



# wwPDB X-ray Structure Validation Summary Report

Jun 6, 2014 – 03:27 AM EDT

PDB ID : 4D0L  
Title : Phosphatidylinositol 4-kinase III beta-PIK93 in a complex with Rab11a- GTP gammaS  
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 : 2014-04-29  
Resolution : 2.94 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>

---

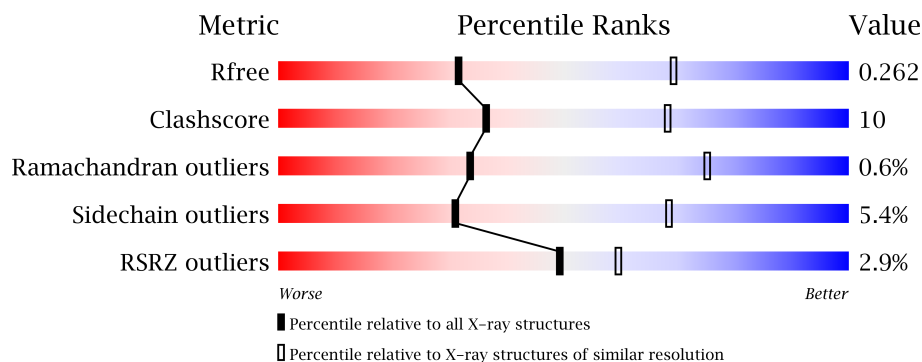
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.94 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	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

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	E	566	
2	B	219	
2	D	219	
2	F	219	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15864 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	476	Total	C	N	O	S	0	0	0
			3833	2456	660	693	24			
1	E	479	Total	C	N	O	S	0	0	0
			3859	2473	666	696	24			

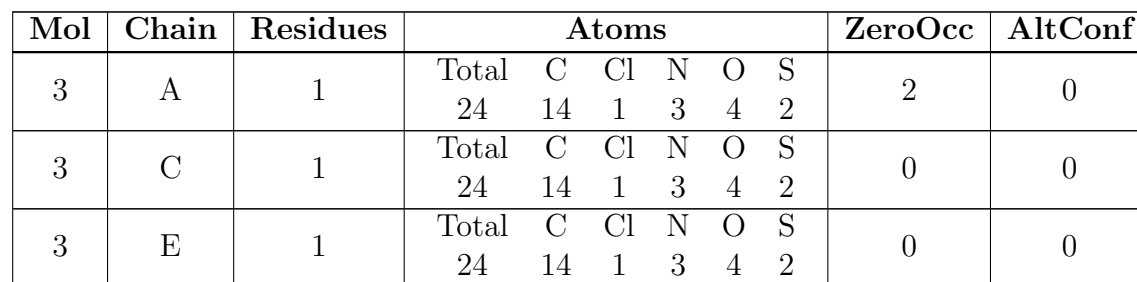
- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

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	177	Total	C	N	O	S	0	0	0
			1409	891	244	272	2			
2	F	177	Total	C	N	O	S	0	0	0
			1409	891	244	272	2			

There are 3 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
F	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491

- Molecule 3 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>).



- 
- The chemical structure of GSP (Guanosine 3'-phosphate) is shown. It consists of a guanine base (a purine ring system with an amino group at position 2 and a carbonyl group at position 6) attached to a ribose sugar (a five-membered ring with hydroxyl groups at positions 2' and 3'). The ribose sugar is linked to a triphosphate chain (three phosphate groups) via a phosphodiester bond. The triphosphate chain is shown with various labels for atoms and bonds, including C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C8

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

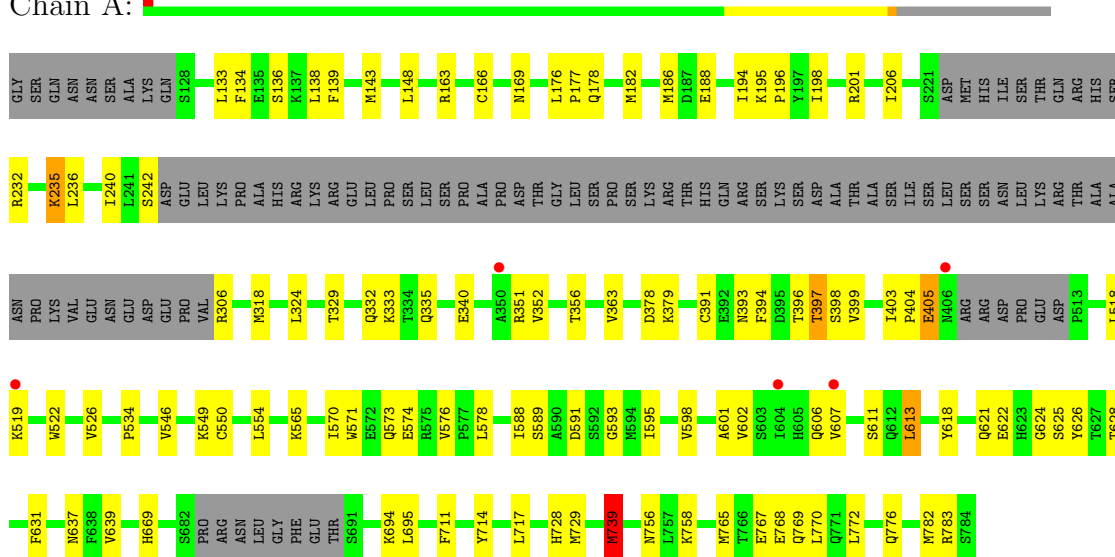
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	2	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			1	1		
6	E	4	Total	O	0	0
			4	4		
6	F	3	Total	O	0	0
			3	3		

### 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.

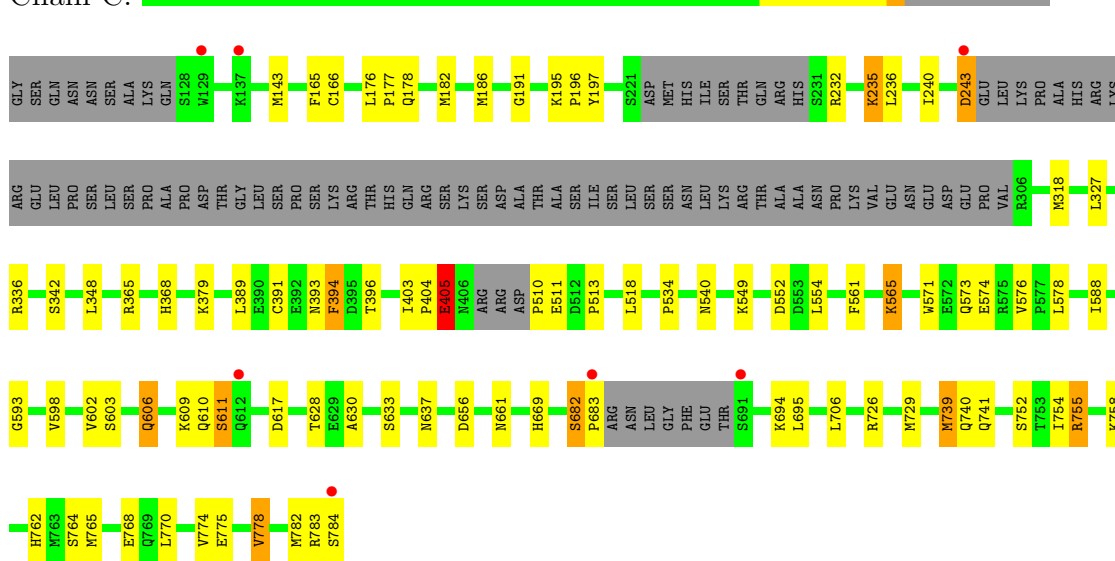
#### • Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain A:



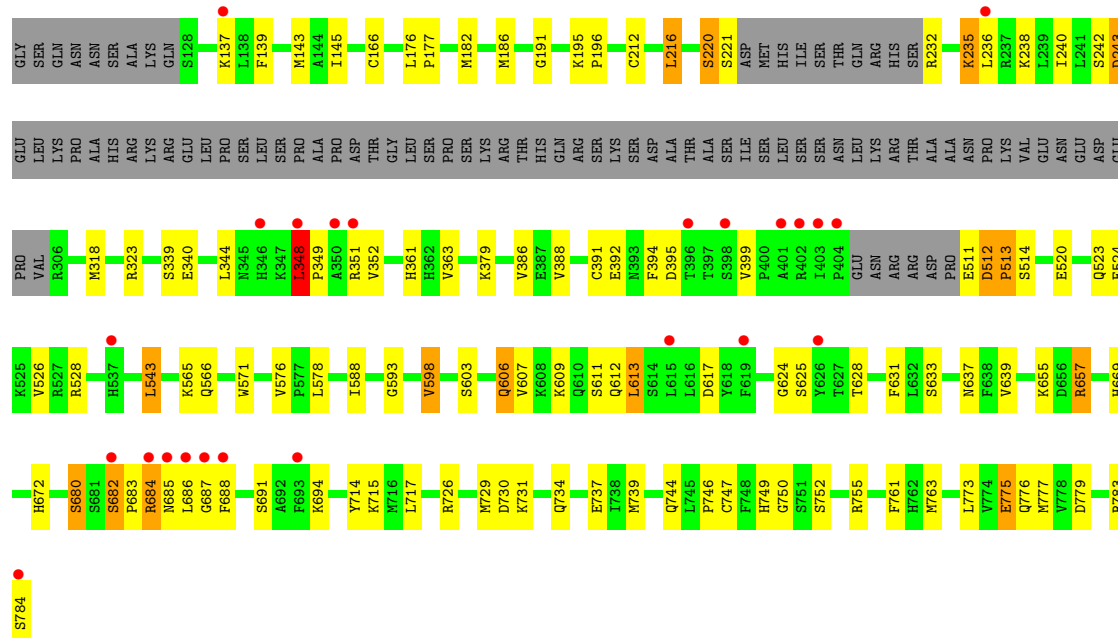
#### • Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain C:



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

## Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.80Å 146.93Å 188.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.84 – 2.94 49.58 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (115.84-2.94) 99.7 (49.58-2.94)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.216 , 0.259 0.218 , 0.262	Depositor DCC
$R_{free}$ test set	3095 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 61151 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.26% 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	0.53	0/3866	0.75	1/5219 (0.0%)
1	C	0.53	0/3913	0.76	2/5285 (0.0%)
1	E	0.53	0/3940	0.75	2/5322 (0.0%)
2	B	0.50	0/1399	0.79	1/1892 (0.1%)
2	D	0.50	0/1431	0.70	0/1933
2	F	0.52	0/1431	0.74	0/1933
All	All	0.53	0/15980	0.75	6/21584 (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	E	0	2
2	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	657	ARG	NE-CZ-NH1	6.79	123.70	120.30
2	B	88	LEU	CB-CG-CD1	6.40	121.89	111.00
1	E	348	LEU	C-N-CA	-5.49	98.94	122.00
1	C	143	MET	CG-SD-CE	5.17	108.48	100.20
1	A	739	MET	CG-SD-CE	-5.12	92.01	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	403	ILE	Peptide
1	E	348	LEU	Peptide
1	E	750	GLY	Peptide
2	F	110	ARG	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	3839	77	1
1	C	3833	0	3870	57	0
1	E	3859	0	3895	106	0
2	B	1377	0	1370	32	0
2	D	1409	0	1405	25	0
2	F	1409	0	1407	23	0
3	A	24	0	16	7	0
3	C	24	0	16	5	0
3	E	24	0	16	7	0
4	B	32	0	12	3	0
4	D	32	0	12	2	0
4	F	32	0	12	3	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	8	0	0	0	0
6	B	2	0	0	1	0
6	C	1	0	0	0	0
6	E	4	0	0	1	0
6	F	3	0	0	0	0
All	All	15864	0	15870	328	1

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 10.

The worst 5 of 328 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:56:ASP:OD2	2:B:174:ARG:NH1	1.72	1.20
1:C:240:ILE:O	1:C:243:ASP:OD1	1.75	1.04
1:E:323:ARG:NH1	1:E:340:GLU:OE2	1.90	1.03
1:E:686:LEU:HD22	1:E:688:PHE:CE2	1.98	0.98
1:C:694:LYS:HD3	1:C:784:SER:HA	1.46	0.95

All (1) 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)
1:A:340:GLU:OE1	1:A:626:TYR:OH[4.595]	2.16	0.04

## 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%)	445 (97%)	13 (3%)	2 (0%)	43	82
1	C	466/566 (82%)	445 (96%)	16 (3%)	5 (1%)	21	60
1	E	471/566 (83%)	446 (95%)	22 (5%)	3 (1%)	33	75
2	B	171/219 (78%)	164 (96%)	6 (4%)	1 (1%)	33	75
2	D	175/219 (80%)	170 (97%)	5 (3%)	0	100	100
2	F	175/219 (80%)	168 (96%)	7 (4%)	0	100	100
All	All	1918/2355 (81%)	1838 (96%)	69 (4%)	11 (1%)	33	75

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	513	PRO
1	E	513	PRO
1	C	405	GLU
2	B	68	ALA
1	C	682	SER

### 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%)	409 (97%)	13 (3%)	52	87
1	C	428/508 (84%)	403 (94%)	25 (6%)	28	64
1	E	429/508 (84%)	398 (93%)	31 (7%)	21	51
2	B	147/191 (77%)	139 (95%)	8 (5%)	31	68
2	D	151/191 (79%)	142 (94%)	9 (6%)	27	63
2	F	151/191 (79%)	144 (95%)	7 (5%)	37	75
All	All	1728/2097 (82%)	1635 (95%)	93 (5%)	31	68

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	764	SER
2	D	177	SER
1	E	776	GLN
1	C	768	GLU
2	D	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	612	GLN
1	E	150	ASN
1	E	540	ASN
1	C	540	ASN
1	E	566	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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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$
3	093	A	2002	-	25,25,25	4.23	9 (36%)	33,36,36	4.74	16 (48%)
4	GSP	B	2000	5	34,34,34	1.55	7 (20%)	52,54,54	3.47	13 (25%)
3	093	C	2002	1	25,25,25	3.72	7 (28%)	33,36,36	5.13	17 (51%)
4	GSP	D	2000	5	34,34,34	1.51	7 (20%)	52,54,54	3.24	18 (34%)
3	093	E	2002	-	25,25,25	3.69	9 (36%)	33,36,36	6.58	11 (33%)
4	GSP	F	2000	5	34,34,34	1.59	6 (17%)	52,54,54	3.40	17 (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
3	093	A	2002	-	-	0/17/19/19	0/2/2/2
4	GSP	B	2000	5	-	0/21/38/38	0/3/3/3
3	093	C	2002	1	-	0/17/19/19	0/2/2/2
4	GSP	D	2000	5	-	0/21/38/38	0/3/3/3
3	093	E	2002	-	-	0/17/19/19	0/2/2/2
4	GSP	F	2000	5	-	0/21/38/38	0/3/3/3

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002	093	CAI-SAP	-15.65	1.55	1.75
3	C	2002	093	CAI-SAP	-12.96	1.58	1.75
3	E	2002	093	CAI-SAP	-12.45	1.59	1.75
3	A	2002	093	CAQ-SAP	-7.70	1.60	1.73
3	C	2002	093	CAQ-SAP	-7.62	1.60	1.73

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2002	093	CAQ-NAK-CAJ	-30.61	109.56	112.36
3	A	2002	093	OAO-SAN-OAM	-19.44	93.89	119.55
4	B	2000	GSP	C6-C5-N7	19.23	136.73	134.14
4	F	2000	GSP	O3B-PG-S1G	-18.42	106.36	114.53
3	C	2002	093	CAQ-NAK-CAJ	-18.36	110.68	112.36

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%)	0.10	5 (1%) 77 85	39, 61, 99, 117	0
1	C	476/566 (84%)	0.07	7 (1%) 70 81	38, 61, 98, 146	0
1	E	479/566 (84%)	0.20	24 (5%) 28 35	42, 67, 110, 171	0
2	B	173/219 (78%)	0.28	4 (2%) 57 68	53, 82, 113, 139	0
2	D	177/219 (80%)	0.34	12 (6%) 17 22	45, 65, 106, 149	0
2	F	177/219 (80%)	0.18	4 (2%) 57 68	41, 65, 109, 136	0
All	All	1952/2355 (82%)	0.16	56 (2%) 49 59	38, 65, 106, 171	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	686	LEU	5.0
1	E	401	ALA	4.0
1	E	687	GLY	3.8
1	C	683	PRO	3.7
1	E	615	LEU	3.3

### 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
3	093	E	2002	24/24	0.21	1.04	65,72,83,124	0
3	093	A	2002	24/24	0.23	0.72	57,75,105,130	2
3	093	C	2002	24/24	0.20	0.50	57,66,75,123	0
4	GSP	D	2000	32/32	0.16	-0.31	46,55,65,72	0
4	GSP	B	2000	32/32	0.13	-1.09	47,58,76,86	0
4	GSP	F	2000	32/32	0.13	-1.25	43,47,58,61	0
5	MG	F	2001	1/1	0.12	-1.31	59,59,59,59	0
5	MG	D	2001	1/1	0.11	-2.88	72,72,72,72	0
5	MG	B	2001	1/1	0.04	-4.62	87,87,87,87	0

## 6.5 Other polymers

There are no such residues in this entry.