



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2017 – 05:50 PM EST

PDB ID : 5M7G
Title : Tubulin-MTD147 complex
Authors : Bohnacker, T.; Protá, A.E.; Steinmetz, M.O.; Wymann, M.P.
Deposited on : 2016-10-27
Resolution : 2.25 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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-20028442

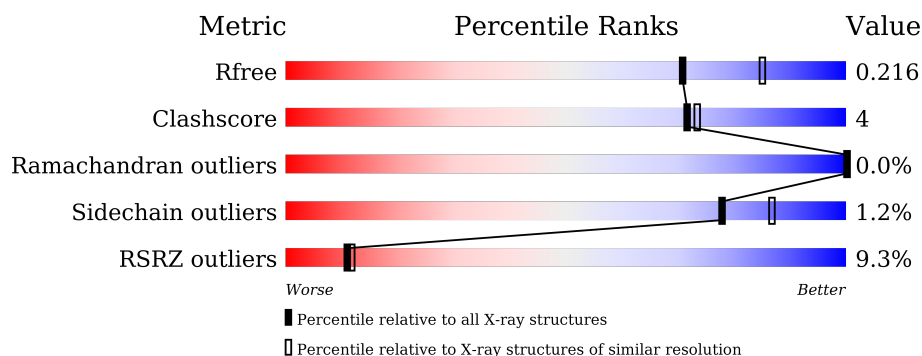
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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>5%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
2	D	445	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
3	E	143	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>14%</div> </div> </div>
4	F	384	<div> <div>27%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>15%</div> </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	A	502	-	-	-	X
9	FB7	D	500	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17780 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	436	Total	C	N	O	S	0	0	0
			3409	2158	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- 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	0	0	0
			3325	2091	567	641	26			
2	D	418	Total	C	N	O	S	0	0	0
			3284	2065	557	636	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	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

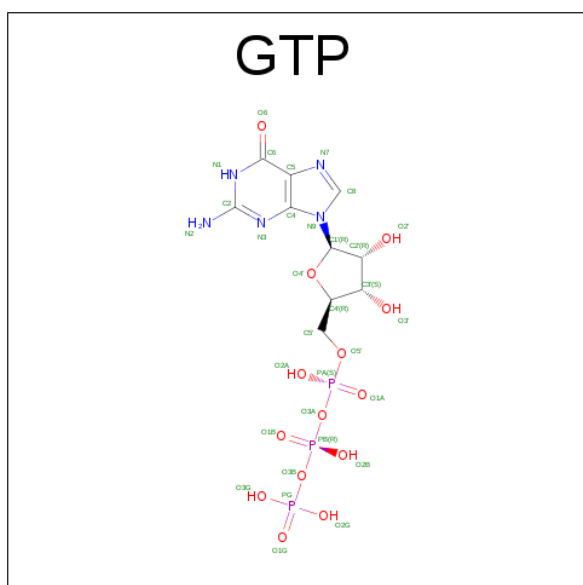
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	326	Total	C	N	O	S	0	0	0
			2647	1707	444	482	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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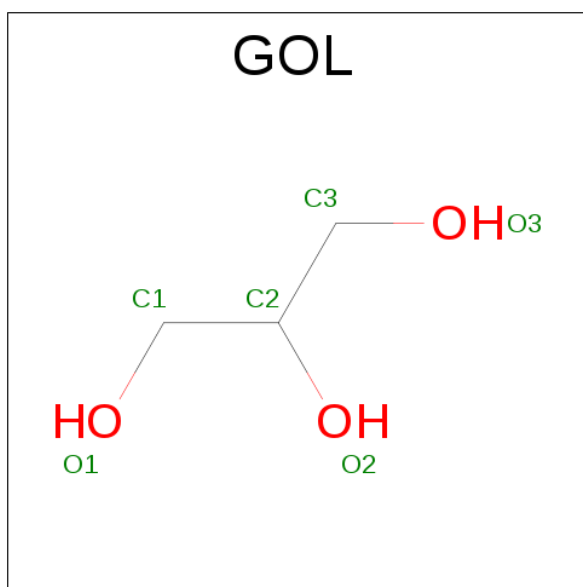
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

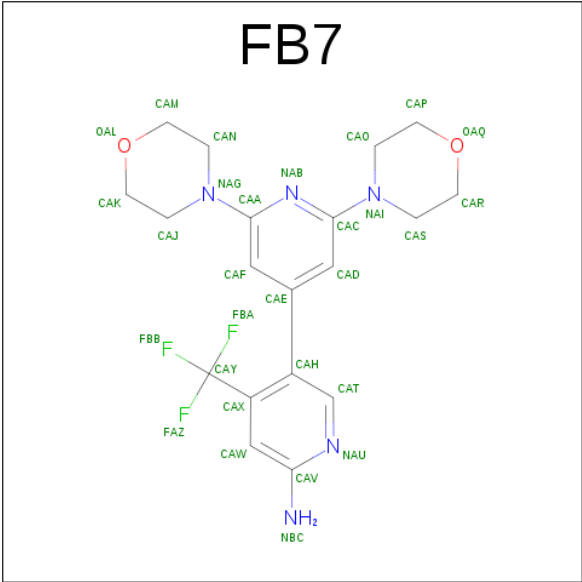
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	2	Total	Ca	0	0
			2	2		
7	C	2	Total	Ca	0	0
			2	2		

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



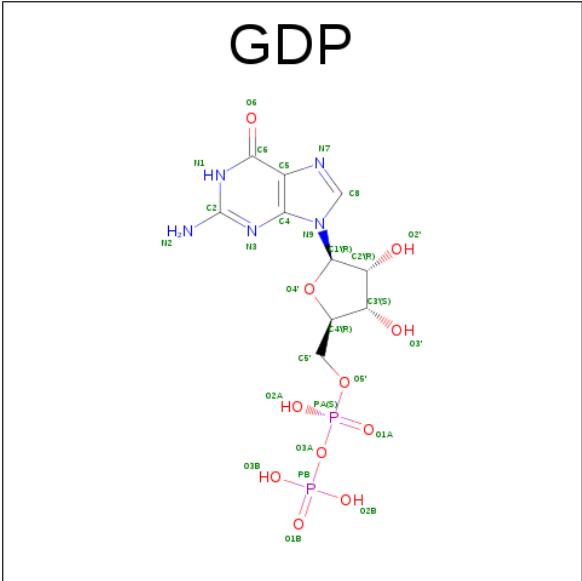
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 5-(2,6-dimorpholin-4-ylpyridin-4-yl)-4-(trifluoromethyl)pyridin-2-amine (three-letter code: FB7) (formula: C₁₉H₂₂F₃N₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	F	N	O	0	0
			29	19	3	5	2		
9	D	1	Total	C	F	N	O	0	0
			29	19	3	5	2		

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



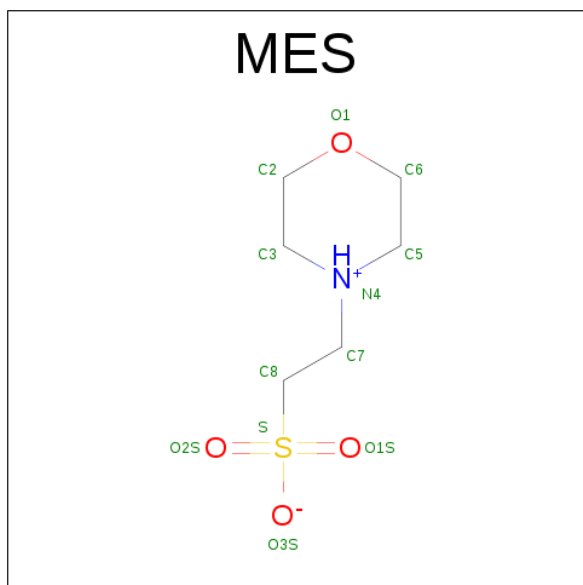
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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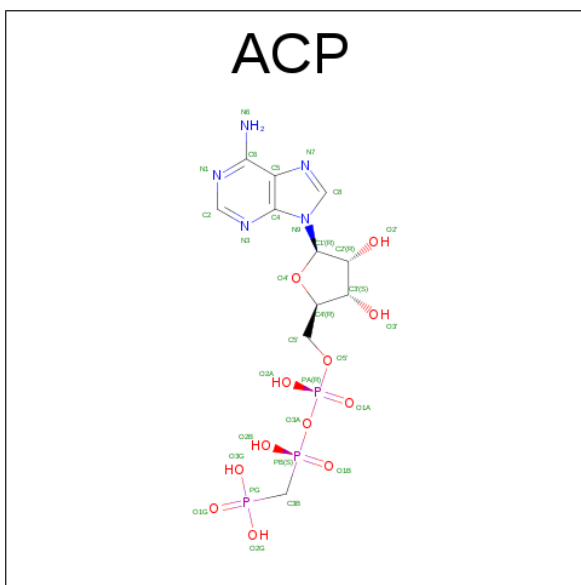
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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		

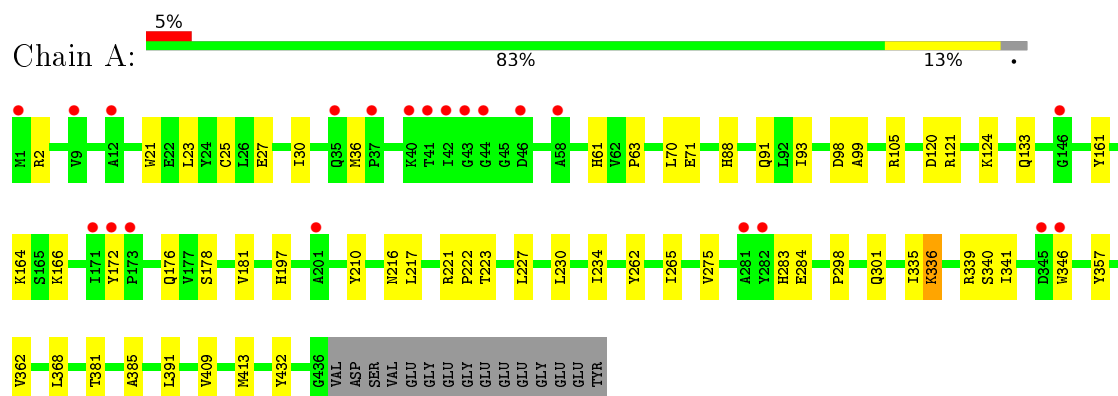
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	82	Total O 82 82	0	0
13	B	76	Total O 76 76	0	0
13	C	175	Total O 175 175	0	0
13	D	45	Total O 45 45	0	0
13	E	15	Total O 15 15	0	0
13	F	28	Total O 28 28	0	0

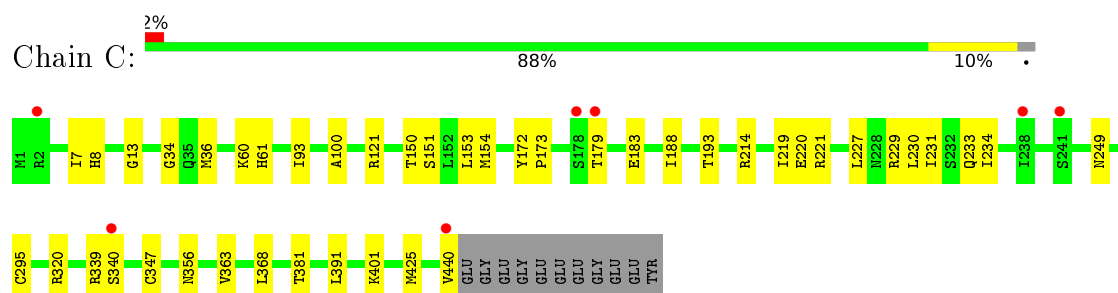
3 Residue-property plots [i](#)

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

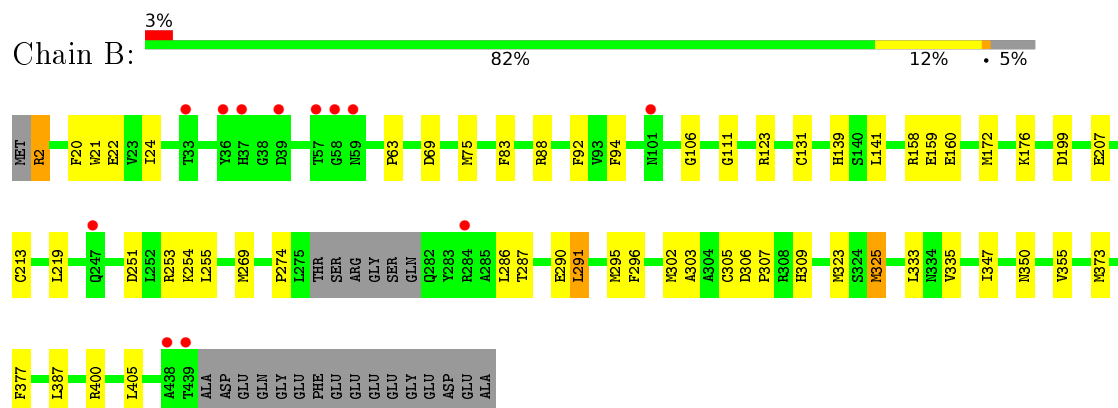
• Molecule 1: Tubulin alpha-1B chain



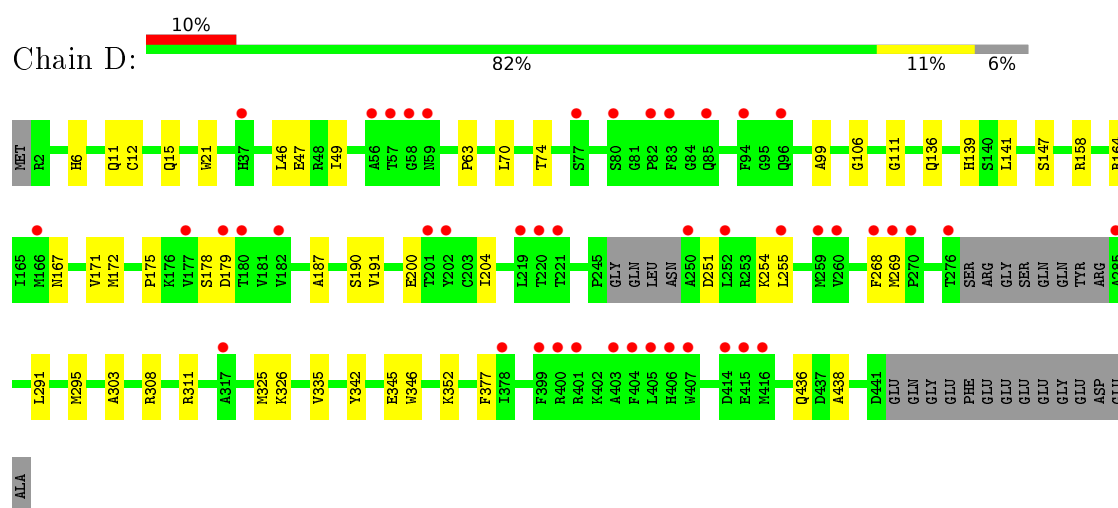
• Molecule 1: Tubulin alpha-1B chain



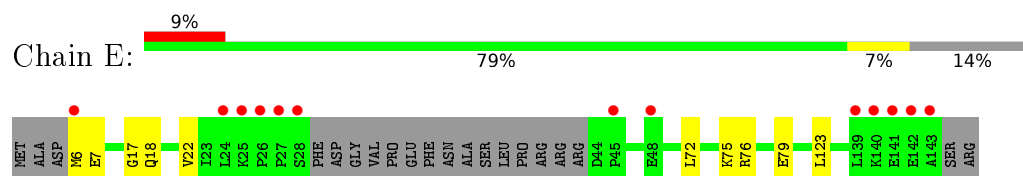
• Molecule 2: Tubulin beta-2B chain



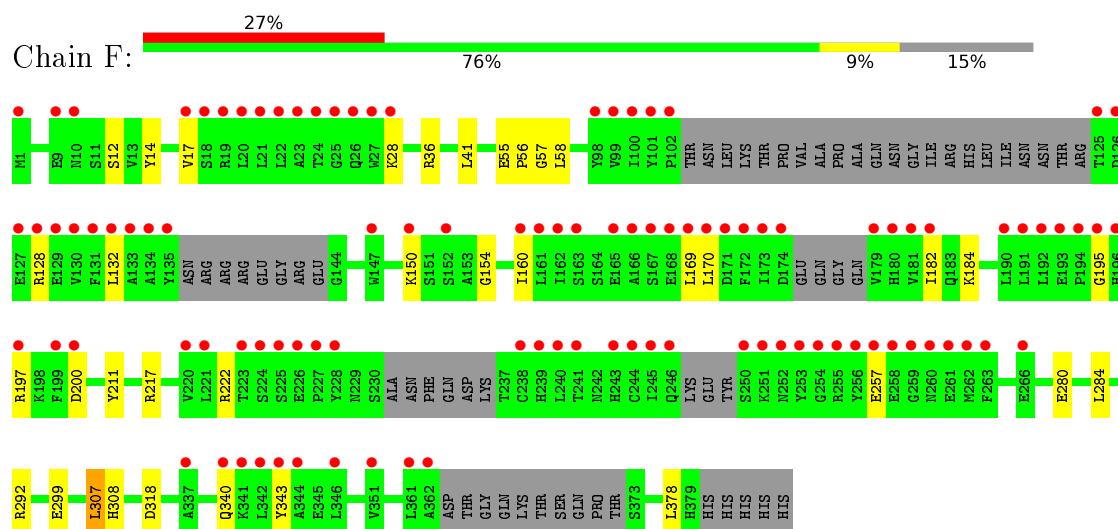
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.08Å 156.86Å 179.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.72 – 2.25 49.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.72-2.25) 99.1 (49.28-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.172 , 0.217 0.170 , 0.216	Depositor DCC
R_{free} test set	6942 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17780	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, FB7, CA, 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	0.41	0/3487	0.54	0/4733
1	C	0.49	1/3515 (0.0%)	0.62	0/4772
2	B	0.42	0/3399	0.56	0/4604
2	D	0.37	0/3356	0.51	0/4546
3	E	0.40	0/1022	0.46	0/1356
4	F	0.35	0/2705	0.50	0/3653
All	All	0.41	1/17484 (0.0%)	0.55	0/23664

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-6.26	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3409	0	3322	37	0
1	C	3437	0	3348	25	0
2	B	3325	0	3203	39	0
2	D	3284	0	3160	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1014	0	1029	6	0
4	F	2647	0	2627	21	0
5	A	32	0	12	0	0
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	2	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
8	A	6	0	8	1	0
8	F	6	0	8	0	0
9	B	29	0	0	0	0
9	D	29	0	0	2	0
10	B	28	0	12	0	0
10	D	28	0	12	2	0
11	B	12	0	12	3	0
12	F	31	0	14	2	0
13	A	82	0	0	1	0
13	B	76	0	0	2	0
13	C	175	0	0	1	0
13	D	45	0	0	3	0
13	E	15	0	0	0	0
13	F	28	0	0	1	0
All	All	17780	0	16779	147	0

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

All (147) 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:253:ARG:NH1	11:B:505:MES:O2S	2.11	0.82
4:F:318:ASP:OD2	12:F:403:ACP:O3G	2.00	0.80
2:B:88:ARG:NH1	13:B:601:HOH:O	2.18	0.75
1:A:221:ARG:HD3	2:B:325:MET:HG3	1.70	0.74
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.69	0.73
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.71	0.70
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:ARG:NH1	13:D:602:HOH:O	2.22	0.70
4:F:154:GLY:O	13:F:501:HOH:O	2.12	0.68
2:D:311:ARG:NH1	2:D:436:GLN:O	2.27	0.66
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.29	0.64
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.31	0.63
2:D:175:PRO:HA	2:D:178:SER:HB2	1.83	0.61
2:B:400:ARG:NH2	1:C:440:VAL:O	2.33	0.61
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.61
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.82	0.60
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.82	0.60
4:F:150:LYS:HG2	4:F:160:ILE:HG12	1.82	0.59
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.84	0.59
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.85	0.58
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.85	0.57
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.19	0.56
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.56
2:D:171:VAL:HA	2:D:204:ILE:O	2.06	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.56
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.87	0.56
1:C:220:GLU:HG2	2:D:326:LYS:HD2	1.87	0.55
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.71	0.55
1:A:216:ASN:ND2	8:A:505:GOL:H2	2.21	0.55
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.90	0.54
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.89	0.54
2:D:11:GLN:HA	2:D:74:THR:HG21	1.90	0.54
4:F:169:LEU:HD13	4:F:182:ILE:HD11	1.90	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.42	0.54
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.43	0.53
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.27	0.52
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.91	0.52
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.89	0.52
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.44	0.52
2:B:325:MET:HE1	2:B:355:VAL:HG11	1.91	0.51
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.93	0.51
2:B:323:MET:HB3	2:B:373:MET:CE	2.40	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.93	0.51
1:C:401:LYS:HE3	2:D:438:ALA:HB1	1.93	0.50
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.92	0.50
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.94	0.49
1:A:23:LEU:O	1:A:27:GLU:HG3	2.13	0.49
4:F:128:ARG:O	4:F:132:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.49
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.94	0.49
2:B:213:CYS:HB3	2:B:219:LEU:HD12	1.94	0.49
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.95	0.49
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.45	0.48
1:A:336:LYS:HE3	1:A:341:ILE:HB	1.96	0.48
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.41	0.48
1:A:298:PRO:HA	1:A:301:GLN:CD	2.34	0.48
2:D:141:LEU:HD12	2:D:172:MET:SD	2.54	0.48
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.45	0.48
1:C:339:ARG:O	13:C:601:HOH:O	2.20	0.47
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.15	0.47
2:B:199:ASP:OD2	11:B:505:MES:H52	2.15	0.47
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.33	0.47
2:B:141:LEU:HD12	2:B:172:MET:SD	2.55	0.46
4:F:14:TYR:HA	4:F:17:VAL:HB	1.96	0.46
2:B:325:MET:H	2:B:325:MET:HG2	1.32	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.51	0.46
1:C:150:THR:O	1:C:154:MET:HG2	2.16	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.16	0.46
2:D:179:ASP:OD2	13:D:601:HOH:O	2.21	0.46
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.50	0.46
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.50	0.45
4:F:211:TYR:CE2	4:F:299:GLU:HB2	2.51	0.45
1:A:25:CYS:HB3	1:A:30:ILE:O	2.16	0.45
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.45
3:E:7:GLU:O	3:E:22:VAL:HA	2.16	0.45
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.52	0.45
1:A:166:LYS:HE2	1:A:197:HIS:O	2.17	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.45
2:B:158:ARG:CZ	11:B:505:MES:H21	2.47	0.45
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.51	0.45
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.99	0.45
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.99	0.45
1:A:340:SER:HA	13:A:655:HOH:O	2.17	0.44
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.52	0.44
4:F:128:ARG:HH11	4:F:170:LEU:HD13	1.82	0.44
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.44
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.53	0.44
1:A:71:GLU:HB3	2:B:2:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:HA	1:A:105:ARG:HG2	1.99	0.44
2:D:187:ALA:O	2:D:191:VAL:HG23	2.18	0.44
2:D:46:LEU:HA	2:D:49:ILE:HB	1.99	0.44
2:D:15:GLN:NE2	10:D:501:GDP:O6	2.51	0.44
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.53	0.43
1:C:173:PRO:HB3	1:C:183:GLU:OE2	2.18	0.43
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.53	0.43
2:B:251:ASP:O	2:B:255:LEU:HG	2.18	0.43
2:D:200:GLU:HB3	2:D:268:PHE:CE2	2.53	0.43
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.43
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.99	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.54	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.01	0.43
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.54	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.19	0.42
2:B:159:GLU:OE2	13:B:602:HOH:O	2.21	0.42
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.54	0.42
1:C:8:HIS:HB3	1:C:13:GLY:O	2.19	0.42
1:A:176:GLN:HG3	4:F:56:PRO:HB3	2.02	0.42
1:C:229:ARG:NE	1:C:363:VAL:HG21	2.34	0.42
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.54	0.42
1:A:230:LEU:O	1:A:234:ILE:HD12	2.20	0.42
2:B:106:GLY:O	2:B:111:GLY:HA3	2.20	0.42
2:B:2:ARG:HG2	2:B:131:CYS:O	2.20	0.42
1:A:223:THR:O	1:A:227:LEU:HG	2.20	0.42
1:A:362:VAL:HG11	1:A:368:LEU:O	2.19	0.42
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.20	0.42
1:C:221:ARG:HG2	2:D:325:MET:HG2	2.00	0.42
1:C:179:THR:HB	9:D:500:FB7:CAP	2.50	0.42
4:F:150:LYS:HE3	12:F:403:ACP:H8	2.01	0.42
2:B:333:LEU:HD13	4:F:57:GLY:HA3	2.02	0.42
1:C:151:SER:HB2	1:C:193:THR:CG2	2.50	0.42
4:F:292:ARG:HD3	4:F:378:LEU:HB3	2.02	0.42
2:B:323:MET:HB3	2:B:373:MET:HE2	2.02	0.41
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.50	0.41
4:F:184:LYS:HB3	4:F:184:LYS:HE2	1.91	0.41
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.02	0.41
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.85	0.41
1:A:262:TYR:CE2	1:A:346:TRP:CH2	3.08	0.41
2:B:405:LEU:HA	2:B:405:LEU:HD23	1.87	0.41
2:D:147:SER:HB2	2:D:190:SER:OG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:GLY:O	2:D:111:GLY:HA3	2.21	0.41
4:F:28:LYS:HD3	4:F:28:LYS:HA	1.92	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.82	0.41
2:B:269:MET:HE1	2:B:307:PRO:HG3	2.03	0.41
2:D:255:LEU:HD22	9:D:500:FB7:CAT	2.51	0.41
1:A:283:HIS:CG	1:A:284:GLU:N	2.89	0.41
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.56	0.41
2:D:251:ASP:O	2:D:255:LEU:HG	2.21	0.41
3:E:72:LEU:O	3:E:76:ARG:HG2	2.20	0.41
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.56	0.40
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.89	0.40
2:D:141:LEU:HD22	2:D:190:SER:HB3	2.02	0.40
2:B:303:ALA:O	2:B:305:CYS:N	2.49	0.40
2:B:323:MET:HB3	2:B:373:MET:HE1	2.03	0.40
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.02	0.40
4:F:55:GLU:HB3	4:F:58:LEU:HD12	2.02	0.40
2:D:352:LYS:HD2	13:D:643:HOH:O	2.21	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	434/451 (96%)	426 (98%)	7 (2%)	1 (0%)	52	60
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	418/445 (94%)	407 (97%)	11 (3%)	0	100	100
2	D	412/445 (93%)	405 (98%)	7 (2%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	312/384 (81%)	307 (98%)	5 (2%)	0	100	100
All	All	2133/2319 (92%)	2093 (98%)	39 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/379 (97%)	364 (99%)	3 (1%)	86	92
1	C	371/379 (98%)	368 (99%)	3 (1%)	86	92
2	B	365/383 (95%)	359 (98%)	6 (2%)	70	80
2	D	361/383 (94%)	356 (99%)	5 (1%)	74	84
3	E	110/127 (87%)	109 (99%)	1 (1%)	84	90
4	F	291/342 (85%)	286 (98%)	5 (2%)	68	78
All	All	1865/1993 (94%)	1842 (99%)	23 (1%)	78	87

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	VAL
1	A	336	LYS
1	A	381	THR
2	B	2	ARG
2	B	139	HIS
2	B	254	LYS
2	B	291	LEU
2	B	302	MET
2	B	325	MET
1	C	340	SER
1	C	347	CYS
1	C	381	THR
2	D	47	GLU
2	D	139	HIS
2	D	291	LEU
2	D	335	VAL

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Mol	Chain	Res	Type
2	D	345	GLU
3	E	6	MET
4	F	12	SER
4	F	36	ARG
4	F	217	ARG
4	F	257	GLU
4	F	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	394	GLN
4	F	239	HIS
4	F	269	GLN

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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	0.86	1 (3%)	29,54,54	1.99	6 (20%)
8	GOL	A	505	-	5,5,5	0.34	0	5,5,5	0.53	0
9	FB7	B	501	-	32,32,32	1.76	4 (12%)	43,46,46	1.70	8 (18%)
10	GDP	B	502	6	24,30,30	1.22	3 (12%)	26,47,47	2.01	6 (23%)
11	MES	B	505	-	12,12,12	2.22	1 (8%)	15,16,16	2.46	5 (33%)
5	GTP	C	501	6	26,34,34	1.00	1 (3%)	29,54,54	1.99	7 (24%)
9	FB7	D	500	-	32,32,32	1.89	4 (12%)	43,46,46	1.72	8 (18%)
10	GDP	D	501	6	24,30,30	1.10	2 (8%)	26,47,47	2.10	6 (23%)
8	GOL	F	401	-	5,5,5	0.38	0	5,5,5	0.41	0
12	ACP	F	403	6	29,33,33	1.90	8 (27%)	29,52,52	1.63	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	505	-	-	0/4/4/4	0/0/0/0
9	FB7	B	501	-	-	0/18/34/34	0/4/4/4
10	GDP	B	502	6	-	0/12/32/32	0/3/3/3
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	FB7	D	500	-	-	0/18/34/34	0/4/4/4
10	GDP	D	501	6	-	0/12/32/32	0/3/3/3
8	GOL	F	401	-	-	0/4/4/4	0/0/0/0
12	ACP	F	403	6	-	0/15/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	MES	C8-S	-7.45	1.66	1.77
9	D	500	FB7	CAH-CAE	-6.64	1.38	1.49
9	B	501	FB7	CAH-CAE	-5.41	1.40	1.49
9	B	501	FB7	CAY-CAX	-4.78	1.40	1.50
9	D	500	FB7	CAY-CAX	-4.48	1.41	1.50
9	D	500	FB7	FBA-CAY	-3.81	1.19	1.32
9	B	501	FB7	FBA-CAY	-3.80	1.19	1.32
9	D	500	FB7	FBB-CAY	-3.65	1.19	1.32
9	B	501	FB7	FBB-CAY	-3.47	1.20	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	403	ACP	PB-O2B	-2.95	1.49	1.56
12	F	403	ACP	PG-O2G	-2.30	1.49	1.54
10	B	502	GDP	O4'-C1'	2.11	1.44	1.41
12	F	403	ACP	PG-O3G	2.23	1.60	1.54
12	F	403	ACP	PG-C3B	2.32	1.82	1.80
10	D	501	GDP	C5-C4	2.52	1.46	1.40
5	A	501	GTP	C6-N1	2.55	1.37	1.33
10	B	502	GDP	C5-C4	2.61	1.46	1.40
5	C	501	GTP	C6-N1	3.03	1.38	1.33
12	F	403	ACP	C5-C4	3.13	1.47	1.40
10	D	501	GDP	C6-C5	3.31	1.48	1.41
12	F	403	ACP	PB-O3A	3.34	1.62	1.58
10	B	502	GDP	C6-C5	3.52	1.48	1.41
12	F	403	ACP	PB-O1B	4.00	1.62	1.51
12	F	403	ACP	PG-O1G	5.13	1.61	1.50

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-6.73	118.40	127.56
12	F	403	ACP	N3-C2-N1	-6.27	123.94	128.87
5	A	501	GTP	N3-C2-N1	-5.60	119.94	127.56
9	D	500	FB7	CAT-CAH-CAE	-4.61	113.45	119.86
9	B	501	FB7	CAT-CAH-CAE	-4.24	113.97	119.86
5	A	501	GTP	C5-C6-N1	-4.23	118.00	123.52
10	B	502	GDP	C6-C5-C4	-4.09	116.19	120.86
10	D	501	GDP	C6-C5-C4	-4.01	116.27	120.86
10	B	502	GDP	C1'-N9-C4	-3.92	122.43	126.81
10	D	501	GDP	C5-C6-N1	-3.90	118.42	123.52
10	B	502	GDP	N3-C2-N1	-3.80	122.39	127.56
10	D	501	GDP	N3-C2-N1	-3.63	122.62	127.56
10	B	502	GDP	C5-C6-N1	-3.34	119.15	123.52
10	D	501	GDP	O4'-C1'-N9	-3.33	101.81	108.11
5	C	501	GTP	C5-C6-N1	-3.16	119.39	123.52
10	D	501	GDP	C1'-N9-C4	-3.03	123.43	126.81
9	B	501	FB7	FBA-CAY-CAX	-2.97	107.62	112.67
9	D	500	FB7	CAD-CAE-CAH	-2.95	115.97	120.68
5	A	501	GTP	O4'-C1'-N9	-2.91	102.61	108.11
5	A	501	GTP	C1'-N9-C4	-2.89	123.58	126.81
5	C	501	GTP	C1'-N9-C4	-2.76	123.73	126.81
9	D	500	FB7	CAD-CAC-NAI	-2.72	118.84	122.27
12	F	403	ACP	O2'-C2'-C1'	-2.11	105.01	111.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C6-C5-C4	-2.06	118.50	120.86
11	B	505	MES	C2-C3-N4	2.11	113.34	110.11
5	C	501	GTP	O2B-PB-O3A	2.15	114.47	105.27
9	B	501	FB7	CAK-CAJ-NAG	2.21	113.94	109.94
5	A	501	GTP	O2A-PA-O3A	2.32	115.20	105.27
11	B	505	MES	C7-N4-C5	2.37	116.40	111.25
5	C	501	GTP	N2-C2-N1	2.45	121.23	117.20
10	B	502	GDP	O2A-PA-O3A	2.47	115.86	105.27
9	B	501	FB7	CAR-CAS-NAI	2.50	114.47	109.94
11	B	505	MES	C7-N4-C3	2.63	116.97	111.25
9	B	501	FB7	CAP-CAO-NAI	2.65	114.74	109.94
9	D	500	FB7	CAA-NAB-CAC	2.75	122.05	117.64
9	D	500	FB7	CAN-NAG-CAJ	2.79	117.31	111.54
11	B	505	MES	O3S-S-C8	2.79	110.78	104.99
12	F	403	ACP	O2G-PG-C3B	2.84	112.85	106.13
9	D	500	FB7	CAF-CAE-CAH	2.87	125.27	120.68
9	B	501	FB7	CAA-NAB-CAC	3.28	122.90	117.64
9	D	500	FB7	CAO-NAI-CAS	3.72	119.23	111.54
9	D	500	FB7	NAB-CAC-NAI	3.88	121.35	116.69
9	B	501	FB7	CAO-NAI-CAS	3.93	119.68	111.54
9	B	501	FB7	CAN-NAG-CAJ	4.33	120.51	111.54
5	C	501	GTP	C6-N1-C2	4.66	121.34	115.88
5	A	501	GTP	C6-N1-C2	4.89	121.61	115.88
10	B	502	GDP	C6-N1-C2	5.02	121.76	115.88
10	D	501	GDP	C6-N1-C2	5.42	122.23	115.88
11	B	505	MES	C5-N4-C3	7.59	125.88	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	505	GOL	1	0
11	B	505	MES	3	0
9	D	500	FB7	2	0
10	D	501	GDP	2	0
12	F	403	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, 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	436/451 (96%)	0.21	21 (4%) 34 36	40, 58, 96, 124	0
1	C	440/451 (97%)	-0.09	7 (1%) 74 76	34, 46, 77, 111	1 (0%)
2	B	422/445 (94%)	0.09	12 (2%) 56 59	35, 56, 96, 139	2 (0%)
2	D	418/445 (93%)	0.43	45 (10%) 8 7	40, 67, 102, 132	5 (1%)
3	E	123/143 (86%)	0.48	13 (10%) 8 8	46, 74, 116, 127	0
4	F	326/384 (84%)	1.26	103 (31%) 1 0	47, 84, 135, 155	0
All	All	2165/2319 (93%)	0.34	201 (9%) 11 12	34, 61, 111, 155	8 (0%)

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	100	ILE	8.9
4	F	173	ILE	7.7
4	F	253	TYR	7.6
4	F	132	LEU	7.4
4	F	130	VAL	7.1
4	F	166	ALA	6.9
4	F	182	ILE	6.8
2	B	59	ASN	6.6
4	F	169	LEU	6.2
4	F	99	VAL	5.9
2	D	57	THR	5.8
4	F	133	ALA	5.7
4	F	225	SER	5.7
4	F	252	ASN	5.7
3	E	26	PRO	5.7
4	F	251	LYS	5.6
1	A	281	ALA	5.5
4	F	21	LEU	5.4
4	F	362	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
4	F	223	THR	5.1
2	D	401	ARG	5.1
4	F	101	TYR	5.0
4	F	170	LEU	5.0
4	F	161	LEU	4.8
4	F	20	LEU	4.7
4	F	179	VAL	4.6
3	E	27	PRO	4.6
2	D	82	PRO	4.6
4	F	25	GLY	4.6
2	B	58	GLY	4.6
4	F	24	THR	4.6
4	F	150	LYS	4.5
4	F	244	CYS	4.5
3	E	143	ALA	4.5
4	F	263	PHE	4.5
4	F	199	PHE	4.4
2	D	415	GLU	4.4
4	F	131	PHE	4.4
4	F	172	PHE	4.3
4	F	17	VAL	4.3
4	F	134	ALA	4.2
4	F	129	GLU	4.2
2	D	400	ARG	4.2
4	F	181	VAL	4.1
4	F	194	PRO	4.1
2	D	250	ALA	4.1
4	F	256	TYR	4.1
4	F	254	GLY	4.0
4	F	1	MET	4.0
4	F	255	ARG	4.0
1	A	42	ILE	3.9
2	D	404	PHE	3.9
2	B	37	HIS	3.8
4	F	259	GLY	3.8
2	B	57	THR	3.8
4	F	152	SER	3.8
4	F	243	HIS	3.8
4	F	227	PRO	3.7
1	C	179	THR	3.7
4	F	197	ARG	3.7
4	F	192	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	E	28	SER	3.6
2	B	439	THR	3.6
2	D	182	VAL	3.6
4	F	165	GLU	3.5
4	F	171	ASP	3.5
4	F	135	TYR	3.5
4	F	128	ARG	3.5
4	F	240	LEU	3.5
2	D	177	VAL	3.5
4	F	28	LYS	3.4
3	E	24	LEU	3.4
4	F	250	SER	3.4
4	F	125	THR	3.4
4	F	228	TYR	3.4
1	A	41	THR	3.4
2	D	179	ASP	3.4
4	F	260	ASN	3.4
2	D	405	LEU	3.3
4	F	200	ASP	3.3
4	F	162	ILE	3.3
3	E	45	PRO	3.3
4	F	22	LEU	3.2
4	F	9	GLU	3.2
4	F	258	GLU	3.2
1	A	171	ILE	3.2
4	F	224	SER	3.2
4	F	167	SER	3.2
4	F	27	TRP	3.1
4	F	337	ALA	3.1
4	F	98	TYR	3.1
2	B	438	ALA	3.1
2	D	37	HIS	3.1
2	B	33	THR	3.1
3	E	48	GLU	3.1
4	F	241	THR	3.1
4	F	262	MET	3.1
4	F	190	LEU	3.0
3	E	140	LYS	3.0
3	E	139	LEU	3.0
2	D	58	GLY	3.0
2	D	56	ALA	3.0
4	F	361	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	260	VAL	2.9
4	F	221	LEU	2.9
4	F	19	ARG	2.9
4	F	26	GLN	2.9
2	D	77	SER	2.9
4	F	346	LEU	2.9
4	F	160	ILE	2.9
4	F	196	HIS	2.8
1	A	43	GLY	2.8
4	F	168	GLU	2.8
2	D	403	ALA	2.8
4	F	18	SER	2.8
4	F	245	ILE	2.8
4	F	102	PRO	2.7
4	F	163	SER	2.7
2	D	268	PHE	2.7
4	F	257	GLU	2.7
4	F	246	GLN	2.7
2	D	202	TYR	2.7
1	A	345	ASP	2.7
2	B	39	ASP	2.7
4	F	147	TRP	2.7
2	D	416	MET	2.7
4	F	174	ASP	2.6
3	E	142	GLU	2.6
2	D	180	THR	2.6
4	F	220	VAL	2.6
2	D	407	TRP	2.6
3	E	141	GLU	2.6
4	F	239	HIS	2.6
1	C	440	VAL	2.5
2	B	284	ARG	2.5
2	D	378	ILE	2.5
2	D	83	PHE	2.5
4	F	238	CYS	2.5
3	E	25	LYS	2.5
1	A	1	MET	2.5
2	D	399	PHE	2.5
2	D	276	THR	2.5
2	D	221	THR	2.5
4	F	341	LYS	2.5
1	A	46	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	252	LEU	2.5
4	F	342	LEU	2.5
2	B	36	TYR	2.4
2	D	219	LEU	2.4
4	F	261	GLU	2.4
4	F	126	ASP	2.4
4	F	344	ALA	2.4
4	F	191	LEU	2.4
1	A	44	GLY	2.4
4	F	180	HIS	2.4
2	B	101	ASN	2.4
2	D	59	ASN	2.4
4	F	226	GLU	2.4
4	F	343	TYR	2.4
4	F	23	ALA	2.3
4	F	193	GLU	2.3
4	F	340	GLN	2.3
1	A	201	ALA	2.3
2	D	201	THR	2.3
2	D	220	THR	2.3
2	D	406	HIS	2.3
1	A	173	PRO	2.3
1	A	282	TYR	2.3
2	D	94	PHE	2.3
2	D	317	ALA	2.3
4	F	127	GLU	2.3
1	C	238	ILE	2.3
2	D	80	SER	2.3
4	F	351	VAL	2.2
1	A	58	ALA	2.2
2	D	269	MET	2.2
1	A	9	VAL	2.2
1	A	146	GLY	2.2
1	A	346	TRP	2.2
1	A	37	PRO	2.2
1	A	35	GLN	2.1
2	B	247	GLN	2.1
2	D	166	MET	2.1
4	F	10	ASN	2.1
2	D	259	MET	2.1
1	A	172	TYR	2.1
2	D	85	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	270	PRO	2.1
2	D	285	ALA	2.1
3	E	6	MET	2.1
4	F	266	GLU	2.0
2	D	414	ASP	2.0
1	C	2	ARG	2.0
1	C	241	SER	2.0
1	A	40	LYS	2.0
2	D	255	LEU	2.0
1	C	178	SER	2.0
1	C	340	SER	2.0
2	D	96	GLN	2.0
4	F	195	GLY	2.0
1	A	12	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
6	MG	A	502	1/1	0.82	0.38	6.71	74,74,74,74	0
9	FB7	D	500	29/29	0.82	0.45	3.70	33,50,65,66	29
11	MES	B	505	12/12	0.96	0.13	0.83	56,66,84,88	0
8	GOL	A	505	6/6	0.91	0.15	0.72	79,83,84,84	0
6	MG	C	502	1/1	0.95	0.17	0.34	40,40,40,40	0
8	GOL	F	401	6/6	0.81	0.14	0.27	76,84,89,94	0
10	GDP	B	502	28/28	0.99	0.18	0.07	29,40,45,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GTP	A	501	32/32	0.99	0.20	0.01	35,43,49,49	0
7	CA	A	504	1/1	0.85	0.14	-0.24	100,100,100,100	0
5	GTP	C	501	32/32	0.99	0.14	-0.32	32,37,43,51	0
10	GDP	D	501	28/28	0.97	0.12	-0.34	45,59,69,74	0
9	FB7	B	501	29/29	0.96	0.15	-0.62	35,49,68,70	0
12	ACP	F	403	31/31	0.91	0.12	-1.14	86,97,122,134	0
7	CA	A	503	1/1	0.98	0.06	-2.38	81,81,81,81	0
7	CA	C	503	1/1	0.99	0.07	-2.61	67,67,67,67	0
6	MG	B	503	1/1	0.95	0.24	-	34,34,34,34	0
7	CA	B	504	1/1	0.95	0.10	-	83,83,83,83	0
6	MG	D	502	1/1	0.92	0.11	-	58,58,58,58	0
6	MG	F	402	1/1	0.89	0.10	-	82,82,82,82	0
7	CA	C	504	1/1	0.80	0.04	-	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.