



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2020 – 01:19 pm BST

PDB ID : 5VIT  
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 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 : 2.11  
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) : 2.11

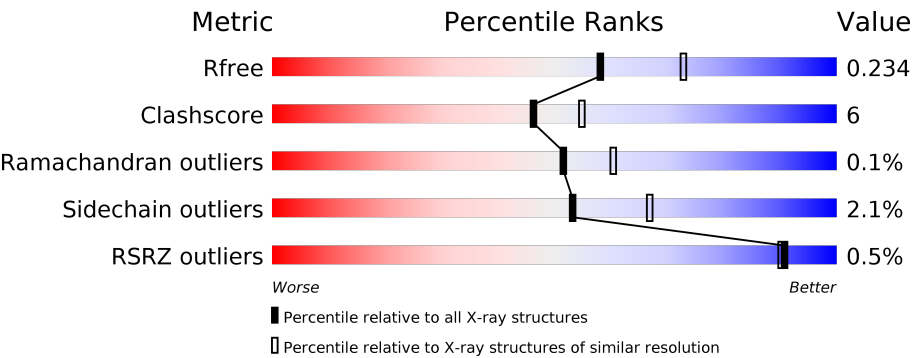
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	<div><div>%</div><div><div></div><div>83%</div><div>15%</div><div>..</div></div></div>
1	I	554	<div><div></div><div>84%</div><div>14%</div><div>..</div></div>
1	P	554	<div><div></div><div>83%</div><div>14%</div><div>..</div></div>
1	V	554	<div><div></div><div>80%</div><div>18%</div><div>..</div></div>
2	C	99	<div><div>%</div><div><div></div><div>81%</div><div>16%</div><div>..</div></div></div>
2	K	99	<div><div></div><div>80%</div><div>17%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
2	R	99	<div><div></div><div>86%12%</div><div></div><div></div></div>
2	X	99	<div><div>%</div><div></div><div>79%18%</div><div></div><div></div></div>
3	D	287	<div><div></div><div>85%11%</div><div></div><div></div></div>
3	L	287	<div><div></div><div>87%9%</div><div></div><div></div></div>
3	S	287	<div><div></div><div>85%11%</div><div></div><div></div></div>
3	Y	287	<div><div></div><div>83%12%</div><div></div><div></div></div>
4	E	284	<div><div>%</div><div></div><div>81%8%10%</div><div></div><div></div></div>
4	M	284	<div><div>%</div><div></div><div>80%10%10%</div><div></div><div></div></div>
4	T	284	<div><div>%</div><div></div><div>82%8%10%</div><div></div><div></div></div>
4	Z	284	<div><div></div><div>80%10%</div><div></div><div></div></div>

## 2 Entry composition

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
1	A	548	Total	C	N	O	S	0	0	0
			4284	2706	780	781	17			
1	P	548	Total	C	N	O	S	0	0	0
			4284	2706	780	781	17			
1	I	548	Total	C	N	O	S	0	0	0
			4284	2706	780	781	17			
1	V	548	Total	C	N	O	S	0	0	0
			4284	2706	780	781	17			

- Molecule 2 is a protein called MdcC.

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

- Molecule 3 is a protein called MdcD.

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

- 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:

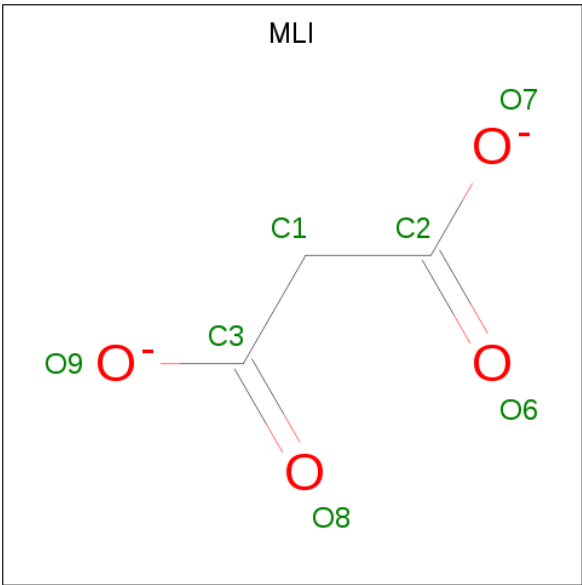
Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	MET	-	initiating methionine	UNP A0A0C6EV56
E	-14	GLY	-	expression tag	UNP A0A0C6EV56
E	-13	SER	-	expression tag	UNP A0A0C6EV56
E	-12	SER	-	expression tag	UNP A0A0C6EV56
E	-11	HIS	-	expression tag	UNP A0A0C6EV56
E	-10	HIS	-	expression tag	UNP A0A0C6EV56
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 (three-letter code: 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	0	0
			7	3	4		
5	P	1	Total	C	O	0	0
			7	3	4		
5	I	1	Total	C	O	0	0
			7	3	4		
5	V	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is water.

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

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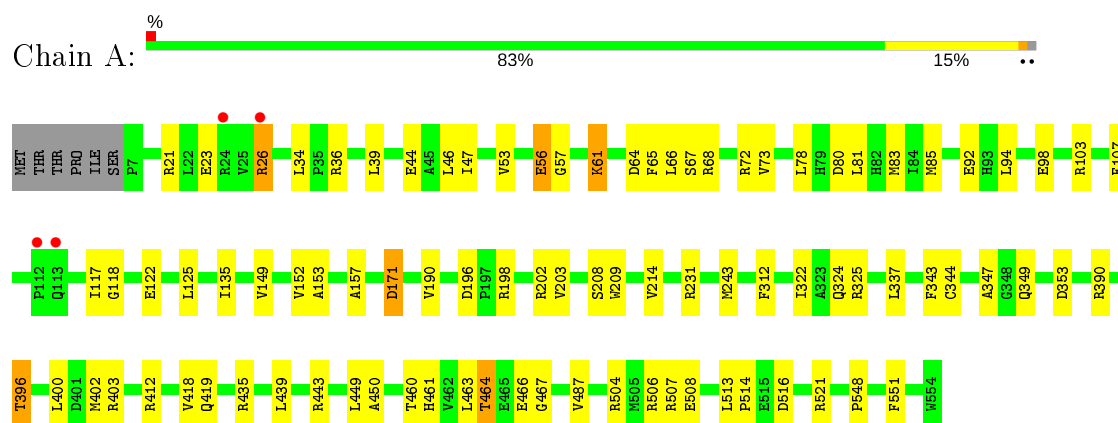
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	165	Total 165	O 165	0	0
6	K	29	Total 29	O 29	0	0
6	L	101	Total 101	O 101	0	0
6	M	66	Total 66	O 66	0	0
6	V	159	Total 159	O 159	0	0
6	X	23	Total 23	O 23	0	0
6	Y	91	Total 91	O 91	0	0
6	Z	78	Total 78	O 78	0	0



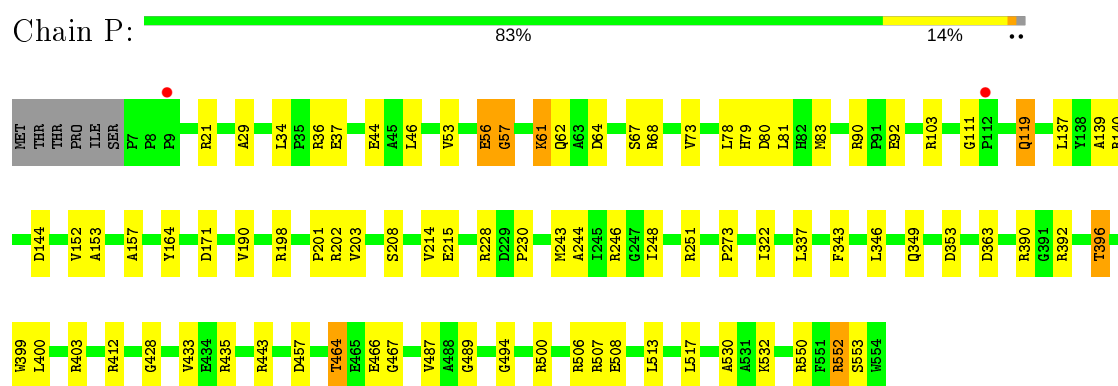
### 3 Residue-property plots [i](#)

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.

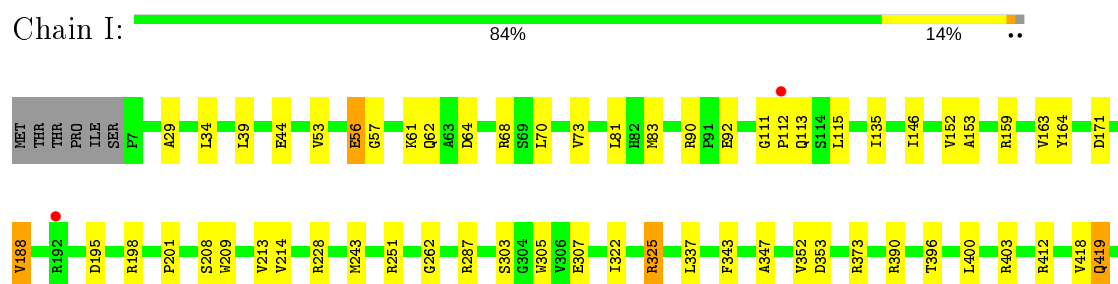
#### • Molecule 1: MdcA

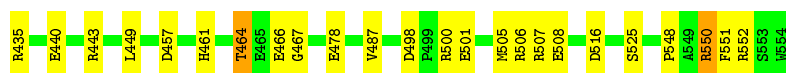


#### • Molecule 1: MdcA



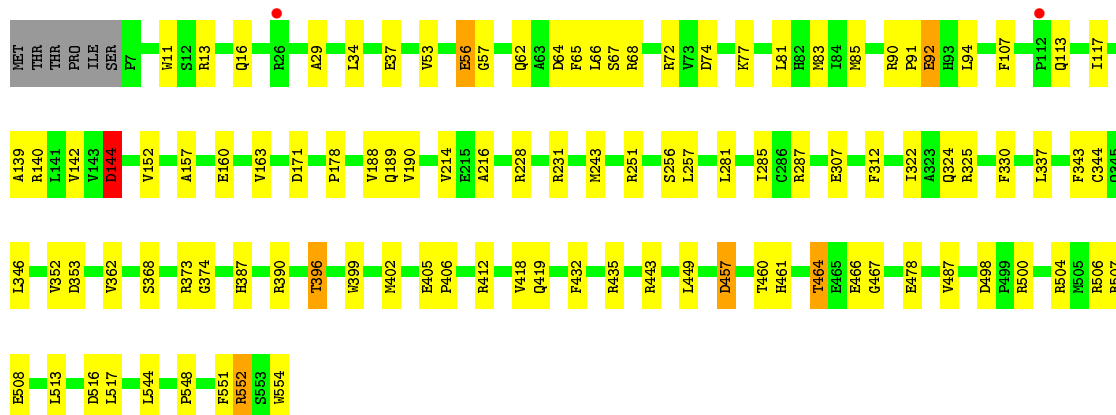
#### • Molecule 1: MdcA





• Molecule 1: MdcA

Chain V: 80% 18% ..



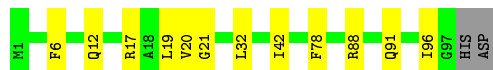
• Molecule 2: MdcC

Chain C: 81% 16% ..



• Molecule 2: MdcC

Chain R: 86% 12% .



• Molecule 2: MdcC

Chain K: 80% 17% ..



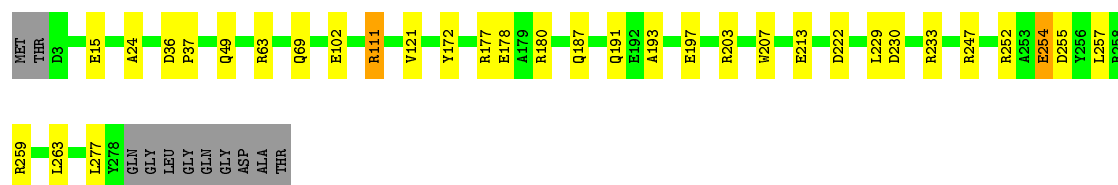
• Molecule 2: MdcC

Chain X: 79% 18% ..

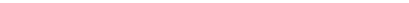


• Molecule 3: MdcD

Chain D:  85% 11% . .



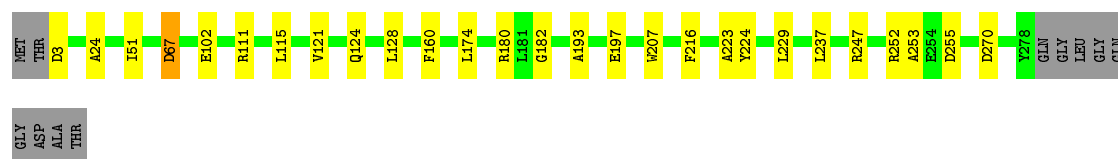
- Molecule 3: MdcD

Chain S:  85% 11% .



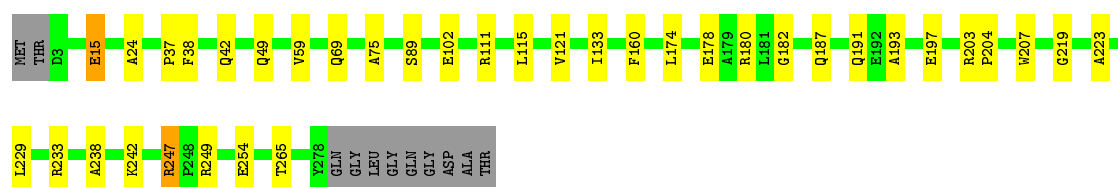
- Molecule 3: MdcD

Chain L:  87% 9% .

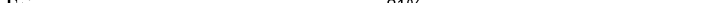


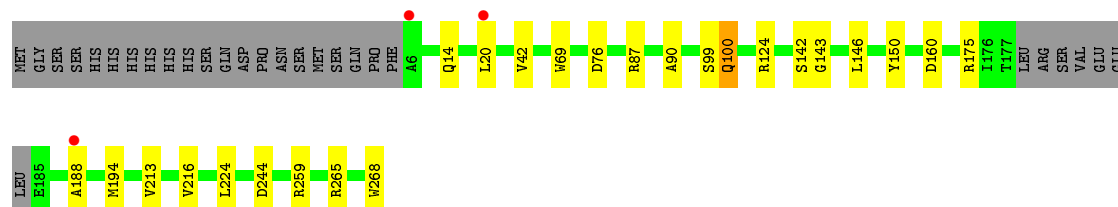
- Molecule 3: MdcD

Chain Y:  83% 12% . .

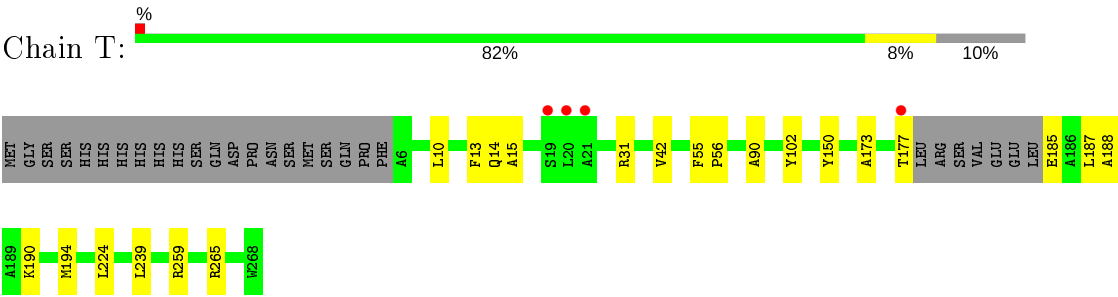


- Molecule 4: MdcE

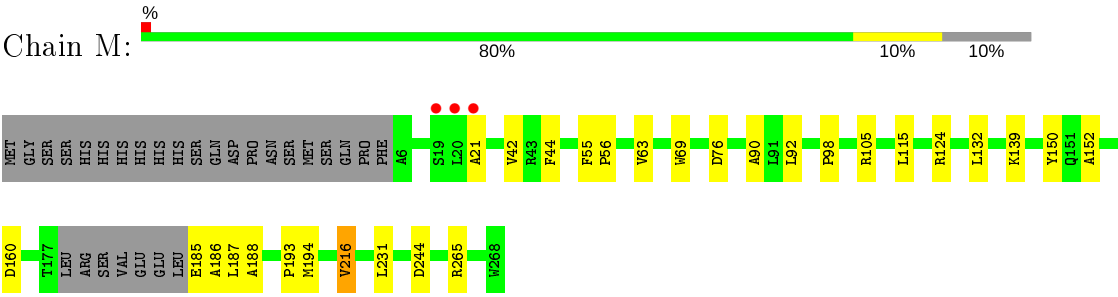
Chain E:  81% 8% 10%



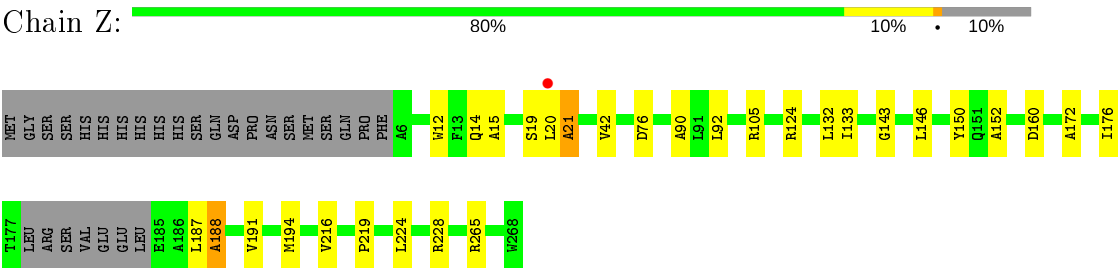
- Molecule 4: MdcE



• Molecule 4: MdcE



• Molecule 4: MdcE



## 4 Data and refinement statistics

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)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.186 , 0.232 0.189 , 0.234	Depositor DCC
$R_{free}$ test set	14611 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 22.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.287 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	37455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage'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	0.43	0/4381	0.63	1/5944 (0.0%)
1	I	0.44	0/4381	0.61	2/5944 (0.0%)
1	P	0.44	0/4381	0.62	1/5944 (0.0%)
1	V	0.43	0/4381	0.61	1/5944 (0.0%)
2	C	0.48	1/751 (0.1%)	0.63	0/1017
2	K	0.48	0/751	0.59	0/1017
2	R	0.46	0/751	0.60	0/1017
2	X	0.44	0/751	0.57	0/1017
3	D	0.43	0/2093	0.58	0/2839
3	L	0.45	0/2093	0.59	1/2839 (0.0%)
3	S	0.43	0/2093	0.56	0/2839
3	Y	0.45	0/2093	0.56	0/2839
4	E	0.38	0/1948	0.55	0/2648
4	M	0.39	0/1948	0.54	0/2648
4	T	0.42	0/1948	0.58	0/2648
4	Z	0.39	0/1948	0.55	0/2648
All	All	0.43	1/36692 (0.0%)	0.59	6/49792 (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	A	0	1
1	I	0	1
1	P	0	1
1	V	0	1
4	E	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	22	CYS	CB-SG	-5.03	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	247	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	I	449	LEU	CA-CB-CG	5.80	128.64	115.30
1	V	144	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	P	57	GLY	N-CA-C	-5.33	99.77	113.10
1	A	57	GLY	N-CA-C	-5.32	99.81	113.10
1	I	57	GLY	N-CA-C	-5.08	100.39	113.10

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	67	0
1	I	4284	0	4281	62	0
1	P	4284	0	4281	71	0
1	V	4284	0	4281	77	0
2	C	735	0	724	8	0
2	K	735	0	724	10	0
2	R	735	0	724	8	0
2	X	735	0	724	9	0
3	D	2063	0	2071	27	0
3	L	2063	0	2071	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	2063	0	2071	23	0
3	Y	2063	0	2071	30	0
4	E	1910	0	1932	25	0
4	M	1910	0	1932	23	0
4	T	1910	0	1932	17	0
4	Z	1910	0	1932	22	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	450	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 6.

All (450) 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:A:507:ARG:NH1	4:E:265:ARG:HH12	1.65	0.95
1:I:419:GLN:HE21	1:I:419:GLN:HA	1.31	0.92
1:V:507:ARG:HH12	4:Z:265:ARG:HH21	1.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:507:ARG:HH12	4:M:265:ARG:HH21	1.13	0.92
1:V:464:THR:HG22	1:V:466:GLU:H	1.34	0.92
1:P:64:ASP:OD2	1:P:68:ARG:NH1	2.05	0.88
3:Y:24:ALA:HB1	3:Y:229:LEU:HD21	1.58	0.85
1:A:72:ARG:NH1	6:A:701:HOH:O	2.08	0.84
1:A:349:GLN:HE22	1:P:349:GLN:HE22	1.25	0.83
1:A:64:ASP:OD2	1:A:68:ARG:NH1	2.13	0.82
3:S:24:ALA:HB1	3:S:229:LEU:HD21	1.62	0.82
1:P:403:ARG:NH1	6:P:701:HOH:O	2.14	0.81
1:I:64:ASP:OD2	1:I:68:ARG:NH1	2.13	0.80
1:A:464:THR:HG22	1:A:466:GLU:H	1.47	0.79
1:A:506:ARG:HD3	1:A:513:LEU:HG	1.64	0.78
3:D:247:ARG:HG2	3:D:252:ARG:HD3	1.64	0.77
1:V:72:ARG:NH1	6:V:702:HOH:O	2.17	0.77
3:D:203:ARG:O	3:D:207:TRP:HD1	1.67	0.76
1:A:80:ASP:HB3	1:A:103:ARG:HH21	1.49	0.76
3:L:24:ALA:HB1	3:L:229:LEU:HD21	1.66	0.76
1:V:13:ARG:NH1	6:V:701:HOH:O	2.18	0.75
1:V:506:ARG:HD3	1:V:513:LEU:HG	1.68	0.75
1:I:353:ASP:OD1	1:I:396:THR:HG21	1.87	0.74
2:R:19:LEU:HD22	3:Y:37:PRO:HG2	1.70	0.74
4:T:42:VAL:HG22	4:T:90:ALA:HB3	1.70	0.73
3:Y:187:GLN:O	3:Y:191:GLN:HG3	1.90	0.71
1:I:34:LEU:HB2	1:I:214:VAL:HG22	1.73	0.71
1:P:506:ARG:HD3	1:P:513:LEU:HG	1.73	0.71
1:V:34:LEU:HB2	1:V:214:VAL:HG22	1.72	0.71
1:A:353:ASP:OD1	1:A:396:THR:HG21	1.91	0.71
1:V:464:THR:HG21	1:V:487:VAL:O	1.90	0.71
3:Y:203:ARG:O	3:Y:207:TRP:HD1	1.73	0.71
3:S:193:ALA:HB1	3:S:197:GLU:HG3	1.72	0.70
1:P:34:LEU:HB2	1:P:214:VAL:HG22	1.73	0.70
1:A:464:THR:HG21	1:A:487:VAL:O	1.92	0.69
3:L:180:ARG:HD2	3:L:207:TRP:CZ2	2.28	0.69
4:Z:15:ALA:HB1	4:Z:224:LEU:HD11	1.74	0.69
4:Z:42:VAL:HG22	4:Z:90:ALA:HB3	1.76	0.68
1:V:353:ASP:OD1	1:V:396:THR:HG21	1.94	0.68
6:I:834:HOH:O	1:V:390:ARG:HG3	1.93	0.68
3:Y:102:GLU:OE2	4:Z:265:ARG:NH2	2.24	0.68
4:E:100:GLN:HE21	4:E:143:GLY:N	1.89	0.67
3:L:197:GLU:OE2	6:L:301:HOH:O	2.12	0.67
1:I:464:THR:HG21	1:I:487:VAL:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:353:ASP:OD1	1:P:396:THR:HG21	1.94	0.67
1:P:73:VAL:HG11	1:P:78:LEU:HD12	1.75	0.67
3:S:180:ARG:HD2	3:S:207:TRP:CZ2	2.30	0.67
1:V:402:MET:HE1	1:V:460:THR:HB	1.76	0.67
1:A:435:ARG:HH22	1:A:443:ARG:HH12	1.42	0.67
3:D:193:ALA:HB1	3:D:197:GLU:HG3	1.77	0.66
1:V:16:GLN:OE1	6:V:701:HOH:O	2.13	0.66
1:P:79:HIS:ND1	1:P:80:ASP:OD1	2.15	0.66
1:I:243:MET:HE1	1:I:467:GLY:HA2	1.76	0.66
4:M:188:ALA:HB1	4:M:194:MET:HB3	1.78	0.66
1:A:435:ARG:HH12	1:A:443:ARG:HH22	1.42	0.66
4:Z:188:ALA:HB1	4:Z:194:MET:HB3	1.78	0.66
1:I:435:ARG:HH22	1:I:443:ARG:HH12	1.44	0.66
1:P:464:THR:HG21	1:P:487:VAL:O	1.96	0.65
1:V:464:THR:HG22	1:V:466:GLU:N	2.09	0.65
1:I:464:THR:HG22	1:I:466:GLU:N	2.07	0.65
3:S:197:GLU:OE2	6:S:301:HOH:O	2.12	0.65
1:I:457:ASP:OD2	1:V:412:ARG:NH2	2.28	0.65
3:D:69:GLN:HG3	3:D:111:ARG:HH21	1.62	0.64
1:P:464:THR:HG22	1:P:466:GLU:N	2.07	0.64
1:A:34:LEU:HB2	1:A:214:VAL:HG22	1.80	0.64
1:V:64:ASP:OD1	1:V:68:ARG:NH1	2.26	0.64
2:K:12:GLN:HG3	2:K:13:PRO:HD2	1.80	0.64
4:T:188:ALA:HB1	4:T:194:MET:HB3	1.80	0.64
1:I:135:ILE:HG12	1:V:346:LEU:HD21	1.80	0.63
1:V:504:ARG:NH2	3:Y:102:GLU:OE1	2.31	0.63
3:S:102:GLU:OE2	4:T:265:ARG:NH2	2.29	0.63
1:I:111:GLY:O	6:I:701:HOH:O	2.15	0.63
3:L:102:GLU:OE2	4:M:265:ARG:NH2	2.24	0.63
2:C:35:GLY:HA2	2:C:72:LEU:HD13	1.82	0.62
1:P:400:LEU:O	1:P:403:ARG:HG3	2.00	0.62
3:L:128:LEU:HG	4:M:193:PRO:HB3	1.82	0.62
3:L:193:ALA:HB1	3:L:197:GLU:HG3	1.82	0.62
4:M:42:VAL:HG22	4:M:90:ALA:HB3	1.81	0.62
3:D:180:ARG:HD2	3:D:207:TRP:CH2	2.34	0.61
1:I:159:ARG:NH1	1:I:195:ASP:OD1	2.33	0.61
1:V:464:THR:CG2	1:V:466:GLU:H	2.10	0.61
3:Y:193:ALA:HB1	3:Y:197:GLU:HG3	1.83	0.61
1:I:435:ARG:HH12	1:I:443:ARG:HH22	1.48	0.61
1:P:80:ASP:OD2	1:P:103:ARG:NH2	2.32	0.61
1:I:111:GLY:N	6:I:704:HOH:O	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:254:GLU:H	3:Y:254:GLU:CD	2.04	0.61
1:I:228:ARG:NH1	6:I:705:HOH:O	2.33	0.60
1:P:507:ARG:HH12	4:T:265:ARG:HH21	1.48	0.60
1:A:81:LEU:HB3	1:A:83:MET:HE3	1.82	0.60
4:E:14:GLN:HB2	4:E:20:LEU:HD13	1.82	0.60
1:I:44:GLU:HG3	1:I:73:VAL:HG22	1.83	0.60
1:A:400:LEU:O	1:A:403:ARG:HG3	2.01	0.60
1:P:435:ARG:HH22	1:P:443:ARG:HH12	1.50	0.60
1:V:74:ASP:HB3	1:V:77:LYS:HG3	1.84	0.59
1:A:73:VAL:HG11	1:A:78:LEU:HD12	1.84	0.59
4:E:76:ASP:OD1	4:E:124:ARG:NH2	2.26	0.59
1:V:435:ARG:HH22	1:V:443:ARG:HH12	1.50	0.59
1:V:68:ARG:HG2	1:V:92:GLU:HG2	1.83	0.59
1:V:81:LEU:HB3	1:V:83:MET:CE	2.33	0.59
3:Y:247:ARG:O	3:Y:247:ARG:HG2	2.03	0.59
2:R:91:GLN:NE2	6:R:103:HOH:O	2.36	0.58
1:A:507:ARG:NH1	4:E:265:ARG:NH1	2.44	0.58
3:S:184:ASN:ND2	4:T:102:TYR:CE1	2.71	0.58
1:A:464:THR:CG2	1:A:466:GLU:H	2.15	0.58
4:E:42:VAL:HG22	4:E:90:ALA:HB3	1.85	0.58
1:P:81:LEU:HB3	1:P:83:MET:CE	2.34	0.57
4:E:100:GLN:NE2	4:E:142:SER:OG	2.37	0.57
1:A:402:MET:HE1	1:A:460:THR:HB	1.86	0.57
1:V:281:LEU:HD13	1:V:285:ILE:HD13	1.87	0.57
2:X:27:ASP:OD2	2:X:88:ARG:NH1	2.38	0.57
1:A:98:GLU:HA	1:A:125:LEU:HD13	1.87	0.56
3:Y:180:ARG:HD2	3:Y:207:TRP:CH2	2.40	0.56
1:A:81:LEU:HB3	1:A:83:MET:CE	2.35	0.56
1:V:507:ARG:HH12	4:Z:265:ARG:NH2	1.96	0.56
1:P:243:MET:HE1	1:P:467:GLY:HA2	1.85	0.56
1:I:412:ARG:NH2	1:V:457:ASP:OD2	2.36	0.56
1:P:119:GLN:NE2	6:P:706:HOH:O	2.37	0.56
1:I:243:MET:CE	1:I:467:GLY:HA2	2.35	0.56
1:V:53:VAL:HB	1:V:83:MET:CE	2.36	0.56
1:I:508:GLU:HA	4:M:265:ARG:HD2	1.87	0.55
1:P:464:THR:CG2	1:P:466:GLU:H	2.11	0.55
3:Y:121:VAL:HG23	6:Y:331:HOH:O	2.06	0.55
1:A:390:ARG:HG3	6:P:864:HOH:O	2.06	0.55
3:D:69:GLN:HG3	3:D:111:ARG:NH2	2.22	0.55
1:V:53:VAL:HB	1:V:83:MET:HE2	1.89	0.55
3:Y:174:LEU:HD22	3:Y:223:ALA:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:213:VAL:HG23	4:E:216:VAL:HG22	1.88	0.55
1:I:508:GLU:HG2	4:M:265:ARG:NE	2.22	0.55
3:L:252:ARG:NH2	3:L:255:ASP:OD2	2.34	0.54
1:A:135:ILE:HG12	1:P:346:LEU:HD21	1.88	0.54
4:Z:76:ASP:OD1	4:Z:124:ARG:NH2	2.32	0.54
1:A:418:VAL:HG22	1:A:461:HIS:HB2	1.90	0.54
1:V:548:PRO:HG2	1:V:551:PHE:HD2	1.72	0.54
1:I:507:ARG:HH12	4:M:265:ARG:NH2	1.93	0.54
4:M:76:ASP:OD1	4:M:124:ARG:NH2	2.32	0.54
1:P:500:ARG:NH2	4:T:239:LEU:O	2.38	0.54
1:I:112:PRO:HG2	1:I:113:GLN:HG2	1.88	0.54
1:V:56:GLU:HG3	1:V:152:VAL:HG12	1.90	0.54
3:Y:238:ALA:O	3:Y:242:LYS:HG3	2.08	0.54
1:I:81:LEU:HB3	1:I:83:MET:CE	2.38	0.53
3:S:11:ARG:HH22	3:S:230:ASP:CG	2.11	0.53
1:V:81:LEU:HB3	1:V:83:MET:HE3	1.90	0.53
1:I:400:LEU:O	1:I:403:ARG:HG3	2.09	0.53
1:P:552:ARG:NH1	3:Y:204:PRO:HB3	2.23	0.53
1:V:29:ALA:HB2	1:V:34:LEU:HD23	1.90	0.53
3:D:177:ARG:NH1	3:D:213:GLU:OE2	2.42	0.53
3:L:121:VAL:HG23	6:L:334:HOH:O	2.08	0.53
1:V:373:ARG:HD2	1:V:374:GLY:N	2.24	0.53
1:I:403:ARG:HG3	1:I:403:ARG:HH11	1.73	0.53
3:S:177:ARG:NH1	6:S:306:HOH:O	2.40	0.53
2:K:12:GLN:HE21	2:K:37:PRO:HB3	1.74	0.53
2:C:91:GLN:NE2	6:C:101:HOH:O	2.41	0.53
1:A:118:GLY:O	1:A:122:GLU:HG3	2.09	0.53
1:A:80:ASP:HB3	1:A:103:ARG:NH2	2.22	0.53
1:I:419:GLN:NE2	1:I:419:GLN:HA	2.11	0.53
1:P:140:ARG:HD2	1:P:144:ASP:HB3	1.92	0.52
1:V:157:ALA:HB2	1:V:190:VAL:HG11	1.90	0.52
3:D:263:LEU:HD13	3:D:277:LEU:HD22	1.92	0.52
1:I:61:LYS:HD3	1:I:153:ALA:HB3	1.91	0.52
1:A:157:ALA:HB2	1:A:190:VAL:HG11	1.91	0.52
4:M:21:ALA:N	6:M:305:HOH:O	2.41	0.52
1:P:392:ARG:HH22	1:P:396:THR:HB	1.75	0.52
3:D:36:ASP:HB2	3:D:37:PRO:HD2	1.92	0.52
1:I:81:LEU:HB3	1:I:83:MET:HE3	1.91	0.52
3:L:174:LEU:HD22	3:L:223:ALA:HB3	1.92	0.52
3:D:63:ARG:NH1	4:E:268:TRP:O	2.43	0.51
4:E:188:ALA:HB1	4:E:194:MET:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:508:GLU:HG2	4:T:265:ARG:NE	2.25	0.51
1:A:322:ILE:HG21	1:A:337:LEU:HB2	1.92	0.51
1:I:464:THR:CG2	1:I:466:GLU:H	2.12	0.51
4:M:98:PRO:HA	4:M:139:LYS:HD2	1.92	0.51
3:L:180:ARG:HD3	6:L:366:HOH:O	2.11	0.51
3:Y:203:ARG:O	3:Y:207:TRP:CD1	2.61	0.51
1:A:508:GLU:HG2	4:E:265:ARG:CZ	2.41	0.51
1:A:61:LYS:HD3	1:A:153:ALA:HB3	1.93	0.51
1:A:439:LEU:HD23	1:A:450:ALA:HB2	1.93	0.50
1:A:435:ARG:NH2	1:A:443:ARG:HH12	2.08	0.50
1:A:506:ARG:HD2	1:A:516:ASP:OD1	2.11	0.50
1:A:53:VAL:HB	1:A:83:MET:CE	2.40	0.50
1:A:464:THR:HG22	1:A:466:GLU:N	2.20	0.50
2:C:10:ALA:O	2:C:38:GLY:HA2	2.11	0.50
3:D:178:GLU:O	3:D:207:TRP:CH2	2.64	0.50
2:K:74:ASP:OD2	6:K:101:HOH:O	2.19	0.50
3:L:270:ASP:OD1	6:L:302:HOH:O	2.20	0.50
1:A:47:ILE:HG12	1:A:149:VAL:HG21	1.93	0.50
1:P:215:GLU:OE1	6:P:702:HOH:O	2.19	0.50
3:S:121:VAL:HG23	6:S:360:HOH:O	2.11	0.50
1:V:228:ARG:CZ	6:V:712:HOH:O	2.58	0.50
2:R:17:ARG:HD3	3:Y:38:PHE:CE1	2.46	0.50
1:A:243:MET:CE	1:A:467:GLY:HA2	2.41	0.50
1:A:324:GLN:O	1:A:325:ARG:HD2	2.12	0.50
3:D:24:ALA:HB1	3:D:229:LEU:HD11	1.93	0.50
1:V:231:ARG:NH1	6:V:705:HOH:O	2.30	0.50
1:I:548:PRO:HG2	1:I:551:PHE:HD2	1.76	0.50
3:L:3:ASP:N	6:L:309:HOH:O	2.44	0.49
1:P:507:ARG:HH12	4:T:265:ARG:NH2	2.10	0.49
3:Y:178:GLU:O	3:Y:207:TRP:CZ3	2.66	0.49
1:I:325:ARG:HD2	1:V:11:TRP:CG	2.47	0.49
1:I:39:LEU:HD13	1:I:214:VAL:HG21	1.93	0.49
1:P:508:GLU:HG2	4:T:265:ARG:HE	1.77	0.49
3:D:187:GLN:H	3:D:187:GLN:CD	2.15	0.49
3:L:111:ARG:NH1	6:L:310:HOH:O	2.44	0.49
1:P:403:ARG:NH2	6:P:709:HOH:O	2.42	0.49
4:T:10:LEU:O	4:T:14:GLN:HG3	2.12	0.49
3:S:111:ARG:HB3	3:S:240:PHE:CE1	2.47	0.49
2:X:14:GLY:O	2:X:34:PRO:HB3	2.12	0.49
3:Y:233:ARG:HD3	6:Y:368:HOH:O	2.11	0.49
3:D:191:GLN:NE2	4:E:175:ARG:HE	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:VAL:HG21	1:I:188:VAL:HG11	1.94	0.49
4:M:160:ASP:OD1	4:M:216:VAL:HG21	2.12	0.49
1:P:44:GLU:HG2	1:P:73:VAL:HG13	1.94	0.48
1:V:140:ARG:HD2	1:V:144:ASP:HB3	1.95	0.48
1:V:508:GLU:HG2	4:Z:265:ARG:NE	2.29	0.48
3:D:102:GLU:OE2	4:E:265:ARG:NH2	2.46	0.48
3:L:253:ALA:HA	4:M:69:TRP:CE3	2.49	0.48
1:P:202:ARG:HG2	1:P:203:VAL:N	2.29	0.48
2:C:30:VAL:HG22	2:C:75:ILE:HG12	1.96	0.48
2:K:29:GLU:HG2	2:K:76:HIS:HB2	1.95	0.48
4:E:100:GLN:NE2	4:E:143:GLY:H	1.93	0.48
6:L:301:HOH:O	4:M:105:ARG:NH2	2.47	0.48
2:R:32:LEU:HB2	2:R:96:ILE:HD13	1.94	0.48
3:S:184:ASN:ND2	4:T:102:TYR:CD1	2.82	0.48
4:M:132:LEU:HB3	4:M:152:ALA:HA	1.96	0.48
3:S:174:LEU:HD22	3:S:223:ALA:HB3	1.95	0.48
3:D:121:VAL:HG23	6:D:308:HOH:O	2.13	0.48
4:M:244:ASP:HB2	6:M:328:HOH:O	2.13	0.48
1:P:29:ALA:HB2	1:P:34:LEU:HD23	1.96	0.48
1:I:146:ILE:HD12	1:V:330:PHE:HZ	1.78	0.47
1:I:53:VAL:HB	1:I:83:MET:HE2	1.96	0.47
1:P:81:LEU:HB3	1:P:83:MET:HE3	1.95	0.47
3:D:172:TYR:HA	3:D:222:ASP:OD2	2.14	0.47
1:V:243:MET:CE	1:V:467:GLY:HA2	2.45	0.47
2:X:29:GLU:HG2	2:X:76:HIS:HB2	1.96	0.47
4:E:160:ASP:OD1	4:E:216:VAL:HG21	2.15	0.47
1:V:85:MET:O	1:V:107:PHE:HA	2.14	0.47
1:V:324:GLN:HG3	1:V:544:LEU:HD13	1.95	0.47
1:A:53:VAL:HB	1:A:83:MET:HE2	1.95	0.47
3:D:180:ARG:HD2	3:D:207:TRP:CZ2	2.49	0.47
3:Y:49:GLN:NE2	4:Z:191:VAL:HG11	2.30	0.47
4:Z:143:GLY:HA2	4:Z:146:LEU:HD12	1.96	0.47
1:P:111:GLY:N	6:P:714:HOH:O	2.47	0.47
1:V:163:VAL:HG21	1:V:188:VAL:HG11	1.96	0.47
1:A:435:ARG:HH22	1:A:443:ARG:NH1	2.11	0.47
3:D:255:ASP:O	3:D:259:ARG:HG3	2.15	0.47
1:P:56:GLU:HG3	1:P:152:VAL:HG12	1.96	0.47
1:P:273:PRO:HG2	1:P:530:ALA:HB2	1.97	0.47
1:V:256:SER:HB2	1:V:352:VAL:HG22	1.95	0.47
4:E:224:LEU:HA	4:E:224:LEU:HD23	1.75	0.47
2:K:16:GLY:O	2:K:34:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:435:ARG:HH12	1:V:443:ARG:HH22	1.61	0.47
3:S:144:GLN:HA	3:S:147:GLN:O	2.15	0.47
3:S:36:ASP:HB2	3:S:37:PRO:HD2	1.96	0.47
1:P:62:GLN:HG3	1:P:90:ARG:HD3	1.97	0.46
4:T:259:ARG:HD2	6:T:353:HOH:O	2.14	0.46
1:P:53:VAL:HB	1:P:83:MET:CE	2.46	0.46
4:T:13:PHE:CE2	4:T:31:ARG:HB3	2.50	0.46
1:V:65:PHE:CD2	1:V:216:ALA:HA	2.51	0.46
1:A:23:GLU:OE2	1:A:26:ARG:HD3	2.14	0.46
1:A:412:ARG:HD2	6:A:751:HOH:O	2.16	0.46
1:P:157:ALA:HB2	1:P:190:VAL:HG11	1.96	0.46
1:I:418:VAL:HG22	1:I:461:HIS:HB2	1.97	0.46
1:V:287:ARG:HD2	1:V:307:GLU:OE1	2.16	0.46
3:D:69:GLN:CG	3:D:111:ARG:HH21	2.27	0.46
4:E:87:ARG:NH1	6:E:301:HOH:O	2.20	0.46
1:P:392:ARG:NH2	1:P:396:THR:HB	2.30	0.46
1:V:435:ARG:NH2	1:V:443:ARG:HH12	2.13	0.46
1:I:62:GLN:HG3	1:I:90:ARG:HD3	1.97	0.46
1:V:94:LEU:HD11	1:V:117:ILE:HG13	1.97	0.46
3:Y:69:GLN:HB3	3:Y:111:ARG:NH1	2.30	0.46
1:P:435:ARG:HH12	1:P:443:ARG:HH22	1.63	0.46
3:Y:180:ARG:HD2	3:Y:207:TRP:CZ2	2.50	0.46
1:A:85:MET:O	1:A:107:PHE:HA	2.16	0.46
1:P:243:MET:CE	1:P:467:GLY:HA2	2.45	0.46
1:V:508:GLU:HA	4:Z:265:ARG:HD2	1.98	0.46
1:P:57:GLY:HA2	1:P:62:GLN:OE1	2.16	0.46
3:S:111:ARG:NH1	6:S:312:HOH:O	2.49	0.46
3:D:178:GLU:O	3:D:207:TRP:CZ3	2.69	0.45
2:R:21:GLY:HA3	2:R:88:ARG:HE	1.82	0.45
4:T:173:ALA:O	4:T:177:THR:OG1	2.30	0.45
1:I:68:ARG:HG2	1:I:92:GLU:HG2	1.98	0.45
2:X:10:ALA:O	2:X:38:GLY:HA2	2.15	0.45
1:I:115:LEU:HB3	6:I:863:HOH:O	2.17	0.45
1:I:209:TRP:N	1:I:209:TRP:CD1	2.85	0.45
4:M:56:PRO:HG2	4:M:105:ARG:NH2	2.31	0.45
1:P:489:GLY:O	1:P:494:GLY:HA3	2.17	0.45
1:P:553:SER:HB3	3:Y:178:GLU:HG3	1.98	0.45
2:C:87:LEU:O	2:C:91:GLN:HG3	2.17	0.45
1:I:390:ARG:HB2	1:V:387:HIS:CD2	2.51	0.45
1:V:81:LEU:HB3	1:V:83:MET:HE1	1.98	0.45
1:A:94:LEU:HD11	1:A:117:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD13	1:A:214:VAL:HG21	1.98	0.45
4:T:55:PHE:HA	4:T:56:PRO:HD3	1.75	0.45
4:Z:228:ARG:NH1	6:Z:303:HOH:O	2.43	0.45
1:A:312:PHE:CD1	1:A:344:CYS:HB3	2.52	0.45
1:A:196:ASP:OD2	1:A:198:ARG:NH2	2.49	0.45
1:A:64:ASP:HA	1:A:67:SER:HB3	1.99	0.45
1:V:548:PRO:HG2	1:V:551:PHE:CD2	2.52	0.45
4:E:244:ASP:HB2	6:E:364:HOH:O	2.17	0.45
1:P:228:ARG:HA	1:P:228:ARG:HD3	1.83	0.45
4:Z:14:GLN:HE21	4:Z:20:LEU:HD22	1.82	0.45
1:V:552:ARG:NH1	1:V:554:TRP:OXT	2.50	0.44
1:I:228:ARG:NH1	1:I:262:GLY:HA2	2.32	0.44
3:Y:75:ALA:HA	3:Y:115:LEU:HB2	1.99	0.44
4:Z:14:GLN:NE2	4:Z:20:LEU:HD22	2.33	0.44
1:V:312:PHE:CD1	1:V:344:CYS:HB3	2.53	0.44
1:V:324:GLN:O	1:V:325:ARG:HD2	2.17	0.44
2:K:53:SER:O	2:K:57:HIS:CD2	2.71	0.44
2:K:57:HIS:H	2:K:57:HIS:CD2	2.34	0.44
3:L:115:LEU:HB3	6:L:372:HOH:O	2.17	0.44
3:D:230:ASP:OD2	3:D:233:ARG:NH2	2.48	0.44
1:P:244:ALA:O	1:P:248:ILE:HB	2.17	0.44
2:X:13:PRO:HA	2:X:70:ALA:HB3	1.99	0.44
2:X:12:GLN:HG3	2:X:13:PRO:HD2	2.00	0.44
4:E:216:VAL:HG23	6:E:306:HOH:O	2.18	0.44
1:P:403:ARG:HH11	1:P:403:ARG:HG3	1.83	0.44
1:A:463:LEU:HD12	1:A:464:THR:N	2.33	0.44
3:D:257:LEU:HG	4:E:69:TRP:HB3	1.99	0.44
2:K:91:GLN:O	2:K:94:GLU:HB3	2.18	0.44
1:P:532:LYS:HG2	3:Y:15:GLU:CG	2.47	0.44
1:A:449:LEU:HD23	6:A:849:HOH:O	2.17	0.44
1:I:56:GLU:HG3	1:I:152:VAL:HG12	2.00	0.44
1:P:390:ARG:HD2	1:P:412:ARG:NH2	2.33	0.44
1:P:532:LYS:HG2	3:Y:15:GLU:HG3	2.00	0.44
1:P:322:ILE:HG21	1:P:337:LEU:HB2	2.00	0.43
2:X:7:GLU:OE1	2:X:39:LYS:HE2	2.17	0.43
1:P:403:ARG:NE	6:P:709:HOH:O	2.43	0.43
2:R:21:GLY:CA	2:R:88:ARG:HE	2.30	0.43
1:V:362:VAL:O	1:V:432:PHE:HA	2.18	0.43
3:Y:265:THR:O	4:Z:105:ARG:NH1	2.51	0.43
3:D:178:GLU:C	3:D:207:TRP:HZ3	2.21	0.43
1:I:188:VAL:HG13	1:I:213:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:21:ARG:HD3	1:P:46:LEU:O	2.18	0.43
1:V:57:GLY:HA2	1:V:62:GLN:OE1	2.17	0.43
1:P:64:ASP:HA	1:P:67:SER:HB3	2.00	0.43
2:X:16:GLY:O	2:X:34:PRO:HD3	2.19	0.43
1:A:171:ASP:OD1	1:A:171:ASP:N	2.51	0.43
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.83	0.43
2:C:14:GLY:O	2:C:34:PRO:HB3	2.18	0.43
2:R:6:PHE:HB2	2:R:42:ILE:HB	2.01	0.43
1:A:21:ARG:HD3	1:A:46:LEU:O	2.19	0.43
1:V:396:THR:HG22	1:V:399:TRP:CB	2.49	0.43
1:V:449:LEU:HD23	6:V:850:HOH:O	2.18	0.43
3:Y:160:PHE:HA	3:Y:182:GLY:O	2.18	0.43
4:Z:12:TRP:CH2	4:Z:219:PRO:HB3	2.54	0.43
1:A:68:ARG:HG2	1:A:92:GLU:HG2	2.00	0.43
1:I:146:ILE:HG12	6:I:817:HOH:O	2.18	0.43
1:V:251:ARG:NH2	6:V:719:HOH:O	2.51	0.43
1:V:478:GLU:HB2	6:V:849:HOH:O	2.18	0.43
1:I:164:TYR:CD2	1:I:201:PRO:HG2	2.54	0.43
1:I:501:GLU:O	1:I:505:MET:HG3	2.19	0.43
4:Z:160:ASP:OD1	4:Z:216:VAL:HG21	2.18	0.43
1:A:202:ARG:HG2	1:A:203:VAL:N	2.34	0.43
1:I:373:ARG:NH2	1:I:440:GLU:HG3	2.34	0.43
2:K:7:GLU:OE1	2:K:39:LYS:HD3	2.19	0.43
1:P:37:GLU:CD	1:P:37:GLU:H	2.22	0.43
3:S:201:ARG:HD2	3:S:201:ARG:HA	1.72	0.43
1:V:243:MET:HE3	1:V:517:LEU:HD12	2.01	0.43
1:V:544:LEU:HA	1:V:544:LEU:HD23	1.80	0.43
3:S:190:GLU:OE1	3:S:200:SER:OG	2.23	0.42
4:T:15:ALA:HB1	4:T:224:LEU:HD11	2.01	0.42
1:I:347:ALA:HA	1:V:139:ALA:HB1	2.00	0.42
1:V:66:LEU:HD21	1:V:189:GLN:HB3	2.00	0.42
3:Y:121:VAL:HG22	3:Y:133:ILE:HD12	2.01	0.42
1:A:521:ARG:NH2	6:A:707:HOH:O	2.39	0.42
3:L:51:ILE:HD12	3:L:124:GLN:HG2	2.01	0.42
1:V:368:SER:OG	1:V:419:GLN:NE2	2.48	0.42
1:I:228:ARG:NH2	6:I:719:HOH:O	2.52	0.42
1:I:506:ARG:HD3	1:I:516:ASP:OD1	2.19	0.42
2:X:87:LEU:O	2:X:91:GLN:HG2	2.18	0.42
1:V:257:LEU:HA	1:V:352:VAL:HG13	2.01	0.42
1:V:322:ILE:HD13	1:V:337:LEU:HD22	2.02	0.42
3:Y:59:VAL:HG23	3:Y:89:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:92:LEU:HD22	4:Z:133:ILE:HB	2.01	0.42
3:D:254:GLU:H	3:D:254:GLU:CD	2.22	0.42
2:K:10:ALA:O	2:K:38:GLY:HA2	2.20	0.42
4:M:185:GLU:HB3	4:M:186:ALA:H	1.60	0.42
4:M:92:LEU:HD13	4:M:231:LEU:HD13	2.02	0.42
1:P:90:ARG:NH1	6:P:710:HOH:O	2.43	0.42
3:L:160:PHE:HA	3:L:182:GLY:O	2.19	0.42
1:A:36:ARG:HG3	1:A:65:PHE:CZ	2.55	0.42
1:I:478:GLU:HB2	6:I:851:HOH:O	2.19	0.42
1:P:36:ARG:HD3	1:P:215:GLU:O	2.19	0.42
1:V:498:ASP:OD1	1:V:500:ARG:HD3	2.20	0.42
1:P:81:LEU:HB3	1:P:83:MET:HE1	1.99	0.42
3:D:203:ARG:O	3:D:207:TRP:CD1	2.59	0.41
4:E:143:GLY:HA2	4:E:146:LEU:HD12	2.02	0.41
3:S:247:ARG:HA	3:S:248:PRO:HD2	1.94	0.41
4:Z:172:ALA:O	4:Z:176:ILE:HG13	2.19	0.41
1:I:322:ILE:HG21	1:I:337:LEU:HB2	2.01	0.41
1:I:70:LEU:O	1:I:73:VAL:HB	2.20	0.41
1:P:246:ARG:HG2	1:P:517:LEU:HB3	2.01	0.41
1:P:90:ARG:HD2	6:P:710:HOH:O	2.20	0.41
1:V:142:VAL:HG12	1:V:178:PRO:HB3	2.02	0.41
1:A:44:GLU:HG2	1:A:73:VAL:HG13	2.02	0.41
1:I:29:ALA:HB2	1:I:34:LEU:HD23	2.02	0.41
1:I:435:ARG:NH2	1:I:443:ARG:HH12	2.14	0.41
4:M:188:ALA:CB	4:M:194:MET:HB3	2.48	0.41
1:V:91:PRO:N	1:V:113:GLN:HE22	2.17	0.41
1:A:209:TRP:N	1:A:209:TRP:CD1	2.87	0.41
1:A:347:ALA:HA	1:P:139:ALA:HB1	2.03	0.41
1:A:390:ARG:NH1	1:P:457:ASP:OD2	2.54	0.41
1:P:53:VAL:HB	1:P:83:MET:HE2	2.02	0.41
3:S:254:GLU:HG2	3:S:255:ASP:N	2.36	0.41
1:V:64:ASP:HA	1:V:67:SER:HB3	2.02	0.41
1:P:363:ASP:HA	1:P:433:VAL:O	2.21	0.41
1:V:418:VAL:HG22	1:V:461:HIS:HB2	2.02	0.41
1:V:90:ARG:HB3	1:V:92:GLU:OE2	2.21	0.41
4:Z:188:ALA:CB	4:Z:194:MET:HB3	2.49	0.41
4:Z:20:LEU:O	4:Z:21:ALA:C	2.59	0.41
1:A:231:ARG:NH1	6:A:720:HOH:O	2.52	0.41
2:C:17:ARG:NH2	6:C:102:HOH:O	2.51	0.41
4:E:175:ARG:NH1	6:E:302:HOH:O	2.31	0.41
3:S:247:ARG:HG2	3:S:252:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:506:ARG:HD2	1:V:516:ASP:OD1	2.21	0.41
3:L:216:PHE:CG	3:L:224:TYR:HB2	2.56	0.41
4:M:55:PHE:HA	4:M:56:PRO:HD3	1.77	0.41
1:V:405:GLU:HA	1:V:406:PRO:HD2	1.91	0.41
1:P:68:ARG:HG2	1:P:92:GLU:HG2	2.03	0.41
3:Y:219:GLY:O	3:Y:249:ARG:HD3	2.20	0.41
1:A:39:LEU:HD21	1:A:66:LEU:HD23	2.03	0.41
3:D:178:GLU:HG2	3:D:178:GLU:O	2.21	0.41
1:P:428:GLY:HA2	6:P:803:HOH:O	2.20	0.41
2:R:21:GLY:HA2	2:R:88:ARG:HH21	1.86	0.41
4:T:185:GLU:C	4:T:187:LEU:H	2.23	0.41
1:P:550:ARG:HB2	6:P:868:HOH:O	2.20	0.41
4:Z:132:LEU:HB3	4:Z:152:ALA:HA	2.03	0.41
4:M:44:PHE:CE2	4:M:92:LEU:HD12	2.56	0.41
3:S:185:GLY:HA2	3:S:186:PRO:HD3	1.92	0.41
1:A:402:MET:HE2	1:A:460:THR:HG21	2.04	0.40
1:I:498:ASP:OD1	1:I:500:ARG:HD3	2.21	0.40
1:I:550:ARG:HD2	1:I:551:PHE:CE2	2.55	0.40
1:P:396:THR:HG22	1:P:399:TRP:CB	2.51	0.40
3:S:254:GLU:HG3	6:S:309:HOH:O	2.20	0.40
1:I:287:ARG:HD2	1:I:307:GLU:OE1	2.20	0.40
1:P:61:LYS:HD3	1:P:153:ALA:HB3	2.04	0.40
1:A:548:PRO:HG2	1:A:551:PHE:HD2	1.87	0.40
2:C:32:LEU:HB2	2:C:96:ILE:HD13	2.03	0.40
4:E:259:ARG:HD2	6:E:336:HOH:O	2.22	0.40
1:V:228:ARG:HD3	1:V:228:ARG:HA	1.83	0.40
1:A:243:MET:HE1	1:A:514:PRO:HD3	2.04	0.40
3:L:67:ASP:HB2	3:L:237:LEU:HD22	2.04	0.40
3:S:59:VAL:CG2	3:S:89:SER:HB2	2.52	0.40
1:A:56:GLU:HG3	1:A:152:VAL:HG12	2.03	0.40
1:I:303:SER:HB2	1:I:305:TRP:HD1	1.86	0.40
4:M:63:VAL:HG12	4:M:115:LEU:HD11	2.03	0.40
1:P:164:TYR:CD2	1:P:201:PRO:HG2	2.56	0.40

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	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%)	13	10
All	All	4668/4896 (95%)	4522 (97%)	143 (3%)	3 (0%)	51	60

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 ⓘ

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%)	442 (98%)	9 (2%)	55	69
1	I	451/457 (99%)	438 (97%)	13 (3%)	42	54
1	P	451/457 (99%)	439 (97%)	12 (3%)	44	57
1	V	451/457 (99%)	441 (98%)	10 (2%)	52	65
2	C	78/80 (98%)	74 (95%)	4 (5%)	24	29
2	K	78/80 (98%)	75 (96%)	3 (4%)	33	42
2	R	78/80 (98%)	75 (96%)	3 (4%)	33	42
2	X	78/80 (98%)	74 (95%)	4 (5%)	24	29
3	D	202/209 (97%)	198 (98%)	4 (2%)	55	69
3	L	202/209 (97%)	201 (100%)	1 (0%)	88	94
3	S	202/209 (97%)	201 (100%)	1 (0%)	88	94
3	Y	202/209 (97%)	199 (98%)	3 (2%)	65	78
4	E	182/209 (87%)	180 (99%)	2 (1%)	73	85
4	M	182/209 (87%)	179 (98%)	3 (2%)	62	76
4	T	182/209 (87%)	180 (99%)	2 (1%)	73	85
4	Z	182/209 (87%)	180 (99%)	2 (1%)	73	85
All	All	3652/3820 (96%)	3576 (98%)	76 (2%)	53	67

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	61	LYS
1	A	171	ASP
1	A	208	SER
1	A	343	PHE
1	A	396	THR
1	A	419	GLN
1	A	464	THR

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Mol	Chain	Res	Type
1	A	504	ARG
2	C	19	LEU
2	C	31	LEU
2	C	78	PHE
2	C	96	ILE
3	D	15	GLU
3	D	49	GLN
3	D	111	ARG
3	D	254	GLU
4	E	100	GLN
4	E	150	TYR
1	P	61	LYS
1	P	119	GLN
1	P	137	LEU
1	P	171	ASP
1	P	198	ARG
1	P	208	SER
1	P	230	PRO
1	P	251	ARG
1	P	343	PHE
1	P	396	THR
1	P	464	THR
1	P	552	ARG
2	R	12	GLN
2	R	20	VAL
2	R	78	PHE
3	S	19	ARG
4	T	150	TYR
4	T	190	LYS
1	I	171	ASP
1	I	188	VAL
1	I	198	ARG
1	I	208	SER
1	I	251	ARG
1	I	325	ARG
1	I	343	PHE
1	I	352	VAL
1	I	419	GLN
1	I	464	THR
1	I	525	SER
1	I	550	ARG
1	I	552	ARG

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Mol	Chain	Res	Type
2	K	12	GLN
2	K	58	LEU
2	K	96	ILE
3	L	67	ASP
4	M	150	TYR
4	M	187	LEU
4	M	216	VAL
1	V	37	GLU
1	V	92	GLU
1	V	144	ASP
1	V	160	GLU
1	V	171	ASP
1	V	343	PHE
1	V	396	THR
1	V	457	ASP
1	V	464	THR
1	V	552	ARG
2	X	12	GLN
2	X	22	CYS
2	X	58	LEU
2	X	78	PHE
3	Y	15	GLU
3	Y	42	GLN
3	Y	247	ARG
4	Z	150	TYR
4	Z	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
3	D	49	GLN
3	D	184	ASN
4	E	100	GLN
1	P	113	GLN
1	P	349	GLN
3	S	49	GLN
1	I	419	GLN
2	K	12	GLN
1	V	113	GLN
4	Z	14	GLN

### 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 ⓘ

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	V	601	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLI	A	601	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLI	P	601	-	0,6,6	0.00	-	0,7,7	0.00	-
5	MLI	I	601	-	0,6,6	0.00	-	0,7,7	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
5	MLI	V	601	-	-	0/0/4/4	-
5	MLI	A	601	-	-	0/0/4/4	-
5	MLI	P	601	-	-	0/0/4/4	-
5	MLI	I	601	-	-	0/0/4/4	-

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

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	548/554 (98%)	-0.52	4 (0%) 87 86	21, 32, 56, 80	0
1	I	548/554 (98%)	-0.52	2 (0%) 92 91	21, 33, 58, 76	0
1	P	548/554 (98%)	-0.53	2 (0%) 92 91	21, 31, 55, 70	0
1	V	548/554 (98%)	-0.51	2 (0%) 92 91	20, 33, 57, 76	0
2	C	97/99 (97%)	-0.45	1 (1%) 82 81	27, 37, 53, 78	0
2	K	97/99 (97%)	-0.43	0 100 100	26, 36, 50, 75	0
2	R	97/99 (97%)	-0.46	0 100 100	25, 36, 50, 77	0
2	X	97/99 (97%)	-0.44	1 (1%) 82 81	25, 36, 52, 76	0
3	D	276/287 (96%)	-0.52	0 100 100	23, 36, 57, 70	0
3	L	276/287 (96%)	-0.59	0 100 100	22, 31, 50, 65	0
3	S	276/287 (96%)	-0.60	0 100 100	21, 30, 49, 65	0
3	Y	276/287 (96%)	-0.55	0 100 100	22, 33, 52, 68	0
4	E	256/284 (90%)	-0.45	3 (1%) 79 77	24, 37, 63, 86	0
4	M	256/284 (90%)	-0.43	3 (1%) 79 77	23, 35, 67, 85	0
4	T	256/284 (90%)	-0.42	4 (1%) 72 70	23, 35, 69, 85	0
4	Z	256/284 (90%)	-0.50	1 (0%) 92 91	23, 33, 63, 85	0
All	All	4708/4896 (96%)	-0.51	23 (0%) 91 90	20, 33, 57, 86	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	T	20	LEU	5.0
4	T	19	SER	4.9
4	M	20	LEU	4.6
1	A	112	PRO	3.5
1	V	26	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
4	Z	20	LEU	2.7
4	M	21	ALA	2.6
4	E	20	LEU	2.6
1	P	112	PRO	2.6
4	T	21	ALA	2.5
2	X	15	ARG	2.5
4	M	19	SER	2.5
1	A	24	ARG	2.3
2	C	15	ARG	2.3
1	I	112	PRO	2.2
1	A	26	ARG	2.2
1	A	113	GLN	2.1
4	E	6	ALA	2.1
4	T	177	THR	2.1
1	V	112	PRO	2.1
1	P	9	PRO	2.1
1	I	192	ARG	2.0
4	E	188	ALA	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
5	MLI	I	601	7/7	0.97	0.12	23,27,32,37	0
5	MLI	A	601	7/7	0.98	0.10	23,25,32,35	0
5	MLI	P	601	7/7	0.98	0.10	21,24,30,31	0
5	MLI	V	601	7/7	0.98	0.08	21,27,29,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.