



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2017 – 08:54 PM EDT

PDB ID : 4PI2  
Title : Crystal structure of particulate methane monooxygenase from *Methylocystis* sp. ATCC 49242 (Rockwell) soaked in zinc  
Authors : Sirajuddin, S.; Rosenzweig, A.C.  
Deposited on : unknown  
Resolution : 3.33 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

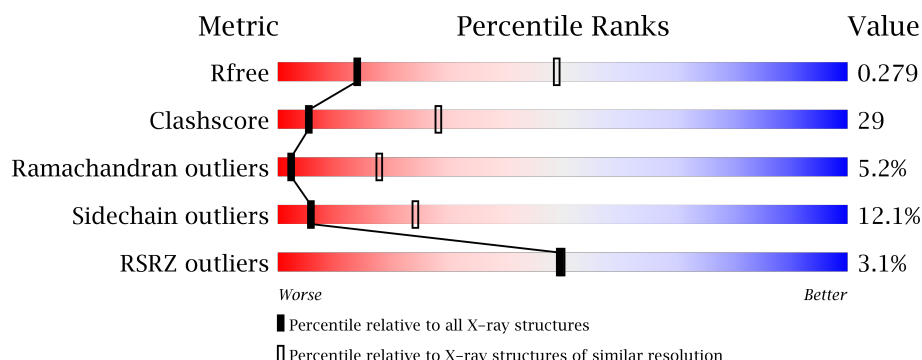
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.33 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))
$R_{free}$	100719	1167 (3.40-3.28)
Clashscore	112137	1239 (3.40-3.28)
Ramachandran outliers	110173	1219 (3.40-3.28)
Sidechain outliers	110143	1218 (3.40-3.28)
RSRZ outliers	101464	1176 (3.40-3.28)

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	
1	H	25	
1	N	25	
2	B	252	
2	F	252	

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Mol	Chain	Length	Quality of chain
2	J	252	<div><div></div><div>2%</div><div>46%</div><div>42%</div><div>8%</div><div></div></div>
3	A	420	<div><div></div><div>7%</div><div>46%</div><div>38%</div><div>9%</div><div>7%</div></div>
3	E	420	<div><div></div><div>%</div><div>47%</div><div>35%</div><div>9%</div><div>7%</div></div>
3	I	420	<div><div></div><div>4%</div><div>46%</div><div>37%</div><div>9%</div><div>7%</div></div>
4	C	256	<div><div></div><div>5%</div><div>39%</div><div>37%</div><div>12%</div><div>11%</div></div>
4	G	256	<div><div></div><div>2%</div><div>38%</div><div>39%</div><div>11%</div><div>11%</div></div>
4	K	256	<div><div></div><div>4%</div><div>34%</div><div>44%</div><div>11%</div><div>11%</div></div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 20979 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 B.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	228	Total	C	N	O	S	0	0	0
			1870	1256	295	310	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	228	Total	C	N	O	S	0	0	0
			1870	1256	295	310	9			
4	C	228	Total	C	N	O	S	0	0	0
			1870	1256	295	310	9			

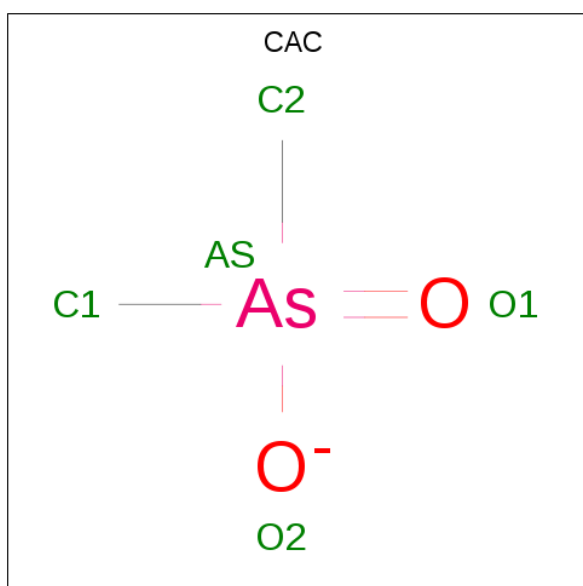
- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total	Zn	0	0
			2	2		
6	K	1	Total	Zn	0	0
			1	1		
6	C	2	Total	Zn	0	0
			2	2		

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



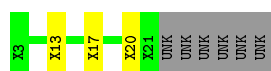
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	As	C	O	0	0
			5	1	2	2		

### 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.

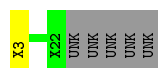
- Molecule 1: unknown peptide

Chain D: 



- Molecule 1: unknown peptide

Chain H: 



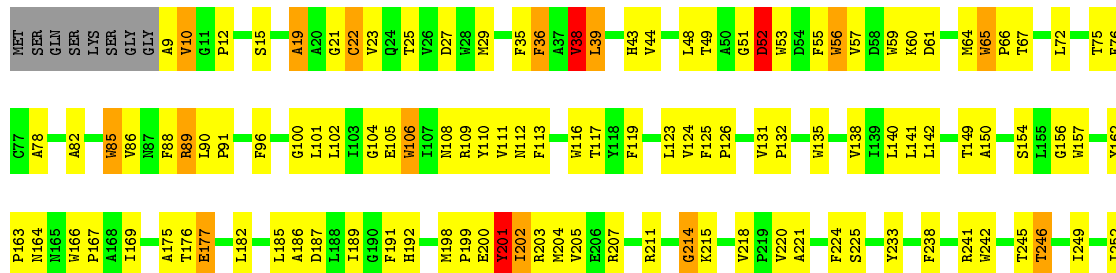
- Molecule 1: unknown peptide

Chain N: 



- Molecule 2: Particulate methane monooxygenase subunit A

Chain F: 

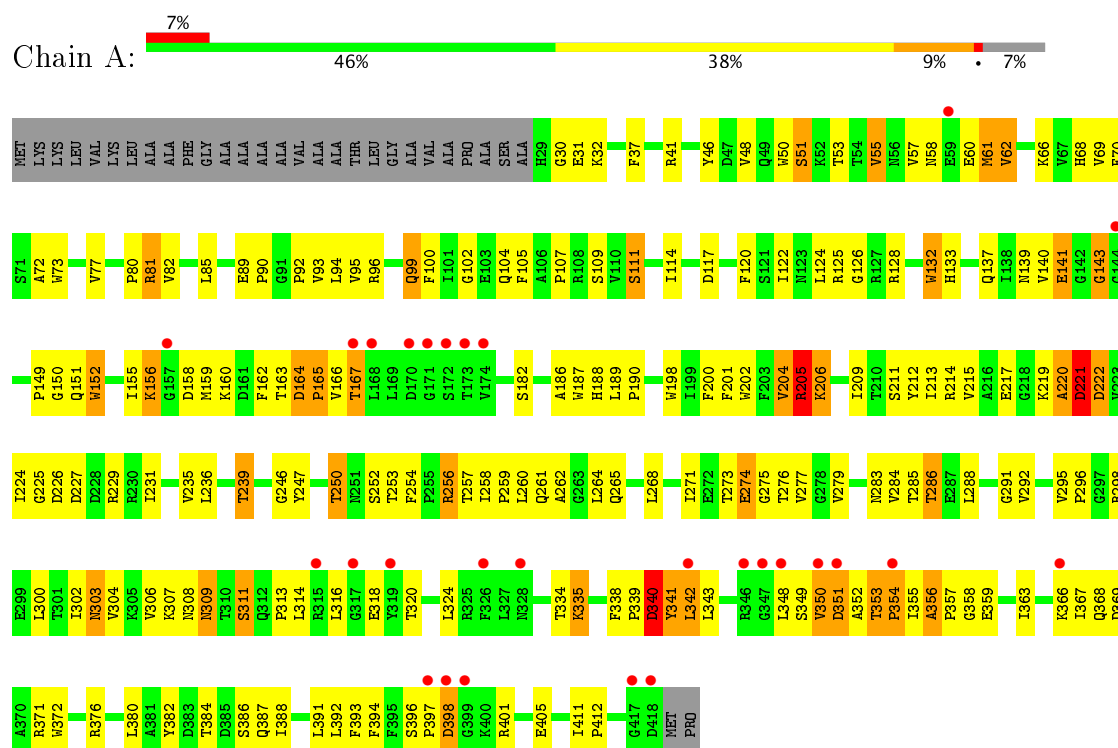


- Molecule 2: Particulate methane monooxygenase subunit A

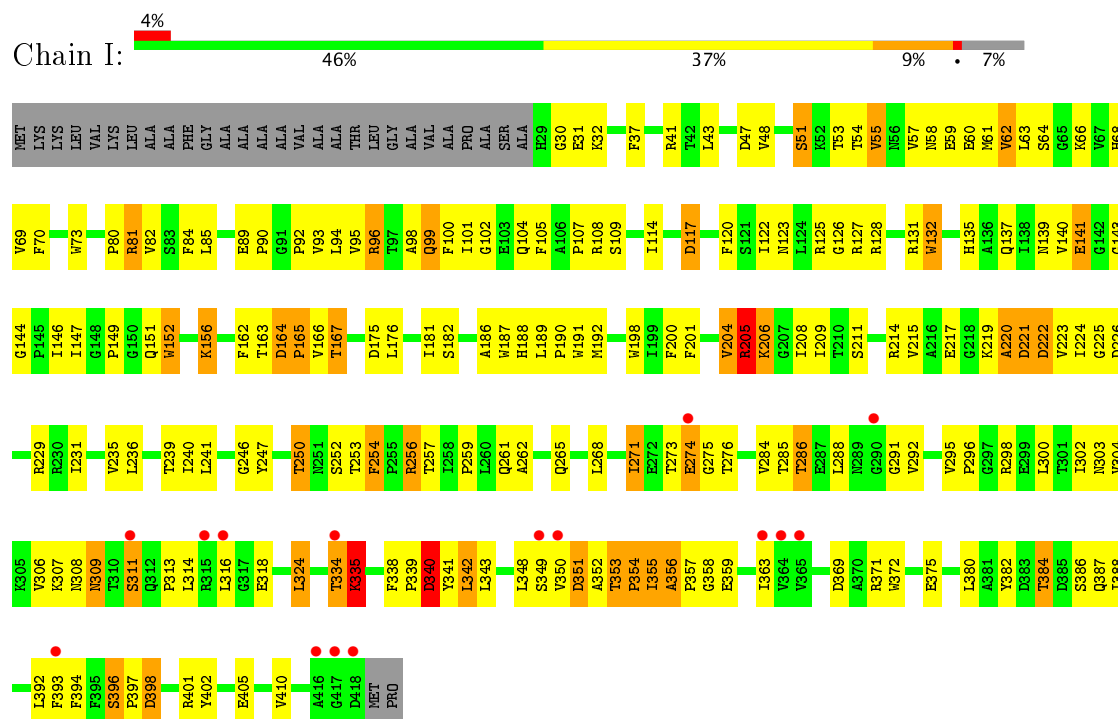
Chain J: 



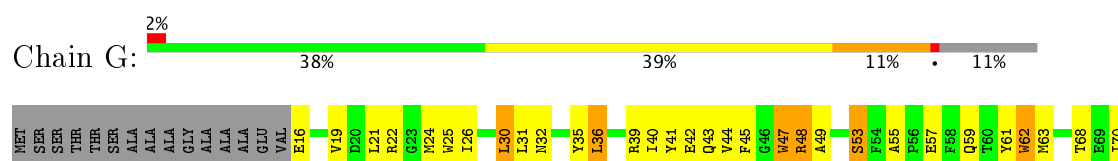


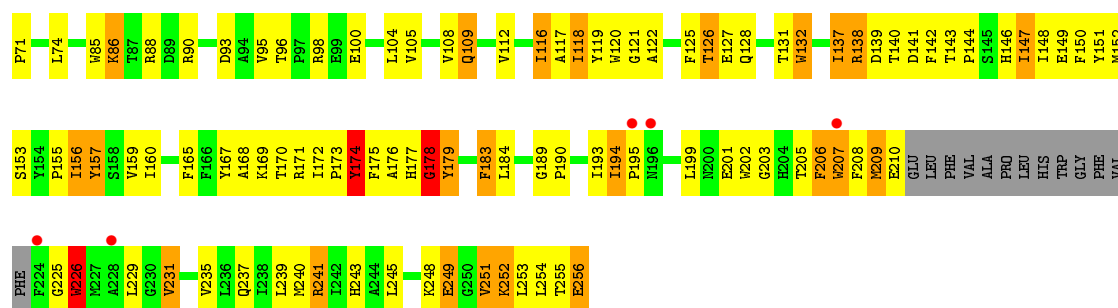


- Molecule 3: Particulate methane monooxygenase subunit B

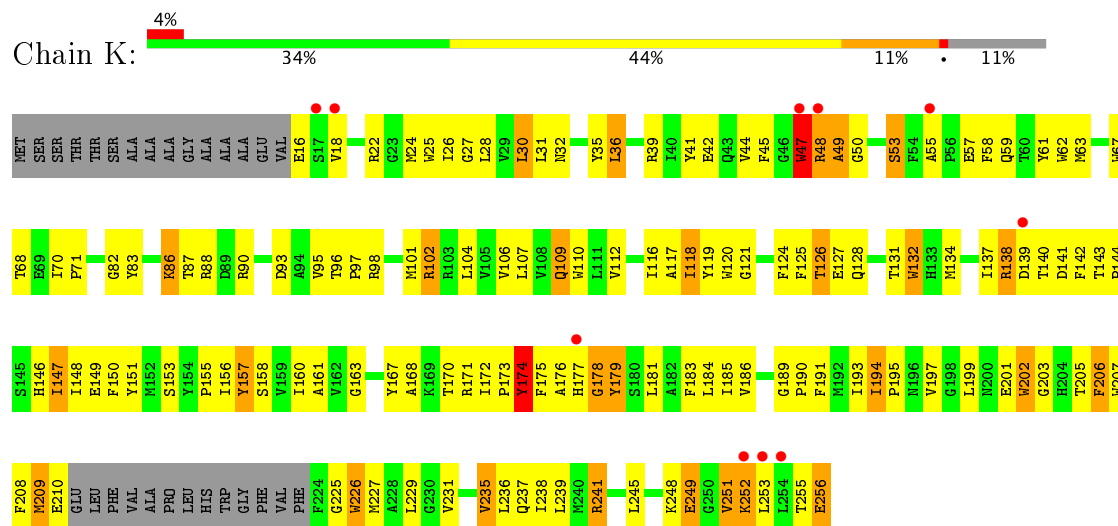


- Molecule 4: Particulate methane monooxygenase subunit C

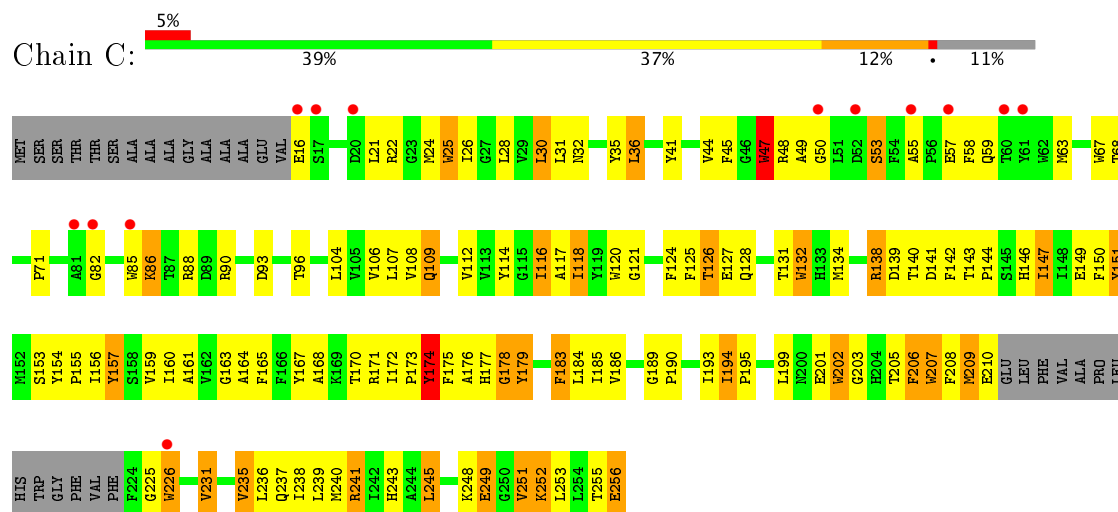




• Molecule 4: Particulate methane monooxygenase subunit C



• Molecule 4: Particulate methane monooxygenase subunit C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.86Å 185.45Å 192.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.33 48.97 – 3.33	Depositor EDS
% Data completeness (in resolution range)	80.7 (50.00-3.33) 80.9 (48.97-3.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.67 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.225 , 0.282 0.223 , 0.279	Depositor DCC
$R_{free}$ test set	2599 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	20979	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 4.27% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN, 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	0.84	6/2052 (0.3%)	0.82	0/2814
2	F	0.91	5/2052 (0.2%)	0.87	1/2814 (0.0%)
2	J	0.91	6/2052 (0.3%)	0.88	0/2814
3	A	0.67	4/3115 (0.1%)	0.82	1/4243 (0.0%)
3	E	0.72	1/3115 (0.0%)	0.84	1/4243 (0.0%)
3	I	0.70	3/3115 (0.1%)	0.85	3/4243 (0.1%)
4	C	0.80	7/1932 (0.4%)	0.80	1/2634 (0.0%)
4	G	0.80	5/1932 (0.3%)	0.85	1/2634 (0.0%)
4	K	0.81	6/1932 (0.3%)	0.89	2/2634 (0.1%)
All	All	0.79	43/21297 (0.2%)	0.84	10/29073 (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	N	0	1
3	A	0	1
3	E	0	2
3	I	0	1
4	C	0	1
4	G	0	1
4	K	0	1
All	All	0	8

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	106	TRP	CD2-CE2	6.74	1.49	1.41
4	K	132	TRP	CD2-CE2	6.64	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	132	TRP	CD2-CE2	6.39	1.49	1.41
3	A	372	TRP	CD2-CE2	5.97	1.48	1.41
2	B	106	TRP	CD2-CE2	5.95	1.48	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	96	ARG	NE-CZ-NH1	-7.62	116.49	120.30
4	G	138	ARG	NE-CZ-NH2	7.53	124.07	120.30
4	K	98	ARG	NE-CZ-NH1	6.15	123.38	120.30
3	I	96	ARG	NE-CZ-NH2	6.01	123.30	120.30
4	K	102	ARG	NE-CZ-NH2	5.60	123.10	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	340	ASP	Peptide
3	E	340	ASP	Peptide
3	E	341	TYR	Peptide
3	I	340	ASP	Peptide
1	N	3	UNK	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	21	4	0
1	H	100	0	23	1	0
1	N	125	0	28	10	0
2	B	1974	0	1932	126	0
2	F	1974	0	1932	126	0
2	J	1974	0	1932	141	0
3	A	3038	0	3022	186	0
3	E	3038	0	3022	191	0
3	I	3038	0	3022	192	0
4	C	1870	0	1854	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1870	0	1854	127	0
4	K	1870	0	1854	133	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
6	C	2	0	0	0	0
6	G	2	0	0	0	0
6	K	1	0	0	0	0
7	C	5	0	0	0	0
All	All	20979	0	20496	1196	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 29.

The worst 5 of 1196 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:B:51:GLY:HA3	2:B:52:ASP:CB	1.70	1.21
3:A:334:THR:HA	3:A:335:LYS:HB2	1.24	1.18
2:J:51:GLY:HA3	2:J:52:ASP:CB	1.73	1.18
2:F:51:GLY:HA3	2:F:52:ASP:CB	1.75	1.16
2:B:51:GLY:CA	2:B:52:ASP:HB2	1.75	1.16

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%)	189 (78%)	48 (20%)	5 (2%)	8	39
2	F	242/252 (96%)	197 (81%)	36 (15%)	9 (4%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	242/252 (96%)	200 (83%)	29 (12%)	13 (5%)	2	17
3	A	388/420 (92%)	307 (79%)	56 (14%)	25 (6%)	1	13
3	E	388/420 (92%)	314 (81%)	44 (11%)	30 (8%)	1	9
3	I	388/420 (92%)	308 (79%)	53 (14%)	27 (7%)	1	11
4	C	224/256 (88%)	169 (75%)	49 (22%)	6 (3%)	6	33
4	G	224/256 (88%)	172 (77%)	44 (20%)	8 (4%)	4	27
4	K	224/256 (88%)	163 (73%)	52 (23%)	9 (4%)	3	25
All	All	2562/2784 (92%)	2019 (79%)	411 (16%)	132 (5%)	2	18

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	52	ASP
3	E	31	GLU
3	E	51	SER
3	E	141	GLU
3	E	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	
2	B	202/208 (97%)	186 (92%)	16 (8%)	14	46
2	F	202/208 (97%)	186 (92%)	16 (8%)	14	46
2	J	202/208 (97%)	186 (92%)	16 (8%)	14	46
3	A	320/336 (95%)	281 (88%)	39 (12%)	6	24
3	E	320/336 (95%)	283 (88%)	37 (12%)	6	26
3	I	320/336 (95%)	280 (88%)	40 (12%)	5	22
4	C	194/213 (91%)	162 (84%)	32 (16%)	2	12
4	G	194/213 (91%)	161 (83%)	33 (17%)	2	11
4	K	194/213 (91%)	163 (84%)	31 (16%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2148/2271 (95%)	1888 (88%)	260 (12%)	6 24

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	256	ARG
4	G	126	THR
4	C	147	ILE
3	I	306	VAL
4	G	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	261	GLN
3	I	58	ASN
4	K	109	GLN
3	A	265	GLN
3	A	283	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 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	$\# Z  > 2$
7	CAC	C	303	6	0,4,4	0.00	-	0,6,6	0.00	-

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
7	CAC	C	303	6	-	0/0/0/0	0/0/0/0

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%)	-0.54	1 (0%) 92 93	27, 51, 92, 117	0
2	F	244/252 (96%)	-0.63	0 100 100	14, 31, 66, 95	0
2	J	244/252 (96%)	-0.58	4 (1%) 72 72	16, 33, 67, 104	0
3	A	390/420 (92%)	0.14	28 (7%) 16 17	35, 72, 112, 153	0
3	E	390/420 (92%)	-0.29	3 (0%) 86 87	24, 47, 85, 129	0
3	I	390/420 (92%)	-0.13	15 (3%) 41 40	25, 64, 117, 179	0
4	C	228/256 (89%)	-0.20	13 (5%) 24 24	31, 59, 111, 148	0
4	G	228/256 (89%)	-0.30	5 (2%) 62 62	20, 48, 101, 153	0
4	K	228/256 (89%)	-0.17	10 (4%) 35 35	24, 47, 115, 160	0
All	All	2586/2859 (90%)	-0.27	79 (3%) 49 50	14, 52, 107, 179	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	418	ASP	6.1
4	K	253	LEU	5.3
3	A	417	GLY	5.0
4	C	17	SER	4.6
4	K	254	LEU	4.2

### 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( $\text{\AA}^2$ )	Q<0.9
7	CAC	C	303	5/5	0.97	0.12	-1.74	92,95,102,107	0
6	ZN	C	301	1/1	0.99	0.07	-2.39	66,66,66,66	0
6	ZN	G	301	1/1	0.99	0.09	-2.55	64,64,64,64	0
6	ZN	K	301	1/1	0.99	0.03	-	67,67,67,67	0
5	CU	A	501	1/1	0.97	0.04	-	85,85,85,85	0
6	ZN	G	302	1/1	0.93	0.04	-	153,153,153,153	0
6	ZN	C	302	1/1	0.98	0.04	-	106,106,106,106	0
5	CU	I	501	1/1	0.99	0.05	-	63,63,63,63	0
5	CU	E	501	1/1	0.99	0.05	-	53,53,53,53	0

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

There are no such residues in this entry.