wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:12 PM GMT

PDB ID	:	4O2A
Title	:	Tubulin-BAL27862 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	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

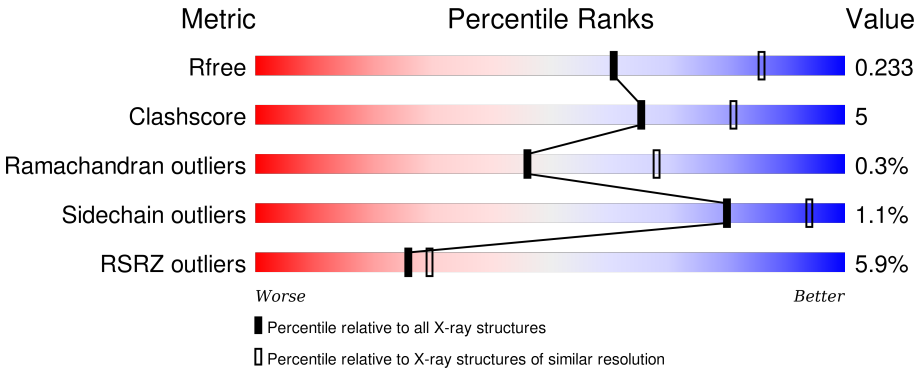
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	87% 10%
1	C	451	88% 9%
2	B	445	82% 12% 6%
2	D	445	3% 79% 14% 5%
3	E	143	3% 83% 13%

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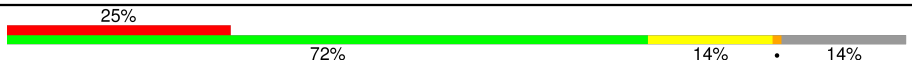
Mol	Chain	Length	Quality of chain
4	F	384	

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	2RR	D	604	-	-	X	X
14	ADP	F	401	-	-	-	X
9	GOL	A	505	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18043 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	12	0
			3487	2214	587	662	24			
1	C	440	Total	C	N	O	S	0	15	0
			3504	2224	587	667	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	418	Total	C	N	O	S	0	16	0
			3371	2127	566	650	28			
2	D	421	Total	C	N	O	S	0	4	0
			3324	2091	562	643	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	5	0
			1045	646	188	205	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

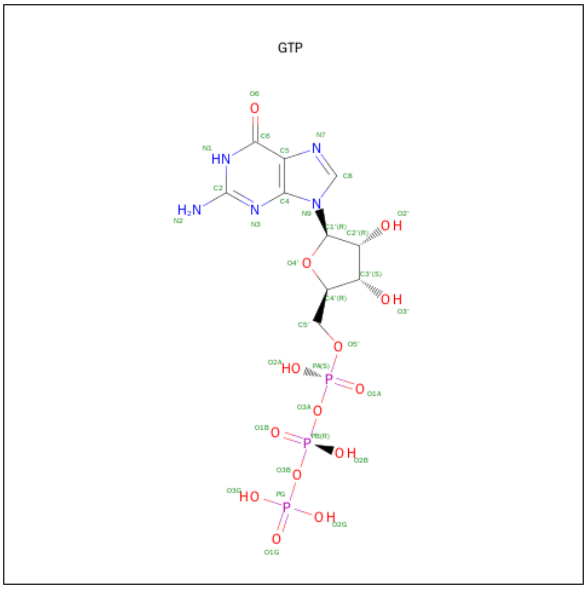
- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	4	0
			2740	1766	465	495	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	2	Total	Mg	0	0
			2	2		
6	A	1	Total	Mg	0	0
			1	1		
6	D	2	Total	Mg	0	0
			2	2		

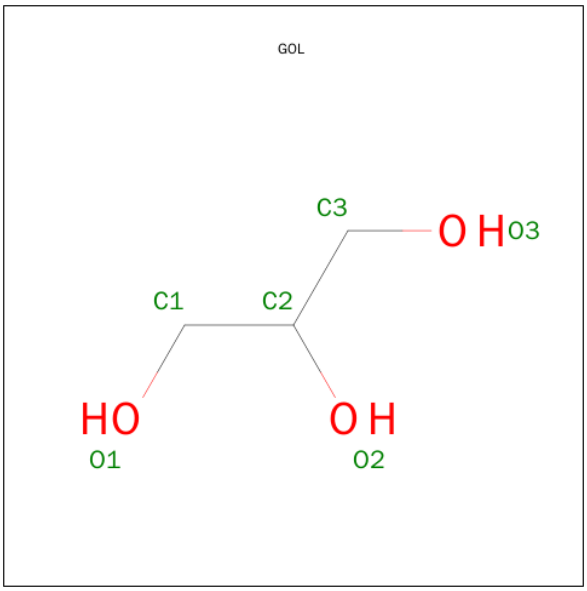
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

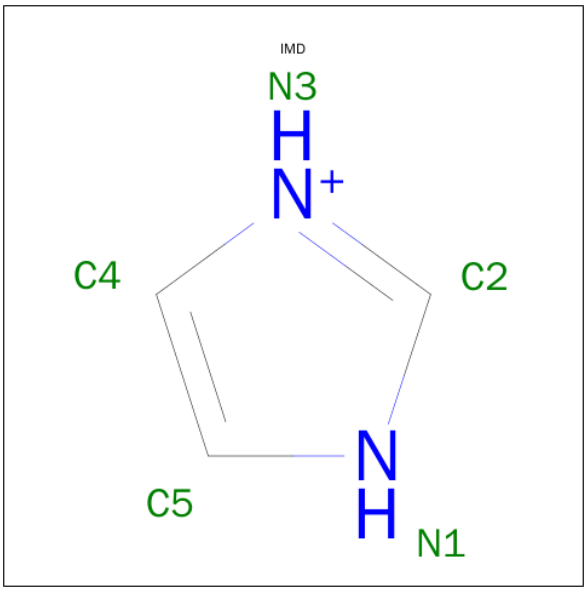
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



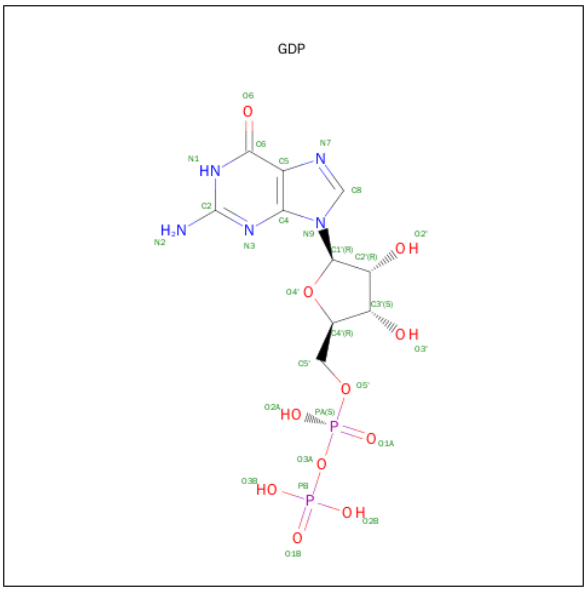
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0

- Molecule 10 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



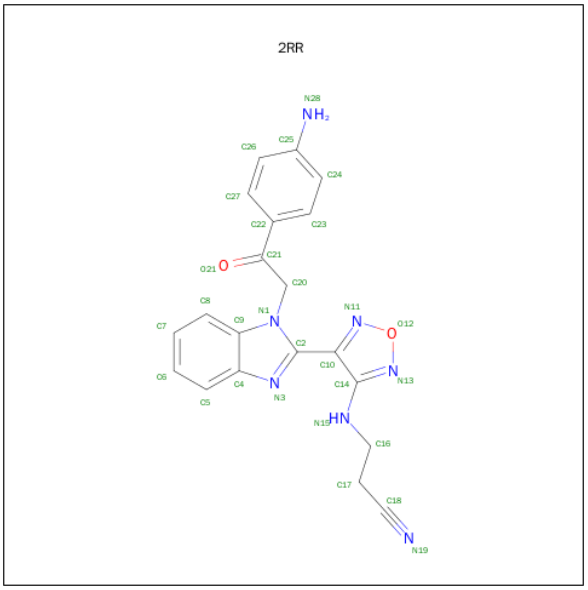
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N 5 3 2	0	0

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



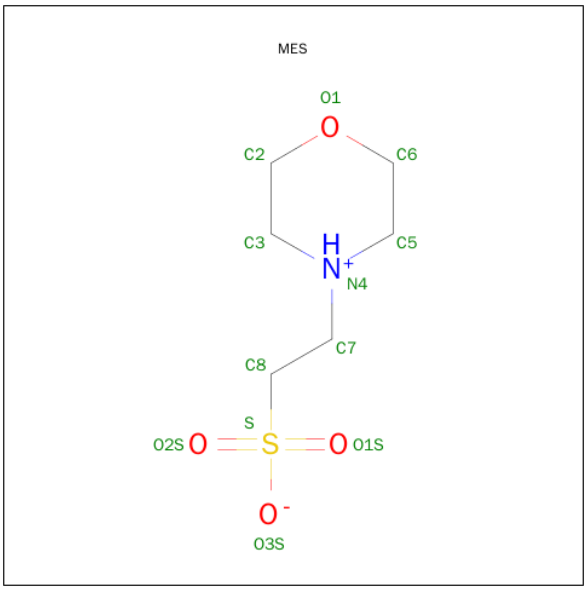
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C N O P 28 10 5 11 2	0	0
11	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 12 is 3-[(4-{1-[2-(4-AMINOPHENYL)-2-OXOETHYL]-1H-BENZIMIDAZOL-2-YL}-1,2,5-OXADIAZOL-3-YL)AMINO]PROPANENITRILE (three-letter code: 2RR) (formula: $C_{20}H_{17}N_7O_2$).



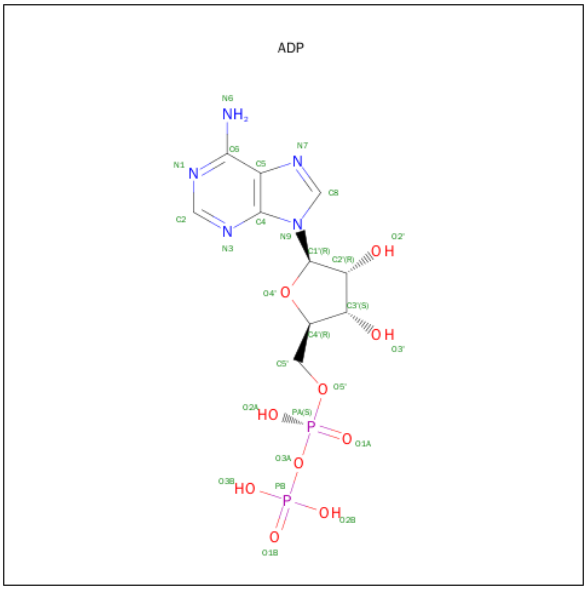
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			29	20	7	2		
12	D	1	Total	C	N	O	0	0
			29	20	7	2		

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



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

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 15 is water.

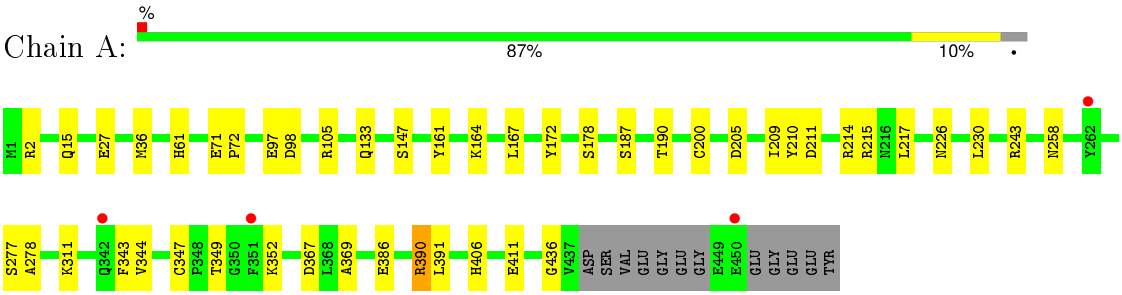
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	63	Total	O	0	0
			63	63		
15	B	70	Total	O	0	0
			70	70		
15	C	144	Total	O	0	0
			144	144		
15	D	26	Total	O	0	0
			26	26		
15	E	13	Total	O	0	0
			13	13		
15	F	18	Total	O	0	0
			18	18		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

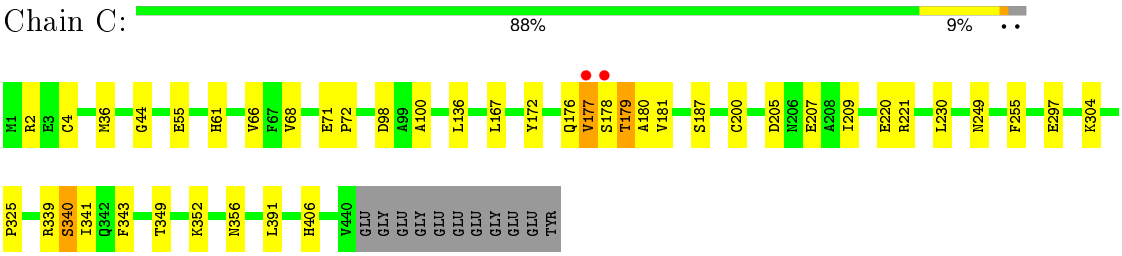
- Molecule 1: Tubulin alpha-1B chain

Chain A:



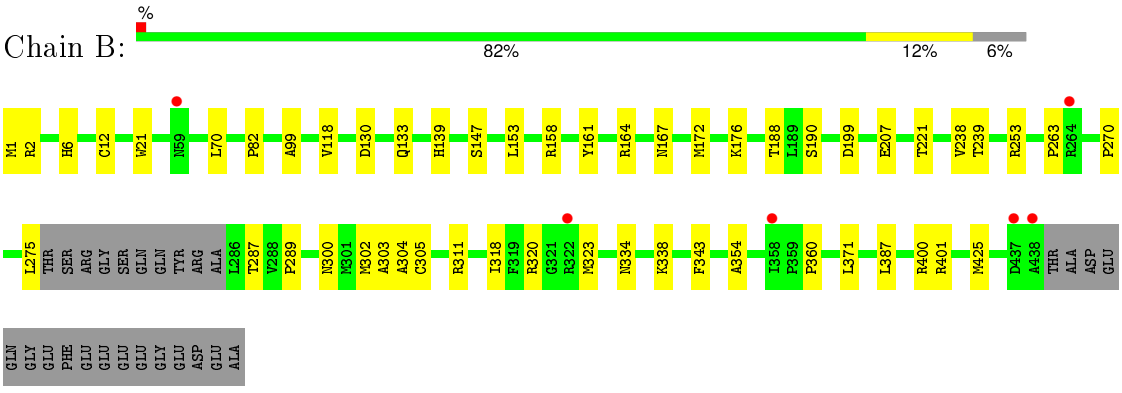
- Molecule 1: Tubulin alpha-1B chain

Chain C:



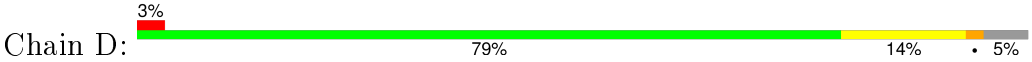
- Molecule 2: Tubulin beta-2B chain

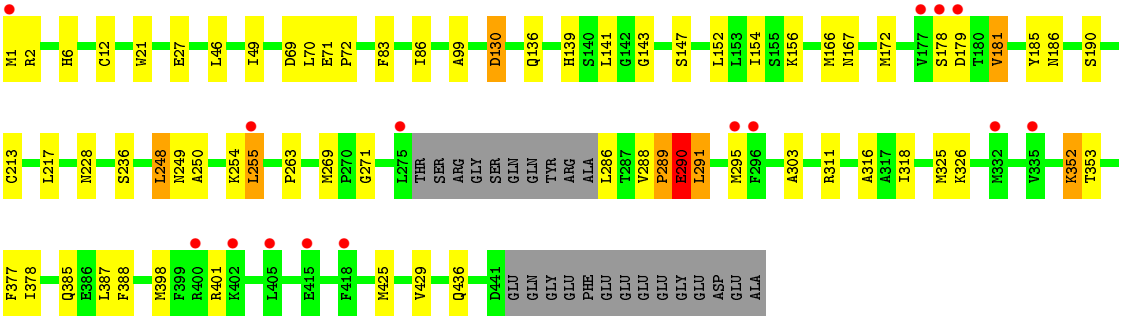
Chain B:



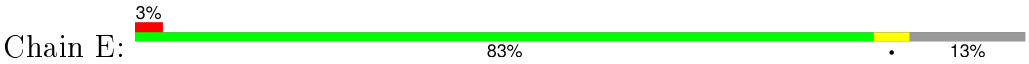
- Molecule 2: Tubulin beta-2B chain

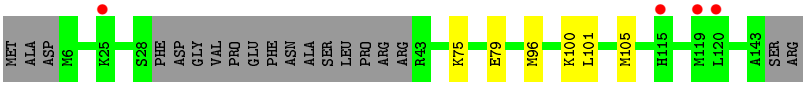
Chain D:



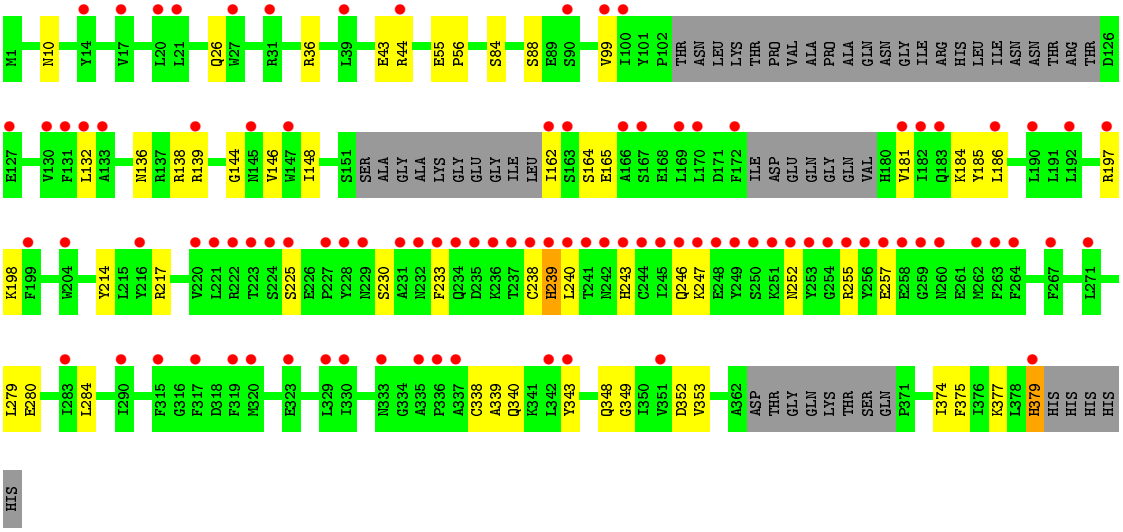


- Molecule 3: Stathmin-4





- Molecule 4: TUBULIN-TYROSINE LIGASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.53Å 158.12Å 179.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.36 – 2.50 78.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.36-2.50) 99.7 (78.45-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.194 , 0.232 0.198 , 0.233	Depositor DCC
R_{free} test set	5151 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 103225 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18043	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, IMD, ADP, CL, CA, GTP, MES, 2RR

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	0.21	0/3600	0.38	0/4886
1	C	0.23	0/3628	0.40	0/4926
2	B	0.22	0/3489	0.38	0/4724
2	D	0.22	0/3409	0.42	2/4619 (0.0%)
3	E	0.20	0/1069	0.31	0/1419
4	F	0.22	0/2815	0.37	0/3801
All	All	0.22	0/18010	0.39	2/24375 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	289	PRO	C-N-CA	5.32	135.00	121.70
2	D	289	PRO	CA-C-N	5.01	128.22	117.20

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	3487	0	3433	25	0
1	C	3504	0	3447	32	0
2	B	3371	0	3289	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3324	0	3215	49	0
3	E	1045	0	1066	3	0
4	F	2740	0	2729	37	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	A	6	0	8	0	0
10	A	5	0	5	0	0
11	B	28	0	12	2	0
11	D	28	0	12	2	0
12	B	29	0	17	2	0
12	D	29	0	17	17	0
13	B	12	0	12	2	0
14	F	27	0	12	3	0
15	A	63	0	0	0	0
15	B	70	0	0	1	0
15	C	144	0	0	1	0
15	D	26	0	0	1	0
15	E	13	0	0	0	0
15	F	18	0	0	2	0
All	All	18043	0	17298	176	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 5.

The worst 5 of 176 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)
4:F:238:CYS:SG	4:F:239:HIS:CE1	2.03	1.50
4:F:238:CYS:SG	4:F:239:HIS:ND1	2.11	1.22
1:C:180:ALA:N	12:D:604:2RR:H16	1.87	0.89
4:F:238:CYS:SG	4:F:239:HIS:HE1	1.67	0.85
4:F:225:SER:H	4:F:246:GLN:HE22	1.30	0.78

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	447/451 (99%)	431 (96%)	15 (3%)	1 (0%)	52 75
1	C	453/451 (100%)	443 (98%)	9 (2%)	1 (0%)	52 75
2	B	430/445 (97%)	417 (97%)	11 (3%)	2 (0%)	34 55
2	D	421/445 (95%)	402 (96%)	17 (4%)	2 (0%)	34 55
3	E	125/143 (87%)	124 (99%)	1 (1%)	0	100 100
4	F	325/384 (85%)	313 (96%)	12 (4%)	0	100 100
All	All	2201/2319 (95%)	2130 (97%)	65 (3%)	6 (0%)	46 68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	290	GLU
2	D	181	VAL
1	C	177	VAL
1	A	178	SER
2	B	304	ALA

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	382/379 (101%)	381 (100%)	1 (0%)	94 99

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	386/379 (102%)	382 (99%)	4 (1%)	82 95
2	B	378/383 (99%)	374 (99%)	4 (1%)	80 94
2	D	368/383 (96%)	357 (97%)	11 (3%)	48 76
3	E	115/127 (91%)	115 (100%)	0	100 100
4	F	303/342 (89%)	301 (99%)	2 (1%)	88 97
All	All	1932/1993 (97%)	1910 (99%)	22 (1%)	80 94

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	130	ASP
2	D	248	LEU
4	F	239	HIS
2	D	139	HIS
2	D	181	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
2	B	8	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	25,34,34	0.91	1 (4%)	34,54,54	1.66	5 (14%)
9	GOL	A	505	-	5,5,5	0.36	0	5,5,5	0.21	0
10	IMD	A	506	-	3,5,5	0.52	0	4,5,5	0.59	0
11	GDP	B	501	-	23,30,30	1.17	2 (8%)	30,47,47	1.77	6 (20%)
12	2RR	B	504	-	26,32,32	1.32	3 (11%)	27,44,44	1.90	3 (11%)
13	MES	B	505	-	11,12,12	0.60	0	14,16,16	2.52	7 (50%)
5	GTP	C	501	6	25,34,34	0.92	1 (4%)	34,54,54	1.63	5 (14%)
11	GDP	D	602	6	23,30,30	1.18	2 (8%)	30,47,47	1.84	7 (23%)
12	2RR	D	604	-	26,32,32	1.32	3 (11%)	27,44,44	1.98	3 (11%)
14	ADP	F	401	-	22,29,29	0.96	1 (4%)	27,45,45	1.99	4 (14%)

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
9	GOL	A	505	-	-	0/4/4/4	0/0/0/0
10	IMD	A	506	-	-	0/0/0/0	0/1/1/1
11	GDP	B	501	-	-	0/12/32/32	0/3/3/3
12	2RR	B	504	-	-	0/11/17/17	0/3/4/4
13	MES	B	505	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
11	GDP	D	602	6	-	0/12/32/32	0/3/3/3
12	2RR	D	604	-	-	0/11/17/17	0/3/4/4
14	ADP	F	401	-	-	0/12/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	504	2RR	C10-C14	-2.74	1.40	1.44
12	D	604	2RR	C10-C14	-2.54	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	604	2RR	C22-C21	-2.28	1.45	1.49
12	B	504	2RR	C22-C21	-2.26	1.45	1.49
5	A	501	GTP	C6-N1	2.76	1.38	1.33

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	604	2RR	C16-N15-C14	-7.78	114.68	123.49
12	B	504	2RR	C16-N15-C14	-7.63	114.85	123.49
14	F	401	ADP	N3-C2-N1	-7.03	123.51	128.89
5	A	501	GTP	N3-C2-N1	-4.78	120.17	127.44
5	C	501	GTP	N3-C2-N1	-4.67	120.34	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
11	B	501	GDP	2	0
12	B	504	2RR	2	0
13	B	505	MES	2	0
11	D	602	GDP	2	0
12	D	604	2RR	17	0
14	F	401	ADP	3	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, 95^{th} 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%)	0.20	4 (0%) 85 88	25, 44, 77, 114	0
1	C	440/451 (97%)	0.17	2 (0%) 91 92	15, 31, 65, 98	0
2	B	418/445 (93%)	0.30	6 (1%) 78 80	19, 41, 78, 112	2 (0%)
2	D	421/445 (94%)	0.32	15 (3%) 46 51	24, 58, 93, 116	6 (1%)
3	E	124/143 (86%)	0.47	4 (3%) 51 56	32, 58, 102, 130	0
4	F	331/384 (86%)	1.44	97 (29%) 1 0	32, 65, 143, 162	0
All	All	2173/2319 (93%)	0.44	128 (5%) 26 29	15, 47, 99, 162	8 (0%)

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	9.4
4	F	249	TYR	8.4
4	F	240	LEU	8.1
4	F	251	LYS	8.0
4	F	253	TYR	7.6

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, 95^{th} 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
12	2RR	D	604	29/29	0.75	0.64	9.26	60,72,78,80	0
14	ADP	F	401	27/27	0.69	0.62	2.38	165,168,234,394	0
9	GOL	A	505	6/6	0.81	0.20	2.36	90,97,99,99	0
11	GDP	B	501	28/28	0.97	0.18	0.49	18,27,36,43	0
7	CA	C	502	1/1	0.98	0.16	0.31	58,58,58,58	0
5	GTP	A	501	32/32	0.97	0.17	0.19	13,31,36,67	0
11	GDP	D	602	28/28	0.95	0.17	0.15	35,44,62,69	0
7	CA	A	503	1/1	0.95	0.13	-0.02	62,62,62,62	0
12	2RR	B	504	29/29	0.95	0.16	-0.34	34,47,54,55	0
5	GTP	C	501	32/32	0.98	0.15	-0.43	11,22,35,62	0
13	MES	B	505	12/12	0.96	0.16	-0.46	41,50,67,67	0
8	CL	A	504	1/1	0.78	0.14	-	78,78,78,78	0
6	MG	D	601	1/1	0.89	0.15	-	23,23,23,23	0
6	MG	B	506	1/1	0.98	0.12	-	42,42,42,42	0
10	IMD	A	506	5/5	0.85	0.23	-	92,92,94,95	0
7	CA	B	503	1/1	0.89	0.31	-	81,81,81,81	0
7	CA	E	700	1/1	0.97	0.19	-	84,84,84,84	0
6	MG	D	603	1/1	0.97	0.08	-	44,44,44,44	0
6	MG	A	502	1/1	0.90	0.16	-	25,25,25,25	0
6	MG	B	502	1/1	0.93	0.33	-	47,47,47,47	0

6.5 Other polymers

There are no such residues in this entry.