Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 08:25 AM EDT

PDB ID	:	3PXG
Title	:	Structure of MecA121 and ClpC1-485 complex
Authors	:	Wang, F.; Mei, Z.Q.; Wang, J.W.; Shi, Y.G.
Deposited on	:	2010-12-09
Resolution	:	3.65 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

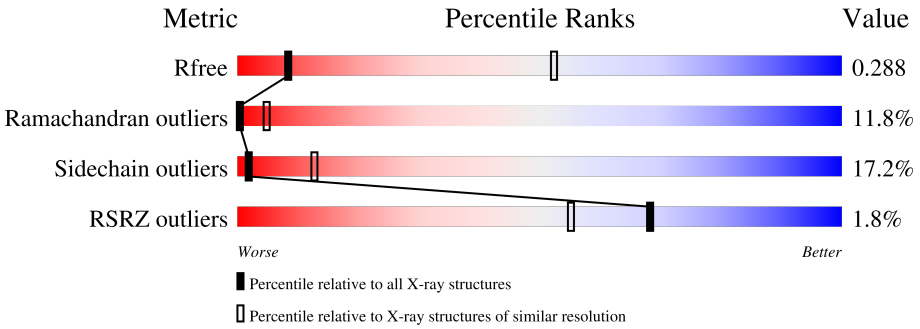
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.65 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	1557 (3.82-3.50)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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	98	73% 22% ·
1	b	98	3% 74% 21% ·
1	c	98	5% 76% 20% ·
1	d	98	73% 23% ·
1	e	98	73% 23% ·
1	f	98	2% 74% 21% ·
2	A	468	3% 72% 21% · 6%

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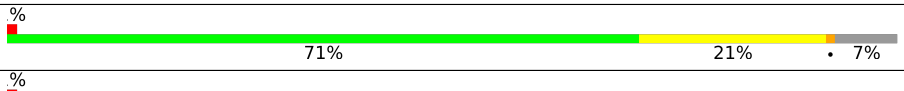
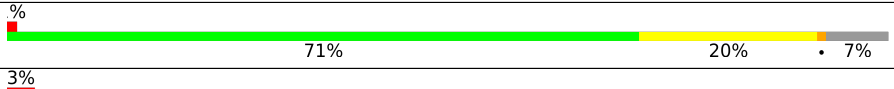
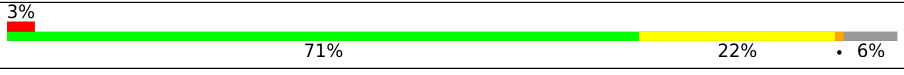
Mol	Chain	Length	Quality of chain
2	B	468	
2	C	468	
2	D	468	
2	E	468	
2	F	468	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24809 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adapter protein mecA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			
1	b	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			
1	c	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			
1	d	95	Total	C	N	O	S	0	0	0
			777	499	123	153	2			
1	e	95	Total	C	N	O	S	0	0	0
			777	499	123	153	2			
1	f	94	Total	C	N	O	S	0	0	0
			772	496	122	152	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	442	Total	C	N	O	S	0	0	0
			3380	2092	621	661	6			
2	B	437	Total	C	N	O	S	0	0	0
			3356	2078	616	656	6			
2	C	444	Total	C	N	O	S	0	0	0
			3386	2095	622	663	6			
2	D	434	Total	C	N	O	S	0	0	0
			3342	2070	613	653	6			
2	E	434	Total	C	N	O	S	0	0	0
			3342	2070	613	653	6			
2	F	438	Total	C	N	O	S	0	0	0
			3361	2081	617	657	6			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P37571
A	?	-	ALA	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	THR	deletion	UNP P37571
A	280	ALA	GLU	engineered mutation	UNP P37571
A	?	-	LEU	deletion	UNP P37571
A	?	-	HIS	deletion	UNP P37571
A	?	-	THR	deletion	UNP P37571
A	?	-	LEU	deletion	UNP P37571
A	?	-	ILE	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	ALA	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	GLU	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	ALA	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	THR	deletion	UNP P37571
B	280	ALA	GLU	engineered mutation	UNP P37571
B	?	-	LEU	deletion	UNP P37571
B	?	-	HIS	deletion	UNP P37571
B	?	-	THR	deletion	UNP P37571
B	?	-	LEU	deletion	UNP P37571
B	?	-	ILE	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	ALA	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	GLU	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	ALA	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	THR	deletion	UNP P37571
C	280	ALA	GLU	engineered mutation	UNP P37571
C	?	-	LEU	deletion	UNP P37571
C	?	-	HIS	deletion	UNP P37571
C	?	-	THR	deletion	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P37571
C	?	-	ILE	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	ALA	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	GLU	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
D	?	-	VAL	deletion	UNP P37571
D	?	-	VAL	deletion	UNP P37571
D	?	-	ALA	deletion	UNP P37571
D	?	-	GLY	deletion	UNP P37571
D	?	-	THR	deletion	UNP P37571
D	280	ALA	GLU	engineered mutation	UNP P37571
D	?	-	LEU	deletion	UNP P37571
D	?	-	HIS	deletion	UNP P37571
D	?	-	THR	deletion	UNP P37571
D	?	-	LEU	deletion	UNP P37571
D	?	-	ILE	deletion	UNP P37571
D	?	-	GLY	deletion	UNP P37571
D	?	-	ALA	deletion	UNP P37571
D	?	-	GLY	deletion	UNP P37571
D	?	-	GLY	deletion	UNP P37571
D	?	-	GLU	deletion	UNP P37571
D	?	-	GLY	deletion	UNP P37571
E	?	-	VAL	deletion	UNP P37571
E	?	-	VAL	deletion	UNP P37571
E	?	-	ALA	deletion	UNP P37571
E	?	-	GLY	deletion	UNP P37571
E	?	-	THR	deletion	UNP P37571
E	280	ALA	GLU	engineered mutation	UNP P37571
E	?	-	LEU	deletion	UNP P37571
E	?	-	HIS	deletion	UNP P37571
E	?	-	THR	deletion	UNP P37571
E	?	-	LEU	deletion	UNP P37571
E	?	-	ILE	deletion	UNP P37571
E	?	-	GLY	deletion	UNP P37571
E	?	-	ALA	deletion	UNP P37571
E	?	-	GLY	deletion	UNP P37571
E	?	-	GLY	deletion	UNP P37571
E	?	-	GLU	deletion	UNP P37571
E	?	-	GLY	deletion	UNP P37571

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	VAL	deletion	UNP P37571
F	?	-	VAL	deletion	UNP P37571
F	?	-	ALA	deletion	UNP P37571
F	?	-	GLY	deletion	UNP P37571
F	?	-	THR	deletion	UNP P37571
F	280	ALA	GLU	engineered mutation	UNP P37571
F	?	-	LEU	deletion	UNP P37571
F	?	-	HIS	deletion	UNP P37571
F	?	-	THR	deletion	UNP P37571
F	?	-	LEU	deletion	UNP P37571
F	?	-	ILE	deletion	UNP P37571
F	?	-	GLY	deletion	UNP P37571
F	?	-	ALA	deletion	UNP P37571
F	?	-	GLY	deletion	UNP P37571
F	?	-	GLY	deletion	UNP P37571
F	?	-	GLU	deletion	UNP P37571
F	?	-	GLY	deletion	UNP P37571

3 Residue-property plots (i)

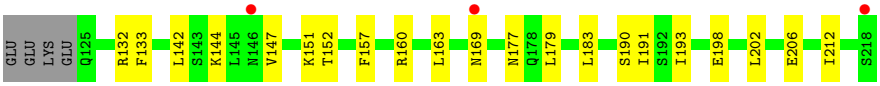
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Adapter protein mecA 1

Chain a:

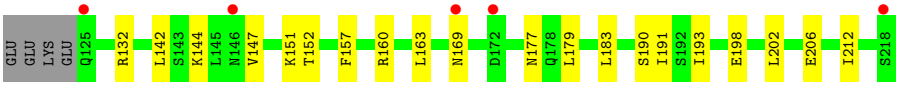
• Molecule 1: Adapter protein mecA 1

Chain b:



• Molecule 1: Adapter protein mecA 1

Chain c:



• Molecule 1: Adapter protein mecA 1

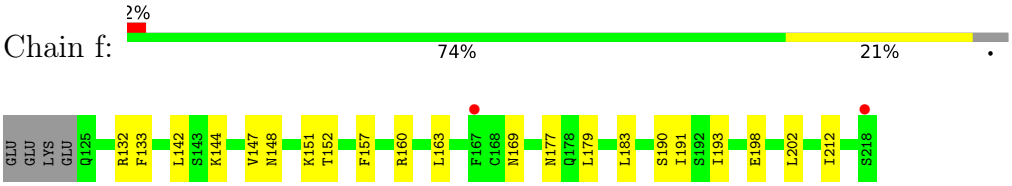
Chain d:

• Molecule 1: Adapter protein mecA 1

Chain e:

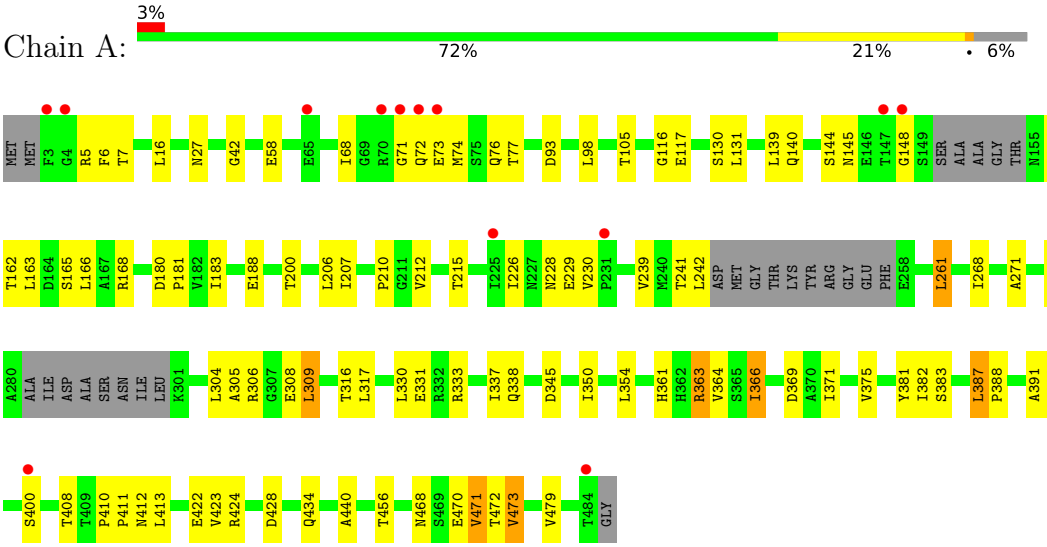
• Molecule 1: Adapter protein mecA 1

Chain f:



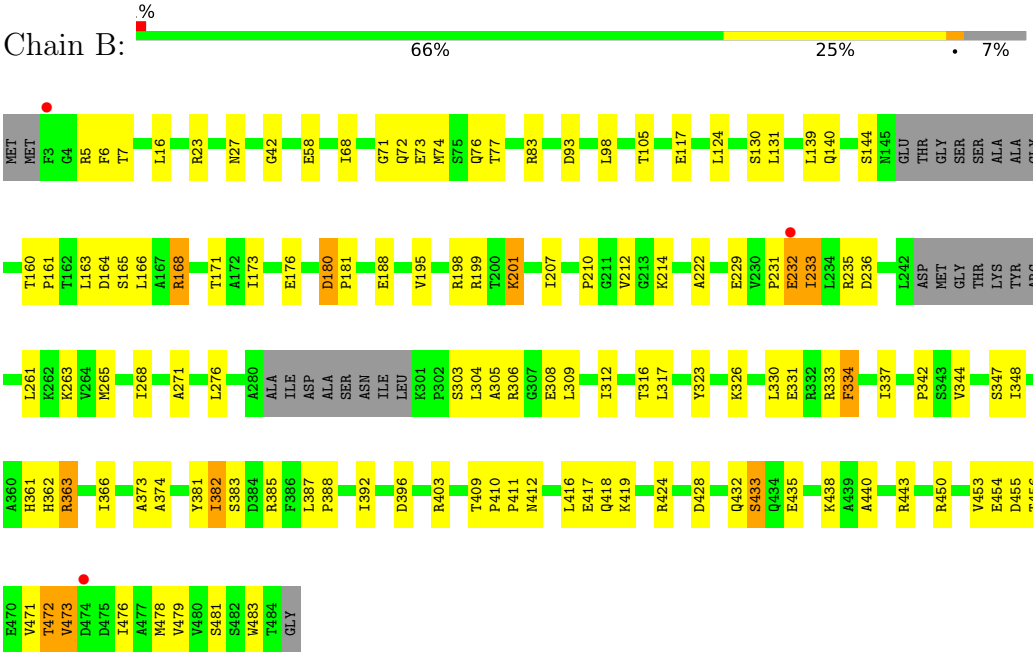
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain A:



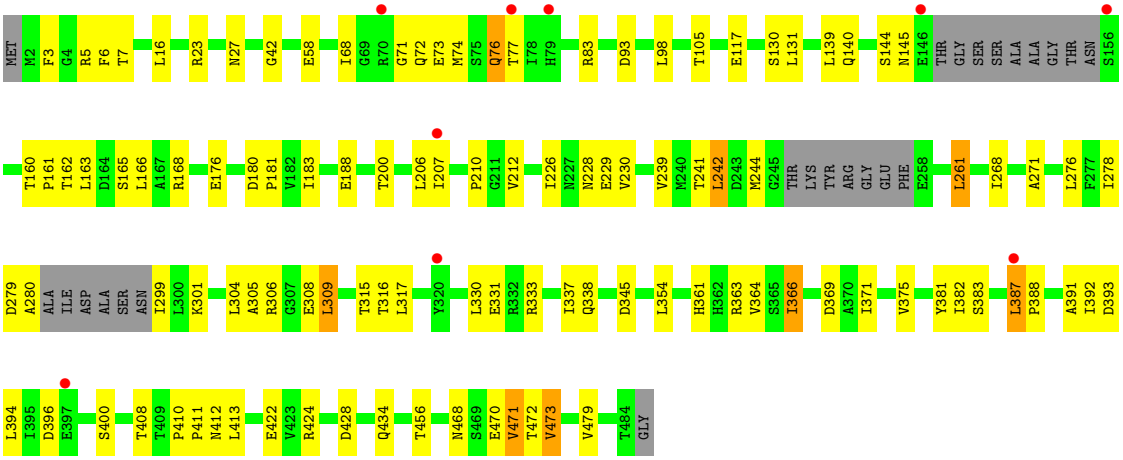
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain B:



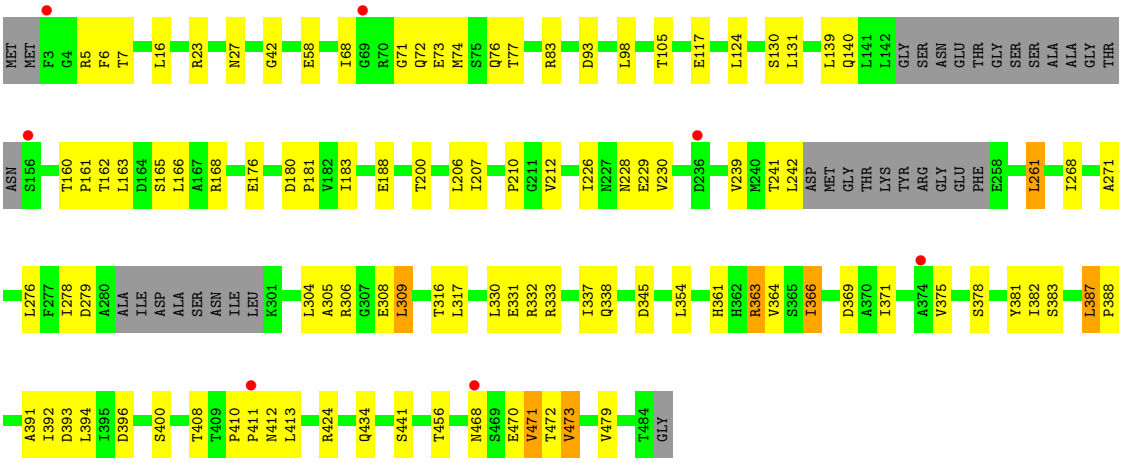
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain C:



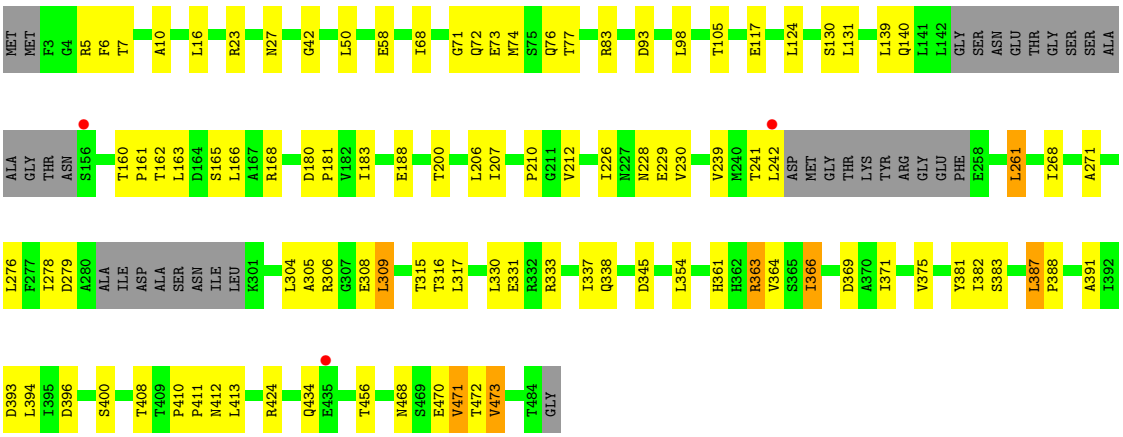
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain D:



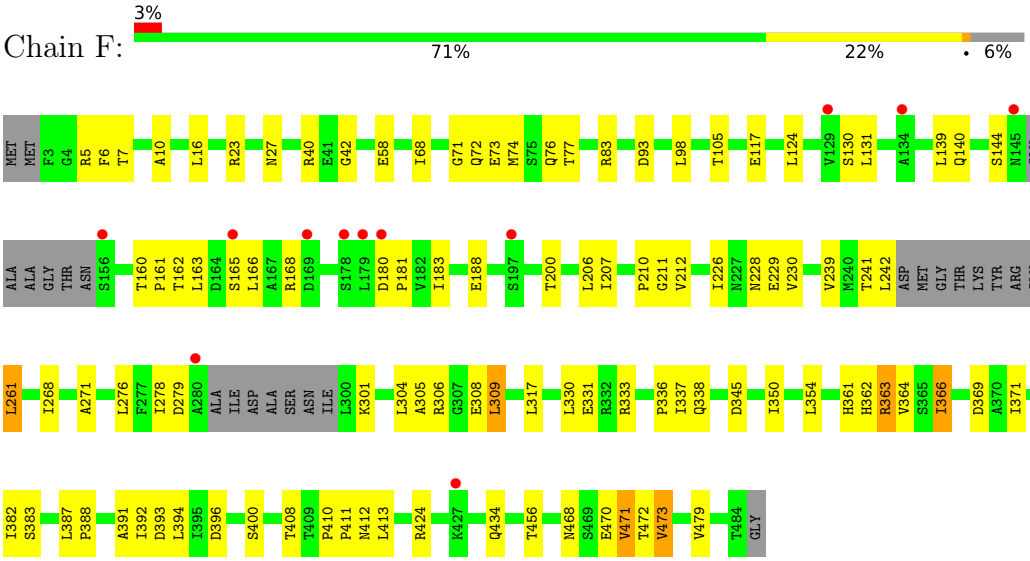
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain E:



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

Chain F:


3%
71%
22%
6%
MET MET F3 G4 R5 F6 T7 A10 L16 R23 N27 R40 E41 G42 E58 I68 G71 Q72 E73 M74 S75 Q76 T77 R83 D93 L98 T105 E117 L124 V129 S130 L131 A134 L139 Q140 S144 N145 GLU THR GLY SER SER
ALA ALA GLY THR ASN S156 T160 P161 T162 L163 D164 S165 L166 A167 R168 D169 S178 L179 D180 P181 V182 I183 E188 S197 T200 L206 I207 P210 G211 V212 I226 N227 N228 E229 V230 V239 M240 T241 L242 ASP MET GLY THR LYS TYR ARG GLY GLU PHE E258
L261 I268 A271 L276 F277 I278 D279 A280 ALA ILE ASP ALA SER ASN ILE L300 K301 L304 A305 R306 G307 E308 L309 L317 L330 E331 R332 R333 P336 I337 Q338 D345 I350 L354 H361 H362 R363 V364 S365 I366 D369 A370 I371 V375 R380 Y381
I382 S383 L387 P388 A391 I392 D393 L394 I395 D396 S400 T408 T409 P410 P411 N412 L413 R424 K427 Q434 T456 N468 S469 E470 V471 T472 V473 V479 T484 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	137.56Å 137.56Å 445.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.52 – 3.65 49.52 – 3.65	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.52-3.65) 96.2 (49.52-3.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.257 , 0.303 0.243 , 0.288	Depositor DCC
R_{free} test set	2858 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å^2)	142.2	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 255.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24809	wwPDB-VP
Average B, all atoms (Å^2)	240.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	a	0.48	0/786	0.66	1/1059 (0.1%)
1	b	0.56	0/786	0.66	0/1059
1	c	0.64	0/786	0.68	0/1059
1	d	0.55	0/791	0.66	0/1066
1	e	0.49	0/791	0.65	0/1066
1	f	0.47	0/786	0.65	0/1059
2	A	0.49	0/3408	0.70	1/4589 (0.0%)
2	B	0.58	1/3384 (0.0%)	0.85	1/4556 (0.0%)
2	C	0.50	0/3415	0.71	1/4602 (0.0%)
2	D	0.48	0/3370	0.69	1/4537 (0.0%)
2	E	0.45	0/3370	0.68	1/4537 (0.0%)
2	F	0.46	0/3389	0.68	1/4563 (0.0%)
All	All	0.50	1/25062 (0.0%)	0.71	7/33752 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
2	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	PHE	CA-CB	5.29	1.65	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	161	PRO	N-CA-CB	6.26	110.81	103.30
2	A	161	PRO	N-CA-CB	6.01	110.51	103.30
2	E	161	PRO	N-CA-CB	5.95	110.44	103.30
2	C	161	PRO	N-CA-CB	5.87	110.34	103.30
2	D	161	PRO	N-CA-CB	5.86	110.33	103.30
2	B	161	PRO	N-CA-CB	5.26	109.61	103.30
1	a	138	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	210	PRO	Peptide
2	C	210	PRO	Peptide
2	D	210	PRO	Peptide
2	E	210	PRO	Peptide
2	F	210	PRO	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	92/98 (94%)	76 (83%)	12 (13%)	4 (4%)	2	24
1	b	92/98 (94%)	76 (83%)	12 (13%)	4 (4%)	2	24
1	c	92/98 (94%)	74 (80%)	14 (15%)	4 (4%)	2	24
1	d	93/98 (95%)	76 (82%)	13 (14%)	4 (4%)	2	24
1	e	93/98 (95%)	76 (82%)	13 (14%)	4 (4%)	2	24
1	f	92/98 (94%)	73 (79%)	15 (16%)	4 (4%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	434/468 (93%)	277 (64%)	98 (23%)	59 (14%)	0 3
2	B	429/468 (92%)	272 (63%)	88 (20%)	69 (16%)	0 3
2	C	438/468 (94%)	274 (63%)	103 (24%)	61 (14%)	0 3
2	D	426/468 (91%)	277 (65%)	97 (23%)	52 (12%)	0 5
2	E	426/468 (91%)	276 (65%)	100 (24%)	50 (12%)	0 5
2	F	430/468 (92%)	273 (64%)	103 (24%)	54 (13%)	0 4
All	All	3137/3396 (92%)	2100 (67%)	668 (21%)	369 (12%)	0 5

All (369) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	169	ASN
2	A	42	GLY
2	A	98	LEU
2	A	144	SER
2	A	183	ILE
2	A	261	LEU
2	A	271	ALA
2	A	306	ARG
2	A	309	LEU
2	A	333	ARG
2	A	363	ARG
2	A	366	ILE
2	A	382	ILE
2	A	410	PRO
2	A	471	VAL
2	A	473	VAL
1	b	169	ASN
2	B	42	GLY
2	B	98	LEU
2	B	130	SER
2	B	144	SER
2	B	157	ASN
2	B	164	ASP
2	B	168	ARG
2	B	180	ASP
2	B	181	PRO
2	B	198	ARG
2	B	201	LYS
2	B	210	PRO

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Mol	Chain	Res	Type
2	B	214	LYS
2	B	231	PRO
2	B	232	GLU
2	B	233	ILE
2	B	261	LEU
2	B	271	ALA
2	B	305	ALA
2	B	308	GLU
2	B	333	ARG
2	B	363	ARG
2	B	366	ILE
2	B	373	ALA
2	B	382	ILE
2	B	410	PRO
2	B	411	PRO
2	B	412	ASN
2	B	438	LYS
2	B	472	THR
1	c	169	ASN
2	C	42	GLY
2	C	98	LEU
2	C	130	SER
2	C	144	SER
2	C	183	ILE
2	C	242	LEU
2	C	244	MET
2	C	261	LEU
2	C	271	ALA
2	C	299	ILE
2	C	306	ARG
2	C	309	LEU
2	C	333	ARG
2	C	363	ARG
2	C	366	ILE
2	C	382	ILE
2	C	391	ALA
2	C	392	ILE
2	C	410	PRO
2	C	411	PRO
2	C	471	VAL
2	C	473	VAL
1	d	169	ASN

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Mol	Chain	Res	Type
2	D	42	GLY
2	D	98	LEU
2	D	183	ILE
2	D	261	LEU
2	D	271	ALA
2	D	306	ARG
2	D	309	LEU
2	D	333	ARG
2	D	363	ARG
2	D	366	ILE
2	D	382	ILE
2	D	383	SER
2	D	410	PRO
2	D	411	PRO
2	D	471	VAL
2	D	473	VAL
1	e	169	ASN
2	E	183	ILE
2	E	261	LEU
2	E	271	ALA
2	E	306	ARG
2	E	309	LEU
2	E	333	ARG
2	E	363	ARG
2	E	366	ILE
2	E	382	ILE
2	E	383	SER
2	E	410	PRO
2	E	411	PRO
2	E	471	VAL
2	E	473	VAL
1	f	169	ASN
2	F	98	LEU
2	F	144	SER
2	F	183	ILE
2	F	261	LEU
2	F	271	ALA
2	F	301	LYS
2	F	306	ARG
2	F	309	LEU
2	F	333	ARG
2	F	363	ARG

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Mol	Chain	Res	Type
2	F	366	ILE
2	F	382	ILE
2	F	383	SER
2	F	410	PRO
2	F	411	PRO
2	F	471	VAL
2	F	473	VAL
1	a	144	LYS
1	a	177	ASN
2	A	156	SER
2	A	163	LEU
2	A	165	SER
2	A	166	LEU
2	A	229	GLU
2	A	383	SER
2	A	391	ALA
2	A	411	PRO
2	B	166	LEU
2	B	171	THR
2	B	199	ARG
2	B	331	GLU
2	B	362	HIS
2	B	433	SER
2	B	440	ALA
2	B	455	ASP
1	c	144	LYS
1	c	206	GLU
2	C	3	PHE
2	C	77	THR
2	C	163	LEU
2	C	165	SER
2	C	166	LEU
2	C	280	ALA
2	C	331	GLU
2	C	383	SER
1	d	144	LYS
2	D	130	SER
2	D	163	LEU
2	D	165	SER
2	D	166	LEU
2	D	229	GLU
2	D	331	GLU

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Mol	Chain	Res	Type
2	D	375	VAL
2	D	391	ALA
2	D	412	ASN
1	e	144	LYS
1	e	177	ASN
2	E	42	GLY
2	E	98	LEU
2	E	130	SER
2	E	165	SER
2	E	166	LEU
2	E	229	GLU
2	E	331	GLU
2	F	42	GLY
2	F	165	SER
2	F	166	LEU
2	F	211	GLY
2	F	229	GLU
2	F	331	GLU
2	F	375	VAL
2	F	391	ALA
2	F	412	ASN
2	F	413	LEU
2	A	73	GLU
2	A	77	THR
2	A	130	SER
2	A	162	THR
2	A	168	ARG
2	A	181	PRO
2	A	200	THR
2	A	228	ASN
2	A	305	ALA
2	A	330	LEU
2	A	331	GLU
2	A	375	VAL
2	A	388	PRO
2	A	412	ASN
2	A	413	LEU
2	A	470	GLU
1	b	144	LYS
1	b	206	GLU
2	B	77	THR
2	B	263	LYS

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Mol	Chain	Res	Type
2	B	334	PHE
2	B	388	PRO
2	B	481	SER
1	c	177	ASN
2	C	23	ARG
2	C	68	ILE
2	C	73	GLU
2	C	140	GLN
2	C	145	ASN
2	C	162	THR
2	C	168	ARG
2	C	181	PRO
2	C	228	ASN
2	C	229	GLU
2	C	330	LEU
2	C	375	VAL
2	C	388	PRO
2	C	412	ASN
2	C	413	LEU
2	C	470	GLU
2	D	77	THR
2	D	162	THR
2	D	168	ARG
2	D	181	PRO
2	D	200	THR
2	D	226	ILE
2	D	316	THR
2	D	330	LEU
2	D	388	PRO
2	D	413	LEU
2	D	434	GLN
2	D	470	GLU
1	e	206	GLU
2	E	73	GLU
2	E	77	THR
2	E	140	GLN
2	E	163	LEU
2	E	168	ARG
2	E	181	PRO
2	E	200	THR
2	E	316	THR
2	E	330	LEU

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Mol	Chain	Res	Type
2	E	375	VAL
2	E	388	PRO
2	E	391	ALA
2	E	412	ASN
2	E	413	LEU
2	E	470	GLU
1	f	144	LYS
1	f	177	ASN
2	F	73	GLU
2	F	77	THR
2	F	130	SER
2	F	162	THR
2	F	163	LEU
2	F	168	ARG
2	F	181	PRO
2	F	200	THR
2	F	212	VAL
2	F	228	ASN
2	F	330	LEU
2	F	388	PRO
2	F	392	ILE
2	F	470	GLU
2	A	71	GLY
2	A	74	MET
2	A	145	ASN
2	A	148	GLY
2	A	212	VAL
2	A	215	THR
2	A	226	ILE
2	A	316	THR
2	A	400	SER
2	A	434	GLN
1	b	177	ASN
2	B	68	ILE
2	B	71	GLY
2	B	73	GLU
2	B	74	MET
2	B	140	GLN
2	B	163	LEU
2	B	165	SER
2	B	176	GLU
2	B	212	VAL

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Mol	Chain	Res	Type
2	B	330	LEU
2	B	344	VAL
2	B	359	GLU
2	B	374	ALA
2	B	385	ARG
2	B	450	ARG
2	B	467	GLU
2	C	71	GLY
2	C	74	MET
2	C	200	THR
2	C	212	VAL
2	C	226	ILE
2	C	301	LYS
2	C	305	ALA
2	C	316	THR
2	C	422	GLU
2	C	434	GLN
1	d	177	ASN
1	d	206	GLU
2	D	68	ILE
2	D	71	GLY
2	D	73	GLU
2	D	74	MET
2	D	140	GLN
2	D	212	VAL
2	D	228	ASN
2	D	305	ALA
2	D	400	SER
2	E	10	ALA
2	E	71	GLY
2	E	74	MET
2	E	162	THR
2	E	226	ILE
2	E	228	ASN
2	E	305	ALA
2	E	400	SER
2	E	434	GLN
2	F	10	ALA
2	F	68	ILE
2	F	71	GLY
2	F	74	MET
2	F	226	ILE

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Mol	Chain	Res	Type
2	F	305	ALA
2	F	400	SER
2	F	434	GLN
1	a	206	GLU
2	A	68	ILE
2	A	140	GLN
2	A	422	GLU
2	B	23	ARG
2	B	160	THR
2	B	306	ARG
2	B	342	PRO
2	C	400	SER
2	D	23	ARG
2	D	332	ARG
2	E	68	ILE
2	E	212	VAL
2	F	23	ARG
2	A	440	ALA
2	B	222	ALA
2	B	383	SER
2	C	76	GLN
2	D	392	ILE
2	E	23	ARG
2	E	387	LEU
1	f	148	ASN
2	F	140	GLN
2	F	362	HIS
2	A	116	GLY
2	A	479	VAL
2	B	473	VAL
2	D	160	THR
2	E	160	THR
2	A	160	THR
2	B	471	VAL
2	B	476	ILE
2	F	160	THR
2	A	392	ILE
2	A	423	VAL
2	C	160	THR
2	C	387	LEU
2	D	479	VAL
2	F	479	VAL

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Mol	Chain	Res	Type
2	A	387	LEU
2	B	392	ILE
2	D	387	LEU
2	C	479	VAL

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	87/92 (95%)	70 (80%)	17 (20%)	1 9
1	b	87/92 (95%)	70 (80%)	17 (20%)	1 9
1	c	87/92 (95%)	71 (82%)	16 (18%)	1 10
1	d	87/92 (95%)	68 (78%)	19 (22%)	1 6
1	e	87/92 (95%)	68 (78%)	19 (22%)	1 6
1	f	87/92 (95%)	70 (80%)	17 (20%)	1 9
2	A	350/394 (89%)	297 (85%)	53 (15%)	3 17
2	B	350/394 (89%)	280 (80%)	70 (20%)	1 8
2	C	349/394 (89%)	294 (84%)	55 (16%)	2 16
2	D	350/394 (89%)	294 (84%)	56 (16%)	2 15
2	E	350/394 (89%)	294 (84%)	56 (16%)	2 15
2	F	350/394 (89%)	294 (84%)	56 (16%)	2 15
All	All	2621/2916 (90%)	2170 (83%)	451 (17%)	2 13

All (451) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	132	ARG
1	a	133	PHE
1	a	142	LEU
1	a	147	VAL
1	a	151	LYS
1	a	152	THR

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Mol	Chain	Res	Type
1	a	157	PHE
1	a	160	ARG
1	a	163	LEU
1	a	179	LEU
1	a	183	LEU
1	a	190	SER
1	a	191	ILE
1	a	193	ILE
1	a	198	GLU
1	a	202	LEU
1	a	212	ILE
2	A	5	ARG
2	A	6	PHE
2	A	7	THR
2	A	16	LEU
2	A	27	ASN
2	A	58	GLU
2	A	72	GLN
2	A	76	GLN
2	A	93	ASP
2	A	105	THR
2	A	117	GLU
2	A	131	LEU
2	A	139	LEU
2	A	180	ASP
2	A	188	GLU
2	A	206	LEU
2	A	207	ILE
2	A	230	VAL
2	A	239	VAL
2	A	241	THR
2	A	242	LEU
2	A	261	LEU
2	A	268	ILE
2	A	276	LEU
2	A	278	ILE
2	A	279	ASP
2	A	304	LEU
2	A	308	GLU
2	A	309	LEU
2	A	317	LEU
2	A	337	ILE

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Mol	Chain	Res	Type
2	A	338	GLN
2	A	345	ASP
2	A	350	ILE
2	A	354	LEU
2	A	361	HIS
2	A	363	ARG
2	A	364	VAL
2	A	366	ILE
2	A	369	ASP
2	A	371	ILE
2	A	381	TYR
2	A	387	LEU
2	A	393	ASP
2	A	396	ASP
2	A	408	THR
2	A	424	ARG
2	A	428	ASP
2	A	456	THR
2	A	468	ASN
2	A	471	VAL
2	A	472	THR
2	A	473	VAL
1	b	132	ARG
1	b	133	PHE
1	b	142	LEU
1	b	147	VAL
1	b	151	LYS
1	b	152	THR
1	b	157	PHE
1	b	160	ARG
1	b	163	LEU
1	b	179	LEU
1	b	183	LEU
1	b	190	SER
1	b	191	ILE
1	b	193	ILE
1	b	198	GLU
1	b	202	LEU
1	b	212	ILE
2	B	5	ARG
2	B	6	PHE
2	B	7	THR

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Mol	Chain	Res	Type
2	B	16	LEU
2	B	27	ASN
2	B	58	GLU
2	B	72	GLN
2	B	76	GLN
2	B	83	ARG
2	B	93	ASP
2	B	105	THR
2	B	117	GLU
2	B	124	LEU
2	B	131	LEU
2	B	139	LEU
2	B	168	ARG
2	B	173	ILE
2	B	180	ASP
2	B	188	GLU
2	B	195	VAL
2	B	201	LYS
2	B	207	ILE
2	B	229	GLU
2	B	232	GLU
2	B	233	ILE
2	B	235	ARG
2	B	236	ASP
2	B	265	MET
2	B	268	ILE
2	B	276	LEU
2	B	303	SER
2	B	304	LEU
2	B	309	LEU
2	B	312	ILE
2	B	316	THR
2	B	317	LEU
2	B	323	TYR
2	B	326	LYS
2	B	337	ILE
2	B	347	SER
2	B	348	ILE
2	B	354	LEU
2	B	355	ARG
2	B	361	HIS
2	B	363	ARG

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Mol	Chain	Res	Type
2	B	381	TYR
2	B	382	ILE
2	B	387	LEU
2	B	396	ASP
2	B	403	ARG
2	B	409	THR
2	B	416	LEU
2	B	417	GLU
2	B	418	GLN
2	B	419	LYS
2	B	424	ARG
2	B	428	ASP
2	B	432	GLN
2	B	433	SER
2	B	435	GLU
2	B	443	ARG
2	B	453	VAL
2	B	454	GLU
2	B	456	THR
2	B	469	SER
2	B	472	THR
2	B	473	VAL
2	B	478	MET
2	B	479	VAL
2	B	483	TRP
1	c	132	ARG
1	c	142	LEU
1	c	147	VAL
1	c	151	LYS
1	c	152	THR
1	c	157	PHE
1	c	160	ARG
1	c	163	LEU
1	c	179	LEU
1	c	183	LEU
1	c	190	SER
1	c	191	ILE
1	c	193	ILE
1	c	198	GLU
1	c	202	LEU
1	c	212	ILE
2	C	5	ARG

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Mol	Chain	Res	Type
2	C	6	PHE
2	C	7	THR
2	C	16	LEU
2	C	27	ASN
2	C	58	GLU
2	C	72	GLN
2	C	76	GLN
2	C	83	ARG
2	C	93	ASP
2	C	105	THR
2	C	117	GLU
2	C	131	LEU
2	C	139	LEU
2	C	176	GLU
2	C	180	ASP
2	C	188	GLU
2	C	206	LEU
2	C	207	ILE
2	C	230	VAL
2	C	239	VAL
2	C	241	THR
2	C	242	LEU
2	C	261	LEU
2	C	268	ILE
2	C	276	LEU
2	C	278	ILE
2	C	279	ASP
2	C	304	LEU
2	C	308	GLU
2	C	309	LEU
2	C	315	THR
2	C	317	LEU
2	C	337	ILE
2	C	338	GLN
2	C	345	ASP
2	C	354	LEU
2	C	361	HIS
2	C	364	VAL
2	C	366	ILE
2	C	369	ASP
2	C	371	ILE
2	C	381	TYR

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Mol	Chain	Res	Type
2	C	387	LEU
2	C	393	ASP
2	C	394	LEU
2	C	396	ASP
2	C	408	THR
2	C	424	ARG
2	C	428	ASP
2	C	456	THR
2	C	468	ASN
2	C	471	VAL
2	C	472	THR
2	C	473	VAL
1	d	131	LEU
1	d	132	ARG
1	d	133	PHE
1	d	142	LEU
1	d	147	VAL
1	d	151	LYS
1	d	152	THR
1	d	157	PHE
1	d	160	ARG
1	d	163	LEU
1	d	179	LEU
1	d	183	LEU
1	d	187	THR
1	d	190	SER
1	d	191	ILE
1	d	193	ILE
1	d	198	GLU
1	d	202	LEU
1	d	212	ILE
2	D	5	ARG
2	D	6	PHE
2	D	7	THR
2	D	16	LEU
2	D	27	ASN
2	D	58	GLU
2	D	72	GLN
2	D	76	GLN
2	D	83	ARG
2	D	93	ASP
2	D	105	THR

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Mol	Chain	Res	Type
2	D	117	GLU
2	D	124	LEU
2	D	131	LEU
2	D	139	LEU
2	D	176	GLU
2	D	180	ASP
2	D	188	GLU
2	D	206	LEU
2	D	207	ILE
2	D	230	VAL
2	D	239	VAL
2	D	241	THR
2	D	242	LEU
2	D	261	LEU
2	D	268	ILE
2	D	276	LEU
2	D	278	ILE
2	D	279	ASP
2	D	304	LEU
2	D	308	GLU
2	D	309	LEU
2	D	317	LEU
2	D	337	ILE
2	D	338	GLN
2	D	345	ASP
2	D	354	LEU
2	D	361	HIS
2	D	363	ARG
2	D	364	VAL
2	D	366	ILE
2	D	369	ASP
2	D	371	ILE
2	D	378	SER
2	D	381	TYR
2	D	387	LEU
2	D	393	ASP
2	D	394	LEU
2	D	396	ASP
2	D	408	THR
2	D	424	ARG
2	D	456	THR
2	D	468	ASN

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Mol	Chain	Res	Type
2	D	471	VAL
2	D	472	THR
2	D	473	VAL
1	e	131	LEU
1	e	132	ARG
1	e	133	PHE
1	e	142	LEU
1	e	147	VAL
1	e	151	LYS
1	e	152	THR
1	e	157	PHE
1	e	160	ARG
1	e	163	LEU
1	e	179	LEU
1	e	183	LEU
1	e	187	THR
1	e	190	SER
1	e	191	ILE
1	e	193	ILE
1	e	198	GLU
1	e	202	LEU
1	e	212	ILE
2	E	5	ARG
2	E	6	PHE
2	E	7	THR
2	E	16	LEU
2	E	27	ASN
2	E	50	LEU
2	E	58	GLU
2	E	72	GLN
2	E	76	GLN
2	E	83	ARG
2	E	93	ASP
2	E	105	THR
2	E	117	GLU
2	E	124	LEU
2	E	131	LEU
2	E	139	LEU
2	E	180	ASP
2	E	188	GLU
2	E	206	LEU
2	E	207	ILE

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Mol	Chain	Res	Type
2	E	230	VAL
2	E	239	VAL
2	E	241	THR
2	E	242	LEU
2	E	261	LEU
2	E	268	ILE
2	E	276	LEU
2	E	278	ILE
2	E	279	ASP
2	E	304	LEU
2	E	308	GLU
2	E	309	LEU
2	E	315	THR
2	E	317	LEU
2	E	337	ILE
2	E	338	GLN
2	E	345	ASP
2	E	354	LEU
2	E	361	HIS
2	E	363	ARG
2	E	364	VAL
2	E	366	ILE
2	E	369	ASP
2	E	371	ILE
2	E	381	TYR
2	E	387	LEU
2	E	393	ASP
2	E	394	LEU
2	E	396	ASP
2	E	408	THR
2	E	424	ARG
2	E	456	THR
2	E	468	ASN
2	E	471	VAL
2	E	472	THR
2	E	473	VAL
1	f	132	ARG
1	f	133	PHE
1	f	142	LEU
1	f	147	VAL
1	f	151	LYS
1	f	152	THR

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Mol	Chain	Res	Type
1	f	157	PHE
1	f	160	ARG
1	f	163	LEU
1	f	179	LEU
1	f	183	LEU
1	f	190	SER
1	f	191	ILE
1	f	193	ILE
1	f	198	GLU
1	f	202	LEU
1	f	212	ILE
2	F	5	ARG
2	F	6	PHE
2	F	7	THR
2	F	16	LEU
2	F	27	ASN
2	F	58	GLU
2	F	72	GLN
2	F	76	GLN
2	F	83	ARG
2	F	93	ASP
2	F	105	THR
2	F	117	GLU
2	F	124	LEU
2	F	131	LEU
2	F	139	LEU
2	F	180	ASP
2	F	188	GLU
2	F	206	LEU
2	F	207	ILE
2	F	230	VAL
2	F	239	VAL
2	F	241	THR
2	F	242	LEU
2	F	261	LEU
2	F	268	ILE
2	F	276	LEU
2	F	278	ILE
2	F	279	ASP
2	F	304	LEU
2	F	308	GLU
2	F	309	LEU

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Mol	Chain	Res	Type
2	F	317	LEU
2	F	336	PRO
2	F	337	ILE
2	F	338	GLN
2	F	345	ASP
2	F	350	ILE
2	F	354	LEU
2	F	361	HIS
2	F	363	ARG
2	F	364	VAL
2	F	366	ILE
2	F	369	ASP
2	F	371	ILE
2	F	381	TYR
2	F	387	LEU
2	F	393	ASP
2	F	394	LEU
2	F	396	ASP
2	F	408	THR
2	F	424	ARG
2	F	456	THR
2	F	468	ASN
2	F	471	VAL
2	F	472	THR
2	F	473	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	159	ASN
1	a	207	HIS
1	a	215	HIS
2	A	28	ASN
2	A	51	GLN
2	A	61	GLN
2	A	72	GLN
2	A	76	GLN
2	A	100	HIS
2	A	126	ASN
2	A	137	GLN
2	A	223	GLN
2	A	228	ASN

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Mol	Chain	Res	Type
2	A	338	GLN
2	A	341	GLN
2	A	362	HIS
2	A	468	ASN
1	b	159	ASN
1	b	207	HIS
1	b	215	HIS
2	B	51	GLN
2	B	61	GLN
2	B	72	GLN
2	B	76	GLN
2	B	100	HIS
2	B	137	GLN
2	B	202	ASN
2	B	203	ASN
2	B	223	GLN
2	B	227	ASN
2	B	228	ASN
2	B	310	GLN
2	B	362	HIS
1	c	159	ASN
1	c	194	HIS
1	c	207	HIS
1	c	215	HIS
2	C	28	ASN
2	C	51	GLN
2	C	61	GLN
2	C	72	GLN
2	C	76	GLN
2	C	100	HIS
2	C	126	ASN
2	C	137	GLN
2	C	190	GLN
2	C	223	GLN
2	C	228	ASN
2	C	338	GLN
2	C	341	GLN
2	C	362	HIS
2	C	468	ASN
1	d	159	ASN
1	d	207	HIS
1	d	215	HIS

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Mol	Chain	Res	Type
2	D	28	ASN
2	D	51	GLN
2	D	61	GLN
2	D	72	GLN
2	D	76	GLN
2	D	100	HIS
2	D	126	ASN
2	D	137	GLN
2	D	223	GLN
2	D	228	ASN
2	D	338	GLN
2	D	341	GLN
2	D	362	HIS
2	D	468	ASN
1	e	159	ASN
1	e	207	HIS
1	e	215	HIS
2	E	28	ASN
2	E	51	GLN
2	E	61	GLN
2	E	72	GLN
2	E	76	GLN
2	E	100	HIS
2	E	126	ASN
2	E	137	GLN
2	E	223	GLN
2	E	228	ASN
2	E	338	GLN
2	E	341	GLN
2	E	362	HIS
2	E	468	ASN
1	f	159	ASN
1	f	207	HIS
1	f	215	HIS
2	F	28	ASN
2	F	51	GLN
2	F	61	GLN
2	F	72	GLN
2	F	76	GLN
2	F	100	HIS
2	F	137	GLN
2	F	223	GLN

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Mol	Chain	Res	Type
2	F	228	ASN
2	F	338	GLN
2	F	341	GLN
2	F	362	HIS
2	F	468	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	a	94/98 (95%)	-0.24	1 (1%) 80 70	180, 227, 340, 398	0
1	b	94/98 (95%)	0.11	3 (3%) 47 34	133, 195, 320, 369	0
1	c	94/98 (95%)	0.29	5 (5%) 26 18	127, 194, 315, 374	0
1	d	95/98 (96%)	-0.20	0 100 100	125, 198, 325, 357	0
1	e	95/98 (96%)	-0.21	0 100 100	139, 196, 317, 357	0
1	f	94/98 (95%)	-0.12	2 (2%) 63 50	174, 224, 366, 376	0
2	A	442/468 (94%)	-0.03	13 (2%) 51 37	120, 243, 393, 613	0
2	B	437/468 (93%)	-0.38	3 (0%) 87 80	106, 210, 317, 493	0
2	C	444/468 (94%)	-0.10	9 (2%) 65 52	97, 240, 364, 533	0
2	D	434/468 (92%)	-0.17	7 (1%) 72 59	112, 240, 368, 489	0
2	E	434/468 (92%)	-0.22	3 (0%) 87 80	115, 241, 368, 465	0
2	F	438/468 (93%)	-0.16	13 (2%) 50 36	133, 251, 376, 477	0
All	All	3195/3396 (94%)	-0.16	59 (1%) 68 55	97, 231, 365, 613	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	147	THR	7.2
2	A	3	PHE	6.1
2	F	156	SER	5.8
1	c	218	SER	5.3
2	B	232	GLU	4.9
1	a	218	SER	4.8
2	A	71	GLY	4.7
2	E	156	SER	4.6
2	C	320	TYR	4.6
1	b	218	SER	4.4
2	A	4	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
2	F	129	VAL	4.2
1	c	125	GLN	3.9
1	f	167	PHE	3.9
1	c	169	ASN	3.6
2	A	400	SER	3.6
2	C	156	SER	3.6
2	D	156	SER	3.3
2	B	3	PHE	3.3
2	E	242	LEU	3.2
2	F	165	SER	3.2
2	D	3	PHE	3.2
2	D	236	ASP	2.9
2	A	73	GLU	2.9
2	D	468	ASN	2.9
2	F	280	ALA	2.9
2	C	77	THR	2.9
1	c	146	ASN	2.8
2	C	146	GLU	2.8
1	b	146	ASN	2.7
2	A	65	GLU	2.6
1	f	218	SER	2.6
2	E	435	GLU	2.5
2	A	148	GLY	2.4
2	F	179	LEU	2.4
2	F	145	ASN	2.4
2	C	387	LEU	2.4
2	F	427	LYS	2.4
2	F	180	ASP	2.4
2	F	178	SER	2.4
2	A	70	ARG	2.3
1	b	169	ASN	2.3
2	C	207	ILE	2.3
2	D	374	ALA	2.3
2	A	225	ILE	2.3
2	F	169	ASP	2.3
2	D	411	PRO	2.3
2	D	69	GLY	2.3
2	C	79	HIS	2.2
2	F	197	SER	2.1
1	c	172	ASP	2.1
2	F	134	ALA	2.1
2	B	474	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	231	PRO	2.1
2	F	380	ARG	2.1
2	A	72	GLN	2.1
2	A	484	THR	2.1
2	C	397	GLU	2.0
2	C	70	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.