



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 15, 2017 – 08:50 AM EST

PDB ID : 5MJS
EMDB ID: : EMD-3522
Title : S. pombe microtubule copolymerized with GTP and Mal3-143
Authors : von Loeffelholz, O.; Moores, C.
Deposited on : unknown
Resolution : 4.60 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

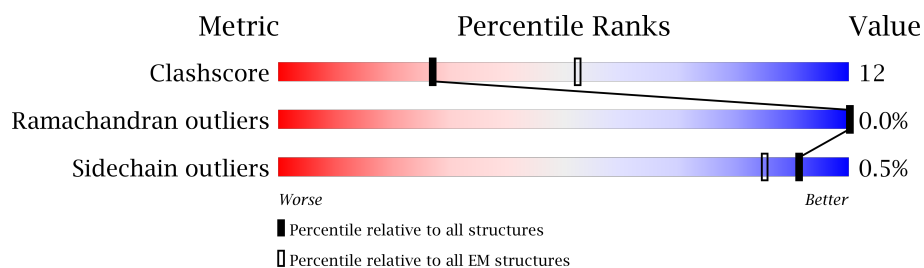
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	429	72% 28%
1	B	429	75% 24%
1	C	429	74% 26%
1	J	429	76% 24%
2	D	143	66% 19% 15%
3	E	444	64% 33% ..
3	F	444	63% 34% ..
3	G	444	64% 33% ..
3	H	444	65% 32% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28114 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	428	Total	C	N	O	S	0	0
			3304	2078	565	639	22		
1	J	428	Total	C	N	O	S	0	0
			3304	2078	565	639	22		
1	B	428	Total	C	N	O	S	0	0
			3304	2078	565	639	22		
1	C	428	Total	C	N	O	S	0	0
			3304	2078	565	639	22		

- Molecule 2 is a protein called Microtubule integrity protein mal3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	121	Total	C	N	O	S	0	0
			1010	643	176	185	6		

- Molecule 3 is a protein called Tubulin alpha-1 chain.

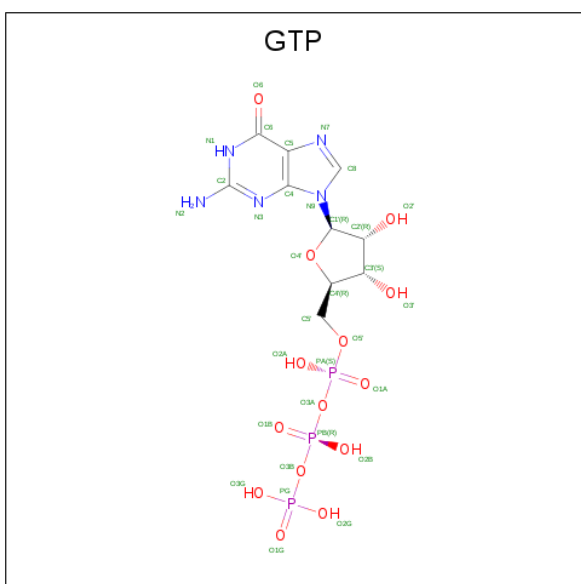
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	434	Total	C	N	O	S	0	0
			3412	2146	587	655	24		
3	F	434	Total	C	N	O	S	0	0
			3412	2146	587	655	24		
3	G	434	Total	C	N	O	S	0	0
			3412	2146	587	655	24		
3	H	434	Total	C	N	O	S	0	0
			3412	2146	587	655	24		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).

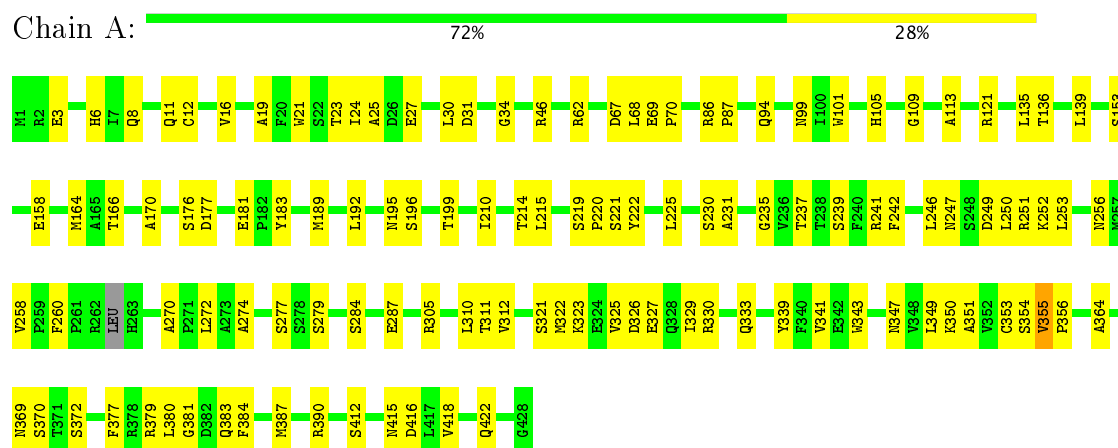


Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	H	1	Total	C	N	O	P	0
			32	10	5	14	3	

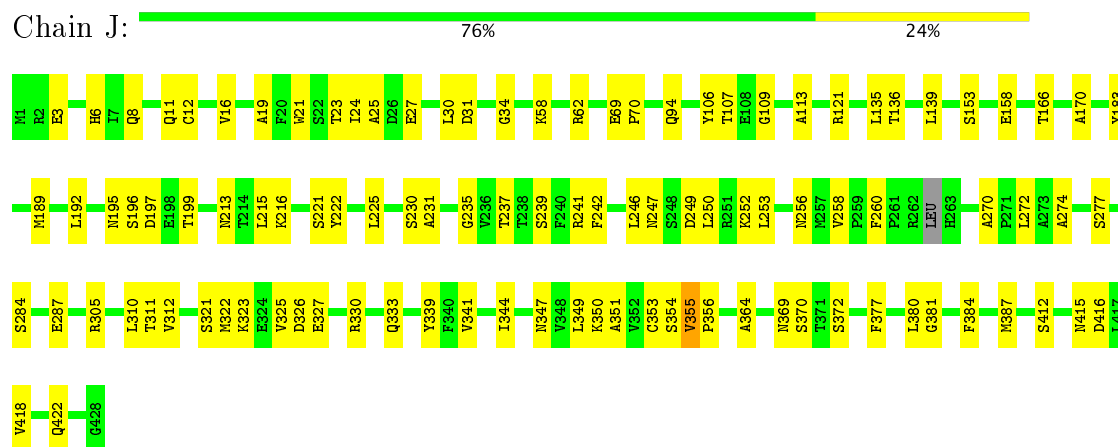
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

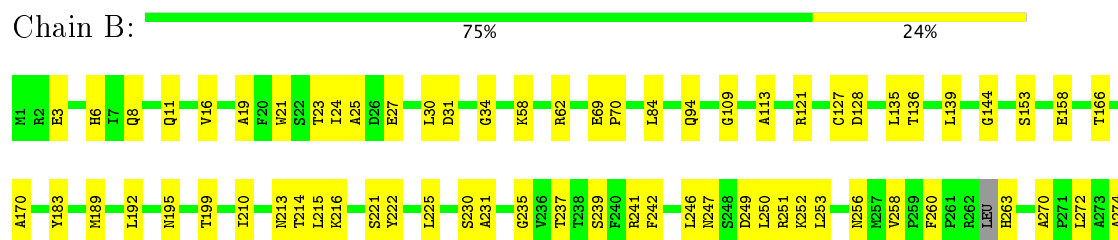
- Molecule 1: Tubulin beta chain

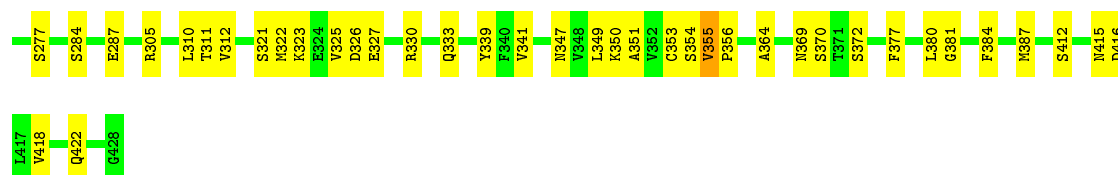


- Molecule 1: Tubulin beta chain

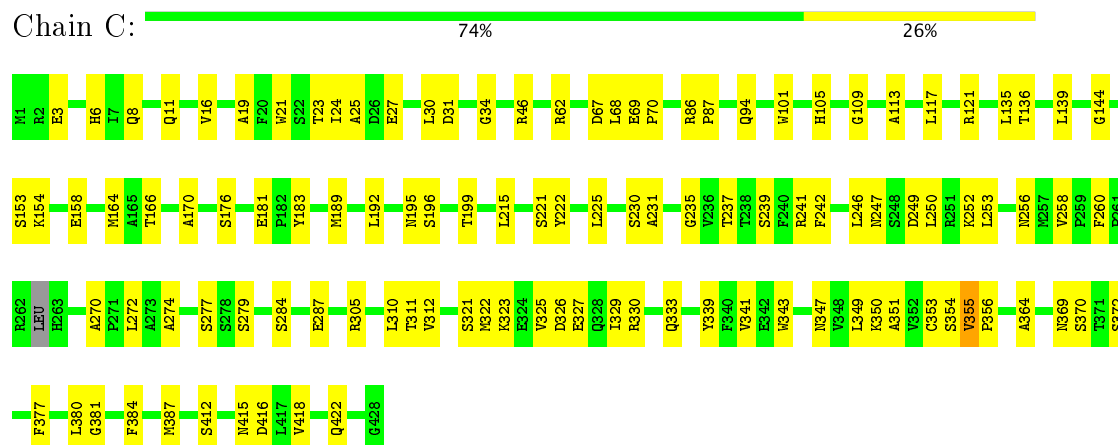


- Molecule 1: Tubulin beta chain

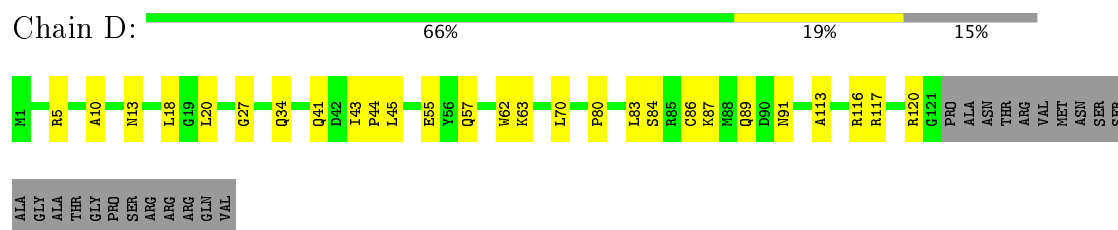


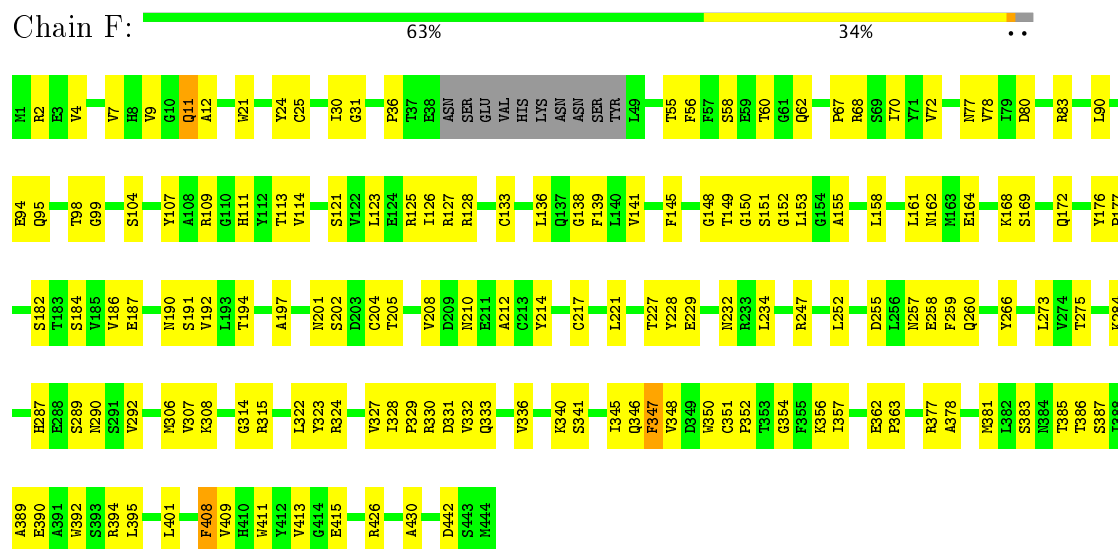


- Molecule 1: Tubulin beta chain

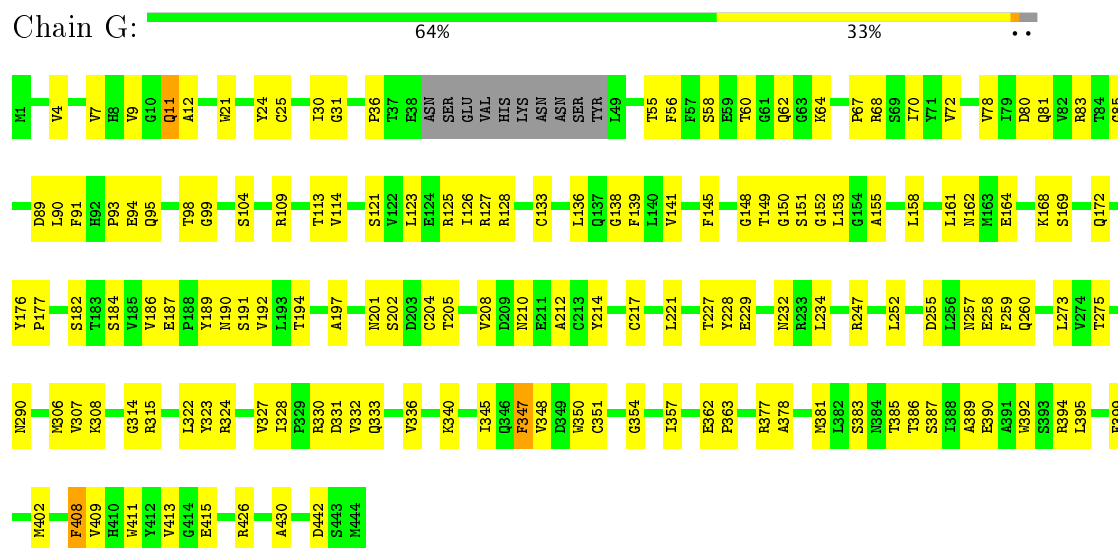


- Molecule 2: Microtubule integrity protein mal3

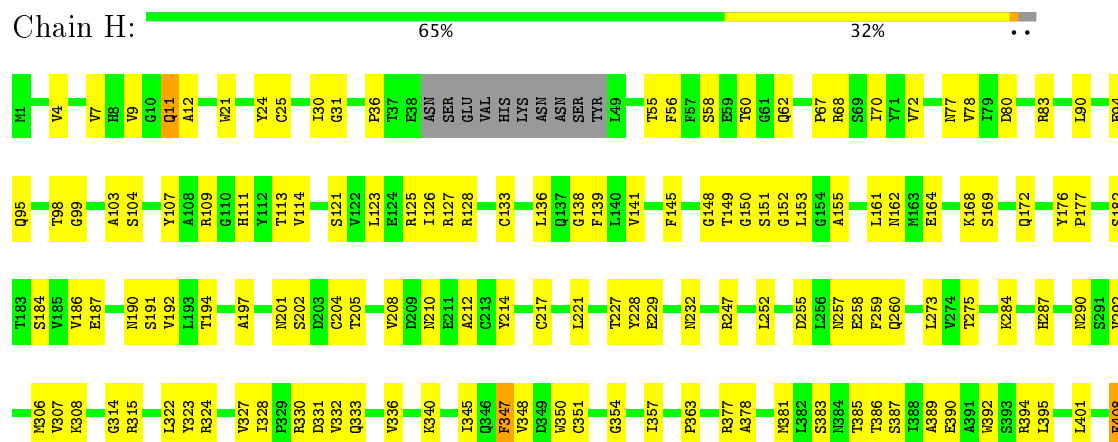




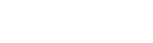
- Molecule 3: Tubulin alpha-1 chain



- Molecule 3: Tubulin alpha-1 chain



1409	1410	1411	1412	1413	1414	1415	1426	1430	1439	1442	1443	1444
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	12763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.48	0/3376	0.63	0/4568
1	B	0.48	0/3376	0.63	0/4568
1	C	0.49	0/3376	0.63	0/4568
1	J	0.49	0/3376	0.63	0/4568
2	D	0.40	0/1032	0.69	0/1390
3	E	0.51	0/3490	0.63	0/4733
3	F	0.51	0/3490	0.63	0/4733
3	G	0.51	0/3490	0.63	0/4733
3	H	0.51	0/3490	0.63	0/4733
All	All	0.50	0/28496	0.63	0/38594

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	J	0	1
3	E	0	1
3	F	0	1
3	G	0	1
3	H	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	LEU	Peptide
3	E	347	PHE	Peptide
3	F	347	PHE	Peptide
3	G	347	PHE	Peptide
3	H	347	PHE	Peptide

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	3304	0	3188	83	0
1	B	3304	0	3188	67	0
1	C	3304	0	3188	68	0
1	J	3304	0	3188	69	0
2	D	1010	0	989	19	0
3	E	3412	0	3284	106	0
3	F	3412	0	3284	119	0
3	G	3412	0	3284	100	0
3	H	3412	0	3284	100	0
4	A	28	0	12	1	0
4	B	28	0	12	1	0
4	C	28	0	12	1	0
4	J	28	0	12	1	0
5	E	32	0	12	4	0
5	F	32	0	12	5	0
5	G	32	0	12	5	0
5	H	32	0	12	4	0
All	All	28114	0	26973	683	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 12.

The worst 5 of 683 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:70:LEU:HB2	3:F:346:GLN:HE22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:31:GLY:H	3:E:36:PRO:HA	1.59	0.68
3:F:31:GLY:H	3:F:36:PRO:HA	1.59	0.68
3:G:31:GLY:H	3:G:36:PRO:HA	1.59	0.68
3:H:31:GLY:H	3:H:36:PRO:HA	1.59	0.67

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 PDB entries followed by that with respect to all EM entries.

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	426/429 (99%)	385 (90%)	41 (10%)	0	100	100
1	B	426/429 (99%)	385 (90%)	41 (10%)	0	100	100
1	C	426/429 (99%)	385 (90%)	41 (10%)	0	100	100
1	J	426/429 (99%)	385 (90%)	41 (10%)	0	100	100
2	D	119/143 (83%)	100 (84%)	18 (15%)	1 (1%)	22	66
3	E	430/444 (97%)	386 (90%)	44 (10%)	0	100	100
3	F	430/444 (97%)	386 (90%)	44 (10%)	0	100	100
3	G	430/444 (97%)	386 (90%)	44 (10%)	0	100	100
3	H	430/444 (97%)	386 (90%)	44 (10%)	0	100	100
All	All	3543/3635 (98%)	3184 (90%)	358 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	55	GLU

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 PDB entries followed by that with respect to all EM entries.

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	351/352 (100%)	350 (100%)	1 (0%)	94	96
1	B	351/352 (100%)	350 (100%)	1 (0%)	94	96
1	C	351/352 (100%)	350 (100%)	1 (0%)	94	96
1	J	351/352 (100%)	350 (100%)	1 (0%)	94	96
2	D	108/125 (86%)	108 (100%)	0	100	100
3	E	374/384 (97%)	371 (99%)	3 (1%)	85	92
3	F	374/384 (97%)	371 (99%)	3 (1%)	85	92
3	G	374/384 (97%)	371 (99%)	3 (1%)	85	92
3	H	374/384 (97%)	371 (99%)	3 (1%)	85	92
All	All	3008/3069 (98%)	2992 (100%)	16 (0%)	91	95

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	11	GLN
3	G	56	PHE
3	H	408	PHE
3	F	408	PHE
1	J	355	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	92	HIS
3	H	95	GLN
1	C	14	ASN
3	G	162	ASN
3	G	210	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 ⓘ

8 ligands are modelled in this entry.

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
4	GDP	A	500	-	25,30,30	1.09	2 (8%)	26,47,47	2.06	7 (26%)
4	GDP	B	500	-	25,30,30	1.08	2 (8%)	26,47,47	2.02	7 (26%)
4	GDP	C	500	-	25,30,30	1.07	2 (8%)	26,47,47	2.01	7 (26%)
5	GTP	E	500	-	27,34,34	1.09	2 (7%)	27,54,54	1.60	4 (14%)
5	GTP	F	500	-	27,34,34	1.11	2 (7%)	27,54,54	1.65	5 (18%)
5	GTP	G	500	-	27,34,34	1.11	2 (7%)	27,54,54	1.42	4 (14%)
5	GTP	H	500	-	27,34,34	1.05	2 (7%)	27,54,54	1.56	6 (22%)
4	GDP	J	500	-	25,30,30	1.07	2 (8%)	26,47,47	2.01	7 (26%)

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
4	GDP	A	500	-	-	0/12/32/32	0/3/3/3
4	GDP	B	500	-	-	0/12/32/32	0/3/3/3
4	GDP	C	500	-	-	0/12/32/32	0/3/3/3
5	GTP	E	500	-	-	0/18/38/38	0/3/3/3
5	GTP	F	500	-	-	0/18/38/38	0/3/3/3
5	GTP	G	500	-	-	0/18/38/38	0/3/3/3
5	GTP	H	500	-	-	0/18/38/38	0/3/3/3
4	GDP	J	500	-	-	0/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	500	GTP	C6-C5	-2.69	1.36	1.41
5	F	500	GTP	C6-C5	-2.40	1.36	1.41
5	E	500	GTP	C6-C5	-2.35	1.36	1.41
5	F	500	GTP	C2'-C1'	-2.26	1.50	1.53
5	H	500	GTP	C2'-C1'	-2.18	1.50	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	500	GDP	C6-C5-C4	-5.30	115.57	120.84
4	A	500	GDP	C6-C5-C4	-5.30	115.58	120.84
4	C	500	GDP	C6-C5-C4	-4.79	116.08	120.84
5	F	500	GTP	N3-C2-N1	-4.74	120.53	127.46
5	E	500	GTP	N3-C2-N1	-4.52	120.85	127.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	GDP	1	0
4	B	500	GDP	1	0
4	C	500	GDP	1	0
5	E	500	GTP	4	0
5	F	500	GTP	5	0
5	G	500	GTP	5	0
5	H	500	GTP	4	0
4	J	500	GDP	1	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.