



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2016 – 11:06 AM EDT

PDB ID : 5CW7  
Title : Crystal structure of the PaaA2-ParE2 antitoxin-toxin complex  
Authors : Sterckx, Y.G.-J.; Loris, R.  
Deposited on : 2015-07-27  
Resolution : 2.83 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027674

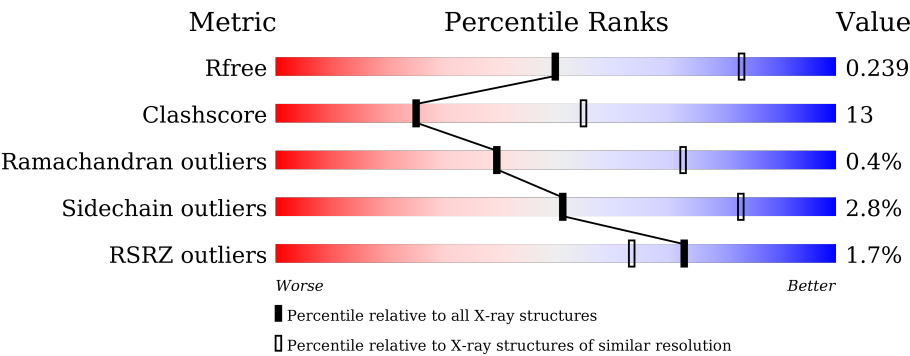
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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))
$R_{free}$	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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  $\geq 3$ , 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	71	<div><div></div><div><div></div><div>75%</div><div>7%</div><div>•</div><div>15%</div></div></div>
1	C	71	<div><div>%</div><div><div></div><div>49%</div><div>30%</div><div>•</div><div>20%</div></div></div>
1	E	71	<div><div>%</div><div><div></div><div>55%</div><div>25%</div><div>•</div><div>17%</div></div></div>
1	G	71	<div><div>%</div><div><div></div><div>66%</div><div>18%</div><div>•</div><div>14%</div></div></div>
1	I	71	<div><div>%</div><div><div></div><div>55%</div><div>28%</div><div>•</div><div>17%</div></div></div>
1	K	71	<div><div></div><div><div></div><div>61%</div><div>23%</div><div>•</div><div>14%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	M	71	
1	O	71	
2	B	100	
2	D	100	
2	F	100	
2	H	100	
2	J	100	
2	L	100	
2	N	100	
2	P	100	

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	GOL	B	201	-	-	-	X
3	GOL	B	202	-	-	-	X
3	GOL	H	201	-	-	-	X
3	GOL	L	202	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10547 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 PAAA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	60	Total	C	N	O	Se	0	0	0
			478	295	89	91	3			
1	C	57	Total	C	N	O	Se	0	0	0
			455	286	83	83	3			
1	E	59	Total	C	N	O	Se	0	1	0
			478	297	90	88	3			
1	G	61	Total	C	N	O	Se	0	0	0
			471	292	87	89	3			
1	I	59	Total	C	N	O	Se	0	0	0
			476	294	89	90	3			
1	K	61	Total	C	N	O	Se	0	0	0
			466	291	86	86	3			
1	M	57	Total	C	N	O	Se	0	0	0
			459	285	83	88	3			
1	O	60	Total	C	N	O	Se	0	0	0
			478	297	89	89	3			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
A	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
A	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
A	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
A	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
A	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
A	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
A	0	ASP	-	expression tag	UNP A0A0F6F6Q9
A	1	LYS	-	expression tag	UNP A0A0F6F6Q9
C	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
C	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
C	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
C	-4	LYS	-	expression tag	UNP A0A0F6F6Q9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
C	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
C	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
C	0	ASP	-	expression tag	UNP A0A0F6F6Q9
C	1	LYS	-	expression tag	UNP A0A0F6F6Q9
E	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
E	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
E	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
E	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
E	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
E	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
E	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
E	0	ASP	-	expression tag	UNP A0A0F6F6Q9
E	1	LYS	-	expression tag	UNP A0A0F6F6Q9
G	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
G	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
G	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
G	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
G	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
G	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
G	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
G	0	ASP	-	expression tag	UNP A0A0F6F6Q9
G	1	LYS	-	expression tag	UNP A0A0F6F6Q9
I	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
I	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
I	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
I	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
I	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
I	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
I	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
I	0	ASP	-	expression tag	UNP A0A0F6F6Q9
I	1	LYS	-	expression tag	UNP A0A0F6F6Q9
K	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
K	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
K	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
K	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
K	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
K	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
K	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
K	0	ASP	-	expression tag	UNP A0A0F6F6Q9
K	1	LYS	-	expression tag	UNP A0A0F6F6Q9
M	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
M	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
M	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
M	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
M	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
M	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
M	0	ASP	-	expression tag	UNP A0A0F6F6Q9
M	1	LYS	-	expression tag	UNP A0A0F6F6Q9
O	-7	MSE	-	initiating methionine	UNP A0A0F6F6Q9
O	-6	ASP	-	expression tag	UNP A0A0F6F6Q9
O	-5	TYR	-	expression tag	UNP A0A0F6F6Q9
O	-4	LYS	-	expression tag	UNP A0A0F6F6Q9
O	-3	ASP	-	expression tag	UNP A0A0F6F6Q9
O	-2	ASP	-	expression tag	UNP A0A0F6F6Q9
O	-1	ASP	-	expression tag	UNP A0A0F6F6Q9
O	0	ASP	-	expression tag	UNP A0A0F6F6Q9
O	1	LYS	-	expression tag	UNP A0A0F6F6Q9

- Molecule 2 is a protein called Plasmid stabilization protein ParE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	95	Total	C	N	O	S	Se	0	0	0
			780	502	136	140	1	1			
2	D	95	Total	C	N	O	S	Se	0	0	0
			776	500	136	138	1	1			
2	F	96	Total	C	N	O	S	Se	0	0	0
			790	508	139	141	1	1			
2	H	95	Total	C	N	O	S	Se	0	0	0
			771	498	133	138	1	1			
2	J	95	Total	C	N	O	S	Se	0	0	0
			776	500	136	138	1	1			
2	L	95	Total	C	N	O	S	Se	0	0	0
			776	500	136	138	1	1			
2	N	95	Total	C	N	O	S	Se	0	0	0
			776	500	136	138	1	1			
2	P	95	Total	C	N	O	S	Se	0	1	0
			786	506	138	140	1	1			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	initiating methionine	UNP A0A0D7C2L1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	93	LEU	-	expression tag	UNP A0A0D7C2L1
B	94	GLU	-	expression tag	UNP A0A0D7C2L1
B	95	HIS	-	expression tag	UNP A0A0D7C2L1
B	96	HIS	-	expression tag	UNP A0A0D7C2L1
B	97	HIS	-	expression tag	UNP A0A0D7C2L1
B	98	HIS	-	expression tag	UNP A0A0D7C2L1
B	99	HIS	-	expression tag	UNP A0A0D7C2L1
B	100	HIS	-	expression tag	UNP A0A0D7C2L1
D	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
D	93	LEU	-	expression tag	UNP A0A0D7C2L1
D	94	GLU	-	expression tag	UNP A0A0D7C2L1
D	95	HIS	-	expression tag	UNP A0A0D7C2L1
D	96	HIS	-	expression tag	UNP A0A0D7C2L1
D	97	HIS	-	expression tag	UNP A0A0D7C2L1
D	98	HIS	-	expression tag	UNP A0A0D7C2L1
D	99	HIS	-	expression tag	UNP A0A0D7C2L1
D	100	HIS	-	expression tag	UNP A0A0D7C2L1
F	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
F	93	LEU	-	expression tag	UNP A0A0D7C2L1
F	94	GLU	-	expression tag	UNP A0A0D7C2L1
F	95	HIS	-	expression tag	UNP A0A0D7C2L1
F	96	HIS	-	expression tag	UNP A0A0D7C2L1
F	97	HIS	-	expression tag	UNP A0A0D7C2L1
F	98	HIS	-	expression tag	UNP A0A0D7C2L1
F	99	HIS	-	expression tag	UNP A0A0D7C2L1
F	100	HIS	-	expression tag	UNP A0A0D7C2L1
H	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
H	93	LEU	-	expression tag	UNP A0A0D7C2L1
H	94	GLU	-	expression tag	UNP A0A0D7C2L1
H	95	HIS	-	expression tag	UNP A0A0D7C2L1
H	96	HIS	-	expression tag	UNP A0A0D7C2L1
H	97	HIS	-	expression tag	UNP A0A0D7C2L1
H	98	HIS	-	expression tag	UNP A0A0D7C2L1
H	99	HIS	-	expression tag	UNP A0A0D7C2L1
H	100	HIS	-	expression tag	UNP A0A0D7C2L1
J	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
J	93	LEU	-	expression tag	UNP A0A0D7C2L1
J	94	GLU	-	expression tag	UNP A0A0D7C2L1
J	95	HIS	-	expression tag	UNP A0A0D7C2L1
J	96	HIS	-	expression tag	UNP A0A0D7C2L1
J	97	HIS	-	expression tag	UNP A0A0D7C2L1
J	98	HIS	-	expression tag	UNP A0A0D7C2L1

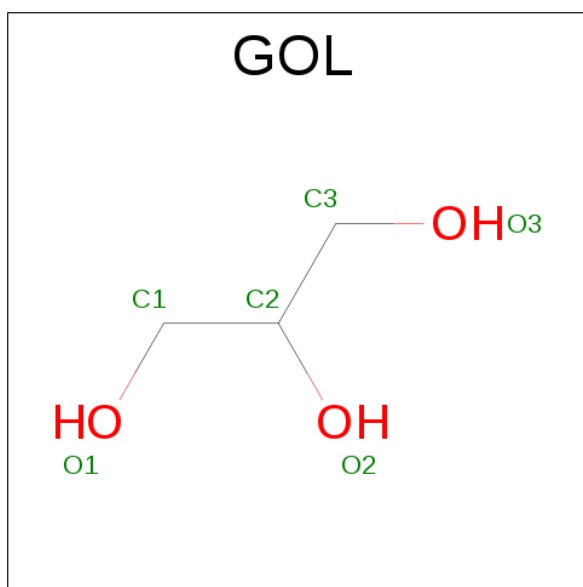
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Chain	Residue	Modelled	Actual	Comment	Reference
J	99	HIS	-	expression tag	UNP A0A0D7C2L1
J	100	HIS	-	expression tag	UNP A0A0D7C2L1
L	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
L	93	LEU	-	expression tag	UNP A0A0D7C2L1
L	94	GLU	-	expression tag	UNP A0A0D7C2L1
L	95	HIS	-	expression tag	UNP A0A0D7C2L1
L	96	HIS	-	expression tag	UNP A0A0D7C2L1
L	97	HIS	-	expression tag	UNP A0A0D7C2L1
L	98	HIS	-	expression tag	UNP A0A0D7C2L1
L	99	HIS	-	expression tag	UNP A0A0D7C2L1
L	100	HIS	-	expression tag	UNP A0A0D7C2L1
N	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
N	93	LEU	-	expression tag	UNP A0A0D7C2L1
N	94	GLU	-	expression tag	UNP A0A0D7C2L1
N	95	HIS	-	expression tag	UNP A0A0D7C2L1
N	96	HIS	-	expression tag	UNP A0A0D7C2L1
N	97	HIS	-	expression tag	UNP A0A0D7C2L1
N	98	HIS	-	expression tag	UNP A0A0D7C2L1
N	99	HIS	-	expression tag	UNP A0A0D7C2L1
N	100	HIS	-	expression tag	UNP A0A0D7C2L1
P	1	MSE	-	initiating methionine	UNP A0A0D7C2L1
P	93	LEU	-	expression tag	UNP A0A0D7C2L1
P	98	GLU	-	expression tag	UNP A0A0D7C2L1
P	99	HIS	-	expression tag	UNP A0A0D7C2L1
P	100	HIS	-	expression tag	UNP A0A0D7C2L1
P	101	HIS	-	expression tag	UNP A0A0D7C2L1
P	102	HIS	-	expression tag	UNP A0A0D7C2L1
P	103	HIS	-	expression tag	UNP A0A0D7C2L1
P	104	HIS	-	expression tag	UNP A0A0D7C2L1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	42	Total	O	0	0
			42	42		
4	C	33	Total	O	0	0
			33	33		
4	D	49	Total	O	0	0
			49	49		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	26	Total 26	O 26	0	0
4	F	47	Total 47	O 47	0	0
4	G	15	Total 15	O 15	0	0
4	H	45	Total 45	O 45	0	0
4	I	12	Total 12	O 12	0	0
4	J	30	Total 30	O 30	0	0
4	K	15	Total 15	O 15	0	0
4	L	28	Total 28	O 28	0	0
4	M	22	Total 22	O 22	0	0
4	N	41	Total 41	O 41	0	0
4	O	26	Total 26	O 26	0	0
4	P	42	Total 42	O 42	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 errors 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: PAAA2

Chain A: 



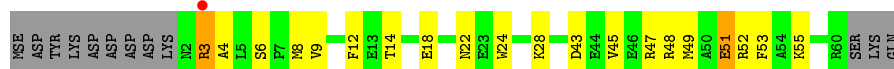
- Molecule 1: PAAA2

Chain C: 



- Molecule 1: PAAA2

Chain E: 



- Molecule 1: PAAA2

Chain G: 



- Molecule 1: PAAA2

Chain I: 



- Molecule 1: PAAA2

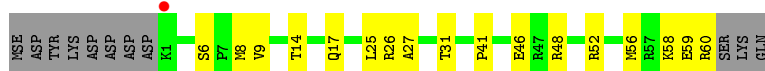
Chain K: 



- Molecule 1: PAAA2



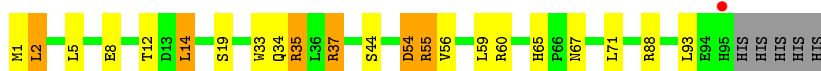
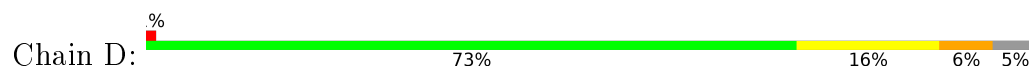
- Molecule 1: PAAA2



- Molecule 2: Plasmid stabilization protein ParE



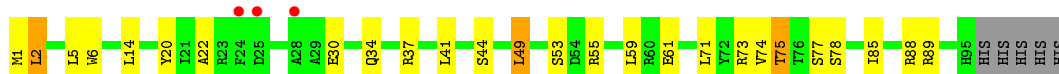
- Molecule 2: Plasmid stabilization protein ParE



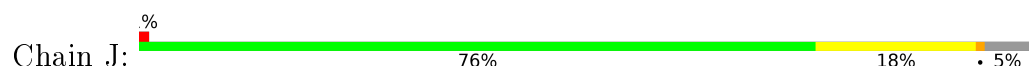
- Molecule 2: Plasmid stabilization protein ParE

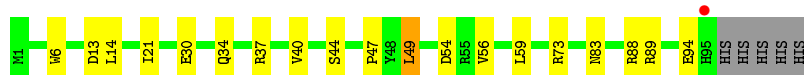


- Molecule 2: Plasmid stabilization protein ParE

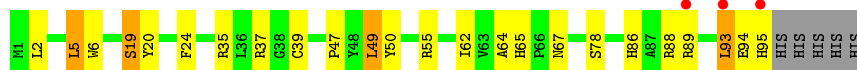


- Molecule 2: Plasmid stabilization protein ParE

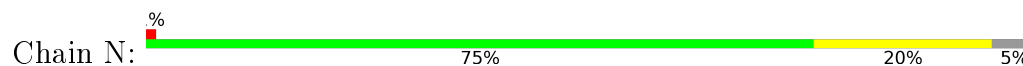




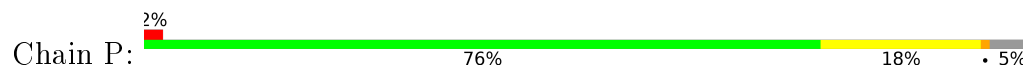
- Molecule 2: Plasmid stabilization protein ParE



- Molecule 2: Plasmid stabilization protein ParE



- Molecule 2: Plasmid stabilization protein ParE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.54Å 90.54Å 412.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.83 49.37 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.37-2.83) 99.8 (49.37-2.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.185 , 0.240 0.183 , 0.239	Depositor DCC
$R_{free}$ test set	2116 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL

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	0.57	0/484	0.68	1/649 (0.2%)
1	C	0.59	0/461	0.65	0/616
1	E	0.63	0/487	0.74	0/651
1	G	0.55	0/477	0.71	1/641 (0.2%)
1	I	0.63	0/482	0.66	0/645
1	K	0.67	0/472	0.71	0/634
1	M	0.69	0/465	0.67	0/623
1	O	0.62	0/484	0.71	0/648
2	B	0.64	0/802	0.69	0/1099
2	D	0.81	2/798 (0.3%)	0.81	2/1094 (0.2%)
2	F	0.64	0/813	0.75	1/1114 (0.1%)
2	H	0.71	0/793	0.73	1/1088 (0.1%)
2	J	0.68	1/798 (0.1%)	0.66	1/1094 (0.1%)
2	L	0.74	2/798 (0.3%)	0.83	2/1094 (0.2%)
2	N	0.70	1/798 (0.1%)	0.71	1/1094 (0.1%)
2	P	0.71	1/811 (0.1%)	0.67	0/1110
All	All	0.67	7/10223 (0.1%)	0.72	10/13894 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	55	ARG	NE-CZ	-7.37	1.23	1.33
2	D	55	ARG	CZ-NH1	-7.21	1.23	1.33
2	L	49	LEU	C-N	-6.86	1.18	1.34
2	P	49	LEU	C-N	-6.09	1.20	1.34
2	L	39	CYS	CB-SG	-5.89	1.72	1.81
2	J	40	VAL	CB-CG1	-5.51	1.41	1.52
2	N	49	LEU	C-N	-5.25	1.22	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	55	ARG	NE-CZ-NH1	-8.25	116.17	120.30
2	F	49	LEU	CB-CG-CD2	-6.10	100.63	111.00
2	L	5	LEU	CA-CB-CG	6.00	129.11	115.30
1	G	8	MSE	CG-SE-CE	5.85	111.77	98.90
2	N	14	LEU	CB-CG-CD2	-5.78	101.18	111.00
2	L	93	LEU	CB-CG-CD2	5.45	120.27	111.00
2	J	14	LEU	CB-CG-CD2	-5.31	101.97	111.00
2	H	49	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	D	14	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	A	8	MSE	CG-SE-CE	5.04	109.99	98.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	93	LEU	Peptide
2	D	93	LEU	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	478	0	449	4	0
1	C	455	0	441	26	0
1	E	478	0	465	13	0
1	G	471	0	437	15	0
1	I	476	0	456	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	466	0	433	20	0
1	M	459	0	436	15	0
1	O	478	0	456	17	0
2	B	780	0	776	28	0
2	D	776	0	772	29	0
2	F	790	0	783	19	0
2	H	771	0	763	30	0
2	J	776	0	772	18	0
2	L	776	0	771	34	0
2	N	776	0	772	26	0
2	P	786	0	779	16	0
3	B	12	0	16	3	0
3	F	6	0	8	1	0
3	H	6	0	8	0	0
3	L	12	0	16	1	0
3	N	6	0	8	0	0
3	P	6	0	8	0	0
4	A	34	0	0	1	0
4	B	42	0	0	1	0
4	C	33	0	0	3	0
4	D	49	0	0	3	0
4	E	26	0	0	2	0
4	F	47	0	0	0	1
4	G	15	0	0	0	0
4	H	45	0	0	0	0
4	I	12	0	0	1	0
4	J	30	0	0	1	0
4	K	15	0	0	2	0
4	L	28	0	0	0	0
4	M	22	0	0	0	0
4	N	41	0	0	3	1
4	O	26	0	0	2	0
4	P	42	0	0	0	0
All	All	10547	0	9825	253	1

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 13.

All (253) 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:I:8:MSE:SE	1:I:8:MSE:CE	2.16	1.43
1:I:8:MSE:SE	2:L:89:ARG:HH22	1.58	1.36
1:I:8:MSE:SE	2:L:89:ARG:HH12	1.65	1.30
1:I:8:MSE:SE	2:L:89:ARG:NH2	2.20	1.25
1:I:8:MSE:SE	2:L:89:ARG:NH1	2.26	1.16
1:I:8:MSE:SE	2:L:89:ARG:CZ	2.52	1.06
1:G:49:MSE:HE3	2:H:14:LEU:HG	1.40	1.03
1:G:49:MSE:HE2	1:G:52:ARG:HH11	1.31	0.95
2:L:93:LEU:HD23	2:L:94:GLU:H	1.29	0.95
1:K:14:THR:HG23	1:K:17:GLN:H	1.31	0.94
1:C:49:MSE:HE2	1:C:52:ARG:HH11	1.35	0.91
1:K:7:PRO:HG2	1:K:8:MSE:HE3	1.53	0.88
2:L:65:HIS:HD2	2:L:67:ASN:H	1.22	0.88
2:F:49:LEU:HD21	2:H:49:LEU:HD21	1.56	0.88
1:G:57:ARG:NH2	2:H:30:GLU:OE1	2.10	0.83
1:M:49:MSE:HE1	1:M:52:ARG:HH21	1.45	0.82
2:B:86:HIS:HD2	2:B:88:ARG:H	1.26	0.81
1:I:8:MSE:CE	2:L:89:ARG:CZ	2.58	0.81
1:I:8:MSE:HE1	2:L:89:ARG:CZ	2.10	0.81
2:L:86:HIS:HD2	2:L:88:ARG:H	1.27	0.81
2:N:35:ARG:NH2	2:N:64:ALA:O	2.13	0.81
2:D:65:HIS:HD2	2:D:67:ASN:H	1.24	0.80
2:L:35:ARG:NH1	2:L:64:ALA:O	2.14	0.80
2:B:89:ARG:HH12	1:C:7:PRO:HB2	1.47	0.79
2:L:93:LEU:CD2	2:L:94:GLU:H	1.97	0.78
2:N:89:ARG:NH2	1:O:8:MSE:HE1	1.99	0.77
1:M:14:THR:HG23	1:M:17:GLN:H	1.50	0.76
1:C:49:MSE:HE2	1:C:52:ARG:NH1	2.01	0.75
1:A:28:LYS:O	1:A:31:THR:HG22	1.87	0.75
1:C:14:THR:HG23	1:C:17:GLN:H	1.50	0.75
2:L:65:HIS:CD2	2:L:67:ASN:H	2.05	0.75
2:D:65:HIS:CD2	2:D:67:ASN:H	2.06	0.73
1:E:43:ASP:OD2	4:E:101:HOH:O	2.05	0.73
2:F:93:LEU:HD23	2:F:94:GLU:O	1.88	0.73
1:K:7:PRO:HG2	1:K:8:MSE:CE	2.18	0.73
1:M:2:ASN:HA	1:M:16:GLU:OE2	1.88	0.73
2:P:65:HIS:HD2	2:P:67:ASN:H	1.34	0.73
2:B:89:ARG:NH1	1:C:7:PRO:HB2	2.04	0.72
1:M:2:ASN:OD1	1:M:3:ARG:N	2.22	0.72
2:P:65:HIS:CD2	2:P:67:ASN:H	2.08	0.71
2:B:65:HIS:HD2	2:B:67:ASN:H	1.35	0.71
1:I:8:MSE:CE	2:L:89:ARG:NH1	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLU:OE1	1:C:26:ARG:NH1	2.24	0.70
2:F:88:ARG:NH2	2:H:88:ARG:HD2	2.06	0.70
1:C:48:ARG:O	1:C:52:ARG:HG3	1.91	0.70
1:G:49:MSE:HE2	1:G:52:ARG:NH1	2.03	0.70
2:L:86:HIS:CD2	2:L:88:ARG:H	2.10	0.70
1:M:49:MSE:CE	1:M:52:ARG:HH21	2.04	0.70
2:B:89:ARG:NH1	4:B:302:HOH:O	2.25	0.69
2:H:75:THR:HG22	2:H:77:SER:H	1.58	0.69
2:B:88:ARG:HD3	2:D:88:ARG:NH2	2.07	0.69
2:N:34:GLN:OE1	2:N:37:ARG:NH2	2.27	0.68
2:N:88:ARG:HD3	2:P:88:ARG:NH2	2.10	0.66
1:K:56:MSE:HE1	2:L:19:SER:HA	1.76	0.65
2:H:34:GLN:HE21	2:H:34:GLN:HA	1.61	0.65
2:N:89:ARG:HD3	1:O:8:MSE:HE1	1.77	0.65
1:E:48:ARG:O	1:E:52:ARG:HG3	1.96	0.65
1:K:46:GLU:OE1	4:K:101:HOH:O	2.15	0.64
1:C:48:ARG:O	1:C:51:GLU:HG2	1.98	0.64
2:H:75:THR:HG22	2:H:78:SER:H	1.63	0.63
1:I:8:MSE:HG3	2:L:20:TYR:CE1	2.33	0.63
2:B:86:HIS:CD2	2:B:88:ARG:H	2.12	0.62
1:K:49:MSE:HE2	1:K:53:PHE:CE2	2.34	0.62
2:D:60:ARG:NH2	1:K:43:ASP:OD1	2.32	0.62
1:E:52:ARG:NH2	2:F:11:ASP:OD1	2.33	0.62
1:I:57:ARG:NH2	2:J:30:GLU:OE1	2.29	0.62
1:C:13:GLU:H	1:C:17:GLN:HE21	1.48	0.61
2:B:7:LEU:HD22	2:B:82:VAL:HA	1.82	0.61
1:E:49:MSE:HE3	1:E:53:PHE:CE2	2.35	0.61
2:B:1:MSE:HE3	2:J:47:PRO:HG3	1.81	0.61
1:E:3:ARG:HG3	1:E:4:ALA:N	2.14	0.61
1:G:44:GLU:OE2	1:G:47:ARG:NH2	2.35	0.59
2:F:20:TYR:CE2	1:G:8:MSE:HG3	2.37	0.59
1:K:46:GLU:OE2	2:L:37:ARG:NH1	2.27	0.59
2:B:88:ARG:HD3	2:D:88:ARG:CZ	2.33	0.58
1:E:8:MSE:HG3	2:H:20:TYR:CE1	2.38	0.58
2:F:67:ASN:OD1	2:F:88:ARG:NH1	2.37	0.58
2:B:65:HIS:CD2	2:B:67:ASN:H	2.19	0.58
1:C:13:GLU:H	1:C:17:GLN:NE2	2.02	0.58
1:M:48:ARG:O	1:M:52:ARG:HG3	2.04	0.58
1:A:26:ARG:NH2	4:A:103:HOH:O	2.36	0.58
1:C:6:SER:HB3	1:C:9:VAL:HG23	1.85	0.57
1:O:26:ARG:NH2	4:O:101:HOH:O	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:89:ARG:NH2	4:J:201:HOH:O	2.36	0.57
2:J:88:ARG:HD2	2:L:88:ARG:NH2	2.18	0.57
1:E:47:ARG:O	1:E:51[B]:GLU:HG2	2.04	0.57
1:K:48:ARG:O	1:K:52:ARG:HG3	2.04	0.57
2:N:89:ARG:CZ	1:O:8:MSE:HE1	2.35	0.56
2:D:12:THR:HG22	4:D:215:HOH:O	2.04	0.56
1:M:44:GLU:OE2	1:M:47:ARG:NH2	2.26	0.56
2:D:2:LEU:O	2:D:44:SER:HB2	2.06	0.56
2:N:88:ARG:HD2	4:N:301:HOH:O	2.05	0.56
1:O:48:ARG:O	1:O:52:ARG:HG3	2.06	0.55
2:P:30:GLU:O	2:P:34:GLN:HG3	2.05	0.55
2:N:93:LEU:HD23	2:N:93:LEU:H	1.71	0.55
1:O:41:PRO:HA	2:P:5:LEU:HD23	1.88	0.55
2:D:1:MSE:CE	2:H:1:MSE:HA	2.36	0.55
2:P:40:VAL:O	2:P:43:LEU:HB2	2.07	0.55
2:J:54:ASP:N	2:J:54:ASP:OD1	2.40	0.55
1:C:14:THR:CG2	1:C:17:GLN:HB3	2.37	0.55
3:F:201:GOL:O3	1:G:11:GLU:OE2	2.25	0.54
2:F:49:LEU:HD21	2:H:49:LEU:CD2	2.33	0.54
2:P:56:VAL:HG11	2:P:59:LEU:HD22	1.90	0.54
1:C:49:MSE:HE3	2:D:14:LEU:HD23	1.90	0.54
1:O:25:LEU:CD1	2:P:85:ILE:HD13	2.38	0.54
2:L:86:HIS:HD2	2:L:89:ARG:H	1.54	0.54
2:N:89:ARG:NH2	4:N:303:HOH:O	2.40	0.54
1:I:48:ARG:O	1:I:52:ARG:HG3	2.08	0.53
2:B:1:MSE:HE3	2:J:47:PRO:CG	2.38	0.53
2:D:65:HIS:HD2	2:D:67:ASN:N	2.01	0.53
1:K:43:ASP:OD2	4:K:102:HOH:O	2.19	0.53
1:I:43:ASP:OD1	2:N:60:ARG:NH1	2.42	0.52
1:G:41:PRO:HA	2:H:5:LEU:HD23	1.92	0.52
1:K:14:THR:CG2	1:K:17:GLN:H	2.14	0.52
2:N:88:ARG:HD3	2:P:88:ARG:CZ	2.40	0.52
1:O:56:MSE:HE1	2:P:19:SER:HA	1.92	0.52
1:K:44:GLU:OE2	1:K:47:ARG:NH2	2.43	0.52
2:L:86:HIS:CD2	2:L:89:ARG:H	2.28	0.52
2:N:21:ILE:HG23	1:O:9:VAL:HG22	1.91	0.52
1:M:52:ARG:NH2	2:N:11:ASP:OD1	2.41	0.52
1:O:58:LYS:O	1:O:60:ARG:N	2.43	0.52
2:D:60:ARG:NH2	1:K:43:ASP:OD2	2.44	0.51
2:B:94:GLU:O	2:B:95:HIS:HB2	2.10	0.51
2:B:5:LEU:HD12	2:B:78:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:MSE:HE3	2:D:14:LEU:CG	2.41	0.50
1:I:23:GLU:OE2	1:I:26:ARG:NH1	2.44	0.50
2:D:54:ASP:OD1	4:D:201:HOH:O	2.19	0.50
2:B:50:TYR:CD2	2:B:62:ILE:HG12	2.46	0.50
2:H:59:LEU:HD22	2:H:73:ARG:HB3	1.93	0.50
2:H:53:SER:HB2	2:H:61:GLU:HG3	1.93	0.50
2:F:61:GLU:HG2	2:F:71:LEU:CD2	2.42	0.49
2:J:34:GLN:HG2	2:J:37:ARG:NH2	2.28	0.49
1:I:29:VAL:HG11	2:J:56:VAL:HG11	1.94	0.49
2:F:5:LEU:HD12	2:F:78:SER:HB2	1.94	0.49
2:H:75:THR:HB	2:H:78:SER:O	2.11	0.49
1:E:24:TRP:CD2	2:F:90:GLN:HG2	2.48	0.49
2:D:1:MSE:N	4:D:206:HOH:O	2.44	0.49
2:D:34:GLN:HG2	2:D:37:ARG:NH2	2.28	0.49
1:O:14:THR:HG22	1:O:17:GLN:H	1.78	0.49
1:I:8:MSE:CE	2:L:89:ARG:NH2	2.76	0.49
1:K:6:SER:C	1:K:8:MSE:H	2.16	0.48
1:O:25:LEU:HD13	2:P:85:ILE:HD13	1.95	0.48
1:K:52:ARG:O	1:K:56:MSE:HG3	2.13	0.48
1:O:58:LYS:C	1:O:60:ARG:H	2.17	0.48
1:I:42:HIS:NE2	4:I:101:HOH:O	2.29	0.48
1:M:25:LEU:HD13	2:N:85:ILE:HD13	1.95	0.48
2:N:35:ARG:HH22	2:N:65:HIS:HA	1.79	0.48
2:N:5:LEU:HD23	2:N:78:SER:HB2	1.96	0.48
2:N:89:ARG:HH21	1:O:8:MSE:HE1	1.78	0.48
2:B:73:ARG:NH1	2:B:80:GLU:OE2	2.39	0.48
2:B:41:LEU:HD23	2:B:41:LEU:HA	1.71	0.47
1:O:6:SER:HB3	1:O:9:VAL:HG23	1.96	0.47
2:B:86:HIS:CD2	2:B:89:ARG:H	2.32	0.47
1:C:58:LYS:O	1:C:60:ARG:N	2.45	0.47
2:F:35:ARG:NH1	2:F:64:ALA:O	2.46	0.47
2:J:59:LEU:HD22	2:J:73:ARG:HB3	1.97	0.47
2:D:14:LEU:HD21	2:D:33:TRP:CZ3	2.49	0.47
2:H:6:TRP:CD1	2:H:6:TRP:N	2.83	0.47
2:H:61:GLU:HG2	2:H:71:LEU:HD23	1.97	0.47
2:H:59:LEU:CD2	2:H:73:ARG:HB3	2.45	0.46
1:M:46:GLU:OE2	2:N:37:ARG:HD2	2.16	0.46
1:M:14:THR:CG2	1:M:17:GLN:HB2	2.45	0.46
2:N:5:LEU:CD2	2:N:78:SER:HB2	2.44	0.46
1:G:22:ASN:O	1:G:26:ARG:HG3	2.15	0.46
2:B:1:MSE:HE3	2:J:47:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:LEU:HD12	2:L:47:PRO:HG3	1.96	0.46
4:E:113:HOH:O	2:F:88:ARG:HD3	2.14	0.46
2:D:1:MSE:HE1	2:H:1:MSE:HA	1.98	0.46
1:C:14:THR:OG1	1:C:15:ILE:N	2.49	0.46
2:J:88:ARG:HD2	2:L:88:ARG:CZ	2.46	0.46
2:N:34:GLN:HE22	2:N:37:ARG:HH21	1.64	0.46
2:L:35:ARG:HH12	2:L:65:HIS:HA	1.81	0.45
2:L:65:HIS:HD2	2:L:67:ASN:N	2.02	0.45
1:K:45:VAL:HG21	2:L:6:TRP:CG	2.52	0.45
2:N:55:ARG:H	2:N:55:ARG:HG2	1.58	0.45
2:L:5:LEU:HD23	2:L:78:SER:HB2	1.98	0.45
1:E:45:VAL:HG21	2:F:6:TRP:CG	2.51	0.45
2:L:20:TYR:CE1	2:L:24:PHE:HE1	2.34	0.45
2:H:2:LEU:O	2:H:44:SER:HB2	2.17	0.45
2:B:61:GLU:HG2	2:B:71:LEU:HD23	1.98	0.45
1:M:21:TYR:OH	2:N:85:ILE:HD12	2.17	0.45
1:E:22:ASN:OD1	2:F:55:ARG:HD2	2.17	0.45
1:I:45:VAL:HG21	2:J:6:TRP:CG	2.52	0.45
2:B:1:MSE:CE	2:J:47:PRO:HG3	2.47	0.44
1:E:4:ALA:HA	1:E:14:THR:HG22	1.99	0.44
2:N:90:GLN:NE2	4:N:305:HOH:O	2.51	0.44
1:O:46:GLU:HG3	4:O:110:HOH:O	2.17	0.44
1:M:45:VAL:HG21	2:N:6:TRP:CG	2.52	0.44
2:P:40:VAL:HA	2:P:43:LEU:HD22	1.99	0.44
2:J:49:LEU:HD21	2:L:49:LEU:HD21	1.99	0.44
2:B:61:GLU:HG2	2:B:71:LEU:CD2	2.48	0.44
2:F:88:ARG:CZ	2:H:88:ARG:HD2	2.46	0.44
2:F:30:GLU:O	2:F:34:GLN:HG3	2.18	0.43
2:J:59:LEU:CD2	2:J:73:ARG:HB3	2.48	0.43
1:C:14:THR:HG23	1:C:17:GLN:HB3	2.01	0.43
1:C:58:LYS:HE2	4:C:103:HOH:O	2.18	0.43
2:H:34:GLN:NE2	2:H:37:ARG:HD3	2.32	0.43
2:P:50:TYR:O	2:P:60:ARG:HD3	2.19	0.43
2:D:56:VAL:HG11	2:D:59:LEU:HD22	1.99	0.43
1:I:60:ARG:HG3	1:I:60:ARG:HH11	1.83	0.43
1:C:49:MSE:HE3	2:D:14:LEU:CD2	2.49	0.43
1:E:12:PHE:CD1	1:E:18:GLU:HB2	2.53	0.43
1:E:6:SER:HB3	1:E:9:VAL:HG23	2.01	0.43
2:H:41:LEU:HD23	2:H:41:LEU:HA	1.81	0.43
2:L:35:ARG:HH22	3:L:201:GOL:C1	2.31	0.43
1:A:6:SER:HB3	1:A:9:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:65:HIS:CD2	2:F:67:ASN:H	2.36	0.43
1:I:14:THR:OG1	1:I:17:GLN:HG3	2.19	0.43
1:M:9:VAL:HG22	2:P:21:ILE:HG23	2.00	0.43
1:G:45:VAL:HG21	2:H:6:TRP:CG	2.54	0.43
2:J:21:ILE:HG23	1:K:9:VAL:HG22	2.01	0.43
1:G:56:MSE:CE	2:H:22:ALA:HB3	2.49	0.42
3:B:202:GOL:O1	2:D:35:ARG:NH2	2.52	0.42
1:M:46:GLU:HG2	2:N:37:ARG:HH11	1.84	0.42
2:H:75:THR:HG22	2:H:77:SER:N	2.31	0.42
2:H:75:THR:CG2	2:H:77:SER:H	2.30	0.42
2:J:13:ASP:OD2	2:J:83:ASN:ND2	2.44	0.42
2:D:60:ARG:NH2	1:K:43:ASP:CG	2.72	0.42
4:C:113:HOH:O	2:H:74:VAL:HG22	2.19	0.42
2:P:35:ARG:NH1	2:P:64:ALA:O	2.43	0.42
2:D:1:MSE:HE3	2:H:1:MSE:HA	2.01	0.42
2:B:35:ARG:NH2	3:B:201:GOL:O1	2.52	0.42
1:I:58:LYS:HE3	1:I:58:LYS:HB2	1.88	0.42
1:I:6:SER:HB3	1:I:9:VAL:HG23	2.00	0.42
1:K:14:THR:HG22	1:K:17:GLN:CD	2.40	0.42
2:B:67:ASN:OD1	2:D:88:ARG:NH1	2.52	0.42
2:B:93:LEU:HD23	2:B:93:LEU:HA	1.74	0.42
2:B:53:SER:HB2	2:B:61:GLU:HG3	2.01	0.41
1:G:56:MSE:HE1	2:H:22:ALA:HB3	2.02	0.41
1:C:25:LEU:HD11	2:D:71:LEU:HD11	2.01	0.41
1:I:27:ALA:O	1:I:31:THR:HG23	2.21	0.41
1:C:39:ALA:HB3	2:D:5:LEU:HD23	2.02	0.41
1:C:44:GLU:O	1:C:48:ARG:HG3	2.20	0.41
1:K:35:ASP:OD1	1:K:37:ARG:HG3	2.20	0.41
2:N:34:GLN:NE2	2:N:37:ARG:HH21	2.18	0.41
2:B:55:ARG:NH2	3:B:202:GOL:H32	2.35	0.41
2:F:20:TYR:O	2:F:23:ARG:HG3	2.20	0.41
2:J:49:LEU:CD2	2:L:49:LEU:HD21	2.51	0.41
1:O:27:ALA:O	1:O:31:THR:HG23	2.21	0.41
1:G:52:ARG:O	1:G:56:MSE:HG3	2.21	0.41
1:C:56:MSE:HE1	2:D:19:SER:HA	2.03	0.40
1:C:49:MSE:HE3	2:D:14:LEU:HB3	2.03	0.40
1:G:48:ARG:O	1:G:52:ARG:HG3	2.20	0.40
1:I:2:ASN:HB2	1:I:16:GLU:HB2	2.04	0.40
2:L:50:TYR:CD2	2:L:62:ILE:HG12	2.56	0.40
2:P:65:HIS:CD2	2:P:67:ASN:HB2	2.57	0.40
1:A:25:LEU:HD11	2:B:71:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:LEU:HD13	2:H:85:ILE:HD13	2.03	0.40
2:L:94:GLU:O	2:L:95:HIS:HB2	2.22	0.40
1:C:26:ARG:NH2	4:C:105:HOH:O	2.55	0.40
1:C:22:ASN:OD1	2:D:55:ARG:HD2	2.20	0.40
2:D:56:VAL:CG1	2:D:59:LEU:HD22	2.52	0.40
2:F:65:HIS:HD2	2:F:67:ASN:HB2	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:318:HOH:O	4:N:308:HOH:O[5_555]	2.10	0.10

## 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	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
1	C	55/71 (78%)	54 (98%)	0	1 (2%)	11	33
1	E	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
1	G	59/71 (83%)	56 (95%)	3 (5%)	0	100	100
1	I	57/71 (80%)	56 (98%)	1 (2%)	0	100	100
1	K	59/71 (83%)	58 (98%)	0	1 (2%)	11	34
1	M	55/71 (78%)	51 (93%)	3 (6%)	1 (2%)	11	33
1	O	58/71 (82%)	57 (98%)	0	1 (2%)	11	34
2	B	93/100 (93%)	90 (97%)	3 (3%)	0	100	100
2	D	93/100 (93%)	91 (98%)	2 (2%)	0	100	100
2	F	94/100 (94%)	91 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	93/100 (93%)	91 (98%)	2 (2%)	0	100	100
2	J	93/100 (93%)	89 (96%)	3 (3%)	1 (1%)	17	48
2	L	93/100 (93%)	89 (96%)	4 (4%)	0	100	100
2	N	93/100 (93%)	91 (98%)	2 (2%)	0	100	100
2	P	92/100 (92%)	90 (98%)	2 (2%)	0	100	100
All	All	1203/1368 (88%)	1167 (97%)	31 (3%)	5 (0%)	39	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	94	GLU
1	M	3	ARG
1	C	59	GLU
1	O	59	GLU
1	K	7	PRO

### 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	47/60 (78%)	45 (96%)	2 (4%)	35	69
1	C	45/60 (75%)	43 (96%)	2 (4%)	35	68
1	E	49/60 (82%)	44 (90%)	5 (10%)	9	26
1	G	46/60 (77%)	46 (100%)	0	100	100
1	I	49/60 (82%)	49 (100%)	0	100	100
1	K	44/60 (73%)	43 (98%)	1 (2%)	58	87
1	M	47/60 (78%)	47 (100%)	0	100	100
1	O	47/60 (78%)	47 (100%)	0	100	100
2	B	87/91 (96%)	84 (97%)	3 (3%)	44	77
2	D	86/91 (94%)	81 (94%)	5 (6%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	88/91 (97%)	86 (98%)	2 (2%)	58	87
2	H	85/91 (93%)	81 (95%)	4 (5%)	32	66
2	J	86/91 (94%)	84 (98%)	2 (2%)	58	87
2	L	86/91 (94%)	84 (98%)	2 (2%)	58	87
2	N	86/91 (94%)	85 (99%)	1 (1%)	78	95
2	P	88/91 (97%)	85 (97%)	3 (3%)	44	77
All	All	1066/1208 (88%)	1034 (97%)	32 (3%)	51	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MSE
1	A	9	VAL
2	B	5	LEU
2	B	35	ARG
2	B	73	ARG
1	C	40	ILE
1	C	58	LYS
2	D	2	LEU
2	D	8	GLU
2	D	35	ARG
2	D	37	ARG
2	D	54	ASP
1	E	3	ARG
1	E	28	LYS
1	E	51[A]	GLU
1	E	51[B]	GLU
1	E	55	LYS
2	F	1	MSE
2	F	5	LEU
2	H	2	LEU
2	H	55	ARG
2	H	75	THR
2	H	89	ARG
2	J	44	SER
2	J	49	LEU
1	K	46	GLU
2	L	19	SER
2	L	55	ARG
2	N	40	VAL

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Mol	Chain	Res	Type
2	P	43	LEU
2	P	54[A]	ASP
2	P	54[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	65	HIS
2	B	86	HIS
2	B	90	GLN
1	C	17	GLN
2	D	65	HIS
2	F	65	HIS
2	H	34	GLN
2	L	34	GLN
2	L	65	HIS
2	L	86	HIS
1	O	19	ASN
2	P	65	HIS

### 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](#)

8 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	GOL	B	201	-	5,5,5	0.36	0	5,5,5	0.55	0
3	GOL	B	202	-	5,5,5	0.43	0	5,5,5	0.41	0
3	GOL	F	201	-	5,5,5	0.51	0	5,5,5	0.28	0
3	GOL	H	201	-	5,5,5	0.46	0	5,5,5	0.33	0
3	GOL	L	201	-	5,5,5	0.39	0	5,5,5	0.57	0
3	GOL	L	202	-	5,5,5	0.54	0	5,5,5	0.46	0
3	GOL	N	201	-	5,5,5	0.34	0	5,5,5	0.34	0
3	GOL	P	201	-	5,5,5	0.37	0	5,5,5	0.39	0

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
3	GOL	B	201	-	-	0/4/4/4	0/0/0/0
3	GOL	B	202	-	-	0/4/4/4	0/0/0/0
3	GOL	F	201	-	-	0/4/4/4	0/0/0/0
3	GOL	H	201	-	-	0/4/4/4	0/0/0/0
3	GOL	L	201	-	-	0/4/4/4	0/0/0/0
3	GOL	L	202	-	-	0/4/4/4	0/0/0/0
3	GOL	N	201	-	-	0/4/4/4	0/0/0/0
3	GOL	P	201	-	-	0/4/4/4	0/0/0/0

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	GOL	1	0
3	B	202	GOL	2	0
3	F	201	GOL	1	0
3	L	201	GOL	1	0

## 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	P	1
2	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	49:LEU	C	50:TYR	N	1.20
1	L	49:LEU	C	50:TYR	N	1.18

## 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	57/71 (80%)	-0.18	0 100 100	39, 44, 93, 124	0
1	C	54/71 (76%)	-0.13	1 (1%) 70 59	34, 46, 87, 137	0
1	E	56/71 (78%)	-0.26	1 (1%) 71 61	36, 44, 86, 96	0
1	G	58/71 (81%)	-0.07	1 (1%) 73 63	41, 55, 99, 149	0
1	I	56/71 (78%)	-0.24	1 (1%) 71 61	37, 56, 92, 116	0
1	K	58/71 (81%)	-0.04	0 100 100	37, 57, 96, 117	0
1	M	54/71 (76%)	-0.17	1 (1%) 70 59	36, 49, 92, 123	0
1	O	57/71 (80%)	0.00	1 (1%) 71 61	41, 48, 87, 94	0
2	B	94/100 (94%)	-0.08	3 (3%) 51 39	32, 39, 75, 119	0
2	D	94/100 (94%)	-0.42	1 (1%) 82 75	30, 36, 56, 111	0
2	F	95/100 (95%)	-0.44	0 100 100	30, 36, 59, 79	0
2	H	94/100 (94%)	-0.24	3 (3%) 51 39	33, 43, 81, 107	0
2	J	94/100 (94%)	-0.29	1 (1%) 82 75	34, 47, 70, 144	0
2	L	94/100 (94%)	-0.11	3 (3%) 51 39	35, 47, 77, 123	0
2	N	94/100 (94%)	-0.31	1 (1%) 82 75	34, 41, 59, 92	0
2	P	94/100 (94%)	-0.27	2 (2%) 67 56	34, 42, 68, 99	0
All	All	1203/1368 (87%)	-0.22	20 (1%) 73 63	30, 45, 86, 149	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	ALA	8.9
2	H	25	ASP	3.7
2	P	100	HIS	3.6
2	L	95	HIS	3.3
2	D	95	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	2	ASN	3.0
1	G	2	ASN	2.9
2	B	23	ARG	2.8
1	E	3	ARG	2.8
1	O	1	LYS	2.7
2	B	24	PHE	2.6
2	N	95	HIS	2.6
2	H	28	ALA	2.5
2	L	89	ARG	2.4
1	I	4	ALA	2.4
2	L	93	LEU	2.2
2	J	95	HIS	2.1
2	P	99	HIS	2.1
2	B	95	HIS	2.0
2	H	24	PHE	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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	L	202	6/6	0.80	0.39	9.47	63,71,74,75	0
3	GOL	B	201	6/6	0.91	0.29	7.74	68,68,70,72	0
3	GOL	H	201	6/6	0.88	0.23	2.73	59,61,65,69	0
3	GOL	B	202	6/6	0.93	0.23	2.41	45,55,58,61	0
3	GOL	P	201	6/6	0.91	0.21	1.88	53,63,68,70	0
3	GOL	F	201	6/6	0.93	0.19	1.18	51,54,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	L	201	6/6	0.87	0.21	0.70	59,60,61,63	0
3	GOL	N	201	6/6	0.85	0.20	0.68	56,66,68,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.