



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:26 AM UTC

PDB ID : 9QVM / pdb_00009qvm
EMDB ID : EMD-53399
Title : Cryo-EM reconstruction of the NEDD1 anchor protein and CDK5RAP2 bound to the gamma-tubulin ring complex
Authors : Munoz-Hernandez, H.; Xu, Y.; Wieczorek, M.
Deposited on : 2025-04-11
Resolution : 6.80 Å(reported)
Based on initial model : .

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

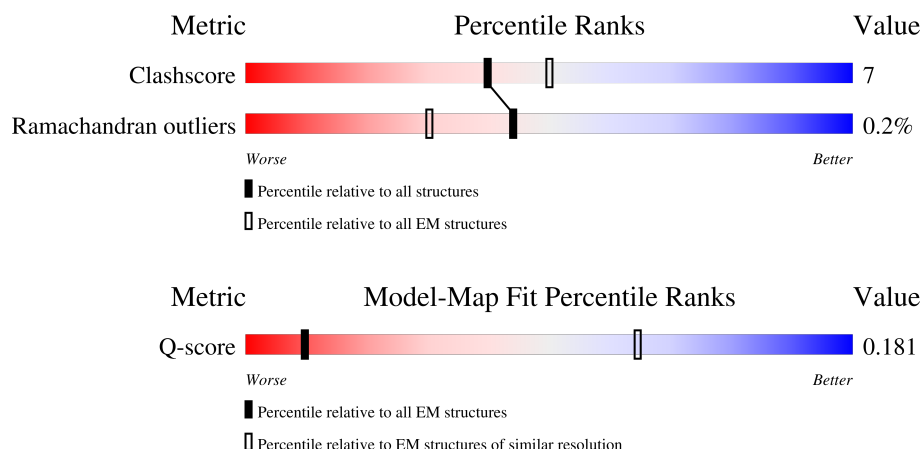
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 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.



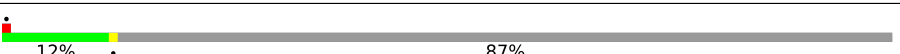
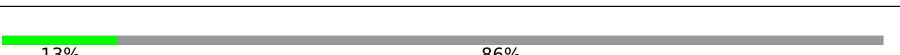
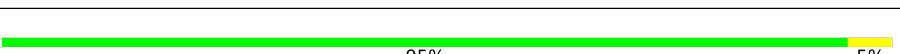
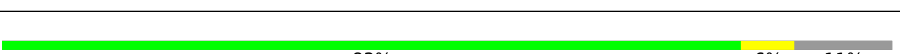
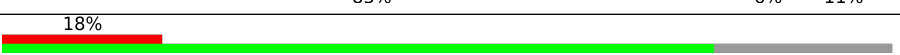
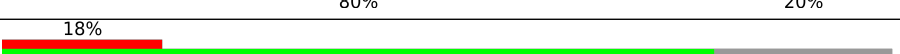
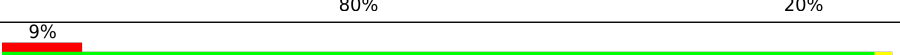
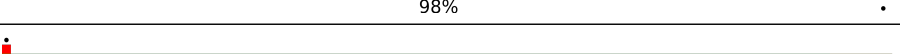
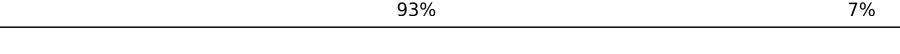
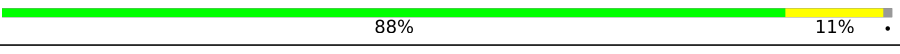
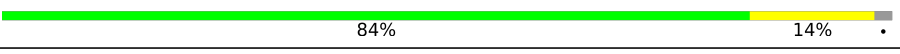
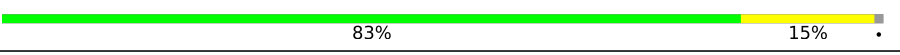
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	503 (6.30 - 7.30)

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	B	907	
1	D	907	
1	F	907	
1	H	907	
1	N	907	

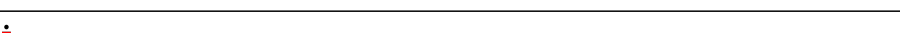
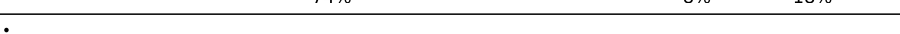
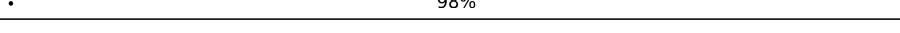
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	r	907	 12% 88%
1	s	907	 12% 87%
1	t	907	 12% 87%
1	u	907	 12% 87%
1	v	907	 13% 86%
2	O	82	 95% 5%
2	P	82	 83% 6% 11%
2	Q	82	 18% 80% 20%
2	R	82	 30% 80% 20%
2	S	82	 18% 80% 20%
2	T	82	 9% 98%
2	U	82	 93% 7%
3	V	660	 12% 88%
3	W	660	 11% 88%
3	X	660	 11% 88%
3	Y	660	 12% 88%
4	Z	375	 82% 18%
5	a	457	 87% 11%
5	b	457	 88% 11%
5	c	457	 84% 14%
5	d	457	 83% 15%
5	e	457	 87% 11%
5	f	457	 84% 15%
5	g	457	 84% 15%
5	h	457	 84% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	i	457	 86% 12%
5	j	457	 85% 13%
5	k	457	 85% 13%
5	l	457	 88% 9%
5	m	457	 93% 5%
5	n	457	 15% 94% 6%
6	I	667	 83% 9% 8%
6	K	667	 84% 8% 8%
7	A	930	 66% 5% 29%
7	C	930	 66% 5% 30%
7	E	930	 68% 5% 27%
7	G	930	 68% 5% 27%
7	M	930	 81% 5% 17%
8	L	1811	 50% 5% 46%
9	J	1024	 74% 8% 18%
10	p	158	 34% 65%
11	w	1663	 98%
11	x	1663	 98%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 88888 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 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	D	657	Total	C	N	O	0	0
			3256	1942	657	657		
1	F	657	Total	C	N	O	0	0
			3256	1942	657	657		
1	H	656	Total	C	N	O	0	0
			3252	1940	656	656		
1	r	113	Total	C	N	O	0	0
			562	336	113	113		
1	s	115	Total	C	N	O	0	0
			572	342	115	115		
1	t	120	Total	C	N	O	0	0
			597	357	120	120		
1	u	120	Total	C	N	O	0	0
			597	357	120	120		
1	v	129	Total	C	N	O	0	0
			642	384	129	129		
1	B	644	Total	C	N	O	0	0
			3192	1904	644	644		
1	N	630	Total	C	N	O	0	0
			3123	1863	630	630		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	82	Total	C	N	O	0	0
			406	242	82	82		
2	P	73	Total	C	N	O	0	0
			363	217	73	73		
2	Q	66	Total	C	N	O	0	0
			328	196	66	66		
2	R	66	Total	C	N	O	0	0
			328	196	66	66		
2	S	66	Total	C	N	O	0	0
			328	196	66	66		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
2	T	82	Total	C	N	O	0	0
			406	242	82	82		
2	U	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 3 is a protein called Protein NEDD1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	W	79	Total	C	N	O	0	0
			394	236	79	79		
3	X	78	Total	C	N	O	0	0
			389	233	78	78		
3	V	77	Total	C	N	O	0	0
			384	230	77	77		
3	Y	78	Total	C	N	O	0	0
			389	233	78	78		

- Molecule 4 is a protein called Actin, cytoplasmic 1, N-terminally processed.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Z	375	Total	C	N	O	0	0
			1847	1097	375	375		

- Molecule 5 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	a	446	Total	C	N	O	0	0
			2204	1312	446	446		
5	b	452	Total	C	N	O	0	0
			2233	1329	452	452		
5	c	448	Total	C	N	O	0	0
			2213	1317	448	448		
5	e	448	Total	C	N	O	0	0
			2213	1317	448	448		
5	f	451	Total	C	N	O	0	0
			2228	1326	451	451		
5	g	450	Total	C	N	O	0	0
			2223	1323	450	450		
5	h	451	Total	C	N	O	0	0
			2228	1326	451	451		
5	i	448	Total	C	N	O	0	0
			2213	1317	448	448		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
5	j	449	Total	C	N	O	0	0
			2218	1320	449	449		
5	k	448	Total	C	N	O	0	0
			2213	1317	448	448		
5	l	447	Total	C	N	O	0	0
			2208	1314	447	447		
5	m	448	Total	C	N	O	0	0
			2213	1317	448	448		
5	n	457	Total	C	N	O	0	0
			2258	1344	457	457		
5	d	451	Total	C	N	O	0	0
			2228	1326	451	451		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	452	GLU	-	expression tag	UNP P23258
a	453	ASN	-	expression tag	UNP P23258
a	454	LEU	-	expression tag	UNP P23258
a	455	TYR	-	expression tag	UNP P23258
a	456	PHE	-	expression tag	UNP P23258
a	457	GLN	-	expression tag	UNP P23258
b	452	GLU	-	expression tag	UNP P23258
b	453	ASN	-	expression tag	UNP P23258
b	454	LEU	-	expression tag	UNP P23258
b	455	TYR	-	expression tag	UNP P23258
b	456	PHE	-	expression tag	UNP P23258
b	457	GLN	-	expression tag	UNP P23258
c	452	GLU	-	expression tag	UNP P23258
c	453	ASN	-	expression tag	UNP P23258
c	454	LEU	-	expression tag	UNP P23258
c	455	TYR	-	expression tag	UNP P23258
c	456	PHE	-	expression tag	UNP P23258
c	457	GLN	-	expression tag	UNP P23258
e	452	GLU	-	expression tag	UNP P23258
e	453	ASN	-	expression tag	UNP P23258
e	454	LEU	-	expression tag	UNP P23258
e	455	TYR	-	expression tag	UNP P23258
e	456	PHE	-	expression tag	UNP P23258
e	457	GLN	-	expression tag	UNP P23258
f	452	GLU	-	expression tag	UNP P23258
f	453	ASN	-	expression tag	UNP P23258
f	454	LEU	-	expression tag	UNP P23258

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
f	455	TYR	-	expression tag	UNP P23258
f	456	PHE	-	expression tag	UNP P23258
f	457	GLN	-	expression tag	UNP P23258
g	452	GLU	-	expression tag	UNP P23258
g	453	ASN	-	expression tag	UNP P23258
g	454	LEU	-	expression tag	UNP P23258
g	455	TYR	-	expression tag	UNP P23258
g	456	PHE	-	expression tag	UNP P23258
g	457	GLN	-	expression tag	UNP P23258
h	452	GLU	-	expression tag	UNP P23258
h	453	ASN	-	expression tag	UNP P23258
h	454	LEU	-	expression tag	UNP P23258
h	455	TYR	-	expression tag	UNP P23258
h	456	PHE	-	expression tag	UNP P23258
h	457	GLN	-	expression tag	UNP P23258
i	452	GLU	-	expression tag	UNP P23258
i	453	ASN	-	expression tag	UNP P23258
i	454	LEU	-	expression tag	UNP P23258
i	455	TYR	-	expression tag	UNP P23258
i	456	PHE	-	expression tag	UNP P23258
i	457	GLN	-	expression tag	UNP P23258
j	452	GLU	-	expression tag	UNP P23258
j	453	ASN	-	expression tag	UNP P23258
j	454	LEU	-	expression tag	UNP P23258
j	455	TYR	-	expression tag	UNP P23258
j	456	PHE	-	expression tag	UNP P23258
j	457	GLN	-	expression tag	UNP P23258
k	452	GLU	-	expression tag	UNP P23258
k	453	ASN	-	expression tag	UNP P23258
k	454	LEU	-	expression tag	UNP P23258
k	455	TYR	-	expression tag	UNP P23258
k	456	PHE	-	expression tag	UNP P23258
k	457	GLN	-	expression tag	UNP P23258
l	452	GLU	-	expression tag	UNP P23258
l	453	ASN	-	expression tag	UNP P23258
l	454	LEU	-	expression tag	UNP P23258
l	455	TYR	-	expression tag	UNP P23258
l	456	PHE	-	expression tag	UNP P23258
l	457	GLN	-	expression tag	UNP P23258
m	452	GLU	-	expression tag	UNP P23258
m	453	ASN	-	expression tag	UNP P23258
m	454	LEU	-	expression tag	UNP P23258

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
m	455	TYR	-	expression tag	UNP P23258
m	456	PHE	-	expression tag	UNP P23258
m	457	GLN	-	expression tag	UNP P23258
n	452	GLU	-	expression tag	UNP P23258
n	453	ASN	-	expression tag	UNP P23258
n	454	LEU	-	expression tag	UNP P23258
n	455	TYR	-	expression tag	UNP P23258
n	456	PHE	-	expression tag	UNP P23258
n	457	GLN	-	expression tag	UNP P23258
d	452	GLU	-	expression tag	UNP P23258
d	453	ASN	-	expression tag	UNP P23258
d	454	LEU	-	expression tag	UNP P23258
d	455	TYR	-	expression tag	UNP P23258
d	456	PHE	-	expression tag	UNP P23258
d	457	GLN	-	expression tag	UNP P23258

- Molecule 6 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	614	Total	C	N	O	0	0
			3037	1809	614	614		
6	I	612	Total	C	N	O	0	0
			3027	1803	612	612		

- Molecule 7 is a protein called Isoform 3 of Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	678	Total	C	N	O	0	0
			3367	2011	678	678		
7	C	653	Total	C	N	O	0	0
			3244	1938	653	653		
7	A	657	Total	C	N	O	0	0
			3264	1950	657	657		
7	E	678	Total	C	N	O	0	0
			3367	2011	678	678		
7	M	771	Total	C	N	O	0	0
			3828	2286	771	771		

- Molecule 8 is a protein called TUBGCP6 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	982	Total	C	N	O	0	0
			4851	2887	982	982		

- Molecule 9 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	842	Total	C	N	O	0	0
			4186	2502	842	842		

- Molecule 10 is a protein called Mitotic-spindle organizing protein 2B.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	p	56	Total	C	N	O	0	0
			277	165	56	56		

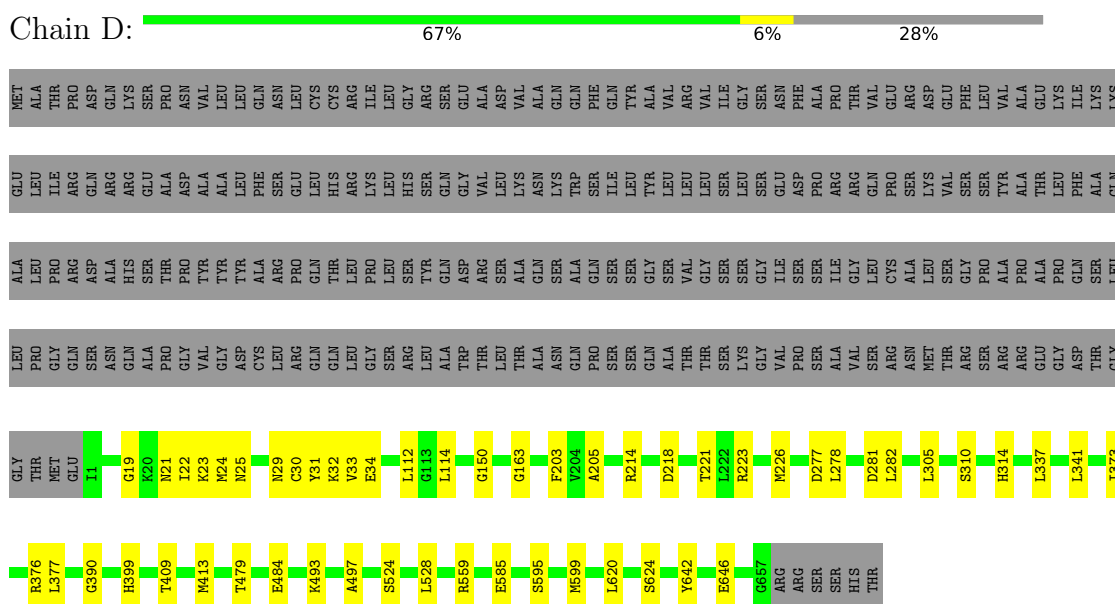
- Molecule 11 is a protein called CDK5 regulatory subunit-associated protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	x	33	Total	C	N	O	0	0
			165	99	33	33		
11	w	33	Total	C	N	O	0	0
			165	99	33	33		

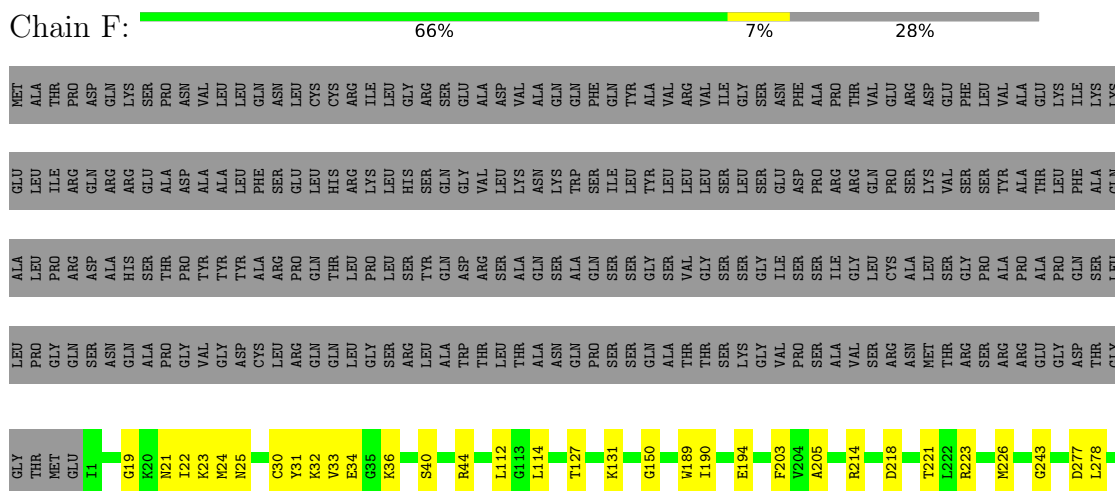
3 Residue-property plots

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 3

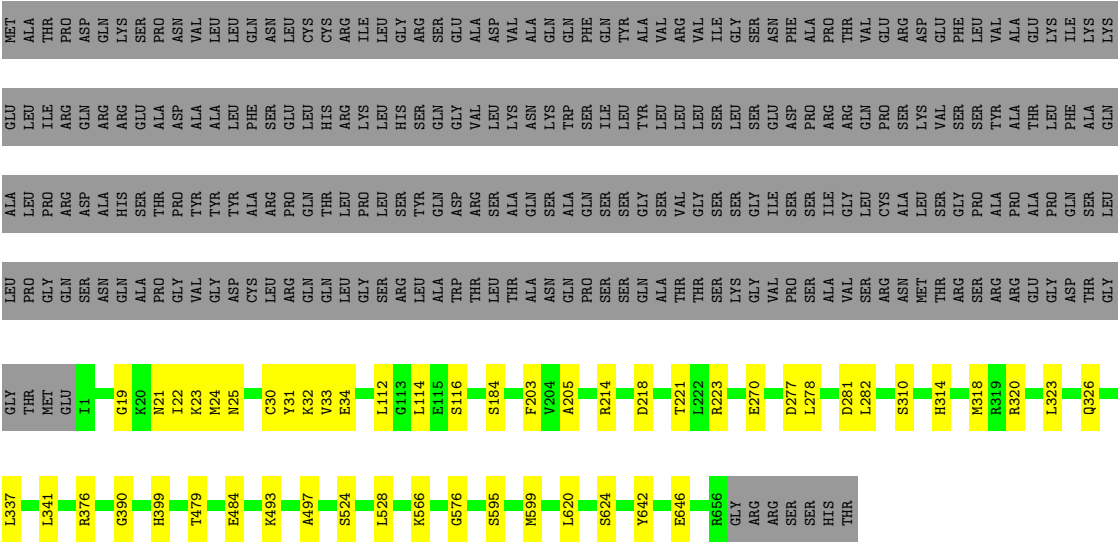


• Molecule 1: Gamma-tubulin complex component 3

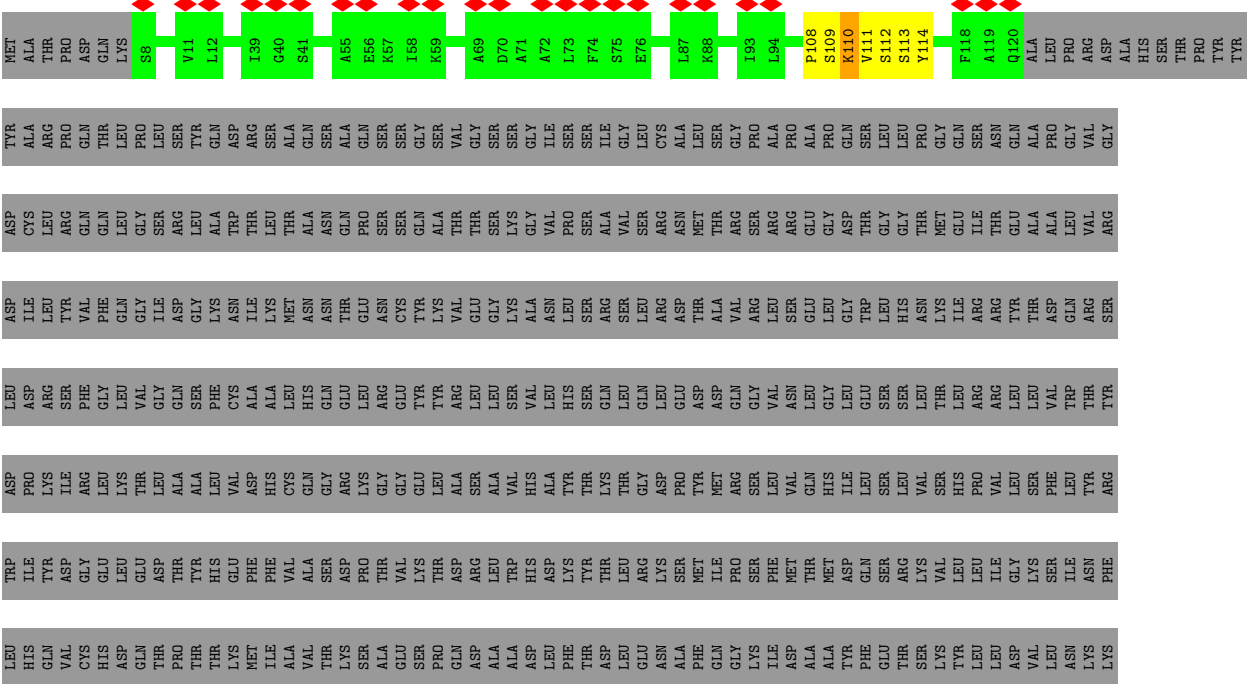




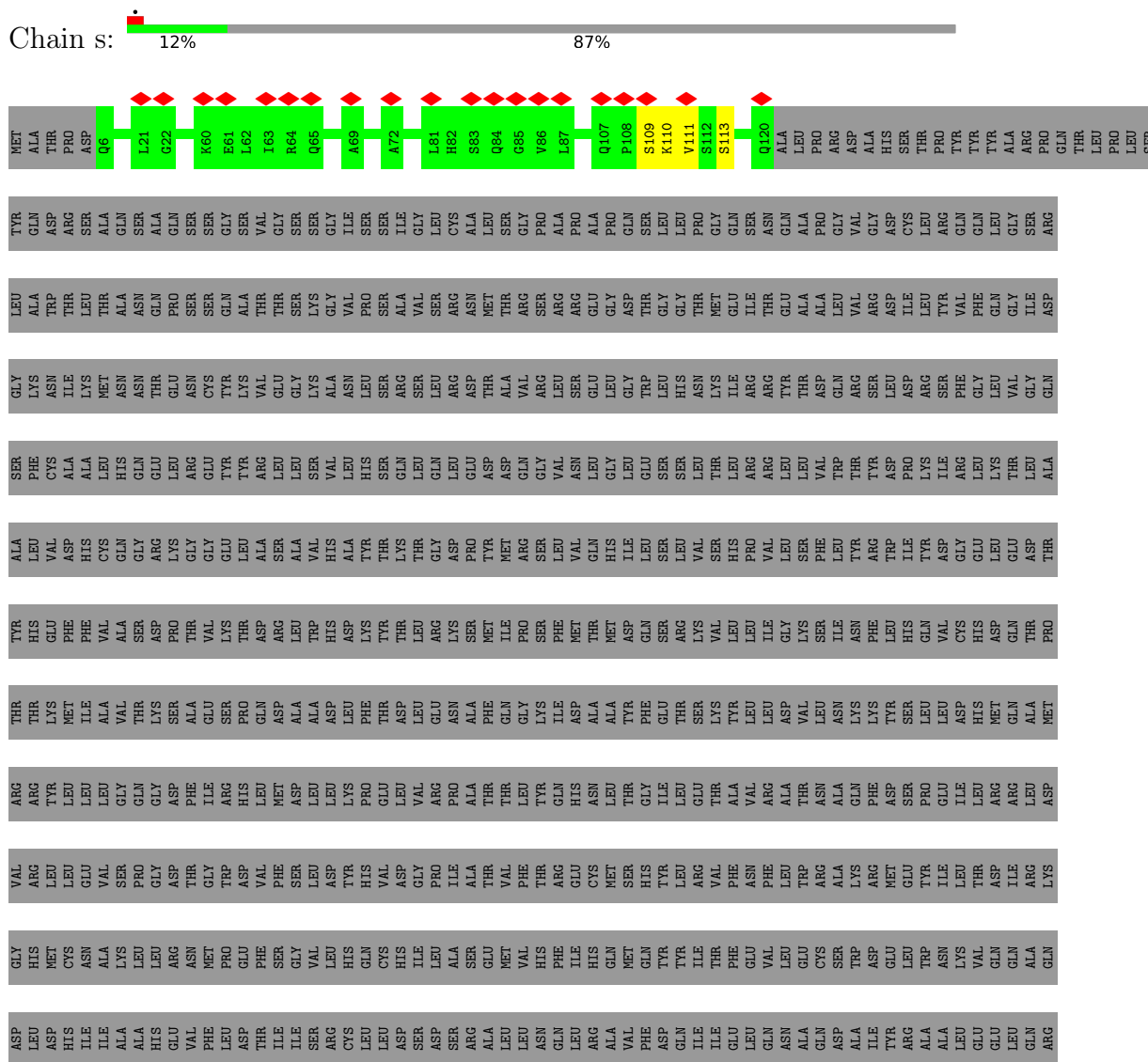
• Molecule 1: Gamma-tubulin complex component 3



• Molecule 1: Gamma-tubulin complex component 3



- Molecule 1: Gamma-tubulin complex component 3



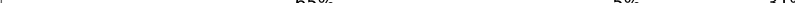
[illegible]

- Molecule 1: Gamma-tubulin complex component 3

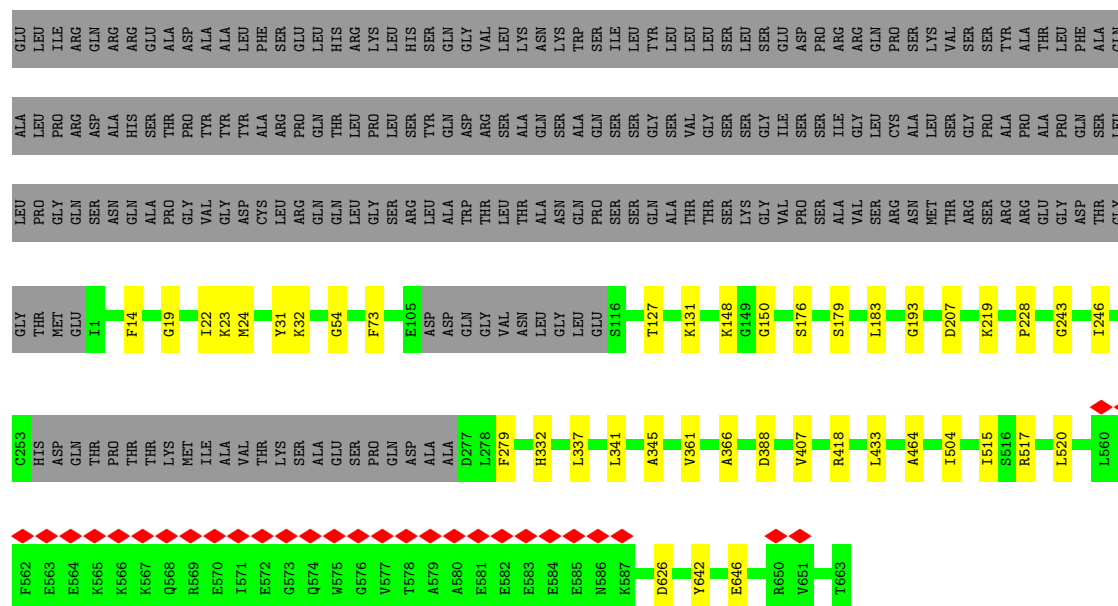
Chain B: 67% . 29%

GLU	THR	GLY	LEU	ALA	GLU	MET
SER	THR	THR	PRO	LEU	LEU	ALA
PRO	GLY	GLY	GLN	PRO	ILE	THR
Q273	GLU	SER	SER	ASP	ARG	PRO
F286	I1	ASN	GLN	ALA	ARG	GLN
I290	K23	GLN	GLN	HIS	ARG	LYS
S310	M24	ALA	PRO	SER	GLU	SER
H314	Y31	GLY	VAL	THR	ALA	PRO
L337	K32	VAL	GLY	TYR	ALA	VAL
L341	L112	ASP	TYR	TYR	LEU	LEU
G390	G113	CYS	ALA	ARG	PHE	GLN
S524	L114	LEU	ARG	PRO	SER	ASN
L528	E115	ARG	GLN	GLN	GLU	LEU
K566	S116	GLN	GLN	THR	LEU	CYS
G576	G150	LEU	GLY	LEU	ARG	CYS
S595	S154	SER	GLY	PRO	ILE	ARG
M599	Y159	LEU	TYR	SER	GLY	LYS
L620	T162	TRP	ALA	ASP	GLN	GLY
S624	G163	THR	LEU	ARG	ASP	SER
K556	D164	THR	ALA	ALA	LYS	VAL
GLY	R168	ALA	ASN	GLN	ASN	VAL
ARG	S179	ASN	GLN	SER	LEU	ARG
ARG	L183	PRO	PRO	GLN	LEU	VAL
SER	F203	SER	SER	SER	ILE	VAL
SER	V204	GLN	GLY	GLY	TYR	GLY
HIS	A205	ALA	SER	ILE	LEU	SER
THR	T221	THR	VAL	VAL	LEU	ASN
ARG	L222	SER	GLY	SER	ASP	PHE
SER	R223	LYS	LYS	GLY	GLU	GLY
HIS	M226	VAL	VAL	ILE	GLU	ASN
THR	D255	PRO	ASN	SER	ASP	PHE
GLY	T260	SER	MET	ILE	PRO	ALA
ALA	LYS	ARG	THR	GLY	ARG	PRO
SER	MET	SER	ARG	LEU	GLN	THR
ILE	ILE	SER	SER	PRO	VAL	VAL
ALA	ALA	ARG	ARG	ALA	ALA	ALA
THR	THR	GLY	GLY	PRO	THR	LYS
LYS	LYS	ASP	GLN	GLN	PHE	ILE
SER	SER	THR	SER	THR	ALA	LYS
ALA	ALA	GLY	THR	THR	GLN	LYS

- Molecule 1: Gamma-tubulin complex component 3

Chain N:  65% 5% 31%

MET	ALA	THR	PRO	ASP	GLN	LYS	SER	PRO	ASN	VAL	LEU	GLN	ASN	LEU	CYS	CYS	ARG	ILE	LEU	GLY	ARG	SER	GLU	ALA	ASP	VAL	GLN	GLN	PHE	GLN	TYR	ALA	ALA	VAL	ARG	VAL	ILE	GLY	SER	ASN	PHE	ALA	PRO	THR	VAL	GLU	ARG	ASP	GLU	PHE	LEU	VAL	ALA	LYS	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



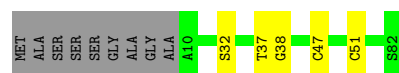
• Molecule 2: Mitotic-spindle organizing protein 1

Chain O: 95% 5%



• Molecule 2: Mitotic-spindle organizing protein 1

Chain P: 83% 6% 11%



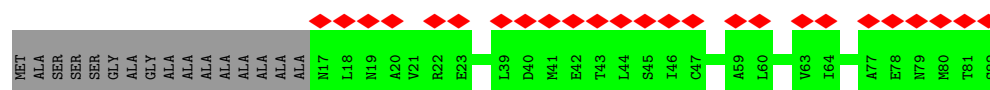
• Molecule 2: Mitotic-spindle organizing protein 1

Chain Q: 18% 80% 20%



• Molecule 2: Mitotic-spindle organizing protein 1

Chain R: 30% 80% 20%



• Molecule 2: Mitotic-spindle organizing protein 1

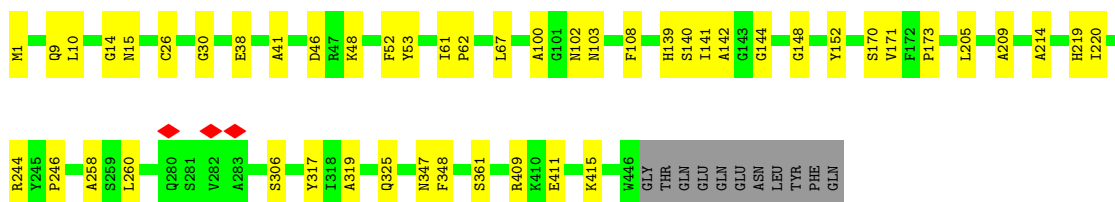
Chain S: 18% 80% 20%



[illegible]

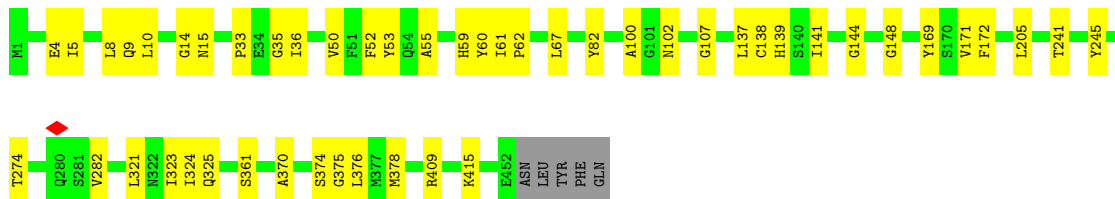
Chain V: 12% 88%

[illegible]



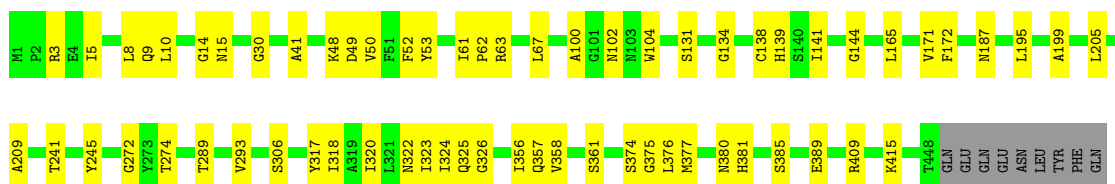
- Molecule 5: Tubulin gamma-1 chain

Chain b: .



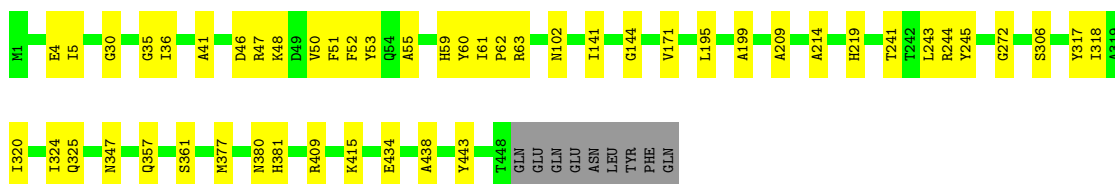
- Molecule 5: Tubulin gamma-1 chain

Chain c: .



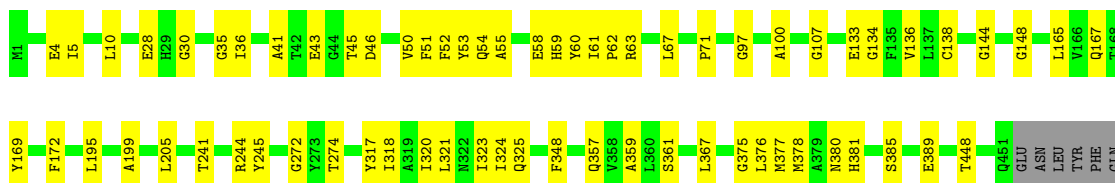
- Molecule 5: Tubulin gamma-1 chain

Chain e: .

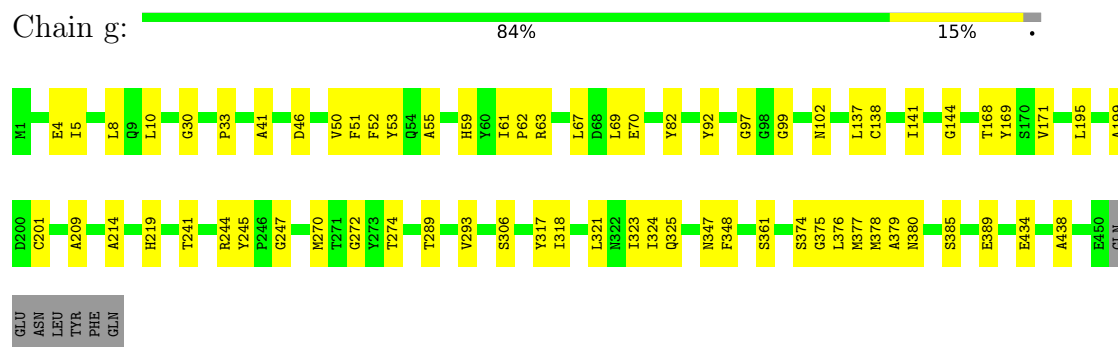


- Molecule 5: Tubulin gamma-1 chain

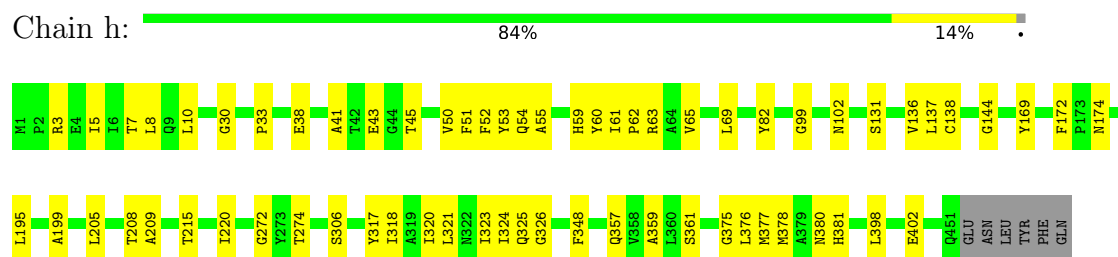
Chain f: .



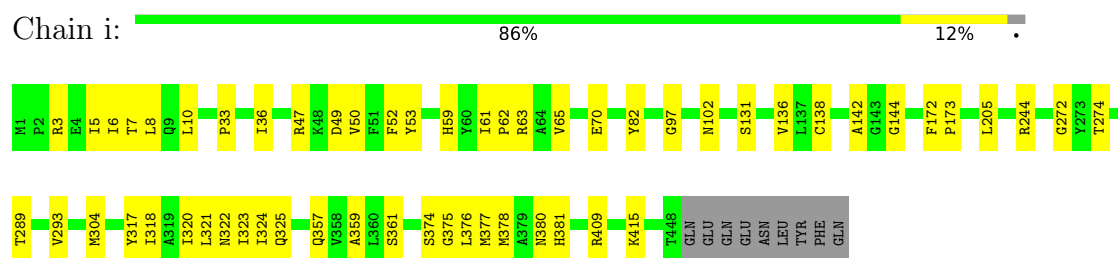
- Molecule 5: Tubulin gamma-1 chain



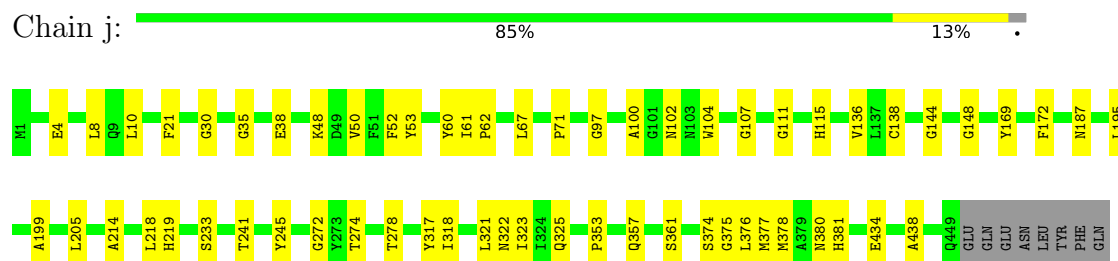
- Molecule 5: Tubulin gamma-1 chain



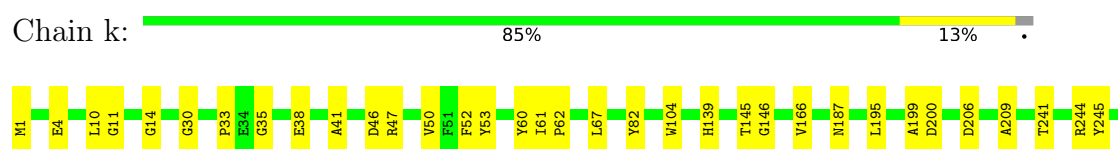
- Molecule 5: Tubulin gamma-1 chain

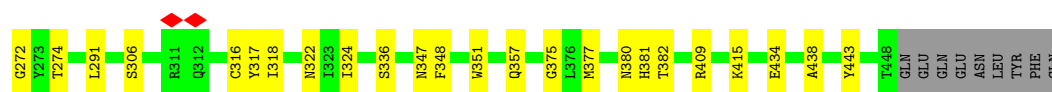


- Molecule 5: Tubulin gamma-1 chain



- Molecule 5: Tubulin gamma-1 chain





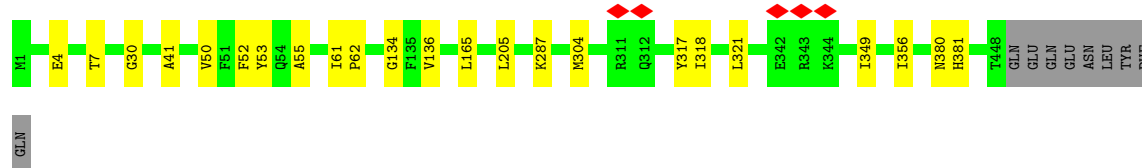
• Molecule 5: Tubulin gamma-1 chain

Chain l: 88% 9% .



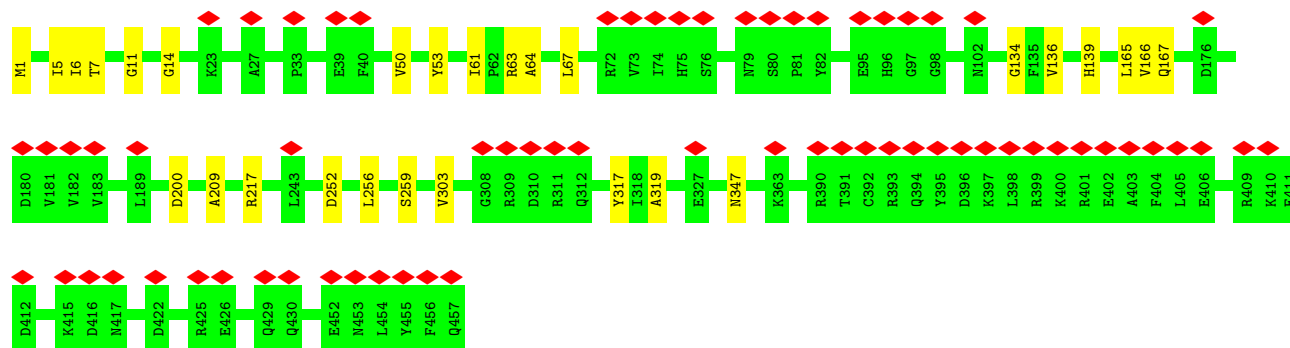
• Molecule 5: Tubulin gamma-1 chain

Chain m: 93% 5% .



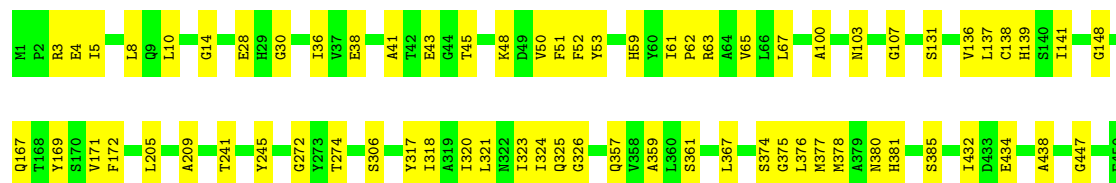
• Molecule 5: Tubulin gamma-1 chain

Chain n: 15% 94% 6% .

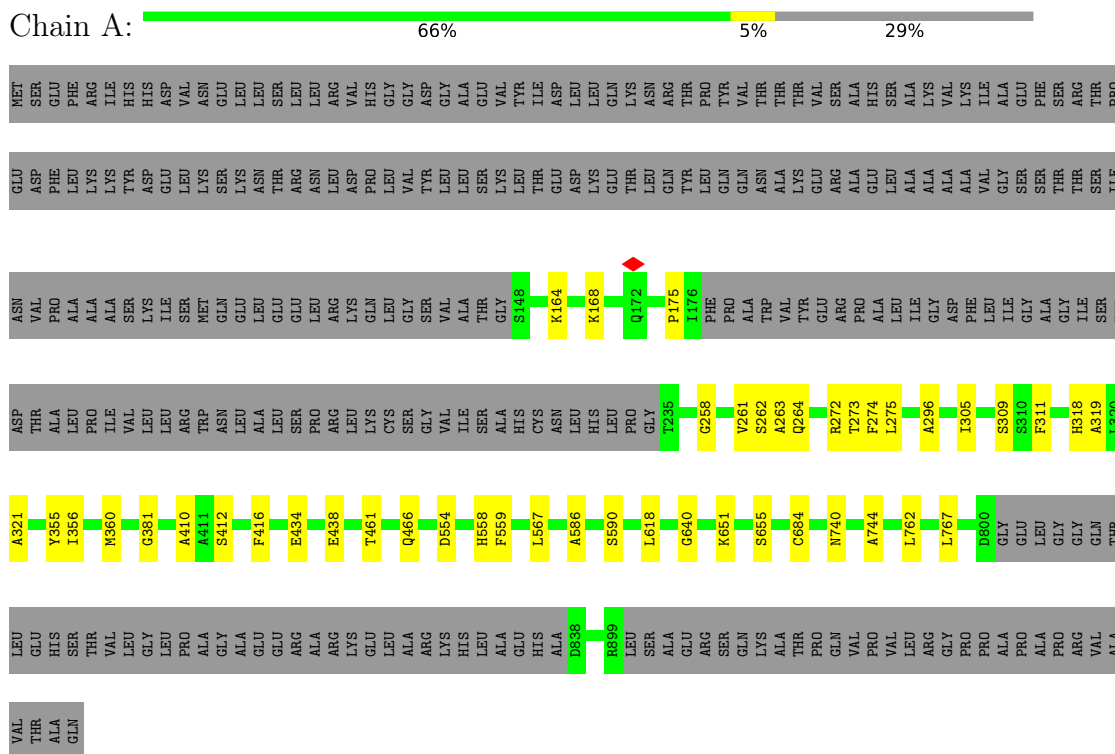


• Molecule 5: Tubulin gamma-1 chain

Chain d: 83% 15% .



- Chain C: 66% 5% 30%



- 

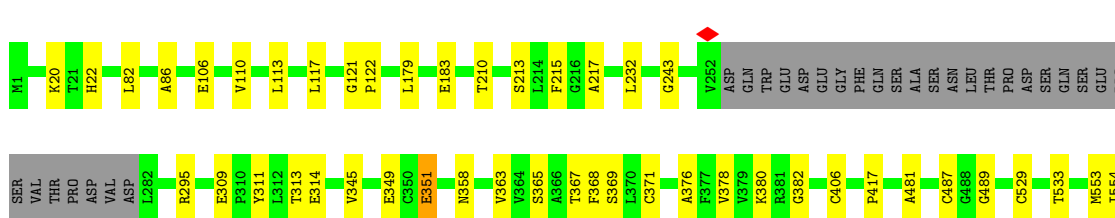
27%

- Molecule 7: Isoform 3 of Gamma-tubulin complex component 2

17%

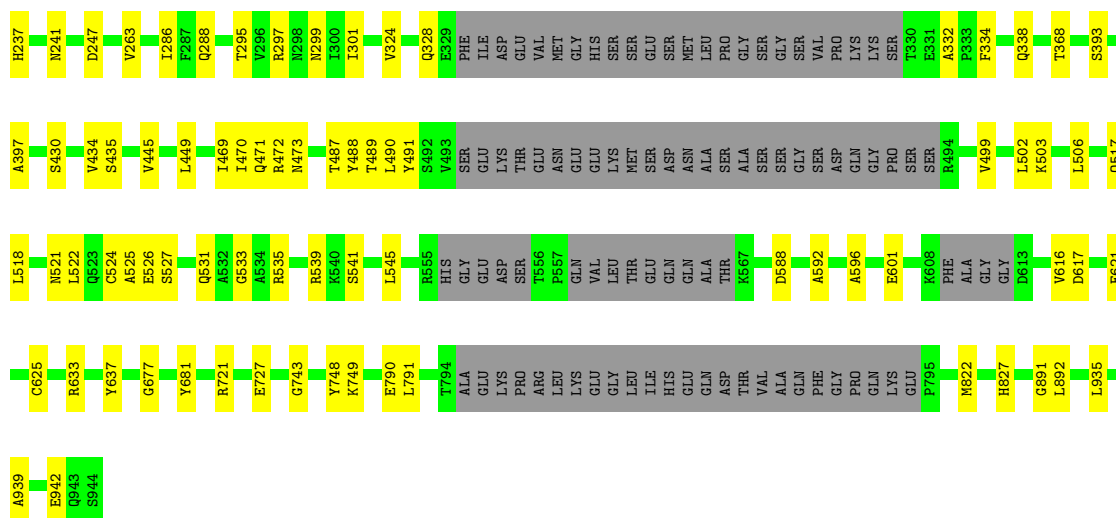
- Molecule 8: TUBGCP6 protein

46%

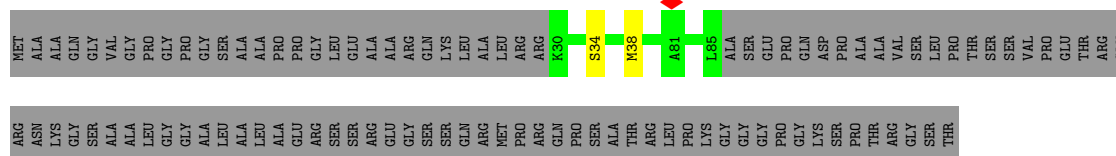


- Molecule 9: Gamma-tubulin complex component 5

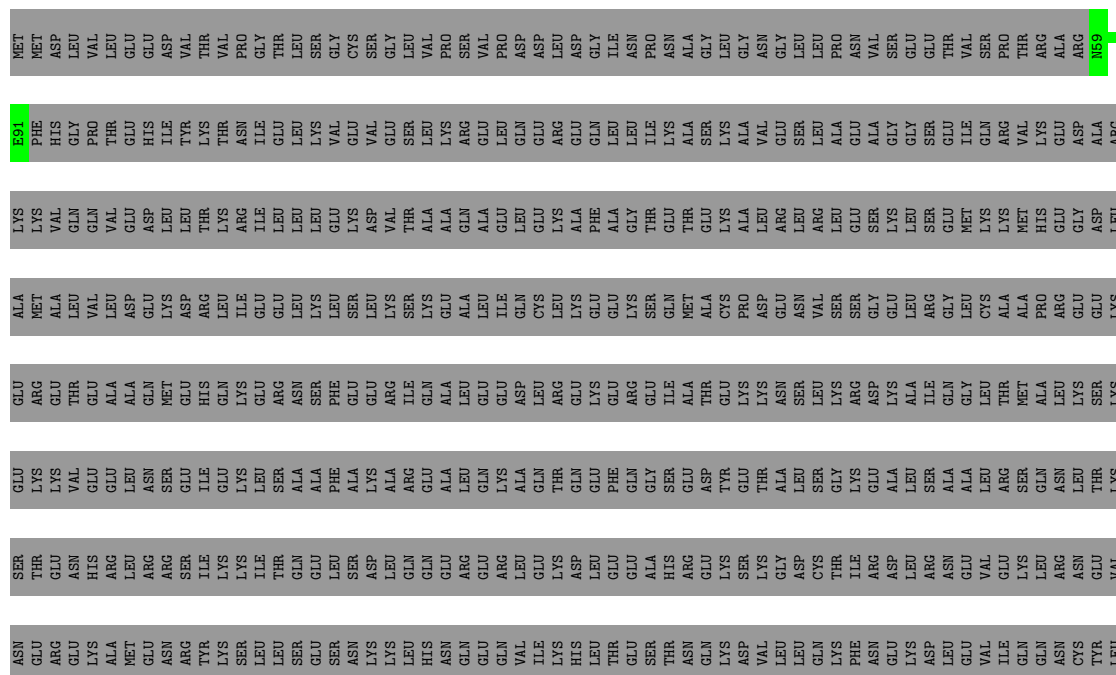
THR	PRO	ASN	GLU	GLU	GLU	GLU	GLU	ASN	ASP	GLN	GLN	PRO	LEU	LEU	SER	ARG	GLU	ASP	SER	GLY	ILE	GLN	GLN	VAL	ASP	ASP	ARG	THR	PRO	LEU	LEU	GLU	GLU	GLN	ASN	ARG	LYS	LEU	ASP	CYS	ILE	SER	TRP	LYS	ASP	ASP	GLU	P210	L216	V220	V221	H222	Q223	T226
MET	ALA	ARG	GLY	P6	P7	W8	S9	G25	P35	F50	H51	R52	D55	I74	S120	S125	TYR	VAL	GLU	THR	PRO	ARG	ASN	GLU	VAL	GLU	LYS	GLY	ASP	ASP	PHE	ASP	TRP	GLY	LYS	TYR	LEU	MET	GLU	ASP	GLU	MET	ASP	ILE	PRO	TYR	MET	ASP						



• Molecule 10: Mitotic-spindle organizing protein 2B



• Molecule 11: CDK5 regulatory subunit-associated protein 2



- Molecule 11: CDK5 regulatory subunit-associated protein 2

98%



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.310	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0363	Depositor
Map size ($\text{\AA}$)	541.44, 541.44, 541.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.41, 1.41, 1.41	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	B	0.15	0/3190	0.35	0/4446
1	D	0.19	0/3255	0.38	0/4538
1	F	0.20	0/3255	0.38	0/4538
1	H	0.23	0/3251	0.37	0/4533
1	N	0.14	0/3120	0.36	0/4347
1	r	0.11	0/561	0.39	0/782
1	s	0.12	0/571	0.41	0/796
1	t	0.15	0/596	0.53	0/831
1	u	0.15	0/596	0.52	0/831
1	v	0.22	0/640	0.45	0/891
2	O	0.24	0/405	0.38	0/563
2	P	0.25	0/362	0.45	0/504
2	Q	0.10	0/327	0.32	0/455
2	R	0.12	0/327	0.30	0/455
2	S	0.09	0/327	0.23	0/455
2	T	0.19	0/405	0.44	0/563
2	U	0.15	0/405	0.43	0/563
3	V	0.12	0/382	0.32	0/531
3	W	0.12	0/393	0.34	0/548
3	X	0.12	0/388	0.30	0/541
3	Y	0.13	0/387	0.30	0/538
4	Z	0.14	0/1846	0.37	0/2566
5	a	0.11	0/2203	0.38	0/3067
5	b	0.13	0/2232	0.38	0/3107
5	c	0.13	0/2212	0.39	0/3079
5	d	0.14	0/2226	0.40	0/3097
5	e	0.13	0/2212	0.39	0/3079
5	f	0.13	0/2227	0.37	0/3100
5	g	0.15	0/2222	0.39	0/3093
5	h	0.16	0/2227	0.39	0/3100
5	i	0.15	0/2212	0.42	0/3079
5	j	0.13	0/2217	0.36	0/3086
5	k	0.13	0/2212	0.42	0/3079
5	l	0.13	0/2207	0.38	0/3072

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	m	0.13	0/2212	0.41	0/3079
5	n	0.11	0/2257	0.38	0/3142
6	I	0.20	0/3024	0.43	1/4209 (0.0%)
6	K	0.18	0/3034	0.42	0/4223
7	A	0.14	0/3261	0.36	0/4548
7	C	0.17	0/3241	0.37	0/4520
7	E	0.19	0/3364	0.37	0/4691
7	G	0.19	0/3364	0.37	0/4691
7	M	0.17	0/3823	0.51	0/5330
8	L	0.17	0/4846	0.42	0/6741
9	J	0.23	1/4182 (0.0%)	0.43	0/5834
10	p	0.14	0/276	0.48	0/383
11	w	0.17	0/164	0.39	0/228
11	x	0.17	0/164	0.39	0/228
All	All	0.17	1/88810 (0.0%)	0.40	1/123700 (0.0%)

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
3	X	0	1
6	I	0	2
6	K	0	3
8	L	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	120	SER	C-O	-8.57	1.19	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	80	GLY	N-CA-C	-5.26	101.40	112.04

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	I	442	ARG	Peptide
6	I	665	GLY	Peptide
6	K	249	MET	Peptide
6	K	417	THR	Peptide
6	K	665	GLY	Peptide
8	L	313	THR	Peptide
3	X	637	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3192	0	1417	22	0
1	D	3256	0	1450	30	0
1	F	3256	0	1450	34	0
1	H	3252	0	1447	28	0
1	N	3123	0	1382	23	0
1	r	562	0	254	4	0
1	s	572	0	258	0	0
1	t	597	0	273	4	0
1	u	597	0	273	5	0
1	v	642	0	295	6	0
2	O	406	0	217	3	0
2	P	363	0	185	6	0
2	Q	328	0	153	0	0
2	R	328	0	150	0	0
2	S	328	0	150	0	0
2	T	406	0	217	2	0
2	U	406	0	217	6	0
3	V	384	0	164	1	0
3	W	394	0	169	4	0
3	X	389	0	165	3	0
3	Y	389	0	166	1	0
4	Z	1847	0	848	40	0
5	a	2204	0	971	33	0
5	b	2233	0	984	30	0
5	c	2213	0	976	39	0
5	d	2228	0	981	46	0
5	e	2213	0	976	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	f	2228	0	982	40	0
5	g	2223	0	980	41	0
5	h	2228	0	982	40	0
5	i	2213	0	976	36	0
5	j	2218	0	978	35	0
5	k	2213	0	976	37	0
5	l	2208	0	974	25	0
5	m	2213	0	976	14	0
5	n	2258	0	994	17	0
6	I	3027	0	1327	33	0
6	K	3037	0	1331	24	0
7	A	3264	0	1445	29	0
7	C	3244	0	1438	24	0
7	E	3367	0	1492	26	0
7	G	3367	0	1492	23	0
7	M	3828	0	1691	10	0
8	L	4851	0	2185	42	0
9	J	4186	0	1817	46	0
10	p	277	0	133	1	0
11	w	165	0	65	0	0
11	x	165	0	65	0	0
All	All	88888	0	39487	906	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 7.

All (906) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:MET:HA	1:F:31:TYR:HA	1.52	0.92
5:a:30:GLY:HA3	5:a:41:ALA:HB2	1.53	0.90
8:L:243:GLY:HA2	7:A:355:TYR:HA	1.56	0.88
5:k:46:ASP:HA	5:k:245:TYR:HA	1.57	0.87
5:m:30:GLY:HA3	5:m:41:ALA:HB2	1.57	0.86
1:H:24:MET:HA	1:H:31:TYR:HA	1.55	0.86
4:Z:150:GLY:HA2	4:Z:293:LEU:HA	1.56	0.86
5:k:30:GLY:HA3	5:k:41:ALA:HB2	1.60	0.84
8:L:369:SER:O	8:L:378:VAL:N	2.11	0.82
4:Z:144:ALA:HB2	4:Z:342:GLY:HA2	1.61	0.82
1:D:24:MET:HA	1:D:31:TYR:HA	1.59	0.81
2:P:38:GLY:H	8:L:122:PRO:HA	1.44	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:24:MET:HA	1:N:31:TYR:HA	1.64	0.80
5:e:46:ASP:HA	5:e:244:ARG:HA	1.64	0.79
9:J:541:SER:O	9:J:545:LEU:N	2.12	0.79
5:d:30:GLY:HA3	5:d:41:ALA:HB2	1.64	0.79
5:c:195:LEU:HA	5:c:199:ALA:HB3	1.64	0.78
5:d:317:TYR:HA	5:d:381:HIS:HA	1.66	0.77
9:J:263:VAL:N	9:J:299:ASN:O	2.15	0.77
7:M:53:ILE:O	7:M:57:SER:N	2.16	0.77
1:D:376:ARG:O	1:D:399:HIS:N	2.17	0.76
5:h:318:ILE:N	5:h:380:ASN:O	2.19	0.76
5:i:53:TYR:O	5:i:61:ILE:N	2.18	0.76
5:e:317:TYR:HA	5:e:381:HIS:HA	1.67	0.76
5:l:317:TYR:HA	5:l:381:HIS:HA	1.68	0.74
1:B:24:MET:HA	1:B:31:TYR:HA	1.68	0.74
5:j:53:TYR:O	5:j:61:ILE:N	2.17	0.74
5:d:107:GLY:HA3	5:d:148:GLY:HA3	1.70	0.74
7:E:262:SER:O	7:E:275:LEU:N	2.21	0.73
5:j:318:ILE:N	5:j:380:ASN:O	2.21	0.73
7:C:263:ALA:HA	7:C:274:PHE:HA	1.70	0.73
1:t:4:PRO:O	1:t:6:GLN:N	2.19	0.73
1:N:418:ARG:HA	9:J:74:ILE:HA	1.71	0.73
5:k:318:ILE:N	5:k:380:ASN:O	2.21	0.73
9:J:332:ALA:HB1	9:J:338:GLN:HA	1.69	0.73
7:C:262:SER:O	7:C:275:LEU:N	2.21	0.73
5:l:409:ARG:HA	5:l:415:LYS:HA	1.70	0.72
5:e:141:ILE:N	5:e:171:VAL:O	2.21	0.72
5:h:8:LEU:O	5:h:138:CYS:N	2.19	0.72
7:G:264:GLN:N	7:G:273:THR:O	2.23	0.72
1:F:620:LEU:O	1:F:624:SER:N	2.22	0.72
7:C:438:GLU:N	7:C:461:THR:O	2.18	0.72
5:e:195:LEU:HA	5:e:199:ALA:HB3	1.70	0.72
1:B:620:LEU:O	1:B:624:SER:N	2.23	0.72
7:G:262:SER:O	7:G:275:LEU:N	2.21	0.71
7:G:263:ALA:HA	7:G:274:PHE:HA	1.71	0.71
9:J:470:ILE:HA	9:J:490:LEU:HA	1.73	0.71
6:K:654:TYR:O	6:K:659:GLY:N	2.18	0.71
5:n:166:VAL:O	5:n:200:ASP:N	2.20	0.71
5:f:317:TYR:HA	5:f:381:HIS:HA	1.73	0.71
7:E:438:GLU:N	7:E:461:THR:O	2.19	0.71
1:H:277:ASP:O	1:H:281:ASP:N	2.22	0.71
5:l:57:ASP:N	5:m:287:LYS:O	2.19	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:h:53:TYR:O	5:h:61:ILE:N	2.22	0.70
5:f:324:ILE:O	5:f:361:SER:N	2.23	0.70
5:i:318:ILE:N	5:i:380:ASN:O	2.24	0.70
5:c:318:ILE:N	5:c:380:ASN:O	2.23	0.70
1:N:515:ILE:O	1:N:520:LEU:N	2.23	0.70
1:H:23:LYS:O	1:H:32:LYS:N	2.18	0.70
7:E:263:ALA:HA	7:E:274:PHE:HA	1.73	0.70
1:D:595:SER:O	1:D:599:MET:N	2.20	0.70
5:k:4:GLU:HA	5:k:50:VAL:HA	1.72	0.70
5:k:195:LEU:HA	5:k:199:ALA:HB3	1.72	0.70
6:I:294:THR:O	6:I:296:LYS:N	2.23	0.70
7:A:412:SER:O	7:A:416:PHE:N	2.19	0.70
5:a:141:ILE:N	5:a:171:VAL:O	2.26	0.69
7:A:559:PHE:HA	7:A:586:ALA:HB1	1.75	0.69
5:a:102:ASN:HA	5:a:144:GLY:HA2	1.74	0.69
7:C:264:GLN:N	7:C:273:THR:O	2.26	0.69
5:b:274:THR:O	5:b:375:GLY:N	2.26	0.69
5:h:324:ILE:O	5:h:361:SER:N	2.26	0.69
1:F:23:LYS:O	1:F:32:LYS:N	2.18	0.68
5:g:274:THR:N	5:g:375:GLY:O	2.26	0.68
1:D:203:PHE:O	1:D:223:ARG:N	2.26	0.68
4:Z:132:MET:O	4:Z:357:ILE:N	2.25	0.68
5:a:53:TYR:N	5:a:61:ILE:O	2.22	0.68
5:c:317:TYR:HA	5:c:381:HIS:HA	1.76	0.68
5:e:272:GLY:O	5:e:377:MET:N	2.26	0.68
5:g:318:ILE:N	5:g:380:ASN:O	2.26	0.68
7:E:264:GLN:N	7:E:273:THR:O	2.27	0.68
5:d:274:THR:O	5:d:375:GLY:N	2.26	0.68
6:I:400:ALA:O	6:I:405:LEU:N	2.23	0.68
5:f:53:TYR:O	5:f:61:ILE:N	2.26	0.68
5:h:5:ILE:N	5:h:50:VAL:O	2.23	0.68
8:L:554:ILE:HA	8:L:575:LEU:HA	1.74	0.68
5:g:5:ILE:N	5:g:50:VAL:O	2.23	0.67
1:t:1:MET:H2	9:J:247:ASP:HA	1.59	0.67
5:g:385:SER:O	5:g:389:GLU:N	2.20	0.67
1:D:205:ALA:N	1:D:221:THR:O	2.21	0.67
4:Z:261:LEU:O	4:Z:274:ILE:N	2.26	0.67
5:b:53:TYR:O	5:b:61:ILE:N	2.24	0.67
1:F:455:GLY:HA2	5:f:448:THR:HA	1.77	0.67
6:I:382:THR:O	6:I:448:GLY:N	2.27	0.67
1:H:337:LEU:O	1:H:341:LEU:N	2.22	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:318:ILE:N	5:f:380:ASN:O	2.28	0.67
7:A:164:LYS:O	7:A:168:LYS:N	2.27	0.67
5:j:274:THR:N	5:j:375:GLY:O	2.28	0.67
6:K:294:THR:O	6:K:296:LYS:N	2.24	0.67
1:D:205:ALA:O	1:D:221:THR:N	2.21	0.66
1:H:376:ARG:O	1:H:399:HIS:N	2.27	0.66
5:c:141:ILE:N	5:c:171:VAL:O	2.24	0.66
8:L:345:VAL:N	8:L:382:GLY:O	2.21	0.66
4:Z:237:GLU:HA	4:Z:251:GLY:HA2	1.78	0.66
5:f:274:THR:O	5:f:375:GLY:N	2.25	0.66
5:l:30:GLY:HA3	5:l:41:ALA:HB2	1.76	0.66
5:m:134:GLY:HA3	5:m:165:LEU:O	1.95	0.66
9:J:822:MET:O	9:J:827:HIS:N	2.27	0.66
5:c:385:SER:O	5:c:389:GLU:N	2.18	0.66
1:v:123:PRO:O	1:v:125:ASP:N	2.23	0.66
1:F:21:ASN:O	1:F:34:GLU:N	2.20	0.66
5:g:195:LEU:HA	5:g:199:ALA:HB3	1.78	0.66
1:H:278:LEU:HA	1:H:282:LEU:HA	1.76	0.66
4:Z:36:GLY:HA2	4:Z:67:LEU:HA	1.76	0.66
5:g:168:THR:N	5:g:201:CYS:O	2.28	0.66
7:A:567:LEU:O	7:A:640:GLY:N	2.29	0.66
10:p:34:SER:O	10:p:38:MET:N	2.22	0.66
5:g:141:ILE:N	5:g:171:VAL:O	2.22	0.65
8:L:210:THR:O	8:L:215:PHE:N	2.26	0.65
4:Z:252:ASN:O	4:Z:256:ARG:N	2.19	0.65
5:j:53:TYR:N	5:j:61:ILE:O	2.25	0.65
1:D:23:LYS:O	1:D:32:LYS:N	2.18	0.65
5:e:434:GLU:O	5:e:438:ALA:N	2.27	0.65
5:g:53:TYR:O	5:g:61:ILE:N	2.26	0.65
5:i:272:GLY:HA2	5:i:304:MET:H	1.61	0.65
4:Z:37:ARG:HA	4:Z:52:SER:HA	1.79	0.65
5:h:323:ILE:O	5:h:376:LEU:N	2.26	0.65
1:H:184:SER:HA	1:H:270:GLU:CB	2.26	0.65
7:G:248:ASP:O	7:G:252:VAL:N	2.26	0.65
4:Z:38:PRO:HA	4:Z:65:LEU:HA	1.78	0.65
5:f:320:ILE:O	5:f:357:GLN:N	2.28	0.65
5:i:53:TYR:N	5:i:61:ILE:O	2.24	0.65
5:j:323:ILE:O	5:j:376:LEU:N	2.29	0.65
5:d:272:GLY:N	5:d:377:MET:O	2.29	0.65
9:J:288:GLN:N	9:J:295:THR:O	2.26	0.65
6:K:400:ALA:O	6:K:405:LEU:N	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ASP:O	1:D:281:ASP:N	2.26	0.64
5:f:323:ILE:HA	5:f:359:ALA:HB3	1.80	0.64
9:J:469:ILE:O	9:J:491:TYR:N	2.25	0.64
9:J:588:ASP:O	9:J:592:ALA:N	2.24	0.64
7:E:651:LYS:O	7:E:655:SER:N	2.30	0.64
1:D:524:SER:O	1:D:528:LEU:N	2.24	0.64
5:h:54:GLN:HA	5:h:60:TYR:HA	1.80	0.64
5:i:8:LEU:O	5:i:138:CYS:N	2.18	0.64
5:j:107:GLY:HA3	5:j:148:GLY:HA3	1.79	0.64
5:k:53:TYR:O	5:k:61:ILE:N	2.26	0.64
6:K:532:GLN:O	6:K:537:GLU:N	2.24	0.64
9:J:621:GLU:O	9:J:625:CYS:N	2.30	0.64
2:P:32:SER:HA	8:L:121:GLY:HA3	1.79	0.64
5:i:323:ILE:O	5:i:376:LEU:N	2.26	0.64
2:O:32:SER:O	2:O:36:ASN:N	2.31	0.63
5:g:8:LEU:O	5:g:138:CYS:N	2.20	0.63
5:j:4:GLU:HA	5:j:50:VAL:HA	1.81	0.63
8:L:406:CYS:HA	8:L:481:ALA:HB2	1.79	0.63
5:g:46:ASP:HA	5:g:244:ARG:HA	1.79	0.63
1:N:23:LYS:O	1:N:32:LYS:N	2.24	0.63
1:F:277:ASP:O	1:F:281:ASP:N	2.26	0.63
1:D:278:LEU:HA	1:D:282:LEU:HA	1.79	0.63
1:B:179:SER:O	1:B:183:LEU:N	2.20	0.63
5:d:209:ALA:HB2	5:d:306:SER:H	1.63	0.63
5:c:8:LEU:O	5:c:138:CYS:N	2.17	0.63
5:d:323:ILE:O	5:d:376:LEU:N	2.26	0.63
9:J:525:ALA:O	9:J:527:SER:N	2.31	0.63
9:J:502:LEU:O	9:J:506:LEU:N	2.31	0.63
7:A:264:GLN:N	7:A:273:THR:O	2.30	0.63
5:f:323:ILE:N	5:f:376:LEU:O	2.32	0.62
5:j:272:GLY:N	5:j:377:MET:O	2.30	0.62
2:O:56:ASN:O	2:O:60:LEU:N	2.21	0.62
5:l:53:TYR:O	5:l:61:ILE:N	2.30	0.62
1:D:620:LEU:O	1:D:624:SER:N	2.32	0.62
8:L:588:LEU:O	8:L:592:ALA:N	2.31	0.62
1:v:105:ARG:HA	1:v:108:PRO:N	2.14	0.62
1:N:19:GLY:N	1:N:22:ILE:O	2.31	0.62
6:I:18:THR:N	6:I:26:GLN:O	2.31	0.62
1:F:205:ALA:N	1:F:221:THR:O	2.26	0.62
5:g:30:GLY:HA3	5:g:41:ALA:HB2	1.82	0.62
5:g:323:ILE:O	5:g:376:LEU:N	2.27	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:473:ASN:N	9:J:487:THR:O	2.32	0.62
5:g:10:LEU:N	5:g:138:CYS:O	2.28	0.62
6:K:157:VAL:O	6:K:161:SER:N	2.31	0.62
9:J:518:LEU:O	9:J:522:LEU:N	2.31	0.62
5:e:53:TYR:O	5:e:61:ILE:N	2.24	0.62
9:J:288:GLN:O	9:J:295:THR:N	2.20	0.62
9:J:791:LEU:HA	9:J:892:LEU:H	1.65	0.62
5:n:134:GLY:HA3	5:n:165:LEU:O	1.99	0.62
1:H:205:ALA:N	1:H:221:THR:O	2.27	0.61
4:Z:131:ALA:HA	4:Z:358:SER:HA	1.82	0.61
8:L:367:THR:O	8:L:380:LYS:N	2.25	0.61
1:F:203:PHE:O	1:F:223:ARG:N	2.34	0.61
5:b:323:ILE:O	5:b:376:LEU:N	2.28	0.61
5:g:324:ILE:O	5:g:361:SER:N	2.32	0.61
5:m:317:TYR:HA	5:m:381:HIS:HA	1.82	0.61
1:B:595:SER:O	1:B:599:MET:N	2.24	0.61
5:e:317:TYR:N	5:e:347:ASN:O	2.34	0.61
5:m:52:PHE:HA	5:m:62:PRO:HA	1.83	0.61
1:B:524:SER:O	1:B:528:LEU:N	2.27	0.61
5:b:325:GLN:N	5:b:374:SER:O	2.25	0.61
5:g:53:TYR:N	5:g:61:ILE:O	2.27	0.61
5:h:30:GLY:HA3	5:h:41:ALA:HB2	1.81	0.61
5:h:172:PHE:N	5:h:205:LEU:O	2.33	0.61
5:e:5:ILE:N	5:e:50:VAL:O	2.24	0.61
5:e:318:ILE:N	5:e:380:ASN:O	2.32	0.61
5:f:272:GLY:N	5:f:377:MET:O	2.33	0.61
1:u:4:PRO:O	1:u:6:GLN:N	2.34	0.61
1:B:310:SER:O	1:B:314:HIS:N	2.26	0.61
9:J:216:LEU:O	9:J:220:VAL:N	2.29	0.61
9:J:445:VAL:O	9:J:449:LEU:N	2.19	0.61
5:h:10:LEU:N	5:h:138:CYS:O	2.31	0.61
5:d:434:GLU:O	5:d:438:ALA:N	2.31	0.61
7:E:436:MET:O	7:E:463:VAL:N	2.31	0.61
5:i:274:THR:N	5:i:375:GLY:O	2.32	0.61
1:D:25:ASN:N	1:D:30:CYS:O	2.29	0.60
5:f:172:PHE:N	5:f:205:LEU:O	2.34	0.60
5:f:385:SER:O	5:f:389:GLU:N	2.23	0.60
9:J:471:GLN:N	9:J:489:THR:O	2.29	0.60
7:A:309:SER:HA	7:A:318:HIS:HA	1.82	0.60
5:k:272:GLY:O	5:k:377:MET:N	2.27	0.60
1:B:23:LYS:O	1:B:32:LYS:N	2.21	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:337:LEU:O	1:F:341:LEU:N	2.20	0.60
9:J:472:ARG:HA	9:J:488:TYR:HA	1.83	0.60
5:b:137:LEU:O	5:b:169:TYR:N	2.26	0.60
5:e:53:TYR:N	5:e:61:ILE:O	2.30	0.60
5:h:317:TYR:HA	5:h:381:HIS:HA	1.83	0.60
5:h:320:ILE:O	5:h:357:GLN:N	2.32	0.60
5:a:317:TYR:N	5:a:347:ASN:O	2.25	0.60
5:d:141:ILE:N	5:d:171:VAL:O	2.31	0.60
1:H:203:PHE:O	1:H:223:ARG:N	2.33	0.60
5:h:323:ILE:N	5:h:376:LEU:O	2.35	0.60
6:K:1:MET:O	6:K:5:LEU:N	2.32	0.60
7:C:438:GLU:O	7:C:461:THR:N	2.21	0.60
6:K:253:SER:O	6:K:256:GLN:N	2.30	0.60
7:G:179:ALA:O	7:G:183:GLU:N	2.34	0.60
5:i:325:GLN:N	5:i:374:SER:O	2.27	0.59
5:k:166:VAL:O	5:k:200:ASP:N	2.29	0.59
1:H:620:LEU:O	1:H:624:SER:N	2.35	0.59
6:K:384:PRO:N	6:K:448:GLY:HA3	2.17	0.59
6:I:157:VAL:O	6:I:161:SER:N	2.35	0.59
5:b:100:ALA:HB3	5:b:144:GLY:HA3	1.84	0.59
5:c:10:LEU:N	5:c:138:CYS:O	2.33	0.59
5:i:5:ILE:N	5:i:50:VAL:O	2.36	0.59
5:k:434:GLU:O	5:k:438:ALA:N	2.35	0.59
9:J:237:HIS:O	9:J:241:ASN:N	2.35	0.59
9:J:334:PHE:O	9:J:338:GLN:N	2.30	0.59
6:I:269:PRO:O	6:I:273:ALA:N	2.30	0.59
5:b:35:GLY:O	5:b:60:TYR:N	2.35	0.59
1:H:320:ARG:O	1:H:326:GLN:N	2.25	0.59
5:b:53:TYR:N	5:b:61:ILE:O	2.27	0.59
6:K:358:LYS:O	6:K:364:GLY:N	2.31	0.59
7:G:438:GLU:N	7:G:461:THR:O	2.26	0.59
5:h:52:PHE:HA	5:h:62:PRO:HA	1.85	0.59
4:Z:70:PRO:O	4:Z:77:THR:N	2.31	0.59
5:a:46:ASP:HA	5:a:244:ARG:HA	1.85	0.59
5:b:10:LEU:HA	5:b:67:LEU:O	2.03	0.59
1:B:337:LEU:O	1:B:341:LEU:N	2.22	0.59
8:L:560:TYR:O	8:L:568:TYR:HA	2.03	0.59
5:i:317:TYR:HA	5:i:381:HIS:HA	1.85	0.59
6:K:20:ASN:O	6:K:24:GLY:N	2.32	0.59
5:i:172:PHE:N	5:i:205:LEU:O	2.30	0.58
1:H:341:LEU:HA	1:H:390:GLY:HA3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:356:ILE:O	7:E:360:MET:N	2.25	0.58
2:P:47:CYS:O	2:P:51:CYS:N	2.32	0.58
5:h:274:THR:O	5:h:375:GLY:N	2.30	0.58
7:C:726:MET:O	7:C:731:GLU:N	2.33	0.58
1:H:25:ASN:N	1:H:30:CYS:O	2.33	0.58
1:D:214:ARG:O	1:D:218:ASP:N	2.32	0.58
5:h:55:ALA:N	5:h:59:HIS:O	2.35	0.58
5:e:272:GLY:N	5:e:377:MET:O	2.35	0.58
5:m:321:LEU:HA	5:m:356:ILE:HA	1.85	0.58
1:N:14:PHE:HA	1:N:54:GLY:HA3	1.86	0.58
4:Z:37:ARG:O	4:Z:66:THR:N	2.33	0.58
5:i:323:ILE:N	5:i:376:LEU:O	2.36	0.58
5:d:53:TYR:O	5:d:61:ILE:N	2.27	0.58
5:d:324:ILE:O	5:d:361:SER:N	2.36	0.58
1:F:25:ASN:N	1:F:30:CYS:O	2.28	0.57
5:m:318:ILE:N	5:m:380:ASN:O	2.35	0.57
5:d:318:ILE:N	5:d:380:ASN:O	2.36	0.57
5:b:36:ILE:HA	5:b:59:HIS:HA	1.85	0.57
9:J:430:SER:O	9:J:434:VAL:N	2.29	0.57
1:F:376:ARG:O	1:F:399:HIS:N	2.33	0.57
5:c:241:THR:O	5:c:245:TYR:N	2.31	0.57
5:e:48:LYS:O	5:e:52:PHE:N	2.25	0.57
5:f:51:PHE:O	5:f:63:ARG:N	2.36	0.57
6:K:604:ASP:O	6:K:608:ALA:N	2.28	0.57
7:G:726:MET:O	7:G:731:GLU:N	2.32	0.57
9:J:471:GLN:O	9:J:489:THR:N	2.33	0.57
5:g:209:ALA:HB1	5:g:306:SER:H	1.69	0.57
5:d:323:ILE:N	5:d:376:LEU:O	2.38	0.57
6:I:20:ASN:O	6:I:24:GLY:N	2.32	0.57
5:a:1:MET:N	7:A:558:HIS:O	2.36	0.57
5:c:53:TYR:N	5:c:61:ILE:O	2.36	0.57
5:c:326:GLY:N	5:c:361:SER:O	2.31	0.57
5:h:195:LEU:HA	5:h:199:ALA:HB3	1.86	0.57
7:M:262:SER:O	7:M:275:LEU:N	2.33	0.57
5:a:141:ILE:H	5:a:171:VAL:C	2.11	0.57
5:f:35:GLY:O	5:f:60:TYR:N	2.32	0.57
5:f:52:PHE:HA	5:f:62:PRO:HA	1.85	0.57
5:f:107:GLY:HA3	5:f:148:GLY:HA3	1.86	0.57
5:k:47:ARG:N	5:k:244:ARG:O	2.32	0.57
7:C:381:GLY:HA3	7:C:466:GLN:O	2.04	0.57
1:F:214:ARG:O	1:F:218:ASP:N	2.32	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:35:VAL:N	4:Z:68:LYS:O	2.30	0.57
5:f:274:THR:N	5:f:375:GLY:O	2.35	0.57
5:d:53:TYR:N	5:d:61:ILE:O	2.30	0.57
1:N:337:LEU:O	1:N:341:LEU:N	2.23	0.57
8:L:113:LEU:O	8:L:117:LEU:N	2.38	0.57
8:L:556:VAL:HA	8:L:573:TYR:HA	1.87	0.57
7:C:567:LEU:O	7:C:640:GLY:N	2.38	0.57
5:j:317:TYR:HA	5:j:381:HIS:HA	1.86	0.56
5:l:53:TYR:N	5:l:61:ILE:O	2.27	0.56
7:G:381:GLY:HA3	7:G:466:GLN:O	2.05	0.56
5:f:323:ILE:O	5:f:376:LEU:N	2.31	0.56
7:C:436:MET:O	7:C:463:VAL:N	2.36	0.56
1:v:123:PRO:C	1:v:125:ASP:H	2.10	0.56
7:C:567:LEU:HA	7:C:640:GLY:HA3	1.86	0.56
7:A:438:GLU:O	7:A:461:THR:N	2.37	0.56
1:D:150:GLY:HA3	1:D:226:MET:HA	1.86	0.56
5:m:55:ALA:HB1	5:m:217:ARG:HA	1.87	0.56
1:N:361:VAL:HA	1:N:366:ALA:HB3	1.87	0.56
7:G:436:MET:O	7:G:463:VAL:N	2.32	0.56
2:T:53:GLN:O	1:r:112:SER:HA	2.06	0.56
7:G:438:GLU:O	7:G:461:THR:N	2.31	0.56
5:h:272:GLY:N	5:h:377:MET:O	2.36	0.56
5:d:51:PHE:O	5:d:63:ARG:N	2.35	0.56
5:j:172:PHE:N	5:j:205:LEU:O	2.38	0.56
5:l:35:GLY:O	5:l:60:TYR:N	2.23	0.56
7:E:264:GLN:H	7:E:274:PHE:HA	1.71	0.56
7:E:412:SER:O	7:E:416:PHE:N	2.25	0.56
1:H:19:GLY:N	1:H:22:ILE:O	2.38	0.56
4:Z:302:GLY:HA2	4:Z:336:LYS:HA	1.88	0.56
5:b:14:GLY:HA3	5:b:139:HIS:HA	1.88	0.56
5:f:241:THR:O	5:f:245:TYR:N	2.31	0.56
6:K:74:SER:HA	6:K:200:HIS:HA	1.88	0.56
1:N:642:TYR:O	1:N:646:GLU:N	2.24	0.56
5:d:5:ILE:N	5:d:50:VAL:O	2.27	0.56
8:L:553:MET:O	8:L:576:ILE:N	2.29	0.56
5:e:30:GLY:HA3	5:e:41:ALA:HB2	1.88	0.56
5:j:322:ASN:N	5:j:357:GLN:O	2.26	0.56
5:d:320:ILE:O	5:d:357:GLN:N	2.36	0.56
7:E:381:GLY:HA3	7:E:466:GLN:O	2.06	0.55
5:a:140:SER:HA	5:a:171:VAL:H	1.70	0.55
5:k:317:TYR:N	5:k:347:ASN:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:35:GLY:O	5:j:60:TYR:N	2.39	0.55
7:E:567:LEU:O	7:E:640:GLY:N	2.39	0.55
5:c:3:ARG:HA	5:c:131:SER:O	2.06	0.55
5:d:36:ILE:HA	5:d:59:HIS:HA	1.87	0.55
8:L:555:GLN:O	8:L:574:VAL:N	2.28	0.55
5:b:324:ILE:O	5:b:361:SER:N	2.40	0.55
4:Z:132:MET:N	4:Z:357:ILE:O	2.37	0.55
5:j:321:LEU:N	5:j:378:MET:O	2.28	0.55
5:d:48:LYS:O	5:d:52:PHE:N	2.26	0.55
5:j:323:ILE:N	5:j:376:LEU:O	2.36	0.55
7:M:436:MET:O	7:M:463:VAL:N	2.34	0.55
1:H:566:LYS:HA	1:H:576:GLY:O	2.07	0.55
8:L:557:ASN:N	8:L:572:GLY:O	2.39	0.55
1:F:479:THR:O	1:F:484:GLU:N	2.39	0.54
5:j:218:LEU:HA	5:j:278:THR:HA	1.89	0.54
1:F:22:ILE:HA	1:F:33:VAL:HA	1.89	0.54
5:l:209:ALA:HB2	5:l:306:SER:N	2.23	0.54
1:B:203:PHE:O	1:B:223:ARG:N	2.36	0.54
6:I:399:SER:O	6:I:403:VAL:N	2.39	0.54
6:I:415:HIS:O	6:I:455:SER:N	2.29	0.54
5:k:317:TYR:O	5:k:348:PHE:HA	2.08	0.54
5:m:317:TYR:O	5:m:349:ILE:N	2.40	0.54
6:K:413:LEU:O	6:K:456:TYR:HA	2.07	0.54
5:d:321:LEU:N	5:d:378:MET:O	2.30	0.54
7:M:264:GLN:N	7:M:273:THR:O	2.32	0.54
5:c:104:TRP:CB	5:c:187:ASN:HA	2.38	0.54
1:H:214:ARG:O	1:H:218:ASP:N	2.35	0.54
4:Z:36:GLY:O	4:Z:53:TYR:N	2.28	0.54
5:a:171:VAL:HA	5:a:205:LEU:O	2.07	0.54
5:b:172:PHE:N	5:b:205:LEU:O	2.40	0.54
5:d:323:ILE:HA	5:d:359:ALA:HB3	1.90	0.54
5:h:326:GLY:N	5:h:361:SER:O	2.33	0.54
5:g:4:GLU:HA	5:g:50:VAL:HA	1.88	0.54
5:g:241:THR:O	5:g:245:TYR:N	2.37	0.54
1:D:305:LEU:O	1:D:310:SER:N	2.41	0.54
5:e:36:ILE:HA	5:e:59:HIS:HA	1.90	0.54
5:f:46:ASP:HA	5:f:244:ARG:HA	1.90	0.54
1:F:566:LYS:HA	1:F:576:GLY:O	2.08	0.53
4:Z:165:ILE:HA	4:Z:170:ALA:HA	1.88	0.53
5:b:141:ILE:N	5:b:171:VAL:O	2.27	0.53
5:c:14:GLY:HA3	5:c:139:HIS:HA	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:7:THR:O	5:i:65:VAL:N	2.30	0.53
1:B:341:LEU:HA	1:B:390:GLY:HA3	1.90	0.53
5:d:30:GLY:O	5:d:38:GLU:N	2.28	0.53
6:I:151:CYS:N	6:I:202:GLU:O	2.42	0.53
5:b:5:ILE:N	5:b:50:VAL:O	2.39	0.53
5:b:321:LEU:N	5:b:378:MET:O	2.34	0.53
5:c:30:GLY:HA3	5:c:41:ALA:HB2	1.90	0.53
5:g:52:PHE:HA	5:g:62:PRO:HA	1.89	0.53
5:h:30:GLY:O	5:h:38:GLU:N	2.29	0.53
5:i:52:PHE:HA	5:i:63:ARG:H	1.73	0.53
5:d:241:THR:O	5:d:245:TYR:N	2.34	0.53
7:G:397:ASP:O	7:G:401:GLN:N	2.37	0.53
5:j:30:GLY:O	5:j:38:GLU:N	2.22	0.53
7:A:319:ALA:HB1	7:A:410:ALA:HB1	1.90	0.53
6:I:16:ILE:O	6:I:28:SER:N	2.25	0.53
5:c:102:ASN:HA	5:c:144:GLY:N	2.23	0.53
8:L:612:HIS:O	8:L:616:TRP:N	2.41	0.53
7:C:651:LYS:O	7:C:655:SER:N	2.39	0.53
5:c:272:GLY:N	5:c:377:MET:O	2.42	0.53
5:d:325:GLN:N	5:d:374:SER:O	2.27	0.53
1:H:524:SER:O	1:H:528:LEU:N	2.27	0.53
4:Z:202:THR:O	4:Z:206:ARG:N	2.34	0.53
5:b:8:LEU:O	5:b:138:CYS:N	2.23	0.53
5:k:30:GLY:O	5:k:38:GLU:N	2.26	0.53
1:v:105:ARG:O	1:v:110:LYS:N	2.42	0.53
5:f:4:GLU:HA	5:f:50:VAL:HA	1.91	0.53
7:M:191:PHE:HA	7:M:255:GLY:O	2.09	0.53
4:Z:11:ASP:N	4:Z:18:LYS:O	2.34	0.53
5:c:323:ILE:O	5:c:376:LEU:N	2.31	0.53
5:j:434:GLU:O	5:j:438:ALA:N	2.34	0.53
7:E:248:ASP:O	7:E:252:VAL:N	2.34	0.53
1:F:341:LEU:O	1:F:391:TRP:N	2.37	0.52
5:i:52:PHE:HA	5:i:62:PRO:HA	1.91	0.52
9:J:677:GLY:O	9:J:681:TYR:CB	2.56	0.52
5:b:102:ASN:HA	5:b:144:GLY:N	2.24	0.52
1:B:162:THR:HA	7:A:311:PHE:CB	2.39	0.52
1:F:205:ALA:O	1:F:221:THR:N	2.24	0.52
5:h:137:LEU:O	5:h:169:TYR:N	2.22	0.52
5:j:52:PHE:HA	5:j:62:PRO:HA	1.91	0.52
8:L:311:TYR:O	8:L:314:GLU:N	2.35	0.52
5:b:241:THR:O	5:b:245:TYR:N	2.36	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:10:LEU:N	5:i:138:CYS:O	2.41	0.52
5:l:104:TRP:CB	5:l:187:ASN:HA	2.40	0.52
7:E:249:LEU:O	7:E:253:LEU:N	2.33	0.52
5:i:320:ILE:O	5:i:357:GLN:N	2.35	0.52
1:B:116:SER:HA	8:L:232:LEU:H	1.74	0.52
9:J:535:ARG:O	9:J:539:ARG:N	2.42	0.52
1:F:112:LEU:C	1:F:114:LEU:H	2.17	0.52
5:j:8:LEU:O	5:j:138:CYS:N	2.21	0.52
7:M:585:LEU:O	7:M:589:MET:CB	2.58	0.52
1:B:154:SER:HA	1:B:229:SER:H	1.75	0.52
5:d:4:GLU:HA	5:d:50:VAL:HA	1.91	0.52
8:L:1652:SER:HA	8:L:1756:GLY:HA3	1.90	0.52
5:n:6:ILE:O	5:n:136:VAL:N	2.26	0.51
6:K:6:LEU:O	6:K:10:SER:N	2.42	0.51
9:J:286:ILE:O	9:J:297:ARG:N	2.37	0.51
1:F:278:LEU:HA	1:F:282:LEU:HA	1.91	0.51
5:g:272:GLY:N	5:g:377:MET:O	2.40	0.51
1:H:21:ASN:O	1:H:34:GLU:N	2.28	0.51
5:b:9:GLN:CB	5:b:15:ASN:HA	2.41	0.51
5:h:323:ILE:HA	5:h:359:ALA:HB3	1.93	0.51
5:i:102:ASN:HA	5:i:144:GLY:N	2.26	0.51
5:k:317:TYR:HA	5:k:381:HIS:HA	1.93	0.51
4:Z:16:MET:HA	4:Z:32:PRO:HA	1.92	0.51
1:D:341:LEU:HA	1:D:390:GLY:HA3	1.93	0.51
1:F:493:LYS:O	1:F:497:ALA:N	2.43	0.51
2:U:2:ALA:HB1	6:I:44:ARG:HA	1.91	0.51
7:E:701:ALA:O	7:E:705:ALA:N	2.43	0.51
7:E:740:ASN:O	7:E:744:ALA:N	2.44	0.51
1:D:21:ASN:O	1:D:34:GLU:N	2.26	0.51
5:i:6:ILE:HA	5:i:63:ARG:O	2.10	0.51
7:A:263:ALA:HA	7:A:274:PHE:HA	1.92	0.51
5:g:52:PHE:HA	5:g:63:ARG:H	1.75	0.51
7:C:454:LYS:O	7:C:459:ARG:N	2.43	0.51
2:P:37:THR:N	8:L:121:GLY:O	2.29	0.51
4:Z:20:GLY:HA3	4:Z:28:ARG:H	1.76	0.51
5:i:409:ARG:HA	5:i:415:LYS:HA	1.92	0.51
4:Z:72:GLU:N	4:Z:75:ILE:O	2.37	0.51
8:L:529:CYS:O	8:L:533:THR:N	2.34	0.51
5:e:241:THR:O	5:e:245:TYR:N	2.30	0.51
5:g:317:TYR:N	5:g:347:ASN:O	2.44	0.51
1:D:337:LEU:O	1:D:341:LEU:N	2.28	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:209:ALA:HB2	5:a:306:SER:N	2.25	0.50
5:c:209:ALA:HB2	5:c:306:SER:H	1.76	0.50
5:e:209:ALA:HB2	5:e:306:SER:H	1.76	0.50
9:J:499:VAL:O	9:J:503:LYS:N	2.43	0.50
5:e:409:ARG:HA	5:e:415:LYS:HA	1.92	0.50
5:j:241:THR:O	5:j:245:TYR:N	2.32	0.50
6:I:343:LEU:O	6:I:348:SER:N	2.44	0.50
5:a:214:ALA:O	5:a:219:HIS:N	2.45	0.50
1:B:286:PHE:O	1:B:290:ILE:N	2.34	0.50
5:d:272:GLY:O	5:d:377:MET:N	2.39	0.50
1:F:19:GLY:N	1:F:22:ILE:O	2.44	0.50
1:H:112:LEU:C	1:H:114:LEU:H	2.20	0.50
8:L:566:LYS:HA	8:L:1606:ILE:HA	1.92	0.50
5:f:317:TYR:O	5:f:348:PHE:HA	2.12	0.50
5:g:102:ASN:HA	5:g:144:GLY:N	2.26	0.50
5:g:323:ILE:N	5:g:376:LEU:O	2.43	0.50
5:k:241:THR:O	5:k:245:TYR:N	2.32	0.50
7:A:762:LEU:O	7:A:767:LEU:N	2.43	0.50
5:c:325:GLN:N	5:c:374:SER:O	2.36	0.50
5:f:30:GLY:HA3	5:f:41:ALA:HB2	1.94	0.50
5:h:317:TYR:O	5:h:348:PHE:HA	2.11	0.50
5:d:10:LEU:HA	5:d:67:LEU:O	2.12	0.50
7:A:740:ASN:O	7:A:744:ALA:N	2.44	0.50
5:f:53:TYR:N	5:f:61:ILE:O	2.32	0.50
5:d:52:PHE:HA	5:d:62:PRO:HA	1.94	0.50
1:D:479:THR:O	1:D:484:GLU:N	2.43	0.50
5:e:209:ALA:HB2	5:e:306:SER:N	2.26	0.50
1:H:22:ILE:HA	1:H:33:VAL:HA	1.92	0.50
4:Z:153:MET:O	4:Z:300:SER:N	2.42	0.50
5:a:52:PHE:HA	5:a:62:PRO:HA	1.93	0.50
9:J:324:VAL:O	9:J:328:GLN:N	2.43	0.50
1:F:320:ARG:O	1:F:326:GLN:N	2.33	0.49
5:j:8:LEU:N	5:j:136:VAL:O	2.25	0.49
5:k:10:LEU:O	5:k:146:GLY:HA2	2.12	0.49
1:N:193:GLY:HA3	1:N:246:ILE:CB	2.42	0.49
7:C:157:LYS:HA	7:C:313:TYR:HA	1.93	0.49
5:j:21:PHE:HA	5:j:233:SER:CB	2.42	0.49
1:B:112:LEU:C	1:B:114:LEU:H	2.20	0.49
7:A:438:GLU:N	7:A:461:THR:O	2.31	0.49
3:W:637:SER:O	3:W:639:ASN:N	2.45	0.49
4:Z:162:THR:N	4:Z:176:LEU:O	2.34	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:GLY:N	1:D:22:ILE:O	2.46	0.49
5:b:323:ILE:N	5:b:376:LEU:O	2.45	0.49
5:e:35:GLY:O	5:e:60:TYR:N	2.46	0.49
1:F:409:THR:O	1:F:413:MET:N	2.23	0.49
1:F:40:SER:O	1:F:44:ARG:N	2.40	0.49
1:F:305:LEU:O	1:F:310:SER:N	2.45	0.49
1:H:595:SER:O	1:H:599:MET:N	2.31	0.49
5:a:409:ARG:HA	5:a:415:LYS:HA	1.93	0.49
5:g:55:ALA:N	5:g:59:HIS:O	2.44	0.49
7:E:726:MET:O	7:E:731:GLU:N	2.38	0.49
5:i:36:ILE:HA	5:i:59:HIS:HA	1.94	0.49
5:j:102:ASN:HA	5:j:144:GLY:N	2.28	0.49
1:N:73:PHE:HA	1:N:148:LYS:CB	2.42	0.49
5:d:326:GLY:N	5:d:361:SER:O	2.37	0.49
9:J:435:SER:CB	9:J:617:ASP:HA	2.42	0.49
9:J:522:LEU:O	9:J:524:CYS:N	2.46	0.49
4:Z:260:ALA:HA	4:Z:263:GLN:O	2.13	0.49
5:c:323:ILE:N	5:c:376:LEU:O	2.44	0.49
5:l:318:ILE:N	5:l:380:ASN:O	2.44	0.49
1:N:193:GLY:HA2	1:N:243:GLY:HA2	1.95	0.49
7:C:356:ILE:O	7:C:360:MET:N	2.31	0.49
7:C:440:HIS:N	7:C:459:ARG:O	2.39	0.49
6:I:417:THR:O	6:I:453:GLY:N	2.37	0.49
5:g:137:LEU:O	5:g:169:TYR:N	2.31	0.49
1:r:112:SER:C	1:r:114:TYR:H	2.21	0.49
9:J:517:GLN:O	9:J:521:ASN:CB	2.61	0.49
7:A:305:ILE:HA	7:A:321:ALA:HB1	1.95	0.49
1:F:524:SER:O	1:F:528:LEU:N	2.27	0.49
5:c:274:THR:N	5:c:375:GLY:O	2.46	0.49
1:H:205:ALA:O	1:H:221:THR:N	2.24	0.48
5:f:10:LEU:HA	5:f:67:LEU:O	2.13	0.48
5:g:247:GLY:O	7:G:553:GLY:HA3	2.12	0.48
7:C:571:VAL:N	7:C:638:LEU:O	2.46	0.48
5:l:8:LEU:HA	5:l:65:VAL:O	2.13	0.48
1:N:207:ASP:N	1:N:219:LYS:O	2.31	0.48
7:E:567:LEU:HA	7:E:640:GLY:HA3	1.96	0.48
5:c:48:LYS:O	5:c:52:PHE:N	2.29	0.48
5:g:214:ALA:O	5:g:219:HIS:N	2.47	0.48
1:B:566:LYS:HA	1:B:576:GLY:O	2.12	0.48
7:A:651:LYS:O	7:A:655:SER:N	2.46	0.48
2:U:6:GLY:HA2	6:I:27:VAL:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:301:GLY:N	4:Z:335:ARG:O	2.47	0.48
5:l:28:GLU:HA	5:l:367:LEU:CB	2.42	0.48
8:L:349:GLU:O	8:L:351:GLU:N	2.47	0.48
1:F:595:SER:O	1:F:599:MET:N	2.34	0.48
5:j:195:LEU:HA	5:j:199:ALA:HB3	1.95	0.48
7:G:249:LEU:O	7:G:253:LEU:N	2.32	0.48
8:L:406:CYS:HA	8:L:481:ALA:CB	2.42	0.48
1:F:150:GLY:HA3	1:F:226:MET:HA	1.95	0.48
5:e:51:PHE:O	5:e:63:ARG:N	2.46	0.48
1:r:112:SER:C	1:r:114:TYR:N	2.72	0.48
9:J:721:ARG:O	9:J:749:LYS:N	2.36	0.48
9:J:935:LEU:O	9:J:939:ALA:N	2.46	0.48
5:f:195:LEU:HA	5:f:199:ALA:HB3	1.96	0.48
6:K:343:LEU:O	6:K:348:SER:N	2.47	0.48
7:G:725:MET:O	7:G:730:MET:N	2.36	0.48
5:a:246:PRO:CB	7:A:554:ASP:H	2.26	0.48
5:e:55:ALA:N	5:e:59:HIS:O	2.45	0.48
5:l:36:ILE:HA	5:l:58:GLU:O	2.14	0.48
7:C:164:LYS:HA	7:C:432:TYR:HA	1.96	0.48
5:c:172:PHE:N	5:c:205:LEU:O	2.46	0.48
5:e:320:ILE:O	5:e:357:GLN:N	2.43	0.48
5:h:8:LEU:N	5:h:136:VAL:O	2.25	0.48
5:l:7:THR:HA	5:l:136:VAL:O	2.13	0.48
1:N:127:THR:O	1:N:131:LYS:N	2.40	0.48
1:B:164:ASP:O	1:B:168:ARG:N	2.36	0.47
9:J:596:ALA:O	9:J:601:GLU:N	2.35	0.47
7:E:179:ALA:O	7:E:183:GLU:N	2.46	0.47
8:L:295:ARG:H	9:J:368:THR:CB	2.26	0.47
5:k:274:THR:O	5:k:375:GLY:N	2.47	0.47
5:k:322:ASN:N	5:k:357:GLN:O	2.33	0.47
1:N:193:GLY:CA	1:N:243:GLY:HA2	2.45	0.47
5:a:214:ALA:O	5:a:220:ILE:N	2.35	0.47
6:K:150:GLY:HA2	6:K:202:GLU:HA	1.95	0.47
7:C:602:LYS:N	7:C:647:ASP:O	2.27	0.47
7:A:356:ILE:O	7:A:360:MET:N	2.33	0.47
7:A:618:LEU:HA	7:A:767:LEU:O	2.15	0.47
6:I:206:LYS:N	6:I:258:SER:O	2.45	0.47
6:I:380:LEU:HA	6:I:448:GLY:HA3	1.97	0.47
5:e:4:GLU:HA	5:e:50:VAL:HA	1.96	0.47
5:h:33:PRO:O	5:h:82:TYR:HA	2.14	0.47
6:K:207:GLN:HA	6:K:257:PHE:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:8:LEU:HA	5:d:65:VAL:O	2.14	0.47
5:d:14:GLY:HA3	5:d:139:HIS:HA	1.95	0.47
5:b:4:GLU:HA	5:b:50:VAL:HA	1.95	0.47
5:f:71:PRO:N	5:f:97:GLY:HA2	2.30	0.47
5:n:317:TYR:N	5:n:347:ASN:O	2.46	0.47
2:U:2:ALA:CB	6:I:44:ARG:HA	2.44	0.47
5:l:322:ASN:HA	5:l:377:MET:HA	1.96	0.47
5:n:7:THR:O	5:n:64:ALA:HA	2.14	0.47
9:J:633:ARG:HA	9:J:637:TYR:CB	2.44	0.47
7:A:381:GLY:HA3	7:A:466:GLN:O	2.14	0.47
3:W:656:LEU:HA	3:X:657:ARG:HA	1.96	0.47
5:l:52:PHE:HA	5:l:62:PRO:HA	1.97	0.47
5:d:172:PHE:N	5:d:205:LEU:O	2.48	0.47
8:L:371:CYS:N	8:L:376:ALA:O	2.38	0.47
5:i:272:GLY:N	5:i:377:MET:O	2.44	0.47
1:N:176:SER:CB	1:N:279:PHE:HA	2.45	0.47
8:L:358:ASN:O	8:L:363:VAL:N	2.42	0.47
5:a:260:LEU:HA	5:a:319:ALA:HB3	1.96	0.47
7:E:600:ASP:O	7:E:648:TYR:HA	2.15	0.47
1:D:642:TYR:O	1:D:646:GLU:N	2.39	0.46
5:e:52:PHE:HA	5:e:62:PRO:HA	1.97	0.46
5:g:272:GLY:O	5:g:377:MET:N	2.39	0.46
5:d:100:ALA:HB1	5:d:103:ASN:O	2.15	0.46
1:F:190:ILE:O	1:F:243:GLY:N	2.48	0.46
4:Z:18:LYS:HA	4:Z:30:VAL:HA	1.98	0.46
4:Z:148:THR:O	4:Z:168:GLY:N	2.26	0.46
5:j:325:GLN:HA	5:j:361:SER:O	2.15	0.46
1:r:108:PRO:O	1:r:110:LYS:N	2.48	0.46
1:N:150:GLY:HA2	1:N:228:PRO:HA	1.96	0.46
5:d:43:GLU:C	5:d:45:THR:H	2.23	0.46
1:H:479:THR:O	1:H:484:GLU:N	2.47	0.46
5:i:49:ASP:HA	5:i:52:PHE:O	2.16	0.46
5:n:14:GLY:HA3	5:n:139:HIS:HA	1.97	0.46
6:K:385:THR:H	6:K:388:THR:CB	2.29	0.46
7:C:740:ASN:O	7:C:744:ALA:N	2.49	0.46
9:J:790:GLU:O	9:J:891:GLY:HA3	2.15	0.46
6:I:358:LYS:O	6:I:364:GLY:N	2.46	0.46
5:b:100:ALA:HB3	5:b:144:GLY:CA	2.46	0.46
1:B:150:GLY:HA3	1:B:226:MET:HA	1.98	0.46
5:f:138:CYS:HA	5:f:169:TYR:O	2.16	0.46
5:k:351:TRP:O	6:K:662:GLY:HA3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:727:GLU:O	9:J:743:GLY:HA3	2.16	0.46
1:D:373:ILE:O	1:D:377:LEU:N	2.45	0.46
3:X:584:LEU:HA	3:Y:584:LEU:H	1.80	0.46
7:G:571:VAL:H	7:G:637:ALA:HB1	1.81	0.46
6:I:6:LEU:O	6:I:10:SER:N	2.47	0.46
5:a:100:ALA:CB	5:a:148:GLY:HA3	2.45	0.46
5:c:10:LEU:HA	5:c:67:LEU:O	2.16	0.46
5:c:322:ASN:O	5:c:358:VAL:HA	2.16	0.46
5:k:324:ILE:HA	5:k:375:GLY:HA2	1.98	0.46
5:l:202:VAL:O	5:l:268:PHE:HA	2.16	0.46
5:l:320:ILE:O	5:l:356:ILE:HA	2.15	0.46
1:N:433:LEU:O	1:N:464:ALA:HB1	2.15	0.46
7:A:272:ARG:N	7:A:296:ALA:HB1	2.30	0.46
3:W:649:LEU:HA	3:X:650:ARG:HA	1.98	0.46
4:Z:162:THR:O	4:Z:176:LEU:N	2.36	0.46
5:c:5:ILE:N	5:c:50:VAL:O	2.41	0.46
5:h:53:TYR:N	5:h:61:ILE:O	2.38	0.46
6:I:206:LYS:O	6:I:258:SER:N	2.38	0.46
1:H:493:LYS:O	1:H:497:ALA:N	2.49	0.46
5:c:52:PHE:HA	5:c:63:ARG:H	1.81	0.46
5:j:325:GLN:N	5:j:374:SER:O	2.30	0.46
5:a:142:ALA:HB2	5:a:173:PRO:N	2.32	0.46
5:b:55:ALA:N	5:b:59:HIS:O	2.49	0.46
5:m:4:GLU:HA	5:m:50:VAL:HA	1.96	0.46
1:D:163:GLY:HA3	7:C:315:GLN:HA	1.97	0.45
1:D:559:ARG:HA	1:D:585:GLU:HA	1.97	0.45
5:g:325:GLN:O	5:g:374:SER:N	2.38	0.45
5:i:33:PRO:O	5:i:82:TYR:HA	2.16	0.45
5:j:111:GLY:O	5:j:115:HIS:N	2.49	0.45
5:k:316:CYS:O	5:k:382:THR:N	2.29	0.45
6:I:194:GLY:HA3	6:I:284:GLN:HA	1.98	0.45
5:c:134:GLY:HA3	5:c:165:LEU:O	2.16	0.45
5:g:270:MET:N	5:g:379:ALA:O	2.37	0.45
5:j:71:PRO:N	5:j:97:GLY:HA2	2.31	0.45
5:k:35:GLY:O	5:k:60:TYR:N	2.50	0.45
5:n:7:THR:N	5:n:63:ARG:O	2.29	0.45
5:d:274:THR:N	5:d:375:GLY:O	2.39	0.45
7:A:262:SER:O	7:A:275:LEU:N	2.33	0.45
5:f:43:GLU:C	5:f:45:THR:H	2.24	0.45
5:j:100:ALA:HB3	5:j:144:GLY:C	2.42	0.45
5:j:138:CYS:HA	5:j:169:TYR:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:397:ASP:O	7:E:401:GLN:N	2.40	0.45
4:Z:174:ALA:HA	4:Z:284:LYS:CB	2.46	0.45
5:a:30:GLY:O	5:a:38:GLU:N	2.30	0.45
5:n:136:VAL:HA	5:n:167:GLN:O	2.16	0.45
5:d:321:LEU:O	5:d:378:MET:N	2.33	0.45
4:Z:19:ALA:N	4:Z:29:ALA:O	2.29	0.45
5:f:134:GLY:HA3	5:f:165:LEU:O	2.16	0.45
5:h:3:ARG:HA	5:h:131:SER:O	2.17	0.45
1:N:517:ARG:HA	1:N:626:ASP:CB	2.47	0.45
7:G:740:ASN:O	7:G:744:ALA:N	2.50	0.45
6:I:496:ALA:O	6:I:500:GLN:N	2.36	0.45
5:d:28:GLU:HA	5:d:367:LEU:CB	2.46	0.45
8:L:179:LEU:O	8:L:183:GLU:N	2.49	0.45
1:H:310:SER:O	1:H:314:HIS:N	2.35	0.45
1:H:642:TYR:O	1:H:646:GLU:N	2.46	0.45
5:c:49:ASP:HA	5:c:52:PHE:O	2.17	0.45
5:l:61:ILE:HA	5:l:85:LEU:O	2.17	0.45
5:d:8:LEU:O	5:d:138:CYS:N	2.21	0.45
8:L:627:ILE:H	8:L:1479:SER:CB	2.30	0.45
9:J:263:VAL:O	9:J:301:ILE:N	2.32	0.45
5:c:9:GLN:CB	5:c:15:ASN:HA	2.47	0.45
5:h:51:PHE:O	5:h:63:ARG:N	2.39	0.45
6:K:18:THR:N	6:K:26:GLN:O	2.50	0.45
7:E:438:GLU:O	7:E:461:THR:N	2.29	0.45
5:f:28:GLU:HA	5:f:367:LEU:CB	2.47	0.45
5:k:206:ASP:CB	5:k:306:SER:H	2.29	0.45
7:G:636:LEU:O	7:G:638:LEU:N	2.50	0.45
2:U:32:SER:O	2:U:36:ASN:N	2.50	0.44
5:g:434:GLU:O	5:g:438:ALA:N	2.43	0.44
5:h:102:ASN:HA	5:h:144:GLY:N	2.32	0.44
5:d:10:LEU:N	5:d:138:CYS:O	2.46	0.44
6:I:338:GLU:HA	6:I:551:ARG:O	2.17	0.44
5:g:69:LEU:CB	5:g:99:GLY:HA2	2.47	0.44
5:n:1:MET:N	1:N:332:HIS:O	2.50	0.44
8:L:213:SER:O	8:L:217:ALA:N	2.51	0.44
7:E:544:ILE:O	7:E:548:PHE:N	2.50	0.44
5:h:7:THR:O	5:h:65:VAL:N	2.27	0.44
8:L:106:GLU:O	8:L:110:VAL:N	2.45	0.44
8:L:557:ASN:O	8:L:572:GLY:HA2	2.18	0.44
5:e:47:ARG:N	5:e:243:LEU:O	2.50	0.44
5:i:289:THR:O	5:i:293:VAL:N	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:353:PRO:CB	9:J:942:GLU:H	2.30	0.44
1:B:205:ALA:N	1:B:221:THR:O	2.33	0.44
5:d:3:ARG:HA	5:d:131:SER:O	2.18	0.44
7:C:412:SER:O	7:C:416:PHE:N	2.28	0.44
6:I:532:GLN:O	6:I:537:GLU:N	2.40	0.44
1:t:112:SER:C	1:t:114:TYR:H	2.26	0.44
9:J:393:SER:HA	9:J:397:ALA:HB3	2.00	0.44
6:I:359:ASP:HA	6:I:364:GLY:HA3	1.99	0.44
2:O:56:ASN:CB	1:v:44:ALA:H	2.31	0.44
5:e:214:ALA:O	5:e:219:HIS:N	2.51	0.44
5:e:325:GLN:HA	5:e:361:SER:O	2.18	0.44
5:i:322:ASN:O	5:i:359:ALA:N	2.32	0.44
5:i:325:GLN:HA	5:i:361:SER:O	2.18	0.44
5:l:262:PRO:HA	8:L:1663:HIS:CB	2.47	0.44
1:D:112:LEU:C	1:D:114:LEU:H	2.25	0.44
1:H:318:MET:O	1:H:323:LEU:N	2.45	0.44
4:Z:71:ILE:HA	4:Z:76:VAL:HA	2.00	0.44
5:e:52:PHE:HA	5:e:63:ARG:H	1.81	0.44
6:I:212:GLY:HA3	6:I:252:PRO:HA	2.00	0.44
2:P:38:GLY:H	8:L:122:PRO:CA	2.23	0.44
5:f:5:ILE:N	5:f:50:VAL:O	2.30	0.44
5:a:108:PHE:HA	5:a:152:TYR:HA	2.00	0.43
5:i:142:ALA:HB2	5:i:173:PRO:CB	2.48	0.43
1:B:249:LEU:O	1:B:255:ASP:N	2.29	0.43
5:h:69:LEU:CB	5:h:99:GLY:HA2	2.47	0.43
7:C:439:GLU:HA	7:C:460:TYR:HA	2.00	0.43
5:c:52:PHE:HA	5:c:62:PRO:HA	1.99	0.43
5:c:289:THR:O	5:c:293:VAL:N	2.32	0.43
5:c:322:ASN:N	5:c:357:GLN:O	2.32	0.43
7:A:586:ALA:O	7:A:590:SER:N	2.52	0.43
4:Z:219:VAL:N	4:Z:307:PRO:O	2.43	0.43
7:G:544:ILE:O	7:G:548:PHE:N	2.51	0.43
1:D:25:ASN:O	1:D:29:ASN:N	2.51	0.43
5:h:321:LEU:O	5:h:378:MET:N	2.36	0.43
5:n:53:TYR:O	5:n:61:ILE:N	2.44	0.43
8:L:365:SER:N	8:L:368:PHE:O	2.51	0.43
1:F:310:SER:O	1:F:314:HIS:N	2.33	0.43
5:j:104:TRP:CB	5:j:187:ASN:HA	2.49	0.43
5:l:10:LEU:C	5:l:146:GLY:HA2	2.43	0.43
1:D:22:ILE:HA	1:D:33:VAL:HA	2.00	0.43
5:a:9:GLN:CB	5:a:15:ASN:HA	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:325:GLN:HA	5:g:361:SER:O	2.17	0.43
5:i:8:LEU:HA	5:i:65:VAL:O	2.19	0.43
1:N:179:SER:O	1:N:183:LEU:N	2.35	0.43
4:Z:299:LEU:N	4:Z:330:ILE:O	2.40	0.43
5:c:100:ALA:HB3	5:c:144:GLY:HA3	2.01	0.43
5:l:70:GLU:HA	5:l:99:GLY:HA2	2.00	0.43
7:G:264:GLN:H	7:G:274:PHE:HA	1.83	0.43
7:G:619:ALA:HB1	7:G:624:GLN:C	2.44	0.43
1:D:310:SER:O	1:D:314:HIS:N	2.36	0.43
5:a:317:TYR:O	5:a:348:PHE:HA	2.19	0.43
5:c:324:ILE:O	5:c:361:SER:N	2.51	0.43
5:e:102:ASN:C	5:e:144:GLY:HA3	2.44	0.43
1:u:3:THR:O	1:u:4:PRO:C	2.62	0.43
7:G:701:ALA:O	7:G:705:ALA:N	2.52	0.43
8:L:82:LEU:O	8:L:86:ALA:N	2.42	0.43
6:I:207:GLN:HA	6:I:257:PHE:HA	2.01	0.43
6:I:413:LEU:O	6:I:456:TYR:HA	2.19	0.43
1:D:493:LYS:O	1:D:497:ALA:N	2.52	0.43
5:a:139:HIS:O	5:a:170:SER:HA	2.18	0.43
6:K:421:HIS:N	6:K:441:PRO:O	2.48	0.43
1:N:407:VAL:HA	1:N:504:ILE:HA	2.01	0.43
5:b:409:ARG:HA	5:b:415:LYS:HA	2.01	0.42
5:c:324:ILE:HA	5:c:375:GLY:HA2	2.01	0.42
5:g:289:THR:O	5:g:293:VAL:N	2.33	0.42
5:i:321:LEU:O	5:i:378:MET:N	2.34	0.42
5:l:323:ILE:N	5:l:376:LEU:O	2.48	0.42
5:n:5:ILE:N	5:n:50:VAL:O	2.52	0.42
7:G:604:ASP:O	7:G:645:SER:N	2.49	0.42
6:K:338:GLU:HA	6:K:551:ARG:O	2.19	0.42
5:a:14:GLY:HA3	5:a:139:HIS:HA	2.01	0.42
5:a:26:CYS:O	5:a:30:GLY:N	2.53	0.42
5:h:321:LEU:N	5:h:378:MET:O	2.28	0.42
5:h:398:LEU:O	5:h:402:GLU:N	2.53	0.42
5:j:48:LYS:O	5:j:52:PHE:N	2.33	0.42
7:A:381:GLY:N	7:A:434:GLU:HA	2.34	0.42
5:c:53:TYR:O	5:c:61:ILE:N	2.37	0.42
5:f:55:ALA:N	5:f:59:HIS:O	2.49	0.42
5:f:136:VAL:HA	5:f:167:GLN:O	2.19	0.42
5:g:321:LEU:N	5:g:378:MET:O	2.27	0.42
5:k:11:GLY:N	5:k:67:LEU:O	2.52	0.42
5:k:33:PRO:O	5:k:82:TYR:HA	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:170:SER:C	7:E:172:GLN:H	2.27	0.42
7:M:426:GLY:HA2	7:M:482:GLY:HA2	2.02	0.42
1:D:409:THR:O	1:D:413:MET:N	2.28	0.42
5:a:10:LEU:HA	5:a:67:LEU:O	2.19	0.42
5:k:52:PHE:HA	5:k:62:PRO:HA	2.00	0.42
5:d:385:SER:CB	5:d:432:ILE:HA	2.49	0.42
4:Z:144:ALA:HB2	4:Z:342:GLY:CA	2.42	0.42
5:c:320:ILE:O	5:c:356:ILE:HA	2.20	0.42
5:m:205:LEU:HA	5:m:304:MET:O	2.20	0.42
1:N:345:ALA:N	1:N:388:ASP:O	2.48	0.42
5:d:138:CYS:HA	5:d:169:TYR:O	2.20	0.42
4:Z:362:TYR:O	4:Z:366:GLY:N	2.45	0.42
5:e:438:ALA:HA	5:e:443:TYR:CB	2.50	0.42
5:g:70:GLU:HA	5:g:97:GLY:HA2	2.01	0.42
5:h:215:THR:HA	5:h:220:ILE:O	2.19	0.42
5:l:10:LEU:HA	5:l:67:LEU:O	2.19	0.42
6:K:269:PRO:O	6:K:273:ALA:N	2.38	0.42
8:L:487:CYS:C	8:L:489:GLY:H	2.28	0.42
7:M:194:GLY:O	7:M:194:GLY:N	2.53	0.42
2:P:38:GLY:N	8:L:122:PRO:HA	2.24	0.42
5:a:258:ALA:HB2	7:A:684:CYS:HA	2.01	0.42
5:i:8:LEU:N	5:i:136:VAL:O	2.30	0.42
5:i:47:ARG:N	5:i:244:ARG:O	2.53	0.42
5:j:10:LEU:HA	5:j:67:LEU:O	2.20	0.42
5:n:259:SER:O	5:n:319:ALA:HB1	2.20	0.42
7:A:305:ILE:O	7:A:321:ALA:HB1	2.19	0.42
1:F:34:GLU:C	1:F:36:LYS:H	2.28	0.42
5:b:52:PHE:HA	5:b:62:PRO:HA	2.02	0.42
5:f:4:GLU:O	5:f:133:GLU:N	2.35	0.42
7:E:381:GLY:HA3	7:E:466:GLN:C	2.45	0.42
5:g:33:PRO:O	5:g:82:TYR:HA	2.19	0.41
5:n:11:GLY:N	5:n:67:LEU:O	2.52	0.41
5:d:324:ILE:HA	5:d:375:GLY:HA2	2.02	0.41
5:k:14:GLY:HA3	5:k:139:HIS:HA	2.02	0.41
1:u:1:MET:O	1:u:3:THR:N	2.53	0.41
7:C:616:ARG:HA	7:C:628:MET:CB	2.50	0.41
1:F:189:TRP:HA	1:F:194:GLU:O	2.21	0.41
4:Z:14:SER:CB	4:Z:158:GLY:H	2.33	0.41
5:a:214:ALA:HB1	5:a:220:ILE:CB	2.51	0.41
5:c:409:ARG:HA	5:c:415:LYS:HA	2.02	0.41
5:k:104:TRP:CB	5:k:187:ASN:HA	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:411:GLU:O	5:a:415:LYS:N	2.53	0.41
5:k:53:TYR:N	5:k:61:ILE:O	2.40	0.41
5:m:55:ALA:CB	5:n:217:ARG:HA	2.50	0.41
1:u:28:VAL:O	1:u:32:PHE:N	2.40	0.41
5:j:214:ALA:O	5:j:219:HIS:N	2.53	0.41
3:W:584:LEU:H	3:V:588:GLN:CB	2.33	0.41
4:Z:102:PRO:HA	4:Z:131:ALA:O	2.20	0.41
5:f:54:GLN:HA	5:f:60:TYR:HA	2.02	0.41
5:g:317:TYR:O	5:g:348:PHE:HA	2.20	0.41
1:B:205:ALA:O	1:B:221:THR:N	2.35	0.41
5:d:447:GLY:H	5:d:452:GLU:N	2.19	0.41
7:C:619:ALA:HB1	7:C:624:GLN:C	2.44	0.41
2:U:3:SER:HA	6:I:43:ASN:CB	2.51	0.41
5:f:100:ALA:HB3	5:f:144:GLY:C	2.44	0.41
5:d:136:VAL:HA	5:d:167:GLN:O	2.21	0.41
5:f:36:ILE:HA	5:f:58:GLU:O	2.21	0.41
5:g:67:LEU:HA	5:g:92:TYR:O	2.21	0.41
5:h:209:ALA:HB2	5:h:306:SER:H	1.85	0.41
5:h:325:GLN:HA	5:h:361:SER:O	2.20	0.41
5:i:70:GLU:HA	5:i:97:GLY:O	2.21	0.41
5:m:7:THR:HA	5:m:136:VAL:O	2.19	0.41
7:M:634:THR:C	7:M:636:LEU:H	2.29	0.41
5:a:48:LYS:O	5:a:52:PHE:N	2.30	0.41
5:b:282:VAL:O	5:b:370:ALA:HB1	2.20	0.41
5:e:324:ILE:O	5:e:361:SER:N	2.38	0.41
5:i:3:ARG:HA	5:i:131:SER:O	2.20	0.41
1:B:159:TYR:HA	7:A:175:PRO:HA	2.03	0.41
5:d:137:LEU:O	5:d:169:TYR:N	2.54	0.41
7:G:606:MET:N	7:G:643:ALA:O	2.34	0.41
9:J:223:GLN:O	9:J:226:THR:N	2.50	0.41
9:J:531:GLN:C	9:J:533:GLY:H	2.29	0.41
1:H:114:LEU:C	1:H:116:SER:N	2.78	0.41
2:U:10:ALA:HB2	6:I:29:GLN:HA	2.03	0.41
5:k:1:MET:N	6:K:371:ALA:HB1	2.36	0.41
5:k:10:LEU:O	5:k:14:GLY:HA3	2.21	0.41
7:M:893:TYR:O	7:M:897:LEU:N	2.45	0.41
4:Z:218:TYR:O	4:Z:255:PHE:HA	2.21	0.40
5:b:33:PRO:O	5:b:82:TYR:HA	2.21	0.40
5:b:107:GLY:HA3	5:b:148:GLY:HA3	2.03	0.40
5:k:11:GLY:HA3	5:k:145:THR:C	2.46	0.40
5:k:409:ARG:HA	5:k:415:LYS:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:438:ALA:HA	5:k:443:TYR:CB	2.51	0.40
5:n:209:ALA:HB1	5:n:303:VAL:O	2.21	0.40
8:L:20:LYS:O	8:L:22:HIS:N	2.54	0.40
7:A:258:GLY:N	7:A:261:VAL:O	2.49	0.40
7:E:619:ALA:HB1	7:E:624:GLN:C	2.46	0.40
1:F:127:THR:O	1:F:131:LYS:N	2.50	0.40
5:h:174:ASN:HA	5:h:208:THR:H	1.86	0.40
5:k:291:LEU:HA	5:k:336:SER:HA	2.03	0.40
1:F:382:LEU:N	1:F:393:VAL:O	2.47	0.40
5:a:325:GLN:HA	5:a:361:SER:O	2.21	0.40
5:i:324:ILE:HA	5:i:375:GLY:HA2	2.03	0.40
5:i:325:GLN:O	5:i:374:SER:N	2.31	0.40
5:m:53:TYR:N	5:m:61:ILE:O	2.43	0.40
5:n:252:ASP:O	5:n:256:LEU:N	2.51	0.40
1:v:123:PRO:C	1:v:125:ASP:N	2.77	0.40
6:I:386:ALA:N	6:I:421:HIS:H	2.19	0.40
2:T:59:ALA:HB2	1:u:43:PHE:CB	2.52	0.40
5:h:324:ILE:N	5:h:359:ALA:O	2.31	0.40
5:l:357:GLN:HA	8:L:1671:VAL:HA	2.02	0.40
8:L:1677:ALA:O	8:L:1682:HIS:N	2.54	0.40
9:J:721:ARG:O	9:J:748:TYR:HA	2.21	0.40
7:E:440:HIS:O	7:E:459:ARG:HA	2.21	0.40
4:Z:19:ALA:O	4:Z:28:ARG:N	2.54	0.40
5:a:100:ALA:HB1	5:a:103:ASN:O	2.22	0.40
5:b:100:ALA:HB3	5:b:144:GLY:C	2.46	0.40
5:f:321:LEU:O	5:f:378:MET:N	2.48	0.40
5:f:325:GLN:HA	5:f:361:SER:O	2.21	0.40
5:g:51:PHE:O	5:g:63:ARG:N	2.49	0.40
5:h:43:GLU:C	5:h:45:THR:H	2.30	0.40
5:k:166:VAL:H	5:k:200:ASP:CB	2.35	0.40
5:k:209:ALA:HB2	5:k:306:SER:N	2.36	0.40
1:t:112:SER:C	1:t:114:TYR:N	2.79	0.40
6:I:212:GLY:H	6:I:253:SER:H	1.69	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	B	640/907 (71%)	629 (98%)	11 (2%)	0	100	100
1	D	655/907 (72%)	642 (98%)	13 (2%)	0	100	100
1	F	655/907 (72%)	645 (98%)	10 (2%)	0	100	100
1	H	654/907 (72%)	641 (98%)	13 (2%)	0	100	100
1	N	624/907 (69%)	618 (99%)	6 (1%)	0	100	100
1	r	111/907 (12%)	102 (92%)	5 (4%)	4 (4%)	2	20
1	s	113/907 (12%)	104 (92%)	5 (4%)	4 (4%)	3	20
1	t	118/907 (13%)	104 (88%)	8 (7%)	6 (5%)	1	15
1	u	118/907 (13%)	103 (87%)	8 (7%)	7 (6%)	1	13
1	v	125/907 (14%)	111 (89%)	10 (8%)	4 (3%)	3	21
2	O	80/82 (98%)	80 (100%)	0	0	100	100
2	P	71/82 (87%)	71 (100%)	0	0	100	100
2	Q	64/82 (78%)	64 (100%)	0	0	100	100
2	R	64/82 (78%)	64 (100%)	0	0	100	100
2	S	64/82 (78%)	64 (100%)	0	0	100	100
2	T	80/82 (98%)	80 (100%)	0	0	100	100
2	U	80/82 (98%)	80 (100%)	0	0	100	100
3	V	73/660 (11%)	73 (100%)	0	0	100	100
3	W	77/660 (12%)	76 (99%)	0	1 (1%)	9	42
3	X	76/660 (12%)	75 (99%)	1 (1%)	0	100	100
3	Y	74/660 (11%)	73 (99%)	1 (1%)	0	100	100
4	Z	373/375 (100%)	365 (98%)	8 (2%)	0	100	100
5	a	444/457 (97%)	437 (98%)	7 (2%)	0	100	100
5	b	450/457 (98%)	442 (98%)	8 (2%)	0	100	100
5	c	446/457 (98%)	438 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	448/457 (98%)	441 (98%)	7 (2%)	0	100	100
5	e	446/457 (98%)	438 (98%)	8 (2%)	0	100	100
5	f	449/457 (98%)	441 (98%)	8 (2%)	0	100	100
5	g	448/457 (98%)	440 (98%)	8 (2%)	0	100	100
5	h	449/457 (98%)	441 (98%)	8 (2%)	0	100	100
5	i	446/457 (98%)	438 (98%)	8 (2%)	0	100	100
5	j	447/457 (98%)	439 (98%)	8 (2%)	0	100	100
5	k	446/457 (98%)	438 (98%)	8 (2%)	0	100	100
5	l	445/457 (97%)	437 (98%)	8 (2%)	0	100	100
5	m	446/457 (98%)	438 (98%)	8 (2%)	0	100	100
5	n	455/457 (100%)	448 (98%)	7 (2%)	0	100	100
6	I	606/667 (91%)	588 (97%)	17 (3%)	1 (0%)	43	78
6	K	608/667 (91%)	589 (97%)	15 (2%)	4 (1%)	18	56
7	A	651/930 (70%)	641 (98%)	10 (2%)	0	100	100
7	C	647/930 (70%)	637 (98%)	10 (2%)	0	100	100
7	E	672/930 (72%)	661 (98%)	11 (2%)	0	100	100
7	G	672/930 (72%)	661 (98%)	11 (2%)	0	100	100
7	M	763/930 (82%)	744 (98%)	18 (2%)	1 (0%)	48	83
8	L	972/1811 (54%)	922 (95%)	46 (5%)	4 (0%)	30	67
9	J	834/1024 (81%)	807 (97%)	23 (3%)	4 (0%)	24	63
10	p	54/158 (34%)	53 (98%)	1 (2%)	0	100	100
11	w	31/1663 (2%)	31 (100%)	0	0	100	100
11	x	31/1663 (2%)	31 (100%)	0	0	100	100
All	All	17795/31360 (57%)	17385 (98%)	370 (2%)	40 (0%)	44	78

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	638	VAL
1	r	109	SER
1	s	109	SER
1	t	5	ASP
1	t	111	VAL
1	u	5	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	v	108	PRO
6	K	295	ARG
8	L	351	GLU
6	I	295	ARG
1	r	111	VAL
1	r	113	SER
1	s	111	VAL
1	s	113	SER
1	t	109	SER
1	t	113	SER
1	u	6	GLN
1	u	109	SER
1	u	111	VAL
1	v	124	ARG
6	K	447	SER
8	L	417	PRO
9	J	221	VAL
1	u	110	LYS
1	u	113	SER
6	K	250	LEU
8	L	1454	GLN
9	J	223	GLN
9	J	526	GLU
1	r	110	LYS
1	s	110	LYS
1	t	6	GLN
1	t	110	LYS
1	v	125	ASP
6	K	445	PRO
7	M	635	GLU
1	u	4	PRO
1	v	123	PRO
8	L	309	GLU
9	J	616	VAL

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	L	2
1	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	106:ARG	C	107:GLN	N	9.43
1	L	123:PRO	C	124:GLN	N	5.75
1	L	311:TYR	C	312:LEU	N	3.96

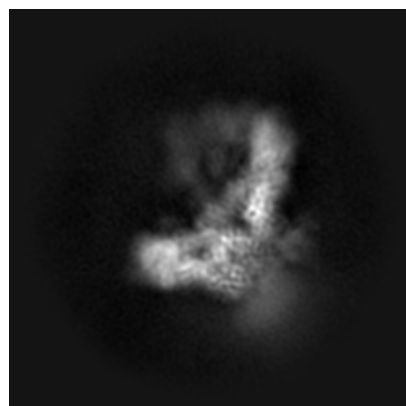
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53399. These allow visual inspection of the internal detail of the map and identification of artifacts.

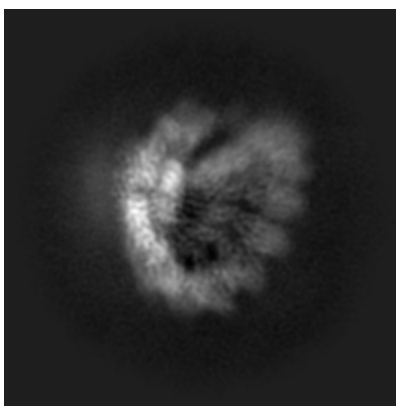
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

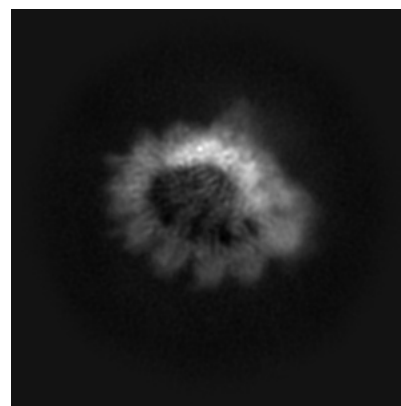
6.1.1 Primary map



X

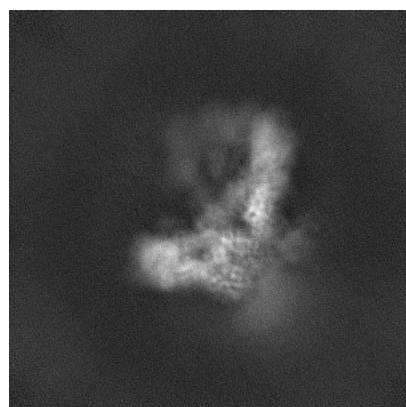


Y

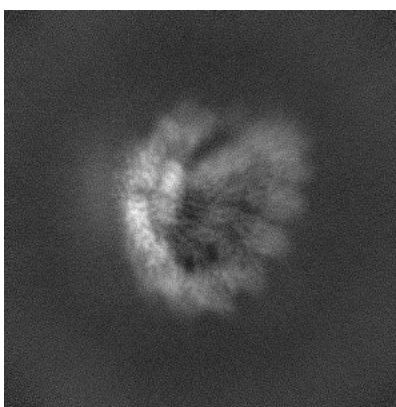


Z

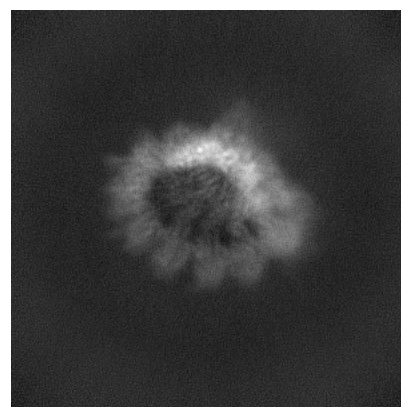
6.1.2 Raw map



X



Y

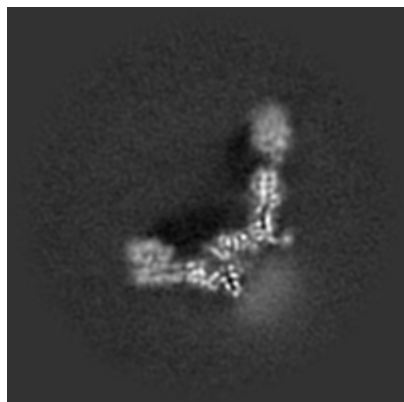


Z

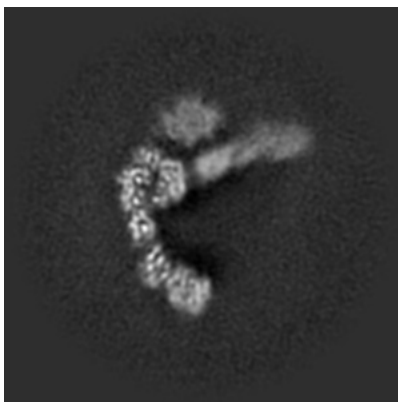
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

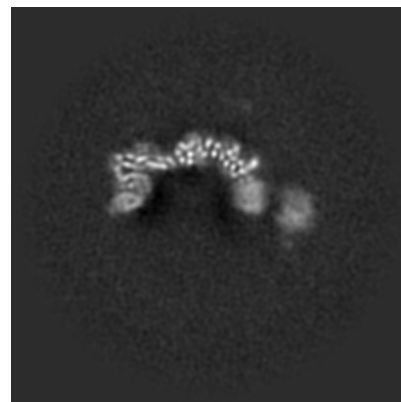
6.2.1 Primary map



X Index: 192

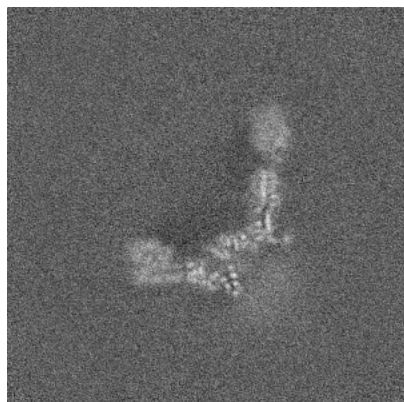


Y Index: 192

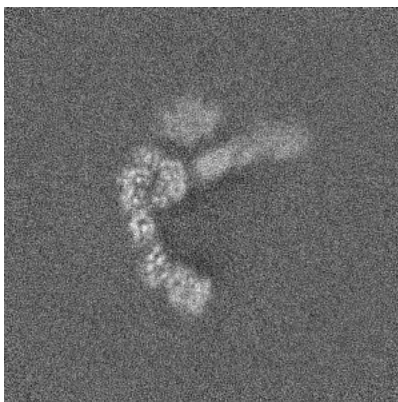


Z Index: 192

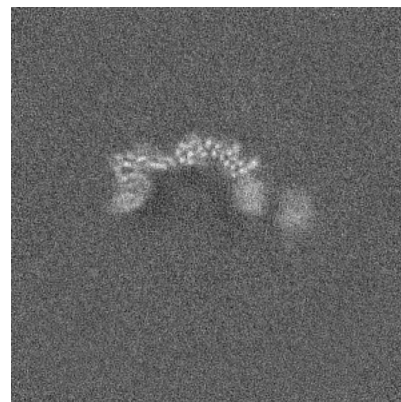
6.2.2 Raw map



X Index: 192



Y Index: 192

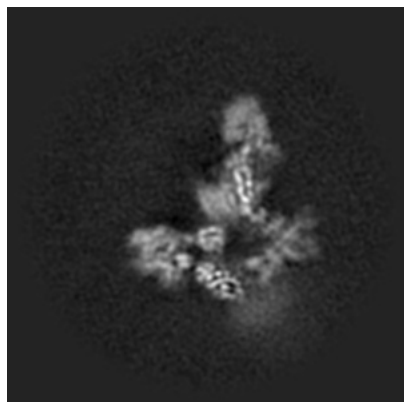


Z Index: 192

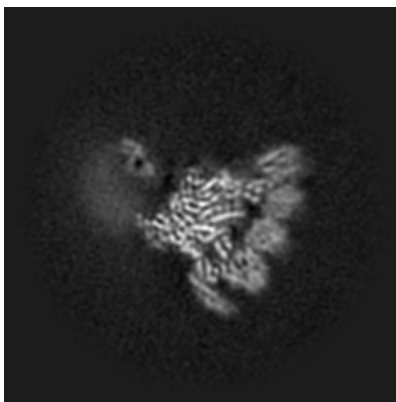
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

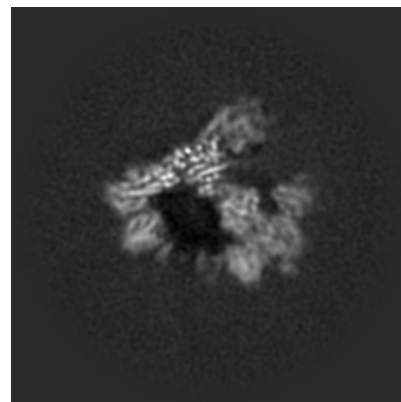
6.3.1 Primary map



X Index: 226

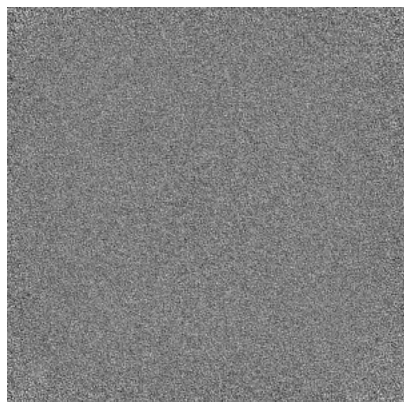


Y Index: 242

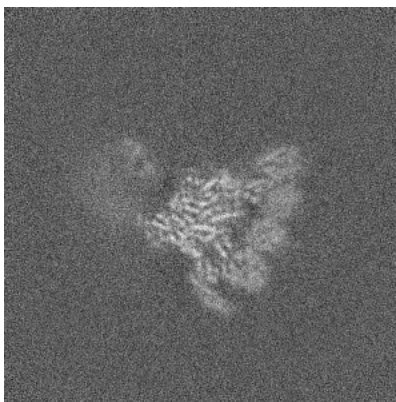


Z Index: 162

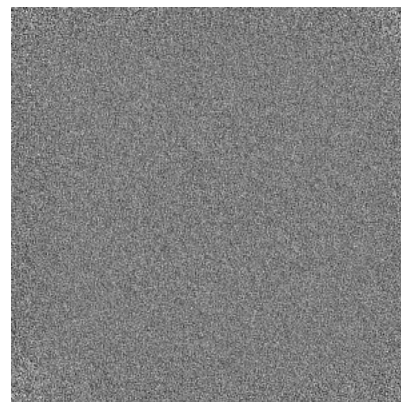
6.3.2 Raw map



X Index: 0



Y Index: 242

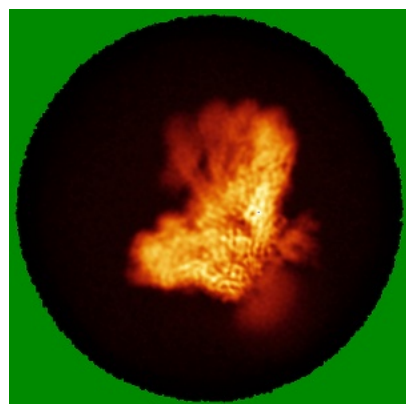


Z Index: 0

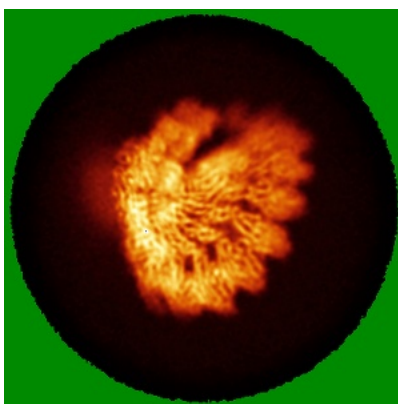
The images above show the largest variance slices of the map in three orthogonal directions.

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

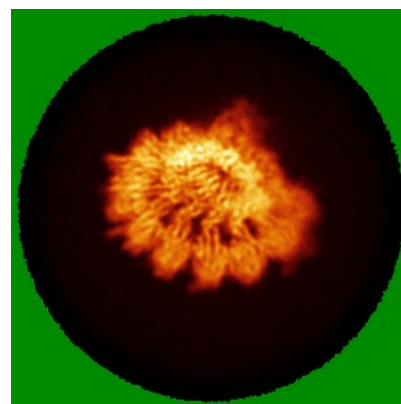
6.4.1 Primary map



X

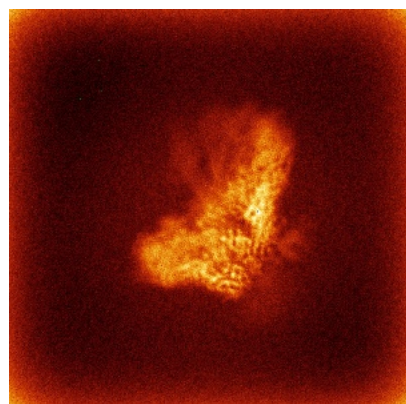


Y

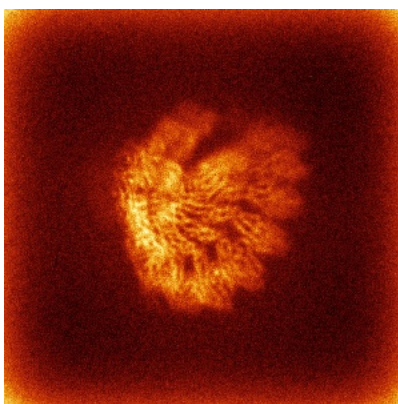


Z

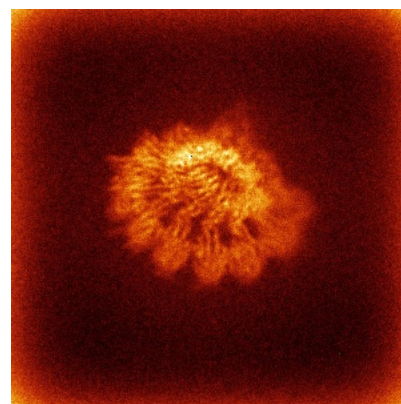
6.4.2 Raw map



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.

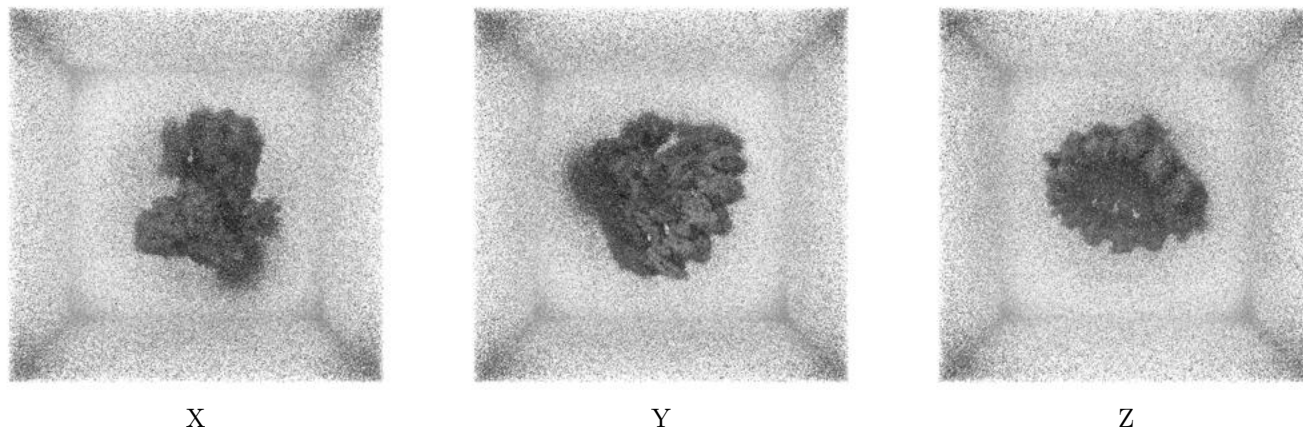
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0363. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

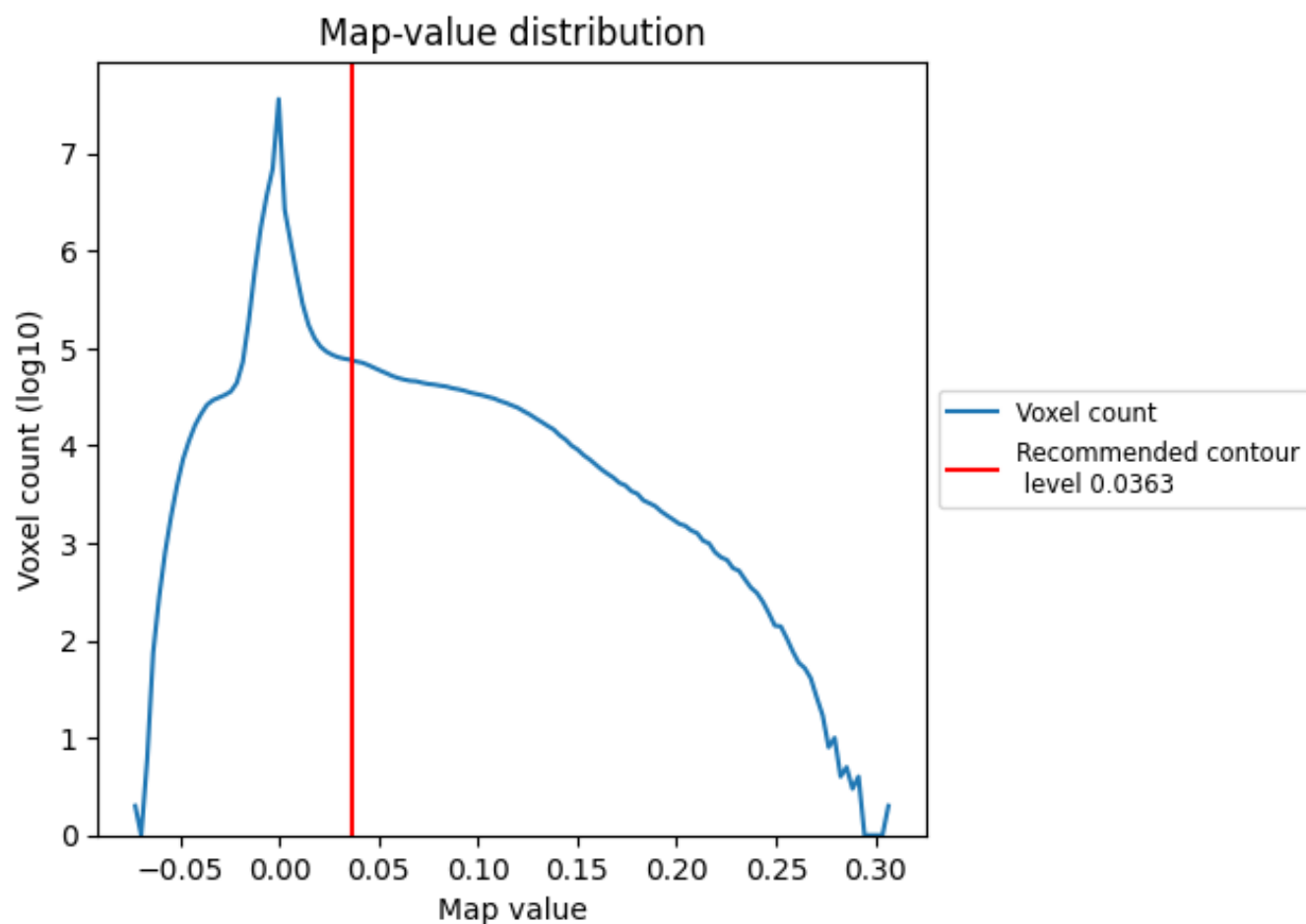
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

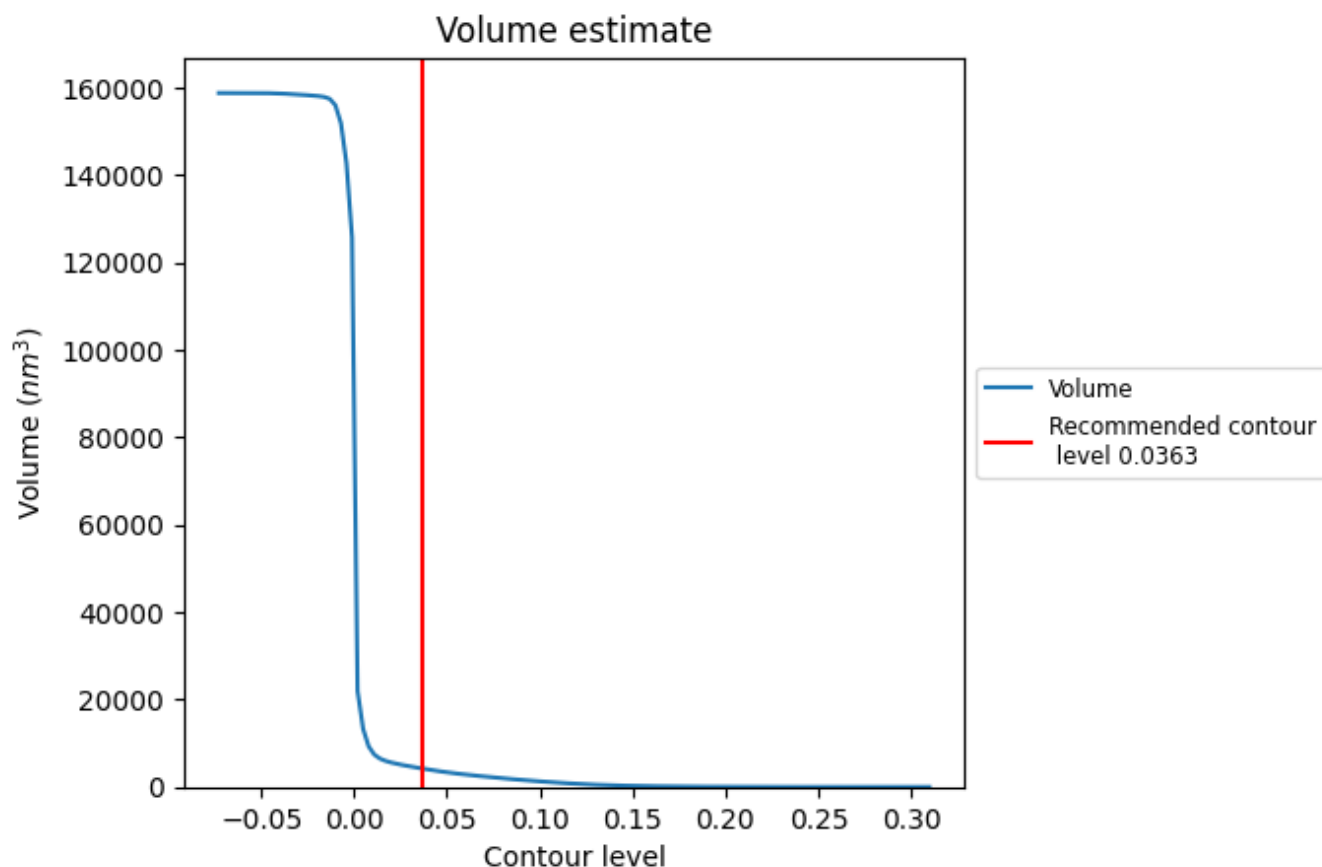
This section contains the results of statistical analysis of the map.

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.

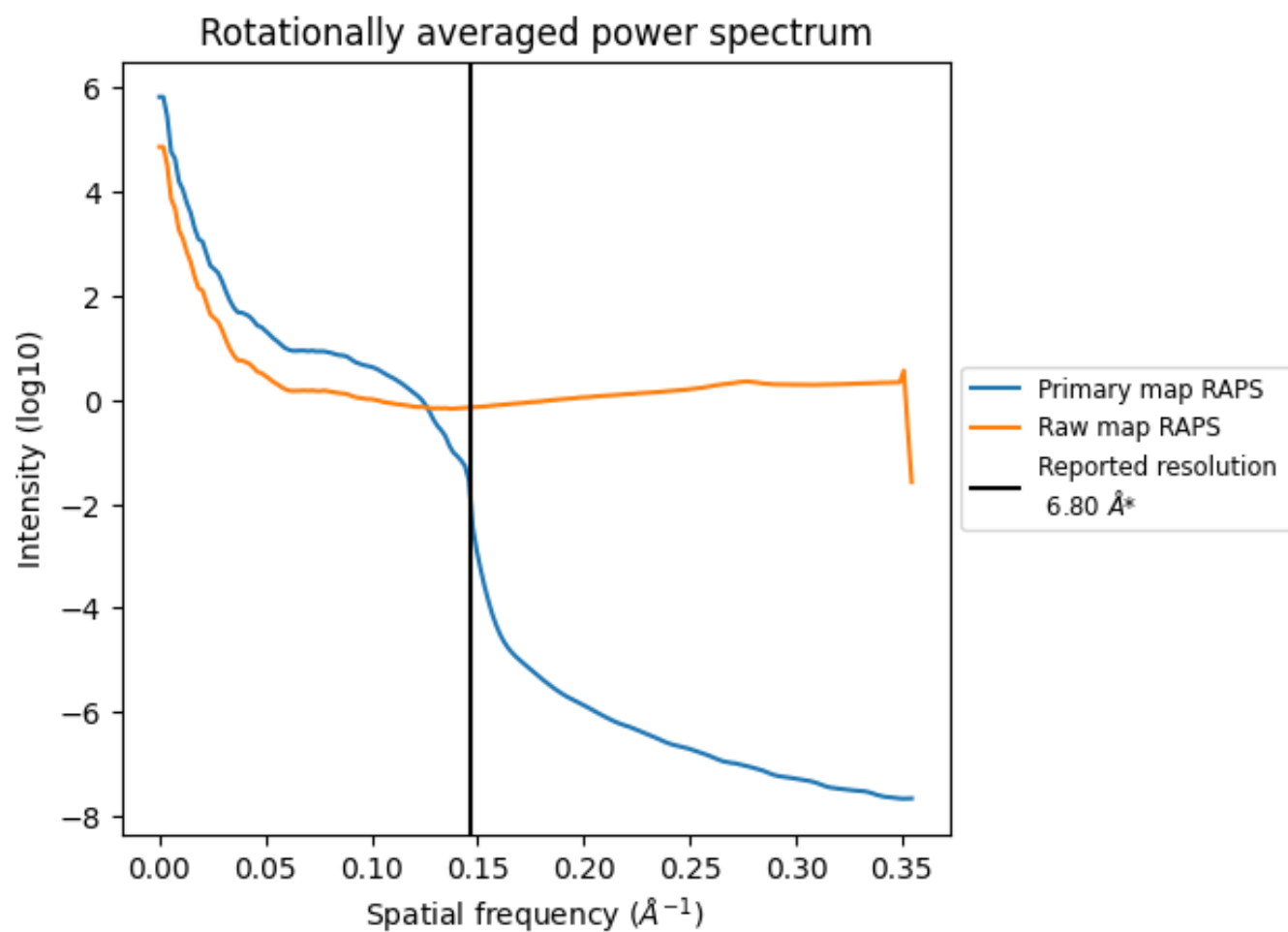
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4247 nm^3 ; this corresponds to an approximate mass of 3836 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 ⓘ

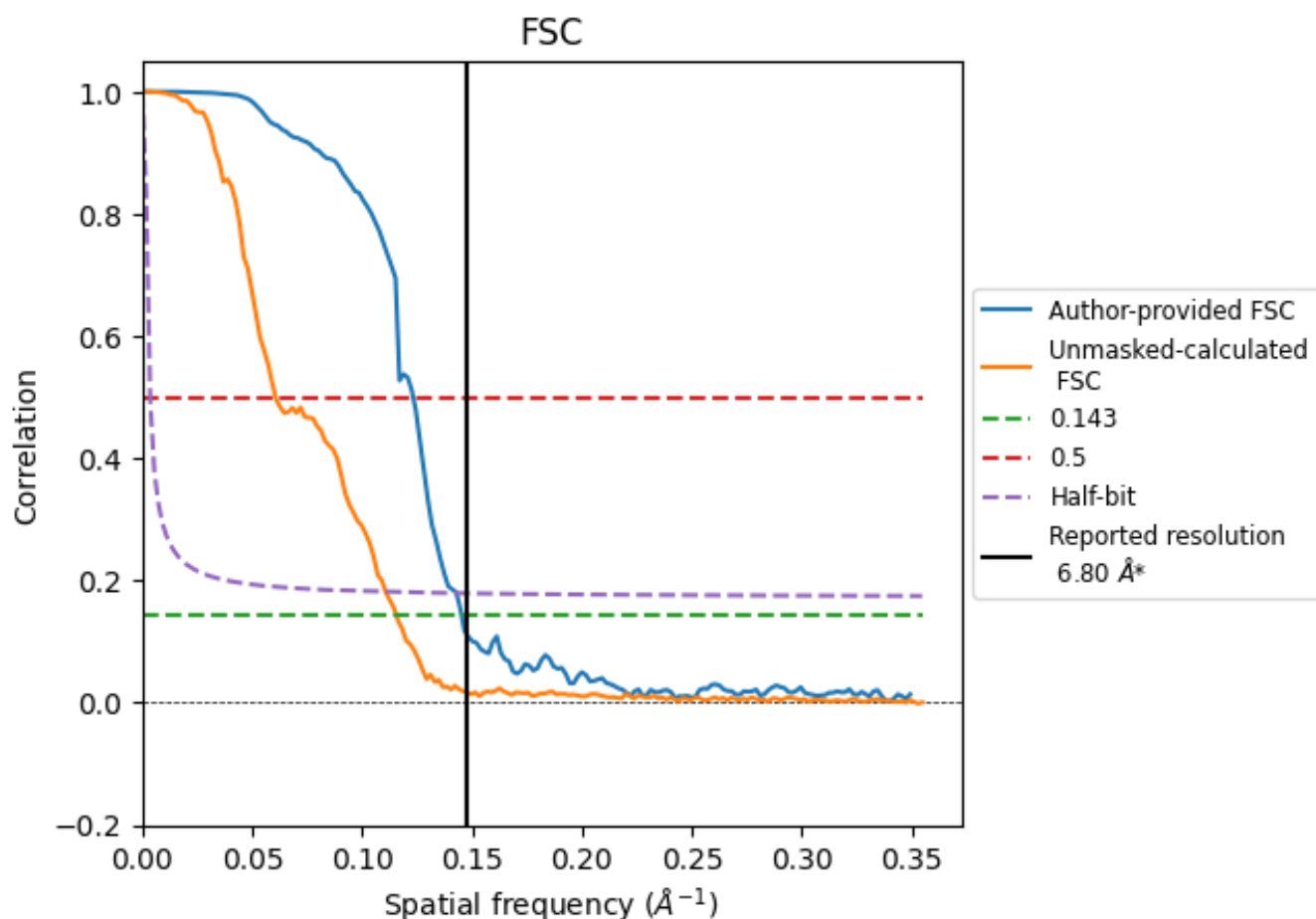


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

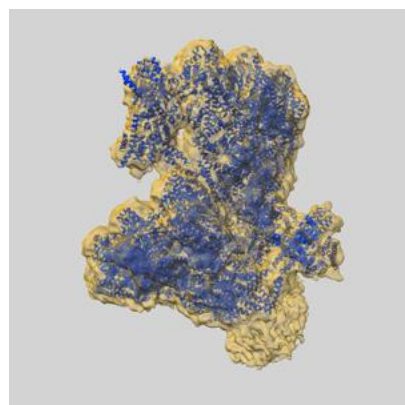
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.89	8.12	7.00
Unmasked-calculated*	8.66	16.47	9.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.66 differs from the reported value 6.8 by more than 10 %

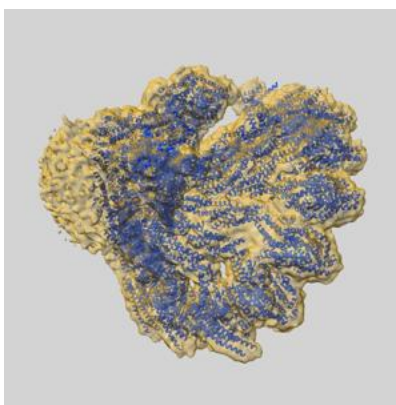
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53399 and PDB model 9QVM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

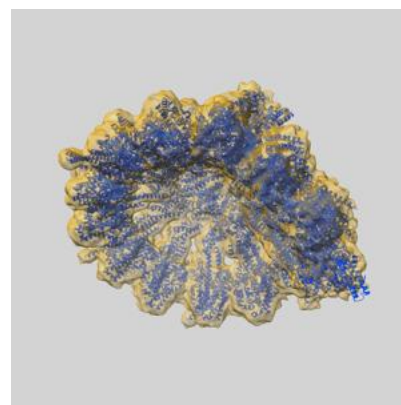
9.1 Map-model overlay [i](#)



X



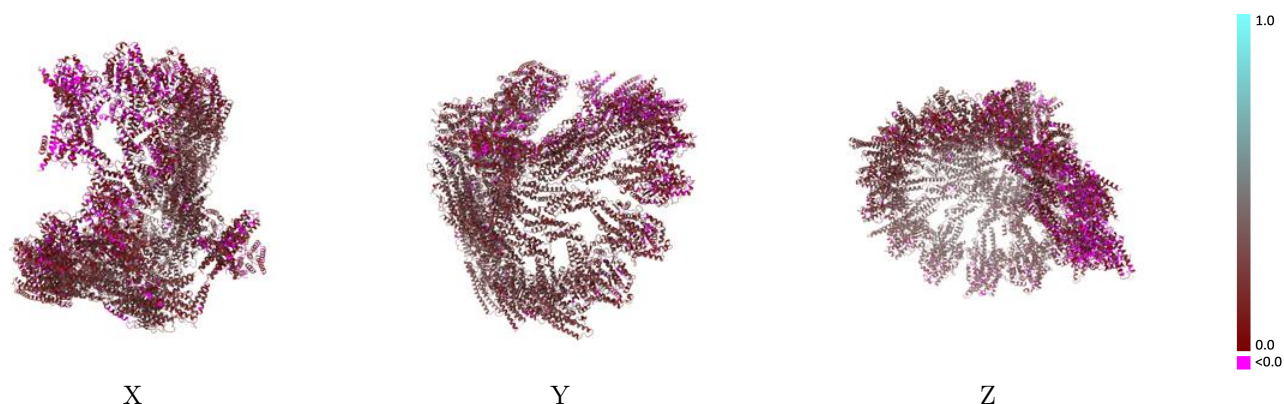
Y



Z

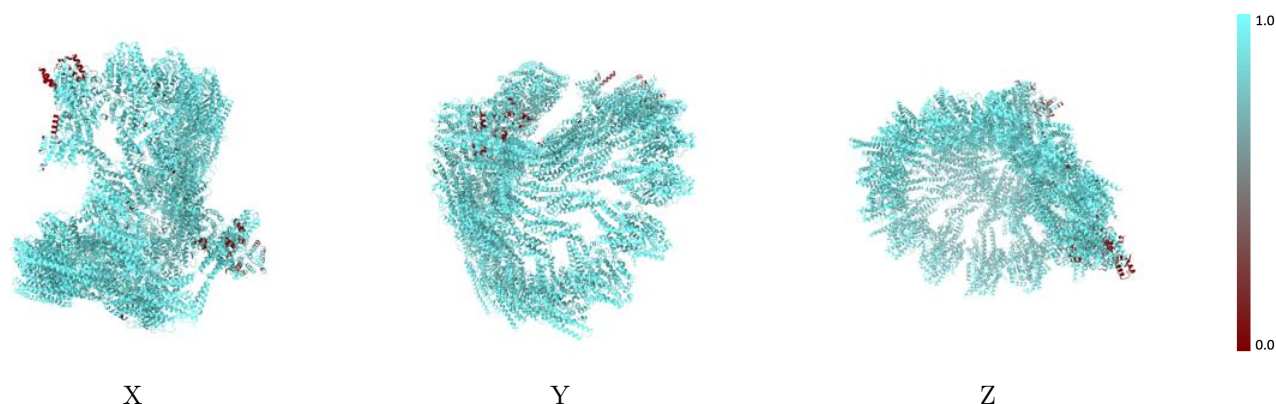
The images above show the 3D surface view of the map at the recommended contour level 0.0363 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



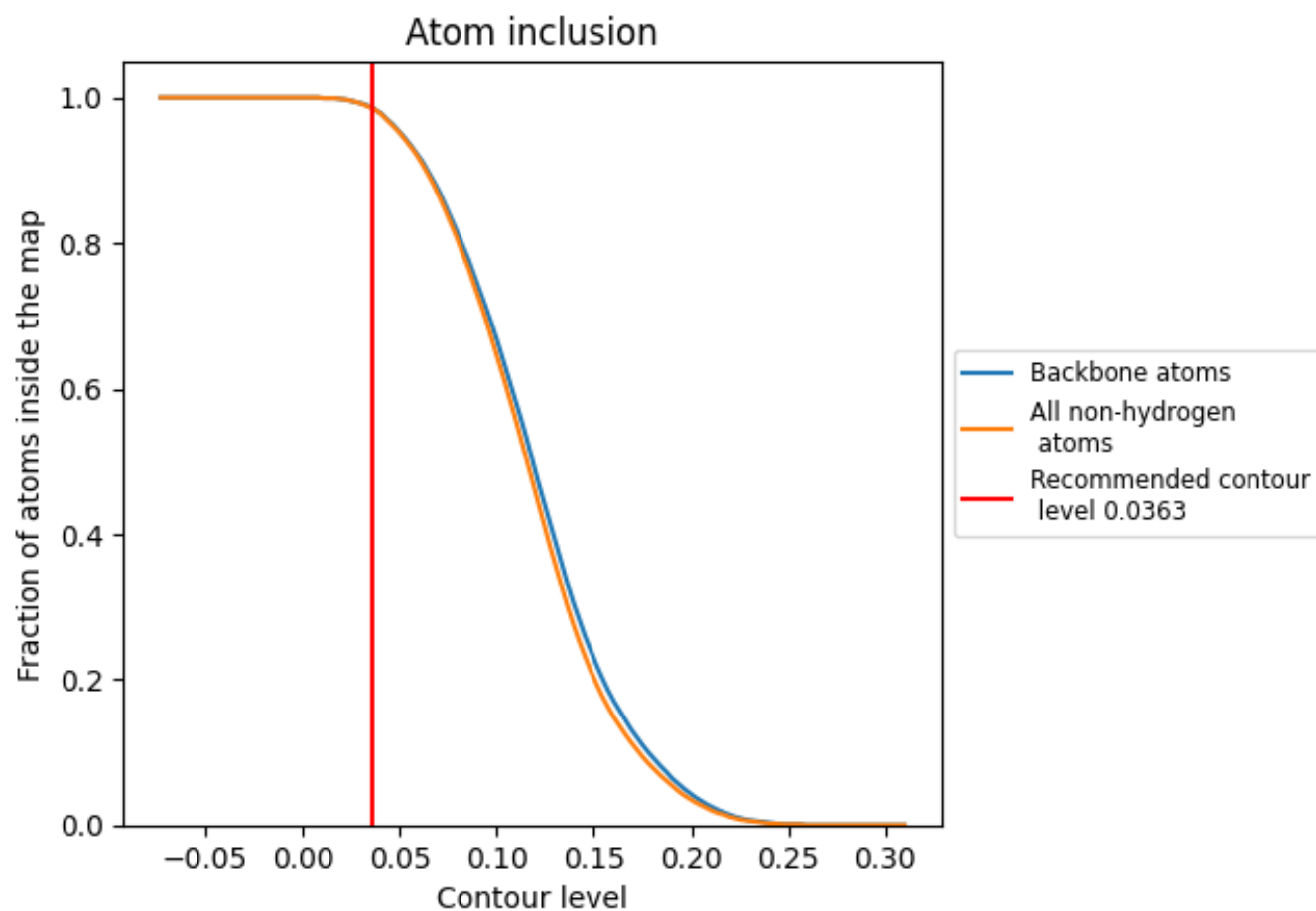
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0363).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.0363) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9850	 0.1810
A	 0.9980	 0.1670
B	 0.9990	 0.2170
C	 0.9980	 0.2310
D	 1.0000	 0.2400
E	 1.0000	 0.2550
F	 1.0000	 0.2570
G	 1.0000	 0.2510
H	 1.0000	 0.2560
I	 1.0000	 0.2520
J	 0.9870	 0.2070
K	 1.0000	 0.2300
L	 0.9980	 0.2100
M	 0.9880	 0.1210
N	 0.9530	 0.0820
O	 0.9900	 0.2590
P	 1.0000	 0.2590
Q	 0.7710	 0.0330
R	 0.6130	 0.1020
S	 0.7620	 0.1030
T	 0.9110	 0.2020
U	 0.9850	 0.1790
V	 0.9920	 0.1510
W	 1.0000	 0.2040
X	 0.9950	 0.1320
Y	 0.9740	 0.1970
Z	 1.0000	 0.2150
a	 0.9910	 0.0950
b	 0.9980	 0.1290
c	 1.0000	 0.1680
d	 1.0000	 0.1630
e	 1.0000	 0.1830
f	 1.0000	 0.2120
g	 1.0000	 0.2070
h	 1.0000	 0.2320



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 1.0000	 0.1910
j	 1.0000	 0.1530
k	 0.9970	 0.0910
l	 0.9990	 0.0750
m	 0.9870	 0.0420
n	 0.8470	 0.0060
p	 0.9680	 0.0310
r	 0.7600	 0.0880
s	 0.7990	 0.0730
t	 0.9670	 0.1490
u	 0.9300	 0.1730
v	 0.9950	 0.2670
w	 1.0000	 0.0810
x	 1.0000	 0.0940