



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3J1T
EMDB ID: : EMD-5439
Title : High 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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

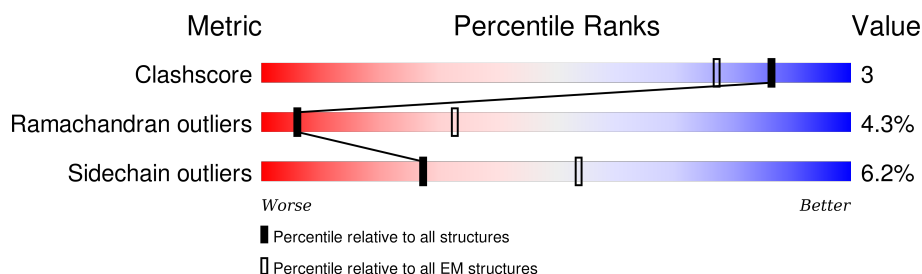
1 Overall quality at a glance

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 ≥ 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	
2	B	451	
3	C	427	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8091 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
			1308	820	227	252	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		

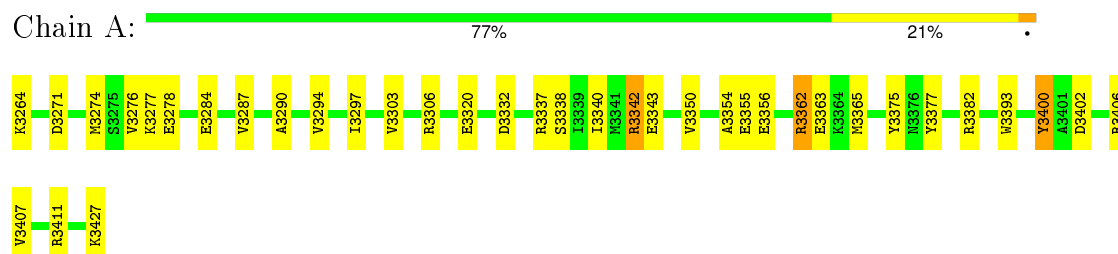
- Molecule 3 is a protein called Tubulin beta-2B chain.

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

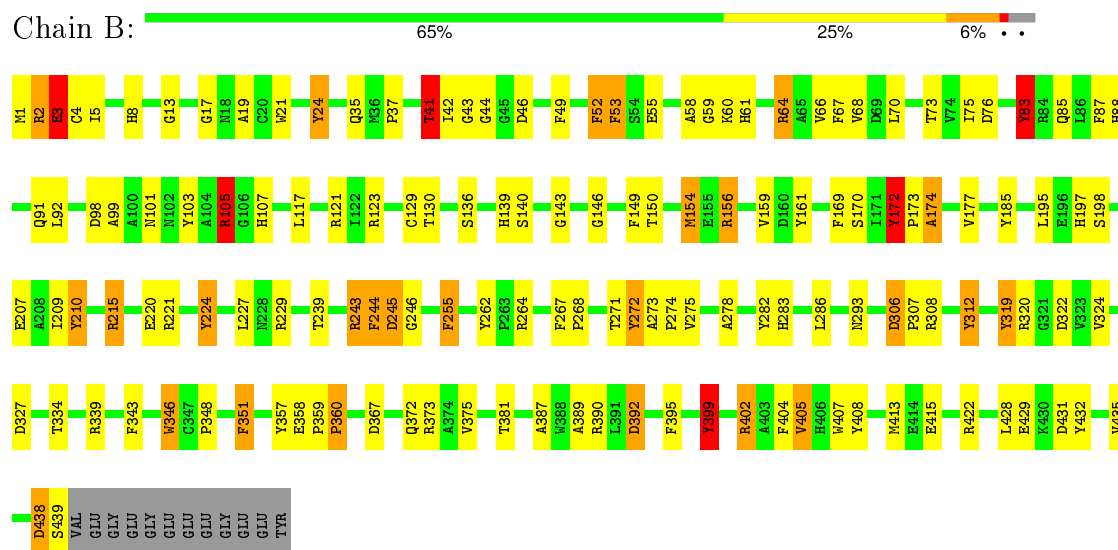
3 Residue-property plots

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.

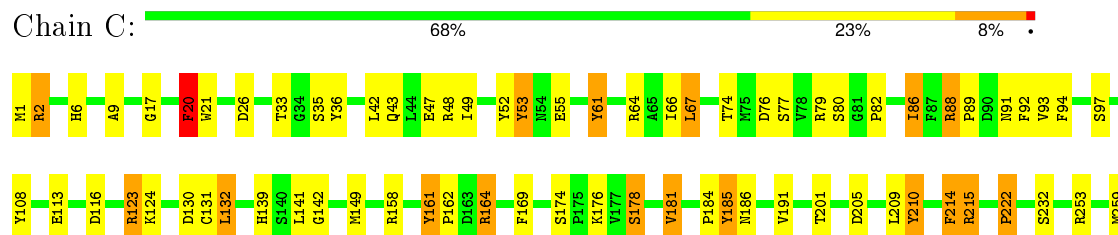
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1, seryl t-RNA synthetase chimera



- Molecule 2: Tubulin alpha-1B chain



- Molecule 3: Tubulin beta-2B chain





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	1.66	9/1325 (0.7%)	1.90	28/1783 (1.6%)
2	B	1.62	23/3501 (0.7%)	2.08	100/4752 (2.1%)
3	C	1.64	25/3435 (0.7%)	1.97	82/4652 (1.8%)
All	All	1.63	57/8261 (0.7%)	2.01	210/11187 (1.9%)

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	4
2	B	0	18
3	C	0	27
All	All	0	49

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3427	LYS	C-OXT	-12.07	1.00	1.23
3	C	437	ASP	C-OXT	-12.06	1.00	1.23
1	A	3427	LYS	C-O	-12.05	1.00	1.23
3	C	437	ASP	C-O	-12.05	1.00	1.23
2	B	439	SER	C-O	-12.02	1.00	1.23
3	C	185	TYR	CG-CD2	7.52	1.49	1.39
3	C	342	TYR	CB-CG	-7.47	1.40	1.51
3	C	340	SER	CA-CB	7.42	1.64	1.52
3	C	346	TRP	CD2-CE2	-7.34	1.32	1.41
1	A	3375	TYR	CG-CD1	7.12	1.48	1.39
3	C	418	PHE	CB-CG	6.85	1.62	1.51
2	B	245	ASP	CA-CB	6.41	1.68	1.53
2	B	24	TYR	CG-CD1	6.37	1.47	1.39
3	C	20	PHE	CE2-CZ	6.35	1.49	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	308	ARG	CD-NE	6.20	1.56	1.46
1	A	3320	GLU	CG-CD	6.18	1.61	1.51
3	C	21	TRP	CE3-CZ3	6.17	1.49	1.38
2	B	59	GLY	N-CA	6.15	1.55	1.46
3	C	131	CYS	CB-SG	6.15	1.92	1.82
2	B	88	HIS	C-N	-6.09	1.22	1.34
1	A	3284	GLU	CB-CG	5.84	1.63	1.52
2	B	136	SER	N-CA	-5.82	1.34	1.46
2	B	360	PRO	N-CA	5.76	1.57	1.47
3	C	35	SER	CA-CB	5.74	1.61	1.52
2	B	244	PHE	CG-CD2	5.73	1.47	1.38
1	A	3264	LYS	N-CA	5.68	1.57	1.46
1	A	3382	ARG	NE-CZ	5.68	1.40	1.33
3	C	232	SER	CA-CB	5.66	1.61	1.52
2	B	262	TYR	CE1-CZ	5.62	1.45	1.38
3	C	113	GLU	C-O	-5.62	1.12	1.23
2	B	136	SER	CA-CB	5.60	1.61	1.52
2	B	170	SER	CA-CB	5.58	1.61	1.52
2	B	339	ARG	CD-NE	5.50	1.55	1.46
3	C	289	PRO	N-CD	-5.48	1.40	1.47
3	C	161	TYR	CD1-CE1	5.47	1.47	1.39
3	C	215	ARG	CD-NE	5.46	1.55	1.46
2	B	13	GLY	N-CA	5.44	1.54	1.46
2	B	172	TYR	CG-CD2	5.42	1.46	1.39
3	C	253	ARG	CZ-NH1	-5.40	1.26	1.33
2	B	161	TYR	CZ-OH	5.40	1.47	1.37
3	C	61	TYR	CE1-CZ	5.39	1.45	1.38
3	C	388	PHE	CG-CD2	5.22	1.46	1.38
2	B	267	PHE	C-N	-5.22	1.24	1.34
3	C	108	TYR	CB-CG	-5.21	1.43	1.51
2	B	91	GLN	N-CA	-5.20	1.35	1.46
2	B	357	TYR	CE2-CZ	5.18	1.45	1.38
3	C	308	ARG	CD-NE	5.18	1.55	1.46
3	C	55	GLU	CB-CG	5.15	1.61	1.52
3	C	53	TYR	CE2-CZ	-5.15	1.31	1.38
2	B	44	GLY	N-CA	5.08	1.53	1.46
3	C	381	SER	CA-CB	5.07	1.60	1.52
2	B	3	GLU	CD-OE1	5.05	1.31	1.25
2	B	169	PHE	CG-CD1	5.04	1.46	1.38
1	A	3278	GLU	CG-CD	5.04	1.59	1.51
2	B	130	THR	C-N	5.03	1.42	1.33
3	C	26	ASP	N-CA	-5.01	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3377	TYR	CZ-OH	5.01	1.46	1.37

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	ARG	NE-CZ-NH2	-20.97	109.81	120.30
2	B	422	ARG	NE-CZ-NH1	18.36	129.48	120.30
2	B	2	ARG	NE-CZ-NH1	16.95	128.78	120.30
3	C	64	ARG	NE-CZ-NH1	15.31	127.95	120.30
3	C	214	PHE	CB-CG-CD1	-15.02	110.28	120.80
2	B	185	TYR	CB-CG-CD1	-13.64	112.81	121.00
2	B	322	ASP	CB-CG-OD2	13.36	130.32	118.30
2	B	83	TYR	CB-CG-CD1	-13.25	113.05	121.00
1	A	3375	TYR	CB-CG-CD2	13.14	128.89	121.00
2	B	121	ARG	NE-CZ-NH1	12.50	126.55	120.30
3	C	210	TYR	CB-CG-CD2	-12.47	113.52	121.00
1	A	3400	TYR	CB-CG-CD2	-11.70	113.98	121.00
2	B	123	ARG	NE-CZ-NH1	11.69	126.14	120.30
3	C	79	ARG	NE-CZ-NH2	-11.26	114.67	120.30
2	B	156	ARG	NE-CZ-NH2	-11.12	114.74	120.30
2	B	312	TYR	CB-CG-CD1	-10.90	114.46	121.00
2	B	21	TRP	CB-CG-CD2	-10.84	112.50	126.60
2	B	320	ARG	NE-CZ-NH2	-10.79	114.91	120.30
2	B	123	ARG	NE-CZ-NH2	-10.61	115.00	120.30
2	B	322	ASP	CB-CG-OD1	-10.49	108.86	118.30
2	B	320	ARG	NE-CZ-NH1	10.34	125.47	120.30
3	C	149	MET	CG-SD-CE	-10.14	83.97	100.20
2	B	221	ARG	NE-CZ-NH2	-10.09	115.26	120.30
3	C	400	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	A	3342	ARG	NE-CZ-NH1	9.79	125.19	120.30
2	B	185	TYR	CB-CG-CD2	9.71	126.83	121.00
2	B	24	TYR	CB-CG-CD2	-9.59	115.25	121.00
1	A	3362	ARG	NE-CZ-NH1	9.58	125.09	120.30
3	C	169	PHE	CB-CG-CD1	-9.51	114.15	120.80
3	C	398	MET	CG-SD-CE	-9.49	85.01	100.20
3	C	400	ARG	NE-CZ-NH1	9.47	125.03	120.30
2	B	408	TYR	CB-CG-CD1	9.39	126.63	121.00
3	C	312	TYR	CB-CG-CD2	-9.25	115.45	121.00
2	B	319	TYR	CB-CG-CD1	-9.13	115.52	121.00
2	B	83	TYR	CB-CG-CD2	9.11	126.47	121.00
2	B	306	ASP	CB-CG-OD1	9.04	126.44	118.30
2	B	408	TYR	CB-CG-CD2	-9.04	115.58	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	296	PHE	CB-CG-CD2	9.01	127.11	120.80
3	C	408	TYR	CB-CG-CD1	-8.96	115.63	121.00
2	B	308	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	3411	ARG	NE-CZ-NH2	8.91	124.76	120.30
3	C	88	ARG	NE-CZ-NH1	8.77	124.69	120.30
2	B	21	TRP	CB-CG-CD1	8.72	138.34	127.00
3	C	76	ASP	CB-CG-OD2	8.71	126.14	118.30
3	C	164	ARG	NE-CZ-NH1	8.61	124.61	120.30
3	C	390	ARG	NE-CZ-NH2	8.52	124.56	120.30
2	B	224	TYR	CB-CG-CD2	-8.47	115.92	121.00
2	B	255	PHE	CB-CG-CD1	8.43	126.70	120.80
1	A	3332	ASP	CB-CG-OD2	8.36	125.82	118.30
3	C	214	PHE	CB-CG-CD2	8.33	126.63	120.80
2	B	49	PHE	CB-CG-CD1	-8.31	114.98	120.80
3	C	67	LEU	CB-CG-CD1	8.15	124.86	111.00
3	C	158	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	B	215	ARG	NE-CZ-NH2	7.99	124.30	120.30
3	C	401	ARG	NE-CZ-NH1	7.93	124.27	120.30
2	B	390	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	B	105	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	B	49	PHE	CB-CG-CD2	7.71	126.20	120.80
1	A	3375	TYR	CG-CD2-CE2	7.62	127.40	121.30
3	C	210	TYR	CG-CD1-CE1	-7.56	115.25	121.30
2	B	432	TYR	CB-CG-CD1	7.56	125.53	121.00
3	C	264	ARG	NE-CZ-NH1	7.54	124.07	120.30
3	C	296	PHE	CB-CG-CD1	-7.48	115.56	120.80
3	C	323	MET	CG-SD-CE	-7.36	88.43	100.20
1	A	3406	ARG	NE-CZ-NH1	7.33	123.96	120.30
3	C	64	ARG	NH1-CZ-NH2	-7.24	111.43	119.40
2	B	407	TRP	CG-CD2-CE3	-7.21	127.41	133.90
1	A	3375	TYR	CB-CG-CD1	-7.19	116.69	121.00
2	B	339	ARG	NE-CZ-NH1	7.08	123.84	120.30
3	C	401	ARG	NE-CZ-NH2	-7.07	116.77	120.30
2	B	46	ASP	CB-CG-OD2	7.06	124.66	118.30
3	C	311	ARG	NE-CZ-NH1	7.05	123.83	120.30
3	C	93	VAL	O-C-N	-6.98	111.53	122.70
2	B	41	THR	N-CA-CB	6.96	123.53	110.30
2	B	431	ASP	CB-CG-OD1	6.96	124.56	118.30
3	C	178	SER	N-CA-CB	6.92	120.88	110.50
2	B	174	ALA	N-CA-CB	6.91	119.78	110.10
2	B	392	ASP	CB-CG-OD1	6.86	124.47	118.30
3	C	52	TYR	CG-CD1-CE1	-6.85	115.82	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3274	MET	CG-SD-CE	6.74	110.99	100.20
2	B	395	PHE	CB-CG-CD1	-6.71	116.10	120.80
3	C	390	ARG	NE-CZ-NH1	-6.71	116.94	120.30
2	B	395	PHE	CB-CG-CD2	6.69	125.48	120.80
1	A	3382	ARG	NE-CZ-NH1	6.66	123.63	120.30
3	C	210	TYR	CB-CG-CD1	6.66	124.99	121.00
3	C	253	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	B	161	TYR	CB-CG-CD2	6.65	124.99	121.00
2	B	49	PHE	C-N-CA	6.59	138.19	121.70
3	C	141	LEU	N-CA-CB	6.53	123.45	110.40
1	A	3277	LYS	N-CA-CB	-6.51	98.88	110.60
2	B	405	VAL	CG1-CB-CG2	6.51	121.31	110.90
2	B	381	THR	CA-CB-CG2	-6.50	103.30	112.40
1	A	3402	ASP	CB-CG-OD1	-6.49	112.46	118.30
2	B	422	ARG	NH1-CZ-NH2	-6.46	112.29	119.40
2	B	149	PHE	CB-CG-CD1	-6.45	116.29	120.80
2	B	198	SER	N-CA-CB	6.43	120.14	110.50
2	B	387	ALA	N-CA-CB	-6.42	101.11	110.10
2	B	413	MET	CG-SD-CE	-6.41	89.94	100.20
3	C	408	TYR	CB-CG-CD2	6.38	124.83	121.00
1	A	3400	TYR	CB-CG-CD1	6.34	124.80	121.00
3	C	20	PHE	CB-CG-CD1	-6.33	116.37	120.80
2	B	83	TYR	CG-CD1-CE1	-6.29	116.27	121.30
3	C	21	TRP	CG-CD2-CE3	-6.27	128.26	133.90
3	C	303	ALA	N-CA-CB	6.27	118.87	110.10
3	C	164	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	B	53	PHE	CB-CG-CD2	6.21	125.15	120.80
2	B	407	TRP	CB-CG-CD1	6.21	135.07	127.00
3	C	431	GLU	O-C-N	-6.18	112.81	122.70
2	B	312	TYR	CB-CG-CD2	6.17	124.70	121.00
3	C	94	PHE	CB-CG-CD2	-6.17	116.48	120.80
2	B	229	ARG	NE-CZ-NH2	6.15	123.37	120.30
3	C	52	TYR	CB-CG-CD1	-6.14	117.32	121.00
2	B	262	TYR	CG-CD2-CE2	-6.13	116.39	121.30
2	B	392	ASP	N-CA-CB	-6.13	99.57	110.60
3	C	344	VAL	O-C-N	-6.12	112.91	122.70
2	B	399	TYR	CA-CB-CG	-6.10	101.81	113.40
2	B	64	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	3290	ALA	N-CA-CB	-6.02	101.68	110.10
3	C	277	SER	N-CA-CB	6.01	119.51	110.50
2	B	308	ARG	NH1-CZ-NH2	-6.00	112.80	119.40
2	B	67	PHE	CB-CG-CD1	6.00	125.00	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	318	VAL	O-C-N	-6.00	113.11	122.70
3	C	388	PHE	CZ-CE2-CD2	-5.97	112.94	120.10
1	A	3407	VAL	CG1-CB-CG2	-5.87	101.51	110.90
3	C	124	LYS	N-CA-CB	-5.87	100.04	110.60
3	C	414	ASP	N-CA-CB	5.83	121.09	110.60
2	B	272	TYR	CB-CG-CD1	5.78	124.47	121.00
3	C	176	LYS	CB-CA-C	5.72	121.83	110.40
3	C	181	VAL	CA-CB-CG1	5.71	119.46	110.90
3	C	36	TYR	CB-CG-CD2	-5.71	117.58	121.00
3	C	43	GLN	C-N-CA	5.71	135.97	121.70
2	B	221	ARG	NE-CZ-NH1	5.70	123.15	120.30
3	C	141	LEU	O-C-N	-5.70	113.51	123.20
3	C	185	TYR	CB-CG-CD2	5.69	124.41	121.00
2	B	121	ARG	NH1-CZ-NH2	-5.67	113.16	119.40
1	A	3303	VAL	CA-CB-CG1	5.66	119.38	110.90
1	A	3362	ARG	NE-CZ-NH2	-5.65	117.48	120.30
3	C	319	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	A	3354	ALA	CB-CA-C	5.61	118.52	110.10
1	A	3400	TYR	CG-CD2-CE2	-5.61	116.81	121.30
2	B	243	ARG	CG-CD-NE	-5.61	100.01	111.80
3	C	262	PHE	CA-C-O	-5.61	108.32	120.10
2	B	293	ASN	N-CA-CB	-5.60	100.52	110.60
3	C	342	TYR	CB-CG-CD2	5.60	124.36	121.00
2	B	239	THR	O-C-N	-5.58	113.77	122.70
3	C	181	VAL	CB-CA-C	5.57	121.98	111.40
3	C	76	ASP	CB-CG-OD1	-5.55	113.30	118.30
3	C	320	ARG	NE-CZ-NH1	5.55	123.08	120.30
3	C	289	PRO	N-CD-CG	5.52	111.49	103.20
2	B	66	VAL	CA-C-O	5.52	131.69	120.10
3	C	382	THR	O-C-N	-5.52	113.87	122.70
3	C	275	LEU	C-N-CA	5.47	135.38	121.70
3	C	77	SER	CB-CA-C	-5.45	99.74	110.10
2	B	185	TYR	CG-CD2-CE2	-5.45	116.94	121.30
2	B	399	TYR	CB-CG-CD1	-5.44	117.73	121.00
2	B	312	TYR	CG-CD1-CE1	-5.43	116.95	121.30
2	B	19	ALA	O-C-N	-5.43	114.01	122.70
1	A	3276	VAL	CB-CA-C	5.41	121.68	111.40
1	A	3271	ASP	CB-CG-OD1	5.40	123.16	118.30
2	B	172	TYR	CG-CD1-CE1	-5.38	117.00	121.30
2	B	87	PHE	CB-CG-CD2	5.37	124.56	120.80
2	B	244	PHE	C-N-CA	5.37	135.12	121.70
2	B	1	MET	CG-SD-CE	-5.36	91.63	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	149	PHE	CZ-CE2-CD2	-5.35	113.68	120.10
2	B	156	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	B	73	THR	O-C-N	-5.34	114.15	122.70
2	B	324	VAL	CA-CB-CG1	5.34	118.92	110.90
2	B	98	ASP	CB-CG-OD2	5.32	123.08	118.30
2	B	372	GLN	CB-CA-C	-5.31	99.78	110.40
2	B	215	ARG	O-C-N	-5.31	114.20	122.70
2	B	60	LYS	C-N-CA	5.31	134.97	121.70
3	C	191	VAL	CG1-CB-CG2	-5.31	102.41	110.90
2	B	76	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	327	ASP	CB-CG-OD2	5.31	123.08	118.30
3	C	268	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	3274	MET	CA-CB-CG	5.29	122.30	113.30
2	B	439	SER	CA-C-O	-5.28	109.00	120.10
3	C	61	TYR	CD1-CE1-CZ	-5.28	115.05	119.80
3	C	437	ASP	CA-C-O	-5.28	109.02	120.10
3	C	205	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	3427	LYS	CA-C-O	-5.27	109.02	120.10
3	C	369	ARG	N-CA-C	5.27	125.24	111.00
3	C	273	ALA	CA-C-N	5.26	131.82	117.10
3	C	214	PHE	CG-CD2-CE2	-5.25	115.02	120.80
3	C	132	LEU	C-N-CA	-5.21	108.66	121.70
2	B	224	TYR	CB-CG-CD1	5.20	124.12	121.00
3	C	123	ARG	NE-CZ-NH1	-5.19	117.71	120.30
2	B	210	TYR	CB-CG-CD2	-5.18	117.89	121.00
2	B	392	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	3306	ARG	NE-CZ-NH2	-5.17	117.72	120.30
2	B	359	PRO	CA-C-N	5.16	131.54	117.10
2	B	435	VAL	O-C-N	-5.15	114.44	123.20
3	C	283	TYR	CG-CD2-CE2	-5.15	117.18	121.30
2	B	68	VAL	CA-CB-CG2	-5.14	103.19	110.90
3	C	283	TYR	CZ-CE2-CD2	5.14	124.43	119.80
2	B	24	TYR	CG-CD1-CE1	-5.13	117.20	121.30
2	B	262	TYR	CZ-CE2-CD2	5.12	124.41	119.80
3	C	319	PHE	CD1-CE1-CZ	-5.12	113.96	120.10
1	A	3350	VAL	CA-CB-CG2	-5.10	103.25	110.90
3	C	33	THR	CA-CB-CG2	-5.10	105.26	112.40
2	B	64	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	B	351	PHE	CB-CG-CD2	-5.08	117.25	120.80
3	C	312	TYR	C-N-CA	5.07	134.37	121.70
2	B	271	THR	O-C-N	-5.06	114.60	122.70
3	C	313	LEU	CB-CG-CD2	-5.06	102.40	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	ARG	NE-CZ-NH2	5.04	122.82	120.30
3	C	116	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	A	3340	ILE	CA-CB-CG2	5.01	120.91	110.90
1	A	3402	ASP	CB-CG-OD2	5.00	122.80	118.30
2	B	121	ARG	CG-CD-NE	-5.00	101.30	111.80

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3337	ARG	Sidechain
1	A	3342	ARG	Sidechain
1	A	3356	GLU	Peptide
1	A	3362	ARG	Sidechain
2	B	103	TYR	Sidechain
2	B	105	ARG	Sidechain
2	B	107	HIS	Sidechain
2	B	156	ARG	Sidechain
2	B	172	TYR	Sidechain
2	B	210	TYR	Sidechain
2	B	215	ARG	Sidechain
2	B	220	GLU	Mainchain
2	B	24	TYR	Sidechain
2	B	255	PHE	Sidechain
2	B	272	TYR	Sidechain
2	B	312	TYR	Sidechain
2	B	343	PHE	Sidechain
2	B	399	TYR	Sidechain
2	B	402	ARG	Sidechain
2	B	52	PHE	Sidechain
2	B	64	ARG	Sidechain
2	B	83	TYR	Sidechain
3	C	123	ARG	Sidechain
3	C	161	TYR	Sidechain
3	C	164	ARG	Sidechain
3	C	2	ARG	Sidechain
3	C	20	PHE	Sidechain
3	C	215	ARG	Sidechain
3	C	274	PRO	Peptide
3	C	277	SER	Peptide
3	C	278	ARG	Sidechain
3	C	284	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	309	HIS	Sidechain
3	C	319	PHE	Sidechain
3	C	322	ARG	Sidechain
3	C	342	TYR	Sidechain
3	C	359	PRO	Mainchain,Peptide
3	C	377	PHE	Sidechain
3	C	398	MET	Peptide
3	C	399	PHE	Sidechain
3	C	406	HIS	Sidechain
3	C	418	PHE	Sidechain
3	C	432	TYR	Sidechain
3	C	435	TYR	Sidechain
3	C	48	ARG	Sidechain
3	C	53	TYR	Peptide
3	C	61	TYR	Sidechain
3	C	80	SER	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	A	1308	0	1342	3	0
2	B	3423	0	3324	24	0
3	C	3360	0	3241	16	0
All	All	8091	0	7907	42	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 3.

All (42) 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)
3:C:259:MET:HB3	3:C:268:PHE:CZ	2.27	0.69
3:C:6:HIS:HE1	3:C:17:GLY:HA2	1.65	0.60
1:A:3338:SER:HB2	3:C:162:PRO:HG3	1.88	0.55
3:C:6:HIS:CE1	3:C:17:GLY:HA2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:ILE:H	3:C:86:ILE:HD13	1.73	0.54
2:B:61:HIS:HB3	2:B:85:GLN:O	2.08	0.54
3:C:306:ASP:O	3:C:309:HIS:CE1	2.60	0.54
1:A:3287:VAL:HG21	1:A:3400:TYR:CD1	2.43	0.52
2:B:139:HIS:CE1	2:B:150:THR:HG23	2.47	0.49
2:B:346:TRP:CH2	2:B:438:ASP:HA	2.47	0.49
3:C:42:LEU:HA	3:C:47:GLU:O	2.13	0.48
2:B:75:ILE:HD12	2:B:92:LEU:HB3	1.96	0.48
2:B:273:ALA:HB2	2:B:375:VAL:HG13	1.96	0.47
2:B:139:HIS:HE1	2:B:150:THR:HG23	1.80	0.47
2:B:139:HIS:CE1	2:B:150:THR:CG2	2.98	0.47
3:C:291:LEU:CD2	3:C:375:ALA:HB3	2.45	0.47
2:B:173:PRO:HB3	2:B:207:GLU:HG2	1.98	0.46
3:C:9:ALA:HB3	3:C:139:HIS:HA	1.98	0.46
2:B:2:ARG:HD2	2:B:55:GLU:HB2	1.98	0.45
2:B:243:ARG:HG3	2:B:244:PHE:H	1.82	0.45
1:A:3294:VAL:HG11	1:A:3393:TRP:CE2	2.53	0.44
2:B:195:LEU:HD21	2:B:428:LEU:HD22	1.99	0.43
2:B:154:MET:SD	2:B:197:HIS:HB2	2.58	0.43
2:B:58:ALA:O	2:B:61:HIS:HA	2.17	0.43
3:C:210:TYR:CD1	3:C:222:PRO:HB2	2.53	0.43
2:B:346:TRP:CZ3	2:B:438:ASP:HA	2.54	0.43
3:C:292:THR:HB	3:C:335:VAL:HG11	2.01	0.42
3:C:67:LEU:HD23	3:C:92:PHE:CE2	2.54	0.42
3:C:210:TYR:HB3	3:C:214:PHE:CZ	2.55	0.42
2:B:389:ALA:HB2	2:B:429:GLU:HG3	2.02	0.42
2:B:273:ALA:HB2	2:B:375:VAL:CG1	2.51	0.41
2:B:70:LEU:HD12	2:B:70:LEU:C	2.40	0.41
2:B:319:TYR:HB3	2:B:373:ARG:HH12	1.84	0.41
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.82	0.41
2:B:8:HIS:CE1	2:B:17:GLY:HA3	2.55	0.41
2:B:101:ASN:HD22	2:B:143:GLY:HA2	1.86	0.41
2:B:278:ALA:HB1	2:B:283:HIS:CD2	2.56	0.41
3:C:371:LEU:HD13	3:C:374:SER:HB2	2.03	0.41
2:B:174:ALA:HB3	2:B:177:VAL:HG21	2.02	0.41
2:B:172:TYR:HA	2:B:173:PRO:HD2	1.91	0.41
3:C:1:MET:CE	3:C:47:GLU:HA	2.50	0.40
3:C:344:VAL:HG22	3:C:346:TRP:CD2	2.57	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	A	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
2	B	437/451 (97%)	372 (85%)	42 (10%)	23 (5%)	2	29
3	C	425/427 (100%)	364 (86%)	40 (9%)	21 (5%)	3	31
All	All	1024/1042 (98%)	888 (87%)	92 (9%)	44 (4%)	6	34

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ALA
2	B	129	CYS
2	B	245	ASP
2	B	264	ARG
3	C	178	SER
3	C	304	ALA
3	C	344	VAL
3	C	369	ARG
2	B	4	CYS
2	B	5	ILE
2	B	282	TYR
3	C	66	ILE
3	C	97	SER
3	C	132	LEU
3	C	181	VAL
3	C	311	ARG
3	C	359	PRO
3	C	385	GLN
2	B	3	GLU
2	B	37	PRO
2	B	146	GLY
2	B	348	PRO
2	B	360	PRO
2	B	404	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	222	PRO
3	C	273	ALA
3	C	303	ALA
2	B	41	THR
2	B	246	GLY
2	B	274	PRO
2	B	286	LEU
2	B	35	GLN
2	B	268	PRO
2	B	275	VAL
3	C	174	SER
3	C	413	MET
3	C	340	SER
3	C	349	ASN
2	B	43	GLY
3	C	306	ASP
3	C	142	GLY
2	B	159	VAL
2	B	306	ASP
3	C	82	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%)	141 (97%)	5 (3%)	44	75
2	B	368/377 (98%)	344 (94%)	24 (6%)	21	58
3	C	368/368 (100%)	342 (93%)	26 (7%)	18	55
All	All	882/891 (99%)	827 (94%)	55 (6%)	27	60

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3297	ILE
1	A	3343	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3355	GLU
1	A	3363	GLU
1	A	3365	MET
2	B	3	GLU
2	B	41	THR
2	B	42	ILE
2	B	52	PHE
2	B	53	PHE
2	B	83	TYR
2	B	105	ARG
2	B	117	LEU
2	B	140	SER
2	B	154	MET
2	B	209	ILE
2	B	224	TYR
2	B	307	PRO
2	B	334	THR
2	B	346	TRP
2	B	351	PHE
2	B	358	GLU
2	B	367	ASP
2	B	392	ASP
2	B	399	TYR
2	B	402	ARG
2	B	405	VAL
2	B	415	GLU
2	B	438	ASP
3	C	20	PHE
3	C	49	ILE
3	C	74	THR
3	C	86	ILE
3	C	88	ARG
3	C	89	PRO
3	C	91	ASN
3	C	130	ASP
3	C	184	PRO
3	C	185	TYR
3	C	186	ASN
3	C	201	THR
3	C	209	LEU
3	C	275	LEU
3	C	292	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	336	GLN
3	C	346	TRP
3	C	356	CYS
3	C	359	PRO
3	C	369	ARG
3	C	396	THR
3	C	413	MET
3	C	416	MET
3	C	424	ASN
3	C	433	GLN
3	C	435	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	61	HIS
2	B	88	HIS
2	B	101	ASN
2	B	283	HIS
3	C	28	HIS
3	C	336	GLN
3	C	433	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.