



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2020 – 01:15 AM EST

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 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

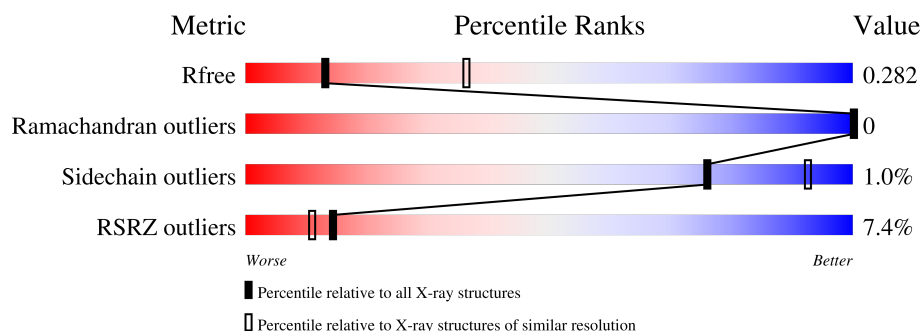
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	108	
1	B	108	
1	C	108	
1	D	108	
1	E	108	
1	F	108	

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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	<div><div></div><div>2%</div><div>91%</div><div>7%</div></div>
2	o	91	<div><div></div><div>3%</div><div>91%</div><div>9%</div></div>
2	p	91	<div><div></div><div>14%</div><div>95%</div><div></div></div>
2	q	91	<div><div></div><div>15%</div><div>93%</div><div>5%</div></div>
2	r	91	<div><div></div><div>9%</div><div>90%</div><div>7%</div></div>

## 2 Entry composition

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

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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.

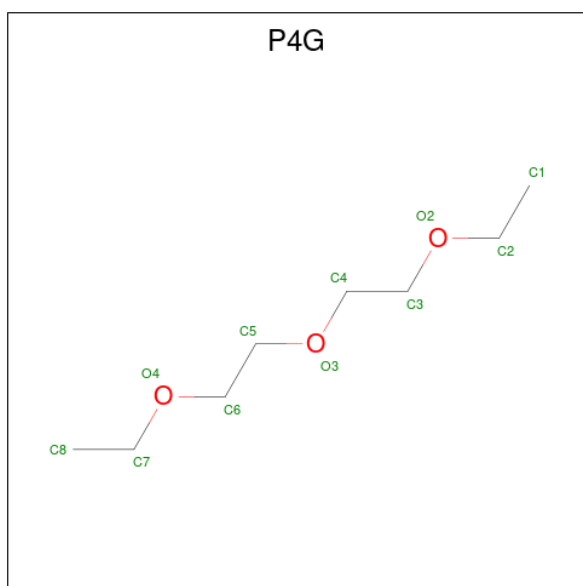
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	a	87	Total	C	H	N	O	S	0	0	0
			1379	429	691	125	132	2			
2	b	87	Total	C	H	N	O	S	0	0	0
			1379	429	691	125	132	2			
2	c	87	Total	C	H	N	O	S	0	0	0
			1379	429	691	125	132	2			
2	d	85	Total	C	H	N	O	S	0	0	0
			1349	420	676	122	129	2			
2	e	79	Total	C	H	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<sub>8</sub>H<sub>18</sub>O<sub>3</sub>).



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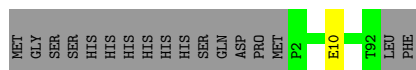
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	H	O	0	0
			29	8	18	3		
3	M	1	Total	C	H	O	0	0
			29	8	18	3		

### 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.

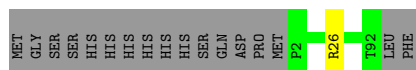
- Molecule 1: Plasmid stabilization system

Chain A:  83% 16%




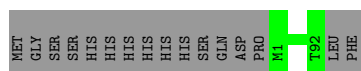
- Molecule 1: Plasmid stabilization system

Chain B:  83% 16%




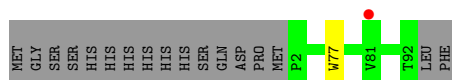
- Molecule 1: Plasmid stabilization system

Chain C:  85% 15%




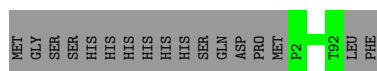
- Molecule 1: Plasmid stabilization system

Chain D:  83% 16%




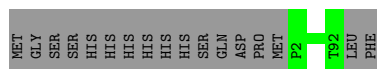
- Molecule 1: Plasmid stabilization system

Chain E:  84% 16%



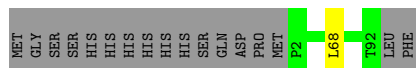
- Molecule 1: Plasmid stabilization system

Chain F:  84% 16%



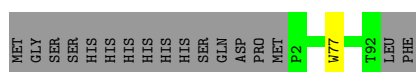
- Molecule 1: Plasmid stabilization system

Chain G: 83% 16%



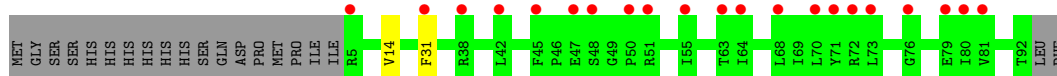
- Molecule 1: Plasmid stabilization system

Chain H: 83% 16%



- Molecule 1: Plasmid stabilization system

Chain I: 19% 80% 19%



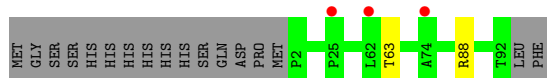
- Molecule 1: Plasmid stabilization system

Chain J: 11% 83% 16%



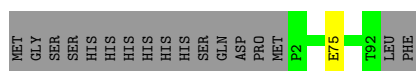
- Molecule 1: Plasmid stabilization system

Chain K: 3% 82% 16%



- Molecule 1: Plasmid stabilization system

Chain L: 83% 16%



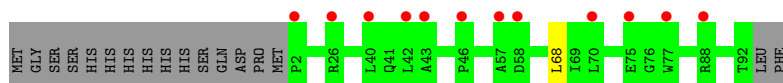
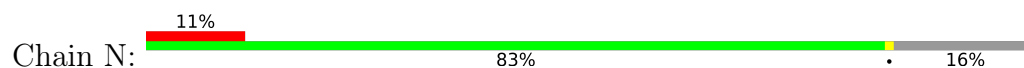
- Molecule 1: Plasmid stabilization system

Chain M: 4% 81% 17%

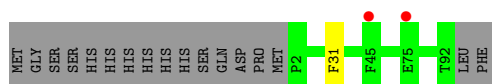
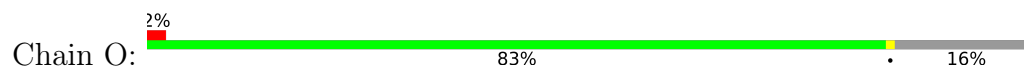




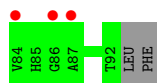
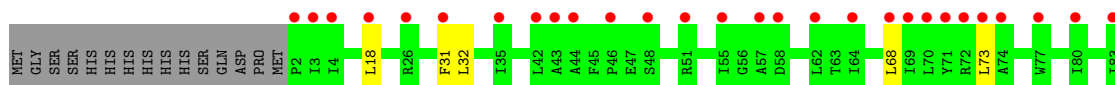
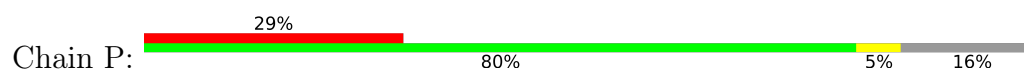
- Molecule 1: Plasmid stabilization system



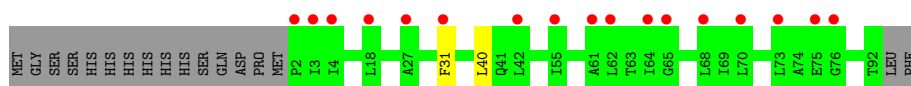
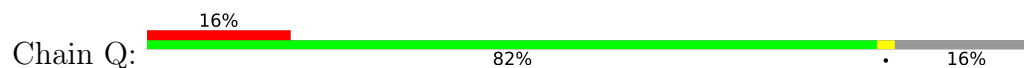
- Molecule 1: Plasmid stabilization system



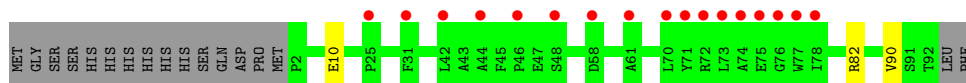
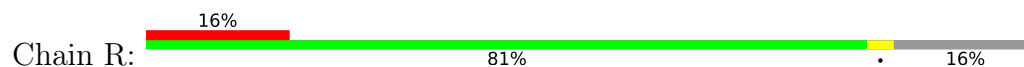
- Molecule 1: Plasmid stabilization system



- Molecule 1: Plasmid stabilization system



- Molecule 1: Plasmid stabilization system

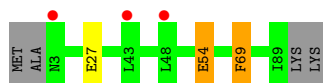
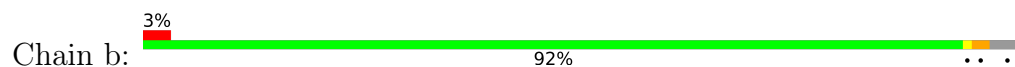


- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera





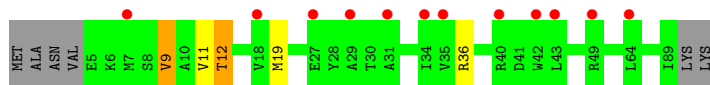
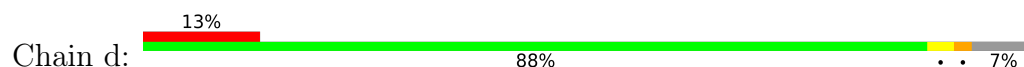
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



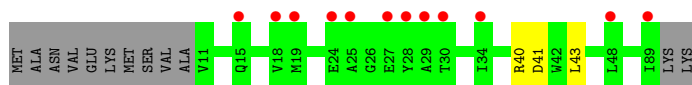
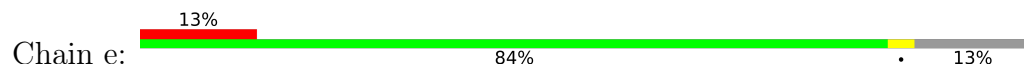
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



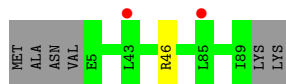
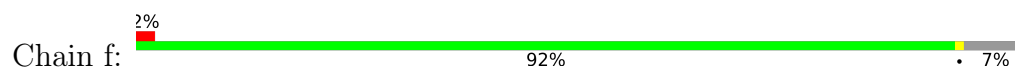
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



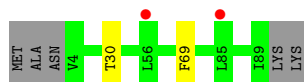
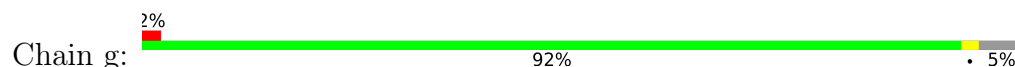
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



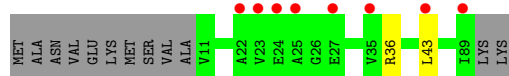
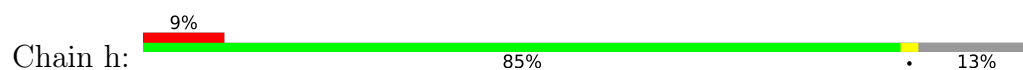
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



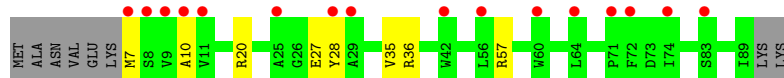
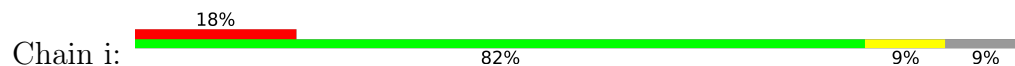
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



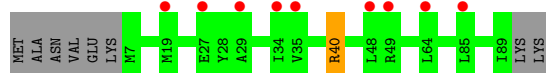
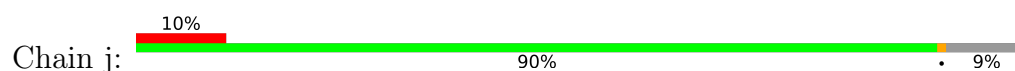
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



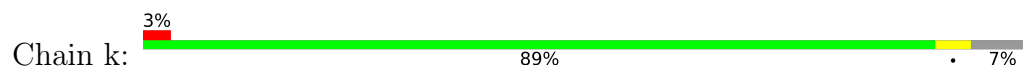
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



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



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



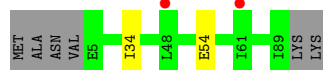
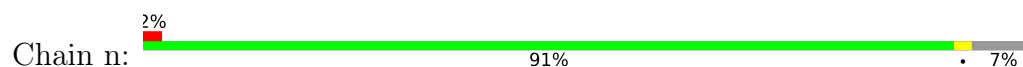
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



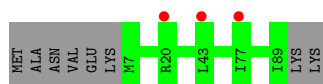
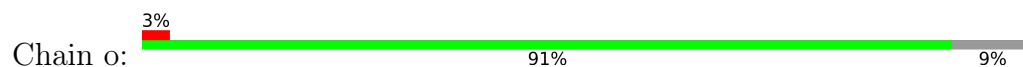
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



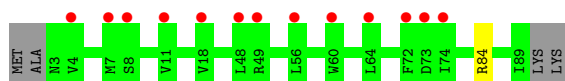
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



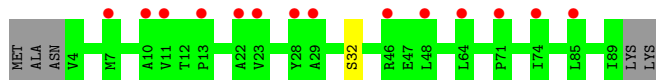
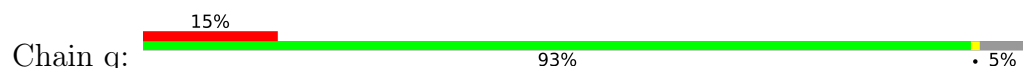
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



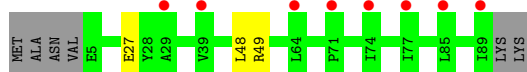
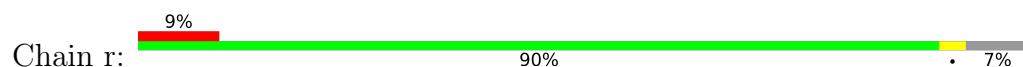
- Molecule 2: Putative addiction module antidote protein, CopG/Arc/MetJ family chimera



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	80.5	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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, 0.333 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

All (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
2	b	69	PHE	CE1-CZ	5.71	1.48	1.37
1	I	31	PHE	CE1-CZ	5.23	1.47	1.37
1	P	31	PHE	CE1-CZ	5.10	1.47	1.37
2	i	28	TYR	CG-CD1	5.09	1.45	1.39

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	i	7	MET	CG-SD-CE	7.85	112.76	100.20
2	a	20	ARG	CG-CD-NE	-7.76	95.50	111.80
1	N	68	LEU	CB-CG-CD1	-7.70	97.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	7	MET	CA-CB-CG	7.69	126.38	113.30
2	e	43	LEU	CB-CG-CD1	-7.58	98.11	111.00
2	p	84	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	h	43	LEU	CB-CG-CD1	-7.53	98.20	111.00
1	N	68	LEU	CB-CG-CD2	7.49	123.74	111.00
2	r	49	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	P	18	LEU	CB-CG-CD1	-7.25	98.67	111.00
1	P	73	LEU	CB-CG-CD1	-7.05	99.02	111.00
2	e	40	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	P	32	LEU	CB-CG-CD2	-6.55	99.86	111.00
1	K	88	ARG	NE-CZ-NH2	-6.53	117.03	120.30
2	k	36	ARG	CG-CD-NE	6.45	125.34	111.80
2	i	36	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	Q	40	LEU	CB-CG-CD1	6.35	121.80	111.00
1	G	68	LEU	CB-CG-CD2	6.35	121.80	111.00
2	b	54	GLU	OE1-CD-OE2	6.33	130.90	123.30
1	R	82	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	R	82	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	c	40	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	i	20	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	Q	31	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	G	68	LEU	CA-CB-CG	5.98	129.06	115.30
2	i	57	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	d	36	ARG	CG-CD-NE	5.87	124.12	111.80
2	l	20	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	b	69	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	M	51	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	h	36	ARG	CG-CD-NE	5.72	123.81	111.80
1	K	63	THR	CA-CB-CG2	5.70	120.38	112.40
1	M	51	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	P	68	LEU	CB-CG-CD1	-5.62	101.44	111.00
1	K	88	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	e	40	ARG	NE-CZ-NH2	-5.59	117.51	120.30
2	i	57	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	i	20	ARG	NE-CZ-NH2	-5.49	117.56	120.30
2	n	54	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	B	26	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	26	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	d	19	MET	CB-CG-SD	-5.12	97.05	112.40
2	e	41	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	l	20	ARG	CA-CB-CG	-5.04	102.31	113.40
2	b	27	GLU	CA-CB-CG	-5.01	102.37	113.40



There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	37	GLU	Mainchain
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	89/108 (82%)	87 (98%)	2 (2%)	0	100	100
1	O	89/108 (82%)	86 (97%)	3 (3%)	0	100	100
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 ⓘ

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

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	D	77	TRP
1	H	77	TRP
1	I	14	VAL
1	M	10	GLU
1	O	31	PHE
1	R	10	GLU
1	R	90	VAL
2	b	54	GLU
2	b	69	PHE
2	c	14	GLN
2	d	9	VAL
2	d	11	VAL
2	d	12	THR
2	f	46	ARG
2	i	35	VAL
2	j	40	ARG
2	k	34	ILE
2	k	50	GLU
2	k	54	GLU
2	l	14	GLN
2	n	34	ILE
2	q	32	SER
2	r	48	LEU

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (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
3	C	102	P4G	O3-C5-C6-O4
3	E	101	P4G	O2-C3-C4-O3
3	M	101	P4G	C6-C5-O3-C4
3	M	101	P4G	O3-C5-C6-O4
3	D	101	P4G	C6-C5-O3-C4
3	B	101	P4G	C6-C5-O3-C4
3	C	101	P4G	O3-C5-C6-O4
3	D	101	P4G	C1-C2-O2-C3
3	A	101	P4G	O2-C3-C4-O3
3	E	101	P4G	C6-C5-O3-C4
3	E	101	P4G	O3-C5-C6-O4

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<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	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	101, 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 <sup>2</sup> )	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

All (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
1	R	74	ALA	6.6
1	J	76	GLY	6.6
2	d	31	ALA	6.2
2	p	8	SER	6.1
2	q	10	ALA	6.0
1	P	80	ILE	5.8
1	N	58	ASP	5.6
1	P	58	ASP	5.6
1	I	70	LEU	5.6
2	d	34	ILE	5.4
1	I	47	GLU	5.4
2	h	27	GLU	5.2
2	i	72	PHE	5.2
2	i	7	MET	5.1
2	i	8	SER	5.0
2	a	3	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	57	ALA	5.0
1	R	75	GLU	5.0
2	h	25	ALA	4.9
1	P	44	ALA	4.9
1	P	42	LEU	4.7
1	I	73	LEU	4.6
1	I	72	ARG	4.5
1	R	76	GLY	4.5
2	p	72	PHE	4.3
2	i	10	ALA	4.3
1	P	55	ILE	4.3
2	p	11	VAL	4.3
1	P	87	ALA	4.1
2	i	60	TRP	4.1
2	p	18	VAL	4.0
2	h	43	LEU	4.0
2	i	29	ALA	3.9
2	i	64	LEU	3.9
2	j	19	MET	3.9
2	p	64	LEU	3.8
1	I	63	THR	3.8
2	e	28	TYR	3.8
1	P	70	LEU	3.8
2	j	64	LEU	3.8
2	r	64	LEU	3.8
1	J	2	PRO	3.7
2	e	19	MET	3.7
1	R	46	PRO	3.7
1	N	46	PRO	3.7
2	d	43	LEU	3.6
1	I	48	SER	3.6
2	d	27	GLU	3.6
2	m	48	LEU	3.6
1	I	42	LEU	3.6
2	r	74	ILE	3.5
1	I	64	ILE	3.5
2	b	3	ASN	3.5
1	I	31	PHE	3.5
1	R	58	ASP	3.4
1	N	2	PRO	3.4
1	I	71	TYR	3.4
2	e	15	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	q	11	VAL	3.4
2	h	22	ALA	3.3
2	q	28	TYR	3.3
2	p	4	VAL	3.3
1	J	75	GLU	3.3
2	p	56	LEU	3.3
2	d	40	ARG	3.3
1	R	72	ARG	3.3
1	Q	75	GLU	3.3
2	d	29	ALA	3.1
2	q	13	PRO	3.1
1	P	74	ALA	3.1
2	e	27	GLU	3.1
1	N	75	GLU	3.1
2	d	7	MET	3.0
1	I	55	ILE	3.0
1	Q	3	ILE	3.0
2	i	9	VAL	3.0
1	N	70	LEU	3.0
1	R	77	TRP	3.0
1	Q	2	PRO	3.0
2	q	23	VAL	2.9
1	P	69	ILE	2.9
1	J	70	LEU	2.9
2	r	29	ALA	2.9
1	P	51	ARG	2.9
2	r	89	ILE	2.9
2	e	34	ILE	2.9
1	Q	31	PHE	2.9
1	M	13	LEU	2.9
1	P	86	GLY	2.9
1	Q	42	LEU	2.9
2	d	42	TRP	2.9
1	M	62	LEU	2.9
1	O	45	PHE	2.8
2	j	29	ALA	2.8
1	N	40	LEU	2.8
1	N	42	LEU	2.8
2	q	7	MET	2.8
2	i	74	ILE	2.8
2	j	48	LEU	2.8
2	d	64	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	e	48	LEU	2.8
2	p	60	TRP	2.8
1	Q	62	LEU	2.8
1	I	51	ARG	2.7
1	P	46	PRO	2.7
1	P	48	SER	2.7
2	h	35	VAL	2.7
1	I	79	GLU	2.7
2	i	71	PRO	2.7
1	Q	18	LEU	2.7
1	Q	73	LEU	2.7
1	J	72	ARG	2.7
2	e	24	GLU	2.7
1	I	80	ILE	2.7
2	e	30	THR	2.7
2	d	35	VAL	2.7
2	g	85	LEU	2.7
1	P	31	PHE	2.7
2	i	56	LEU	2.7
1	I	50	PRO	2.7
1	R	31	PHE	2.6
2	r	77	ILE	2.6
1	Q	70	LEU	2.6
1	N	57	ALA	2.6
2	q	29	ALA	2.6
2	e	25	ALA	2.6
1	P	4	ILE	2.6
1	Q	68	LEU	2.6
1	P	18	LEU	2.6
1	R	73	LEU	2.6
2	f	85	LEU	2.6
2	i	42	TRP	2.6
1	Q	64	ILE	2.6
2	q	74	ILE	2.6
2	q	22	ALA	2.6
1	Q	61	ALA	2.6
1	I	76	GLY	2.6
1	N	88	ARG	2.6
2	i	83	SER	2.6
1	R	78	ILE	2.5
2	g	56	LEU	2.5
1	P	73	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	b	43	LEU	2.5
2	q	85	LEU	2.5
2	h	24	GLU	2.5
1	R	44	ALA	2.5
2	f	43	LEU	2.5
1	R	25	PRO	2.5
2	e	89	ILE	2.5
1	P	72	ARG	2.5
1	P	64	ILE	2.5
1	R	70	LEU	2.5
2	k	64	LEU	2.5
2	i	25	ALA	2.4
1	K	74	ALA	2.4
1	J	90	VAL	2.4
1	I	81	VAL	2.4
2	q	71	PRO	2.4
2	p	73	ASP	2.4
2	e	29	ALA	2.4
2	q	64	LEU	2.4
1	J	25	PRO	2.4
1	P	35	ILE	2.4
2	n	61	ILE	2.4
1	R	48	SER	2.4
2	q	46	ARG	2.3
2	a	77	ILE	2.3
1	P	62	LEU	2.3
1	P	83	ILE	2.3
2	q	48	LEU	2.3
2	m	45	LYS	2.3
2	j	34	ILE	2.3
2	i	28	TYR	2.3
1	P	77	TRP	2.3
2	j	85	LEU	2.3
2	r	85	LEU	2.3
1	N	77	TRP	2.3
2	p	7	MET	2.3
2	d	49	ARG	2.3
1	P	43	ALA	2.3
2	n	48	LEU	2.3
1	J	73	LEU	2.2
2	p	74	ILE	2.2
1	P	3	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	71	TYR	2.2
2	j	49	ARG	2.2
2	h	23	VAL	2.2
1	O	75	GLU	2.2
1	P	57	ALA	2.2
1	Q	27	ALA	2.2
1	Q	55	ILE	2.2
2	o	77	ILE	2.2
2	r	71	PRO	2.2
2	o	43	LEU	2.2
1	I	38	ARG	2.2
1	M	69	ILE	2.2
1	D	81	VAL	2.2
1	P	84	VAL	2.2
2	p	49	ARG	2.2
1	R	61	ALA	2.2
1	N	26	ARG	2.2
1	J	77	TRP	2.1
2	j	35	VAL	2.1
2	k	85	LEU	2.1
1	J	78	ILE	2.1
2	h	89	ILE	2.1
1	M	45	PHE	2.1
2	b	48	LEU	2.1
1	Q	4	ILE	2.1
1	K	25	PRO	2.1
2	d	18	VAL	2.1
1	R	42	LEU	2.1
2	k	72	PHE	2.1
1	P	26	ARG	2.1
2	j	27	GLU	2.1
1	J	42	LEU	2.1
1	Q	65	GLY	2.1
2	r	39	VAL	2.1
2	e	18	VAL	2.1
1	I	45	PHE	2.1
1	P	71	TYR	2.0
2	p	48	LEU	2.0
1	Q	76	GLY	2.0
2	a	4	VAL	2.0
1	I	5	ARG	2.0
1	K	62	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	o	20	ARG	2.0
1	N	43	ALA	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](#)

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<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	B-factors(Å <sup>2</sup> )	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	C	101	11/11	0.90	0.25	74,97,138,138	0
3	P4G	B	101	11/11	0.90	0.25	64,89,137,137	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.