



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 10:56 PM EDT

PDB ID : 6FKL
Title : Tubulin-TUB015 complex
Authors : Prota, A.E.; Steinmetz, M.O.; Priego, E.-M.
Deposited on : 2018-01-24
Resolution : 2.10 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-20030736
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-20030736

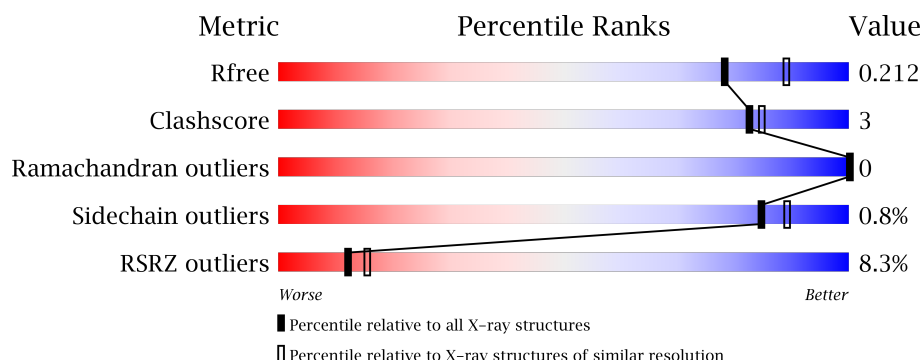
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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>3%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	C	451	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
2	B	445	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
2	D	445	<div> <div>8%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
3	E	143	<div> <div>9%</div> <div>78%</div> <div>7%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div> <div>26%</div> <div>82%</div> <div>9%</div> <div>9%</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
10	MES	B	506	-	-	-	X
11	DLK	B	507	X	-	-	-
11	DLK	D	503	X	-	-	-
8	GOL	A	505	-	-	-	X
8	GOL	B	505	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18310 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	8	0
			3463	2196	583	660	24			
1	C	439	Total	C	N	O	S	0	14	0
			3496	2216	592	666	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	4	0
			3363	2114	573	649	27			
2	D	422	Total	C	N	O	S	0	2	0
			3317	2085	563	643	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	3	0
			1022	632	184	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	-	cloning artifact	UNP P63043

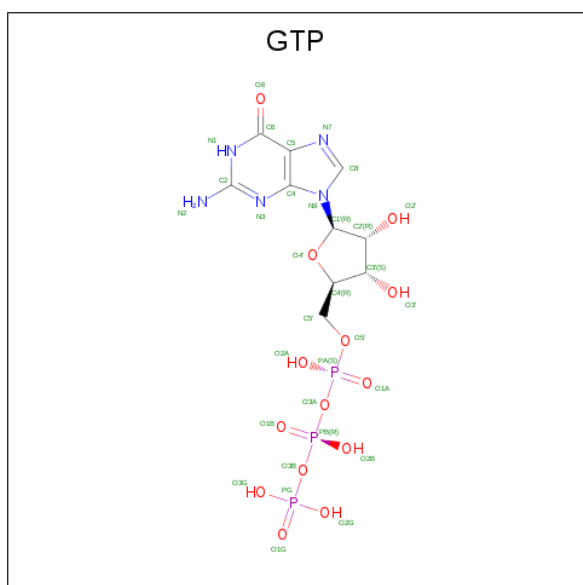
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	1	0
			2852	1827	488	523	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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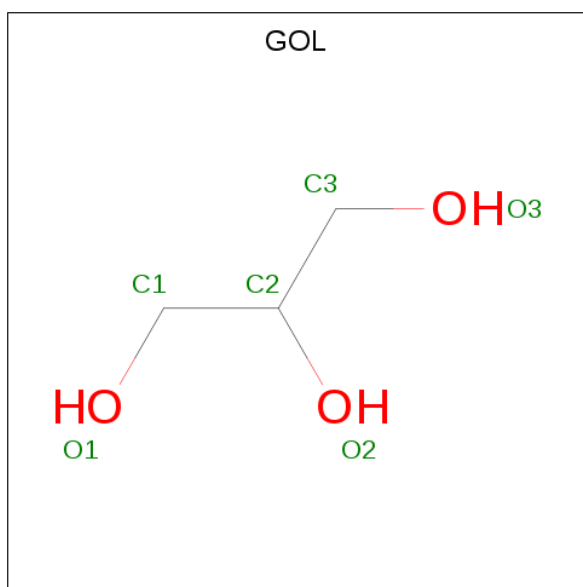
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

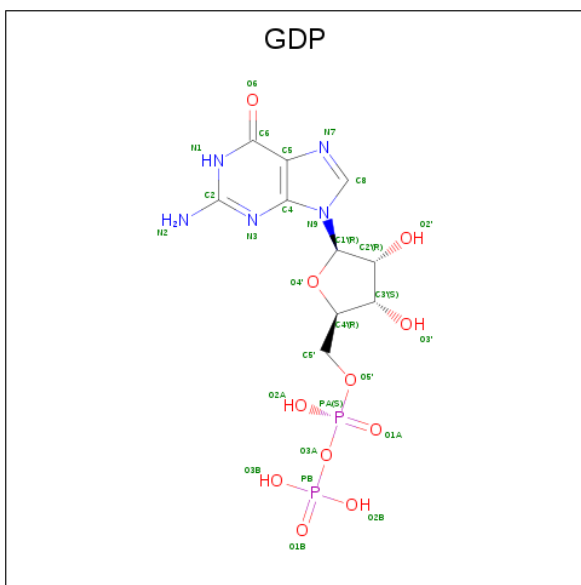
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

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



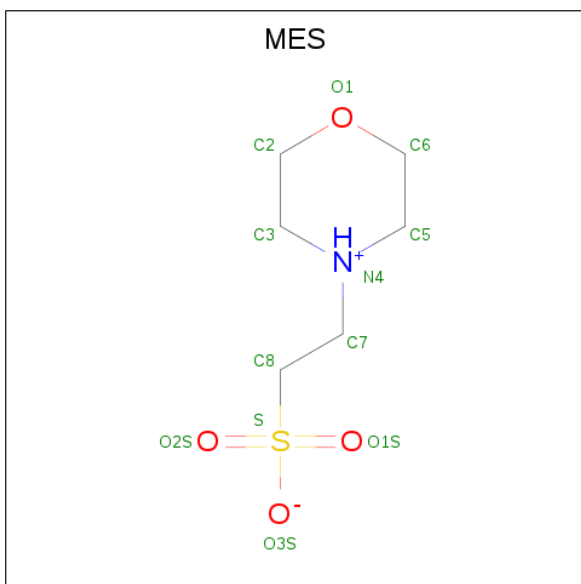
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

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



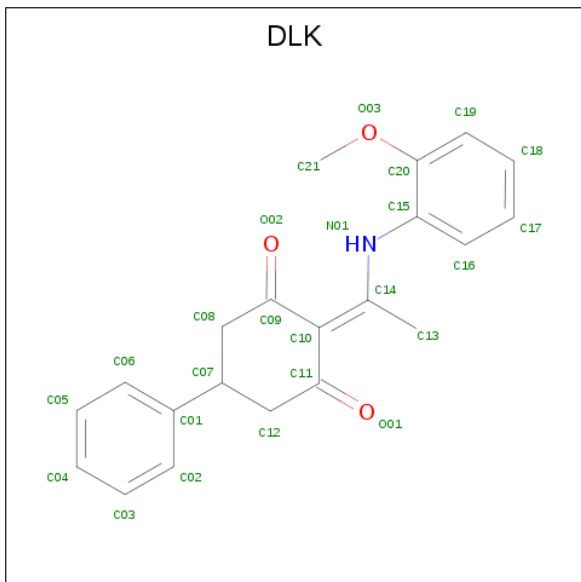
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



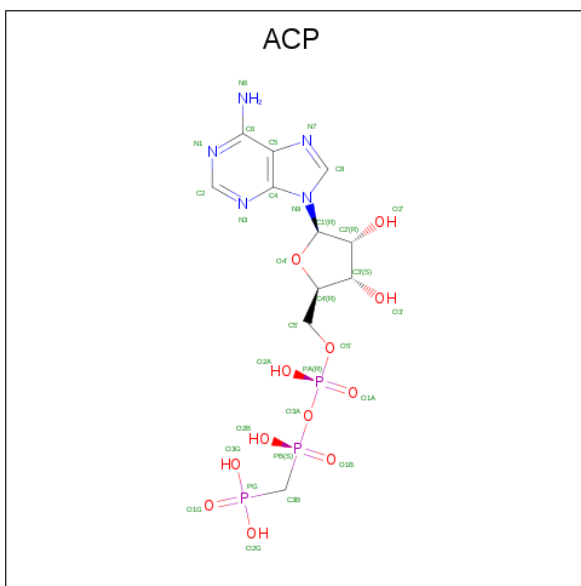
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 2-{1-[(2-Methoxyphenyl)amino]ethylidene}-5-phenyl-1,3-cyclohexanedione (three-letter code: DLK) (formula: $C_{21}H_{21}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			25	21	1	3		
11	D	1	Total	C	N	O	0	0
			25	21	1	3		

- 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		

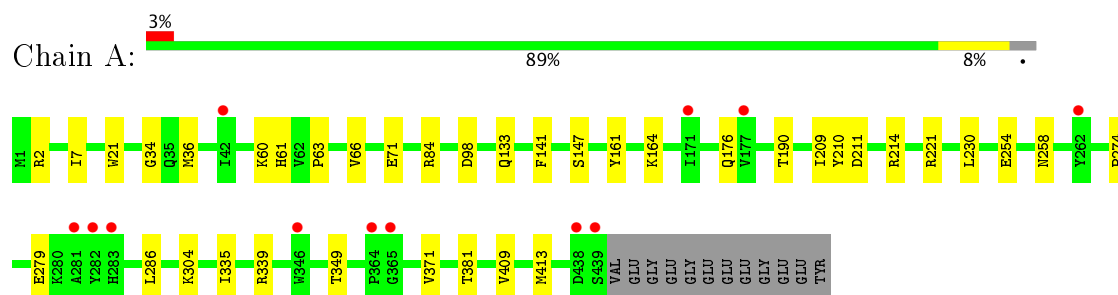
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	125	Total	O	0	0
			125	125		
13	B	120	Total	O	0	0
			120	120		
13	C	212	Total	O	0	0
			212	212		
13	D	53	Total	O	0	0
			53	53		
13	E	20	Total	O	0	0
			20	20		
13	F	32	Total	O	0	0
			32	32		

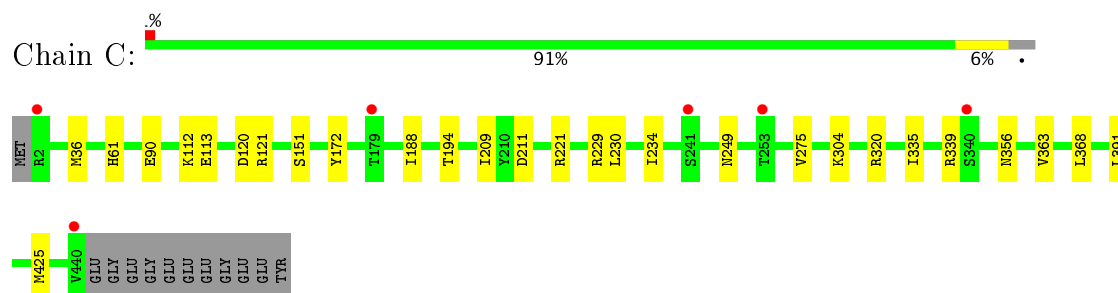
3 Residue-property plots [i](#)

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.

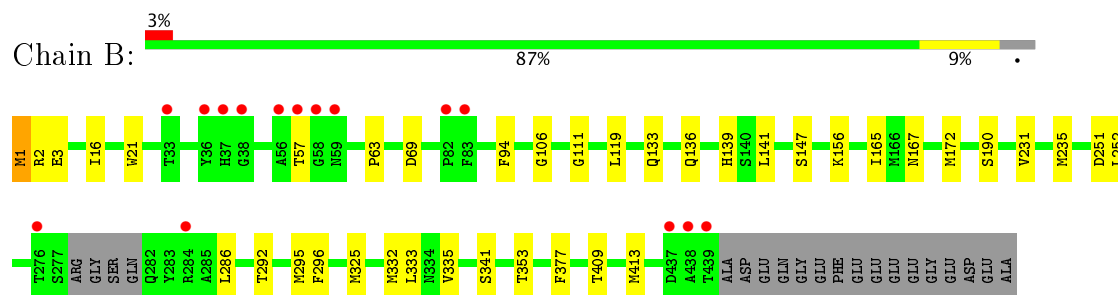
• Molecule 1: Tubulin alpha-1B chain



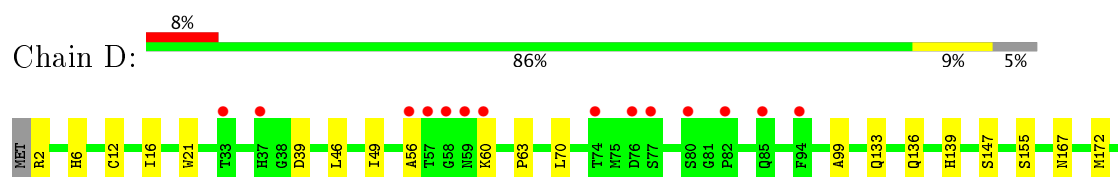
• Molecule 1: Tubulin alpha-1B chain

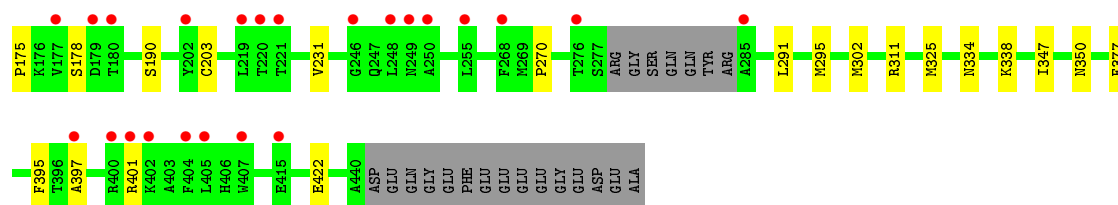


• Molecule 2: Tubulin beta-2B chain

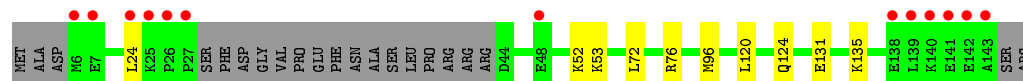
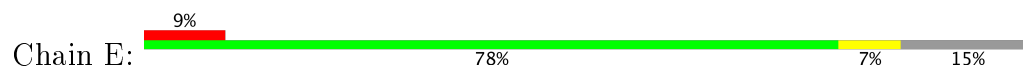


• Molecule 2: Tubulin beta-2B chain

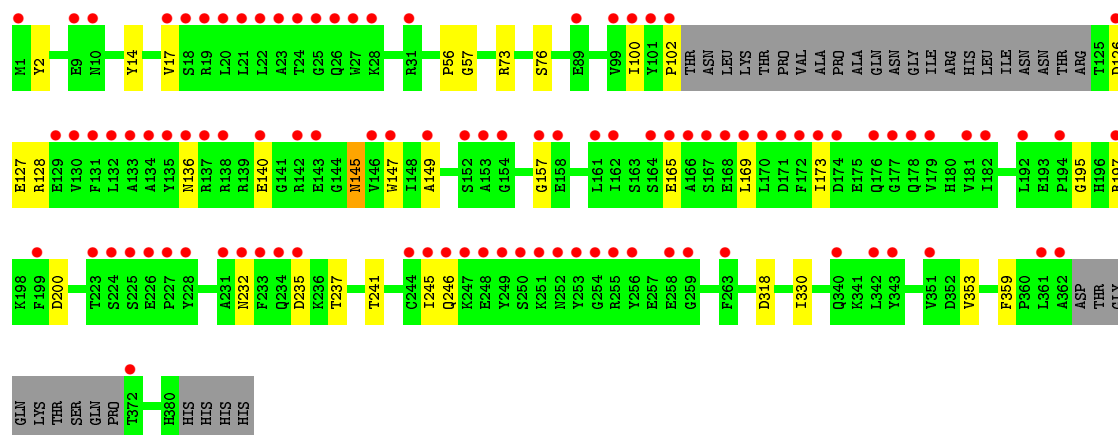
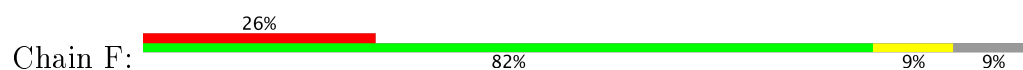




• Molecule 3: Stathmin-4



• 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	104.75Å 157.76Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 2.10 49.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.44-2.10) 98.4 (49.44-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2863: ???)	Depositor
R, R_{free}	0.178 , 0.217 0.172 , 0.212	Depositor DCC
R_{free} test set	8574 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18310	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, DLK, 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	0.27	0/3565	0.45	0/4840
1	C	0.29	0/3616	0.46	0/4911
2	B	0.27	0/3449	0.45	0/4670
2	D	0.26	0/3396	0.44	0/4601
3	E	0.25	0/1040	0.37	0/1381
4	F	0.25	0/2920	0.42	0/3944
All	All	0.27	0/17986	0.44	0/24347

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	3463	0	3393	20	0
1	C	3496	0	3436	18	0
2	B	3363	0	3255	20	0
2	D	3317	0	3200	23	0
3	E	1022	0	1043	5	0
4	F	2852	0	2821	21	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	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
8	B	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	12	0	0
11	B	25	0	0	0	0
11	D	25	0	0	0	0
12	F	31	0	14	2	0
13	A	125	0	0	0	0
13	B	120	0	0	0	0
13	C	212	0	0	1	0
13	D	53	0	0	1	0
13	E	20	0	0	0	0
13	F	32	0	0	1	0
All	All	18310	0	17238	101	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 (101) 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:147[A]:SER:HG	2:D:190:SER:HG	1.39	0.69
1:C:120[B]:ASP:OD2	1:C:121[B]:ARG:NH2	2.24	0.68
2:B:332:MET:HG3	2:B:353:THR:HG21	1.80	0.63
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.80	0.63
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.29	0.62
4:F:145:ASN:HD22	4:F:147:TRP:HE1	1.48	0.61
4:F:318:ASP:OD2	12:F:402:ACP:O3G	2.18	0.60
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.71	0.56
1:A:176:GLN:HG2	4:F:56:PRO:HB3	1.87	0.55
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.71	0.55
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.89	0.54
4:F:232:ASN:ND2	4:F:235:ASP:OD1	2.40	0.54
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.89	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.53
2:B:133:GLN:HG3	2:B:251:ASP:HB2	1.91	0.52
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.91	0.52
4:F:241:THR:OG1	12:F:402:ACP:O3'	2.21	0.52
2:D:147[A]:SER:OG	2:D:190:SER:OG	2.17	0.51
2:D:311:ARG:NH1	13:D:601:HOH:O	2.42	0.51
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.46	0.51
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.33	0.51
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.93	0.51
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.45	0.50
4:F:145:ASN:ND2	4:F:147:TRP:HE1	2.09	0.50
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.45	0.50
2:D:16:ILE:HD13	2:D:231:VAL:HG11	1.94	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.30	0.50
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.46	0.50
1:C:230:LEU:O	1:C:234:ILE:HD12	2.12	0.50
1:A:349:THR:HG22	3:E:24:LEU:HD12	1.94	0.49
1:C:221:ARG:HG2	2:D:325:MET:HG2	1.94	0.49
2:B:69:ASP:O	2:B:94:PHE:HA	2.12	0.49
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.93	0.48
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.96	0.48
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.94	0.48
2:D:175:PRO:HA	2:D:178:SER:HB2	1.94	0.48
4:F:237:THR:O	4:F:246:GLN:NE2	2.44	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.48
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.49	0.48
4:F:169:LEU:O	4:F:173:ILE:HG12	2.14	0.47
2:B:1:MET:N	2:B:3:GLU:OE1	2.32	0.47
4:F:100:ILE:HG23	4:F:128:ARG:HG3	1.97	0.47
2:B:147[B]:SER:HB2	2:B:190:SER:HG	1.79	0.47
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.96	0.47
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.97	0.46
2:D:39:ASP:N	2:D:39:ASP:OD1	2.48	0.46
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.46
1:C:221:ARG:HG2	2:D:325:MET:CG	2.45	0.46
2:D:2:ARG:HB3	2:D:133:GLN:NE2	2.31	0.46
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356[B]:ASN:ND2	13:C:605:HOH:O	2.49	0.45
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.51	0.45
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.98	0.45
4:F:157:GLY:HA3	4:F:245:ILE:HD11	1.98	0.45
4:F:149:ALA:HB1	4:F:173:ILE:HD11	1.99	0.45
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG23	2.00	0.44
2:D:397:ALA:O	2:D:401:ARG:HD3	2.17	0.44
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.53	0.44
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.53	0.44
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.00	0.44
4:F:14:TYR:HA	4:F:17:VAL:HB	1.99	0.44
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.99	0.43
2:D:46:LEU:HA	2:D:49:ILE:HB	2.00	0.43
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.36	0.43
2:B:296:PHE:CG	2:B:335:VAL:HG11	2.54	0.43
2:B:136:GLN:HA	2:B:167:ASN:O	2.17	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.43
2:B:235:MET:HE2	2:B:235:MET:HB3	1.87	0.43
2:D:136:GLN:HA	2:D:167:ASN:O	2.19	0.43
1:A:221:ARG:HG2	2:B:325:MET:HG2	2.01	0.43
2:D:172:MET:HE2	2:D:203:CYS:HA	2.01	0.42
2:B:119:LEU:HD11	2:B:156:LYS:HB3	2.00	0.42
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.42
1:A:274:PRO:HG2	1:A:371:VAL:HG11	2.02	0.42
2:D:56:ALA:HB3	2:D:60:LYS:HB2	2.01	0.42
4:F:126:ASP:OD1	4:F:127:GLU:N	2.53	0.42
2:B:141:LEU:HD12	2:B:172:MET:SD	2.60	0.42
2:D:295:MET:CG	2:D:377:PHE:HB2	2.49	0.42
2:D:395:PHE:CE1	2:D:422:GLU:HB2	2.54	0.42
2:B:295:MET:CG	2:B:377:PHE:HB2	2.50	0.42
4:F:136:ASN:O	4:F:140:GLU:HG3	2.20	0.42
1:C:90:GLU:O	1:C:121[B]:ARG:HG2	2.20	0.42
3:E:131:GLU:O	3:E:135:LYS:HG2	2.19	0.42
3:E:52:LYS:HG2	3:E:53:LYS:NZ	2.35	0.42
1:C:229:ARG:NE	1:C:363:VAL:HG21	2.35	0.42
4:F:102:PRO:O	13:F:501:HOH:O	2.22	0.41
4:F:330:ILE:HA	4:F:330:ILE:HD13	1.91	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.21	0.41
4:F:73:ARG:HB2	4:F:76:SER:OG	2.21	0.41
2:B:409:THR:HA	2:B:413:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.57	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.56	0.40
4:F:195:GLY:HA3	4:F:197:ARG:HD3	2.01	0.40
3:E:120:LEU:O	3:E:124:GLN:HG3	2.22	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.03	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	445/451 (99%)	439 (99%)	6 (1%)	0	100	100
1	C	450/451 (100%)	439 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	420/445 (94%)	413 (98%)	7 (2%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	344/384 (90%)	333 (97%)	11 (3%)	0	100	100
All	All	2205/2319 (95%)	2161 (98%)	44 (2%)	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	378/379 (100%)	375 (99%)	3 (1%)	85	89
1	C	384/379 (101%)	384 (100%)	0	100	100
2	B	372/383 (97%)	366 (98%)	6 (2%)	68	74
2	D	366/383 (96%)	362 (99%)	4 (1%)	78	83
3	E	112/127 (88%)	111 (99%)	1 (1%)	82	87
4	F	312/342 (91%)	309 (99%)	3 (1%)	80	85
All	All	1924/1993 (96%)	1907 (99%)	17 (1%)	85	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	279	GLU
1	A	381	THR
2	B	1	MET
2	B	2	ARG
2	B	57	THR
2	B	139	HIS
2	B	286	LEU
2	B	341	SER
2	D	139	HIS
2	D	155[A]	SER
2	D	155[B]	SER
2	D	291	LEU
3	E	96	MET
4	F	145	ASN
4	F	165	GLU
4	F	353	VAL

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

Mol	Chain	Res	Type
1	A	301	GLN
2	D	294	GLN
4	F	145	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 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	0.94	1 (3%)	27,54,54	1.69	5 (18%)
8	GOL	A	505	-	5,5,5	0.87	0	5,5,5	1.00	0
9	GDP	B	501	6	25,30,30	1.12	2 (8%)	26,47,47	2.04	6 (23%)
8	GOL	B	505	-	5,5,5	1.04	0	5,5,5	0.83	0
10	MES	B	506	-	12,12,12	2.13	1 (8%)	14,16,16	2.36	8 (57%)
11	DLK	B	507	-	27,27,27	1.57	4 (14%)	33,37,37	1.50	6 (18%)
5	GTP	C	501	6	27,34,34	0.96	1 (3%)	27,54,54	1.70	4 (14%)
9	GDP	D	501	6	25,30,30	1.17	2 (8%)	26,47,47	1.99	6 (23%)
11	DLK	D	503	-	27,27,27	1.63	4 (14%)	33,37,37	1.59	8 (24%)
12	ACP	F	402	6	27,33,33	1.65	6 (22%)	30,52,52	1.51	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	GDP	B	501	6	-	0/12/32/32	0/3/3/3
8	GOL	B	505	-	-	0/4/4/4	0/0/0/0
10	MES	B	506	-	-	0/6/14/14	0/1/1/1
11	DLK	B	507	-	1/1/5/6	0/14/30/30	0/3/3/3
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
11	DLK	D	503	-	1/1/5/6	0/14/30/30	0/3/3/3
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)
10	B	506	MES	C8-S	-7.05	1.66	1.77
12	F	402	ACP	PB-O2B	-3.18	1.48	1.56
11	B	507	DLK	C10-C09	-3.06	1.38	1.46
11	D	503	DLK	C10-C09	-3.06	1.38	1.46
11	B	507	DLK	C14-N01	-2.12	1.29	1.34
11	D	503	DLK	C14-N01	-2.04	1.29	1.34
12	F	402	ACP	PG-O3G	2.68	1.61	1.54
9	B	501	GDP	C5-C4	2.71	1.46	1.40
12	F	402	ACP	PG-O2G	2.83	1.61	1.54
5	A	501	GTP	C6-N1	2.94	1.38	1.33
9	D	501	GDP	C5-C4	3.02	1.47	1.40
12	F	402	ACP	PB-O3A	3.09	1.61	1.58
11	B	507	DLK	C10-C14	3.10	1.48	1.42
5	C	501	GTP	C6-N1	3.10	1.38	1.33
12	F	402	ACP	C5-C4	3.21	1.47	1.40
11	D	503	DLK	C10-C14	3.34	1.48	1.42
9	B	501	GDP	C6-C5	3.59	1.48	1.41
9	D	501	GDP	C6-C5	3.85	1.48	1.41
12	F	402	ACP	PB-O1B	3.85	1.61	1.51
11	B	507	DLK	O02-C09	5.84	1.35	1.23
11	D	503	DLK	O02-C09	6.13	1.35	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	N3-C2-N1	-5.65	123.93	128.86
5	C	501	GTP	N3-C2-N1	-4.99	120.17	127.46
5	A	501	GTP	N3-C2-N1	-4.94	120.24	127.46
9	B	501	GDP	C6-C5-C4	-4.36	116.51	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C5-C6-N1	-3.95	117.86	123.48
9	D	501	GDP	C6-C5-C4	-3.67	117.19	120.84
9	B	501	GDP	C5-C6-N1	-3.60	118.35	123.48
9	B	501	GDP	N3-C2-N1	-3.55	122.27	127.46
9	D	501	GDP	C4-C5-N7	-3.22	106.30	109.41
9	D	501	GDP	N3-C2-N1	-3.19	122.80	127.46
12	F	402	ACP	PA-O3A-PB	-3.19	122.11	132.39
5	C	501	GTP	C5-C6-N1	-3.16	118.99	123.48
5	A	501	GTP	C5-C6-N1	-3.11	119.06	123.48
12	F	402	ACP	C4-C5-N7	-2.89	106.61	109.41
11	D	503	DLK	O03-C20-C19	-2.82	119.64	124.37
11	B	507	DLK	O03-C20-C19	-2.72	119.81	124.37
9	B	501	GDP	C4-C5-N7	-2.67	106.83	109.41
10	B	506	MES	C2-C3-N4	-2.43	106.70	110.11
11	B	507	DLK	O02-C09-C08	-2.26	111.19	120.68
11	D	503	DLK	O02-C09-C08	-2.21	111.40	120.68
11	D	503	DLK	C13-C14-C10	-2.04	119.65	122.50
11	B	507	DLK	C13-C14-C10	-2.04	119.66	122.50
11	D	503	DLK	C16-C15-N01	-2.04	117.04	121.84
10	B	506	MES	C6-O1-C2	2.03	116.75	109.89
5	A	501	GTP	N2-C2-N1	2.06	120.54	117.24
11	D	503	DLK	C12-C11-C10	2.18	120.57	116.12
10	B	506	MES	O1S-S-C8	2.30	108.77	106.79
10	B	506	MES	C7-N4-C3	2.69	118.16	111.26
10	B	506	MES	C7-N4-C5	2.72	118.22	111.26
10	B	506	MES	O3S-S-C8	2.74	109.43	106.06
5	A	501	GTP	C6-N1-C2	2.93	120.27	116.06
5	C	501	GTP	C6-N1-C2	3.09	120.50	116.06
11	B	507	DLK	O03-C20-C15	3.30	119.11	114.81
11	B	507	DLK	C08-C09-C10	3.73	123.76	116.12
11	D	503	DLK	C08-C09-C10	3.77	123.83	116.12
11	B	507	DLK	C20-C15-N01	3.77	123.62	116.70
11	D	503	DLK	O03-C20-C15	3.86	119.84	114.81
10	B	506	MES	C5-N4-C3	3.87	117.64	108.87
5	C	501	GTP	C2-N3-C4	3.91	119.72	115.16
5	A	501	GTP	C2-N3-C4	4.00	119.83	115.16
10	B	506	MES	O2S-S-C8	4.21	110.41	106.79
11	D	503	DLK	C20-C15-N01	4.25	124.51	116.70
9	D	501	GDP	C6-N1-C2	4.44	122.45	116.06
9	B	501	GDP	C6-N1-C2	4.44	122.45	116.06
9	D	501	GDP	C2-N3-C4	4.97	120.96	115.16
9	B	501	GDP	C2-N3-C4	5.01	121.02	115.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	B	507	DLK	C10
11	D	503	DLK	C10

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
12	F	402	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	439/451 (97%)	0.28	12 (2%) 55 61	32, 49, 81, 138	0
1	C	439/451 (97%)	0.06	6 (1%) 75 79	26, 38, 65, 95	0
2	B	425/445 (95%)	0.26	15 (3%) 44 51	26, 45, 82, 115	0
2	D	422/445 (94%)	0.48	37 (8%) 11 14	34, 58, 89, 143	0
3	E	122/143 (85%)	0.46	13 (10%) 7 8	38, 64, 100, 122	0
4	F	349/384 (90%)	1.25	100 (28%) 1 1	39, 78, 143, 170	0
All	All	2196/2319 (94%)	0.44	183 (8%) 12 15	26, 51, 103, 170	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.6
2	D	57	THR	8.6
4	F	130	VAL	7.6
4	F	249	TYR	7.0
4	F	233	PHE	6.8
4	F	20	LEU	6.7
2	D	59	ASN	6.7
1	A	282	TYR	6.2
4	F	253	TYR	6.2
4	F	177	GLY	6.1
4	F	132	LEU	6.1
1	A	439	SER	6.0
4	F	250	SER	5.8
4	F	231	ALA	5.8
2	D	285	ALA	5.6
4	F	251	LYS	5.3
2	B	59	ASN	5.3
4	F	182	ILE	5.3
4	F	167	SER	5.2

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Mol	Chain	Res	Type	RSRZ
4	F	22	LEU	5.0
4	F	170	LEU	5.0
2	B	439	THR	4.9
4	F	361	LEU	4.9
3	E	139	LEU	4.9
4	F	99	VAL	4.9
4	F	21	LEU	4.8
4	F	131	PHE	4.8
4	F	161	LEU	4.8
4	F	169	LEU	4.7
2	B	58	GLY	4.7
3	E	27	PRO	4.6
1	A	281	ALA	4.5
4	F	174	ASP	4.5
2	B	438	ALA	4.4
2	B	57	THR	4.4
4	F	179	VAL	4.3
4	F	372	THR	4.3
4	F	172	PHE	4.3
4	F	362	ALA	4.3
4	F	142	ARG	4.2
1	C	2[A]	ARG	4.2
4	F	227	PRO	4.2
4	F	157	GLY	4.0
4	F	259	GLY	4.0
1	C	179	THR	4.0
4	F	101	TYR	4.0
4	F	133	ALA	4.0
3	E	26	PRO	4.0
4	F	100	ILE	4.0
4	F	24	THR	3.9
4	F	137	ARG	3.9
3	E	142	GLU	3.9
1	C	440	VAL	3.9
2	D	37	HIS	3.9
4	F	248	GLU	3.8
1	A	262	TYR	3.8
4	F	263	PHE	3.8
4	F	244	CYS	3.8
4	F	17	VAL	3.7
4	F	136	ASN	3.7
2	B	284	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	232	ASN	3.6
2	B	37	HIS	3.6
4	F	252	ASN	3.6
4	F	18	SER	3.6
4	F	234	GLN	3.6
1	C	340	SER	3.6
2	B	276	THR	3.6
3	E	24	LEU	3.5
4	F	256	TYR	3.5
2	D	56	ALA	3.4
4	F	135	TYR	3.4
4	F	168	GLU	3.4
2	B	56	ALA	3.3
4	F	23	ALA	3.3
4	F	176	GLN	3.3
4	F	194	PRO	3.2
4	F	245	ILE	3.2
4	F	178	GLN	3.2
2	D	246	GLY	3.2
2	D	276	THR	3.2
2	D	401	ARG	3.2
4	F	25	GLY	3.1
4	F	166	ALA	3.1
3	E	140	LYS	3.1
2	D	220	THR	3.1
1	A	438	ASP	3.1
2	D	94	PHE	3.1
4	F	126	ASP	3.1
4	F	134	ALA	3.0
3	E	6	MET	3.0
4	F	138	ARG	3.0
4	F	171	ASP	3.0
4	F	143	GLU	2.9
2	D	404	PHE	2.9
4	F	164	SER	2.9
4	F	255	ARG	2.9
2	D	400	ARG	2.9
4	F	89	GLU	2.9
3	E	7	GLU	2.8
2	D	82	PRO	2.7
1	A	346	TRP	2.7
4	F	153	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	2.7
3	E	143	ALA	2.7
4	F	129	GLU	2.7
2	D	221	THR	2.7
2	D	250	ALA	2.6
2	D	249	ASN	2.6
2	D	407	TRP	2.6
2	B	83	PHE	2.6
4	F	247	LYS	2.6
4	F	235	ASP	2.6
4	F	102	PRO	2.6
3	E	25	LYS	2.5
4	F	162	ILE	2.5
4	F	158	GLU	2.5
2	B	437	ASP	2.5
4	F	31	ARG	2.5
2	D	255	LEU	2.5
2	B	38	GLY	2.5
4	F	165	GLU	2.5
4	F	181	VAL	2.5
4	F	149	ALA	2.5
4	F	19	ARG	2.5
4	F	340	GLN	2.5
4	F	147	TRP	2.4
4	F	246	GLN	2.4
2	B	82	PRO	2.4
1	A	171	ILE	2.4
2	D	248	LEU	2.4
4	F	9	GLU	2.4
2	D	58	GLY	2.4
4	F	254	GLY	2.4
2	D	179	ASP	2.4
2	B	33	THR	2.4
2	D	60	LYS	2.4
4	F	192	LEU	2.3
4	F	1	MET	2.3
4	F	228	TYR	2.3
1	A	364	PRO	2.3
2	D	80	SER	2.3
2	D	219	LEU	2.3
4	F	224	SER	2.3
4	F	140	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	27	TRP	2.3
2	D	77	SER	2.2
2	D	76	ASP	2.2
2	D	33	THR	2.2
2	B	36	TYR	2.2
2	D	268	PHE	2.2
4	F	258	GLU	2.2
4	F	152	SER	2.2
3	E	138	GLU	2.2
4	F	197	ARG	2.2
3	E	141	GLU	2.2
2	D	85	GLN	2.2
3	E	48	GLU	2.2
2	D	405	LEU	2.1
1	A	177	VAL	2.1
4	F	226	GLU	2.1
2	D	397	ALA	2.1
2	D	415	GLU	2.1
2	D	402	LYS	2.1
4	F	28	LYS	2.1
4	F	351	VAL	2.1
1	C	253	THR	2.1
4	F	10	ASN	2.1
1	C	241	SER	2.1
4	F	225	SER	2.1
4	F	146	VAL	2.1
2	D	74	THR	2.1
4	F	26	GLN	2.1
4	F	199	PHE	2.1
2	D	202	TYR	2.1
4	F	343	TYR	2.1
2	D	180	THR	2.0
1	A	283	HIS	2.0
4	F	223	THR	2.0
1	A	365	GLY	2.0
4	F	154	GLY	2.0
4	F	342	LEU	2.0
2	D	177	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	GOL	B	505	6/6	0.70	0.29	6.62	51,72,73,77	0
8	GOL	A	505	6/6	0.91	0.18	2.65	59,68,72,76	0
10	MES	B	506	12/12	0.95	0.15	2.01	41,51,77,89	0
11	DLK	D	503	25/25	0.87	0.26	1.35	48,69,77,79	0
9	GDP	B	501	28/28	0.99	0.16	0.11	27,31,36,36	0
5	GTP	A	501	32/32	0.98	0.18	0.06	24,33,40,42	0
11	DLK	B	507	25/25	0.97	0.14	0.03	30,36,43,47	0
5	GTP	C	501	32/32	0.99	0.14	0.02	21,29,32,38	0
9	GDP	D	501	28/28	0.97	0.11	-0.38	44,51,56,62	0
6	MG	C	502	1/1	0.99	0.14	-0.58	28,28,28,28	0
12	ACP	F	402	31/31	0.86	0.14	-0.95	68,78,107,108	0
6	MG	A	502	1/1	0.98	0.12	-1.03	32,32,32,32	0
7	CA	A	504	1/1	0.91	0.08	-1.78	101,101,101,101	0
7	CA	A	503	1/1	0.97	0.04	-2.32	63,63,63,63	0
7	CA	C	503	1/1	0.99	0.04	-3.79	49,49,49,49	0
7	CA	B	503	1/1	0.95	0.08	-	94,94,94,94	0
7	CA	B	504	1/1	0.92	0.11	-	122,122,122,122	0
6	MG	F	401	1/1	0.86	0.06	-	76,76,76,76	0
6	MG	D	502	1/1	0.89	0.09	-	55,55,55,55	0
6	MG	B	502	1/1	1.00	0.21	-	24,24,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.