



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3J1U  
EMDB ID: : EMD-5439  
Title : Low affinity dynein microtubule binding domain - tubulin complex  
Authors : Redwine, W.B.; Hernandez-Lopez, R.; Zou, S.; Huang, J.; Reck-Peterson, S.L.;  
Leschziner, A.E.  
Deposited on : 2012-06-25  
Resolution : 9.70 Å(reported)  
Based on PDB ID : 3ERR, 1JFF

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>

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MolProbity : 4.02b-467  
Mogul : unknown  
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

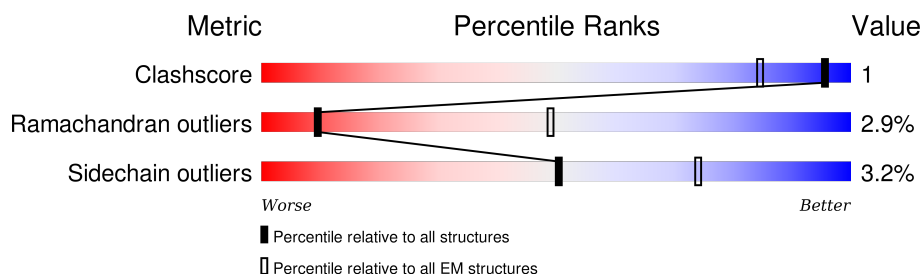
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.70 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	A	164	<div> <div style="width: 85%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>85% 13% .</div>
2	B	451	<div> <div style="width: 72%; background-color: green;"></div> <div style="width: 19%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>72% 19% 6% .</div>
3	C	427	<div> <div style="width: 73%; background-color: green;"></div> <div style="width: 22%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>73% 22% . .</div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8089 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 Cytoplasmic dynein 1 heavy chain 1, seryl t-RNA synthetase chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	164	Total	C	N	O	S	0	0
			1306	820	227	250	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	439	Total	C	N	O	S	0	0
			3423	2163	582	656	22		


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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	427	Total	C	N	O	S	0	0
			3360	2110	576	648	26		

### 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.

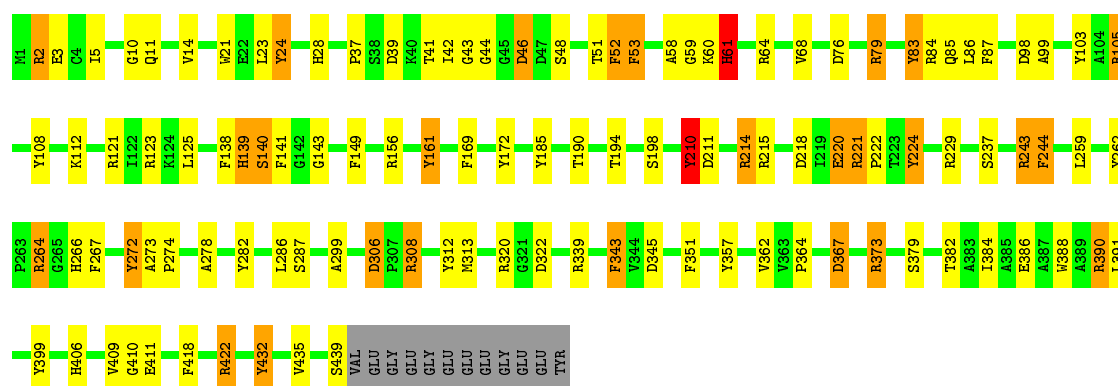
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1, seryl t-RNA synthetase chimera

Chain A: 



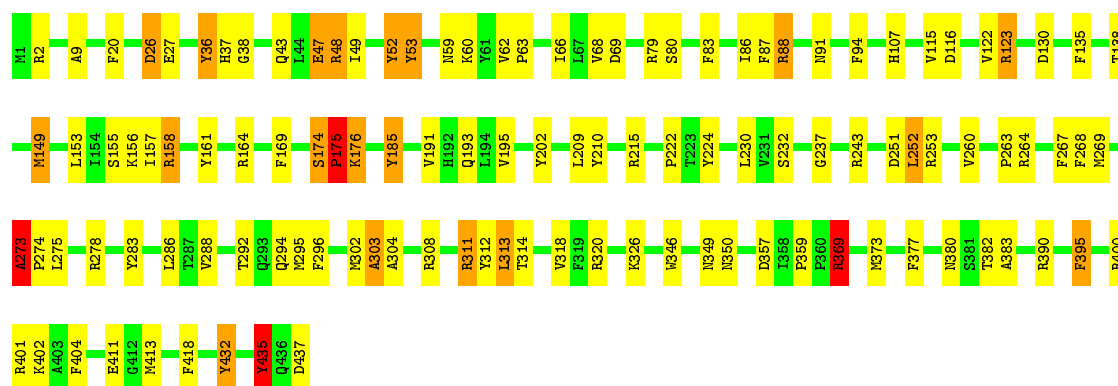
- Molecule 2: Tubulin alpha-1B chain

Chain B: 



- Molecule 3: Tubulin beta-2B chain

Chain C: 



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	10419	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	phase and amplitude correction using Fre-align	Depositor
Microscope	FEI Tecnai F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	62000	Depositor
Image detector	Kodak SO-163 film	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	1.58	3/1323 (0.2%)	1.84	24/1782 (1.3%)
2	B	1.64	21/3501 (0.6%)	2.04	108/4752 (2.3%)
3	C	1.67	18/3435 (0.5%)	2.07	98/4652 (2.1%)
All	All	1.64	42/8259 (0.5%)	2.02	230/11186 (2.1%)

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	6
2	B	0	20
3	C	0	18
All	All	0	44

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	439	SER	C-O	-12.05	1.00	1.23
3	C	437	ASP	C-OXT	-12.04	1.00	1.23
3	C	437	ASP	C-O	-12.03	1.00	1.23
2	B	224	TYR	CE2-CZ	8.84	1.50	1.38
2	B	224	TYR	CE1-CZ	8.35	1.49	1.38
3	C	411	GLU	CD-OE1	7.70	1.34	1.25
3	C	377	PHE	CG-CD1	6.62	1.48	1.38
1	A	3369	TYR	CD1-CE1	6.59	1.49	1.39
3	C	237	GLY	CA-C	-6.54	1.41	1.51
2	B	198	SER	CA-CB	6.54	1.62	1.52
3	C	185	TYR	CG-CD2	6.33	1.47	1.39
3	C	36	TYR	CG-CD2	6.21	1.47	1.39
2	B	237	SER	CB-OG	6.16	1.50	1.42
2	B	169	PHE	CG-CD2	5.93	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	TYR	CG-CD1	5.91	1.46	1.39
2	B	143	GLY	C-N	5.85	1.43	1.33
3	C	185	TYR	CG-CD1	5.85	1.46	1.39
3	C	48	ARG	CD-NE	5.80	1.56	1.46
2	B	221	ARG	CD-NE	5.79	1.56	1.46
2	B	21	TRP	NE1-CE2	5.70	1.45	1.37
3	C	83	PHE	CE2-CZ	5.62	1.48	1.37
2	B	58	ALA	CA-CB	5.57	1.64	1.52
3	C	155	SER	CA-CB	5.53	1.61	1.52
2	B	411	GLU	CD-OE2	-5.52	1.19	1.25
1	A	3321	SER	CB-OG	5.50	1.49	1.42
3	C	232	SER	CB-OG	5.49	1.49	1.42
2	B	399	TYR	CD1-CE1	5.45	1.47	1.39
2	B	272	TYR	CG-CD1	5.43	1.46	1.39
3	C	63	PRO	N-CD	-5.43	1.40	1.47
2	B	48	SER	CA-CB	5.38	1.61	1.52
2	B	287	SER	CA-CB	5.35	1.60	1.52
3	C	195	VAL	CB-CG1	5.34	1.64	1.52
2	B	10	GLY	CA-C	-5.33	1.43	1.51
2	B	272	TYR	CE2-CZ	5.21	1.45	1.38
3	C	169	PHE	CG-CD1	5.20	1.46	1.38
3	C	435	TYR	CZ-OH	5.19	1.46	1.37
2	B	410	GLY	CA-C	-5.19	1.43	1.51
3	C	346	TRP	CE2-CZ2	5.14	1.48	1.39
2	B	357	TYR	CB-CG	5.06	1.59	1.51
1	A	3400	TYR	CG-CD1	5.05	1.45	1.39
2	B	121	ARG	CD-NE	5.02	1.54	1.46
3	C	20	PHE	CG-CD2	5.01	1.46	1.38

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	253	ARG	NE-CZ-NH1	16.85	128.72	120.30
3	C	185	TYR	CB-CG-CD2	16.69	131.01	121.00
3	C	401	ARG	NE-CZ-NH1	16.59	128.59	120.30
2	B	224	TYR	CD1-CE1-CZ	16.50	134.65	119.80
2	B	84	ARG	NE-CZ-NH2	-14.29	113.15	120.30
3	C	210	TYR	CB-CG-CD1	14.15	129.49	121.00
3	C	185	TYR	CB-CG-CD1	-14.09	112.55	121.00
3	C	243	ARG	NE-CZ-NH2	-13.10	113.75	120.30
2	B	243	ARG	NE-CZ-NH1	13.02	126.81	120.30
2	B	224	TYR	CE1-CZ-CE2	-12.94	99.10	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	268	PHE	CB-CG-CD2	12.19	129.33	120.80
2	B	224	TYR	CZ-CE2-CD2	12.16	130.74	119.80
3	C	2	ARG	NE-CZ-NH2	-11.43	114.59	120.30
3	C	210	TYR	CB-CG-CD2	-11.17	114.30	121.00
3	C	308	ARG	NE-CZ-NH2	-11.15	114.72	120.30
3	C	320	ARG	NE-CZ-NH1	11.12	125.86	120.30
3	C	432	TYR	CB-CG-CD1	-11.11	114.33	121.00
3	C	311	ARG	NE-CZ-NH2	-11.07	114.77	120.30
3	C	390	ARG	NE-CZ-NH1	11.05	125.82	120.30
2	B	210	TYR	CB-CG-CD1	10.99	127.59	121.00
3	C	253	ARG	NE-CZ-NH2	-10.73	114.93	120.30
3	C	395	PHE	CB-CG-CD2	-10.69	113.32	120.80
2	B	264	ARG	NE-CZ-NH1	10.49	125.55	120.30
2	B	262	TYR	CB-CG-CD2	10.27	127.16	121.00
3	C	312	TYR	CB-CG-CD1	-10.25	114.85	121.00
2	B	221	ARG	NE-CZ-NH2	-10.24	115.18	120.30
2	B	224	TYR	CB-CG-CD2	10.21	127.12	121.00
3	C	308	ARG	NE-CZ-NH1	10.16	125.38	120.30
2	B	262	TYR	CB-CG-CD1	-10.03	114.98	121.00
2	B	172	TYR	CB-CG-CD1	-9.98	115.01	121.00
3	C	320	ARG	NE-CZ-NH2	-9.88	115.36	120.30
2	B	52	PHE	CB-CG-CD2	9.79	127.65	120.80
1	A	3279	ASP	CB-CG-OD2	-9.67	109.59	118.30
2	B	210	TYR	CB-CG-CD2	-9.59	115.25	121.00
2	B	320	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	A	3345	PHE	CB-CG-CD2	-9.47	114.17	120.80
3	C	169	PHE	CB-CG-CD1	9.46	127.42	120.80
3	C	164	ARG	NE-CZ-NH2	-9.34	115.63	120.30
3	C	202	TYR	CB-CG-CD1	-9.18	115.49	121.00
3	C	311	ARG	NE-CZ-NH1	9.15	124.88	120.30
2	B	308	ARG	NE-CZ-NH1	9.10	124.85	120.30
3	C	224	TYR	CB-CG-CD1	-9.09	115.54	121.00
2	B	84	ARG	NE-CZ-NH1	9.08	124.84	120.30
2	B	215	ARG	NE-CZ-NH2	8.88	124.74	120.30
3	C	401	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	3279	ASP	CB-CG-OD1	8.61	126.05	118.30
2	B	299	ALA	N-CA-CB	8.45	121.93	110.10
3	C	164	ARG	NE-CZ-NH1	8.41	124.50	120.30
2	B	312	TYR	CB-CG-CD1	-8.35	115.99	121.00
2	B	218	ASP	CB-CG-OD2	-8.33	110.80	118.30
3	C	53	TYR	CB-CG-CD2	-8.24	116.06	121.00
2	B	264	ARG	NE-CZ-NH2	-8.15	116.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	43	GLN	C-N-CA	8.09	141.93	121.70
3	C	404	PHE	CB-CG-CD2	-8.02	115.19	120.80
2	B	87	PHE	CB-CG-CD2	-7.94	115.24	120.80
3	C	215	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	3400	TYR	CB-CG-CD2	-7.85	116.29	121.00
2	B	308	ARG	NH1-CZ-NH2	-7.79	110.83	119.40
2	B	218	ASP	CB-CG-OD1	7.79	125.31	118.30
3	C	295	MET	CG-SD-CE	-7.76	87.79	100.20
2	B	185	TYR	CB-CG-CD1	-7.71	116.37	121.00
2	B	229	ARG	NE-CZ-NH1	-7.70	116.45	120.30
3	C	243	ARG	NE-CZ-NH1	7.69	124.14	120.30
3	C	296	PHE	CB-CG-CD2	-7.64	115.45	120.80
2	B	367	ASP	CB-CG-OD1	7.63	125.17	118.30
2	B	224	TYR	CE1-CZ-OH	7.60	140.63	120.10
2	B	422	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	B	422	ARG	NE-CZ-NH2	-7.57	116.51	120.30
2	B	343	PHE	CB-CG-CD2	-7.52	115.54	120.80
2	B	215	ARG	NE-CZ-NH1	-7.45	116.57	120.30
2	B	194	THR	N-CA-CB	7.43	124.41	110.30
3	C	303	ALA	N-CA-CB	7.40	120.46	110.10
3	C	395	PHE	CB-CG-CD1	7.39	125.97	120.80
1	A	3377	TYR	CB-CG-CD1	-7.34	116.59	121.00
2	B	214	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	3342	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	3411	ARG	NE-CZ-NH1	7.30	123.95	120.30
3	C	357	ASP	CB-CG-OD1	7.25	124.83	118.30
2	B	185	TYR	CB-CG-CD2	7.23	125.34	121.00
3	C	123	ARG	NE-CZ-NH1	7.19	123.89	120.30
3	C	302	MET	CA-CB-CG	7.12	125.41	113.30
2	B	161	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	A	3408	GLU	OE1-CD-OE2	-7.10	114.78	123.30
2	B	156	ARG	NE-CZ-NH1	7.09	123.85	120.30
2	B	24	TYR	CB-CG-CD2	-7.06	116.77	121.00
1	A	3290	ALA	CB-CA-C	-7.05	99.52	110.10
3	C	43	GLN	O-C-N	7.01	133.92	122.70
2	B	138	PHE	CB-CG-CD2	6.99	125.69	120.80
3	C	87	PHE	C-N-CA	6.91	138.99	121.70
2	B	220	GLU	OE1-CD-OE2	-6.90	115.02	123.30
2	B	2	ARG	NE-CZ-NH2	-6.89	116.86	120.30
3	C	224	TYR	CB-CG-CD2	6.87	125.12	121.00
2	B	39	ASP	CB-CG-OD1	6.79	124.42	118.30
3	C	318	VAL	CA-CB-CG2	-6.74	100.79	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	382	THR	CA-CB-CG2	-6.70	103.02	112.40
2	B	53	PHE	CB-CG-CD2	6.64	125.45	120.80
1	A	3377	TYR	CZ-CE2-CD2	-6.64	113.82	119.80
2	B	244	PHE	CB-CG-CD1	-6.63	116.16	120.80
3	C	20	PHE	CB-CG-CD2	6.62	125.44	120.80
2	B	14	VAL	CG1-CB-CG2	-6.62	100.31	110.90
2	B	79	ARG	NE-CZ-NH2	-6.60	117.00	120.30
2	B	399	TYR	CB-CG-CD2	6.59	124.95	121.00
3	C	373	MET	CG-SD-CE	-6.58	89.67	100.20
1	A	3271	ASP	CB-CG-OD1	-6.56	112.39	118.30
2	B	243	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	B	267	PHE	CB-CG-CD1	6.53	125.37	120.80
3	C	268	PHE	CB-CG-CD1	-6.51	116.24	120.80
3	C	130	ASP	CB-CG-OD1	6.49	124.14	118.30
2	B	123	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	3377	TYR	CB-CG-CD2	6.42	124.85	121.00
2	B	60	LYS	C-N-CA	6.40	137.69	121.70
3	C	69	ASP	CB-CG-OD1	-6.39	112.55	118.30
2	B	244	PHE	CB-CG-CD2	6.39	125.27	120.80
3	C	149	MET	CG-SD-CE	-6.38	89.99	100.20
1	A	3297	ILE	O-C-N	-6.35	112.53	122.70
3	C	311	ARG	CG-CD-NE	-6.35	98.46	111.80
2	B	322	ASP	CB-CG-OD1	6.34	124.01	118.30
3	C	359	PRO	CA-C-N	6.32	134.79	117.10
2	B	121	ARG	NE-CZ-NH2	6.31	123.45	120.30
3	C	20	PHE	CB-CG-CD1	-6.30	116.39	120.80
3	C	191	VAL	CA-CB-CG1	6.29	120.33	110.90
2	B	388	TRP	CH2-CZ2-CE2	6.28	123.68	117.40
2	B	224	TYR	CB-CG-CD1	-6.27	117.24	121.00
3	C	158	ARG	NE-CZ-NH2	6.26	123.43	120.30
2	B	267	PHE	CB-CG-CD2	-6.22	116.44	120.80
2	B	172	TYR	CG-CD1-CE1	-6.21	116.33	121.30
2	B	108	TYR	CG-CD1-CE1	-6.19	116.35	121.30
3	C	26	ASP	CB-CG-OD2	6.18	123.86	118.30
3	C	209	LEU	CB-CA-C	6.15	121.89	110.20
2	B	21	TRP	CG-CD2-CE3	-6.14	128.37	133.90
3	C	135	PHE	CB-CG-CD1	6.12	125.08	120.80
2	B	432	TYR	CB-CG-CD2	-6.12	117.33	121.00
2	B	409	VAL	CA-CB-CG2	-6.09	101.76	110.90
2	B	422	ARG	CA-CB-CG	6.08	126.78	113.40
2	B	339	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	B	149	PHE	CB-CG-CD2	-6.07	116.55	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	292	THR	OG1-CB-CG2	-6.05	96.09	110.00
3	C	9	ALA	N-CA-CB	-6.03	101.66	110.10
1	A	3369	TYR	CD1-CE1-CZ	-5.89	114.50	119.80
2	B	60	LYS	O-C-N	5.88	132.11	122.70
3	C	80	SER	O-C-N	-5.88	113.21	123.20
3	C	252	LEU	CB-CG-CD1	5.84	120.94	111.00
3	C	68	VAL	CG1-CB-CG2	5.83	120.23	110.90
2	B	211	ASP	CB-CG-OD1	5.82	123.54	118.30
3	C	288	VAL	O-C-N	-5.82	110.04	121.10
2	B	313	MET	CG-SD-CE	-5.78	90.95	100.20
1	A	3369	TYR	CZ-CE2-CD2	5.78	125.00	119.80
3	C	312	TYR	CD1-CG-CD2	5.78	124.26	117.90
2	B	345	ASP	CB-CG-OD1	5.77	123.49	118.30
2	B	379	SER	N-CA-CB	5.73	119.09	110.50
3	C	264	ARG	N-CA-C	-5.70	95.62	111.00
3	C	138	THR	N-CA-CB	5.69	121.11	110.30
3	C	380	ASN	O-C-N	-5.69	113.59	122.70
2	B	432	TYR	CZ-CE2-CD2	-5.69	114.68	119.80
3	C	88	ARG	NE-CZ-NH2	5.69	123.14	120.30
2	B	282	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	3400	TYR	CG-CD2-CE2	-5.63	116.79	121.30
3	C	359	PRO	O-C-N	-5.63	110.40	121.10
2	B	273	ALA	N-CA-C	5.63	126.19	111.00
2	B	210	TYR	CG-CD2-CE2	5.62	125.80	121.30
3	C	94	PHE	CD1-CE1-CZ	-5.62	113.35	120.10
2	B	399	TYR	CB-CG-CD1	-5.59	117.64	121.00
2	B	61	HIS	N-CA-CB	5.54	120.57	110.60
1	A	3369	TYR	CB-CG-CD1	5.54	124.32	121.00
2	B	83	TYR	N-CA-CB	5.53	120.55	110.60
3	C	43	GLN	CA-C-N	-5.52	105.05	117.20
2	B	418	PHE	CB-CG-CD2	-5.51	116.94	120.80
3	C	47	GLU	CA-C-N	5.51	129.32	117.20
3	C	294	GLN	CG-CD-OE1	5.48	132.55	121.60
3	C	122	VAL	O-C-N	-5.46	113.95	122.70
3	C	302	MET	CG-SD-CE	-5.46	91.47	100.20
2	B	194	THR	O-C-N	-5.40	114.06	122.70
2	B	68	VAL	CG1-CB-CG2	-5.39	102.27	110.90
3	C	156	LYS	O-C-N	-5.38	114.09	122.70
2	B	406	HIS	CA-CB-CG	5.38	122.75	113.60
3	C	191	VAL	CG1-CB-CG2	-5.36	102.32	110.90
3	C	404	PHE	CB-CG-CD1	5.35	124.55	120.80
3	C	2	ARG	NE-CZ-NH1	5.33	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	278	ARG	NE-CZ-NH2	5.31	122.95	120.30
2	B	139	HIS	C-N-CA	5.29	134.94	121.70
3	C	357	ASP	CB-CG-OD2	-5.29	113.54	118.30
3	C	116	ASP	CB-CG-OD1	-5.28	113.55	118.30
3	C	437	ASP	CA-C-O	-5.28	109.02	120.10
2	B	23	LEU	CB-CA-C	5.27	120.21	110.20
2	B	439	SER	CA-C-O	-5.27	109.04	120.10
1	A	3369	TYR	CG-CD2-CE2	-5.26	117.09	121.30
3	C	296	PHE	CB-CG-CD1	5.25	124.48	120.80
3	C	175	PRO	C-N-CA	5.25	134.82	121.70
2	B	272	TYR	CB-CG-CD1	5.24	124.15	121.00
2	B	52	PHE	CB-CG-CD1	-5.24	117.13	120.80
2	B	112	LYS	O-C-N	-5.24	114.32	122.70
2	B	351	PHE	CB-CG-CD1	-5.22	117.15	120.80
2	B	244	PHE	CB-CA-C	-5.21	99.97	110.40
1	A	3281	ASP	CB-CG-OD1	5.21	122.98	118.30
2	B	362	VAL	CA-CB-CG1	5.19	118.69	110.90
3	C	350	ASN	N-CA-CB	-5.19	101.26	110.60
3	C	383	ALA	O-C-N	-5.19	114.40	122.70
2	B	105	ARG	CG-CD-NE	-5.19	100.91	111.80
3	C	359	PRO	N-CD-CG	5.15	110.93	103.20
3	C	49	ILE	CA-CB-CG1	5.14	120.78	111.00
2	B	382	THR	CA-CB-CG2	-5.13	105.22	112.40
3	C	176	LYS	CG-CD-CE	5.13	127.30	111.90
2	B	46	ASP	CB-CG-OD1	5.13	122.92	118.30
2	B	384	ILE	N-CA-CB	5.13	122.59	110.80
2	B	390	ARG	NE-CZ-NH2	5.12	122.86	120.30
3	C	320	ARG	O-C-N	-5.12	114.49	123.20
2	B	86	LEU	CB-CG-CD1	5.12	119.71	111.00
1	A	3375	TYR	CB-CG-CD1	-5.11	117.94	121.00
3	C	157	ILE	O-C-N	-5.10	114.55	122.70
2	B	418	PHE	CB-CG-CD1	5.09	124.37	120.80
2	B	435	VAL	CG1-CB-CG2	-5.09	102.75	110.90
3	C	269	MET	CG-SD-CE	-5.09	92.06	100.20
2	B	51	THR	CA-CB-OG1	5.08	119.67	109.00
2	B	141	PHE	CB-CG-CD1	-5.08	117.25	120.80
3	C	390	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	3369	TYR	CB-CG-CD2	-5.07	117.96	121.00
2	B	282	TYR	CG-CD2-CE2	-5.06	117.25	121.30
1	A	3377	TYR	CG-CD1-CE1	-5.06	117.25	121.30
2	B	229	ARG	CD-NE-CZ	5.06	130.68	123.60
3	C	432	TYR	CB-CG-CD2	5.06	124.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	THR	O-C-N	-5.05	114.62	122.70
3	C	53	TYR	CG-CD2-CE2	-5.04	117.27	121.30
3	C	52	TYR	O-C-N	-5.04	114.64	122.70
1	A	3359	ASP	CB-CG-OD1	5.03	122.83	118.30
3	C	273	ALA	O-C-N	-5.03	111.55	121.10
2	B	391	LEU	N-CA-CB	5.03	120.45	110.40
1	A	3314	ALA	CB-CA-C	5.01	117.62	110.10
2	B	278	ALA	CB-CA-C	5.01	117.62	110.10
2	B	14	VAL	O-C-N	-5.01	114.68	122.70
2	B	76	ASP	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3342	ARG	Sidechain
1	A	3362	ARG	Sidechain
1	A	3369	TYR	Sidechain
1	A	3400	TYR	Sidechain
1	A	3406	ARG	Sidechain
1	A	3411	ARG	Sidechain
2	B	103	TYR	Sidechain
2	B	105	ARG	Sidechain
2	B	161	TYR	Sidechain
2	B	210	TYR	Sidechain
2	B	214	ARG	Sidechain
2	B	221	ARG	Sidechain
2	B	224	TYR	Sidechain
2	B	24	TYR	Sidechain
2	B	243	ARG	Sidechain
2	B	272	TYR	Sidechain
2	B	28	HIS	Sidechain
2	B	308	ARG	Sidechain
2	B	343	PHE	Sidechain
2	B	373	ARG	Sidechain
2	B	390	ARG	Sidechain
2	B	432	TYR	Sidechain
2	B	64	ARG	Sidechain
2	B	79	ARG	Sidechain
2	B	83	TYR	Sidechain
2	B	98	ASP	Peptide
3	C	123	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	158	ARG	Sidechain
3	C	161	TYR	Sidechain
3	C	185	TYR	Sidechain
3	C	263	PRO	Peptide
3	C	267	PHE	Sidechain
3	C	273	ALA	Peptide
3	C	283	TYR	Sidechain
3	C	36	TYR	Sidechain
3	C	369	ARG	Sidechain
3	C	37	HIS	Sidechain
3	C	400	ARG	Sidechain
3	C	432	TYR	Sidechain
3	C	435	TYR	Sidechain
3	C	52	TYR	Sidechain
3	C	53	TYR	Sidechain
3	C	79	ARG	Sidechain
3	C	88	ARG	Sidechain

## 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	1306	0	1342	2	0
2	B	3423	0	3324	9	0
3	C	3360	0	3241	11	0
All	All	8089	0	7907	21	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 1.

All (21) 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:B:5:ILE:HG12	2:B:125:LEU:HD21	1.83	0.59
3:C:313:LEU:HG	3:C:314:THR:H	1.69	0.57
2:B:5:ILE:CG1	2:B:125:LEU:HD21	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:273:ALA:HB3	3:C:274:PRO:HD3	1.87	0.55
2:B:61:HIS:HB3	2:B:85:GLN:O	2.07	0.54
3:C:107:HIS:CE1	3:C:193:GLN:OE1	2.64	0.51
2:B:259:LEU:O	2:B:266:HIS:CD2	2.68	0.47
2:B:5:ILE:HG12	2:B:125:LEU:CD2	2.46	0.45
2:B:61:HIS:CB	2:B:85:GLN:O	2.66	0.44
2:B:139:HIS:HA	2:B:140:SER:HB3	2.01	0.43
2:B:42:ILE:HG22	2:B:46:ASP:HA	2.01	0.43
1:A:3302:LEU:HD22	1:A:3340:ILE:HB	2.01	0.43
3:C:230:LEU:C	3:C:230:LEU:HD23	2.40	0.42
3:C:27:GLU:OE2	3:C:369:ARG:HB2	2.19	0.41
3:C:26:ASP:CG	3:C:369:ARG:HH21	2.24	0.41
3:C:413:MET:HG2	3:C:418:PHE:CZ	2.56	0.41
3:C:115:VAL:HG23	3:C:153:LEU:HD12	2.02	0.41
1:A:3413:GLU:O	1:A:3417:LEU:HB2	2.20	0.40
3:C:174:SER:HA	3:C:175:PRO:HD3	1.95	0.40
3:C:47:GLU:O	3:C:48:ARG:HB2	2.21	0.40
2:B:222:PRO:HB2	3:C:326:LYS:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	30	74
2	B	437/451 (97%)	379 (87%)	43 (10%)	15 (3%)	5	40
3	C	425/427 (100%)	378 (89%)	33 (8%)	14 (3%)	5	40
All	All	1024/1042 (98%)	913 (89%)	81 (8%)	30 (3%)	9	43

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	252	LEU
3	C	273	ALA
3	C	349	ASN
3	C	369	ARG
2	B	2	ARG
2	B	61	HIS
2	B	244	PHE
3	C	59	ASN
3	C	303	ALA
3	C	304	ALA
1	A	3327	GLY
2	B	37	PRO
2	B	44	GLY
2	B	99	ALA
2	B	140	SER
2	B	264	ARG
2	B	274	PRO
2	B	364	PRO
3	C	313	LEU
3	C	402	LYS
2	B	41	THR
3	C	176	LYS
2	B	59	GLY
2	B	306	ASP
3	C	311	ARG
2	B	286	LEU
2	B	43	GLY
3	C	66	ILE
3	C	38	GLY
3	C	222	PRO

### 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	146/146 (100%)	144 (99%)	2 (1%)	74	89
2	B	368/377 (98%)	356 (97%)	12 (3%)	45	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	368/368 (100%)	354 (96%)	14 (4%)	40	73
All	All	882/891 (99%)	854 (97%)	28 (3%)	50	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3268	VAL
1	A	3278	GLU
2	B	3	GLU
2	B	11	GLN
2	B	52	PHE
2	B	53	PHE
2	B	190	THR
2	B	210	TYR
2	B	220	GLU
2	B	306	ASP
2	B	367	ASP
2	B	373	ARG
2	B	386	GLU
2	B	422	ARG
3	C	60	LYS
3	C	62	VAL
3	C	86	ILE
3	C	91	ASN
3	C	149	MET
3	C	174	SER
3	C	175	PRO
3	C	251	ASP
3	C	260	VAL
3	C	275	LEU
3	C	286	LEU
3	C	369	ARG
3	C	395	PHE
3	C	435	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	85	GLN
2	B	216	ASN
2	B	266	HIS

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Mol	Chain	Res	Type
3	C	37	HIS
3	C	59	ASN
3	C	107	HIS
3	C	192	HIS
3	C	193	GLN
3	C	331	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](#)

There are no ligands in this entry.

### 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.