	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	b	21/45 (47%)	21 (100%)	0	100	100
3	e	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	f	21/45 (47%)	21 (100%)	0	100	100
3	i	31/45 (69%)	30 (97%)	1 (3%)	46	76
3	j	21/45 (47%)	21 (100%)	0	100	100
All	All	7140/8928 (80%)	6931 (97%)	209 (3%)	50	78

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 molecules 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	-	21,25,25	2.00	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	B	2000	6	25,34,34	1.49	4 (16%)	31,54,54	2.00	7 (22%)
4	093	C	2002	-	21,25,25	2.02	6 (28%)	24,36,36	4.52	10 (41%)
5	GSP	D	2000	6	25,34,34	1.59	5 (20%)	31,54,54	2.18	10 (32%)
4	093	G	2002	1	21,25,25	2.01	6 (28%)	24,36,36	4.53	11 (45%)
5	GSP	H	2000	6	25,34,34	1.39	4 (16%)	31,54,54	2.10	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	093	I	2002	-	21,25,25	2.01	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	J	2000	6	25,34,34	1.62	5 (20%)	31,54,54	2.28	10 (32%)
4	093	M	2002	-	21,25,25	2.03	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	N	2000	6	25,34,34	1.32	4 (16%)	31,54,54	2.27	11 (35%)
4	093	O	2002	1	21,25,25	2.04	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	P	2000	6	25,34,34	1.36	5 (20%)	31,54,54	2.16	10 (32%)
4	093	Q	2002	1	21,25,25	2.02	6 (28%)	24,36,36	4.53	11 (45%)
5	GSP	R	2000	6	25,34,34	1.43	4 (16%)	31,54,54	2.17	8 (25%)
4	093	S	2002	1	21,25,25	2.02	6 (28%)	24,36,36	4.54	11 (45%)
5	GSP	T	2000	6	25,34,34	1.33	4 (16%)	31,54,54	2.14	8 (25%)
4	093	W	2002	1	21,25,25	2.01	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	X	2000	6	25,34,34	1.52	5 (20%)	31,54,54	2.07	10 (32%)
4	093	Y	2002	1	21,25,25	2.02	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	Z	2000	6	25,34,34	1.47	5 (20%)	31,54,54	2.08	8 (25%)
4	093	c	2002	1	21,25,25	2.04	6 (28%)	24,36,36	4.52	11 (45%)
5	GSP	d	2000	6	25,34,34	1.49	5 (20%)	31,54,54	2.25	11 (35%)
4	093	g	2002	1	21,25,25	2.02	6 (28%)	24,36,36	4.53	11 (45%)
5	GSP	h	2000	6	25,34,34	1.64	6 (24%)	31,54,54	2.08	10 (32%)

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	-	0/15/38/38	0/3/3/3
4	093	C	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	D	2000	6	-	0/15/38/38	0/3/3/3
4	093	G	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	H	2000	6	-	0/15/38/38	0/3/3/3
4	093	I	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	J	2000	6	-	0/15/38/38	0/3/3/3
4	093	M	2002	-	-	0/17/19/19	0/2/2/2
5	GSP	N	2000	6	-	0/15/38/38	0/3/3/3
4	093	O	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	P	2000	6	-	0/15/38/38	0/3/3/3
4	093	Q	2002	1	-	0/17/19/19	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GSP	R	2000	6	-	0/15/38/38	0/3/3/3
4	093	S	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	T	2000	6	-	0/15/38/38	0/3/3/3
4	093	W	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	X	2000	6	-	0/15/38/38	0/3/3/3
4	093	Y	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	Z	2000	6	-	0/15/38/38	0/3/3/3
4	093	c	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	d	2000	6	-	0/15/38/38	0/3/3/3
4	093	g	2002	1	-	0/17/19/19	0/2/2/2
5	GSP	h	2000	6	-	0/15/38/38	0/3/3/3

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	2002	093	OAM-SAN	-3.20	1.40	1.43
4	O	2002	093	OAM-SAN	-3.16	1.40	1.43
4	M	2002	093	OAM-SAN	-3.14	1.40	1.43
4	g	2002	093	OAM-SAN	-3.12	1.40	1.43
4	W	2002	093	OAM-SAN	-3.11	1.40	1.43

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2002	093	OAO-SAN-OAM	-18.87	94.51	119.54
4	g	2002	093	OAO-SAN-OAM	-18.85	94.53	119.54
4	Q	2002	093	OAO-SAN-OAM	-18.84	94.55	119.54
4	G	2002	093	OAO-SAN-OAM	-18.83	94.56	119.54
4	C	2002	093	OAO-SAN-OAM	-18.83	94.56	119.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2000	GSP	6	0
5	D	2000	GSP	11	0
5	H	2000	GSP	7	0
5	J	2000	GSP	4	0
5	N	2000	GSP	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	2000	GSP	7	0
5	R	2000	GSP	5	0
5	T	2000	GSP	5	0
5	X	2000	GSP	6	0
5	Z	2000	GSP	6	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 ⓘ

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	470/566 (83%)	-0.07	6 (1%) 79 73	95, 212, 331, 500	0
1	C	470/566 (83%)	0.58	53 (11%) 7 12	126, 300, 456, 500	0
1	G	470/566 (83%)	-0.05	10 (2%) 67 62	98, 214, 342, 500	0
1	I	470/566 (83%)	0.65	62 (13%) 4 10	124, 306, 474, 500	0
1	M	470/566 (83%)	-0.02	13 (2%) 56 52	95, 217, 341, 500	0
1	O	470/566 (83%)	-0.03	13 (2%) 56 52	102, 208, 335, 500	0
1	Q	470/566 (83%)	0.10	21 (4%) 37 36	102, 247, 364, 498	0
1	S	470/566 (83%)	0.11	17 (3%) 46 43	114, 251, 389, 500	0
1	W	470/566 (83%)	0.14	11 (2%) 64 59	99, 253, 387, 500	0
1	Y	470/566 (83%)	-0.07	11 (2%) 64 59	115, 250, 365, 474	0
1	c	470/566 (83%)	0.38	40 (8%) 13 17	119, 305, 478, 500	0
1	g	470/566 (83%)	0.27	24 (5%) 32 31	126, 268, 416, 500	0
2	B	173/219 (78%)	0.12	5 (2%) 55 50	94, 201, 375, 493	0
2	D	173/219 (78%)	0.05	1 (0%) 90 87	95, 220, 341, 488	0
2	H	173/219 (78%)	0.15	4 (2%) 64 59	94, 207, 382, 499	0
2	J	173/219 (78%)	0.05	2 (1%) 81 75	92, 198, 338, 500	0
2	N	173/219 (78%)	0.59	14 (8%) 15 18	137, 282, 424, 496	0
2	P	173/219 (78%)	0.65	16 (9%) 11 15	132, 277, 432, 496	0
2	R	173/219 (78%)	0.74	22 (12%) 5 10	139, 269, 415, 496	0
2	T	173/219 (78%)	0.61	19 (10%) 7 12	136, 266, 407, 493	0
2	X	173/219 (78%)	0.45	16 (9%) 11 15	146, 282, 453, 500	0
2	Z	173/219 (78%)	0.62	20 (11%) 6 11	165, 262, 362, 494	0
2	d	173/219 (78%)	0.91	28 (16%) 3 8	146, 308, 447, 500	0
2	h	173/219 (78%)	0.55	18 (10%) 8 13	158, 294, 440, 500	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
3	E	41/48 (85%)	0.02	0	100	100	153, 251, 365, 489	0
3	F	32/48 (66%)	-0.46	0	100	100	169, 285, 399, 466	0
3	K	41/48 (85%)	0.05	0	100	100	131, 240, 410, 465	0
3	L	32/48 (66%)	-0.45	0	100	100	170, 263, 384, 436	0
3	U	41/48 (85%)	0.19	0	100	100	175, 284, 408, 494	0
3	V	32/48 (66%)	-0.47	0	100	100	170, 260, 403, 435	0
3	a	41/48 (85%)	-0.08	0	100	100	195, 318, 423, 476	0
3	b	32/48 (66%)	-0.22	0	100	100	213, 309, 428, 479	0
3	e	41/48 (85%)	0.09	0	100	100	175, 255, 384, 478	0
3	f	32/48 (66%)	-0.48	0	100	100	194, 288, 337, 363	0
3	i	41/48 (85%)	0.08	1 (2%)	62	57	202, 325, 441, 500	0
3	j	32/48 (66%)	-0.20	0	100	100	194, 282, 404, 462	0
All	All	8154/9996 (81%)	0.22	447 (5%)	29	29	92, 255, 416, 500	0

The worst 5 of 447 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	382	TYR	6.1
1	g	515	ALA	6.0
2	H	46	VAL	5.7
1	I	513	PRO	5.5
1	M	513	PRO	5.4

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 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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	GSP	N	2000	32/32	0.95	0.23	-0.49	97,151,255,301	0
5	GSP	J	2000	32/32	0.94	0.27	-0.50	94,165,285,323	0
5	GSP	h	2000	32/32	0.94	0.24	-0.55	123,249,350,363	0
5	GSP	D	2000	32/32	0.95	0.24	-0.69	110,193,250,272	0
5	GSP	T	2000	32/32	0.93	0.23	-0.71	123,205,238,264	0
5	GSP	R	2000	32/32	0.88	0.22	-0.72	108,197,262,274	0
5	GSP	Z	2000	32/32	0.90	0.21	-0.73	176,212,274,298	0
6	MG	d	2001	1/1	0.76	0.23	-0.77	167,167,167,167	0
5	GSP	P	2000	32/32	0.94	0.22	-0.78	111,168,247,275	0
5	GSP	B	2000	32/32	0.93	0.20	-0.81	141,197,232,249	0
5	GSP	d	2000	32/32	0.83	0.23	-0.88	174,212,349,391	0
5	GSP	H	2000	32/32	0.92	0.18	-0.89	141,183,247,282	0
6	MG	P	2001	1/1	0.93	0.16	-1.16	244,244,244,244	0
5	GSP	X	2000	32/32	0.95	0.20	-1.21	134,226,322,330	0
6	MG	T	2001	1/1	0.99	0.13	-1.24	127,127,127,127	0
6	MG	J	2001	1/1	0.93	0.13	-1.24	142,142,142,142	0
6	MG	H	2001	1/1	0.94	0.12	-1.25	139,139,139,139	0
6	MG	B	2001	1/1	0.95	0.13	-1.27	159,159,159,159	0
6	MG	N	2001	1/1	0.91	0.12	-1.39	240,240,240,240	0
6	MG	Z	2001	1/1	0.85	0.10	-1.43	178,178,178,178	0
6	MG	R	2001	1/1	0.97	0.09	-1.49	106,106,106,106	0
6	MG	X	2001	1/1	0.89	0.12	-1.60	255,255,255,255	0
6	MG	D	2001	1/1	0.92	0.11	-1.92	64,64,64,64	0
6	MG	h	2001	1/1	0.75	0.12	-1.97	190,190,190,190	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 [i](#)

There are no such residues in this entry.