



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 03:01 AM EDT

PDB ID : 5M8G
Title : Tubulin-MTD265 complex
Authors : Bohnacker, T.; Protá, A.E.; Steinmetz, M.O.; Wymann, M.P.
Deposited on : unknown
Resolution : 2.15 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

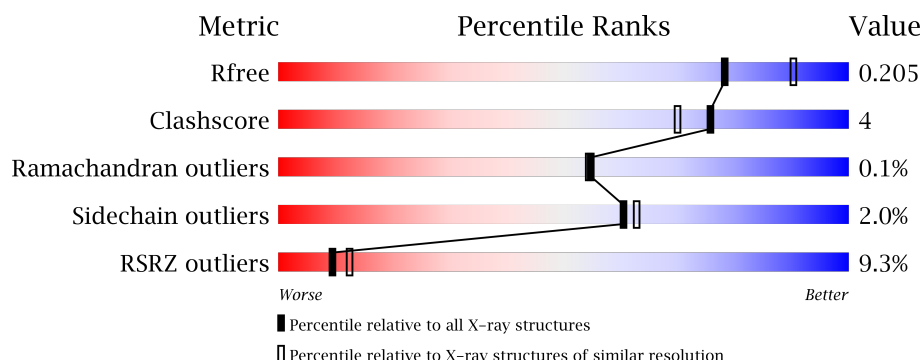
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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>86% 12% .</div> </div>
1	C	451	<div> <div>2%</div> <div>89% 8% ..</div> </div>
2	B	445	<div> <div>4%</div> <div>84% 11% 5%</div> </div>
2	D	445	<div> <div>9%</div> <div>83% 13% .</div> </div>
3	E	143	<div> <div>9%</div> <div>77% 9% 14%</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
7	CA	B	505	-	-	-	X
8	GOL	A	505	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18016 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	440	Total	C	N	O	S	0	1	0
			3436	2172	584	657	23			
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	423	Total	C	N	O	S	0	0	0
			3331	2094	568	643	26			
2	D	427	Total	C	N	O	S	0	0	0
			3349	2101	572	650	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

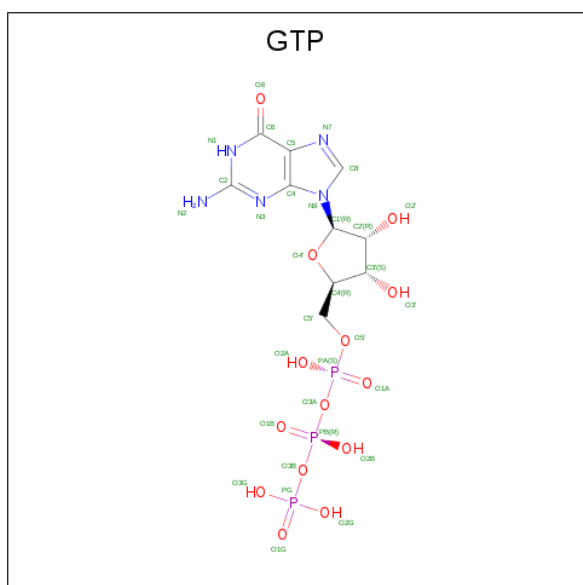
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	0	0
			2724	1756	461	493	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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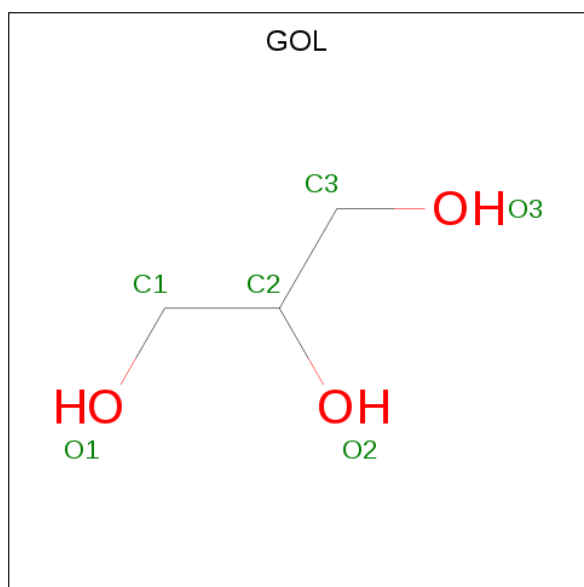
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

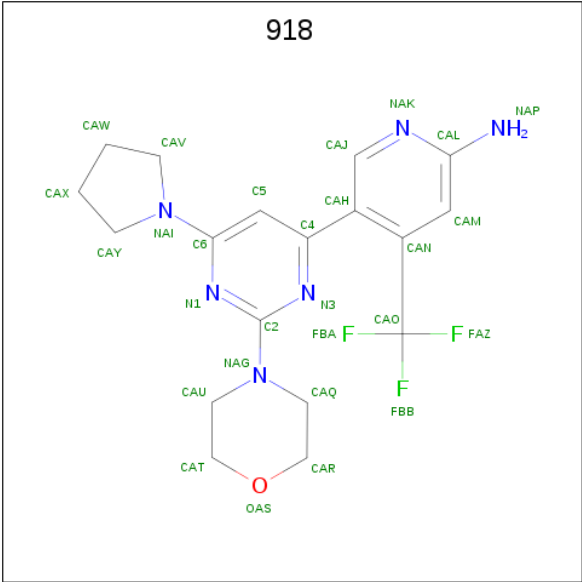
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

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



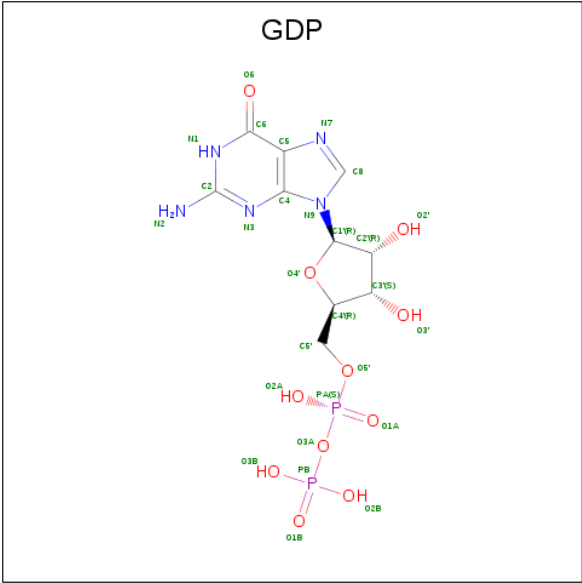
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 5-(2-morpholin-4-yl-6-pyrrolidin-1-yl-pyrimidin-4-yl)-4-(trifluoromethyl)pyridine-2-amine (three-letter code: 918) (formula: C₁₈H₂₁F₃N₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	F	N	O	0	0
			28	18	3	6	1		
9	D	1	Total	C	F	N	O	0	0
			28	18	3	6	1		

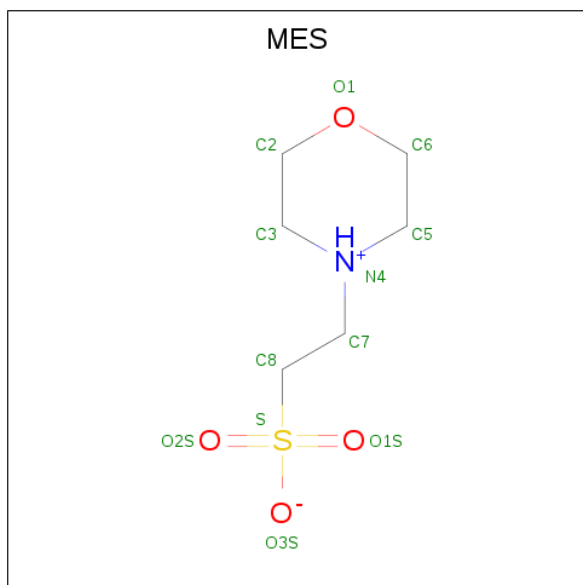
- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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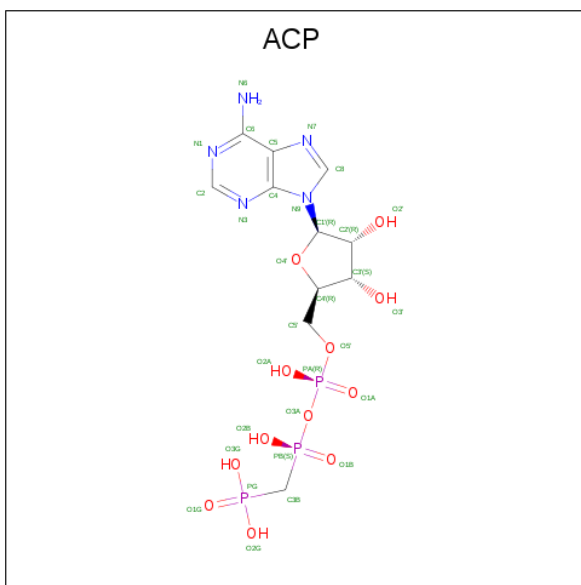
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
11	D	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: C₁₁H₁₈N₅O₁₂P₃).



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

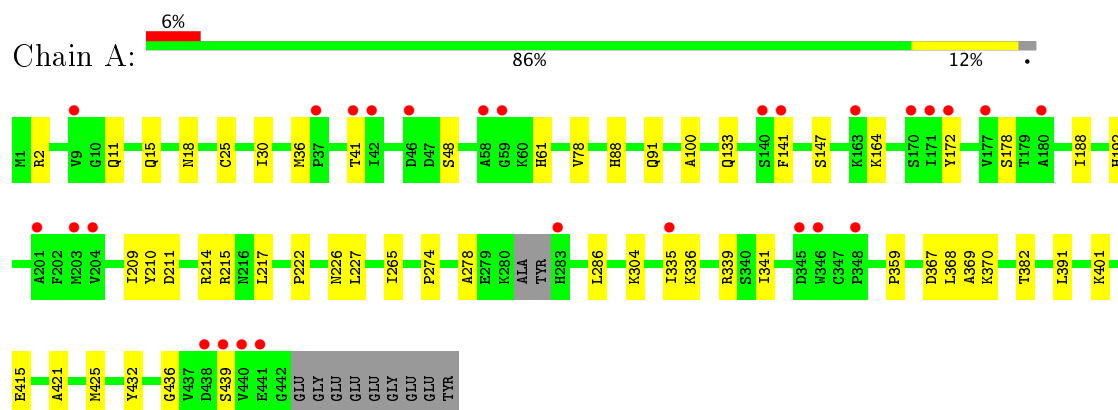
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	95	Total O 95 95	0	0
13	B	93	Total O 93 93	0	0
13	C	186	Total O 186 186	0	0
13	D	51	Total O 51 51	0	0
13	E	17	Total O 17 17	0	0
13	F	36	Total O 36 36	0	0

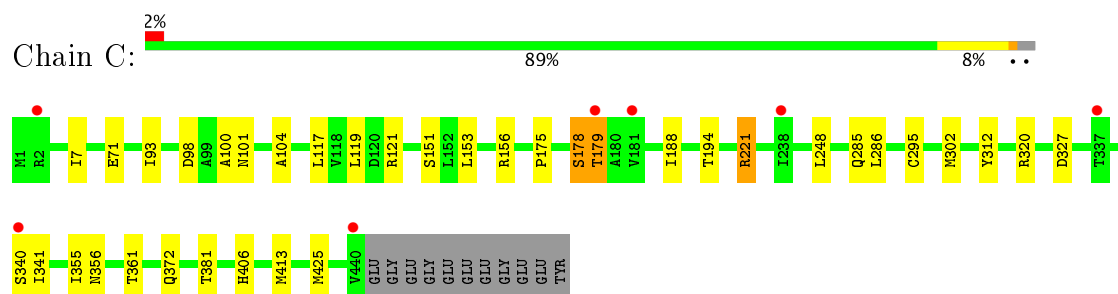
3 Residue-property plots [i](#)

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.

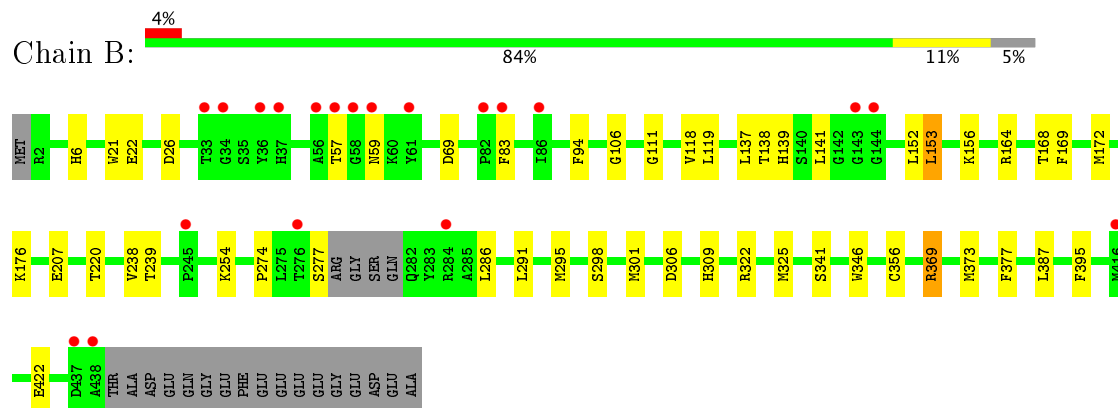
- Molecule 1: Tubulin alpha-1B chain



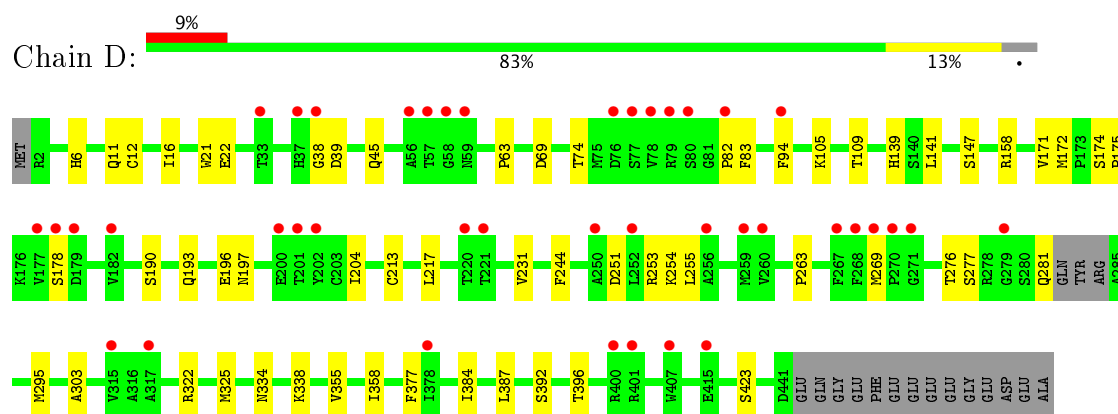
- Molecule 1: Tubulin alpha-1B chain



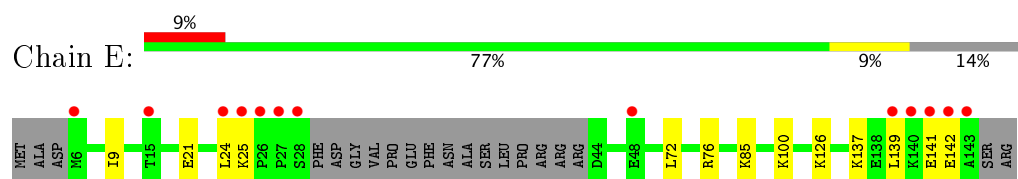
- Molecule 2: Tubulin beta-2B chain



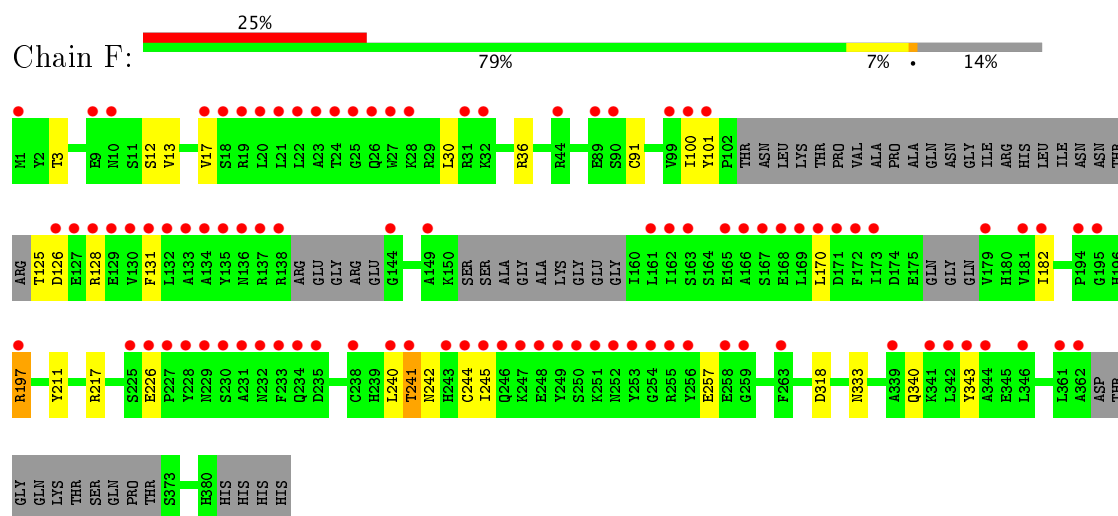
- Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-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	104.77Å 157.51Å 179.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.15 49.29 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-2.15) 99.7 (49.29-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.171 , 0.208 0.164 , 0.205	Depositor DCC
R_{free} test set	8069 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.5	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	0.97	EDS
Total number of atoms	18016	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, CA, GTP, ACP, 918, 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	0.39	0/3515	0.53	0/4769
1	C	0.48	1/3515 (0.0%)	0.58	0/4772
2	B	0.41	0/3405	0.56	0/4612
2	D	0.36	0/3422	0.52	0/4635
3	E	0.37	0/1022	0.48	0/1356
4	F	0.33	0/2786	0.50	0/3763
All	All	0.40	1/17665 (0.0%)	0.54	0/23907

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-8.23	1.68	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	3436	0	3348	29	0
1	C	3437	0	3349	19	0
2	B	3331	0	3208	26	0
2	D	3349	0	3223	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1014	0	1029	9	0
4	F	2724	0	2698	15	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	2	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	0	0	0
9	D	28	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	12	0	12	0	0
11	D	12	0	12	1	0
12	F	31	0	14	1	0
13	A	95	0	0	0	0
13	B	93	0	0	2	0
13	C	186	0	0	1	0
13	D	51	0	0	1	0
13	E	17	0	0	1	0
13	F	36	0	0	0	0
All	All	18016	0	16949	124	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 (124) 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:D:158:ARG:NH1	2:D:197:ASN:OD1	2.22	0.73
4:F:318:ASP:OD2	12:F:402:ACP:O3G	2.06	0.72
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.65
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.79	0.64
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.80	0.64
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.81	0.63
4:F:101:TYR:O	4:F:128:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:ARG:NH1	11:D:504:MES:O3S	2.33	0.62
2:D:11:GLN:HA	2:D:74:THR:HG21	1.83	0.61
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.67	0.60
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.84	0.60
3:E:85:LYS:NZ	13:E:201:HOH:O	2.28	0.59
1:A:88:HIS:N	1:A:91:GLN:OE1	2.27	0.59
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.84	0.58
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.85	0.58
2:B:152:LEU:HD11	2:B:156:LYS:HZ1	1.69	0.58
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.84	0.58
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.37	0.58
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.34	0.57
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.57
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.85	0.56
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.40	0.56
1:C:221:ARG:HD2	2:D:325:MET:HB3	1.87	0.56
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.88	0.55
3:E:137:LYS:O	3:E:141:GLU:HG2	2.07	0.55
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.88	0.55
3:E:139:LEU:O	3:E:142:GLU:HG2	2.08	0.54
2:B:106:GLY:O	2:B:111:GLY:HA3	2.08	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.43	0.54
2:D:325:MET:SD	2:D:355:VAL:HG21	2.48	0.53
1:C:175:PRO:HA	1:C:179:THR:OG1	2.08	0.53
2:B:220:THR:O	13:B:601:HOH:O	2.19	0.53
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.08	0.52
2:D:193:GLN:OE1	3:E:126:LYS:HE2	2.09	0.52
2:D:16:ILE:HD13	2:D:231:VAL:HG11	1.91	0.52
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.46	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.50
2:B:118:VAL:HG11	2:B:153:LEU:HD21	1.94	0.49
2:D:12:CYS:HB2	10:D:502:GDP:C8	2.47	0.49
1:C:101:ASN:ND2	2:D:254:LYS:HE2	2.26	0.49
1:A:336:LYS:NZ	1:A:341:ILE:O	2.46	0.49
3:E:24:LEU:O	3:E:25:LYS:HD2	2.13	0.48
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.28	0.48
4:F:241:THR:O	4:F:241:THR:OG1	2.30	0.48
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.48	0.48
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.48
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.95	0.48
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.95	0.48
1:C:327:ASP:OD2	13:C:601:HOH:O	2.19	0.47
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.97	0.47
3:E:72:LEU:O	3:E:76:ARG:HG2	2.15	0.47
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.95	0.47
1:A:359:PRO:HB2	1:A:370:LYS:HE2	1.96	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.46
2:D:325:MET:CE	2:D:355:VAL:HG21	2.45	0.46
4:F:240:LEU:HB3	4:F:242:ASN:HD22	1.80	0.46
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.50	0.46
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.98	0.46
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.42	0.46
1:A:192:HIS:CG	1:A:421:ALA:HA	2.51	0.46
2:D:171:VAL:HA	2:D:204:ILE:O	2.16	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.45
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.97	0.45
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.48	0.45
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.99	0.44
2:D:82:PRO:O	2:D:83:PHE:HB2	2.18	0.44
4:F:128:ARG:HH11	4:F:170:LEU:HD23	1.82	0.44
1:A:211:ASP:HB3	1:A:215:ARG:NH2	2.32	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.44
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.98	0.44
2:D:174:SER:O	2:D:178:SER:N	2.51	0.44
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.18	0.44
2:B:141:LEU:HD12	2:B:172:MET:SD	2.57	0.44
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.53	0.44
2:B:176:LYS:HD3	2:B:207:GLU:CG	2.47	0.44
2:B:298:SER:HA	2:B:301:MET:HG3	2.00	0.43
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.00	0.43
1:A:11:GLN:O	1:A:15:GLN:HG3	2.18	0.43
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
2:B:138:THR:HG22	2:B:169:PHE:HB2	2.00	0.43
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.54	0.43
4:F:240:LEU:HB3	4:F:242:ASN:ND2	2.34	0.43
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.01	0.43
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.43
1:C:151:SER:HA	1:C:194:THR:HG22	2.01	0.43
2:D:392:SER:O	2:D:396:THR:HG22	2.19	0.43
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.54	0.42
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.42
2:D:251:ASP:O	2:D:255:LEU:HG	2.18	0.42
2:D:105:LYS:HA	2:D:109:THR:OG1	2.20	0.42
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.42
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.87	0.42
2:D:22:GLU:OE1	2:D:82:PRO:HG2	2.19	0.42
3:E:100:LYS:HB2	3:E:100:LYS:HE3	1.85	0.42
4:F:126:ASP:OD2	4:F:128:ARG:HB2	2.19	0.42
2:D:175:PRO:HA	2:D:178:SER:HB3	2.02	0.42
1:A:25:CYS:HB3	1:A:30:ILE:O	2.19	0.42
1:A:211:ASP:HB3	1:A:215:ARG:HH22	1.85	0.42
2:B:238:VAL:HG23	2:B:239:THR:HG23	2.01	0.41
2:D:147:SER:HB2	2:D:190:SER:OG	2.20	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.41
4:F:13:VAL:O	4:F:17:VAL:HG23	2.20	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.55	0.41
2:D:334:ASN:HD21	2:D:338:LYS:NZ	2.18	0.41
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.86	0.41
2:B:322:ARG:O	2:B:373:MET:HE1	2.20	0.41
1:A:382:THR:HG21	1:A:436:GLY:HA3	2.01	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.55	0.41
2:B:164:ARG:HD2	13:B:685:HOH:O	2.20	0.41
2:D:39:ASP:N	2:D:39:ASP:OD1	2.54	0.41
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.03	0.41
1:C:104:ALA:HB2	1:C:413:MET:SD	2.61	0.41
2:D:281:GLN:NE2	13:D:602:HOH:O	2.39	0.40
4:F:3:THR:HB	4:F:30:LEU:HD11	2.02	0.40
2:B:295:MET:HE2	2:B:377:PHE:HB2	2.02	0.40
2:D:141:LEU:HD12	2:D:172:MET:SD	2.62	0.40
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.20	0.40
2:B:286:LEU:HD23	2:B:291:LEU:HG	2.04	0.40
1:C:286:LEU:HA	1:C:286:LEU:HD23	1.80	0.40
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.03	0.40
2:D:69:ASP:O	2:D:94:PHE:HA	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	437/451 (97%)	427 (98%)	9 (2%)	1 (0%)	51	48
1	C	438/451 (97%)	431 (98%)	6 (1%)	1 (0%)	51	48
2	B	419/445 (94%)	409 (98%)	10 (2%)	0	100	100
2	D	423/445 (95%)	416 (98%)	7 (2%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	319/384 (83%)	314 (98%)	5 (2%)	0	100	100
All	All	2155/2319 (93%)	2115 (98%)	38 (2%)	2 (0%)	55	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
1	C	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	372/379 (98%)	367 (99%)	5 (1%)	73	77
1	C	371/379 (98%)	364 (98%)	7 (2%)	62	65
2	B	366/383 (96%)	357 (98%)	9 (2%)	53	53
2	D	368/383 (96%)	361 (98%)	7 (2%)	62	65
3	E	110/127 (87%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	300/342 (88%)	290 (97%)	10 (3%)	43	41
All	All	1887/1993 (95%)	1849 (98%)	38 (2%)	60	63

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	SER
1	A	164	LYS
1	A	415	GLU
1	A	439	SER
2	B	57	THR
2	B	59	ASN
2	B	139	HIS
2	B	153	LEU
2	B	277	SER
2	B	325	MET
2	B	341	SER
2	B	356	CYS
2	B	369	ARG
1	C	178	SER
1	C	179	THR
1	C	221	ARG
1	C	302	MET
1	C	340	SER
1	C	361	THR
1	C	381	THR
2	D	139	HIS
2	D	196	GLU
2	D	276	THR
2	D	277	SER
2	D	322	ARG
2	D	384	ILE
2	D	423	SER
4	F	12	SER
4	F	36	ARG
4	F	91	CYS
4	F	125	THR
4	F	197	ARG
4	F	211	TYR
4	F	217	ARG
4	F	226	GLU

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Mol	Chain	Res	Type
4	F	241	THR
4	F	333	ASN

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

Mol	Chain	Res	Type
4	F	242	ASN
4	F	252	ASN
4	F	348	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	27,34,34	0.91	1 (3%)	27,54,54	1.76	5 (18%)
8	GOL	A	505	-	5,5,5	0.30	0	5,5,5	0.35	0
9	918	B	501	-	31,31,31	1.30	3 (9%)	40,45,45	1.67	8 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GDP	B	502	6	25,30,30	1.07	2 (8%)	26,47,47	2.17	7 (26%)
11	MES	B	506	-	12,12,12	1.80	1 (8%)	14,16,16	2.25	4 (28%)
5	GTP	C	501	6	27,34,34	0.92	1 (3%)	27,54,54	1.90	6 (22%)
9	918	D	501	-	31,31,31	1.20	4 (12%)	40,45,45	1.86	8 (20%)
10	GDP	D	502	6	25,30,30	1.15	2 (8%)	26,47,47	2.04	6 (23%)
11	MES	D	504	-	12,12,12	2.01	1 (8%)	14,16,16	2.22	5 (35%)
12	ACP	F	402	6	27,33,33	1.69	6 (22%)	30,52,52	1.51	4 (13%)

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	918	B	501	-	-	0/18/33/33	0/4/4/4
10	GDP	B	502	6	-	0/12/32/32	0/3/3/3
11	MES	B	506	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	918	D	501	-	-	0/18/33/33	0/4/4/4
10	GDP	D	502	6	-	0/12/32/32	0/3/3/3
11	MES	D	504	-	-	0/6/14/14	0/1/1/1
12	ACP	F	402	6	-	0/15/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	504	MES	C8-S	-6.67	1.67	1.77
11	B	506	MES	C8-S	-5.83	1.68	1.77
9	D	501	918	CAO-CAN	-3.78	1.41	1.50
9	B	501	918	C6-NAI	-3.64	1.30	1.37
9	B	501	918	CAO-CAN	-3.54	1.42	1.50
12	F	402	ACP	PB-O2B	-3.05	1.48	1.56
9	B	501	918	CAH-C4	-2.85	1.40	1.48
9	D	501	918	CAH-C4	-2.74	1.40	1.48
9	D	501	918	C6-NAI	-2.13	1.33	1.37
9	D	501	918	CAJ-NAK	2.18	1.39	1.34
10	B	502	GDP	C5-C4	2.34	1.45	1.40
12	F	402	ACP	PG-O3G	2.67	1.61	1.54
5	C	501	GTP	C6-N1	2.67	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C6-N1	2.72	1.38	1.33
12	F	402	ACP	PG-O2G	2.86	1.61	1.54
10	B	502	GDP	C6-C5	3.04	1.47	1.41
10	D	502	GDP	C5-C4	3.04	1.47	1.40
12	F	402	ACP	C5-C4	3.10	1.47	1.40
10	D	502	GDP	C6-C5	3.60	1.48	1.41
12	F	402	ACP	PB-O3A	3.71	1.62	1.58
12	F	402	ACP	PB-O1B	3.80	1.61	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	N3-C2-N1	-5.50	124.07	128.86
5	C	501	GTP	N3-C2-N1	-5.31	119.71	127.46
10	B	502	GDP	C6-C5-C4	-4.65	116.22	120.84
5	A	501	GTP	N3-C2-N1	-4.42	121.01	127.46
10	D	502	GDP	C5-C6-N1	-4.22	117.47	123.48
5	A	501	GTP	C5-C6-N1	-4.08	117.67	123.48
10	B	502	GDP	N3-C2-N1	-4.06	121.53	127.46
9	B	501	918	N1-C2-N3	-3.92	119.78	126.32
10	D	502	GDP	C6-C5-C4	-3.89	116.98	120.84
9	D	501	918	CAJ-CAH-C4	-3.86	114.16	120.86
9	D	501	918	N1-C2-N3	-3.81	119.96	126.32
10	B	502	GDP	C5-C6-N1	-3.60	118.36	123.48
9	B	501	918	CAJ-CAH-C4	-3.57	114.67	120.86
10	D	502	GDP	C4-C5-N7	-3.53	106.00	109.41
5	C	501	GTP	C5-C6-N1	-3.26	118.84	123.48
12	F	402	ACP	C4-C5-N7	-3.22	106.30	109.41
9	D	501	918	C5-C4-N3	-3.21	118.52	122.38
10	B	502	GDP	C4-C5-N7	-2.94	106.56	109.41
9	B	501	918	C5-C4-N3	-2.67	119.16	122.38
10	D	502	GDP	N3-C2-N1	-2.62	123.63	127.46
11	B	506	MES	O3S-S-O1S	-2.51	105.62	111.37
5	A	501	GTP	C4-C5-N7	-2.45	107.04	109.41
12	F	402	ACP	PA-O3A-PB	-2.35	124.83	132.39
5	C	501	GTP	C6-C5-C4	-2.27	118.59	120.84
9	B	501	918	CAH-CAJ-NAK	-2.18	121.15	124.49
12	F	402	ACP	O2'-C2'-C1'	-2.05	105.22	111.61
10	B	502	GDP	C1'-N9-C4	-2.04	123.12	126.64
11	D	504	MES	C7-N4-C5	2.00	116.39	111.26
5	C	501	GTP	N2-C2-N1	2.05	120.52	117.24
9	D	501	918	CAW-CAV-NAI	2.06	106.04	103.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	918	N3-C2-NAG	2.66	120.07	117.11
9	B	501	918	N1-C2-NAG	2.72	120.14	117.11
11	D	504	MES	O2S-S-C8	2.78	109.18	106.79
5	A	501	GTP	C2-N3-C4	2.84	118.47	115.16
11	B	506	MES	O3S-S-C8	2.86	109.57	106.06
9	B	501	918	C2-N1-C6	2.89	120.25	115.26
9	D	501	918	CAT-CAU-NAG	2.96	115.31	109.98
5	C	501	GTP	C6-N1-C2	3.56	121.18	116.06
11	D	504	MES	O3S-S-C8	3.58	110.46	106.06
9	D	501	918	N3-C2-NAG	3.65	121.16	117.11
9	D	501	918	C2-N1-C6	3.73	121.70	115.26
5	A	501	GTP	C6-N1-C2	3.77	121.49	116.06
11	D	504	MES	O1S-S-C8	4.15	110.35	106.79
10	D	502	GDP	C2-N3-C4	4.19	120.05	115.16
5	C	501	GTP	C2-N3-C4	4.20	120.06	115.16
11	D	504	MES	C5-N4-C3	4.29	118.58	108.87
9	D	501	918	CAQ-NAG-CAU	4.33	120.75	111.57
10	D	502	GDP	C6-N1-C2	4.49	122.51	116.06
9	B	501	918	CAQ-NAG-CAU	4.60	121.33	111.57
10	B	502	GDP	C6-N1-C2	4.84	123.03	116.06
11	B	506	MES	O1S-S-C8	4.96	111.06	106.79
10	B	502	GDP	C2-N3-C4	5.12	121.14	115.16
11	B	506	MES	C5-N4-C3	5.16	120.56	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	GDP	1	0
11	D	504	MES	1	0
12	F	402	ACP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	440/451 (97%)	0.36	27 (6%)	22 27	37, 56, 95, 136	0
1	C	440/451 (97%)	0.03	7 (1%)	72 77	31, 44, 77, 119	0
2	B	423/445 (95%)	0.24	20 (4%)	32 39	32, 52, 88, 132	2 (0%)
2	D	427/445 (95%)	0.46	41 (9%)	9 11	38, 65, 100, 132	4 (0%)
3	E	123/143 (86%)	0.37	13 (10%)	7 8	40, 70, 113, 131	0
4	F	331/384 (86%)	1.18	95 (28%)	1 1	47, 83, 141, 168	0
All	All	2184/2319 (94%)	0.42	203 (9%)	9 12	31, 59, 110, 168	6 (0%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	8.7
4	F	173	ILE	8.2
4	F	249	TYR	7.7
4	F	169	LEU	7.1
4	F	130	VAL	6.9
4	F	250	SER	6.6
4	F	233	PHE	6.3
4	F	100	ILE	6.3
4	F	161	LEU	6.2
4	F	179	VAL	6.1
4	F	132	LEU	6.0
2	D	57	THR	5.9
4	F	253	TYR	5.7
3	E	26	PRO	5.5
4	F	252	ASN	5.4
1	A	440	VAL	5.3
2	B	57	THR	5.2
2	D	82	PRO	5.2
4	F	182	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	5.0
4	F	101	TYR	4.9
4	F	20	LEU	4.9
4	F	227	PRO	4.9
4	F	133	ALA	4.9
4	F	248	GLU	4.9
4	F	134	ALA	4.8
2	D	58	GLY	4.8
4	F	251	LYS	4.8
2	D	56	ALA	4.8
4	F	170	LEU	4.6
4	F	167	SER	4.6
4	F	232	ASN	4.6
2	B	245	PRO	4.6
4	F	166	ALA	4.6
4	F	17	VAL	4.5
1	A	439	SER	4.4
4	F	362	ALA	4.4
3	E	143	ALA	4.4
4	F	99	VAL	4.3
1	C	340	SER	4.2
4	F	244	CYS	4.1
4	F	263	PHE	4.1
1	A	346	TRP	4.0
3	E	24	LEU	4.0
2	D	407	TRP	4.0
3	E	142	GLU	4.0
3	E	139	LEU	4.0
4	F	361	LEU	3.9
1	A	441	GLU	3.9
4	F	22	LEU	3.8
2	B	37	HIS	3.8
4	F	259	GLY	3.8
2	B	58	GLY	3.8
2	B	284	ARG	3.8
1	A	171	ILE	3.7
2	B	59	ASN	3.7
4	F	165	GLU	3.7
4	F	194	PRO	3.7
4	F	25	GLY	3.7
4	F	172	PHE	3.7
4	F	137	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	37	HIS	3.6
2	B	36	TYR	3.6
4	F	129	GLU	3.6
4	F	131	PHE	3.5
1	C	440	VAL	3.5
4	F	24	THR	3.5
1	A	163	LYS	3.4
4	F	32	LYS	3.4
4	F	344	ALA	3.4
4	F	31	ARG	3.4
1	A	42	ILE	3.3
4	F	163	SER	3.3
4	F	149	ALA	3.3
4	F	135	TYR	3.3
2	D	268	PHE	3.3
4	F	234	GLN	3.3
4	F	18	SER	3.2
4	F	255	ARG	3.2
4	F	256	TYR	3.2
2	B	33	THR	3.2
2	B	61	TYR	3.1
4	F	341	LYS	3.1
2	B	56	ALA	3.0
4	F	168	GLU	3.0
4	F	27	TRP	3.0
4	F	144	GLY	3.0
1	A	201	ALA	3.0
3	E	6	MET	3.0
2	D	317	ALA	2.9
3	E	140	LYS	2.9
3	E	25	LYS	2.9
2	D	279	GLY	2.9
4	F	342	LEU	2.9
2	B	438	ALA	2.9
2	D	220	THR	2.9
2	D	260	VAL	2.8
2	B	437	ASP	2.8
2	B	276	THR	2.8
2	D	202	TYR	2.8
2	D	77	SER	2.8
4	F	128	ARG	2.7
4	F	136	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	229	ASN	2.7
2	D	33	THR	2.7
4	F	90	SER	2.7
4	F	247	LYS	2.7
4	F	21	LEU	2.7
4	F	181	VAL	2.7
3	E	28	SER	2.7
2	D	59	ASN	2.7
2	D	80	SER	2.7
1	A	283	HIS	2.7
4	F	254	GLY	2.7
4	F	126	ASP	2.7
4	F	241	THR	2.7
2	D	378	ILE	2.6
1	A	438	ASP	2.6
4	F	171	ASP	2.6
2	D	79	ARG	2.6
4	F	138	ARG	2.6
2	D	78	VAL	2.6
2	D	259	MET	2.6
4	F	195	GLY	2.6
1	A	345	ASP	2.6
1	C	2	ARG	2.6
3	E	15	THR	2.6
3	E	141	GLU	2.6
2	D	178	SER	2.5
1	C	179	THR	2.5
4	F	9	GLU	2.5
2	D	400	ARG	2.5
4	F	238	CYS	2.5
4	F	225	SER	2.5
2	D	38	GLY	2.5
2	D	94	PHE	2.5
2	D	415	GLU	2.5
2	D	182	VAL	2.5
4	F	197	ARG	2.4
4	F	246	GLN	2.4
4	F	1	MET	2.4
4	F	339	ALA	2.4
1	A	9	VAL	2.4
2	B	83	PHE	2.4
2	D	401	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	86	ILE	2.4
2	D	76	ASP	2.4
4	F	26	GLN	2.3
4	F	346	LEU	2.3
1	C	181	VAL	2.3
4	F	230	SER	2.3
4	F	23	ALA	2.3
2	D	221	THR	2.3
2	D	201	THR	2.3
4	F	235	ASP	2.3
4	F	228	TYR	2.2
1	A	41	THR	2.2
1	A	141	PHE	2.2
2	D	267	PHE	2.2
1	A	37	PRO	2.2
1	A	335	ILE	2.2
2	D	252	LEU	2.2
2	B	82	PRO	2.2
2	B	143	GLY	2.2
2	D	250	ALA	2.2
2	B	144	GLY	2.2
4	F	243	HIS	2.2
2	B	416	MET	2.2
1	C	238	ILE	2.2
2	D	271	GLY	2.2
4	F	258	GLU	2.2
4	F	162	ILE	2.2
1	A	46	ASP	2.2
2	D	179	ASP	2.2
2	D	270	PRO	2.2
2	D	200	GLU	2.2
4	F	127	GLU	2.2
1	A	204	VAL	2.1
4	F	343	TYR	2.1
2	B	34	GLY	2.1
4	F	226	GLU	2.1
4	F	240	LEU	2.1
1	A	140	SER	2.1
1	A	180	ALA	2.1
4	F	89	GLU	2.1
4	F	19	ARG	2.1
1	A	203	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	2.1
1	A	348	PRO	2.1
3	E	48	GLU	2.1
4	F	10	ASN	2.1
4	F	44	ARG	2.0
2	D	269	MET	2.0
1	C	337	THR	2.0
2	D	177	VAL	2.0
4	F	28	LYS	2.0
2	D	256	ALA	2.0
1	A	177	VAL	2.0
2	D	315	VAL	2.0
1	A	170	SER	2.0
1	A	172	TYR	2.0
4	F	245	ILE	2.0
1	A	59	GLY	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
7	CA	B	505	1/1	0.87	0.24	4.16	92,92,92,92	0
8	GOL	A	505	6/6	0.90	0.17	3.26	78,81,88,89	0
11	MES	D	504	12/12	0.91	0.21	1.36	89,100,103,107	0
11	MES	B	506	12/12	0.97	0.12	0.58	36,47,67,75	0
6	MG	A	502	1/1	0.95	0.17	0.28	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	GDP	B	502	28/28	0.99	0.18	0.15	31,37,43,43	0
5	GTP	A	501	32/32	0.98	0.19	-0.12	32,40,44,54	0
5	GTP	C	501	32/32	0.98	0.14	-0.20	27,34,40,44	0
9	918	B	501	28/28	0.95	0.16	-0.34	34,44,55,60	0
6	MG	C	502	1/1	0.97	0.12	-0.53	39,39,39,39	0
10	GDP	D	502	28/28	0.97	0.10	-0.57	46,56,66,72	0
9	918	D	501	28/28	0.92	0.17	-0.78	44,50,57,60	0
7	CA	A	504	1/1	0.87	0.09	-1.14	114,114,114,114	0
12	ACP	F	402	31/31	0.91	0.12	-1.29	82,96,119,130	0
7	CA	A	503	1/1	0.97	0.04	-2.35	75,75,75,75	0
7	CA	C	503	1/1	0.99	0.06	-2.98	59,59,59,59	0
7	CA	B	504	1/1	0.83	0.10	-	112,112,112,112	0
6	MG	B	503	1/1	0.99	0.24	-	30,30,30,30	0
6	MG	D	503	1/1	0.93	0.04	-	61,61,61,61	0
6	MG	F	401	1/1	0.85	0.05	-	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.