



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:50 PM UTC

PDB ID : 7QJ1 / pdb_00007qj1
EMDB ID : EMD-14006
Title : Structure of the recombinant human gamma-Tubulin Ring Complex 6-spoked assembly intermediate (spokes 7-12, homogeneous dataset)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 7.00 Å (reported)
Based on initial models : 7AS4, 6X0U, 6V6S, 6L81

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

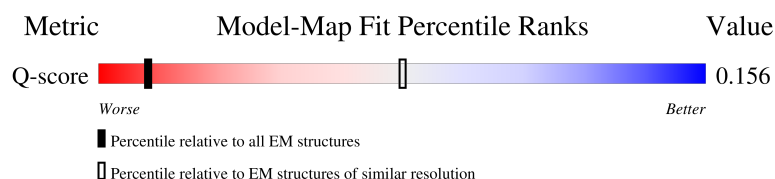
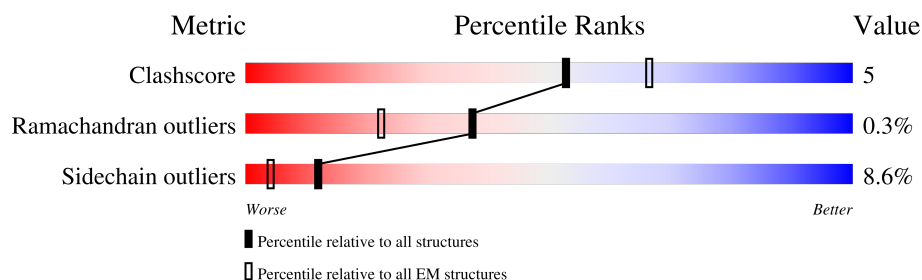
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 7.00 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.



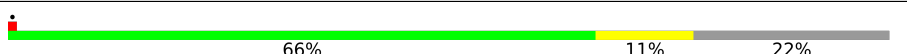
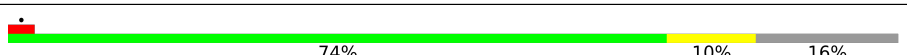
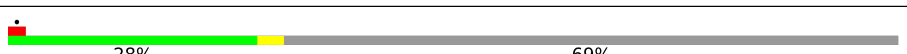
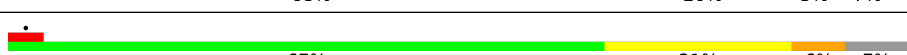
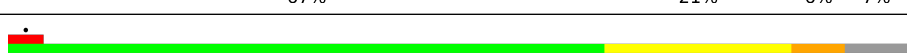
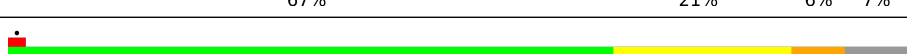
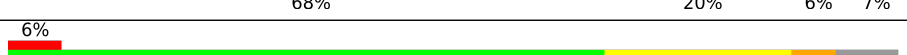
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	483 (6.50 - 7.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	J	1024	
1	l	1024	
2	b	82	
2	m	82	

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Mol	Chain	Length	Quality of chain
3	H	907	
3	a	907	
4	G	902	
5	I	667	
5	K	667	
6	L	1819	
7	U	451	
7	V	451	
7	W	451	
7	X	451	
7	Y	451	
7	Z	451	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 50899 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 Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	108	Total	C	N	O	S	0	0
			847	539	150	157	1		
1	J	534	Total	C	N	O	S	0	0
			4429	2893	737	776	23		

- Molecule 2 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
2	b	65	Total	C	N	O	S	0	0
			484	299	85	96	4		

- Molecule 3 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
3	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		

- Molecule 4 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	636	Total	C	N	O	S	0	0
			5186	3342	871	940	33		

- Molecule 5 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	521	Total	C	N	O	S	0	0
			4225	2737	720	750	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	562	Total	C	N	O	S	0	0
			4579	2964	781	816	18		

- Molecule 6 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	566	Total	C	N	O	S	0	0
			4587	3000	773	789	25		

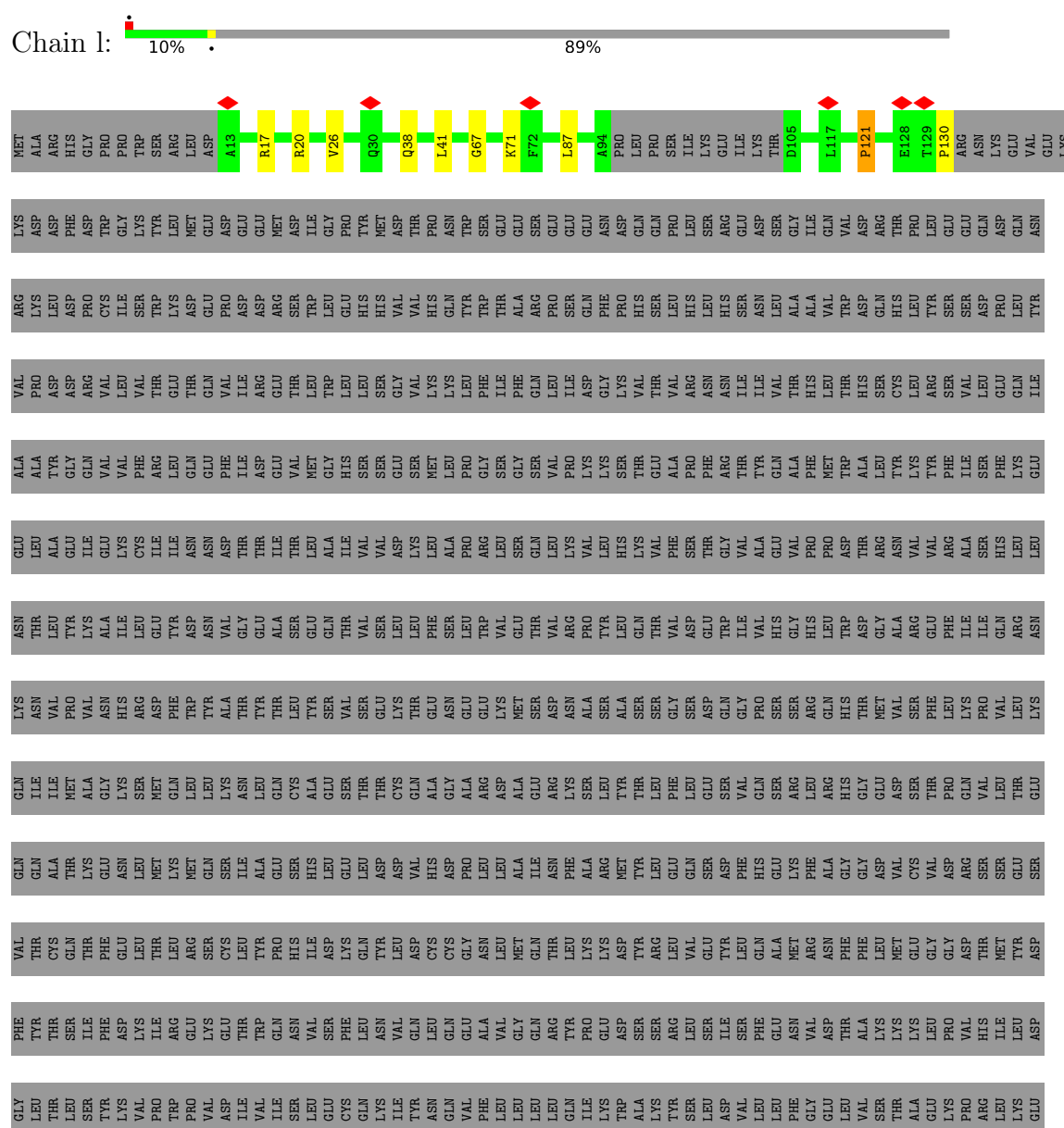
- Molecule 7 is a protein called Tubulin gamma-1 chain.

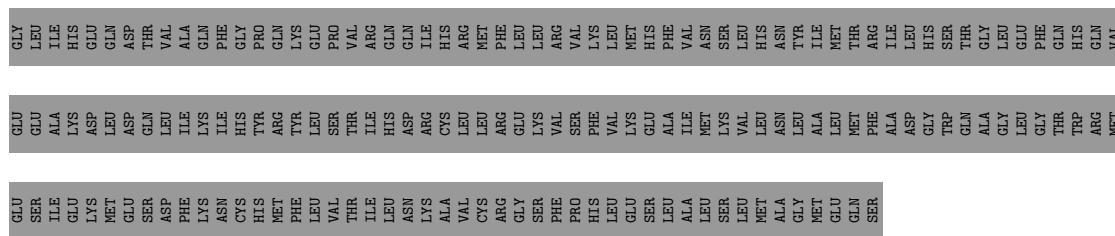
Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	V	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	W	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	X	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	Y	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	Z	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		

3 Residue-property plots

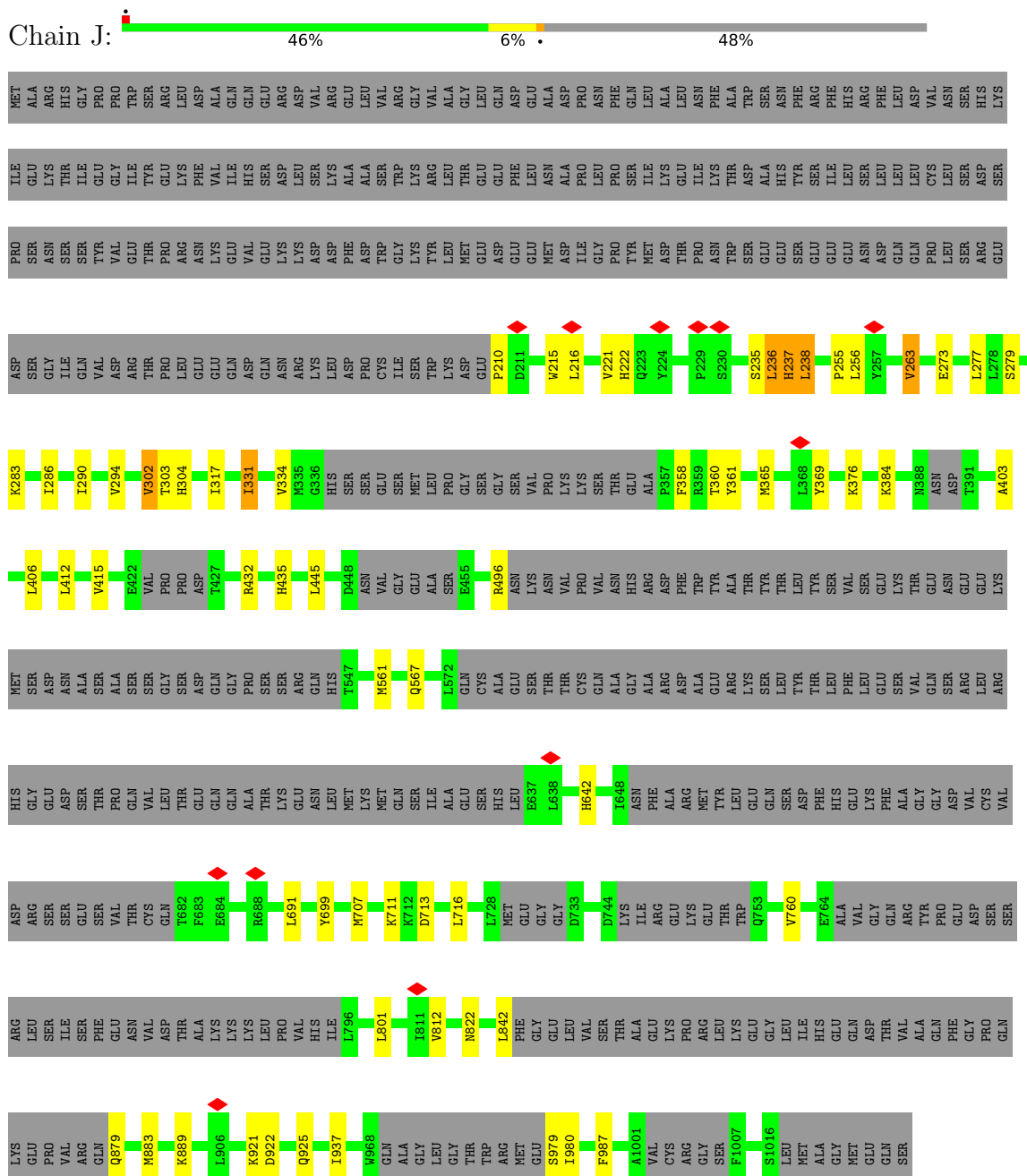
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Gamma-tubulin complex component 5





- Molecule 1: Gamma-tubulin complex component 5



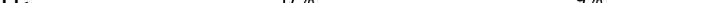
- Molecule 2: Mitotic-spindle organizing protein 1





THR	SER	SER	ASP	GLU	SER	LEU	ARG	PHE	LEU	SER	PHE	ARG	LEU	PHE	ASN	GLU	HIS	TYR	LYS	ALA	ARG	GLU	PRO	ARG	LEU	ARG	VAL	SER	LEU	GLY	THR	ARG	GLY	ARG	ARG	SER	SER	HIS	THR
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- Molecule 3: Gamma-tubulin complex component 3

Chain H:  57% 9% 35%

LEU PRO GLY GLN SER ASN GLN ALA GLA PRO PRO GLY GLY VAL ASP CYS LEU ARG ARG SER LEU GLN GLN LEU GLY ASP LEU LEU THR ALA ASN GLN PRO PRO SER SER SER GLN GLN THR THR THR THR LYS GLY VAL PRO SER SER ALA VAL SER ARG ASN MET THR THR ARG ARG GLU GLY ASP THR

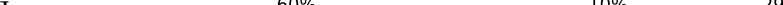
LEU	GLU	GLY	S361	L362	T363	L364	R365	R366	T380	Y403	G407	L421	L439	S450	V454	K455	Y464	V483	I486	P502	T503	T504	K505	NET	ILE	ALA	ALA	VAL	THR	LYS	SER	GLU	ALA	SER	PRO	PRO	GLN	ASP	ALA	ALA	ASP	LEU	PHE	T524	H558	R564	T570
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Year	Value	Category
1957	1578	Green
1958	1579	Green
1959	1580	Green
1960	1581	Green
1961	1582	Green
1962	1583	Green
1963	1584	Green
1964	1589	Green
1965	1592	Green
1966	1603	Green
1967	1608	Green
1968	1609	Green
1969	1610	Green
1970	1613	Orange
1971	1616	Green
1972	1621	Red
1973	1626	Green
1974	1632	Green
1975	1637	Green
1976	1642	Red
1977	1649	Red
1978	1681	Green
1979	1686	Green
1980	1689	Green
1981	1690	Green
1982	1691	Red
1983	1698	Green
1984	1702	Green
1985	1712	Green
1986	1715	Green
1987	1716	Green
1988	1717	Green
1989	1718	Green
1990	1730	Green
1991	1733	Green
1992	1737	Green

Year	Value	Category
Q7'40	1740	Green
L744	1744	Yellow
I747	1747	Yellow
R761	1761	Red
C762	1762	Red
L763	1763	Yellow
S768	1768	Yellow
L771	1771	Yellow
F779	1779	Yellow
I782	1782	Yellow
R811	1811	Green
GLN	1811	Grey
ARG	1811	Grey
GLU	1811	Grey
ILE	1811	Grey
GLU	1811	Grey
GLY	1811	Grey
GLN	1811	Grey
TRP	1811	Grey
GLY	1811	Grey
VAL	1811	Grey
THR	1811	Grey
ALA	1811	Grey
ALA	1811	Grey
GLU	1811	Grey
GLU	1811	Grey
ES27	1827	Green
R842	1842	Yellow
Q859	1859	Yellow
L862	1862	Yellow
L865	1865	Yellow
S869	1869	Yellow
L873	1873	Yellow
R879	1879	Red
L880	1880	Yellow
D881	1881	Yellow
F882	1882	Yellow
N883	1883	Yellow
E884	1884	Yellow
H885	1885	Yellow
Y886	1886	Red
K887	1887	Yellow
F890	1890	Green

PRO
ARG
LEU
ARG
VAL
SER
LEU
GLY
THR
ARG
GLY
ARG
ARG
SER
SER
HIS
THR

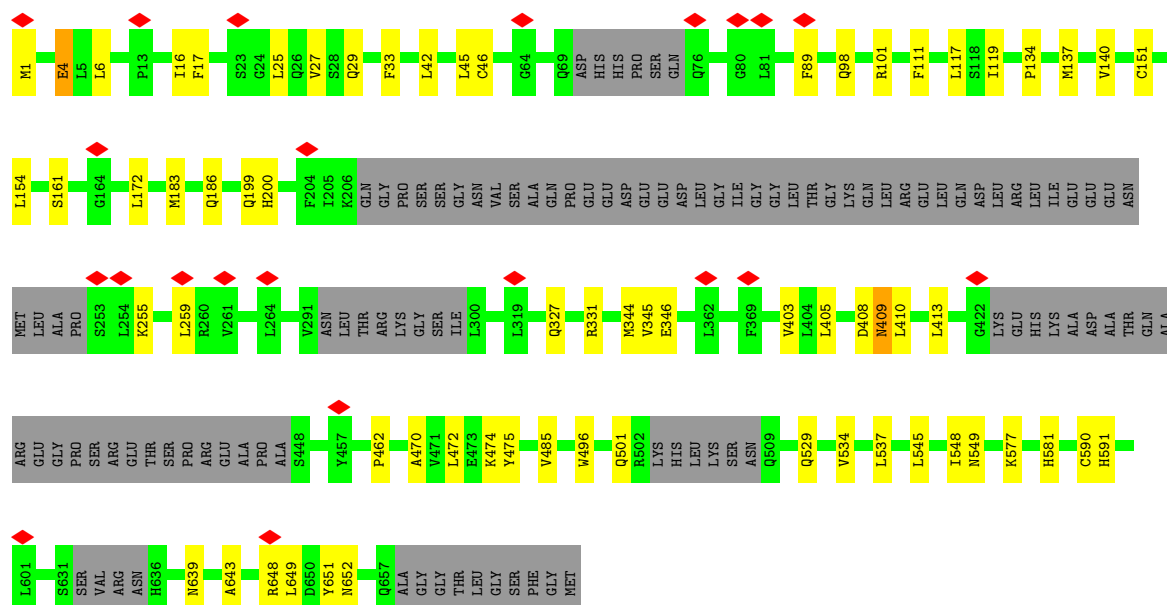
- Molecule 4: Gamma-tubulin complex component 2

Chain G: 

MET	GLU	GLU	PHE	ARG	ILE	HIS	HIS	HIS	ASP	VAL	ASN	GLU	LEU	LEU	LEU	LEU	ARG	VAL	HIS	GLY	GLY	ASP	GLY	ALA	GLU	GLU	TYR	ILE	ASP	LEU	LEU	GLN	LYS	ASN	ARG	THR	PRO	TYR	VAL	VAL	THR	THR	THR	VAL	SER	ALA	HIS	SER	ALA	LYS	VAL	VAL	LYS	ILE	ALA	ALA	GLU	PHE	ARG	ARG	THR	PRO
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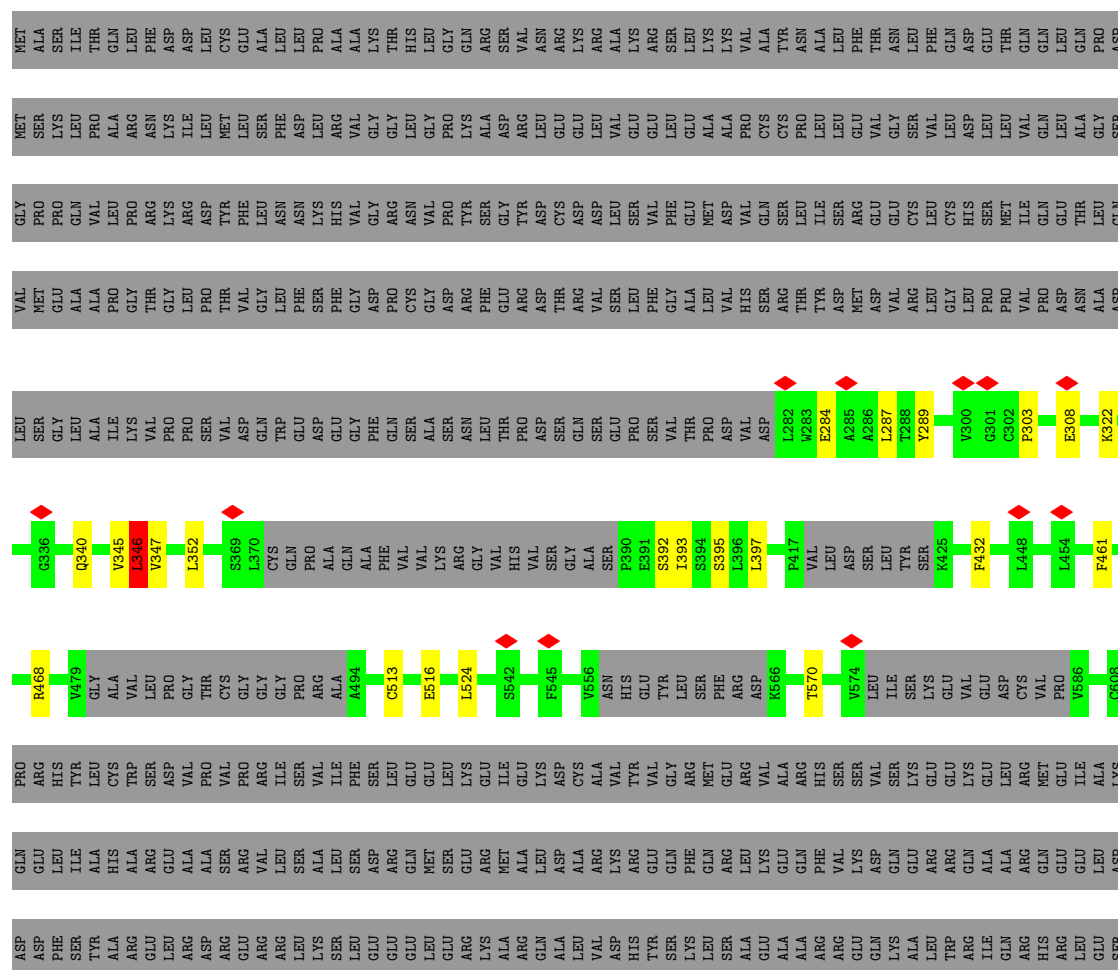
GLU	ASP	PHE	LEU	LYS	TYR	ASP	GLU	LEU	LYS	SER	LYS	ASN	THR	ARG	ASN	LEU	ASP	PRO	LEU	VAL	TYR	LEU	LEU	SER	LYS	LEU	THR	GLN	TYR	LEU	GLN	ASP	LYS	GLU	THR	ALA	ASN	ALA	LYS	GLU	ARG	ALA	ALA	VAL	GLY	SER	SER	THR	THR	SER	ILE
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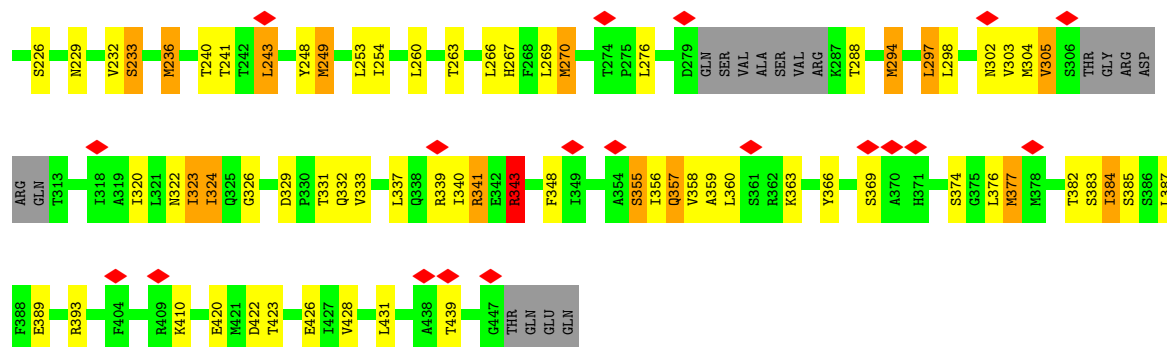
ASN	PRO	VAL	ALA	ALA	ALA	ALA	SER	LYS	SER	SER	SER	MET	GLN	GLU	LEU	GLU	GLU	GLU	LEU	ARG	LYS	GLN	LEU	GLY	SER	SER	VAL	ALA	THR	GLY	SER	THR	L150	R158	K164	Q165	N169	S170	H173	L174	F177	V181	Y182	P185	L188	G189	D190	F191	LEU	ILE	GLY	ALA	GLY	ILE
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• Molecule 6: Gamma-tubulin complex component 6

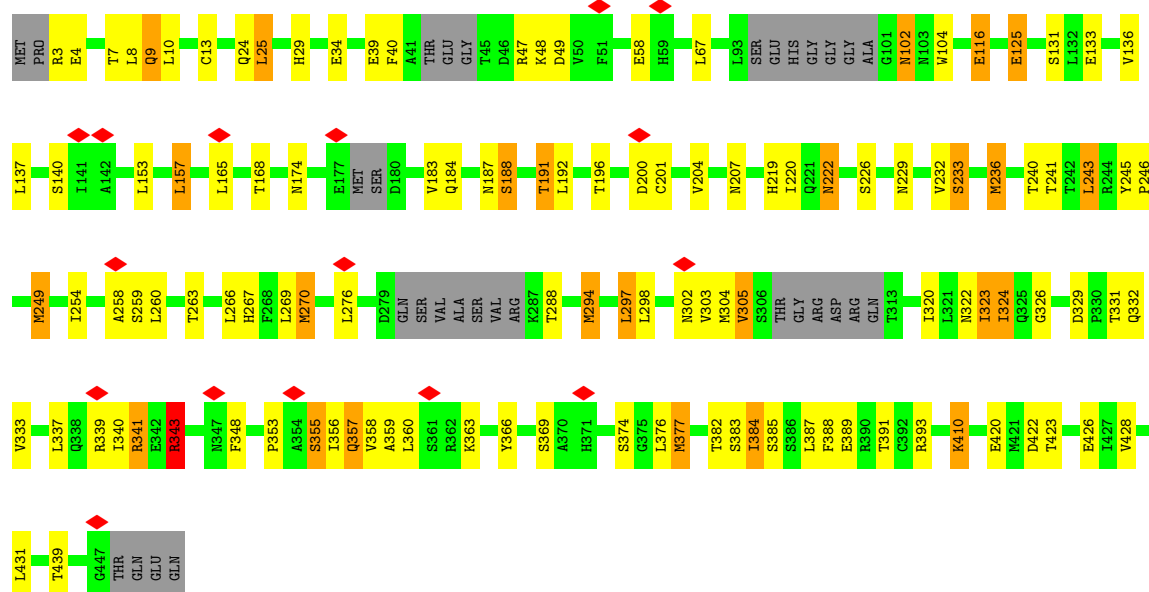
Chain L: 28% 69%





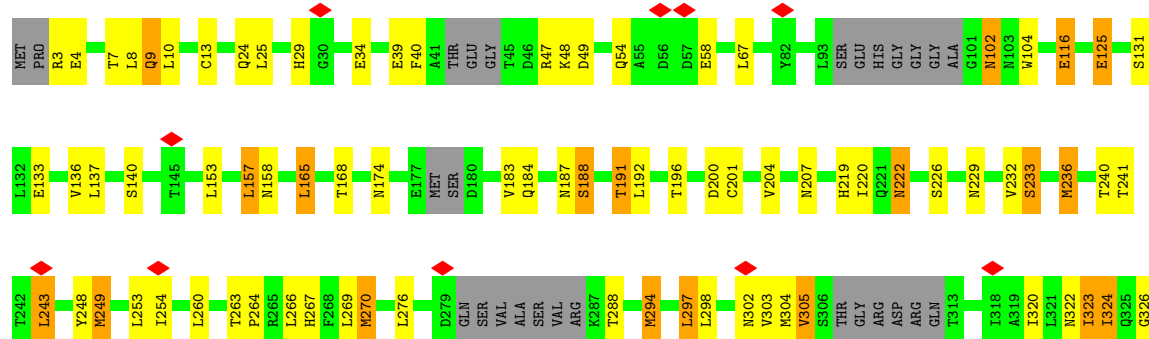
• Molecule 7: Tubulin gamma-1 chain

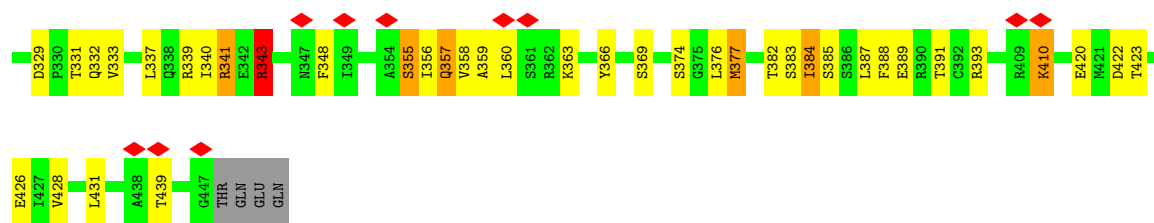
Chain V: 67% 21% 6% 7%



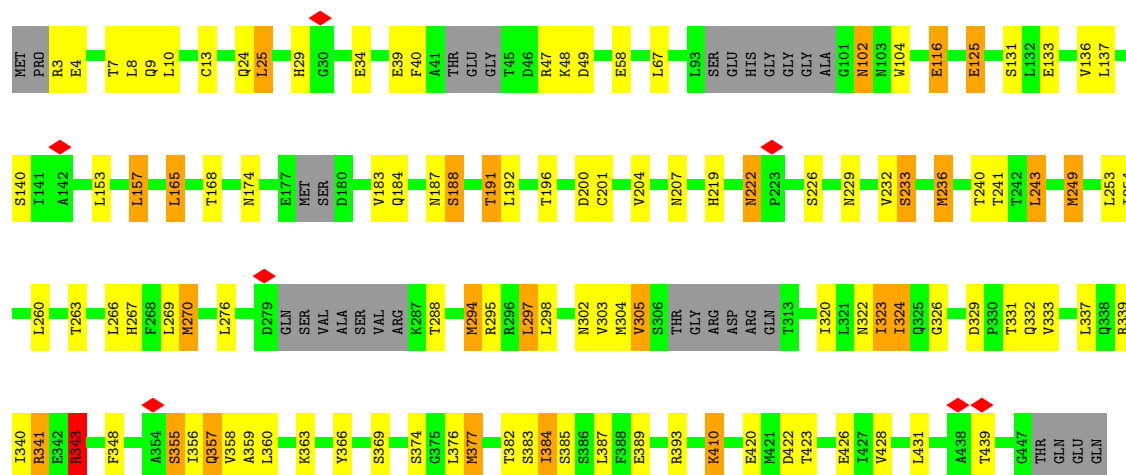
• Molecule 7: Tubulin gamma-1 chain

Chain W: 67% 21% 6% 7%

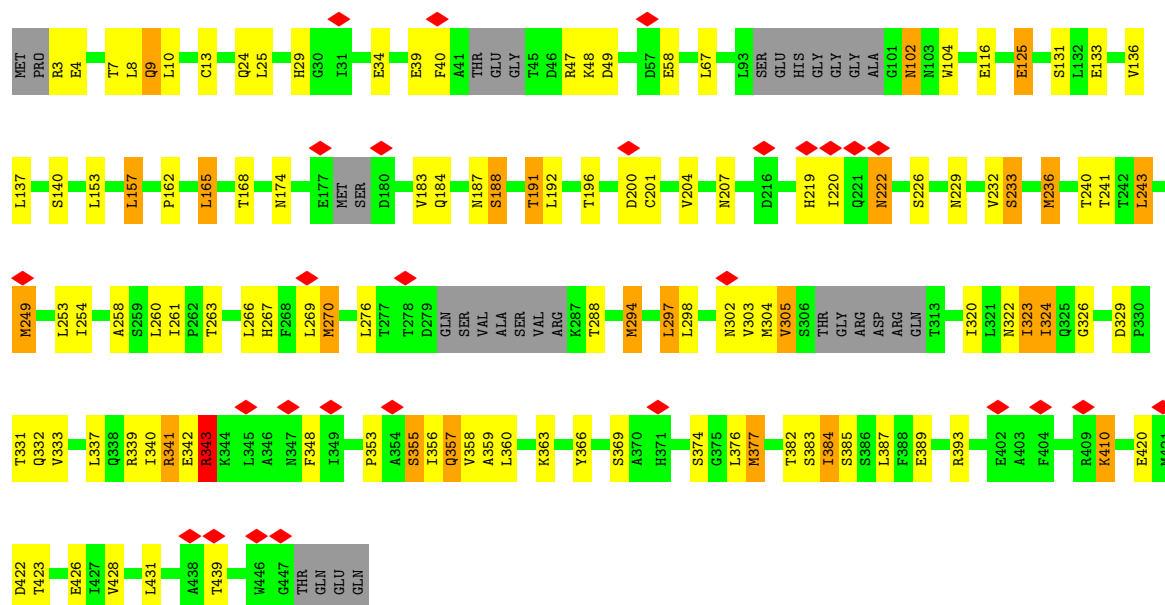




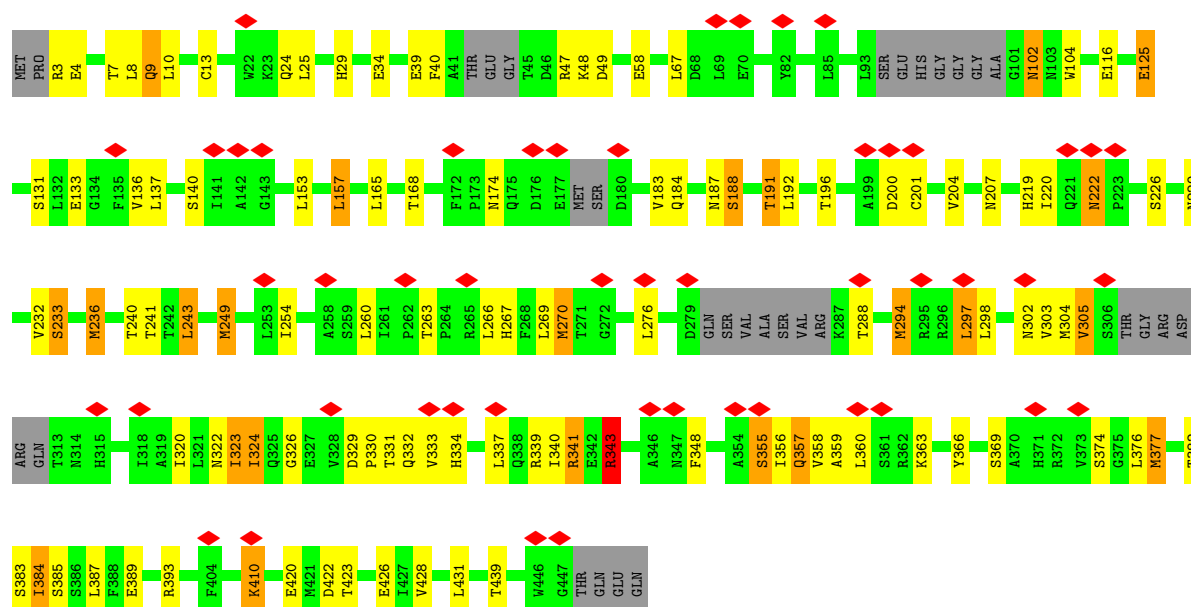
• Molecule 7: Tubulin gamma-1 chain



• Molecule 7: Tubulin gamma-1 chain



• Molecule 7: Tubulin gamma-1 chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59861	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.338	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0571	Depositor
Map size ($\text{\AA}$)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.66, 2.66, 2.66	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 > 5$	RMSZ	# $ Z > 5$
1	J	0.32	0/4525	0.77	10/6119 (0.2%)
1	l	0.30	0/863	0.75	2/1166 (0.2%)
2	b	0.40	0/484	0.97	0/653
2	m	0.40	0/484	0.97	0/653
3	H	0.32	0/5009	0.72	5/6761 (0.1%)
3	a	0.33	0/948	0.74	0/1277
4	G	0.32	0/5295	0.75	14/7147 (0.2%)
5	I	0.35	1/4322 (0.0%)	0.75	4/5853 (0.1%)
5	K	0.32	0/4683	0.67	0/6338
6	L	0.32	0/4697	0.72	6/6348 (0.1%)
7	U	0.28	0/3441	0.74	6/4661 (0.1%)
7	V	0.28	0/3441	0.74	6/4661 (0.1%)
7	W	0.28	0/3441	0.74	6/4661 (0.1%)
7	X	0.28	0/3441	0.74	6/4661 (0.1%)
7	Y	0.28	0/3441	0.74	6/4661 (0.1%)
7	Z	0.28	0/3441	0.74	6/4661 (0.1%)
All	All	0.31	1/51956 (0.0%)	0.74	77/70281 (0.1%)

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	J	0	7
3	H	0	1
4	G	0	2
5	I	0	4
5	K	0	2
6	L	0	1
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	361	TYR	CB-CG	-5.25	1.40	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	557	LEU	CB-CG-CD2	8.52	136.26	110.70
1	I	121	PRO	N-CA-CB	8.46	112.13	103.25
6	L	1787	VAL	N-CA-C	-7.96	105.73	113.53
1	J	237	HIS	CA-C-N	7.51	135.89	121.54
1	J	237	HIS	C-N-CA	7.51	135.89	121.54
7	X	343	ARG	NE-CZ-NH2	7.37	125.83	119.20
7	W	343	ARG	NE-CZ-NH2	7.37	125.83	119.20
7	V	343	ARG	NE-CZ-NH2	7.35	125.81	119.20
7	U	343	ARG	NE-CZ-NH2	7.33	125.80	119.20
7	Z	343	ARG	NE-CZ-NH2	7.33	125.80	119.20
7	Y	343	ARG	NE-CZ-NH2	7.32	125.78	119.20
4	G	557	LEU	CB-CG-CD1	-7.25	88.95	110.70
4	G	173	HIS	CA-C-N	6.97	130.38	120.49
4	G	173	HIS	C-N-CA	6.97	130.38	120.49
5	I	600	ASN	CA-C-N	6.79	134.51	121.54
5	I	600	ASN	C-N-CA	6.79	134.51	121.54
4	G	240	GLY	N-CA-C	-6.56	100.89	111.59
1	I	130	PRO	N-CA-CB	6.38	110.02	103.00
6	L	1689	ARG	N-CA-C	-6.17	106.98	114.75
7	Y	125	GLU	CA-CB-CG	6.08	126.26	114.10
7	V	125	GLU	CA-CB-CG	6.08	126.26	114.10
7	X	125	GLU	CA-CB-CG	6.07	126.24	114.10
7	W	125	GLU	CA-CB-CG	6.07	126.24	114.10
7	Z	125	GLU	CA-CB-CG	6.05	126.21	114.10
7	U	125	GLU	CA-CB-CG	6.05	126.20	114.10
1	J	238	LEU	N-CA-C	6.00	123.58	110.80
7	U	294	MET	CB-CG-SD	5.94	130.53	112.70
7	V	294	MET	CB-CG-SD	5.94	130.51	112.70
7	Z	294	MET	CB-CG-SD	5.93	130.50	112.70
7	W	294	MET	CB-CG-SD	5.93	130.49	112.70
7	X	294	MET	CB-CG-SD	5.92	130.47	112.70
7	Y	294	MET	CB-CG-SD	5.92	130.46	112.70
1	J	303	THR	N-CA-C	-5.92	105.64	114.64
1	J	255	PRO	CA-C-N	5.81	132.15	121.70
1	J	255	PRO	C-N-CA	5.81	132.15	121.70
6	L	1691	ARG	N-CA-C	-5.76	107.24	114.56
6	L	570	THR	N-CA-C	-5.72	105.23	114.09
5	I	132	LEU	CA-C-N	5.64	127.82	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	132	LEU	C-N-CA	5.64	127.82	120.26
6	L	340	GLN	N-CA-C	5.55	117.40	110.91
3	H	691	LEU	CA-CB-CG	5.54	135.69	116.30
6	L	345	VAL	CA-C-O	-5.53	115.23	121.75
4	G	557	LEU	CA-CB-CG	-5.46	97.19	116.30
4	G	613	LEU	N-CA-C	-5.42	106.54	114.39
4	G	240	GLY	CA-C-O	-5.41	115.42	121.21
7	Y	157	LEU	CA-CB-CG	5.38	135.15	116.30
7	X	157	LEU	CA-CB-CG	5.37	135.10	116.30
7	Z	157	LEU	CA-CB-CG	5.37	135.10	116.30
7	W	157	LEU	CA-CB-CG	5.37	135.09	116.30
7	U	157	LEU	CA-CB-CG	5.37	135.08	116.30
7	V	157	LEU	CA-CB-CG	5.37	135.08	116.30
4	G	240	GLY	CA-C-N	5.27	131.61	121.54
4	G	240	GLY	C-N-CA	5.27	131.61	121.54
7	X	343	ARG	NE-CZ-NH1	-5.25	116.25	121.50
7	Y	343	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	J	713	ASP	CA-C-N	5.21	131.49	121.54
1	J	713	ASP	C-N-CA	5.21	131.49	121.54
7	V	343	ARG	NE-CZ-NH1	-5.21	116.29	121.50
7	W	343	ARG	NE-CZ-NH1	-5.19	116.31	121.50
3	H	454	VAL	CA-C-N	5.18	131.44	121.54
3	H	454	VAL	C-N-CA	5.18	131.44	121.54
7	U	343	ARG	NE-CZ-NH1	-5.18	116.32	121.50
7	Z	343	ARG	NE-CZ-NH1	-5.17	116.33	121.50
3	H	613	ASP	CA-C-N	5.14	127.97	120.51
3	H	613	ASP	C-N-CA	5.14	127.97	120.51
4	G	401	HIS	CA-C-N	5.14	128.38	122.83
4	G	401	HIS	C-N-CA	5.14	128.38	122.83
4	G	419	ILE	CA-C-N	5.10	132.82	124.31
4	G	419	ILE	C-N-CA	5.10	132.82	124.31
7	U	343	ARG	CD-NE-CZ	5.07	131.50	124.40
7	Z	343	ARG	CD-NE-CZ	5.07	131.50	124.40
7	W	343	ARG	CD-NE-CZ	5.07	131.50	124.40
1	J	263	VAL	CA-C-N	5.06	131.21	121.54
1	J	263	VAL	C-N-CA	5.06	131.21	121.54
7	V	343	ARG	CD-NE-CZ	5.05	131.47	124.40
7	Y	343	ARG	CD-NE-CZ	5.05	131.47	124.40
7	X	343	ARG	CD-NE-CZ	5.02	131.43	124.40

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	240	GLY	Peptide
4	G	580	HIS	Peptide
3	H	454	VAL	Peptide
5	I	407	ASP	Peptide
5	I	503	LYS	Peptide
5	I	600	ASN	Peptide
5	I	601	LEU	Peptide
1	J	210	PRO	Peptide
1	J	221	VAL	Peptide
1	J	235	SER	Peptide
1	J	236	LEU	Mainchain
1	J	237	HIS	Peptide
1	J	256	LEU	Peptide
1	J	263	VAL	Peptide
5	K	408	ASP	Peptide
5	K	409	ASN	Mainchain
6	L	346	LEU	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	J	4429	0	4482	29	0
1	l	847	0	789	7	0
2	b	484	0	512	16	0
2	m	484	0	512	9	0
3	H	4907	0	4896	49	0
3	a	933	0	953	12	0
4	G	5186	0	5219	48	0
5	I	4225	0	4259	49	0
5	K	4579	0	4586	44	0
6	L	4587	0	4636	36	0
7	U	3373	0	3325	47	0
7	V	3373	0	3325	48	0
7	W	3373	0	3325	47	0
7	X	3373	0	3325	45	0
7	Y	3373	0	3325	49	0
7	Z	3373	0	3325	46	0
All	All	50899	0	50794	536	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 5.

All (536) 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)
5:I:527:ASN:O	5:I:530:TYR:HB3	1.70	0.91
5:K:4:GLU:OE1	5:K:17:PHE:CE1	2.27	0.87
1:I:71:LYS:HE3	3:H:626:LEU:HB3	1.64	0.79
6:L:284:GLU:HA	6:L:287:LEU:HG	1.64	0.79
5:K:4:GLU:CD	5:K:17:PHE:CE1	2.61	0.78
5:K:4:GLU:CD	5:K:17:PHE:HE1	1.92	0.77
5:K:4:GLU:OE1	5:K:17:PHE:HE1	1.70	0.74
5:I:412:PRO:HB3	5:I:455:LEU:HD11	1.76	0.66
7:W:54:GLN:O	7:X:295:ARG:NH2	2.25	0.65
5:K:4:GLU:OE1	5:K:17:PHE:CD1	2.49	0.65
2:b:22:ARG:HH11	6:L:287:LEU:HA	1.61	0.65
7:V:329:ASP:HB2	7:V:332:GLN:HE21	1.62	0.65
7:X:329:ASP:HB2	7:X:332:GLN:HE21	1.62	0.65
7:Z:329:ASP:HB2	7:Z:332:GLN:HE21	1.62	0.64
3:H:564:ARG:HH21	3:H:570:GLN:HG2	1.64	0.63
2:m:19:ASN:HA	2:m:22:ARG:HE	1.62	0.63
2:b:19:ASN:HA	2:b:22:ARG:HE	1.62	0.63
7:U:329:ASP:HB2	7:U:332:GLN:HE21	1.62	0.63
7:Y:329:ASP:HB2	7:Y:332:GLN:HE21	1.62	0.63
7:W:329:ASP:HB2	7:W:332:GLN:HE21	1.62	0.63
4:G:280:LYS:HB3	4:G:289:ASN:HD21	1.64	0.63
7:U:263:THR:HB	7:U:266:LEU:HG	1.81	0.63
7:V:263:THR:HB	7:V:266:LEU:HG	1.81	0.62
6:L:513:CYS:HG	6:L:1474:VAL:N	1.97	0.62
7:U:382:THR:O	7:U:385:SER:OG	2.18	0.62
7:V:382:THR:O	7:V:385:SER:OG	2.17	0.62
7:W:183:VAL:HG13	7:W:187:ASN:HD21	1.65	0.62
7:X:183:VAL:HG13	7:X:187:ASN:HD21	1.65	0.62
3:H:768:SER:O	3:H:771:LEU:HB2	1.99	0.62
7:W:382:THR:O	7:W:385:SER:OG	2.18	0.62
7:Y:263:THR:HB	7:Y:266:LEU:HG	1.81	0.62
4:G:741:ASN:HD22	4:G:839:ARG:HH21	1.48	0.62
7:W:323:ILE:HG13	7:W:359:ALA:HB3	1.81	0.62
7:X:263:THR:HB	7:X:266:LEU:HG	1.81	0.62
7:W:263:THR:HB	7:W:266:LEU:HG	1.81	0.62
7:Y:183:VAL:HG13	7:Y:187:ASN:HD21	1.65	0.62
7:Z:263:THR:HB	7:Z:266:LEU:HG	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:590:CYS:SG	5:K:591:HIS:N	2.72	0.62
7:V:183:VAL:HG13	7:V:187:ASN:HD21	1.65	0.62
7:Z:183:VAL:HG13	7:Z:187:ASN:HD21	1.65	0.62
7:U:323:ILE:HG13	7:U:359:ALA:HB3	1.81	0.62
7:X:201:CYS:HA	7:X:267:HIS:HB2	1.82	0.62
3:H:363:THR:HB	3:H:366:ARG:HE	1.63	0.61
7:Y:201:CYS:HA	7:Y:267:HIS:HB2	1.82	0.61
7:V:276:LEU:HD21	7:V:302:ASN:HA	1.82	0.61
2:b:49:ARG:HH21	6:L:284:GLU:HB2	1.64	0.61
7:Z:323:ILE:HG13	7:Z:359:ALA:HB3	1.81	0.61
7:X:276:LEU:HD21	7:X:302:ASN:HA	1.82	0.61
7:Y:382:THR:O	7:Y:385:SER:OG	2.18	0.61
7:Z:276:LEU:HD21	7:Z:302:ASN:HA	1.82	0.61
7:V:201:CYS:HA	7:V:267:HIS:HB2	1.82	0.61
7:V:323:ILE:HG13	7:V:359:ALA:HB3	1.81	0.61
7:W:276:LEU:HD21	7:W:302:ASN:HA	1.83	0.61
7:X:323:ILE:HG13	7:X:359:ALA:HB3	1.81	0.61
7:Z:196:THR:HG21	7:Z:431:LEU:HD11	1.83	0.61
7:Z:382:THR:O	7:Z:385:SER:OG	2.17	0.61
7:Y:276:LEU:HD21	7:Y:302:ASN:HA	1.82	0.61
7:U:183:VAL:HG13	7:U:187:ASN:HD21	1.65	0.60
7:Y:323:ILE:HG13	7:Y:359:ALA:HB3	1.81	0.60
4:G:254:LEU:HA	4:G:257:ARG:HD3	1.83	0.60
7:Y:196:THR:HG21	7:Y:431:LEU:HD11	1.83	0.60
5:I:530:TYR:OH	7:W:248:TYR:O	2.20	0.60
1:J:642:HIS:HD2	1:J:691:LEU:HD13	1.66	0.60
5:K:639:ASN:O	5:K:643:ALA:HB2	2.02	0.60
7:X:196:THR:HG21	7:X:431:LEU:HD11	1.83	0.60
7:U:276:LEU:HD21	7:U:302:ASN:HA	1.83	0.59
5:I:500:MET:O	5:I:504:HIS:ND1	2.32	0.59
7:V:355:SER:OG	7:V:356:ILE:N	2.35	0.59
3:H:862:LEU:HA	3:H:865:LEU:HD12	1.85	0.59
7:U:201:CYS:HA	7:U:267:HIS:HB2	1.82	0.59
7:X:382:THR:O	7:X:385:SER:OG	2.17	0.59
5:I:157:VAL:HB	5:I:172:LEU:HD21	1.84	0.59
7:Y:355:SER:OG	7:Y:356:ILE:N	2.35	0.59
5:I:361:TYR:CE2	5:I:475:TYR:HB3	2.38	0.59
6:L:468:ARG:NH1	6:L:516:GLU:OE2	2.33	0.59
6:L:1800:LEU:HD11	7:Z:341:ARG:HD3	1.84	0.59
7:W:196:THR:HG21	7:W:431:LEU:HD11	1.83	0.59
7:W:201:CYS:HA	7:W:267:HIS:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:249:ASP:O	4:G:257:ARG:NH1	2.34	0.59
7:V:187:ASN:O	7:V:191:THR:OG1	2.21	0.59
7:Z:201:CYS:HA	7:Z:267:HIS:HB2	1.82	0.59
7:W:187:ASN:O	7:W:191:THR:OG1	2.21	0.59
7:U:187:ASN:O	7:U:191:THR:OG1	2.21	0.59
7:Z:187:ASN:O	7:Z:191:THR:OG1	2.21	0.59
7:U:196:THR:HG21	7:U:431:LEU:HD11	1.83	0.58
7:V:196:THR:HG21	7:V:431:LEU:HD11	1.83	0.58
7:X:355:SER:OG	7:X:356:ILE:N	2.35	0.58
7:V:249:MET:SD	7:V:249:MET:N	2.77	0.58
4:G:293:ALA:HA	4:G:296:MET:HE2	1.85	0.58
7:U:249:MET:SD	7:U:249:MET:N	2.77	0.58
7:X:249:MET:SD	7:X:249:MET:N	2.77	0.58
5:I:471:VAL:HG21	5:I:561:HIS:HE1	1.69	0.57
7:Y:249:MET:SD	7:Y:249:MET:N	2.77	0.57
7:Y:102:ASN:OD1	7:Y:102:ASN:N	2.37	0.57
7:Y:187:ASN:O	7:Y:191:THR:OG1	2.21	0.57
1:J:331:ILE:HD11	1:J:369:TYR:HB2	1.86	0.57
7:W:249:MET:SD	7:W:249:MET:N	2.77	0.57
7:W:102:ASN:OD1	7:W:102:ASN:N	2.37	0.57
4:G:518:ARG:HA	4:G:523:ASP:HB3	1.86	0.57
3:H:558:HIS:HE1	3:H:616:GLU:HG3	1.68	0.57
7:Z:249:MET:SD	7:Z:249:MET:N	2.77	0.57
7:U:3:ARG:HB2	7:U:133:GLU:HB2	1.87	0.57
7:X:187:ASN:O	7:X:191:THR:OG1	2.21	0.57
1:J:922:ASP:HB3	1:J:925:GLN:HG2	1.86	0.57
7:U:102:ASN:N	7:U:102:ASN:OD1	2.37	0.57
7:V:102:ASN:OD1	7:V:102:ASN:N	2.37	0.57
7:X:326:GLY:HA2	7:X:363:LYS:HB2	1.87	0.57
7:V:3:ARG:HB2	7:V:133:GLU:HB2	1.87	0.57
7:V:339:ARG:HD2	7:V:343:ARG:HH12	1.70	0.57
4:G:555:LEU:HD21	4:G:573:LEU:HD22	1.87	0.56
6:L:1677:ALA:O	6:L:1682:HIS:ND1	2.38	0.56
7:U:355:SER:OG	7:U:356:ILE:N	2.35	0.56
7:Y:339:ARG:HD2	7:Y:343:ARG:HH12	1.70	0.56
7:W:326:GLY:HA2	7:W:363:LYS:HB2	1.87	0.56
7:W:355:SER:OG	7:W:356:ILE:N	2.35	0.56
7:Y:3:ARG:HB2	7:Y:133:GLU:HB2	1.87	0.56
7:Z:102:ASN:N	7:Z:102:ASN:OD1	2.37	0.56
1:l:26:VAL:HG11	2:m:64:ILE:HG23	1.87	0.56
5:K:161:SER:HB3	5:K:172:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:557:LEU:O	4:G:560:ARG:N	2.39	0.56
1:J:279:SER:HB2	1:J:376:LYS:HE3	1.88	0.56
7:Z:339:ARG:HD2	7:Z:343:ARG:HH12	1.70	0.56
7:Z:355:SER:OG	7:Z:356:ILE:N	2.35	0.56
5:I:357:ILE:O	5:I:361:TYR:CB	2.53	0.56
1:J:273:GLU:HG2	1:J:286:ILE:HD13	1.87	0.56
7:V:326:GLY:HA2	7:V:363:LYS:HB2	1.87	0.56
7:X:102:ASN:OD1	7:X:102:ASN:N	2.37	0.56
4:G:696:TYR:O	4:G:700:GLU:HB3	2.06	0.56
7:Z:326:GLY:HA2	7:Z:363:LYS:HB2	1.87	0.56
5:K:27:VAL:HG13	5:K:29:GLN:HB2	1.88	0.56
6:L:1499:PHE:HB3	6:L:1505:LEU:HD11	1.88	0.56
7:X:3:ARG:HB2	7:X:133:GLU:HB2	1.87	0.56
3:H:608:THR:HG23	3:H:610:ALA:H	1.71	0.56
6:L:461:PHE:HA	6:L:464:LYS:HD2	1.88	0.56
6:L:1534:LYS:HD3	6:L:1544:LEU:HB2	1.87	0.56
7:W:339:ARG:HD2	7:W:343:ARG:HH12	1.70	0.56
7:Y:326:GLY:HA2	7:Y:363:LYS:HB2	1.87	0.55
5:I:529:GLN:O	5:I:532:LEU:HB3	2.06	0.55
1:J:412:LEU:HA	1:J:415:VAL:HG22	1.87	0.55
7:X:339:ARG:HD2	7:X:343:ARG:HH12	1.70	0.55
5:I:191:MET:HE1	5:I:276:ILE:HA	1.89	0.55
7:U:326:GLY:HA2	7:U:363:LYS:HB2	1.87	0.55
7:Z:3:ARG:HB2	7:Z:133:GLU:HB2	1.87	0.55
4:G:372:ALA:HA	4:G:375:LEU:HD12	1.88	0.55
5:K:1:MET:HA	5:K:4:GLU:HG2	1.89	0.55
7:U:339:ARG:HD2	7:U:343:ARG:HH12	1.70	0.54
7:W:3:ARG:HB2	7:W:133:GLU:HB2	1.87	0.54
5:I:506:LYS:HB3	5:I:508:ASN:HD22	1.73	0.54
5:I:515:TRP:HE1	5:I:519:ASN:H	1.56	0.54
7:X:324:ILE:HG22	7:X:360:LEU:HA	1.90	0.54
3:H:737:LYS:HA	3:H:740:GLN:HE21	1.72	0.54
1:I:26:VAL:HG21	2:m:64:ILE:HD12	1.89	0.54
6:L:1652:SER:O	6:L:1656:ARG:NE	2.40	0.54
3:H:885:HIS:HB2	7:V:353:PRO:HB3	1.89	0.54
7:U:324:ILE:HG22	7:U:360:LEU:HA	1.90	0.54
4:G:646:PHE:HA	4:G:649:LYS:HD2	1.90	0.54
5:I:161:SER:HB3	5:I:172:LEU:HD22	1.89	0.54
7:V:339:ARG:HB3	7:V:343:ARG:HH22	1.73	0.54
7:Y:324:ILE:HG22	7:Y:360:LEU:HA	1.90	0.54
5:I:279:VAL:HG13	5:I:336:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:28:LEU:HA	2:m:31:ILE:HG13	1.90	0.53
2:b:28:LEU:HA	2:b:31:ILE:HG13	1.90	0.53
7:W:324:ILE:HG22	7:W:360:LEU:HA	1.90	0.53
7:W:339:ARG:HB3	7:W:343:ARG:HH22	1.73	0.53
7:Z:324:ILE:HG22	7:Z:360:LEU:HA	1.90	0.53
7:Z:339:ARG:HB3	7:Z:343:ARG:HH22	1.74	0.53
7:W:322:ASN:ND2	7:W:357:GLN:O	2.42	0.53
5:K:648:ARG:NH2	7:Y:353:PRO:O	2.41	0.53
7:U:322:ASN:ND2	7:U:357:GLN:O	2.42	0.53
7:Y:184:GLN:O	7:Y:188:SER:OG	2.27	0.53
7:V:184:GLN:O	7:V:188:SER:OG	2.27	0.53
7:W:184:GLN:O	7:W:188:SER:OG	2.27	0.53
7:V:322:ASN:ND2	7:V:357:GLN:O	2.42	0.53
3:H:869:SER:H	3:H:873:LEU:HD12	1.74	0.53
7:X:184:GLN:O	7:X:188:SER:OG	2.27	0.53
4:G:559:LEU:HD21	4:G:570:LYS:HB2	1.92	0.52
7:X:339:ARG:HB3	7:X:343:ARG:HH22	1.74	0.52
5:I:486:ARG:HA	5:I:489:GLN:HE21	1.74	0.52
7:V:324:ILE:HG22	7:V:360:LEU:HA	1.90	0.52
7:Y:322:ASN:ND2	7:Y:357:GLN:O	2.42	0.52
4:G:311:GLU:OE2	3:H:365:ARG:NH2	2.43	0.52
7:Y:40:PHE:HB2	7:Y:366:TYR:HE1	1.75	0.52
7:Z:322:ASN:ND2	7:Z:357:GLN:O	2.42	0.52
7:X:40:PHE:HB2	7:X:366:TYR:HE1	1.75	0.52
7:X:322:ASN:ND2	7:X:357:GLN:O	2.42	0.52
7:Y:320:ILE:HB	7:Y:356:ILE:HG13	1.92	0.52
4:G:692:ASN:OD1	7:U:357:GLN:NE2	2.42	0.52
1:J:277:LEU:HD11	1:J:294:VAL:HG21	1.90	0.52
7:Y:339:ARG:HB3	7:Y:343:ARG:HH22	1.74	0.52
4:G:392:GLU:HA	4:G:395:ILE:HG12	1.91	0.51
7:U:339:ARG:HB3	7:U:343:ARG:HH22	1.74	0.51
3:H:439:LEU:HD23	3:H:450:SER:HB2	1.92	0.51
7:X:320:ILE:HB	7:X:356:ILE:HG13	1.92	0.51
7:V:320:ILE:HB	7:V:356:ILE:HG13	1.92	0.51
3:H:483:VAL:HA	3:H:486:ILE:HD12	1.91	0.51
1:J:801:LEU:O	1:J:822:ASN:ND2	2.44	0.51
5:K:183:MET:HG2	5:K:186:GLN:HE21	1.76	0.51
7:U:184:GLN:O	7:U:188:SER:OG	2.27	0.51
7:W:40:PHE:HB2	7:W:366:TYR:HE1	1.75	0.51
7:Z:320:ILE:HB	7:Z:356:ILE:HG13	1.92	0.51
7:Z:184:GLN:O	7:Z:188:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:87:LEU:HD13	2:m:31:ILE:HG12	1.92	0.51
3:H:254:ILE:HA	3:H:257:VAL:HG22	1.93	0.51
5:K:496:TRP:HZ2	7:Y:261:ILE:HD12	1.76	0.51
5:K:545:LEU:O	5:K:549:ASN:ND2	2.45	0.50
7:U:320:ILE:HB	7:U:356:ILE:HG13	1.92	0.50
7:Z:40:PHE:HB2	7:Z:366:TYR:HE1	1.75	0.50
5:K:42:LEU:HA	5:K:45:LEU:HG	1.93	0.50
5:K:485:VAL:HB	5:K:529:GLN:HE22	1.76	0.50
7:V:40:PHE:HB2	7:V:366:TYR:HE1	1.75	0.50
2:b:22:ARG:NH1	6:L:287:LEU:HA	2.24	0.50
5:I:154:LEU:O	5:I:158:TYR:HB3	2.11	0.50
4:G:242:GLN:HE21	4:G:343:THR:HG23	1.76	0.50
1:J:216:LEU:HD11	5:K:33:PHE:HB3	1.94	0.50
5:K:410:LEU:HD23	5:K:413:LEU:HD12	1.93	0.50
7:W:320:ILE:HB	7:W:356:ILE:HG13	1.92	0.50
3:H:255:LEU:HD11	3:H:343:HIS:HA	1.93	0.50
3:H:715:ILE:HA	3:H:718:MET:HG2	1.94	0.50
4:G:607:GLU:N	4:G:610:LEU:O	2.44	0.50
3:H:768:SER:HA	3:H:771:LEU:HD23	1.94	0.50
7:U:40:PHE:HB2	7:U:366:TYR:HE1	1.75	0.50
1:l:17:ARG:HA	1:l:20:ARG:HD2	1.93	0.50
5:I:499:GLN:HG3	7:W:264:PRO:HB3	1.94	0.50
1:J:334:VAL:HG21	1:J:365:MET:HG2	1.94	0.50
6:L:1662:LYS:O	6:L:1662:LYS:NZ	2.37	0.49
5:I:51:ASP:HB2	5:I:133:PHE:HD1	1.78	0.49
6:L:1676:ILE:HG23	6:L:1680:ILE:HD12	1.94	0.49
4:G:641:LEU:HD21	4:G:734:LEU:HA	1.95	0.49
3:H:842:LYS:O	3:H:842:LYS:NZ	2.42	0.49
5:I:361:TYR:HE2	5:I:475:TYR:HB3	1.76	0.49
4:G:307:VAL:HA	4:G:310:LEU:HG	1.94	0.49
3:H:779:PHE:HA	3:H:782:ILE:HD12	1.95	0.49
5:I:621:ARG:O	5:I:624:SER:OG	2.31	0.49
2:b:27:VAL:HG13	3:a:77:LEU:HD22	1.95	0.49
3:H:862:LEU:HD21	3:H:880:LEU:HB2	1.95	0.49
5:I:357:ILE:O	5:I:361:TYR:HB3	2.13	0.49
1:J:707:MET:SD	1:J:711:LYS:NZ	2.86	0.49
5:I:191:MET:HB2	5:I:192:LEU:HD12	1.95	0.48
1:J:760:VAL:HG21	7:Y:342:GLU:HG3	1.94	0.48
4:G:523:ASP:OD1	7:U:248:TYR:OH	2.32	0.48
3:H:716:HIS:CE1	7:V:259:SER:HB3	2.49	0.48
5:K:134:PRO:HA	5:K:137:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:240:THR:HA	7:V:243:LEU:HD12	1.96	0.48
7:X:240:THR:HA	7:X:243:LEU:HD12	1.96	0.48
3:H:681:ARG:HG2	7:V:258:ALA:HA	1.94	0.48
1:J:302:VAL:HG23	1:J:304:HIS:H	1.78	0.48
2:m:48:VAL:O	2:m:52:GLU:HG3	2.14	0.48
4:G:613:LEU:HD12	4:G:614:GLU:HG2	1.95	0.48
5:K:501:GLN:HE21	7:Y:162:PRO:HB2	1.77	0.48
6:L:1633:LEU:HB2	6:L:1662:LYS:HE2	1.95	0.48
3:H:879:ARG:HA	3:H:882:PHE:CZ	2.49	0.48
2:b:48:VAL:O	2:b:52:GLU:HG3	2.14	0.47
5:K:4:GLU:OE2	5:K:16:ILE:HB	2.13	0.47
7:Y:240:THR:HA	7:Y:243:LEU:HD12	1.96	0.47
3:H:268:MET:HE3	3:H:271:THR:HA	1.95	0.47
7:Z:240:THR:HA	7:Z:243:LEU:HD12	1.96	0.47
5:K:17:PHE:HE2	5:K:42:LEU:HD21	1.79	0.47
5:K:651:TYR:CE1	7:Y:355:SER:HA	2.49	0.47
3:H:329:HIS:CE1	5:I:131:LEU:HD11	2.50	0.47
7:Z:222:ASN:OD1	7:Z:222:ASN:N	2.48	0.47
4:G:761:CYS:HA	4:G:764:LYS:HE2	1.97	0.47
3:H:884:GLU:HB3	3:H:887:LYS:HB3	1.97	0.47
7:V:343:ARG:HA	7:V:343:ARG:HD3	1.46	0.47
3:a:67:ARG:HH12	3:a:104:PRO:HG2	1.79	0.47
7:U:389:GLU:O	7:U:393:ARG:N	2.48	0.47
7:X:222:ASN:OD1	7:X:222:ASN:N	2.48	0.47
3:a:16:LEU:HD23	3:a:19:ARG:HH21	1.79	0.47
5:I:380:LEU:HG	5:I:450:TRP:HE1	1.80	0.47
5:I:601:LEU:HD23	5:I:601:LEU:HA	1.82	0.47
1:J:215:TRP:HB3	6:L:322:LYS:HE3	1.97	0.47
5:K:151:CYS:HA	5:K:154:LEU:HD13	1.96	0.47
7:Y:222:ASN:N	7:Y:222:ASN:OD1	2.48	0.47
7:W:389:GLU:O	7:W:393:ARG:N	2.48	0.47
7:X:389:GLU:O	7:X:393:ARG:N	2.48	0.47
4:G:684:GLN:O	4:G:688:ASN:ND2	2.48	0.46
7:V:388:PHE:O	7:V:391:THR:OG1	2.27	0.46
3:H:716:HIS:HE1	7:V:259:SER:HB3	1.80	0.46
5:I:43:ASN:O	5:I:46:CYS:HB3	2.15	0.46
7:U:377:MET:HE2	7:U:377:MET:HB2	1.86	0.46
7:Z:324:ILE:HD12	7:Z:324:ILE:HA	1.80	0.46
3:H:859:GLN:HE21	3:H:859:GLN:HB2	1.57	0.46
5:K:577:LYS:O	5:K:581:HIS:HB2	2.15	0.46
7:U:222:ASN:OD1	7:U:222:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:240:THR:HA	7:U:243:LEU:HD12	1.96	0.46
7:V:222:ASN:OD1	7:V:222:ASN:N	2.48	0.46
7:V:389:GLU:O	7:V:393:ARG:N	2.48	0.46
7:Y:104:TRP:HE1	7:Y:191:THR:HG23	1.81	0.46
2:b:37:THR:HG22	3:a:100:LEU:HB2	1.98	0.46
5:I:92:GLY:HA3	5:I:175:ILE:HG12	1.97	0.46
7:V:104:TRP:HE1	7:V:191:THR:HG23	1.81	0.46
7:X:384:ILE:O	7:X:387:LEU:HB2	2.16	0.46
3:H:712:VAL:O	3:H:716:HIS:HB2	2.15	0.46
5:K:199:GLN:O	5:K:200:HIS:ND1	2.48	0.46
7:W:104:TRP:HE1	7:W:191:THR:HG23	1.81	0.46
7:W:240:THR:HA	7:W:243:LEU:HD12	1.96	0.46
5:I:63:THR:HG22	5:I:87:ARG:HG2	1.97	0.46
5:I:357:ILE:O	5:I:361:TYR:HB2	2.15	0.46
7:V:384:ILE:O	7:V:387:LEU:HB2	2.16	0.46
7:W:174:ASN:H	7:W:207:ASN:HD21	1.64	0.46
7:X:174:ASN:H	7:X:207:ASN:HD21	1.64	0.46
7:Y:384:ILE:O	7:Y:387:LEU:HB2	2.16	0.46
5:I:59:ILE:HD13	5:I:90:CYS:HB2	1.97	0.46
7:V:174:ASN:H	7:V:207:ASN:HD21	1.64	0.46
1:J:496:ARG:HH11	1:J:567:GLN:HG2	1.81	0.46
1:J:979:SER:HB2	1:J:980:ILE:HD12	1.98	0.46
7:U:104:TRP:HE1	7:U:191:THR:HG23	1.81	0.46
7:W:222:ASN:N	7:W:222:ASN:OD1	2.48	0.46
7:X:104:TRP:HE1	7:X:191:THR:HG23	1.80	0.46
7:V:29:HIS:HB3	7:V:48:LYS:HD3	1.98	0.46
7:W:29:HIS:HB3	7:W:48:LYS:HD3	1.98	0.46
7:U:384:ILE:O	7:U:387:LEU:HB2	2.16	0.46
4:G:221:LEU:HD11	4:G:260:VAL:HG22	1.97	0.45
5:K:472:LEU:HD13	5:K:475:TYR:HD2	1.81	0.45
7:U:324:ILE:HD12	7:U:324:ILE:HA	1.80	0.45
2:b:22:ARG:HG3	6:L:287:LEU:HD22	1.97	0.45
7:U:29:HIS:HB3	7:U:48:LYS:HD3	1.98	0.45
7:Y:343:ARG:HA	7:Y:343:ARG:HD3	1.46	0.45
7:Z:104:TRP:HE1	7:Z:191:THR:HG23	1.81	0.45
7:Z:174:ASN:H	7:Z:207:ASN:HD21	1.64	0.45
6:L:1554:LEU:HD13	6:L:1574:LEU:HD22	1.98	0.45
7:V:337:LEU:HB2	7:V:341:ARG:NH1	2.32	0.45
7:W:297:LEU:HD11	7:W:377:MET:HB3	1.99	0.45
7:W:384:ILE:O	7:W:387:LEU:HB2	2.16	0.45
7:X:297:LEU:HD11	7:X:377:MET:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:337:LEU:HB2	7:X:341:ARG:NH1	2.32	0.45
3:a:113:SER:OG	3:a:114:TYR:N	2.46	0.45
4:G:555:LEU:HD22	4:G:575:ILE:HG13	1.98	0.45
6:L:1800:LEU:HD21	7:Z:341:ARG:NE	2.31	0.45
7:W:229:ASN:O	7:W:233:SER:OG	2.34	0.45
7:W:337:LEU:HB2	7:W:341:ARG:NH1	2.32	0.45
7:Z:389:GLU:O	7:Z:393:ARG:N	2.48	0.45
1:J:561:MET:HG3	1:J:699:TYR:CZ	2.51	0.45
5:K:344:MET:HE1	5:K:462:PRO:HB2	1.97	0.45
6:L:1800:LEU:HD21	7:Z:341:ARG:CZ	2.46	0.45
7:X:29:HIS:HB3	7:X:48:LYS:HD3	1.98	0.45
7:Z:384:ILE:O	7:Z:387:LEU:HB2	2.16	0.45
2:b:39:LEU:HD13	2:b:44:LEU:HD13	1.99	0.45
4:G:695:TYR:CE1	7:U:249:MET:HG3	2.52	0.45
3:H:589:ALA:N	3:H:632:ASP:OD2	2.50	0.45
5:I:406:ASP:OD1	5:I:406:ASP:N	2.43	0.45
7:V:428:VAL:HA	7:V:431:LEU:HB2	1.99	0.45
7:W:232:VAL:O	7:W:236:MET:HG2	2.17	0.45
7:U:229:ASN:O	7:U:233:SER:OG	2.34	0.45
7:U:337:LEU:HB2	7:U:341:ARG:NH1	2.32	0.45
7:V:229:ASN:O	7:V:233:SER:OG	2.34	0.45
7:V:232:VAL:O	7:V:236:MET:HG2	2.17	0.45
7:W:343:ARG:HA	7:W:343:ARG:HD3	1.46	0.45
7:Y:337:LEU:HB2	7:Y:341:ARG:NH1	2.32	0.45
7:Z:29:HIS:HB3	7:Z:48:LYS:HD3	1.98	0.45
2:b:46:ILE:HG21	3:a:19:ARG:NH2	2.32	0.45
4:G:521:LEU:HD23	4:G:702:MET:HB3	1.98	0.45
7:U:428:VAL:HA	7:U:431:LEU:HB2	1.99	0.45
7:X:229:ASN:O	7:X:233:SER:OG	2.34	0.45
3:H:339:LEU:HA	3:H:342:LEU:HD12	1.99	0.45
7:Y:389:GLU:O	7:Y:393:ARG:N	2.48	0.45
4:G:282:SER:OG	4:G:284:GLU:OE1	2.31	0.44
5:I:543:GLN:O	5:I:546:HIS:HB3	2.17	0.44
7:Z:337:LEU:HB2	7:Z:341:ARG:NH1	2.32	0.44
5:K:534:VAL:HA	5:K:537:LEU:HG	1.99	0.44
6:L:1732:ILE:O	6:L:1736:VAL:HG23	2.16	0.44
7:U:232:VAL:O	7:U:236:MET:HG2	2.17	0.44
2:m:39:LEU:HD13	2:m:44:LEU:HD13	1.99	0.44
3:a:7:LYS:HB2	3:a:12:LEU:HD21	1.99	0.44
3:H:589:ALA:HA	3:H:592:LEU:HD13	1.98	0.44
5:I:45:LEU:HD12	5:I:48:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:480:LYS:HA	5:I:483:LEU:HD12	1.99	0.44
7:W:341:ARG:HH11	7:W:341:ARG:HD2	1.63	0.44
7:Y:229:ASN:O	7:Y:233:SER:OG	2.34	0.44
7:Y:232:VAL:O	7:Y:236:MET:HG2	2.17	0.44
7:Z:232:VAL:O	7:Z:236:MET:HG2	2.17	0.44
7:Z:343:ARG:HA	7:Z:343:ARG:HD3	1.46	0.44
2:b:46:ILE:HG13	3:a:19:ARG:CZ	2.47	0.44
3:H:763:LEU:HD21	3:H:771:LEU:HB3	1.99	0.44
5:K:6:LEU:HD21	5:K:111:PHE:HE2	1.81	0.44
5:K:183:MET:HG2	5:K:186:GLN:NE2	2.32	0.44
7:U:174:ASN:H	7:U:207:ASN:HD21	1.64	0.44
7:X:377:MET:HE2	7:X:377:MET:HB2	1.85	0.44
7:Y:174:ASN:H	7:Y:207:ASN:HD21	1.64	0.44
7:Z:297:LEU:HD11	7:Z:377:MET:HB3	1.99	0.44
7:W:410:LYS:H	7:W:410:LYS:HG2	1.62	0.44
7:X:232:VAL:O	7:X:236:MET:HG2	2.17	0.44
7:Y:29:HIS:HB3	7:Y:48:LYS:HD3	1.98	0.44
3:H:329:HIS:HA	3:H:332:LEU:HG	2.00	0.44
2:b:36:ASN:HD21	3:a:104:PRO:HB3	1.81	0.44
4:G:858:ARG:NH1	7:U:357:GLN:OE1	2.51	0.44
7:U:343:ARG:HA	7:U:343:ARG:HD3	1.46	0.44
7:X:324:ILE:HD12	7:X:324:ILE:HA	1.80	0.44
7:Z:229:ASN:O	7:Z:233:SER:OG	2.34	0.44
4:G:285:TYR:HB3	4:G:289:ASN:HD22	1.83	0.44
3:H:301:HIS:HA	3:H:304:ILE:HG12	1.99	0.44
5:I:42:LEU:O	5:I:46:CYS:N	2.50	0.44
7:W:339:ARG:HB3	7:W:343:ARG:NH2	2.33	0.44
7:Y:297:LEU:HD11	7:Y:377:MET:HB3	1.99	0.44
7:Y:339:ARG:HB3	7:Y:343:ARG:NH2	2.33	0.44
1:J:432:ARG:HA	1:J:435:HIS:CD2	2.52	0.44
6:L:393:ILE:O	6:L:397:LEU:N	2.50	0.44
7:U:297:LEU:HD11	7:U:377:MET:HB3	1.99	0.44
7:V:297:LEU:HD11	7:V:377:MET:HB3	1.99	0.44
7:X:25:LEU:HD13	7:X:25:LEU:HA	1.82	0.44
6:L:1797:ASP:HA	7:Z:334:HIS:CE1	2.52	0.43
7:W:428:VAL:HA	7:W:431:LEU:HB2	1.99	0.43
7:Z:339:ARG:HB3	7:Z:343:ARG:NH2	2.33	0.43
4:G:499:LEU:HB3	4:G:719:ILE:HD11	1.99	0.43
7:U:270:MET:HE2	7:U:305:VAL:HB	2.00	0.43
2:b:60:LEU:O	2:b:64:ILE:HG12	2.19	0.43
6:L:1634:LYS:HE3	6:L:1634:LYS:HB3	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:270:MET:HE2	7:Z:305:VAL:HB	2.00	0.43
6:L:1632:ALA:HB1	6:L:1740:ARG:HG3	2.01	0.43
7:X:343:ARG:HA	7:X:343:ARG:HD3	1.46	0.43
2:b:23:GLU:OE2	2:b:24:THR:N	2.51	0.43
3:H:744:LEU:HA	3:H:747:ILE:HG12	2.00	0.43
3:H:887:LYS:HA	3:H:887:LYS:HD3	1.75	0.43
7:Y:428:VAL:HA	7:Y:431:LEU:HB2	1.99	0.43
7:Z:428:VAL:HA	7:Z:431:LEU:HB2	1.99	0.43
1:l:38:GLN:HE22	1:l:41:LEU:HD22	1.82	0.43
5:K:345:VAL:HG23	5:K:346:GLU:HG3	2.01	0.43
7:W:270:MET:HE2	7:W:305:VAL:HB	2.00	0.43
2:m:23:GLU:OE2	2:m:24:THR:N	2.51	0.43
2:m:60:LEU:O	2:m:64:ILE:HG12	2.19	0.43
3:H:266:ILE:HD13	3:H:277:VAL:HA	2.00	0.43
3:H:698:SER:O	3:H:702:HIS:HB3	2.19	0.43
5:I:190:TRP:CE2	5:I:280:GLY:HA3	2.54	0.43
6:L:1779:LEU:HA	6:L:1782:VAL:HG12	2.00	0.43
7:X:428:VAL:HA	7:X:431:LEU:HB2	1.99	0.43
7:Z:410:LYS:H	7:Z:410:LYS:HG2	1.62	0.43
5:K:98:GLN:HA	5:K:101:ARG:HD2	2.00	0.43
1:J:358:PHE:HD2	1:J:361:TYR:H	1.66	0.43
6:L:1550:LEU:HA	6:L:1553:VAL:HB	2.01	0.43
7:X:116:GLU:H	7:X:116:GLU:HG2	1.49	0.43
5:I:466:LEU:HD12	5:I:554:PHE:HE1	1.84	0.43
1:J:921:LYS:H	1:J:925:GLN:HE21	1.67	0.43
7:U:339:ARG:HB3	7:U:343:ARG:NH2	2.33	0.43
7:X:339:ARG:HB3	7:X:343:ARG:NH2	2.33	0.43
3:a:117:LEU:HD13	4:G:375:LEU:HD23	2.01	0.42
5:I:510:THR:HG23	5:I:513:ILE:HB	2.01	0.42
7:X:270:MET:HE2	7:X:305:VAL:HB	2.00	0.42
7:Y:47:ARG:HE	7:Y:49:ASP:HB2	1.84	0.42
5:I:414:LEU:HD22	5:I:453:LEU:HD11	2.00	0.42
5:K:327:GLN:HB3	5:K:331:ARG:HH21	1.84	0.42
7:W:47:ARG:HE	7:W:49:ASP:HB2	1.84	0.42
7:X:410:LYS:H	7:X:410:LYS:HG2	1.63	0.42
4:G:219:GLU:HB2	4:G:314:HIS:HE1	1.83	0.42
7:U:47:ARG:HE	7:U:49:ASP:HB2	1.84	0.42
6:L:392:SER:O	6:L:395:SER:OG	2.28	0.42
6:L:1670:LYS:HA	6:L:1670:LYS:HD3	1.94	0.42
7:V:339:ARG:HB3	7:V:343:ARG:NH2	2.33	0.42
7:Y:270:MET:HE2	7:Y:305:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:53:LEU:HD12	4:G:309:GLN:NE2	2.35	0.42
4:G:513:LEU:HD23	4:G:630:ILE:HD11	2.01	0.42
4:G:543:VAL:HG12	4:G:611:SER:HB3	2.01	0.42
5:I:553:ASP:O	5:I:556:SER:OG	2.35	0.42
1:J:716:LEU:HD22	1:J:812:VAL:HG11	2.02	0.42
5:K:25:LEU:HB2	5:K:46:CYS:HB2	2.01	0.42
5:K:470:ALA:O	5:K:474:LYS:HG2	2.19	0.42
3:a:73:LEU:O	3:a:76:GLU:HG2	2.20	0.42
4:G:861:PHE:CE1	7:U:341:ARG:HG3	2.54	0.42
7:V:270:MET:HE2	7:V:305:VAL:HB	2.00	0.42
4:G:277:ILE:HD12	4:G:277:ILE:HA	1.88	0.42
4:G:393:LYS:HG2	4:G:397:ARG:HH11	1.85	0.42
4:G:522:MET:HG3	4:G:528:PHE:CD2	2.55	0.42
1:l:67:GLY:O	1:l:71:LYS:NZ	2.53	0.42
3:H:581:LEU:HD12	3:H:584:GLU:HB2	2.02	0.42
3:H:686:CYS:HA	3:H:689:LYS:NZ	2.35	0.42
5:I:131:LEU:O	5:I:135:SER:OG	2.30	0.42
5:I:196:LEU:HD23	5:I:196:LEU:HA	1.96	0.42
6:L:1660:LEU:HA	6:L:1660:LEU:HD13	1.78	0.42
7:X:47:ARG:HE	7:X:49:ASP:HB2	1.84	0.42
7:Z:47:ARG:HE	7:Z:49:ASP:HB2	1.84	0.42
4:G:577:LEU:HD12	4:G:579:PRO:HD3	2.01	0.41
4:G:709:LEU:HG	4:G:713:LEU:HD23	2.01	0.41
3:H:578:MET:HE3	3:H:578:MET:HA	2.01	0.41
3:H:613:ASP:HB3	3:H:617:ILE:HD11	2.02	0.41
1:J:842:LEU:HD23	1:J:842:LEU:HA	1.85	0.41
5:K:89:PHE:HE2	5:K:140:VAL:HG12	1.85	0.41
7:X:428:VAL:HA	7:X:431:LEU:HD12	2.02	0.41
7:Y:324:ILE:HD12	7:Y:324:ILE:HA	1.80	0.41
3:H:365:ARG:NH2	3:H:366:ARG:HH22	2.18	0.41
7:V:47:ARG:HE	7:V:49:ASP:HB2	1.84	0.41
5:I:515:TRP:CD1	5:I:518:ARG:H	2.39	0.41
5:K:403:VAL:HG23	5:K:405:LEU:H	1.85	0.41
6:L:352:LEU:HD21	6:L:397:LEU:HD13	2.01	0.41
6:L:1680:ILE:HD11	6:L:1716:GLY:HA2	2.02	0.41
4:G:363:SER:HA	4:G:376:CYS:SG	2.60	0.41
5:I:199:GLN:NE2	1:J:445:LEU:O	2.53	0.41
7:V:25:LEU:HA	7:V:25:LEU:HD13	1.82	0.41
7:Z:428:VAL:HA	7:Z:431:LEU:HD12	2.02	0.41
5:K:111:PHE:HD1	5:K:117:LEU:HD12	1.86	0.41
5:K:545:LEU:HA	5:K:548:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:639:ASN:O	5:K:643:ALA:CB	2.68	0.41
6:L:1682:HIS:HB3	7:Z:330:PRO:CB	2.51	0.41
4:G:276:PHE:HD2	4:G:296:MET:HE1	1.86	0.41
1:J:384:LYS:HA	1:J:384:LYS:HD2	1.88	0.41
5:K:496:TRP:CE2	7:Y:258:ALA:HA	2.55	0.41
7:W:388:PHE:O	7:W:391:THR:OG1	2.27	0.41
7:Y:377:MET:HE2	7:Y:377:MET:HB2	1.85	0.41
2:b:22:ARG:CZ	6:L:289:TYR:HE1	2.34	0.41
4:G:359:LEU:HG	4:G:380:THR:HB	2.03	0.41
5:I:350:LEU:HD13	5:I:464:HIS:CE1	2.56	0.41
1:J:889:LYS:HE2	1:J:987:PHE:CD2	2.55	0.41
7:U:9:GLN:OE1	7:U:9:GLN:N	2.54	0.41
7:U:165:LEU:HD13	7:U:253:LEU:HG	2.03	0.41
4:G:414:LEU:HB2	4:G:426:LYS:HD3	2.03	0.41
4:G:610:LEU:HD13	4:G:613:LEU:HD11	2.02	0.41
3:H:258:PHE:HD1	3:H:297:LEU:HD22	1.86	0.41
7:W:165:LEU:HD13	7:W:253:LEU:HG	2.03	0.41
7:Y:165:LEU:HD13	7:Y:253:LEU:HG	2.03	0.41
3:H:254:ILE:HD11	3:H:294:LEU:HB2	2.03	0.40
3:H:730:SER:HA	3:H:733:GLU:HG3	2.03	0.40
1:J:403:ALA:HA	1:J:406:LEU:HG	2.02	0.40
5:K:255:LYS:HD2	5:K:255:LYS:HA	1.81	0.40
6:L:432:PHE:HE2	6:L:524:LEU:HD13	1.86	0.40
7:V:9:GLN:N	7:V:9:GLN:OE1	2.54	0.40
7:X:165:LEU:HD13	7:X:253:LEU:HG	2.03	0.40
7:Y:428:VAL:HA	7:Y:431:LEU:HD12	2.02	0.40
7:Z:9:GLN:OE1	7:Z:9:GLN:N	2.54	0.40
5:K:649:LEU:HD12	5:K:652:ASN:HA	2.03	0.40
6:L:1669:VAL:HA	6:L:1672:ILE:HG22	2.02	0.40
7:V:428:VAL:HA	7:V:431:LEU:HD12	2.02	0.40
4:G:259:LEU:HB3	4:G:321:LEU:HD21	2.02	0.40
3:H:579:ASP:O	3:H:582:LYS:NZ	2.51	0.40
3:H:626:LEU:HB2	3:H:637:VAL:HG13	2.03	0.40
5:I:282:SER:HB3	5:I:340:LEU:HD21	2.04	0.40
7:U:428:VAL:HA	7:U:431:LEU:HD12	2.02	0.40
7:V:116:GLU:H	7:V:116:GLU:HG2	1.49	0.40
7:V:245:TYR:HA	7:V:246:PRO:HD3	1.92	0.40
7:W:9:GLN:N	7:W:9:GLN:OE1	2.54	0.40
7:W:116:GLU:H	7:W:116:GLU:HG2	1.49	0.40
7:Y:410:LYS:H	7:Y:410:LYS:HG2	1.63	0.40
5:I:504:HIS:CE1	7:W:158:ASN:HD21	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:283:LYS:HA	1:J:283:LYS:HD2	1.89	0.40
1:J:937:ILE:HD12	1:J:937:ILE:HA	1.91	0.40
7:Y:9:GLN:N	7:Y:9:GLN:OE1	2.54	0.40
5:I:400:ALA:HB1	5:I:405:LEU:HD22	2.04	0.40
5:I:484:SER:HB2	5:I:587:LEU:HD11	2.02	0.40
1:J:879:GLN:HB3	1:J:883:MET:HE3	2.03	0.40
7:V:410:LYS:H	7:V:410:LYS:HG2	1.63	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	J	506/1024 (49%)	469 (93%)	34 (7%)	3 (1%)	21	59
1	l	104/1024 (10%)	98 (94%)	5 (5%)	1 (1%)	12	48
2	b	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
2	m	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
3	H	584/907 (64%)	572 (98%)	11 (2%)	1 (0%)	43	78
3	a	112/907 (12%)	108 (96%)	4 (4%)	0	100	100
4	G	624/902 (69%)	597 (96%)	22 (4%)	5 (1%)	16	54
5	I	511/667 (77%)	489 (96%)	20 (4%)	2 (0%)	30	67
5	K	548/667 (82%)	530 (97%)	17 (3%)	1 (0%)	43	78
6	L	540/1819 (30%)	509 (94%)	27 (5%)	4 (1%)	18	56
7	U	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	V	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
7	W	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	X	408/451 (90%)	392 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Y	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	Z	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
All	All	6103/10787 (57%)	5845 (96%)	241 (4%)	17 (0%)	37	72

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	l	121	PRO
4	G	241	ARG
4	G	581	ASP
3	H	455	LYS
5	I	601	LEU
1	J	236	LEU
1	J	238	LEU
5	K	409	ASN
6	L	308	GLU
4	G	557	LEU
5	I	600	ASN
1	J	222	HIS
6	L	1800	LEU
4	G	582	LEU
4	G	854	SER
6	L	346	LEU
6	L	303	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	J	498/933 (53%)	493 (99%)	5 (1%)	68	78
1	l	84/933 (9%)	84 (100%)	0	100	100
2	b	53/62 (86%)	39 (74%)	14 (26%)	0	3
2	m	53/62 (86%)	39 (74%)	14 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	539/798 (68%)	536 (99%)	3 (1%)	78	83
3	a	101/798 (13%)	97 (96%)	4 (4%)	28	49
4	G	572/791 (72%)	563 (98%)	9 (2%)	55	70
5	I	472/594 (80%)	469 (99%)	3 (1%)	78	83
5	K	509/594 (86%)	506 (99%)	3 (1%)	78	83
6	L	501/1546 (32%)	497 (99%)	4 (1%)	73	80
7	U	376/400 (94%)	305 (81%)	71 (19%)	1	8
7	V	376/400 (94%)	305 (81%)	71 (19%)	1	8
7	W	376/400 (94%)	305 (81%)	71 (19%)	1	8
7	X	376/400 (94%)	306 (81%)	70 (19%)	1	8
7	Y	376/400 (94%)	305 (81%)	71 (19%)	1	8
7	Z	376/400 (94%)	305 (81%)	71 (19%)	1	8
All	All	5638/9511 (59%)	5154 (91%)	484 (9%)	12	29

All (484) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	m	22	ARG
2	m	23	GLU
2	m	28	LEU
2	m	31	ILE
2	m	34	ILE
2	m	39	LEU
2	m	41	MET
2	m	43	THR
2	m	45	SER
2	m	48	VAL
2	m	61	SER
2	m	69	LYS
2	m	71	THR
2	m	74	LEU
2	b	22	ARG
2	b	23	GLU
2	b	28	LEU
2	b	31	ILE
2	b	34	ILE
2	b	39	LEU
2	b	41	MET

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Mol	Chain	Res	Type
2	b	43	THR
2	b	45	SER
2	b	48	VAL
2	b	61	SER
2	b	69	LYS
2	b	71	THR
2	b	74	LEU
3	a	12	LEU
3	a	38	VAL
3	a	39	ILE
3	a	86	VAL
4	G	233	VAL
4	G	260	VAL
4	G	328	ILE
4	G	355	THR
4	G	414	LEU
4	G	469	CYS
4	G	557	LEU
4	G	563	THR
4	G	751	LEU
3	H	380	THR
3	H	421	LEU
3	H	603	THR
5	I	59	ILE
5	I	403	VAL
5	I	475	TYR
1	J	290	ILE
1	J	302	VAL
1	J	317	ILE
1	J	331	ILE
1	J	360	THR
5	K	4	GLU
5	K	119	ILE
5	K	259	LEU
6	L	346	LEU
6	L	347	VAL
6	L	1636	VAL
6	L	1660	LEU
7	U	4	GLU
7	U	7	THR
7	U	8	LEU
7	U	9	GLN

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Mol	Chain	Res	Type
7	U	10	LEU
7	U	13	CYS
7	U	24	GLN
7	U	25	LEU
7	U	34	GLU
7	U	39	GLU
7	U	58	GLU
7	U	67	LEU
7	U	102	ASN
7	U	116	GLU
7	U	125	GLU
7	U	131	SER
7	U	136	VAL
7	U	137	LEU
7	U	140	SER
7	U	153	LEU
7	U	157	LEU
7	U	165	LEU
7	U	168	THR
7	U	188	SER
7	U	191	THR
7	U	192	LEU
7	U	200	ASP
7	U	204	VAL
7	U	219	HIS
7	U	220	ILE
7	U	222	ASN
7	U	226	SER
7	U	233	SER
7	U	236	MET
7	U	241	THR
7	U	243	LEU
7	U	249	MET
7	U	254	ILE
7	U	260	LEU
7	U	269	LEU
7	U	270	MET
7	U	288	THR
7	U	294	MET
7	U	297	LEU
7	U	298	LEU
7	U	303	VAL

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Mol	Chain	Res	Type
7	U	304	MET
7	U	305	VAL
7	U	323	ILE
7	U	324	ILE
7	U	331	THR
7	U	333	VAL
7	U	340	ILE
7	U	341	ARG
7	U	343	ARG
7	U	348	PHE
7	U	355	SER
7	U	357	GLN
7	U	358	VAL
7	U	369	SER
7	U	374	SER
7	U	376	LEU
7	U	377	MET
7	U	383	SER
7	U	384	ILE
7	U	410	LYS
7	U	420	GLU
7	U	422	ASP
7	U	423	THR
7	U	426	GLU
7	U	439	THR
7	V	4	GLU
7	V	7	THR
7	V	8	LEU
7	V	9	GLN
7	V	10	LEU
7	V	13	CYS
7	V	24	GLN
7	V	25	LEU
7	V	34	GLU
7	V	39	GLU
7	V	58	GLU
7	V	67	LEU
7	V	102	ASN
7	V	116	GLU
7	V	125	GLU
7	V	131	SER
7	V	136	VAL

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Mol	Chain	Res	Type
7	V	137	LEU
7	V	140	SER
7	V	153	LEU
7	V	157	LEU
7	V	165	LEU
7	V	168	THR
7	V	188	SER
7	V	191	THR
7	V	192	LEU
7	V	200	ASP
7	V	204	VAL
7	V	219	HIS
7	V	220	ILE
7	V	222	ASN
7	V	226	SER
7	V	233	SER
7	V	236	MET
7	V	241	THR
7	V	243	LEU
7	V	249	MET
7	V	254	ILE
7	V	260	LEU
7	V	269	LEU
7	V	270	MET
7	V	288	THR
7	V	294	MET
7	V	297	LEU
7	V	298	LEU
7	V	303	VAL
7	V	304	MET
7	V	305	VAL
7	V	323	ILE
7	V	324	ILE
7	V	331	THR
7	V	333	VAL
7	V	340	ILE
7	V	341	ARG
7	V	343	ARG
7	V	348	PHE
7	V	355	SER
7	V	357	GLN
7	V	358	VAL

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Mol	Chain	Res	Type
7	V	369	SER
7	V	374	SER
7	V	376	LEU
7	V	377	MET
7	V	383	SER
7	V	384	ILE
7	V	410	LYS
7	V	420	GLU
7	V	422	ASP
7	V	423	THR
7	V	426	GLU
7	V	439	THR
7	W	4	GLU
7	W	7	THR
7	W	8	LEU
7	W	9	GLN
7	W	10	LEU
7	W	13	CYS
7	W	24	GLN
7	W	25	LEU
7	W	34	GLU
7	W	39	GLU
7	W	58	GLU
7	W	67	LEU
7	W	102	ASN
7	W	116	GLU
7	W	125	GLU
7	W	131	SER
7	W	136	VAL
7	W	137	LEU
7	W	140	SER
7	W	153	LEU
7	W	157	LEU
7	W	165	LEU
7	W	168	THR
7	W	188	SER
7	W	191	THR
7	W	192	LEU
7	W	200	ASP
7	W	204	VAL
7	W	219	HIS
7	W	220	ILE

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Mol	Chain	Res	Type
7	W	222	ASN
7	W	226	SER
7	W	233	SER
7	W	236	MET
7	W	241	THR
7	W	243	LEU
7	W	249	MET
7	W	254	ILE
7	W	260	LEU
7	W	269	LEU
7	W	270	MET
7	W	288	THR
7	W	294	MET
7	W	297	LEU
7	W	298	LEU
7	W	303	VAL
7	W	304	MET
7	W	305	VAL
7	W	323	ILE
7	W	324	ILE
7	W	331	THR
7	W	333	VAL
7	W	340	ILE
7	W	341	ARG
7	W	343	ARG
7	W	348	PHE
7	W	355	SER
7	W	357	GLN
7	W	358	VAL
7	W	369	SER
7	W	374	SER
7	W	376	LEU
7	W	377	MET
7	W	383	SER
7	W	384	ILE
7	W	410	LYS
7	W	420	GLU
7	W	422	ASP
7	W	423	THR
7	W	426	GLU
7	W	439	THR
7	X	4	GLU

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Mol	Chain	Res	Type
7	X	7	THR
7	X	8	LEU
7	X	9	GLN
7	X	10	LEU
7	X	13	CYS
7	X	24	GLN
7	X	25	LEU
7	X	34	GLU
7	X	39	GLU
7	X	58	GLU
7	X	67	LEU
7	X	102	ASN
7	X	116	GLU
7	X	125	GLU
7	X	131	SER
7	X	136	VAL
7	X	137	LEU
7	X	140	SER
7	X	153	LEU
7	X	157	LEU
7	X	165	LEU
7	X	168	THR
7	X	188	SER
7	X	191	THR
7	X	192	LEU
7	X	200	ASP
7	X	204	VAL
7	X	219	HIS
7	X	222	ASN
7	X	226	SER
7	X	233	SER
7	X	236	MET
7	X	241	THR
7	X	243	LEU
7	X	249	MET
7	X	254	ILE
7	X	260	LEU
7	X	269	LEU
7	X	270	MET
7	X	288	THR
7	X	294	MET
7	X	297	LEU

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Mol	Chain	Res	Type
7	X	298	LEU
7	X	303	VAL
7	X	304	MET
7	X	305	VAL
7	X	323	ILE
7	X	324	ILE
7	X	331	THR
7	X	333	VAL
7	X	340	ILE
7	X	341	ARG
7	X	343	ARG
7	X	348	PHE
7	X	355	SER
7	X	357	GLN
7	X	358	VAL
7	X	369	SER
7	X	374	SER
7	X	376	LEU
7	X	377	MET
7	X	383	SER
7	X	384	ILE
7	X	410	LYS
7	X	420	GLU
7	X	422	ASP
7	X	423	THR
7	X	426	GLU
7	X	439	THR
7	Y	4	GLU
7	Y	7	THR
7	Y	8	LEU
7	Y	9	GLN
7	Y	10	LEU
7	Y	13	CYS
7	Y	24	GLN
7	Y	25	LEU
7	Y	34	GLU
7	Y	39	GLU
7	Y	58	GLU
7	Y	67	LEU
7	Y	102	ASN
7	Y	116	GLU
7	Y	125	GLU

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Mol	Chain	Res	Type
7	Y	131	SER
7	Y	136	VAL
7	Y	137	LEU
7	Y	140	SER
7	Y	153	LEU
7	Y	157	LEU
7	Y	165	LEU
7	Y	168	THR
7	Y	188	SER
7	Y	191	THR
7	Y	192	LEU
7	Y	200	ASP
7	Y	204	VAL
7	Y	219	HIS
7	Y	220	ILE
7	Y	222	ASN
7	Y	226	SER
7	Y	233	SER
7	Y	236	MET
7	Y	241	THR
7	Y	243	LEU
7	Y	249	MET
7	Y	254	ILE
7	Y	260	LEU
7	Y	269	LEU
7	Y	270	MET
7	Y	288	THR
7	Y	294	MET
7	Y	297	LEU
7	Y	298	LEU
7	Y	303	VAL
7	Y	304	MET
7	Y	305	VAL
7	Y	323	ILE
7	Y	324	ILE
7	Y	331	THR
7	Y	333	VAL
7	Y	340	ILE
7	Y	341	ARG
7	Y	343	ARG
7	Y	348	PHE
7	Y	355	SER

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Mol	Chain	Res	Type
7	Y	357	GLN
7	Y	358	VAL
7	Y	369	SER
7	Y	374	SER
7	Y	376	LEU
7	Y	377	MET
7	Y	383	SER
7	Y	384	ILE
7	Y	410	LYS
7	Y	420	GLU
7	Y	422	ASP
7	Y	423	THR
7	Y	426	GLU
7	Y	439	THR
7	Z	4	GLU
7	Z	7	THR
7	Z	8	LEU
7	Z	9	GLN
7	Z	10	LEU
7	Z	13	CYS
7	Z	24	GLN
7	Z	25	LEU
7	Z	34	GLU
7	Z	39	GLU
7	Z	58	GLU
7	Z	67	LEU
7	Z	102	ASN
7	Z	116	GLU
7	Z	125	GLU
7	Z	131	SER
7	Z	136	VAL
7	Z	137	LEU
7	Z	140	SER
7	Z	153	LEU
7	Z	157	LEU
7	Z	165	LEU
7	Z	168	THR
7	Z	188	SER
7	Z	191	THR
7	Z	192	LEU
7	Z	200	ASP
7	Z	204	VAL

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Mol	Chain	Res	Type
7	Z	219	HIS
7	Z	220	ILE
7	Z	222	ASN
7	Z	226	SER
7	Z	233	SER
7	Z	236	MET
7	Z	241	THR
7	Z	243	LEU
7	Z	249	MET
7	Z	254	ILE
7	Z	260	LEU
7	Z	269	LEU
7	Z	270	MET
7	Z	288	THR
7	Z	294	MET
7	Z	297	LEU
7	Z	298	LEU
7	Z	303	VAL
7	Z	304	MET
7	Z	305	VAL
7	Z	323	ILE
7	Z	324	ILE
7	Z	331	THR
7	Z	333	VAL
7	Z	340	ILE
7	Z	341	ARG
7	Z	343	ARG
7	Z	348	PHE
7	Z	355	SER
7	Z	357	GLN
7	Z	358	VAL
7	Z	369	SER
7	Z	374	SER
7	Z	376	LEU
7	Z	377	MET
7	Z	383	SER
7	Z	384	ILE
7	Z	410	LYS
7	Z	420	GLU
7	Z	422	ASP
7	Z	423	THR
7	Z	426	GLU

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Mol	Chain	Res	Type
7	Z	439	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	l	30	GLN
1	l	36	ASN
1	l	38	GLN
2	m	56	ASN
2	b	56	ASN
3	a	84	GLN
3	a	127	HIS
4	G	172	GLN
4	G	289	ASN
4	G	312	GLN
4	G	424	ASN
4	G	436	GLN
4	G	438	GLN
4	G	465	HIS
4	G	493	ASN
4	G	524	GLN
4	G	580	HIS
4	G	662	ASN
4	G	688	ASN
4	G	725	HIS
4	G	726	HIS
4	G	741	ASN
4	G	862	ASN
3	H	310	GLN
3	H	322	GLN
3	H	329	HIS
3	H	347	GLN
3	H	389	GLN
3	H	491	ASN
3	H	528	ASN
3	H	609	ASN
3	H	684	HIS
3	H	716	HIS
3	H	739	GLN
3	H	740	GLN
3	H	774	GLN
3	H	787	ASN

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Mol	Chain	Res	Type
3	H	830	ASN
3	H	855	GLN
3	H	859	GLN
3	H	883	ASN
5	I	29	GLN
5	I	193	HIS
5	I	398	GLN
5	I	401	HIS
5	I	460	GLN
5	I	464	HIS
5	I	489	GLN
5	I	493	GLN
5	I	508	ASN
5	I	520	HIS
5	I	540	GLN
5	I	543	GLN
5	I	561	HIS
5	I	571	GLN
5	I	584	ASN
1	J	222	HIS
1	J	288	GLN
1	J	316	GLN
1	J	413	HIS
1	J	642	HIS
1	J	754	ASN
1	J	818	GLN
1	J	822	ASN
1	J	916	GLN
1	J	989	ASN
5	K	3	HIS
5	K	43	ASN
5	K	67	GLN
5	K	82	HIS
5	K	102	GLN
5	K	130	GLN
5	K	152	GLN
5	K	199	GLN
5	K	284	GLN
5	K	339	HIS
5	K	377	GLN
5	K	390	HIS
5	K	397	GLN

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Mol	Chain	Res	Type
5	K	501	GLN
5	K	519	ASN
5	K	529	GLN
5	K	543	GLN
5	K	549	ASN
5	K	622	GLN
5	K	652	ASN
6	L	340	GLN
6	L	358	ASN
6	L	469	GLN
6	L	1492	ASN
6	L	1525	GLN
6	L	1654	GLN
6	L	1673	GLN
6	L	1678	ASN
6	L	1679	GLN
6	L	1710	HIS
6	L	1788	ASN
7	U	12	GLN
7	U	16	GLN
7	U	158	ASN
7	U	187	ASN
7	U	197	GLN
7	U	198	ASN
7	U	229	ASN
7	U	322	ASN
7	U	332	GLN
7	U	347	ASN
7	V	12	GLN
7	V	16	GLN
7	V	187	ASN
7	V	197	GLN
7	V	198	ASN
7	V	229	ASN
7	V	322	ASN
7	V	332	GLN
7	V	334	HIS
7	V	347	ASN
7	W	12	GLN
7	W	16	GLN
7	W	187	ASN
7	W	197	GLN

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Mol	Chain	Res	Type
7	W	198	ASN
7	W	229	ASN
7	W	322	ASN
7	W	332	GLN
7	W	347	ASN
7	X	12	GLN
7	X	16	GLN
7	X	187	ASN
7	X	197	GLN
7	X	198	ASN
7	X	229	ASN
7	X	322	ASN
7	X	332	GLN
7	X	347	ASN
7	Y	12	GLN
7	Y	16	GLN
7	Y	158	ASN
7	Y	187	ASN
7	Y	197	GLN
7	Y	198	ASN
7	Y	229	ASN
7	Y	322	ASN
7	Y	332	GLN
7	Y	334	HIS
7	Y	347	ASN
7	Z	12	GLN
7	Z	16	GLN
7	Z	187	ASN
7	Z	197	GLN
7	Z	198	ASN
7	Z	229	ASN
7	Z	267	HIS
7	Z	322	ASN
7	Z	332	GLN
7	Z	334	HIS
7	Z	347	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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.

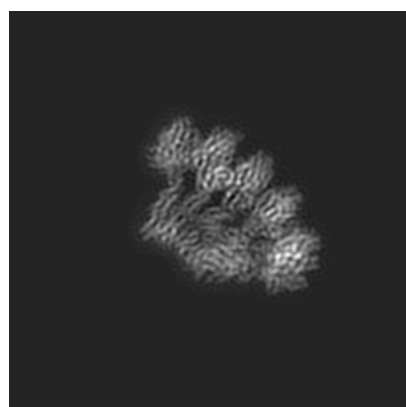
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14006. These allow visual inspection of the internal detail of the map and identification of artifacts.

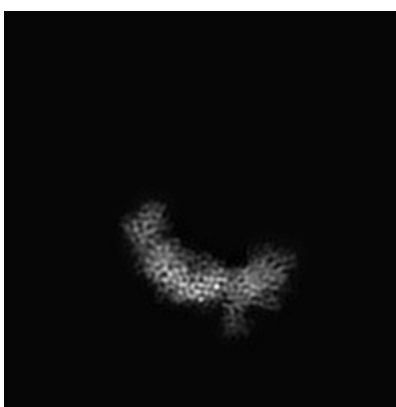
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

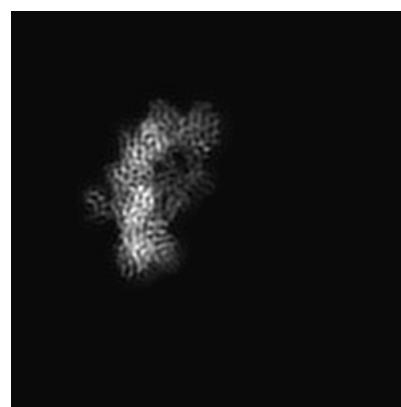
6.1.1 Primary map



X



Y

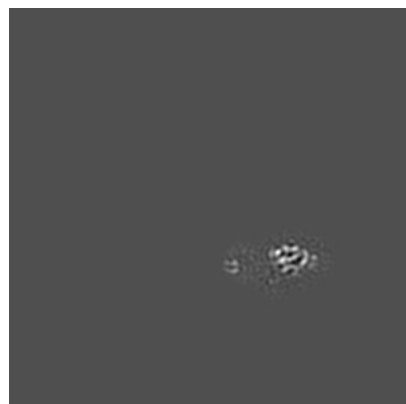


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 62



Y Index: 101

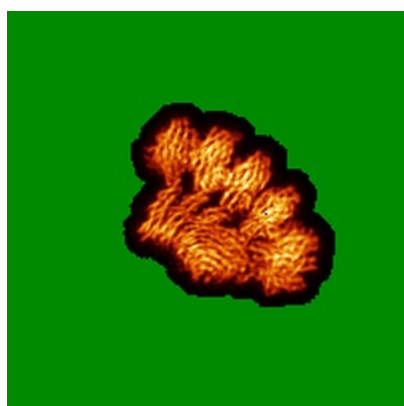


Z Index: 77

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

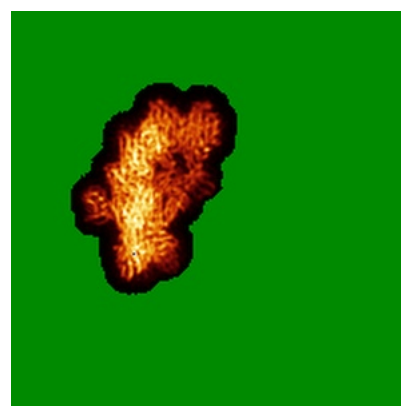
6.4.1 Primary map



X



Y

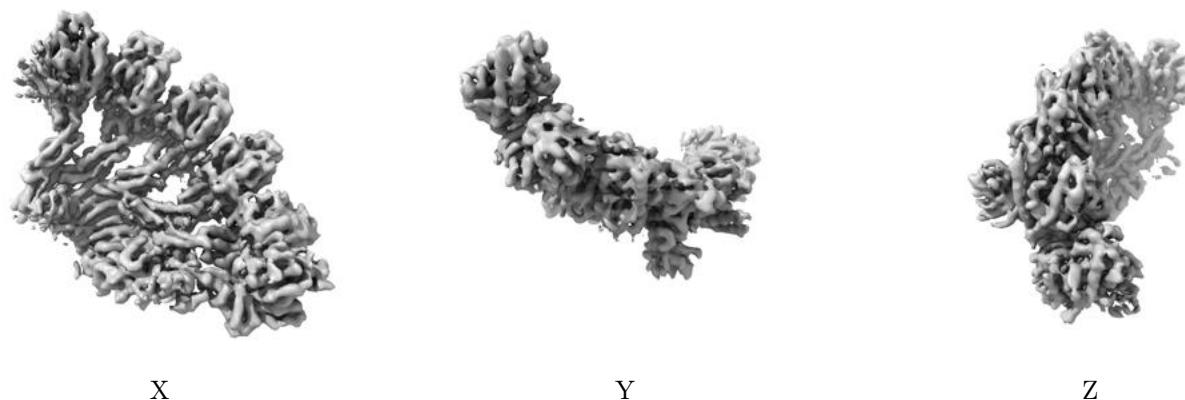


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0571. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

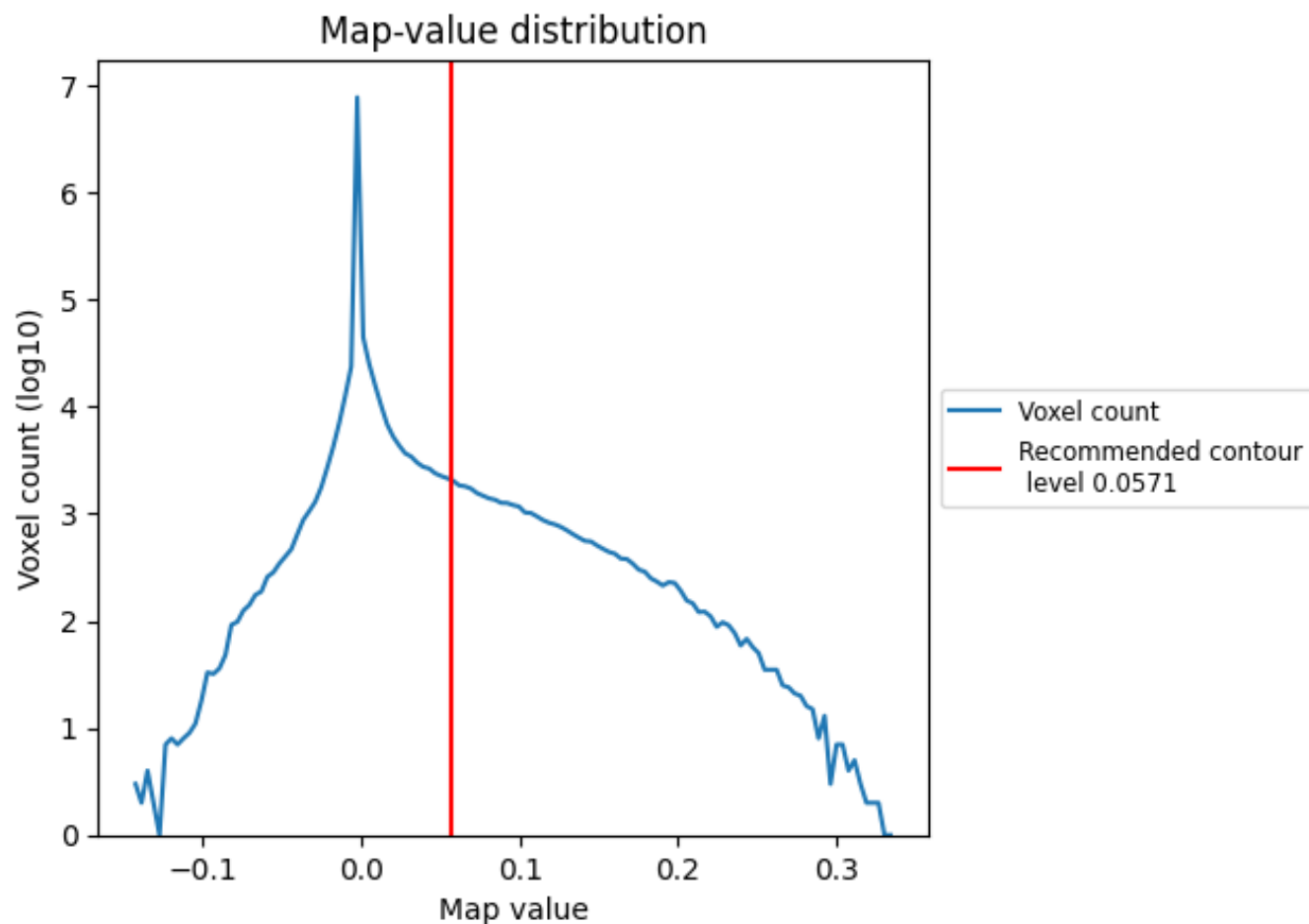
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

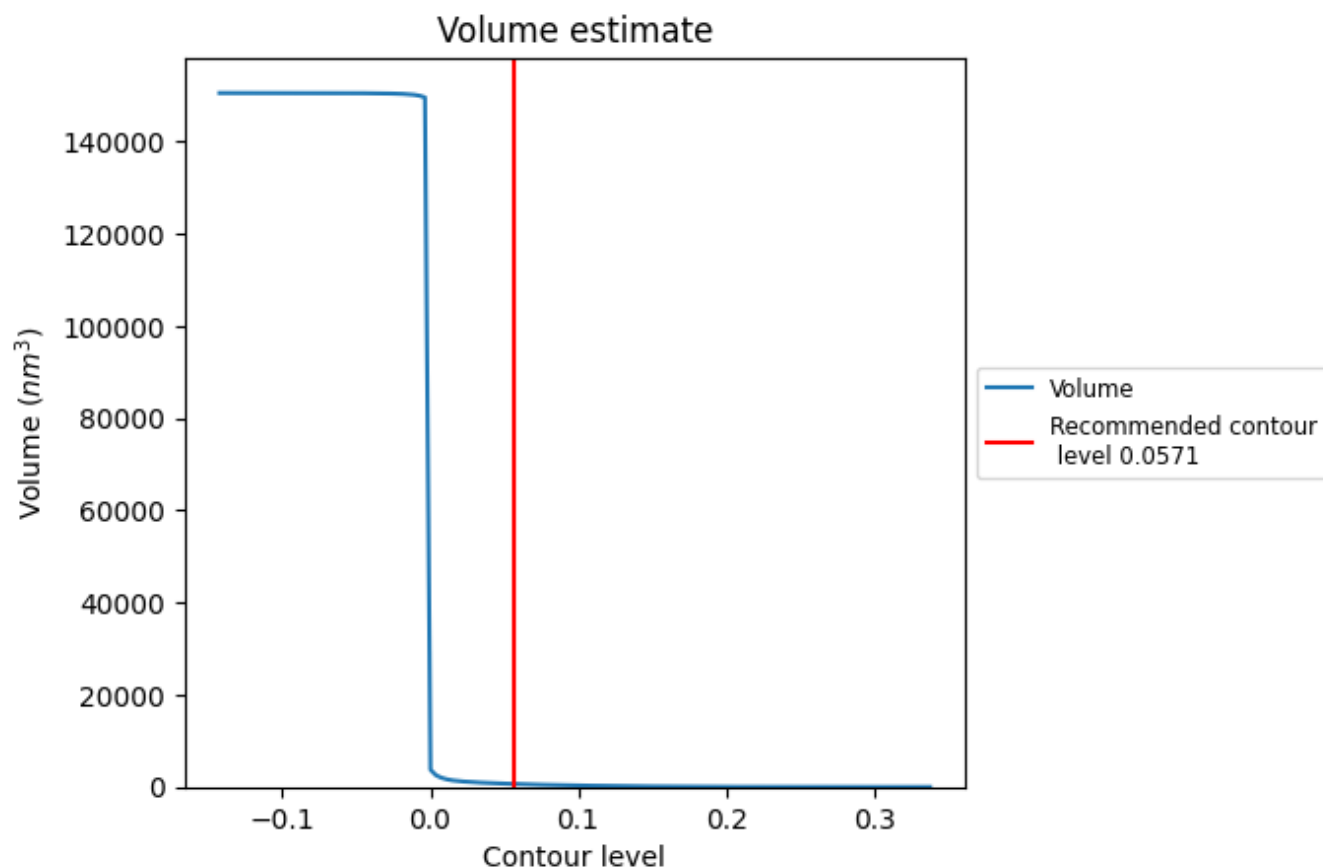
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

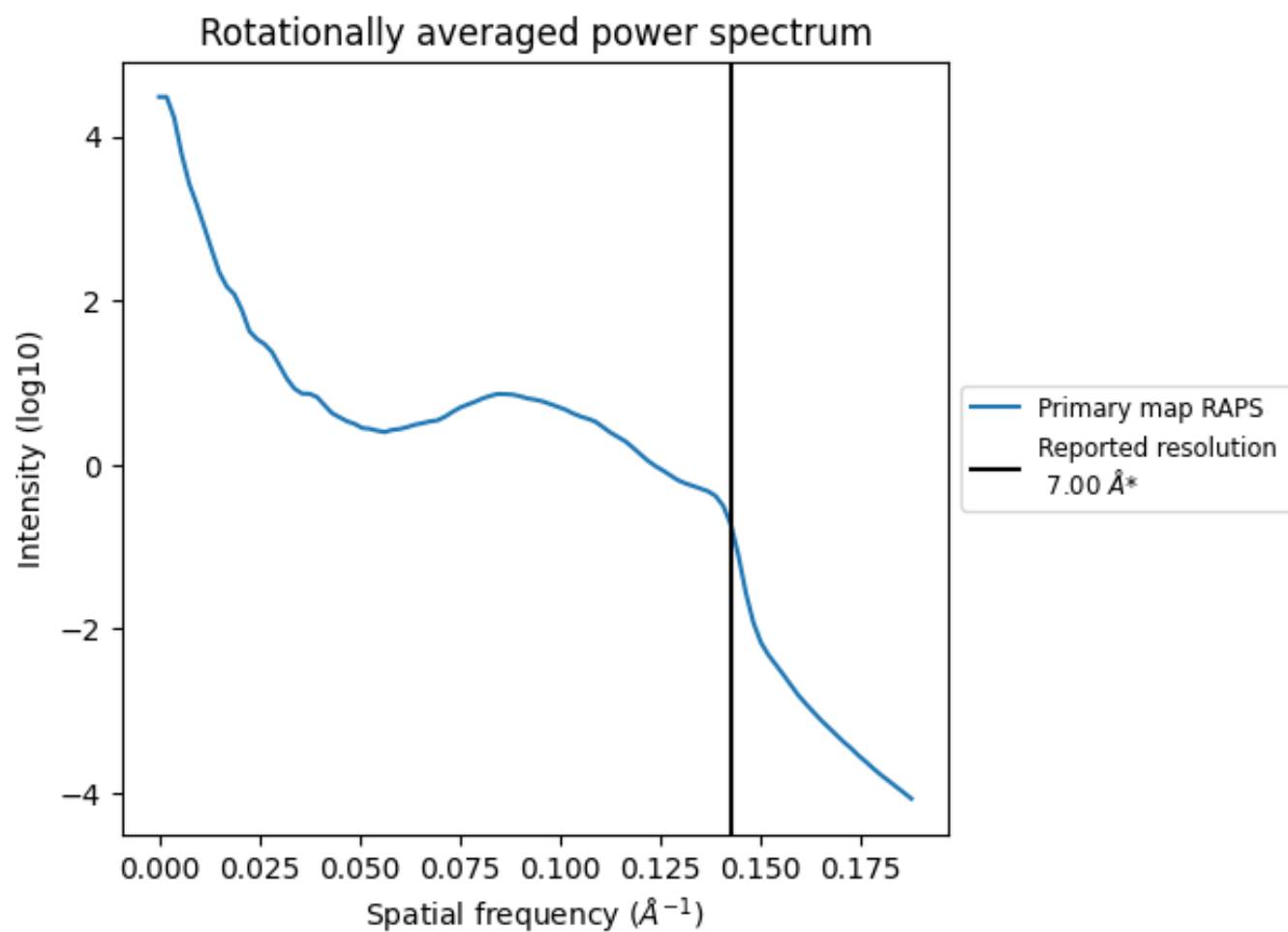
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 646 nm³; this corresponds to an approximate mass of 584 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

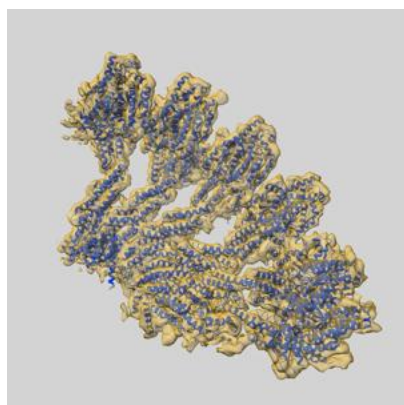
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

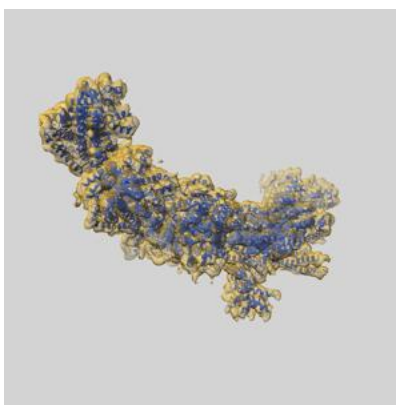
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14006 and PDB model 7QJ1. Per-residue inclusion information can be found in section [3](#) on page [6](#).

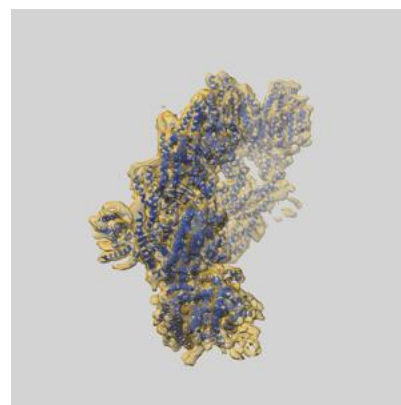
9.1 Map-model overlay [i](#)



X



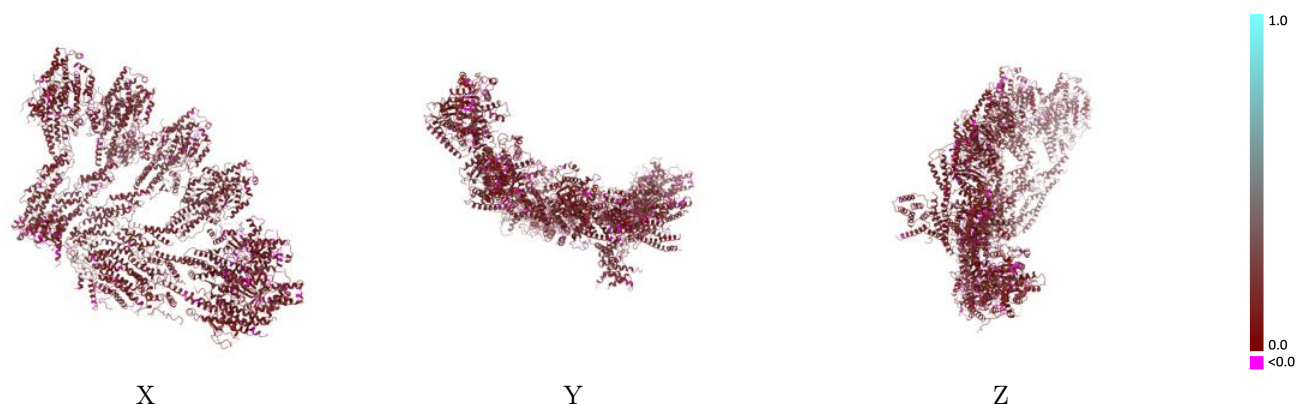
Y



Z

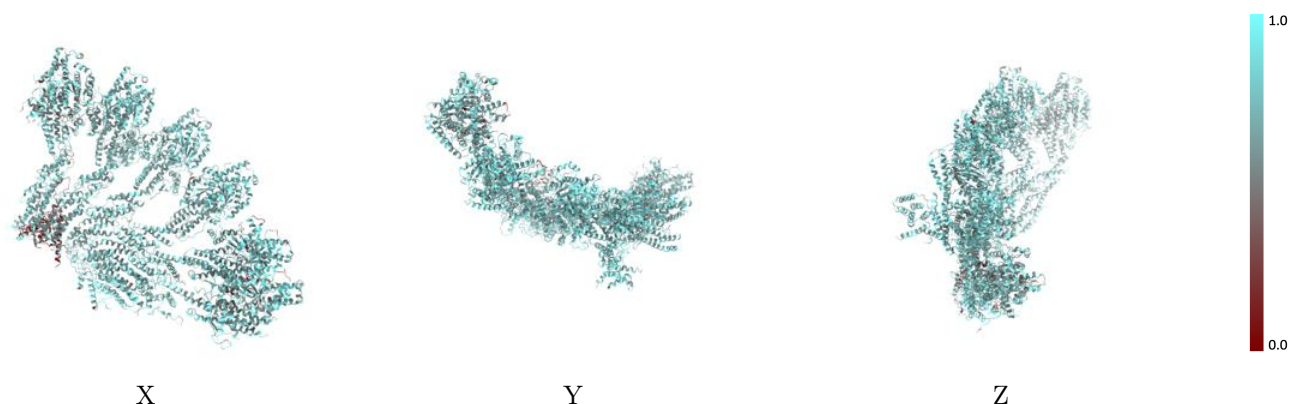
The images above show the 3D surface view of the map at the recommended contour level 0.0571 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



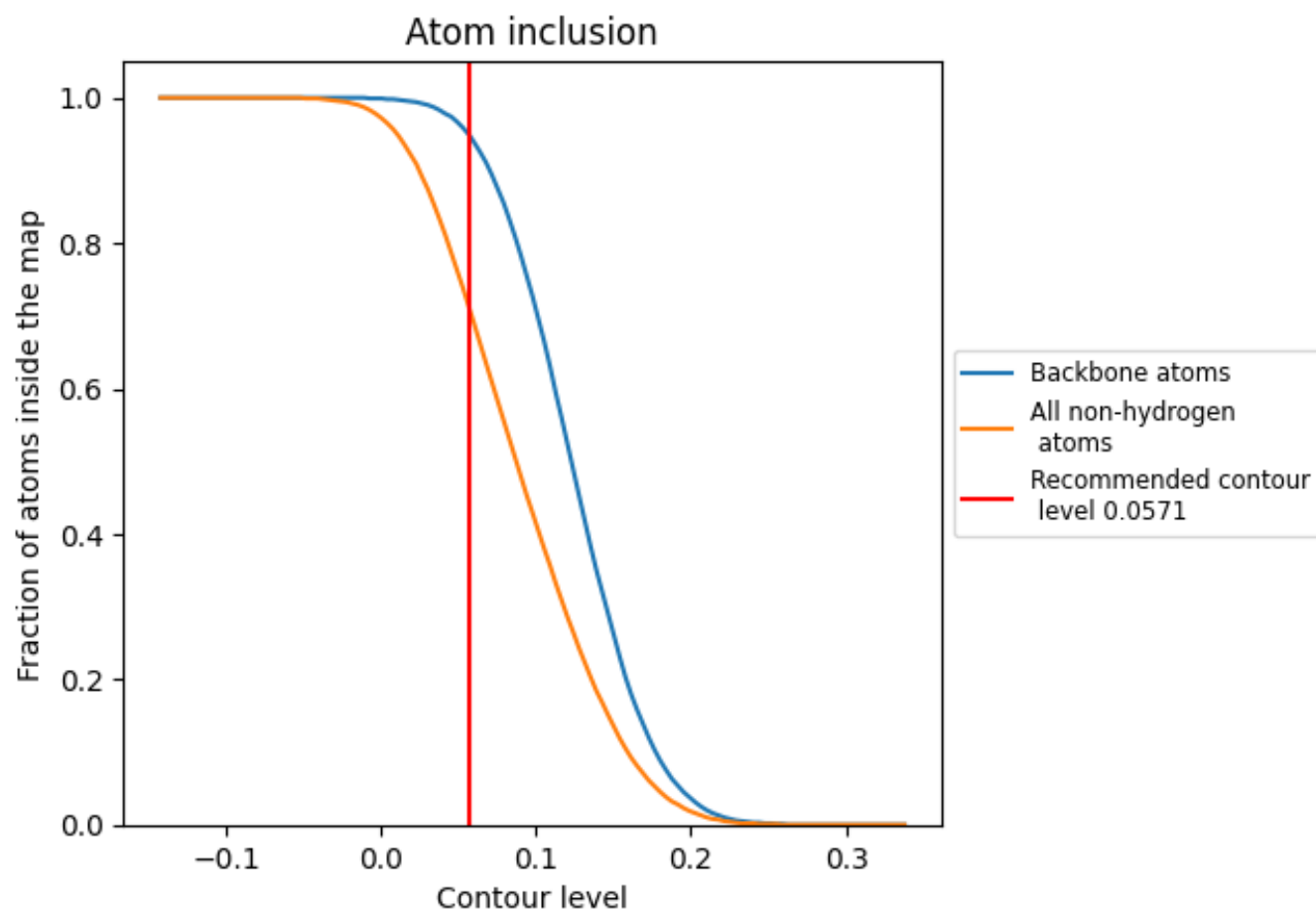
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0571).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0571) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7090	 0.1560
G	 0.6840	 0.1600
H	 0.7190	 0.1520
I	 0.7350	 0.1660
J	 0.7370	 0.1610
K	 0.7300	 0.1600
L	 0.7110	 0.1590
U	 0.6820	 0.1470
V	 0.7410	 0.1560
W	 0.7480	 0.1520
X	 0.7560	 0.1700
Y	 0.7270	 0.1350
Z	 0.6590	 0.1460
a	 0.3490	 0.1300
b	 0.3890	 0.1390
l	 0.7540	 0.1680
m	 0.7460	 0.1740

