



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2016 – 11:02 PM EDT

PDB ID : 5BMV  
Title : CRYSTAL STRUCTURE OF TUBULIN-STATHMIN-TTL-Vinblastine  
COMPLEX  
Authors : Wang, Y.; Chen, Q.; Zhang, R.  
Deposited on : 2015-05-23  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027790

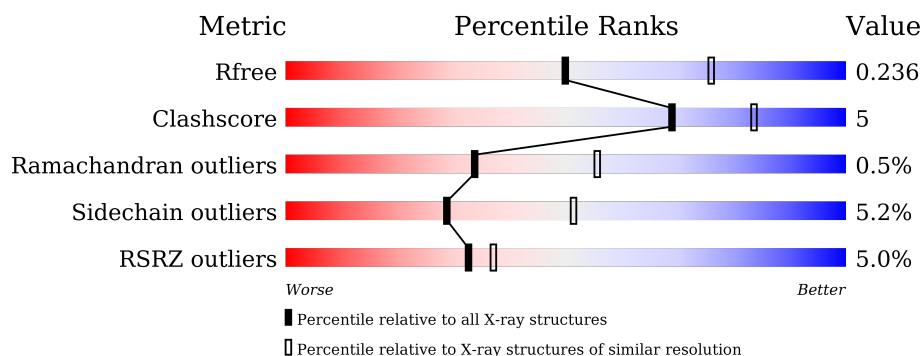
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	451	<div> <div>2%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	C	451	<div> <div>88%</div> <div>9%</div> <div>.</div> </div>
2	B	445	<div> <div>%</div> <div>80%</div> <div>14%</div> <div>.</div> <div>.</div> </div>
2	D	445	<div> <div>7%</div> <div>76%</div> <div>17%</div> <div>.</div> <div>5%</div> </div>
3	E	143	<div> <div>10%</div> <div>73%</div> <div>10%</div> <div>.</div> <div>14%</div> </div>
4	F	384	<div> <div>13%</div> <div>74%</div> <div>14%</div> <div>.</div> <div>10%</div> </div>

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
6	MG	D	502	-	-	-	X
8	GOL	A	506	-	-	-	X
8	GOL	C	504	-	-	X	-
8	GOL	C	505	-	-	X	X
8	GOL	C	506	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 17912 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	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	1	0
			3446	2180	585	659	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3360	2111	576	647	26			
2	D	422	Total	C	N	O	S	0	0	0
			3311	2082	563	640	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

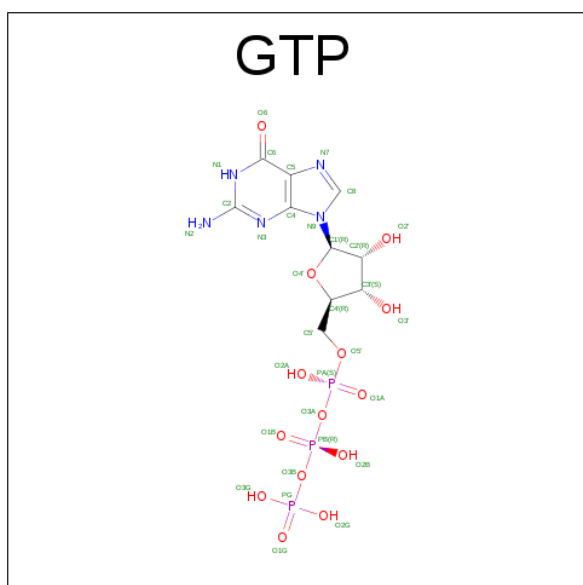
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	0	0
			2849	1825	492	518	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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		

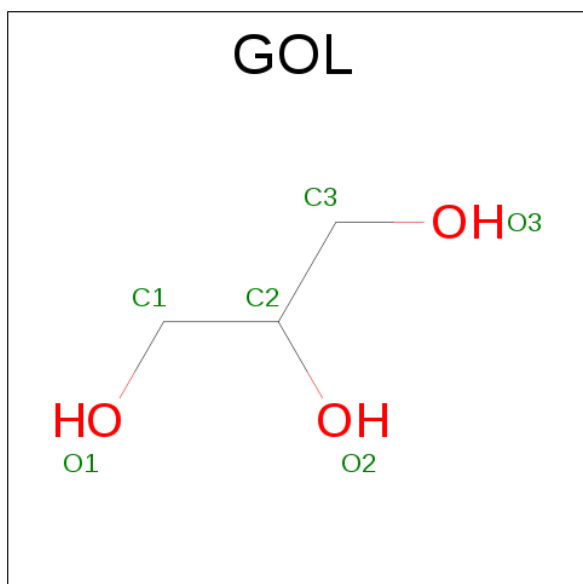
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

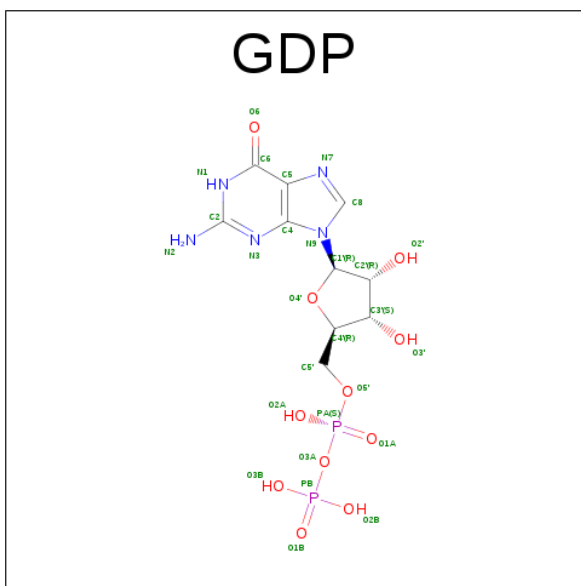
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



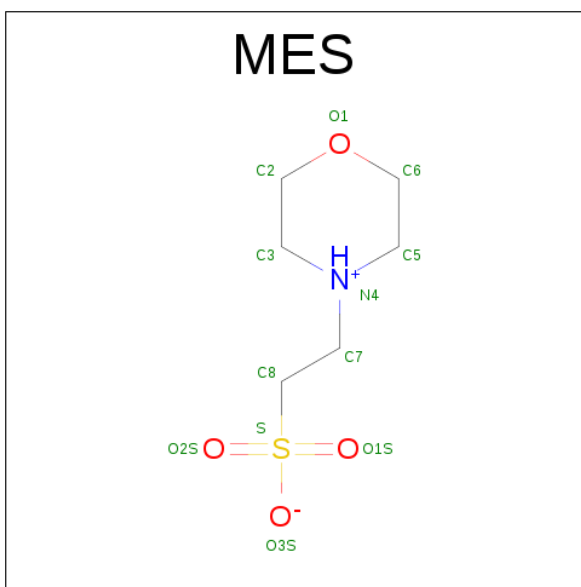
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:

$$\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2).$$


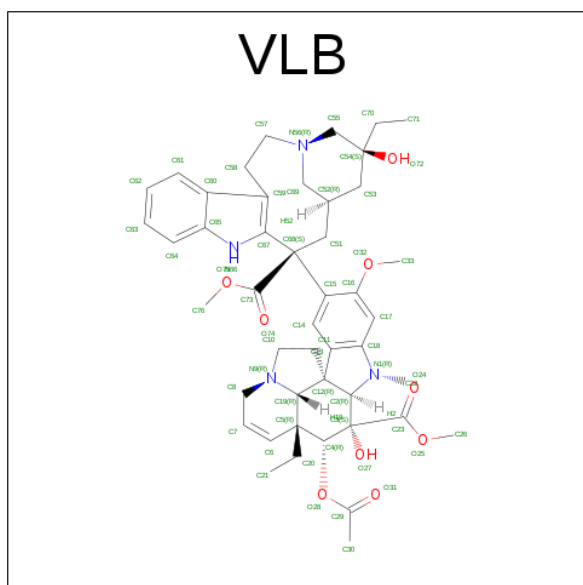
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- 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		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

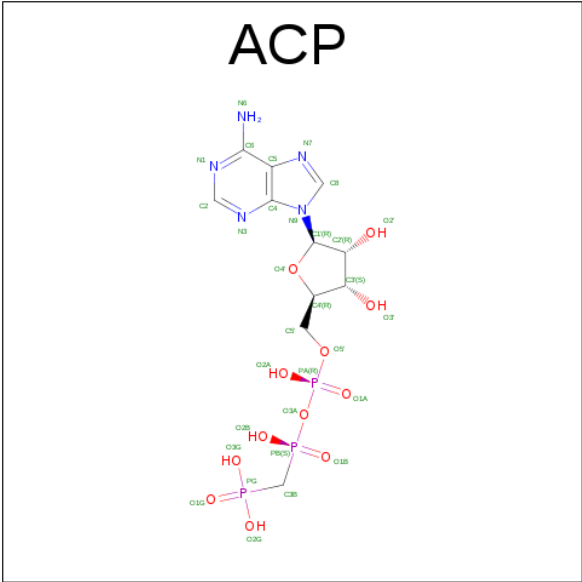
- Molecule 11 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula:  $C_{46}H_{58}N_4O_9$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O		0	0
			59	46	4	9			

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

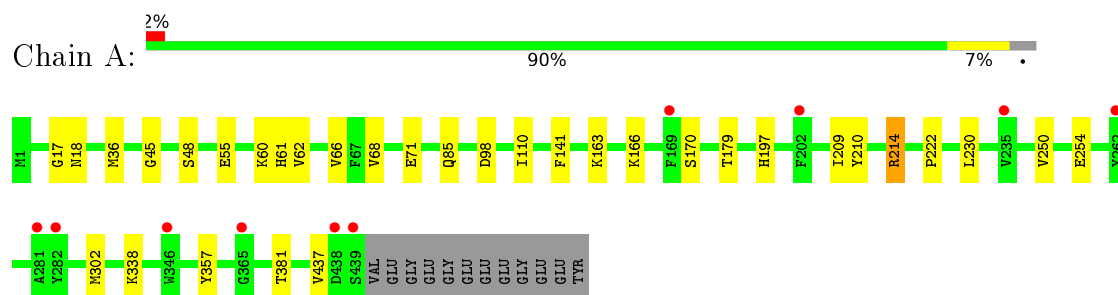
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	47	Total	O	0	0
			47	47		
13	B	56	Total	O	0	0
			56	56		
13	C	83	Total	O	0	0
			83	83		
13	D	8	Total	O	0	0
			8	8		
13	E	1	Total	O	0	0
			1	1		
13	F	24	Total	O	0	0
			24	24		

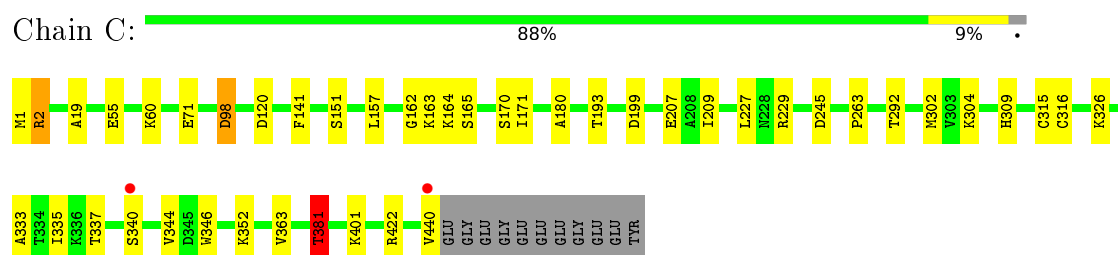
### 3 Residue-property plots [i](#)

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

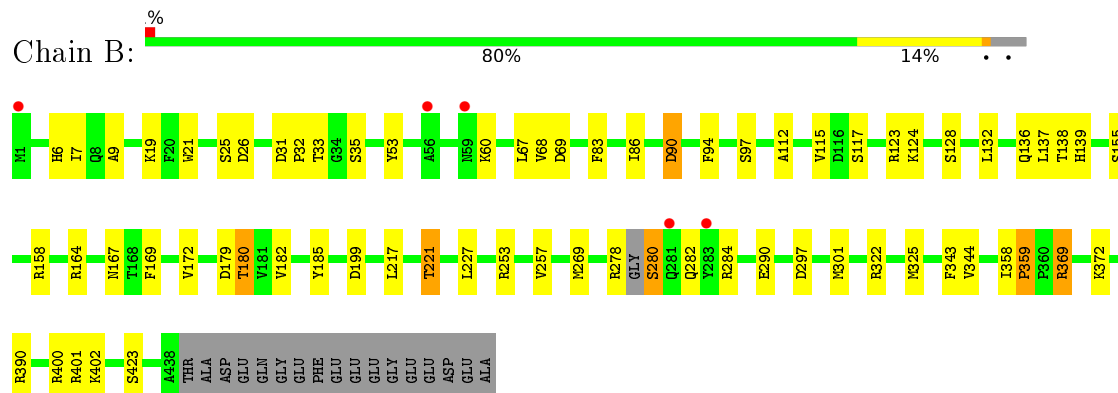
- Molecule 1: Tubulin alpha-1B chain



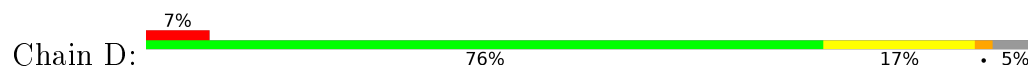
- Molecule 1: Tubulin alpha-1B chain

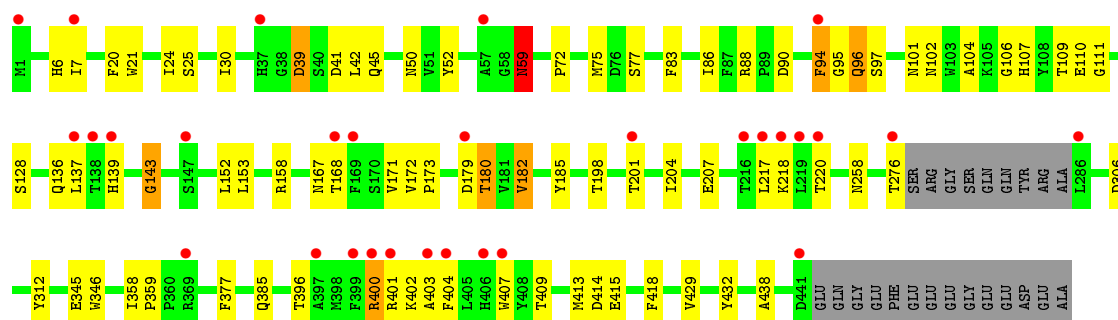


- Molecule 2: Tubulin beta chain

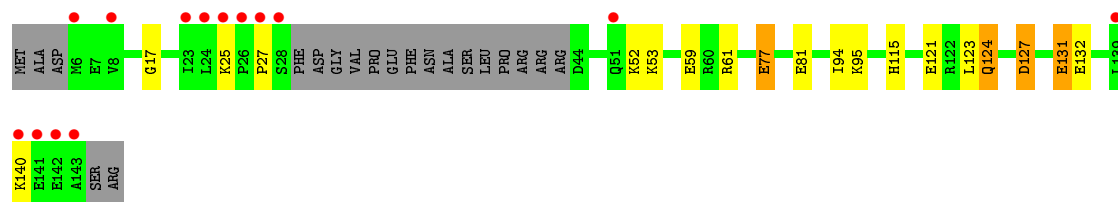


- Molecule 2: Tubulin beta chain

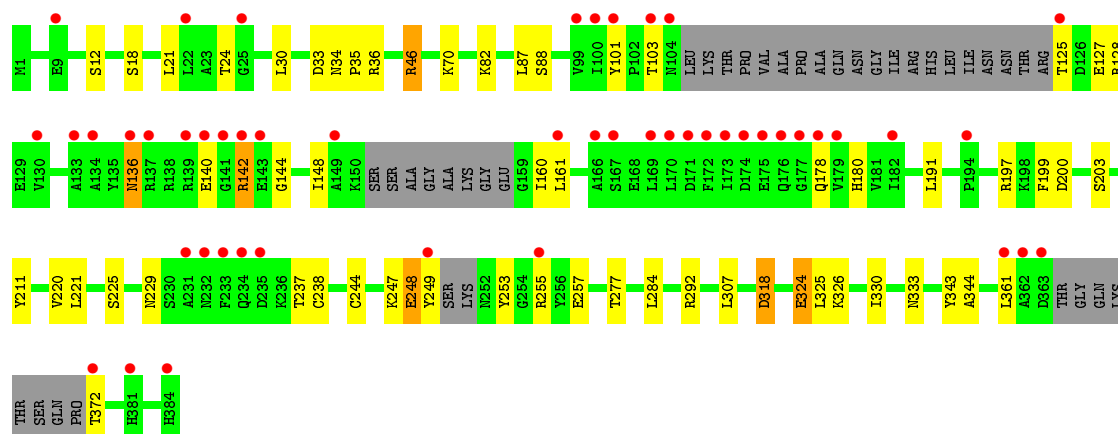
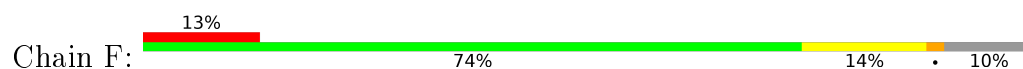




• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.47Å 157.42Å 183.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 39.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.50) 99.5 (39.91-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.184 , 0.235 0.192 , 0.236	Depositor DCC
$R_{free}$ test set	4906 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, CA, VLB, GTP, ACP, MES

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	0.71	0/3508	0.82	1/4762 (0.0%)
1	C	0.78	0/3524	0.85	4/4785 (0.1%)
2	B	0.80	1/3434 (0.0%)	0.87	7/4651 (0.2%)
2	D	0.68	2/3384 (0.1%)	0.81	4/4586 (0.1%)
3	E	0.71	0/1022	0.81	1/1356 (0.1%)
4	F	0.59	0/2916	0.78	3/3940 (0.1%)
All	All	0.72	3/17788 (0.0%)	0.83	20/24080 (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	C	0	1
4	F	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	179	ASP	CB-CG	-6.36	1.38	1.51
2	D	173	PRO	N-CD	5.23	1.55	1.47
2	D	359	PRO	N-CD	5.20	1.55	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	61	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	C	98	ASP	CB-CG-OD2	-6.31	112.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	306	ASP	CB-CG-OD1	6.28	123.95	118.30
2	D	359	PRO	C-N-CD	6.27	141.58	128.40
2	B	179	ASP	CB-CG-OD1	-6.21	112.71	118.30
2	B	390	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	358	ILE	C-N-CD	6.00	141.01	128.40
1	C	381	THR	CB-CA-C	-5.92	95.63	111.60
2	B	359	PRO	C-N-CD	5.87	140.72	128.40
2	B	297	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	98	ASP	CB-CG-OD1	5.73	123.45	118.30
2	D	358	ILE	C-N-CD	5.66	140.28	128.40
4	F	36	ARG	NE-CZ-NH2	-5.51	117.54	120.30
4	F	36	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	422	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	B	179	ASP	CB-CA-C	-5.41	99.58	110.40
2	D	172	VAL	C-N-CD	5.22	139.36	128.40
2	B	172	VAL	C-N-CD	5.16	139.24	128.40
4	F	318	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	214	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	163	LYS	Peptide
4	F	136	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	3430	0	3340	16	0
1	C	3446	0	3354	33	0
2	B	3360	0	3242	40	0
2	D	3311	0	3192	40	0
3	E	1014	0	1029	9	0
4	F	2849	0	2796	22	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	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
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	18	0	24	0	0
8	B	6	0	8	1	0
8	C	18	0	24	12	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	24	0	26	4	0
11	C	59	0	58	5	0
12	F	31	0	14	2	0
13	A	47	0	0	1	0
13	B	56	0	0	1	0
13	C	83	0	0	6	0
13	D	8	0	0	2	0
13	E	1	0	0	0	0
13	F	24	0	0	1	0
All	All	17912	0	17155	159	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 5.

All (159) 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)
2:B:35:SER:OG	2:B:60:LYS:NZ	1.65	1.30
2:D:432:TYR:OH	13:D:601:HOH:O	1.71	1.09
11:C:507:VLB:H511	11:C:507:VLB:H582	1.43	1.01
2:B:33:THR:HG22	2:B:60:LYS:HE3	1.58	0.85
2:B:83:PHE:O	2:B:86:ILE:HG22	1.79	0.82
2:B:33:THR:CG2	2:B:60:LYS:HE3	2.14	0.77
2:D:96:GLN:HG2	2:D:97:SER:N	1.99	0.77
1:C:381:THR:HG23	13:C:667:HOH:O	1.87	0.73
8:C:506:GOL:O1	8:C:506:GOL:O3	2.11	0.69
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.75	0.68
11:C:507:VLB:C51	11:C:507:VLB:H582	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:TYR:CD1	2:D:418:PHE:HE2	2.12	0.67
13:C:663:HOH:O	3:E:115:HIS:HE1	1.76	0.67
2:B:278:ARG:C	2:B:280:SER:N	2.49	0.66
2:B:33:THR:HG22	2:B:60:LYS:CE	2.26	0.64
2:D:7:ILE:O	2:D:137:LEU:HD12	1.96	0.63
3:E:131:GLU:HA	3:E:131:GLU:OE2	1.96	0.63
4:F:148:ILE:HD11	4:F:160:ILE:HD11	1.79	0.63
2:B:35:SER:HG	2:B:60:LYS:NZ	1.95	0.63
1:A:60:LYS:NZ	1:A:85:GLN:O	2.18	0.62
2:B:199:ASP:OD1	10:B:504:MES:H32	1.99	0.62
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.36	0.61
11:C:507:VLB:O32	11:C:507:VLB:C73	2.47	0.61
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.35	0.61
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.33	0.61
2:B:132:LEU:O	2:B:164:ARG:NH1	2.30	0.61
2:D:414:ASP:OD1	2:D:415:GLU:N	2.34	0.60
2:B:401:ARG:HH21	8:B:506:GOL:H11	1.66	0.60
2:D:136:GLN:HA	2:D:167:ASN:O	2.01	0.60
1:C:309:HIS:CE1	13:C:612:HOH:O	2.55	0.59
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.38	0.59
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.85	0.58
1:C:229:ARG:HG2	8:C:505:GOL:O2	2.04	0.57
2:D:21:TRP:O	2:D:25:SER:OG	2.09	0.57
2:B:221:THR:CG2	2:B:221:THR:O	2.53	0.56
2:D:143:GLY:HA3	9:D:501:GDP:O3A	2.05	0.56
2:D:217:LEU:C	2:D:218:LYS:HG2	2.27	0.55
4:F:324:GLU:O	4:F:325:LEU:HB2	2.05	0.55
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.42	0.55
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.26	0.54
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.89	0.54
2:B:31:ASP:OD1	2:B:33:THR:HB	2.07	0.54
3:E:124:GLN:O	3:E:127:ASP:N	2.40	0.54
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.89	0.53
2:D:401:ARG:O	2:D:403:ALA:N	2.41	0.53
2:D:59:ASN:OD1	2:D:59:ASN:N	2.40	0.53
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.12	0.53
2:B:284:ARG:NH2	2:B:290:GLU:OE1	2.43	0.52
1:C:229:ARG:CG	8:C:505:GOL:O2	2.57	0.52
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.44	0.52
3:E:124:GLN:HA	3:E:124:GLN:OE1	2.10	0.52
1:C:207:GLU:OE2	8:C:504:GOL:H11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:THR:HB	13:C:608:HOH:O	2.09	0.51
2:B:90:ASP:OD1	2:B:90:ASP:N	2.44	0.51
1:C:363:VAL:HG21	8:C:505:GOL:H11	1.93	0.51
2:D:39:ASP:N	2:D:39:ASP:OD1	2.41	0.51
1:C:304:LYS:HG3	8:C:504:GOL:H12	1.93	0.51
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.29	0.50
2:B:253:ARG:O	2:B:257:VAL:HG23	2.12	0.50
4:F:191:LEU:HA	4:F:197:ARG:O	2.10	0.50
2:B:269:MET:HE1	2:B:301:MET:HG3	1.93	0.50
1:C:171:ILE:HD13	1:C:171:ILE:N	2.25	0.50
1:C:1:MET:O	1:C:2:ARG:HB2	2.11	0.50
2:D:182:VAL:HG22	2:D:185:TYR:HD2	1.76	0.50
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.94	0.50
4:F:200:ASP:OD2	12:F:401:ACP:O3'	2.30	0.49
1:C:229:ARG:HG2	8:C:505:GOL:C2	2.41	0.49
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.42	0.49
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.12	0.49
1:C:209:ILE:HD11	1:C:302:MET:HG2	1.93	0.49
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.12	0.48
4:F:21:LEU:O	4:F:24:THR:OG1	2.27	0.48
4:F:248:GLU:O	4:F:249:TYR:CD2	2.66	0.48
1:C:19:ALA:HA	8:C:505:GOL:H12	1.95	0.48
3:E:121:GLU:O	3:E:124:GLN:HB2	2.13	0.48
2:D:96:GLN:HG2	2:D:97:SER:H	1.76	0.48
2:B:164:ARG:HD2	13:B:614:HOH:O	2.13	0.48
11:C:507:VLB:H19	11:C:507:VLB:H213	1.72	0.48
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.96	0.47
2:D:400:ARG:HG3	2:D:401:ARG:N	2.30	0.47
1:C:304:LYS:HE3	8:C:504:GOL:H31	1.95	0.47
1:A:110:ILE:O	1:A:110:ILE:HG22	2.15	0.47
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.15	0.47
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.50	0.47
2:B:7:ILE:O	2:B:137:LEU:HA	2.15	0.46
1:C:55:GLU:HA	1:C:60:LYS:O	2.14	0.46
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.98	0.46
2:D:102:ASN:ND2	2:D:407:TRP:O	2.47	0.46
2:B:227:LEU:HD22	11:C:507:VLB:H711	1.97	0.46
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.46
2:B:158:ARG:NE	10:B:504:MES:O1	2.49	0.46
1:C:381:THR:CG2	13:C:667:HOH:O	2.53	0.46
2:B:199:ASP:OD2	10:B:504:MES:H52	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:O	2:B:280:SER:N	2.50	0.45
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.99	0.45
2:D:83:PHE:O	2:D:86:ILE:HG22	2.16	0.45
4:F:247:LYS:HE3	4:F:253:TYR:CZ	2.52	0.45
4:F:343:TYR:O	4:F:344:ALA:C	2.55	0.45
2:B:25:SER:HA	2:B:53:TYR:OH	2.17	0.44
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.17	0.44
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.44
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
2:D:107:HIS:O	2:D:152:LEU:HD22	2.18	0.44
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.52	0.44
2:B:343:PHE:O	2:B:344:VAL:C	2.53	0.44
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.53	0.44
8:C:506:GOL:HO1	8:C:506:GOL:HO3	1.61	0.44
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.44
4:F:46:ARG:NH2	4:F:46:ARG:HB3	2.33	0.43
2:B:158:ARG:HG3	10:B:504:MES:H62	2.00	0.43
1:A:166:LYS:HE2	1:A:197:HIS:O	2.18	0.43
1:A:55:GLU:HA	1:A:60:LYS:O	2.18	0.43
1:A:17:GLY:O	1:A:18:ASN:C	2.56	0.43
4:F:330:ILE:HD13	4:F:330:ILE:HA	1.77	0.43
2:B:269:MET:HE2	2:B:301:MET:SD	2.58	0.43
4:F:333:ASN:HB3	13:F:518:HOH:O	2.18	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.19	0.43
1:C:304:LYS:HB3	8:C:504:GOL:H31	2.01	0.42
2:D:101:ASN:ND2	2:D:180:THR:HG21	2.34	0.42
1:A:209:ILE:HD11	1:A:302:MET:SD	2.59	0.42
2:B:112:ALA:O	2:B:115:VAL:HG12	2.19	0.42
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.42
2:D:438:ALA:O	13:D:602:HOH:O	2.21	0.42
2:B:269:MET:CE	2:B:301:MET:HG3	2.49	0.42
3:E:77:GLU:O	3:E:81:GLU:HG3	2.19	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
4:F:101:TYR:O	4:F:128:ARG:NH2	2.52	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.54	0.42
2:B:9:ALA:HA	2:B:68:VAL:O	2.20	0.42
1:C:304:LYS:CB	8:C:504:GOL:H31	2.50	0.42
1:C:333:ALA:O	1:C:337:THR:HG23	2.20	0.41
2:B:138:THR:HG22	2:B:169:PHE:HB2	2.02	0.41
1:C:157:LEU:HA	1:C:157:LEU:HD23	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:PRO:HD2	13:C:641:HOH:O	2.20	0.41
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.51	0.41
2:D:102:ASN:OD1	2:D:102:ASN:C	2.59	0.41
2:B:97:SER:O	1:C:2:ARG:NH2	2.53	0.41
1:C:316:CYS:HA	1:C:352:LYS:O	2.20	0.41
2:D:168:THR:HG23	2:D:198:THR:HG21	2.02	0.41
2:D:52:TYR:OH	2:D:136:GLN:OE1	2.32	0.41
4:F:136:ASN:O	4:F:140:GLU:HG2	2.21	0.41
4:F:178:GLN:OE1	4:F:178:GLN:N	2.54	0.41
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.55	0.41
1:A:45:GLY:HA3	13:A:624:HOH:O	2.21	0.41
2:D:41:ASP:C	2:D:45:GLN:N	2.73	0.41
2:D:171:VAL:HA	2:D:204:ILE:O	2.21	0.41
2:D:168:THR:OG1	2:D:201:THR:HG23	2.21	0.40
2:D:41:ASP:C	2:D:45:GLN:H	2.24	0.40
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.40
2:B:182:VAL:O	2:B:185:TYR:HB2	2.20	0.40
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.40
2:D:185:TYR:CD1	2:D:418:PHE:CE2	3.02	0.40
2:B:180:THR:HG22	1:C:352:LYS:NZ	2.37	0.40
2:D:72:PRO:HG3	2:D:95:GLY:O	2.22	0.40
2:B:69:ASP:O	2:B:94:PHE:HA	2.21	0.40
1:C:151:SER:HB2	1:C:193:THR:HG22	2.03	0.40
4:F:244:CYS:O	4:F:247:LYS:N	2.55	0.40
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.97	0.40

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	437/451 (97%)	417 (95%)	20 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	439/451 (97%)	423 (96%)	14 (3%)	2 (0%)	34	55
2	B	423/445 (95%)	417 (99%)	6 (1%)	0	100	100
2	D	418/445 (94%)	390 (93%)	23 (6%)	5 (1%)	16	29
3	E	119/143 (83%)	111 (93%)	7 (6%)	1 (1%)	24	41
4	F	336/384 (88%)	306 (91%)	27 (8%)	3 (1%)	21	37
All	All	2172/2319 (94%)	2064 (95%)	97 (4%)	11 (0%)	34	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	402	LYS
3	E	27	PRO
1	C	2	ARG
1	C	164	LYS
2	D	143	GLY
2	D	404	PHE
4	F	142	ARG
2	D	59	ASN
2	D	180	THR
4	F	88	SER
4	F	144	GLY

### 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	370/379 (98%)	360 (97%)	10 (3%)	52	79
1	C	372/379 (98%)	365 (98%)	7 (2%)	65	87
2	B	368/381 (97%)	347 (94%)	21 (6%)	25	46
2	D	363/381 (95%)	341 (94%)	22 (6%)	23	42
3	E	110/127 (87%)	99 (90%)	11 (10%)	9	18
4	F	312/342 (91%)	284 (91%)	28 (9%)	12	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1895/1989 (95%)	1796 (95%)	99 (5%)	29 51

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	62	VAL
1	A	66	VAL
1	A	68	VAL
1	A	71	GLU
1	A	163	LYS
1	A	179	THR
1	A	338	LYS
1	A	381	THR
1	A	437	VAL
2	B	19	LYS
2	B	90	ASP
2	B	117	SER
2	B	123	ARG
2	B	124	LYS
2	B	128	SER
2	B	139	HIS
2	B	155	SER
2	B	180	THR
2	B	217	LEU
2	B	221	THR
2	B	280	SER
2	B	282	GLN
2	B	322	ARG
2	B	325	MET
2	B	359	PRO
2	B	369	ARG
2	B	372	LYS
2	B	400	ARG
2	B	402	LYS
2	B	423	SER
1	C	120	ASP
1	C	245	ASP
1	C	315	CYS
1	C	326	LYS
1	C	340	SER
1	C	381	THR

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Mol	Chain	Res	Type
1	C	440	VAL
2	D	30	ILE
2	D	39	ASP
2	D	42	LEU
2	D	50	ASN
2	D	59	ASN
2	D	77	SER
2	D	88	ARG
2	D	90	ASP
2	D	94	PHE
2	D	96	GLN
2	D	128	SER
2	D	139	HIS
2	D	153	LEU
2	D	179	ASP
2	D	182	VAL
2	D	207	GLU
2	D	220	THR
2	D	276	THR
2	D	345	GLU
2	D	396	THR
2	D	400	ARG
2	D	409	THR
3	E	25	LYS
3	E	52	LYS
3	E	53	LYS
3	E	59	GLU
3	E	77	GLU
3	E	95	LYS
3	E	124	GLN
3	E	127	ASP
3	E	131	GLU
3	E	132	GLU
3	E	140	LYS
4	F	12	SER
4	F	18	SER
4	F	30	LEU
4	F	33	ASP
4	F	46	ARG
4	F	70	LYS
4	F	87	LEU
4	F	103	THR

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Mol	Chain	Res	Type
4	F	125	THR
4	F	142	ARG
4	F	161	LEU
4	F	180	HIS
4	F	203	SER
4	F	211	TYR
4	F	220	VAL
4	F	225	SER
4	F	229	ASN
4	F	237	THR
4	F	238	CYS
4	F	248	GLU
4	F	255	ARG
4	F	277	THR
4	F	292	ARG
4	F	307	LEU
4	F	324	GLU
4	F	326	LYS
4	F	361	LEU
4	F	372	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	281	GLN
2	D	96	GLN
2	D	101	ASN
3	E	18	GLN
4	F	229	ASN
4	F	269	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	26,34,34	1.14	2 (7%)	29,54,54	1.74	5 (17%)
8	GOL	A	504	-	5,5,5	0.46	0	5,5,5	0.47	0
8	GOL	A	505	-	5,5,5	0.41	0	5,5,5	1.02	0
8	GOL	A	506	-	5,5,5	0.70	0	5,5,5	0.54	0
9	GDP	B	501	6	24,30,30	1.23	3 (12%)	26,47,47	1.89	4 (15%)
10	MES	B	504	-	12,12,12	2.19	3 (25%)	15,16,16	8.17	8 (53%)
10	MES	B	505	-	12,12,12	2.24	1 (8%)	15,16,16	2.03	1 (6%)
8	GOL	B	506	-	5,5,5	0.36	0	5,5,5	0.34	0
5	GTP	C	501	6	26,34,34	1.26	4 (15%)	29,54,54	2.21	8 (27%)
8	GOL	C	504	-	5,5,5	0.57	0	5,5,5	0.99	0
8	GOL	C	505	-	5,5,5	0.61	0	5,5,5	0.70	0
8	GOL	C	506	-	5,5,5	0.40	0	5,5,5	0.50	0
11	VLB	C	507	-	63,67,67	2.67	18 (28%)	71,108,108	2.09	17 (23%)
9	GDP	D	501	6	24,30,30	1.20	3 (12%)	26,47,47	1.66	5 (19%)
12	ACP	F	401	-	29,33,33	2.03	7 (24%)	29,52,52	1.81	3 (10%)

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
8	GOL	A	504	-	-	0/4/4/4	0/0/0/0
8	GOL	A	505	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	506	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
8	GOL	B	506	-	-	0/4/4/4	0/0/0/0
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GOL	C	504	-	-	0/4/4/4	0/0/0/0
8	GOL	C	505	-	-	0/4/4/4	0/0/0/0
8	GOL	C	506	-	-	0/4/4/4	0/0/0/0
11	VLB	C	507	-	-	0/38/131/131	0/7/9/9
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
12	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	507	VLB	C68-C67	-7.77	1.44	1.53
10	B	505	MES	C8-S	-7.37	1.66	1.77
11	C	507	VLB	C12-C13	-6.54	1.41	1.51
10	B	504	MES	C8-S	-6.23	1.68	1.77
11	C	507	VLB	C58-C59	-5.79	1.44	1.52
11	C	507	VLB	C68-C73	-5.72	1.45	1.53
11	C	507	VLB	C18-C13	-3.74	1.34	1.39
5	C	501	GTP	C4-N3	-3.35	1.30	1.35
11	C	507	VLB	C60-C65	-3.24	1.33	1.42
11	C	507	VLB	C61-C60	-3.09	1.36	1.42
11	C	507	VLB	C17-C18	-3.08	1.34	1.39
11	C	507	VLB	C14-C13	-3.06	1.34	1.39
11	C	507	VLB	C20-C5	-3.02	1.49	1.55
11	C	507	VLB	C59-C60	-2.95	1.36	1.41
11	C	507	VLB	C64-C65	-2.88	1.36	1.41
12	F	401	ACP	PG-O2G	-2.73	1.48	1.54
11	C	507	VLB	C18-N1	-2.20	1.35	1.39
11	C	507	VLB	C68-C15	-2.18	1.45	1.54
5	C	501	GTP	C2'-C1'	-2.13	1.50	1.53
9	D	501	GDP	C2'-C1'	-2.07	1.50	1.53
5	C	501	GTP	C5-C4	2.02	1.45	1.40
10	B	504	MES	O1S-S	2.04	1.51	1.45
12	F	401	ACP	PB-C3B	2.15	1.82	1.80
5	C	501	GTP	C2-N2	2.15	1.38	1.34
12	F	401	ACP	PB-O2B	2.29	1.61	1.56
5	A	501	GTP	C5-C4	2.65	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	O4'-C1'	2.67	1.45	1.41
10	B	504	MES	O2S-S	2.75	1.53	1.45
11	C	507	VLB	C57-C58	2.77	1.61	1.52
9	D	501	GDP	C5-C4	2.77	1.46	1.40
9	B	501	GDP	C5-C4	2.81	1.46	1.40
9	B	501	GDP	C6-C5	2.84	1.47	1.41
12	F	401	ACP	PG-O3G	2.91	1.62	1.54
5	A	501	GTP	C6-C5	2.95	1.47	1.41
11	C	507	VLB	O75-C73	2.96	1.38	1.33
12	F	401	ACP	C5-C4	3.15	1.47	1.40
9	D	501	GDP	C6-C5	3.18	1.47	1.41
11	C	507	VLB	C19-N9	3.39	1.53	1.47
12	F	401	ACP	PG-O1G	5.42	1.62	1.50
12	F	401	ACP	PB-O3A	5.85	1.65	1.58
11	C	507	VLB	C6-C7	10.74	1.54	1.32

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O3S-S-O1S	-14.13	79.98	111.26
10	B	504	MES	O3S-S-O2S	-9.17	90.97	111.26
10	B	504	MES	O3S-S-C8	-8.82	86.66	104.99
12	F	401	ACP	N3-C2-N1	-7.38	123.07	128.87
11	C	507	VLB	C8-C7-C6	-6.52	109.72	122.73
5	C	501	GTP	C5-C6-N1	-5.24	116.67	123.52
11	C	507	VLB	C11-C12-C13	-4.86	103.53	112.40
5	A	501	GTP	C1'-N9-C4	-4.78	121.47	126.81
9	B	501	GDP	C5-C6-N1	-4.76	117.31	123.52
5	A	501	GTP	C5-C6-N1	-4.33	117.86	123.52
5	C	501	GTP	N3-C2-N1	-4.10	121.98	127.56
5	C	501	GTP	C1'-N9-C4	-3.95	122.40	126.81
9	D	501	GDP	C5-C6-N1	-3.49	118.96	123.52
5	C	501	GTP	C6-C5-C4	-3.47	116.89	120.86
9	B	501	GDP	C1'-N9-C4	-3.39	123.02	126.81
9	B	501	GDP	C6-C5-C4	-3.21	117.19	120.86
11	C	507	VLB	C63-C62-C61	-2.54	116.79	120.45
12	F	401	ACP	C1'-N9-C4	-2.26	124.29	126.81
11	C	507	VLB	C17-C18-C13	-2.23	119.18	122.04
5	A	501	GTP	N3-C2-N1	-2.15	124.63	127.56
11	C	507	VLB	C17-C16-C15	-2.08	120.17	122.14
9	D	501	GDP	C6-C5-C4	-2.07	118.50	120.86
11	C	507	VLB	C11-C10-N9	-2.07	100.22	104.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	O2G-PG-C3B	2.00	110.88	106.13
5	C	501	GTP	O2A-PA-O3A	2.02	113.92	105.27
11	C	507	VLB	C54-C55-N56	2.06	116.84	111.74
5	C	501	GTP	O2A-PA-O1A	2.37	124.88	112.56
9	D	501	GDP	C4'-O4'-C1'	2.38	112.16	109.64
10	B	504	MES	O2S-S-O1S	2.38	120.68	113.96
11	C	507	VLB	C2-C12-C19	2.48	118.55	114.10
5	C	501	GTP	N2-C2-N1	2.78	121.79	117.20
11	C	507	VLB	C53-C52-C69	2.78	111.82	108.66
10	B	504	MES	C6-C5-N4	2.81	114.41	110.11
5	A	501	GTP	O3G-PG-O1G	2.83	119.85	110.63
11	C	507	VLB	C13-C18-N1	2.97	113.90	111.06
10	B	504	MES	C5-N4-C3	3.12	115.86	108.87
9	D	501	GDP	C6-N1-C2	3.47	119.95	115.88
11	C	507	VLB	C4-O28-C29	3.67	124.13	117.75
11	C	507	VLB	C13-C12-C2	3.67	107.46	102.09
11	C	507	VLB	O75-C73-C68	3.69	115.48	111.16
9	D	501	GDP	O3B-PB-O1B	3.94	123.47	110.63
5	A	501	GTP	C6-N1-C2	3.94	120.50	115.88
11	C	507	VLB	O28-C4-C3	4.46	112.93	106.44
11	C	507	VLB	O28-C29-C30	4.55	119.75	111.09
11	C	507	VLB	C52-C69-N56	4.91	117.24	110.69
11	C	507	VLB	C19-C5-C6	5.20	115.39	108.36
9	B	501	GDP	C6-N1-C2	5.36	122.16	115.88
5	C	501	GTP	C6-N1-C2	6.01	122.93	115.88
10	B	505	MES	O2S-S-C8	6.48	111.45	106.87
10	B	504	MES	O2S-S-C8	12.97	116.03	106.87
10	B	504	MES	O1S-S-C8	20.93	121.66	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
10	B	504	MES	4	0
8	B	506	GOL	1	0
8	C	504	GOL	5	0
8	C	505	GOL	5	0
8	C	506	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	507	VLB	5	0
9	D	501	GDP	1	0
12	F	401	ACP	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 ⓘ

### 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	439/451 (97%)	0.03	10 (2%) 64 67	26, 45, 74, 106	0
1	C	440/451 (97%)	-0.25	2 (0%) 91 92	24, 38, 66, 97	0
2	B	427/445 (95%)	-0.14	5 (1%) 81 83	24, 38, 75, 109	0
2	D	422/445 (94%)	0.23	30 (7%) 19 21	33, 58, 89, 111	0
3	E	123/143 (86%)	0.50	14 (11%) 7 6	35, 62, 101, 125	0
4	F	346/384 (90%)	0.49	49 (14%) 4 3	33, 68, 121, 136	0
All	All	2197/2319 (94%)	0.08	110 (5%) 32 37	24, 49, 95, 136	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	104	ASN	7.7
3	E	143	ALA	6.8
4	F	177	GLY	5.3
1	A	282	TYR	5.2
4	F	139	ARG	5.1
4	F	133	ALA	4.9
2	D	400	ARG	4.5
2	D	404	PHE	4.3
4	F	169	LEU	4.3
4	F	362	ALA	4.3
4	F	101	TYR	4.3
4	F	140	GLU	4.1
4	F	173	ILE	4.1
2	D	218	LYS	4.0
4	F	137	ARG	4.0
4	F	149	ALA	4.0
2	D	407	TRP	4.0
4	F	175	GLU	4.0
4	F	232	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	142	ARG	3.9
4	F	171	ASP	3.8
4	F	100	ILE	3.7
1	A	438	ASP	3.7
2	D	1	MET	3.7
2	D	37	HIS	3.6
1	A	439	SER	3.6
4	F	233	PHE	3.5
4	F	103	THR	3.4
4	F	372	THR	3.4
4	F	172	PHE	3.4
4	F	167	SER	3.4
1	A	281	ALA	3.4
3	E	139	LEU	3.2
4	F	176	GLN	3.2
1	C	440	VAL	3.2
2	B	59	ASN	3.2
1	A	262	TYR	3.2
2	B	281	GLN	3.1
4	F	381	HIS	3.1
3	E	140	LYS	3.1
4	F	235	ASP	3.1
4	F	178	GLN	3.1
4	F	234	GLN	3.1
4	F	361	LEU	3.0
2	B	1	MET	3.0
2	D	401	ARG	3.0
4	F	363	ASP	2.9
2	B	283	TYR	2.9
3	E	24	LEU	2.9
4	F	170	LEU	2.9
4	F	99	VAL	2.9
3	E	8	VAL	2.8
4	F	249	TYR	2.8
2	D	216	THR	2.7
2	D	94	PHE	2.7
3	E	28	SER	2.7
3	E	27	PRO	2.7
1	C	340	SER	2.6
2	D	276	THR	2.6
3	E	25	LYS	2.6
2	D	137	LEU	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	26	PRO	2.6
4	F	136	ASN	2.6
3	E	142	GLU	2.6
2	D	169	PHE	2.5
4	F	231	ALA	2.5
4	F	182	ILE	2.5
2	D	168	THR	2.5
4	F	161	LEU	2.5
4	F	141	GLY	2.5
2	D	201	THR	2.5
4	F	134	ALA	2.5
4	F	125	THR	2.4
4	F	255	ARG	2.4
4	F	179	VAL	2.4
4	F	194	PRO	2.4
1	A	365	GLY	2.4
4	F	174	ASP	2.4
2	D	147	SER	2.4
3	E	51	GLN	2.4
2	D	179	ASP	2.3
2	D	138	THR	2.3
1	A	235	VAL	2.3
3	E	23	ILE	2.3
2	B	56	ALA	2.3
2	D	220	THR	2.3
2	D	217	LEU	2.3
4	F	166	ALA	2.2
3	E	6	MET	2.2
4	F	130	VAL	2.2
2	D	406	HIS	2.2
2	D	286	LEU	2.2
2	D	7	ILE	2.2
1	A	169	PHE	2.2
2	D	399	PHE	2.2
4	F	384	HIS	2.2
4	F	9	GLU	2.2
4	F	25	GLY	2.2
2	D	219	LEU	2.2
3	E	141	GLU	2.1
4	F	143	GLU	2.1
2	D	397	ALA	2.1
2	D	57	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	PHE	2.1
2	D	441	ASP	2.1
2	D	139	HIS	2.1
1	A	346	TRP	2.1
4	F	22	LEU	2.0
2	D	403	ALA	2.0
2	D	369	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
8	GOL	C	505	6/6	0.63	0.67	18.81	81,96,107,130	0
6	MG	D	502	1/1	0.87	0.43	16.00	53,53,53,53	0
8	GOL	A	506	6/6	0.80	0.29	8.68	56,64,70,71	0
8	GOL	C	506	6/6	0.93	0.21	6.02	49,62,65,74	0
8	GOL	A	505	6/6	0.92	0.13	1.47	61,65,68,69	0
8	GOL	A	504	6/6	0.76	0.22	1.37	70,74,80,86	0
10	MES	B	505	12/12	0.95	0.14	1.08	65,71,76,76	0
10	MES	B	504	12/12	0.91	0.17	0.16	53,63,74,82	0
9	GDP	B	501	28/28	0.99	0.14	-0.40	23,26,28,29	0
5	GTP	C	501	32/32	0.99	0.12	-0.54	25,28,32,33	0
5	GTP	A	501	32/32	0.99	0.15	-0.55	25,30,34,34	0
11	VLB	C	507	59/59	0.96	0.12	-0.76	28,35,44,49	0
12	ACP	F	401	31/31	0.92	0.14	-0.93	72,85,113,115	0
9	GDP	D	501	28/28	0.95	0.13	-0.97	44,48,60,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	502	1/1	0.98	0.07	-2.13	28,28,28,28	0
6	MG	A	502	1/1	0.99	0.07	-2.20	36,36,36,36	0
7	CA	A	503	1/1	0.99	0.04	-2.45	62,62,62,62	0
7	CA	C	503	1/1	0.99	0.02	-4.54	49,49,49,49	0
7	CA	B	503	1/1	0.98	0.07	-	76,76,76,76	0
8	GOL	B	506	6/6	0.84	0.23	-	80,84,88,88	0
8	GOL	C	504	6/6	0.84	0.35	-	55,69,70,72	0
6	MG	B	502	1/1	0.54	0.33	-	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.