

May 24, 2025 - 07:46 am BST

PDB ID	:	$9 \mathrm{QVN} \ / \ \mathrm{pdb} \ 00009 \mathrm{qvn}$
EMDB ID	:	EMD-53400
Title	:	Cryo-EM reconstruction of the NEDD1 anchor protein bound to the gamma-
		tubulin ring complex
Authors	:	Munoz-Hernandez, H.; Xu, Y.; Wieczorek, M.
Deposited on	:	2025-04-11
Resolution	:	4.70 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

The following versions of software and data (see references (1)) were used in the production of this report:

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 4.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	(#Entries)	$\mathop{{\rm EM}}\limits_{{\rm (\#Entries)}}$
Clashscore	210492	15764
Ramachandran outliers	207382	16835

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 <=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	В	907	•		66%		5%	29%		
1	D	907	•		68%		•	28%		
1	F	907			66%		6%	28%		
1	Н	907			67%		5%	28%		
1	Ν	907		42%	66%		•	31%		
1	r	907	12% 12%	-		88%				
1	s	907	13% 12%			87%				
1	t	907	7% 12%	•		87%				
1	u	907	6% 12%	•		87%				



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Continued	from	previous	page

Mol	Chain	Length	Quality of chain	
1	V	907	13% 86%	
2	Ο	82	9%	5%
2	Р	82	83%	6% 11%
2	Q	82	80% 79%	20%
2	R	82	80%	20%
2	S	82	80% 79%	20%
2	Т	82	13%	
2	U	82	50% 98%	•
3	V	660	5% 12% 88%	
3	W	660	6% 12% 88%	
3	Х	660	7% 12% 88%	
3	Y	660	11% 88%	
4	Z	375	85%	15%
5	a	457	<b>•</b> 86%	11% •
5	b	457	91%	8% •
5	с	457	88%	10% •
5	d	457	85%	13% •
5	е	457	86%	12% ·
5	f	457	88%	10% •
5	g	457	<b>•</b> 86%	13% ·
5	h	457	90%	9% •
5	i	457		10% •
5	j	457		11% •
5	k	457	85%	13% •
5	1	457	91%	6% •



Mol	Chain	Length	Quality of chain					
5	m	457	42%		• •			
5	n	457	91%		6%			
6	Ι	667	85%		7% 8%			
6	Κ	667	85%		7% 8%			
7	А	930	<b>6</b> 5%	6%	29%			
7	С	930	65%	5%	30%			
7	Е	930	<b>•</b> 70%	•	27%			
7	G	930	<b>6</b> 9%	•	27%			
7	М	930	67%	•	28%			
8	L	1811	<b>•</b> 51% •		46%			
9	J	1024	12%		7% 18%			



## 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 87756 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.

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mol	Chain	Residues	Aton	ns	AltConf	Trace
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	657	Total C	N O	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				3256 1942	<u>657 657</u>		
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	F	657	Total C	N O	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				3256 1942	657 657	_	-
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	Н	656	Total C	N O	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				3252 1940	$656  ext{ } 656  ext{ }$		0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	r	113	Total C	N O	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	110	562  336	113 113	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	G	115	Total C	N O	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		5	115	572 342	$115 \ 115$	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	+	190	Total C	N O	0	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		U	120	597  357	120 120	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1		190	Total C	N O	0	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		u	120	597  357	120 120	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1		190	Total C	N O	0	0
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		V	129	642 384	129 129	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	D	644	Total C	N O	0	0
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		D	044	3192 1904	644 644	U	U
1 $1$ $1$ $1$ $1$ $1$ $1$ $1$ $1$ $1$	1	N	620	Total C	N O	0	0
		IN	030	3123 1863	630 630	U	U

• Molecule 1 is a protein called Gamma-tubulin complex component 3.

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

Mol	Chain	Residues	Atom	ıs	AltConf	Trace
2	P	73	Total C	N O	0	0
	1	15	363  217	$73  ext{ }73$	0	0
2	В	66	Total C	N O	0	0
2	10	00	328 196	66 66	0	0
2	S	66	Total C	N O	0	0
2	0	00	328 196	66 66	0	0
2	т	82	Total C	N O	0	0
2	T	02	406 242	82 82	0	0
2	T	82	Total C	N O	0	0
	U	02	406 242	82 82	0	0



Mol	Chain	Residues	Atoms	AltConf	Trace	
2	0	82	Total C N	0	0	0
	0	02	406  242  82	82	0	0
2	0	66	Total C N	Ο	0	0
	V V	00	328  196  66	66		0

• Molecule 3 is a protein called Protein NEDD1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	W	70	Total	С	Ν	0	0	0
5	vv	19	394	236	79	79	0	0
3	v	78	Total	С	Ν	0	0	0
0	Λ	10	389	233	78	78	0	0
3	V	77	Total	С	Ν	0	0	0
0	v	11	384	230	77	77	0	0
	70	Total	С	Ν	Ο	0	0	
0	I	10	389	233	78	78	0	0

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

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

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

Mol	Chain	Residues		Ator	AltConf	Trace		
5	0	446	Total	С	Ν	Ο	0	0
0	a	440	2204	1312	446	446	0	0
5	h	459	Total	С	Ν	Ο	0	0
0	U	402	2233	1329	452	452	0	0
5	0	118	Total	С	Ν	Ο	0	0
0	C	440	2213	1317	448	448	0	0
5	0	118	Total	С	Ν	Ο	0	0
0	е	440	2213	1317	448	448	0	0
5	f	451	Total	С	Ν	Ο	0	0
0	L	401	2228	1326	451	451	0	0
5	ď	450	Total	С	Ν	Ο	0	0
0	g	400	2223	1323	450	450	0	0
5	h	451	Total	С	Ν	Ο	0	0
0	11	401	2228	1326	451	451	0	0
5	i	118	Total	$\overline{\mathbf{C}}$	N	Ō	0	0
	1	440	2213	1317	448	448	U	



Mol	Chain	Residues		Ator	$\mathbf{ns}$		AltConf	Trace
5	;	440	Total	С	Ν	Ο	0	0
5	J	449	2218	1320	449	449	0	0
5	ŀ	118	Total	С	Ν	Ο	0	0
5	K	440	2213	1317	448	448	0	0
5	1	447	Total	С	Ν	Ο	0	0
5	1	447	2208	1314	447	447	0	0
5	m	118	Total	С	Ν	Ο	0	0
5	111	440	2213	1317	448	448	0	0
5	n	457	Total	С	Ν	Ο	0	0
5	11	407	2258	1344	457	457	0	0
5	d	451	Total	С	Ν	Ο	0	0
5	u	401	2228	1326	451	451	0	0

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
с	452	GLU	-	expression tag	UNP P23258
с	453	ASN	-	expression tag	UNP P23258
с	454	LEU	-	expression tag	UNP P23258
с	455	TYR	-	expression tag	UNP P23258
с	456	PHE	-	expression tag	UNP P23258
с	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



Continu	ied from pre	vious 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						
1	452	GLU	-	expression tag	UNP P23258						
1	453	ASN	-	expression tag	UNP P23258						
1	454	LEU	-	expression tag	UNP P23258						
1	455	TYR	-	expression tag	UNP P23258						
1	456	PHE	-	expression tag	UNP P23258						
1	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						

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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		Ator	ns		AltConf	Trace		
6	K	614	Total 3037	C 1809	N 614	O 614	0	0		
6	Ι	612	Total 3027	C 1803	N 612	O 612	0	0		

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

Mol	Chain	Residues		Ator	AltConf	Trace		
7	C	678	Total	С	Ν	Ο	0	0
1	G	010	3367	2011	678	678	0	0
7	М	665	Total	С	Ν	Ο	0	0
1	111	005	3303	1973	665	665	0	0
7	C	652	Total	С	Ν	Ο	0	0
1	U	000	3244	1938	653	653	0	0
7	Δ	657	Total	С	Ν	Ο	0	0
1	Л	001	3264	1950	657	657	0	0
7	F	678	Total	С	Ν	Ο	0	0
	Ľ	010	3367	2011	678	678	0	0

• Molecule 8 is a protein called TUBGCP6 protein.



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

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

Mol	Chain	Residues		Ator	$\mathbf{ns}$		AltConf	Trace		
9	J	842	Total 4186	C 2502	N 842	O 842	0	0		



### 3 Residue-property plots (i)

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



# Q273 Q273 A275 L282 L282 L337 L337 L337 L332 Q390 Q326 L332 L332 Q390 Q393 Q392 Q393 Q392 Q393 L337 L382 L337 L343 M413 Q326 L483 L483 K493 K493 K566 G576 G576 G576 G576 G576 G576 A10 SE24 A10 S524 S524 S524 S524 S526 S524 S524 S524 S524 S524 S524</td

### SER HIS THR

• Molecule 1: Gamma-tubulin complex component 3

















### PRO LEU ARG VAL SER LEU GLY ARG GLY ARG GLY ARG SER ARG SER ARG SER ARG SER THR

• Molecule 1: Gamma-tubulin complex component 3

Cha	in <sup>.</sup>	v:		13	3%																		86	5%																		
M1 A44	R105	50 50 50	P108	A119	P123	R124 D105	07 T/	T129	PRO	TYR	TVB	ALA	ARG	PRO	GLN	THR	PRO	LEU	SER	TYR	ASP	ARG	SER AT A	GLN	SER	ALA	SER	SER	GLY SER	VAL	GLY	SER	GLY	ILE SED	SER	ILE	GLY	CYS	ALA	SER	GLY	PRU ALA
PRO ALA PRO	GLN SER	LEU LEU	PRO	GLN	SER	GLN	ALA	PRO	GLY	CT V	ASP	CYS	LEU	ARG	CL.N	LEU	GLY	SER	ARG I FII	ALA	TRP	THR	THR	ALA	ASN	PRO	SER	SER	ALA	THR	THR SER	LYS	GLY	PRO	SER	ALA	SER	ARG	ASN MET	THR	ARG	ARG
ARG GLU GLY	ASP THR	GLY GLY	THR	GLU	ILE	GLU	ALA	ALA	LEU	VAL	ASP	ILE	LEU	JYYL MAT	V AL PHF.	GLN	GLY	ILE	ASP CI V	TVS	ASN	ILE	MET	ASN	ASN	GLU	ASN	CYS	LYS	VAL	GLY	LYS	ALA	LEU	SER	ARG	LEU	ARG	ASP THR	ALA	VAL	LEU
SER GLU LEU	GLY TRP	LEU	ASN	ILE	ARG	TYR	THR	ASP	GLN	SFR	LEU	ASP	ARG	SER	CI.Y	LEU	VAL	GLY GLY	GLN	DHE	CYS	ALA	LEU	HIS	GLN GLN	GLU	ARG	GLU	TYR	ARG	LEU	SER	VAL	HIS	SER	GLN	GLN	LEU	GLU ASP	ASP	GLN	VAL
ASN LEU GLY	GLU	SER	TEU	LEU	ARG	AKG	LEU	VAL	TRP	TVR	ASP	PRO	LYS	TLE	ARG LEU	LYS	THR	LEU	ALA AT A	LEU	VAL	ASP	CIS	GLN	GLY	LYS	GLY	GL Y	LEU	ALA	SER	VAL	HIS	TYR	THR	LYS	GLY	ASP	PRO TYR	MET	ARG	LEU
VAL GLN HIS	LEU	SER	VAL	SIH	PRO 	V AL LEU	SER	PHE	LEU	ARG	TRP	ILE	TYR	ASP	GLII GLII	LEU	GLU	ASP	TVB	NIT	GLU	PHE	VAL	ALA	SER	PRO	THR	VAL T VS	THR	ASP	ARG LEU	TRP	HIS	LYS	TYR	THR	ARG	LYS	SER	ILE	PRO	PHE
MET THR MET	GLN	SER ARG	LYS	LEU	LEU	GLY	LYS	SER	ILE	ASN	TEU	HIS	GLN	VAL	HTS	ASP	GLN	THR	THR	THR	LYS	MET	ALA	VAL	THR	LYS	ALA	GLU	PRO	GLN	ASP ALA	ALA	ASP	PHE	THR	ASP	GLU	ASN	ALA PHE	GLN	GLY	ILE
ASP ALA ALA	TYR PHE	GLU THR	SER	TYR	LEU	ASP	VAL	LEU	ASN	LYS	TYR	SER	LEU	UEU VED	HTS	MET	GLN	ALA	1 TEM	ARG	TYR	LEU	LEU	GLY	GLN	GL Y ASP	PHE	ILE	SIH	LEU	ASP	LEU	LEU	PRO	GLU	LEU	ARG	PRO	ALA THR	THR	LEU	GLN
HIS ASN LEU	THR GLY	ILEU LEU	GLU	ALA	VAL	ALA	THR	ASN	ALA	GLN	ASP	SER	PR0	GLU GLU	T.EU	ARG	ARG	LEU	VAL	ARG	LEU	LEU	VAL	SER	PRO CT V	GL Y ASP	THR	GLY	ASP	VAL	PHE SER	LEU	ASP	HIS	VAL	ASP	PRO	ILE	ALA THR	VAL	PHE	ARG
GLU CYS MET	SER HIS	TYR LEU	ARG	PHE	ASN	LEU	TRP	ARG	ALA	ARG	MET	GLU	TYR	ITE I	THR	ASP	ILE	ARG	CI V	SIH	MET	CYS	ALA	LYS	LEU	ARG	ASN	MET	GLU	PHE	GLY	VAL	LEU	CTU	CYS	HIS	LEU	ALA	GLU	MET	VAL	PHE
ILE HIS GLN	GLN	TYR TYR	ILE	THE	GLU	V AL LEU	GLU	CYS	SER	dsh A	GLU	LEU	TRP	ASN	UAL.	GLN	GLN	ALA	USD V	LEU	ASP	SIH	TLE	ALA	ALA	GLU	VAL	PHE	ASP	THR	ILE	SER	ARG	LEU	LEU	ASP	ASP	SER	ARG ALA	LEU	LEU	GLN
LEU ARG ALA	VAL PHE	GLN	ILE	GLU	LEU	ASN	ALA	GLN	ASP	ALA TIF	TYR	ARG	ALA	ALA	CI.II	GLU	LEU	CLN	ARG	LEU	GLN	PHE	GLU	LYS	LYS	GLN	ARG	GLU	GLU	GLY	GLN	GLY	VAL	ALA	ALA	GLU	GLU	GLU	GLU	LYS	ARG	GLY
GLU CLS GLU	GLU SER	TLE PRO	LYS	CYS	SER	GLN	ARG	ILE	LEU	TTS	PHE	TYR	GLN	2T 7	VAL.	GLN	GLN	PHE		LEU	LEU	THR	SER	SER	ASP	GLU SER	LEU	ARG	LEU	SER	PHE	LEU	ASP	ASN	GLU	HIS	LYS	ALA	ARG GLU	PRO	ARG	ARG
VAL SER LEU	GLY THR	ARG GLY	ARG	SER	SER	THR																																				

• Molecule 1: Gamma-tubulin complex component 3

Chain B:
66%
5%
29%

Image: State of the state of th









• Molecule 2: Mitotic-spindle organizing protein 1







		*********	*******
CVS CUV PRO TILE PRO TILE ASN SER ASN PRO LVS SER ASN TILE SER TILE SER TILE SER ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	VAL VAL ALA ALA ALA SER SER CUU LEU CUU LUY CUU LIY ALA ASN ASN ASN ASN ASN ASN	A500 A582 P583 F583 F583 F591 F591	1595 1596 1596 1596 1596 1596 1599 1599
D601 ♦ D610 ♦ M629 ♦ N639 ♦ N639 ♦ D641 ♦ L642 ♦ N644 ♦ A644 ♦ E645 ♦ E645 ♦	E552 N653 K654 R655 R655 R655 R655 H659 H659		
• Molecule 3: Protein NEDD	01		
Chain X: 12%	88%		
MET MET GLU GLU GLU GLU ALAS PHE ALA ALA ASP CLY ASP TLE CLY ASP ASP ASP ASP TLE SER SER SER SER	MET THR LEU VAL CEU VAS PAS PHE ASN PHE ASN PHE ASN PHE ASN THR SER RSER SER SER SER SER SER SER SER CUV	TRP SER SER ASN ASN ASN ASN PHE LEU VAL LEU THR ALA SER SER	GLY ASP LYS ILE VAL
SER SER SER CYS CYS CYS CYS PRO CYS PRO LEU LEU LEU LEU CLU CLU CLU CLU CLU CLU CLU CLU CLU CL	CYS VAL ASN ASN ASN ASN SER SER SER MET TYR CIY VAL CIY CIY ASN ASN ASN	AND AND TRP ASP ASP LEU LYS SER ARG ARG ARG SER ARG SER LEU	LYS ASP HIS LYS ASP
VALN VALN THR VAL THR TTR TTR ASN ASN ASN ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	CLU CLU CLU TLE TLEU TLEU TLEU TLEU TLEU TRR TTRR TRR TRR TRR TRR TRR TRR TRR T	ASN ASN GLN SER ARG HIS LEU LYS SER LEU PHE LEU PHE LYS	SER LEU GLY SER
VAL SER ASP ASP ASP CLF TLE TLEU TLEU TRP ASR SER SER SER PR0 GLN SER ASN ASN SER PR0 ASN SER PR0 ASN SER PR0 ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	ASP SER VAL HIS LYS ALA ALA ALA ALA ALA CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	PHE VAL THR THR THR THR CLY CLY CLEU CLEU LEU TLE TLE TLEU TYR ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	THR SER SER LYS LYS
VLEU VLAL LYRS LYRS LTHR VAL ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	THR LIEU ALA CLF CLF CLF CLF SER SER SER SER ARG CLN TTF ARG CLN TTF ARG ARG CLN TTF CLEU	SLIS SLIS PRO VAL LYS THR TLA ALA ALA ALA HIS LYS SER VAL GLN	CYS ILE ALA PHE GLN
TYR TYR THR THR LEU LAR SER SER SER SER CYS CYS CYS CYS CYS CYS CYS THR THR VAL	ASN ASN AND AND AND AND ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	ARAL AVAL GLU GLU GLU ALA ALA ALA ALA ALA ALA ALA ALA ALA CLU CAL CLU CAL	PRO MET THR SER ALA
MET CLY CLY CLY CLY CLY VAL ALA VAL CLU CLU CLU CLV CLV CLV CLV CLV CLV CLY CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	THR LEU SEU SEU SEU CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ALTA CLYS SER SER SER SER CLY GLY GLY MET PHE SER SER SER ARG ARG	ASP ALA VAL VAL ASN
LY/S SER ASP ASP ASP ASP ASP ASP LU YS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	VAL PROE PROE PRO PRO PRO PRO PRO ASN VAL TTR TTR TTR TTR TTR TTR TTR TTR TTR SER SER SER SER SER SER SER	LEU LEU ASN AASN PHE MET MET MET GLY GLY GLU GLU GLU GLU GLU	ASN ARG ASP LEU THR
ALA SERU LLYS SERU LLYS TLYS TLYS LLYS SER ALA ALA ALA ALA	LVS VALEU VALEU VALEU VALEU VALEU ALS ALA ALA ALA ALA ALA SER SER SER SER SER SER ALS	T GLM ARG ASN ASN C C C C C C C C C C C C C C C C C C C	GLU ALA GLN ILEU ILE
		********	****
CYS CYS PRO PRO PRO PRO ASN GLY CHE PRO PRO PRO PRO PRO PRO PRO PRO AILA AILA ALA	GLY ALA ALA SER SER SER LEU SER LEU CLU CLU CLU SER ALA ASN ASN ASN ASN ASN ASN	A.S.N ALA P583 L584 L584 L585 S586 I587 Q588 I589 R590 R590 F591 I592	q593 N594 M595 1596 q597 E598 T599 L600
D601 F603 F603 R604 E605 A606 A606 C607 C607 E612 E617 S637 V638 N639 B640	G641 L642 A644 E643 E645 E645 E645 E645 E645 E645 E645 R648 K654 K654 K655	L656 R657 A658 H659 F660	
• Molecule 3: Protein NEDD	01		
Chain V: 12%	88%		
MET MET GLU GLU GLU ARG ARG ARG SER ASP TLE TLP SER ASP ASP ASP SER SER SER	MET THE LEU VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL	TTRP SER SER ASN ASN ASN ASN PHE LEU VAL LEU VAL THR SER SER SER	GLY ASP LYS ILE VAL
AL SER VYS VYS VYS VYS AL AL LU LLU LLU LLU LLU LLU LLU HR YYS YYS YYS	YYS AAL EEN SSN EER HRR HR EET EEU EEU SSN SSN HR	LE ALL SER VS VS SER SER ALL LE RG ER ER ER	XS ASP ASP ASP ASP





LUYS SEER ASP SEER ASP CLIV SEER ASP CLIV CLIVE CLIVE



### 

### D601 D602 F603 F635 Y635 S637 VAL ASA ASA ASA ASA F660

• Molecule 4: Actin, cytoplasmic 1, N-terminally processed





### 

 $\bullet$  Molecule 5: Tubulin gamma-1 chain









• Molecule 5: Tubu	llin gamma-1 chain	
Chain d:	85%	13% •
82 82 82 83 83 83 83 83 83 83 83 83 83 83 83 83	C35 C35 C35 C38 C38 C38 C38 C38 C43 C43 C44 C44 C44 C44 C44 C44 C44 C44	L666 L67 L67 L67 C100 N102 N102 N102 C138 C138 C138 C138 C138 C138 C138 C138
A199 L205 A209 T241 Y245 C272 C272 T274	2779 Q280 Q285 Q 285 Q285	A350 L360 S374 C375 C375 C375 C375 A377 A377 A377 A377 A377 A377 A377 A
• Molecule 6: Gam	ma-tubulin complex component	nt 4
Chain K:	85%	7% 8%
M1 L5 L6 31 0 81 0 24 24 57 4 57 4 57 4	VI 57 S161 S161 S161 H200 R212 SER ALA ALA ALA ALU CLU CLU CLU CLU CLU CLU CLU CLU CLU C	TLE GLY GLY CLY LEU THR CLY CLV CLV CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
8253 8256 9269 9269 7295 7294 7295 7295 7295 8238	L343 S348 K388 K388 A371 A371 P383 P383 P383 P383 P383 P383 P383 P38	L405 T41 T41 T41 T421 C423 C423 C423 C423 C423 C423 C423 C423
8440 8441 8445 8446 8446 6448 9532 9532 8537 8551 8551	D604 A608 N634 C659 C662 C665 C666	
• Molecule 6: Gam	ma-tubulin complex component	nt 4
Chain I:	85%	7% 8%
M1 16 116 116 118 118 118 118 118 118 118	426 227 227 227 228 228 229 229 229 230 44 44 44 44 44 421 2 206 421 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	ASP ASP GLU GLU GLU GLU CLZ CLZ CLZ CLZ CLZ CLZ CLZ CLZ CLZ CLZ
6LU 6LU 6LU 6LU 6LU 725 7252 8253 8253 8253 8256 8256 8258	P269 A273 A273 T294 R296 K296 K296 C348 C348 C348 C364 C364 C364 C364 C368 C368 C368 C368 C368 C368 C368 C368	A400 V403 L404 L404 C404 C404 C405 C405 C405 C404 C404 C
8440 8444 8441 8441 8448 9448 9532 8532 8622 8622	V632 4656 4656 4656 4656 4656 4666 4666	
• Molecule 7: Isofo	rm 3 of Gamma-tubulin comp	lex component 2
Chain G:	69%	• 27%
MET SER GLU PHE ARG HIS HIS ASP ASP ASP ASN CLU LEU	SER LEU LEU LEU ARG ARG ARG ALY ASP ALA ASP ALA ASP ALA ASP ASP ASP ASP ASN ASP ASP ASP ASP ASP ASP ASP ASP ASS ASP ASS ASS	THR THR TYR THR THR THR THR THR THR SER ALA ALA ALA ALA ALA ALA ALA ALA ALA TLE TLF SER TLE TLF SER THR THR THR THR THR THR THR THR THR TH
GLU ASP PHE LEU LYS LYS ASP GLU LEU LEU LYS SER ASN	THR ARG ASP ASP PRO LEU TEU LEU TTR ASP CLU ASP CLU ASP CLU CSC CLU CSC CCU CCC CCU CCC CCC CCC CCC CCC CC	TYR CLEU CLN CLN CLN CLN CLN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
VAL VAL PRO ALA ALA ALA ALA ALA SER ILE SER SER GLN GLN CLU	GLU GLU LEU LEU LARG CLN GLN GLY SER ALA ALA CLY SER T149 CLY ALA A179 A179 A179	E183 A186 F191 CL192 A18 CL7 CL92 A1A ALA ALA ALA ALA ALA ALA ALA ALA ALA
		D W I D E







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









# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	266675	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 $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.796	Depositor
Minimum map value	-0.165	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	485.76, 485.76, 485.76	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

![](_page_30_Picture_5.jpeg)

# 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).

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	В	0.18	0/3190	0.34	0/4446
1	D	0.23	0/3255	0.37	0/4538
1	F	0.24	0/3255	0.36	0/4538
1	Н	0.25	0/3251	0.36	0/4533
1	Ν	0.11	0/3120	0.33	0/4347
1	r	0.08	0/561	0.32	0/782
1	s	0.09	0/571	0.34	0/796
1	t	0.12	0/596	0.42	0/831
1	u	0.13	0/596	0.42	0/831
1	V	0.29	0/640	0.51	0/891
2	0	0.33	0/405	0.39	0/563
2	Р	0.30	0/362	0.49	0/504
2	Q	0.12	0/327	0.40	0/455
2	R	0.09	0/327	0.28	0/455
2	S	0.07	0/327	0.20	0/455
2	Т	0.15	0/405	0.33	0/563
2	U	0.11	0/405	0.34	0/563
3	V	0.11	0/382	0.28	0/531
3	W	0.11	0/393	0.32	0/548
3	Х	0.10	0/388	0.25	0/541
3	Y	0.11	0/387	0.24	0/538
4	Ζ	0.16	0/1846	0.35	0/2566
5	a	0.12	0/2203	0.40	0/3067
5	b	0.14	0/2232	0.36	0/3107
5	с	0.15	0/2212	0.37	0/3079
5	d	0.15	0/2226	0.37	0/3097
5	е	0.15	0/2212	0.42	0/3079
5	f	0.16	0/2227	0.37	0/3100
5	g	0.15	0/2222	0.37	0/3093
5	h	0.16	$0/2\overline{227}$	$0.\overline{37}$	$0/3\overline{100}$
5	i	0.14	$0/2\overline{212}$	0.36	0/3079
5	j	0.13	0/2217	0.34	0/3086
5	k	0.12	0/2212	0.38	0/3079
5	1	0.11	0/2207	0.35	0/3072

![](_page_31_Picture_7.jpeg)

Mol Chain		Bond lengths		Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
5	m	0.10	0/2212	0.37	0/3079
5	n	0.10	0/2257	0.38	0/3142
6	Ι	0.23	0/3024	0.42	2/4209~(0.0%)
6	Κ	0.19	0/3034	0.40	1/4223~(0.0%)
7	А	0.17	0/3261	0.39	0/4548
7	С	0.23	0/3241	0.37	0/4520
7	Е	0.23	0/3364	0.36	0/4691
7	G	0.23	0/3364	0.36	0/4691
7	М	0.11	0/3300	0.34	0/4602
8	L	0.18	0/4846	0.40	0/6741
9	J	0.21	0/4182	0.42	0/5834
All	All	0.18	0/87683	0.37	3/122133~(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	Х	0	1
6	Ι	0	2
6	Κ	0	3
8	L	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	Ι	79	GLY	N-CA-C	-6.40	98.02	113.18
6	Ι	80	GLY	N-CA-C	-5.44	101.06	112.04
6	Κ	79	GLY	N-CA-C	-5.17	100.92	113.18

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	Ι	442	ARG	Peptide
6	Ι	665	GLY	Peptide
6	Κ	249	MET	Peptide
6	Κ	417	THR	Peptide

![](_page_32_Picture_13.jpeg)

Continued from previous page...

Mol	Chain	Res	Type	Group
6	Κ	665	GLY	Peptide
8	L	313	THR	Peptide
3	Х	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	В	3192	0	1417	25	0
1	D	3256	0	1450	19	0
1	F	3256	0	1450	33	0
1	Н	3252	0	1447	26	0
1	N	3123	0	1382	19	0
1	r	562	0	254	1	0
1	s	572	0	258	2	0
1	t	597	0	273	2	0
1	u	597	0	273	3	0
1	V	642	0	295	4	0
2	0	406	0	217	3	0
2	Р	363	0	185	7	0
2	Q	328	0	153	1	0
2	R	328	0	150	0	0
2	S	328	0	150	1	0
2	Т	406	0	217	0	0
2	U	406	0	217	4	0
3	V	384	0	164	1	0
3	W	394	0	169	1	0
3	Х	389	0	165	1	0
3	Y	389	0	166	3	0
4	Ζ	1847	0	848	33	0
5	a	2204	0	971	34	0
5	b	2233	0	984	26	0
5	с	2213	0	976	26	0
5	d	2228	0	981	43	0
5	е	2213	0	976	40	0
5	f	2228	0	982	31	0
5	g	2223	0	980	36	0
5	h	2228	0	982	27	0

![](_page_33_Picture_9.jpeg)

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	i	2213	0	976	31	0
5	i	2218	0	978	30	0
5	k	2213	0	976	39	0
5	1	2208	0	974	16	0
5	m	2213	0	976	10	0
5	n	2258	0	994	16	0
6	Ι	3027	0	1327	24	0
6	К	3037	0	1331	22	0
7	А	3264	0	1445	34	0
7	С	3244	0	1438	26	0
7	Е	3367	0	1492	15	0
7	G	3367	0	1492	18	0
7	М	3303	0	1464	22	0
8	L	4851	0	2185	35	0
9	J	4186	0	1817	41	0
All	All	87756	0	38997	796	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 6.

All (796) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:24:MET:HA	1:H:31:TYR:HA	1.56	0.86
4:Z:237:GLU:HA	4:Z:251:GLY:HA2	1.58	0.84
4:Z:36:GLY:HA2	4:Z:67:LEU:HA	1.58	0.83
1:F:24:MET:HA	1:F:31:TYR:HA	1.59	0.83
1:D:24:MET:HA	1:D:31:TYR:HA	1.60	0.83
1:t:4:PRO:O	1:t:6:GLN:N	2.12	0.82
7:M:385:SER:HA	7:M:468:PRO:HA	1.62	0.81
1:B:24:MET:HA	1:B:31:TYR:HA	1.63	0.80
5:a:30:GLY:HA3	5:a:41:ALA:HB2	1.62	0.79
5:e:317:TYR:N	5:e:347:ASN:O	2.16	0.79
5:k:195:LEU:HA	5:k:199:ALA:HB3	1.65	0.78
7:C:262:SER:O	7:C:275:LEU:N	2.18	0.77
5:h:274:THR:O	5:h:375:GLY:N	2.16	0.76
5:i:318:ILE:N	5:i:380:ASN:O	2.18	0.76
7:E:262:SER:O	7:E:275:LEU:N	2.18	0.76
8:L:243:GLY:HA2	7:A:355:TYR:HA	1.68	0.76
5:b:323:ILE:O	5:b:376:LEU:N	2.16	0.75
1:N:642:TYR:O	1:N:646:GLU:N	2.19	0.74

![](_page_34_Picture_9.jpeg)

		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
5:k:4:GLU:HA	5:k:50:VAL:HA	1.69	0.74
5:g:318:ILE:N	5:g:380:ASN:O	2.21	0.74
5:a:102:ASN:HA	5:a:144:GLY:HA2	1.70	0.73
5:i:318:ILE:N	5:i:380:ASN:O	2.20	0.73
7:A:356:ILE:O	7:A:360:MET:N	2.19	0.73
1:D:277:ASP:O	1:D:281:ASP:N	2.19	0.73
2:P:38:GLY:H	8:L:122:PRO:HA	1.53	0.73
4:Z:36:GLY:N	4:Z:53:TYR:O	2.21	0.73
5:h:53:TYR:O	5:h:61:ILE:N	2.20	0.73
5:g:274:THR:N	5:g:375:GLY:O	2.22	0.72
7:C:264:GLN:N	7:C:273:THR:O	2.23	0.72
8:L:369:SER:O	8:L:378:VAL:N	2.23	0.72
1:H:524:SER:O	1:H:528:LEU:N	2.17	0.72
2:P:32:SER:HA	8:L:121:GLY:HA3	1.71	0.72
5:c:323:ILE:O	5:c:376:LEU:N	2.19	0.72
7:G:262:SER:O	7:G:275:LEU:N	2.20	0.71
9:J:822:MET:O	9:J:827:HIS:N	2.24	0.71
5:c:318:ILE:N	5:c:380:ASN:O	2.24	0.71
5:i:274:THR:N	5:i:375:GLY:O	2.23	0.71
5:f:4:GLU:HA	5:f:50:VAL:HA	1.73	0.71
5:k:318:ILE:N	5:k:380:ASN:O	2.24	0.71
1:N:24:MET:HA	1:N:31:TYR:HA	1.73	0.71
5:f:324:ILE:O	5:f:361:SER:N	2.24	0.70
5:k:272:GLY:O	5:k:377:MET:N	2.22	0.70
7:A:164:LYS:O	7:A:168:LYS:N	2.21	0.70
7:A:262:SER:O	7:A:275:LEU:N	2.22	0.70
5:h:318:ILE:N	5:h:380:ASN:O	2.22	0.70
1:v:123:PRO:O	1:v:125:ASP:N	2.20	0.70
1:N:19:GLY:N	1:N:22:ILE:O	2.25	0.70
5:d:107:GLY:HA3	5:d:148:GLY:HA3	1.73	0.70
5:i:323:ILE:O	5:i:376:LEU:N	2.24	0.70
1:u:4:PRO:0	1:u:6:GLN:N	2.25	0.70
5:g:70:GLU:HA	5:g:97:GLY:HA2	1.74	0.70
9:J:263:VAL:N	9:J:299:ASN:O	2.19	0.70
4:Z:36:GLY:O	4:Z:53:TYR:N	2.19	0.70
5:f:272:GLY:N	5:f:377:MET:O	2.25	0.69
5:1:409:ARG:HA	5:l:415:LYS:HA	1.74	0.69
1:N:515:ILE:O	1:N:520:LEU:N	2.24	0.69
5:l:317:TYR:HA	5:l:381:HIS:HA	1.74	0.69
5:e:141:ILE:N	5:e:171:VAL:O	2.19	0.69
1:F:524:SER:O	1:F:528:LEU:N	2.20	0.69

![](_page_35_Picture_6.jpeg)
		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:Z:37:ARG:O	4:Z:66:THR:N	2.24	0.69
7:E:264:GLN:N	7:E:273:THR:O	2.25	0.69
5:f:320:ILE:O	5:f:357:GLN:N	2.26	0.69
5:k:30:GLY:HA3	5:k:41:ALA:HB2	1.73	0.69
5:k:46:ASP:HA	5:k:245:TYR:HA	1.75	0.69
5:d:317:TYR:HA	5:d:381:HIS:HA	1.74	0.69
6:I:294:THR:O	6:I:296:LYS:N	2.25	0.69
9:J:791:LEU:HA	9:J:892:LEU:H	1.57	0.68
2:P:37:THR:N	8:L:121:GLY:O	2.17	0.68
5:d:324:ILE:O	5:d:361:SER:N	2.26	0.68
5:c:5:ILE:N	5:c:50:VAL:O	2.26	0.68
5:i:325:GLN:N	5:i:374:SER:O	2.23	0.68
1:B:203:PHE:O	1:B:223:ARG:N	2.26	0.68
1:B:286:PHE:O	1:B:290:ILE:N	2.22	0.68
5:d:321:LEU:N	5:d:378:MET:O	2.19	0.68
5:h:272:GLY:N	5:h:377:MET:O	2.27	0.68
5:h:324:ILE:O	5:h:361:SER:N	2.26	0.68
5:i:172:PHE:N	5:i:205:LEU:O	2.23	0.68
1:D:23:LYS:O	1:D:32:LYS:N	2.21	0.68
5:b:53:TYR:O	5:b:61:ILE:N	2.23	0.68
7:A:264:GLN:N	7:A:273:THR:O	2.27	0.68
5:d:323:ILE:O	5:d:376:LEU:N	2.24	0.68
5:e:53:TYR:O	5:e:61:ILE:N	2.24	0.67
5:k:317:TYR:HA	5:k:381:HIS:HA	1.76	0.67
5:d:30:GLY:HA3	5:d:41:ALA:HB2	1.76	0.67
7:C:438:GLU:N	7:C:461:THR:O	2.23	0.67
5:e:321:LEU:N	5:e:378:MET:O	2.19	0.67
5:c:274:THR:N	5:c:375:GLY:O	2.27	0.67
5:d:272:GLY:N	5:d:377:MET:O	2.27	0.67
7:M:157:LYS:HA	7:M:313:TYR:HA	1.74	0.67
5:d:318:ILE:N	5:d:380:ASN:O	2.28	0.67
1:H:277:ASP:O	1:H:281:ASP:N	2.23	0.67
1:H:278:LEU:HA	1:H:282:LEU:HA	1.76	0.67
5:e:317:TYR:HA	5:e:381:HIS:HA	1.75	0.67
5:k:324:ILE:HA	5:k:375:GLY:HA2	1.77	0.66
1:H:21:ASN:O	1:H:34:GLU:N	2.23	0.66
9:J:518:LEU:O	9:J:522:LEU:N	2.29	0.66
5:c:325:GLN:N	5:c:374:SER:O	2.24	0.66
5:a:141:ILE:N	5:a:171:VAL:O	2.28	0.66
1:D:203:PHE:O	1:D:223:ARG:N	2.28	0.66
9:J:471:GLN:N	9:J:489:THR:O	2.25	0.66



	lite as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:I:399:SER:O	6:I:403:VAL:N	2.29	0.66
5:f:53:TYR:O	5:f:61:ILE:N	2.24	0.66
1:B:620:LEU:O	1:B:624:SER:N	2.28	0.66
5:e:195:LEU:HA	5:e:199:ALA:HB3	1.77	0.66
8:L:367:THR:O	8:L:380:LYS:N	2.28	0.66
7:E:438:GLU:N	7:E:461:THR:O	2.26	0.66
5:h:54:GLN:HA	5:h:60:TYR:HA	1.76	0.66
7:E:651:LYS:O	7:E:655:SER:N	2.29	0.66
1:F:277:ASP:O	1:F:281:ASP:N	2.23	0.66
9:J:541:SER:O	9:J:545:LEU:N	2.18	0.65
5:b:274:THR:N	5:b:375:GLY:O	2.29	0.65
5:g:195:LEU:HA	5:g:199:ALA:HB3	1.77	0.65
1:N:23:LYS:O	1:N:32:LYS:N	2.21	0.65
7:C:164:LYS:HA	7:C:432:TYR:HA	1.77	0.65
1:D:620:LEU:O	1:D:624:SER:N	2.29	0.65
1:B:179:SER:O	1:B:183:LEU:N	2.19	0.65
6:K:400:ALA:O	6:K:405:LEU:N	2.28	0.65
5:h:320:ILE:O	5:h:357:GLN:N	2.28	0.65
1:F:205:ALA:N	1:F:221:THR:O	2.27	0.65
4:Z:238:LYS:N	4:Z:250:ILE:O	2.24	0.65
2:0:56:ASN:O	2:O:60:LEU:N	2.22	0.65
1:D:524:SER:O	1:D:528:LEU:N	2.22	0.65
5:g:323:ILE:O	5:g:376:LEU:N	2.29	0.65
9:J:470:ILE:HA	9:J:490:LEU:HA	1.78	0.65
4:Z:37:ARG:HA	4:Z:52:SER:HA	1.79	0.65
7:G:726:MET:O	7:G:731:GLU:N	2.26	0.65
1:F:203:PHE:O	1:F:223:ARG:N	2.29	0.65
1:v:105:ARG:HA	1:v:108:PRO:N	2.12	0.65
1:F:21:ASN:O	1:F:34:GLU:N	2.24	0.65
5:i:317:TYR:HA	5:i:381:HIS:HA	1.79	0.65
9:J:288:GLN:N	9:J:295:THR:O	2.27	0.65
5:b:324:ILE:O	5:b:361:SER:N	2.28	0.64
5:j:272:GLY:N	5:j:377:MET:O	2.29	0.64
6:K:253:SER:O	6:K:256:GLN:N	2.29	0.64
7:G:263:ALA:HA	7:G:274:PHE:HA	1.78	0.64
5:e:318:ILE:N	5:e:380:ASN:O	2.30	0.64
5:f:35:GLY:O	5:f:60:TYR:N	2.29	0.64
5:m:4:GLU:HA	5:m:50:VAL:HA	1.79	0.64
5:e:324:ILE:O	5:e:361:SER:N	2.27	0.64
5:d:53:TYR:O	5:d:61:ILE:N	2.21	0.64
1:B:524:SER:O	1:B:528:LEU:N	2.20	0.64



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:d:5:ILE:N	5:d:50:VAL:O	2.29	0.64
1:H:203:PHE:O	1:H:223:ARG:N	2.30	0.64
5:b:35:GLY:O	5:b:60:TYR:N	2.30	0.64
6:K:294:THR:O	6:K:296:LYS:N	2.27	0.64
7:C:356:ILE:O	7:C:360:MET:N	2.25	0.64
1:H:620:LEU:O	1:H:624:SER:N	2.30	0.64
4:Z:165:ILE:HA	4:Z:170:ALA:HA	1.79	0.64
5:g:53:TYR:O	5:g:61:ILE:N	2.27	0.64
1:H:205:ALA:N	1:H:221:THR:O	2.29	0.64
5:j:317:TYR:HA	5:j:381:HIS:HA	1.79	0.64
7:A:263:ALA:HA	7:A:274:PHE:HA	1.80	0.64
7:E:263:ALA:HA	7:E:274:PHE:HA	1.80	0.64
5:d:323:ILE:N	5:d:376:LEU:O	2.29	0.64
8:L:345:VAL:N	8:L:382:GLY:O	2.20	0.64
1:F:320:ARG:O	1:F:326:GLN:N	2.28	0.63
5:b:325:GLN:N	5:b:374:SER:O	2.22	0.63
5:k:323:ILE:N	5:k:376:LEU:O	2.32	0.63
1:B:23:LYS:O	1:B:32:LYS:N	2.22	0.63
7:C:263:ALA:HA	7:C:274:PHE:HA	1.78	0.63
7:C:651:LYS:O	7:C:655:SER:N	2.32	0.63
1:B:150:GLY:HA3	1:B:226:MET:HA	1.81	0.63
1:D:278:LEU:HA	1:D:282:LEU:HA	1.80	0.63
5:c:195:LEU:HA	5:c:199:ALA:HB3	1.80	0.63
5:e:53:TYR:N	5:e:61:ILE:O	2.25	0.63
5:f:318:ILE:N	5:f:380:ASN:O	2.30	0.62
1:D:21:ASN:O	1:D:34:GLU:N	2.27	0.62
9:J:588:ASP:O	9:J:592:ALA:N	2.24	0.62
7:G:264:GLN:N	7:G:273:THR:O	2.30	0.62
1:F:620:LEU:O	1:F:624:SER:N	2.33	0.62
5:j:323:ILE:O	5:j:376:LEU:N	2.29	0.62
5:j:274:THR:N	5:j:375:GLY:O	2.32	0.62
1:F:382:LEU:N	1:F:393:VAL:O	2.30	0.62
5:m:318:ILE:N	5:m:380:ASN:O	2.29	0.62
5:a:270:MET:N	5:a:379:ALA:O	2.30	0.62
5:a:272:GLY:O	5:a:377:MET:N	2.23	0.62
5:f:323:ILE:N	5:f:376:LEU:O	2.29	0.62
5:l:47:ARG:N	5:l:244:ARG:O	2.27	0.62
7:M:264:GLN:N	7:M:273:THR:O	2.25	0.62
7:C:436:MET:O	7:C:463:VAL:N	2.30	0.62
5:j:325:GLN:N	5:j:374:SER:O	2.25	0.62
7:M:707:ALA:HB1	7:M:790:MET:HA	1.82	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
7:E:453:ASP:O	7:E:457:ASP:N	2.20	0.62
5:e:35:GLY:O	5:e:60:TYR:N	2.31	0.62
5:d:36:ILE:HA	5:d:59:HIS:HA	1.82	0.62
5:c:317:TYR:HA	5:c:381:HIS:HA	1.81	0.62
6:K:604:ASP:O	6:K:608:ALA:N	2.25	0.61
9:J:621:GLU:O	9:J:625:CYS:N	2.33	0.61
5:e:272:GLY:O	5:e:377:MET:N	2.32	0.61
1:N:418:ARG:HA	9:J:74:ILE:HA	1.82	0.61
5:a:409:ARG:HA	5:a:415:LYS:HA	1.81	0.61
5:d:325:GLN:N	5:d:374:SER:O	2.25	0.61
1:H:184:SER:HA	1:H:270:GLU:CB	2.30	0.61
5:n:269:LEU:HA	5:n:380:ASN:HA	1.83	0.61
7:A:412:SER:O	7:A:416:PHE:N	2.21	0.61
2:0:32:SER:O	2:O:36:ASN:N	2.33	0.61
5:f:323:ILE:O	5:f:376:LEU:N	2.31	0.61
5:f:323:ILE:HA	5:f:359:ALA:HB3	1.82	0.61
5:n:166:VAL:O	5:n:200:ASP:N	2.28	0.61
6:I:269:PRO:O	6:I:273:ALA:N	2.27	0.61
5:g:324:ILE:O	5:g:361:SER:N	2.33	0.61
5:g:141:ILE:N	5:g:171:VAL:O	2.22	0.61
7:C:157:LYS:HA	7:C:313:TYR:HA	1.83	0.61
5:n:134:GLY:HA3	5:n:165:LEU:O	1.99	0.61
1:H:214:ARG:O	1:H:218:ASP:N	2.32	0.61
5:n:270:MET:N	5:n:379:ALA:O	2.34	0.61
5:i:272:GLY:N	5:i:377:MET:O	2.34	0.60
4:Z:132:MET:O	4:Z:357:ILE:N	2.34	0.60
4:Z:150:GLY:O	4:Z:165:ILE:N	2.31	0.60
6:I:400:ALA:O	6:I:405:LEU:N	2.32	0.60
5:f:317:TYR:HA	5:f:381:HIS:HA	1.84	0.60
1:v:123:PRO:C	1:v:125:ASP:H	2.07	0.60
8:L:113:LEU:O	8:L:117:LEU:N	2.35	0.60
5:k:53:TYR:O	5:k:61:ILE:N	2.31	0.60
6:K:654:TYR:O	6:K:659:GLY:N	2.22	0.60
9:J:502:LEU:O	9:J:506:LEU:N	2.35	0.60
5:c:53:TYR:O	5:c:61:ILE:N	2.29	0.60
5:m:317:TYR:HA	5:m:381:HIS:HA	1.83	0.60
5:n:317:TYR:N	5:n:347:ASN:O	2.35	0.60
1:F:23:LYS:O	1:F:32:LYS:N	2.29	0.60
5:h:5:ILE:N	5:h:50:VAL:O	2.33	0.60
1:B:205:ALA:N	1:B:221:THR:O	2.29	0.60
7:M:424:TYR:HA	7:M:496:THR:HA	1.83	0.60



	tio as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:c:385:SER:O	5:c:389:GLU:N	2.21	0.59
5:e:209:ALA:HB2	5:e:306:SER:H	1.66	0.59
6:K:384:PRO:N	6:K:448:GLY:HA3	2.17	0.59
1:D:205:ALA:N	1:D:221:THR:O	2.27	0.59
6:K:6:LEU:O	6:K:10:SER:N	2.36	0.59
9:J:288:GLN:O	9:J:295:THR:N	2.25	0.59
5:f:172:PHE:N	5:f:205:LEU:O	2.35	0.59
1:B:566:LYS:HA	1:B:576:GLY:O	2.03	0.59
2:U:2:ALA:HB1	6:I:44:ARG:HA	1.84	0.59
5:b:323:ILE:N	5:b:376:LEU:O	2.36	0.59
6:I:343:LEU:O	6:I:348:SER:N	2.36	0.59
5:1:53:TYR:N	5:l:61:ILE:O	2.33	0.58
1:B:382:LEU:N	1:B:393:VAL:O	2.33	0.58
4:Z:38:PRO:HA	4:Z:65:LEU:HA	1.85	0.58
5:a:53:TYR:N	5:a:61:ILE:O	2.27	0.58
7:E:397:ASP:O	7:E:401:GLN:N	2.33	0.58
5:e:320:ILE:O	5:e:357:GLN:N	2.34	0.58
5:b:409:ARG:HA	5:b:415:LYS:HA	1.85	0.58
5:e:323:ILE:N	5:e:376:LEU:O	2.32	0.58
5:h:52:PHE:HA	5:h:62:PRO:HA	1.86	0.58
5:k:434:GLU:O	5:k:438:ALA:N	2.34	0.58
5:d:321:LEU:O	5:d:378:MET:N	2.28	0.58
5:g:272:GLY:N	5:g:377:MET:O	2.36	0.58
6:I:382:THR:O	6:I:448:GLY:N	2.36	0.58
2:P:47:CYS:O	2:P:51:CYS:N	2.30	0.58
5:c:172:PHE:N	5:c:205:LEU:O	2.36	0.58
7:A:651:LYS:O	7:A:655:SER:N	2.37	0.58
1:D:559:ARG:HA	1:D:585:GLU:HA	1.86	0.58
5:c:272:GLY:N	5:c:377:MET:O	2.36	0.57
6:I:20:ASN:O	6:I:24:GLY:N	2.33	0.57
1:H:566:LYS:HA	1:H:576:GLY:O	2.04	0.57
5:e:52:PHE:HA	5:e:62:PRO:HA	1.86	0.57
5:h:323:ILE:HA	5:h:359:ALA:HB3	1.86	0.57
5:n:1:MET:N	1:N:332:HIS:O	2.36	0.57
5:d:10:LEU:HA	5:d:67:LEU:O	2.04	0.57
5:d:323:ILE:HA	5:d:359:ALA:HB3	1.86	0.57
9:J:216:LEU:O	9:J:220:VAL:N	2.33	0.57
5:j:324:ILE:O	5:j:361:SER:N	2.37	0.57
6:I:6:LEU:O	6:I:10:SER:N	2.38	0.57
4:Z:252:ASN:O	4:Z:256:ARG:N	2.21	0.57
4:Z:369:ILE:O	4:Z:373:LYS:N	2.21	0.57



	eve as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
9:J:334:PHE:O	9:J:338:GLN:N	2.32	0.57
5:f:321:LEU:O	5:f:378:MET:N	2.30	0.57
5:i:323:ILE:N	5:i:376:LEU:O	2.35	0.57
1:D:163:GLY:HA3	7:C:315:GLN:HA	1.85	0.56
5:g:4:GLU:HA	5:g:50:VAL:HA	1.87	0.56
5:g:5:ILE:N	5:g:50:VAL:O	2.24	0.56
5:b:289:THR:O	5:b:293:VAL:N	2.30	0.56
5:k:1:MET:N	6:K:371:ALA:HB1	2.20	0.56
4:Z:8:LEU:N	4:Z:102:PRO:O	2.30	0.56
5:h:323:ILE:O	5:h:376:LEU:N	2.28	0.56
1:B:116:SER:HA	8:L:232:LEU:H	1.69	0.56
9:J:237:HIS:O	9:J:241:ASN:N	2.34	0.56
4:Z:72:GLU:N	4:Z:75:ILE:O	2.34	0.56
4:Z:202:THR:O	4:Z:206:ARG:N	2.32	0.56
5:m:260:LEU:HA	5:m:319:ALA:HB3	1.86	0.56
6:K:1:MET:O	6:K:5:LEU:N	2.31	0.56
8:L:612:HIS:O	8:L:616:TRP:N	2.39	0.56
1:H:320:ARG:O	1:H:326:GLN:N	2.36	0.56
5:c:324:ILE:O	5:c:361:SER:N	2.38	0.56
5:f:272:GLY:O	5:f:377:MET:N	2.33	0.56
9:J:525:ALA:O	9:J:527:SER:N	2.39	0.56
5:c:326:GLY:N	5:c:361:SER:O	2.33	0.56
5:j:107:GLY:HA3	5:j:148:GLY:HA3	1.87	0.56
5:k:47:ARG:N	5:k:244:ARG:O	2.35	0.56
5:d:274:THR:O	5:d:375:GLY:N	2.26	0.56
3:X:584:LEU:HA	3:Y:584:LEU:H	1.70	0.56
4:Z:35:VAL:HA	4:Z:54:VAL:HA	1.87	0.56
1:N:337:LEU:O	1:N:341:LEU:N	2.21	0.56
5:d:274:THR:N	5:d:375:GLY:O	2.35	0.56
7:G:248:ASP:O	7:G:252:VAL:N	2.33	0.56
7:A:567:LEU:O	7:A:640:GLY:N	2.39	0.56
5:e:321:LEU:O	5:e:378:MET:N	2.30	0.56
5:d:241:THR:O	5:d:245:TYR:N	2.31	0.56
7:M:356:ILE:O	7:M:360:MET:N	2.30	0.56
1:F:278:LEU:HA	1:F:282:LEU:HA	1.88	0.55
1:H:23:LYS:O	1:H:32:LYS:N	2.25	0.55
5:g:8:LEU:O	5:g:138:CYS:N	2.24	0.55
7:A:385:SER:HA	7:A:469:SER:H	1.71	0.55
5:b:36:ILE:HA	5:b:59:HIS:HA	1.88	0.55
5:j:53:TYR:O	5:j:61:ILE:N	2.25	0.55
$1:N:407:VAL:H\overline{A}$	1:N:504:ILE:HA	1.88	0.55



	A la C	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
9:J:332:ALA:HB1	9:J:338:GLN:HA	1.87	0.55
5:k:11:GLY:N	5:k:67:LEU:O	2.40	0.55
5:k:166:VAL:O	5:k:200:ASP:N	2.32	0.55
4:Z:301:GLY:N	4:Z:335:ARG:O	2.39	0.55
5:e:137:LEU:O	5:e:169:TYR:N	2.31	0.55
6:I:18:THR:N	6:I:26:GLN:O	2.40	0.55
1:D:214:ARG:O	1:D:218:ASP:N	2.35	0.55
1:F:305:LEU:O	1:F:310:SER:N	2.40	0.55
1:F:566:LYS:HA	1:F:576:GLY:O	2.06	0.55
5:c:323:ILE:N	5:c:376:LEU:O	2.36	0.55
7:M:252:VAL:C	7:M:295:ALA:HB1	2.32	0.55
5:h:172:PHE:N	5:h:205:LEU:O	2.40	0.55
5:k:405:LEU:O	5:k:409:ARG:N	2.36	0.55
5:d:10:LEU:N	5:d:138:CYS:O	2.36	0.55
9:J:499:VAL:O	9:J:503:LYS:N	2.41	0.54
9:J:727:GLU:O	9:J:743:GLY:HA3	2.08	0.54
7:A:249:LEU:O	7:A:253:LEU:N	2.31	0.54
4:Z:70:PRO:O	4:Z:77:THR:N	2.32	0.54
1:B:159:TYR:HA	7:A:175:PRO:HA	1.88	0.54
1:D:409:THR:O	1:D:413:MET:N	2.25	0.54
5:h:3:ARG:HA	5:h:131:SER:O	2.07	0.54
5:i:325:GLN:O	5:i:374:SER:N	2.29	0.54
6:K:74:SER:HA	6:K:200:HIS:HA	1.89	0.54
5:b:274:THR:O	5:b:375:GLY:N	2.19	0.54
5:k:241:THR:O	5:k:245:TYR:N	2.35	0.54
7:C:740:ASN:O	7:C:744:ALA:N	2.41	0.54
1:H:318:MET:O	1:H:323:LEU:N	2.40	0.54
5:k:316:CYS:O	5:k:382:THR:N	2.25	0.54
5:1:30:GLY:HA3	5:l:41:ALA:HB2	1.89	0.54
1:F:409:THR:O	1:F:413:MET:N	2.25	0.54
5:a:100:ALA:CB	5:a:148:GLY:HA3	2.38	0.54
2:P:38:GLY:H	8:L:122:PRO:CA	2.20	0.54
6:K:358:LYS:O	6:K:364:GLY:N	2.38	0.54
7:A:319:ALA:HB1	7:A:410:ALA:HB1	1.90	0.53
4:Z:131:ALA:HA	4:Z:358:SER:HA	1.91	0.53
5:n:11:GLY:N	5:n:67:LEU:O	2.41	0.53
1:N:127:THR:O	1:N:131:LYS:N	2.39	0.53
5:c:241:THR:O	5:c:245:TYR:N	2.33	0.53
9:J:471:GLN:O	9:J:489:THR:N	2.37	0.53
5:b:241:THR:O	5:b:245:TYR:N	2.31	0.53
9:J:473:ASN:N	9:J:487:THR:O	2.41	0.53



	tio de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:b:55:ALA:N	5:b:59:HIS:O	2.40	0.53
7:E:726:MET:O	7:E:731:GLU:N	2.36	0.53
2:S:76:ALA:HB1	1:s:113:SER:HA	1.90	0.53
5:d:30:GLY:O	5:d:38:GLU:N	2.31	0.53
2:U:10:ALA:HB2	6:I:29:GLN:HA	1.91	0.53
5:b:172:PHE:N	5:b:205:LEU:O	2.40	0.53
5:f:138:CYS:HA	5:f:169:TYR:O	2.08	0.53
5:j:7:THR:O	5:j:65:VAL:N	2.26	0.53
5:d:320:ILE:O	5:d:357:GLN:N	2.35	0.53
7:G:438:GLU:O	7:G:461:THR:N	2.38	0.53
8:L:1577:LYS:N	8:L:1593:CYS:O	2.29	0.53
5:h:274:THR:N	5:h:375:GLY:O	2.38	0.52
1:N:13:VAL:O	1:N:54:GLY:HA3	2.08	0.52
7:G:438:GLU:N	7:G:461:THR:O	2.30	0.52
8:L:588:LEU:O	8:L:592:ALA:N	2.43	0.52
7:M:657:ILE:HA	7:M:751:LEU:HA	1.90	0.52
5:g:274:THR:O	5:g:375:GLY:N	2.27	0.52
5:i:317:TYR:O	5:i:348:PHE:HA	2.09	0.52
5:d:8:LEU:O	5:d:138:CYS:N	2.28	0.52
8:L:311:TYR:O	8:L:314:GLU:N	2.40	0.52
5:a:141:ILE:H	5:a:171:VAL:C	2.16	0.52
5:g:55:ALA:N	5:g:59:HIS:O	2.42	0.52
5:j:241:THR:O	5:j:245:TYR:N	2.34	0.52
2:P:32:SER:CA	8:L:121:GLY:HA3	2.39	0.52
5:i:289:THR:O	5:i:293:VAL:N	2.30	0.52
5:k:291:LEU:HA	5:k:336:SER:HA	1.92	0.52
5:k:324:ILE:O	5:k:361:SER:N	2.42	0.52
7:M:314:GLY:HA2	7:M:432:TYR:CB	2.39	0.52
9:J:535:ARG:O	9:J:539:ARG:N	2.41	0.52
4:Z:11:ASP:N	4:Z:18:LYS:O	2.33	0.52
5:f:321:LEU:N	5:f:378:MET:O	2.24	0.52
5:k:323:ILE:O	5:k:376:LEU:N	2.40	0.52
1:B:162:THR:HA	7:A:311:PHE:CB	2.40	0.52
5:d:141:ILE:N	5:d:171:VAL:O	2.30	0.52
6:I:532:GLN:O	6:I:537:GLU:N	2.34	0.52
1:D:479:THR:O	1:D:484:GLU:N	2.43	0.52
5:a:1:MET:N	7:A:558:HIS:O	2.40	0.52
1:r:108:PRO:O	1:r:110:LYS:N	2.43	0.52
9:J:721:ARG:O	9:J:749:LYS:N	2.41	0.52
6:K:20:ASN:O	6:K:24:GLY:N	2.33	0.51
5:j:172:PHE:N	5:j:205:LEU:O	2.43	0.51



	tional page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:g:168:THR:N	5:g:201:CYS:O	2.40	0.51
5:j:57:ASP:N	5:k:285:VAL:O	2.43	0.51
7:M:468:PRO:O	7:M:472:GLN:N	2.43	0.51
5:b:102:ASN:HA	5:b:144:GLY:N	2.25	0.51
5:i:324:ILE:O	5:i:361:SER:N	2.41	0.51
5:j:434:GLU:O	5:j:438:ALA:N	2.39	0.51
5:m:166:VAL:O	5:m:200:ASP:N	2.38	0.51
4:Z:144:ALA:HB2	4:Z:342:GLY:HA2	1.91	0.51
5:j:323:ILE:N	5:j:376:LEU:O	2.42	0.51
5:d:53:TYR:N	5:d:61:ILE:O	2.32	0.51
1:D:22:ILE:HA	1:D:33:VAL:HA	1.92	0.51
7:E:740:ASN:O	7:E:744:ALA:N	2.44	0.51
5:e:10:LEU:N	5:e:138:CYS:O	2.32	0.51
5:i:323:ILE:HA	5:i:359:ALA:HB3	1.93	0.51
8:L:106:GLU:O	8:L:110:VAL:N	2.40	0.51
2:U:2:ALA:CB	6:I:44:ARG:HA	2.40	0.51
5:g:385:SER:O	5:g:389:GLU:N	2.28	0.51
5:k:326:GLY:N	5:k:361:SER:O	2.44	0.51
7:A:586:ALA:O	7:A:590:SER:N	2.43	0.51
5:a:100:ALA:HB2	5:a:148:GLY:HA3	1.93	0.51
5:g:172:PHE:N	5:g:205:LEU:O	2.44	0.51
5:h:70:GLU:HA	5:h:97:GLY:HA2	1.93	0.51
6:K:343:LEU:O	6:K:348:SER:N	2.43	0.51
5:d:209:ALA:HB2	5:d:306:SER:H	1.75	0.51
5:e:8:LEU:O	5:e:138:CYS:N	2.32	0.50
7:G:571:VAL:H	7:G:637:ALA:HB1	1.76	0.50
9:J:430:SER:O	9:J:434:VAL:N	2.34	0.50
9:J:517:GLN:O	9:J:521:ASN:CB	2.58	0.50
5:a:10:LEU:HA	5:a:67:LEU:O	2.11	0.50
5:a:214:ALA:O	5:a:220:ILE:N	2.33	0.50
6:I:253:SER:O	6:I:256:GLN:N	2.44	0.50
1:H:112:LEU:C	1:H:114:LEU:H	2.19	0.50
5:a:317:TYR:N	5:a:347:ASN:O	2.30	0.50
1:H:205:ALA:O	1:H:221:THR:N	2.29	0.50
5:a:52:PHE:HA	5:a:62:PRO:HA	1.92	0.50
4:Z:20:GLY:HA3	4:Z:28:ARG:H	1.76	0.50
5:h:323:ILE:N	5:h:376:LEU:O	2.39	0.50
1:B:19:GLY:N	1:B:22:ILE:O	2.45	0.50
9:J:723:SER:N	9:J:747:SER:O	2.33	0.50
7:A:341:LEU:O	7:A:346:LEU:N	2.38	0.50
5:c:3:ARG:HA	5:c:131:SER:O	2.11	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:c:141:ILE:N	5:c:171:VAL:O	2.35	0.50
5:i:46:ASP:HA	5:i:244:ARG:O	2.12	0.50
1:F:310:SER:O	1:F:314:HIS:N	2.34	0.49
5:j:320:ILE:O	5:j:357:GLN:N	2.41	0.49
5:k:10:LEU:O	5:k:146:GLY:HA2	2.12	0.49
5:1:209:ALA:HB2	5:1:306:SER:N	2.27	0.49
5:n:6:ILE:O	5:n:136:VAL:N	2.30	0.49
5:n:163:LYS:HA	1:N:439:GLY:HA2	1.94	0.49
7:A:762:LEU:O	7:A:767:LEU:N	2.45	0.49
9:J:522:LEU:O	9:J:524:CYS:N	2.42	0.49
1:F:191:TYR:CB	1:F:266:THR:HA	2.43	0.49
5:k:35:GLY:O	5:k:60:TYR:N	2.45	0.49
7:C:619:ALA:HB1	7:C:624:GLN:C	2.38	0.49
2:U:10:ALA:HB2	6:I:30:ASP:H	1.77	0.49
5:a:48:LYS:O	5:a:52:PHE:N	2.24	0.49
5:f:325:GLN:HA	5:f:361:SER:O	2.13	0.49
5:h:55:ALA:N	5:h:59:HIS:O	2.44	0.49
5:k:14:GLY:CA	5:k:139:HIS:HA	2.42	0.49
1:N:578:THR:O	1:N:582:GLU:N	2.33	0.49
7:A:381:GLY:N	7:A:434:GLU:HA	2.28	0.49
5:h:53:TYR:N	5:h:61:ILE:O	2.40	0.49
8:L:295:ARG:H	9:J:368:THR:CB	2.26	0.49
1:F:341:LEU:HA	1:F:390:GLY:HA3	1.93	0.49
5:a:71:PRO:N	5:a:97:GLY:HA2	2.27	0.49
1:B:214:ARG:O	1:B:218:ASP:N	2.35	0.49
3:W:637:SER:O	3:W:639:ASN:N	2.46	0.49
5:f:322:ASN:O	5:f:359:ALA:N	2.24	0.49
5:n:14:GLY:HA3	5:n:139:HIS:HA	1.95	0.49
7:C:567:LEU:O	7:C:640:GLY:N	2.45	0.49
5:g:53:TYR:N	5:g:61:ILE:O	2.34	0.48
8:L:179:LEU:O	8:L:183:GLU:N	2.46	0.48
8:L:349:GLU:O	8:L:351:GLU:N	2.45	0.48
7:C:567:LEU:HA	7:C:640:GLY:HA3	1.95	0.48
1:D:595:SER:O	1:D:599:MET:N	2.30	0.48
5:a:269:LEU:HA	5:a:380:ASN:HA	1.95	0.48
5:e:4:GLU:HA	5:e:50:VAL:HA	1.94	0.48
1:B:341:LEU:HA	1:B:390:GLY:HA3	1.95	0.48
7:E:381:GLY:HA3	7:E:466:GLN:O	2.13	0.48
5:a:214:ALA:O	5:a:219:HIS:N	2.47	0.48
5:b:282:VAL:O	5:b:370:ALA:HB1	2.14	0.48
5:a:46:ASP:HA	5:a:244:ARG:HA	1.94	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:e:320:ILE:HA	5:e:379:ALA:HA	1.96	0.48
1:B:310:SER:O	1:B:314:HIS:N	2.33	0.48
1:F:22:ILE:HA	1:F:33:VAL:HA	1.94	0.48
1:F:205:ALA:O	1:F:221:THR:N	2.28	0.48
1:F:214:ARG:O	1:F:218:ASP:N	2.35	0.48
1:H:22:ILE:HA	1:H:33:VAL:HA	1.95	0.48
5:a:385:SER:O	5:a:389:GLU:N	2.27	0.48
5:h:272:GLY:O	5:h:377:MET:N	2.36	0.48
1:H:455:GLY:HA2	5:h:448:THR:HA	1.95	0.48
5:e:434:GLU:O	5:e:438:ALA:N	2.36	0.48
6:K:157:VAL:O	6:K:161:SER:N	2.47	0.48
1:F:112:LEU:C	1:F:114:LEU:H	2.22	0.48
1:H:595:SER:O	1:H:599:MET:N	2.35	0.48
4:Z:19:ALA:O	4:Z:28:ARG:N	2.47	0.48
5:e:438:ALA:HA	5:e:443:TYR:CB	2.44	0.48
5:g:241:THR:O	5:g:245:TYR:N	2.41	0.48
5:h:137:LEU:O	5:h:169:TYR:N	2.35	0.48
7:C:161:LEU:N	7:C:312:GLU:O	2.46	0.48
9:J:627:THR:O	9:J:631:THR:N	2.25	0.48
6:I:16:ILE:O	6:I:28:SER:N	2.26	0.48
1:H:25:ASN:N	1:H:30:CYS:O	2.39	0.48
5:c:53:TYR:N	5:c:61:ILE:O	2.41	0.48
5:g:274:THR:C	5:g:375:GLY:H	2.20	0.48
5:f:107:GLY:HA3	5:f:148:GLY:HA3	1.95	0.48
7:A:272:ARG:N	7:A:296:ALA:HB1	2.29	0.48
6:I:632:VAL:O	6:I:636:GLN:N	2.47	0.48
5:e:272:GLY:N	5:e:377:MET:O	2.43	0.47
5:d:35:GLY:O	5:d:60:TYR:N	2.47	0.47
7:E:619:ALA:HB1	7:E:624:GLN:C	2.39	0.47
7:M:157:LYS:HA	7:M:313:TYR:CA	2.44	0.47
5:a:289:THR:O	5:a:293:VAL:N	2.34	0.47
5:b:53:TYR:N	5:b:61:ILE:O	2.38	0.47
5:f:52:PHE:HA	5:f:62:PRO:HA	1.95	0.47
5:i:274:THR:O	5:i:375:GLY:N	2.33	0.47
5:n:259:SER:O	5:n:319:ALA:HB1	2.14	0.47
5:d:195:LEU:HA	5:d:199:ALA:HB3	1.96	0.47
7:A:618:LEU:HA	7:A:767:LEU:O	2.13	0.47
5:f:241:THR:O	5:f:245:TYR:N	2.36	0.47
5:k:8:LEU:O	5:k:138:CYS:N	2.35	0.47
7:G:740:ASN:O	7:G:744:ALA:N	2.48	0.47
8:L:244:LEU:N	7:A:355:TYR:O	2.47	0.47



	tio as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:k:317:TYR:O	5:k:348:PHE:HA	2.14	0.47
1:B:25:ASN:N	1:B:30:CYS:O	2.38	0.47
1:N:207:ASP:N	1:N:219:LYS:O	2.34	0.47
8:L:349:GLU:O	8:L:352:LEU:N	2.47	0.47
5:g:10:LEU:N	5:g:138:CYS:O	2.41	0.47
5:i:274:THR:C	5:i:375:GLY:H	2.20	0.47
5:j:4:GLU:HA	5:j:50:VAL:HA	1.97	0.47
5:m:55:ALA:HB1	5:n:217:ARG:HA	1.95	0.47
8:L:210:THR:O	8:L:215:PHE:N	2.36	0.47
7:E:436:MET:O	7:E:463:VAL:N	2.41	0.47
1:F:478:ILE:O	1:F:483:LEU:N	2.31	0.47
5:e:325:GLN:HA	5:e:361:SER:O	2.14	0.47
5:j:136:VAL:HA	5:j:167:GLN:O	2.14	0.47
9:J:469:ILE:O	9:J:491:TYR:N	2.30	0.47
7:A:309:SER:HA	7:A:318:HIS:HA	1.96	0.47
5:f:324:ILE:N	5:f:359:ALA:O	2.29	0.47
5:g:321:LEU:N	5:g:378:MET:O	2.24	0.47
5:g:434:GLU:O	5:g:438:ALA:N	2.44	0.47
5:i:324:ILE:HA	5:i:375:GLY:HA2	1.95	0.47
7:G:179:ALA:O	7:G:183:GLU:N	2.43	0.47
1:F:25:ASN:N	1:F:30:CYS:O	2.41	0.47
5:e:5:ILE:N	5:e:50:VAL:O	2.26	0.47
7:A:619:ALA:HB1	7:A:624:GLN:C	2.40	0.47
5:j:195:LEU:HA	5:j:199:ALA:HB3	1.97	0.47
5:k:322:ASN:HA	5:k:377:MET:HA	1.97	0.46
5:i:53:TYR:O	5:i:61:ILE:N	2.36	0.46
5:i:320:ILE:O	5:i:357:GLN:N	2.33	0.46
5:1:52:PHE:HA	5:1:63:ARG:H	1.81	0.46
1:B:493:LYS:O	1:B:497:ALA:N	2.49	0.46
5:d:320:ILE:HA	5:d:379:ALA:HA	1.98	0.46
7:A:610:LEU:H	7:A:642:GLU:CB	2.28	0.46
1:H:337:LEU:O	1:H:341:LEU:N	2.33	0.46
5:b:324:ILE:HA	5:b:375:GLY:HA2	1.97	0.46
5:c:321:LEU:O	5:c:378:MET:N	2.37	0.46
9:J:324:VAL:O	9:J:328:GLN:N	2.48	0.46
1:F:341:LEU:O	1:F:390:GLY:N	2.48	0.46
5:g:325:GLN:HA	5:g:361:SER:O	2.15	0.46
5:1:7:THR:O	5:1:65:VAL:N	2.29	0.46
5:k:11:GLY:HA2	5:k:68:ASP:HA	1.98	0.46
8:L:20:LYS:O	8:L:22:HIS:N	2.49	0.46
5:g:102:ASN:HA	5:g:144:GLY:N	2.30	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:i:409:ARG:HA	5:i:415:LYS:HA	1.97	0.46
5:j:317:TYR:N	5:j:347:ASN:O	2.47	0.46
5:l:52:PHE:HA	5:l:62:PRO:HA	1.98	0.46
6:K:269:PRO:O	6:K:273:ALA:N	2.39	0.46
7:G:397:ASP:O	7:G:401:GLN:N	2.39	0.46
5:g:325:GLN:N	5:g:374:SER:O	2.34	0.46
5:i:321:LEU:O	5:i:378:MET:N	2.33	0.46
5:j:4:GLU:O	5:j:132:LEU:HA	2.15	0.46
1:u:1:MET:O	1:u:3:THR:N	2.48	0.46
4:Z:144:ALA:HB2	4:Z:342:GLY:CA	2.46	0.46
5:c:102:ASN:HA	5:c:144:GLY:N	2.31	0.46
5:l:4:GLU:HA	5:l:50:VAL:HA	1.98	0.46
5:d:272:GLY:O	5:d:377:MET:N	2.44	0.46
4:Z:166:TYR:N	4:Z:169:TYR:O	2.31	0.46
5:f:51:PHE:O	5:f:63:ARG:N	2.43	0.46
5:k:14:GLY:HA3	5:k:139:HIS:HA	1.97	0.46
1:t:112:SER:C	1:t:114:TYR:H	2.24	0.46
1:N:179:SER:O	1:N:183:LEU:N	2.35	0.46
7:G:249:LEU:O	7:G:253:LEU:N	2.35	0.46
7:G:701:ALA:O	7:G:705:ALA:N	2.48	0.46
4:Z:240:TYR:N	4:Z:248:ILE:O	2.31	0.46
5:k:104:TRP:CB	5:k:187:ASN:HA	2.46	0.46
5:m:52:PHE:HA	5:m:62:PRO:HA	1.97	0.46
1:B:337:LEU:O	1:B:341:LEU:N	2.30	0.46
7:M:248:ASP:CB	7:M:258:GLY:HA3	2.46	0.46
7:A:248:ASP:O	7:A:252:VAL:N	2.34	0.45
5:a:52:PHE:HA	5:a:63:ARG:H	1.81	0.45
5:c:49:ASP:HA	5:c:52:PHE:O	2.16	0.45
1:B:566:LYS:HA	1:B:576:GLY:C	2.41	0.45
7:E:356:ILE:O	7:E:360:MET:N	2.35	0.45
5:h:317:TYR:O	5:h:348:PHE:HA	2.16	0.45
5:k:351:TRP:O	6:K:662:GLY:HA3	2.17	0.45
5:1:57:ASP:N	5:m:287:LYS:O	2.47	0.45
5:1:320:ILE:O	5:1:356:ILE:HA	2.16	0.45
1:B:249:LEU:O	1:B:255:ASP:N	2.30	0.45
7:G:619:ALA:HB1	7:G:624:GLN:C	2.41	0.45
7:M:262:SER:O	7:M:275:LEU:N	2.31	0.45
5:l:318:ILE:N	5:1:380:ASN:O	2.45	0.45
1:H:19:GLY:N	1:H:22:ILE:O	2.50	0.45
2:P:32:SER:CB	8:L:121:GLY:HA3	2.46	0.45
1:F:493:LYS:O	1:F:497:ALA:N	2.50	0.45



	lious page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:h:325:GLN:HA	5:h:361:SER:O	2.16	0.45
7:M:316:VAL:H	7:M:434:GLU:CB	2.30	0.45
7:C:164:LYS:HA	7:C:431:PRO:O	2.16	0.45
5:c:70:GLU:HA	5:c:97:GLY:O	2.16	0.45
5:j:317:TYR:O	5:j:348:PHE:HA	2.17	0.45
8:L:553:MET:O	8:L:576:ILE:N	2.26	0.45
5:m:5:ILE:N	5:m:50:VAL:O	2.42	0.45
6:I:359:ASP:HA	6:I:364:GLY:HA3	1.99	0.45
5:j:325:GLN:HA	5:j:361:SER:O	2.16	0.45
5:k:202:VAL:O	5:k:268:PHE:HA	2.17	0.45
5:b:61:ILE:HA	5:b:85:LEU:O	2.18	0.45
5:i:438:ALA:HA	5:i:443:TYR:CB	2.47	0.45
8:L:20:LYS:C	8:L:22:HIS:H	2.26	0.45
7:M:567:LEU:CB	7:M:641:LEU:H	2.30	0.45
5:b:100:ALA:HB3	5:b:144:GLY:HA3	1.99	0.44
5:l:274:THR:O	5:l:375:GLY:N	2.50	0.44
7:G:453:ASP:O	7:G:457:ASP:N	2.31	0.44
7:C:610:LEU:H	7:C:642:GLU:CB	2.30	0.44
5:a:49:ASP:HA	5:a:52:PHE:O	2.17	0.44
5:g:137:LEU:O	5:g:169:TYR:N	2.26	0.44
5:k:10:LEU:O	5:k:14:GLY:HA3	2.17	0.44
4:Z:148:THR:O	4:Z:168:GLY:N	2.29	0.44
5:f:55:ALA:N	5:f:59:HIS:O	2.47	0.44
5:n:53:TYR:O	5:n:61:ILE:N	2.39	0.44
6:K:383:PRO:HA	6:K:448:GLY:HA3	1.98	0.44
7:C:381:GLY:HA3	7:C:466:GLN:O	2.17	0.44
7:A:740:ASN:O	7:A:744:ALA:N	2.50	0.44
7:C:157:LYS:HA	7:C:313:TYR:CA	2.46	0.44
5:f:30:GLY:HA3	5:f:41:ALA:HB2	2.00	0.44
5:f:274:THR:O	5:f:375:GLY:N	2.42	0.44
3:V:584:LEU:H	3:Y:588:GLN:CB	2.30	0.44
7:M:604:ASP:N	7:M:645:SER:O	2.35	0.44
7:C:249:LEU:O	7:C:253:LEU:N	2.35	0.44
9:J:72:PHE:O	9:J:77:ASP:N	2.50	0.44
1:F:12:TYR:O	1:F:17:ILE:N	2.34	0.44
5:e:214:ALA:O	5:e:219:HIS:N	2.50	0.44
5:h:102:ASN:HA	5:h:144:GLY:N	2.32	0.44
5:h:434:GLU:O	5:h:438:ALA:N	2.39	0.44
5:d:172:PHE:N	5:d:205:LEU:O	2.50	0.44
5:d:325:GLN:O	5:d:374:SER:N	2.42	0.44
7:G:604:ASP:0	7:G:645:SER:N	2.49	0.44



	tio ao page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:A:438:GLU:N	7:A:461:THR:O	2.33	0.44
7:E:544:ILE:O	7:E:548:PHE:N	2.50	0.44
7:E:604:ASP:O	7:E:645:SER:N	2.47	0.44
1:D:25:ASN:N	1:D:30:CYS:O	2.41	0.44
5:b:320:ILE:O	5:b:357:GLN:N	2.51	0.44
5:c:319:ALA:O	5:c:380:ASN:N	2.39	0.44
5:g:52:PHE:HA	5:g:63:ARG:H	1.83	0.44
1:N:361:VAL:HA	1:N:366:ALA:HB3	1.99	0.44
1:F:108:GLN:C	1:F:110:VAL:H	2.25	0.44
5:e:49:ASP:HA	5:e:52:PHE:O	2.18	0.44
5:i:138:CYS:HA	5:i:169:TYR:O	2.18	0.44
5:n:7:THR:O	5:n:64:ALA:HA	2.17	0.44
7:C:262:SER:N	7:C:275:LEU:O	2.41	0.44
7:C:341:LEU:O	7:C:346:LEU:N	2.45	0.44
9:J:119:ASP:N	2:Q:19:LEU:O	2.31	0.44
5:g:320:ILE:O	5:g:356:ILE:HA	2.17	0.44
5:i:174:ASN:HA	5:i:208:THR:N	2.33	0.44
1:v:44:ALA:H	2:O:56:ASN:CB	2.31	0.44
6:K:532:GLN:O	6:K:537:GLU:N	2.40	0.44
8:L:346:LEU:HA	8:L:384:HIS:O	2.17	0.44
4:Z:71:ILE:HA	4:Z:76:VAL:HA	1.99	0.43
5:i:325:GLN:HA	5:i:361:SER:O	2.18	0.43
5:1:340:ILE:O	5:l:344:LYS:N	2.51	0.43
5:m:205:LEU:HA	5:m:304:MET:O	2.17	0.43
5:n:252:ASP:O	5:n:256:LEU:N	2.48	0.43
1:D:493:LYS:O	1:D:497:ALA:N	2.51	0.43
4:Z:150:GLY:N	4:Z:165:ILE:O	2.37	0.43
5:a:171:VAL:HA	5:a:205:LEU:O	2.18	0.43
6:K:338:GLU:HA	6:K:551:ARG:O	2.18	0.43
5:d:8:LEU:HA	5:d:65:VAL:O	2.19	0.43
7:C:452:ASN:O	7:C:454:LYS:N	2.50	0.43
4:Z:229:THR:O	4:Z:233:SER:N	2.49	0.43
5:e:209:ALA:HB2	5:e:306:SER:N	2.32	0.43
5:i:53:TYR:N	5:i:61:ILE:O	2.45	0.43
5:i:321:LEU:N	5:i:378:MET:O	2.28	0.43
6:K:421:HIS:N	6:K:441:PRO:O	2.47	0.43
7:M:416:PHE:CB	7:M:503:ILE:H	2.32	0.43
1:D:337:LEU:O	1:D:341:LEU:N	2.30	0.43
5:g:52:PHE:HA	5:g:62:PRO:HA	1.99	0.43
5:j:325:GLN:O	5:j:374:SER:N	2.23	0.43
8:L:371:CYS:N	8:L:376:ALA:O	2.34	0.43



	tio ao pagoini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:108:GLN:C	1:H:110:VAL:H	2.27	0.43
5:a:108:PHE:HA	5:a:152:TYR:HA	2.01	0.43
5:e:52:PHE:HA	5:e:63:ARG:H	1.83	0.43
5:d:52:PHE:HA	5:d:62:PRO:HA	2.00	0.43
6:I:380:LEU:HA	6:I:448:GLY:HA3	2.00	0.43
8:L:406:CYS:HA	8:L:481:ALA:HB2	2.00	0.43
7:C:616:ARG:HA	7:C:628:MET:CB	2.48	0.43
4:Z:260:ALA:HA	4:Z:263:GLN:O	2.18	0.43
8:L:365:SER:N	8:L:368:PHE:O	2.51	0.43
7:M:272:ARG:N	7:M:296:ALA:HB1	2.34	0.43
5:e:241:THR:O	5:e:245:TYR:N	2.33	0.43
5:l:325:GLN:N	5:l:374:SER:O	2.42	0.43
5:a:260:LEU:HA	5:a:319:ALA:HB3	2.00	0.43
5:i:385:SER:O	5:i:389:GLU:N	2.27	0.43
5:k:409:ARG:HA	5:k:415:LYS:HA	2.01	0.43
5:d:319:ALA:O	5:d:380:ASN:N	2.38	0.43
7:A:438:GLU:O	7:A:461:THR:N	2.43	0.43
5:a:11:GLY:HA3	5:a:146:GLY:N	2.34	0.43
5:b:10:LEU:HA	5:b:67:LEU:O	2.19	0.43
5:b:272:GLY:N	5:b:377:MET:O	2.52	0.43
1:H:187:TYR:CB	1:H:269:ALA:HB3	2.49	0.42
1:F:337:LEU:O	1:F:341:LEU:N	2.25	0.42
5:a:140:SER:HA	5:a:171:VAL:H	1.85	0.42
5:f:49:ASP:HA	5:f:52:PHE:O	2.18	0.42
7:M:544:ILE:O	7:M:548:PHE:N	2.51	0.42
7:M:602:LYS:O	7:M:647:ASP:N	2.36	0.42
7:A:157:LYS:HA	7:A:313:TYR:CA	2.49	0.42
7:A:437:VAL:HA	7:A:461:THR:O	2.19	0.42
5:b:5:ILE:N	5:b:50:VAL:O	2.53	0.42
5:c:209:ALA:HB2	5:c:306:SER:H	1.84	0.42
5:g:289:THR:O	5:g:293:VAL:N	2.32	0.42
1:N:150:GLY:HA2	1:N:228:PRO:HA	2.01	0.42
7:G:659:ASN:O	7:G:663:LEU:N	2.30	0.42
8:L:1558:LEU:HA	8:L:1564:GLY:HA3	2.02	0.42
7:C:453:ASP:O	7:C:457:ASP:N	2.26	0.42
6:K:399:SER:O	6:K:403:VAL:N	2.45	0.42
5:d:9:GLN:CB	5:d:15:ASN:HA	2.48	0.42
9:J:223:GLN:O	9:J:226:THR:N	2.48	0.42
9:J:531:GLN:C	9:J:533:GLY:H	2.26	0.42
7:G:571:VAL:N	7:G:637:ALA:HB1	2.35	0.42
1:s:112:SER:C	1:s:114:TYR:H	2.26	0.42



	tio as page	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
5:d:325:GLN:HA	5:d:361:SER:O	2.20	0.42
6:I:358:LYS:O	6:I:364:GLY:N	2.51	0.42
1:F:40:SER:O	1:F:44:ARG:N	2.44	0.42
1:H:341:LEU:HA	1:H:390:GLY:HA3	2.00	0.42
5:a:26:CYS:O	5:a:30:GLY:N	2.53	0.42
5:f:61:ILE:HA	5:f:85:LEU:O	2.20	0.42
5:f:409:ARG:O	5:f:415:LYS:HA	2.20	0.42
5:g:174:ASN:HA	5:g:208:THR:H	1.84	0.42
5:d:322:ASN:O	5:d:359:ALA:N	2.29	0.42
5:c:320:ILE:O	5:c:356:ILE:HA	2.20	0.42
5:e:215:THR:O	5:e:219:HIS:HA	2.19	0.42
1:u:3:THR:O	1:u:4:PRO:C	2.63	0.42
6:I:206:LYS:O	6:I:258:SER:N	2.40	0.42
5:g:323:ILE:N	5:g:376:LEU:O	2.44	0.42
5:k:274:THR:O	5:k:375:GLY:N	2.53	0.42
5:e:51:PHE:O	5:e:63:ARG:N	2.50	0.42
5:l:405:LEU:O	5:1:409:ARG:N	2.44	0.42
9:J:577:ALA:O	9:J:581:LEU:N	2.31	0.42
7:A:157:LYS:HA	7:A:313:TYR:HA	2.02	0.42
5:e:102:ASN:C	5:e:144:GLY:HA3	2.45	0.41
5:e:214:ALA:O	5:e:220:ILE:N	2.37	0.41
5:j:142:ALA:HB2	5:j:173:PRO:CB	2.50	0.41
9:J:472:ARG:HA	9:J:488:TYR:HA	2.01	0.41
5:j:100:ALA:HB3	5:j:144:GLY:C	2.45	0.41
5:j:104:TRP:CB	5:j:187:ASN:HA	2.50	0.41
5:n:438:ALA:HA	5:n:443:TYR:CB	2.50	0.41
4:Z:219:VAL:O	4:Z:308:GLY:HA3	2.19	0.41
5:e:30:GLY:HA3	5:e:41:ALA:HB2	2.02	0.41
5:j:61:ILE:HA	5:j:85:LEU:O	2.20	0.41
1:F:455:GLY:HA2	5:f:448:THR:HA	2.02	0.41
5:g:30:GLY:HA3	5:g:41:ALA:HB2	2.02	0.41
5:e:322:ASN:O	5:e:359:ALA:N	2.33	0.41
1:N:14:PHE:HA	1:N:54:GLY:HA3	2.02	0.41
5:d:3:ARG:HA	5:d:131:SER:O	2.21	0.41
5:d:43:GLU:C	5:d:45:THR:H	2.29	0.41
1:H:493:LYS:O	1:H:497:ALA:N	2.53	0.41
5:e:317:TYR:O	5:e:348:PHE:HA	2.21	0.41
5:j:321:LEU:N	5:j:378:MET:O	2.34	0.41
8:L:311:TYR:HA	9:J:220:VAL:O	2.21	0.41
5:g:209:ALA:HB1	5:g:306:SER:H	1.86	0.41
8:L:1652:SER:HA	8:L:1756:GLY:HA3	2.02	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1.F.189.TRP.HA	1·F·194·GLU·O	2.20	0.41
5:a:51:PHE:O	5:a:63:ARG:N	2.50	0.41
5:c:35:GLY:O	5:c:60:TYR:N	2.54	0.41
5:g:8:LEU:N	5:g:136:VAL:O	2.28	0.41
5:i:70:GLU:HA	5:i:97:GLY:HA2	2.03	0.41
5:k:438:ALA:HA	5:k:443:TYR:CB	2.51	0.41
5:d:322:ASN:N	5:d:357:GLN:O	2.36	0.41
7:M:412:SER:O	7:M:416:PHE:N	2.34	0.41
7:M:779:LEU:HA	7:M:857:PHE:HA	2.03	0.41
7:C:544:ILE:O	7:C:548:PHE:N	2.54	0.41
7:A:161:LEU:N	7:A:312:GLU:O	2.53	0.41
6:I:508:GLN:O	6:I:666:MET:HA	2.21	0.41
6:I:652:LYS:O	6:I:656:GLN:N	2.39	0.41
1:F:105:GLU:CB	1:F:117:SER:HA	2.51	0.41
5:e:273:TYR:HA	5:e:376:LEU:HA	2.02	0.41
5:f:4:GLU:O	5:f:133:GLU:N	2.34	0.41
5:a:325:GLN:HA	5:a:361:SER:O	2.20	0.40
5:i:136:VAL:HA	5:i:167:GLN:O	2.21	0.40
1:B:112:LEU:C	1:B:114:LEU:H	2.28	0.40
6:K:385:THR:H	6:K:388:THR:CB	2.34	0.40
8:L:368:PHE:HA	8:L:378:VAL:O	2.21	0.40
9:J:723:SER:O	9:J:747:SER:N	2.26	0.40
5:e:324:ILE:N	5:e:359:ALA:O	2.33	0.40
5:j:35:GLY:O	5:j:60:TYR:N	2.31	0.40
5:k:206:ASP:CB	5:k:306:SER:H	2.34	0.40
5:a:11:GLY:HA3	5:a:146:GLY:HA2	2.04	0.40
5:b:325:GLN:HA	5:b:361:SER:O	2.22	0.40
5:h:138:CYS:HA	5:h:169:TYR:O	2.21	0.40
5:h:317:TYR:HA	5:h:381:HIS:HA	2.03	0.40
1:B:205:ALA:O	1:B:221:THR:N	2.30	0.40
1:N:345:ALA:N	1:N:388:ASP:O	2.48	0.40
5:b:272:GLY:HA2	5:b:304:MET:H	1.86	0.40
5:d:102:ASN:HA	5:d:144:GLY:N	2.37	0.40
7:A:636:LEU:O	7:A:638:LEU:N	2.55	0.40
1:F:19:GLY:N	1:F:22:ILE:O	2.54	0.40
5:a:100:ALA:HB1	5:a:103:ASN:O	2.22	0.40
5:d:100:ALA:HB3	5:d:144:GLY:C	2.46	0.40
3:Y:660:PHE:C	8:L:230:LEU:HA	2.47	0.40
9:J:935:LEU:O	9:J:939:ALA:N	2.55	0.40
6:I:622:SER:CB	6:I:661:LEU:H	2.35	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	Perce	entiles
1	В	640/907~(71%)	628~(98%)	12 (2%)	0	100	100
1	D	655/907~(72%)	644 (98%)	11 (2%)	0	100	100
1	F	655/907~(72%)	644 (98%)	11 (2%)	0	100	100
1	Н	654/907~(72%)	642 (98%)	12 (2%)	0	100	100
1	Ν	624/907~(69%)	617 (99%)	7 (1%)	0	100	100
1	r	111/907~(12%)	102 (92%)	5 (4%)	4 (4%)	3	20
1	s	113/907~(12%)	104 (92%)	5 (4%)	4 (4%)	3	20
1	t	118/907~(13%)	103 (87%)	9 (8%)	6 (5%)	1	16
1	u	118/907~(13%)	103 (87%)	8 (7%)	7 (6%)	1	14
1	v	125/907~(14%)	111 (89%)	9 (7%)	5 (4%)	2	18
2	Ο	80/82~(98%)	80 (100%)	0	0	100	100
2	Р	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	Т	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%)	10	42
3	Х	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	$\overline{444/457}~(97\%)$	437 (98%)	7 (2%)	0	100	100
5	b	$\overline{450/457}~(98\%)$	442 (98%)	8 (2%)	0	100	100
5	с	446/457~(98%)	439 (98%)	7 (2%)	0	100	100
					Continued a	on next	page

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
5	d	448/457~(98%)	440 (98%)	8 (2%)	0	100	100
5	е	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	1	445/457~(97%)	438 (98%)	7 (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	Ι	606/667~(91%)	586~(97%)	19 (3%)	1 (0%)	44	78
6	K	608/667~(91%)	589~(97%)	15 (2%)	4 (1%)	19	56
7	А	651/930~(70%)	640 (98%)	11 (2%)	0	100	100
7	С	647/930~(70%)	637~(98%)	10 (2%)	0	100	100
7	Е	672/930~(72%)	661 (98%)	11 (2%)	0	100	100
7	G	672/930~(72%)	661 (98%)	11 (2%)	0	100	100
7	М	659/930~(71%)	650 (99%)	9 (1%)	0	100	100
8	L	972/1811~(54%)	923~(95%)	45 (5%)	4 (0%)	30	68
9	J	834/1024 (81%)	807 (97%)	23 (3%)	4 (0%)	25	64
All	All	17575/27876~(63%)	17174 (98%)	361 (2%)	40 (0%)	45	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	s	111	VAL
1	t	5	ASP
1	t	109	SER
1	t	111	VAL
1	u	5	ASP
1	u	111	VAL
1	V	108	PRO



Mol	Chain	Res	Type
6	K	295	ARG
6	K	447	SER
8	L	351	GLU
6	Ι	295	ARG
1	r	111	VAL
1	r	113	SER
1	s	113	SER
1	t	6	GLN
1	t	113	SER
1	u	6	GLN
1	u	109	SER
1	u	113	SER
1	V	124	ARG
1	V	125	ASP
6	K	250	LEU
8	L	417	PRO
9	J	221	VAL
1	r	110	LYS
1	t	110	LYS
1	u	110	LYS
8	L	1454	GLN
9	J	223	GLN
9	J	526	GLU
1	s	110	LYS
6	К	445	PRO
1	u	4	PRO
1	v	119	ALA
1	V	123	PRO
8	L	309	GLU
9	J	616	VAL

$\alpha$ $\cdot$ $\cdot$ $\cdot$	r	•	
Continued	from	previous	page

#### 5.3.2 Protein sidechains (i)

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

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.



# 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

# 5.5 Carbohydrates (i)

There are no 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	С	107:GLN	N	8.98
1	L	123:PRO	С	124:GLN	N	5.52
1	L	311:TYR	С	312:LEU	N	3.84



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-53400. 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



6.1.2 Raw map



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



# 6.2 Central slices (i)

# 6.2.1 Primary map



X Index: 184



Y Index: 184



Z Index: 184

#### 6.2.2 Raw map



X Index: 184

Y Index: 184

Z Index: 184

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: 149



Y Index: 196



Z Index: 175

#### 6.3.2 Raw map



X Index: 149

Y Index: 196



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







2

6.4.2 Raw map



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 0.15. 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.



#### Mask visualisation (i) 6.6

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

#### $emd_{53400}msk_{1.map}$ (i) 6.6.1





# 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 2190  $\rm nm^3;$  this corresponds to an approximate mass of 1978 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 (i)



\*Reported resolution corresponds to spatial frequency of 0.213  ${\rm \AA^{-1}}$ 



# 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 0.213  $\text{\AA}^{-1}$ 



# 8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estim	timation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	4.70	-	-	
Author-provided FSC curve	4.69	6.82	4.81	
Unmasked-calculated*	7.25	8.80	7.45	

\*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 7.25 differs from the reported value 4.7 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-53400 and PDB model 9QVN. Per-residue inclusion information can be found in section 3 on page 11.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.15 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 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 (0.15).



# 9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.


1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} ext{-score}$
All	0.8680	0.2270
А	0.9740	0.2350
В	0.9840	0.2660
С	0.9860	0.2760
D	0.9860	0.2780
E	0.9780	0.2830
F	0.9920	0.2860
G	0.9860	0.2790
Н	0.9970	0.2950
I	0.9990	0.2850
J	0.8500	0.2510
K	0.9940	0.2540
L	0.9690	0.2470
М	0.7240	0.1350
Ν	0.4040	0.0870
0	0.8990	0.2870
Р	0.9810	0.2800
Q	0.0000	0.0710
R	0.0000	0.1830
S	0.0000	0.1520
Т	0.7780	0.2340
U	0.4700	0.2380
V	0.5650	0.2420
W	0.4310	0.2260
Х	0.3910	0.2160
Y	0.5730	0.2340
Z	0.9720	0.2750
a	0.9740	0.1620
b	0.9840	0.2180
с	0.9820	0.2450
d	0.9860	0.2350
e	0.9890	0.2280
f	0.9970	0.2640
g	0.9730	0.2480
h	0.9920	0.2820

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Chain	Atom inclusion	Q-score
i	0.9830	0.2480
j	0.9770	0.2270
k	0.9720	0.1480
l	0.8940	0.1090
m	0.5730	0.0610
n	0.0860	0.0490
r	0.0000	0.1660
S	0.0090	0.1350
t	0.4120	0.2310
u	0.5490	0.2660
V	0.9910	0.3160

