



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:00 PM BST

PDB ID : 3JAK
EMDB ID: : EMD-6349
Title : Cryo-EM structure of GTPgammaS-microtubule co-polymerized with EB3
(merged dataset with and without kinesin bound)
Authors : Zhang, R.; Nogales, E.
Deposited on : 2015-06-16
Resolution : 3.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

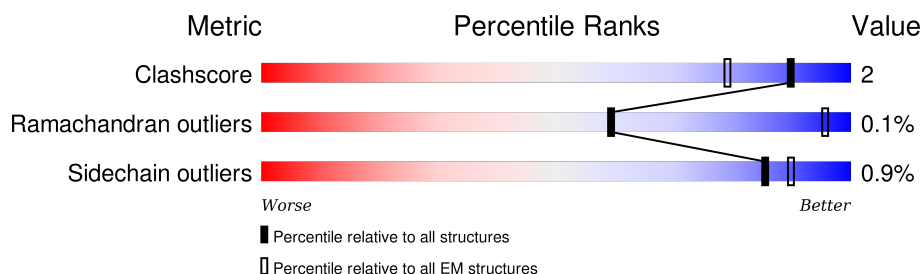
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	451	90% 6% .
1	C	451	90% 5% .
1	E	451	90% 6% .
1	J	451	90% 5% .
1	K	451	91% 5% .
1	L	451	91% 5% .
2	B	445	90% 7% .
2	D	445	90% 7% .
2	F	445	90% 7% .

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Mol	Chain	Length	Quality of chain
2	G	445	<div><div></div><div>91%</div><div>6%</div><div></div></div>
2	H	445	<div><div></div><div>90%</div><div>6%</div><div></div></div>
2	I	445	<div><div></div><div>90%</div><div>6%</div><div></div></div>
3	M	203	<div><div></div><div>59%</div><div>5%</div><div>35%</div><div></div></div>
3	N	203	<div><div></div><div>59%</div><div>5%</div><div>35%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43066 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 alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	432	Total	C	N	O	S	0	0
			3385	2145	575	644	21		
1	J	432	Total	C	N	O	S	0	0
			3385	2145	575	644	21		
1	C	432	Total	C	N	O	S	0	0
			3385	2145	575	644	21		
1	L	432	Total	C	N	O	S	0	0
			3385	2145	575	644	21		
1	A	432	Total	C	N	O	S	0	0
			3385	2145	575	644	21		
1	K	432	Total	C	N	O	S	0	0
			3385	2145	575	644	21		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	G	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	D	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	I	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	B	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	H	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		

- Molecule 3 is a protein called Microtubule-associated protein RP/EB family member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	131	Total	C	N	O	S	0	0
			1079	702	181	189	7		

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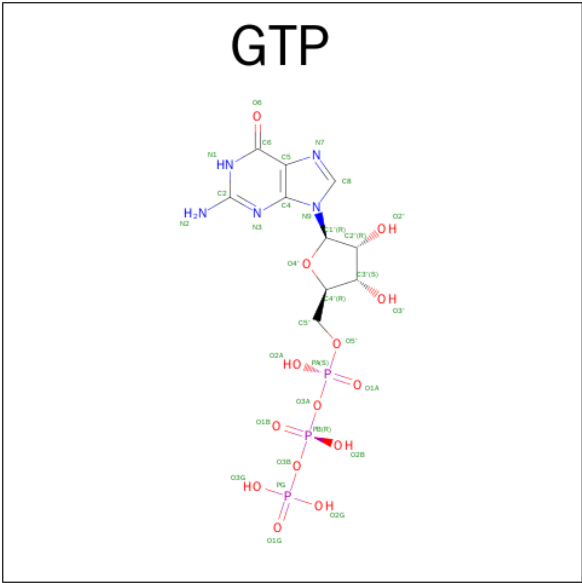
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	131	Total	C	N	O	S	0	0
			1079	702	181	189	7		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-2	SER	-	EXPRESSION TAG	UNP Q9UPY8
N	-1	ASN	-	EXPRESSION TAG	UNP Q9UPY8
N	0	ALA	-	EXPRESSION TAG	UNP Q9UPY8
M	-2	SER	-	EXPRESSION TAG	UNP Q9UPY8
M	-1	ASN	-	EXPRESSION TAG	UNP Q9UPY8
M	0	ALA	-	EXPRESSION TAG	UNP Q9UPY8

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



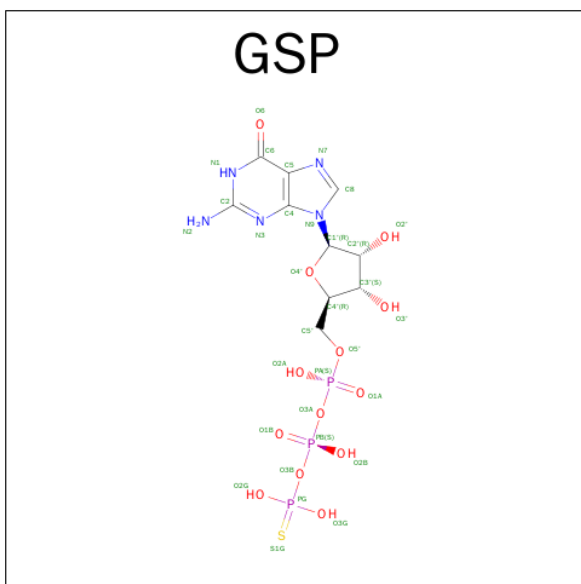
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Mol	Chain	Residues	Atoms					AltConf
4	K	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	J	1	Total	Mg	0
			1	1	
5	K	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	A	1	Total	Mg	0
			1	1	
5	L	1	Total	Mg	0
			1	1	

- Molecule 6 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						AltConf
6	F	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
6	G	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

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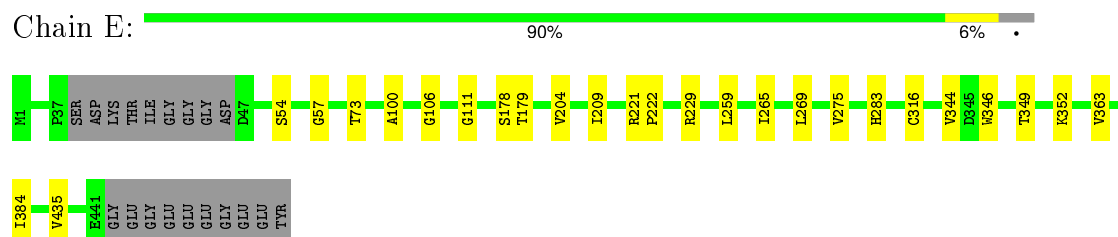
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Mol	Chain	Residues	Atoms						AltConf
6	D	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
6	I	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
6	B	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
6	H	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

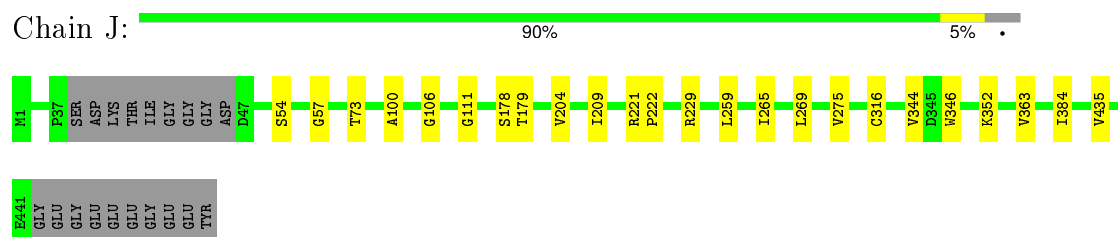
3 Residue-property plots [i](#)

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. 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.

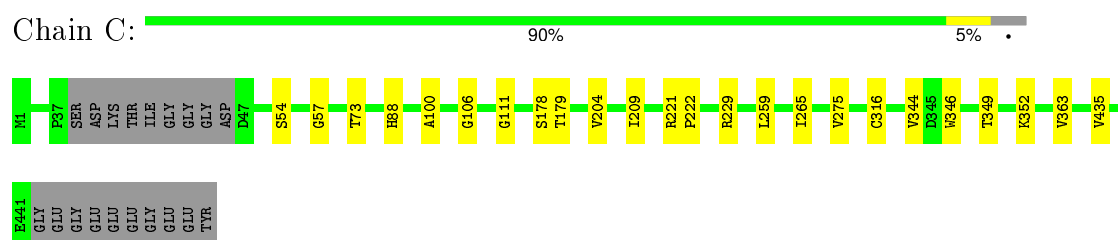
- Molecule 1: Tubulin alpha-1B chain



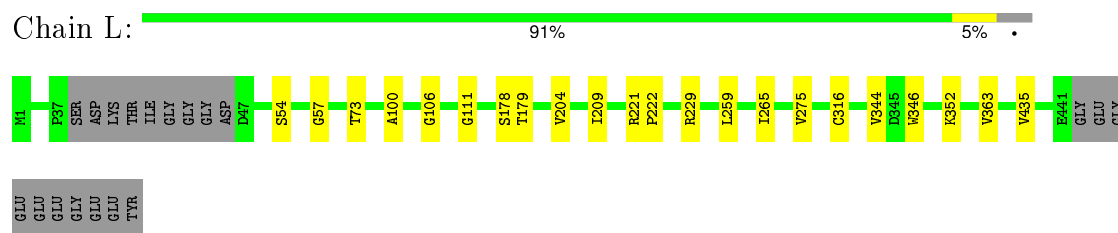
- Molecule 1: Tubulin alpha-1B chain



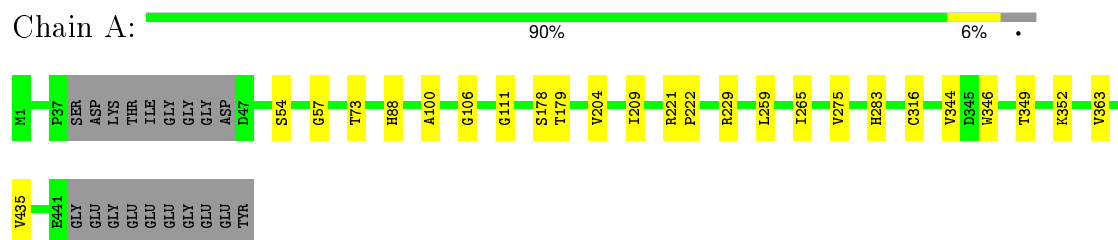
- Molecule 1: Tubulin alpha-1B chain



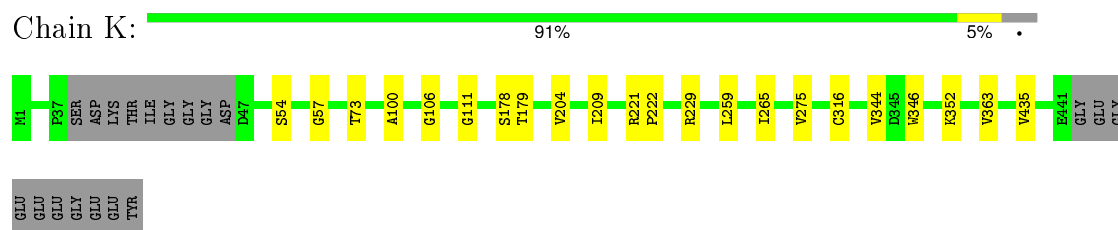
- Molecule 1: Tubulin alpha-1B chain



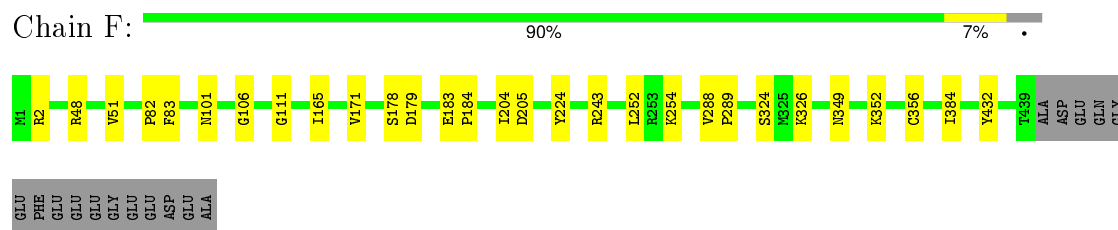
- Molecule 1: Tubulin alpha-1B chain



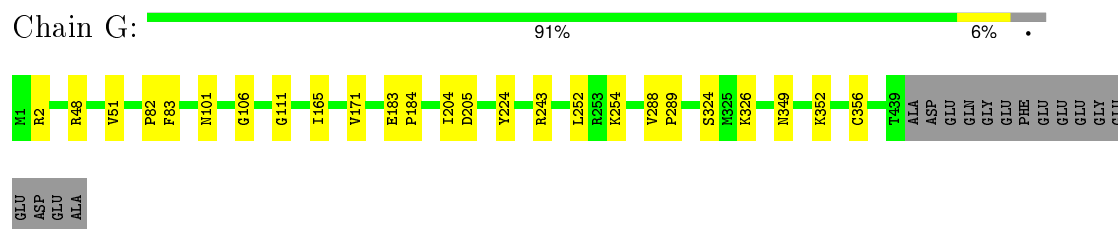
- Molecule 1: Tubulin alpha-1B chain



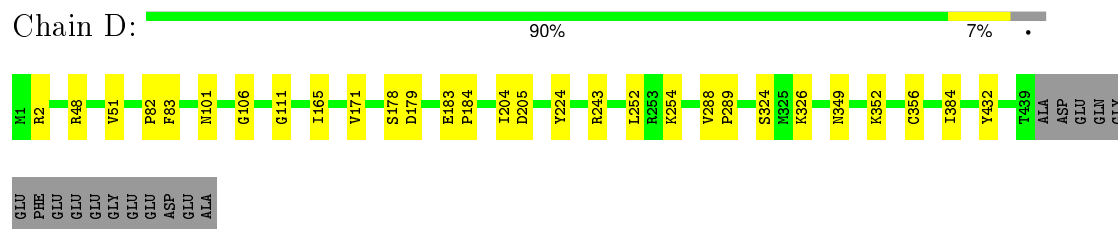
- Molecule 2: Tubulin beta chain



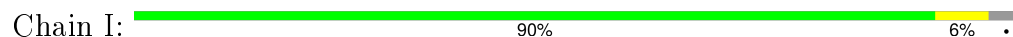
- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain



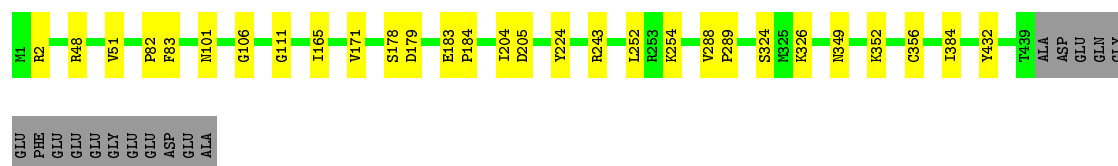
- Molecule 2: Tubulin beta chain





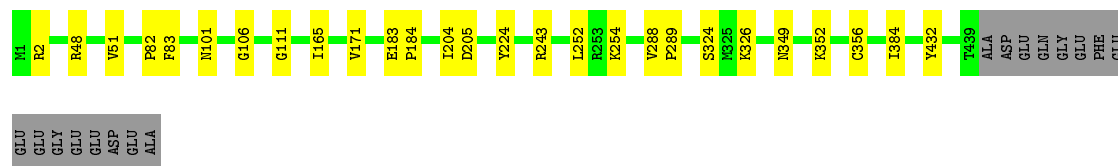
- Molecule 2: Tubulin beta chain

Chain B: 90% 7%



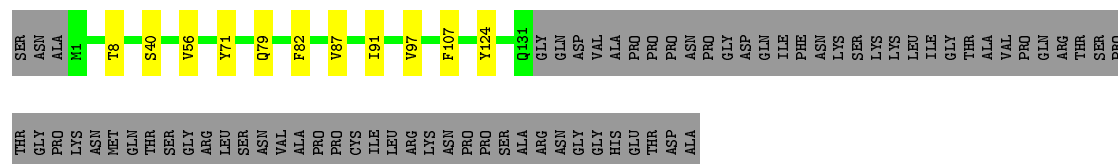
- Molecule 2: Tubulin beta chain

Chain H: 90% 6%



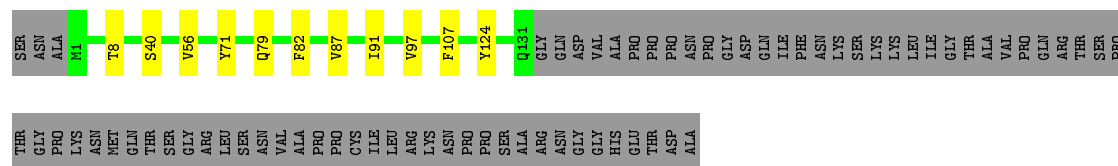
- Molecule 3: Microtubule-associated protein RP/EB family member 3

Chain N: 59% 5% 35%



- Molecule 3: Microtubule-associated protein RP/EB family member 3

Chain M: 59% 5% 35%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTFFIND4, each particle	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

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: GTP, GSP, MG

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	0.43	0/3462	0.68	0/4701
1	C	0.43	0/3462	0.68	0/4701
1	E	0.43	0/3462	0.68	0/4701
1	J	0.43	0/3462	0.68	0/4701
1	K	0.43	0/3462	0.68	0/4701
1	L	0.43	0/3462	0.68	0/4701
2	B	0.41	0/3443	0.68	0/4666
2	D	0.41	0/3443	0.68	0/4666
2	F	0.41	0/3443	0.68	0/4666
2	G	0.41	0/3443	0.68	0/4666
2	H	0.42	0/3443	0.68	0/4666
2	I	0.41	0/3443	0.68	0/4666
3	M	0.41	0/1107	0.57	0/1490
3	N	0.41	0/1107	0.57	0/1490
All	All	0.42	0/43644	0.67	0/59182

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	3385	0	3294	22	0
1	C	3385	0	3294	20	0
1	E	3385	0	3294	22	0
1	J	3385	0	3294	19	0
1	K	3385	0	3294	18	0
1	L	3385	0	3294	18	0
2	B	3368	0	3246	21	0
2	D	3368	0	3246	21	0
2	F	3368	0	3246	21	0
2	G	3368	0	3246	18	0
2	H	3368	0	3246	19	0
2	I	3368	0	3246	19	0
3	M	1079	0	1065	8	0
3	N	1079	0	1065	8	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	E	32	0	12	0	0
4	J	32	0	12	0	0
4	K	32	0	12	0	0
4	L	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	B	32	0	12	0	0
6	D	32	0	12	0	0
6	F	32	0	12	0	0
6	G	32	0	12	0	0
6	H	32	0	12	0	0
6	I	32	0	12	0	0
All	All	43066	0	41514	186	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 2.

The worst 5 of 186 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)
1:E:179:THR:O	2:G:352:LYS:HA	1.97	0.65
1:C:179:THR:O	2:I:352:LYS:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:352:LYS:HA	1:J:179:THR:O	1.97	0.64
2:D:352:LYS:HA	1:L:179:THR:O	1.97	0.64
1:A:179:THR:O	2:H:352:LYS:HA	1.97	0.62

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	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	52	88
1	C	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	52	88
1	E	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	52	88
1	J	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	52	88
1	K	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	52	88
1	L	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	52	88
2	B	427/445 (96%)	419 (98%)	8 (2%)	0	100	100
2	D	427/445 (96%)	419 (98%)	8 (2%)	0	100	100
2	F	427/445 (96%)	419 (98%)	8 (2%)	0	100	100
2	G	427/445 (96%)	419 (98%)	8 (2%)	0	100	100
2	H	427/445 (96%)	419 (98%)	8 (2%)	0	100	100
2	I	427/445 (96%)	419 (98%)	8 (2%)	0	100	100
3	M	129/203 (64%)	127 (98%)	2 (2%)	0	100	100
3	N	129/203 (64%)	127 (98%)	2 (2%)	0	100	100
All	All	5388/5782 (93%)	5264 (98%)	118 (2%)	6 (0%)	59	90

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	57	GLY
1	J	57	GLY
1	C	57	GLY
1	L	57	GLY
1	A	57	GLY

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	365/379 (96%)	363 (100%)	2 (0%)	92	97
1	C	365/379 (96%)	363 (100%)	2 (0%)	92	97
1	E	365/379 (96%)	363 (100%)	2 (0%)	92	97
1	J	365/379 (96%)	363 (100%)	2 (0%)	92	97
1	K	365/379 (96%)	363 (100%)	2 (0%)	92	97
1	L	365/379 (96%)	363 (100%)	2 (0%)	92	97
2	B	368/381 (97%)	364 (99%)	4 (1%)	80	92
2	D	368/381 (97%)	364 (99%)	4 (1%)	80	92
2	F	368/381 (97%)	364 (99%)	4 (1%)	80	92
2	G	368/381 (97%)	364 (99%)	4 (1%)	80	92
2	H	368/381 (97%)	364 (99%)	4 (1%)	80	92
2	I	368/381 (97%)	364 (99%)	4 (1%)	80	92
3	M	116/176 (66%)	113 (97%)	3 (3%)	54	83
3	N	116/176 (66%)	113 (97%)	3 (3%)	54	83
All	All	4630/4912 (94%)	4588 (99%)	42 (1%)	85	94

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	205	ASP
2	I	101	ASN
2	H	101	ASN

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Mol	Chain	Res	Type
2	D	224	TYR
1	L	54	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	309	HIS
1	L	358	GLN
2	H	14	ASN
1	L	88	HIS
2	I	14	ASN

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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\# Z > 2$
4	GTP	A	501	5	26,34,34	1.13	2 (7%)	29,54,54	1.65	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GSP	B	501	-	26,34,34	1.34	5 (19%)	27,54,54	1.95	7 (25%)
4	GTP	C	501	5	26,34,34	1.15	2 (7%)	29,54,54	1.67	5 (17%)
6	GSP	D	501	-	26,34,34	1.33	4 (15%)	27,54,54	1.94	7 (25%)
4	GTP	E	501	5	26,34,34	1.15	2 (7%)	29,54,54	1.66	4 (13%)
6	GSP	F	501	-	26,34,34	1.34	5 (19%)	27,54,54	1.97	7 (25%)
6	GSP	G	501	-	26,34,34	1.48	5 (19%)	27,54,54	1.91	7 (25%)
6	GSP	H	501	-	26,34,34	1.48	6 (23%)	27,54,54	1.96	7 (25%)
6	GSP	I	501	-	26,34,34	1.47	5 (19%)	27,54,54	1.92	7 (25%)
4	GTP	J	501	5	26,34,34	1.13	2 (7%)	29,54,54	1.69	4 (13%)
4	GTP	K	501	5	26,34,34	1.16	2 (7%)	29,54,54	1.70	4 (13%)
4	GTP	L	501	5	26,34,34	1.17	2 (7%)	29,54,54	1.69	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	501	5	-	0/18/38/38	0/3/3/3
6	GSP	B	501	-	-	0/17/38/38	0/3/3/3
4	GTP	C	501	5	-	0/18/38/38	0/3/3/3
6	GSP	D	501	-	-	0/17/38/38	0/3/3/3
4	GTP	E	501	5	-	0/18/38/38	0/3/3/3
6	GSP	F	501	-	-	0/17/38/38	0/3/3/3
6	GSP	G	501	-	-	0/17/38/38	0/3/3/3
6	GSP	H	501	-	-	0/17/38/38	0/3/3/3
6	GSP	I	501	-	-	0/17/38/38	0/3/3/3
4	GTP	J	501	5	-	0/18/38/38	0/3/3/3
4	GTP	K	501	5	-	0/18/38/38	0/3/3/3
4	GTP	L	501	5	-	0/18/38/38	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	501	GSP	O4'-C1'	2.00	1.44	1.41
6	B	501	GSP	PG-S1G	2.11	1.94	1.90
6	F	501	GSP	PG-S1G	2.17	1.94	1.90
6	F	501	GSP	PG-O2G	2.24	1.61	1.55
6	D	501	GSP	PG-O2G	2.26	1.61	1.55

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	F	501	GSP	C5-C6-N1	-4.03	118.25	123.52
6	D	501	GSP	C5-C6-N1	-3.98	118.32	123.52
4	K	501	GTP	C5-C6-N1	-3.97	118.33	123.52
4	A	501	GTP	C5-C6-N1	-3.94	118.37	123.52
4	C	501	GTP	C5-C6-N1	-3.94	118.37	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.