



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:12 PM GMT

PDB ID : 4O2B
Title : Tubulin-Colchicine complex
Authors : Prota, A.E.; Franck, D.; Bachmann, F.; Bargsten, K.; Buey, R.M.; Pohlmann, J.; Reinelt, S.; Lane, H.; Steinmetz, M.O.
Deposited on : 2013-12-17
Resolution : 2.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

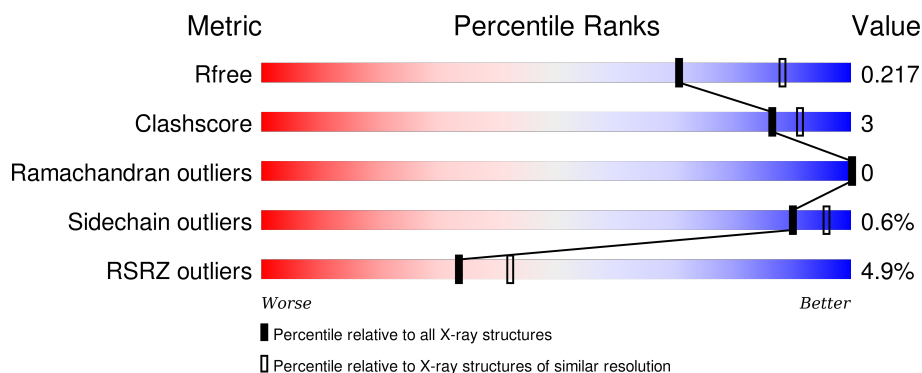
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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>90%</div> <div>7%</div> <div>•</div> </div>
1	C	451	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
2	B	445	<div> <div>%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
2	D	445	<div> <div>3%</div> <div>89%</div> <div>5%</div> <div>5%</div> </div>
3	E	143	<div> <div>4%</div> <div>83%</div> <div>•</div> <div>15%</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
12	PEG	C	506	-	-	-	X
12	PEG	C	507	-	-	-	X
13	IMD	C	510	-	-	-	X
6	MG	A	502	-	-	-	X
7	GOL	A	503	-	-	-	X
7	GOL	A	505	-	-	-	X
7	GOL	B	504	-	-	-	X
7	GOL	B	505	-	-	-	X
7	GOL	B	507	-	-	-	X
7	GOL	C	503	-	-	-	X
7	GOL	C	504	-	-	-	X
7	GOL	C	505	-	-	-	X
7	GOL	D	505	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

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

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

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

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	CLONING ARTIFACT	UNP P63043
E	4	ALA	-	CLONING ARTIFACT	UNP P63043

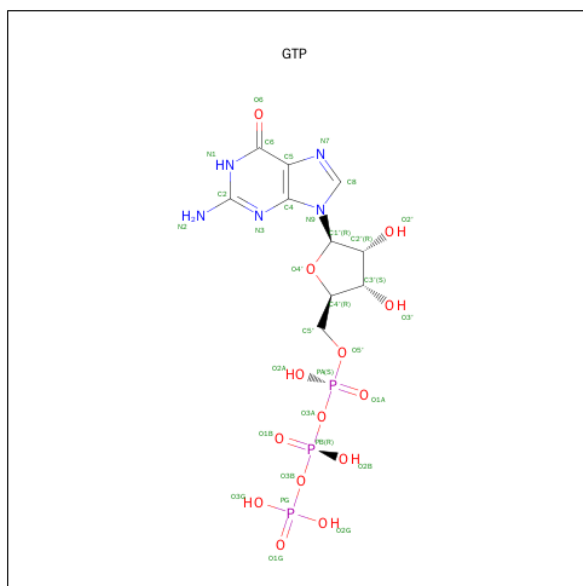
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	319	Total	C	N	O	S	0	5	0
			2633	1706	436	477	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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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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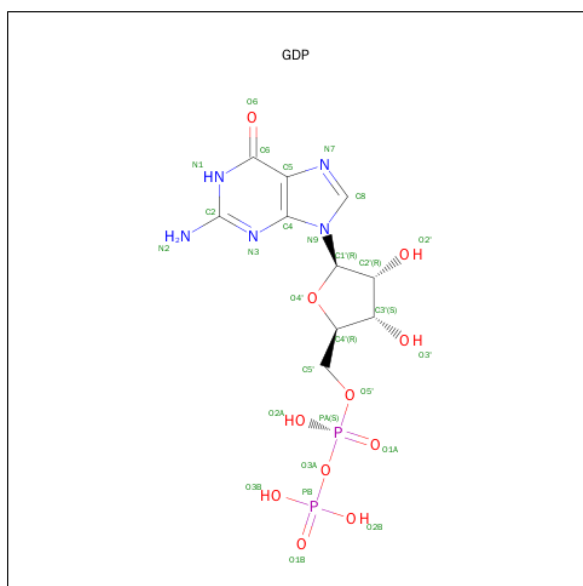
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

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

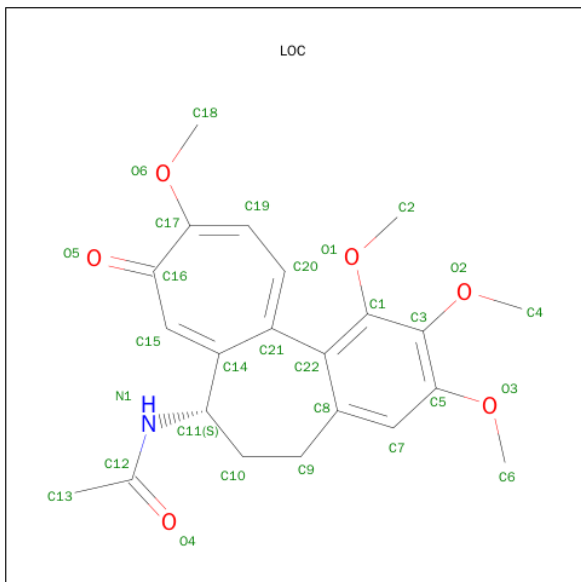
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



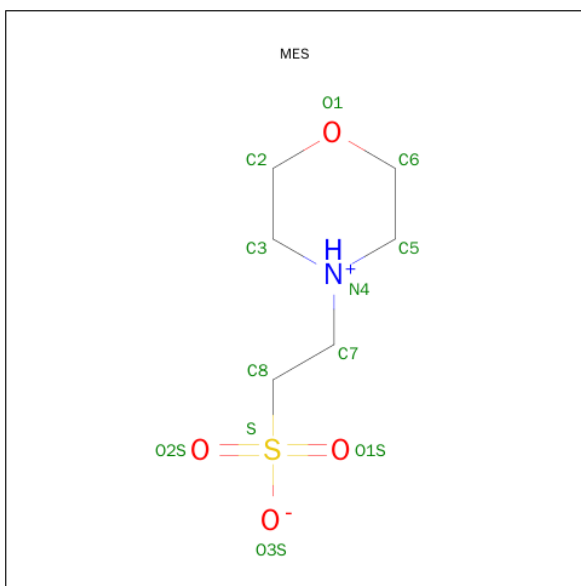
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is N-[(7S)-1,2,3,10-TETRAMETHOXY-9-OXO-6,7-DIHYDRO-5H-BENZO[D]HEPTALEN-7-YL]ETHANAMIDE (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$).



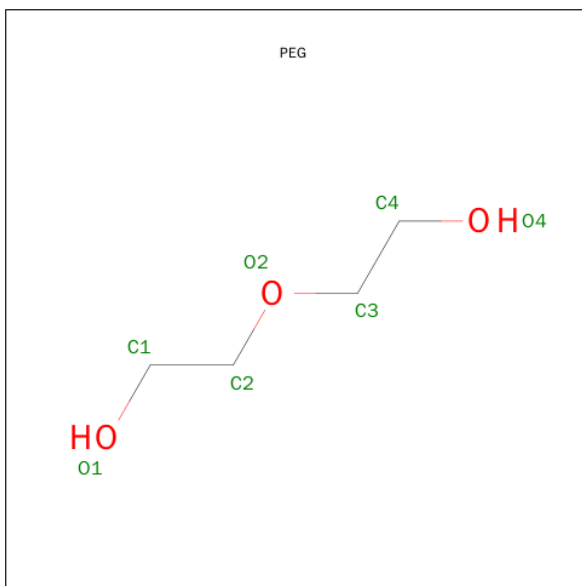
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			29	22	1	6		
10	D	1	Total	C	N	O	0	0
			29	22	1	6		

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



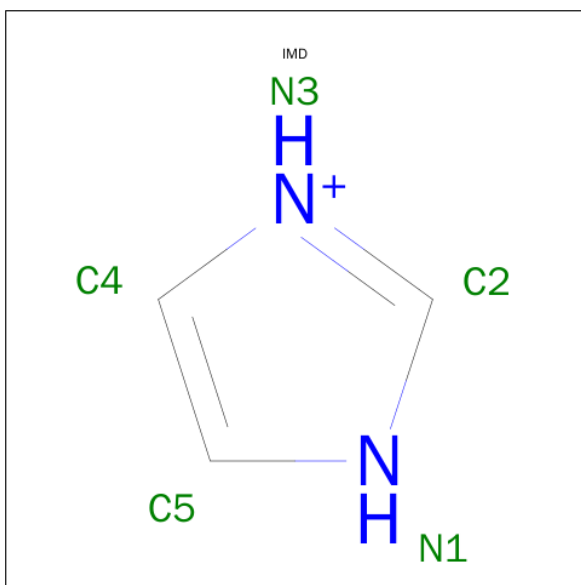
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



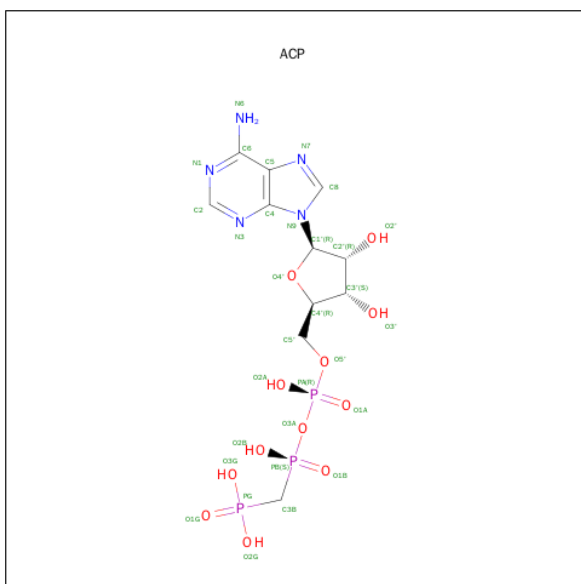
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

- Molecule 14 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
14	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

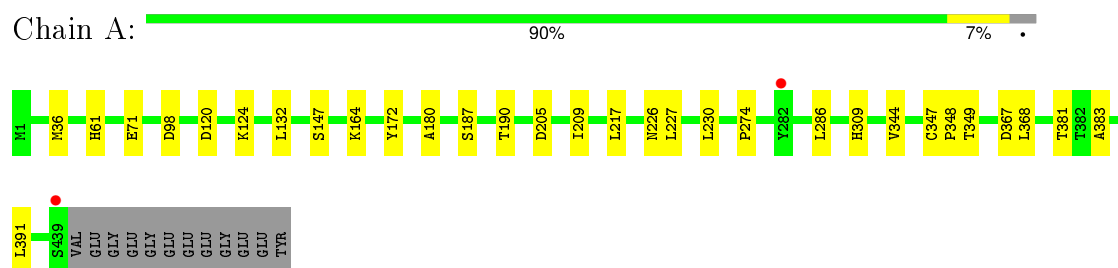
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	127	Total	O	0	0
			127	127		
15	B	132	Total	O	0	0
			132	132		
15	C	219	Total	O	0	0
			219	219		
15	D	84	Total	O	0	0
			84	84		
15	E	29	Total	O	0	0
			29	29		
15	F	35	Total	O	0	0
			35	35		

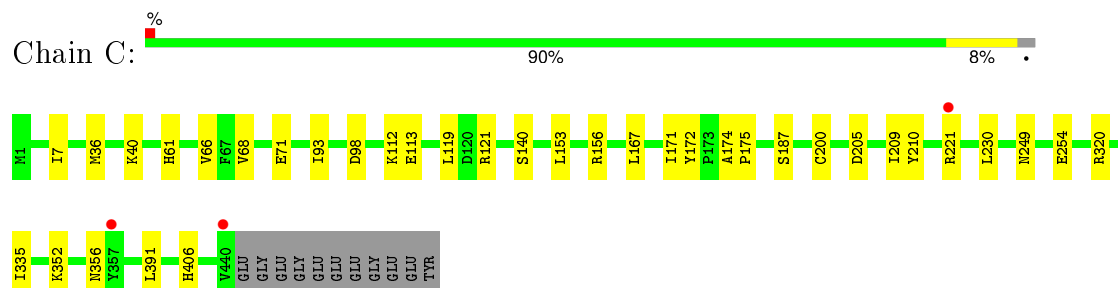
3 Residue-property plots

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.

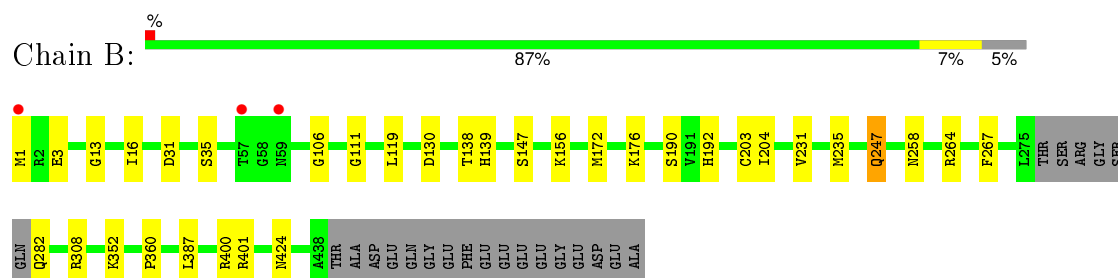
• Molecule 1: Tubulin alpha-1B chain



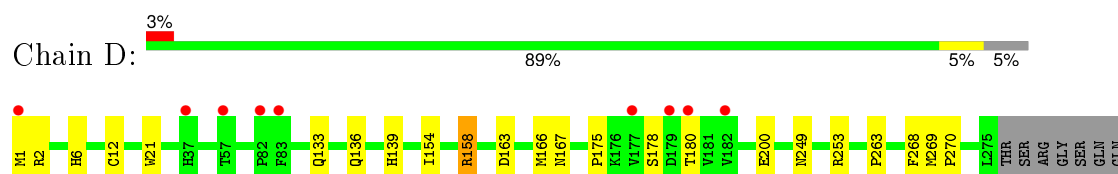
• Molecule 1: Tubulin alpha-1B chain



• Molecule 2: Tubulin beta-2B chain

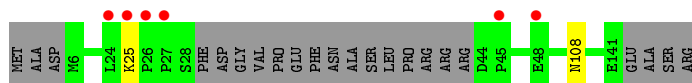
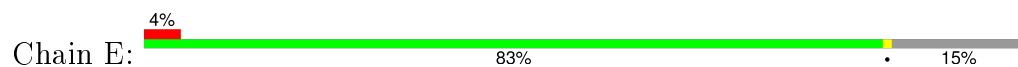


• Molecule 2: Tubulin beta-2B chain

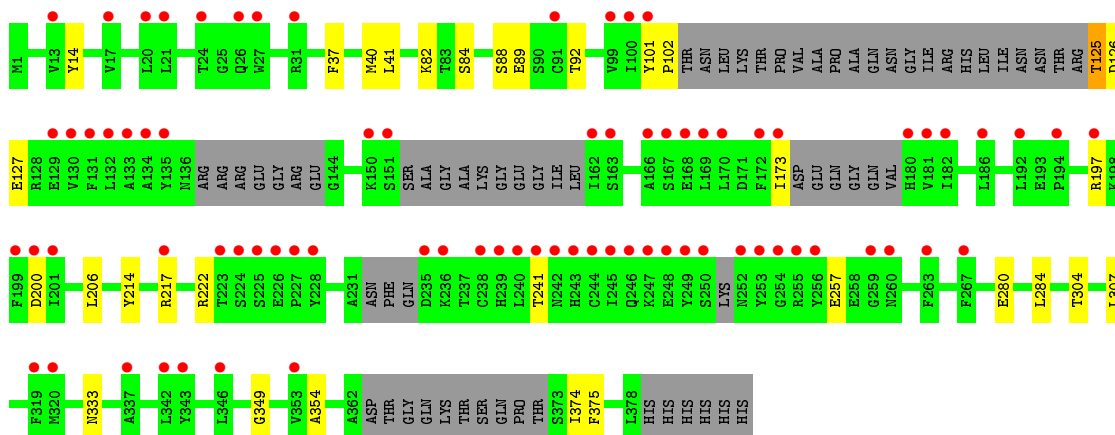
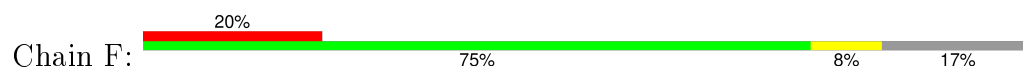




● Molecule 3: Stathmin-4



● 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	104.31Å 157.01Å 180.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.70 – 2.30 78.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.70-2.30) 97.8 (78.50-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.182 , 0.213 0.187 , 0.217	Depositor DCC
R_{free} test set	1792 reflections (1.38%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	43 of 146979 reflections (0.029%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18288	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, LOC, MG, IMD, GOL, CA, GTP, ACP, MES, PEG

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	0.22	0/3605	0.39	0/4895
1	C	0.22	0/3597	0.40	0/4885
2	B	0.22	0/3478	0.38	0/4710
2	D	0.21	0/3411	0.37	0/4622
3	E	0.20	0/1033	0.31	0/1370
4	F	0.21	0/2704	0.37	0/3650
All	All	0.21	0/17828	0.38	0/24132

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	3488	0	3441	18	0
1	C	3489	0	3413	20	0
2	B	3374	0	3270	22	0
2	D	3326	0	3221	16	0
3	E	1016	0	1041	2	0
4	F	2633	0	2631	18	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	18	0	24	1	0
7	B	24	0	32	1	0
7	C	18	0	24	0	0
7	D	12	0	16	2	0
7	E	6	0	8	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	29	0	25	1	0
10	D	29	0	25	0	0
11	B	12	0	12	1	0
12	C	14	0	20	0	0
13	C	15	0	15	0	0
14	F	31	0	14	1	0
15	A	127	0	0	0	0
15	B	132	0	0	3	0
15	C	219	0	0	1	0
15	D	84	0	0	1	0
15	E	29	0	0	1	0
15	F	35	0	0	1	0
All	All	18288	0	17280	93	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 3.

All (93) 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:264:ARG:HH12	2:B:424[B]:ASN:HD21	1.40	0.69
2:D:175:PRO:HA	2:D:178:SER:HB2	1.76	0.67
2:D:158:ARG:NH1	7:D:505:GOL:O2	2.30	0.65
1:C:210:TYR:OH	1:C:221:ARG:NH2	2.31	0.64
3:E:108[A]:ASN:ND2	15:E:301:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:102:PRO:HB3	4:F:173:ILE:HG22	1.83	0.61
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.82	0.61
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.34	0.61
4:F:217:ARG:HE	4:F:374:ILE:HA	1.66	0.60
4:F:101:TYR:HD2	4:F:126:ASP:HB3	1.67	0.60
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.83	0.60
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.48	0.59
1:A:132:LEU:O	1:A:164:LYS:NZ	2.36	0.58
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.86	0.57
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.87	0.57
1:C:40:LYS:NZ	15:C:737:HOH:O	2.38	0.56
1:A:309:HIS:O	7:A:505:GOL:O1	2.24	0.56
1:A:344:VAL:HG23	1:A:347:CYS:HB2	1.89	0.54
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.90	0.54
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.21	0.54
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.41	0.54
1:A:381:THR:HG22	1:A:383:ALA:H	1.73	0.53
2:B:308:ARG:NH1	15:B:691:HOH:O	2.41	0.53
2:D:163:ASP:O	2:D:253:ARG:NH2	2.41	0.53
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.90	0.53
1:A:349:THR:HB	3:E:25:LYS:HB3	1.90	0.52
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.41	0.52
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.37	0.51
2:B:360:PRO:HG3	7:B:507:GOL:O2	2.11	0.51
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.93	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.51
2:B:247:GLN:NE2	15:B:663:HOH:O	2.33	0.50
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.93	0.50
2:D:253:ARG:NH1	7:D:505:GOL:O3	2.31	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.94	0.49
2:B:31:ASP:OD1	2:B:35:SER:N	2.45	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.49	0.48
4:F:200:ASP:OD1	4:F:222:ARG:NH2	2.46	0.48
2:B:352:LYS:HG3	10:B:503:LOC:C16	2.44	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.48
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.41	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.96	0.47
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.48	0.47
2:D:2:ARG:HB3	2:D:133:GLN:HE21	1.80	0.46
4:F:333:ASN:ND2	14:F:402:ACP:O2G	2.38	0.46
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.46
4:F:125:THR:HA	4:F:126:ASP:HA	1.56	0.46
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.49	0.46
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.98	0.46
4:F:14:TYR:OH	15:F:531:HOH:O	2.20	0.45
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.99	0.45
2:D:2:ARG:HB3	2:D:133:GLN:NE2	2.31	0.45
2:D:158:ARG:NH2	15:D:633:HOH:O	2.47	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.44
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.99	0.44
2:D:167:ASN:ND2	2:D:200:GLU:O	2.49	0.44
11:B:509:MES:H81	11:B:509:MES:H51	1.82	0.44
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.99	0.44
2:D:136:GLN:HA	2:D:167:ASN:O	2.18	0.43
2:B:119:LEU:HD11	2:B:156:LYS:HB3	2.00	0.43
4:F:37:PHE:CE2	4:F:40:MET:HB2	2.53	0.43
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.99	0.43
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	2.01	0.43
2:B:235:MET:HE2	2:B:235:MET:HB3	1.90	0.43
2:B:176:LYS:HA	2:B:176:LYS:HD2	1.78	0.43
2:B:282:GLN:N	15:B:628:HOH:O	2.52	0.42
2:B:1:MET:HB2	2:B:3:GLU:OE1	2.19	0.42
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.00	0.42
4:F:304:THR:HG22	4:F:307:LEU:HD12	2.00	0.42
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.24	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.42
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.01	0.42
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.01	0.41
2:B:1:MET:HG3	2:B:130:ASP:OD2	2.19	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	2.03	0.41
1:C:71:GLU:OE1	2:D:249:ASN:ND2	2.50	0.41
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.01	0.41
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.21	0.41
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.56	0.41
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.03	0.41
1:A:347:CYS:HA	1:A:348:PRO:HD3	1.95	0.41
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.61	0.41
4:F:84:SER:O	4:F:88:SER:N	2.45	0.40
1:C:174:ALA:HA	1:C:175:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	2.04	0.40
1:A:180:ALA:HB1	2:B:258:ASN:OD1	2.20	0.40
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.04	0.40
2:D:268:PHE:O	2:D:270:PRO:HD3	2.21	0.40
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/451 (100%)	438 (97%)	12 (3%)	0	100	100
1	C	449/451 (100%)	440 (98%)	9 (2%)	0	100	100
2	B	429/445 (96%)	420 (98%)	9 (2%)	0	100	100
2	D	421/445 (95%)	406 (96%)	15 (4%)	0	100	100
3	E	120/143 (84%)	120 (100%)	0	0	100	100
4	F	307/384 (80%)	293 (95%)	14 (5%)	0	100	100
All	All	2176/2319 (94%)	2117 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/379 (101%)	383 (100%)	0	100	100
1	C	382/379 (101%)	381 (100%)	1 (0%)	94	98
2	B	375/383 (98%)	372 (99%)	3 (1%)	86	94
2	D	368/383 (96%)	363 (99%)	5 (1%)	74	86
3	E	112/127 (88%)	112 (100%)	0	100	100
4	F	293/342 (86%)	290 (99%)	3 (1%)	82	91
All	All	1913/1993 (96%)	1901 (99%)	12 (1%)	90	96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	HIS
2	B	192	HIS
2	B	247	GLN
1	C	335	ILE
2	D	1	MET
2	D	139	HIS
2	D	158	ARG
2	D	180	THR
2	D	345	GLU
4	F	89	GLU
4	F	92	THR
4	F	125	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	247	GLN
1	C	133	GLN
1	C	406	HIS
3	E	18	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 8 are monoatomic - leaving 26 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	25,34,34	0.92	1 (4%)	34,54,54	1.62	5 (14%)
7	GOL	A	503	-	5,5,5	0.41	0	5,5,5	0.21	0
7	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.23	0
7	GOL	A	505	-	5,5,5	0.34	0	5,5,5	0.25	0
9	GDP	B	501	6	23,30,30	1.19	2 (8%)	30,47,47	1.74	6 (20%)
10	LOC	B	503	-	29,31,31	2.29	9 (31%)	27,44,44	1.10	1 (3%)
7	GOL	B	504	-	5,5,5	0.32	0	5,5,5	0.25	0
7	GOL	B	505	-	5,5,5	0.35	0	5,5,5	0.24	0
7	GOL	B	506	-	5,5,5	0.34	0	5,5,5	0.21	0
7	GOL	B	507	-	5,5,5	0.38	0	5,5,5	0.14	0
11	MES	B	509	-	11,12,12	0.60	0	14,16,16	2.06	5 (35%)
5	GTP	C	501	6	25,34,34	0.94	1 (4%)	34,54,54	1.60	5 (14%)
7	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.25	0
7	GOL	C	504	-	5,5,5	0.36	0	5,5,5	0.19	0
7	GOL	C	505	-	5,5,5	0.35	0	5,5,5	0.20	0
12	PEG	C	506	-	6,6,6	0.44	0	5,5,5	0.29	0
12	PEG	C	507	-	6,6,6	0.42	0	5,5,5	0.33	0
13	IMD	C	509	-	3,5,5	0.50	0	4,5,5	0.59	0
13	IMD	C	510	-	3,5,5	0.52	0	4,5,5	0.55	0
13	IMD	C	511	-	3,5,5	0.51	0	4,5,5	0.56	0
9	GDP	D	501	6	23,30,30	1.18	2 (8%)	30,47,47	1.78	6 (20%)
10	LOC	D	503	-	29,31,31	2.31	9 (31%)	27,44,44	1.12	1 (3%)
7	GOL	D	504	-	5,5,5	0.33	0	5,5,5	0.22	0
7	GOL	D	505	-	5,5,5	0.36	0	5,5,5	0.23	0
7	GOL	E	201	-	5,5,5	0.33	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	ACP	F	402	6	25,33,33	1.61	6 (24%)	31,52,52	2.82	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
7	GOL	A	503	-	-	0/4/4/4	0/0/0/0
7	GOL	A	504	-	-	0/4/4/4	0/0/0/0
7	GOL	A	505	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	LOC	B	503	-	-	0/10/25/25	0/3/3/3
7	GOL	B	504	-	-	0/4/4/4	0/0/0/0
7	GOL	B	505	-	-	0/4/4/4	0/0/0/0
7	GOL	B	506	-	-	0/4/4/4	0/0/0/0
7	GOL	B	507	-	-	0/4/4/4	0/0/0/0
11	MES	B	509	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
7	GOL	C	503	-	-	0/4/4/4	0/0/0/0
7	GOL	C	504	-	-	0/4/4/4	0/0/0/0
7	GOL	C	505	-	-	0/4/4/4	0/0/0/0
12	PEG	C	506	-	-	0/4/4/4	0/0/0/0
12	PEG	C	507	-	-	0/4/4/4	0/0/0/0
13	IMD	C	509	-	-	0/0/0/0	0/1/1/1
13	IMD	C	510	-	-	0/0/0/0	0/1/1/1
13	IMD	C	511	-	-	0/0/0/0	0/1/1/1
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
10	LOC	D	503	-	-	0/10/25/25	0/3/3/3
7	GOL	D	504	-	-	0/4/4/4	0/0/0/0
7	GOL	D	505	-	-	0/4/4/4	0/0/0/0
7	GOL	E	201	-	-	0/4/4/4	0/0/0/0
14	ACP	F	402	6	-	0/15/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	LOC	C20-C21	-3.56	1.34	1.40
10	B	503	LOC	C20-C21	-3.50	1.34	1.40
10	D	503	LOC	C19-C17	-3.07	1.34	1.39
10	B	503	LOC	C19-C17	-3.06	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	402	ACP	C2'-C3'	-3.00	1.45	1.53
14	F	402	ACP	O3'-C3'	-2.23	1.37	1.43
14	F	402	ACP	O5'-C5'	-2.08	1.36	1.44
10	D	503	LOC	C19-C20	2.10	1.46	1.40
10	B	503	LOC	C19-C20	2.15	1.46	1.40
14	F	402	ACP	PG-O3G	2.20	1.60	1.54
14	F	402	ACP	PG-O2G	2.72	1.61	1.54
5	A	501	GTP	C6-N1	2.78	1.38	1.33
5	C	501	GTP	C6-N1	2.88	1.38	1.33
9	B	501	GDP	C5-C4	3.02	1.47	1.40
9	D	501	GDP	C5-C4	3.04	1.47	1.40
10	B	503	LOC	C22-C1	3.26	1.48	1.40
10	D	503	LOC	C22-C1	3.28	1.48	1.40
9	D	501	GDP	C6-C5	3.64	1.48	1.41
9	B	501	GDP	C6-C5	3.66	1.48	1.41
10	B	503	LOC	C5-C3	3.83	1.48	1.40
10	D	503	LOC	C5-C3	3.89	1.49	1.40
10	B	503	LOC	C15-C16	4.23	1.48	1.39
14	F	402	ACP	C6-N6	4.25	1.48	1.34
10	D	503	LOC	C15-C16	4.36	1.48	1.39
10	B	503	LOC	C22-C8	4.64	1.48	1.40
10	D	503	LOC	C22-C8	4.70	1.48	1.40
10	B	503	LOC	C1-C3	4.97	1.48	1.39
10	D	503	LOC	C1-C3	5.01	1.48	1.39
10	D	503	LOC	O6-C17	5.36	1.45	1.37
10	B	503	LOC	O6-C17	5.38	1.45	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	402	ACP	N3-C2-N1	-9.35	121.73	128.89
14	F	402	ACP	O4'-C1'-N9	-6.08	95.37	108.10
5	C	501	GTP	N3-C2-N1	-4.79	120.15	127.44
5	A	501	GTP	N3-C2-N1	-4.78	120.16	127.44
9	D	501	GDP	C5-C6-N1	-4.15	117.92	123.59
14	F	402	ACP	PA-O3A-PB	-4.11	121.18	132.73
9	B	501	GDP	C5-C6-N1	-3.94	118.20	123.59
5	A	501	GTP	PA-O3A-PB	-3.69	122.35	132.73
5	C	501	GTP	PA-O3A-PB	-3.52	122.85	132.73
9	B	501	GDP	C6-C5-C4	-3.44	116.79	120.90
9	D	501	GDP	C4-C5-N7	-3.22	106.52	109.48
9	D	501	GDP	C6-C5-C4	-3.18	117.09	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C4-C5-N7	-3.13	106.60	109.48
9	B	501	GDP	N3-C2-N1	-3.13	122.68	127.44
9	D	501	GDP	N3-C2-N1	-3.08	122.76	127.44
5	A	501	GTP	C5-C6-N1	-3.03	119.45	123.59
5	C	501	GTP	C5-C6-N1	-3.03	119.45	123.59
9	D	501	GDP	PA-O3A-PB	-2.99	122.64	132.67
9	B	501	GDP	PA-O3A-PB	-2.97	122.70	132.67
5	C	501	GTP	PB-O3B-PG	-2.96	122.74	132.67
5	A	501	GTP	PB-O3B-PG	-2.91	122.91	132.67
11	B	509	MES	C6-C5-N4	-2.64	106.12	110.12
10	D	503	LOC	O3-C5-C7	-2.14	120.56	124.21
10	B	503	LOC	C6-O3-C5	2.06	120.66	117.54
11	B	509	MES	C7-N4-C5	2.18	116.85	111.27
14	F	402	ACP	O5'-C5'-C4'	2.82	119.51	109.12
14	F	402	ACP	O3A-PA-O5'	2.85	110.50	102.94
5	C	501	GTP	C6-N1-C2	2.96	120.05	115.94
5	A	501	GTP	C6-N1-C2	2.97	120.07	115.94
11	B	509	MES	O2S-S-C8	3.06	109.52	106.91
11	B	509	MES	O1S-S-C8	3.14	109.58	106.91
11	B	509	MES	C5-N4-C3	4.18	117.96	108.90
9	B	501	GDP	C6-N1-C2	4.62	122.36	115.94
9	D	501	GDP	C6-N1-C2	4.69	122.45	115.94
14	F	402	ACP	C2'-C1'-N9	8.02	126.54	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	505	GOL	1	0
10	B	503	LOC	1	0
7	B	507	GOL	1	0
11	B	509	MES	1	0
9	D	501	GDP	1	0
7	D	505	GOL	2	0
14	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	439/451 (97%)	-0.01	2 (0%) 91 94	30, 47, 85, 126	0
1	C	440/451 (97%)	0.14	3 (0%) 89 92	22, 36, 66, 90	0
2	B	422/445 (94%)	0.09	3 (0%) 89 92	25, 43, 75, 123	1 (0%)
2	D	421/445 (94%)	0.16	14 (3%) 50 59	30, 56, 89, 111	4 (0%)
3	E	121/143 (84%)	0.50	6 (4%) 32 41	35, 64, 104, 117	0
4	F	319/384 (83%)	1.24	78 (24%) 1 1	43, 74, 132, 155	0
All	All	2162/2319 (93%)	0.29	106 (4%) 33 42	22, 50, 98, 155	5 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	10.2
4	F	173	ILE	8.4
4	F	130	VAL	8.1
4	F	244	CYS	7.2
4	F	240	LEU	6.8
4	F	169	LEU	5.6
4	F	236	LYS	5.6
4	F	245	ILE	5.6
4	F	253	TYR	5.2
4	F	132	LEU	5.2
4	F	100	ILE	5.0
4	F	166	ALA	4.9
2	B	1	MET	4.7
4	F	20	LEU	4.7
4	F	250	SER	4.5
2	D	82	PRO	4.5
4	F	182	ILE	4.5
4	F	248	GLU	4.2
4	F	17	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	439	SER	4.0
3	E	26	PRO	3.9
2	D	405	LEU	3.9
4	F	353[A]	VAL	3.8
4	F	238	CYS	3.7
2	B	57	THR	3.7
4	F	259	GLY	3.7
4	F	21	LEU	3.6
4	F	99	VAL	3.6
4	F	167	SER	3.5
4	F	133	ALA	3.4
2	D	83	PHE	3.4
4	F	246	GLN	3.4
4	F	170	LEU	3.4
4	F	247	LYS	3.3
4	F	199	PHE	3.3
4	F	263	PHE	3.3
4	F	225	SER	3.3
4	F	134	ALA	3.3
2	B	59	ASN	3.2
2	D	57	THR	3.2
3	E	25	LYS	3.2
4	F	101	TYR	3.2
4	F	320	MET	3.1
4	F	342	LEU	3.1
2	D	177	VAL	3.1
2	D	400	ARG	3.1
4	F	241	THR	3.1
4	F	243	HIS	3.1
4	F	256	TYR	3.1
4	F	337	ALA	3.0
4	F	181	VAL	3.0
4	F	254	GLY	3.0
4	F	226	GLU	2.8
3	E	27	PRO	2.8
4	F	163	SER	2.8
2	D	180	THR	2.8
4	F	26	GLN	2.8
3	E	24	LEU	2.7
4	F	172	PHE	2.7
4	F	27	TRP	2.7
4	F	260	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	186	LEU	2.7
2	D	179	ASP	2.7
4	F	151	SER	2.6
1	A	282	TYR	2.6
1	C	440	VAL	2.6
4	F	346	LEU	2.6
4	F	224	SER	2.6
4	F	223	THR	2.6
4	F	235	ASP	2.6
2	D	404	PHE	2.6
4	F	228	TYR	2.5
4	F	162	ILE	2.5
4	F	267	PHE	2.5
4	F	31	ARG	2.5
4	F	252	ASN	2.5
2	D	401	ARG	2.5
2	D	1	MET	2.5
2	D	37	HIS	2.5
4	F	180	HIS	2.4
4	F	192	LEU	2.4
2	D	415	GLU	2.4
3	E	45	PRO	2.4
2	D	182	VAL	2.3
4	F	201	ILE	2.3
4	F	129	GLU	2.3
4	F	242	ASN	2.3
4	F	227	PRO	2.3
4	F	24	THR	2.3
4	F	131	PHE	2.3
4	F	319	PHE	2.3
3	E	48	GLU	2.3
4	F	194	PRO	2.2
4	F	135	TYR	2.2
4	F	197	ARG	2.2
4	F	217	ARG	2.2
4	F	255	ARG	2.2
4	F	13	VAL	2.2
4	F	200	ASP	2.1
4	F	239	HIS	2.1
4	F	91	CYS	2.1
4	F	168	GLU	2.0
1	C	221	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	150	LYS	2.0
1	C	357	TYR	2.0
4	F	343	TYR	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
7	GOL	B	507	6/6	0.71	0.50	20.01	89,97,98,100	0
7	GOL	C	504	6/6	0.89	0.27	7.19	60,72,75,79	0
7	GOL	B	505	6/6	0.80	0.28	5.78	76,86,86,88	0
6	MG	A	502	1/1	0.83	0.19	4.83	33,33,33,33	0
12	PEG	C	506	7/7	0.72	0.24	4.80	56,74,84,84	0
7	GOL	D	505	6/6	0.84	0.23	4.70	71,74,77,79	0
13	IMD	C	510	5/5	0.88	0.25	4.67	84,85,86,86	0
12	PEG	C	507	7/7	0.64	0.31	3.98	94,95,98,98	0
7	GOL	A	503	6/6	0.91	0.31	3.88	67,72,77,77	0
7	GOL	B	504	6/6	0.75	0.26	3.87	68,77,79,81	0
7	GOL	C	505	6/6	0.85	0.22	3.40	63,72,74,76	0
7	GOL	A	505	6/6	0.86	0.24	3.17	71,78,83,85	0
7	GOL	C	503	6/6	0.92	0.28	3.02	62,64,70,75	0
13	IMD	C	511	5/5	0.81	0.20	1.94	78,79,81,81	0
11	MES	B	509	12/12	0.90	0.16	1.92	58,68,87,94	0
7	GOL	A	504	6/6	0.89	0.17	1.75	69,71,73,74	0
7	GOL	E	201	6/6	0.62	0.18	1.67	70,82,85,86	0
7	GOL	B	506	6/6	0.88	0.17	1.58	72,73,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	IMD	C	509	5/5	0.93	0.14	0.77	52,54,55,55	0
5	GTP	A	501	32/32	0.98	0.14	0.75	20,32,38,52	0
5	GTP	C	501	32/32	0.98	0.14	0.68	19,24,33,41	0
10	LOC	D	503	29/29	0.96	0.14	0.67	29,34,42,45	0
9	GDP	B	501	28/28	0.98	0.16	0.32	20,30,37,37	0
6	MG	C	502	1/1	0.97	0.14	0.31	26,26,26,26	0
9	GDP	D	501	28/28	0.95	0.14	-0.26	42,49,60,65	0
10	LOC	B	503	29/29	0.97	0.13	-0.40	30,35,40,42	0
8	CA	A	506	1/1	0.93	0.11	-0.74	75,75,75,75	0
14	ACP	F	402	31/31	0.91	0.17	-1.17	67,84,150,199	0
6	MG	F	401	1/1	0.94	0.07	-2.84	77,77,77,77	0
6	MG	B	502	1/1	0.99	0.15	-	22,22,22,22	0
7	GOL	D	504	6/6	0.87	0.21	-	76,79,80,80	0
8	CA	C	508	1/1	0.85	0.15	-	95,95,95,95	0
6	MG	D	502	1/1	0.85	0.07	-	54,54,54,54	0
8	CA	B	508	1/1	0.95	0.14	-	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.