



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 01:41 AM UTC

PDB ID : 5VIT / pdb\_00005vit  
Title : Crystal structure of a Pseudomonas malonate decarboxylase hetero-tetramer  
in complex with malonate  
Authors : Maderbocus, R.; Tong, L.  
Deposited on : 2017-04-17  
Resolution : 2.20 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

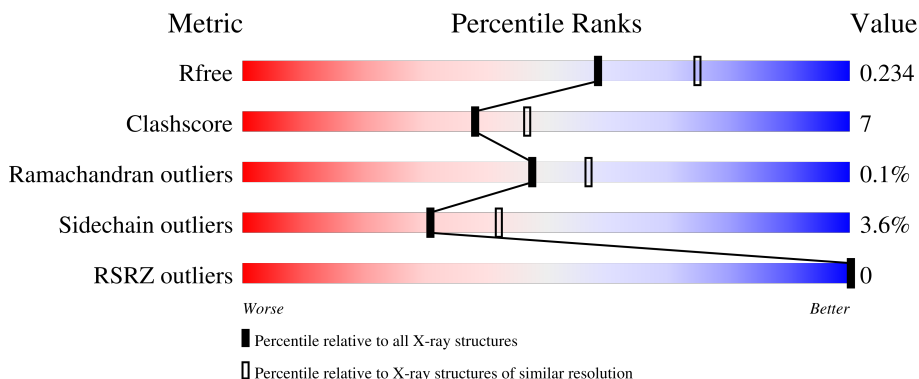
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


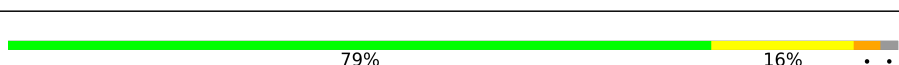

The reported resolution of this entry is 2.20 Å.

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))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	554	 79% 18% ..
1	I	554	 82% 14% ..
1	P	554	 81% 16% ..
1	V	554	 78% 19% ..
2	C	99	 79% 16% ..

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Mol	Chain	Length	Quality of chain
2	K	99	 78% 19% ..
2	R	99	 83% 14% ..
2	X	99	 75% 21% ..
3	D	287	 84% 11% ..
3	L	287	 85% 11% .
3	S	287	 84% 11% ..
3	Y	287	 81% 14% ..
4	E	284	 80% 9% . 10%
4	M	284	 79% 10% . 10%
4	T	284	 80% 10% . 10%
4	Z	284	 76% 12% . 10%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 37455 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 MdcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4284	2706	780	781	17	0	0	0
1	P	548	4284	2706	780	781	17	0	0	0
1	I	548	4284	2706	780	781	17	0	0	0
1	V	548	4284	2706	780	781	17	0	0	0

- Molecule 2 is a protein called MdcC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	97	735	465	129	139	2	0	0	0
2	R	97	735	465	129	139	2	0	0	0
2	K	97	735	465	129	139	2	0	0	0
2	X	97	735	465	129	139	2	0	0	0

- Molecule 3 is a protein called MdcD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	276	2063	1292	376	391	4	0	0	0
3	S	276	2063	1292	376	391	4	0	0	0
3	L	276	2063	1292	376	391	4	0	0	0
3	Y	276	2063	1292	376	391	4	0	0	0

- Molecule 4 is a protein called MdcE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	256	Total	C	N	O	S	0	0	0
			1910	1203	358	344	5			
4	T	256	Total	C	N	O	S	0	0	0
			1910	1203	358	344	5			
4	M	256	Total	C	N	O	S	0	0	0
			1910	1203	358	344	5			
4	Z	256	Total	C	N	O	S	0	0	0
			1910	1203	358	344	5			

There are 64 discrepancies between the modelled and reference sequences:

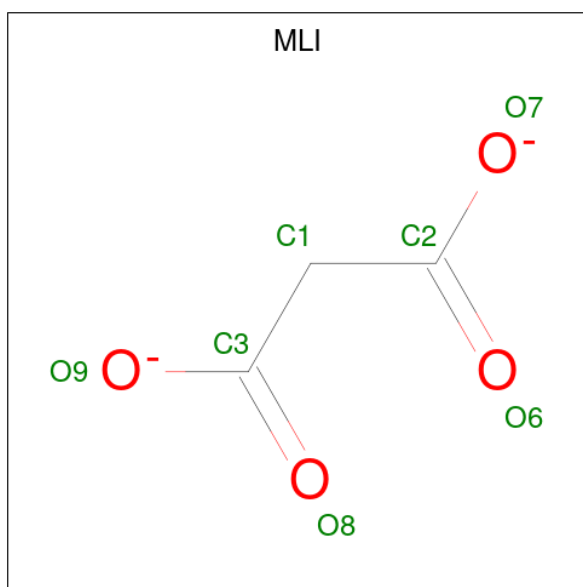
Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	MET	-	initiating methionine	UNP A0A0C6EV56
E	-14	GLY	-	expression tag	UNP A0A0C6EV56
E	-13	SER	-	expression tag	UNP A0A0C6EV56
E	-12	SER	-	expression tag	UNP A0A0C6EV56
E	-11	HIS	-	expression tag	UNP A0A0C6EV56
E	-10	HIS	-	expression tag	UNP A0A0C6EV56
E	-9	HIS	-	expression tag	UNP A0A0C6EV56
E	-8	HIS	-	expression tag	UNP A0A0C6EV56
E	-7	HIS	-	expression tag	UNP A0A0C6EV56
E	-6	HIS	-	expression tag	UNP A0A0C6EV56
E	-5	SER	-	expression tag	UNP A0A0C6EV56
E	-4	GLN	-	expression tag	UNP A0A0C6EV56
E	-3	ASP	-	expression tag	UNP A0A0C6EV56
E	-2	PRO	-	expression tag	UNP A0A0C6EV56
E	-1	ASN	-	expression tag	UNP A0A0C6EV56
E	0	SER	-	expression tag	UNP A0A0C6EV56
T	-15	MET	-	initiating methionine	UNP A0A0C6EV56
T	-14	GLY	-	expression tag	UNP A0A0C6EV56
T	-13	SER	-	expression tag	UNP A0A0C6EV56
T	-12	SER	-	expression tag	UNP A0A0C6EV56
T	-11	HIS	-	expression tag	UNP A0A0C6EV56
T	-10	HIS	-	expression tag	UNP A0A0C6EV56
T	-9	HIS	-	expression tag	UNP A0A0C6EV56
T	-8	HIS	-	expression tag	UNP A0A0C6EV56
T	-7	HIS	-	expression tag	UNP A0A0C6EV56
T	-6	HIS	-	expression tag	UNP A0A0C6EV56
T	-5	SER	-	expression tag	UNP A0A0C6EV56
T	-4	GLN	-	expression tag	UNP A0A0C6EV56
T	-3	ASP	-	expression tag	UNP A0A0C6EV56
T	-2	PRO	-	expression tag	UNP A0A0C6EV56

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	ASN	-	expression tag	UNP A0A0C6EV56
T	0	SER	-	expression tag	UNP A0A0C6EV56
M	-15	MET	-	initiating methionine	UNP A0A0C6EV56
M	-14	GLY	-	expression tag	UNP A0A0C6EV56
M	-13	SER	-	expression tag	UNP A0A0C6EV56
M	-12	SER	-	expression tag	UNP A0A0C6EV56
M	-11	HIS	-	expression tag	UNP A0A0C6EV56
M	-10	HIS	-	expression tag	UNP A0A0C6EV56
M	-9	HIS	-	expression tag	UNP A0A0C6EV56
M	-8	HIS	-	expression tag	UNP A0A0C6EV56
M	-7	HIS	-	expression tag	UNP A0A0C6EV56
M	-6	HIS	-	expression tag	UNP A0A0C6EV56
M	-5	SER	-	expression tag	UNP A0A0C6EV56
M	-4	GLN	-	expression tag	UNP A0A0C6EV56
M	-3	ASP	-	expression tag	UNP A0A0C6EV56
M	-2	PRO	-	expression tag	UNP A0A0C6EV56
M	-1	ASN	-	expression tag	UNP A0A0C6EV56
M	0	SER	-	expression tag	UNP A0A0C6EV56
Z	-15	MET	-	initiating methionine	UNP A0A0C6EV56
Z	-14	GLY	-	expression tag	UNP A0A0C6EV56
Z	-13	SER	-	expression tag	UNP A0A0C6EV56
Z	-12	SER	-	expression tag	UNP A0A0C6EV56
Z	-11	HIS	-	expression tag	UNP A0A0C6EV56
Z	-10	HIS	-	expression tag	UNP A0A0C6EV56
Z	-9	HIS	-	expression tag	UNP A0A0C6EV56
Z	-8	HIS	-	expression tag	UNP A0A0C6EV56
Z	-7	HIS	-	expression tag	UNP A0A0C6EV56
Z	-6	HIS	-	expression tag	UNP A0A0C6EV56
Z	-5	SER	-	expression tag	UNP A0A0C6EV56
Z	-4	GLN	-	expression tag	UNP A0A0C6EV56
Z	-3	ASP	-	expression tag	UNP A0A0C6EV56
Z	-2	PRO	-	expression tag	UNP A0A0C6EV56
Z	-1	ASN	-	expression tag	UNP A0A0C6EV56
Z	0	SER	-	expression tag	UNP A0A0C6EV56

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 3 4	0	0
5	P	1	Total C O 7 3 4	0	0
5	I	1	Total C O 7 3 4	0	0
5	V	1	Total C O 7 3 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	171	Total O 171 171	0	0
6	C	21	Total O 21 21	0	0
6	D	80	Total O 80 80	0	0
6	E	72	Total O 72 72	0	0
6	P	193	Total O 193 193	0	0
6	R	30	Total O 30 30	0	0
6	S	110	Total O 110 110	0	0
6	T	70	Total O 70 70	0	0

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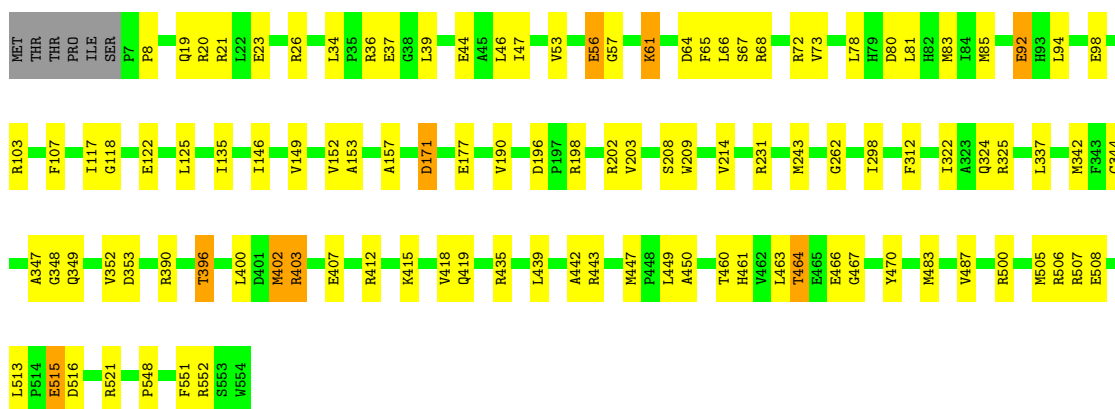
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	I	165	Total 165	O 165	0	0
6	K	29	Total 29	O 29	0	0
6	L	101	Total 101	O 101	0	0
6	M	66	Total 66	O 66	0	0
6	V	159	Total 159	O 159	0	0
6	X	23	Total 23	O 23	0	0
6	Y	91	Total 91	O 91	0	0
6	Z	78	Total 78	O 78	0	0

### 3 Residue-property plots


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.

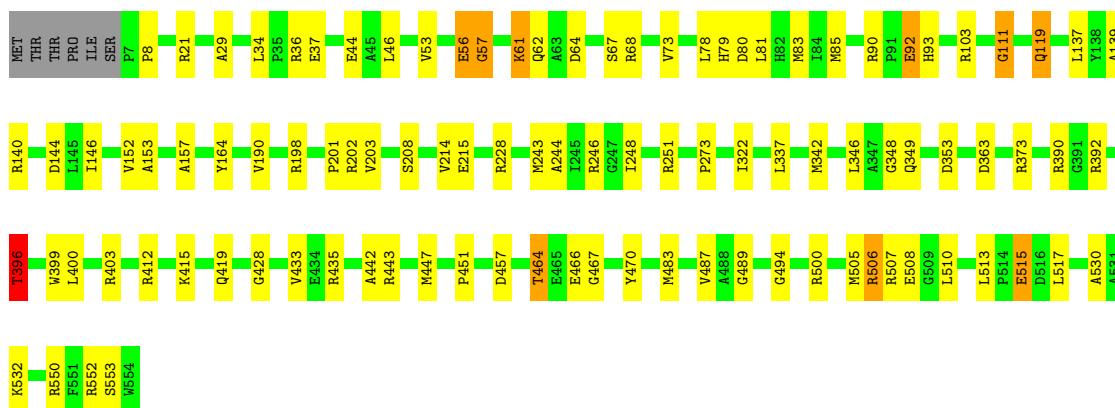
- Molecule 1: MdcA

Chain A:  79% 18%




- Molecule 1: MdcA

Chain P:  81% 16%



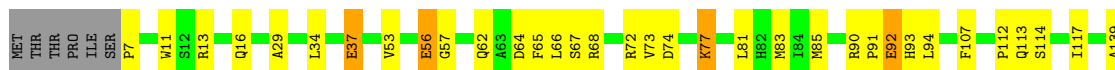
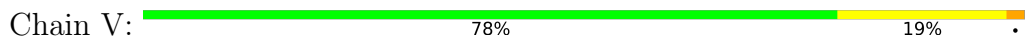
- Molecule 1: MdcA

Chain I:  82% 14%

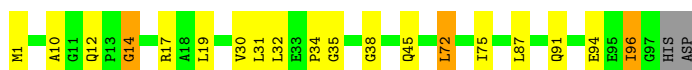
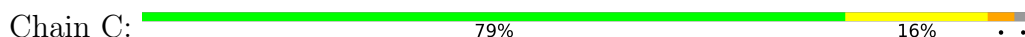




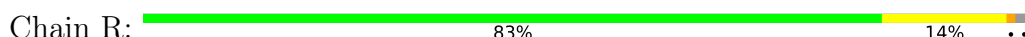
• Molecule 1: MdcA



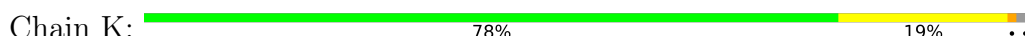
• Molecule 2: MdcC



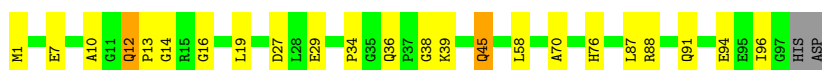
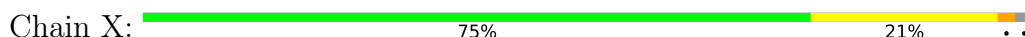
• Molecule 2: MdcC




• Molecule 2: MdcC



• Molecule 2: MdcC




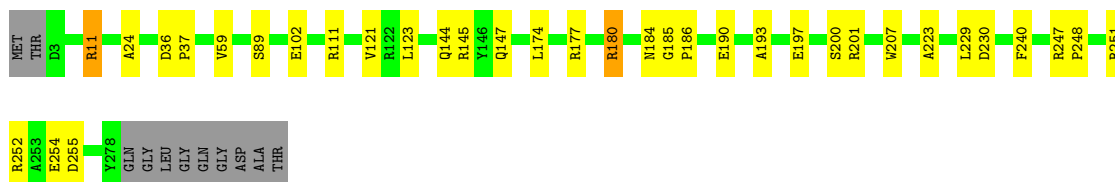
- Molecule 3: MdcD

Chain D:  84% 11% . .




- Molecule 3: MdcD

Chain S:  84% 11% . .




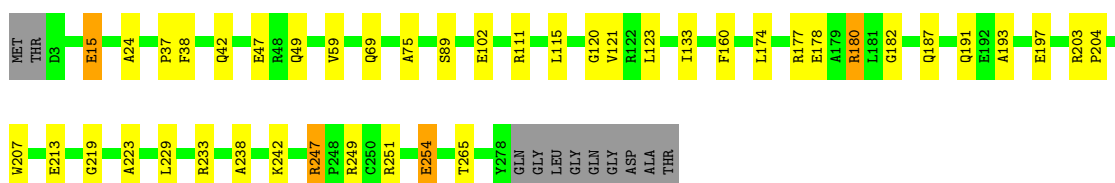
- Molecule 3: MdcD

Chain L:  85% 11% .




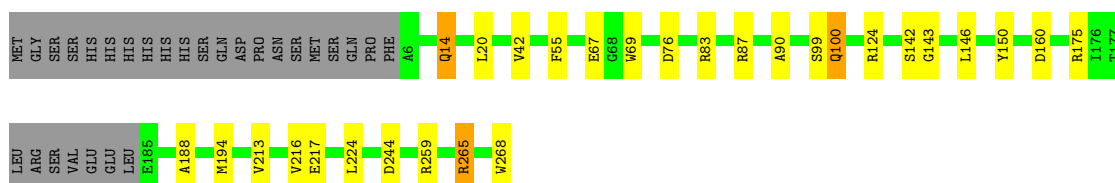
- Molecule 3: MdcD

Chain Y:  81% 14% . .




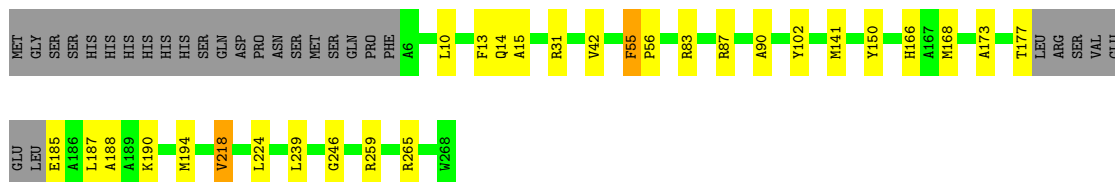
- Molecule 4: MdcE

Chain E:  80% 9% . 10%




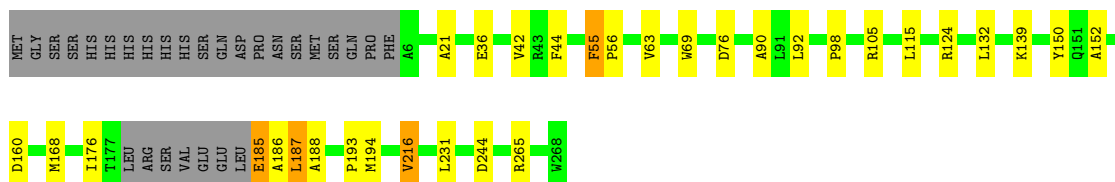
- Molecule 4: MdcE

Chain T:  80% 10% 10%



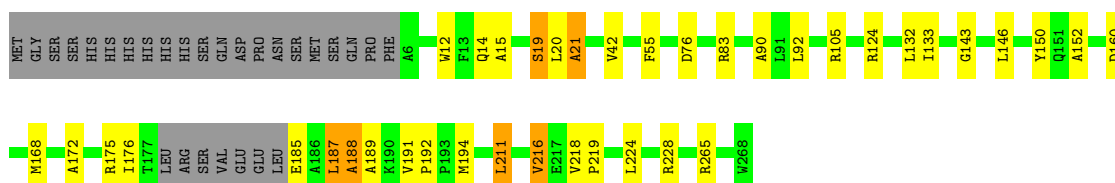
- Molecule 4: MdcE

Chain M:  79% 10% 10%



- Molecule 4: MdcE

Chain Z:  76% 12% 10%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.51Å 161.45Å 102.72Å 90.80° 93.76° 90.11°	Depositor
Resolution (Å)	49.04 – 2.20 49.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.04-2.20) 89.7 (49.04-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.186 , 0.232 0.191 , 0.234	Depositor DCC
$R_{free}$ test set	14611 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 18.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.287 for -h,k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	37455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: MLI

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	0.55	1/4381 (0.0%)	0.88	8/5944 (0.1%)
1	I	0.56	0/4381	0.86	7/5944 (0.1%)
1	P	0.56	0/4381	0.87	7/5944 (0.1%)
1	V	0.55	0/4381	0.87	5/5944 (0.1%)
2	C	0.55	0/751	0.90	1/1017 (0.1%)
2	K	0.54	0/751	0.80	0/1017
2	R	0.55	0/751	0.82	0/1017
2	X	0.53	0/751	0.83	0/1017
3	D	0.52	0/2093	0.84	2/2839 (0.1%)
3	L	0.55	0/2093	0.85	4/2839 (0.1%)
3	S	0.55	0/2093	0.84	1/2839 (0.0%)
3	Y	0.56	0/2093	0.82	1/2839 (0.0%)
4	E	0.49	0/1948	0.84	2/2648 (0.1%)
4	M	0.51	0/1948	0.83	2/2648 (0.1%)
4	T	0.56	1/1948 (0.1%)	0.87	3/2648 (0.1%)
4	Z	0.51	0/1948	0.88	6/2648 (0.2%)
All	All	0.55	2/36692 (0.0%)	0.86	49/49792 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	I	0	1
1	P	0	1
1	V	0	1
4	E	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	218	VAL	CA-CB	5.13	1.60	1.54
1	A	402	MET	SD-CE	-5.01	1.67	1.79

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	247	ARG	CA-C-N	8.25	128.19	120.03
3	L	247	ARG	C-N-CA	8.25	128.19	120.03
1	A	262	GLY	N-CA-C	8.12	120.46	111.85
1	I	111	GLY	CA-C-N	7.88	127.55	119.19
1	I	111	GLY	C-N-CA	7.88	127.55	119.19

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	GLU	Peptide
4	E	99	SER	Peptide
1	I	56	GLU	Peptide
1	P	56	GLU	Peptide
1	V	56	GLU	Peptide

## 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	4284	0	4281	74	0
1	I	4284	0	4281	68	0
1	P	4284	0	4281	81	0
1	V	4284	0	4281	86	0
2	C	735	0	724	9	0
2	K	735	0	724	11	0
2	R	735	0	724	10	0
2	X	735	0	724	10	0
3	D	2063	0	2071	28	0
3	L	2063	0	2071	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	2063	0	2071	24	0
3	Y	2063	0	2071	33	0
4	E	1910	0	1932	26	0
4	M	1910	0	1932	26	0
4	T	1910	0	1932	19	0
4	Z	1910	0	1932	25	0
5	A	7	0	2	0	0
5	I	7	0	2	0	0
5	P	7	0	2	0	0
5	V	7	0	2	0	0
6	A	171	0	0	5	0
6	C	21	0	0	2	0
6	D	80	0	0	1	0
6	E	72	0	0	5	0
6	I	165	0	0	8	0
6	K	29	0	0	1	0
6	L	101	0	0	8	0
6	M	66	0	0	2	0
6	P	193	0	0	11	0
6	R	30	0	0	1	0
6	S	110	0	0	5	0
6	T	70	0	0	1	0
6	V	159	0	0	8	0
6	X	23	0	0	0	0
6	Y	91	0	0	2	0
6	Z	78	0	0	1	0
All	All	37455	0	36040	496	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 7.

The worst 5 of 496 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:507:ARG:HH12	4:E:265:ARG:HH12	1.09	0.98
1:P:464:THR:HG22	1:P:466:GLU:H	1.26	0.98
1:I:464:THR:HG22	1:I:466:GLU:H	1.26	0.96
4:E:100:GLN:HE21	4:E:143:GLY:H	1.09	0.96
1:I:243:MET:HE1	1:I:467:GLY:HA2	1.48	0.95

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	546/554 (99%)	528 (97%)	18 (3%)	0	100	100
1	I	546/554 (99%)	533 (98%)	13 (2%)	0	100	100
1	P	546/554 (99%)	533 (98%)	13 (2%)	0	100	100
1	V	546/554 (99%)	528 (97%)	18 (3%)	0	100	100
2	C	95/99 (96%)	92 (97%)	3 (3%)	0	100	100
2	K	95/99 (96%)	91 (96%)	4 (4%)	0	100	100
2	R	95/99 (96%)	92 (97%)	3 (3%)	0	100	100
2	X	95/99 (96%)	92 (97%)	3 (3%)	0	100	100
3	D	274/287 (96%)	270 (98%)	4 (2%)	0	100	100
3	L	274/287 (96%)	267 (97%)	7 (3%)	0	100	100
3	S	274/287 (96%)	268 (98%)	6 (2%)	0	100	100
3	Y	274/287 (96%)	268 (98%)	6 (2%)	0	100	100
4	E	252/284 (89%)	241 (96%)	11 (4%)	0	100	100
4	M	252/284 (89%)	238 (94%)	14 (6%)	0	100	100
4	T	252/284 (89%)	243 (96%)	9 (4%)	0	100	100
4	Z	252/284 (89%)	238 (94%)	11 (4%)	3 (1%)	10	8
All	All	4668/4896 (95%)	4522 (97%)	143 (3%)	3 (0%)	48	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Z	19	SER
4	Z	188	ALA
4	Z	21	ALA

### 5.3.2 Protein sidechains [i](#)

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	451/457 (99%)	434 (96%)	17 (4%)	29	40
1	I	451/457 (99%)	430 (95%)	21 (5%)	23	31
1	P	451/457 (99%)	437 (97%)	14 (3%)	35	48
1	V	451/457 (99%)	438 (97%)	13 (3%)	37	51
2	C	78/80 (98%)	72 (92%)	6 (8%)	12	13
2	K	78/80 (98%)	75 (96%)	3 (4%)	29	40
2	R	78/80 (98%)	73 (94%)	5 (6%)	16	19
2	X	78/80 (98%)	71 (91%)	7 (9%)	9	9
3	D	202/209 (97%)	196 (97%)	6 (3%)	36	49
3	L	202/209 (97%)	197 (98%)	5 (2%)	42	56
3	S	202/209 (97%)	199 (98%)	3 (2%)	57	73
3	Y	202/209 (97%)	196 (97%)	6 (3%)	36	49
4	E	182/209 (87%)	176 (97%)	6 (3%)	33	45
4	M	182/209 (87%)	176 (97%)	6 (3%)	33	45
4	T	182/209 (87%)	177 (97%)	5 (3%)	39	53
4	Z	182/209 (87%)	174 (96%)	8 (4%)	25	34
All	All	3652/3820 (96%)	3521 (96%)	131 (4%)	31	42

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	94	GLU
3	Y	180	ARG
4	Z	218	VAL
1	P	515	GLU
1	P	506	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	419	GLN
3	L	191	GLN
3	L	42	GLN
1	V	113	GLN
3	D	49	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 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
5	MLI	P	601	-	6,6,6	1.24	0	7,7,7	1.35	1 (14%)
5	MLI	I	601	-	6,6,6	1.00	0	7,7,7	1.42	1 (14%)
5	MLI	V	601	-	6,6,6	1.23	0	7,7,7	1.39	1 (14%)
5	MLI	A	601	-	6,6,6	1.16	0	7,7,7	1.45	1 (14%)

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
5	MLI	P	601	-	-	0/4/4/4	-
5	MLI	I	601	-	-	2/4/4/4	-
5	MLI	V	601	-	-	2/4/4/4	-
5	MLI	A	601	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	601	MLI	O9-C3-C1	2.18	121.27	114.51
5	P	601	MLI	O9-C3-C1	2.15	121.16	114.51
5	A	601	MLI	O7-C2-C1	2.14	121.14	114.51
5	V	601	MLI	O9-C3-C1	2.01	120.74	114.51

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	V	601	MLI	C2-C1-C3-O9
5	V	601	MLI	C2-C1-C3-O8
5	A	601	MLI	C3-C1-C2-O6
5	A	601	MLI	C3-C1-C2-O7
5	I	601	MLI	C2-C1-C3-O8

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	A	548/554 (98%)	-1.59	0 100 100	21, 32, 56, 80	0
1	I	548/554 (98%)	-1.59	0 100 100	21, 33, 58, 76	0
1	P	548/554 (98%)	-1.61	0 100 100	21, 31, 55, 70	0
1	V	548/554 (98%)	-1.57	0 100 100	20, 33, 57, 76	0
2	C	97/99 (97%)	-1.53	0 100 100	27, 37, 53, 78	0
2	K	97/99 (97%)	-1.54	0 100 100	26, 36, 50, 75	0
2	R	97/99 (97%)	-1.54	0 100 100	25, 36, 50, 77	0
2	X	97/99 (97%)	-1.55	0 100 100	25, 36, 52, 76	0
3	D	276/287 (96%)	-1.56	0 100 100	23, 36, 57, 70	0
3	L	276/287 (96%)	-1.61	0 100 100	22, 31, 50, 65	0
3	S	276/287 (96%)	-1.63	0 100 100	21, 30, 49, 65	0
3	Y	276/287 (96%)	-1.59	0 100 100	22, 33, 52, 68	0
4	E	256/284 (90%)	-1.46	0 100 100	24, 37, 63, 86	0
4	M	256/284 (90%)	-1.48	0 100 100	23, 35, 67, 85	0
4	T	256/284 (90%)	-1.51	0 100 100	23, 35, 69, 85	0
4	Z	256/284 (90%)	-1.52	0 100 100	23, 33, 63, 85	0
All	All	4708/4896 (96%)	-1.57	0 100 100	20, 33, 57, 86	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
5	MLI	I	601	7/7	0.99	0.04	23,27,32,37	0
5	MLI	V	601	7/7	0.99	0.03	21,27,29,31	0
5	MLI	A	601	7/7	1.00	0.03	23,25,32,35	0
5	MLI	P	601	7/7	1.00	0.02	21,24,30,31	0

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

There are no such residues in this entry.