



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 05:49 AM EDT

PDB ID : 6HSV  
Title : Engineered higher-order assembly of Cholera Toxin B subunits via the addition of C-terminal parallel coiled-coiled domains  
Authors : Pearson, A.R.; Turnbull, W.B.; Ross, J.F.; Trinh, C.H.; Webb, M.E.  
Deposited on : 2018-10-01  
Resolution : 2.45 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
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)	:	2.37.1

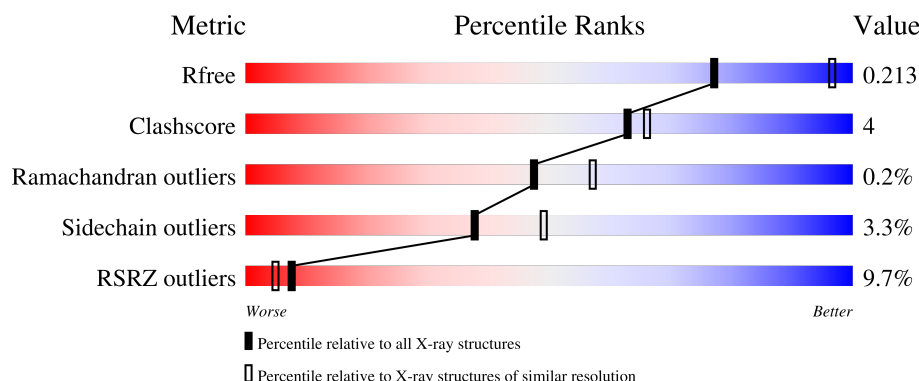
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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	124	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>6%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	124	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>6%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	124	<div> <div>0%</div> <div> <div></div> <div>63%</div> <div>15%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	124	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>7%</div> <div>••</div> <div>17%</div> </div> </div>
1	E	124	<div> <div>18%</div> <div> <div></div> <div>94%</div> <div>•••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	124	
1	G	124	
1	H	124	
1	I	124	
1	J	124	
1	K	124	
1	L	124	
1	M	124	
1	N	124	
1	O	124	
1	P	124	
1	Q	124	
1	R	124	
1	S	124	
1	T	124	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	P	203	-	-	-	X
3	MPD	S	201	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Toxin B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			820	518	141	156	5			
1	B	103	Total	C	N	O	S	0	0	0
			816	516	140	155	5			
1	C	97	Total	C	N	O	S	0	0	0
			771	490	131	145	5			
1	D	103	Total	C	N	O	S	0	0	0
			816	516	140	155	5			
1	E	123	Total	C	N	O	S	0	0	0
			915	575	160	175	5			
1	F	123	Total	C	N	O	S	0	0	0
			917	577	160	175	5			
1	G	123	Total	C	N	O	S	0	0	0
			915	575	160	175	5			
1	H	104	Total	C	N	O	S	0	0	0
			820	518	141	156	5			
1	I	103	Total	C	N	O	S	0	0	0
			816	516	140	155	5			
1	J	123	Total	C	N	O	S	0	1	0
			921	578	161	176	6			
1	K	103	Total	C	N	O	S	0	0	0
			816	516	140	155	5			
1	L	123	Total	C	N	O	S	0	0	0
			915	575	160	175	5			
1	M	123	Total	C	N	O	S	0	1	0
			927	583	161	176	7			
1	N	123	Total	C	N	O	S	0	0	0
			915	575	160	175	5			
1	O	123	Total	C	N	O	S	0	0	0
			915	575	160	175	5			
1	P	123	Total	C	N	O	S	0	1	0
			923	580	163	175	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	103	Total	C	N	O	S	0	0	0
			816	516	140	155	5			
1	R	104	Total	C	N	O	S	0	0	0
			820	518	141	156	5			
1	S	103	Total	C	N	O	S	0	1	0
			828	522	142	157	7			
1	T	103	Total	C	N	O	S	0	0	0
			816	516	140	155	5			

There are 400 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	VAL	-	expression tag	UNP Q7X2D2
A	106	SER	-	expression tag	UNP Q7X2D2
A	107	ALA	-	expression tag	UNP Q7X2D2
A	108	LEU	-	expression tag	UNP Q7X2D2
A	109	GLU	-	expression tag	UNP Q7X2D2
A	110	LYS	-	expression tag	UNP Q7X2D2
A	111	GLU	-	expression tag	UNP Q7X2D2
A	112	VAL	-	expression tag	UNP Q7X2D2
A	113	SER	-	expression tag	UNP Q7X2D2
A	114	ALA	-	expression tag	UNP Q7X2D2
A	115	LEU	-	expression tag	UNP Q7X2D2
A	116	LYS	-	expression tag	UNP Q7X2D2
A	117	GLU	-	expression tag	UNP Q7X2D2
A	118	LYS	-	expression tag	UNP Q7X2D2
A	119	VAL	-	expression tag	UNP Q7X2D2
A	120	SER	-	expression tag	UNP Q7X2D2
A	121	ALA	-	expression tag	UNP Q7X2D2
A	122	LEU	-	expression tag	UNP Q7X2D2
A	123	GLU	-	expression tag	UNP Q7X2D2
A	124	PHE	-	expression tag	UNP Q7X2D2
B	105	VAL	-	expression tag	UNP Q7X2D2
B	106	SER	-	expression tag	UNP Q7X2D2
B	107	ALA	-	expression tag	UNP Q7X2D2
B	108	LEU	-	expression tag	UNP Q7X2D2
B	109	GLU	-	expression tag	UNP Q7X2D2
B	110	LYS	-	expression tag	UNP Q7X2D2
B	111	GLU	-	expression tag	UNP Q7X2D2
B	112	VAL	-	expression tag	UNP Q7X2D2
B	113	SER	-	expression tag	UNP Q7X2D2
B	114	ALA	-	expression tag	UNP Q7X2D2
B	115	LEU	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	116	LYS	-	expression tag	UNP Q7X2D2
B	117	GLU	-	expression tag	UNP Q7X2D2
B	118	LYS	-	expression tag	UNP Q7X2D2
B	119	VAL	-	expression tag	UNP Q7X2D2
B	120	SER	-	expression tag	UNP Q7X2D2
B	121	ALA	-	expression tag	UNP Q7X2D2
B	122	LEU	-	expression tag	UNP Q7X2D2
B	123	GLU	-	expression tag	UNP Q7X2D2
B	124	PHE	-	expression tag	UNP Q7X2D2
C	105	VAL	-	expression tag	UNP Q7X2D2
C	106	SER	-	expression tag	UNP Q7X2D2
C	107	ALA	-	expression tag	UNP Q7X2D2
C	108	LEU	-	expression tag	UNP Q7X2D2
C	109	GLU	-	expression tag	UNP Q7X2D2
C	110	LYS	-	expression tag	UNP Q7X2D2
C	111	GLU	-	expression tag	UNP Q7X2D2
C	112	VAL	-	expression tag	UNP Q7X2D2
C	113	SER	-	expression tag	UNP Q7X2D2
C	114	ALA	-	expression tag	UNP Q7X2D2
C	115	LEU	-	expression tag	UNP Q7X2D2
C	116	LYS	-	expression tag	UNP Q7X2D2
C	117	GLU	-	expression tag	UNP Q7X2D2
C	118	LYS	-	expression tag	UNP Q7X2D2
C	119	VAL	-	expression tag	UNP Q7X2D2
C	120	SER	-	expression tag	UNP Q7X2D2
C	121	ALA	-	expression tag	UNP Q7X2D2
C	122	LEU	-	expression tag	UNP Q7X2D2
C	123	GLU	-	expression tag	UNP Q7X2D2
C	124	PHE	-	expression tag	UNP Q7X2D2
D	105	VAL	-	expression tag	UNP Q7X2D2
D	106	SER	-	expression tag	UNP Q7X2D2
D	107	ALA	-	expression tag	UNP Q7X2D2
D	108	LEU	-	expression tag	UNP Q7X2D2
D	109	GLU	-	expression tag	UNP Q7X2D2
D	110	LYS	-	expression tag	UNP Q7X2D2
D	111	GLU	-	expression tag	UNP Q7X2D2
D	112	VAL	-	expression tag	UNP Q7X2D2
D	113	SER	-	expression tag	UNP Q7X2D2
D	114	ALA	-	expression tag	UNP Q7X2D2
D	115	LEU	-	expression tag	UNP Q7X2D2
D	116	LYS	-	expression tag	UNP Q7X2D2
D	117	GLU	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	118	LYS	-	expression tag	UNP Q7X2D2
D	119	VAL	-	expression tag	UNP Q7X2D2
D	120	SER	-	expression tag	UNP Q7X2D2
D	121	ALA	-	expression tag	UNP Q7X2D2
D	122	LEU	-	expression tag	UNP Q7X2D2
D	123	GLU	-	expression tag	UNP Q7X2D2
D	124	PHE	-	expression tag	UNP Q7X2D2
E	105	VAL	-	expression tag	UNP Q7X2D2
E	106	SER	-	expression tag	UNP Q7X2D2
E	107	ALA	-	expression tag	UNP Q7X2D2
E	108	LEU	-	expression tag	UNP Q7X2D2
E	109	GLU	-	expression tag	UNP Q7X2D2
E	110	LYS	-	expression tag	UNP Q7X2D2
E	111	GLU	-	expression tag	UNP Q7X2D2
E	112	VAL	-	expression tag	UNP Q7X2D2
E	113	SER	-	expression tag	UNP Q7X2D2
E	114	ALA	-	expression tag	UNP Q7X2D2
E	115	LEU	-	expression tag	UNP Q7X2D2
E	116	LYS	-	expression tag	UNP Q7X2D2
E	117	GLU	-	expression tag	UNP Q7X2D2
E	118	LYS	-	expression tag	UNP Q7X2D2
E	119	VAL	-	expression tag	UNP Q7X2D2
E	120	SER	-	expression tag	UNP Q7X2D2
E	121	ALA	-	expression tag	UNP Q7X2D2
E	122	LEU	-	expression tag	UNP Q7X2D2
E	123	GLU	-	expression tag	UNP Q7X2D2
E	124	PHE	-	expression tag	UNP Q7X2D2
F	105	VAL	-	expression tag	UNP Q7X2D2
F	106	SER	-	expression tag	UNP Q7X2D2
F	107	ALA	-	expression tag	UNP Q7X2D2
F	108	LEU	-	expression tag	UNP Q7X2D2
F	109	GLU	-	expression tag	UNP Q7X2D2
F	110	LYS	-	expression tag	UNP Q7X2D2
F	111	GLU	-	expression tag	UNP Q7X2D2
F	112	VAL	-	expression tag	UNP Q7X2D2
F	113	SER	-	expression tag	UNP Q7X2D2
F	114	ALA	-	expression tag	UNP Q7X2D2
F	115	LEU	-	expression tag	UNP Q7X2D2
F	116	LYS	-	expression tag	UNP Q7X2D2
F	117	GLU	-	expression tag	UNP Q7X2D2
F	118	LYS	-	expression tag	UNP Q7X2D2
F	119	VAL	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	120	SER	-	expression tag	UNP Q7X2D2
F	121	ALA	-	expression tag	UNP Q7X2D2
F	122	LEU	-	expression tag	UNP Q7X2D2
F	123	GLU	-	expression tag	UNP Q7X2D2
F	124	PHE	-	expression tag	UNP Q7X2D2
G	105	VAL	-	expression tag	UNP Q7X2D2
G	106	SER	-	expression tag	UNP Q7X2D2
G	107	ALA	-	expression tag	UNP Q7X2D2
G	108	LEU	-	expression tag	UNP Q7X2D2
G	109	GLU	-	expression tag	UNP Q7X2D2
G	110	LYS	-	expression tag	UNP Q7X2D2
G	111	GLU	-	expression tag	UNP Q7X2D2
G	112	VAL	-	expression tag	UNP Q7X2D2
G	113	SER	-	expression tag	UNP Q7X2D2
G	114	ALA	-	expression tag	UNP Q7X2D2
G	115	LEU	-	expression tag	UNP Q7X2D2
G	116	LYS	-	expression tag	UNP Q7X2D2
G	117	GLU	-	expression tag	UNP Q7X2D2
G	118	LYS	-	expression tag	UNP Q7X2D2
G	119	VAL	-	expression tag	UNP Q7X2D2
G	120	SER	-	expression tag	UNP Q7X2D2
G	121	ALA	-	expression tag	UNP Q7X2D2
G	122	LEU	-	expression tag	UNP Q7X2D2
G	123	GLU	-	expression tag	UNP Q7X2D2
G	124	PHE	-	expression tag	UNP Q7X2D2
H	105	VAL	-	expression tag	UNP Q7X2D2
H	106	SER	-	expression tag	UNP Q7X2D2
H	107	ALA	-	expression tag	UNP Q7X2D2
H	108	LEU	-	expression tag	UNP Q7X2D2
H	109	GLU	-	expression tag	UNP Q7X2D2
H	110	LYS	-	expression tag	UNP Q7X2D2
H	111	GLU	-	expression tag	UNP Q7X2D2
H	112	VAL	-	expression tag	UNP Q7X2D2
H	113	SER	-	expression tag	UNP Q7X2D2
H	114	ALA	-	expression tag	UNP Q7X2D2
H	115	LEU	-	expression tag	UNP Q7X2D2
H	116	LYS	-	expression tag	UNP Q7X2D2
H	117	GLU	-	expression tag	UNP Q7X2D2
H	118	LYS	-	expression tag	UNP Q7X2D2
H	119	VAL	-	expression tag	UNP Q7X2D2
H	120	SER	-	expression tag	UNP Q7X2D2
H	121	ALA	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	122	LEU	-	expression tag	UNP Q7X2D2
H	123	GLU	-	expression tag	UNP Q7X2D2
H	124	PHE	-	expression tag	UNP Q7X2D2
I	105	VAL	-	expression tag	UNP Q7X2D2
I	106	SER	-	expression tag	UNP Q7X2D2
I	107	ALA	-	expression tag	UNP Q7X2D2
I	108	LEU	-	expression tag	UNP Q7X2D2
I	109	GLU	-	expression tag	UNP Q7X2D2
I	110	LYS	-	expression tag	UNP Q7X2D2
I	111	GLU	-	expression tag	UNP Q7X2D2
I	112	VAL	-	expression tag	UNP Q7X2D2
I	113	SER	-	expression tag	UNP Q7X2D2
I	114	ALA	-	expression tag	UNP Q7X2D2
I	115	LEU	-	expression tag	UNP Q7X2D2
I	116	LYS	-	expression tag	UNP Q7X2D2
I	117	GLU	-	expression tag	UNP Q7X2D2
I	118	LYS	-	expression tag	UNP Q7X2D2
I	119	VAL	-	expression tag	UNP Q7X2D2
I	120	SER	-	expression tag	UNP Q7X2D2
I	121	ALA	-	expression tag	UNP Q7X2D2
I	122	LEU	-	expression tag	UNP Q7X2D2
I	123	GLU	-	expression tag	UNP Q7X2D2
I	124	PHE	-	expression tag	UNP Q7X2D2
J	105	VAL	-	expression tag	UNP Q7X2D2
J	106	SER	-	expression tag	UNP Q7X2D2
J	107	ALA	-	expression tag	UNP Q7X2D2
J	108	LEU	-	expression tag	UNP Q7X2D2
J	109	GLU	-	expression tag	UNP Q7X2D2
J	110	LYS	-	expression tag	UNP Q7X2D2
J	111	GLU	-	expression tag	UNP Q7X2D2
J	112	VAL	-	expression tag	UNP Q7X2D2
J	113	SER	-	expression tag	UNP Q7X2D2
J	114	ALA	-	expression tag	UNP Q7X2D2
J	115	LEU	-	expression tag	UNP Q7X2D2
J	116	LYS	-	expression tag	UNP Q7X2D2
J	117	GLU	-	expression tag	UNP Q7X2D2
J	118	LYS	-	expression tag	UNP Q7X2D2
J	119	VAL	-	expression tag	UNP Q7X2D2
J	120	SER	-	expression tag	UNP Q7X2D2
J	121	ALA	-	expression tag	UNP Q7X2D2
J	122	LEU	-	expression tag	UNP Q7X2D2
J	123	GLU	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	124	PHE	-	expression tag	UNP Q7X2D2
K	105	VAL	-	expression tag	UNP Q7X2D2
K	106	SER	-	expression tag	UNP Q7X2D2
K	107	ALA	-	expression tag	UNP Q7X2D2
K	108	LEU	-	expression tag	UNP Q7X2D2
K	109	GLU	-	expression tag	UNP Q7X2D2
K	110	LYS	-	expression tag	UNP Q7X2D2
K	111	GLU	-	expression tag	UNP Q7X2D2
K	112	VAL	-	expression tag	UNP Q7X2D2
K	113	SER	-	expression tag	UNP Q7X2D2
K	114	ALA	-	expression tag	UNP Q7X2D2
K	115	LEU	-	expression tag	UNP Q7X2D2
K	116	LYS	-	expression tag	UNP Q7X2D2
K	117	GLU	-	expression tag	UNP Q7X2D2
K	118	LYS	-	expression tag	UNP Q7X2D2
K	119	VAL	-	expression tag	UNP Q7X2D2
K	120	SER	-	expression tag	UNP Q7X2D2
K	121	ALA	-	expression tag	UNP Q7X2D2
K	122	LEU	-	expression tag	UNP Q7X2D2
K	123	GLU	-	expression tag	UNP Q7X2D2
K	124	PHE	-	expression tag	UNP Q7X2D2
L	105	VAL	-	expression tag	UNP Q7X2D2
L	106	SER	-	expression tag	UNP Q7X2D2
L	107	ALA	-	expression tag	UNP Q7X2D2
L	108	LEU	-	expression tag	UNP Q7X2D2
L	109	GLU	-	expression tag	UNP Q7X2D2
L	110	LYS	-	expression tag	UNP Q7X2D2
L	111	GLU	-	expression tag	UNP Q7X2D2
L	112	VAL	-	expression tag	UNP Q7X2D2
L	113	SER	-	expression tag	UNP Q7X2D2
L	114	ALA	-	expression tag	UNP Q7X2D2
L	115	LEU	-	expression tag	UNP Q7X2D2
L	116	LYS	-	expression tag	UNP Q7X2D2
L	117	GLU	-	expression tag	UNP Q7X2D2
L	118	LYS	-	expression tag	UNP Q7X2D2
L	119	VAL	-	expression tag	UNP Q7X2D2
L	120	SER	-	expression tag	UNP Q7X2D2
L	121	ALA	-	expression tag	UNP Q7X2D2
L	122	LEU	-	expression tag	UNP Q7X2D2
L	123	GLU	-	expression tag	UNP Q7X2D2
L	124	PHE	-	expression tag	UNP Q7X2D2
M	105	VAL	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	106	SER	-	expression tag	UNP Q7X2D2
M	107	ALA	-	expression tag	UNP Q7X2D2
M	108	LEU	-	expression tag	UNP Q7X2D2
M	109	GLU	-	expression tag	UNP Q7X2D2
M	110	LYS	-	expression tag	UNP Q7X2D2
M	111	GLU	-	expression tag	UNP Q7X2D2
M	112	VAL	-	expression tag	UNP Q7X2D2
M	113	SER	-	expression tag	UNP Q7X2D2
M	114	ALA	-	expression tag	UNP Q7X2D2
M	115	LEU	-	expression tag	UNP Q7X2D2
M	116	LYS	-	expression tag	UNP Q7X2D2
M	117	GLU	-	expression tag	UNP Q7X2D2
M	118	LYS	-	expression tag	UNP Q7X2D2
M	119	VAL	-	expression tag	UNP Q7X2D2
M	120	SER	-	expression tag	UNP Q7X2D2
M	121	ALA	-	expression tag	UNP Q7X2D2
M	122	LEU	-	expression tag	UNP Q7X2D2
M	123	GLU	-	expression tag	UNP Q7X2D2
M	124	PHE	-	expression tag	UNP Q7X2D2
N	105	VAL	-	expression tag	UNP Q7X2D2
N	106	SER	-	expression tag	UNP Q7X2D2
N	107	ALA	-	expression tag	UNP Q7X2D2
N	108	LEU	-	expression tag	UNP Q7X2D2
N	109	GLU	-	expression tag	UNP Q7X2D2
N	110	LYS	-	expression tag	UNP Q7X2D2
N	111	GLU	-	expression tag	UNP Q7X2D2
N	112	VAL	-	expression tag	UNP Q7X2D2
N	113	SER	-	expression tag	UNP Q7X2D2
N	114	ALA	-	expression tag	UNP Q7X2D2
N	115	LEU	-	expression tag	UNP Q7X2D2
N	116	LYS	-	expression tag	UNP Q7X2D2
N	117	GLU	-	expression tag	UNP Q7X2D2
N	118	LYS	-	expression tag	UNP Q7X2D2
N	119	VAL	-	expression tag	UNP Q7X2D2
N	120	SER	-	expression tag	UNP Q7X2D2
N	121	ALA	-	expression tag	UNP Q7X2D2
N	122	LEU	-	expression tag	UNP Q7X2D2
N	123	GLU	-	expression tag	UNP Q7X2D2
N	124	PHE	-	expression tag	UNP Q7X2D2
O	105	VAL	-	expression tag	UNP Q7X2D2
O	106	SER	-	expression tag	UNP Q7X2D2
O	107	ALA	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
O	108	LEU	-	expression tag	UNP Q7X2D2
O	109	GLU	-	expression tag	UNP Q7X2D2
O	110	LYS	-	expression tag	UNP Q7X2D2
O	111	GLU	-	expression tag	UNP Q7X2D2
O	112	VAL	-	expression tag	UNP Q7X2D2
O	113	SER	-	expression tag	UNP Q7X2D2
O	114	ALA	-	expression tag	UNP Q7X2D2
O	115	LEU	-	expression tag	UNP Q7X2D2
O	116	LYS	-	expression tag	UNP Q7X2D2
O	117	GLU	-	expression tag	UNP Q7X2D2
O	118	LYS	-	expression tag	UNP Q7X2D2
O	119	VAL	-	expression tag	UNP Q7X2D2
O	120	SER	-	expression tag	UNP Q7X2D2
O	121	ALA	-	expression tag	UNP Q7X2D2
O	122	LEU	-	expression tag	UNP Q7X2D2
O	123	GLU	-	expression tag	UNP Q7X2D2
O	124	PHE	-	expression tag	UNP Q7X2D2
P	105	VAL	-	expression tag	UNP Q7X2D2
P	106	SER	-	expression tag	UNP Q7X2D2
P	107	ALA	-	expression tag	UNP Q7X2D2
P	108	LEU	-	expression tag	UNP Q7X2D2
P	109	GLU	-	expression tag	UNP Q7X2D2
P	110	LYS	-	expression tag	UNP Q7X2D2
P	111	GLU	-	expression tag	UNP Q7X2D2
P	112	VAL	-	expression tag	UNP Q7X2D2
P	113	SER	-	expression tag	UNP Q7X2D2
P	114	ALA	-	expression tag	UNP Q7X2D2
P	115	LEU	-	expression tag	UNP Q7X2D2
P	116	LYS	-	expression tag	UNP Q7X2D2
P	117	GLU	-	expression tag	UNP Q7X2D2
P	118	LYS	-	expression tag	UNP Q7X2D2
P	119	VAL	-	expression tag	UNP Q7X2D2
P	120	SER	-	expression tag	UNP Q7X2D2
P	121	ALA	-	expression tag	UNP Q7X2D2
P	122	LEU	-	expression tag	UNP Q7X2D2
P	123	GLU	-	expression tag	UNP Q7X2D2
P	124	PHE	-	expression tag	UNP Q7X2D2
Q	105	VAL	-	expression tag	UNP Q7X2D2
Q	106	SER	-	expression tag	UNP Q7X2D2
Q	107	ALA	-	expression tag	UNP Q7X2D2
Q	108	LEU	-	expression tag	UNP Q7X2D2
Q	109	GLU	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	110	LYS	-	expression tag	UNP Q7X2D2
Q	111	GLU	-	expression tag	UNP Q7X2D2
Q	112	VAL	-	expression tag	UNP Q7X2D2
Q	113	SER	-	expression tag	UNP Q7X2D2
Q	114	ALA	-	expression tag	UNP Q7X2D2
Q	115	LEU	-	expression tag	UNP Q7X2D2
Q	116	LYS	-	expression tag	UNP Q7X2D2
Q	117	GLU	-	expression tag	UNP Q7X2D2
Q	118	LYS	-	expression tag	UNP Q7X2D2
Q	119	VAL	-	expression tag	UNP Q7X2D2
Q	120	SER	-	expression tag	UNP Q7X2D2
Q	121	ALA	-	expression tag	UNP Q7X2D2
Q	122	LEU	-	expression tag	UNP Q7X2D2
Q	123	GLU	-	expression tag	UNP Q7X2D2
Q	124	PHE	-	expression tag	UNP Q7X2D2
R	105	VAL	-	expression tag	UNP Q7X2D2
R	106	SER	-	expression tag	UNP Q7X2D2
R	107	ALA	-	expression tag	UNP Q7X2D2
R	108	LEU	-	expression tag	UNP Q7X2D2
R	109	GLU	-	expression tag	UNP Q7X2D2
R	110	LYS	-	expression tag	UNP Q7X2D2
R	111	GLU	-	expression tag	UNP Q7X2D2
R	112	VAL	-	expression tag	UNP Q7X2D2
R	113	SER	-	expression tag	UNP Q7X2D2
R	114	ALA	-	expression tag	UNP Q7X2D2
R	115	LEU	-	expression tag	UNP Q7X2D2
R	116	LYS	-	expression tag	UNP Q7X2D2
R	117	GLU	-	expression tag	UNP Q7X2D2
R	118	LYS	-	expression tag	UNP Q7X2D2
R	119	VAL	-	expression tag	UNP Q7X2D2
R	120	SER	-	expression tag	UNP Q7X2D2
R	121	ALA	-	expression tag	UNP Q7X2D2
R	122	LEU	-	expression tag	UNP Q7X2D2
R	123	GLU	-	expression tag	UNP Q7X2D2
R	124	PHE	-	expression tag	UNP Q7X2D2
S	105	VAL	-	expression tag	UNP Q7X2D2
S	106	SER	-	expression tag	UNP Q7X2D2
S	107	ALA	-	expression tag	UNP Q7X2D2
S	108	LEU	-	expression tag	UNP Q7X2D2
S	109	GLU	-	expression tag	UNP Q7X2D2
S	110	LYS	-	expression tag	UNP Q7X2D2
S	111	GLU	-	expression tag	UNP Q7X2D2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	112	VAL	-	expression tag	UNP Q7X2D2
S	113	SER	-	expression tag	UNP Q7X2D2
S	114	ALA	-	expression tag	UNP Q7X2D2
S	115	LEU	-	expression tag	UNP Q7X2D2
S	116	LYS	-	expression tag	UNP Q7X2D2
S	117	GLU	-	expression tag	UNP Q7X2D2
S	118	LYS	-	expression tag	UNP Q7X2D2
S	119	VAL	-	expression tag	UNP Q7X2D2
S	120	SER	-	expression tag	UNP Q7X2D2
S	121	ALA	-	expression tag	UNP Q7X2D2
S	122	LEU	-	expression tag	UNP Q7X2D2
S	123	GLU	-	expression tag	UNP Q7X2D2
S	124	PHE	-	expression tag	UNP Q7X2D2
T	105	VAL	-	expression tag	UNP Q7X2D2
T	106	SER	-	expression tag	UNP Q7X2D2
T	107	ALA	-	expression tag	UNP Q7X2D2
T	108	LEU	-	expression tag	UNP Q7X2D2
T	109	GLU	-	expression tag	UNP Q7X2D2
T	110	LYS	-	expression tag	UNP Q7X2D2
T	111	GLU	-	expression tag	UNP Q7X2D2
T	112	VAL	-	expression tag	UNP Q7X2D2
T	113	SER	-	expression tag	UNP Q7X2D2
T	114	ALA	-	expression tag	UNP Q7X2D2
T	115	LEU	-	expression tag	UNP Q7X2D2
T	116	LYS	-	expression tag	UNP Q7X2D2
T	117	GLU	-	expression tag	UNP Q7X2D2
T	118	LYS	-	expression tag	UNP Q7X2D2
T	119	VAL	-	expression tag	UNP Q7X2D2
T	120	SER	-	expression tag	UNP Q7X2D2
T	121	ALA	-	expression tag	UNP Q7X2D2
T	122	LEU	-	expression tag	UNP Q7X2D2
T	123	GLU	-	expression tag	UNP Q7X2D2
T	124	PHE	-	expression tag	UNP Q7X2D2

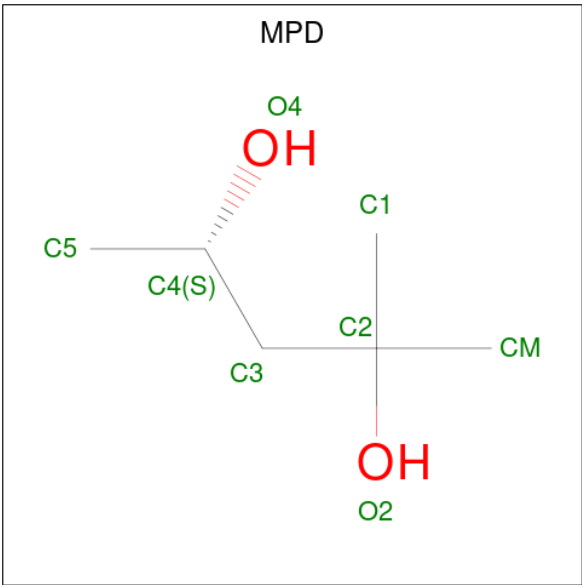
- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	J	1	Total	C	O	0	0
			8	6	2		
3	J	1	Total	C	O	0	0
			8	6	2		
3	L	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total C O 8 6 2	0	0
3	N	1	Total C O 8 6 2	0	0
3	O	1	Total C O 8 6 2	0	0
3	O	1	Total C O 8 6 2	0	0
3	P	1	Total C O 8 6 2	0	0
3	P	1	Total C O 8 6 2	0	0
3	Q	1	Total C O 8 6 2	0	0
3	R	1	Total C O 8 6 2	0	0
3	R	1	Total C O 8 6 2	0	0
3	R	1	Total C O 8 6 2	0	0
3	S	1	Total C O 8 6 2	0	0
3	S	1	Total C O 8 6 2	0	0
3	T	1	Total C O 8 6 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	T	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0
5	B	14	Total O 14 14	0	0
5	C	14	Total O 14 14	0	0

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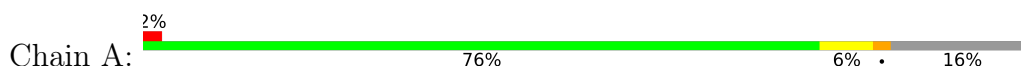
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	22	Total 22	O 22	0	0
5	E	22	Total 22	O 22	0	0
5	F	31	Total 31	O 31	0	0
5	G	24	Total 24	O 24	0	0
5	H	28	Total 28	O 28	0	0
5	I	35	Total 35	O 35	0	0
5	J	42	Total 42	O 42	0	0
5	K	24	Total 24	O 24	0	0
5	L	23	Total 23	O 23	0	0
5	M	28	Total 28	O 28	0	0
5	N	22	Total 22	O 22	0	0
5	O	22	Total 22	O 22	0	0
5	P	41	Total 41	O 41	0	0
5	Q	34	Total 34	O 34	0	0
5	R	34	Total 34	O 34	0	0
5	S	50	Total 50	O 50	0	0
5	T	57	Total 57	O 57	0	0

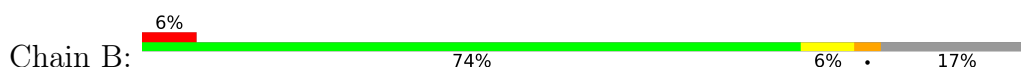
### 3 Residue-property plots [i](#)

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

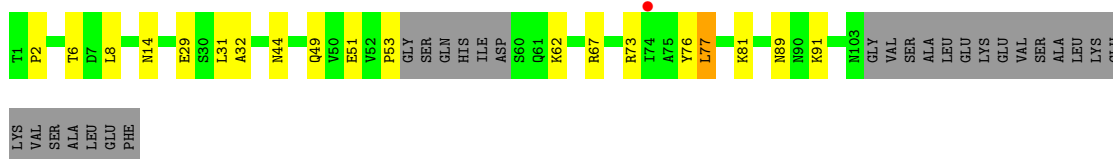
- Molecule 1: Toxin B subunit



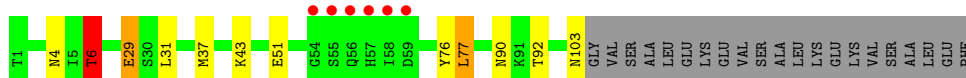
- Molecule 1: Toxin B subunit



- Molecule 1: Toxin B subunit



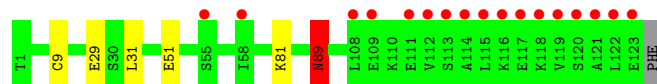
- Molecule 1: Toxin B subunit



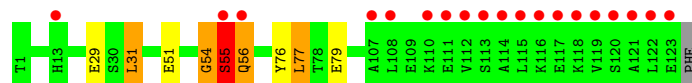
- Molecule 1: Toxin B subunit



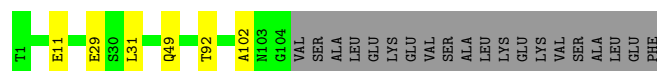
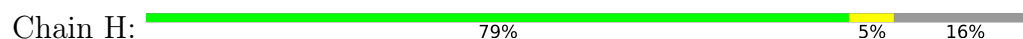
- Molecule 1: Toxin B subunit



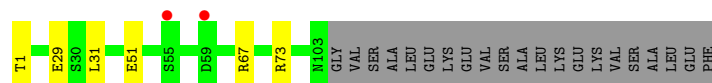
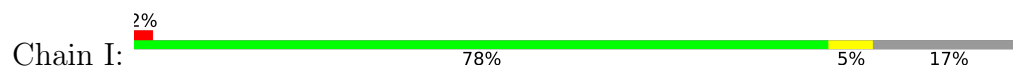
- Molecule 1: Toxin B subunit



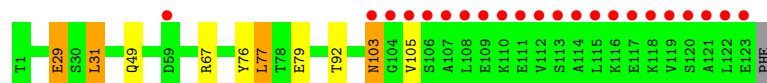
- Molecule 1: Toxin B subunit



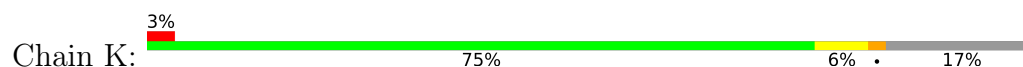
- Molecule 1: Toxin B subunit



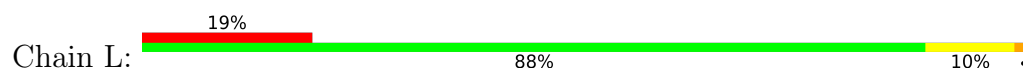
- Molecule 1: Toxin B subunit




- Molecule 1: Toxin B subunit

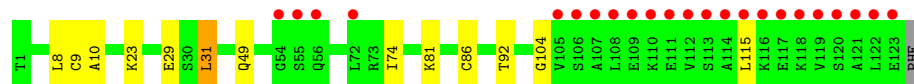


- Molecule 1: Toxin B subunit




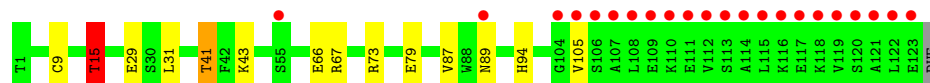
- Molecule 1: Toxin B subunit

Chain M: 




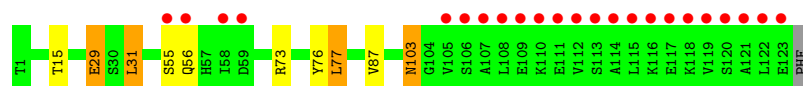
- Molecule 1: Toxin B subunit

Chain N: 



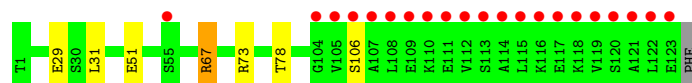
- Molecule 1: Toxin B subunit

Chain O: 




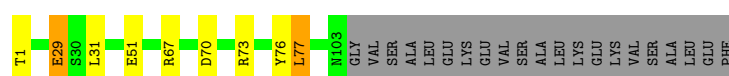
- Molecule 1: Toxin B subunit

Chain P: 




- Molecule 1: Toxin B subunit

Chain Q: 



- Molecule 1: Toxin B subunit

Chain R: 

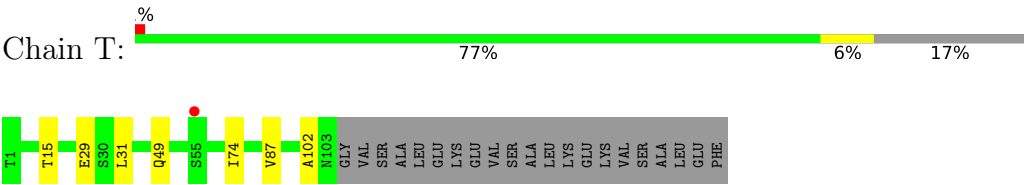


- Molecule 1: Toxin B subunit

Chain S: 



● Molecule 1: Toxin B subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.16Å 179.16Å 192.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.28 – 2.45 37.28 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.28-2.45) 100.0 (37.28-2.45)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.195 , 0.214 0.197 , 0.213	Depositor DCC
$R_{free}$ test set	6304 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.879	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: MPD, CL, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.83	2/834 (0.2%)	0.90	1/1127 (0.1%)
1	B	0.76	0/830	0.94	2/1122 (0.2%)
1	C	0.77	1/783 (0.1%)	1.00	4/1057 (0.4%)
1	D	0.78	1/830 (0.1%)	0.98	4/1122 (0.4%)
1	E	0.79	0/929	0.93	1/1260 (0.1%)
1	F	0.86	1/931 (0.1%)	0.94	1/1263 (0.1%)
1	G	0.90	3/929 (0.3%)	1.00	4/1260 (0.3%)
1	H	0.81	1/834 (0.1%)	0.92	2/1127 (0.2%)
1	I	0.80	1/830 (0.1%)	0.90	1/1122 (0.1%)
1	J	0.84	1/935 (0.1%)	0.90	0/1268
1	K	0.78	1/830 (0.1%)	0.90	2/1122 (0.2%)
1	L	0.83	1/929 (0.1%)	0.94	2/1260 (0.2%)
1	M	0.78	0/944	0.90	1/1280 (0.1%)
1	N	0.94	3/929 (0.3%)	1.02	4/1260 (0.3%)
1	O	0.80	0/929	0.94	1/1260 (0.1%)
1	P	0.82	0/940	0.93	1/1274 (0.1%)
1	Q	0.83	1/830 (0.1%)	0.91	1/1122 (0.1%)
1	R	0.78	0/834	0.93	1/1127 (0.1%)
1	S	0.91	0/842	0.97	0/1138
1	T	0.84	0/830	0.94	0/1122
All	All	0.82	17/17502 (0.1%)	0.94	33/23693 (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	A	0	1
1	C	0	1
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	J	0	1
1	M	0	1
1	N	0	1
1	S	0	1
1	T	0	2
All	All	0	10

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GLU	CD-OE1	-9.91	1.14	1.25
1	J	79	GLU	CD-OE2	-8.38	1.16	1.25
1	G	55	SER	C-O	7.58	1.37	1.23
1	Q	51	GLU	CD-OE1	7.56	1.33	1.25
1	N	66	GLU	CD-OE1	7.37	1.33	1.25

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	ASN	CB-CA-C	-8.58	93.25	110.40
1	N	41	THR	CA-CB-OG1	-8.41	91.34	109.00
1	B	90	ASN	CB-CA-C	-7.90	94.59	110.40
1	I	73	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	L	73	ARG	NE-CZ-NH2	-7.87	116.37	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ALA	Peptide
1	C	49	GLN	Peptide
1	G	54	GLY	Peptide
1	H	49	GLN	Peptide
1	J	49	GLN	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	820	0	826	5	0
1	B	816	0	823	10	0
1	C	771	0	784	12	0
1	D	816	0	823	11	0
1	E	915	0	873	6	0
1	F	917	0	880	4	0
1	G	915	0	873	7	0
1	H	820	0	826	2	0
1	I	816	0	823	3	0
1	J	921	0	876	8	0
1	K	816	0	823	5	0
1	L	915	0	873	12	0
1	M	927	0	888	8	0
1	N	915	0	871	8	0
1	O	915	0	873	6	0
1	P	923	0	886	5	0
1	Q	816	0	823	6	0
1	R	820	0	826	13	0
1	S	828	0	831	9	0
1	T	816	0	823	3	0
2	A	5	0	0	1	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
2	I	5	0	0	0	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
3	A	16	0	28	2	0
3	B	16	0	28	2	0
3	D	16	0	28	1	0
3	G	16	0	28	2	0
3	H	24	0	42	2	0
3	J	16	0	28	4	0
3	L	8	0	14	1	0
3	M	8	0	14	2	0
3	N	8	0	14	3	0
3	O	16	0	28	0	0
3	P	16	0	28	3	0
3	Q	8	0	14	1	0
3	R	24	0	42	5	0
3	S	16	0	28	9	0
3	T	8	0	14	1	0
4	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	17	0	0	0	0
5	B	14	0	0	0	0
5	C	14	0	0	1	0
5	D	22	0	0	3	0
5	E	22	0	0	1	0
5	F	31	0	0	0	0
5	G	24	0	0	0	0
5	H	28	0	0	0	0
5	I	35	0	0	0	0
5	J	42	0	0	2	0
5	K	24	0	0	0	0
5	L	23	0	0	0	0
5	M	28	0	0	0	0
5	N	22	0	0	0	0
5	O	22	0	0	0	0
5	P	41	0	0	1	0
5	Q	34	0	0	1	0
5	R	34	0	0	0	0
5	S	50	0	0	1	0
5	T	57	0	0	0	0
All	All	18049	0	17302	150	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 150 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:GLN:HG2	1:G:56:GLN:O	1.52	1.05
1:L:87:VAL:HG11	1:L:94:HIS:HB3	1.52	0.91
3:S:201:MPD:H52	3:S:201:MPD:H12	1.54	0.86
3:P:202:MPD:O4	3:P:202:MPD:H12	1.76	0.85
1:M:8:LEU:C	1:M:9[B]:CYS:CA	2.47	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	102/124 (82%)	100 (98%)	1 (1%)	1 (1%)	15	16
1	B	101/124 (82%)	100 (99%)	1 (1%)	0	100	100
1	C	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
1	D	101/124 (82%)	100 (99%)	1 (1%)	0	100	100
1	E	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
1	F	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
1	G	121/124 (98%)	113 (93%)	7 (6%)	1 (1%)	19	22
1	H	102/124 (82%)	101 (99%)	1 (1%)	0	100	100
1	I	101/124 (82%)	100 (99%)	1 (1%)	0	100	100
1	J	122/124 (98%)	118 (97%)	3 (2%)	1 (1%)	19	22
1	K	101/124 (82%)	100 (99%)	1 (1%)	0	100	100
1	L	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
1	M	123/124 (99%)	116 (94%)	6 (5%)	1 (1%)	19	22
1	N	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
1	O	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
1	P	122/124 (98%)	117 (96%)	4 (3%)	1 (1%)	19	22
1	Q	101/124 (82%)	100 (99%)	1 (1%)	0	100	100
1	R	102/124 (82%)	101 (99%)	1 (1%)	0	100	100
1	S	103/124 (83%)	102 (99%)	1 (1%)	0	100	100
1	T	101/124 (82%)	100 (99%)	1 (1%)	0	100	100
All	All	2201/2480 (89%)	2138 (97%)	58 (3%)	5 (0%)	47	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	105	VAL

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Mol	Chain	Res	Type
1	G	55	SER
1	M	104	GLY
1	A	103	ASN
1	P	106	SER

### 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	89/106 (84%)	87 (98%)	2 (2%)	52	64
1	B	89/106 (84%)	85 (96%)	4 (4%)	27	36
1	C	84/106 (79%)	79 (94%)	5 (6%)	19	24
1	D	89/106 (84%)	85 (96%)	4 (4%)	27	36
1	E	89/106 (84%)	86 (97%)	3 (3%)	37	48
1	F	90/106 (85%)	86 (96%)	4 (4%)	28	37
1	G	89/106 (84%)	85 (96%)	4 (4%)	27	36
1	H	89/106 (84%)	88 (99%)	1 (1%)	73	82
1	I	89/106 (84%)	88 (99%)	1 (1%)	73	82
1	J	90/106 (85%)	86 (96%)	4 (4%)	28	37
1	K	89/106 (84%)	86 (97%)	3 (3%)	37	48
1	L	89/106 (84%)	85 (96%)	4 (4%)	27	36
1	M	92/106 (87%)	90 (98%)	2 (2%)	52	64
1	N	89/106 (84%)	85 (96%)	4 (4%)	27	36
1	O	89/106 (84%)	83 (93%)	6 (7%)	16	20
1	P	90/106 (85%)	87 (97%)	3 (3%)	38	49
1	Q	89/106 (84%)	87 (98%)	2 (2%)	52	64
1	R	89/106 (84%)	88 (99%)	1 (1%)	73	82
1	S	91/106 (86%)	89 (98%)	2 (2%)	52	64
1	T	89/106 (84%)	88 (99%)	1 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1783/2120 (84%)	1723 (97%)	60 (3%)	38 48

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	29	GLU
1	Q	77	LEU
1	L	29	GLU
1	Q	29	GLU
1	T	29	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	103	ASN
1	K	3	GLN
1	T	3	GLN
1	O	3	GLN
1	S	103	ASN

### 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](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

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	$\# Z  > 2$
2	PO4	I	201	-	4,4,4	0.62	0	6,6,6	0.49	0
2	PO4	F	201	-	4,4,4	1.21	1 (25%)	6,6,6	0.49	0
3	MPD	T	201	-	7,7,7	0.11	0	9,10,10	0.59	0
2	PO4	A	201	-	4,4,4	0.53	0	6,6,6	0.56	0
3	MPD	D	203	-	7,7,7	0.13	0	9,10,10	0.43	0
3	MPD	O	201	-	7,7,7	0.16	0	9,10,10	0.48	0
3	MPD	G	201	-	7,7,7	0.11	0	9,10,10	0.44	0
3	MPD	L	201	-	7,7,7	0.11	0	9,10,10	0.51	0
2	PO4	D	201	-	4,4,4	0.68	0	6,6,6	0.44	0
3	MPD	A	203	-	7,7,7	0.14	0	9,10,10	0.47	0
3	MPD	D	202	-	7,7,7	0.14	0	9,10,10	0.48	0
3	MPD	H	203	-	7,7,7	0.62	0	9,10,10	1.40	2 (22%)
2	PO4	Q	201	-	4,4,4	0.81	0	6,6,6	0.38	0
3	MPD	M	201	-	7,7,7	0.16	0	9,10,10	0.69	0
3	MPD	Q	202	-	7,7,7	0.27	0	9,10,10	0.69	0
3	MPD	R	201	-	7,7,7	0.12	0	9,10,10	0.65	0
3	MPD	R	202	-	7,7,7	0.14	0	9,10,10	0.69	0
3	MPD	B	202	-	7,7,7	0.12	0	9,10,10	0.56	0
3	MPD	J	201	-	7,7,7	0.24	0	9,10,10	0.57	0
2	PO4	P	201	-	4,4,4	0.87	0	6,6,6	0.38	0
3	MPD	J	202	-	7,7,7	0.10	0	9,10,10	0.57	0
3	MPD	P	203	-	7,7,7	0.38	0	9,10,10	0.58	0
3	MPD	A	202	-	7,7,7	0.28	0	9,10,10	0.59	0
3	MPD	B	201	-	7,7,7	0.17	0	9,10,10	0.61	0
3	MPD	S	202	-	7,7,7	0.20	0	9,10,10	0.66	0
3	MPD	H	201	-	7,7,7	0.10	0	9,10,10	0.62	0
3	MPD	P	202	-	7,7,7	0.16	0	9,10,10	0.62	0
3	MPD	H	202	-	7,7,7	0.22	0	9,10,10	0.31	0
3	MPD	R	203	-	7,7,7	0.24	0	9,10,10	0.58	0
3	MPD	G	202	-	7,7,7	0.17	0	9,10,10	0.60	0
3	MPD	O	202	-	7,7,7	0.41	0	9,10,10	0.67	0
3	MPD	S	201	-	7,7,7	0.37	0	9,10,10	0.68	0
3	MPD	N	201	-	7,7,7	0.25	0	9,10,10	0.67	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	MPD	T	201	-	-	1/5/5/5	-
3	MPD	D	203	-	-	2/5/5/5	-
3	MPD	O	201	-	-	2/5/5/5	-
3	MPD	G	201	-	-	0/5/5/5	-
3	MPD	L	201	-	-	2/5/5/5	-
3	MPD	A	203	-	-	0/5/5/5	-
3	MPD	D	202	-	-	1/5/5/5	-
3	MPD	H	203	-	-	2/5/5/5	-
3	MPD	M	201	-	-	0/5/5/5	-
3	MPD	Q	202	-	-	0/5/5/5	-
3	MPD	R	201	-	-	2/5/5/5	-
3	MPD	R	202	-	-	1/5/5/5	-
3	MPD	B	202	-	-	1/5/5/5	-
3	MPD	J	201	-	-	3/5/5/5	-
3	MPD	J	202	-	-	2/5/5/5	-
3	MPD	P	203	-	-	0/5/5/5	-
3	MPD	A	202	-	-	3/5/5/5	-
3	MPD	B	201	-	-	1/5/5/5	-
3	MPD	S	202	-	-	3/5/5/5	-
3	MPD	H	201	-	-	5/5/5/5	-
3	MPD	P	202	-	-	0/5/5/5	-
3	MPD	H	202	-	-	2/5/5/5	-
3	MPD	R	203	-	-	1/5/5/5	-
3	MPD	G	202	-	-	1/5/5/5	-
3	MPD	O	202	-	-	2/5/5/5	-
3	MPD	S	201	-	-	1/5/5/5	-
3	MPD	N	201	-	-	1/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201	PO4	P-O1	2.22	1.56	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	203	MPD	O2-C2-C1	-2.51	100.03	108.08
3	H	203	MPD	C5-C4-C3	2.11	121.62	111.69

There are no chirality outliers.



5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	201	MPD	C1-C2-C3-C4
3	H	201	MPD	O2-C2-C3-C4
3	H	201	MPD	C2-C3-C4-O4
3	J	201	MPD	O2-C2-C3-C4
3	J	201	MPD	CM-C2-C3-C4

There are no ring outliers.

19 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	201	MPD	1	0
2	A	201	PO4	1	0
3	D	203	MPD	1	0
3	L	201	MPD	1	0
3	A	203	MPD	2	0
3	M	201	MPD	2	0
3	Q	202	MPD	1	0
3	R	201	MPD	1	0
3	R	202	MPD	1	0
3	J	201	MPD	3	0
3	J	202	MPD	1	0
3	B	201	MPD	2	0
3	S	202	MPD	2	0
3	P	202	MPD	3	0
3	H	202	MPD	2	0
3	R	203	MPD	3	0
3	G	202	MPD	2	0
3	S	201	MPD	7	0
3	N	201	MPD	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	104/124 (83%)	-0.02	3 (2%) 51 47	49, 62, 82, 102	0
1	B	103/124 (83%)	0.24	7 (6%) 17 13	52, 69, 99, 136	0
1	C	97/124 (78%)	0.03	1 (1%) 82 83	50, 67, 90, 98	0
1	D	103/124 (83%)	0.00	6 (5%) 23 20	45, 61, 92, 124	0
1	E	123/124 (99%)	0.64	22 (17%) 1 0	46, 58, 181, 198	0
1	F	123/124 (99%)	0.60	17 (13%) 2 1	42, 53, 181, 195	0
1	G	123/124 (99%)	0.84	19 (15%) 2 1	40, 57, 186, 196	0
1	H	104/124 (83%)	-0.39	0 100 100	39, 51, 74, 88	0
1	I	103/124 (83%)	-0.23	2 (1%) 66 64	37, 48, 71, 81	0
1	J	123/124 (99%)	1.04	22 (17%) 1 0	40, 52, 186, 200	0
1	K	103/124 (83%)	-0.11	4 (3%) 39 36	43, 58, 83, 101	1 (0%)
1	L	123/124 (99%)	1.10	24 (19%) 1 0	43, 64, 175, 193	0
1	M	123/124 (99%)	1.15	23 (18%) 1 0	45, 59, 180, 195	0
1	N	123/124 (99%)	0.79	22 (17%) 1 0	42, 61, 179, 195	0
1	O	123/124 (99%)	0.88	23 (18%) 1 0	42, 60, 173, 191	0
1	P	123/124 (99%)	0.76	21 (17%) 1 1	28, 47, 180, 204	0
1	Q	103/124 (83%)	-0.24	0 100 100	39, 53, 67, 93	0
1	R	104/124 (83%)	-0.26	1 (0%) 82 83	35, 50, 65, 82	0
1	S	103/124 (83%)	-0.46	0 100 100	29, 38, 49, 74	0
1	T	103/124 (83%)	-0.29	1 (0%) 82 83	27, 35, 54, 80	0
All	All	2237/2480 (90%)	0.35	218 (9%) 7 5	27, 56, 173, 204	1 (0%)

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	119	VAL	12.5
1	P	105	VAL	12.4
1	J	114	ALA	12.4
1	G	119	VAL	11.9
1	M	113	SER	11.7

## 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( $\text{\AA}^2$ )	Q<0.9
2	PO4	F	201	5/5	0.66	0.36	65,75,102,104	0
3	MPD	P	203	8/8	0.69	0.45	69,83,99,100	0
3	MPD	O	202	8/8	0.71	0.35	59,81,83,88	0
3	MPD	J	201	8/8	0.78	0.24	59,67,85,90	0
3	MPD	G	201	8/8	0.78	0.29	66,78,102,105	0
3	MPD	G	202	8/8	0.78	0.20	64,76,77,84	0
3	MPD	H	203	8/8	0.81	0.28	57,64,70,74	0
3	MPD	B	202	8/8	0.82	0.28	74,80,98,102	0
3	MPD	D	202	8/8	0.82	0.22	75,83,96,102	0
3	MPD	S	202	8/8	0.84	0.27	59,64,69,71	0
3	MPD	P	202	8/8	0.85	0.19	63,77,83,83	0
3	MPD	M	201	8/8	0.85	0.24	71,76,84,85	0
2	PO4	I	201	5/5	0.85	0.33	81,88,102,104	0
3	MPD	A	203	8/8	0.86	0.34	70,81,95,97	0
3	MPD	O	201	8/8	0.87	0.21	57,68,80,82	0
2	PO4	D	201	5/5	0.88	0.34	83,84,102,103	0
3	MPD	R	201	8/8	0.88	0.20	60,69,94,96	0
3	MPD	H	201	8/8	0.88	0.14	59,72,84,87	0
3	MPD	H	202	8/8	0.89	0.20	70,75,78,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MPD	T	201	8/8	0.89	0.16	66,73,86,93	0
3	MPD	Q	202	8/8	0.90	0.22	61,70,73,77	0
3	MPD	D	203	8/8	0.90	0.32	77,86,88,90	0
3	MPD	B	201	8/8	0.91	0.18	70,89,101,107	0
3	MPD	R	203	8/8	0.91	0.32	60,69,78,81	0
3	MPD	J	202	8/8	0.92	0.22	78,83,93,95	0
3	MPD	A	202	8/8	0.92	0.27	60,71,79,79	0
3	MPD	R	202	8/8	0.92	0.21	60,71,88,91	0
2	PO4	A	201	5/5	0.94	0.10	65,69,76,78	0
3	MPD	N	201	8/8	0.94	0.27	73,78,88,88	0
3	MPD	L	201	8/8	0.94	0.20	62,70,75,78	0
2	PO4	Q	201	5/5	0.95	0.11	60,60,69,70	0
3	MPD	S	201	8/8	0.95	0.19	42,51,56,60	0
2	PO4	P	201	5/5	0.97	0.09	58,66,68,74	0
4	CL	T	202	1/1	0.98	0.08	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.