



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2018 – 04:54 PM EST

PDB ID : 4FDG
Title : Crystal Structure of an Archaeal MCM Filament
Authors : Slaymaker, I.M.; Fu, Y.; Brewster, A.B.; Chen, X.S.
Deposited on : 2012-05-28
Resolution : 4.10 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

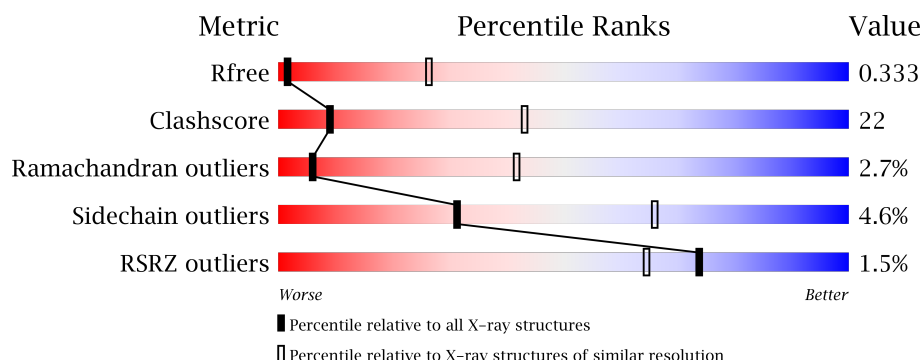
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1153 (4.60-3.60)
Clashscore	112137	1002 (4.54-3.66)
Ramachandran outliers	110173	1000 (4.58-3.62)
Sidechain outliers	110143	1191 (4.60-3.60)
RSRZ outliers	101464	1165 (4.60-3.60)

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. 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	692	<div> <div>2%</div> <div>52%</div> <div>29%</div> <div>• •</div> <div>14%</div> </div>
1	B	692	<div> <div>%</div> <div>51%</div> <div>30%</div> <div>• •</div> <div>14%</div> </div>
1	C	692	<div> <div>%</div> <div>51%</div> <div>31%</div> <div>• •</div> <div>14%</div> </div>
1	D	692	<div> <div>%</div> <div>51%</div> <div>30%</div> <div>• •</div> <div>14%</div> </div>
1	E	692	<div> <div>%</div> <div>52%</div> <div>30%</div> <div>• •</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23585 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 Minichromosome maintenance protein MCM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			
1	A	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			
1	C	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			
1	D	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			
1	E	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP Q9UXG1
B	-4	HIS	-	EXPRESSION TAG	UNP Q9UXG1
B	-3	HIS	-	EXPRESSION TAG	UNP Q9UXG1
B	-2	HIS	-	EXPRESSION TAG	UNP Q9UXG1
B	-1	HIS	-	EXPRESSION TAG	UNP Q9UXG1
B	0	HIS	-	EXPRESSION TAG	UNP Q9UXG1
B	1	MET	-	EXPRESSION TAG	UNP Q9UXG1
B	2	GLU	-	EXPRESSION TAG	UNP Q9UXG1
B	3	ILE	-	EXPRESSION TAG	UNP Q9UXG1
B	4	PRO	-	EXPRESSION TAG	UNP Q9UXG1
B	5	SER	-	EXPRESSION TAG	UNP Q9UXG1
B	6	LYS	-	EXPRESSION TAG	UNP Q9UXG1
A	-5	HIS	-	EXPRESSION TAG	UNP Q9UXG1
A	-4	HIS	-	EXPRESSION TAG	UNP Q9UXG1
A	-3	HIS	-	EXPRESSION TAG	UNP Q9UXG1
A	-2	HIS	-	EXPRESSION TAG	UNP Q9UXG1
A	-1	HIS	-	EXPRESSION TAG	UNP Q9UXG1
A	0	HIS	-	EXPRESSION TAG	UNP Q9UXG1
A	1	MET	-	EXPRESSION TAG	UNP Q9UXG1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	-	EXPRESSION TAG	UNP Q9UXG1
A	3	ILE	-	EXPRESSION TAG	UNP Q9UXG1
A	4	PRO	-	EXPRESSION TAG	UNP Q9UXG1
A	5	SER	-	EXPRESSION TAG	UNP Q9UXG1
A	6	LYS	-	EXPRESSION TAG	UNP Q9UXG1
C	-5	HIS	-	EXPRESSION TAG	UNP Q9UXG1
C	-4	HIS	-	EXPRESSION TAG	UNP Q9UXG1
C	-3	HIS	-	EXPRESSION TAG	UNP Q9UXG1
C	-2	HIS	-	EXPRESSION TAG	UNP Q9UXG1
C	-1	HIS	-	EXPRESSION TAG	UNP Q9UXG1
C	0	HIS	-	EXPRESSION TAG	UNP Q9UXG1
C	1	MET	-	EXPRESSION TAG	UNP Q9UXG1
C	2	GLU	-	EXPRESSION TAG	UNP Q9UXG1
C	3	ILE	-	EXPRESSION TAG	UNP Q9UXG1
C	4	PRO	-	EXPRESSION TAG	UNP Q9UXG1
C	5	SER	-	EXPRESSION TAG	UNP Q9UXG1
C	6	LYS	-	EXPRESSION TAG	UNP Q9UXG1
D	-5	HIS	-	EXPRESSION TAG	UNP Q9UXG1
D	-4	HIS	-	EXPRESSION TAG	UNP Q9UXG1
D	-3	HIS	-	EXPRESSION TAG	UNP Q9UXG1
D	-2	HIS	-	EXPRESSION TAG	UNP Q9UXG1
D	-1	HIS	-	EXPRESSION TAG	UNP Q9UXG1
D	0	HIS	-	EXPRESSION TAG	UNP Q9UXG1
D	1	MET	-	EXPRESSION TAG	UNP Q9UXG1
D	2	GLU	-	EXPRESSION TAG	UNP Q9UXG1
D	3	ILE	-	EXPRESSION TAG	UNP Q9UXG1
D	4	PRO	-	EXPRESSION TAG	UNP Q9UXG1
D	5	SER	-	EXPRESSION TAG	UNP Q9UXG1
D	6	LYS	-	EXPRESSION TAG	UNP Q9UXG1
E	-5	HIS	-	EXPRESSION TAG	UNP Q9UXG1
E	-4	HIS	-	EXPRESSION TAG	UNP Q9UXG1
E	-3	HIS	-	EXPRESSION TAG	UNP Q9UXG1
E	-2	HIS	-	EXPRESSION TAG	UNP Q9UXG1
E	-1	HIS	-	EXPRESSION TAG	UNP Q9UXG1
E	0	HIS	-	EXPRESSION TAG	UNP Q9UXG1
E	1	MET	-	EXPRESSION TAG	UNP Q9UXG1
E	2	GLU	-	EXPRESSION TAG	UNP Q9UXG1
E	3	ILE	-	EXPRESSION TAG	UNP Q9UXG1
E	4	PRO	-	EXPRESSION TAG	UNP Q9UXG1
E	5	SER	-	EXPRESSION TAG	UNP Q9UXG1
E	6	LYS	-	EXPRESSION TAG	UNP Q9UXG1

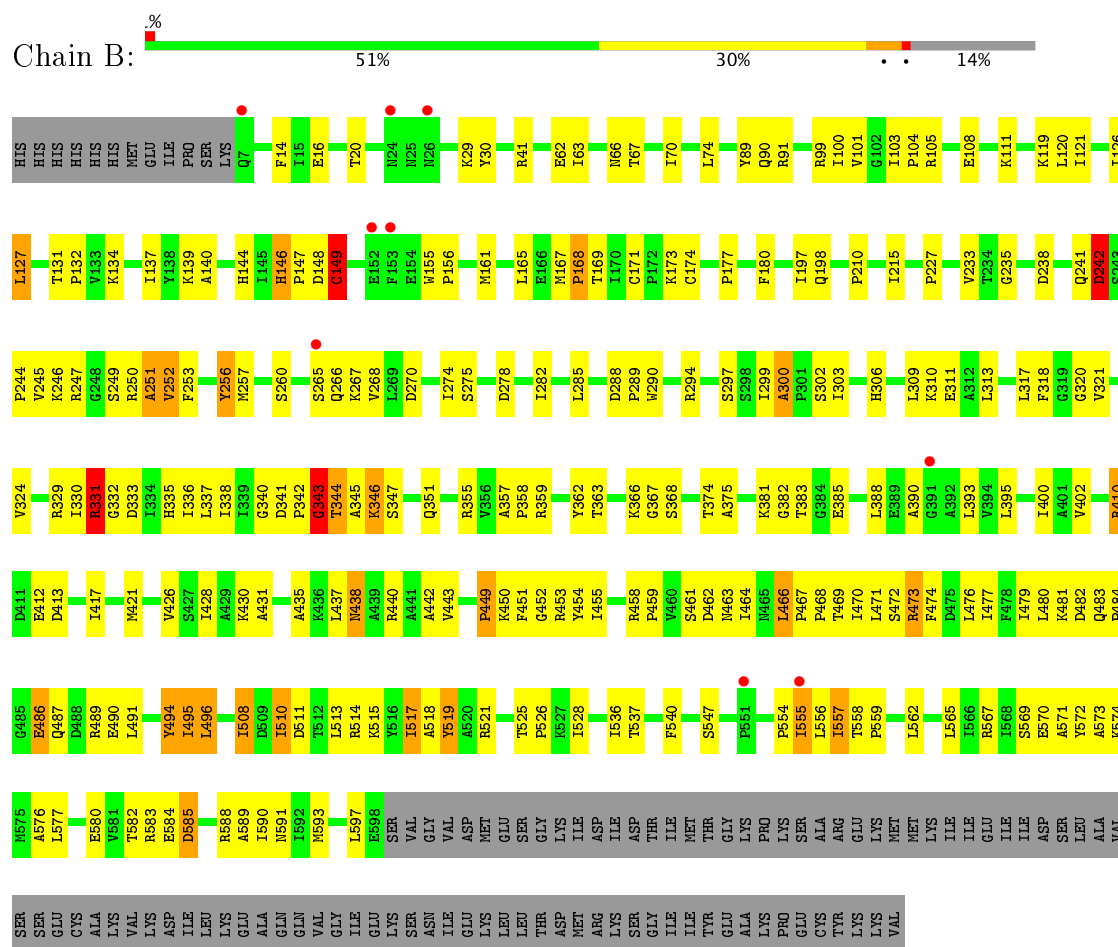
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0

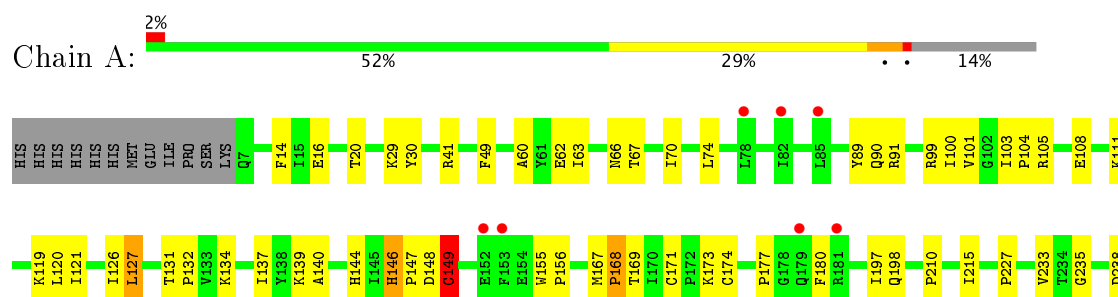
3 Residue-property plots [i](#)

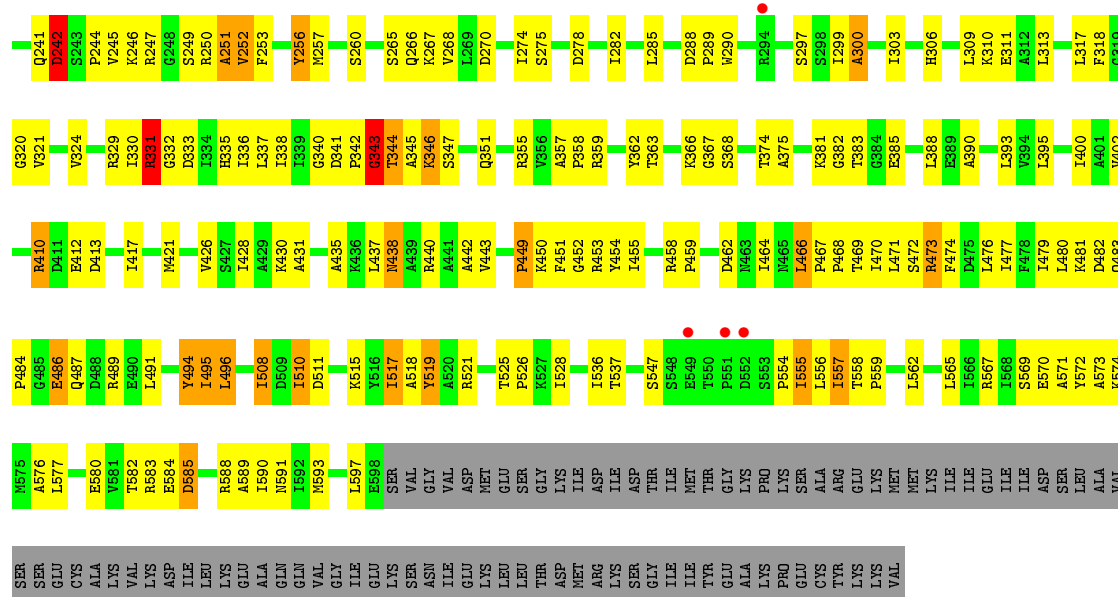
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Minichromosome maintenance protein MCM

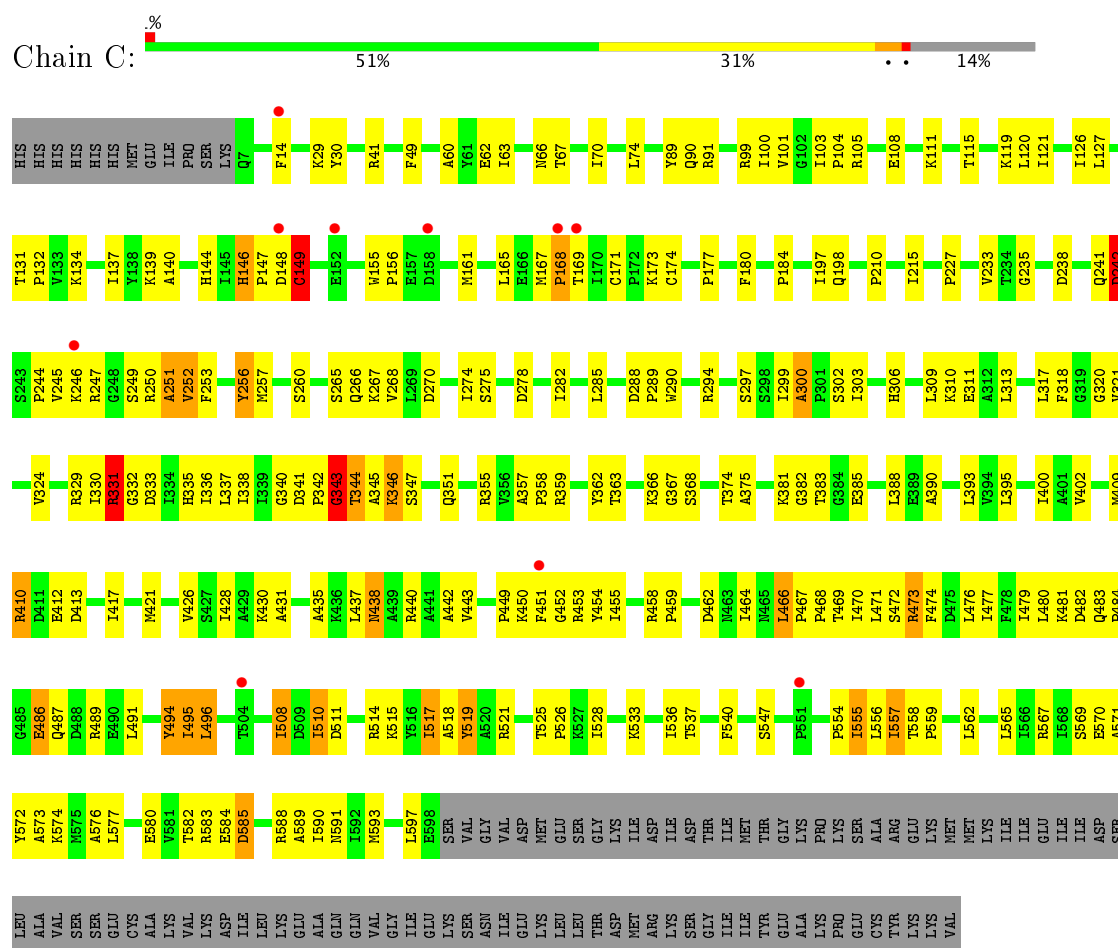


- Molecule 1: Minichromosome maintenance protein MCM





• Molecule 1: Minichromosome maintenance protein MCM



• Molecule 1: Minichromosome maintenance protein MCM





GLN	GLN	VAL	GLY	ILE	GLU	LYS	SER	ASN	ILE	GLU	LYS	LEU	LEU	THR	ASP	MET	ARG	LYS	SER	GLY	ILE	ILE	TYR	GLU	ALA	LYS	PRO	GLU	CYS	TYR	LYS	LYS	VAL
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	169.66Å 107.74Å 170.21Å 90.00° 107.89° 90.00°	Depositor
Resolution (Å)	47.58 – 4.10 48.15 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.58-4.10) 90.9 (48.15-4.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.7.2_863	Depositor
R, R_{free}	0.331 , 0.341 0.312 , 0.333	Depositor DCC
R_{free} test set	1827 reflections (4.34%)	DCC
Wilson B-factor (Å ²)	144.4	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 109.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.047 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	23585	wwPDB-VP
Average B, all atoms (Å ²)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.04 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.6353e-03.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.41	0/4796	0.42	0/6486
1	B	0.40	0/4796	0.42	0/6486
1	C	0.40	0/4796	0.42	0/6486
1	D	0.40	0/4796	0.42	0/6486
1	E	0.40	0/4796	0.42	0/6486
All	All	0.40	0/23980	0.42	0/32430

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	9
1	B	0	9
1	C	0	9
1	D	0	9
1	E	0	9
All	All	0	45

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	168	PRO	Peptide
1	B	242	ASP	Peptide
1	B	247	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	249	SER	Peptide
1	B	251	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4716	0	4865	216	0
1	B	4716	0	4865	217	0
1	C	4716	0	4865	220	0
1	D	4716	0	4865	218	0
1	E	4716	0	4865	214	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
All	All	23585	0	24325	1069	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 22.

The worst 5 of 1069 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:547:SER:HB2	1:A:557:ILE:HD12	1.38	1.05
1:D:547:SER:HB2	1:D:557:ILE:HD12	1.38	1.04
1:C:547:SER:HB2	1:C:557:ILE:HD12	1.38	1.03
1:B:547:SER:HB2	1:B:557:ILE:HD12	1.38	1.02
1:E:547:SER:HB2	1:E:557:ILE:HD12	1.38	1.01

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	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	6	42
1	B	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	6	42
1	C	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	6	42
1	D	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	6	42
1	E	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	6	42
All	All	2950/3460 (85%)	2475 (84%)	395 (13%)	80 (3%)	6	42

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	CYS
1	B	557	ILE
1	A	149	CYS
1	A	557	ILE
1	C	149	CYS

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	518/608 (85%)	494 (95%)	24 (5%)	31	66
1	B	518/608 (85%)	494 (95%)	24 (5%)	31	66
1	C	518/608 (85%)	495 (96%)	23 (4%)	33	67
1	D	518/608 (85%)	495 (96%)	23 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	518/608 (85%)	494 (95%)	24 (5%)	31	66
All	All	2590/3040 (85%)	2472 (95%)	118 (5%)	31	66

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	252	VAL
1	C	494	TYR
1	E	454	TYR
1	C	256	TYR
1	C	410	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	90	GLN
1	C	306	HIS
1	E	90	GLN
1	A	438	ASN
1	D	438	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 [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	592/692 (85%)	-0.15	11 (1%) 67 58	126, 198, 269, 306	0
1	B	592/692 (85%)	-0.24	9 (1%) 74 64	116, 188, 259, 300	0
1	C	592/692 (85%)	-0.17	10 (1%) 70 61	114, 192, 273, 324	0
1	D	592/692 (85%)	-0.18	6 (1%) 82 74	129, 201, 270, 375	0
1	E	592/692 (85%)	-0.26	7 (1%) 79 71	118, 181, 253, 349	0
All	All	2960/3460 (85%)	-0.20	43 (1%) 74 64	114, 193, 267, 375	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	551	PRO	4.7
1	C	168	PRO	4.4
1	E	551	PRO	4.3
1	A	552	ASP	4.3
1	D	24	ASN	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	E	701	1/1	0.98	0.18	-0.77	283,283,283,283	0
2	ZN	C	701	1/1	0.78	0.17	-1.30	281,281,281,281	0
2	ZN	B	701	1/1	0.97	0.06	-1.47	200,200,200,200	0
2	ZN	D	701	1/1	0.95	0.08	-2.15	255,255,255,255	0
2	ZN	A	701	1/1	0.82	0.17	-2.44	260,260,260,260	0

6.5 Other polymers

There are no such residues in this entry.