



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2022 – 12:05 PM EDT

PDB ID : 6NM1  
Title : The crystal structure of the Staphylococcus aureus Fatty acid Kinase (Fak) B1 protein A158L mutant to 2.33 Angstrom resolution exhibits a conformation change compared to the wild type form  
Authors : Cuypers, M.G.; Gullett, J.M.; Subramanian, C.; Ericson, M.; White, S.W.; Rock, C.O.  
Deposited on : 2019-01-10  
Resolution : 2.33 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

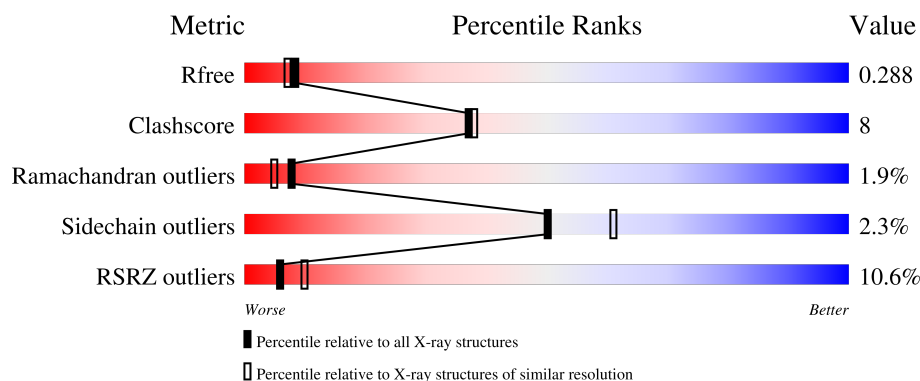
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div>9%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	B	288	<div> <div>12%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4649 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.

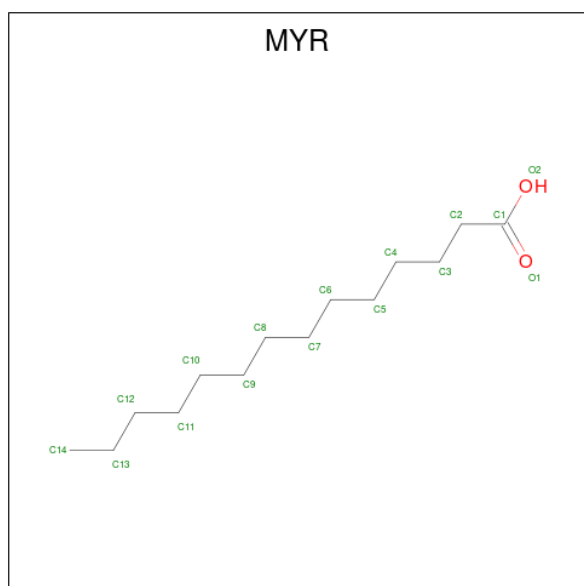
- Molecule 1 is a protein called Fatty acid Kinase (Fak) B1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	3	0
			2278	1447	371	448	12			
1	B	285	Total	C	N	O	S	0	0	0
			2205	1400	356	437	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	LEU	ALA	engineered mutation	UNP X5EH37
B	158	LEU	ALA	engineered mutation	UNP X5EH37

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			16	14	2		

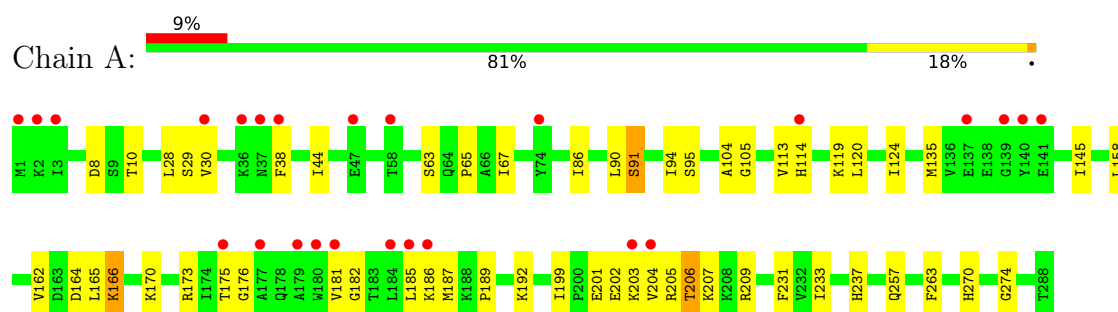
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	64	Total	O	0	0
			64	64		

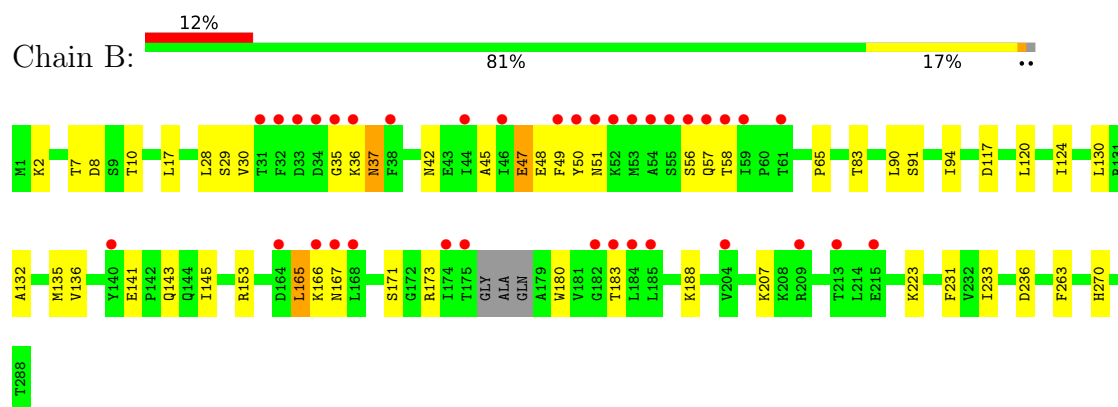
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Fatty acid Kinase (Fak) B1 protein



- Molecule 1: Fatty acid Kinase (Fak) B1 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	33.35Å 53.52Å 86.15Å 76.88° 89.36° 72.27°	Depositor
Resolution (Å)	31.71 – 2.33 31.71 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.1 (31.71-2.33) 98.2 (31.71-2.33)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.34Å)	Xtriage
Refinement program	PHENIX (dev_3354: ???)	Depositor
R, $R_{free}$	0.237 , 0.288 0.236 , 0.288	Depositor DCC
$R_{free}$ test set	1118 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 70.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for h,h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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: MYR

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	0.26	0/2316	0.43	0/3125
1	B	0.24	0/2240	0.42	0/3025
All	All	0.25	0/4556	0.42	0/6150

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	2278	0	2274	37	0
1	B	2205	0	2178	32	0
2	A	16	0	27	4	0
2	B	16	0	27	5	0
3	A	70	0	0	0	0
3	B	64	0	0	0	0
All	All	4649	0	4506	70	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 8.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HD12	1:A:44:ILE:O	1.87	0.74
1:A:201:GLU:HG3	1:A:202:GLU:HG3	1.75	0.69
1:A:94:ILE:HD12	2:A:301:MYR:H51	1.74	0.68
1:B:173:ARG:HD2	2:B:301:MYR:H51	1.75	0.68
1:A:44:ILE:HD12	1:A:44:ILE:C	2.18	0.64
1:A:192:LYS:HE3	1:A:199:ILE:HD11	1.83	0.61
1:A:166:LYS:HG2	1:A:170:LYS:HE3	1.81	0.61
1:A:120:LEU:HD13	1:A:124:ILE:HG21	1.85	0.58
1:A:207:LYS:NZ	1:A:274:GLY:O	2.37	0.58
1:B:120:LEU:HD13	1:B:124:ILE:HG21	1.84	0.58
1:B:2:LYS:H	1:B:83:THR:HG22	1.68	0.57
1:A:28:LEU:HG	1:A:65:PRO:HD3	1.87	0.56
1:A:162:VAL:HB	1:A:189:PRO:HG2	1.87	0.56
1:A:206:THR:HG23	1:A:209:ARG:H	1.70	0.56
1:B:29:SER:OG	1:B:37:ASN:OD1	2.24	0.55
1:A:10:THR:HG21	1:A:90:LEU:HD22	1.89	0.55
1:A:182:GLY:O	1:A:186:LYS:N	2.41	0.54
1:A:270:HIS:CG	2:A:301:MYR:H61	2.43	0.54
1:A:91:SER:OG	1:A:94:ILE:HG12	2.07	0.53
1:A:10:THR:HG23	1:A:28:LEU:HD13	1.91	0.53
1:B:47:GLU:O	1:B:50:TYR:N	2.29	0.53
1:B:10:THR:HG23	1:B:28:LEU:HD13	1.90	0.53
1:B:165:LEU:O	1:B:167:ASN:N	2.42	0.52
1:A:120:LEU:HD21	1:A:158:LEU:HB3	1.91	0.52
1:A:44:ILE:C	1:A:44:ILE:CD1	2.79	0.51
1:B:135:MET:HE2	1:B:145:ILE:HD13	1.94	0.50
1:B:28:LEU:HG	1:B:65:PRO:HD3	1.94	0.50
1:B:270:HIS:CD2	2:B:301:MYR:H52	2.47	0.50
1:A:91:SER:HB2	1:A:119:LYS:HA	1.93	0.50
1:A:204:VAL:HG12	1:A:205:ARG:O	2.12	0.49
1:B:48:GLU:HA	1:B:51:ASN:HB2	1.94	0.49
1:B:10:THR:HG21	1:B:90:LEU:HD22	1.93	0.49
1:B:143:GLN:H	1:B:143:GLN:CD	2.15	0.49
1:A:181:VAL:O	1:A:185:LEU:HD22	2.12	0.49
1:B:91:SER:HB3	1:B:94:ILE:HG12	1.95	0.49
1:A:205:ARG:O	1:A:206:THR:HG22	2.12	0.48
1:A:67:ILE:HG23	1:A:104:ALA:HB2	1.95	0.48
1:A:105:GLY:HA3	1:A:113:VAL:HG11	1.95	0.48
1:A:90:LEU:HD11	1:A:94:ILE:HD11	1.94	0.48
1:B:233:ILE:HG22	1:B:263:PHE:HD2	1.77	0.48
1:A:29:SER:OG	1:A:63:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG22	1:A:263:PHE:HD2	1.79	0.47
1:B:56:SER:C	1:B:58:THR:H	2.18	0.46
1:B:17:LEU:HD13	1:B:130:LEU:HD11	1.98	0.46
1:B:188:LYS:HD3	1:B:207:LYS:HA	1.98	0.45
1:A:29:SER:HG	1:A:63:SER:HG	1.62	0.45
2:B:301:MYR:H61	2:B:301:MYR:H92	1.83	0.45
1:A:8:ASP:OD1	1:A:10:THR:OG1	2.35	0.45
1:A:158:LEU:HD21	2:A:301:MYR:H131	1.98	0.45
1:A:165:LEU:H	1:A:165:LEU:HG	1.61	0.44
1:B:167:ASN:O	1:B:171:SER:OG	2.21	0.44
1:A:30:VAL:HG13	1:A:38:PHE:HB2	2.00	0.43
1:B:30:VAL:HG11	1:B:49:PHE:HE2	1.82	0.43
1:B:141:GLU:O	1:B:145:ILE:HG12	2.19	0.43
1:B:47:GLU:O	1:B:49:PHE:N	2.52	0.43
1:B:56:SER:O	1:B:57:GLN:HB2	2.19	0.43
1:A:86:ILE:HD13	1:A:114:HIS:HB2	2.01	0.42
1:A:175:THR:OG1	1:A:176:GLY:N	2.52	0.42
1:A:166:LYS:HB3	1:A:166:LYS:HE2	1.90	0.42
1:A:135:MET:HE1	1:A:145:ILE:HG23	2.01	0.42
1:B:117:ASP:O	1:B:153:ARG:NH1	2.49	0.42
1:B:48:GLU:H	1:B:48:GLU:CD	2.23	0.41
1:B:270:HIS:HB2	2:B:301:MYR:H72	2.01	0.41
1:B:30:VAL:O	1:B:37:ASN:HA	2.20	0.41
1:A:95:SER:HB2	2:A:301:MYR:H31	2.02	0.41
1:B:7:THR:OG1	1:B:8:ASP:N	2.54	0.41
1:B:35:GLY:O	1:B:37:ASN:N	2.54	0.41
1:B:56:SER:HB3	1:B:57:GLN:H	1.75	0.41
1:B:132:ALA:O	1:B:136:VAL:HG13	2.21	0.41
1:B:94:ILE:HD12	2:B:301:MYR:H62	2.02	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/288 (100%)	276 (96%)	10 (4%)	3 (1%)	15	14
1	B	281/288 (98%)	249 (89%)	24 (8%)	8 (3%)	5	2
All	All	570/576 (99%)	525 (92%)	34 (6%)	11 (2%)	8	5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	THR
1	B	166	LYS
1	B	36	LYS
1	B	47	GLU
1	B	165	LEU
1	B	180	TRP
1	A	166	LYS
1	B	45	ALA
1	B	183	THR
1	B	37	ASN
1	A	164	ASP

### 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	249/247 (101%)	241 (97%)	8 (3%)	39	47
1	B	239/247 (97%)	235 (98%)	4 (2%)	60	72
All	All	488/494 (99%)	476 (98%)	12 (2%)	50	58

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	173	ARG
1	A	187	MET
1	A	203[A]	LYS
1	A	203[B]	LYS

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Mol	Chain	Res	Type
1	A	231	PHE
1	A	237	HIS
1	A	257	GLN
1	B	42	ASN
1	B	223	LYS
1	B	231	PHE
1	B	236	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MYR	B	301	-	12,15,15	0.27	0	11,15,15	0.94	0
2	MYR	A	301	-	12,15,15	0.27	0	11,15,15	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	B	301	-	-	6/11/13/13	-
2	MYR	A	301	-	-	4/11/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MYR	C6-C7-C8-C9
2	B	301	MYR	C10-C11-C12-C13
2	A	301	MYR	C5-C6-C7-C8
2	B	301	MYR	C9-C10-C11-C12
2	B	301	MYR	C11-C10-C9-C8
2	A	301	MYR	C11-C12-C13-C14
2	B	301	MYR	C11-C12-C13-C14
2	B	301	MYR	C7-C8-C9-C10
2	B	301	MYR	C6-C7-C8-C9
2	A	301	MYR	C4-C5-C6-C7

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	MYR	5	0
2	A	301	MYR	4	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, 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	288/288 (100%)	0.67	25 (8%)	10 15	26, 47, 74, 96	0
1	B	285/288 (98%)	0.90	36 (12%)	3 6	34, 52, 96, 112	0
All	All	573/576 (99%)	0.79	61 (10%)	6 10	26, 50, 86, 112	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	TRP	7.7
1	B	183	THR	6.9
1	B	38	PHE	6.8
1	B	32	PHE	6.8
1	A	184	LEU	6.5
1	B	49	PHE	6.3
1	B	167	ASN	6.0
1	A	179	ALA	5.0
1	A	181	VAL	5.0
1	B	58	THR	4.6
1	A	175	THR	4.5
1	B	55	SER	4.3
1	B	51	ASN	4.2
1	A	38	PHE	4.1
1	B	57	GLN	4.1
1	B	50	TYR	4.1
1	B	168	LEU	4.0
1	B	52	LYS	3.8
1	A	37	ASN	3.8
1	B	56	SER	3.8
1	B	44	ILE	3.7
1	A	177	ALA	3.7
1	B	184	LEU	3.6
1	A	186	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	204	VAL	3.2
1	B	36	LYS	3.1
1	B	46	ILE	3.1
1	B	34	ASP	3.1
1	B	31	THR	3.0
1	B	53	MET	3.0
1	A	58	THR	3.0
1	B	215	GLU	3.0
1	B	174	ILE	2.8
1	B	175	THR	2.7
1	B	61	THR	2.7
1	A	204	VAL	2.6
1	A	141	GLU	2.6
1	B	33	ASP	2.6
1	A	185	LEU	2.5
1	A	47	GLU	2.4
1	B	182	GLY	2.4
1	A	1	MET	2.4
1	B	209	ARG	2.3
1	A	74	TYR	2.3
1	A	2	LYS	2.2
1	A	36	LYS	2.2
1	B	35	GLY	2.2
1	B	54	ALA	2.2
1	A	139	GLY	2.2
1	B	164	ASP	2.2
1	B	213	THR	2.2
1	B	140	TYR	2.1
1	A	140	TYR	2.1
1	A	3	ILE	2.1
1	A	203[A]	LYS	2.1
1	B	166	LYS	2.1
1	B	185	LEU	2.1
1	A	30	VAL	2.1
1	A	137	GLU	2.0
1	A	114	HIS	2.0
1	B	59	ILE	2.0

## 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 [i](#)

There are no monosaccharides 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
2	MYR	A	301	16/16	0.88	0.19	38,47,51,51	0
2	MYR	B	301	16/16	0.89	0.19	40,46,62,64	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.