



Full wwPDB EM Validation Report ⓘ

Jan 29, 2022 – 06:15 am GMT

PDB ID : 7QJ6
EMDB ID : EMD-14011
Title : Structure of recombinant human gamma-Tubulin Ring Complex 10-spoked assembly intermediate (spokes 3-12, substoichiometric spokes 13-14)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 7.80 Å (reported)
Based on initial models : 6L81, 6X0U, 7AS4, 6V6S

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

EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

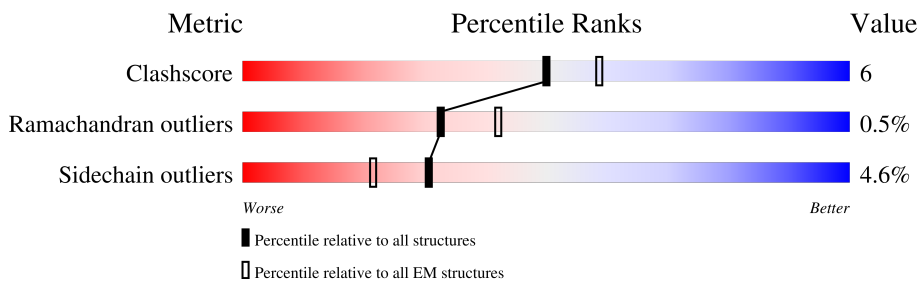
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	e	375	
2	b	82	
2	d	82	
2	i	82	
2	k	82	
2	m	82	
3	D	907	
3	F	907	

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Mol	Chain	Length	Quality of chain
3	H	907	59% 7% 35%
3	a	907	13% 87%
3	h	907	11% 88%
3	j	907	12% 88%
4	C	902	6% 59% 9% 31%
4	E	902	64% 6% 29%
4	G	902	62% 9% 29%
5	I	667	68% 9% 22%
5	K	667	76% 8% 16%
6	J	1024	45% 7% 48%
6	l	1024	10% 89%
7	L	1819	28% 69%
7	c	1819	9% 91%
8	Q	451	29% 65% 24% 7%
8	R	451	12% 65% 25% 7%
8	S	451	64% 25% 7%
8	T	451	65% 25% 7%
8	U	451	65% 25% 7%
8	V	451	64% 25% 7%
8	W	451	65% 25% 7%
8	X	451	63% 26% 7%
8	Y	451	65% 24% 7%
8	Z	451	65% 25% 7%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 91575 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 actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	e	364	2847	1803	476	548	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	65	484	299	85	96	4	0	0
2	k	65	484	299	85	96	4	0	0
2	m	65	484	299	85	96	4	0	0
2	i	65	484	299	85	96	4	0	0
2	d	59	454	281	79	90	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	a	116	933	591	171	169	2	0	0
3	D	581	4796	3061	842	868	25	0	0
3	F	599	4941	3151	871	894	25	0	0
3	H	594	4907	3130	864	888	25	0	0
3	h	107	843	533	156	152	2	0	0
3	j	107	843	533	156	152	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
4	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		
4	G	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	521	Total	C	N	O	S	0	0
			4225	2737	720	750	18		
5	K	562	Total	C	N	O	S	0	0
			4579	2964	781	816	18		

- Molecule 6 is a protein called Gamma-tubulin complex component 5.

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

- Molecule 7 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	566	Total	C	N	O	S	0	0
			4587	3000	773	789	25		
7	c	158	Total	C	N	O	S	0	0
			1220	771	209	232	8		

- Molecule 8 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	R	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	S	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	T	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	1	6	Total	O	0
			6	6	

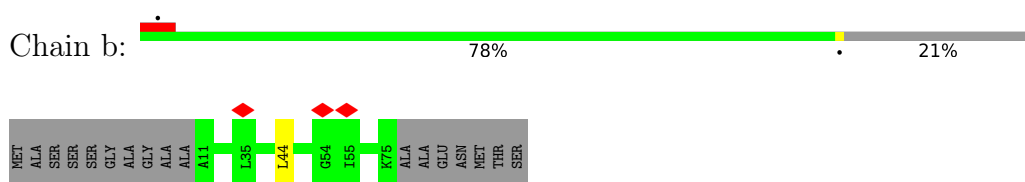
3 Residue-property plots [i](#)

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: actin, cytoplasmic 1



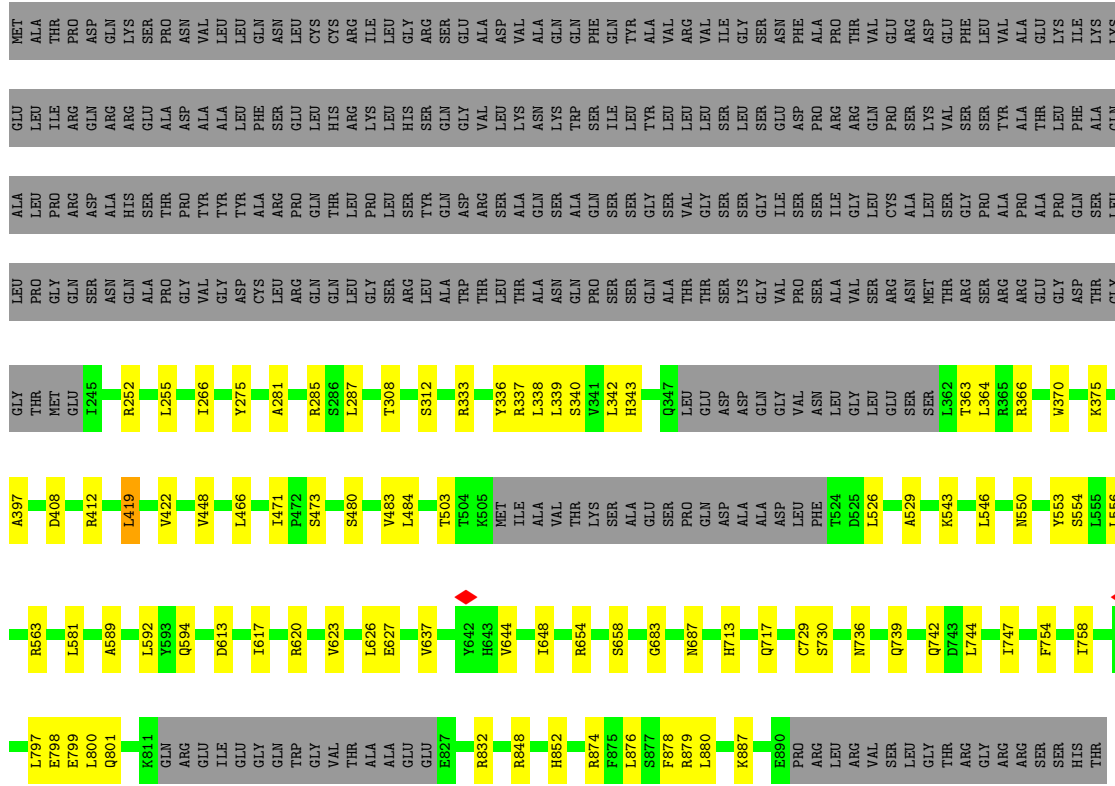
- Molecule 2: Mitotic-spindle organizing protein 1



- Molecule 2: Mitotic-spindle organizing protein 1

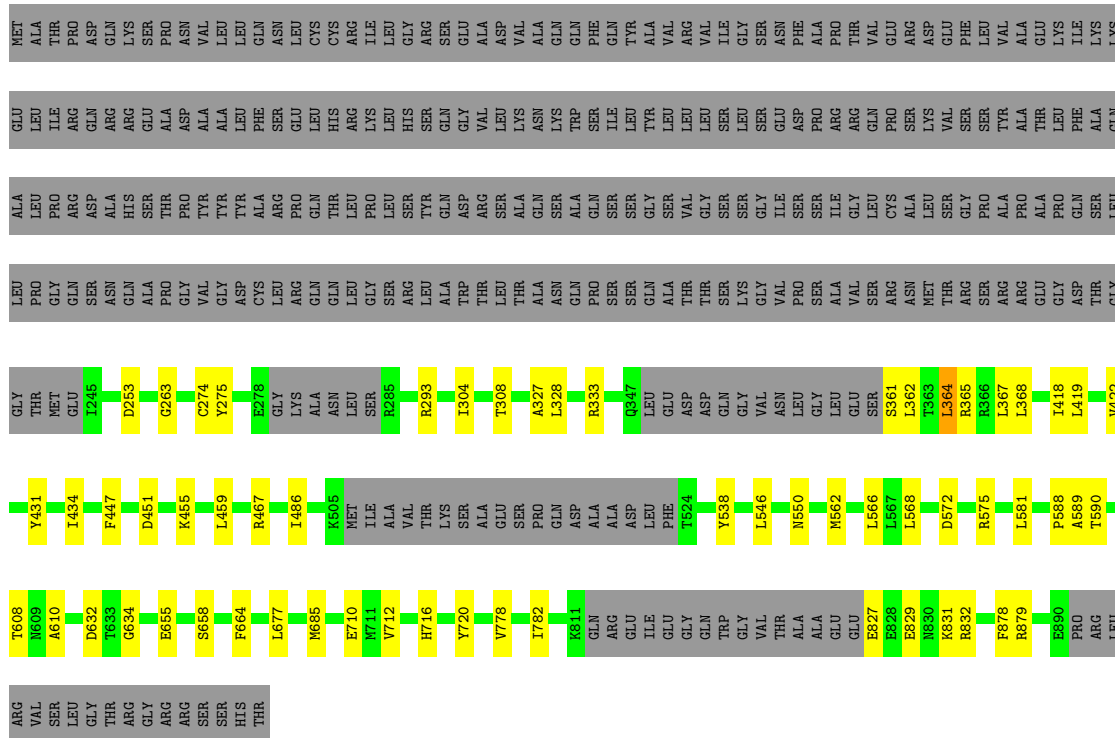


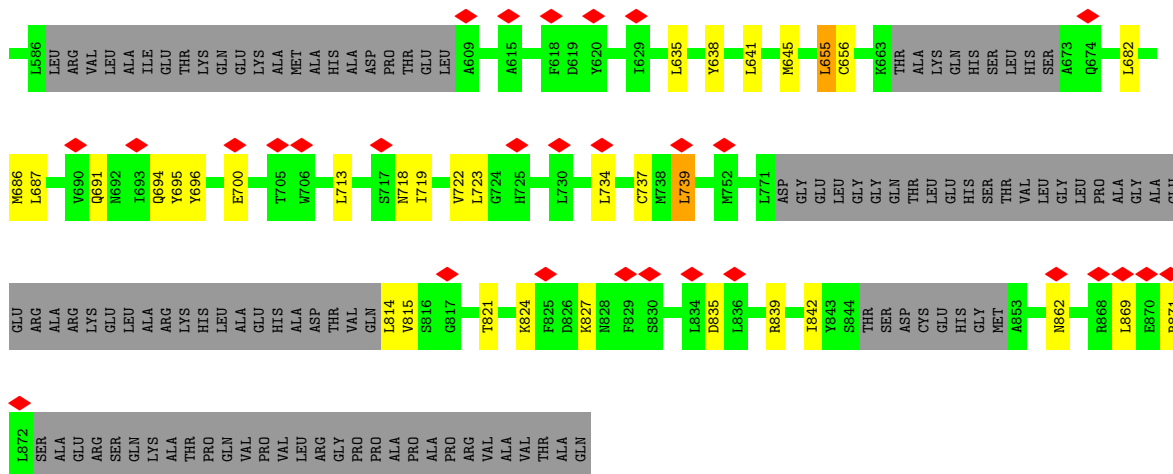
Chain F: 57% 9% 34%



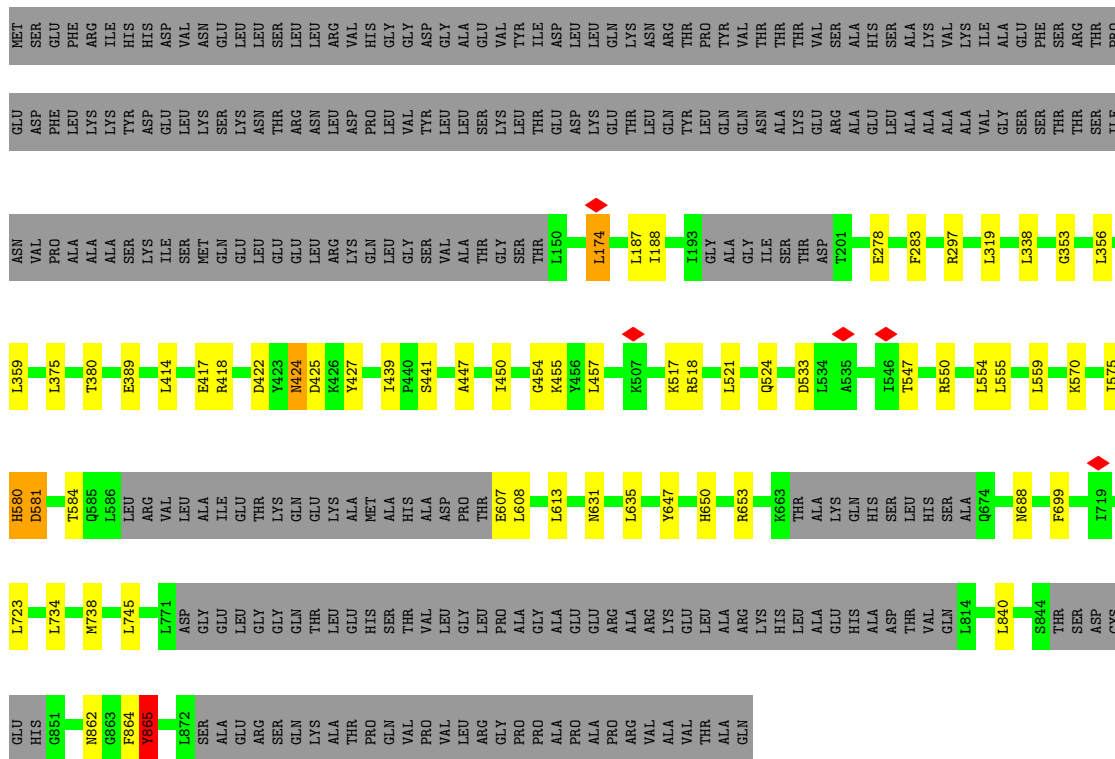
• Molecule 3: Gamma-tubulin complex component 3

Chain H: 59% 7% 35%

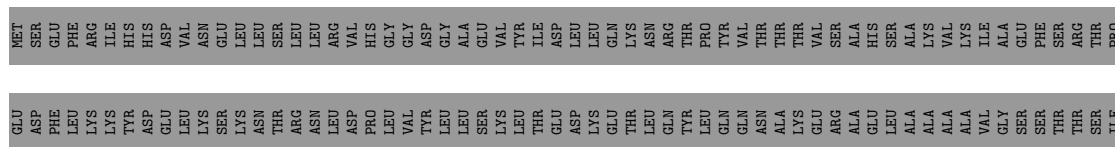


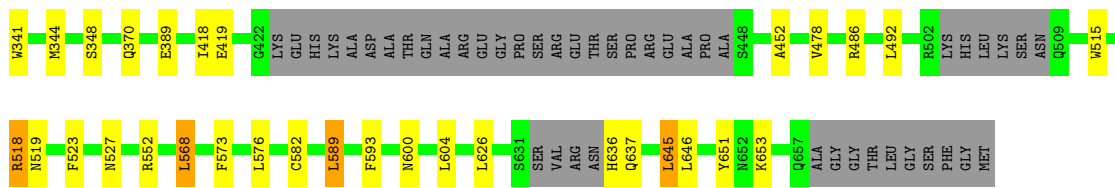


• Molecule 4: Gamma-tubulin complex component 2

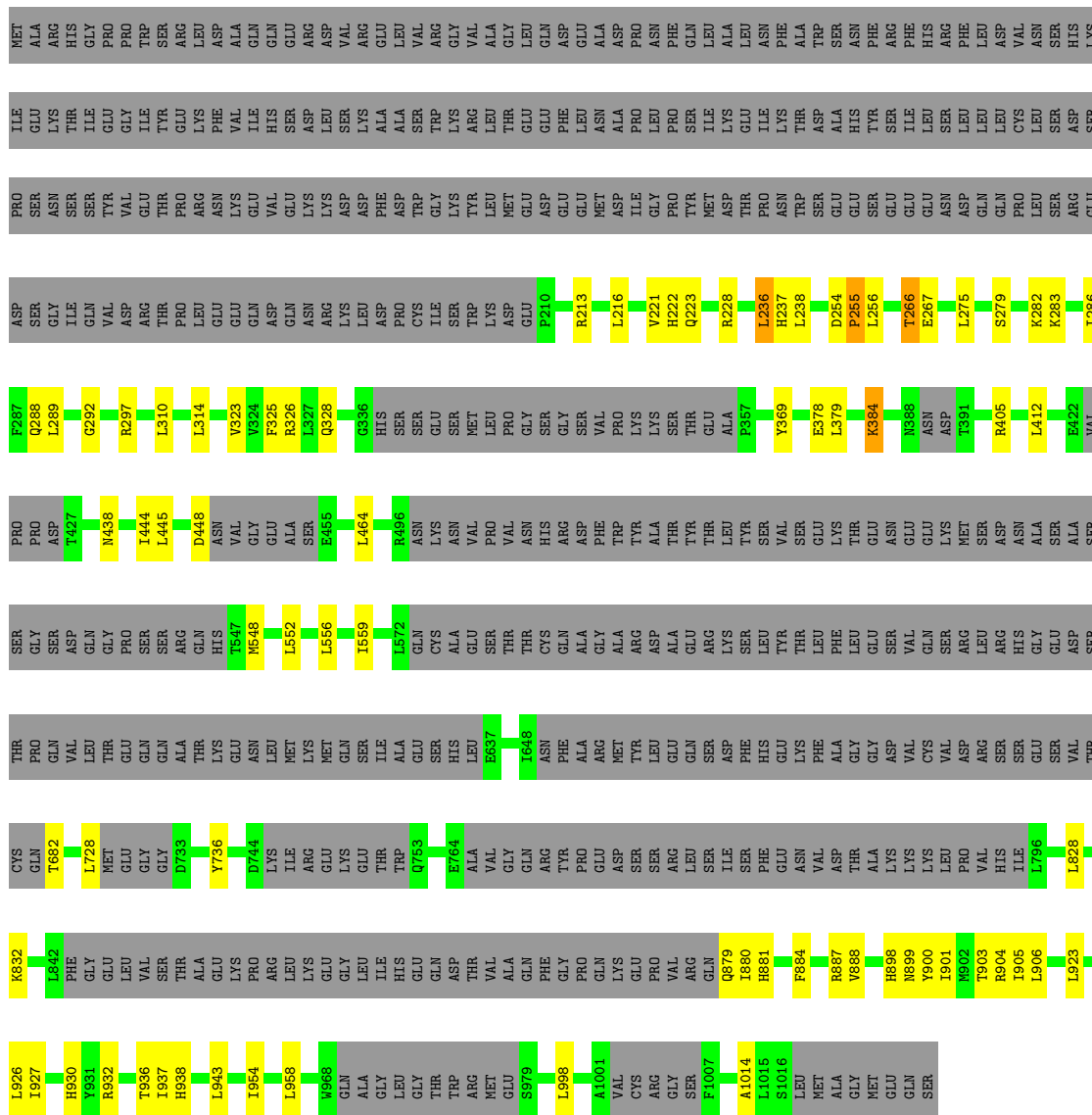


• Molecule 4: Gamma-tubulin complex component 2



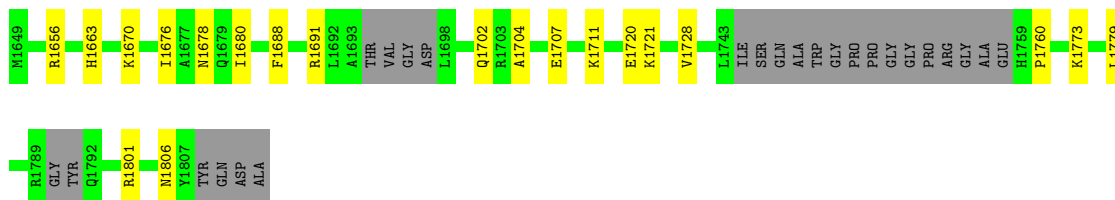


• Molecule 6: Gamma-tubulin complex component 5

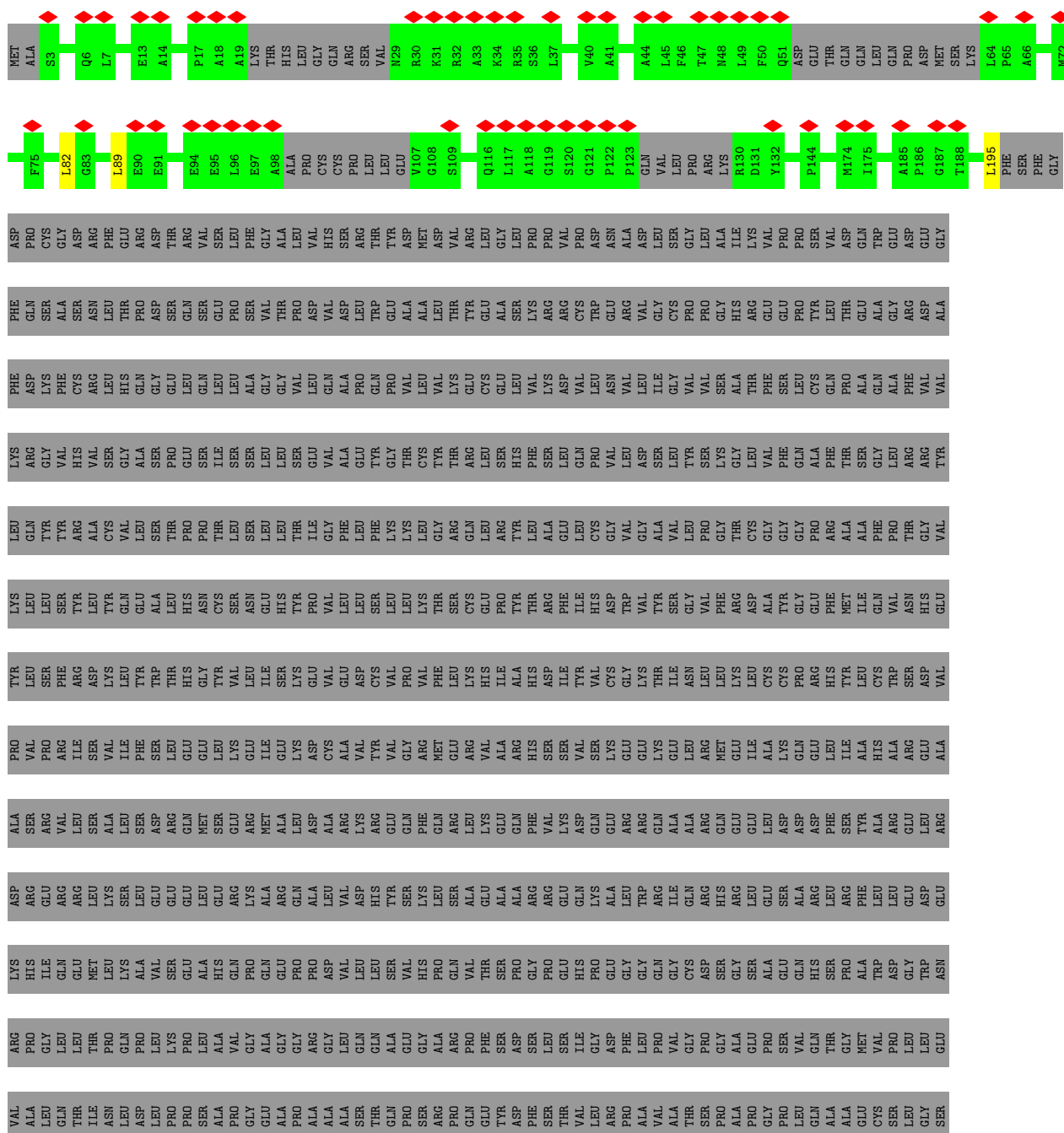


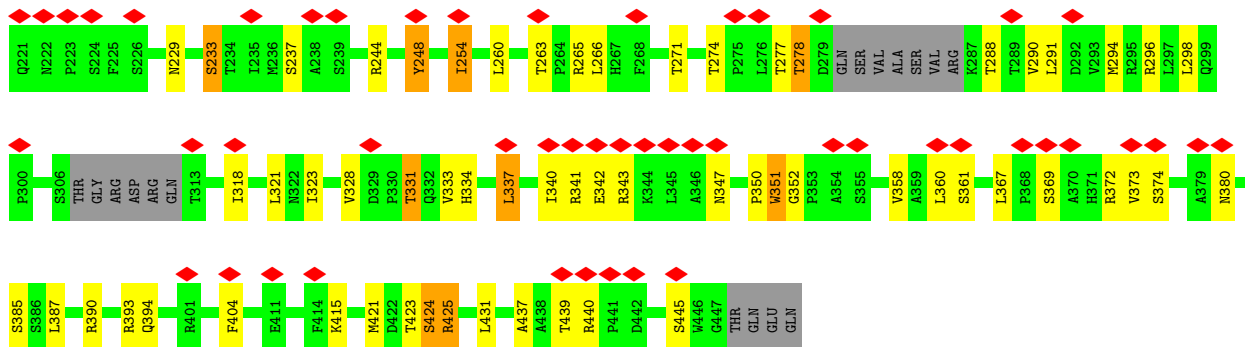
• Molecule 6: Gamma-tubulin complex component 5



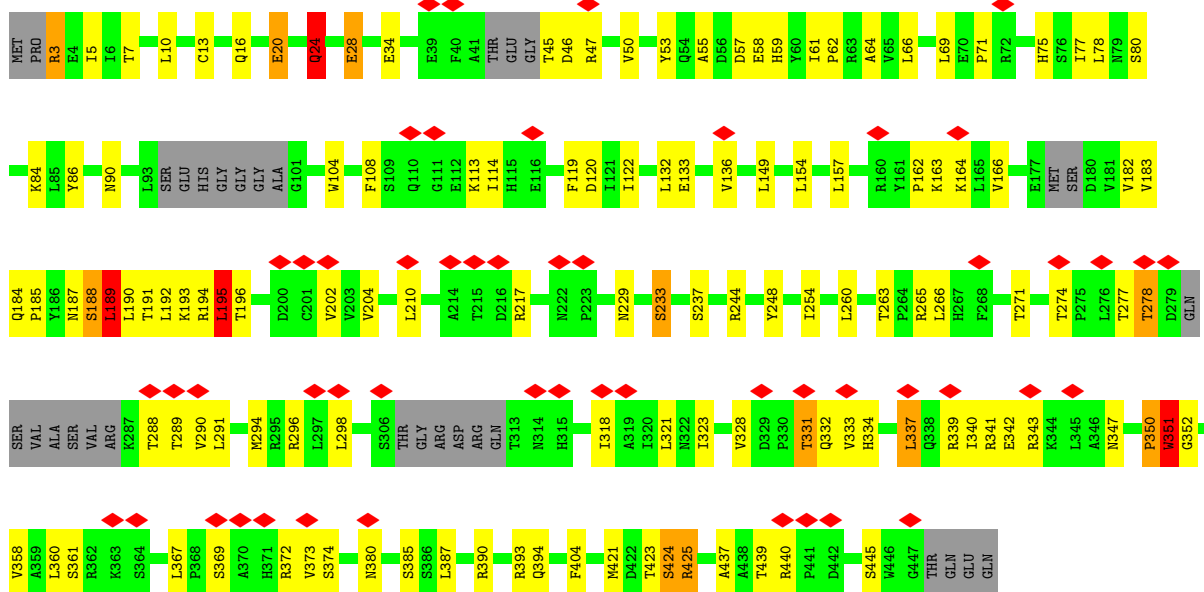


• Molecule 7: Gamma-tubulin complex component 6

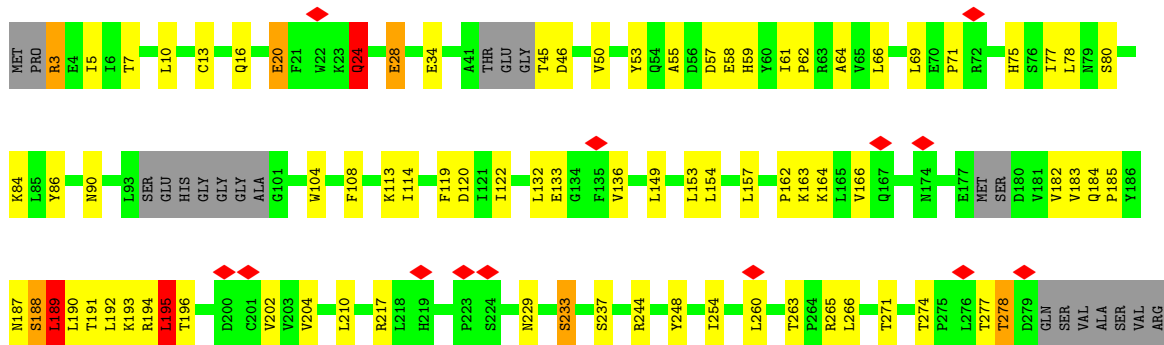


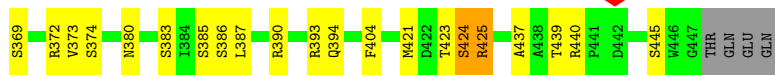
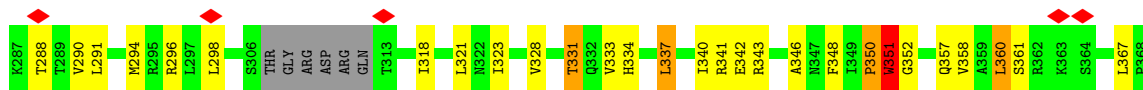


• Molecule 8: Tubulin gamma-1 chain

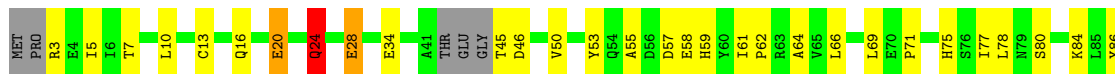


• Molecule 8: Tubulin gamma-1 chain

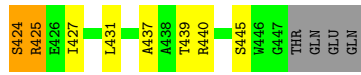
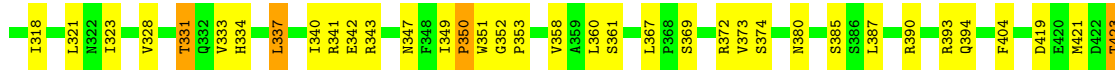
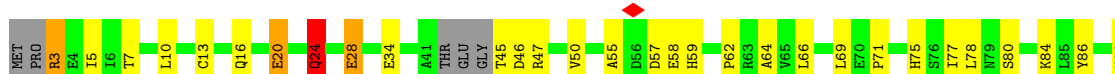




• Molecule 8: Tubulin gamma-1 chain

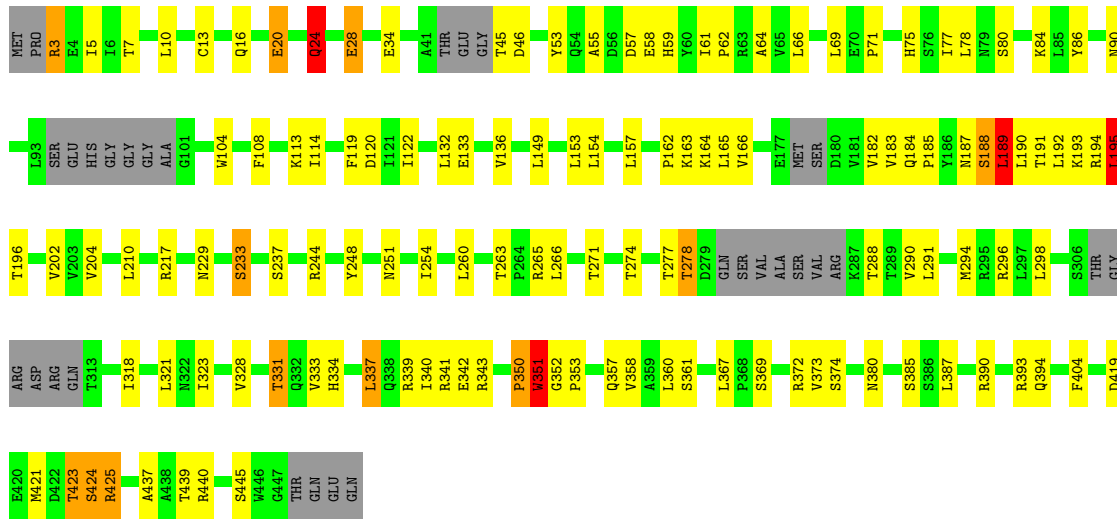


• Molecule 8: Tubulin gamma-1 chain



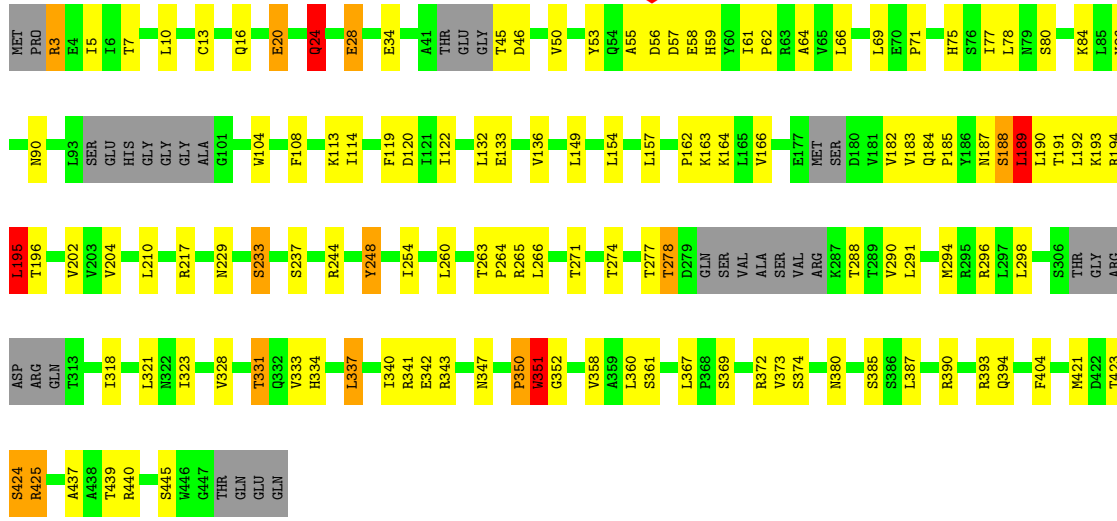
• Molecule 8: Tubulin gamma-1 chain

Chain V: 64% 25% 7%



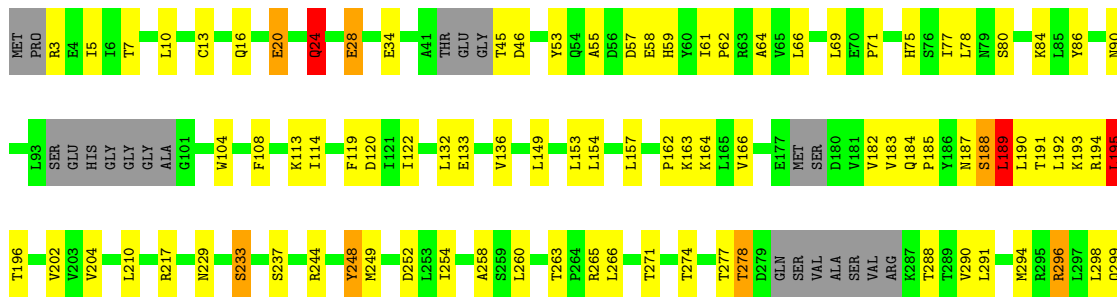
• Molecule 8: Tubulin gamma-1 chain

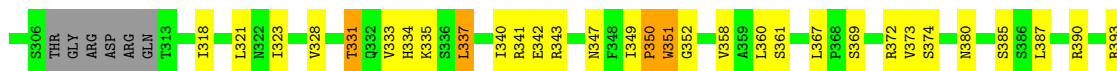
Chain W: 65% 25% 7%



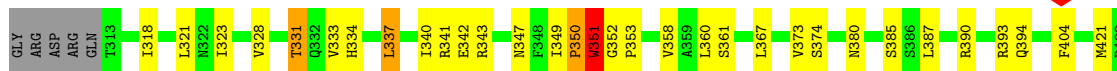
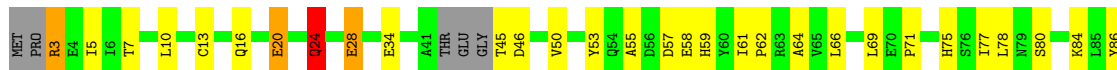
• Molecule 8: Tubulin gamma-1 chain

Chain X: 63% 26% 7%

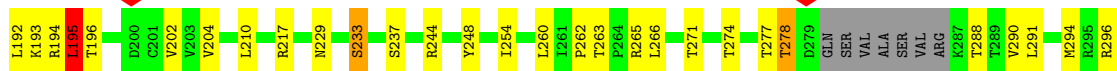
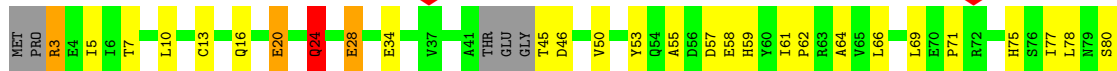




• Molecule 8: Tubulin gamma-1 chain



• Molecule 8: Tubulin gamma-1 chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28611	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.247	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0308	Depositor
Map size (\AA)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.66, 2.66, 2.66	Depositor

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	e	0.58	1/2908 (0.0%)	0.72	4/3938 (0.1%)
2	b	0.39	0/484	0.63	0/653
2	d	0.40	0/454	0.67	0/611
2	i	0.37	0/484	0.81	0/653
2	k	0.31	0/484	0.56	0/653
2	m	0.33	0/484	0.63	1/653 (0.2%)
3	D	0.38	0/4897	0.66	4/6610 (0.1%)
3	F	0.36	0/5044	0.65	4/6809 (0.1%)
3	H	0.37	0/5009	0.63	1/6761 (0.0%)
3	a	0.37	0/948	0.64	1/1277 (0.1%)
3	h	0.34	0/855	0.70	1/1152 (0.1%)
3	j	0.37	0/855	0.65	1/1152 (0.1%)
4	C	0.40	0/5151	0.71	7/6955 (0.1%)
4	E	0.45	4/5311 (0.1%)	0.70	11/7169 (0.2%)
4	G	0.40	0/5315	0.65	0/7175
5	I	0.39	0/4322	0.67	3/5853 (0.1%)
5	K	0.39	0/4683	0.65	3/6338 (0.0%)
6	J	0.41	0/4525	0.69	1/6119 (0.0%)
6	l	0.39	0/863	0.66	2/1166 (0.2%)
7	L	0.36	0/4697	0.65	2/6348 (0.0%)
7	c	0.37	0/1235	0.76	3/1664 (0.2%)
8	Q	0.33	0/3441	0.61	5/4661 (0.1%)
8	R	0.33	0/3441	0.61	5/4661 (0.1%)
8	S	0.33	0/3441	0.61	5/4661 (0.1%)
8	T	0.33	0/3441	0.61	5/4661 (0.1%)
8	U	0.34	0/3441	0.60	5/4661 (0.1%)
8	V	0.33	0/3441	0.61	5/4661 (0.1%)
8	W	0.33	0/3441	0.61	5/4661 (0.1%)
8	X	0.33	0/3441	0.61	5/4661 (0.1%)
8	Y	0.33	0/3441	0.61	5/4661 (0.1%)
8	Z	0.34	0/3441	0.61	5/4661 (0.1%)
All	All	0.38	5/93418 (0.0%)	0.65	99/126319 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	1
4	E	0	2
4	G	0	2
5	I	0	4
5	K	0	1
6	J	0	1
7	L	0	2
8	Q	0	1
8	R	0	1
8	S	0	1
8	T	0	1
8	V	0	1
8	W	0	1
8	X	0	1
8	Y	0	1
All	All	0	21

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	243	PRO	N-CD	22.77	1.79	1.47
4	E	865	TYR	CD2-CE2	-11.80	1.21	1.39
4	E	865	TYR	CE2-CZ	-9.06	1.26	1.38
4	E	865	TYR	CG-CD2	-5.94	1.31	1.39
4	E	865	TYR	CZ-OH	-5.27	1.28	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	840	LEU	CB-CG-CD2	-10.35	93.40	111.00
3	D	581	LEU	CA-CB-CG	9.99	138.27	115.30
3	j	108	PRO	N-CA-CB	9.81	115.08	103.30
7	c	195	LEU	CA-CB-CG	9.72	137.65	115.30
8	V	189	LEU	CA-CB-CG	9.14	136.33	115.30
8	Q	189	LEU	CA-CB-CG	9.14	136.33	115.30
8	R	189	LEU	CA-CB-CG	9.14	136.32	115.30
8	S	189	LEU	CA-CB-CG	9.14	136.32	115.30
8	U	189	LEU	CA-CB-CG	9.14	136.32	115.30
8	W	189	LEU	CA-CB-CG	9.14	136.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	X	189	LEU	CA-CB-CG	9.13	136.30	115.30
8	T	189	LEU	CA-CB-CG	9.13	136.29	115.30
8	Y	189	LEU	CA-CB-CG	9.13	136.29	115.30
8	Z	189	LEU	CA-CB-CG	9.12	136.28	115.30
7	c	82	LEU	CA-CB-CG	8.70	135.32	115.30
8	T	189	LEU	CB-CG-CD1	8.54	125.53	111.00
8	X	189	LEU	CB-CG-CD1	8.54	125.52	111.00
8	Z	189	LEU	CB-CG-CD1	8.53	125.50	111.00
8	Y	189	LEU	CB-CG-CD1	8.52	125.49	111.00
8	V	189	LEU	CB-CG-CD1	8.52	125.49	111.00
8	R	189	LEU	CB-CG-CD1	8.51	125.47	111.00
8	U	189	LEU	CB-CG-CD1	8.51	125.47	111.00
8	Q	189	LEU	CB-CG-CD1	8.51	125.47	111.00
8	S	189	LEU	CB-CG-CD1	8.51	125.47	111.00
8	W	189	LEU	CB-CG-CD1	8.51	125.47	111.00
4	E	865	TYR	OH-CZ-CE2	-7.90	98.77	120.10
3	h	108	PRO	N-CA-CB	7.77	112.63	103.30
4	E	174	LEU	CA-CB-CG	7.67	132.95	115.30
3	F	581	LEU	CA-CB-CG	7.56	132.69	115.30
3	D	368	LEU	CA-CB-CG	7.33	132.17	115.30
4	C	655	LEU	CA-CB-CG	7.15	131.74	115.30
4	E	865	TYR	CD1-CE1-CZ	-7.09	113.42	119.80
4	E	865	TYR	CB-CG-CD2	-7.09	116.75	121.00
4	E	840	LEU	CA-CB-CG	6.88	131.12	115.30
4	E	580	HIS	C-N-CA	6.61	138.22	121.70
5	K	645	LEU	CA-CB-CG	6.46	130.16	115.30
6	l	121	PRO	N-CA-CB	6.32	110.88	103.30
5	I	530	TYR	CA-CB-CG	6.21	125.19	113.40
5	I	583	LEU	CA-CB-CG	6.20	129.57	115.30
7	L	312	LEU	CA-CB-CG	6.20	129.56	115.30
6	l	130	PRO	N-CA-CB	6.20	110.73	103.30
4	E	865	TYR	CE1-CZ-OH	6.17	136.77	120.10
3	D	297	LEU	CA-CB-CG	6.16	129.46	115.30
1	e	243	PRO	CA-N-CD	-6.09	102.97	111.50
5	I	104	LEU	CA-CB-CG	6.07	129.25	115.30
3	H	581	LEU	CA-CB-CG	6.03	129.17	115.30
3	F	333	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	m	18	LEU	CA-CB-CG	5.86	128.77	115.30
8	S	195	LEU	CA-CB-CG	5.80	128.65	115.30
8	U	195	LEU	CA-CB-CG	5.80	128.63	115.30
8	X	195	LEU	CA-CB-CG	5.80	128.63	115.30
8	Y	195	LEU	CA-CB-CG	5.79	128.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	195	LEU	CA-CB-CG	5.79	128.61	115.30
8	W	195	LEU	CA-CB-CG	5.79	128.61	115.30
4	C	723	LEU	CA-CB-CG	5.79	128.61	115.30
8	R	195	LEU	CA-CB-CG	5.79	128.60	115.30
8	Q	195	LEU	CA-CB-CG	5.78	128.60	115.30
8	Z	195	LEU	CA-CB-CG	5.78	128.60	115.30
8	T	195	LEU	CA-CB-CG	5.78	128.59	115.30
4	E	723	LEU	CA-CB-CG	5.71	128.43	115.30
5	K	589	LEU	CB-CG-CD1	5.63	120.57	111.00
8	Q	24	GLN	CA-CB-CG	5.61	125.73	113.40
8	T	24	GLN	CA-CB-CG	5.61	125.73	113.40
8	S	24	GLN	CA-CB-CG	5.60	125.72	113.40
8	Z	24	GLN	CA-CB-CG	5.60	125.72	113.40
8	U	24	GLN	CA-CB-CG	5.60	125.72	113.40
8	V	24	GLN	CA-CB-CG	5.60	125.71	113.40
8	W	24	GLN	CA-CB-CG	5.59	125.70	113.40
8	R	24	GLN	CA-CB-CG	5.59	125.69	113.40
8	X	24	GLN	CA-CB-CG	5.58	125.69	113.40
8	Y	24	GLN	CA-CB-CG	5.58	125.67	113.40
4	C	264	LEU	CA-CB-CG	5.57	128.11	115.30
5	K	255	LYS	N-CA-CB	5.53	120.55	110.60
3	D	439	LEU	CA-CB-CG	5.52	128.00	115.30
1	e	267	LEU	CA-CB-CG	5.44	127.81	115.30
7	L	1531	LEU	CA-CB-CG	5.43	127.79	115.30
8	Y	24	GLN	CB-CG-CD	5.38	125.59	111.60
8	X	24	GLN	CB-CG-CD	5.38	125.59	111.60
8	W	24	GLN	CB-CG-CD	5.37	125.57	111.60
8	U	24	GLN	CB-CG-CD	5.37	125.56	111.60
8	Q	24	GLN	CB-CG-CD	5.37	125.55	111.60
8	Z	24	GLN	CB-CG-CD	5.36	125.53	111.60
8	R	24	GLN	CB-CG-CD	5.36	125.53	111.60
8	V	24	GLN	CB-CG-CD	5.36	125.53	111.60
8	S	24	GLN	CB-CG-CD	5.36	125.52	111.60
8	T	24	GLN	CB-CG-CD	5.36	125.53	111.60
3	a	27	ASP	CB-CG-OD1	5.33	123.09	118.30
4	E	174	LEU	CB-CG-CD2	-5.32	101.96	111.00
3	F	556	LEU	CA-CB-CG	5.31	127.52	115.30
6	J	464	LEU	CA-CB-CG	5.30	127.50	115.30
7	c	89	LEU	CA-CB-CG	5.30	127.50	115.30
4	C	221	LEU	CA-CB-CG	5.28	127.45	115.30
4	C	739	LEU	CA-CB-CG	5.24	127.36	115.30
4	C	306	LEU	CA-CB-CG	5.22	127.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	869	LEU	CA-CB-CG	5.22	127.31	115.30
4	E	319	LEU	CB-CG-CD1	-5.18	102.19	111.00
3	F	419	LEU	CA-CB-CG	5.15	127.14	115.30
1	e	216	LEU	CA-CB-CG	5.12	127.06	115.30
1	e	299	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	581	ASP	Mainchain
4	E	865	TYR	Peptide
4	G	240	GLY	Peptide
4	G	580	HIS	Peptide
3	H	364	LEU	Peptide
5	I	407	ASP	Peptide
5	I	408	ASP	Mainchain
5	I	499	GLN	Peptide
5	I	507	SER	Peptide
6	J	255	PRO	Peptide
5	K	254	LEU	Peptide
7	L	306	HIS	Peptide
7	L	346	LEU	Peptide
8	Q	351	TRP	Peptide
8	R	351	TRP	Peptide
8	S	351	TRP	Peptide
8	T	351	TRP	Peptide
8	V	351	TRP	Peptide
8	W	351	TRP	Peptide
8	X	351	TRP	Peptide
8	Y	351	TRP	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	e	2847	0	2810	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	484	0	512	0	0
2	d	454	0	482	0	0
2	i	484	0	512	0	0
2	k	484	0	512	0	0
2	m	484	0	512	0	0
3	D	4796	0	4775	35	0
3	F	4941	0	4935	46	0
3	H	4907	0	4896	33	0
3	a	933	0	953	0	0
3	h	843	0	846	0	0
3	j	843	0	846	0	0
4	C	5044	0	5081	50	0
4	E	5202	0	5241	35	0
4	G	5206	0	5230	48	0
5	I	4225	0	4259	36	0
5	K	4579	0	4586	36	0
6	J	4429	0	4482	44	0
6	l	847	0	789	0	0
7	L	4587	0	4636	32	0
7	c	1220	0	1231	0	0
8	Q	3373	0	3325	58	0
8	R	3373	0	3325	66	0
8	S	3373	0	3325	63	0
8	T	3373	0	3325	58	0
8	U	3373	0	3325	61	0
8	V	3373	0	3325	64	0
8	W	3373	0	3325	60	0
8	X	3373	0	3325	67	0
8	Y	3373	0	3325	60	0
8	Z	3373	0	3325	57	0
9	l	6	0	0	0	0
All	All	91575	0	91376	952	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 (952) 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)
4:C:656:CYS:HB3	8:Q:254:ILE:HD11	1.63	0.80
7:L:1806:ASN:HD22	8:Z:353:PRO:HB3	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:414:LEU:HG	4:E:424:ASN:HB2	1.65	0.78
4:E:688:ASN:HD21	8:S:357:GLN:HE22	1.32	0.78
4:C:482:ARG:HH11	4:C:486:GLU:HG2	1.52	0.75
6:J:881:HIS:NE2	8:X:444:ILE:O	2.20	0.74
4:E:865:TYR:OH	8:S:350:PRO:O	2.03	0.74
5:I:184:TYR:HB3	5:I:315:LYS:HZ2	1.53	0.73
3:F:543:LYS:HD3	3:F:742:GLN:HG2	1.72	0.72
8:V:185:PRO:O	8:V:189:LEU:HB3	1.92	0.70
8:Z:185:PRO:O	8:Z:189:LEU:HB3	1.92	0.70
3:D:739:GLN:HE21	3:D:740:GLN:HE22	1.39	0.70
8:W:185:PRO:O	8:W:189:LEU:HB3	1.92	0.70
8:Q:185:PRO:O	8:Q:189:LEU:HB3	1.92	0.70
8:S:185:PRO:O	8:S:189:LEU:HB3	1.92	0.70
8:R:185:PRO:O	8:R:189:LEU:HB3	1.92	0.70
3:F:363:THR:OG1	3:F:366:ARG:NH2	2.25	0.69
3:H:829:GLU:HA	3:H:832:ARG:HD3	1.75	0.69
8:T:185:PRO:O	8:T:189:LEU:HB3	1.92	0.69
8:U:185:PRO:O	8:U:189:LEU:HB3	1.92	0.69
8:X:185:PRO:O	8:X:189:LEU:HB3	1.92	0.68
8:Y:185:PRO:O	8:Y:189:LEU:HB3	1.92	0.68
8:S:62:PRO:HD2	8:S:86:TYR:HB3	1.76	0.68
8:Y:62:PRO:HD2	8:Y:86:TYR:HB3	1.76	0.68
8:X:62:PRO:HD2	8:X:86:TYR:HB3	1.76	0.68
4:E:613:LEU:HD11	4:E:647:TYR:HA	1.75	0.68
8:R:62:PRO:HD2	8:R:86:TYR:HB3	1.76	0.68
4:C:526:ASP:HB3	4:C:562:SER:HB2	1.75	0.67
8:T:62:PRO:HD2	8:T:86:TYR:HB3	1.76	0.67
8:W:56:ASP:O	8:X:296:ARG:NE	2.28	0.67
3:H:365:ARG:HB2	3:H:368:LEU:HB2	1.77	0.67
5:K:518:ARG:HH12	5:K:589:LEU:HD13	1.60	0.67
8:W:62:PRO:HD2	8:W:86:TYR:HB3	1.76	0.67
5:I:312:HIS:HA	5:I:315:LYS:HD2	1.76	0.66
8:Q:62:PRO:HD2	8:Q:86:TYR:HB3	1.76	0.66
8:Z:62:PRO:HD2	8:Z:86:TYR:HB3	1.76	0.66
5:I:85:TYR:OH	5:I:151:CYS:SG	2.54	0.66
8:U:62:PRO:HD2	8:U:86:TYR:HB3	1.76	0.66
8:V:62:PRO:HD2	8:V:86:TYR:HB3	1.76	0.66
6:J:279:SER:HB3	6:J:379:LEU:HD22	1.76	0.66
4:C:334:THR:OG1	4:C:371:GLN:NE2	2.30	0.65
5:I:515:TRP:HE1	5:I:519:ASN:H	1.44	0.65
6:J:222:HIS:HE1	5:K:33:PHE:HA	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:646:LEU:HB3	8:Y:341:ARG:HD2	1.79	0.65
6:J:898:HIS:NE2	8:X:249:MET:SD	2.69	0.64
8:S:217:ARG:HE	8:S:277:THR:HA	1.63	0.64
8:Q:217:ARG:HE	8:Q:277:THR:HA	1.63	0.63
8:V:217:ARG:HE	8:V:277:THR:HA	1.63	0.63
8:Z:217:ARG:HE	8:Z:277:THR:HA	1.63	0.63
8:U:217:ARG:HE	8:U:277:THR:HA	1.63	0.63
8:W:217:ARG:HE	8:W:277:THR:HA	1.63	0.63
4:G:863:GLY:HA2	8:U:353:PRO:HB3	1.79	0.63
8:V:24:GLN:HE21	8:V:24:GLN:HA	1.64	0.62
4:C:696:TYR:O	4:C:700:GLU:HB2	1.99	0.62
8:T:217:ARG:HE	8:T:277:THR:HA	1.63	0.62
8:Z:24:GLN:HE21	8:Z:24:GLN:HA	1.64	0.62
8:U:24:GLN:HE21	8:U:24:GLN:HA	1.65	0.62
8:Y:217:ARG:HE	8:Y:277:THR:HA	1.63	0.62
4:C:534:LEU:HD13	4:C:557:LEU:HG	1.81	0.62
8:R:24:GLN:HE21	8:R:24:GLN:HA	1.64	0.62
8:X:217:ARG:HE	8:X:277:THR:HA	1.63	0.62
8:Y:24:GLN:HE21	8:Y:24:GLN:HA	1.64	0.62
8:Q:24:GLN:HA	8:Q:24:GLN:HE21	1.64	0.62
8:V:193:LYS:HB2	8:V:424:SER:HB2	1.82	0.62
8:T:193:LYS:HB2	8:T:424:SER:HB2	1.82	0.62
8:T:24:GLN:HE21	8:T:24:GLN:HA	1.64	0.61
8:X:193:LYS:HB2	8:X:424:SER:HB2	1.82	0.61
8:R:193:LYS:HB2	8:R:424:SER:HB2	1.82	0.61
8:R:217:ARG:HE	8:R:277:THR:HA	1.63	0.61
8:Y:193:LYS:HB2	8:Y:424:SER:HB2	1.82	0.61
4:E:688:ASN:HD21	8:S:357:GLN:NE2	1.98	0.61
8:W:193:LYS:HB2	8:W:424:SER:HB2	1.82	0.61
8:Q:193:LYS:HB2	8:Q:424:SER:HB2	1.82	0.61
8:Z:193:LYS:HB2	8:Z:424:SER:HB2	1.82	0.61
8:S:24:GLN:HE21	8:S:24:GLN:HA	1.64	0.61
8:U:193:LYS:HB2	8:U:424:SER:HB2	1.82	0.61
8:X:24:GLN:HA	8:X:24:GLN:HE21	1.65	0.61
3:F:553:TYR:HB3	3:F:648:ILE:HD11	1.82	0.60
8:S:193:LYS:HB2	8:S:424:SER:HB2	1.82	0.60
4:G:578:MET:H	4:G:615:ALA:HB1	1.66	0.60
8:W:24:GLN:HE21	8:W:24:GLN:HA	1.64	0.60
5:I:363:LEU:HD13	5:I:486:ARG:HH21	1.66	0.60
5:I:131:LEU:HB3	5:I:165:LEU:HD21	1.84	0.60
6:J:900:TYR:O	6:J:904:ARG:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:589:ALA:HA	3:F:592:LEU:HD13	1.82	0.59
4:E:862:ASN:ND2	8:S:346:ALA:O	2.34	0.59
3:H:720:TYR:HE2	8:V:357:GLN:HB3	1.67	0.59
4:G:511:ALA:HA	4:G:514:ARG:HE	1.68	0.59
5:I:154:LEU:O	5:I:158:TYR:HB2	2.03	0.59
7:L:1607:VAL:HG12	7:L:1702:GLN:HG2	1.83	0.59
3:H:431:TYR:HA	3:H:434:ILE:HG22	1.84	0.58
5:I:486:ARG:HH22	8:W:248:TYR:HE1	1.48	0.58
4:G:563:THR:HG21	8:U:47:ARG:HB2	1.85	0.58
5:K:582:CYS:HB2	5:K:626:LEU:HD13	1.86	0.58
6:J:266:THR:OG1	6:J:267:GLU:N	2.36	0.58
8:V:183:VAL:HG13	8:V:187:ASN:HD21	1.69	0.58
8:Y:64:ALA:O	8:Y:90:ASN:ND2	2.37	0.58
8:X:64:ALA:O	8:X:90:ASN:ND2	2.37	0.58
4:G:242:GLN:HE21	4:G:343:THR:HG23	1.68	0.58
5:K:62:TYR:HB3	5:K:86:LEU:HD21	1.86	0.58
8:R:183:VAL:HG13	8:R:187:ASN:HD21	1.69	0.58
8:S:183:VAL:HG13	8:S:187:ASN:HD21	1.69	0.58
8:X:183:VAL:HG13	8:X:187:ASN:HD21	1.69	0.58
6:J:438:ASN:ND2	6:J:548:MET:O	2.37	0.58
5:K:7:LEU:HD23	7:L:392:SER:HB3	1.84	0.58
8:T:183:VAL:HG13	8:T:187:ASN:HD21	1.69	0.58
8:Z:64:ALA:O	8:Z:90:ASN:ND2	2.37	0.58
5:K:653:LYS:HG2	8:Y:353:PRO:HB3	1.85	0.58
4:G:356:LEU:HG	4:G:440:PRO:HB3	1.87	0.57
8:R:64:ALA:O	8:R:90:ASN:ND2	2.37	0.57
8:Z:183:VAL:HG13	8:Z:187:ASN:HD21	1.69	0.57
8:S:64:ALA:O	8:S:90:ASN:ND2	2.37	0.57
8:T:217:ARG:HH21	8:T:278:THR:H	1.53	0.57
8:U:64:ALA:O	8:U:90:ASN:ND2	2.37	0.57
8:U:217:ARG:HH21	8:U:278:THR:H	1.53	0.57
4:E:356:LEU:HD23	4:E:359:LEU:HD21	1.85	0.57
8:Q:64:ALA:O	8:Q:90:ASN:ND2	2.37	0.57
8:V:64:ALA:O	8:V:90:ASN:ND2	2.37	0.57
7:L:294:ARG:HH11	7:L:305:GLY:HA2	1.67	0.57
8:Q:217:ARG:HH21	8:Q:278:THR:H	1.52	0.57
8:Y:217:ARG:HH21	8:Y:278:THR:H	1.53	0.57
8:U:183:VAL:HG13	8:U:187:ASN:HD21	1.69	0.57
8:W:217:ARG:HH21	8:W:278:THR:H	1.53	0.57
4:E:559:LEU:HD21	4:E:570:LYS:HG3	1.86	0.57
5:K:17:PHE:HE1	5:K:42:LEU:HD21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:709:LEU:HD13	4:G:729:PHE:HB2	1.87	0.57
8:T:64:ALA:O	8:T:90:ASN:ND2	2.37	0.57
8:V:217:ARG:HH21	8:V:278:THR:H	1.53	0.57
8:W:183:VAL:HG13	8:W:187:ASN:HD21	1.69	0.57
3:F:266:ILE:HD11	3:F:275:TYR:HB3	1.87	0.57
8:Y:183:VAL:HG13	8:Y:187:ASN:HD21	1.69	0.57
8:Y:318:ILE:HB	8:Y:380:ASN:HB3	1.87	0.57
3:F:797:LEU:HA	3:F:800:LEU:HD12	1.85	0.57
8:Q:183:VAL:HG13	8:Q:187:ASN:HD21	1.69	0.57
8:S:318:ILE:HB	8:S:380:ASN:HB3	1.87	0.57
8:T:318:ILE:HB	8:T:380:ASN:HB3	1.87	0.57
8:W:64:ALA:O	8:W:90:ASN:ND2	2.37	0.57
8:Z:318:ILE:HB	8:Z:380:ASN:HB3	1.87	0.57
3:D:710:GLU:OE1	3:D:855:GLN:NE2	2.38	0.56
8:X:13:CYS:HA	8:X:16:GLN:HE21	1.71	0.56
4:E:359:LEU:HD13	4:E:380:THR:HG22	1.88	0.56
5:K:519:ASN:HD22	5:K:593:PHE:HE2	1.52	0.56
8:Q:13:CYS:HA	8:Q:16:GLN:HE21	1.71	0.56
8:R:318:ILE:HB	8:R:380:ASN:HB3	1.87	0.56
8:W:13:CYS:HA	8:W:16:GLN:HE21	1.71	0.56
8:X:217:ARG:HH21	8:X:278:THR:H	1.53	0.56
8:X:318:ILE:HB	8:X:380:ASN:HB3	1.87	0.56
3:D:320:VAL:HG21	3:D:393:GLY:H	1.70	0.56
8:Q:318:ILE:HB	8:Q:380:ASN:HB3	1.87	0.56
8:S:13:CYS:HA	8:S:16:GLN:HE21	1.71	0.56
3:F:879:ARG:NH1	8:T:355:SER:OG	2.39	0.56
5:K:523:PHE:O	5:K:527:ASN:ND2	2.38	0.56
8:R:13:CYS:HA	8:R:16:GLN:HE21	1.71	0.56
8:Z:217:ARG:HH21	8:Z:278:THR:H	1.52	0.56
4:C:335:MET:HG3	4:C:338:LEU:HD12	1.87	0.56
8:V:13:CYS:HA	8:V:16:GLN:HE21	1.71	0.56
3:F:798:GLU:HA	3:F:801:GLN:HE21	1.70	0.55
8:V:318:ILE:HB	8:V:380:ASN:HB3	1.87	0.55
3:D:566:LEU:HD21	3:D:660:TYR:HB3	1.88	0.55
6:J:288:GLN:HE21	6:J:297:ARG:HG3	1.71	0.55
8:W:182:VAL:HB	8:W:404:PHE:HB3	1.89	0.55
3:H:655:GLU:O	3:H:658:SER:OG	2.23	0.55
6:J:879:GLN:HG2	6:J:880:ILE:HG13	1.87	0.55
5:K:34:LEU:HD12	5:K:38:GLU:HG3	1.88	0.55
8:R:217:ARG:HH21	8:R:278:THR:H	1.53	0.55
8:U:13:CYS:HA	8:U:16:GLN:HE21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:13:CYS:HA	8:Z:16:GLN:HE21	1.71	0.55
4:C:821:THR:HA	4:C:824:LYS:HG2	1.88	0.55
5:K:651:TYR:CE2	8:Y:349:ILE:HG22	2.41	0.55
8:X:182:VAL:HB	8:X:404:PHE:HB3	1.89	0.55
4:C:413:GLU:OE1	4:C:431:ARG:NH2	2.35	0.55
8:T:13:CYS:HA	8:T:16:GLN:HE21	1.71	0.55
8:W:318:ILE:HB	8:W:380:ASN:HB3	1.87	0.55
8:Y:13:CYS:HA	8:Y:16:GLN:HE21	1.71	0.55
3:D:323:SER:HB3	3:D:421:LEU:HG	1.87	0.55
8:V:182:VAL:HB	8:V:404:PHE:HB3	1.89	0.55
8:U:318:ILE:HB	8:U:380:ASN:HB3	1.87	0.55
4:E:353:GLY:HA2	4:E:356:LEU:HD12	1.87	0.55
4:E:555:LEU:HD13	4:E:575:ILE:HD11	1.87	0.55
3:F:654:ARG:HH22	3:F:658:SER:HB3	1.70	0.55
3:H:455:LYS:HB3	3:H:459:LEU:HG	1.88	0.55
7:L:1801:ARG:HH11	8:Z:337:LEU:HD21	1.72	0.55
8:S:217:ARG:HH21	8:S:278:THR:H	1.52	0.55
8:T:182:VAL:HB	8:T:404:PHE:HB3	1.89	0.55
8:S:182:VAL:HB	8:S:404:PHE:HB3	1.89	0.55
8:Y:182:VAL:HB	8:Y:404:PHE:HB3	1.89	0.55
4:C:560:ARG:NH1	8:R:289:THR:OG1	2.40	0.54
8:U:182:VAL:HB	8:U:404:PHE:HB3	1.89	0.54
8:W:341:ARG:NH1	8:W:342:GLU:OE1	2.40	0.54
7:L:461:PHE:HA	7:L:464:LYS:HD2	1.88	0.54
7:L:1485:ALA:HA	7:L:1488:ILE:HD12	1.89	0.54
8:X:184:GLN:O	8:X:188:SER:OG	2.25	0.54
8:X:341:ARG:NH1	8:X:342:GLU:OE1	2.41	0.54
8:Y:341:ARG:NH1	8:Y:342:GLU:OE1	2.40	0.54
4:C:556:GLU:HB3	8:R:339:ARG:HH11	1.73	0.54
4:G:320:SER:HG	4:G:323:LYS:HZ3	1.51	0.54
8:T:45:THR:OG1	8:T:46:ASP:N	2.41	0.54
8:W:56:ASP:HB3	8:X:299:GLN:OE1	2.06	0.54
8:Y:184:GLN:O	8:Y:188:SER:OG	2.25	0.54
8:S:71:PRO:O	8:S:75:HIS:NE2	2.41	0.54
8:V:71:PRO:O	8:V:75:HIS:NE2	2.41	0.54
6:J:901:ILE:HA	6:J:905:ILE:HD12	1.88	0.54
8:Q:71:PRO:O	8:Q:75:HIS:NE2	2.41	0.54
8:R:182:VAL:HB	8:R:404:PHE:HB3	1.89	0.54
8:R:341:ARG:NH1	8:R:342:GLU:OE1	2.40	0.54
8:X:71:PRO:O	8:X:75:HIS:NE2	2.41	0.54
8:Z:45:THR:OG1	8:Z:46:ASP:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:359:LEU:HD21	4:C:379:LEU:HB3	1.88	0.54
3:F:594:GLN:NE2	3:F:623:VAL:O	2.36	0.54
8:R:229:ASN:O	8:R:233:SER:OG	2.25	0.54
5:K:27:VAL:HG13	5:K:29:GLN:HB3	1.90	0.54
8:Q:182:VAL:HB	8:Q:404:PHE:HB3	1.89	0.54
8:U:437:ALA:HA	8:U:440:ARG:HG2	1.90	0.54
8:X:45:THR:OG1	8:X:46:ASP:N	2.41	0.54
8:Y:437:ALA:HA	8:Y:440:ARG:HG2	1.90	0.54
3:F:337:ARG:O	3:F:340:SER:OG	2.23	0.53
5:I:98:GLN:HA	5:I:101:ARG:HD2	1.90	0.53
8:Q:341:ARG:NH1	8:Q:342:GLU:OE1	2.40	0.53
8:U:45:THR:OG1	8:U:46:ASP:N	2.41	0.53
8:V:341:ARG:NH1	8:V:342:GLU:OE1	2.40	0.53
8:Z:182:VAL:HB	8:Z:404:PHE:HB3	1.89	0.53
3:D:548:VAL:HG22	3:D:552:LYS:HE2	1.90	0.53
3:D:586:VAL:HG12	3:D:635:TRP:HE1	1.72	0.53
5:K:515:TRP:O	5:K:519:ASN:HB2	2.08	0.53
8:T:341:ARG:NH1	8:T:342:GLU:OE1	2.40	0.53
8:T:437:ALA:HA	8:T:440:ARG:HG2	1.90	0.53
8:U:341:ARG:NH1	8:U:342:GLU:OE1	2.40	0.53
8:W:437:ALA:HA	8:W:440:ARG:HG2	1.90	0.53
7:L:1676:ILE:HG23	7:L:1680:ILE:HD12	1.89	0.53
8:Z:184:GLN:O	8:Z:188:SER:OG	2.25	0.53
8:Q:45:THR:OG1	8:Q:46:ASP:N	2.41	0.53
8:Y:71:PRO:O	8:Y:75:HIS:NE2	2.41	0.53
8:Z:71:PRO:O	8:Z:75:HIS:NE2	2.41	0.53
8:Z:341:ARG:NH1	8:Z:342:GLU:OE1	2.40	0.53
4:G:158:ARG:HA	4:G:161:LEU:HD12	1.90	0.53
6:J:881:HIS:ND1	8:X:446:TRP:HB3	2.24	0.53
8:Q:229:ASN:O	8:Q:233:SER:OG	2.25	0.53
8:W:71:PRO:O	8:W:75:HIS:NE2	2.41	0.53
4:C:473:LYS:HE2	4:C:474:GLU:HG3	1.91	0.53
8:S:341:ARG:NH1	8:S:342:GLU:OE1	2.40	0.53
8:T:71:PRO:O	8:T:75:HIS:NE2	2.41	0.53
8:R:71:PRO:O	8:R:75:HIS:NE2	2.41	0.53
8:U:71:PRO:O	8:U:75:HIS:NE2	2.41	0.53
4:E:297:ARG:NH1	3:F:408:ASP:OD2	2.39	0.53
8:S:437:ALA:HA	8:S:440:ARG:HG2	1.90	0.53
8:W:45:THR:OG1	8:W:46:ASP:N	2.41	0.53
4:C:835:ASP:OD1	4:C:871:ARG:NH2	2.42	0.53
4:E:454:GLY:HA2	4:E:457:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:736:ASN:HA	3:F:739:GLN:HE21	1.73	0.53
6:J:887:ARG:NH1	8:X:258:ALA:O	2.42	0.53
8:Q:184:GLN:O	8:Q:188:SER:OG	2.25	0.53
8:Q:437:ALA:HA	8:Q:440:ARG:HG2	1.90	0.53
8:R:45:THR:OG1	8:R:46:ASP:N	2.41	0.53
8:S:45:THR:OG1	8:S:46:ASP:N	2.41	0.53
8:V:437:ALA:HA	8:V:440:ARG:HG2	1.90	0.53
8:X:437:ALA:HA	8:X:440:ARG:HG2	1.90	0.53
3:H:712:VAL:O	3:H:716:HIS:ND1	2.33	0.53
5:I:305:ASP:N	5:I:305:ASP:OD1	2.41	0.53
7:L:1720:GLU:HG3	7:L:1721:LYS:HD2	1.89	0.53
8:Q:337:LEU:HD11	8:Q:358:VAL:HG11	1.92	0.53
4:C:638:TYR:HA	4:C:641:LEU:HD12	1.92	0.52
8:T:337:LEU:HD11	8:T:358:VAL:HG11	1.91	0.52
8:U:337:LEU:HD11	8:U:358:VAL:HG11	1.92	0.52
8:V:184:GLN:O	8:V:188:SER:OG	2.25	0.52
8:Y:77:ILE:O	8:Y:80:SER:OG	2.27	0.52
3:H:589:ALA:HB2	3:H:634:GLY:HA2	1.91	0.52
8:T:184:GLN:O	8:T:188:SER:OG	2.25	0.52
8:V:77:ILE:O	8:V:80:SER:OG	2.28	0.52
7:L:1688:PHE:HB2	7:L:1691:ARG:HH21	1.75	0.52
8:U:229:ASN:O	8:U:233:SER:OG	2.25	0.52
8:V:337:LEU:HD11	8:V:358:VAL:HG11	1.92	0.52
8:Q:77:ILE:O	8:Q:80:SER:OG	2.27	0.52
8:V:45:THR:OG1	8:V:46:ASP:N	2.41	0.52
8:Y:45:THR:OG1	8:Y:46:ASP:N	2.41	0.52
8:Z:437:ALA:HA	8:Z:440:ARG:HG2	1.90	0.52
4:E:417:GLU:HG2	4:E:418:ARG:HG3	1.92	0.52
4:C:557:LEU:HA	8:R:339:ARG:HD3	1.92	0.52
4:C:694:GLN:HB3	8:Q:248:TYR:CE2	2.44	0.52
4:E:427:TYR:HE2	4:E:455:LYS:HG3	1.75	0.52
8:X:77:ILE:O	8:X:80:SER:OG	2.27	0.52
5:I:526:ASP:O	5:I:530:TYR:HB2	2.10	0.52
3:H:677:LEU:HB2	3:H:782:ILE:HD11	1.92	0.52
8:R:337:LEU:HD11	8:R:358:VAL:HG11	1.92	0.52
8:S:337:LEU:HD11	8:S:358:VAL:HG11	1.91	0.52
6:J:828:LEU:O	6:J:832:LYS:NZ	2.28	0.52
8:S:184:GLN:O	8:S:188:SER:OG	2.25	0.52
8:Z:77:ILE:O	8:Z:80:SER:OG	2.27	0.52
3:D:783:ILE:HD12	3:D:786:GLN:HG3	1.91	0.52
4:E:518:ARG:HG3	4:E:524:GLN:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:34:LEU:HD21	7:L:312:LEU:HD22	1.92	0.52
8:X:337:LEU:HD11	8:X:358:VAL:HG11	1.92	0.52
3:H:608:THR:HG23	3:H:610:ALA:H	1.75	0.51
8:R:184:GLN:O	8:R:188:SER:OG	2.25	0.51
8:V:343:ARG:O	8:V:343:ARG:NH2	2.42	0.51
3:H:590:THR:OG1	3:H:632:ASP:OD1	2.23	0.51
8:U:77:ILE:O	8:U:80:SER:OG	2.27	0.51
8:V:28:GLU:HA	8:V:367:LEU:HD13	1.93	0.51
8:V:229:ASN:O	8:V:233:SER:OG	2.25	0.51
8:W:184:GLN:O	8:W:188:SER:OG	2.25	0.51
4:C:203:LEU:HD11	4:C:231:ARG:HD2	1.92	0.51
5:K:344:MET:O	5:K:348:SER:OG	2.27	0.51
8:S:343:ARG:O	8:S:343:ARG:NH2	2.42	0.51
4:G:478:THR:HG21	4:G:483:ALA:H	1.75	0.51
8:Q:28:GLU:HA	8:Q:367:LEU:HD13	1.93	0.51
8:R:437:ALA:HA	8:R:440:ARG:HG2	1.90	0.51
4:G:415:ARG:NH2	4:G:427:TYR:OH	2.36	0.51
8:T:28:GLU:HA	8:T:367:LEU:HD13	1.93	0.51
8:T:77:ILE:O	8:T:80:SER:OG	2.27	0.51
8:W:337:LEU:HD11	8:W:358:VAL:HG11	1.91	0.51
4:C:177:PHE:HE2	4:C:282:SER:HA	1.76	0.51
8:W:77:ILE:O	8:W:80:SER:OG	2.27	0.51
8:Z:337:LEU:HD11	8:Z:358:VAL:HG11	1.92	0.51
5:K:89:PHE:HE1	5:K:157:VAL:HG11	1.75	0.51
8:S:77:ILE:O	8:S:80:SER:OG	2.28	0.51
8:R:77:ILE:O	8:R:80:SER:OG	2.27	0.51
8:S:28:GLU:HA	8:S:367:LEU:HD13	1.93	0.51
8:W:28:GLU:HA	8:W:367:LEU:HD13	1.93	0.51
8:Y:337:LEU:HD11	8:Y:358:VAL:HG11	1.92	0.51
5:K:45:LEU:HD22	5:K:126:LEU:HD12	1.93	0.51
5:I:128:GLN:HA	5:I:131:LEU:HD12	1.91	0.50
6:J:221:VAL:HG12	6:J:223:GLN:HG2	1.94	0.50
8:T:162:PRO:HG2	8:T:163:LYS:HZ2	1.76	0.50
8:X:28:GLU:HA	8:X:367:LEU:HD13	1.93	0.50
7:L:1678:ASN:OD1	7:L:1801:ARG:NH1	2.45	0.50
4:E:517:LYS:HG3	4:E:521:LEU:HD12	1.93	0.50
4:G:408:MET:HG3	4:G:409:VAL:HG23	1.93	0.50
6:J:899:ASN:O	6:J:903:THR:OG1	2.23	0.50
8:U:28:GLU:HA	8:U:367:LEU:HD13	1.93	0.50
8:X:229:ASN:O	8:X:233:SER:OG	2.25	0.50
8:Z:28:GLU:HA	8:Z:367:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:738:MET:HG3	4:E:745:LEU:HD12	1.93	0.50
8:Q:119:PHE:HA	8:Q:122:ILE:HD12	1.94	0.50
5:I:499:GLN:HE22	8:W:265:ARG:HH12	1.59	0.50
8:R:119:PHE:HA	8:R:122:ILE:HD12	1.94	0.50
8:V:119:PHE:HA	8:V:122:ILE:HD12	1.94	0.50
8:U:119:PHE:HA	8:U:122:ILE:HD12	1.94	0.50
3:F:419:LEU:HA	3:F:422:VAL:HG22	1.93	0.50
4:G:241:ARG:HG3	4:G:243:SER:H	1.76	0.50
3:H:304:ILE:HG22	3:H:328:LEU:HD21	1.93	0.50
3:H:327:ALA:HB1	3:H:418:ILE:HD12	1.94	0.50
5:I:586:ILE:HD13	5:I:622:GLN:HE21	1.77	0.50
8:R:28:GLU:HA	8:R:367:LEU:HD13	1.93	0.50
8:S:191:THR:O	8:S:195:LEU:HB2	2.12	0.50
8:V:393:ARG:HH12	8:V:394:GLN:HE21	1.60	0.50
4:C:655:LEU:HD11	4:C:687:LEU:HD13	1.94	0.50
7:L:1545:LEU:HD11	7:L:1580:PRO:HD2	1.94	0.50
8:S:119:PHE:HA	8:S:122:ILE:HD12	1.94	0.50
8:T:191:THR:O	8:T:195:LEU:HB2	2.12	0.50
8:U:387:LEU:HD13	8:U:390:ARG:HD3	1.94	0.50
8:U:393:ARG:HH12	8:U:394:GLN:HE21	1.60	0.50
8:W:387:LEU:HD13	8:W:390:ARG:HD3	1.94	0.50
8:X:119:PHE:HA	8:X:122:ILE:HD12	1.94	0.50
8:Y:387:LEU:HD13	8:Y:390:ARG:HD3	1.94	0.50
6:J:213:ARG:HA	6:J:216:LEU:HD12	1.93	0.50
8:Q:191:THR:O	8:Q:195:LEU:HB2	2.12	0.50
8:R:191:THR:O	8:R:195:LEU:HB2	2.12	0.50
8:R:387:LEU:HD13	8:R:390:ARG:HD3	1.94	0.50
8:U:191:THR:O	8:U:195:LEU:HB2	2.12	0.50
8:Y:28:GLU:HA	8:Y:367:LEU:HD13	1.93	0.50
8:Z:119:PHE:HA	8:Z:122:ILE:HD12	1.94	0.50
4:G:277:ILE:HD11	4:G:296:MET:HB2	1.94	0.49
6:J:938:HIS:CE1	6:J:943:LEU:HB2	2.47	0.49
5:K:389:GLU:HB2	5:K:418:ILE:HG22	1.94	0.49
8:Q:113:LYS:HG3	8:Q:114:ILE:HG23	1.94	0.49
8:Q:290:VAL:HG11	8:Q:333:VAL:HG12	1.94	0.49
8:Y:113:LYS:HG3	8:Y:114:ILE:HG23	1.94	0.49
5:K:1:MET:HA	5:K:5:LEU:HD23	1.93	0.49
8:Z:290:VAL:HG11	8:Z:333:VAL:HG12	1.95	0.49
8:Z:387:LEU:HD13	8:Z:390:ARG:HD3	1.94	0.49
4:C:484:TYR:C	4:C:486:GLU:H	2.15	0.49
3:F:448:VAL:HG22	3:F:484:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:387:LEU:HD13	8:Q:390:ARG:HD3	1.94	0.49
8:R:347:ASN:OD1	8:R:347:ASN:N	2.45	0.49
8:T:387:LEU:HD13	8:T:390:ARG:HD3	1.94	0.49
8:W:191:THR:O	8:W:195:LEU:HB2	2.12	0.49
4:E:422:ASP:OD2	4:E:422:ASP:N	2.42	0.49
4:G:201:THR:OG1	4:G:202:ALA:N	2.39	0.49
8:Q:393:ARG:HH12	8:Q:394:GLN:HE21	1.60	0.49
8:T:290:VAL:HG11	8:T:333:VAL:HG12	1.95	0.49
8:U:343:ARG:O	8:U:343:ARG:NH2	2.42	0.49
8:Z:191:THR:O	8:Z:195:LEU:HB2	2.12	0.49
8:X:191:THR:O	8:X:195:LEU:HB2	2.12	0.49
8:Y:290:VAL:HG11	8:Y:333:VAL:HG12	1.95	0.49
3:F:848:ARG:HH21	3:F:852:HIS:HE1	1.59	0.49
4:G:452:SER:HA	4:G:455:LYS:HE2	1.95	0.49
8:Q:55:ALA:HB3	8:Q:59:HIS:HB2	1.95	0.49
8:R:113:LYS:HG3	8:R:114:ILE:HG23	1.95	0.49
8:S:290:VAL:HG11	8:S:333:VAL:HG12	1.95	0.49
8:S:387:LEU:HD13	8:S:390:ARG:HD3	1.94	0.49
8:X:55:ALA:HB3	8:X:59:HIS:HB2	1.95	0.49
8:R:290:VAL:HG11	8:R:333:VAL:HG12	1.95	0.49
8:U:113:LYS:HG3	8:U:114:ILE:HG23	1.95	0.49
3:D:275:TYR:HB2	3:D:295:SER:HB2	1.95	0.49
8:V:55:ALA:HB3	8:V:59:HIS:HB2	1.95	0.49
8:Y:191:THR:O	8:Y:195:LEU:HB2	2.12	0.49
3:D:676:ILE:HD12	3:D:786:GLN:HE21	1.78	0.49
3:F:554:SER:O	3:F:554:SER:OG	2.31	0.49
6:J:289:LEU:HD23	6:J:292:GLY:HA2	1.95	0.49
8:T:119:PHE:HA	8:T:122:ILE:HD12	1.94	0.49
8:U:34:GLU:HG3	8:U:84:LYS:HE3	1.95	0.49
8:U:290:VAL:HG11	8:U:333:VAL:HG12	1.95	0.49
8:W:343:ARG:O	8:W:343:ARG:NH2	2.42	0.49
4:C:687:LEU:O	4:C:691:GLN:HB2	2.13	0.49
8:Q:34:GLU:HG3	8:Q:84:LYS:HE3	1.95	0.49
8:Q:343:ARG:O	8:Q:343:ARG:NH2	2.42	0.49
8:S:162:PRO:HG2	8:S:163:LYS:HZ2	1.78	0.49
8:S:393:ARG:HH12	8:S:394:GLN:HE21	1.60	0.49
8:V:113:LYS:HG3	8:V:114:ILE:HG23	1.94	0.49
3:H:568:LEU:HD11	3:H:664:PHE:HA	1.95	0.48
8:S:34:GLU:HG3	8:S:84:LYS:HE3	1.95	0.48
8:W:290:VAL:HG11	8:W:333:VAL:HG12	1.95	0.48
8:Y:229:ASN:O	8:Y:233:SER:OG	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:113:LYS:HG3	8:Z:114:ILE:HG23	1.94	0.48
5:K:59:ILE:HD11	5:K:93:LEU:HD22	1.95	0.48
8:S:113:LYS:HG3	8:S:114:ILE:HG23	1.94	0.48
8:U:347:ASN:OD1	8:U:347:ASN:N	2.45	0.48
8:V:387:LEU:HD13	8:V:390:ARG:HD3	1.94	0.48
8:X:343:ARG:O	8:X:343:ARG:NH2	2.42	0.48
3:H:419:LEU:HA	3:H:422:VAL:HG22	1.94	0.48
8:T:55:ALA:HB3	8:T:59:HIS:HB2	1.95	0.48
8:T:393:ARG:HH12	8:T:394:GLN:HE21	1.60	0.48
8:U:55:ALA:HB3	8:U:59:HIS:HB2	1.95	0.48
8:V:34:GLU:HG3	8:V:84:LYS:HE3	1.95	0.48
8:V:191:THR:O	8:V:195:LEU:HB2	2.12	0.48
8:Y:55:ALA:HB3	8:Y:59:HIS:HB2	1.95	0.48
8:Y:119:PHE:HA	8:Y:122:ILE:HD12	1.94	0.48
8:T:34:GLU:HG3	8:T:84:LYS:HE3	1.95	0.48
8:X:34:GLU:HG3	8:X:84:LYS:HE3	1.95	0.48
8:X:393:ARG:HH12	8:X:394:GLN:HE21	1.60	0.48
8:Z:55:ALA:HB3	8:Z:59:HIS:HB2	1.95	0.48
3:F:281:ALA:HB3	3:F:287:LEU:HD11	1.95	0.48
8:S:55:ALA:HB3	8:S:59:HIS:HB2	1.95	0.48
8:U:184:GLN:O	8:U:188:SER:OG	2.25	0.48
8:W:113:LYS:HG3	8:W:114:ILE:HG23	1.95	0.48
8:Z:393:ARG:HH12	8:Z:394:GLN:HE21	1.60	0.48
8:T:343:ARG:O	8:T:343:ARG:NH2	2.42	0.48
8:W:119:PHE:HA	8:W:122:ILE:HD12	1.94	0.48
8:W:229:ASN:O	8:W:233:SER:OG	2.25	0.48
8:Y:34:GLU:HG3	8:Y:84:LYS:HE3	1.95	0.48
8:Y:393:ARG:HH12	8:Y:394:GLN:HE21	1.60	0.48
3:F:626:LEU:HB2	3:F:637:VAL:HG13	1.95	0.48
5:K:478:VAL:HG21	5:K:568:LEU:HD21	1.95	0.48
8:T:113:LYS:HG3	8:T:114:ILE:HG23	1.94	0.48
8:W:34:GLU:HG3	8:W:84:LYS:HE3	1.95	0.48
8:W:55:ALA:HB3	8:W:59:HIS:HB2	1.95	0.48
8:Z:34:GLU:HG3	8:Z:84:LYS:HE3	1.95	0.48
8:X:113:LYS:HG3	8:X:114:ILE:HG23	1.94	0.48
6:J:275:LEU:HB3	6:J:379:LEU:HD21	1.96	0.48
8:X:387:LEU:HD13	8:X:390:ARG:HD3	1.94	0.48
4:G:460:VAL:HB	4:G:499:LEU:HD13	1.96	0.48
7:L:1493:LYS:HD2	7:L:1493:LYS:HA	1.66	0.48
8:V:290:VAL:HG11	8:V:333:VAL:HG12	1.94	0.48
8:X:290:VAL:HG11	8:X:333:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:609:ASN:HB2	8:R:47:ARG:HA	1.96	0.47
3:F:683:GLY:O	3:F:687:ASN:HB2	2.13	0.47
5:I:621:ARG:O	5:I:624:SER:OG	2.32	0.47
8:Q:195:LEU:HD21	8:Q:202:VAL:HG11	1.97	0.47
8:Y:343:ARG:O	8:Y:343:ARG:NH2	2.42	0.47
8:Y:347:ASN:OD1	8:Y:347:ASN:N	2.45	0.47
4:G:418:ARG:HE	4:G:424:ASN:HB2	1.78	0.47
8:W:393:ARG:HH12	8:W:394:GLN:HE21	1.60	0.47
4:E:864:PHE:CZ	8:S:348:PHE:HB2	2.49	0.47
3:F:799:GLU:HG2	3:F:832:ARG:HE	1.78	0.47
5:I:102:GLN:HE22	5:I:105:LEU:HD23	1.78	0.47
8:R:55:ALA:HB3	8:R:59:HIS:HB2	1.95	0.47
8:R:393:ARG:HH12	8:R:394:GLN:HE21	1.60	0.47
8:V:350:PRO:HB2	8:V:351:TRP:H	1.49	0.47
3:D:738:VAL:HG23	3:D:747:ILE:HG12	1.95	0.47
6:J:221:VAL:O	6:J:228:ARG:NH2	2.47	0.47
7:L:1663:HIS:CG	8:Z:262:PRO:HA	2.49	0.47
8:R:237:SER:O	8:R:244:ARG:NH2	2.41	0.47
8:Z:195:LEU:HD21	8:Z:202:VAL:HG11	1.97	0.47
4:G:709:LEU:HD12	4:G:709:LEU:HA	1.79	0.47
8:W:195:LEU:HD21	8:W:202:VAL:HG11	1.96	0.47
8:Z:343:ARG:O	8:Z:343:ARG:NH2	2.42	0.47
4:E:650:HIS:HA	4:E:653:ARG:HE	1.79	0.47
5:K:370:GLN:HG3	5:K:486:ARG:HH21	1.79	0.47
7:L:433:THR:HA	7:L:436:LEU:HD12	1.96	0.47
4:C:641:LEU:HG	4:C:734:LEU:HD13	1.96	0.47
3:D:799:GLU:OE1	3:D:803:ARG:NH1	2.48	0.47
4:G:624:TRP:O	4:G:627:SER:OG	2.32	0.47
7:L:1691:ARG:HG2	7:L:1704:ALA:HB1	1.97	0.47
8:T:195:LEU:HD21	8:T:202:VAL:HG11	1.96	0.47
8:U:162:PRO:HG2	8:U:163:LYS:HZ2	1.79	0.47
8:V:195:LEU:HD21	8:V:202:VAL:HG11	1.96	0.47
8:W:347:ASN:OD1	8:W:347:ASN:N	2.45	0.47
8:X:347:ASN:OD1	8:X:347:ASN:N	2.45	0.47
8:Y:237:SER:O	8:Y:244:ARG:NH2	2.41	0.47
4:E:447:ALA:HA	4:E:450:ILE:HD12	1.96	0.47
4:G:221:LEU:HA	4:G:224:VAL:HG22	1.95	0.47
4:G:737:CYS:SG	4:G:738:MET:N	2.88	0.47
8:R:34:GLU:HG3	8:R:84:LYS:HE3	1.95	0.47
8:R:195:LEU:HD21	8:R:202:VAL:HG11	1.96	0.47
8:Z:347:ASN:OD1	8:Z:347:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:560:ARG:HH22	8:R:332:GLN:HB3	1.78	0.47
3:D:394:GLY:H	3:D:470:MET:HA	1.80	0.47
4:E:738:MET:SD	4:E:738:MET:N	2.87	0.47
3:F:713:HIS:O	3:F:717:GLN:HG2	2.15	0.47
8:U:195:LEU:HD21	8:U:202:VAL:HG11	1.96	0.47
4:C:560:ARG:NE	8:R:339:ARG:HH22	2.13	0.47
3:H:588:PRO:HB3	3:H:632:ASP:HB3	1.97	0.47
6:J:923:LEU:HA	6:J:926:LEU:HD12	1.96	0.47
6:J:998:LEU:HD23	6:J:1014:ALA:HB2	1.97	0.47
8:V:263:THR:HB	8:V:266:LEU:HD12	1.97	0.47
4:C:289:ASN:HA	4:C:292:LEU:HD12	1.96	0.46
4:G:562:SER:OG	4:G:563:THR:N	2.48	0.46
4:G:655:LEU:HD22	4:G:687:LEU:HD13	1.97	0.46
8:Q:263:THR:HB	8:Q:266:LEU:HD12	1.98	0.46
8:S:53:TYR:N	8:S:61:ILE:O	2.44	0.46
8:X:195:LEU:HD21	8:X:202:VAL:HG11	1.97	0.46
3:H:572:ASP:OD1	8:V:251:ASN:ND2	2.42	0.46
8:S:263:THR:HB	8:S:266:LEU:HD12	1.98	0.46
8:Q:162:PRO:HG2	8:Q:163:LYS:HZ2	1.81	0.46
8:V:90:ASN:OD1	8:V:90:ASN:N	2.49	0.46
8:W:263:THR:HB	8:W:266:LEU:HD12	1.98	0.46
8:X:53:TYR:N	8:X:61:ILE:O	2.44	0.46
4:C:517:LYS:HA	4:C:521:LEU:HD13	1.98	0.46
4:C:713:LEU:HG	4:C:722:VAL:HG13	1.96	0.46
5:K:107:LEU:HD11	5:K:126:LEU:HD21	1.98	0.46
3:D:464:TYR:OH	3:D:491:ASN:ND2	2.48	0.46
3:D:746:HIS:HA	3:D:749:ALA:HB3	1.96	0.46
5:I:34:LEU:HD22	5:I:38:GLU:HG2	1.97	0.46
8:R:90:ASN:OD1	8:R:90:ASN:N	2.49	0.46
8:R:343:ARG:O	8:R:343:ARG:NH2	2.42	0.46
8:W:294:MET:HE2	8:W:340:ILE:HG13	1.98	0.46
7:L:295:ARG:HD3	7:L:303:PRO:HD2	1.96	0.46
8:R:162:PRO:HG2	8:R:163:LYS:HZ2	1.81	0.46
8:S:154:LEU:HD23	8:S:194:ARG:HB3	1.98	0.46
8:T:154:LEU:HD23	8:T:194:ARG:HB3	1.98	0.46
8:Z:53:TYR:N	8:Z:61:ILE:O	2.44	0.46
3:H:710:GLU:HG2	8:V:353:PRO:HD2	1.98	0.46
3:H:827:GLU:OE2	3:H:831:LYS:NZ	2.44	0.46
8:S:195:LEU:HD21	8:S:202:VAL:HG11	1.97	0.46
8:Z:154:LEU:HD23	8:Z:194:ARG:HB3	1.98	0.46
4:C:737:CYS:HB2	4:C:739:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:439:ILE:HG22	4:G:441:SER:H	1.81	0.46
3:H:451:ASP:HB3	3:H:455:LYS:HZ1	1.81	0.46
5:K:63:THR:HG23	5:K:87:ARG:HG3	1.98	0.46
8:S:229:ASN:O	8:S:233:SER:OG	2.25	0.46
8:S:383:SER:O	8:S:386:SER:OG	2.30	0.46
8:X:263:THR:HB	8:X:266:LEU:HD12	1.98	0.46
8:X:294:MET:HE2	8:X:340:ILE:HG13	1.98	0.46
6:J:378:GLU:HG2	6:J:405:ARG:HH11	1.81	0.45
5:K:651:TYR:CD2	8:Y:349:ILE:HG22	2.51	0.45
8:X:154:LEU:HD23	8:X:194:ARG:HB3	1.98	0.45
8:Y:263:THR:HB	8:Y:266:LEU:HD12	1.98	0.45
8:Q:323:ILE:HD11	8:Q:361:SER:HB3	1.98	0.45
8:R:154:LEU:HD23	8:R:194:ARG:HB3	1.98	0.45
8:R:263:THR:HB	8:R:266:LEU:HD12	1.98	0.45
8:R:294:MET:HE2	8:R:340:ILE:HG13	1.98	0.45
8:V:162:PRO:HG2	8:V:163:LYS:HZ2	1.81	0.45
8:W:323:ILE:HD11	8:W:361:SER:HB3	1.98	0.45
8:Y:195:LEU:HD21	8:Y:202:VAL:HG11	1.97	0.45
8:Z:229:ASN:O	8:Z:233:SER:OG	2.25	0.45
4:G:864:PHE:CG	8:U:351:TRP:HA	2.51	0.45
8:T:263:THR:HB	8:T:266:LEU:HD12	1.98	0.45
4:E:580:HIS:O	4:E:584:THR:OG1	2.21	0.45
3:H:364:LEU:H	3:H:367:LEU:H	1.65	0.45
6:J:310:LEU:HG	6:J:314:LEU:HD13	1.97	0.45
8:S:90:ASN:OD1	8:S:90:ASN:N	2.49	0.45
4:E:188:ILE:HG12	4:E:278:GLU:HG3	1.98	0.45
4:G:305:ILE:O	4:G:308:SER:OG	2.34	0.45
5:K:419:GLU:HG2	5:K:452:ALA:HB1	1.98	0.45
8:R:323:ILE:HD11	8:R:361:SER:HB3	1.98	0.45
8:T:294:MET:HE2	8:T:340:ILE:HG13	1.99	0.45
8:T:323:ILE:HD11	8:T:361:SER:HB3	1.98	0.45
8:U:3:ARG:NH1	8:U:132:LEU:O	2.35	0.45
3:H:361:SER:OG	3:H:362:LEU:N	2.47	0.45
7:L:307:ARG:HD2	7:L:307:ARG:HA	1.64	0.45
8:U:294:MET:HE2	8:U:340:ILE:HG13	1.98	0.45
8:V:154:LEU:HD23	8:V:194:ARG:HB3	1.98	0.45
8:X:162:PRO:HG2	8:X:163:LYS:HZ2	1.82	0.45
4:G:186:ALA:HB1	3:H:293:ARG:HG2	1.99	0.45
8:U:263:THR:HB	8:U:266:LEU:HD12	1.98	0.45
8:Z:263:THR:HB	8:Z:266:LEU:HD12	1.98	0.45
3:D:803:ARG:HH11	3:D:829:GLU:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:550:ARG:HE	4:E:554:LEU:HD11	1.82	0.45
4:E:699:PHE:CZ	8:S:360:LEU:HB3	2.52	0.45
6:J:444:ILE:HG13	6:J:445:LEU:HG	1.99	0.45
6:J:552:LEU:HG	6:J:556:LEU:HG	1.99	0.45
8:T:350:PRO:HB2	8:T:351:TRP:H	1.49	0.45
4:G:499:LEU:HD23	4:G:719:ILE:HD13	1.99	0.45
4:G:633:LYS:O	4:G:637:ARG:HG2	2.16	0.45
4:G:719:ILE:HA	4:G:722:VAL:HG22	1.97	0.45
6:J:286:ILE:HD12	6:J:297:ARG:HD2	1.99	0.45
4:C:461:ARG:HD3	4:C:467:VAL:HG21	2.00	0.45
4:C:550:ARG:O	4:C:553:ALA:HB3	2.17	0.45
3:D:647:PRO:HG2	3:D:648:ILE:HD12	1.99	0.45
8:U:323:ILE:HD11	8:U:361:SER:HB3	1.98	0.45
8:X:237:SER:O	8:X:244:ARG:NH2	2.41	0.45
4:C:555:LEU:HD21	4:C:573:LEU:HD22	1.99	0.44
8:T:5:ILE:HG12	8:T:133:GLU:HB3	1.99	0.44
8:T:229:ASN:O	8:T:233:SER:OG	2.25	0.44
3:F:480:SER:HA	3:F:483:VAL:HG12	1.99	0.44
4:G:542:PRO:HA	4:G:610:LEU:HG	1.99	0.44
4:G:556:GLU:HB3	8:V:339:ARG:HE	1.82	0.44
5:I:59:ILE:HD11	5:I:93:LEU:HD22	1.99	0.44
5:K:573:PHE:HD1	5:K:576:LEU:HD13	1.82	0.44
7:L:1688:PHE:HD1	7:L:1691:ARG:HE	1.66	0.44
7:L:1728:VAL:HB	7:L:1779:LEU:HD12	1.98	0.44
8:Q:5:ILE:HG12	8:Q:133:GLU:HB3	1.99	0.44
8:T:347:ASN:OD1	8:T:347:ASN:N	2.45	0.44
8:V:3:ARG:NH1	8:V:132:LEU:O	2.35	0.44
8:X:323:ILE:HD11	8:X:361:SER:HB3	1.98	0.44
8:Z:5:ILE:HG12	8:Z:133:GLU:HB3	1.99	0.44
8:Z:294:MET:HE2	8:Z:340:ILE:HG13	1.99	0.44
3:F:546:LEU:HD23	3:F:546:LEU:HA	1.83	0.44
8:R:5:ILE:HG12	8:R:133:GLU:HB3	1.99	0.44
8:X:5:ILE:HG12	8:X:133:GLU:HB3	1.99	0.44
4:C:429:ASP:OD1	4:C:429:ASP:N	2.50	0.44
7:L:1691:ARG:HH12	7:L:1711:LYS:HD2	1.82	0.44
8:Q:237:SER:O	8:Q:244:ARG:NH2	2.41	0.44
8:S:323:ILE:HD11	8:S:361:SER:HB3	1.98	0.44
8:W:154:LEU:HD23	8:W:194:ARG:HB3	1.98	0.44
8:X:132:LEU:HD23	8:X:164:LYS:HE3	2.00	0.44
8:X:189:LEU:HD12	8:X:190:LEU:HG	2.00	0.44
8:Y:132:LEU:HD23	8:Y:164:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:445:LEU:HA	6:J:448:ASP:HB2	2.00	0.44
5:K:636:HIS:HB2	5:K:637:GLN:H	1.60	0.44
7:L:1656:ARG:H	7:L:1656:ARG:HG2	1.65	0.44
8:Q:154:LEU:HD23	8:Q:194:ARG:HB3	1.98	0.44
8:Q:189:LEU:HD12	8:Q:190:LEU:HG	2.00	0.44
8:U:196:THR:O	8:U:265:ARG:NH1	2.51	0.44
8:V:189:LEU:HD12	8:V:190:LEU:HG	2.00	0.44
8:V:323:ILE:HD11	8:V:361:SER:HB3	1.98	0.44
8:Z:196:THR:O	8:Z:265:ARG:NH1	2.51	0.44
3:D:837:LYS:HA	3:D:837:LYS:HD3	1.91	0.44
4:G:503:LEU:HD11	4:G:625:PRO:HB2	1.98	0.44
6:J:323:VAL:HG13	6:J:326:ARG:HH22	1.82	0.44
5:K:515:TRP:HE1	5:K:604:LEU:HD11	1.82	0.44
8:R:196:THR:O	8:R:265:ARG:NH1	2.51	0.44
8:S:5:ILE:HG12	8:S:133:GLU:HB3	1.99	0.44
8:T:132:LEU:HD23	8:T:164:LYS:HE3	2.00	0.44
8:V:196:THR:O	8:V:265:ARG:NH1	2.51	0.44
8:V:237:SER:O	8:V:244:ARG:NH2	2.41	0.44
8:X:90:ASN:OD1	8:X:90:ASN:N	2.49	0.44
8:Y:5:ILE:HG12	8:Y:133:GLU:HB3	1.99	0.44
7:L:1773:LYS:HA	7:L:1773:LYS:HD2	1.85	0.44
8:R:3:ARG:NH1	8:R:132:LEU:O	2.35	0.44
8:V:294:MET:HE2	8:V:340:ILE:HG13	2.00	0.44
8:Y:154:LEU:HD23	8:Y:194:ARG:HB3	1.98	0.44
8:Y:323:ILE:HD11	8:Y:361:SER:HB3	1.98	0.44
8:Z:237:SER:O	8:Z:244:ARG:NH2	2.41	0.44
4:C:522:MET:HG2	4:C:528:PHE:CZ	2.52	0.44
3:D:383:ALA:O	3:D:387:HIS:ND1	2.46	0.44
8:Q:132:LEU:HD23	8:Q:164:LYS:HE3	2.00	0.44
8:S:196:THR:O	8:S:265:ARG:NH1	2.51	0.44
8:S:294:MET:HE2	8:S:340:ILE:HG13	1.99	0.44
8:U:154:LEU:HD23	8:U:194:ARG:HB3	1.98	0.44
8:V:132:LEU:HD23	8:V:164:LYS:HE3	2.00	0.44
8:W:196:THR:O	8:W:265:ARG:NH1	2.51	0.44
4:C:482:ARG:HA	4:C:485:VAL:HG23	2.00	0.44
4:C:691:GLN:HG2	4:C:695:TYR:CZ	2.53	0.44
4:E:187:LEU:HD23	3:F:375:LYS:HE2	2.00	0.44
6:J:556:LEU:HD23	6:J:559:ILE:HD12	2.00	0.44
8:S:3:ARG:NH1	8:S:132:LEU:O	2.35	0.44
8:U:431:LEU:HD13	8:U:431:LEU:HA	1.87	0.44
8:X:196:THR:O	8:X:265:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:323:ILE:HD11	8:Z:361:SER:HB3	1.98	0.44
5:I:165:LEU:HD12	5:I:166:PRO:HD2	1.99	0.43
8:R:132:LEU:HD23	8:R:164:LYS:HE3	2.00	0.43
8:R:189:LEU:HD12	8:R:190:LEU:HG	2.00	0.43
8:T:189:LEU:HD12	8:T:190:LEU:HG	2.00	0.43
8:V:5:ILE:HG12	8:V:133:GLU:HB3	1.99	0.43
8:W:132:LEU:HD23	8:W:164:LYS:HE3	2.00	0.43
3:F:620:ARG:HH11	3:F:644:VAL:HA	1.83	0.43
3:F:744:LEU:HA	3:F:747:ILE:HD12	2.00	0.43
3:H:562:MET:HG2	3:H:566:LEU:HD12	2.00	0.43
8:T:202:VAL:HG12	8:T:204:VAL:HG22	2.00	0.43
8:U:28:GLU:HG2	8:U:367:LEU:HD22	2.01	0.43
8:U:132:LEU:HD23	8:U:164:LYS:HE3	2.00	0.43
8:W:5:ILE:HG12	8:W:133:GLU:HB3	1.99	0.43
8:X:153:LEU:HD13	8:X:153:LEU:HA	1.92	0.43
8:Y:28:GLU:HG2	8:Y:367:LEU:HD22	2.01	0.43
3:D:615:PRO:O	3:D:619:ARG:HB2	2.18	0.43
8:Q:196:THR:O	8:Q:265:ARG:NH1	2.51	0.43
8:Y:162:PRO:HG2	8:Y:163:LYS:HZ2	1.84	0.43
4:C:298:THR:HA	4:C:301:LYS:HD2	2.00	0.43
4:G:530:HIS:CE1	8:U:47:ARG:HH12	2.36	0.43
3:H:486:ILE:HD11	3:H:538:TYR:HB2	1.99	0.43
7:L:531:PRO:HA	7:L:534:ARG:HE	1.83	0.43
8:Q:187:ASN:O	8:Q:191:THR:OG1	2.34	0.43
8:Q:294:MET:HE2	8:Q:340:ILE:HG13	2.00	0.43
8:Q:369:SER:O	8:Q:372:ARG:NE	2.49	0.43
8:T:196:THR:O	8:T:265:ARG:NH1	2.51	0.43
8:U:20:GLU:O	8:U:24:GLN:HB2	2.19	0.43
8:U:189:LEU:HD12	8:U:190:LEU:HG	2.00	0.43
8:X:202:VAL:HG12	8:X:204:VAL:HG22	2.00	0.43
8:Y:196:THR:O	8:Y:265:ARG:NH1	2.51	0.43
8:Y:202:VAL:HG12	8:Y:204:VAL:HG22	2.00	0.43
4:E:439:ILE:HG22	4:E:441:SER:H	1.83	0.43
3:F:336:TYR:HA	3:F:339:LEU:HD12	2.00	0.43
8:U:5:ILE:HG12	8:U:133:GLU:HB3	1.99	0.43
3:D:848:ARG:HD2	3:D:848:ARG:HA	1.82	0.43
4:G:823:ASN:HD21	4:G:827:LYS:HE3	1.84	0.43
3:H:546:LEU:O	3:H:550:ASN:ND2	2.52	0.43
5:I:345:VAL:HG22	5:I:350:LEU:HD12	2.00	0.43
5:I:408:ASP:HB2	5:I:409:ASN:H	1.62	0.43
8:S:132:LEU:HD23	8:S:164:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:237:SER:O	8:S:244:ARG:NH2	2.41	0.43
8:W:53:TYR:N	8:W:61:ILE:O	2.44	0.43
8:W:56:ASP:HA	8:X:296:ARG:NH1	2.34	0.43
8:Z:3:ARG:NH1	8:Z:132:LEU:O	2.35	0.43
4:G:427:TYR:HD1	4:G:431:ARG:HD3	1.83	0.43
3:H:878:PHE:HB2	3:H:879:ARG:NH2	2.34	0.43
6:J:221:VAL:HG22	7:L:309:GLU:HB3	2.00	0.43
6:J:728:LEU:HA	8:X:248:TYR:CZ	2.54	0.43
8:R:20:GLU:O	8:R:24:GLN:HB2	2.19	0.43
8:S:20:GLU:O	8:S:24:GLN:HB2	2.19	0.43
8:S:369:SER:O	8:S:372:ARG:NE	2.49	0.43
8:Z:28:GLU:HG2	8:Z:367:LEU:HD22	2.00	0.43
4:C:862:ASN:HB3	8:Q:341:ARG:HG3	2.00	0.43
3:F:364:LEU:HD13	3:F:370:TRP:HE1	1.84	0.43
8:W:189:LEU:HD12	8:W:190:LEU:HG	2.00	0.43
8:X:28:GLU:HG2	8:X:367:LEU:HD22	2.00	0.43
8:Z:202:VAL:HG12	8:Z:204:VAL:HG22	2.00	0.43
8:Z:431:LEU:HD13	8:Z:431:LEU:HA	1.87	0.43
4:C:346:ASP:OD2	4:C:347:LYS:N	2.52	0.43
4:G:613:LEU:HA	4:G:613:LEU:HD23	1.70	0.43
5:I:351:LEU:HA	5:I:354:LEU:HD12	1.99	0.43
5:K:492:LEU:HD22	5:K:523:PHE:HB2	2.00	0.43
8:Q:28:GLU:HG2	8:Q:367:LEU:HD22	2.01	0.43
8:Q:57:ASP:HB3	8:Q:59:HIS:CD2	2.54	0.43
8:S:28:GLU:HG2	8:S:367:LEU:HD22	2.01	0.43
8:T:90:ASN:OD1	8:T:90:ASN:N	2.49	0.43
8:V:28:GLU:HG2	8:V:367:LEU:HD22	2.01	0.43
8:W:28:GLU:HG2	8:W:367:LEU:HD22	2.00	0.43
8:Y:20:GLU:O	8:Y:24:GLN:HB2	2.19	0.43
8:Y:90:ASN:OD1	8:Y:90:ASN:N	2.49	0.43
8:Z:132:LEU:HD23	8:Z:164:LYS:HE3	2.00	0.43
4:G:610:LEU:HD23	4:G:613:LEU:HD12	2.00	0.43
5:I:564:PHE:O	5:I:568:LEU:HG	2.19	0.43
5:I:578:PRO:HA	5:I:581:HIS:CD2	2.54	0.43
6:J:736:TYR:OH	8:X:252:ASP:OD2	2.20	0.43
8:R:28:GLU:HG2	8:R:367:LEU:HD22	2.01	0.43
8:S:57:ASP:HB3	8:S:59:HIS:CD2	2.54	0.43
8:T:20:GLU:O	8:T:24:GLN:HB2	2.19	0.43
8:T:28:GLU:HG2	8:T:367:LEU:HD22	2.01	0.43
8:T:57:ASP:HB3	8:T:59:HIS:CD2	2.54	0.43
8:T:369:SER:O	8:T:372:ARG:NE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:20:GLU:O	8:X:24:GLN:HB2	2.19	0.43
4:C:635:LEU:HA	4:C:638:TYR:HD2	1.84	0.42
4:C:814:LEU:HB3	4:C:815:VAL:H	1.63	0.42
3:F:754:PHE:O	3:F:758:ILE:HG12	2.19	0.42
4:G:556:GLU:HB3	8:V:339:ARG:NE	2.34	0.42
4:G:694:GLN:O	4:G:698:MET:HG2	2.19	0.42
5:I:511:ASP:HA	5:I:514:LYS:HD3	2.01	0.42
7:L:1575:ALA:HB3	7:L:1595:GLU:HB2	2.00	0.42
8:Q:20:GLU:O	8:Q:24:GLN:HB2	2.19	0.42
8:R:202:VAL:HG12	8:R:204:VAL:HG22	2.00	0.42
8:S:189:LEU:HD12	8:S:190:LEU:HG	2.00	0.42
8:X:57:ASP:HB3	8:X:59:HIS:CD2	2.54	0.42
8:Y:57:ASP:HB3	8:Y:59:HIS:CD2	2.54	0.42
8:Y:294:MET:HE2	8:Y:340:ILE:HG13	2.01	0.42
8:Z:57:ASP:HB3	8:Z:59:HIS:CD2	2.54	0.42
3:D:707:LEU:HD13	3:D:851:THR:HG22	2.00	0.42
4:G:518:ARG:HA	4:G:523:ASP:HB3	2.00	0.42
8:V:369:SER:O	8:V:372:ARG:NE	2.49	0.42
8:W:237:SER:O	8:W:244:ARG:NH2	2.41	0.42
4:C:556:GLU:HB3	8:R:339:ARG:HE	1.83	0.42
3:D:692:ARG:NH1	8:R:265:ARG:HG2	2.35	0.42
4:E:533:ASP:N	4:E:533:ASP:OD1	2.50	0.42
3:H:253:ASP:HB3	3:H:263:GLY:HA3	2.00	0.42
8:W:20:GLU:O	8:W:24:GLN:HB2	2.19	0.42
4:C:326:PHE:O	4:C:329:GLN:HG2	2.20	0.42
4:E:174:LEU:HD21	4:E:283:PHE:HB3	2.02	0.42
5:I:190:TRP:CE2	5:I:280:GLY:HA3	2.55	0.42
5:K:143:ILE:HA	5:K:148:ILE:HD12	2.01	0.42
8:R:57:ASP:HB3	8:R:59:HIS:CD2	2.54	0.42
8:S:202:VAL:HG12	8:S:204:VAL:HG22	2.00	0.42
8:V:20:GLU:O	8:V:24:GLN:HB2	2.19	0.42
8:W:202:VAL:HG12	8:W:204:VAL:HG22	2.00	0.42
6:J:828:LEU:HD13	6:J:832:LYS:HE2	2.01	0.42
8:T:153:LEU:HD13	8:T:153:LEU:HA	1.92	0.42
8:T:237:SER:O	8:T:244:ARG:NH2	2.41	0.42
8:V:202:VAL:HG12	8:V:204:VAL:HG22	2.00	0.42
8:Z:189:LEU:HD12	8:Z:190:LEU:HG	2.00	0.42
3:D:394:GLY:O	3:D:398:SER:OG	2.30	0.42
4:G:497:LYS:HD3	4:G:497:LYS:HA	1.86	0.42
6:J:954:ILE:O	6:J:958:LEU:HG	2.18	0.42
8:S:260:LEU:HD21	8:S:321:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:104:TRP:O	8:T:108:PHE:HB2	2.20	0.42
8:U:202:VAL:HG12	8:U:204:VAL:HG22	2.00	0.42
8:Y:189:LEU:HD12	8:Y:190:LEU:HG	2.00	0.42
3:F:543:LYS:HA	3:F:543:LYS:HD2	1.79	0.42
4:G:521:LEU:HD21	4:G:702:MET:HB3	2.01	0.42
3:H:685:MET:SD	8:V:165:LEU:HD21	2.59	0.42
8:Q:260:LEU:HD21	8:Q:321:LEU:HB2	2.02	0.42
8:V:421:MET:O	8:V:425:ARG:HB2	2.20	0.42
8:W:421:MET:O	8:W:425:ARG:HB2	2.20	0.42
8:Y:104:TRP:O	8:Y:108:PHE:HB2	2.20	0.42
4:E:389:GLU:OE2	3:F:412:ARG:NH1	2.51	0.42
3:F:255:LEU:HD21	3:F:343:HIS:HB2	2.02	0.42
3:F:874:ARG:HG2	3:F:878:PHE:CE2	2.55	0.42
3:H:447:PHE:HA	3:H:467:ARG:HB3	2.01	0.42
8:S:421:MET:O	8:S:425:ARG:HB2	2.20	0.42
8:T:331:THR:O	8:T:334:HIS:NE2	2.53	0.42
8:U:104:TRP:O	8:U:108:PHE:HB2	2.20	0.42
8:V:260:LEU:HD21	8:V:321:LEU:HB2	2.02	0.42
8:Z:20:GLU:O	8:Z:24:GLN:HB2	2.19	0.42
3:D:677:LEU:HB2	3:D:782:ILE:HD11	2.01	0.42
3:F:397:ALA:O	3:F:473:SER:OG	2.37	0.42
6:J:283:LYS:HD2	6:J:283:LYS:HA	1.70	0.42
8:Q:347:ASN:OD1	8:Q:347:ASN:N	2.45	0.42
8:Q:431:LEU:HD13	8:Q:431:LEU:HA	1.87	0.42
8:R:369:SER:O	8:R:372:ARG:NE	2.49	0.42
8:S:331:THR:O	8:S:334:HIS:NE2	2.53	0.42
8:V:104:TRP:O	8:V:108:PHE:HB2	2.20	0.42
8:X:421:MET:O	8:X:425:ARG:HB2	2.20	0.42
3:F:338:LEU:O	3:F:342:LEU:HG	2.20	0.42
5:I:37:SER:O	5:I:40:SER:OG	2.38	0.42
8:R:331:THR:O	8:R:334:HIS:NE2	2.53	0.42
8:V:57:ASP:HB3	8:V:59:HIS:CD2	2.54	0.42
4:C:718:ASN:OD1	4:C:719:ILE:N	2.48	0.41
3:F:613:ASP:HB3	3:F:617:ILE:HD11	2.02	0.41
3:H:333:ARG:HH11	5:I:127:ASP:HB3	1.85	0.41
7:L:448:LEU:HD23	7:L:448:LEU:HA	1.87	0.41
7:L:1691:ARG:HH11	7:L:1707:GLU:HG3	1.85	0.41
8:R:421:MET:O	8:R:425:ARG:HB2	2.20	0.41
8:S:350:PRO:HB2	8:S:351:TRP:H	1.49	0.41
8:T:53:TYR:N	8:T:61:ILE:O	2.44	0.41
8:U:421:MET:O	8:U:425:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:3:ARG:NH1	8:W:132:LEU:O	2.35	0.41
8:Z:104:TRP:O	8:Z:108:PHE:HB2	2.20	0.41
3:F:308:THR:O	3:F:312:SER:OG	2.30	0.41
8:Q:202:VAL:HG12	8:Q:204:VAL:HG22	2.00	0.41
8:V:53:TYR:N	8:V:61:ILE:O	2.44	0.41
8:W:331:THR:O	8:W:334:HIS:NE2	2.53	0.41
8:X:349:ILE:HA	8:X:350:PRO:HD2	1.93	0.41
4:C:236:GLN:HG3	4:C:245:THR:HG23	2.01	0.41
8:Q:104:TRP:O	8:Q:108:PHE:HB2	2.20	0.41
8:R:350:PRO:HB2	8:R:351:TRP:H	1.49	0.41
8:U:57:ASP:HB3	8:U:59:HIS:CD2	2.54	0.41
8:V:331:THR:O	8:V:334:HIS:NE2	2.53	0.41
8:Y:260:LEU:HD21	8:Y:321:LEU:HB2	2.02	0.41
3:D:688:ALA:HB3	3:D:689:LYS:HZ2	1.85	0.41
5:I:184:TYR:O	5:I:188:SER:OG	2.24	0.41
8:U:331:THR:O	8:U:334:HIS:NE2	2.53	0.41
8:U:369:SER:O	8:U:372:ARG:NE	2.49	0.41
8:W:57:ASP:HB3	8:W:59:HIS:CD2	2.54	0.41
8:X:260:LEU:HD21	8:X:321:LEU:HB2	2.02	0.41
8:Y:331:THR:O	8:Y:334:HIS:NE2	2.53	0.41
4:C:522:MET:HB2	4:C:645:MET:HE1	2.03	0.41
6:J:325:PHE:O	6:J:328:GLN:HG2	2.20	0.41
6:J:884:PHE:O	6:J:888:VAL:HG23	2.21	0.41
6:J:927:ILE:HA	6:J:930:HIS:CE1	2.56	0.41
6:J:932:ARG:HH21	6:J:936:THR:HB	1.85	0.41
8:R:53:TYR:N	8:R:61:ILE:O	2.44	0.41
8:U:90:ASN:OD1	8:U:90:ASN:N	2.49	0.41
8:X:331:THR:O	8:X:334:HIS:NE2	2.53	0.41
8:X:369:SER:O	8:X:372:ARG:NE	2.49	0.41
8:Y:349:ILE:HA	8:Y:350:PRO:HD2	1.93	0.41
4:C:682:LEU:O	4:C:686:MET:HG2	2.21	0.41
3:D:416:GLN:HA	3:D:419:LEU:HG	2.02	0.41
3:F:876:LEU:HG	3:F:880:LEU:HD11	2.03	0.41
5:I:339:HIS:HA	5:I:342:LYS:HE2	2.01	0.41
8:Q:421:MET:O	8:Q:425:ARG:HB2	2.20	0.41
8:S:104:TRP:O	8:S:108:PHE:HB2	2.20	0.41
8:W:162:PRO:HG2	8:W:163:LYS:HZ2	1.85	0.41
8:Y:50:VAL:HG21	8:Y:244:ARG:HG2	2.03	0.41
8:Z:421:MET:O	8:Z:425:ARG:HB2	2.20	0.41
4:C:219:GLU:OE2	4:C:314:HIS:ND1	2.53	0.41
3:D:703:GLN:HA	3:D:706:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:876:LEU:HD12	3:D:876:LEU:HA	1.89	0.41
7:L:459:ILE:HG13	7:L:460:GLY:N	2.36	0.41
8:Q:337:LEU:HD12	8:Q:337:LEU:HA	1.92	0.41
8:R:337:LEU:HD12	8:R:337:LEU:HA	1.92	0.41
8:Z:162:PRO:HG2	8:Z:163:LYS:HZ2	1.84	0.41
4:E:607:GLU:HG3	4:E:608:LEU:HD23	2.02	0.41
3:H:274:CYS:SG	3:H:275:TYR:N	2.91	0.41
8:Q:50:VAL:HG21	8:Q:244:ARG:HG2	2.03	0.41
8:Q:415:LYS:HD2	8:Q:415:LYS:HA	1.92	0.41
8:R:425:ARG:HA	8:R:425:ARG:HD2	1.91	0.41
8:T:260:LEU:HD21	8:T:321:LEU:HB2	2.02	0.41
8:W:104:TRP:O	8:W:108:PHE:HB2	2.20	0.41
8:Z:260:LEU:HD21	8:Z:321:LEU:HB2	2.02	0.41
3:D:548:VAL:O	3:D:552:LYS:HG2	2.21	0.41
3:F:466:LEU:HD11	3:F:471:ILE:HD11	2.03	0.41
3:F:546:LEU:O	3:F:550:ASN:HB2	2.20	0.41
4:G:427:TYR:CD1	4:G:431:ARG:HD3	2.55	0.41
4:G:444:GLN:H	4:G:444:GLN:HG3	1.70	0.41
6:J:906:LEU:HD22	6:J:937:ILE:HD11	2.03	0.41
5:K:645:LEU:HB2	5:K:646:LEU:HD22	2.02	0.41
8:Q:331:THR:O	8:Q:334:HIS:NE2	2.53	0.41
8:R:260:LEU:HD21	8:R:321:LEU:HB2	2.02	0.41
8:T:50:VAL:HG21	8:T:244:ARG:HG2	2.03	0.41
8:T:421:MET:O	8:T:425:ARG:HB2	2.20	0.41
8:U:50:VAL:HG21	8:U:244:ARG:HG2	2.03	0.41
8:U:349:ILE:HA	8:U:350:PRO:HD2	1.93	0.41
8:W:260:LEU:HD21	8:W:321:LEU:HB2	2.02	0.41
8:W:350:PRO:HB2	8:W:351:TRP:H	1.49	0.41
8:Z:331:THR:O	8:Z:334:HIS:NE2	2.53	0.41
3:D:577:LEU:O	3:D:581:LEU:HB3	2.21	0.41
4:E:338:LEU:HD21	4:E:375:LEU:HD11	2.03	0.41
3:H:677:LEU:HD11	3:H:712:VAL:HA	2.03	0.41
5:K:600:ASN:HD22	5:K:604:LEU:HD23	1.85	0.41
7:L:1546:ASN:OD1	7:L:1546:ASN:N	2.54	0.41
7:L:1670:LYS:HA	7:L:1670:LYS:HD2	1.89	0.41
8:R:50:VAL:HG21	8:R:244:ARG:HG2	2.03	0.41
8:R:104:TRP:O	8:R:108:PHE:HB2	2.20	0.41
8:V:153:LEU:HD13	8:V:153:LEU:HA	1.92	0.41
8:X:189:LEU:HD13	8:X:424:SER:OG	2.21	0.41
8:Y:3:ARG:NH1	8:Y:132:LEU:O	2.35	0.41
4:E:425:ASP:HB2	4:E:631:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:627:GLU:HG3	3:F:627:GLU:H	1.71	0.40
3:F:879:ARG:HH21	3:F:879:ARG:HD2	1.76	0.40
8:U:189:LEU:HD13	8:U:424:SER:OG	2.22	0.40
8:U:419:ASP:O	8:U:423:THR:OG1	2.39	0.40
8:X:104:TRP:O	8:X:108:PHE:HB2	2.20	0.40
8:X:431:LEU:HD13	8:X:431:LEU:HA	1.87	0.40
8:Y:421:MET:O	8:Y:425:ARG:HB2	2.20	0.40
4:G:306:LEU:O	4:G:310:LEU:HG	2.21	0.40
5:I:165:LEU:HG	5:I:167:PRO:HD2	2.03	0.40
5:I:594:CYS:SG	5:I:595:SER:N	2.94	0.40
8:S:153:LEU:HD13	8:S:153:LEU:HA	1.92	0.40
8:V:84:LYS:HE3	8:V:84:LYS:HB2	1.94	0.40
8:V:189:LEU:HD13	8:V:424:SER:OG	2.22	0.40
8:V:343:ARG:HA	8:V:343:ARG:HD2	1.90	0.40
8:X:419:ASP:O	8:X:423:THR:OG1	2.39	0.40
8:Z:90:ASN:OD1	8:Z:90:ASN:N	2.49	0.40
4:C:252:LEU:HD22	4:C:257:ARG:HG3	2.04	0.40
3:D:688:ALA:HB3	3:D:689:LYS:NZ	2.35	0.40
3:F:526:LEU:HB3	3:F:529:ALA:HB3	2.03	0.40
4:G:164:LYS:HD2	4:G:404:TYR:HB3	2.02	0.40
5:I:346:GLU:OE2	5:I:346:GLU:N	2.53	0.40
5:I:478:VAL:O	5:I:482:LEU:HG	2.21	0.40
6:J:369:TYR:OH	5:K:127:ASP:O	2.38	0.40
8:R:189:LEU:HD13	8:R:424:SER:OG	2.21	0.40
8:S:189:LEU:HD13	8:S:424:SER:OG	2.22	0.40
8:T:435:TYR:O	8:T:439:THR:OG1	2.40	0.40
8:X:335:LYS:H	8:X:335:LYS:HG2	1.73	0.40
8:Y:53:TYR:N	8:Y:61:ILE:O	2.44	0.40
8:Y:189:LEU:HD13	8:Y:424:SER:OG	2.22	0.40
3:D:552:LYS:HG3	3:D:553:TYR:CD1	2.56	0.40
3:F:729:CYS:SG	3:F:730:SER:N	2.95	0.40
5:K:341:TRP:CE2	5:K:552:ARG:HA	2.55	0.40
8:T:220:ILE:H	8:T:220:ILE:HG13	1.77	0.40
8:U:260:LEU:HD21	8:U:321:LEU:HB2	2.02	0.40
8:Z:50:VAL:HG21	8:Z:244:ARG:HG2	2.03	0.40
4:C:839:ARG:HA	4:C:842:ILE:HG12	2.04	0.40
3:D:535:ASP:OD1	3:D:535:ASP:N	2.55	0.40
3:F:887:LYS:HA	3:F:887:LYS:HD2	1.83	0.40
5:I:179:CYS:O	5:I:183:MET:HG2	2.21	0.40
5:I:499:GLN:HB2	8:W:264:PRO:HB3	2.04	0.40
6:J:282:LYS:HE3	6:J:328:GLN:HE21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:384:LYS:HB3	6:J:384:LYS:HE3	1.79	0.40
8:S:50:VAL:HG21	8:S:244:ARG:HG2	2.03	0.40
8:U:427:ILE:HD13	8:U:427:ILE:HA	1.96	0.40
8:V:419:ASP:O	8:V:423:THR:OG1	2.39	0.40
8:W:50:VAL:HG21	8:W:244:ARG:HG2	2.03	0.40
8:W:369:SER:O	8:W:372:ARG:NE	2.49	0.40
8:Y:350:PRO:HB2	8:Y:351:TRP:H	1.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	360/375 (96%)	336 (93%)	23 (6%)	1 (0%)	41	77
2	b	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
2	d	57/82 (70%)	55 (96%)	2 (4%)	0	100	100
2	i	63/82 (77%)	57 (90%)	5 (8%)	1 (2%)	9	44
2	k	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
2	m	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
3	D	571/907 (63%)	552 (97%)	19 (3%)	0	100	100
3	F	591/907 (65%)	563 (95%)	28 (5%)	0	100	100
3	H	584/907 (64%)	565 (97%)	19 (3%)	0	100	100
3	a	112/907 (12%)	104 (93%)	8 (7%)	0	100	100
3	h	105/907 (12%)	94 (90%)	8 (8%)	3 (3%)	4	29
3	j	105/907 (12%)	100 (95%)	4 (4%)	1 (1%)	15	55
4	C	606/902 (67%)	567 (94%)	38 (6%)	1 (0%)	47	81
4	E	626/902 (69%)	587 (94%)	38 (6%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	628/902 (70%)	590 (94%)	34 (5%)	4 (1%)	25	66
5	I	511/667 (77%)	490 (96%)	15 (3%)	6 (1%)	13	50
5	K	548/667 (82%)	533 (97%)	14 (3%)	1 (0%)	47	81
6	J	506/1024 (49%)	466 (92%)	35 (7%)	5 (1%)	15	55
6	l	104/1024 (10%)	96 (92%)	7 (7%)	1 (1%)	15	55
7	L	540/1819 (30%)	498 (92%)	39 (7%)	3 (1%)	25	66
7	c	148/1819 (8%)	142 (96%)	6 (4%)	0	100	100
8	Q	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	22	63
8	R	408/451 (90%)	381 (93%)	24 (6%)	3 (1%)	22	63
8	S	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	22	63
8	T	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	22	63
8	U	408/451 (90%)	382 (94%)	24 (6%)	2 (0%)	29	69
8	V	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	22	63
8	W	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	22	63
8	X	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	22	63
8	Y	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	22	63
8	Z	408/451 (90%)	383 (94%)	24 (6%)	1 (0%)	47	81
All	All	11034/20463 (54%)	10397 (94%)	582 (5%)	55 (0%)	32	69

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	581	ASP
5	I	408	ASP
6	J	238	LEU
5	K	255	LYS
2	i	36	ASN
8	Q	350	PRO
8	Q	351	TRP
8	R	350	PRO
8	R	351	TRP
8	S	350	PRO
8	S	351	TRP
8	T	350	PRO
8	T	351	TRP
8	U	350	PRO

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Mol	Chain	Res	Type
8	V	350	PRO
8	V	351	TRP
8	W	350	PRO
8	W	351	TRP
8	X	350	PRO
8	X	351	TRP
8	Y	350	PRO
8	Y	351	TRP
3	h	107	GLN
3	h	108	PRO
3	j	108	PRO
5	I	508	ASN
7	L	307	ARG
8	Q	352	GLY
8	R	352	GLY
8	S	352	GLY
8	T	352	GLY
8	U	352	GLY
8	V	352	GLY
8	W	352	GLY
8	X	352	GLY
8	Y	352	GLY
5	I	405	LEU
6	J	236	LEU
6	J	237	HIS
6	J	255	PRO
4	G	241	ARG
4	G	370	SER
6	l	121	PRO
1	e	37	ARG
4	G	741	ASN
5	I	404	LEU
5	I	409	ASN
5	I	603	PRO
4	C	466	ASP
8	Z	350	PRO
3	h	104	PRO
4	G	742	PRO
6	J	254	ASP
7	L	452	PRO
7	L	1760	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	310/318 (98%)	305 (98%)	5 (2%)	62	79
2	b	53/62 (86%)	52 (98%)	1 (2%)	57	75
2	d	53/62 (86%)	52 (98%)	1 (2%)	57	75
2	i	53/62 (86%)	53 (100%)	0	100	100
2	k	53/62 (86%)	50 (94%)	3 (6%)	20	45
2	m	53/62 (86%)	53 (100%)	0	100	100
3	D	525/798 (66%)	521 (99%)	4 (1%)	81	89
3	F	542/798 (68%)	538 (99%)	4 (1%)	84	90
3	H	539/798 (68%)	536 (99%)	3 (1%)	86	92
3	a	101/798 (13%)	101 (100%)	0	100	100
3	h	88/798 (11%)	88 (100%)	0	100	100
3	j	88/798 (11%)	88 (100%)	0	100	100
4	C	556/791 (70%)	554 (100%)	2 (0%)	91	94
4	E	574/791 (73%)	570 (99%)	4 (1%)	84	90
4	G	572/791 (72%)	570 (100%)	2 (0%)	92	95
5	I	472/594 (80%)	469 (99%)	3 (1%)	86	92
5	K	509/594 (86%)	506 (99%)	3 (1%)	86	92
6	J	498/933 (53%)	492 (99%)	6 (1%)	71	83
6	l	84/933 (9%)	83 (99%)	1 (1%)	71	83
7	L	501/1546 (32%)	499 (100%)	2 (0%)	91	94
7	c	135/1546 (9%)	135 (100%)	0	100	100
8	Q	376/400 (94%)	334 (89%)	42 (11%)	6	22
8	R	376/400 (94%)	334 (89%)	42 (11%)	6	22
8	S	376/400 (94%)	334 (89%)	42 (11%)	6	22
8	T	376/400 (94%)	334 (89%)	42 (11%)	6	22
8	U	376/400 (94%)	334 (89%)	42 (11%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	376/400 (94%)	334 (89%)	42 (11%)	6	22
8	W	376/400 (94%)	334 (89%)	42 (11%)	6	22
8	X	376/400 (94%)	334 (89%)	42 (11%)	6	22
8	Y	376/400 (94%)	334 (89%)	42 (11%)	6	22
8	Z	376/400 (94%)	333 (89%)	43 (11%)	5	21
All	All	10119/17935 (56%)	9654 (95%)	465 (5%)	31	52

All (465) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	39	ARG
1	e	132	MET
1	e	200	PHE
1	e	247	VAL
1	e	369	ILE
2	b	44	LEU
4	C	485	VAL
4	C	827	LYS
3	D	385	VAL
3	D	575	ARG
3	D	775	LEU
3	D	809	LYS
4	E	424	ASN
4	E	547	THR
4	E	635	LEU
4	E	734	LEU
3	F	252	ARG
3	F	285	ARG
3	F	503	THR
3	F	563	ARG
4	G	478	THR
4	G	551	LEU
3	H	308	THR
3	H	575	ARG
3	H	778	VAL
5	I	18	THR
5	I	530	TYR
5	I	594	CYS
6	J	236	LEU
6	J	256	LEU

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Mol	Chain	Res	Type
6	J	266	THR
6	J	384	LYS
6	J	412	LEU
6	J	682	THR
5	K	86	LEU
5	K	518	ARG
5	K	568	LEU
7	L	570	THR
7	L	1607	VAL
2	k	24	THR
2	k	43	THR
2	k	65	LYS
8	Q	3	ARG
8	Q	7	THR
8	Q	10	LEU
8	Q	20	GLU
8	Q	24	GLN
8	Q	28	GLU
8	Q	58	GLU
8	Q	66	LEU
8	Q	69	LEU
8	Q	78	LEU
8	Q	120	ASP
8	Q	136	VAL
8	Q	149	LEU
8	Q	157	LEU
8	Q	166	VAL
8	Q	188	SER
8	Q	189	LEU
8	Q	192	LEU
8	Q	195	LEU
8	Q	210	LEU
8	Q	233	SER
8	Q	248	TYR
8	Q	254	ILE
8	Q	271	THR
8	Q	274	THR
8	Q	278	THR
8	Q	288	THR
8	Q	291	LEU
8	Q	296	ARG
8	Q	298	LEU

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Mol	Chain	Res	Type
8	Q	328	VAL
8	Q	331	THR
8	Q	337	LEU
8	Q	360	LEU
8	Q	373	VAL
8	Q	374	SER
8	Q	385	SER
8	Q	423	THR
8	Q	424	SER
8	Q	425	ARG
8	Q	439	THR
8	Q	445	SER
8	R	3	ARG
8	R	7	THR
8	R	10	LEU
8	R	20	GLU
8	R	24	GLN
8	R	28	GLU
8	R	58	GLU
8	R	66	LEU
8	R	69	LEU
8	R	78	LEU
8	R	120	ASP
8	R	136	VAL
8	R	149	LEU
8	R	157	LEU
8	R	166	VAL
8	R	188	SER
8	R	189	LEU
8	R	192	LEU
8	R	195	LEU
8	R	210	LEU
8	R	233	SER
8	R	248	TYR
8	R	254	ILE
8	R	271	THR
8	R	274	THR
8	R	278	THR
8	R	288	THR
8	R	291	LEU
8	R	296	ARG
8	R	298	LEU

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Mol	Chain	Res	Type
8	R	328	VAL
8	R	331	THR
8	R	337	LEU
8	R	360	LEU
8	R	373	VAL
8	R	374	SER
8	R	385	SER
8	R	423	THR
8	R	424	SER
8	R	425	ARG
8	R	439	THR
8	R	445	SER
8	S	3	ARG
8	S	7	THR
8	S	10	LEU
8	S	20	GLU
8	S	24	GLN
8	S	28	GLU
8	S	58	GLU
8	S	66	LEU
8	S	69	LEU
8	S	78	LEU
8	S	120	ASP
8	S	136	VAL
8	S	149	LEU
8	S	157	LEU
8	S	166	VAL
8	S	188	SER
8	S	189	LEU
8	S	192	LEU
8	S	195	LEU
8	S	210	LEU
8	S	233	SER
8	S	248	TYR
8	S	254	ILE
8	S	271	THR
8	S	274	THR
8	S	278	THR
8	S	288	THR
8	S	291	LEU
8	S	296	ARG
8	S	298	LEU

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Mol	Chain	Res	Type
8	S	328	VAL
8	S	331	THR
8	S	337	LEU
8	S	360	LEU
8	S	373	VAL
8	S	374	SER
8	S	385	SER
8	S	423	THR
8	S	424	SER
8	S	425	ARG
8	S	439	THR
8	S	445	SER
8	T	3	ARG
8	T	7	THR
8	T	10	LEU
8	T	20	GLU
8	T	24	GLN
8	T	28	GLU
8	T	58	GLU
8	T	66	LEU
8	T	69	LEU
8	T	78	LEU
8	T	120	ASP
8	T	136	VAL
8	T	149	LEU
8	T	157	LEU
8	T	166	VAL
8	T	188	SER
8	T	189	LEU
8	T	192	LEU
8	T	195	LEU
8	T	210	LEU
8	T	233	SER
8	T	248	TYR
8	T	254	ILE
8	T	271	THR
8	T	274	THR
8	T	278	THR
8	T	288	THR
8	T	291	LEU
8	T	296	ARG
8	T	298	LEU

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Mol	Chain	Res	Type
8	T	328	VAL
8	T	331	THR
8	T	337	LEU
8	T	360	LEU
8	T	373	VAL
8	T	374	SER
8	T	385	SER
8	T	423	THR
8	T	424	SER
8	T	425	ARG
8	T	439	THR
8	T	445	SER
8	U	3	ARG
8	U	7	THR
8	U	10	LEU
8	U	20	GLU
8	U	24	GLN
8	U	28	GLU
8	U	58	GLU
8	U	66	LEU
8	U	69	LEU
8	U	78	LEU
8	U	120	ASP
8	U	136	VAL
8	U	149	LEU
8	U	157	LEU
8	U	166	VAL
8	U	188	SER
8	U	189	LEU
8	U	192	LEU
8	U	195	LEU
8	U	210	LEU
8	U	233	SER
8	U	248	TYR
8	U	254	ILE
8	U	271	THR
8	U	274	THR
8	U	278	THR
8	U	288	THR
8	U	291	LEU
8	U	296	ARG
8	U	298	LEU

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Mol	Chain	Res	Type
8	U	328	VAL
8	U	331	THR
8	U	337	LEU
8	U	360	LEU
8	U	373	VAL
8	U	374	SER
8	U	385	SER
8	U	423	THR
8	U	424	SER
8	U	425	ARG
8	U	439	THR
8	U	445	SER
8	V	3	ARG
8	V	7	THR
8	V	10	LEU
8	V	20	GLU
8	V	24	GLN
8	V	28	GLU
8	V	58	GLU
8	V	66	LEU
8	V	69	LEU
8	V	78	LEU
8	V	120	ASP
8	V	136	VAL
8	V	149	LEU
8	V	157	LEU
8	V	166	VAL
8	V	188	SER
8	V	189	LEU
8	V	192	LEU
8	V	195	LEU
8	V	210	LEU
8	V	233	SER
8	V	248	TYR
8	V	254	ILE
8	V	271	THR
8	V	274	THR
8	V	278	THR
8	V	288	THR
8	V	291	LEU
8	V	296	ARG
8	V	298	LEU

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Mol	Chain	Res	Type
8	V	328	VAL
8	V	331	THR
8	V	337	LEU
8	V	360	LEU
8	V	373	VAL
8	V	374	SER
8	V	385	SER
8	V	423	THR
8	V	424	SER
8	V	425	ARG
8	V	439	THR
8	V	445	SER
8	W	3	ARG
8	W	7	THR
8	W	10	LEU
8	W	20	GLU
8	W	24	GLN
8	W	28	GLU
8	W	58	GLU
8	W	66	LEU
8	W	69	LEU
8	W	78	LEU
8	W	120	ASP
8	W	136	VAL
8	W	149	LEU
8	W	157	LEU
8	W	166	VAL
8	W	188	SER
8	W	189	LEU
8	W	192	LEU
8	W	195	LEU
8	W	210	LEU
8	W	233	SER
8	W	248	TYR
8	W	254	ILE
8	W	271	THR
8	W	274	THR
8	W	278	THR
8	W	288	THR
8	W	291	LEU
8	W	296	ARG
8	W	298	LEU

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Mol	Chain	Res	Type
8	W	328	VAL
8	W	331	THR
8	W	337	LEU
8	W	360	LEU
8	W	373	VAL
8	W	374	SER
8	W	385	SER
8	W	423	THR
8	W	424	SER
8	W	425	ARG
8	W	439	THR
8	W	445	SER
8	X	3	ARG
8	X	7	THR
8	X	10	LEU
8	X	20	GLU
8	X	24	GLN
8	X	28	GLU
8	X	58	GLU
8	X	66	LEU
8	X	69	LEU
8	X	78	LEU
8	X	120	ASP
8	X	136	VAL
8	X	149	LEU
8	X	157	LEU
8	X	166	VAL
8	X	188	SER
8	X	189	LEU
8	X	192	LEU
8	X	195	LEU
8	X	210	LEU
8	X	233	SER
8	X	248	TYR
8	X	254	ILE
8	X	271	THR
8	X	274	THR
8	X	278	THR
8	X	288	THR
8	X	291	LEU
8	X	296	ARG
8	X	298	LEU

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Mol	Chain	Res	Type
8	X	328	VAL
8	X	331	THR
8	X	337	LEU
8	X	360	LEU
8	X	373	VAL
8	X	374	SER
8	X	385	SER
8	X	423	THR
8	X	424	SER
8	X	425	ARG
8	X	439	THR
8	X	445	SER
8	Y	3	ARG
8	Y	7	THR
8	Y	10	LEU
8	Y	20	GLU
8	Y	24	GLN
8	Y	28	GLU
8	Y	58	GLU
8	Y	66	LEU
8	Y	69	LEU
8	Y	78	LEU
8	Y	120	ASP
8	Y	136	VAL
8	Y	149	LEU
8	Y	157	LEU
8	Y	166	VAL
8	Y	188	SER
8	Y	189	LEU
8	Y	192	LEU
8	Y	195	LEU
8	Y	210	LEU
8	Y	233	SER
8	Y	248	TYR
8	Y	254	ILE
8	Y	271	THR
8	Y	274	THR
8	Y	278	THR
8	Y	288	THR
8	Y	291	LEU
8	Y	296	ARG
8	Y	298	LEU

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Mol	Chain	Res	Type
8	Y	328	VAL
8	Y	331	THR
8	Y	337	LEU
8	Y	360	LEU
8	Y	373	VAL
8	Y	374	SER
8	Y	385	SER
8	Y	423	THR
8	Y	424	SER
8	Y	425	ARG
8	Y	439	THR
8	Y	445	SER
8	Z	3	ARG
8	Z	7	THR
8	Z	10	LEU
8	Z	20	GLU
8	Z	24	GLN
8	Z	28	GLU
8	Z	58	GLU
8	Z	66	LEU
8	Z	69	LEU
8	Z	78	LEU
8	Z	120	ASP
8	Z	136	VAL
8	Z	149	LEU
8	Z	157	LEU
8	Z	166	VAL
8	Z	188	SER
8	Z	189	LEU
8	Z	192	LEU
8	Z	195	LEU
8	Z	210	LEU
8	Z	233	SER
8	Z	248	TYR
8	Z	254	ILE
8	Z	271	THR
8	Z	274	THR
8	Z	278	THR
8	Z	288	THR
8	Z	291	LEU
8	Z	296	ARG
8	Z	298	LEU

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Mol	Chain	Res	Type
8	Z	328	VAL
8	Z	331	THR
8	Z	337	LEU
8	Z	351	TRP
8	Z	360	LEU
8	Z	373	VAL
8	Z	374	SER
8	Z	385	SER
8	Z	423	THR
8	Z	424	SER
8	Z	425	ARG
8	Z	439	THR
8	Z	445	SER
2	d	65	LYS
6	l	85	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	12	ASN
1	e	92	ASN
1	e	111	ASN
1	e	314	GLN
2	b	19	ASN
4	C	151	GLN
4	C	242	GLN
4	C	371	GLN
4	C	674	GLN
4	C	684	GLN
4	C	688	ASN
4	C	691	GLN
4	C	862	ASN
3	D	322	GLN
3	D	491	ASN
3	D	495	GLN
3	D	558	HIS
3	D	703	GLN
3	D	705	HIS
3	D	740	GLN
3	D	786	GLN
3	D	852	HIS
4	E	303	HIS

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Mol	Chain	Res	Type
4	E	329	GLN
4	E	401	HIS
4	E	412	HIS
4	E	420	GLN
4	E	430	GLN
4	E	662	ASN
4	E	688	ASN
3	F	301	HIS
3	F	302	ASN
3	F	345	GLN
3	F	717	GLN
3	F	736	ASN
3	F	739	GLN
3	F	742	GLN
3	F	786	GLN
3	F	801	GLN
3	F	852	HIS
4	G	289	ASN
4	G	694	GLN
4	G	823	ASN
3	H	273	ASN
3	H	329	HIS
3	H	751	HIS
3	H	830	ASN
3	H	883	ASN
5	I	102	GLN
5	I	339	HIS
5	I	398	GLN
5	I	489	GLN
5	I	529	GLN
5	I	571	GLN
5	I	581	HIS
5	I	622	GLN
6	J	222	HIS
6	J	288	GLN
6	J	299	ASN
6	J	456	GLN
6	J	705	ASN
6	J	725	ASN
6	J	938	HIS
5	K	3	HIS
5	K	29	GLN

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Mol	Chain	Res	Type
5	K	61	GLN
5	K	67	GLN
5	K	78	GLN
5	K	123	ASN
5	K	519	ASN
5	K	591	HIS
7	L	327	HIS
7	L	571	HIS
7	L	1508	HIS
7	L	1568	HIS
7	L	1666	GLN
7	L	1730	HIS
7	L	1788	ASN
2	k	53	GLN
8	Q	16	GLN
8	Q	24	GLN
8	Q	187	ASN
8	Q	229	ASN
8	Q	332	GLN
8	R	16	GLN
8	R	24	GLN
8	R	187	ASN
8	R	229	ASN
8	R	332	GLN
8	S	16	GLN
8	S	24	GLN
8	S	87	ASN
8	S	187	ASN
8	S	229	ASN
8	S	332	GLN
8	T	16	GLN
8	T	24	GLN
8	T	187	ASN
8	T	229	ASN
8	T	332	GLN
8	U	16	GLN
8	U	24	GLN
8	U	87	ASN
8	U	187	ASN
8	U	229	ASN
8	U	332	GLN
8	V	16	GLN

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Mol	Chain	Res	Type
8	V	24	GLN
8	V	187	ASN
8	V	229	ASN
8	V	314	ASN
8	V	332	GLN
8	W	16	GLN
8	W	24	GLN
8	W	187	ASN
8	W	229	ASN
8	W	332	GLN
8	X	16	GLN
8	X	24	GLN
8	X	187	ASN
8	X	229	ASN
8	X	332	GLN
8	Y	16	GLN
8	Y	24	GLN
8	Y	187	ASN
8	Y	229	ASN
8	Y	332	GLN
8	Z	16	GLN
8	Z	24	GLN
8	Z	87	ASN
8	Z	187	ASN
8	Z	229	ASN
8	Z	332	GLN
2	d	56	ASN
7	c	48	ASN
3	h	14	GLN
3	h	65	GLN
3	j	14	GLN
3	j	15	ASN
6	l	107	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

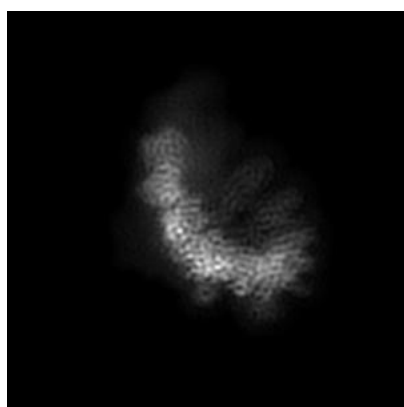
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14011. These allow visual inspection of the internal detail of the map and identification of artifacts.

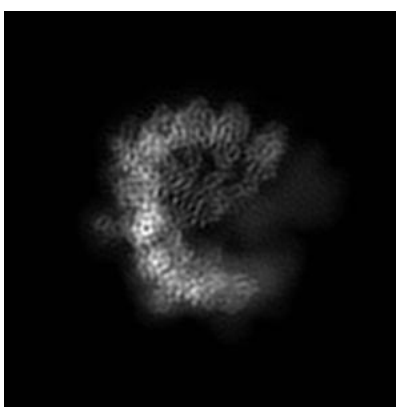
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

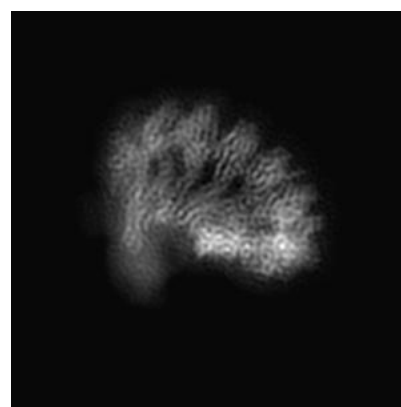
6.1.1 Primary map



X



Y



Z

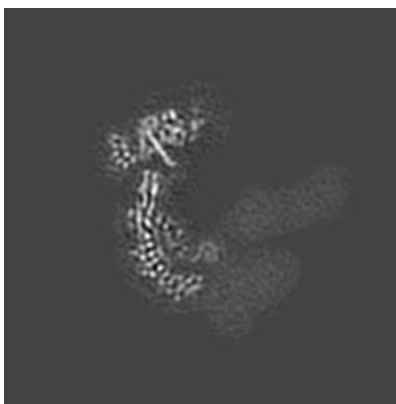
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

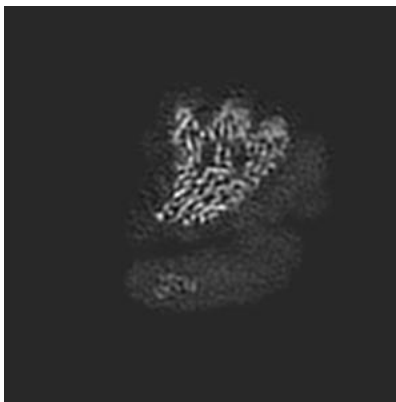
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

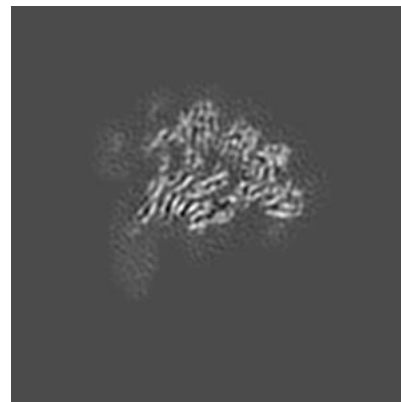
6.3.1 Primary map



X Index: 135



Y Index: 81



Z Index: 72

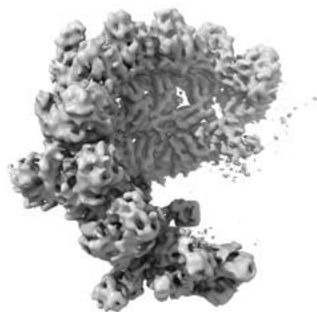
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0308. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

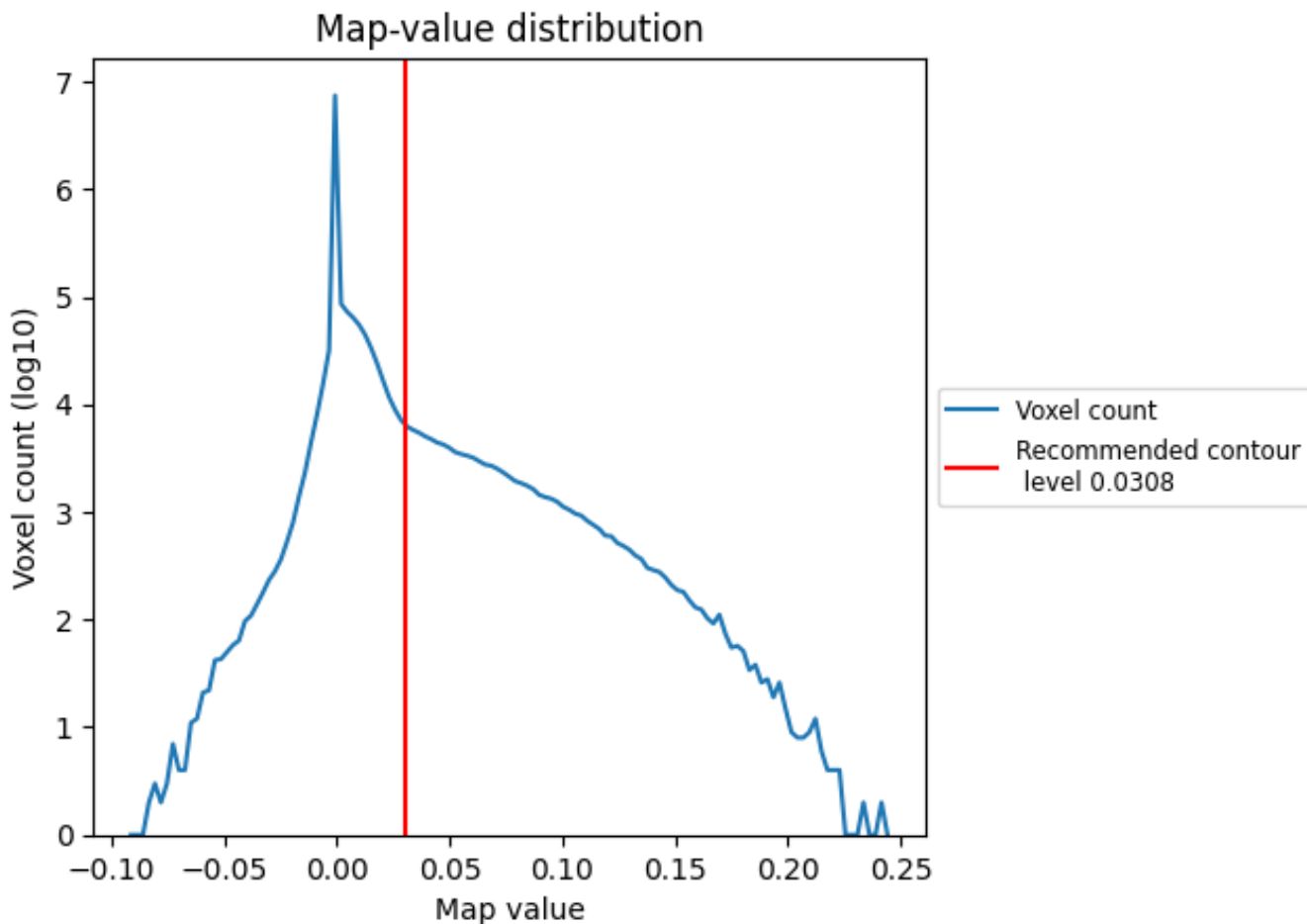
6.5 Mask visualisation

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

7 Map analysis [i](#)

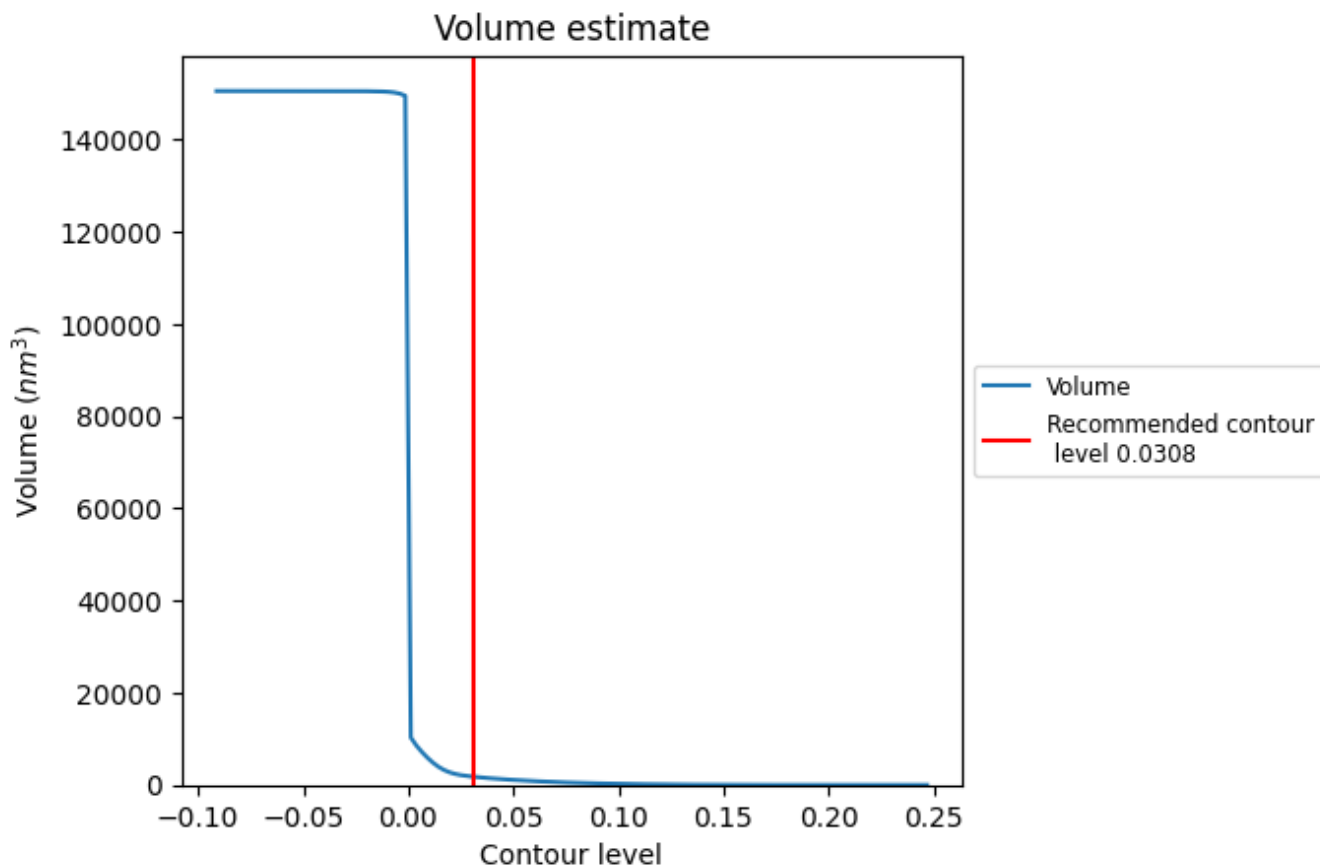
This section contains the results of statistical analysis of the map.

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.

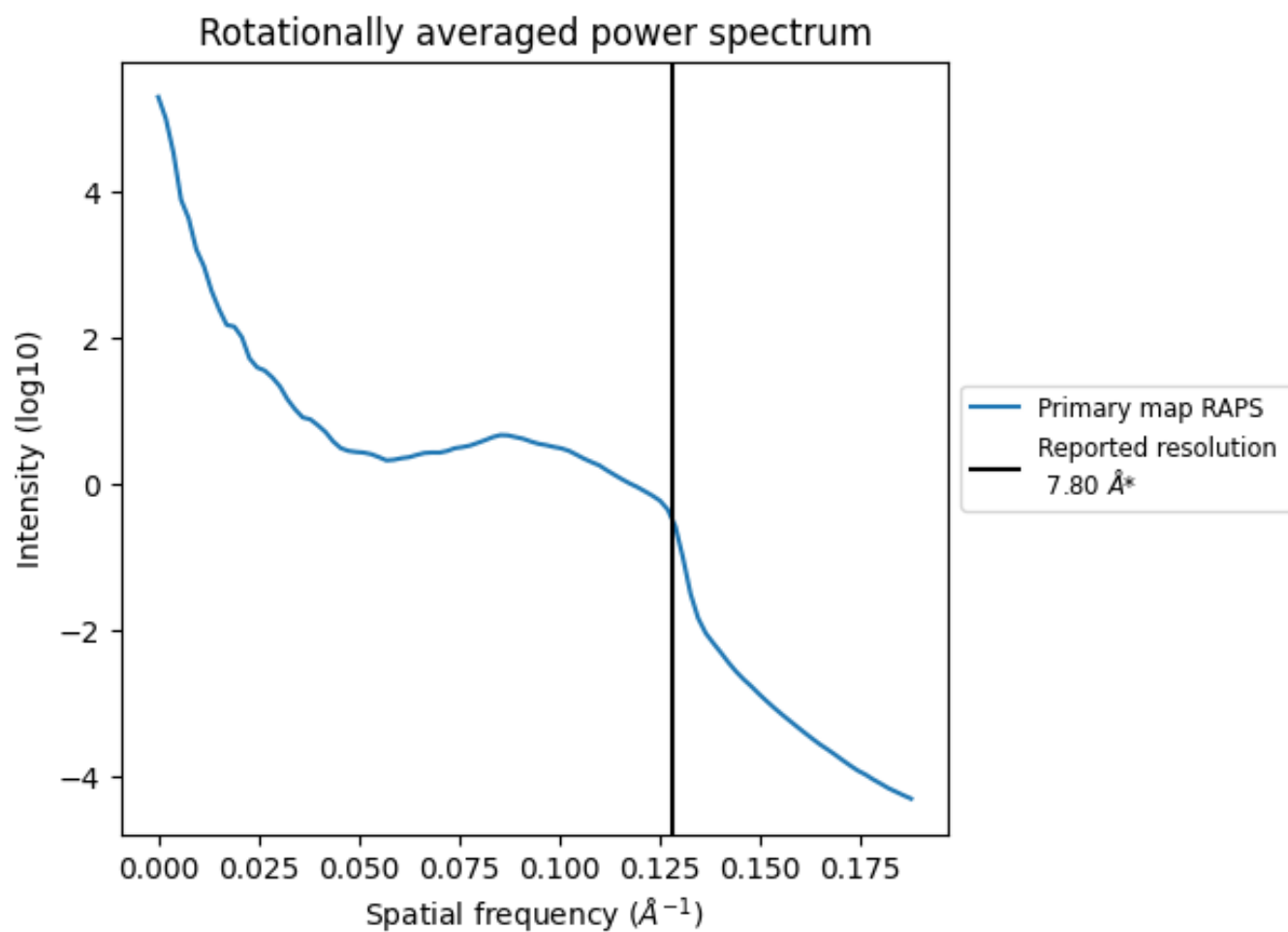
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1794 nm^3 ; this corresponds to an approximate mass of 1620 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 0.128 Å⁻¹

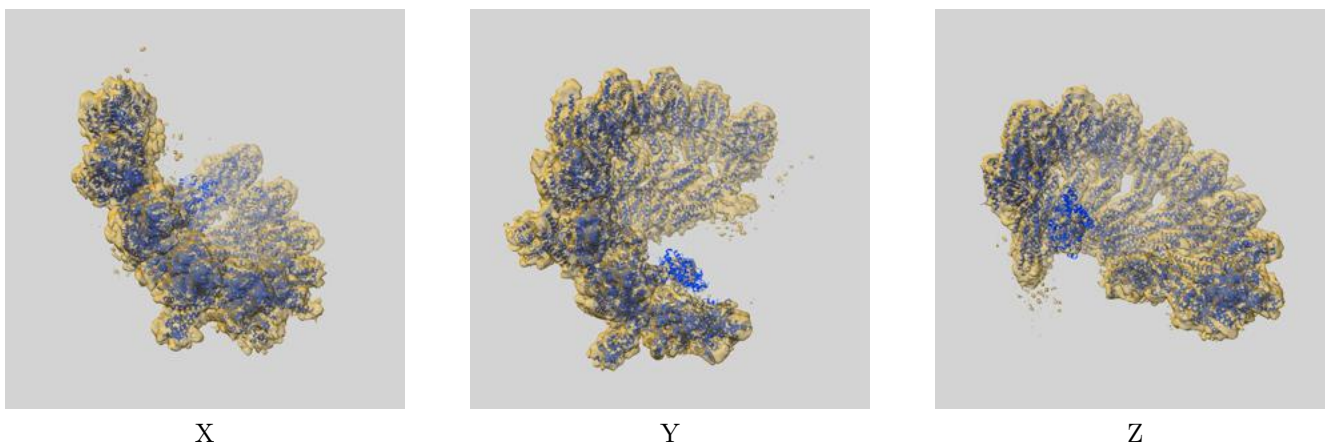
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

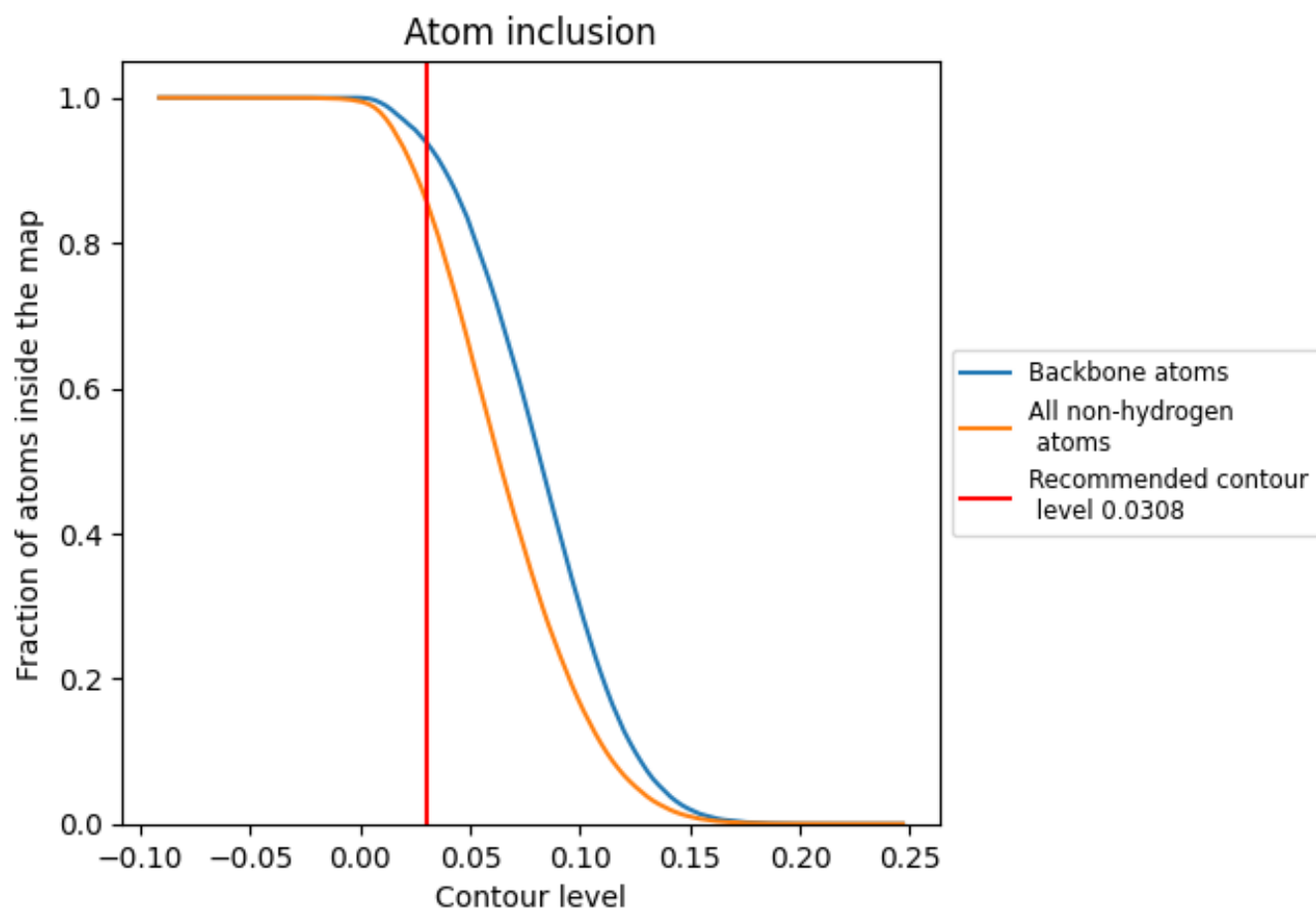
This section contains information regarding the fit between EMDB map EMD-14011 and PDB model 7QJ6. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0308 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 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.