



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2017 – 09:04 AM EDT

PDB ID : 5JVD
Title : Tubulin-TUB092 complex
Authors : Canela, M.-D.; Noppen, S.; Bueno, O.; Prota, A.E.; Bargsten, K.; Saez-Calvo, G.; Jimeno, M.-L.; Benkheil, M.; Ribatti, D.; Velazquez, S.; Camarasa, M.-J.; Diaz, J.F.; Steinmetz, M.O.; Priego, E.-M.; Perez-Perez, M.-J.; Liekens, S.
Deposited on : unknown
Resolution : 2.39 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

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-20029824
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-20029824

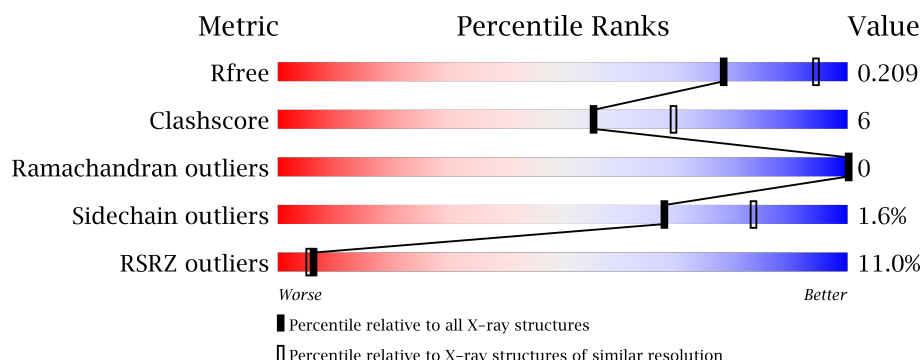
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 ≥ 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>6%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>• •</div> </div> </div>
1	C	451	<div> <div>•</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>•</div> </div> </div>
2	D	445	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div> </div>
3	E	143	<div> <div>14%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

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
8	GOL	A	505	-	-	-	X
8	GOL	B	504	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17853 atoms, of which 36 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	438	Total	C	N	O	S	0	0	0
			3422	2165	582	654	21			
1	C	439	Total	C	N	O	S	0	0	0
			3429	2170	583	655	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	1	0
			3346	2103	570	647	26			
2	D	422	Total	C	N	O	S	0	0	0
			3313	2082	563	642	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	0	0
			1008	622	182	199	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	conflict	UNP P63043
E	4	ALA	SER	conflict	UNP P63043

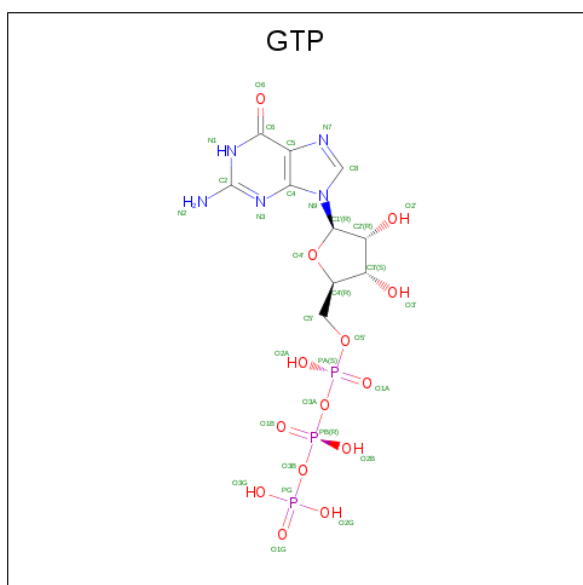
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	348	Total	C	N	O	S	0	0	0
			2842	1821	487	520	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		

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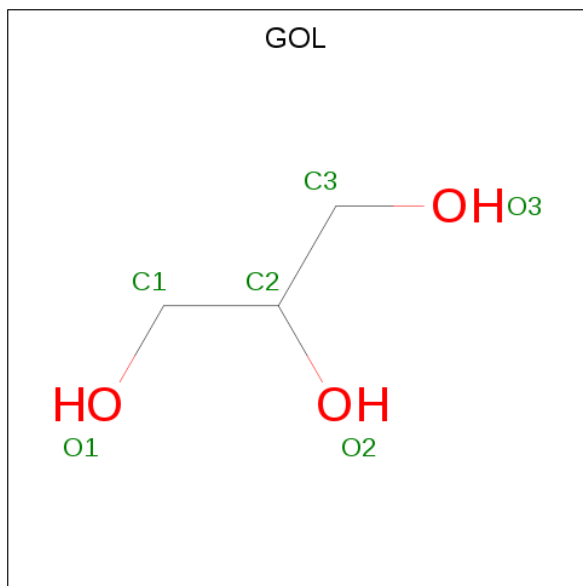
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- 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		
7	E	1	Total	Ca	0	0
			1	1		

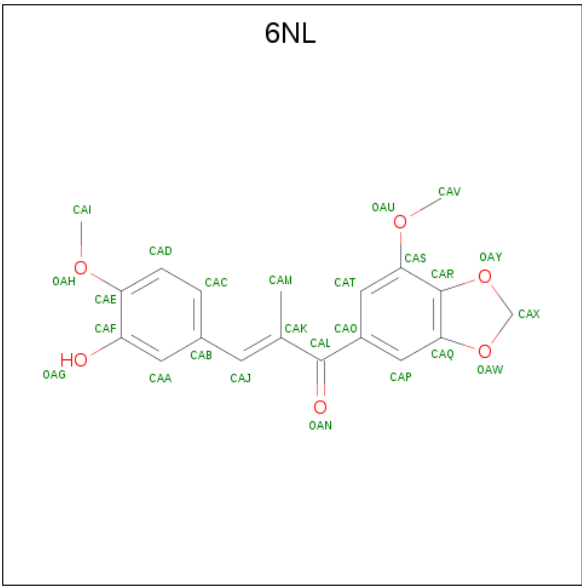
- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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	B	1	Total	C	O	0	0
			6	3	3		

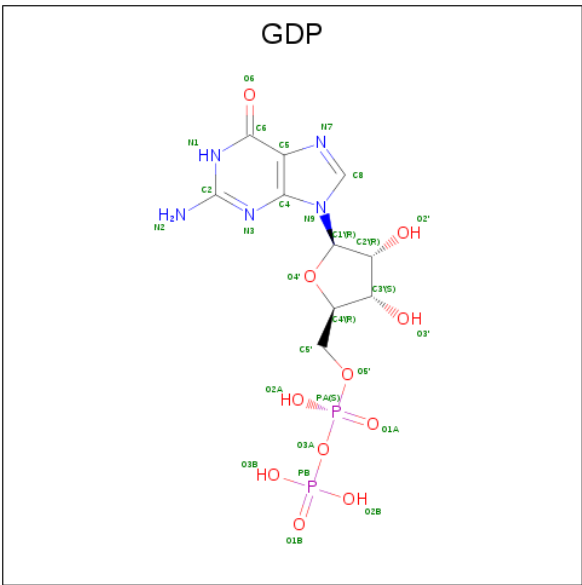
- Molecule 9 is (2E)-3-(3-hydroxy-4-methoxyphenyl)-1-(7-methoxy-2H-1,3-benzodioxol-5-yl)-

2-methylprop-2-en-1-one (three-letter code: 6NL) (formula: C₁₉H₁₈O₆).



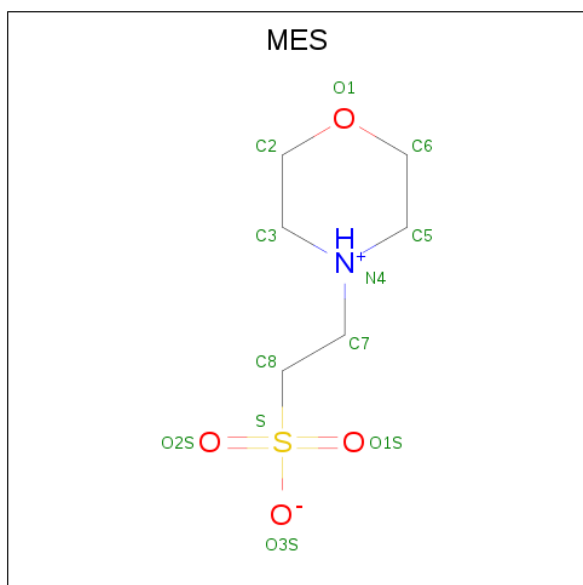
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			43	19	18	6		
9	D	1	Total	C	H	O	0	0
			43	19	18	6		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



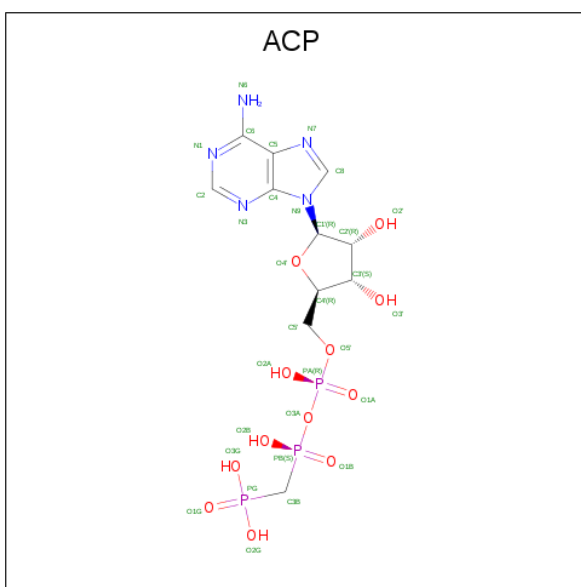
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
10	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- 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		

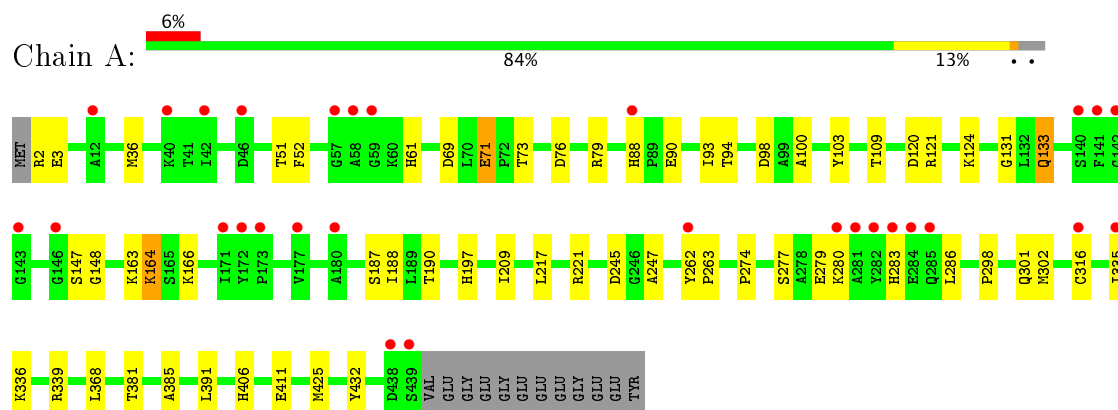
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	43	Total O 43 43	0	0
13	B	43	Total O 43 43	0	0
13	C	95	Total O 95 95	0	0
13	D	18	Total O 18 18	0	0
13	E	9	Total O 9 9	0	0
13	F	9	Total O 9 9	0	0

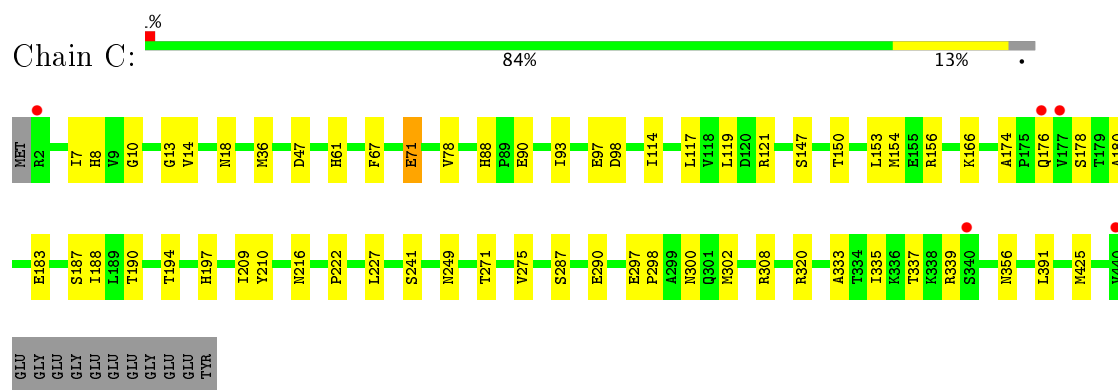
3 Residue-property plots [i](#)

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.

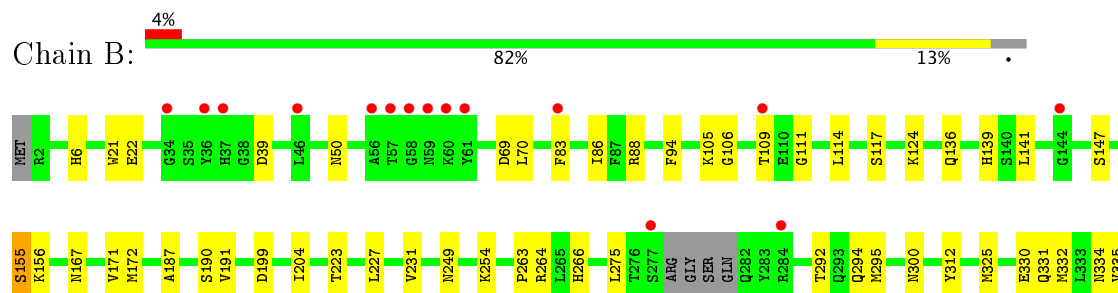
- Molecule 1: Tubulin alpha-1B chain

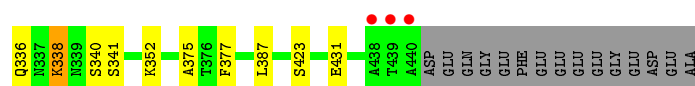


- Molecule 1: Tubulin alpha-1B chain

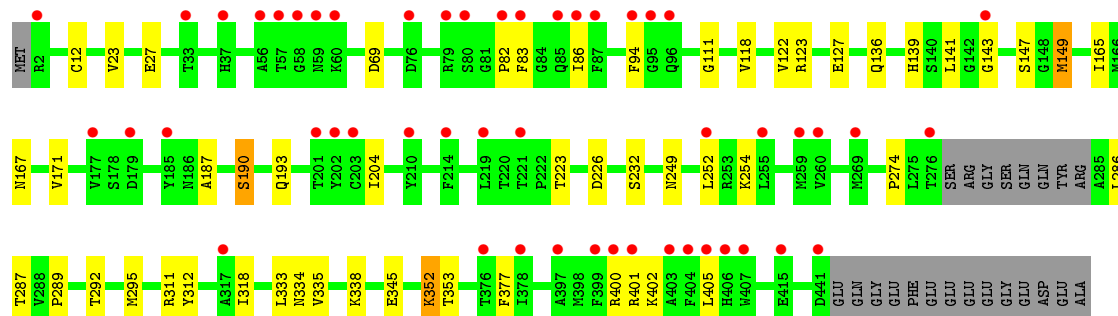
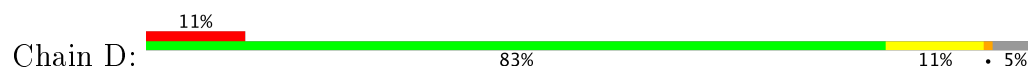


- Molecule 2: Tubulin beta-2B chain

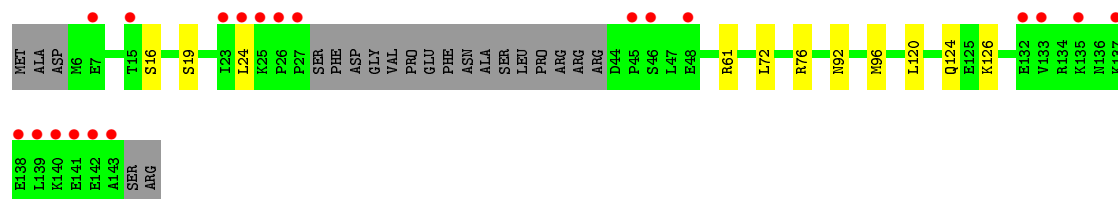
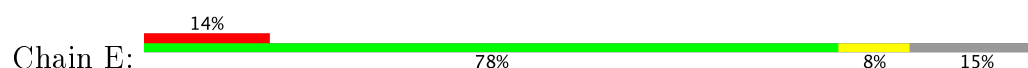




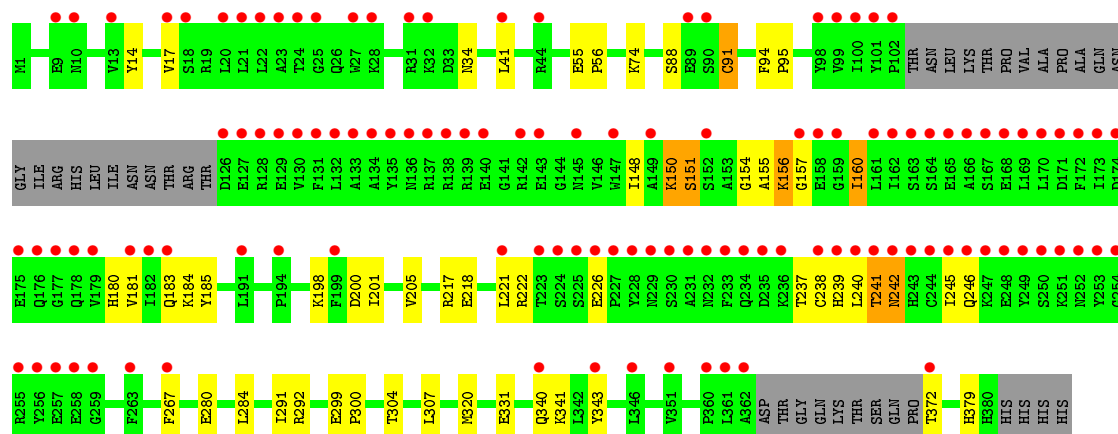
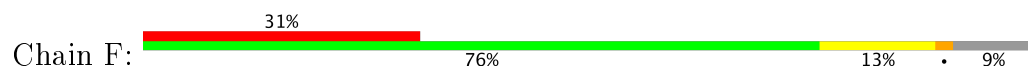
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.25Å 156.32Å 180.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 2.39 49.46 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.46-2.39) 99.7 (49.46-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.169 , 0.208 0.169 , 0.209	Depositor DCC
R_{free} test set	5815 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17853	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 6NL, 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	0.28	0/3500	0.45	0/4752
1	C	0.34	0/3507	0.48	0/4762
2	B	0.31	0/3423	0.46	0/4637
2	D	0.27	0/3386	0.44	0/4588
3	E	0.27	0/1016	0.38	0/1348
4	F	0.24	0/2907	0.44	0/3926
All	All	0.29	0/17739	0.45	0/24013

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3422	0	3327	38	0
1	C	3429	0	3337	36	0
2	B	3346	0	3225	45	0
2	D	3313	0	3189	36	0
3	E	1008	0	1024	10	0
4	F	2842	0	2809	50	0
5	A	32	0	12	0	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
6	F	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
7	E	1	0	0	0	0
8	A	12	0	16	2	0
8	B	6	0	8	0	0
9	B	25	18	0	0	0
9	D	25	18	0	2	0
10	B	28	0	12	0	0
10	D	28	0	12	2	0
11	B	12	0	12	1	0
12	F	31	0	14	5	0
13	A	43	0	0	0	0
13	B	43	0	0	1	0
13	C	95	0	0	1	0
13	D	18	0	0	1	0
13	E	9	0	0	0	0
13	F	9	0	0	0	0
All	All	17817	36	17009	205	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 6.

All (205) 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:334:ASN:ND2	2:B:338:LYS:HE3	1.73	1.02
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.03	0.91
4:F:241:THR:HG1	12:F:402:ACP:HO3'	1.12	0.90
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.08	0.86
4:F:151:SER:HB2	4:F:154:GLY:H	1.39	0.86
2:B:334:ASN:HD21	2:B:338:LYS:HE3	1.38	0.83
4:F:150:LYS:NZ	12:F:402:ACP:O2A	2.11	0.83
4:F:155:ALA:HB1	4:F:156:LYS:HD3	1.64	0.80
2:D:223:THR:N	2:D:226:ASP:OD2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.18	0.76
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.32	0.74
2:B:334:ASN:CG	2:B:338:LYS:HE3	2.09	0.73
1:A:164:LYS:HD2	1:A:164:LYS:N	2.04	0.72
1:A:221:ARG:HD3	2:B:325:MET:HB3	1.71	0.72
4:F:241:THR:OG1	12:F:402:ACP:O3'	2.00	0.69
1:A:280:LYS:O	1:A:283:HIS:NE2	2.29	0.66
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.12	0.65
1:A:280:LYS:HB2	1:A:283:HIS:HE2	1.62	0.64
2:B:334:ASN:O	2:B:338:LYS:HD2	1.97	0.64
4:F:155:ALA:C	4:F:156:LYS:HE3	2.18	0.64
2:D:274:PRO:HB3	2:D:286:LEU:HD21	1.81	0.63
4:F:157:GLY:HA2	4:F:160:ILE:HD11	1.81	0.63
4:F:221:LEU:HD11	4:F:267:PHE:CG	2.34	0.63
4:F:156:LYS:HB2	4:F:156:LYS:NZ	2.14	0.62
4:F:151:SER:HG	4:F:180:HIS:CE1	2.17	0.62
2:B:249:ASN:O	2:B:254:LYS:NZ	2.33	0.62
2:D:352:LYS:HG3	9:D:500:6NL:CAF	2.32	0.60
4:F:292:ARG:NH1	4:F:379:HIS:O	2.34	0.59
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.84	0.59
3:E:92:ASN:O	3:E:96:MET:HG2	2.02	0.59
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.67	0.59
4:F:156:LYS:HB2	4:F:156:LYS:HZ2	1.68	0.59
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.85	0.58
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.84	0.58
2:B:294:GLN:OE1	13:B:601:HOH:O	2.17	0.58
1:C:190:THR:O	1:C:194:THR:HG23	2.04	0.58
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.86	0.58
1:C:241:SER:HA	1:C:249:ASN:HD21	1.69	0.57
4:F:148:ILE:HG22	4:F:183:GLN:O	2.04	0.57
2:B:332:MET:O	2:B:336:GLN:HG3	2.04	0.57
4:F:201:ILE:HG12	4:F:221:LEU:CD2	2.34	0.57
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.87	0.57
1:C:176:GLN:NE2	2:D:333:LEU:HD21	2.20	0.57
1:A:280:LYS:HB2	1:A:283:HIS:NE2	2.20	0.56
8:A:504:GOL:O3	8:A:504:GOL:O1	2.19	0.56
1:A:166:LYS:HE2	1:A:197:HIS:O	2.06	0.55
2:B:50:ASN:ND2	2:B:50:ASN:H	2.04	0.55
4:F:200:ASP:N	4:F:241:THR:HG21	2.21	0.55
1:A:3:GLU:O	1:A:133:GLN:HG3	2.07	0.55
2:B:136:GLN:HA	2:B:167:ASN:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.89	0.54
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.89	0.54
1:C:98:ASP:OD2	2:D:254:LYS:NZ	2.41	0.54
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.89	0.54
3:E:72:LEU:O	3:E:76:ARG:HG2	2.07	0.54
1:C:47:ASP:OD2	13:C:601:HOH:O	2.18	0.54
1:C:320:ARG:HA	1:C:356:ASN:O	2.07	0.54
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.88	0.54
2:B:83:PHE:O	2:B:86:ILE:HG22	2.07	0.54
2:D:171:VAL:HA	2:D:204:ILE:O	2.08	0.54
4:F:157:GLY:HA3	4:F:245:ILE:HD11	1.90	0.54
4:F:160:ILE:HD12	4:F:240:LEU:CD1	2.38	0.54
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.91	0.53
4:F:237:THR:O	4:F:246:GLN:NE2	2.35	0.53
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.91	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.09	0.52
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.44	0.52
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.74	0.52
4:F:155:ALA:O	4:F:156:LYS:HE3	2.09	0.52
2:D:83:PHE:O	2:D:86:ILE:HG22	2.09	0.52
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.45	0.52
1:A:2:ARG:HA	1:A:131:GLY:O	2.10	0.51
4:F:150:LYS:HG3	4:F:181:VAL:HG23	1.93	0.51
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.93	0.51
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.76	0.51
1:A:221:ARG:NH1	2:B:325:MET:SD	2.84	0.50
1:C:209:ILE:HD11	1:C:302:MET:SD	2.51	0.50
2:D:143:GLY:HA3	10:D:501:GDP:O5'	2.10	0.50
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.92	0.50
4:F:88:SER:O	4:F:91:CYS:HB3	2.11	0.50
1:A:298:PRO:HA	1:A:301:GLN:CD	2.33	0.50
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.94	0.50
2:B:141:LEU:HD12	2:B:172:MET:SD	2.52	0.49
2:D:82:PRO:O	2:D:83:PHE:HB2	2.12	0.49
4:F:160:ILE:HD12	4:F:240:LEU:HD11	1.94	0.49
4:F:320:MET:HE2	12:F:402:ACP:C2	2.42	0.49
1:A:109:THR:OG1	1:A:411:GLU:OE2	2.19	0.49
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.94	0.49
2:D:147:SER:HB2	2:D:190:SER:OG	2.13	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.49
4:F:222:ARG:O	4:F:241:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:ARG:NH2	2:D:345:GLU:OE2	2.45	0.48
4:F:14:TYR:HA	4:F:17:VAL:HB	1.95	0.48
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.95	0.48
4:F:239:HIS:C	4:F:240:LEU:HD23	2.34	0.48
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.46	0.48
4:F:95:PRO:HB2	4:F:183:GLN:HG3	1.96	0.48
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.31	0.48
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.46	0.47
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.48	0.47
1:C:333:ALA:O	1:C:337:THR:HG23	2.15	0.47
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.96	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.15	0.47
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.96	0.47
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.96	0.47
2:D:141:LEU:HB3	2:D:187:ALA:HA	1.96	0.47
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.46
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.30	0.46
2:D:111:GLY:HA3	2:D:149:MET:HG3	1.97	0.46
2:B:264:ARG:HE	2:B:431:GLU:CD	2.18	0.46
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.97	0.46
1:C:10:GLY:O	1:C:14:VAL:HG23	2.16	0.46
4:F:155:ALA:HB1	4:F:156:LYS:CD	2.38	0.46
2:D:400:ARG:HG3	2:D:401:ARG:HG2	1.98	0.46
2:B:295:MET:CE	2:B:375:ALA:HB1	2.45	0.46
4:F:242:ASN:N	4:F:242:ASN:OD1	2.37	0.45
2:B:114:LEU:O	2:B:114:LEU:HG	2.16	0.45
2:B:105:LYS:HA	2:B:109:THR:OG1	2.17	0.45
2:D:223:THR:OG1	2:D:226:ASP:OD2	2.27	0.45
4:F:201:ILE:HG12	4:F:221:LEU:HD23	1.98	0.45
2:B:50:ASN:H	2:B:50:ASN:HD22	1.64	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.17	0.45
1:C:147:SER:HB2	1:C:190:THR:HB	1.98	0.45
2:B:331:GLN:O	2:B:335:VAL:HG23	2.16	0.45
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.98	0.45
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.52	0.45
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.81	0.45
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.81	0.45
1:C:150:THR:O	1:C:154:MET:HG2	2.17	0.45
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.52	0.45
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:THR:CG2	2:D:335:VAL:HG21	2.47	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.44
1:A:98:ASP:OD1	1:A:100:ALA:N	2.40	0.44
2:B:334:ASN:OD1	2:B:338:LYS:HE3	2.17	0.44
4:F:155:ALA:CB	4:F:156:LYS:HD3	2.43	0.44
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.52	0.44
2:D:69:ASP:O	2:D:94:PHE:HA	2.18	0.44
1:C:216:ASN:HB3	1:C:275:VAL:O	2.17	0.43
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.53	0.43
1:C:297:GLU:OE2	1:C:339:ARG:NH2	2.51	0.43
2:D:141:LEU:HA	2:D:147:SER:HB3	1.98	0.43
1:C:287:SER:OG	1:C:290:GLU:HG3	2.19	0.43
2:B:227:LEU:O	2:B:231:VAL:HG23	2.19	0.43
1:C:298:PRO:HG2	1:C:308:ARG:CZ	2.49	0.43
2:D:118:VAL:O	2:D:122:VAL:HG23	2.19	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.42
2:B:199:ASP:O	2:B:266:HIS:HB2	2.19	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.42
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.42
8:A:504:GOL:H31	3:E:61:ARG:HD2	2.00	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.42
2:D:352:LYS:HG3	9:D:500:6NL:CAA	2.49	0.42
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.54	0.42
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.01	0.42
2:B:88:ARG:HH12	2:B:124:LYS:HZ3	1.67	0.42
2:B:223:THR:O	2:B:227:LEU:HD13	2.20	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.42
2:D:167:ASN:ND2	13:D:603:HOH:O	2.52	0.42
2:D:287:THR:HB	2:D:289:PRO:HD2	2.00	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.42
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.81	0.42
2:B:340:SER:OG	4:F:34:ASN:ND2	2.48	0.42
2:D:123:ARG:O	2:D:127:GLU:HG2	2.19	0.42
3:E:120:LEU:O	3:E:124:GLN:HG3	2.20	0.42
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.55	0.42
2:D:23:VAL:O	2:D:27:GLU:HG3	2.19	0.42
2:B:39:ASP:OD1	2:B:39:ASP:N	2.53	0.41
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.41
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.02	0.41
1:A:209:ILE:HD11	1:A:302:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:55:GLU:HA	4:F:56:PRO:HD2	1.82	0.41
1:A:187:SER:CB	1:A:391:LEU:HD21	2.50	0.41
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.38	0.41
2:B:330:GLU:O	2:B:334:ASN:HB2	2.21	0.41
1:C:271:THR:HG23	1:C:300:ASN:O	2.19	0.41
2:D:295:MET:CG	2:D:377:PHE:HB2	2.50	0.41
2:B:275:LEU:HG	2:B:300:ASN:ND2	2.36	0.41
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.51	0.41
1:C:8:HIS:HB3	1:C:13:GLY:O	2.20	0.41
4:F:184:LYS:HE2	4:F:185:TYR:O	2.20	0.41
1:A:51:THR:HG22	1:A:52:PHE:CD1	2.54	0.41
2:B:156:LYS:NZ	3:E:76:ARG:NE	2.68	0.41
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.02	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.02	0.41
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.02	0.41
1:A:391:LEU:HA	1:A:391:LEU:HD12	1.80	0.41
11:B:505:MES:H81	11:B:505:MES:H51	1.81	0.41
4:F:239:HIS:O	4:F:240:LEU:HD23	2.20	0.41
1:A:247:ALA:HB3	3:E:19:SER:OG	2.21	0.41
1:A:336:LYS:HG3	3:E:24:LEU:HD13	2.03	0.41
1:C:174:ALA:O	1:C:178:SER:HB3	2.21	0.41
4:F:240:LEU:HD12	4:F:245:ILE:HD13	2.03	0.41
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.84	0.41
1:A:245:ASP:HB3	3:E:16:SER:OG	2.22	0.40
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.03	0.40
1:A:277:SER:OG	1:A:279:GLU:OE1	2.39	0.40
2:B:187:ALA:O	2:B:191:VAL:HG23	2.22	0.40
2:B:295:MET:HE3	2:B:375:ALA:HB1	2.04	0.40
2:B:70:LEU:HA	2:B:70:LEU:HD23	1.86	0.40
4:F:155:ALA:CB	4:F:156:LYS:CE	2.99	0.40
2:D:352:LYS:HD3	2:D:353:THR:N	2.36	0.40
4:F:320:MET:CE	12:F:402:ACP:C2	3.00	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	436/451 (97%)	428 (98%)	8 (2%)	0	100	100
1	C	437/451 (97%)	429 (98%)	8 (2%)	0	100	100
2	B	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
2	D	418/445 (94%)	414 (99%)	4 (1%)	0	100	100
3	E	118/143 (82%)	116 (98%)	2 (2%)	0	100	100
4	F	342/384 (89%)	335 (98%)	7 (2%)	0	100	100
All	All	2173/2319 (94%)	2136 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	363 (98%)	6 (2%)	68	83
1	C	370/379 (98%)	368 (100%)	2 (0%)	91	96
2	B	368/383 (96%)	361 (98%)	7 (2%)	62	80
2	D	364/383 (95%)	358 (98%)	6 (2%)	68	83
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	310/342 (91%)	301 (97%)	9 (3%)	48	68
All	All	1890/1993 (95%)	1860 (98%)	30 (2%)	68	83

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	133	GLN
1	A	163	LYS

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Mol	Chain	Res	Type
1	A	164	LYS
1	A	316	CYS
1	A	381	THR
2	B	117	SER
2	B	139	HIS
2	B	155	SER
2	B	338	LYS
2	B	341	SER
2	B	352	LYS
2	B	423	SER
1	C	71	GLU
1	C	97	GLU
2	D	139	HIS
2	D	149	MET
2	D	190	SER
2	D	232	SER
2	D	249	ASN
2	D	352	LYS
4	F	91	CYS
4	F	150	LYS
4	F	151	SER
4	F	156	LYS
4	F	160	ILE
4	F	241	THR
4	F	242	ASN
4	F	341	LYS
4	F	372	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
2	B	167	ASN
1	C	249	ASN
2	D	406	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 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	0.99	1 (3%)	27,54,54	1.73	4 (14%)
8	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.31	0
8	GOL	A	505	-	5,5,5	0.31	0	5,5,5	0.41	0
9	6NL	B	501	-	27,27,27	1.03	1 (3%)	37,38,38	1.54	6 (16%)
10	GDP	B	502	6	25,30,30	1.17	2 (8%)	26,47,47	2.08	7 (26%)
8	GOL	B	504	-	5,5,5	0.35	0	5,5,5	0.30	0
11	MES	B	505	-	12,12,12	2.16	1 (8%)	14,16,16	2.13	5 (35%)
5	GTP	C	501	6	27,34,34	0.94	1 (3%)	27,54,54	1.79	5 (18%)
9	6NL	D	500	-	27,27,27	0.97	1 (3%)	37,38,38	1.67	6 (16%)
10	GDP	D	501	6	25,30,30	1.15	2 (8%)	26,47,47	2.06	6 (23%)
12	ACP	F	402	6	27,33,33	1.48	2 (7%)	30,52,52	1.57	6 (20%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	505	-	-	0/4/4/4	0/0/0/0
9	6NL	B	501	-	-	0/16/22/22	0/3/3/3
10	GDP	B	502	6	-	0/12/32/32	0/3/3/3
8	GOL	B	504	-	-	0/4/4/4	0/0/0/0
11	MES	B	505	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	6NL	D	500	-	-	0/16/22/22	0/3/3/3
10	GDP	D	501	6	-	0/12/32/32	0/3/3/3
12	ACP	F	402	6	-	0/15/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	MES	C8-S	-7.21	1.66	1.77
12	F	402	ACP	C8-N7	-2.10	1.30	1.34
10	B	502	GDP	C5-C4	2.83	1.46	1.40
5	C	501	GTP	C6-N1	2.94	1.38	1.33
10	D	501	GDP	C5-C4	2.97	1.47	1.40
5	A	501	GTP	C6-N1	3.02	1.38	1.33
9	D	500	6NL	CAJ-CAK	3.21	1.37	1.34
9	B	501	6NL	CAJ-CAK	3.60	1.38	1.34
10	D	501	GDP	C6-C5	3.79	1.48	1.41
10	B	502	GDP	C6-C5	3.86	1.48	1.41
12	F	402	ACP	PB-O3A	5.88	1.65	1.58

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.36	119.63	127.46
5	A	501	GTP	N3-C2-N1	-5.16	119.92	127.46
10	B	502	GDP	C6-C5-C4	-4.79	116.08	120.84
9	D	500	6NL	CAX-OAY-CAR	-4.54	99.27	105.08
9	D	500	6NL	CAX-OAW-CAQ	-4.47	99.38	105.35
12	F	402	ACP	N3-C2-N1	-4.23	125.17	128.86
10	D	501	GDP	C5-C6-N1	-4.01	117.77	123.48
10	D	501	GDP	C6-C5-C4	-3.66	117.20	120.84
10	B	502	GDP	N3-C2-N1	-3.45	122.42	127.46
10	B	502	GDP	C5-C6-N1	-3.41	118.63	123.48
12	F	402	ACP	O1G-PG-C3B	-3.40	103.72	111.22
9	B	501	6NL	CAX-OAY-CAR	-3.39	100.73	105.08
10	D	501	GDP	C4-C5-N7	-3.26	106.26	109.41
10	D	501	GDP	N3-C2-N1	-3.22	122.75	127.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	6NL	CAX-OAW-CAQ	-3.02	101.31	105.35
10	B	502	GDP	C4-C5-N7	-2.99	106.53	109.41
5	A	501	GTP	C5-C6-N1	-2.91	119.34	123.48
5	C	501	GTP	C5-C6-N1	-2.88	119.38	123.48
9	B	501	6NL	OAH-CAE-CAD	-2.65	119.92	124.37
9	D	500	6NL	OAH-CAE-CAD	-2.60	120.00	124.37
12	F	402	ACP	PA-O3A-PB	-2.47	124.43	132.39
10	B	502	GDP	C1'-N9-C4	-2.46	122.38	126.64
9	D	500	6NL	CAT-CAS-CAR	-2.45	117.40	120.22
9	B	501	6NL	CAB-CAA-CAF	-2.40	119.06	120.80
9	B	501	6NL	CAT-CAS-CAR	-2.40	117.45	120.22
11	B	505	MES	C6-C5-N4	-2.28	106.92	110.11
12	F	402	ACP	O2G-PG-C3B	-2.06	101.41	106.40
9	D	500	6NL	CAB-CAA-CAF	-2.04	119.32	120.80
5	C	501	GTP	N2-C2-N1	2.14	120.67	117.24
12	F	402	ACP	O2B-PB-O1B	2.22	117.54	110.09
11	B	505	MES	O3S-S-C8	2.52	109.15	106.06
11	B	505	MES	O2S-S-C8	2.56	108.99	106.79
5	A	501	GTP	C6-N1-C2	2.95	120.31	116.06
5	C	501	GTP	C6-N1-C2	3.09	120.50	116.06
12	F	402	ACP	C4-C5-N7	3.71	113.00	109.41
11	B	505	MES	O1S-S-C8	4.13	110.34	106.79
5	A	501	GTP	C2-N3-C4	4.23	120.09	115.16
9	B	501	6NL	OAH-CAE-CAF	4.34	119.83	114.55
10	B	502	GDP	C6-N1-C2	4.37	122.35	116.06
11	B	505	MES	C5-N4-C3	4.39	118.81	108.87
5	C	501	GTP	C2-N3-C4	4.49	120.41	115.16
9	D	500	6NL	OAH-CAE-CAF	4.50	120.03	114.55
10	D	501	GDP	C6-N1-C2	4.52	122.56	116.06
10	B	502	GDP	C2-N3-C4	4.89	120.86	115.16
10	D	501	GDP	C2-N3-C4	5.11	121.12	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	504	GOL	2	0
11	B	505	MES	1	0
9	D	500	6NL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	501	GDP	2	0
12	F	402	ACP	5	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.56	29 (6%)	19 17	45, 66, 105, 177	0
1	C	439/451 (97%)	0.15	5 (1%)	80 79	38, 53, 84, 110	0
2	B	425/445 (95%)	0.36	18 (4%)	37 35	40, 58, 96, 134	1 (0%)
2	D	422/445 (94%)	0.73	50 (11%)	5 4	45, 77, 113, 144	5 (1%)
3	E	122/143 (85%)	0.82	20 (16%)	2 2	50, 80, 116, 130	0
4	F	348/384 (90%)	1.60	120 (34%)	0 0	56, 95, 165, 186	0
All	All	2194/2319 (94%)	0.65	242 (11%)	6 5	38, 69, 128, 186	6 (0%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	9.1
1	A	282	TYR	8.5
4	F	132	LEU	7.8
4	F	173	ILE	7.7
2	B	59	ASN	7.5
4	F	231	ALA	7.5
4	F	249	TYR	7.3
4	F	100	ILE	7.2
4	F	134	ALA	7.1
1	A	439	SER	7.0
4	F	251	LYS	6.7
4	F	253	TYR	6.5
4	F	166	ALA	6.5
4	F	130	VAL	6.4
3	E	143	ALA	6.1
4	F	250	SER	6.1
4	F	182	ILE	5.9
4	F	177	GLY	5.9
2	D	58	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
2	D	57	THR	5.8
3	E	139	LEU	5.8
4	F	248	GLU	5.5
4	F	245	ILE	5.5
4	F	101	TYR	5.4
4	F	167	SER	5.3
1	A	283	HIS	5.2
4	F	225	SER	5.2
4	F	255	ARG	5.2
4	F	133	ALA	5.2
4	F	131	PHE	5.1
4	F	362	ALA	5.1
4	F	179	VAL	5.0
1	A	281	ALA	5.0
4	F	135	TYR	5.0
2	B	57	THR	4.9
4	F	172	PHE	4.8
4	F	238	CYS	4.8
2	D	405	LEU	4.8
4	F	169	LEU	4.7
1	A	42	ILE	4.7
4	F	199	PHE	4.7
3	E	140	LYS	4.6
4	F	20	LEU	4.6
4	F	178	GLN	4.5
2	D	401	ARG	4.5
4	F	129	GLU	4.5
4	F	244	CYS	4.4
4	F	128	ARG	4.4
2	D	400	ARG	4.3
4	F	89	GLU	4.3
4	F	21	LEU	4.2
2	D	82	PRO	4.2
4	F	247	LYS	4.2
3	E	24	LEU	4.2
4	F	170	LEU	4.2
4	F	157	GLY	4.1
4	F	256	TYR	4.1
4	F	232	ASN	4.1
4	F	252	ASN	4.1
4	F	136	ASN	4.0
4	F	234	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	90	SER	4.0
2	D	404	PHE	4.0
4	F	164	SER	4.0
4	F	137	ARG	3.9
2	B	439	THR	3.9
3	E	26	PRO	3.9
4	F	240	LEU	3.8
4	F	17	VAL	3.7
2	D	59	ASN	3.7
3	E	142	GLU	3.7
4	F	127	GLU	3.7
2	B	284	ARG	3.7
4	F	176	GLN	3.7
2	D	94	PHE	3.7
2	B	58	GLY	3.7
2	B	440	ALA	3.6
4	F	143	GLU	3.6
4	F	174	ASP	3.6
4	F	149	ALA	3.6
1	C	340	SER	3.6
2	B	37	HIS	3.6
4	F	228	TYR	3.5
4	F	139	ARG	3.5
4	F	24	THR	3.5
4	F	28	LYS	3.5
4	F	372	THR	3.5
2	D	96	GLN	3.5
4	F	98	TYR	3.5
4	F	162	ILE	3.4
4	F	246	GLN	3.4
3	E	133	VAL	3.4
4	F	147	TRP	3.4
4	F	165	GLU	3.4
2	B	438	ALA	3.4
4	F	229	ASN	3.3
3	E	141	GLU	3.3
4	F	254	GLY	3.3
4	F	99	VAL	3.3
4	F	13	VAL	3.3
2	B	36	TYR	3.3
1	C	440	VAL	3.3
2	D	85	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	219	LEU	3.2
4	F	152	SER	3.2
3	E	48	GLU	3.2
2	D	80	SER	3.2
4	F	138	ARG	3.2
2	D	56	ALA	3.2
2	D	415	GLU	3.2
2	B	83	PHE	3.2
3	E	138	GLU	3.1
4	F	9	GLU	3.1
2	D	179	ASP	3.1
4	F	159	GLY	3.1
4	F	44	ARG	3.1
4	F	142	ARG	3.1
2	D	203	CYS	3.1
2	D	276	THR	3.1
3	E	45	PRO	3.1
4	F	259	GLY	3.1
2	D	79	ARG	3.1
4	F	102	PRO	3.0
1	A	88	HIS	3.0
4	F	223	THR	3.0
4	F	236	LYS	3.0
4	F	31	ARG	3.0
4	F	161	LEU	2.9
4	F	140	GLU	2.9
4	F	226	GLU	2.9
4	F	145	ASN	2.9
2	D	441	ASP	2.9
1	A	280	LYS	2.9
4	F	343	TYR	2.9
2	D	83	PHE	2.9
4	F	263	PHE	2.9
1	A	57	GLY	2.8
2	B	56	ALA	2.8
4	F	227	PRO	2.8
4	F	163	SER	2.8
1	A	12	ALA	2.8
4	F	22	LEU	2.8
3	E	7	GLU	2.8
2	B	34	GLY	2.7
2	D	406	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	397	ALA	2.7
4	F	340	GLN	2.7
2	D	37	HIS	2.7
1	A	171	ILE	2.7
1	A	146	GLY	2.7
2	B	277	SER	2.7
1	A	177	VAL	2.7
3	E	25	LYS	2.7
1	A	143	GLY	2.7
4	F	32	LYS	2.7
2	D	255	LEU	2.7
2	D	407	TRP	2.6
4	F	171	ASP	2.6
2	D	60	LYS	2.6
2	D	210	TYR	2.6
4	F	181	VAL	2.6
4	F	239	HIS	2.6
2	D	76	ASP	2.6
2	D	252	LEU	2.6
3	E	132	GLU	2.6
4	F	168	GLU	2.6
4	F	224	SER	2.6
4	F	230	SER	2.6
1	A	335	ILE	2.6
1	C	2	ARG	2.6
2	D	95	GLY	2.6
4	F	257	GLU	2.6
2	D	399	PHE	2.5
1	A	262	TYR	2.5
1	A	142	GLY	2.5
4	F	221	LEU	2.5
4	F	361	LEU	2.5
1	A	285	GLN	2.5
4	F	235	ASP	2.5
4	F	175	GLU	2.5
3	E	137	LYS	2.5
4	F	346	LEU	2.5
1	A	173	PRO	2.4
2	B	61	TYR	2.4
2	D	201	THR	2.4
4	F	10	ASN	2.4
3	E	27	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	60	LYS	2.4
4	F	41	LEU	2.4
2	D	403	ALA	2.4
1	A	46	ASP	2.4
2	D	221	THR	2.4
4	F	242	ASN	2.4
4	F	158	GLU	2.4
2	D	143	GLY	2.4
1	A	438	ASP	2.4
1	A	40	LYS	2.3
4	F	126	ASP	2.3
3	E	23	ILE	2.3
2	B	144	GLY	2.3
3	E	15	THR	2.3
1	A	59	GLY	2.3
2	D	202	TYR	2.3
2	D	269	MET	2.3
4	F	27	TRP	2.3
1	A	141	PHE	2.2
4	F	243	HIS	2.2
2	D	185	TYR	2.2
2	D	378	ILE	2.2
4	F	25	GLY	2.2
4	F	241	THR	2.2
3	E	46	SER	2.2
2	D	259	MET	2.2
4	F	183	GLN	2.2
2	D	260	VAL	2.1
2	D	214	PHE	2.1
4	F	23	ALA	2.1
4	F	18	SER	2.1
4	F	194	PRO	2.1
4	F	360	PRO	2.1
1	A	284	GLU	2.1
4	F	258	GLU	2.1
2	D	87	PHE	2.1
2	B	109	THR	2.1
4	F	351	VAL	2.1
1	A	58	ALA	2.1
2	D	33	THR	2.1
3	E	135	LYS	2.1
1	A	140	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	177	VAL	2.1
2	B	46	LEU	2.0
2	D	86	ILE	2.0
4	F	191	LEU	2.0
2	D	376	THR	2.0
2	D	177	VAL	2.0
4	F	267	PHE	2.0
1	A	180	ALA	2.0
1	C	176	GLN	2.0
2	D	317	ALA	2.0
2	D	2	ARG	2.0
1	A	172	TYR	2.0
1	A	316	CYS	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, 95th 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 ²)	Q<0.9
8	GOL	A	505	6/6	0.91	0.19	2.88	83,85,91,94	0
8	GOL	B	504	6/6	0.88	0.21	2.30	103,106,108,110	0
5	GTP	A	501	32/32	0.99	0.24	0.35	39,48,55,73	0
10	GDP	B	502	28/28	0.98	0.19	0.25	35,43,50,61	0
9	6NL	D	500	25/25	0.96	0.22	0.09	42,59,84,85	0
8	GOL	A	504	6/6	0.94	0.16	0.06	87,89,94,97	0
5	GTP	C	501	32/32	0.99	0.16	0.04	31,40,53,68	0
7	CA	E	201	1/1	0.77	0.16	-0.28	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	6NL	B	501	25/25	0.98	0.16	-0.55	36,50,60,67	0
10	GDP	D	501	28/28	0.96	0.13	-0.64	56,68,83,92	0
11	MES	B	505	12/12	0.97	0.14	-1.04	49,63,77,78	0
7	CA	C	503	1/1	0.98	0.08	-1.32	78,78,78,78	0
12	ACP	F	402	31/31	0.86	0.12	-1.66	86,105,139,156	0
7	CA	A	503	1/1	0.93	0.04	-2.12	89,89,89,89	0
6	MG	F	401	1/1	0.95	0.06	-	104,104,104,104	0
6	MG	C	502	1/1	0.99	0.18	-	39,39,39,39	0
6	MG	D	502	1/1	0.95	0.10	-	75,75,75,75	0
7	CA	B	506	1/1	0.62	0.58	-	163,163,163,163	0
6	MG	A	502	1/1	0.77	0.28	-	74,74,74,74	0
6	MG	B	503	1/1	0.97	0.22	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.