



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3J8X  
EMDB ID: : EMD-6187  
Title : High-resolution structure of no-nucleotide kinesin on microtubules  
Authors : Shang, Z.; Zhou, K.; Xu, C.; Csencsits, R.; Cochran, J.C.; Sindelar, C.V.  
Deposited on : 2014-11-20  
Resolution : 5.00 Å(reported)  
Based on PDB ID : 4HNA

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](mailto: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

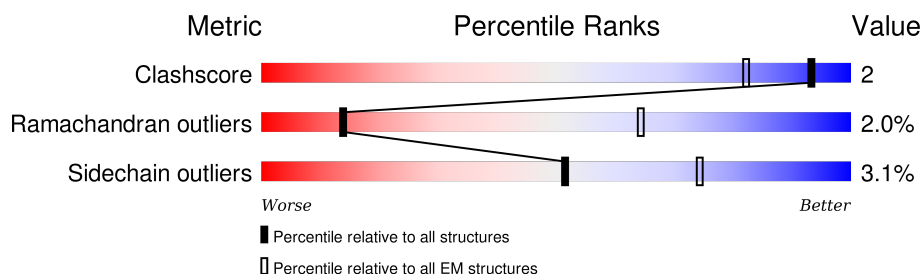
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.00 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  $\geq 3$ , 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	K	349	<div> <div style="width: 67%;">67%</div> <div style="width: 21%;">21%</div> <div style="width: 9%;">9%</div> <div style="width: 3%;">•</div> </div>
2	A	451	<div> <div style="width: 68%;">68%</div> <div style="width: 23%;">23%</div> <div style="width: 5%;">5%</div> <div style="width: 4%;">•</div> </div>
3	B	445	<div> <div style="width: 67%;">67%</div> <div style="width: 25%;">25%</div> <div style="width: 5%;">5%</div> <div style="width: 3%;">•</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9295 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 Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	316	Total	C	N	O	S	0	0
			2474	1543	423	498	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	7	SER	CYS	CONFLICT	UNP P33176
K	168	ALA	CYS	CONFLICT	UNP P33176
K	174	SER	CYS	CONFLICT	UNP P33176
K	330	SER	CYS	CONFLICT	UNP P33176

- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		

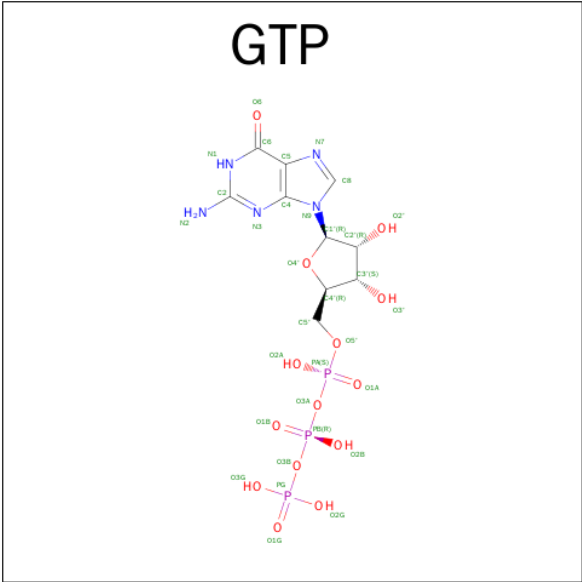
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	431	Total	C	N	O	S	0	0
			3389	2126	580	657	26		

There is a discrepancy between the modelled and reference sequences:

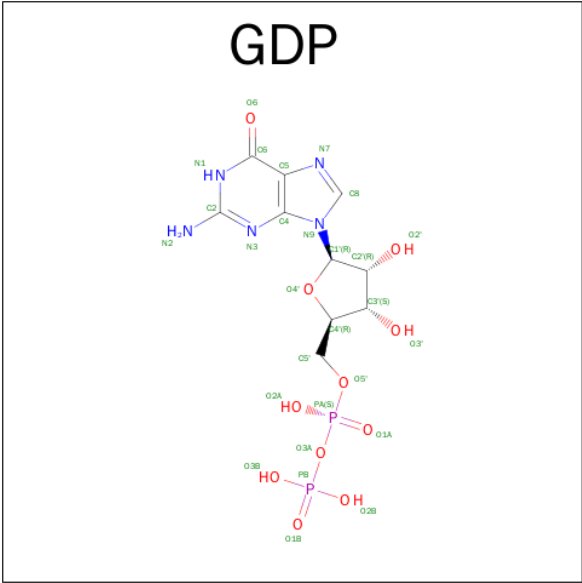
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	SER	CYS	CONFLICT	UNP F2Z5B2

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

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

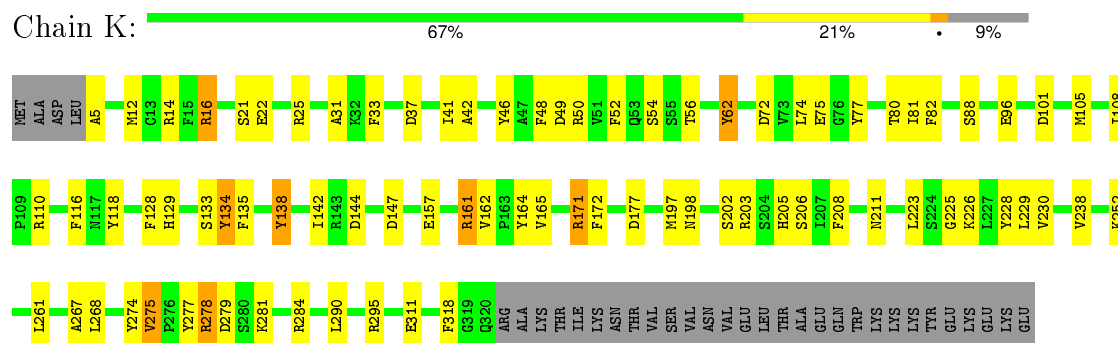


Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

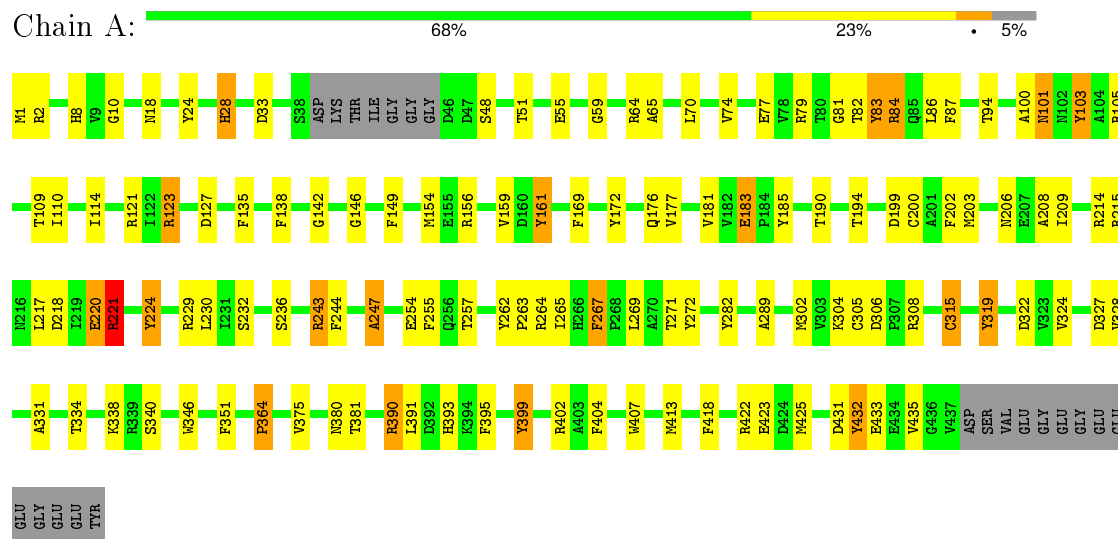
### 3 Residue-property plots

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

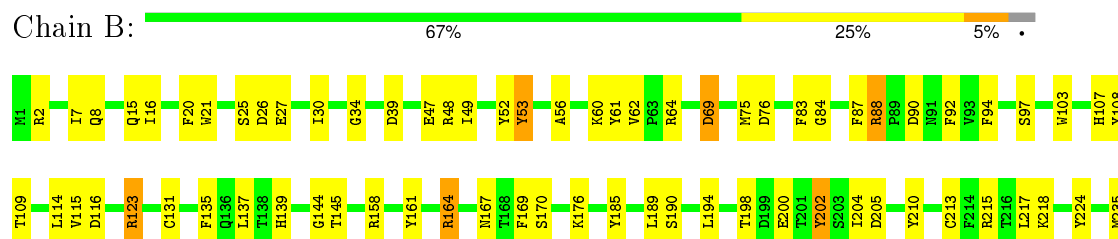
#### • Molecule 1: Kinesin-1 heavy chain



#### • Molecule 2: Tubulin alpha-1B chain



#### • Molecule 3: Tubulin beta-2B chain



S236	G237	V238	F244	I249	A250	D251	L252	R253	V257	F262	P263	R264	F267	F268	I269	F272	T276	Q281	Q282	Y283	R284	F286	D297	S298	R301	R302	R311	Y312	A316	F319	R320	E321	R322	P323	S324	R325	R326	E327	R332	L333	Y342	F343	V344
U349	R350	V351	K352	T353	A354	I358	P359	P360	R369	F377	R390	A397	R398	F399	R400	R401	K402	W407	Y408	T409	G412	F418	E422	D427	E431	Q434	Y435	A440	D441	GLU	GLN	GLY	GLU	PHE	GLU	GLU	GLU	GLU	GLY	GLU	ASP	GLU	ALA

## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	120783	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	done within FREALIGN	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 (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	K	1.64	15/2513 (0.6%)	1.96	67/3389 (2.0%)
2	A	1.64	21/3450 (0.6%)	2.01	92/4685 (2.0%)
3	B	1.61	16/3464 (0.5%)	2.06	119/4692 (2.5%)
All	All	1.63	52/9427 (0.6%)	2.02	278/12766 (2.2%)

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	K	0	10
2	A	1	19
3	B	0	18
All	All	1	47

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	412	GLY	CA-C	-7.85	1.39	1.51
1	K	277	TYR	CG-CD2	7.84	1.49	1.39
2	A	282	TYR	CG-CD2	7.35	1.48	1.39
1	K	206	SER	CA-CB	7.00	1.63	1.52
2	A	305	CYS	CB-SG	6.45	1.93	1.82
3	B	213	CYS	CB-SG	6.24	1.92	1.82
2	A	10	GLY	CA-C	-6.12	1.42	1.51
1	K	5	ALA	CA-CB	6.03	1.65	1.52
2	A	346	TRP	CD2-CE3	-6.02	1.31	1.40
3	B	97	SER	CA-CB	6.00	1.61	1.52
2	A	423	GLU	CB-CG	5.96	1.63	1.52
2	A	315	CYS	CB-SG	5.96	1.92	1.82

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	272	TYR	CE1-CZ	5.96	1.46	1.38
2	A	185	TYR	CG-CD2	5.93	1.46	1.39
2	A	24	TYR	CG-CD1	5.90	1.46	1.39
3	B	237	GLY	CA-C	-5.88	1.42	1.51
3	B	190	SER	CA-CB	5.87	1.61	1.52
3	B	407	TRP	N-CA	-5.85	1.34	1.46
1	K	22	GLU	CB-CG	5.81	1.63	1.52
1	K	105	MET	CG-SD	5.59	1.95	1.81
2	A	319	TYR	CE2-CZ	5.55	1.45	1.38
2	A	267	PHE	CG-CD2	5.49	1.47	1.38
1	K	16	ARG	NE-CZ	5.46	1.40	1.33
2	A	432	TYR	CG-CD2	5.46	1.46	1.39
3	B	39	ASP	CA-CB	5.46	1.66	1.53
1	K	172	PHE	CE1-CZ	5.45	1.47	1.37
2	A	10	GLY	N-CA	5.44	1.54	1.46
3	B	21	TRP	CB-CG	5.43	1.60	1.50
1	K	134	TYR	CZ-OH	5.42	1.47	1.37
3	B	185	TYR	CB-CG	5.37	1.59	1.51
2	A	200	CYS	CB-SG	5.36	1.91	1.82
1	K	54	SER	CB-OG	5.36	1.49	1.42
2	A	169	PHE	CG-CD2	5.34	1.46	1.38
3	B	25	SER	CA-CB	5.32	1.60	1.52
2	A	77	GLU	CG-CD	-5.32	1.44	1.51
2	A	399	TYR	CE1-CZ	5.32	1.45	1.38
2	A	254	GLU	CD-OE1	5.31	1.31	1.25
3	B	20	PHE	CG-CD1	5.30	1.46	1.38
3	B	103	TRP	CE3-CZ3	5.27	1.47	1.38
1	K	46	TYR	CG-CD1	5.24	1.46	1.39
1	K	157	GLU	CG-CD	-5.24	1.44	1.51
1	K	275	VAL	CB-CG2	5.22	1.63	1.52
2	A	142	GLY	C-N	5.21	1.42	1.33
2	A	183	GLU	CD-OE2	5.17	1.31	1.25
3	B	312	TYR	CZ-OH	5.15	1.46	1.37
3	B	47	GLU	CD-OE1	-5.14	1.20	1.25
3	B	210	TYR	CG-CD1	-5.13	1.32	1.39
1	K	164	TYR	CD2-CE2	5.13	1.47	1.39
3	B	52	TYR	CE1-CZ	5.12	1.45	1.38
2	A	236	SER	CA-CB	5.11	1.60	1.52
1	K	88	SER	CB-OG	5.05	1.48	1.42
1	K	208	PHE	CB-CG	5.00	1.59	1.51

All (278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	278	ARG	NE-CZ-NH2	-17.75	111.43	120.30
2	A	272	TYR	CB-CG-CD2	-17.55	110.47	121.00
2	A	243	ARG	NE-CZ-NH1	17.17	128.88	120.30
3	B	108	TYR	CB-CG-CD1	16.12	130.68	121.00
1	K	25	ARG	NE-CZ-NH1	15.52	128.06	120.30
3	B	322	ARG	NE-CZ-NH2	15.38	127.99	120.30
2	A	255	PHE	CB-CG-CD2	-15.35	110.05	120.80
2	A	264	ARG	NE-CZ-NH1	15.21	127.91	120.30
2	A	402	ARG	NE-CZ-NH1	14.74	127.67	120.30
2	A	24	TYR	CB-CG-CD1	-13.97	112.62	121.00
3	B	202	TYR	CB-CG-CD2	-13.04	113.17	121.00
3	B	88	ARG	NE-CZ-NH1	12.96	126.78	120.30
3	B	53	TYR	CB-CG-CD1	12.88	128.73	121.00
1	K	278	ARG	NE-CZ-NH1	12.68	126.64	120.30
3	B	108	TYR	CB-CG-CD2	-12.67	113.40	121.00
3	B	53	TYR	CB-CG-CD2	-12.09	113.74	121.00
3	B	158	ARG	NE-CZ-NH1	11.43	126.01	120.30
3	B	435	TYR	CB-CG-CD2	-11.41	114.16	121.00
2	A	24	TYR	CB-CG-CD2	10.79	127.47	121.00
2	A	432	TYR	CB-CG-CD1	10.45	127.27	121.00
3	B	202	TYR	CB-CG-CD1	10.32	127.19	121.00
3	B	75	MET	CG-SD-CE	-10.25	83.79	100.20
3	B	135	PHE	CB-CG-CD2	-10.08	113.75	120.80
2	A	214	ARG	NE-CZ-NH1	9.90	125.25	120.30
3	B	210	TYR	CB-CG-CD2	-9.86	115.08	121.00
1	K	284	ARG	NE-CZ-NH2	9.52	125.06	120.30
2	A	322	ASP	CB-CG-OD2	9.49	126.84	118.30
3	B	418	PHE	CB-CG-CD1	-9.48	114.17	120.80
2	A	185	TYR	CB-CG-CD2	9.29	126.58	121.00
1	K	295	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	A	123	ARG	NE-CZ-NH1	9.05	124.82	120.30
3	B	244	PHE	CB-CG-CD1	-8.95	114.54	120.80
2	A	399	TYR	CB-CG-CD1	-8.94	115.64	121.00
2	A	255	PHE	CB-CG-CD1	8.85	127.00	120.80
3	B	158	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	K	49	ASP	CB-CG-OD2	8.81	126.22	118.30
3	B	311	ARG	NE-CZ-NH2	8.59	124.60	120.30
2	A	224	TYR	CB-CG-CD2	-8.51	115.89	121.00
1	K	72	ASP	CB-CG-OD2	-8.39	110.75	118.30
2	A	395	PHE	CB-CG-CD2	-8.39	114.92	120.80
3	B	401	ARG	NE-CZ-NH1	8.39	124.49	120.30
2	A	127	ASP	CB-CG-OD1	8.36	125.82	118.30
3	B	342	TYR	CB-CG-CD1	8.29	125.98	121.00

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	161	TYR	CB-CG-CD1	-8.15	116.11	121.00
3	B	342	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	K	147	ASP	CB-CG-OD2	-8.07	111.04	118.30
2	A	308	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	K	77	TYR	CB-CG-CD2	-8.04	116.18	121.00
3	B	390	ARG	NE-CZ-NH2	-8.02	116.29	120.30
3	B	92	PHE	CB-CG-CD1	-7.95	115.24	120.80
3	B	397	ALA	N-CA-CB	-7.71	99.30	110.10
1	K	134	TYR	CB-CG-CD2	-7.66	116.40	121.00
1	K	82	PHE	CB-CG-CD2	-7.65	115.44	120.80
2	A	64	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	A	105	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	K	177	ASP	CB-CG-OD1	-7.60	111.46	118.30
2	A	264	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	K	318	PHE	CB-CG-CD2	-7.57	115.50	120.80
3	B	311	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	A	306	ASP	CB-CG-OD2	7.55	125.10	118.30
3	B	272	PHE	N-CA-CB	-7.55	97.00	110.60
3	B	343	PHE	CB-CG-CD1	-7.41	115.61	120.80
3	B	268	PHE	CB-CG-CD2	7.40	125.98	120.80
2	A	1	MET	CG-SD-CE	-7.35	88.43	100.20
3	B	311	ARG	NH1-CZ-NH2	-7.35	111.31	119.40
2	A	418	PHE	CB-CG-CD1	7.33	125.93	120.80
2	A	390	ARG	NE-CZ-NH1	7.31	123.95	120.30
2	A	161	TYR	CA-CB-CG	-7.27	99.58	113.40
2	A	199	ASP	CB-CG-OD2	7.23	124.80	118.30
2	A	65	ALA	O-C-N	-7.19	111.20	122.70
3	B	400	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	A	282	TYR	CB-CG-CD2	7.14	125.28	121.00
1	K	228	TYR	CB-CG-CD1	-7.13	116.72	121.00
1	K	77	TYR	CB-CG-CD1	7.08	125.25	121.00
3	B	103	TRP	CG-CD2-CE3	-7.08	127.53	133.90
2	A	247	ALA	CB-CA-C	7.07	120.71	110.10
2	A	156	ARG	NE-CZ-NH2	-7.07	116.77	120.30
2	A	83	TYR	CB-CG-CD2	-7.06	116.76	121.00
3	B	164	ARG	NE-CZ-NH1	7.03	123.82	120.30
2	A	433	GLU	O-C-N	-7.03	111.45	122.70
1	K	277	TYR	CB-CG-CD1	7.01	125.20	121.00
3	B	170	SER	N-CA-CB	7.00	121.00	110.50
1	K	50	ARG	NE-CZ-NH1	-6.96	116.82	120.30
3	B	322	ARG	NH1-CZ-NH2	-6.93	111.77	119.40
1	K	274	TYR	CB-CG-CD1	6.93	125.16	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	26	ASP	CB-CG-OD1	6.91	124.52	118.30
3	B	251	ASP	CB-CG-OD1	-6.90	112.09	118.30
2	A	202	PHE	CB-CG-CD2	-6.84	116.02	120.80
3	B	319	PHE	CB-CG-CD2	-6.82	116.03	120.80
1	K	48	PHE	CB-CG-CD1	-6.78	116.06	120.80
3	B	21	TRP	CB-CG-CD1	6.77	135.80	127.00
3	B	262	PHE	CB-CG-CD1	6.77	125.54	120.80
2	A	404	PHE	CB-CG-CD2	-6.77	116.06	120.80
2	A	272	TYR	CB-CG-CD1	6.77	125.06	121.00
2	A	395	PHE	CB-CG-CD1	6.76	125.53	120.80
3	B	167	ASN	O-C-N	-6.75	111.89	122.70
2	A	404	PHE	CB-CG-CD1	6.73	125.51	120.80
1	K	42	ALA	CB-CA-C	6.71	120.16	110.10
1	K	205	HIS	N-CA-CB	6.70	122.65	110.60
1	K	161	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	K	105	MET	CG-SD-CE	6.66	110.85	100.20
3	B	296	PHE	CB-CG-CD1	6.63	125.44	120.80
3	B	161	TYR	CB-CG-CD2	6.60	124.96	121.00
1	K	21	SER	N-CA-CB	6.59	120.38	110.50
2	A	319	TYR	CB-CG-CD1	-6.56	117.06	121.00
3	B	114	LEU	O-C-N	-6.54	112.24	122.70
2	A	262	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	K	311	GLU	OE1-CD-OE2	-6.50	115.50	123.30
2	A	269	LEU	O-C-N	-6.47	112.34	122.70
1	K	52	PHE	CB-CG-CD1	-6.46	116.28	120.80
2	A	215	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	A	159	VAL	CA-CB-CG1	6.42	120.53	110.90
3	B	2	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	A	154	MET	CG-SD-CE	-6.42	89.93	100.20
3	B	123	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	K	31	ALA	N-CA-CB	-6.35	101.21	110.10
3	B	431	GLU	O-C-N	-6.31	112.61	122.70
2	A	121	ARG	NE-CZ-NH1	-6.30	117.15	120.30
3	B	61	TYR	CB-CG-CD2	-6.30	117.22	121.00
3	B	390	ARG	CB-CA-C	6.29	122.99	110.40
2	A	105	ARG	NE-CZ-NH1	6.28	123.44	120.30
3	B	397	ALA	CB-CA-C	6.26	119.48	110.10
3	B	210	TYR	CB-CG-CD1	6.25	124.75	121.00
3	B	185	TYR	CG-CD1-CE1	-6.25	116.30	121.30
2	A	87	PHE	CB-CG-CD2	-6.25	116.43	120.80
3	B	235	MET	CG-SD-CE	-6.24	90.21	100.20
1	K	171	ARG	NE-CZ-NH1	6.23	123.41	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	76	ASP	CB-CG-OD1	6.22	123.90	118.30
2	A	243	ARG	CG-CD-NE	-6.21	98.75	111.80
1	K	37	ASP	CB-CG-OD1	-6.21	112.71	118.30
3	B	103	TRP	CB-CG-CD2	6.16	134.61	126.60
3	B	320	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	K	164	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	K	25	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	K	12	MET	CG-SD-CE	-6.12	90.41	100.20
3	B	90	ASP	CB-CG-OD2	6.11	123.80	118.30
3	B	244	PHE	CB-CG-CD2	6.11	125.07	120.80
3	B	267	PHE	CB-CG-CD1	6.07	125.05	120.80
2	A	224	TYR	CB-CG-CD1	6.04	124.63	121.00
1	K	101	ASP	CB-CG-OD2	-6.04	112.86	118.30
3	B	205	ASP	CB-CG-OD2	-6.04	112.86	118.30
3	B	401	ARG	NH1-CZ-NH2	-6.03	112.76	119.40
1	K	46	TYR	CB-CG-CD2	6.03	124.62	121.00
3	B	323	MET	CG-SD-CE	-6.03	90.56	100.20
3	B	253	ARG	NE-CZ-NH1	6.01	123.31	120.30
3	B	399	PHE	CG-CD1-CE1	-6.01	114.19	120.80
2	A	169	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	K	197	MET	CG-SD-CE	-5.99	90.61	100.20
3	B	116	ASP	CB-CG-OD1	-5.97	112.93	118.30
3	B	402	LYS	N-CA-CB	5.97	121.34	110.60
3	B	354	ALA	CB-CA-C	5.96	119.04	110.10
2	A	138	PHE	CZ-CE2-CD2	5.96	127.25	120.10
3	B	224	TYR	CG-CD1-CE1	-5.91	116.57	121.30
1	K	62	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	K	144	ASP	CB-CG-OD2	-5.89	112.99	118.30
3	B	21	TRP	CB-CG-CD2	-5.87	118.97	126.60
2	A	402	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	K	202	SER	N-CA-CB	5.86	119.29	110.50
2	A	24	TYR	CZ-CE2-CD2	-5.86	114.53	119.80
3	B	316	ALA	N-CA-CB	-5.86	101.90	110.10
3	B	302	MET	CG-SD-CE	-5.81	90.90	100.20
3	B	88	ARG	NE-CZ-NH2	-5.81	117.40	120.30
2	A	181	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	K	62	TYR	CG-CD2-CE2	-5.79	116.67	121.30
3	B	320	ARG	NE-CZ-NH1	5.78	123.19	120.30
3	B	377	PHE	CB-CG-CD1	-5.76	116.77	120.80
2	A	203	MET	CG-SD-CE	-5.76	90.99	100.20
2	A	331	ALA	N-CA-CB	5.75	118.15	110.10
2	A	172	TYR	CG-CD2-CE2	-5.75	116.70	121.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	215	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	A	272	TYR	CD1-CG-CD2	5.74	124.22	117.90
3	B	399	PHE	CD1-CE1-CZ	5.74	126.98	120.10
1	K	72	ASP	CB-CG-OD1	5.72	123.45	118.30
3	B	369	ARG	NE-CZ-NH1	-5.72	117.44	120.30
3	B	409	THR	N-CA-CB	5.72	121.17	110.30
2	A	94	THR	CA-CB-CG2	-5.71	104.40	112.40
3	B	251	ASP	CB-CG-OD2	5.71	123.44	118.30
3	B	27	GLU	O-C-N	-5.71	113.57	122.70
1	K	128	PHE	CB-CG-CD1	-5.69	116.81	120.80
2	A	324	VAL	CA-CB-CG1	5.69	119.44	110.90
3	B	262	PHE	CB-CG-CD2	-5.68	116.82	120.80
3	B	88	ARG	CD-NE-CZ	-5.67	115.67	123.60
2	A	55	GLU	CA-CB-CG	5.66	125.85	113.40
3	B	264	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	A	243	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	K	108	ILE	CA-C-N	5.62	132.82	117.10
3	B	47	GLU	CB-CA-C	5.61	121.62	110.40
2	A	232	SER	N-CA-CB	5.61	118.91	110.50
1	K	33	PHE	CB-CG-CD1	-5.61	116.88	120.80
3	B	94	PHE	CB-CG-CD2	-5.61	116.88	120.80
2	A	334	THR	O-C-N	-5.60	113.73	122.70
3	B	301	MET	CG-SD-CE	-5.60	91.24	100.20
3	B	224	TYR	CB-CG-CD1	-5.59	117.64	121.00
2	A	64	ARG	NE-CZ-NH1	5.57	123.08	120.30
3	B	26	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	K	277	TYR	CB-CA-C	-5.53	99.33	110.40
3	B	39	ASP	CB-CG-OD2	5.53	123.28	118.30
1	K	147	ASP	CB-CG-OD1	5.53	123.28	118.30
3	B	62	VAL	CG1-CB-CG2	-5.53	102.05	110.90
3	B	296	PHE	CB-CA-C	-5.53	99.34	110.40
1	K	164	TYR	CB-CG-CD1	5.53	124.31	121.00
1	K	268	LEU	CB-CG-CD1	-5.51	101.64	111.00
2	A	172	TYR	CB-CG-CD2	-5.48	117.71	121.00
3	B	2	ARG	NE-CZ-NH1	-5.47	117.56	120.30
3	B	435	TYR	CD1-CG-CD2	5.47	123.92	117.90
1	K	25	ARG	NH1-CZ-NH2	-5.46	113.39	119.40
3	B	189	LEU	O-C-N	-5.46	113.96	122.70
2	A	229	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	B	94	PHE	CB-CG-CD1	5.46	124.62	120.80
3	B	276	THR	CA-CB-CG2	-5.45	104.77	112.40
3	B	351	VAL	O-C-N	-5.44	113.99	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	139	HIS	N-CA-CB	-5.44	100.81	110.60
3	B	400	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	B	281	GLN	C-N-CA	5.41	135.22	121.70
2	A	48	SER	N-CA-CB	5.39	118.58	110.50
2	A	161	TYR	CD1-CE1-CZ	-5.38	114.95	119.80
3	B	69	ASP	CB-CG-OD1	5.38	123.14	118.30
2	A	177	VAL	O-C-N	-5.36	114.12	122.70
2	A	84	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	K	134	TYR	CG-CD1-CE1	-5.36	117.01	121.30
2	A	271	THR	N-CA-CB	5.36	120.48	110.30
1	K	223	LEU	CB-CG-CD1	-5.35	101.91	111.00
2	A	79	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	A	123	ARG	CD-NE-CZ	5.31	131.03	123.60
3	B	377	PHE	CG-CD2-CE2	-5.31	114.96	120.80
1	K	21	SER	CB-CA-C	-5.30	100.02	110.10
1	K	80	THR	CA-CB-CG2	-5.29	105.00	112.40
3	B	48	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	A	103	TYR	CB-CG-CD1	-5.28	117.83	121.00
3	B	297	ASP	CB-CG-OD2	5.27	123.04	118.30
1	K	116	PHE	O-C-N	-5.26	114.28	122.70
2	A	289	ALA	N-CA-CB	-5.26	102.73	110.10
2	A	263	PRO	N-CA-CB	5.25	109.60	103.30
2	A	433	GLU	CA-C-O	5.24	131.11	120.10
3	B	217	LEU	CB-CA-C	5.24	120.16	110.20
3	B	200	GLU	N-CA-CB	5.24	120.02	110.60
2	A	431	ASP	CB-CG-OD2	5.23	123.00	118.30
1	K	228	TYR	CG-CD1-CE1	-5.23	117.12	121.30
2	A	432	TYR	CA-CB-CG	-5.22	103.47	113.40
3	B	135	PHE	CA-CB-CG	-5.22	101.38	113.90
1	K	133	SER	N-CA-CB	5.21	118.32	110.50
3	B	327	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	K	252	LYS	CD-CE-NZ	5.21	123.69	111.70
1	K	177	ASP	CB-CG-OD2	5.21	122.98	118.30
2	A	380	ASN	CB-CA-C	5.20	120.80	110.40
1	K	49	ASP	CB-CG-OD1	-5.18	113.64	118.30
2	A	84	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	B	269	MET	N-CA-CB	-5.17	101.29	110.60
1	K	96	GLU	O-C-N	-5.16	114.43	123.20
2	A	135	PHE	CB-CG-CD1	-5.15	117.19	120.80
2	A	221	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	K	238	VAL	O-C-N	-5.14	114.48	122.70
3	B	64	ARG	O-C-N	5.11	130.88	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	338	LYS	O-C-N	-5.11	114.52	122.70
3	B	107	HIS	CA-CB-CG	5.11	122.29	113.60
1	K	274	TYR	CZ-CE2-CD2	5.11	124.40	119.80
2	A	375	VAL	CA-CB-CG2	5.11	118.56	110.90
3	B	344	VAL	N-CA-CB	5.10	122.73	111.50
1	K	267	ALA	N-CA-CB	5.10	117.24	110.10
2	A	364	PRO	CA-N-CD	5.09	118.83	111.70
2	A	220	GLU	OE1-CD-OE2	-5.09	117.19	123.30
3	B	64	ARG	NE-CZ-NH1	5.09	122.84	120.30
3	B	90	ASP	CB-CG-OD1	-5.08	113.72	118.30
2	A	74	VAL	CA-CB-CG1	5.08	118.52	110.90
3	B	15	GLN	N-CA-CB	5.08	119.75	110.60
2	A	156	ARG	N-CA-CB	5.06	119.70	110.60
1	K	198	ASN	CA-CB-CG	-5.05	102.28	113.40
3	B	353	THR	CA-CB-CG2	-5.05	105.33	112.40
1	K	277	TYR	CA-CB-CG	-5.04	103.82	113.40
2	A	308	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
1	K	230	VAL	N-CA-CB	-5.03	100.43	111.50
3	B	16	ILE	CA-CB-CG1	5.03	120.56	111.00
3	B	135	PHE	CB-CG-CD1	5.02	124.31	120.80
3	B	427	ASP	N-CA-CB	5.02	119.63	110.60
1	K	138	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	K	16	ARG	NE-CZ-NH2	-5.01	117.79	120.30
3	B	283	TYR	CG-CD2-CE2	-5.01	117.29	121.30
2	A	257	THR	N-CA-CB	5.00	119.81	110.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	46	ASP	CA

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	100	ALA	Peptide
2	A	101	ASN	Peptide
2	A	103	TYR	Sidechain
2	A	114	ILE	Peptide
2	A	123	ARG	Sidechain
2	A	146	GLY	Peptide
2	A	149	PHE	Sidechain
2	A	161	TYR	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	A	2	ARG	Sidechain
2	A	218	ASP	Peptide
2	A	224	TYR	Sidechain
2	A	243	ARG	Sidechain
2	A	267	PHE	Sidechain
2	A	28	HIS	Sidechain
2	A	390	ARG	Sidechain
2	A	399	TYR	Sidechain
2	A	422	ARG	Sidechain
2	A	83	TYR	Sidechain
2	A	84	ARG	Sidechain
3	B	123	ARG	Sidechain
3	B	164	ARG	Sidechain
3	B	169	PHE	Sidechain
3	B	202	TYR	Sidechain
3	B	250	ALA	Peptide
3	B	264	ARG	Sidechain
3	B	281	GLN	Peptide
3	B	284	ARG	Peptide
3	B	311	ARG	Sidechain
3	B	312	TYR	Sidechain
3	B	342	TYR	Sidechain
3	B	377	PHE	Sidechain
3	B	400	ARG	Sidechain
3	B	401	ARG	Sidechain
3	B	435	TYR	Sidechain
3	B	53	TYR	Sidechain
3	B	87	PHE	Sidechain
3	B	88	ARG	Sidechain
1	K	110	ARG	Sidechain
1	K	129	HIS	Sidechain
1	K	138	TYR	Sidechain
1	K	16	ARG	Sidechain
1	K	161	ARG	Sidechain
1	K	171	ARG	Sidechain
1	K	203	ARG	Sidechain
1	K	278	ARG	Sidechain
1	K	62	TYR	Sidechain
1	K	75	GLU	Peptide

## 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	K	2474	0	2434	6	0
2	A	3372	0	3287	16	0
3	B	3389	0	3266	13	0
4	A	32	0	12	0	0
5	B	28	0	12	0	0
All	All	9295	0	9011	31	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.

All (31) 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:A:208:ALA:HB2	2:A:304:LYS:HB2	1.87	0.56
3:B:332:MET:HG3	3:B:351:VAL:HG11	1.87	0.56
2:A:407:TRP:CE3	3:B:257:VAL:HG22	2.41	0.55
3:B:69:ASP:HA	3:B:145:THR:HG21	1.87	0.55
3:B:30:ILE:HD11	3:B:49:ILE:HD11	1.90	0.53
2:A:407:TRP:CE2	3:B:257:VAL:HA	2.44	0.52
1:K:142:ILE:HD11	1:K:281:LYS:HE2	1.92	0.51
2:A:109:THR:HG22	2:A:110:ILE:HD13	1.92	0.51
2:A:265:ILE:HG23	2:A:432:TYR:CZ	2.47	0.49
2:A:217:LEU:O	2:A:217:LEU:HD23	2.14	0.48
3:B:320:ARG:HB3	3:B:359:PRO:HA	1.96	0.47
2:A:190:THR:O	2:A:194:THR:HG23	2.15	0.47
2:A:18:ASN:HD21	2:A:82:THR:HG21	1.81	0.46
2:A:28:HIS:CE1	2:A:244:PHE:CZ	3.04	0.46
3:B:7:ILE:HD12	3:B:137:LEU:HD12	2.00	0.44
1:K:135:PHE:CZ	1:K:165:VAL:HG21	2.51	0.44
2:A:315:CYS:HB2	2:A:351:PHE:CD1	2.52	0.44
2:A:221:ARG:HH12	3:B:325:MET:HB2	1.83	0.44
3:B:253:ARG:HG3	3:B:257:VAL:HG23	2.00	0.44
1:K:162:VAL:HG11	1:K:226:LYS:NZ	2.32	0.43
2:A:176:GLN:HG2	3:B:333:LEU:HD22	2.00	0.43
3:B:194:LEU:HD22	3:B:198:THR:HG21	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:319:TYR:CE1	2:A:328:VAL:HG13	2.55	0.42
2:A:208:ALA:HB3	2:A:302:MET:O	2.20	0.41
1:K:41:ILE:HD13	1:K:41:ILE:HA	1.87	0.41
3:B:358:ILE:HG22	3:B:359:PRO:O	2.20	0.41
3:B:34:GLY:O	3:B:60:LYS:HA	2.21	0.41
1:K:81:ILE:HB	1:K:229:LEU:HD23	2.01	0.41
2:A:265:ILE:HG23	2:A:432:TYR:CE2	2.55	0.41
1:K:261:LEU:HD11	1:K:290:LEU:HD21	2.03	0.41
2:A:391:LEU:HD23	2:A:425:MET:HG3	2.04	0.40

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 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	K	314/349 (90%)	273 (87%)	39 (12%)	2 (1%)	30	74
2	A	428/451 (95%)	374 (87%)	44 (10%)	10 (2%)	8	49
3	B	429/445 (96%)	367 (86%)	51 (12%)	11 (3%)	7	46
All	All	1171/1245 (94%)	1014 (87%)	134 (11%)	23 (2%)	14	52

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	220	GLU
3	B	84	GLY
3	B	282	GLN
3	B	349	ASN
2	A	59	GLY
2	A	247	ALA
3	B	325	MET
2	A	101	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	340	SER
3	B	109	THR
3	B	298	SER
3	B	440	ALA
2	A	70	LEU
3	B	56	ALA
3	B	218	LYS
3	B	249	ASN
2	A	81	GLY
2	A	364	PRO
3	B	144	GLY
2	A	393	HIS
2	A	435	VAL
1	K	225	GLY
1	K	275	VAL

### 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	K	279/311 (90%)	272 (98%)	7 (2%)	55	82
2	A	364/379 (96%)	352 (97%)	12 (3%)	45	77
3	B	372/383 (97%)	360 (97%)	12 (3%)	46	77
All	All	1015/1073 (95%)	984 (97%)	31 (3%)	51	78

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	14	ARG
1	K	56	THR
1	K	74	LEU
1	K	118	TYR
1	K	134	TYR
1	K	211	ASN
1	K	279	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	8	HIS
2	A	33	ASP
2	A	51	THR
2	A	86	LEU
2	A	183	GLU
2	A	206	ASN
2	A	209	ILE
2	A	221	ARG
2	A	230	LEU
2	A	327	ASP
2	A	381	THR
2	A	413	MET
3	B	8	GLN
3	B	83	PHE
3	B	115	VAL
3	B	131	CYS
3	B	176	LYS
3	B	204	ILE
3	B	238	VAL
3	B	302	MET
3	B	323	MET
3	B	332	MET
3	B	422	GLU
3	B	434	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	61	HIS

### 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

2 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	GTP	A	600	-	26,34,34	1.91	6 (23%)	29,54,54	3.09	10 (34%)
5	GDP	B	501	-	24,30,30	1.93	6 (25%)	26,47,47	3.68	9 (34%)

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	600	-	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	C2'-C1'	-6.30	1.43	1.53
5	B	501	GDP	C8-N7	-3.14	1.28	1.34
4	A	600	GTP	PA-O2A	-2.28	1.45	1.55
5	B	501	GDP	C2-N2	-2.17	1.29	1.34
5	B	501	GDP	O6-C6	-2.05	1.19	1.24
4	A	600	GTP	C2'-C3'	2.09	1.59	1.53
5	B	501	GDP	O4'-C4'	2.16	1.50	1.45
5	B	501	GDP	O2'-C2'	2.78	1.49	1.43
4	A	600	GTP	O4'-C1'	3.15	1.45	1.41
4	A	600	GTP	O4'-C4'	3.30	1.52	1.45
4	A	600	GTP	C3'-C4'	4.37	1.64	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	C6-N1	4.72	1.41	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C5-C6-N1	-9.96	110.51	123.52
4	A	600	GTP	C5-C6-N1	-9.29	111.38	123.52
5	B	501	GDP	N3-C2-N1	-5.57	119.99	127.56
4	A	600	GTP	C6-C5-C4	-4.97	115.18	120.86
5	B	501	GDP	O4'-C4'-C3'	-3.45	98.17	105.16
4	A	600	GTP	N2-C2-N1	-3.26	111.83	117.20
4	A	600	GTP	N3-C2-N1	-2.93	123.58	127.56
4	A	600	GTP	C4'-O4'-C1'	-2.67	106.82	109.64
5	B	501	GDP	C6-C5-C4	-2.25	118.28	120.86
5	B	501	GDP	O3B-PB-O1B	2.12	117.54	110.63
5	B	501	GDP	C4'-O4'-C1'	2.13	111.90	109.64
4	A	600	GTP	O2'-C2'-C3'	2.34	119.41	111.86
4	A	600	GTP	O4'-C1'-N9	2.79	113.37	108.11
4	A	600	GTP	O2B-PB-O3A	2.80	117.27	105.27
5	B	501	GDP	O3'-C3'-C2'	3.08	121.80	111.86
5	B	501	GDP	O4'-C1'-N9	3.10	113.97	108.11
4	A	600	GTP	N2-C2-N3	3.50	124.29	117.72
4	A	600	GTP	C6-N1-C2	9.23	126.69	115.88
5	B	501	GDP	C6-N1-C2	12.44	130.46	115.88

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.