



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 02:35 PM BST

PDB ID : 3PXI
Title : Structure of MecA108:ClpC
Authors : Wang, F.; Mei, Z.Q.; Wang, J.W.; Shi, Y.G.
Deposited on : 2010-12-09
Resolution : 6.93 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

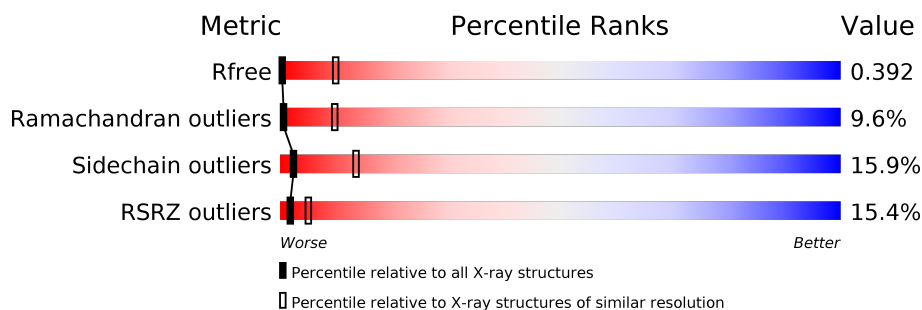
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.93 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	1003 (9.70-3.90)
Ramachandran outliers	138981	1001 (9.70-3.90)
Sidechain outliers	138945	1001 (9.70-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 ≥ 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	111	<div> <div>8%</div> <div>61%</div> <div>23%</div> <div>15%</div> </div>
1	b	111	<div> <div>30%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
1	c	111	<div> <div>18%</div> <div>67%</div> <div>18%</div> <div>15%</div> </div>
2	A	758	<div> <div>14%</div> <div>73%</div> <div>19%</div> <div>7%</div> </div>
2	B	758	<div> <div>15%</div> <div>71%</div> <div>20%</div> <div>7%</div> </div>
2	C	758	<div> <div>12%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18645 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 Adapter protein mecA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	94	Total	C	N	O	S	0	0	0
			755	486	118	149	2			
1	b	94	Total	C	N	O	S	0	0	0
			756	485	120	149	2			
1	c	94	Total	C	N	O	S	0	0	0
			763	491	120	150	2			

- Molecule 2 is a protein called Negative regulator of genetic competence ClpC/MecB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	708	Total	C	N	O	S	0	0	0
			5455	3394	993	1055	13			
2	B	704	Total	C	N	O	S	0	0	0
			5437	3385	985	1054	13			
2	C	711	Total	C	N	O	S	0	0	0
			5479	3410	993	1063	13			

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	ALA	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	THR	DELETION	UNP P37571
A	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	HIS	DELETION	UNP P37571
A	?	-	THR	DELETION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	ILE	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	ALA	DELETION	UNP P37571
A	?	-	GLU	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	ARG	DELETION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	SER	DELETION	UNP P37571
A	?	-	PRO	DELETION	UNP P37571
A	?	-	PRO	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	TYR	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	TYR	DELETION	UNP P37571
A	?	-	ASP	DELETION	UNP P37571
A	?	-	GLU	DELETION	UNP P37571
A	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
A	?	-	LEU	DELETION	UNP P37571
A	?	-	LYS	DELETION	UNP P37571
A	?	-	ARG	DELETION	UNP P37571
A	?	-	ASN	DELETION	UNP P37571
A	?	-	LYS	DELETION	UNP P37571
A	?	-	TYR	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	GLY	DELETION	UNP P37571
A	?	-	PHE	DELETION	UNP P37571
A	?	-	ASN	DELETION	UNP P37571
A	?	-	VAL	DELETION	UNP P37571
A	?	-	GLN	DELETION	UNP P37571
A	?	-	ASP	DELETION	UNP P37571
A	?	-	GLU	DELETION	UNP P37571
A	?	-	THR	DELETION	UNP P37571
A	?	-	GLN	DELETION	UNP P37571
A	?	-	ASN	DELETION	UNP P37571
A	?	-	HIS	DELETION	UNP P37571
A	?	-	LYS	DELETION	UNP P37571
A	?	-	ASP	DELETION	UNP P37571
A	?	-	MET	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	ALA	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	THR	DELETION	UNP P37571
B	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	HIS	DELETION	UNP P37571
B	?	-	THR	DELETION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	ILE	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	ALA	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	ALA	DELETION	UNP P37571
B	?	-	GLU	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	ARG	DELETION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	SER	DELETION	UNP P37571
B	?	-	PRO	DELETION	UNP P37571
B	?	-	PRO	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	TYR	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	TYR	DELETION	UNP P37571
B	?	-	ASP	DELETION	UNP P37571
B	?	-	GLU	DELETION	UNP P37571
B	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	?	-	LEU	DELETION	UNP P37571
B	?	-	LYS	DELETION	UNP P37571
B	?	-	ARG	DELETION	UNP P37571
B	?	-	ASN	DELETION	UNP P37571
B	?	-	LYS	DELETION	UNP P37571
B	?	-	TYR	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	GLY	DELETION	UNP P37571
B	?	-	PHE	DELETION	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	DELETION	UNP P37571
B	?	-	VAL	DELETION	UNP P37571
B	?	-	GLN	DELETION	UNP P37571
B	?	-	ASP	DELETION	UNP P37571
B	?	-	GLU	DELETION	UNP P37571
B	?	-	THR	DELETION	UNP P37571
B	?	-	GLN	DELETION	UNP P37571
B	?	-	ASN	DELETION	UNP P37571
B	?	-	HIS	DELETION	UNP P37571
B	?	-	LYS	DELETION	UNP P37571
B	?	-	ASP	DELETION	UNP P37571
B	?	-	MET	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	ALA	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	THR	DELETION	UNP P37571
C	280	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	HIS	DELETION	UNP P37571
C	?	-	THR	DELETION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	ILE	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	ALA	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	ALA	DELETION	UNP P37571
C	?	-	GLU	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	ARG	DELETION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	SER	DELETION	UNP P37571
C	?	-	PRO	DELETION	UNP P37571
C	?	-	PRO	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	TYR	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	TYR	DELETION	UNP P37571

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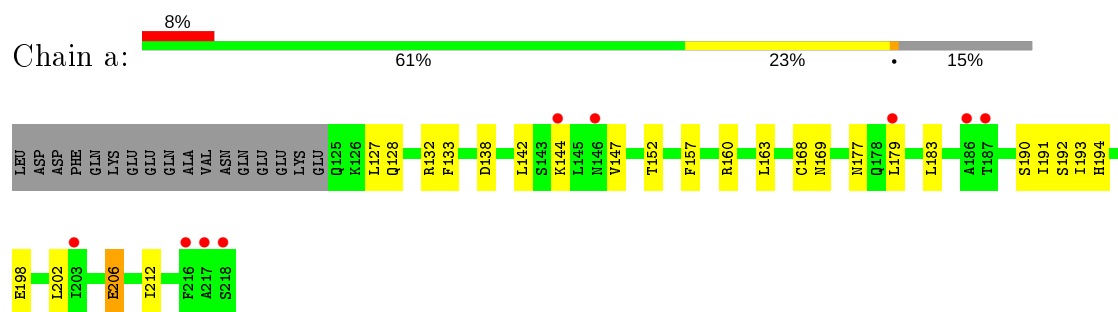
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	DELETION	UNP P37571
C	?	-	GLU	DELETION	UNP P37571
C	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
C	?	-	LEU	DELETION	UNP P37571
C	?	-	LYS	DELETION	UNP P37571
C	?	-	ARG	DELETION	UNP P37571
C	?	-	ASN	DELETION	UNP P37571
C	?	-	LYS	DELETION	UNP P37571
C	?	-	TYR	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	GLY	DELETION	UNP P37571
C	?	-	PHE	DELETION	UNP P37571
C	?	-	ASN	DELETION	UNP P37571
C	?	-	VAL	DELETION	UNP P37571
C	?	-	GLN	DELETION	UNP P37571
C	?	-	ASP	DELETION	UNP P37571
C	?	-	GLU	DELETION	UNP P37571
C	?	-	THR	DELETION	UNP P37571
C	?	-	GLN	DELETION	UNP P37571
C	?	-	ASN	DELETION	UNP P37571
C	?	-	HIS	DELETION	UNP P37571
C	?	-	LYS	DELETION	UNP P37571
C	?	-	ASP	DELETION	UNP P37571
C	?	-	MET	DELETION	UNP P37571

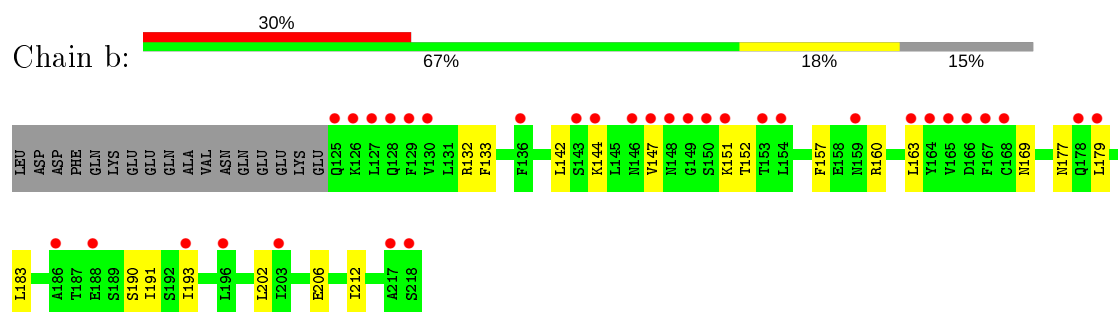
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

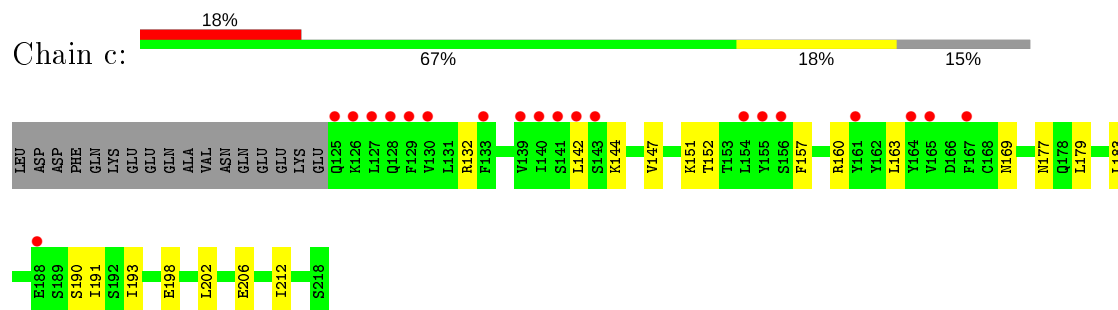
- Molecule 1: Adapter protein mecA 1



- Molecule 1: Adapter protein mecA 1



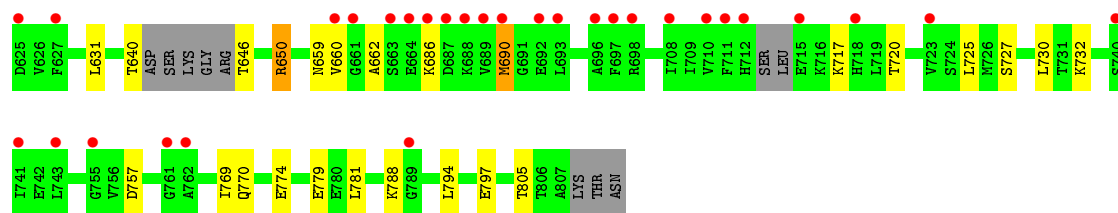
- Molecule 1: Adapter protein mecA 1



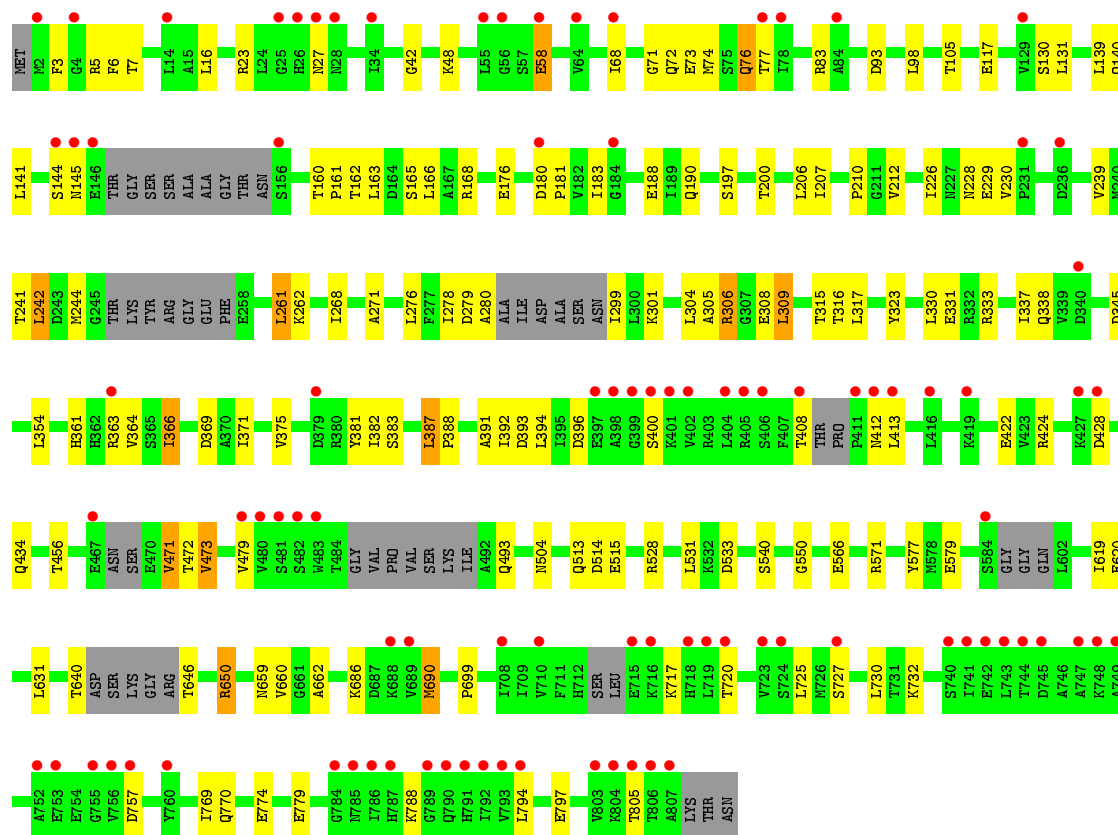
- Molecule 2: Negative regulator of genetic competence ClpC/MecB







• Molecule 2: Negative regulator of genetic competence ClpC/MecB



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	141.81Å 141.81Å 656.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.15 – 6.93 49.15 – 6.93	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.15-6.93) 99.6 (49.15-6.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.84 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.407 , 0.422 0.372 , 0.392	Depositor DCC
R_{free} test set	333 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	188.0	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 751.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	18645	wwPDB-VP
Average B, all atoms (Å ²)	642.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.48	0/768	0.66	1/1035 (0.1%)
1	b	0.56	0/768	0.67	0/1035
1	c	0.64	0/776	0.68	0/1046
2	A	0.52	1/5498 (0.0%)	0.70	2/7386 (0.0%)
2	B	0.58	2/5483 (0.0%)	0.80	2/7369 (0.0%)
2	C	0.53	1/5526 (0.0%)	0.72	2/7431 (0.0%)
All	All	0.55	4/18819 (0.0%)	0.73	7/25302 (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
2	A	0	1
2	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	515	GLU	CG-CD	5.50	1.60	1.51
2	A	515	GLU	CG-CD	5.49	1.60	1.51
2	C	515	GLU	CG-CD	5.42	1.60	1.51
2	B	334	PHE	CA-CB	5.26	1.65	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	161	PRO	N-CA-CB	6.09	110.61	103.30
2	C	161	PRO	N-CA-CB	5.88	110.35	103.30
2	B	161	PRO	N-CA-CB	5.25	109.60	103.30
1	a	138	ASP	CB-CG-OD1	5.23	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	515	GLU	OE1-CD-OE2	-5.15	117.12	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	210	PRO	Peptide
2	C	210	PRO	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	2	22
1	b	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	2	22
1	c	92/111 (83%)	75 (82%)	13 (14%)	4 (4%)	2	22
2	A	686/758 (90%)	493 (72%)	127 (18%)	66 (10%)	0	10
2	B	682/758 (90%)	491 (72%)	115 (17%)	76 (11%)	0	7
2	C	691/758 (91%)	492 (71%)	130 (19%)	69 (10%)	0	9
All	All	2335/2607 (90%)	1703 (73%)	409 (18%)	223 (10%)	0	10

5 of 223 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	169	ASN
2	A	42	GLY

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Mol	Chain	Res	Type
2	A	98	LEU
2	A	144	SER
2	A	183	ILE

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	83/104 (80%)	67 (81%)	16 (19%)	1	8
1	b	84/104 (81%)	68 (81%)	16 (19%)	1	8
1	c	85/104 (82%)	69 (81%)	16 (19%)	1	9
2	A	571/645 (88%)	487 (85%)	84 (15%)	3	15
2	B	573/645 (89%)	476 (83%)	97 (17%)	2	12
2	C	576/645 (89%)	492 (85%)	84 (15%)	3	15
All	All	1972/2247 (88%)	1659 (84%)	313 (16%)	2	13

5 of 313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	235	ARG
2	B	443	ARG
2	C	571	ARG
2	B	276	LEU
2	B	355	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	126	ASN
2	B	310	GLN
2	C	362	HIS
2	B	137	GLN
2	B	203	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	A	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	664:GLU	C	686:LYS	N	7.77
1	B	664:GLU	C	686:LYS	N	7.77
1	C	664:GLU	C	686:LYS	N	7.77

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, 95th 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 ²)	Q<0.9
1	a	94/111 (84%)	0.76	9 (9%) 8 11	583, 624, 738, 792	0
1	b	94/111 (84%)	1.55	33 (35%) 0 2	543, 603, 730, 756	0
1	c	94/111 (84%)	1.14	20 (21%) 0 3	523, 590, 707, 731	0
2	A	708/758 (93%)	0.97	104 (14%) 2 5	508, 632, 810, 849	0
2	B	704/758 (92%)	0.92	110 (15%) 2 5	523, 661, 747, 823	0
2	C	711/758 (93%)	0.86	94 (13%) 3 7	426, 601, 842, 889	0
All	All	2405/2607 (92%)	0.94	370 (15%) 2 5	426, 636, 815, 889	0

The worst 5 of 370 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	411	PRO	7.9
2	A	231	PRO	7.4
2	A	465	GLY	7.2
2	A	466	GLN	6.9
2	C	720	THR	6.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.