wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 05:52 AM EDT

PDB ID	:	4U39
Title	:	Crystal Structure of FtsZ:MciZ Complex from Bacillus subtilis
Authors	:	Bisson-Filho, A.W.; Discola, K.F.; Castellen, P.; Blasios, V.; Martins, A.; Sforca, M.L.; Garcia, W.; Zeri, A.C.; Erickson, H.P.; Dessen, A.; Gueiros-Filho, F.J.
Deposited on	:	2014-07-19
Resolution	:	3.19 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

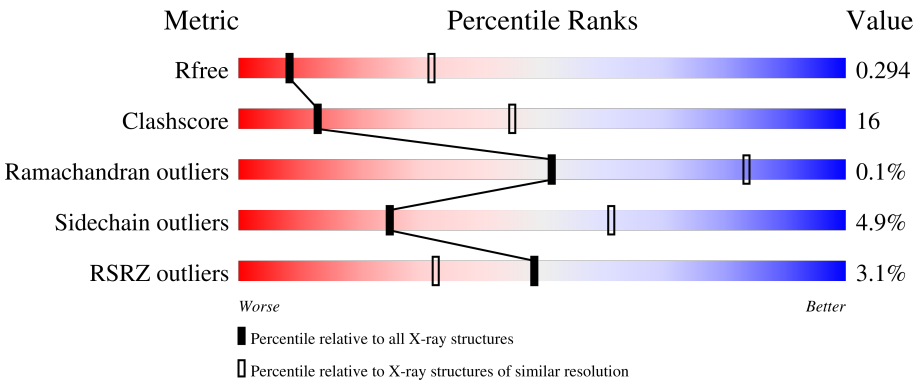
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 >=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 <=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	305	56% 39% • •
1	B	305	4% 67% 28% • 5%
1	C	305	% 60% 32% • 6%
1	D	305	3% 64% 26% • 8%
1	E	305	2% 60% 31% • 6%

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Mol	Chain	Length	Quality of chain
1	F	305	2%, 62%, 30%, 7%
1	G	305	5%, 61%, 30%, 9%
1	H	305	3%, 59%, 29%, 12%
1	I	305	6%, 62%, 25%, 11%
2	J	60	33%, 23%, 40%
2	K	60	17%, 8%, 75%
2	L	60	2%, 35%, 13%, 50%
2	M	60	32%, 8%, 58%
2	N	60	32%, 10%, 55%
2	O	60	28%, 17%, 53%
2	P	60	27%, 8%, 65%
2	Q	60	2%, 38%, 5%, 55%
2	R	60	5%, 25%, 5%, 70%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	H	402	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19225 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 Cell division protein FtsZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2074	1288	360	417	9	0	0	0
1	B	289	1951	1205	349	389	8	0	0	0
1	C	288	2030	1259	356	406	9	0	0	0
1	D	280	1951	1211	342	389	9	0	0	0
1	E	286	1970	1223	346	392	9	0	0	0
1	F	284	1991	1235	350	396	10	0	0	0
1	G	279	1935	1197	338	390	10	0	0	0
1	H	269	1854	1151	331	363	9	0	0	0
1	I	270	1849	1151	326	362	10	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP P17865
B	11	MET	-	initiating methionine	UNP P17865
C	11	MET	-	initiating methionine	UNP P17865
D	11	MET	-	initiating methionine	UNP P17865
E	11	MET	-	initiating methionine	UNP P17865
F	11	MET	-	initiating methionine	UNP P17865
G	11	MET	-	initiating methionine	UNP P17865
H	11	MET	-	initiating methionine	UNP P17865
I	11	MET	-	initiating methionine	UNP P17865

- Molecule 2 is a protein called Cell division factor.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	J	36	Total C N O S 268 178 44 45 1	0	0	0
2	K	15	Total C N O 86 55 16 15	0	0	0
2	L	30	Total C N O 221 149 33 39	0	0	0
2	M	25	Total C N O 147 90 29 28	0	0	0
2	N	27	Total C N O 189 127 32 30	0	0	0
2	O	28	Total C N O 205 137 34 34	0	0	0
2	P	21	Total C N O 149 99 25 25	0	0	0
2	Q	27	Total C N O 161 106 28 27	0	0	0
2	R	18	Total C N O 114 73 22 19	0	0	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-19	MET	-	expression tag	UNP L8EBJ9
J	-18	GLY	-	expression tag	UNP L8EBJ9
J	-17	SER	-	expression tag	UNP L8EBJ9
J	-16	SER	-	expression tag	UNP L8EBJ9
J	-15	HIS	-	expression tag	UNP L8EBJ9
J	-14	HIS	-	expression tag	UNP L8EBJ9
J	-13	HIS	-	expression tag	UNP L8EBJ9
J	-12	HIS	-	expression tag	UNP L8EBJ9
J	-11	HIS	-	expression tag	UNP L8EBJ9
J	-10	HIS	-	expression tag	UNP L8EBJ9
J	-9	SER	-	expression tag	UNP L8EBJ9
J	-8	SER	-	expression tag	UNP L8EBJ9
J	-7	GLY	-	expression tag	UNP L8EBJ9
J	-6	LEU	-	expression tag	UNP L8EBJ9
J	-5	VAL	-	expression tag	UNP L8EBJ9
J	-4	PRO	-	expression tag	UNP L8EBJ9
J	-3	ARG	-	expression tag	UNP L8EBJ9
J	-2	GLY	-	expression tag	UNP L8EBJ9
J	-1	SER	-	expression tag	UNP L8EBJ9
J	0	HIS	-	expression tag	UNP L8EBJ9
K	-19	MET	-	expression tag	UNP L8EBJ9
K	-18	GLY	-	expression tag	UNP L8EBJ9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-17	SER	-	expression tag	UNP L8EBJ9
K	-16	SER	-	expression tag	UNP L8EBJ9
K	-15	HIS	-	expression tag	UNP L8EBJ9
K	-14	HIS	-	expression tag	UNP L8EBJ9
K	-13	HIS	-	expression tag	UNP L8EBJ9
K	-12	HIS	-	expression tag	UNP L8EBJ9
K	-11	HIS	-	expression tag	UNP L8EBJ9
K	-10	HIS	-	expression tag	UNP L8EBJ9
K	-9	SER	-	expression tag	UNP L8EBJ9
K	-8	SER	-	expression tag	UNP L8EBJ9
K	-7	GLY	-	expression tag	UNP L8EBJ9
K	-6	LEU	-	expression tag	UNP L8EBJ9
K	-5	VAL	-	expression tag	UNP L8EBJ9
K	-4	PRO	-	expression tag	UNP L8EBJ9
K	-3	ARG	-	expression tag	UNP L8EBJ9
K	-2	GLY	-	expression tag	UNP L8EBJ9
K	-1	SER	-	expression tag	UNP L8EBJ9
K	0	HIS	-	expression tag	UNP L8EBJ9
L	-19	MET	-	expression tag	UNP L8EBJ9
L	-18	GLY	-	expression tag	UNP L8EBJ9
L	-17	SER	-	expression tag	UNP L8EBJ9
L	-16	SER	-	expression tag	UNP L8EBJ9
L	-15	HIS	-	expression tag	UNP L8EBJ9
L	-14	HIS	-	expression tag	UNP L8EBJ9
L	-13	HIS	-	expression tag	UNP L8EBJ9
L	-12	HIS	-	expression tag	UNP L8EBJ9
L	-11	HIS	-	expression tag	UNP L8EBJ9
L	-10	HIS	-	expression tag	UNP L8EBJ9
L	-9	SER	-	expression tag	UNP L8EBJ9
L	-8	SER	-	expression tag	UNP L8EBJ9
L	-7	GLY	-	expression tag	UNP L8EBJ9
L	-6	LEU	-	expression tag	UNP L8EBJ9
L	-5	VAL	-	expression tag	UNP L8EBJ9
L	-4	PRO	-	expression tag	UNP L8EBJ9
L	-3	ARG	-	expression tag	UNP L8EBJ9
L	-2	GLY	-	expression tag	UNP L8EBJ9
L	-1	SER	-	expression tag	UNP L8EBJ9
L	0	HIS	-	expression tag	UNP L8EBJ9
M	-19	MET	-	expression tag	UNP L8EBJ9
M	-18	GLY	-	expression tag	UNP L8EBJ9
M	-17	SER	-	expression tag	UNP L8EBJ9
M	-16	SER	-	expression tag	UNP L8EBJ9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-15	HIS	-	expression tag	UNP L8EBJ9
M	-14	HIS	-	expression tag	UNP L8EBJ9
M	-13	HIS	-	expression tag	UNP L8EBJ9
M	-12	HIS	-	expression tag	UNP L8EBJ9
M	-11	HIS	-	expression tag	UNP L8EBJ9
M	-10	HIS	-	expression tag	UNP L8EBJ9
M	-9	SER	-	expression tag	UNP L8EBJ9
M	-8	SER	-	expression tag	UNP L8EBJ9
M	-7	GLY	-	expression tag	UNP L8EBJ9
M	-6	LEU	-	expression tag	UNP L8EBJ9
M	-5	VAL	-	expression tag	UNP L8EBJ9
M	-4	PRO	-	expression tag	UNP L8EBJ9
M	-3	ARG	-	expression tag	UNP L8EBJ9
M	-2	GLY	-	expression tag	UNP L8EBJ9
M	-1	SER	-	expression tag	UNP L8EBJ9
M	0	HIS	-	expression tag	UNP L8EBJ9
N	-19	MET	-	expression tag	UNP L8EBJ9
N	-18	GLY	-	expression tag	UNP L8EBJ9
N	-17	SER	-	expression tag	UNP L8EBJ9
N	-16	SER	-	expression tag	UNP L8EBJ9
N	-15	HIS	-	expression tag	UNP L8EBJ9
N	-14	HIS	-	expression tag	UNP L8EBJ9
N	-13	HIS	-	expression tag	UNP L8EBJ9
N	-12	HIS	-	expression tag	UNP L8EBJ9
N	-11	HIS	-	expression tag	UNP L8EBJ9
N	-10	HIS	-	expression tag	UNP L8EBJ9
N	-9	SER	-	expression tag	UNP L8EBJ9
N	-8	SER	-	expression tag	UNP L8EBJ9
N	-7	GLY	-	expression tag	UNP L8EBJ9
N	-6	LEU	-	expression tag	UNP L8EBJ9
N	-5	VAL	-	expression tag	UNP L8EBJ9
N	-4	PRO	-	expression tag	UNP L8EBJ9
N	-3	ARG	-	expression tag	UNP L8EBJ9
N	-2	GLY	-	expression tag	UNP L8EBJ9
N	-1	SER	-	expression tag	UNP L8EBJ9
N	0	HIS	-	expression tag	UNP L8EBJ9
O	-19	MET	-	expression tag	UNP L8EBJ9
O	-18	GLY	-	expression tag	UNP L8EBJ9
O	-17	SER	-	expression tag	UNP L8EBJ9
O	-16	SER	-	expression tag	UNP L8EBJ9
O	-15	HIS	-	expression tag	UNP L8EBJ9
O	-14	HIS	-	expression tag	UNP L8EBJ9

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-13	HIS	-	expression tag	UNP L8EBJ9
O	-12	HIS	-	expression tag	UNP L8EBJ9
O	-11	HIS	-	expression tag	UNP L8EBJ9
O	-10	HIS	-	expression tag	UNP L8EBJ9
O	-9	SER	-	expression tag	UNP L8EBJ9
O	-8	SER	-	expression tag	UNP L8EBJ9
O	-7	GLY	-	expression tag	UNP L8EBJ9
O	-6	LEU	-	expression tag	UNP L8EBJ9
O	-5	VAL	-	expression tag	UNP L8EBJ9
O	-4	PRO	-	expression tag	UNP L8EBJ9
O	-3	ARG	-	expression tag	UNP L8EBJ9
O	-2	GLY	-	expression tag	UNP L8EBJ9
O	-1	SER	-	expression tag	UNP L8EBJ9
O	0	HIS	-	expression tag	UNP L8EBJ9
P	-19	MET	-	expression tag	UNP L8EBJ9
P	-18	GLY	-	expression tag	UNP L8EBJ9
P	-17	SER	-	expression tag	UNP L8EBJ9
P	-16	SER	-	expression tag	UNP L8EBJ9
P	-15	HIS	-	expression tag	UNP L8EBJ9
P	-14	HIS	-	expression tag	UNP L8EBJ9
P	-13	HIS	-	expression tag	UNP L8EBJ9
P	-12	HIS	-	expression tag	UNP L8EBJ9
P	-11	HIS	-	expression tag	UNP L8EBJ9
P	-10	HIS	-	expression tag	UNP L8EBJ9
P	-9	SER	-	expression tag	UNP L8EBJ9
P	-8	SER	-	expression tag	UNP L8EBJ9
P	-7	GLY	-	expression tag	UNP L8EBJ9
P	-6	LEU	-	expression tag	UNP L8EBJ9
P	-5	VAL	-	expression tag	UNP L8EBJ9
P	-4	PRO	-	expression tag	UNP L8EBJ9
P	-3	ARG	-	expression tag	UNP L8EBJ9
P	-2	GLY	-	expression tag	UNP L8EBJ9
P	-1	SER	-	expression tag	UNP L8EBJ9
P	0	HIS	-	expression tag	UNP L8EBJ9
Q	-19	MET	-	expression tag	UNP L8EBJ9
Q	-18	GLY	-	expression tag	UNP L8EBJ9
Q	-17	SER	-	expression tag	UNP L8EBJ9
Q	-16	SER	-	expression tag	UNP L8EBJ9
Q	-15	HIS	-	expression tag	UNP L8EBJ9
Q	-14	HIS	-	expression tag	UNP L8EBJ9
Q	-13	HIS	-	expression tag	UNP L8EBJ9
Q	-12	HIS	-	expression tag	UNP L8EBJ9

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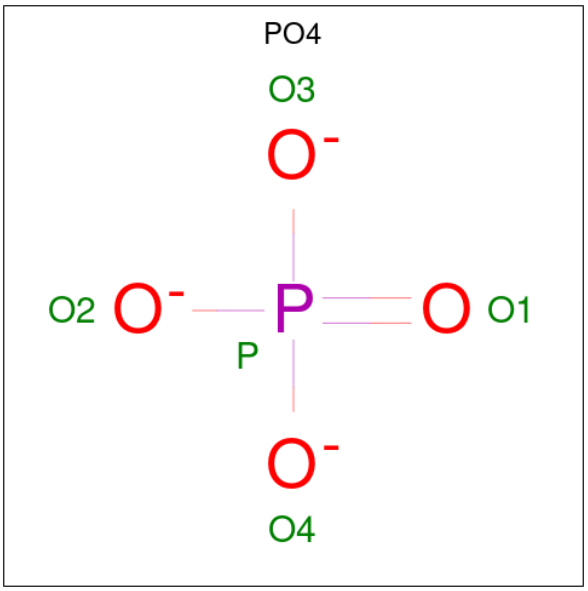
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-11	HIS	-	expression tag	UNP L8EBJ9
Q	-10	HIS	-	expression tag	UNP L8EBJ9
Q	-9	SER	-	expression tag	UNP L8EBJ9
Q	-8	SER	-	expression tag	UNP L8EBJ9
Q	-7	GLY	-	expression tag	UNP L8EBJ9
Q	-6	LEU	-	expression tag	UNP L8EBJ9
Q	-5	VAL	-	expression tag	UNP L8EBJ9
Q	-4	PRO	-	expression tag	UNP L8EBJ9
Q	-3	ARG	-	expression tag	UNP L8EBJ9
Q	-2	GLY	-	expression tag	UNP L8EBJ9
Q	-1	SER	-	expression tag	UNP L8EBJ9
Q	0	HIS	-	expression tag	UNP L8EBJ9
R	-19	MET	-	expression tag	UNP L8EBJ9
R	-18	GLY	-	expression tag	UNP L8EBJ9
R	-17	SER	-	expression tag	UNP L8EBJ9
R	-16	SER	-	expression tag	UNP L8EBJ9
R	-15	HIS	-	expression tag	UNP L8EBJ9
R	-14	HIS	-	expression tag	UNP L8EBJ9
R	-13	HIS	-	expression tag	UNP L8EBJ9
R	-12	HIS	-	expression tag	UNP L8EBJ9
R	-11	HIS	-	expression tag	UNP L8EBJ9
R	-10	HIS	-	expression tag	UNP L8EBJ9
R	-9	SER	-	expression tag	UNP L8EBJ9
R	-8	SER	-	expression tag	UNP L8EBJ9
R	-7	GLY	-	expression tag	UNP L8EBJ9
R	-6	LEU	-	expression tag	UNP L8EBJ9
R	-5	VAL	-	expression tag	UNP L8EBJ9
R	-4	PRO	-	expression tag	UNP L8EBJ9
R	-3	ARG	-	expression tag	UNP L8EBJ9
R	-2	GLY	-	expression tag	UNP L8EBJ9
R	-1	SER	-	expression tag	UNP L8EBJ9
R	0	HIS	-	expression tag	UNP L8EBJ9

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	I	1	5	4	1	0	0
			Total	O	P		
3	I	1	5	4	1	0	0

3 Residue-property plots (i)

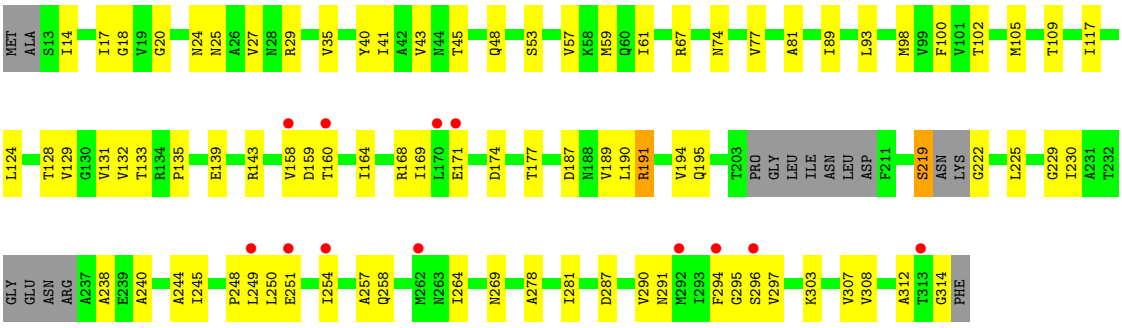
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

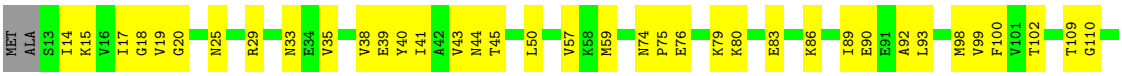
• Molecule 1: Cell division protein FtsZ

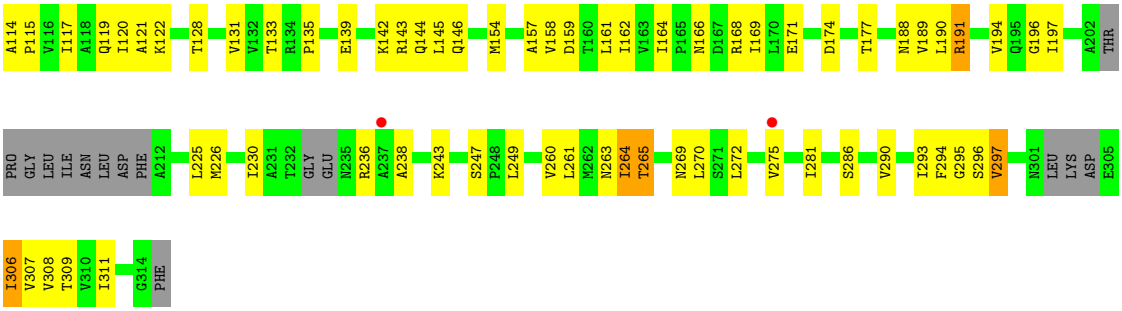
Chain B:



• Molecule 1: Cell division protein FtsZ

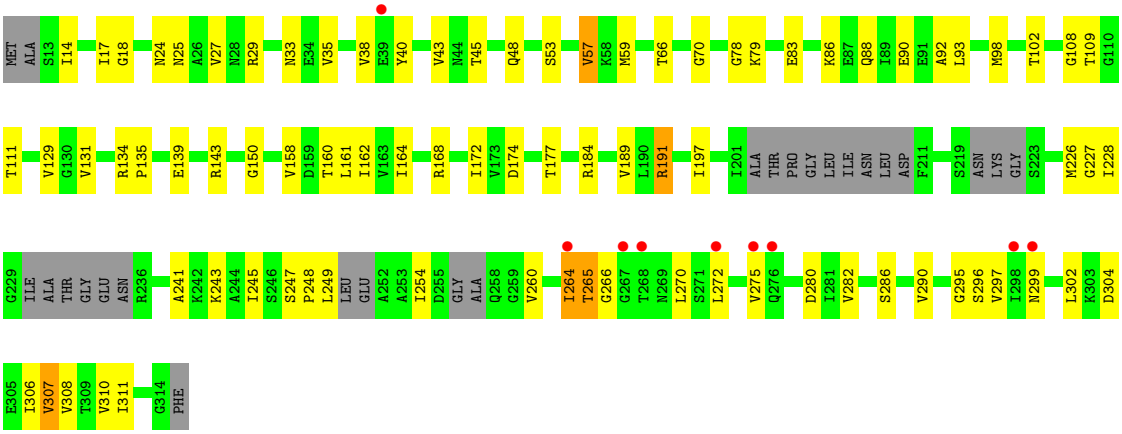
Chain C:





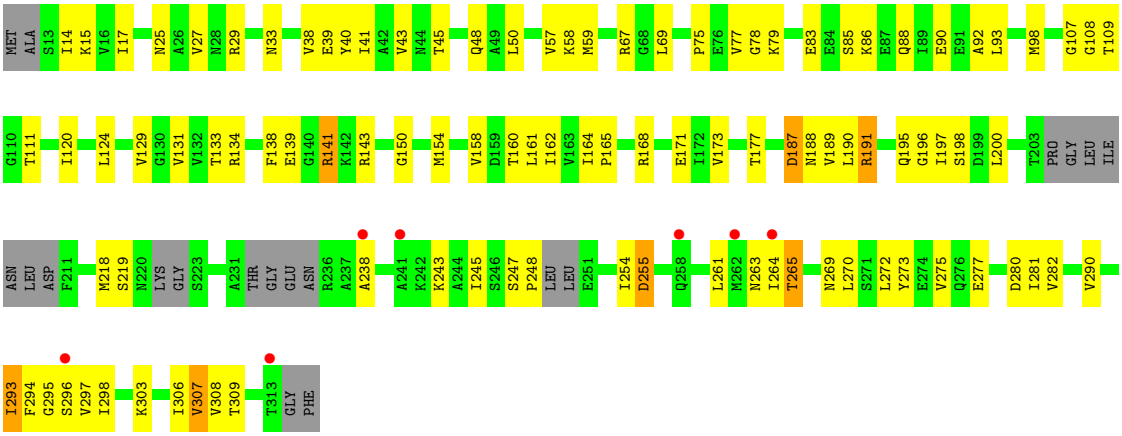
• Molecule 1: Cell division protein FtsZ

Chain D:



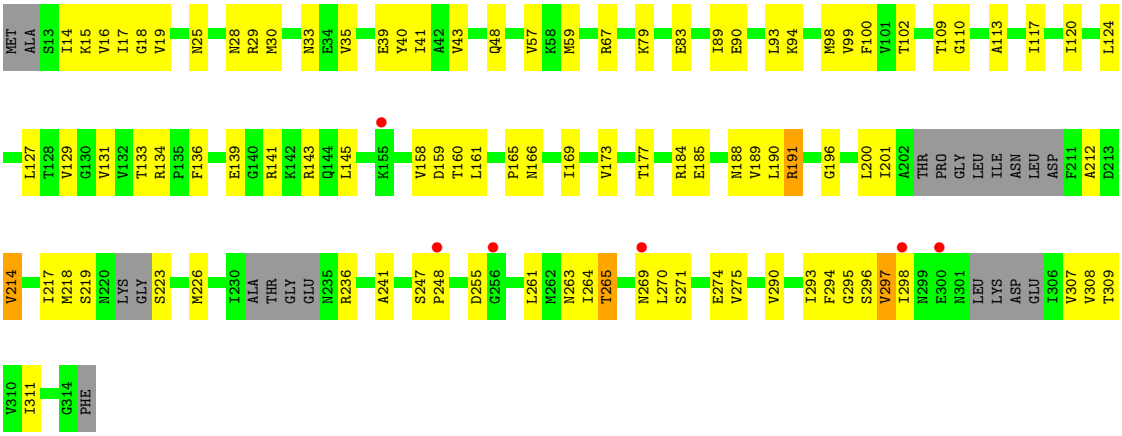
• Molecule 1: Cell division protein FtsZ

Chain E:



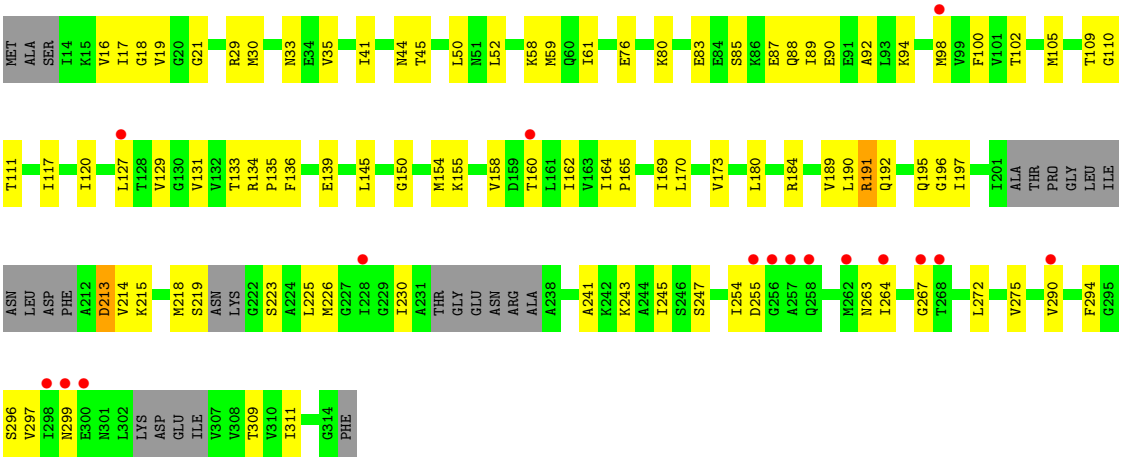
• Molecule 1: Cell division protein FtsZ

Chain F:



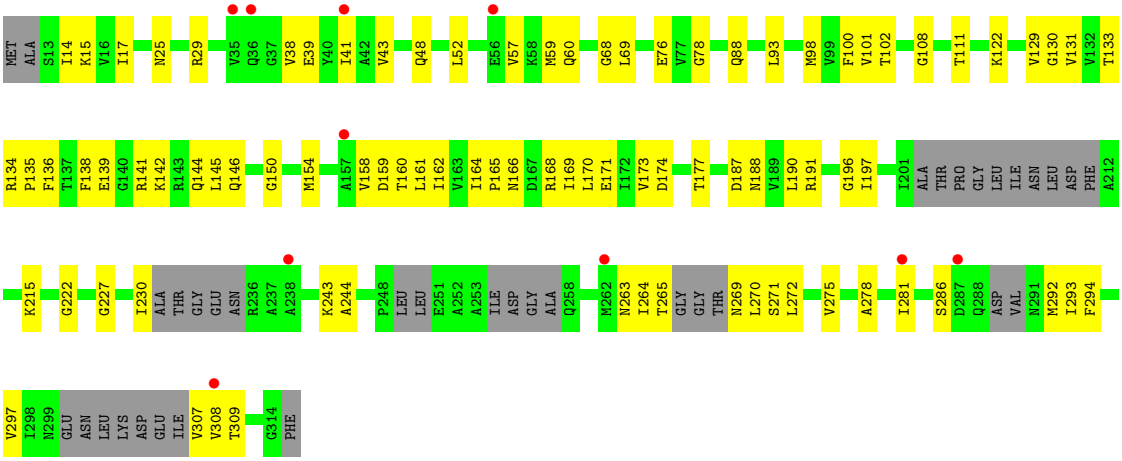
• Molecule 1: Cell division protein FtsZ

Chain G:



• Molecule 1: Cell division protein FtsZ

Chain H:



• Molecule 1: Cell division protein FtsZ

Chain I: 6% 62% 25% • 11%

MET ALA S13 I14 I17 G18 N25 A26 V27 N28 R29 V35 V38 E39 Y40 I41 L52 V57 Q60 R67 G68 E76 V77 G78 K79 K80 S85 Q88 I89 E90 L93 K94 D97 M98 V99 F100 V101 T102 G108 T111 I117 L127 T128

V129 G130 V131 V132 T133 F136 E139 R143 G150 K155 V158 D159 T160 L161 I162 V163 I164 P165 N166 D167 R168 I169 L170 E171 V189 L190 R191 Q192 G193 V194 Q195 G196 I197 S198 D199 L200 I201 ALA THR PRO GLY LEU ILE ASN LEU ASP PHE ALA ASP VAL K215 M218

G222 S223 A224 L225 M226 G227 I228 G229 I230 A231 T232 GLY GLU ASN ARG ALA ALA GLU A240 A241 P248 L249 I254 D255 V260 L261 M262 N263 I264 T265 GLY GLY THR ASN LEU SER L272 A278 I281 V290 N291 M292 I293 N301 LEU LYS ASP GLU ILE V307 V308 T309

V310 I311 A312 T313 GLY PHE

- Molecule 2: Cell division factor

Chain J: 33% 23% • 40%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET K2 V3 H4 R5 G9 V10 V11 L12 A16 I19 R20 L23 K24 E25 Y26 G27 R28 T29 F30 Q31 Y32 W36 I37 SER LYS PRO

- Molecule 2: Cell division factor

Chain K: 17% 8% 75%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET LYS VAL HIS ARG MET PRO LYS GLY V10 V11 L12 V13 GLY LYS A16 W17 Y26 GLY ARG THR PHE GLN TYR VAL LYS ASP TRP ILE SER LYS PRO

- Molecule 2: Cell division factor

Chain L: 2% 35% 13% • 50%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET LYS VAL HIS ARG MET PRO LYS G9 V10 V11 L12 V13 A21 K22 L23 Y26 F30 S38 LYS PRO

- Molecule 2: Cell division factor

Chain M: 32% 8% • 58%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET LYS VAL HIS ARG MET PRO LYS GLY V10 V11 L12 V13 GLY LYS A16 R20 E25 T29 F30 GLN Y32 V33 I37 SER LYS PRO

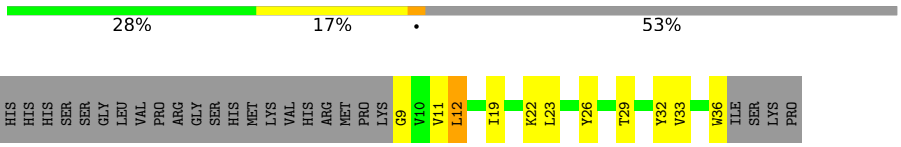
- Molecule 2: Cell division factor

Chain N: 32% 10% • 55%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET LYS VAL HIS ARG MET PRO LYS G9 V10 V11 L12 V13 GLY LYS A16 I19 R20 L23 K24 E25 T29 V33 I37 SER LYS PRO

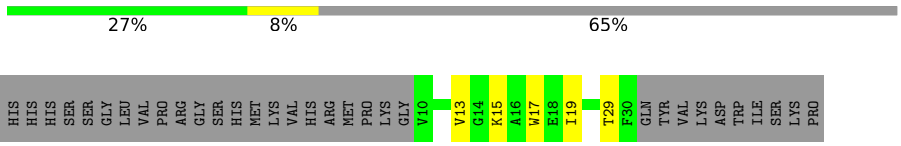
• Molecule 2: Cell division factor

Chain O:



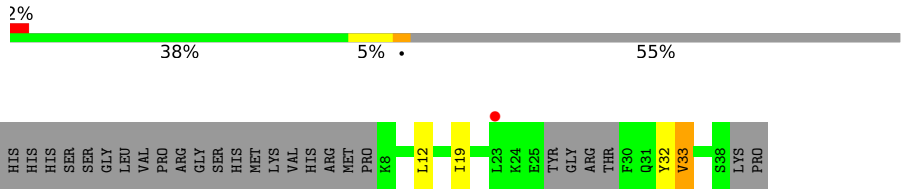
• Molecule 2: Cell division factor

Chain P:



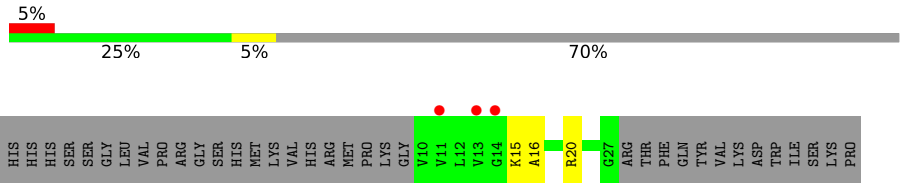
• Molecule 2: Cell division factor

Chain Q:



• Molecule 2: Cell division factor

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	167.36Å 167.36Å 528.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.59 – 3.19 46.59 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.59-3.19) 98.0 (46.59-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	10.94 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.232 , 0.292 0.236 , 0.294	Depositor DCC
R_{free} test set	3667 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 82.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19225	wwPDB-VP
Average B, all atoms (Å^2)	93.0	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 20.89 % 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 7.8760e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4

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	0.59	0/2085	0.76	0/2819
1	B	0.49	0/1959	0.68	0/2653
1	C	0.57	0/2039	0.70	0/2755
1	D	0.53	0/1957	0.71	0/2643
1	E	0.51	0/1977	0.67	0/2677
1	F	0.48	0/1999	0.68	0/2700
1	G	0.49	0/1942	0.69	0/2626
1	H	0.49	0/1858	0.68	0/2505
1	I	0.50	0/1856	0.68	0/2512
2	J	0.51	0/276	0.64	0/378
2	K	0.48	0/86	0.52	0/118
2	L	0.46	0/227	0.59	0/311
2	M	0.39	0/146	0.58	0/198
2	N	0.44	0/194	0.58	0/266
2	O	0.45	0/210	0.61	0/287
2	P	0.42	0/152	0.71	0/208
2	Q	0.45	0/162	0.61	0/222
2	R	0.43	0/116	0.74	0/159
All	All	0.51	0/19241	0.69	0/26037

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2074	0	2080	92	0
1	B	1951	0	1875	60	0
1	C	2030	0	2042	78	0
1	D	1951	0	1946	56	0
1	E	1970	0	1946	74	0
1	F	1991	0	1999	73	0
1	G	1935	0	1917	65	0
1	H	1854	0	1827	53	0
1	I	1849	0	1819	56	0
2	J	268	0	235	16	0
2	K	86	0	49	4	0
2	L	221	0	193	8	0
2	M	147	0	89	5	0
2	N	189	0	145	10	0
2	O	205	0	184	14	0
2	P	149	0	130	2	0
2	Q	161	0	116	3	0
2	R	114	0	83	2	0
3	A	10	0	0	2	0
3	B	10	0	0	0	0
3	C	10	0	0	2	0
3	D	10	0	0	2	0
3	E	5	0	0	1	0
3	F	5	0	0	1	0
3	G	10	0	0	1	0
3	H	10	0	0	2	0
3	I	10	0	0	1	0
All	All	19225	0	18675	620	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 16.

The worst 5 of 620 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:17:ILE:HD11	1:A:93:LEU:HD21	1.36	1.07
1:D:17:ILE:HD11	1:D:93:LEU:HD21	1.45	0.98
1:C:17:ILE:HD11	1:C:93:LEU:HD21	1.45	0.95
1:I:263:ASN:HB3	1:I:309:THR:HB	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:ILE:HD12	1:F:293:ILE:HG13	1.55	0.88

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	288/305 (94%)	283 (98%)	5 (2%)	0	100	100
1	B	281/305 (92%)	276 (98%)	5 (2%)	0	100	100
1	C	280/305 (92%)	273 (98%)	7 (2%)	0	100	100
1	D	268/305 (88%)	266 (99%)	2 (1%)	0	100	100
1	E	276/305 (90%)	271 (98%)	5 (2%)	0	100	100
1	F	274/305 (90%)	270 (98%)	4 (2%)	0	100	100
1	G	269/305 (88%)	265 (98%)	4 (2%)	0	100	100
1	H	253/305 (83%)	247 (98%)	5 (2%)	1 (0%)	34	69
1	I	260/305 (85%)	255 (98%)	4 (2%)	1 (0%)	34	69
2	J	34/60 (57%)	34 (100%)	0	0	100	100
2	K	11/60 (18%)	11 (100%)	0	0	100	100
2	L	28/60 (47%)	27 (96%)	1 (4%)	0	100	100
2	M	19/60 (32%)	19 (100%)	0	0	100	100
2	N	23/60 (38%)	23 (100%)	0	0	100	100
2	O	26/60 (43%)	25 (96%)	1 (4%)	0	100	100
2	P	19/60 (32%)	18 (95%)	1 (5%)	0	100	100
2	Q	23/60 (38%)	22 (96%)	1 (4%)	0	100	100
2	R	16/60 (27%)	15 (94%)	0	1 (6%)	1	10
All	All	2648/3285 (81%)	2600 (98%)	45 (2%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	15	LYS
1	I	222	GLY
1	H	222	GLY

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	205/227 (90%)	197 (96%)	8 (4%)	32	67
1	B	174/227 (77%)	169 (97%)	5 (3%)	42	74
1	C	200/227 (88%)	190 (95%)	10 (5%)	24	60
1	D	190/227 (84%)	181 (95%)	9 (5%)	26	62
1	E	187/227 (82%)	175 (94%)	12 (6%)	17	52
1	F	196/227 (86%)	188 (96%)	8 (4%)	30	66
1	G	188/227 (83%)	180 (96%)	8 (4%)	29	64
1	H	173/227 (76%)	167 (96%)	6 (4%)	36	69
1	I	172/227 (76%)	165 (96%)	7 (4%)	30	66
2	J	22/52 (42%)	20 (91%)	2 (9%)	9	34
2	K	2/52 (4%)	0	2 (100%)	0	0
2	L	18/52 (35%)	16 (89%)	2 (11%)	6	25
2	M	5/52 (10%)	4 (80%)	1 (20%)	1	6
2	N	11/52 (21%)	9 (82%)	2 (18%)	1	8
2	O	16/52 (31%)	14 (88%)	2 (12%)	4	21
2	P	11/52 (21%)	9 (82%)	2 (18%)	1	8
2	Q	7/52 (14%)	5 (71%)	2 (29%)	0	1
2	R	5/52 (10%)	5 (100%)	0	100	100
All	All	1782/2511 (71%)	1694 (95%)	88 (5%)	25	61

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	255	ASP
1	I	290	VAL
1	G	297	VAL
1	H	286	SER
2	K	10	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	B	263	ASN
1	C	144	GLN
1	H	144	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
3	PO4	D	402	-	4,4,4	0.90	0	6,6,6	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	B	402	-	4,4,4	0.76	0	6,6,6	0.62	0
3	PO4	A	402	-	4,4,4	0.99	0	6,6,6	0.57	0
3	PO4	H	402	-	4,4,4	1.09	0	6,6,6	0.85	0
3	PO4	E	401	-	4,4,4	0.90	0	6,6,6	0.48	0
3	PO4	D	401	-	4,4,4	0.87	0	6,6,6	0.80	0
3	PO4	B	401	-	4,4,4	0.93	0	6,6,6	0.90	0
3	PO4	I	401	-	4,4,4	0.85	0	6,6,6	0.90	0
3	PO4	I	402	-	4,4,4	1.25	0	6,6,6	0.83	0
3	PO4	G	401	-	4,4,4	0.97	0	6,6,6	0.58	0
3	PO4	H	401	-	4,4,4	1.04	0	6,6,6	1.07	0
3	PO4	C	402	-	4,4,4	1.10	0	6,6,6	1.04	0
3	PO4	F	401	-	4,4,4	0.90	0	6,6,6	0.50	0
3	PO4	A	401	-	4,4,4	0.82	0	6,6,6	0.72	0
3	PO4	G	402	-	4,4,4	0.82	0	6,6,6	0.91	0
3	PO4	C	401	-	4,4,4	1.04	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	PO4	1	0
3	A	402	PO4	1	0
3	H	402	PO4	2	0
3	E	401	PO4	1	0
3	D	401	PO4	1	0
3	I	401	PO4	1	0
3	G	401	PO4	1	0
3	C	402	PO4	1	0
3	F	401	PO4	1	0
3	A	401	PO4	1	0
3	C	401	PO4	1	0

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, 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	294/305 (96%)	0.04	1 (0%)	94	92	43, 72, 125, 180	0
1	B	289/305 (94%)	0.22	12 (4%)	36	23	48, 102, 158, 209	0
1	C	288/305 (94%)	0.08	2 (0%)	87	81	43, 77, 137, 197	0
1	D	280/305 (91%)	0.20	9 (3%)	47	31	50, 83, 153, 193	0
1	E	286/305 (93%)	0.14	7 (2%)	59	44	50, 93, 150, 198	0
1	F	284/305 (93%)	0.17	6 (2%)	63	49	52, 92, 146, 233	0
1	G	279/305 (91%)	0.29	16 (5%)	23	13	50, 93, 151, 229	0
1	H	269/305 (88%)	0.19	10 (3%)	41	26	52, 91, 148, 188	0
1	I	270/305 (88%)	0.33	18 (6%)	17	10	46, 94, 150, 204	0
2	J	36/60 (60%)	-0.03	0	100	100	61, 84, 122, 145	0
2	K	15/60 (25%)	-0.42	0	100	100	84, 101, 118, 130	0
2	L	30/60 (50%)	-0.17	1 (3%)	46	30	62, 97, 119, 170	0
2	M	25/60 (41%)	-0.07	0	100	100	69, 106, 138, 145	0
2	N	27/60 (45%)	-0.16	0	100	100	73, 104, 138, 189	0
2	O	28/60 (46%)	-0.27	0	100	100	65, 89, 127, 161	0
2	P	21/60 (35%)	0.05	0	100	100	63, 90, 113, 158	0
2	Q	27/60 (45%)	-0.43	1 (3%)	41	26	75, 100, 114, 157	0
2	R	18/60 (30%)	0.36	3 (16%)	1	1	81, 105, 141, 184	0
All	All	2766/3285 (84%)	0.16	86 (3%)	49	32	43, 90, 147, 233	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	256	GLY	6.1
1	G	267	GLY	5.1
1	D	298	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	G	298	ILE	5.0
1	I	292	MET	4.5

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)

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, 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	B-factors(Å^2)	Q<0.9
3	PO4	B	402	5/5	0.94	0.10	120,125,129,132	0
3	PO4	I	401	5/5	0.94	0.31	83,84,85,90	0
3	PO4	D	402	5/5	0.95	0.20	57,62,68,69	0
3	PO4	G	401	5/5	0.95	0.27	76,77,82,84	0
3	PO4	H	401	5/5	0.95	0.26	63,67,74,75	0
3	PO4	C	401	5/5	0.95	0.36	69,72,74,84	0
3	PO4	E	401	5/5	0.96	0.21	72,77,84,87	0
3	PO4	C	402	5/5	0.96	0.21	60,62,71,73	0
3	PO4	I	402	5/5	0.96	0.20	59,63,72,78	0
3	PO4	B	401	5/5	0.97	0.27	77,78,83,83	0
3	PO4	H	402	5/5	0.97	0.25	64,67,72,76	0
3	PO4	A	402	5/5	0.97	0.21	47,55,59,64	0
3	PO4	D	401	5/5	0.97	0.29	62,62,68,69	0
3	PO4	A	401	5/5	0.98	0.21	59,63,65,70	0
3	PO4	G	402	5/5	0.98	0.18	50,59,62,67	0
3	PO4	F	401	5/5	0.98	0.22	72,73,79,80	0

6.5 Other polymers (i)

There are no such residues in this entry.