



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2016 – 05:07 PM EDT

PDB ID : 4PI0  
Title : Crystal structure of particulate methane monooxygenase from *Methylocystis* sp. ATCC 49242 (Rockwell) soaked in copper  
Authors : Sirajuddin, S.; Rosenzweig, A.C.  
Deposited on : 2014-05-07  
Resolution : 3.15 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](mailto: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.

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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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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) : rb-20027107

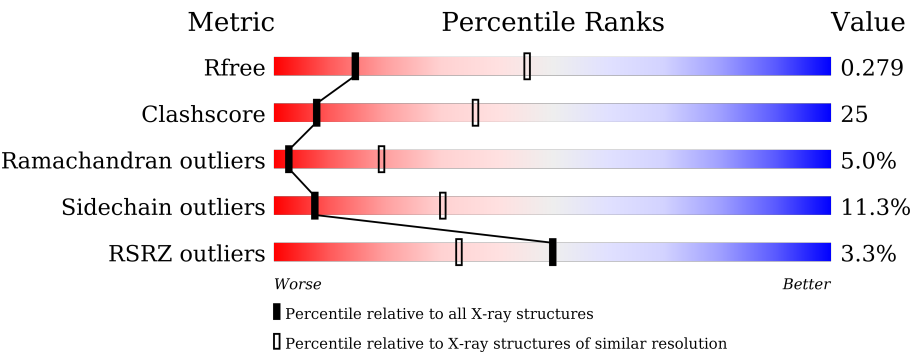
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	D	25	<div><div></div><div>60%16%24%</div></div>
1	H	25	<div><div></div><div>64%16%20%</div></div>
1	N	25	<div><div></div><div>60%40%</div></div>
2	B	252	<div><div>%</div><div>56%36%. . .</div></div>
2	F	252	<div><div>%</div><div>57%34%5%. . .</div></div>
2	J	252	<div><div></div><div>55%37%. . .</div></div>

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Mol	Chain	Length	Quality of chain
3	C	256	<div><div></div><div>3%</div><div>46%</div><div>29%</div><div>10%</div><div>15%</div></div>
3	G	256	<div><div></div><div>4%</div><div>43%</div><div>32%</div><div>8%</div><div>17%</div></div>
3	K	256	<div><div></div><div>5%</div><div>43%</div><div>32%</div><div>11%</div><div>15%</div></div>
4	A	420	<div><div></div><div>7%</div><div>51%</div><div>33%</div><div>7%</div><div>7%</div></div>
4	E	420	<div><div></div><div></div><div>51%</div><div>33%</div><div>8%</div><div>7%</div></div>
4	I	420	<div><div></div><div>4%</div><div>52%</div><div>34%</div><div>6%</div><div>7%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20630 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 unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	D	19	Total	C	N	O	0	0	0
			95	57	19	19			
1	H	20	Total	C	N	O	0	0	0
			100	60	20	20			
1	N	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 2 is a protein called Particulate methane monooxygenase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			
2	J	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			
2	B	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			

- Molecule 3 is a protein called Particulate methane monooxygenase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	217	Total	C	N	O	S	0	0	0
			1765	1185	279	293	8			
3	C	217	Total	C	N	O	S	0	0	0
			1765	1185	279	293	8			
3	G	213	Total	C	N	O	S	0	0	0
			1738	1168	274	288	8			

- Molecule 4 is a protein called Particulate methane monooxygenase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	390	Total	C	N	O	S	0	0	0
			3038	1952	523	559	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	390	Total	C	N	O	S	0	0	0
			3038	1952	523	559	4			
4	I	390	Total	C	N	O	S	0	0	0
			3038	1952	523	559	4			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

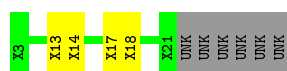
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cu	0	0
			1	1		
5	K	1	Total	Cu	0	0
			1	1		
5	E	1	Total	Cu	0	0
			1	1		
5	I	1	Total	Cu	0	0
			1	1		
5	C	1	Total	Cu	0	0
			1	1		
5	A	1	Total	Cu	0	0
			1	1		

### 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 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: unknown peptide

Chain D: 



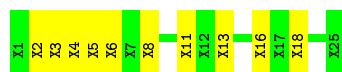
- Molecule 1: unknown peptide

Chain H: 



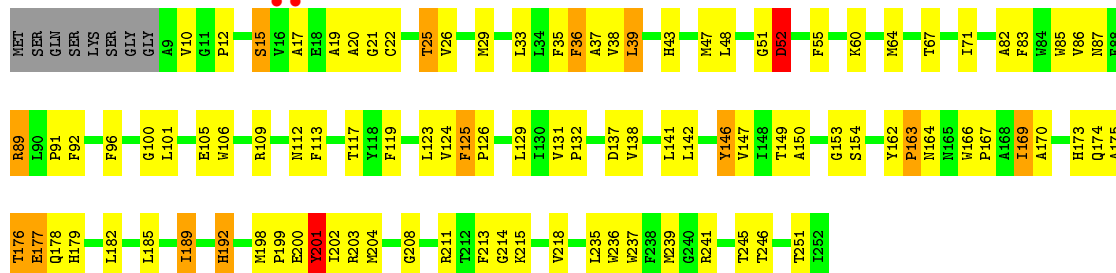
- Molecule 1: unknown peptide

Chain N: 



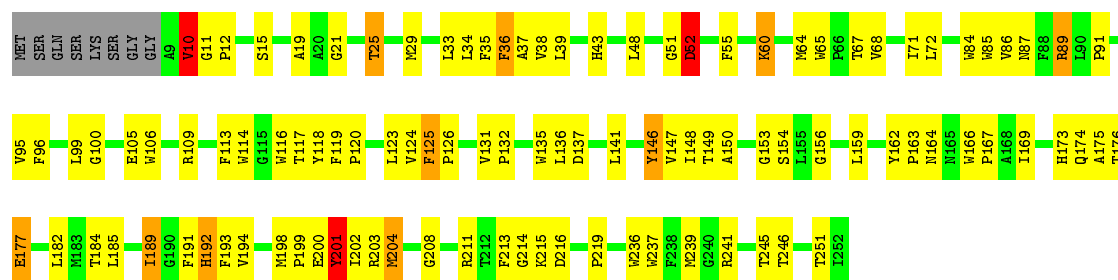
- Molecule 2: Particulate methane monooxygenase subunit A

Chain F: 

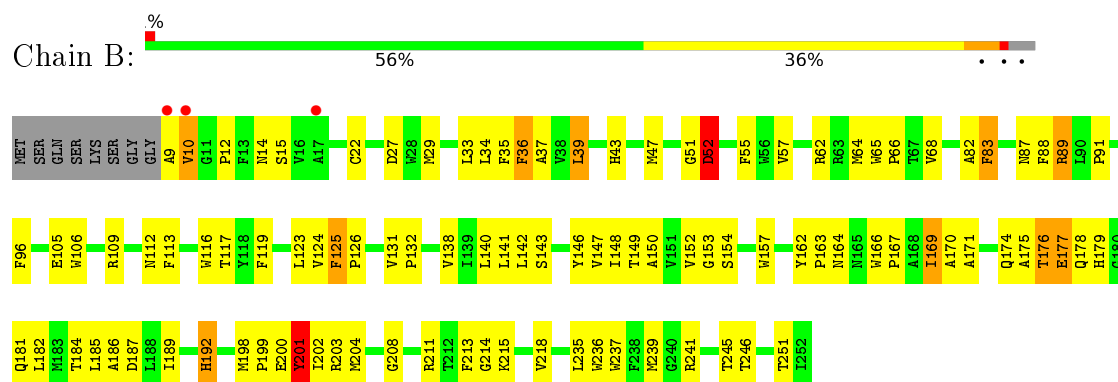


- Molecule 2: Particulate methane monooxygenase subunit A

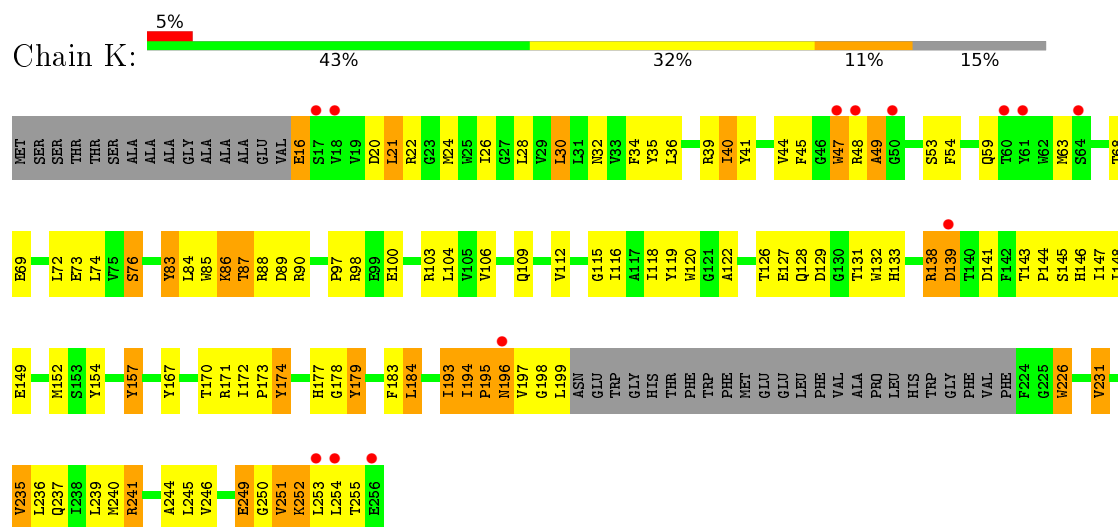
Chain J: 



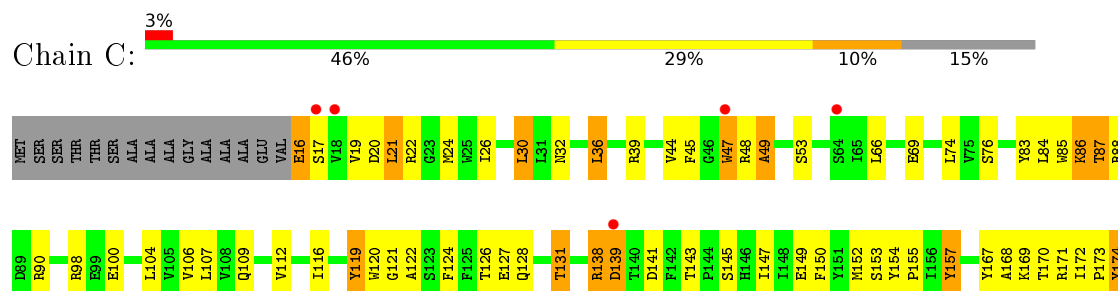
• Molecule 2: Particulate methane monooxygenase subunit A

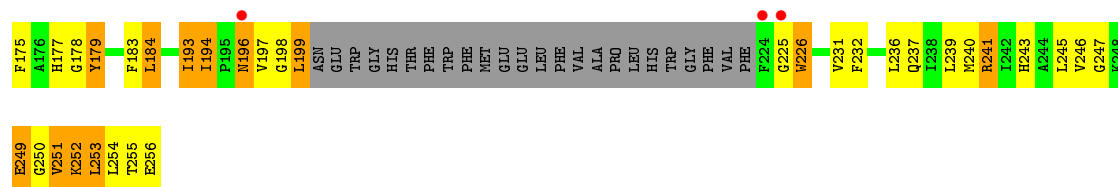


• Molecule 3: Particulate methane monooxygenase subunit C

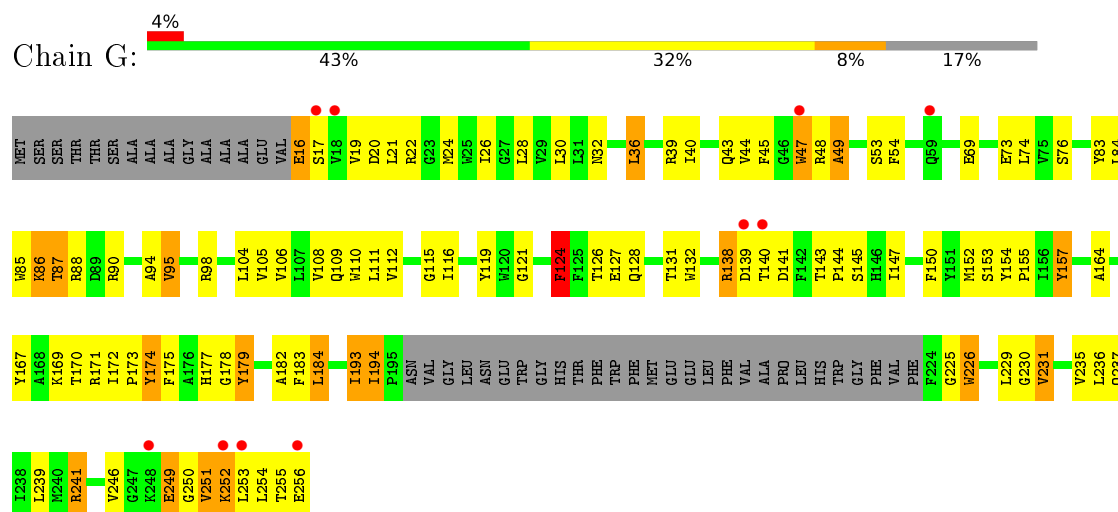


• Molecule 3: Particulate methane monooxygenase subunit C

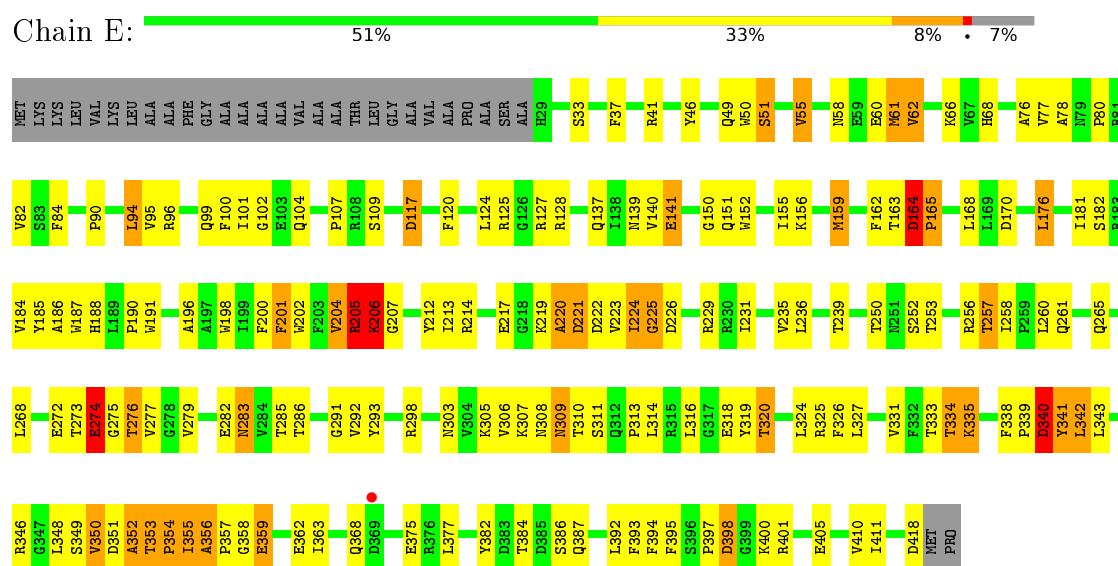




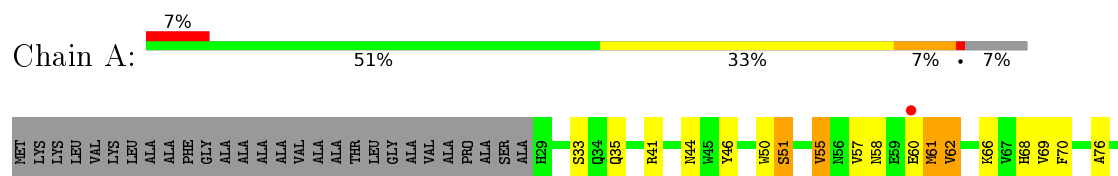
• Molecule 3: Particulate methane monooxygenase subunit C



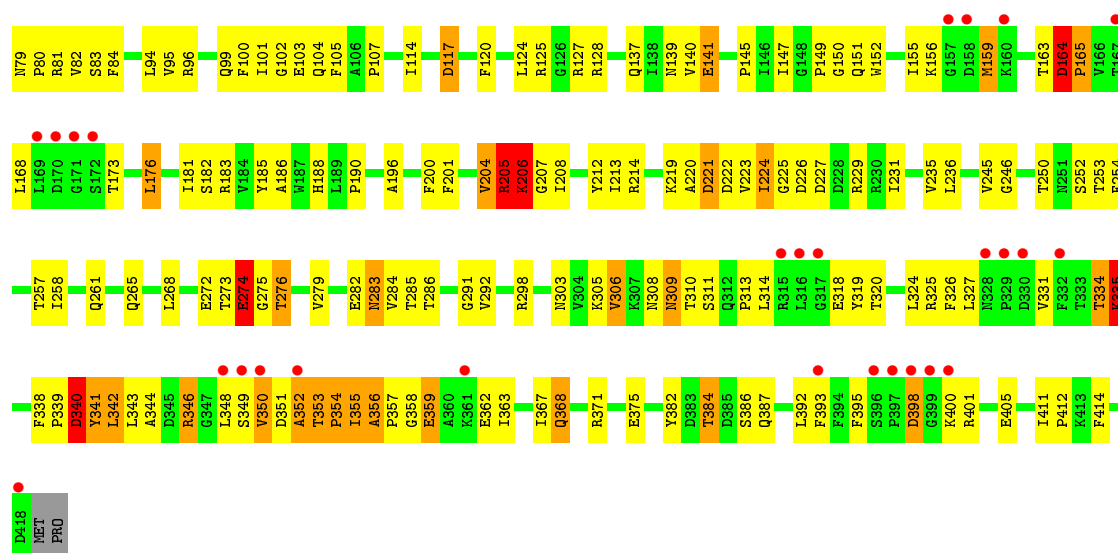
• Molecule 4: Particulate methane monooxygenase subunit B



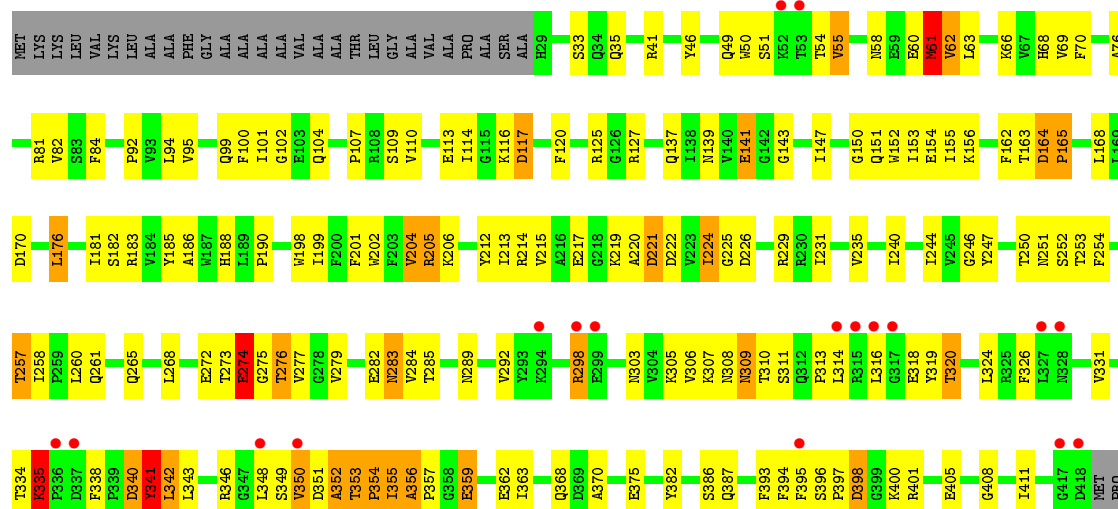
• Molecule 4: Particulate methane monooxygenase subunit B







• Molecule 4: Particulate methane monooxygenase subunit B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.36Å 184.74Å 188.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.15 49.52 – 3.15	Depositor EDS
% Data completeness (in resolution range)	78.2 (50.00-3.15) 78.5 (49.52-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.221 , 0.280 0.221 , 0.279	Depositor DCC
$R_{free}$ test set	2796 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 42.2	EDS
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 55807 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	20630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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, 0.375 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: CU

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
2	B	0.64	0/2052	0.79	0/2814
2	F	0.75	1/2052 (0.0%)	0.84	0/2814
2	J	0.74	0/2052	0.86	0/2814
3	C	0.61	2/1820 (0.1%)	0.75	1/2481 (0.0%)
3	G	0.65	2/1793 (0.1%)	0.78	1/2444 (0.0%)
3	K	0.67	0/1820	0.82	1/2481 (0.0%)
4	A	0.60	0/3115	0.80	0/4243
4	E	0.67	0/3115	0.83	0/4243
4	I	0.60	0/3115	0.81	0/4243
All	All	0.66	5/20934 (0.0%)	0.81	3/28577 (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
4	A	0	2
4	E	0	3
4	I	0	2
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	119	TYR	CE1-CZ	-6.83	1.29	1.38
3	C	119	TYR	CG-CD2	-6.31	1.30	1.39
3	G	119	TYR	CG-CD1	-5.63	1.31	1.39
3	C	119	TYR	CE1-CZ	-5.62	1.31	1.38
2	F	83	PHE	CG-CD1	-5.54	1.30	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	229	LEU	CA-CB-CG	5.37	127.65	115.30
3	K	199	LEU	CA-CB-CG	5.14	127.13	115.30
3	C	199	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	340	ASP	Peptide
4	A	341	TYR	Peptide
4	E	333	THR	Peptide
4	E	340	ASP	Peptide
4	E	341	TYR	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	D	95	0	22	4	0
1	H	100	0	23	3	0
1	N	125	0	27	7	0
2	B	1974	0	1932	116	0
2	F	1974	0	1932	110	0
2	J	1974	0	1932	115	0
3	C	1765	0	1772	94	0
3	G	1738	0	1743	91	0
3	K	1765	0	1772	103	0
4	A	3038	0	3022	182	0
4	E	3038	0	3022	178	0
4	I	3038	0	3022	160	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20630	0	20221	1032	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 25.

The worst 5 of 1032 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:F:51:GLY:CA	2:F:52:ASP:HB2	1.63	1.26
2:J:51:GLY:CA	2:J:52:ASP:HB2	1.72	1.16
2:B:51:GLY:CA	2:B:52:ASP:HB2	1.76	1.15
2:J:146:TYR:HD2	2:J:237:TRP:CE2	1.63	1.15
4:E:352:ALA:O	4:E:354:PRO:HD3	1.46	1.13

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	
2	B	242/252 (96%)	197 (81%)	40 (16%)	5 (2%)	9	44
2	F	242/252 (96%)	204 (84%)	32 (13%)	6 (2%)	7	39
2	J	242/252 (96%)	200 (83%)	35 (14%)	7 (3%)	6	35
3	C	213/256 (83%)	171 (80%)	31 (15%)	11 (5%)	2	18
3	G	209/256 (82%)	172 (82%)	28 (13%)	9 (4%)	3	23
3	K	213/256 (83%)	167 (78%)	36 (17%)	10 (5%)	3	21
4	A	388/420 (92%)	310 (80%)	53 (14%)	25 (6%)	2	12
4	E	388/420 (92%)	315 (81%)	43 (11%)	30 (8%)	1	7
4	I	388/420 (92%)	315 (81%)	50 (13%)	23 (6%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2525/2784 (91%)	2051 (81%)	348 (14%)	126 (5%)	3	19

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	52	ASP
3	K	174	TYR
3	K	179	TYR
3	K	251	VAL
4	E	141	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	
2	B	202/208 (97%)	184 (91%)	18 (9%)	12	42
2	F	202/208 (97%)	179 (89%)	23 (11%)	7	30
2	J	202/208 (97%)	181 (90%)	21 (10%)	9	33
3	C	184/213 (86%)	155 (84%)	29 (16%)	3	14
3	G	181/213 (85%)	156 (86%)	25 (14%)	4	20
3	K	184/213 (86%)	156 (85%)	28 (15%)	3	16
4	A	320/336 (95%)	289 (90%)	31 (10%)	10	37
4	E	320/336 (95%)	289 (90%)	31 (10%)	10	37
4	I	320/336 (95%)	288 (90%)	32 (10%)	9	36
All	All	2115/2271 (93%)	1877 (89%)	238 (11%)	7	30

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	335	LYS
4	I	277	VAL
2	J	251	THR
4	A	368	GLN

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Mol	Chain	Res	Type
4	I	117	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	151	GLN
4	I	44	ASN
2	J	174	GLN
4	A	261	GLN
4	I	58	ASN

### 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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	D	0/25	-	-	-	-
1	H	0/25	-	-	-	-
1	N	0/25	-	-	-	-
2	B	244/252 (96%)	-0.40	3 (1%) 81 69	29, 55, 88, 135	0
2	F	244/252 (96%)	-0.53	2 (0%) 87 79	19, 37, 78, 118	0
2	J	244/252 (96%)	-0.55	0 100 100	21, 38, 69, 115	0
3	C	217/256 (84%)	-0.18	8 (3%) 45 28	35, 67, 127, 170	0
3	G	213/256 (83%)	-0.19	10 (4%) 35 20	26, 56, 108, 176	0
3	K	217/256 (84%)	-0.26	13 (5%) 25 13	23, 50, 123, 166	0
4	A	390/420 (92%)	0.03	28 (7%) 18 9	30, 66, 102, 159	0
4	E	390/420 (92%)	-0.43	1 (0%) 94 92	22, 41, 71, 120	0
4	I	390/420 (92%)	-0.12	18 (4%) 36 21	27, 60, 106, 160	0
All	All	2549/2859 (89%)	-0.28	83 (3%) 50 33	19, 52, 102, 176	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	418	ASP	5.7
3	G	253	LEU	5.3
3	C	18	VAL	5.3
3	G	252	LYS	5.2
4	A	328	ASN	5.1

### 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CU	C	301	1/1	0.99	0.06	-	71,71,71,71	0
5	CU	E	501	1/1	0.99	0.07	-	53,53,53,53	0
5	CU	A	501	1/1	0.95	0.06	-	108,108,108,108	0
5	CU	K	301	1/1	0.98	0.11	-	85,85,85,85	0
5	CU	I	501	1/1	0.97	0.06	-	85,85,85,85	0
5	CU	G	301	1/1	0.97	0.08	-	69,69,69,69	0

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

There are no such residues in this entry.