



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 11:15 am GMT

PDB ID : 4LX0  
Title : Crystal structure of Myo5b globular tail domain in complex with active Rab11a  
Authors : Pylypenko, O.; Attanda, W.; Gauquelin, C.; Houdusse, A.  
Deposited on : 2013-07-29  
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

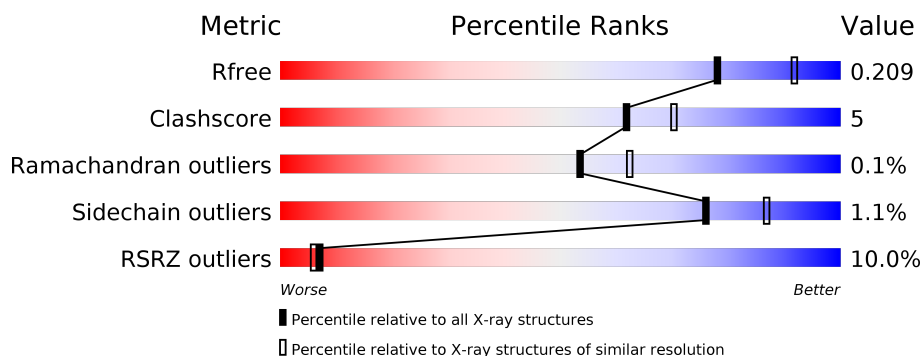
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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. 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	177	<div> <div>3%</div> <div>90%</div> <div>6%</div> <div>••</div> </div>
1	C	177	<div> <div>16%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>
2	B	427	<div> <div>9%</div> <div>82%</div> <div>7%</div> <div>11%</div> </div>
2	D	427	<div> <div>9%</div> <div>77%</div> <div>12%</div> <div>11%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9344 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 Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1352	856	232	263	1			
1	C	171	Total	C	N	O	S	0	0	0
			1317	835	223	258	1			

- Molecule 2 is a protein called Unconventional myosin-Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	382	Total	C	N	O	S	0	1	0
			2979	1892	509	553	25			
2	D	380	Total	C	N	O	S	0	2	0
			2973	1888	501	559	25			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1423	MET	-	EXPRESSION TAG	UNP Q9ULV0
B	1424	ARG	-	EXPRESSION TAG	UNP Q9ULV0
B	1425	SER	-	EXPRESSION TAG	UNP Q9ULV0
B	1426	GLU	-	EXPRESSION TAG	UNP Q9ULV0
B	1427	THR	-	EXPRESSION TAG	UNP Q9ULV0
B	1428	MET	-	EXPRESSION TAG	UNP Q9ULV0
B	1429	SER	-	EXPRESSION TAG	UNP Q9ULV0
B	1430	TYR	-	EXPRESSION TAG	UNP Q9ULV0
B	1431	TYR	-	EXPRESSION TAG	UNP Q9ULV0
B	1432	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1433	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1434	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1435	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1436	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1437	HIS	-	EXPRESSION TAG	UNP Q9ULV0
B	1438	ASP	-	EXPRESSION TAG	UNP Q9ULV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1439	TYR	-	EXPRESSION TAG	UNP Q9ULV0
B	1440	ASP	-	EXPRESSION TAG	UNP Q9ULV0
B	1441	ILE	-	EXPRESSION TAG	UNP Q9ULV0
B	1442	PRO	-	EXPRESSION TAG	UNP Q9ULV0
B	1443	THR	-	EXPRESSION TAG	UNP Q9ULV0
B	1444	THR	-	EXPRESSION TAG	UNP Q9ULV0
B	1445	GLU	-	EXPRESSION TAG	UNP Q9ULV0
B	1446	ASN	-	EXPRESSION TAG	UNP Q9ULV0
B	1447	LEU	-	EXPRESSION TAG	UNP Q9ULV0
B	1448	TYR	-	EXPRESSION TAG	UNP Q9ULV0
B	1449	PHE	-	EXPRESSION TAG	UNP Q9ULV0
B	1450	GLN	-	EXPRESSION TAG	UNP Q9ULV0
B	1451	GLY	-	EXPRESSION TAG	UNP Q9ULV0
B	1452	ALA	-	EXPRESSION TAG	UNP Q9ULV0
B	1452A	MET	-	EXPRESSION TAG	UNP Q9ULV0
B	1452B	GLY	-	EXPRESSION TAG	UNP Q9ULV0
B	1452C	SER	-	EXPRESSION TAG	UNP Q9ULV0
B	1455	MET	-	EXPRESSION TAG	UNP Q9ULV0
D	1420	MET	-	EXPRESSION TAG	UNP Q9ULV0
D	1421	ARG	-	EXPRESSION TAG	UNP Q9ULV0
D	1422	SER	-	EXPRESSION TAG	UNP Q9ULV0
D	1423	GLU	-	EXPRESSION TAG	UNP Q9ULV0
D	1424	THR	-	EXPRESSION TAG	UNP Q9ULV0
D	1425	MET	-	EXPRESSION TAG	UNP Q9ULV0
D	1426	SER	-	EXPRESSION TAG	UNP Q9ULV0
D	1427	TYR	-	EXPRESSION TAG	UNP Q9ULV0
D	1428	TYR	-	EXPRESSION TAG	UNP Q9ULV0
D	1429	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1430	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1431	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1432	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1433	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1434	HIS	-	EXPRESSION TAG	UNP Q9ULV0
D	1435	ASP	-	EXPRESSION TAG	UNP Q9ULV0
D	1436	TYR	-	EXPRESSION TAG	UNP Q9ULV0
D	1437	ASP	-	EXPRESSION TAG	UNP Q9ULV0
D	1438	ILE	-	EXPRESSION TAG	UNP Q9ULV0
D	1439	PRO	-	EXPRESSION TAG	UNP Q9ULV0
D	1440	THR	-	EXPRESSION TAG	UNP Q9ULV0
D	1441	THR	-	EXPRESSION TAG	UNP Q9ULV0
D	1442	GLU	-	EXPRESSION TAG	UNP Q9ULV0
D	1443	ASN	-	EXPRESSION TAG	UNP Q9ULV0

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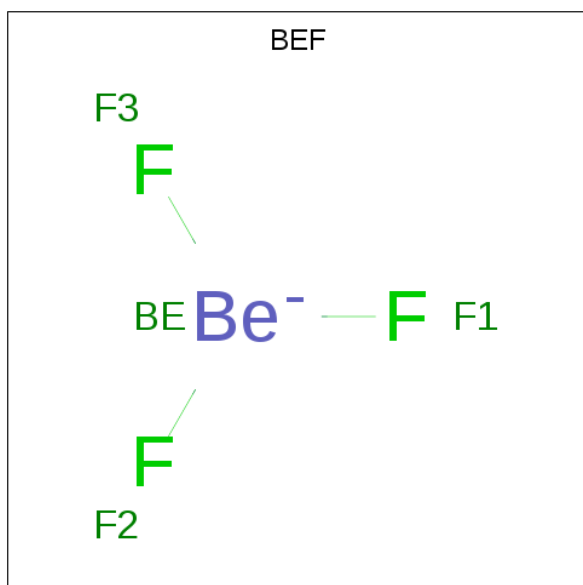
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1444	LEU	-	EXPRESSION TAG	UNP Q9ULV0
D	1445	TYR	-	EXPRESSION TAG	UNP Q9ULV0
D	1446	PHE	-	EXPRESSION TAG	UNP Q9ULV0
D	1447	GLN	-	EXPRESSION TAG	UNP Q9ULV0
D	1448	GLY	-	EXPRESSION TAG	UNP Q9ULV0
D	1449	ALA	-	EXPRESSION TAG	UNP Q9ULV0
D	1450	MET	-	EXPRESSION TAG	UNP Q9ULV0
D	1451	GLY	-	EXPRESSION TAG	UNP Q9ULV0
D	1454	SER	-	EXPRESSION TAG	UNP Q9ULV0
D	1455	MET	-	EXPRESSION TAG	UNP Q9ULV0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Be F 4 1 3	0	0
4	C	1	Total Be F 4 1 3	0	0

- 
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including the amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group being a diphosphate moiety. The structure is labeled with various atoms and bonds, including the nitrogenous base, the sugar, and the phosphate groups, with labels like O6, C6, N7, C8, N9, 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, C8

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
5	C	1	Total 28	C 10	N 5	O 11	P 2	0	0

- GOL
- 
- Chemical structure of GOL (Glycerol) showing a three-carbon chain with hydroxyl groups. The carbons are labeled C1, C2, and C3 in green. The hydroxyl groups are labeled HO O1, OH O2, and OH O3 in red. C1 is connected to HO O1, C2 is connected to OH O2, and C3 is connected to OH O3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		


- Molecule 7 is water.

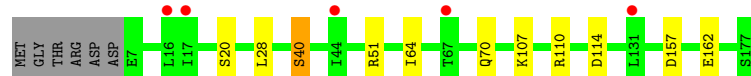
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	187	Total	O	0	0
			187	187		
7	B	225	Total	O	0	0
			225	225		
7	C	51	Total	O	0	0
			51	51		
7	D	188	Total	O	0	0
			188	188		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

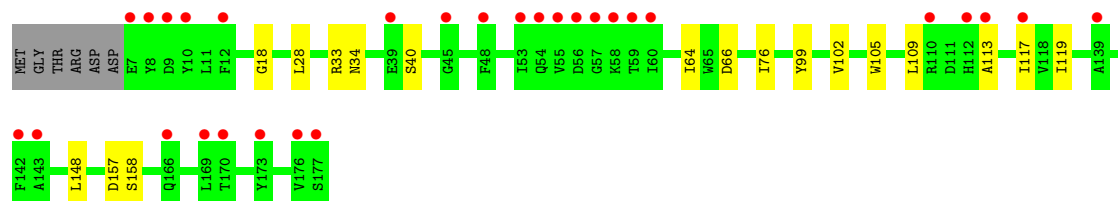
- Molecule 1: Ras-related protein Rab-11A

Chain A: 




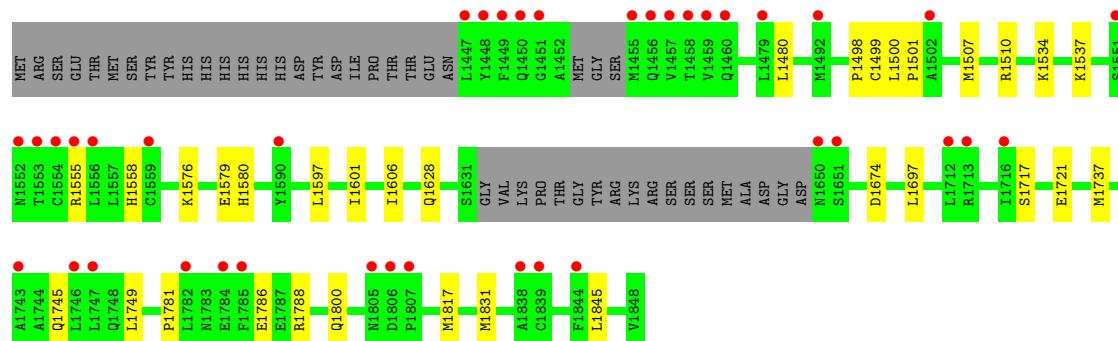
- Molecule 1: Ras-related protein Rab-11A

Chain C: 




- Molecule 2: Unconventional myosin-Vb

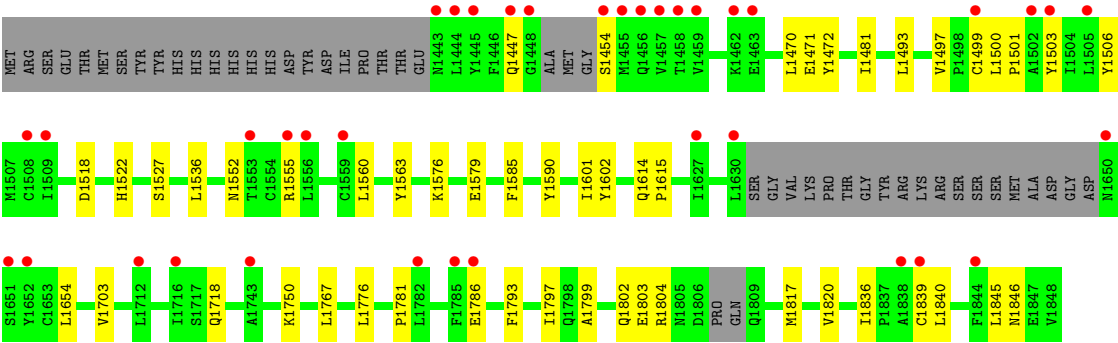
Chain B: 



- Molecule 2: Unconventional myosin-Vb

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.10Å 125.92Å 157.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 2.19 31.52 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.50-2.19) 100.0 (31.52-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.181 , 0.218 0.173 , 0.209	Depositor DCC
$R_{free}$ test set	4890 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, BEF

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	0.76	0/1374	0.75	0/1859
1	C	0.48	0/1338	0.62	0/1815
2	B	0.60	0/3032	0.62	0/4112
2	D	0.58	0/3026	0.63	0/4101
All	All	0.61	0/8770	0.65	0/11887

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1352	0	1333	8	0
1	C	1317	0	1268	13	0
2	B	2979	0	2928	21	0
2	D	2973	0	2913	41	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
5	A	28	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	28	0	12	0	0
6	A	6	0	8	0	0
7	A	187	0	0	3	0
7	B	225	0	0	2	0
7	C	51	0	0	1	0
7	D	188	0	0	1	0
All	All	9344	0	8474	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (82) 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:D:1767:LEU:O	2:D:1804:ARG:NH2	2.24	0.69
2:D:1776:LEU:CD1	2:D:1797:ILE:HD13	2.23	0.69
1:C:117:ILE:HD11	7:C:312:HOH:O	1.95	0.67
2:D:1839:CYS:SG	2:D:1840:LEU:HD12	2.35	0.67
2:D:1776:LEU:HD11	2:D:1797:ILE:HD13	1.76	0.66
2:B:1781:PRO:HB3	2:B:1786:GLU:HB2	1.78	0.65
1:C:113:ALA:HB1	1:C:117:ILE:HD12	1.79	0.64
1:C:28:LEU:HD13	1:C:64:ILE:HG21	1.79	0.64
2:B:1507:MET:HG3	2:B:1831:MET:HE2	1.81	0.61
2:D:1602:TYR:CD2	2:D:1820:VAL:HG21	2.36	0.60
2:D:1781:PRO:HB3	2:D:1786:GLU:HB2	1.82	0.60
2:B:1534:LYS:HA	2:B:1537:LYS:HE3	1.86	0.58
1:C:99:TYR:O	1:C:102:VAL:HG22	2.03	0.58
2:B:1576:LYS:O	2:B:1579:GLU:HG2	2.03	0.58
2:D:1602:TYR:CE2	2:D:1820:VAL:HG22	2.39	0.57
2:D:1471:GLU:HG2	2:D:1846:ASN:HB2	1.88	0.56
2:D:1614:GLN:HB3	2:D:1615:PRO:HD3	1.88	0.55
2:D:1839:CYS:SG	2:D:1840:LEU:CD1	2.94	0.55
2:D:1536:LEU:CD1	2:D:1601:ILE:HG12	2.37	0.54
2:B:1507:MET:HG3	2:B:1831:MET:CE	2.39	0.53
2:D:1472:TYR:HB3	2:D:1845:LEU:HD22	1.90	0.52
2:B:1597:LEU:O	2:B:1601:ILE:HG13	2.10	0.52
2:B:1788:ARG:HG3	7:B:1916:HOH:O	2.09	0.52
2:D:1500:LEU:N	2:D:1501:PRO:CD	2.73	0.51
2:D:1497:VAL:CG2	2:D:1500:LEU:HD13	2.41	0.51
2:D:1793:PHE:CE2	2:D:1797:ILE:HD11	2.46	0.51
2:D:1576:LYS:O	2:D:1579:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LEU:CD1	1:C:64:ILE:HG21	2.42	0.50
2:D:1803:GLU:HB2	7:D:2047:HOH:O	2.12	0.50
1:C:28:LEU:HD22	1:C:66:ASP:HB2	1.93	0.49
2:B:1534:LYS:HA	2:B:1537:LYS:CE	2.43	0.49
1:C:109:LEU:O	1:C:113:ALA:HB3	2.12	0.49
2:D:1614:GLN:HB3	2:D:1615:PRO:CD	2.42	0.48
2:D:1793:PHE:CE2	2:D:1797:ILE:CD1	2.96	0.48
2:D:1471:GLU:CG	2:D:1846:ASN:HB2	2.42	0.48
1:A:28:LEU:HD13	1:A:64:ILE:HG21	1.96	0.48
2:D:1493:LEU:HD21	2:D:1840:LEU:HD11	1.96	0.47
1:C:119:ILE:CG2	1:C:148:LEU:HD22	2.45	0.47
2:B:1606:ILE:HG21	2:B:1817:MET:SD	2.55	0.47
2:B:1480:LEU:HD13	2:B:1845:LEU:HD11	1.97	0.46
2:D:1781:PRO:HB3	2:D:1786:GLU:CB	2.44	0.46
2:D:1522:HIS:HD1	2:D:1590:TYR:HH	1.63	0.46
2:D:1602:TYR:CE2	2:D:1820:VAL:CG2	2.99	0.46
2:B:1697:LEU:C	2:B:1697:LEU:HD23	2.36	0.45
2:B:1580:HIS:HD2	7:B:1947:HOH:O	1.99	0.45
1:A:51:ARG:NH1	1:A:162:GLU:OE2	2.39	0.44
2:D:1470:LEU:HD13	2:D:1836:ILE:HD11	1.99	0.44
2:D:1614:GLN:N	2:D:1615:PRO:HD2	2.33	0.44
1:A:110:ARG:NH1	7:A:344:HOH:O	2.52	0.43
2:B:1507:MET:CG	2:B:1831:MET:CE	2.96	0.43
1:A:40:SER:HB3	5:A:203:GDP:O2A	2.18	0.43
1:A:157:ASP:C	1:A:157:ASP:OD1	2.57	0.43
2:B:1745:GLN:O	2:B:1749:LEU:HG	2.18	0.43
1:C:28:LEU:HD11	1:C:64:ILE:HB	2.01	0.43
1:A:20:SER:CB	1:A:70:GLN:HG3	2.50	0.42
2:D:1799:ALA:O	2:D:1802:GLN:HG2	2.19	0.42
2:B:1717:SER:O	2:B:1721:GLU:HG3	2.19	0.42
2:D:1472:TYR:HB3	2:D:1845:LEU:CD2	2.49	0.42
1:A:110:ARG:NH2	7:A:399:HOH:O	2.52	0.42
2:D:1497:VAL:HG22	2:D:1500:LEU:HD13	2.01	0.42
1:C:76:ILE:HG22	2:D:1750:LYS:HG2	2.00	0.42
2:D:1654:LEU:HD21	2:D:1718:GLN:HB2	2.02	0.42
2:B:1500:LEU:HB3	2:B:1501:PRO:HD3	2.01	0.41
2:D:1447:GLN:O	2:D:1454:SER:HA	2.20	0.41
2:D:1602:TYR:CD2	2:D:1820:VAL:CG2	3.02	0.41
2:B:1555:ARG:HD3	2:B:1555:ARG:O	2.21	0.41
1:A:20:SER:HB2	1:A:70:GLN:HG3	2.03	0.41
1:C:18:GLY:HA2	1:C:105:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1560:LEU:HD23	2:D:1560:LEU:HA	1.91	0.41
2:D:1506:TYR:OH	2:D:1563:TYR:HB3	2.21	0.41
7:A:398:HOH:O	2:B:1628:GLN:HG2	2.20	0.41
1:C:109:LEU:HD12	1:C:109:LEU:HA	1.91	0.41
1:C:157:ASP:O	1:C:158:SER:CB	2.68	0.41
2:D:1503:TYR:CZ	2:D:1555:ARG:HD2	2.55	0.41
2:D:1500:LEU:HA	2:D:1500:LEU:HD12	1.97	0.41
2:D:1499:CYS:HA	2:D:1552:ASN:OD1	2.21	0.41
2:D:1518:ASP:HB3	2:D:1585:PHE:CZ	2.55	0.41
2:D:1614:GLN:CB	2:D:1615:PRO:CD	3.00	0.41
2:B:1507:MET:CG	2:B:1831:MET:HE2	2.48	0.40
2:D:1481:ILE:HG13	2:D:1527:SER:HB3	2.03	0.40
2:B:1498:PRO:O	2:B:1499:CYS:HB2	2.20	0.40
2:B:1558:HIS:HE1	2:B:1674:ASP:OD2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/177 (96%)	164 (97%)	5 (3%)	0	100	100
1	C	169/177 (96%)	162 (96%)	6 (4%)	1 (1%)	27	28
2	B	377/427 (88%)	368 (98%)	9 (2%)	0	100	100
2	D	374/427 (88%)	367 (98%)	7 (2%)	0	100	100
All	All	1089/1208 (90%)	1061 (97%)	27 (2%)	1 (0%)	53	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	ASN

### 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	143/150 (95%)	140 (98%)	3 (2%)	56	70
1	C	134/150 (89%)	132 (98%)	2 (2%)	67	80
2	B	323/391 (83%)	320 (99%)	3 (1%)	81	90
2	D	324/391 (83%)	322 (99%)	2 (1%)	87	94
All	All	924/1082 (85%)	914 (99%)	10 (1%)	76	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	107	LYS
1	A	114	ASP
2	B	1510	ARG
2	B	1737	MET
2	B	1800	GLN
1	C	33	ARG
1	C	40	SER
2	D	1703	VAL
2	D	1817	MET

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

Mol	Chain	Res	Type
2	B	1511	HIS
2	B	1558	HIS
2	B	1800	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	BEF	A	202	5	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	A	203	3,4	25,30,30	1.19	3 (12%)	27,47,47	2.09	7 (25%)
6	GOL	A	204	-	5,5,5	0.33	0	5,5,5	0.41	0
4	BEF	C	202	5	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	C	203	3,4	25,30,30	1.18	3 (12%)	27,47,47	1.99	8 (29%)

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	BEF	A	202	5	-	0/0/0/0	0/0/0/0
5	GDP	A	203	3,4	-	0/12/32/32	0/3/3/3
6	GOL	A	204	-	-	0/4/4/4	0/0/0/0
4	BEF	C	202	5	-	0/0/0/0	0/0/0/0
5	GDP	C	203	3,4	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	203	GDP	O4'-C1'	2.11	1.44	1.41
5	C	203	GDP	C5-C4	2.25	1.45	1.40
5	A	203	GDP	PB-O3A	2.46	1.63	1.60
5	A	203	GDP	C5-C4	2.64	1.46	1.40
5	A	203	GDP	C6-C5	2.67	1.46	1.41
5	C	203	GDP	C6-C5	3.55	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	203	GDP	C6-C5-C4	-4.63	116.31	120.85
5	A	203	GDP	C5-C6-N1	-4.38	117.23	123.47
5	C	203	GDP	C5-C6-N1	-3.77	118.10	123.47
5	A	203	GDP	C1'-N9-C4	-3.43	120.71	126.64
5	C	203	GDP	C6-C5-C4	-3.21	117.69	120.85
5	C	203	GDP	N3-C2-N1	-3.03	122.97	127.41
5	C	203	GDP	O3'-C3'-C2'	-2.99	102.24	111.83
5	A	203	GDP	N3-C2-N1	-2.45	123.82	127.41
5	C	203	GDP	PA-O3A-PB	-2.42	124.51	132.63
5	C	203	GDP	C4'-O4'-C1'	-2.09	107.65	109.83
5	A	203	GDP	C2-N3-C4	2.88	118.52	115.16
5	A	203	GDP	O2'-C2'-C3'	3.40	122.71	111.83
5	C	203	GDP	C6-N1-C2	3.93	121.71	116.06
5	A	203	GDP	C6-N1-C2	4.58	122.65	116.06
5	C	203	GDP	C2-N3-C4	4.96	120.95	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	203	GDP	1	0

## 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	171/177 (96%)	0.01	5 (2%)	51	49	36, 49, 75, 113	0
1	C	171/177 (96%)	0.95	29 (16%)	1	1	47, 89, 143, 168	0
2	B	382/427 (89%)	0.34	39 (10%)	7	6	37, 67, 120, 173	0
2	D	380/427 (88%)	0.30	37 (9%)	8	6	40, 68, 120, 154	0
All	All	1104/1208 (91%)	0.37	110 (9%)	7	6	36, 67, 124, 173	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1457	VAL	8.6
1	C	173	TYR	7.6
1	C	55	VAL	7.3
2	D	1454	SER	6.9
1	C	176	VAL	6.6
2	D	1444	LEU	6.5
1	C	10	TYR	6.5
2	D	1456	GLN	6.0
1	C	59	THR	6.0
1	C	170	THR	6.0
2	D	1782	LEU	5.7
2	B	1448	TYR	5.3
2	D	1455	MET	5.3
1	C	8	TYR	5.3
2	D	1445	TYR	5.2
1	C	177	SER	5.1
2	D	1785	PHE	5.1
2	D	1556	LEU	4.9
2	B	1785	PHE	4.9
1	C	9	ASP	4.6
1	C	12	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	1458	THR	4.5
2	D	1447	GLN	4.4
2	B	1556	LEU	4.3
1	C	57	GLY	4.1
2	B	1455	MET	4.1
2	B	1447	LEU	4.1
2	B	1456	GLN	4.0
2	B	1559	CYS	4.0
2	D	1505	LEU	4.0
1	C	169	LEU	3.9
2	B	1650	ASN	3.9
2	B	1449	PHE	3.9
2	B	1459	VAL	3.8
2	B	1554	CYS	3.8
1	C	54	GLN	3.7
1	C	7	GLU	3.7
1	C	56	ASP	3.7
2	D	1502	ALA	3.7
1	C	143	ALA	3.6
2	D	1459	VAL	3.6
2	D	1463	GLU	3.6
2	B	1838	ALA	3.6
1	C	58	LYS	3.6
2	B	1844	PHE	3.2
2	B	1458	THR	3.2
1	C	48	PHE	3.2
1	C	113	ALA	3.2
2	D	1838	ALA	3.1
2	B	1805	ASN	3.1
2	D	1508	CYS	3.1
2	B	1651	SER	3.1
2	B	1553	THR	3.0
2	B	1457	VAL	3.0
2	B	1460	GLN	3.0
2	B	1712	LEU	2.9
2	B	1746	LEU	2.9
1	A	16	LEU	2.9
1	C	117	ILE	2.9
1	C	60	ILE	2.8
2	B	1747	LEU	2.8
2	D	1651	SER	2.8
2	B	1716	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	1451	GLY	2.7
2	D	1712	LEU	2.7
1	C	53	ILE	2.6
2	D	1652	TYR	2.6
2	D	1448	GLY	2.5
1	A	17	ILE	2.5
1	C	142	PHE	2.5
2	D	1844	PHE	2.5
2	B	1502	ALA	2.5
2	B	1782	LEU	2.5
2	B	1839	CYS	2.5
2	D	1509	ILE	2.5
2	B	1450	GLN	2.4
1	C	39	GLU	2.4
2	D	1499	CYS	2.4
2	D	1627	ILE	2.4
2	B	1743	ALA	2.4
2	B	1806	ASP	2.4
2	B	1492	MET	2.3
2	D	1555	ARG	2.3
2	D	1839	CYS	2.3
1	C	139	ALA	2.2
2	B	1479	LEU	2.2
2	B	1555	ARG	2.2
2	D	1559	CYS	2.2
2	D	1743	ALA	2.2
2	B	1807	PRO	2.2
1	C	112	HIS	2.2
2	B	1552	ASN	2.2
2	D	1443	ASN	2.2
1	A	67	THR	2.2
2	B	1784	GLU	2.2
2	D	1650	ASN	2.1
2	D	1716	ILE	2.1
2	D	1462	LYS	2.1
1	C	45	GLY	2.1
2	B	1590	TYR	2.1
2	D	1553	THR	2.1
1	A	131	LEU	2.1
2	B	1551	SER	2.1
1	C	166	GLN	2.1
2	D	1630	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1713	ARG	2.1
2	D	1786	GLU	2.1
2	D	1503	TYR	2.1
1	A	44	ILE	2.0
1	C	110	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BEF	C	202	4/4	0.93	0.07	49,50,52,54	0
6	GOL	A	204	6/6	0.94	0.09	57,67,71,80	0
4	BEF	A	202	4/4	0.96	0.09	42,43,44,45	0
3	MG	C	201	1/1	0.98	0.12	58,58,58,58	0
3	MG	A	201	1/1	0.99	0.18	42,42,42,42	0
5	GDP	C	203	28/28	0.99	0.09	43,50,62,65	0
5	GDP	A	203	28/28	0.99	0.09	37,43,52,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.