



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2017 – 02:33 PM EDT

PDB ID : 5GON  
Title : Structures of a beta-lactam bridged analogue in complex with tubulin  
Authors : Zhou, L.; Liu, Y.; Cheng, L.; Wang, Y.  
Deposited on : 2016-07-28  
Resolution : 2.48 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

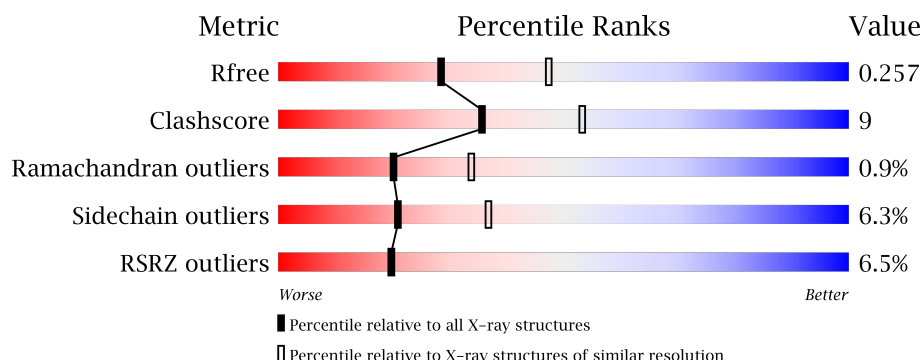
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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))
$R_{free}$	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>
1	C	440	<div> <div>87%</div> <div>12%</div> <div>•</div> </div>
2	B	431	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>••</div> </div> </div>
2	D	431	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>••</div> </div> </div>
3	E	136	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	F	378	

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
12	IMD	C	509	-	-	-	X
12	IMD	C	510	-	-	-	X
6	MG	A	502	-	-	-	X
6	MG	C	504	-	-	-	X
7	GOL	A	504	-	-	-	X
7	GOL	B	503	-	-	-	X
7	GOL	B	504	-	-	-	X
7	GOL	B	505	-	-	X	X
7	GOL	C	502	-	-	-	X
7	GOL	C	506	-	-	-	X
7	GOL	C	507	-	-	-	X
7	GOL	D	504	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17847 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	13	0
			3488	2217	585	661	25			
1	C	440	Total	C	N	O	S	0	11	0
			3489	2209	588	668	24			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	1	11	0
			3374	2126	568	653	27			
2	D	421	Total	C	N	O	S	0	4	0
			3326	2094	562	642	28			

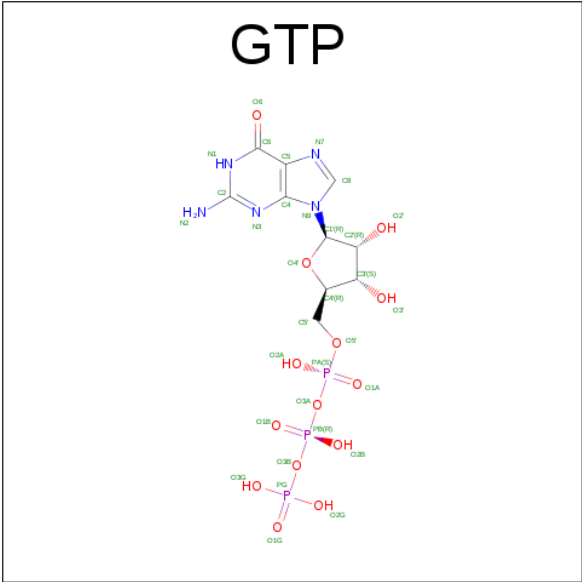
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	3	0
			1016	628	183	199	6			

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	319	Total	C	N	O	S	0	5	0
			2633	1706	436	477	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

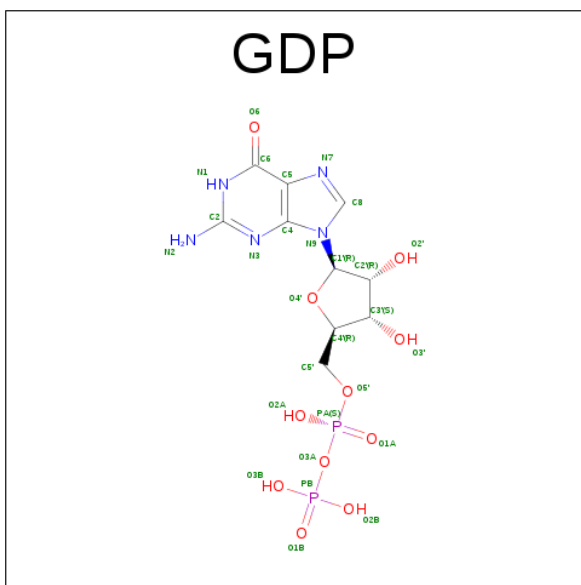


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

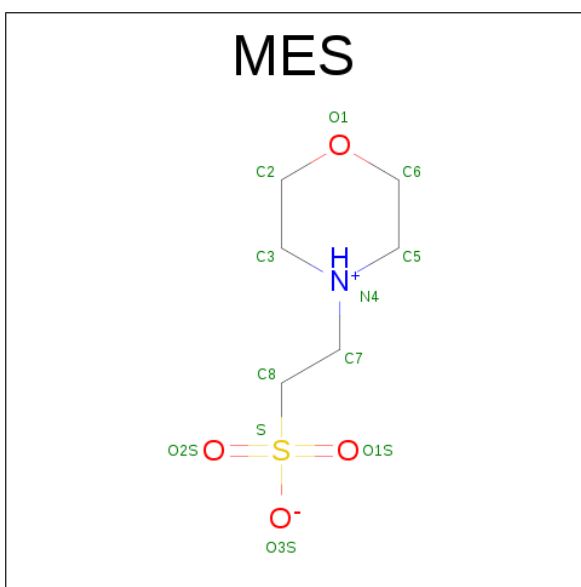
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Ca 1 1	0	0
8	A	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



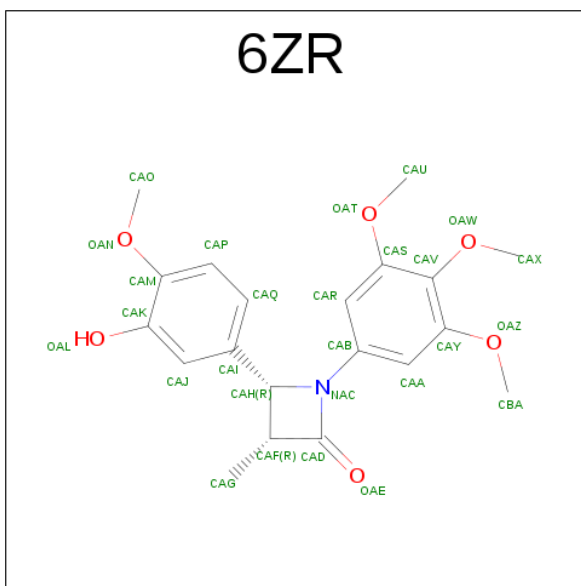
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

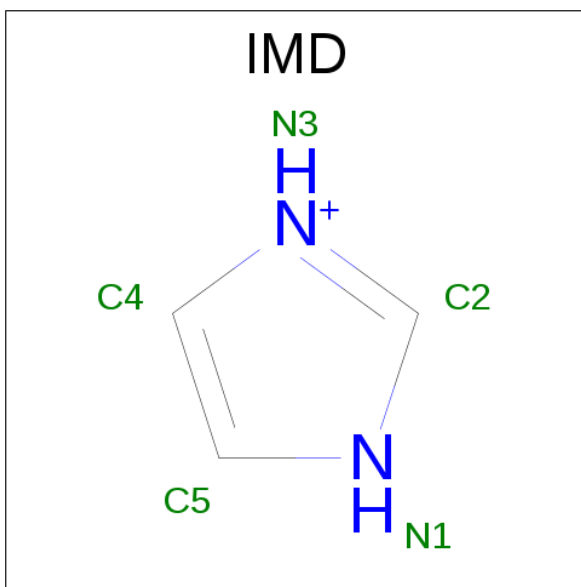
- Molecule 11 is (3R,4R)-4-(4-methoxy-3-oxidanyl-phenyl)-3-methyl-1-(3,4,5-trimethoxyphenyl)azetidin-2-one (three-letter code: 6ZR) (formula: C<sub>20</sub>H<sub>23</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			27	20	1	6		

- Molecule 12 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C N 5 3 2	0	0
12	C	1	Total C N 5 3 2	0	0
12	C	1	Total C N 5 3 2	0	0

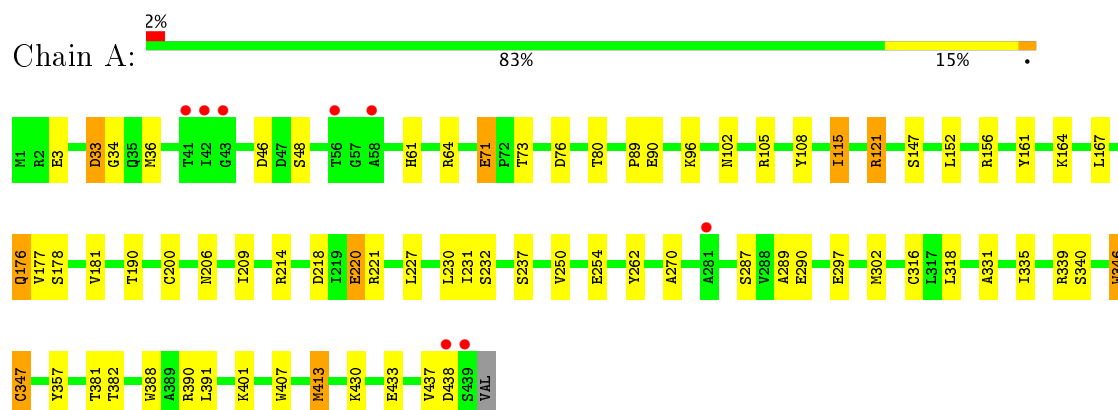
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	44	Total O 44 44	0	0
13	B	52	Total O 52 52	0	0
13	C	110	Total O 110 110	0	0
13	D	25	Total O 25 25	0	0
13	E	16	Total O 16 16	0	0
13	F	20	Total O 20 20	0	0

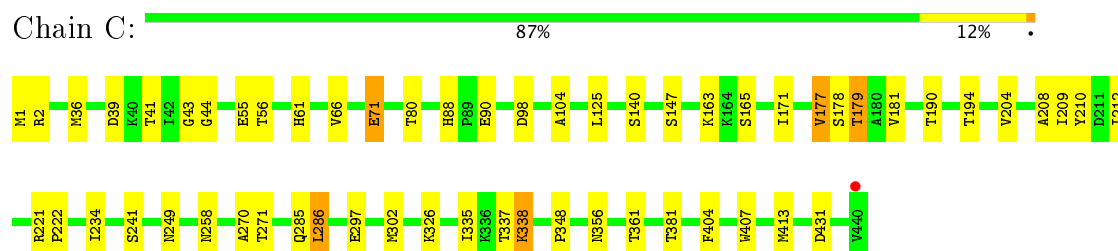
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

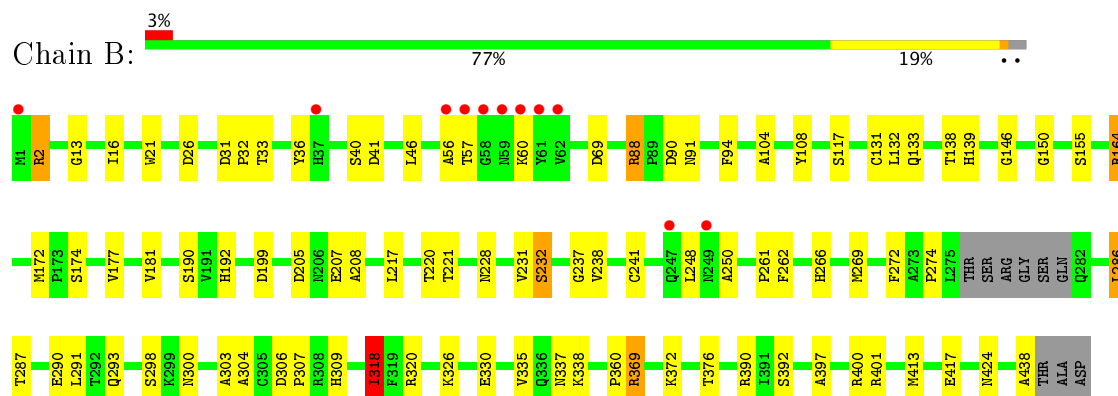
- Molecule 1: Tubulin alpha-1B chain



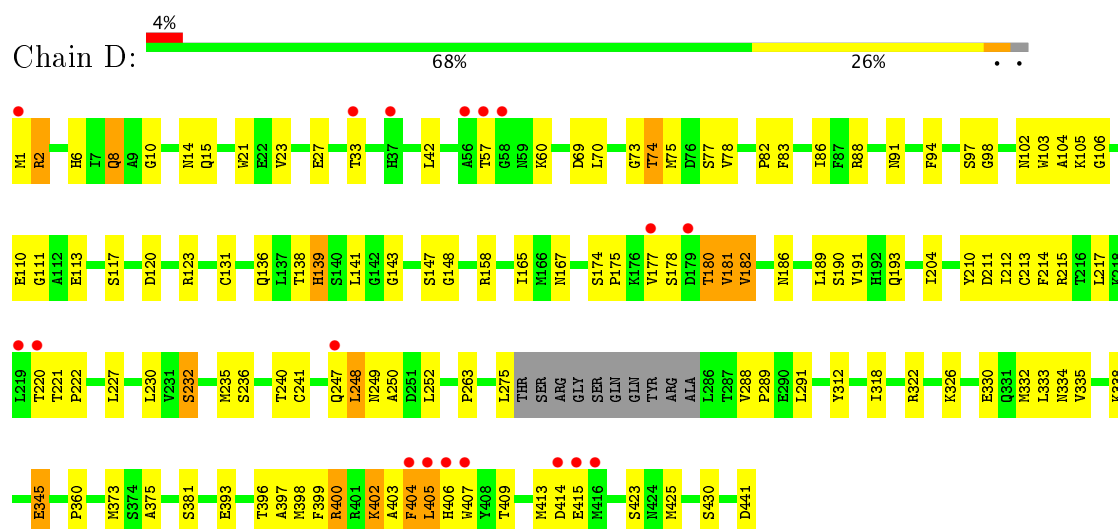
- Molecule 1: Tubulin alpha-1B chain



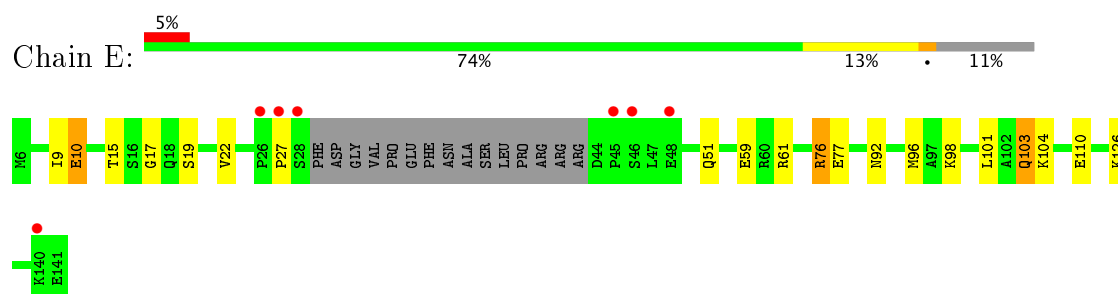
- Molecule 2: Tubulin beta-2B chain



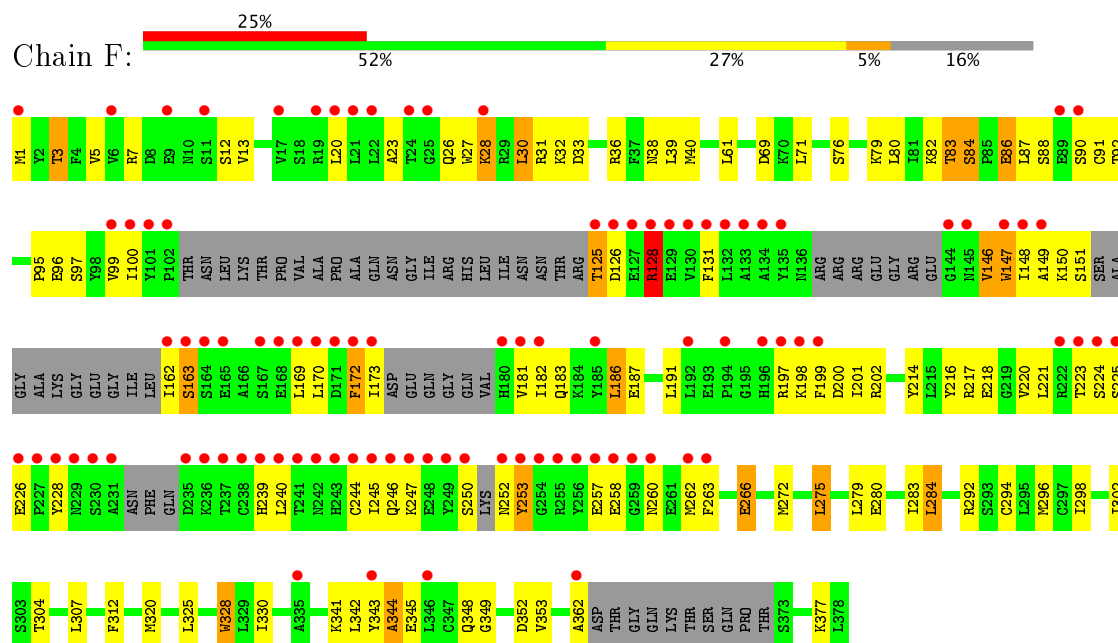
- Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.51Å 156.46Å 181.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.60 – 2.48 49.71 – 2.48	Depositor EDS
% Data completeness (in resolution range)	92.9 (118.60-2.48) 92.9 (49.71-2.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.205 , 0.257 0.205 , 0.257	Depositor DCC
$R_{free}$ test set	4912 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: GDP, GOL, MG, IMD, CA, GTP, MES, 6ZR

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	0.75	3/3605 (0.1%)	0.75	1/4895 (0.0%)
1	C	0.88	1/3597 (0.0%)	0.82	0/4885
2	B	0.81	1/3478 (0.0%)	0.78	2/4710 (0.0%)
2	D	0.74	2/3411 (0.1%)	0.78	2/4622 (0.0%)
3	E	0.77	0/1033	0.81	2/1370 (0.1%)
4	F	0.82	5/2704 (0.2%)	0.77	2/3650 (0.1%)
All	All	0.80	12/17828 (0.1%)	0.78	9/24132 (0.0%)

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

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	LEU	C-N	9.96	1.56	1.34
2	D	360	PRO	C-N	9.08	1.54	1.34
4	F	226	GLU	CD-OE1	-8.86	1.16	1.25
4	F	27	TRP	CD2-CE2	6.11	1.48	1.41
1	A	346	TRP	CD2-CE2	5.96	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	405	LEU	CB-CG-CD1	-9.60	94.67	111.00
2	D	2	ARG	NE-CZ-NH1	-7.99	116.31	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	61	ARG	NE-CZ-NH1	7.42	124.01	120.30
4	F	36	ARG	NE-CZ-NH1	5.63	123.11	120.30
3	E	76	ARG	NE-CZ-NH1	-5.61	117.50	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	249	ASN	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	3488	0	3441	40	0
1	C	3489	0	3413	43	0
2	B	3374	0	3270	71	0
2	D	3326	0	3221	78	0
3	E	1016	0	1041	11	0
4	F	2633	0	2631	80	0
5	A	32	0	12	0	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	18	0	24	1	0
7	B	18	0	24	12	0
7	C	24	0	32	6	0
7	D	12	0	16	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	12	0	13	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	27	0	0	3	0
12	C	15	0	15	4	0
13	A	44	0	0	2	0
13	B	52	0	0	0	0
13	C	110	0	0	3	0
13	D	25	0	0	1	0
13	E	16	0	0	0	0
13	F	20	0	0	0	0
All	All	17847	0	17189	321	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 9.

The worst 5 of 321 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)
4:F:240:LEU:HD23	4:F:245:ILE:HD12	1.30	1.13
2:B:320:ARG:HH11	7:B:505:GOL:H11	1.05	1.10
4:F:1:MET:HG2	4:F:28:LYS:HD2	1.19	1.09
2:B:320:ARG:NH1	7:B:505:GOL:H11	1.68	1.06
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.34	1.05

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	450/440 (102%)	431 (96%)	19 (4%)	0	100	100
1	C	449/440 (102%)	437 (97%)	12 (3%)	0	100	100
2	B	429/431 (100%)	409 (95%)	18 (4%)	2 (0%)	32	51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	421/431 (98%)	395 (94%)	18 (4%)	8 (2%)	9	14
3	E	120/136 (88%)	111 (92%)	8 (7%)	1 (1%)	22	37
4	F	307/378 (81%)	264 (86%)	34 (11%)	9 (3%)	5	7
All	All	2176/2256 (96%)	2047 (94%)	109 (5%)	20 (1%)	20	34

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	177	VAL
2	D	399	PHE
4	F	343	TYR
2	B	337	ASN
2	D	181	VAL

### 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	383/371 (103%)	365 (95%)	18 (5%)	30	52
1	C	382/371 (103%)	369 (97%)	13 (3%)	42	67
2	B	375/372 (101%)	350 (93%)	25 (7%)	19	33
2	D	368/372 (99%)	342 (93%)	26 (7%)	17	30
3	E	112/122 (92%)	103 (92%)	9 (8%)	14	25
4	F	293/336 (87%)	261 (89%)	32 (11%)	7	13
All	All	1913/1944 (98%)	1790 (94%)	123 (6%)	21	36

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	381	THR
2	D	204	ILE
4	F	244	CYS
2	D	8	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	D	117	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	406	HIS
3	E	92	ASN
4	F	196	HIS
2	D	101	ASN
4	F	145	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 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
5	GTP	A	501	6	27,34,34	1.02	2 (7%)	27,54,54	1.75	8 (29%)
7	GOL	A	503	-	5,5,5	0.50	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	A	504	-	5,5,5	0.84	0	5,5,5	0.66	0
7	GOL	A	506	-	5,5,5	0.53	0	5,5,5	0.77	0
9	GDP	B	501	6	25,30,30	1.39	3 (12%)	26,47,47	1.83	6 (23%)
7	GOL	B	503	-	5,5,5	0.47	0	5,5,5	1.04	0
7	GOL	B	504	-	5,5,5	0.57	0	5,5,5	0.29	0
7	GOL	B	505	-	5,5,5	0.62	0	5,5,5	0.37	0
10	MES	B	507	-	12,12,12	2.09	1 (8%)	14,16,16	3.77	7 (50%)
11	6ZR	B	508	-	28,29,29	2.20	7 (25%)	38,42,42	2.58	13 (34%)
7	GOL	C	502	-	5,5,5	0.92	0	5,5,5	0.59	0
5	GTP	C	503	6	27,34,34	1.19	1 (3%)	27,54,54	2.03	7 (25%)
7	GOL	C	505	-	5,5,5	0.59	0	5,5,5	0.57	0
7	GOL	C	506	-	5,5,5	0.51	0	5,5,5	0.54	0
7	GOL	C	507	-	5,5,5	0.90	0	5,5,5	0.73	0
12	IMD	C	508	-	3,5,5	0.50	0	4,5,5	0.47	0
12	IMD	C	509	-	3,5,5	0.43	0	4,5,5	0.95	0
12	IMD	C	510	-	3,5,5	0.45	0	4,5,5	0.58	0
9	GDP	D	501	6	25,30,30	1.25	2 (8%)	26,47,47	1.93	6 (23%)
7	GOL	D	503	-	5,5,5	0.50	0	5,5,5	0.26	0
7	GOL	D	504	-	5,5,5	0.29	0	5,5,5	0.43	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
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
7	GOL	A	503	-	-	0/4/4/4	0/0/0/0
7	GOL	A	504	-	-	0/4/4/4	0/0/0/0
7	GOL	A	506	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
7	GOL	B	503	-	-	0/4/4/4	0/0/0/0
7	GOL	B	504	-	-	0/4/4/4	0/0/0/0
7	GOL	B	505	-	-	0/4/4/4	0/0/0/0
10	MES	B	507	-	-	0/6/14/14	0/1/1/1
11	6ZR	B	508	-	-	0/16/32/32	0/3/3/3
7	GOL	C	502	-	-	0/4/4/4	0/0/0/0
5	GTP	C	503	6	-	0/18/38/38	0/3/3/3
7	GOL	C	505	-	-	0/4/4/4	0/0/0/0
7	GOL	C	506	-	-	0/4/4/4	0/0/0/0
7	GOL	C	507	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	IMD	C	508	-	-	0/0/0/0	0/1/1/1
12	IMD	C	509	-	-	0/0/0/0	0/1/1/1
12	IMD	C	510	-	-	0/0/0/0	0/1/1/1
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
7	GOL	D	503	-	-	0/4/4/4	0/0/0/0
7	GOL	D	504	-	-	0/4/4/4	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	507	MES	C8-S	-6.84	1.67	1.77
11	B	508	6ZR	CAB-NAC	-5.86	1.32	1.43
11	B	508	6ZR	CAF-CAH	-5.42	1.50	1.57
11	B	508	6ZR	CAI-CAH	-4.47	1.45	1.51
9	B	501	GDP	C2'-C1'	-3.71	1.47	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	508	6ZR	OAN-CAM-CAP	-6.13	114.08	124.37
11	B	508	6ZR	CAH-NAC-CAD	-4.31	90.84	95.27
10	B	507	MES	C6-C5-N4	-4.02	104.48	110.11
11	B	508	6ZR	CAU-OAT-CAS	-3.97	111.83	117.54
5	C	503	GTP	C6-C5-C4	-3.96	116.91	120.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	504	GOL	1	0
7	B	503	GOL	2	0
7	B	505	GOL	10	0
10	B	507	MES	1	0
11	B	508	6ZR	3	0
5	C	503	GTP	1	0
7	C	505	GOL	3	0
7	C	506	GOL	1	0
7	C	507	GOL	2	0
12	C	508	IMD	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	509	IMD	2	0
12	C	510	IMD	1	0
7	D	504	GOL	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	439/440 (99%)	0.05	8 (1%) 69 70	18, 38, 62, 99	0
1	C	440/440 (100%)	-0.42	1 (0%) 94 95	10, 23, 43, 59	0
2	B	422/431 (97%)	-0.08	11 (2%) 56 58	12, 33, 66, 99	1 (0%)
2	D	421/431 (97%)	0.18	18 (4%) 36 38	22, 45, 73, 93	2 (0%)
3	E	121/136 (88%)	0.18	7 (5%) 24 24	20, 44, 76, 96	0
4	F	319/378 (84%)	1.53	96 (30%) 1 0	27, 62, 143, 176	0
All	All	2162/2256 (95%)	0.18	141 (6%) 20 20	10, 39, 79, 176	3 (0%)

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	13.3
4	F	256	TYR	12.0
4	F	252	ASN	11.9
4	F	253	TYR	9.2
4	F	243	HIS	8.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	B	505	6/6	0.84	0.48	12.04	54,55,62,68	0
7	GOL	C	506	6/6	0.90	0.31	9.64	47,52,65,65	0
7	GOL	B	503	6/6	0.88	0.38	8.01	42,49,52,72	0
6	MG	A	502	1/1	0.97	0.33	7.22	37,37,37,37	0
7	GOL	B	504	6/6	0.65	0.33	7.03	53,62,69,71	0
6	MG	C	504	1/1	0.91	0.34	6.74	38,38,38,38	0
12	IMD	C	510	5/5	0.83	0.28	4.94	56,64,66,67	0
7	GOL	C	502	6/6	0.76	0.30	4.77	46,52,64,67	0
7	GOL	A	504	6/6	0.81	0.29	4.54	56,71,73,79	0
7	GOL	D	504	6/6	0.89	0.29	4.26	51,53,65,77	0
12	IMD	C	509	5/5	0.86	0.23	3.48	64,66,73,76	0
7	GOL	C	507	6/6	0.88	0.19	2.14	34,47,48,57	0
7	GOL	A	503	6/6	0.93	0.19	1.46	47,56,58,59	0
7	GOL	C	505	6/6	0.86	0.33	1.32	61,65,73,81	0
7	GOL	A	506	6/6	0.80	0.22	0.97	52,63,69,73	0
5	GTP	C	503	32/32	0.98	0.15	0.89	12,16,20,22	0
9	GDP	B	501	28/28	0.99	0.15	0.32	13,18,21,24	0
11	6ZR	B	508	27/27	0.93	0.16	-0.10	35,47,53,58	0
10	MES	B	507	12/12	0.97	0.12	-0.16	26,38,47,52	0
5	GTP	A	501	32/32	0.99	0.19	-0.22	18,23,30,33	0
9	GDP	D	501	28/28	0.97	0.13	-0.38	33,42,57,61	0
8	CA	A	505	1/1	0.95	0.06	-2.08	59,59,59,59	0
6	MG	F	401	1/1	0.77	0.83	-	86,86,86,86	0
6	MG	B	502	1/1	0.98	0.34	-	16,16,16,16	0
12	IMD	C	508	5/5	0.95	0.21	-	32,35,36,42	0
8	CA	C	501	1/1	0.96	0.06	-	82,82,82,82	0
6	MG	D	502	1/1	0.95	0.12	-	40,40,40,40	0
7	GOL	D	503	6/6	0.76	0.44	-	74,81,86,87	0
8	CA	B	506	1/1	0.95	0.09	-	81,81,81,81	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.