wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2023 – 04:46 PM EDT

PDB ID	:	6X0A
Title	:	X-ray structure of a chimeric ParDE toxin-antitoxin complex from Mesorhizobium opportunistum
Authors	:	Lite, T.L.; Grant, R.A.; Laub, M.T.
Deposited on	:	2020-05-15
Resolution	:	2.90 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:

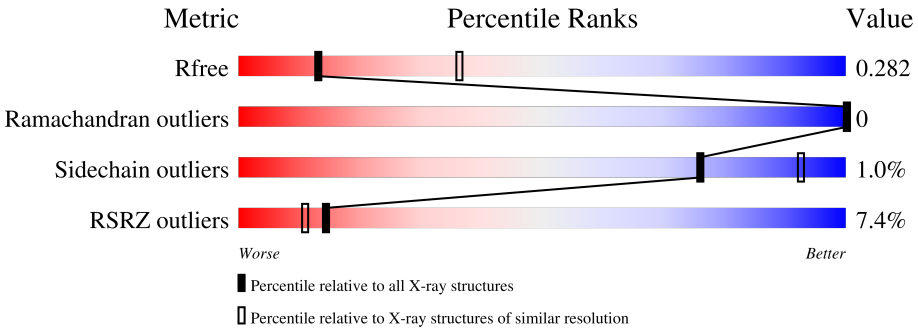
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.90 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	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	108	83% · 16%
1	B	108	83% · 16%
1	C	108	85% 15%
1	D	108	% 83% · 16%
1	E	108	84% 16%
1	F	108	84% 16%

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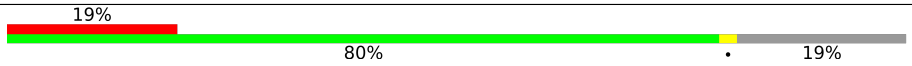
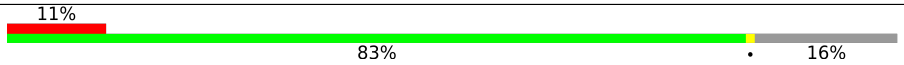
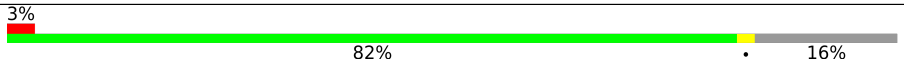
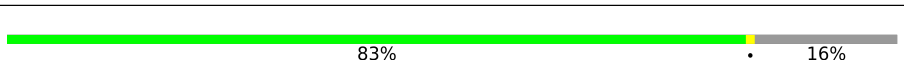
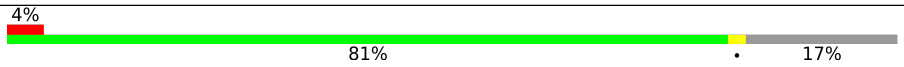
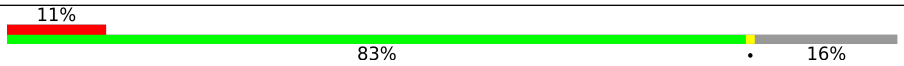
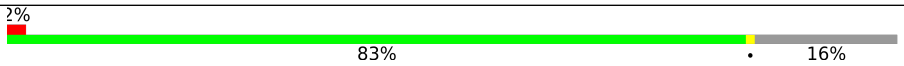
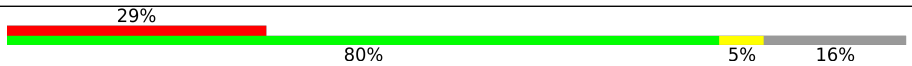
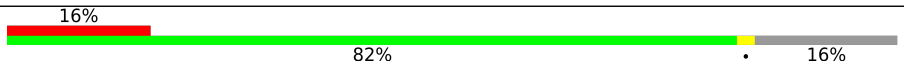
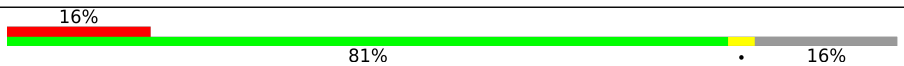
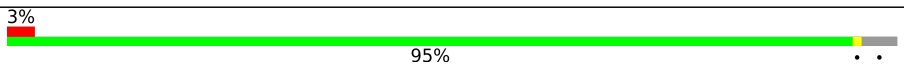
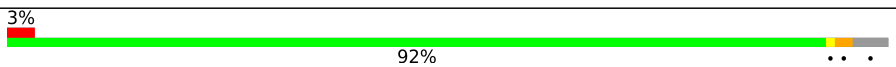
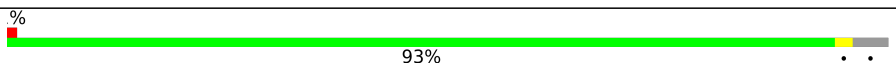
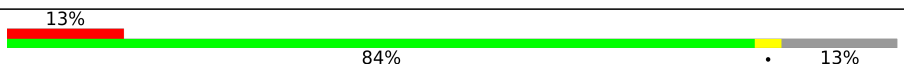
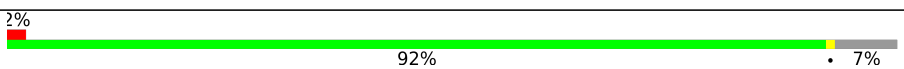
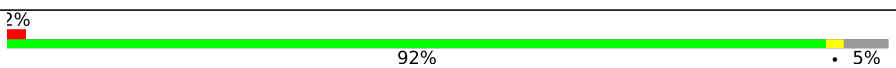
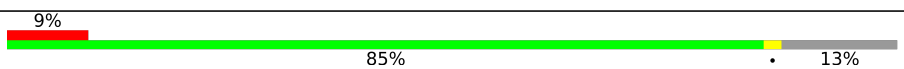
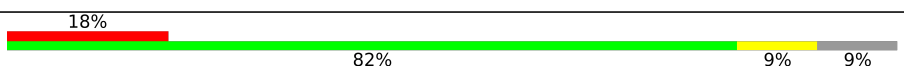
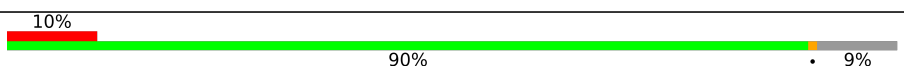
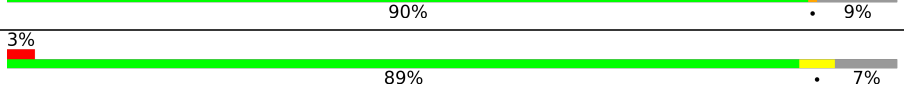
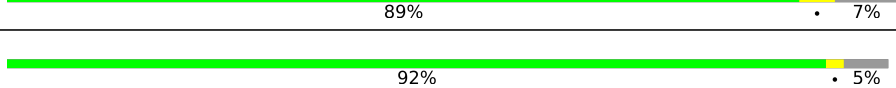
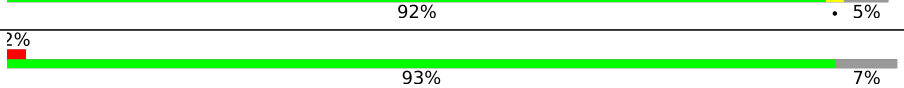
Mol	Chain	Length	Quality of chain
1	G	108	
1	H	108	
1	I	108	
1	J	108	
1	K	108	
1	L	108	
1	M	108	
1	N	108	
1	O	108	
1	P	108	
1	Q	108	
1	R	108	
2	a	91	
2	b	91	
2	c	91	
2	d	91	
2	e	91	
2	f	91	
2	g	91	
2	h	91	
2	i	91	
2	j	91	
2	k	91	
2	l	91	
2	m	91	

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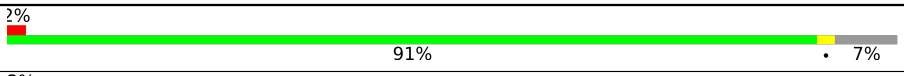
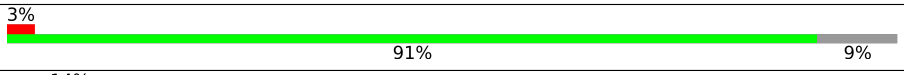
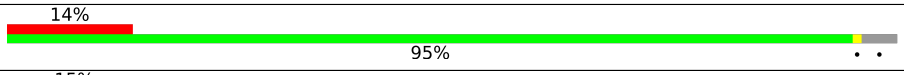
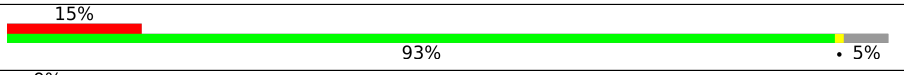
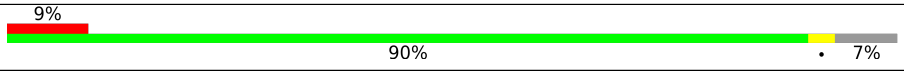
Mol	Chain	Length	Quality of chain
2	n	91	
2	o	91	
2	p	91	
2	q	91	
2	r	91	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 49728 atoms, of which 24951 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 Plasmid stabilization system.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	91	Total C H N O 1407 447 705 127 128	0	0	0
1	B	91	Total C H N O 1407 447 705 127 128	0	0	0
1	C	92	Total C H N O S 1425 452 715 128 129 1	0	0	0
1	D	91	Total C H N O 1407 447 705 127 128	0	0	0
1	E	91	Total C H N O 1408 447 706 127 128	0	0	0
1	F	91	Total C H N O 1408 447 706 127 128	0	0	0
1	G	91	Total C H N O 1407 447 705 127 128	0	0	0
1	H	91	Total C H N O 1407 447 705 127 128	0	0	0
1	I	88	Total C H N O 1355 430 676 124 125	0	0	0
1	J	91	Total C H N O 1408 447 706 127 128	0	0	0
1	K	91	Total C H N O 1407 447 705 127 128	0	0	0
1	L	91	Total C H N O 1408 447 706 127 128	0	0	0
1	M	90	Total C H N O 1392 442 697 126 127	0	0	0
1	N	91	Total C H N O 1408 447 706 127 128	0	0	0
1	O	91	Total C H N O 1407 447 705 127 128	0	0	0
1	P	91	Total C H N O 1407 447 705 127 128	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	91	Total	C	H	N	O	0	0	0
			1407	447	705	127	128			
1	R	91	Total	C	H	N	O	0	0	0
			1407	447	705	127	128			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP F7Y4W0
A	-12	GLY	-	expression tag	UNP F7Y4W0
A	-11	SER	-	expression tag	UNP F7Y4W0
A	-10	SER	-	expression tag	UNP F7Y4W0
A	-9	HIS	-	expression tag	UNP F7Y4W0
A	-8	HIS	-	expression tag	UNP F7Y4W0
A	-7	HIS	-	expression tag	UNP F7Y4W0
A	-6	HIS	-	expression tag	UNP F7Y4W0
A	-5	HIS	-	expression tag	UNP F7Y4W0
A	-4	HIS	-	expression tag	UNP F7Y4W0
A	-3	SER	-	expression tag	UNP F7Y4W0
A	-2	GLN	-	expression tag	UNP F7Y4W0
A	-1	ASP	-	expression tag	UNP F7Y4W0
A	0	PRO	-	expression tag	UNP F7Y4W0
B	-13	MET	-	initiating methionine	UNP F7Y4W0
B	-12	GLY	-	expression tag	UNP F7Y4W0
B	-11	SER	-	expression tag	UNP F7Y4W0
B	-10	SER	-	expression tag	UNP F7Y4W0
B	-9	HIS	-	expression tag	UNP F7Y4W0
B	-8	HIS	-	expression tag	UNP F7Y4W0
B	-7	HIS	-	expression tag	UNP F7Y4W0
B	-6	HIS	-	expression tag	UNP F7Y4W0
B	-5	HIS	-	expression tag	UNP F7Y4W0
B	-4	HIS	-	expression tag	UNP F7Y4W0
B	-3	SER	-	expression tag	UNP F7Y4W0
B	-2	GLN	-	expression tag	UNP F7Y4W0
B	-1	ASP	-	expression tag	UNP F7Y4W0
B	0	PRO	-	expression tag	UNP F7Y4W0
C	-13	MET	-	initiating methionine	UNP F7Y4W0
C	-12	GLY	-	expression tag	UNP F7Y4W0
C	-11	SER	-	expression tag	UNP F7Y4W0
C	-10	SER	-	expression tag	UNP F7Y4W0
C	-9	HIS	-	expression tag	UNP F7Y4W0
C	-8	HIS	-	expression tag	UNP F7Y4W0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	HIS	-	expression tag	UNP F7Y4W0
C	-6	HIS	-	expression tag	UNP F7Y4W0
C	-5	HIS	-	expression tag	UNP F7Y4W0
C	-4	HIS	-	expression tag	UNP F7Y4W0
C	-3	SER	-	expression tag	UNP F7Y4W0
C	-2	GLN	-	expression tag	UNP F7Y4W0
C	-1	ASP	-	expression tag	UNP F7Y4W0
C	0	PRO	-	expression tag	UNP F7Y4W0
D	-13	MET	-	initiating methionine	UNP F7Y4W0
D	-12	GLY	-	expression tag	UNP F7Y4W0
D	-11	SER	-	expression tag	UNP F7Y4W0
D	-10	SER	-	expression tag	UNP F7Y4W0
D	-9	HIS	-	expression tag	UNP F7Y4W0
D	-8	HIS	-	expression tag	UNP F7Y4W0
D	-7	HIS	-	expression tag	UNP F7Y4W0
D	-6	HIS	-	expression tag	UNP F7Y4W0
D	-5	HIS	-	expression tag	UNP F7Y4W0
D	-4	HIS	-	expression tag	UNP F7Y4W0
D	-3	SER	-	expression tag	UNP F7Y4W0
D	-2	GLN	-	expression tag	UNP F7Y4W0
D	-1	ASP	-	expression tag	UNP F7Y4W0
D	0	PRO	-	expression tag	UNP F7Y4W0
E	-13	MET	-	initiating methionine	UNP F7Y4W0
E	-12	GLY	-	expression tag	UNP F7Y4W0
E	-11	SER	-	expression tag	UNP F7Y4W0
E	-10	SER	-	expression tag	UNP F7Y4W0
E	-9	HIS	-	expression tag	UNP F7Y4W0
E	-8	HIS	-	expression tag	UNP F7Y4W0
E	-7	HIS	-	expression tag	UNP F7Y4W0
E	-6	HIS	-	expression tag	UNP F7Y4W0
E	-5	HIS	-	expression tag	UNP F7Y4W0
E	-4	HIS	-	expression tag	UNP F7Y4W0
E	-3	SER	-	expression tag	UNP F7Y4W0
E	-2	GLN	-	expression tag	UNP F7Y4W0
E	-1	ASP	-	expression tag	UNP F7Y4W0
E	0	PRO	-	expression tag	UNP F7Y4W0
F	-13	MET	-	initiating methionine	UNP F7Y4W0
F	-12	GLY	-	expression tag	UNP F7Y4W0
F	-11	SER	-	expression tag	UNP F7Y4W0
F	-10	SER	-	expression tag	UNP F7Y4W0
F	-9	HIS	-	expression tag	UNP F7Y4W0
F	-8	HIS	-	expression tag	UNP F7Y4W0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	HIS	-	expression tag	UNP F7Y4W0
F	-6	HIS	-	expression tag	UNP F7Y4W0
F	-5	HIS	-	expression tag	UNP F7Y4W0
F	-4	HIS	-	expression tag	UNP F7Y4W0
F	-3	SER	-	expression tag	UNP F7Y4W0
F	-2	GLN	-	expression tag	UNP F7Y4W0
F	-1	ASP	-	expression tag	UNP F7Y4W0
F	0	PRO	-	expression tag	UNP F7Y4W0
G	-13	MET	-	initiating methionine	UNP F7Y4W0
G	-12	GLY	-	expression tag	UNP F7Y4W0
G	-11	SER	-	expression tag	UNP F7Y4W0
G	-10	SER	-	expression tag	UNP F7Y4W0
G	-9	HIS	-	expression tag	UNP F7Y4W0
G	-8	HIS	-	expression tag	UNP F7Y4W0
G	-7	HIS	-	expression tag	UNP F7Y4W0
G	-6	HIS	-	expression tag	UNP F7Y4W0
G	-5	HIS	-	expression tag	UNP F7Y4W0
G	-4	HIS	-	expression tag	UNP F7Y4W0
G	-3	SER	-	expression tag	UNP F7Y4W0
G	-2	GLN	-	expression tag	UNP F7Y4W0
G	-1	ASP	-	expression tag	UNP F7Y4W0
G	0	PRO	-	expression tag	UNP F7Y4W0
H	-13	MET	-	initiating methionine	UNP F7Y4W0
H	-12	GLY	-	expression tag	UNP F7Y4W0
H	-11	SER	-	expression tag	UNP F7Y4W0
H	-10	SER	-	expression tag	UNP F7Y4W0
H	-9	HIS	-	expression tag	UNP F7Y4W0
H	-8	HIS	-	expression tag	UNP F7Y4W0
H	-7	HIS	-	expression tag	UNP F7Y4W0
H	-6	HIS	-	expression tag	UNP F7Y4W0
H	-5	HIS	-	expression tag	UNP F7Y4W0
H	-4	HIS	-	expression tag	UNP F7Y4W0
H	-3	SER	-	expression tag	UNP F7Y4W0
H	-2	GLN	-	expression tag	UNP F7Y4W0
H	-1	ASP	-	expression tag	UNP F7Y4W0
H	0	PRO	-	expression tag	UNP F7Y4W0
I	-13	MET	-	initiating methionine	UNP F7Y4W0
I	-12	GLY	-	expression tag	UNP F7Y4W0
I	-11	SER	-	expression tag	UNP F7Y4W0
I	-10	SER	-	expression tag	UNP F7Y4W0
I	-9	HIS	-	expression tag	UNP F7Y4W0
I	-8	HIS	-	expression tag	UNP F7Y4W0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-7	HIS	-	expression tag	UNP F7Y4W0
I	-6	HIS	-	expression tag	UNP F7Y4W0
I	-5	HIS	-	expression tag	UNP F7Y4W0
I	-4	HIS	-	expression tag	UNP F7Y4W0
I	-3	SER	-	expression tag	UNP F7Y4W0
I	-2	GLN	-	expression tag	UNP F7Y4W0
I	-1	ASP	-	expression tag	UNP F7Y4W0
I	0	PRO	-	expression tag	UNP F7Y4W0
J	-13	MET	-	initiating methionine	UNP F7Y4W0
J	-12	GLY	-	expression tag	UNP F7Y4W0
J	-11	SER	-	expression tag	UNP F7Y4W0
J	-10	SER	-	expression tag	UNP F7Y4W0
J	-9	HIS	-	expression tag	UNP F7Y4W0
J	-8	HIS	-	expression tag	UNP F7Y4W0
J	-7	HIS	-	expression tag	UNP F7Y4W0
J	-6	HIS	-	expression tag	UNP F7Y4W0
J	-5	HIS	-	expression tag	UNP F7Y4W0
J	-4	HIS	-	expression tag	UNP F7Y4W0
J	-3	SER	-	expression tag	UNP F7Y4W0
J	-2	GLN	-	expression tag	UNP F7Y4W0
J	-1	ASP	-	expression tag	UNP F7Y4W0
J	0	PRO	-	expression tag	UNP F7Y4W0
K	-13	MET	-	initiating methionine	UNP F7Y4W0
K	-12	GLY	-	expression tag	UNP F7Y4W0
K	-11	SER	-	expression tag	UNP F7Y4W0
K	-10	SER	-	expression tag	UNP F7Y4W0
K	-9	HIS	-	expression tag	UNP F7Y4W0
K	-8	HIS	-	expression tag	UNP F7Y4W0
K	-7	HIS	-	expression tag	UNP F7Y4W0
K	-6	HIS	-	expression tag	UNP F7Y4W0
K	-5	HIS	-	expression tag	UNP F7Y4W0
K	-4	HIS	-	expression tag	UNP F7Y4W0
K	-3	SER	-	expression tag	UNP F7Y4W0
K	-2	GLN	-	expression tag	UNP F7Y4W0
K	-1	ASP	-	expression tag	UNP F7Y4W0
K	0	PRO	-	expression tag	UNP F7Y4W0
L	-13	MET	-	initiating methionine	UNP F7Y4W0
L	-12	GLY	-	expression tag	UNP F7Y4W0
L	-11	SER	-	expression tag	UNP F7Y4W0
L	-10	SER	-	expression tag	UNP F7Y4W0
L	-9	HIS	-	expression tag	UNP F7Y4W0
L	-8	HIS	-	expression tag	UNP F7Y4W0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	HIS	-	expression tag	UNP F7Y4W0
L	-6	HIS	-	expression tag	UNP F7Y4W0
L	-5	HIS	-	expression tag	UNP F7Y4W0
L	-4	HIS	-	expression tag	UNP F7Y4W0
L	-3	SER	-	expression tag	UNP F7Y4W0
L	-2	GLN	-	expression tag	UNP F7Y4W0
L	-1	ASP	-	expression tag	UNP F7Y4W0
L	0	PRO	-	expression tag	UNP F7Y4W0
M	-13	MET	-	initiating methionine	UNP F7Y4W0
M	-12	GLY	-	expression tag	UNP F7Y4W0
M	-11	SER	-	expression tag	UNP F7Y4W0
M	-10	SER	-	expression tag	UNP F7Y4W0
M	-9	HIS	-	expression tag	UNP F7Y4W0
M	-8	HIS	-	expression tag	UNP F7Y4W0
M	-7	HIS	-	expression tag	UNP F7Y4W0
M	-6	HIS	-	expression tag	UNP F7Y4W0
M	-5	HIS	-	expression tag	UNP F7Y4W0
M	-4	HIS	-	expression tag	UNP F7Y4W0
M	-3	SER	-	expression tag	UNP F7Y4W0
M	-2	GLN	-	expression tag	UNP F7Y4W0
M	-1	ASP	-	expression tag	UNP F7Y4W0
M	0	PRO	-	expression tag	UNP F7Y4W0
N	-13	MET	-	initiating methionine	UNP F7Y4W0
N	-12	GLY	-	expression tag	UNP F7Y4W0
N	-11	SER	-	expression tag	UNP F7Y4W0
N	-10	SER	-	expression tag	UNP F7Y4W0
N	-9	HIS	-	expression tag	UNP F7Y4W0
N	-8	HIS	-	expression tag	UNP F7Y4W0
N	-7	HIS	-	expression tag	UNP F7Y4W0
N	-6	HIS	-	expression tag	UNP F7Y4W0
N	-5	HIS	-	expression tag	UNP F7Y4W0
N	-4	HIS	-	expression tag	UNP F7Y4W0
N	-3	SER	-	expression tag	UNP F7Y4W0
N	-2	GLN	-	expression tag	UNP F7Y4W0
N	-1	ASP	-	expression tag	UNP F7Y4W0
N	0	PRO	-	expression tag	UNP F7Y4W0
O	-13	MET	-	initiating methionine	UNP F7Y4W0
O	-12	GLY	-	expression tag	UNP F7Y4W0
O	-11	SER	-	expression tag	UNP F7Y4W0
O	-10	SER	-	expression tag	UNP F7Y4W0
O	-9	HIS	-	expression tag	UNP F7Y4W0
O	-8	HIS	-	expression tag	UNP F7Y4W0

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-7	HIS	-	expression tag	UNP F7Y4W0
O	-6	HIS	-	expression tag	UNP F7Y4W0
O	-5	HIS	-	expression tag	UNP F7Y4W0
O	-4	HIS	-	expression tag	UNP F7Y4W0
O	-3	SER	-	expression tag	UNP F7Y4W0
O	-2	GLN	-	expression tag	UNP F7Y4W0
O	-1	ASP	-	expression tag	UNP F7Y4W0
O	0	PRO	-	expression tag	UNP F7Y4W0
P	-13	MET	-	initiating methionine	UNP F7Y4W0
P	-12	GLY	-	expression tag	UNP F7Y4W0
P	-11	SER	-	expression tag	UNP F7Y4W0
P	-10	SER	-	expression tag	UNP F7Y4W0
P	-9	HIS	-	expression tag	UNP F7Y4W0
P	-8	HIS	-	expression tag	UNP F7Y4W0
P	-7	HIS	-	expression tag	UNP F7Y4W0
P	-6	HIS	-	expression tag	UNP F7Y4W0
P	-5	HIS	-	expression tag	UNP F7Y4W0
P	-4	HIS	-	expression tag	UNP F7Y4W0
P	-3	SER	-	expression tag	UNP F7Y4W0
P	-2	GLN	-	expression tag	UNP F7Y4W0
P	-1	ASP	-	expression tag	UNP F7Y4W0
P	0	PRO	-	expression tag	UNP F7Y4W0
Q	-13	MET	-	initiating methionine	UNP F7Y4W0
Q	-12	GLY	-	expression tag	UNP F7Y4W0
Q	-11	SER	-	expression tag	UNP F7Y4W0
Q	-10	SER	-	expression tag	UNP F7Y4W0
Q	-9	HIS	-	expression tag	UNP F7Y4W0
Q	-8	HIS	-	expression tag	UNP F7Y4W0
Q	-7	HIS	-	expression tag	UNP F7Y4W0
Q	-6	HIS	-	expression tag	UNP F7Y4W0
Q	-5	HIS	-	expression tag	UNP F7Y4W0
Q	-4	HIS	-	expression tag	UNP F7Y4W0
Q	-3	SER	-	expression tag	UNP F7Y4W0
Q	-2	GLN	-	expression tag	UNP F7Y4W0
Q	-1	ASP	-	expression tag	UNP F7Y4W0
Q	0	PRO	-	expression tag	UNP F7Y4W0
R	-13	MET	-	initiating methionine	UNP F7Y4W0
R	-12	GLY	-	expression tag	UNP F7Y4W0
R	-11	SER	-	expression tag	UNP F7Y4W0
R	-10	SER	-	expression tag	UNP F7Y4W0
R	-9	HIS	-	expression tag	UNP F7Y4W0
R	-8	HIS	-	expression tag	UNP F7Y4W0

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-7	HIS	-	expression tag	UNP F7Y4W0
R	-6	HIS	-	expression tag	UNP F7Y4W0
R	-5	HIS	-	expression tag	UNP F7Y4W0
R	-4	HIS	-	expression tag	UNP F7Y4W0
R	-3	SER	-	expression tag	UNP F7Y4W0
R	-2	GLN	-	expression tag	UNP F7Y4W0
R	-1	ASP	-	expression tag	UNP F7Y4W0
R	0	PRO	-	expression tag	UNP F7Y4W0

- Molecule 2 is a protein called Putative addiction module antidote protein, CopG/Arc/MetJ family chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	a	87	Total	C	H	N	O	S	0	0	0
			1379	429	691	125	132	2			
2	b	87	Total	C	H	N	O	S	0	0	0
			1379	429	691	125	132	2			
2	c	87	Total	C	H	N	O	S	0	0	0
			1379	429	691	125	132	2			
2	d	85	Total	C	H	N	O	S	0	0	0
			1349	420	676	122	129	2			
2	e	79	Total	C	H	N	O	S	0	0	0
			1258	393	629	115	120	1			
2	f	85	Total	C	H	N	O	S	0	0	0
			1349	420	676	122	129	2			
2	g	86	Total	C	H	N	O	S	0	0	0
			1365	425	685	123	130	2			
2	h	79	Total	C	H	N	O	S	0	0	0
			1258	393	629	115	120	1			
2	i	83	Total	C	H	N	O	S	0	0	0
			1312	409	657	119	125	2			
2	j	83	Total	C	H	N	O	S	0	0	0
			1312	409	657	119	125	2			
2	k	85	Total	C	H	N	O	S	0	0	0
			1349	420	676	122	129	2			
2	l	86	Total	C	H	N	O	S	0	0	0
			1366	425	686	123	130	2			
2	m	85	Total	C	H	N	O	S	0	0	0
			1349	420	676	122	129	2			
2	n	85	Total	C	H	N	O	S	0	0	0
			1349	420	676	122	129	2			
2	o	83	Total	C	H	N	O	S	0	0	0
			1312	409	657	119	125	2			

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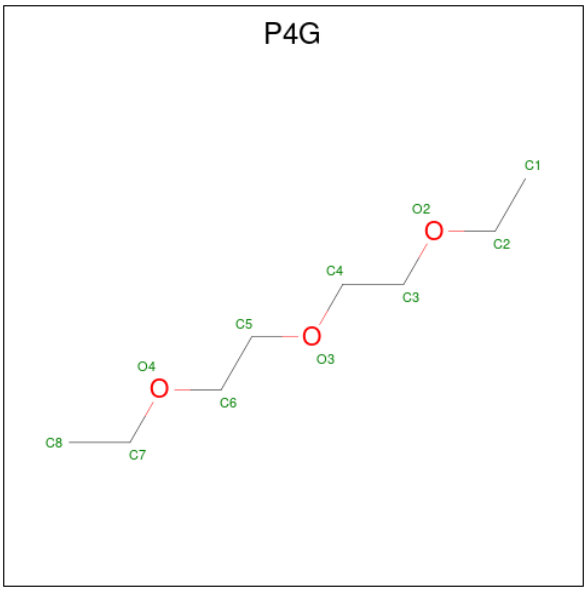
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	p	87	Total	C	H	N	O	S	0	0	0
			1379	429	691	125	132	2			
2	q	86	Total	C	H	N	O	S	0	0	0
			1365	425	685	123	130	2			
2	r	85	Total	C	H	N	O	S	0	0	0
			1347	420	674	122	129	2			

- Molecule 3 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			29	8	18	3		
3	A	1	Total	C	H	O	0	0
			29	8	18	3		
3	B	1	Total	C	H	O	0	0
			29	8	18	3		
3	C	1	Total	C	H	O	0	0
			29	8	18	3		
3	C	1	Total	C	H	O	0	0
			29	8	18	3		
3	D	1	Total	C	H	O	0	0
			29	8	18	3		
3	D	1	Total	C	H	O	0	0
			29	8	18	3		
3	E	1	Total	C	H	O	0	0
			29	8	18	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	H	O	0	0
			29	8	18	3		
3	M	1	Total	C	H	O	0	0
			29	8	18	3		

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: Plasmid stabilization system

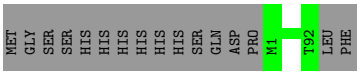
Chain A:

- Molecule 1: Plasmid stabilization system

Chain B:

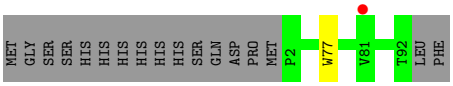
- Molecule 1: Plasmid stabilization system

Chain C:



- Molecule 1: Plasmid stabilization system

Chain D:



- Molecule 1: Plasmid stabilization system

Chain E:

- Molecule 1: Plasmid stabilization system

Chain F:

• Molecule 1: Plasmid stabilization system

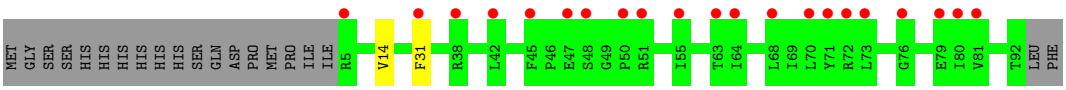
Chain G:

• Molecule 1: Plasmid stabilization system

Chain H:

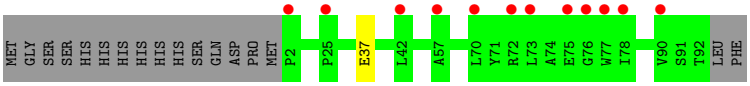
• Molecule 1: Plasmid stabilization system

Chain I:



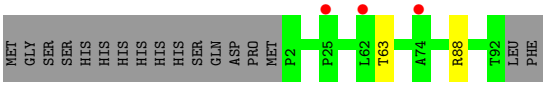
• Molecule 1: Plasmid stabilization system

Chain J:



• Molecule 1: Plasmid stabilization system

Chain K:

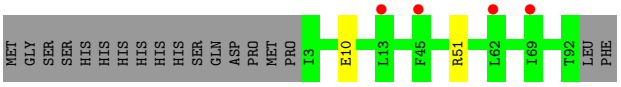


• Molecule 1: Plasmid stabilization system

Chain L:

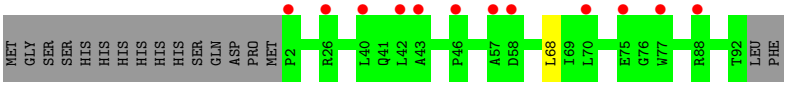
• Molecule 1: Plasmid stabilization system

Chain M:



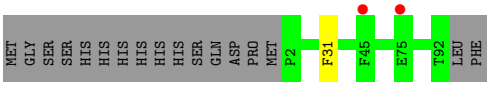
• Molecule 1: Plasmid stabilization system

Chain N:



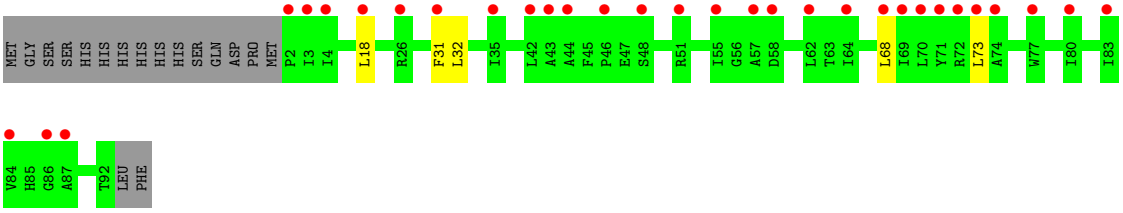
• Molecule 1: Plasmid stabilization system

Chain O:



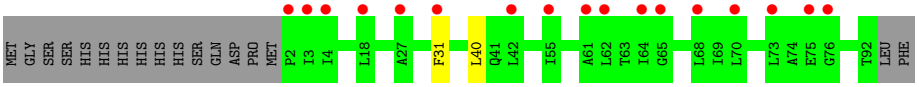
• Molecule 1: Plasmid stabilization system

Chain P:



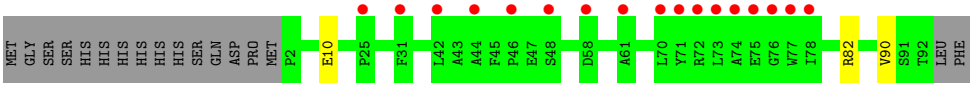
• Molecule 1: Plasmid stabilization system

Chain Q:



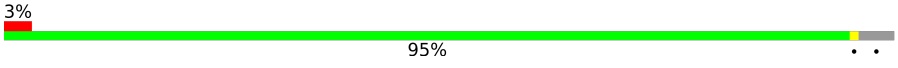
• Molecule 1: Plasmid stabilization system

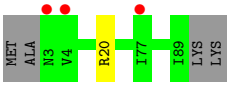
Chain R:



• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

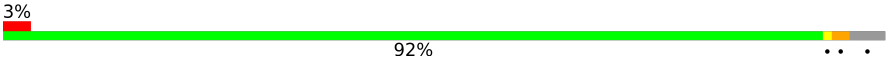
Chain a:

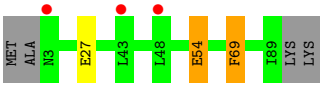




• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

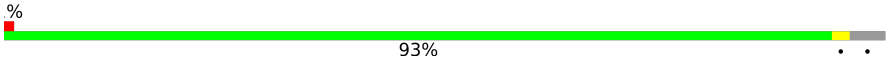
Chain b:





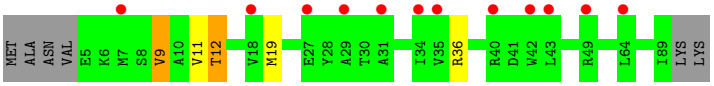
• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

Chain c:



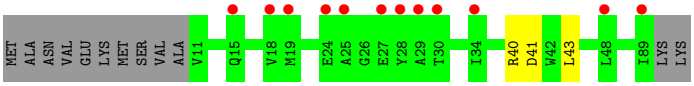
• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

Chain d:



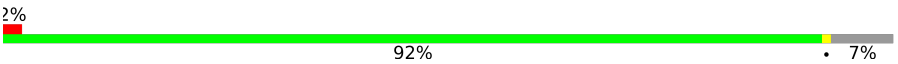
• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

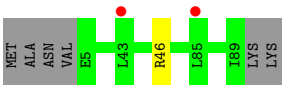
Chain e:



• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

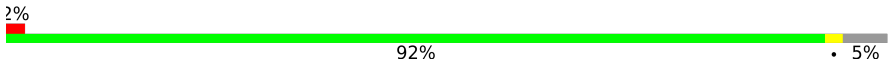
Chain f:

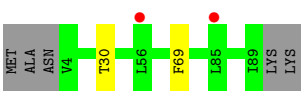




• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

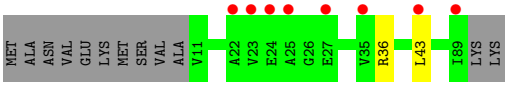
Chain g:





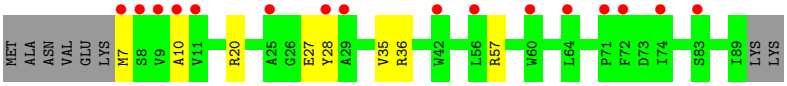
• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

Chain h:



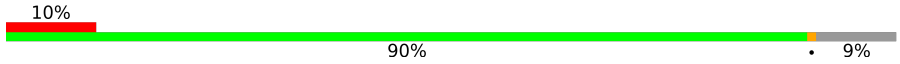
• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

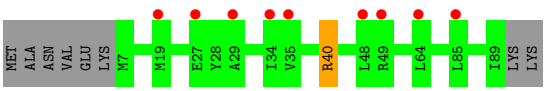
Chain i:



• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

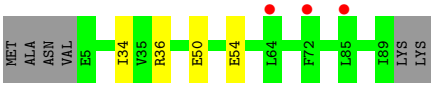
Chain j:





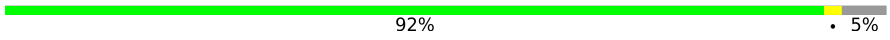
• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

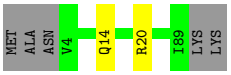
Chain k:



• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

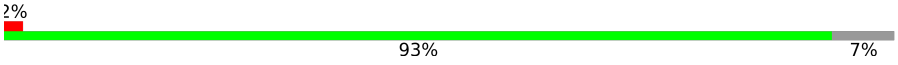
Chain l:

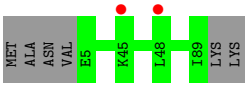




• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

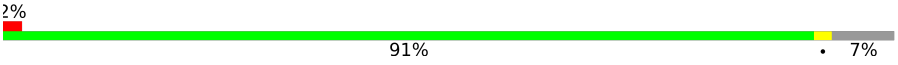
Chain m:

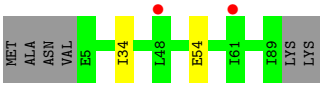




• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

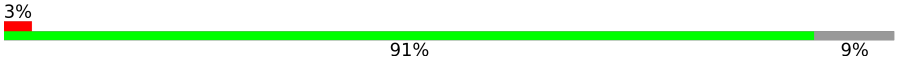
Chain n:

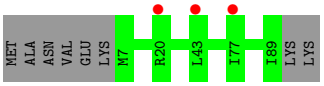




• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

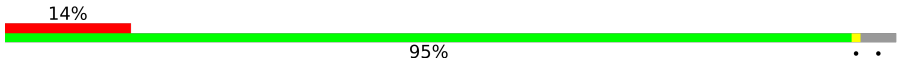
Chain o:

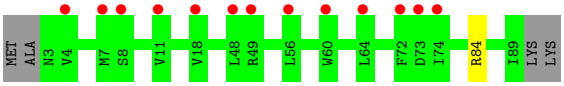




• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

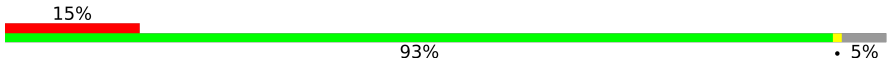
Chain p:

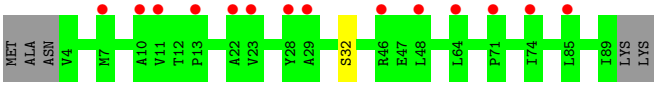




• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

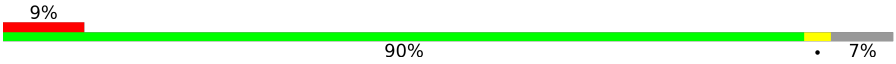
Chain q:

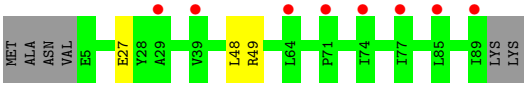




• Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera

Chain r:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	148.54Å 148.54Å 195.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.81 – 2.90 29.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.81-2.90) 90.6 (29.81-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.255 , 0.282 0.255 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å^2)	80.5	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.032 for h,-h-k,-l 0.049 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49728	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.50% 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

Bond lengths and bond angles in the following residue types are not validated in this section: P4G

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	0.32	0/717	0.54	0/978
1	B	0.32	0/717	0.63	2/978 (0.2%)
1	C	0.33	0/725	0.53	0/989
1	D	0.31	0/717	0.56	0/978
1	E	0.36	0/717	0.60	0/978
1	F	0.31	0/717	0.55	0/978
1	G	0.31	0/717	0.74	3/978 (0.3%)
1	H	0.34	0/717	0.63	0/978
1	I	0.49	2/693 (0.3%)	0.65	0/945
1	J	0.32	0/717	0.60	0/978
1	K	0.42	0/717	0.68	3/978 (0.3%)
1	L	0.35	0/717	0.60	0/978
1	M	0.32	0/709	0.59	2/967 (0.2%)
1	N	0.43	0/717	0.74	2/978 (0.2%)
1	O	0.30	0/717	0.54	0/978
1	P	0.42	1/717 (0.1%)	0.81	4/978 (0.4%)
1	Q	0.56	0/717	0.78	2/978 (0.2%)
1	R	0.36	0/717	0.67	2/978 (0.2%)
2	a	0.40	0/697	0.63	1/939 (0.1%)
2	b	0.71	3/697 (0.4%)	0.77	3/939 (0.3%)
2	c	0.39	0/697	0.63	1/939 (0.1%)
2	d	0.58	0/682	0.87	3/918 (0.3%)
2	e	0.45	0/638	0.76	4/860 (0.5%)
2	f	0.54	0/682	0.65	0/918
2	g	0.56	1/689 (0.1%)	0.65	0/928
2	h	0.49	0/638	0.82	2/860 (0.2%)
2	i	0.70	2/664 (0.3%)	1.03	7/895 (0.8%)
2	j	0.53	0/664	1.05	2/895 (0.2%)
2	k	0.55	0/682	0.69	1/918 (0.1%)
2	l	0.47	0/689	0.60	2/928 (0.2%)
2	m	0.43	0/682	0.60	0/918
2	n	0.43	0/682	0.66	1/918 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	o	0.38	0/664	0.54	0/895
2	p	0.41	0/697	0.76	2/939 (0.2%)
2	q	0.40	0/689	0.65	0/928
2	r	0.55	0/682	0.80	1/918 (0.1%)
All	All	0.44	9/25097 (0.0%)	0.69	50/34024 (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
1	J	0	1
2	d	0	1
2	i	0	2
2	r	0	1
All	All	0	5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	69	PHE	CE2-CZ	8.09	1.52	1.37
1	I	31	PHE	CE2-CZ	6.64	1.50	1.37
2	b	27	GLU	CG-CD	-6.23	1.42	1.51
2	i	28	TYR	CE1-CZ	5.91	1.46	1.38
2	g	69	PHE	CE2-CZ	5.84	1.48	1.37

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	40	ARG	NE-CZ-NH2	16.69	128.65	120.30
2	j	40	ARG	NE-CZ-NH1	-13.52	113.54	120.30
1	G	68	LEU	CB-CG-CD1	-11.08	92.17	111.00
2	p	84	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	d	12	THR	OG1-CB-CG2	7.95	128.29	110.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	37	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	d	9	VAL	Peptide
2	i	10	ALA	Peptide
2	i	27	GLU	Peptide
2	r	27	GLU	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	89/108 (82%)	87 (98%)	2 (2%)	0	100	100
1	B	89/108 (82%)	88 (99%)	1 (1%)	0	100	100
1	C	90/108 (83%)	89 (99%)	1 (1%)	0	100	100
1	D	89/108 (82%)	87 (98%)	2 (2%)	0	100	100
1	E	89/108 (82%)	88 (99%)	1 (1%)	0	100	100
1	F	89/108 (82%)	87 (98%)	2 (2%)	0	100	100
1	G	89/108 (82%)	87 (98%)	2 (2%)	0	100	100
1	H	89/108 (82%)	87 (98%)	2 (2%)	0	100	100
1	I	86/108 (80%)	85 (99%)	1 (1%)	0	100	100
1	J	89/108 (82%)	87 (98%)	2 (2%)	0	100	100
1	K	89/108 (82%)	88 (99%)	1 (1%)	0	100	100
1	L	89/108 (82%)	88 (99%)	1 (1%)	0	100	100
1	M	88/108 (82%)	86 (98%)	2 (2%)	0	100	100
1	N	89/108 (82%)	87 (98%)	2 (2%)	0	100	100
1	O	89/108 (82%)	86 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	89/108 (82%)	88 (99%)	1 (1%)	0	100	100
1	Q	89/108 (82%)	88 (99%)	1 (1%)	0	100	100
1	R	89/108 (82%)	88 (99%)	1 (1%)	0	100	100
2	a	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
2	b	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
2	c	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
2	d	83/91 (91%)	80 (96%)	3 (4%)	0	100	100
2	e	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
2	f	83/91 (91%)	82 (99%)	1 (1%)	0	100	100
2	g	84/91 (92%)	83 (99%)	1 (1%)	0	100	100
2	h	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
2	i	81/91 (89%)	80 (99%)	1 (1%)	0	100	100
2	j	81/91 (89%)	80 (99%)	1 (1%)	0	100	100
2	k	83/91 (91%)	82 (99%)	1 (1%)	0	100	100
2	l	84/91 (92%)	83 (99%)	1 (1%)	0	100	100
2	m	83/91 (91%)	82 (99%)	1 (1%)	0	100	100
2	n	83/91 (91%)	82 (99%)	1 (1%)	0	100	100
2	o	81/91 (89%)	80 (99%)	1 (1%)	0	100	100
2	p	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
2	q	84/91 (92%)	81 (96%)	3 (4%)	0	100	100
2	r	83/91 (91%)	80 (96%)	3 (4%)	0	100	100
All	All	3086/3582 (86%)	3031 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	70/86 (81%)	69 (99%)	1 (1%)	67 89
1	B	70/86 (81%)	70 (100%)	0	100 100
1	C	71/86 (83%)	71 (100%)	0	100 100
1	D	70/86 (81%)	69 (99%)	1 (1%)	67 89
1	E	70/86 (81%)	70 (100%)	0	100 100
1	F	70/86 (81%)	70 (100%)	0	100 100
1	G	70/86 (81%)	70 (100%)	0	100 100
1	H	70/86 (81%)	69 (99%)	1 (1%)	67 89
1	I	67/86 (78%)	66 (98%)	1 (2%)	65 87
1	J	70/86 (81%)	70 (100%)	0	100 100
1	K	70/86 (81%)	70 (100%)	0	100 100
1	L	70/86 (81%)	70 (100%)	0	100 100
1	M	69/86 (80%)	68 (99%)	1 (1%)	67 89
1	N	70/86 (81%)	70 (100%)	0	100 100
1	O	70/86 (81%)	69 (99%)	1 (1%)	67 89
1	P	70/86 (81%)	70 (100%)	0	100 100
1	Q	70/86 (81%)	70 (100%)	0	100 100
1	R	70/86 (81%)	68 (97%)	2 (3%)	42 76
2	a	69/72 (96%)	69 (100%)	0	100 100
2	b	69/72 (96%)	67 (97%)	2 (3%)	42 76
2	c	69/72 (96%)	68 (99%)	1 (1%)	67 89
2	d	67/72 (93%)	64 (96%)	3 (4%)	27 61
2	e	62/72 (86%)	62 (100%)	0	100 100
2	f	67/72 (93%)	66 (98%)	1 (2%)	65 87
2	g	68/72 (94%)	68 (100%)	0	100 100
2	h	62/72 (86%)	62 (100%)	0	100 100
2	i	65/72 (90%)	64 (98%)	1 (2%)	65 87
2	j	65/72 (90%)	64 (98%)	1 (2%)	65 87
2	k	67/72 (93%)	64 (96%)	3 (4%)	27 61
2	l	68/72 (94%)	67 (98%)	1 (2%)	65 87
2	m	67/72 (93%)	67 (100%)	0	100 100
2	n	67/72 (93%)	66 (98%)	1 (2%)	65 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	o	65/72 (90%)	65 (100%)	0	100	100
2	p	69/72 (96%)	69 (100%)	0	100	100
2	q	68/72 (94%)	67 (98%)	1 (2%)	65	87
2	r	67/72 (93%)	66 (98%)	1 (2%)	65	87
All	All	2458/2844 (86%)	2434 (99%)	24 (1%)	76	92

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	f	46	ARG
2	k	34	ILE
2	j	40	ARG
2	k	50	GLU
1	R	10	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	P4G	D	102	-	10,10,10	0.49	0	9,9,9	0.29	0
3	P4G	B	101	-	10,10,10	0.50	0	9,9,9	0.47	0
3	P4G	A	101	-	10,10,10	0.49	0	9,9,9	0.25	0
3	P4G	E	101	-	10,10,10	0.49	0	9,9,9	0.24	0
3	P4G	M	101	-	10,10,10	0.50	0	9,9,9	0.35	0
3	P4G	A	102	-	10,10,10	0.50	0	9,9,9	0.21	0
3	P4G	D	101	-	10,10,10	0.49	0	9,9,9	0.29	0
3	P4G	L	101	-	10,10,10	0.52	0	9,9,9	0.26	0
3	P4G	C	101	-	10,10,10	0.50	0	9,9,9	0.29	0
3	P4G	C	102	-	10,10,10	0.50	0	9,9,9	0.22	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	P4G	D	102	-	-	1/8/8/8	-
3	P4G	B	101	-	-	2/8/8/8	-
3	P4G	A	101	-	-	1/8/8/8	-
3	P4G	E	101	-	-	3/8/8/8	-
3	P4G	M	101	-	-	2/8/8/8	-
3	P4G	A	102	-	-	0/8/8/8	-
3	P4G	D	101	-	-	2/8/8/8	-
3	P4G	L	101	-	-	2/8/8/8	-
3	P4G	C	101	-	-	2/8/8/8	-
3	P4G	C	102	-	-	1/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	101	P4G	O2-C3-C4-O3
3	D	102	P4G	O3-C5-C6-O4
3	L	101	P4G	O3-C5-C6-O4
3	B	101	P4G	O2-C3-C4-O3
3	C	101	P4G	O2-C3-C4-O3

There are no ring outliers.

No monomer is involved in short contacts.

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

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	91/108 (84%)	0.47	0 100 100	57, 77, 101, 108	0
1	B	91/108 (84%)	0.57	0 100 100	67, 85, 117, 130	0
1	C	92/108 (85%)	0.46	0 100 100	63, 79, 104, 128	0
1	D	91/108 (84%)	0.41	1 (1%) 80 80	70, 85, 129, 148	0
1	E	91/108 (84%)	0.38	0 100 100	72, 91, 123, 134	0
1	F	91/108 (84%)	0.52	0 100 100	56, 79, 109, 117	0
1	G	91/108 (84%)	0.48	0 100 100	61, 87, 117, 125	0
1	H	91/108 (84%)	0.36	0 100 100	71, 87, 130, 142	0
1	I	88/108 (81%)	1.14	21 (23%) 0 0	114, 177, 246, 275	0
1	J	91/108 (84%)	0.62	12 (13%) 3 2	100, 127, 176, 186	0
1	K	91/108 (84%)	0.45	3 (3%) 46 41	78, 99, 143, 165	0
1	L	91/108 (84%)	0.44	0 100 100	68, 85, 108, 117	0
1	M	90/108 (83%)	0.45	4 (4%) 34 30	72, 116, 157, 167	0
1	N	91/108 (84%)	0.67	12 (13%) 3 2	106, 135, 180, 206	0
1	O	91/108 (84%)	0.40	2 (2%) 62 59	73, 106, 135, 162	0
1	P	91/108 (84%)	1.52	31 (34%) 0 0	141, 195, 245, 272	0
1	Q	91/108 (84%)	0.84	17 (18%) 1 0	111, 165, 201, 209	0
1	R	91/108 (84%)	0.80	17 (18%) 1 0	126, 151, 208, 233	0
2	a	87/91 (95%)	0.57	3 (3%) 45 40	71, 89, 130, 166	0
2	b	87/91 (95%)	0.53	3 (3%) 45 40	71, 100, 129, 181	0
2	c	87/91 (95%)	0.50	1 (1%) 80 80	72, 90, 132, 155	0
2	d	85/91 (93%)	0.75	12 (14%) 2 2	75, 148, 211, 214	0
2	e	79/91 (86%)	0.76	12 (15%) 2 1	91, 126, 252, 260	0
2	f	85/91 (93%)	0.49	2 (2%) 59 56	70, 94, 111, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	g	86/91 (94%)	0.47	2 (2%) 60 58	72, 105, 130, 152	0
2	h	79/91 (86%)	0.70	8 (10%) 7 5	76, 131, 202, 207	0
2	i	83/91 (91%)	0.98	16 (19%) 1 0	108, 181, 215, 233	0
2	j	83/91 (91%)	0.63	9 (10%) 5 4	97, 132, 167, 187	0
2	k	85/91 (93%)	0.38	3 (3%) 44 38	73, 109, 139, 166	0
2	l	86/91 (94%)	0.45	0 100 100	74, 93, 124, 146	0
2	m	85/91 (93%)	0.47	2 (2%) 59 56	77, 108, 134, 140	0
2	n	85/91 (93%)	0.30	2 (2%) 59 56	72, 114, 146, 153	0
2	o	83/91 (91%)	0.48	3 (3%) 42 37	70, 101, 133, 159	0
2	p	87/91 (95%)	0.75	13 (14%) 2 1	118, 192, 229, 238	0
2	q	86/91 (94%)	0.59	14 (16%) 1 1	129, 162, 220, 229	0
2	r	85/91 (93%)	0.51	8 (9%) 8 6	114, 147, 171, 180	0
All	All	3158/3582 (88%)	0.59	233 (7%) 14 11	56, 108, 205, 275	0

The worst 5 of 233 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	2	PRO	18.3
2	c	3	ASN	7.6
2	i	11	VAL	7.5
1	P	68	LEU	7.3
1	I	68	LEU	6.6

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, 95^{th} 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	P4G	L	101	11/11	0.78	0.22	72,90,98,98	0
3	P4G	D	102	11/11	0.83	0.26	99,119,135,135	0
3	P4G	A	101	11/11	0.85	0.26	75,100,148,148	0
3	P4G	D	101	11/11	0.85	0.29	80,96,113,113	0
3	P4G	A	102	11/11	0.86	0.25	74,92,102,102	0
3	P4G	M	101	11/11	0.89	0.25	99,120,126,126	0
3	P4G	B	101	11/11	0.90	0.25	64,89,137,137	0
3	P4G	C	101	11/11	0.90	0.25	74,97,138,138	0
3	P4G	C	102	11/11	0.91	0.25	68,86,128,128	0
3	P4G	E	101	11/11	0.92	0.30	89,107,125,125	0

6.5 Other polymers (i)

There are no such residues in this entry.