



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:43 AM UTC

PDB ID : 8Q62 / pdb_00008q62
EMDB ID : EMD-18181
Title : Early closed conformation of the g-tubulin ring complex
Authors : Llorca, O.; Serna, M.; Fernandez-Leiro, R.
Deposited on : 2023-08-10
Resolution : 3.72 Å (reported)
Based on initial models : 7AS4, 6X0U

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

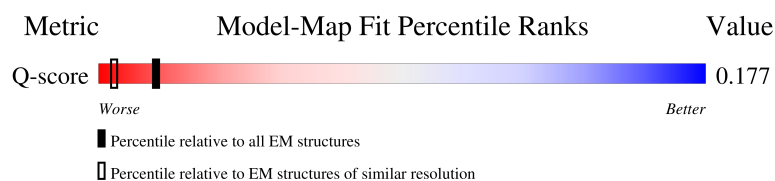
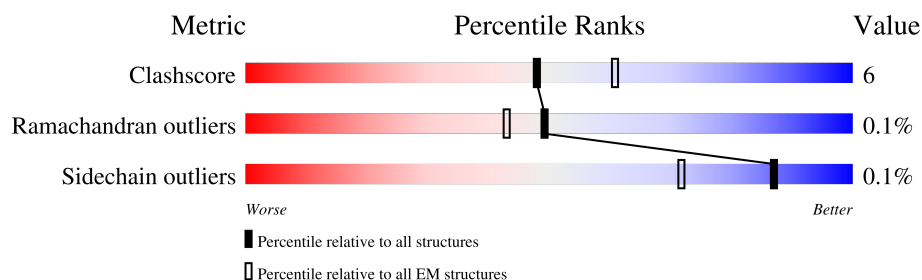
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.72 Å.

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



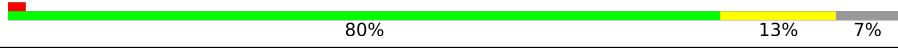
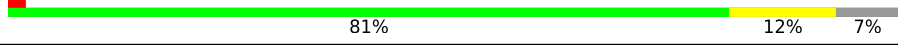
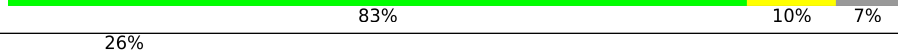
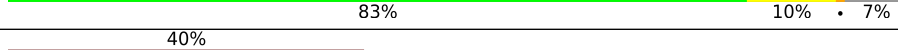
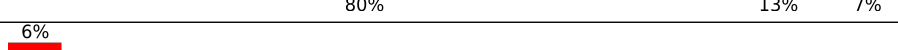
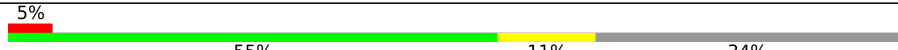
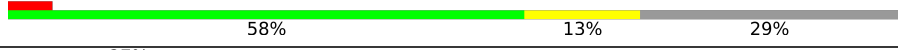
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10474 (3.22 - 4.22)

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	a	451	
1	b	451	
1	c	451	
1	d	451	

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Mol	Chain	Length	Quality of chain
1	e	451	
1	f	451	
1	g	451	
1	h	451	
1	i	451	
1	j	451	
1	k	451	
1	l	451	
1	m	451	
1	n	451	
2	J	1024	
3	I	667	
3	K	667	
4	B	907	
4	D	907	
4	F	907	
4	H	907	
4	N	907	
5	A	902	
5	C	902	
5	E	902	
5	G	902	
5	M	902	
6	L	1819	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 230788 atoms, of which 115024 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 Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	k	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		
1	a	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		
1	b	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		
1	c	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		
1	d	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		
1	e	420	Total	C	H	N	O	S	2	0
			6685	2138	3305	587	640	15		
1	f	420	Total	C	H	N	O	S	2	0
			6690	2135	3316	584	640	15		
1	g	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		
1	h	420	Total	C	H	N	O	S	2	0
			6679	2135	3305	584	640	15		
1	i	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		
1	j	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		
1	l	420	Total	C	H	N	O	S	2	0
			6696	2138	3316	587	640	15		
1	m	420	Total	C	H	N	O	S	2	0
			6696	2138	3316	587	640	15		
1	n	420	Total	C	H	N	O	S	2	0
			6707	2138	3327	587	640	15		

- Molecule 2 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	594	Total	C	H	N	O	S	0	0
			9558	3093	4769	807	863	26		

- Molecule 3 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	553	Total	C	H	N	O	S	0	0
			9010	2918	4507	768	800	17		
3	I	521	Total	C	H	N	O	S	0	0
			8472	2734	4250	720	750	18		

- Molecule 4 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B	610	Total	C	H	N	O	S	0	0
			9984	3195	4969	885	910	25		
4	D	581	Total	C	H	N	O	S	0	0
			9560	3061	4764	842	868	25		
4	F	599	Total	C	H	N	O	S	0	0
			9852	3146	4919	871	891	25		
4	H	586	Total	C	H	N	O	S	0	0
			9655	3087	4820	852	871	25		
4	N	594	Total	C	H	N	O	S	0	0
			9779	3125	4880	864	885	25		

- Molecule 5 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	C	620	Total	C	H	N	O	S	0	0
			10108	3254	5070	842	910	32		
5	E	638	Total	C	H	N	O	S	0	0
			10443	3354	5241	873	942	33		
5	G	636	Total	C	H	N	O	S	0	0
			10394	3342	5208	871	940	33		
5	M	636	Total	C	H	N	O	S	0	0
			10405	3342	5219	871	940	33		
5	A	609	Total	C	H	N	O	S	0	0
			9890	3181	4956	825	896	32		

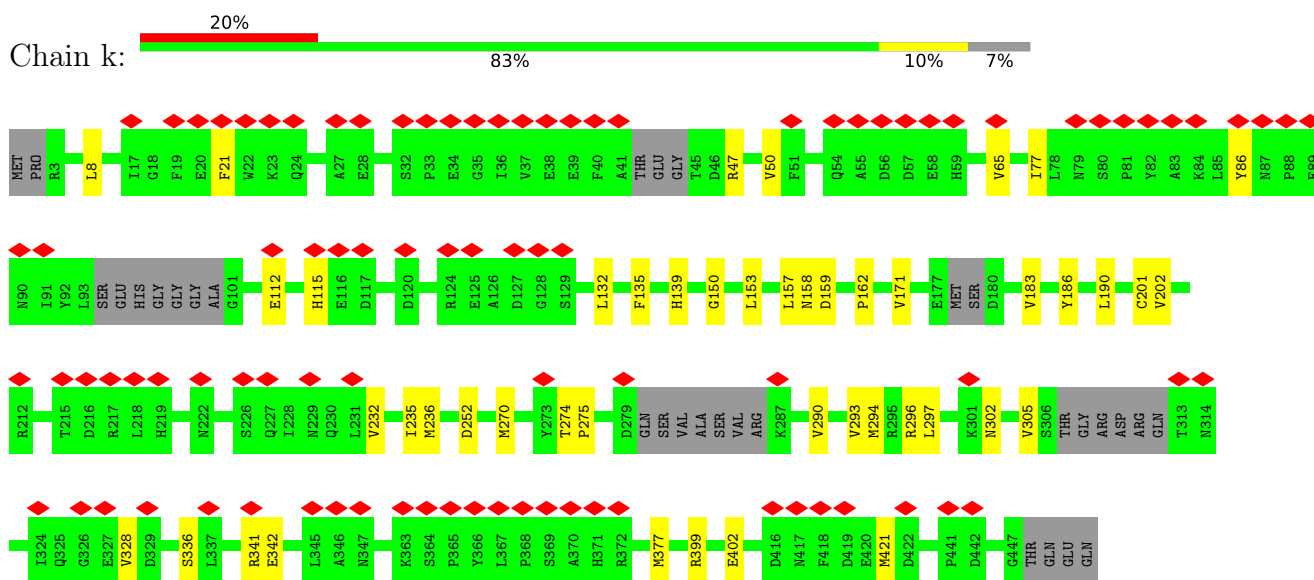
- Molecule 6 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	616	Total	C	H	N	O	S	0	0
			9869	3211	4951	826	855	26		

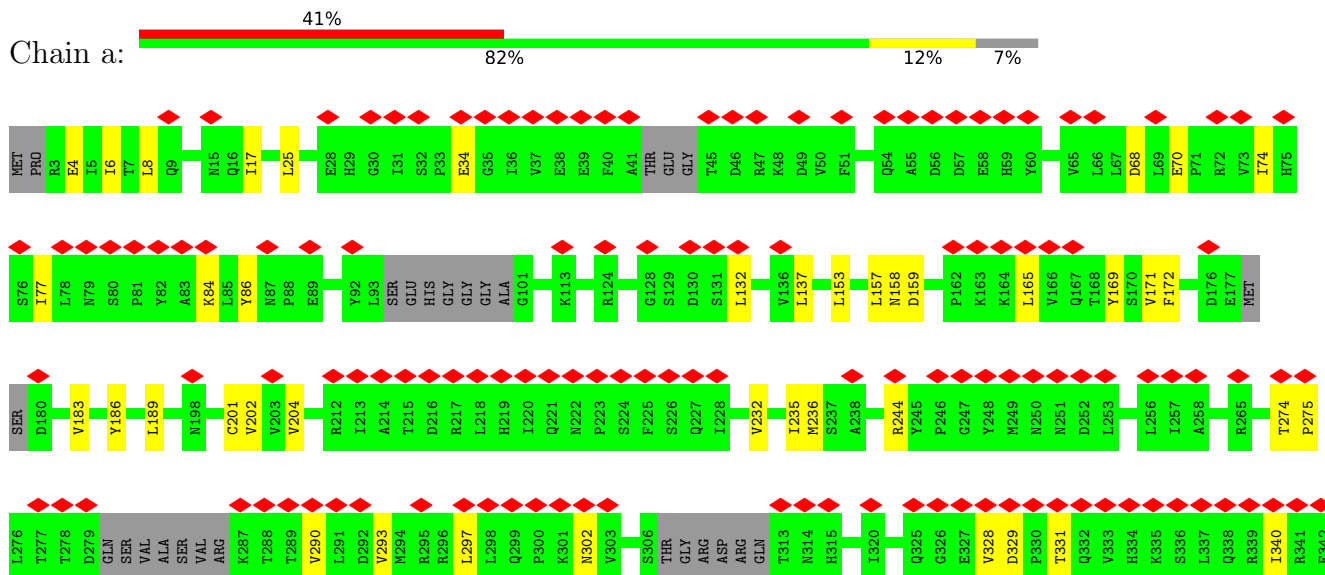
3 Residue-property plots [i](#)

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: Tubulin gamma-1 chain

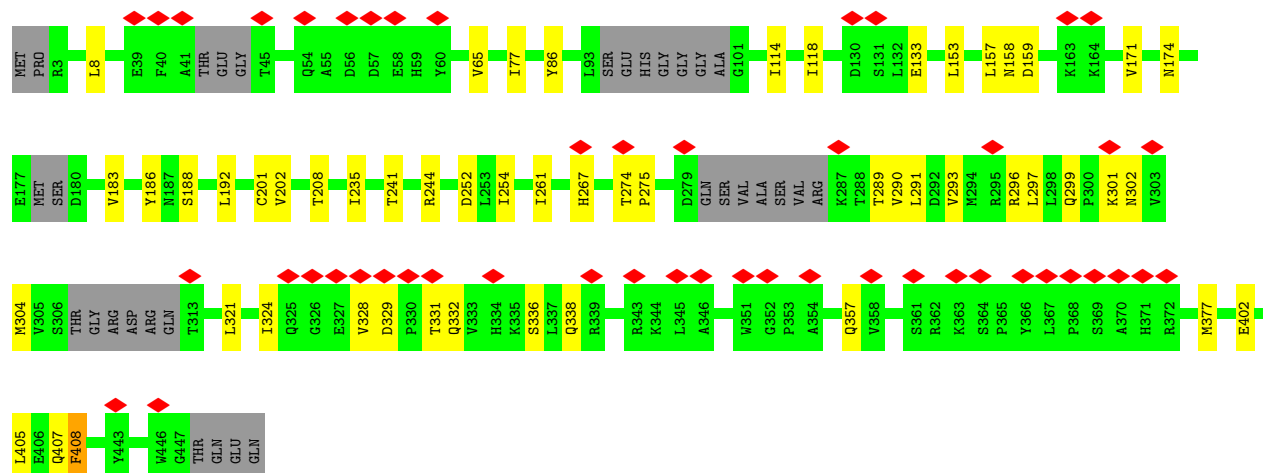
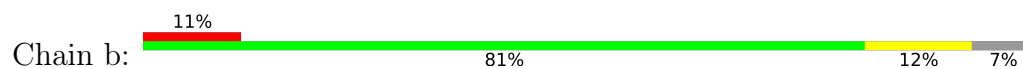


- Molecule 1: Tubulin gamma-1 chain

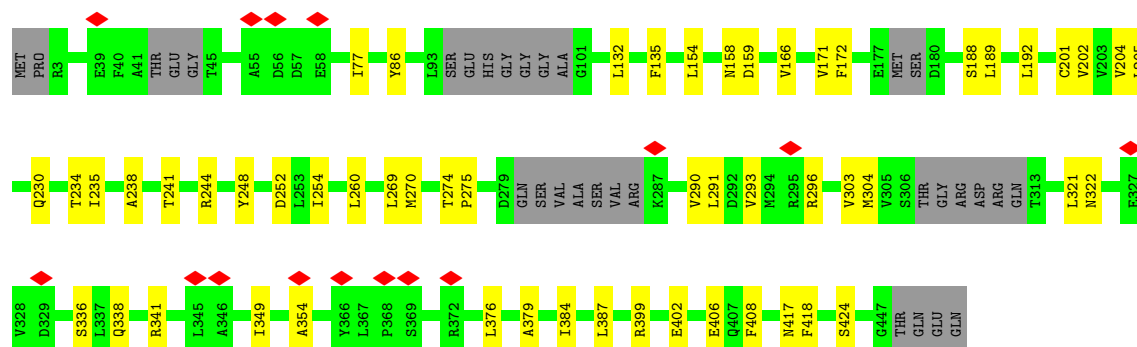
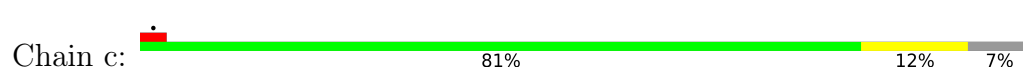




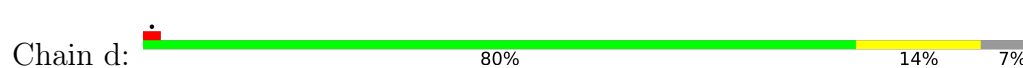
• Molecule 1: Tubulin gamma-1 chain

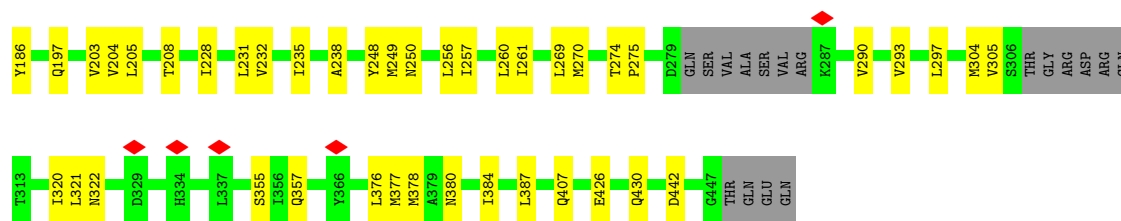


• Molecule 1: Tubulin gamma-1 chain



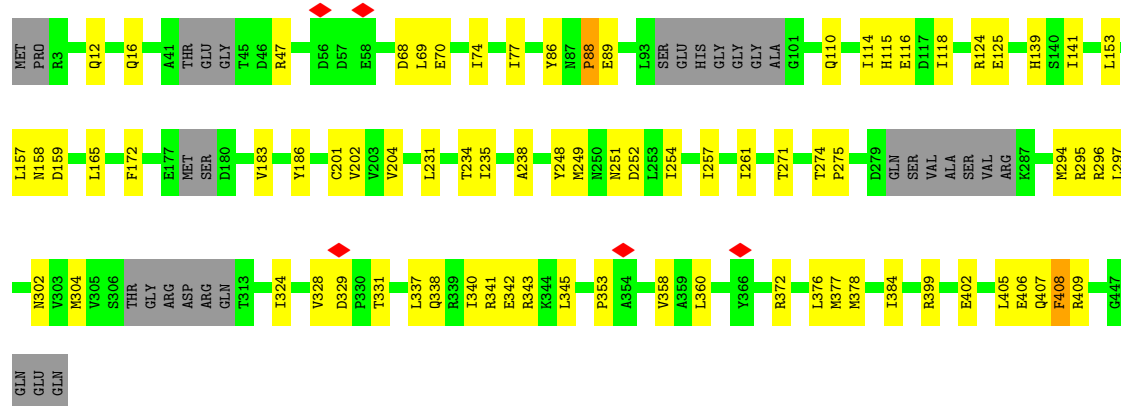
• Molecule 1: Tubulin gamma-1 chain





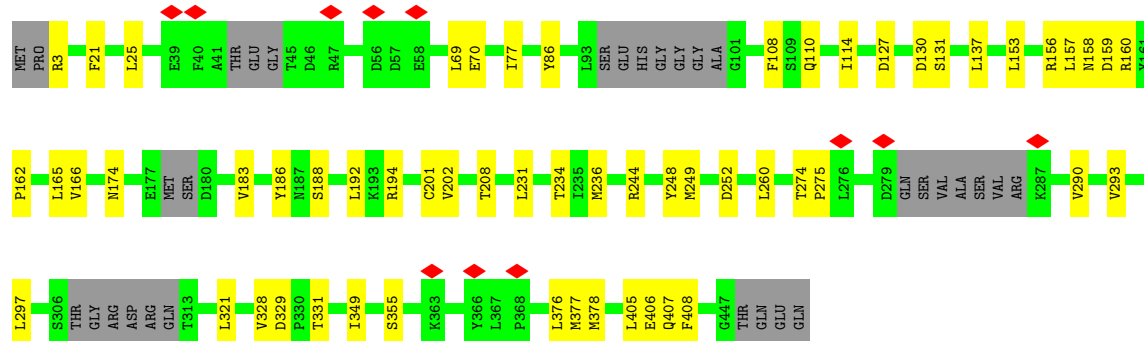
- Molecule 1: Tubulin gamma-1 chain

Chain e: 76% 17% 7%



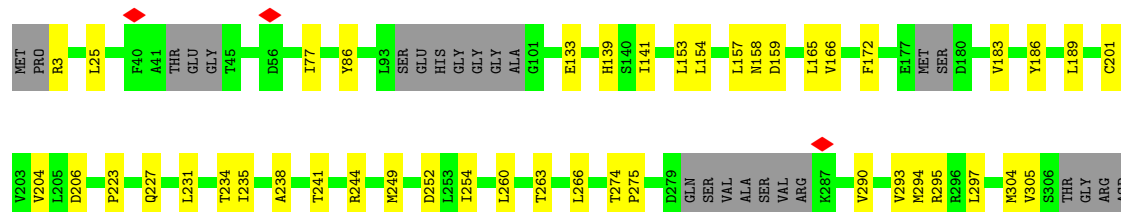
- Molecule 1: Tubulin gamma-1 chain

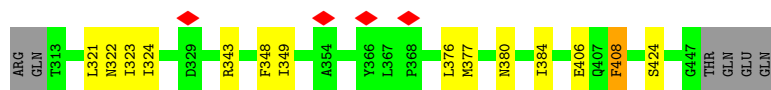
Chain f: 80% 13% 7%



- Molecule 1: Tubulin gamma-1 chain

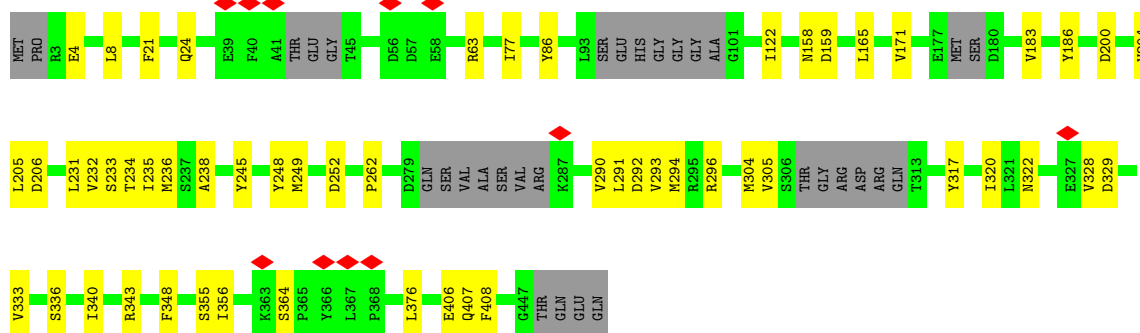
Chain g: 80% 13% 7%





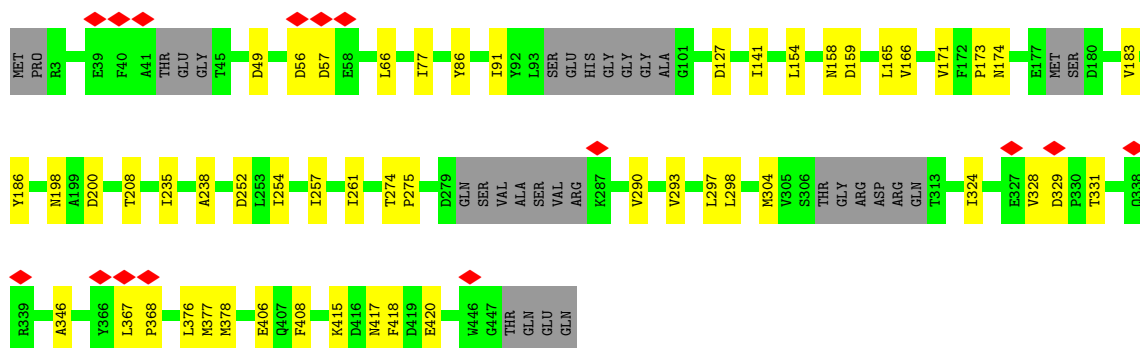
- Molecule 1: Tubulin gamma-1 chain

Chain h: 81% 12% 7%



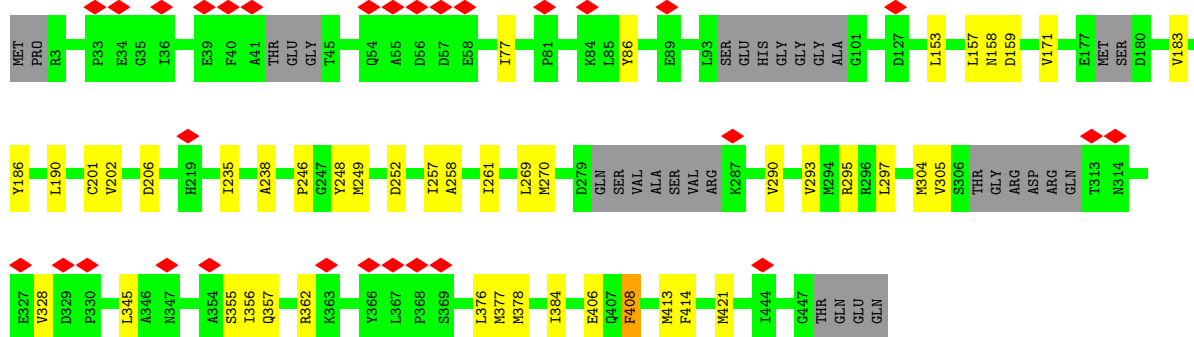
- Molecule 1: Tubulin gamma-1 chain

Chain i: 82% 11% 7%

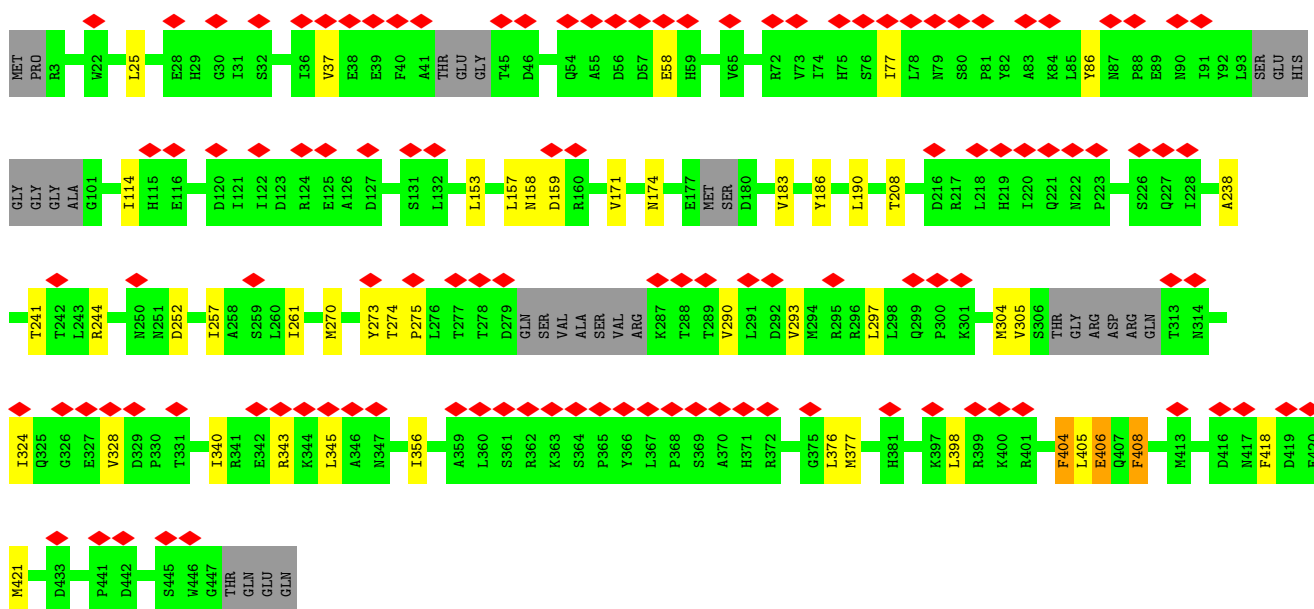
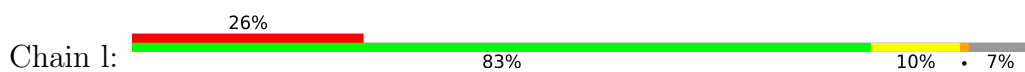


- Molecule 1: Tubulin gamma-1 chain

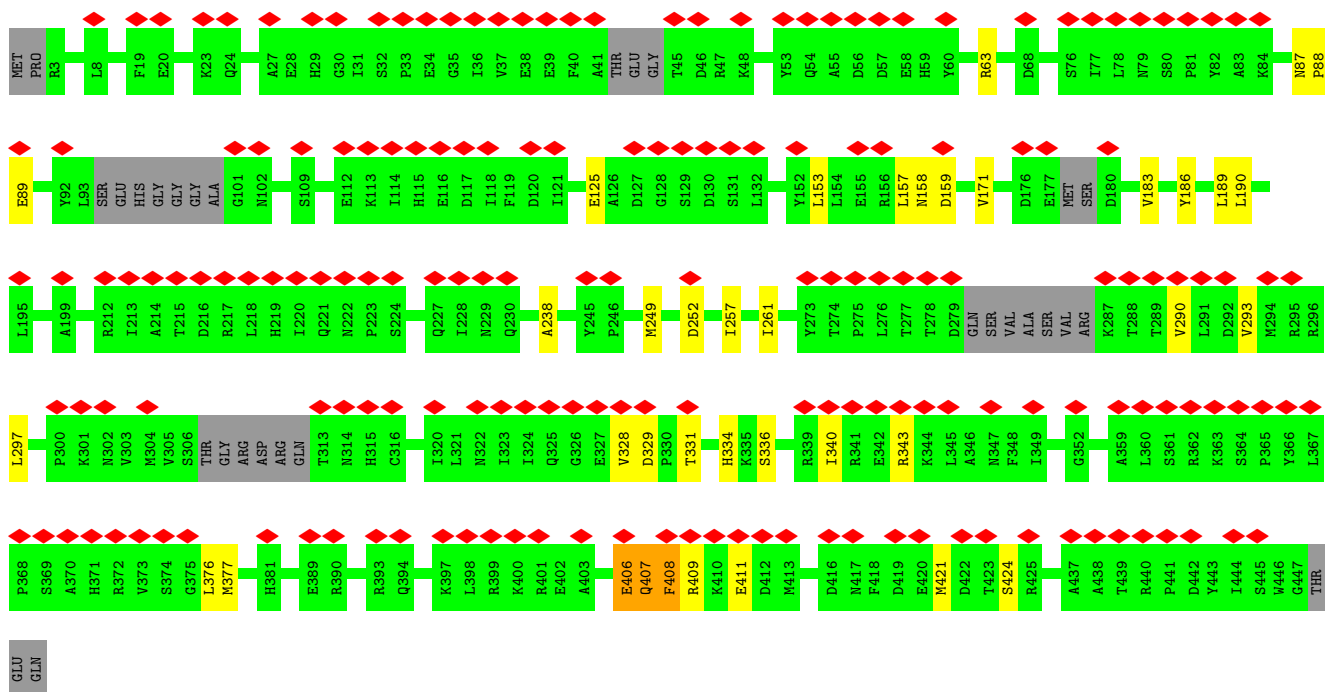
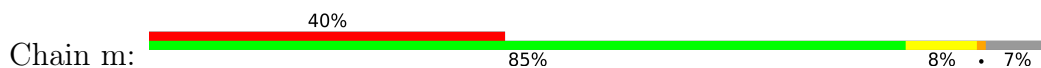
Chain j: 7% 83% 10% 7%



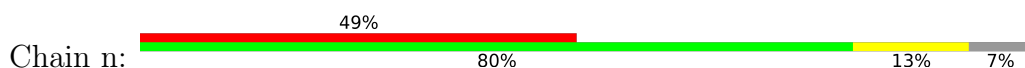
- Molecule 1: Tubulin gamma-1 chain

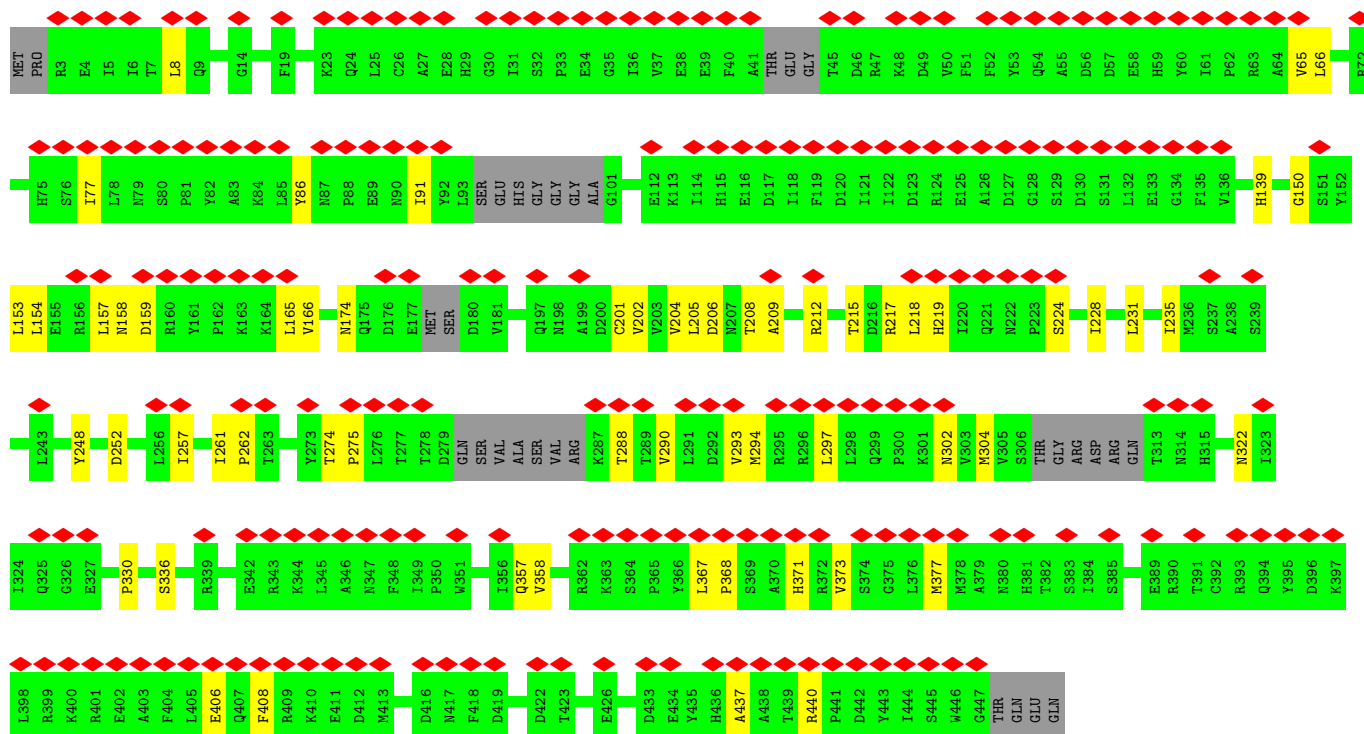


• Molecule 1: Tubulin gamma-1 chain

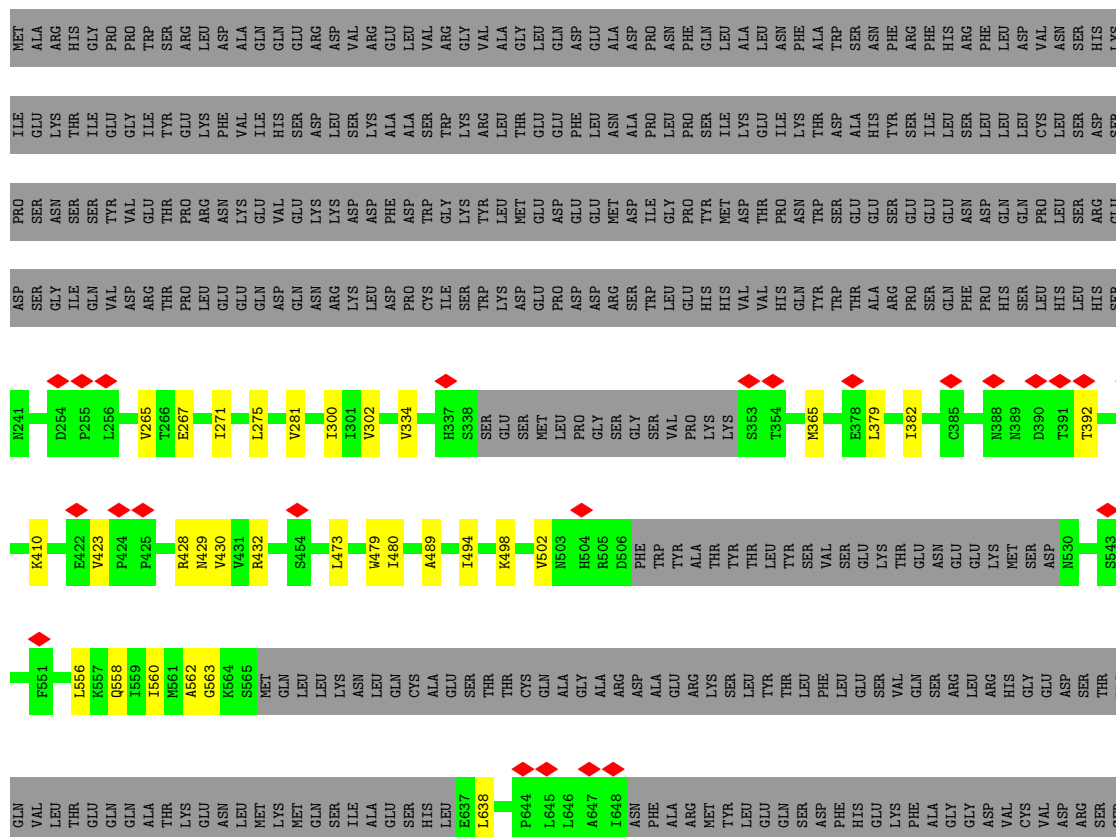


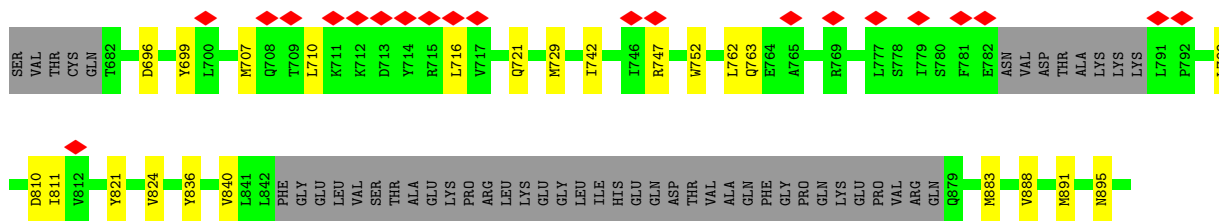
• Molecule 1: Tubulin gamma-1 chain



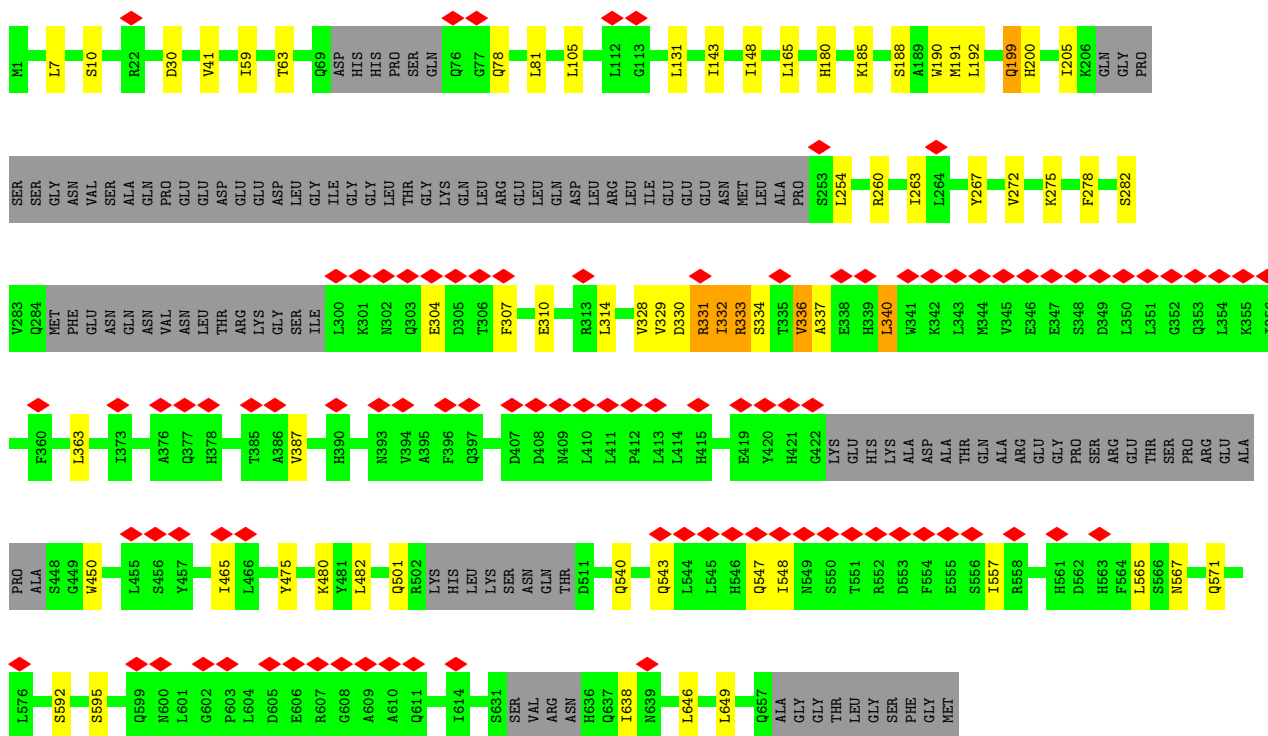


• Molecule 2: Gamma-tubulin complex component 5

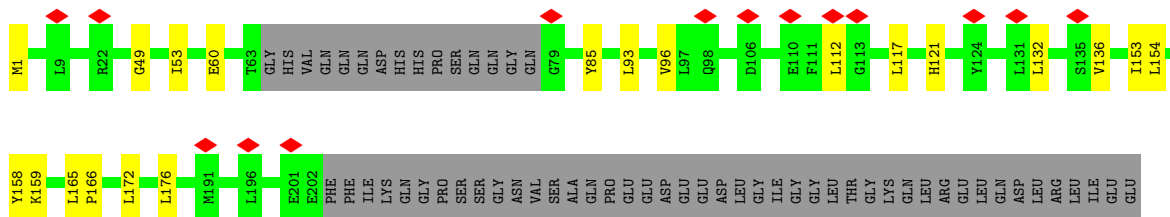


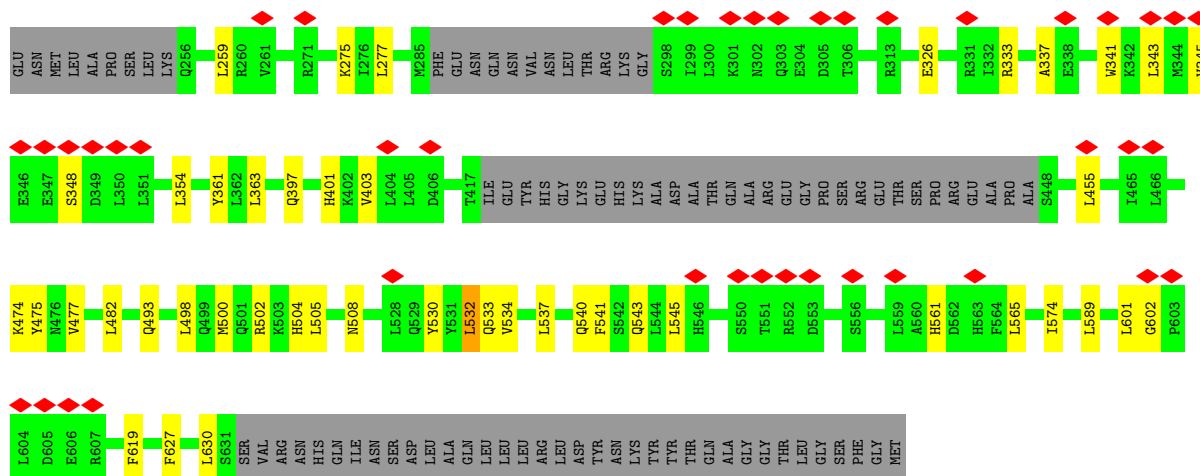


• Molecule 3: Gamma-tubulin complex component 4

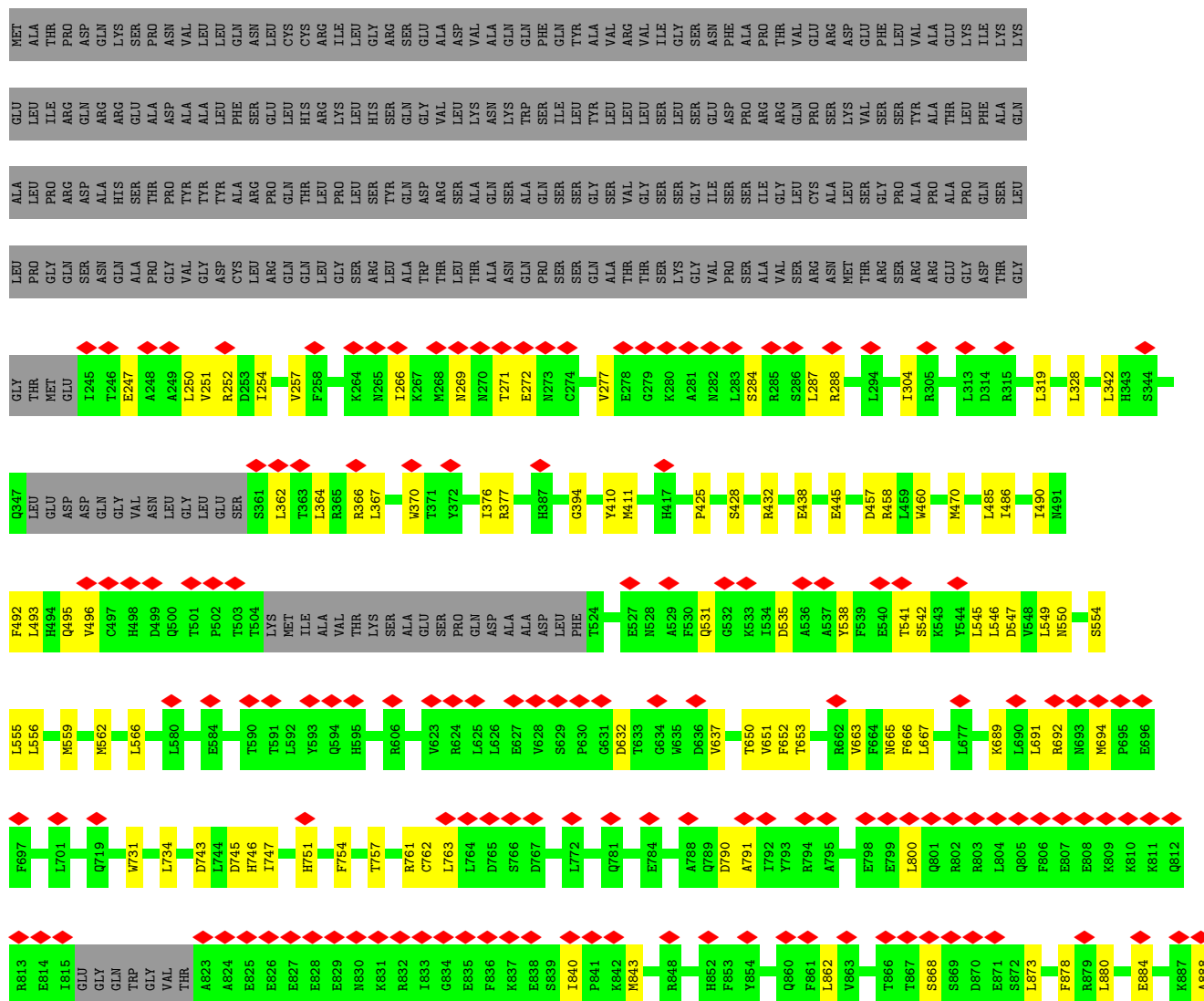


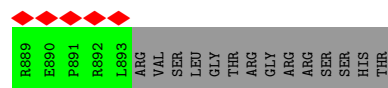
• Molecule 3: Gamma-tubulin complex component 4



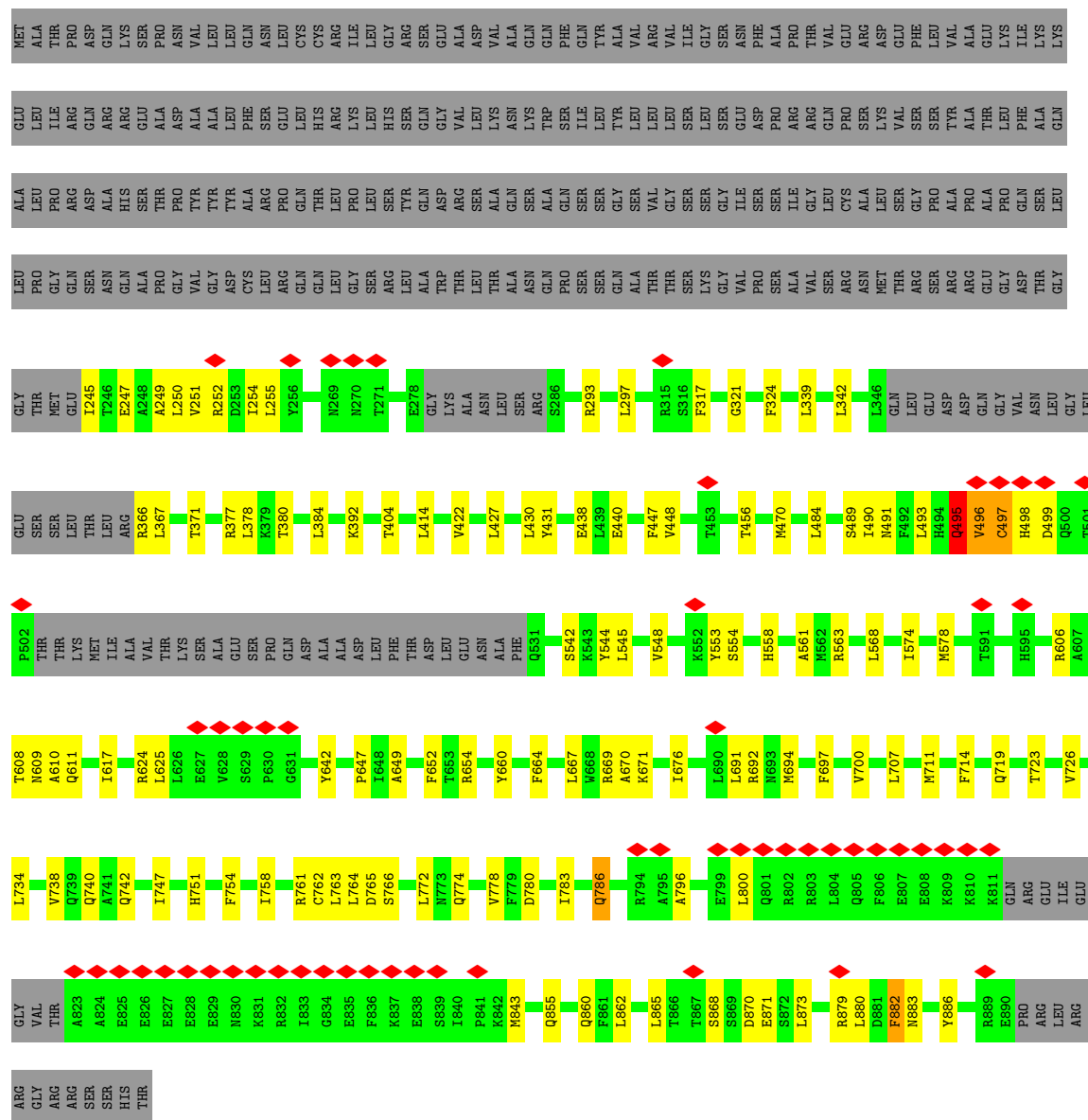


• Molecule 4: Gamma-tubulin complex component 3

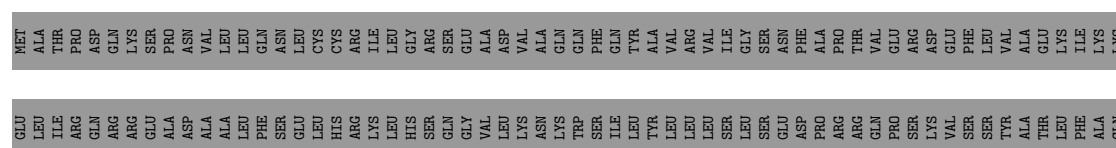




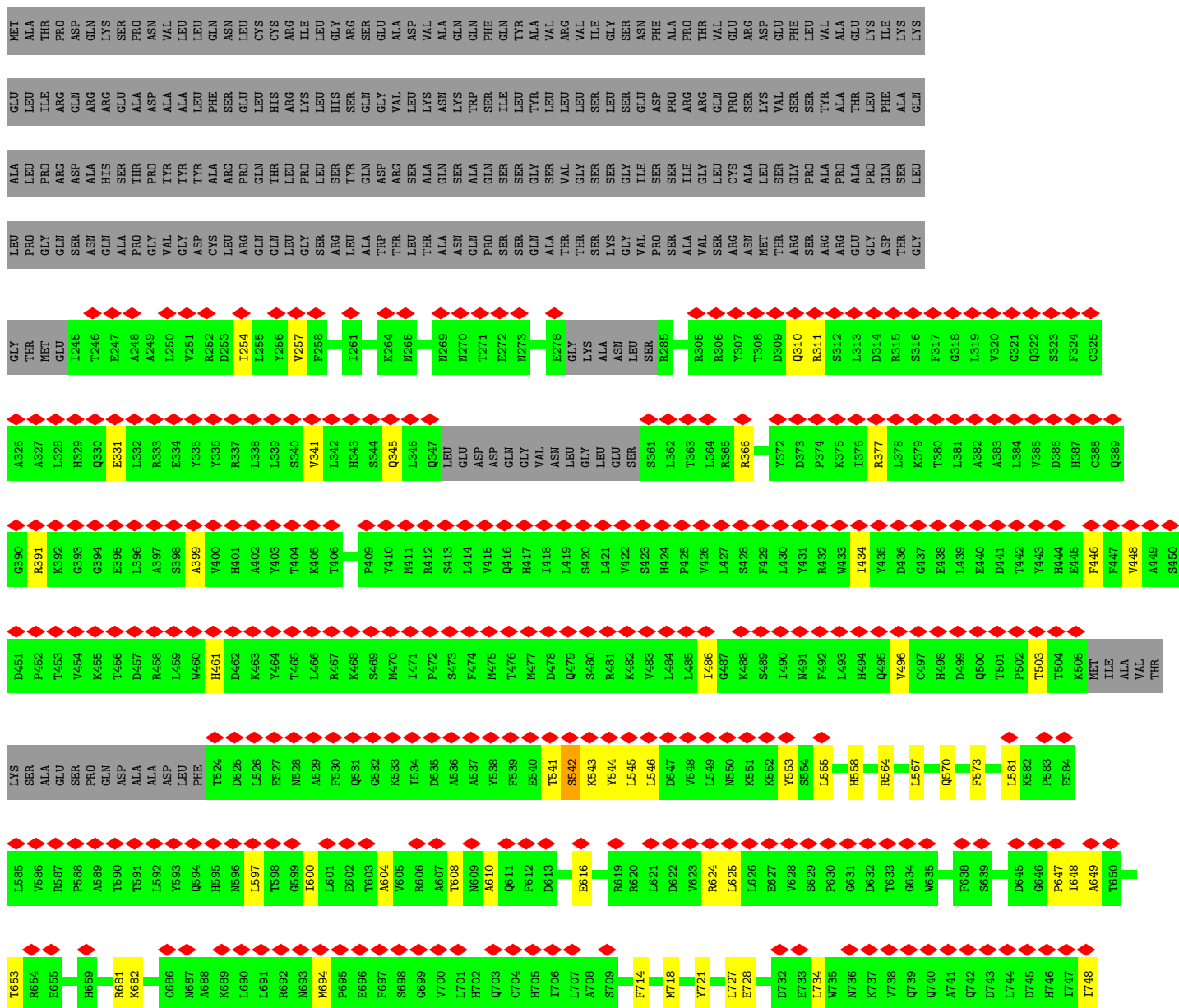
• Molecule 4: Gamma-tubulin complex component 3



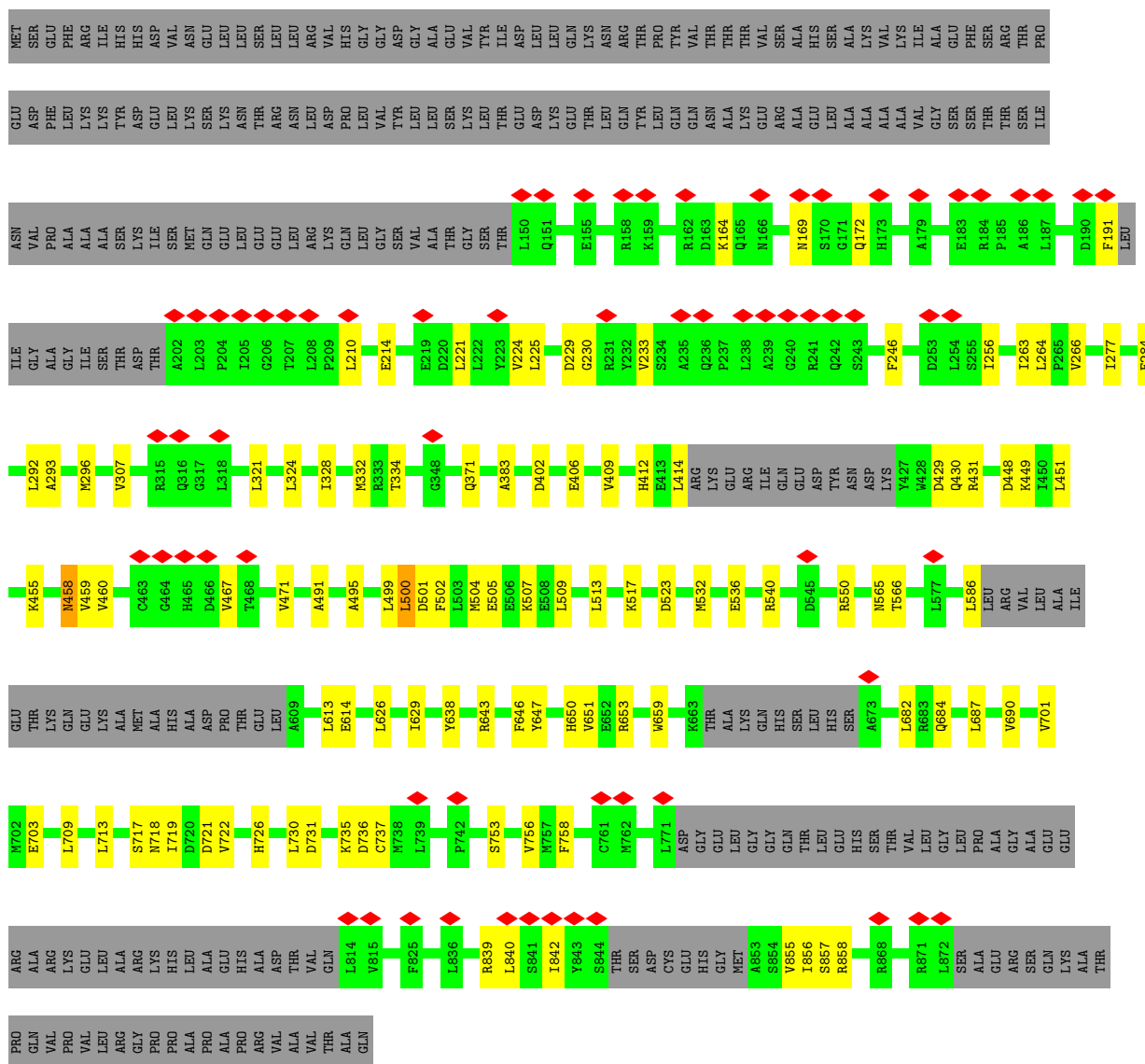
• Molecule 4: Gamma-tubulin complex component 3





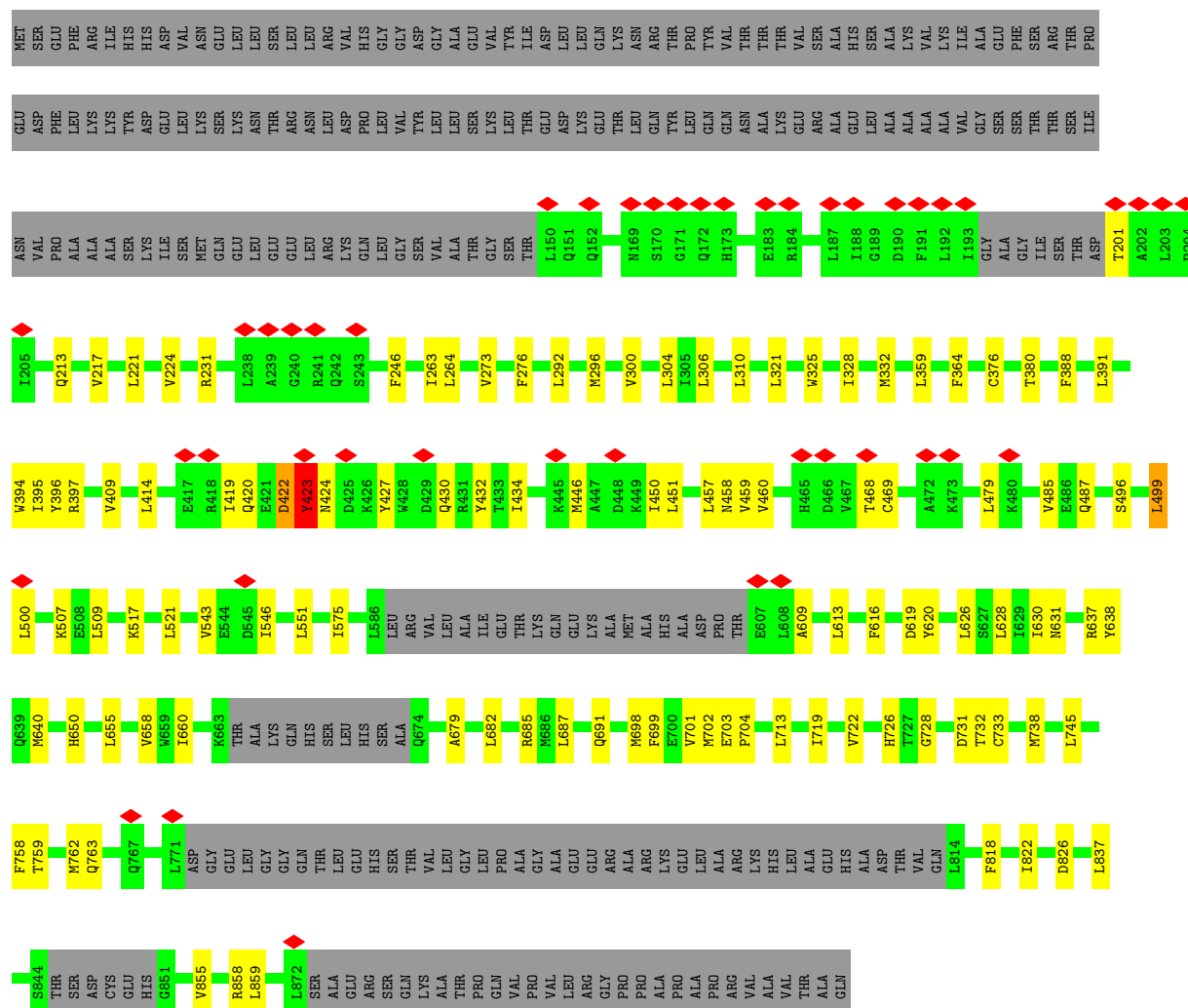


- Molecule 5: Gamma-tubulin complex component 2

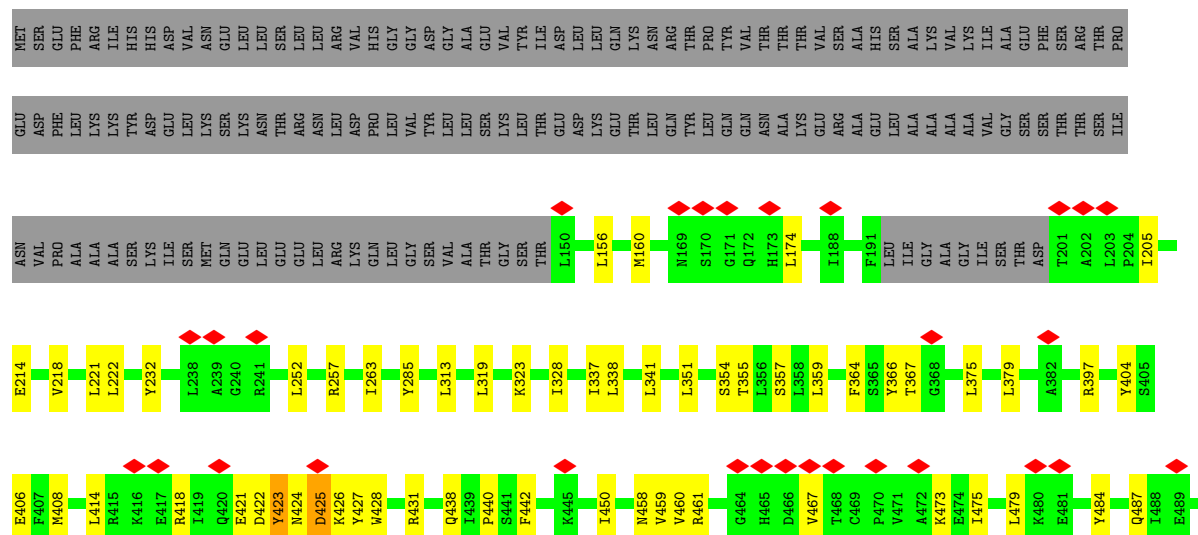


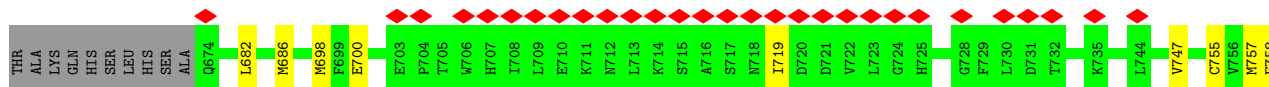
- Molecule 5: Gamma-tubulin complex component 2

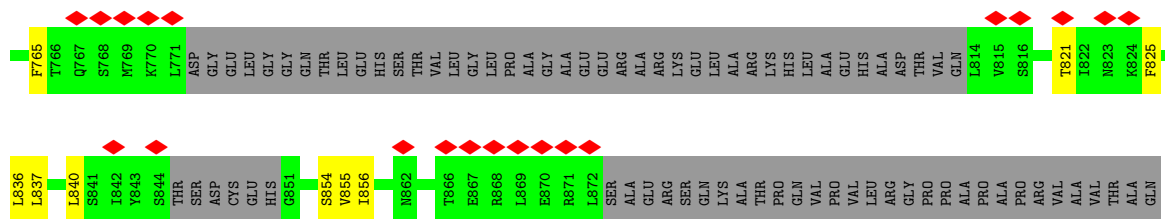




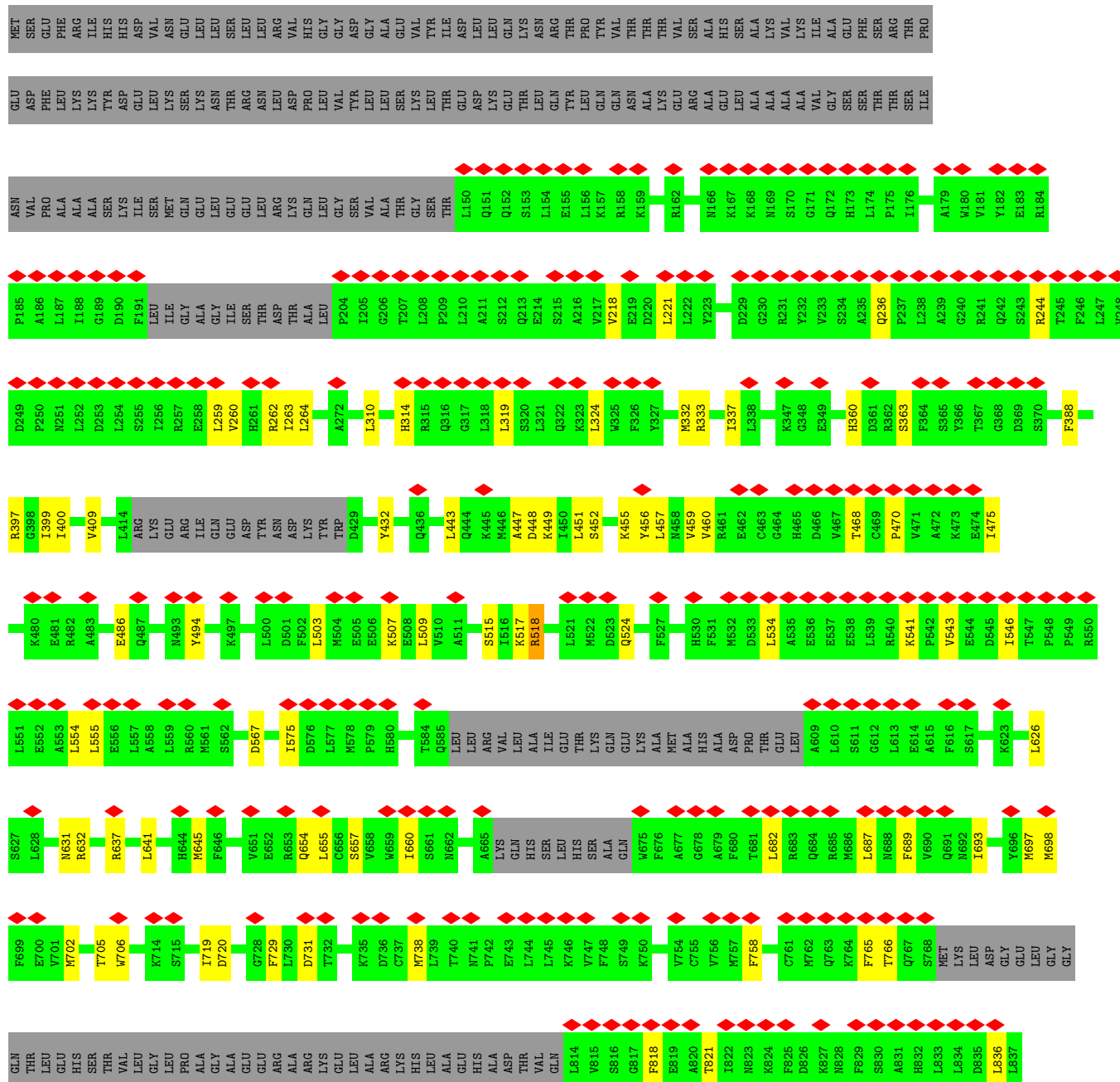
• Molecule 5: Gamma-tubulin complex component 2

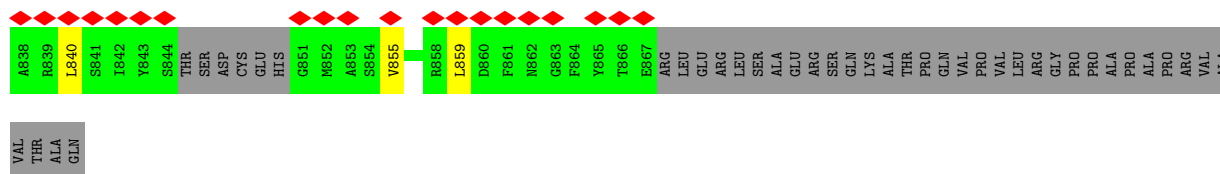




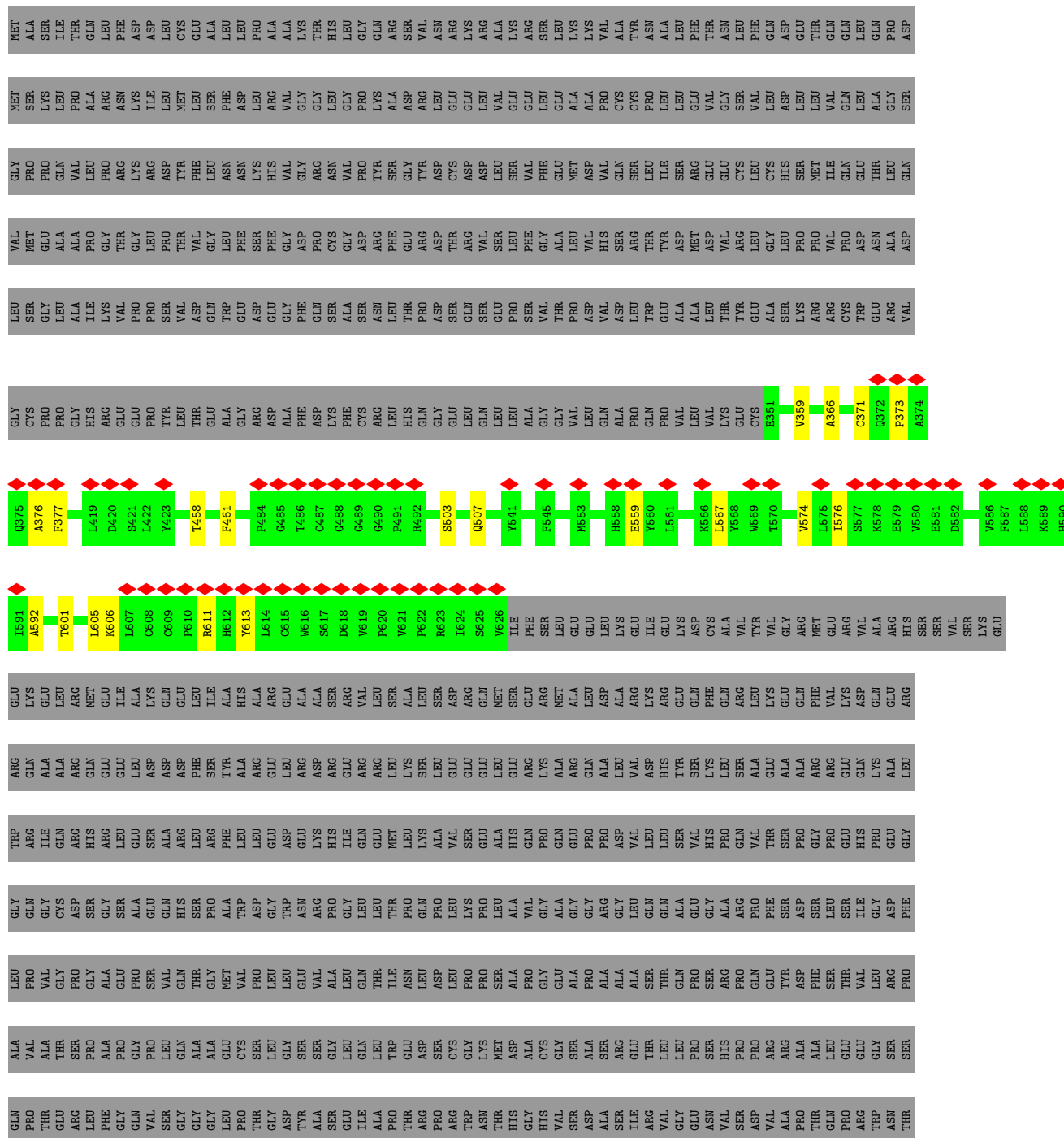


• Molecule 5: Gamma-tubulin complex component 2





• Molecule 6: Gamma-tubulin complex component 6



G1761	A1658	G1572	Y1506	GLU	LEU	ARG	VAL	VAL	GLY	HIS
P1762	G1659	D1573	F1507	PRO	SER	SER	PRO	THR	SER	GLY
R1763	S1660	T1574	F1508	ILE	ASN	ARG	VAL	VAL	ILE	HIS
G1764	V1661	P1575	V1509	ALA	TRP	GLU	PRO	ASP	VAL	SER
A1765	Q1662	H1576	E1510	HIS	PRO	VAL	VAL	ARG	GLY	ASN
E1766	F1663	A1577	L1511	LEU	LEU	GLY	GLY	ALA	ALA	SER
H1767	Q1667	S1578	H1512	LEU	ASN	SER	PRO	THR	ASN	ILE
P1768	M1673	N1579	L1513	PRO	GLN	SER	HIS	SER	SER	ILE
M1769	M1673	L1580	E1514	VAL	GLU	SER	VAL	PRO	ASP	LEU
F1770	V1677	S1581	A1515	LEU	ASP	SER	PRO	ARG	VAL	GLY
A1771		L1582	H1516	PRO	THR	THR	ILE	TRP	ALA	GLU
L1772		A1583	Y1517	ARG	ALA	SER	PRO	ASN	PRO	SER
M1773	A1685	L1584	E1518	ALA	GLN	GLY	PRO	HIS	THR	THR
Q1774	M1696	K1585	A1519	ALA	SER	CYS	PRO	GLY	ARG	SER
G1775	I1687	L1586	L1520	PHE	SER	SER	MET	HIS	ARG	VAL
	L1689	L1587		PRO	PRO	GLY	VAL	VAL	ALA	ALA
		L1588	L1524	VAL	GLY	GLY	VAL	VAL	ASP	PRO
	T1692	P1588	L1525	ASP	ARG	ILE	GLY	SER	ASN	THR
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				VAL	GLU	VAL	VAL	SER	HIS	TRP
		F1531		GLN	ALA	GLY	PRO	ARG	VAL	ASN
		A1532		GLU	GLU	GLY	GLU	VAL	VAL	SER
		Q1533		ALA	ALA	ASN	ALA	GLY	ILE	ASP
		S1534		ALA	SER	VAL	GLU	GLY	ALA	HIS
		L1535		ASP	ALA	SER	PRO	ASN	GLY	GLY
		S1536		GLU	ALA	ASP	ASN	VAL	VAL	HIS
		D1537		THR	GLU	VAL	THR	SER	SER	VAL
		L1538		ALA	ALA	ALA	PRO	ASP	LEU	SER
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				LEU	GLY	GLN	GLN	PRO	SER	ILE
				SER	GLU	TRP	SER	ILE	VAL	SER
					GLN	TRP	ARG	ARG	SER	ARG
				E1476	ALA	ALA	THR	ASP	ASP	VAL
				L1477	TYR	PRO	PRO	MET	GLY	GLY
				T1478	LEU	ASN	GLY	CYS	ALA	ASN
				T1479	ALA	ALA	HIS	PRO	PRO	ASN
				L1480	GLY	THR	THR	THR	ALA	VAL
				P1481	LEU	PRO	GLY	HIS	ARG	SER
					ALA	ASP	GLN	GLN	PRO	ASP
					GLY	SER	SER	HIS	ARG	VAL
					TYR	VAL	ALA	VAL	TRP	ALA
					HIS	GLU	LEU	ASP	ASN	THR
					LEU	GLU	LEU	ALA	HIS	ARG
					GLU	LEU	GLY	SER	GLY	PRO
					ARG	ARG	ILE	ILE	HIS	ASN
					PRO	GLY	GLN	PRO	VAL	TRP
					ASP	ASP	GLY	LEU	SER	ASN
					THR	THR	THR	GLY	ASP	THR
					SER	SER	VAL	GLU	ALA	HIS
					TYR	GLY	PRO	PRO	SER	GLY
					GLU	ASP	VAL	VAL	ILE	GLY
					SER	THR	CYS	ASP	SER	HIS
					MET	GLU	GLY	GLY	VAL	GLY
					SER	SER	PRO	ASP	LEU	ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	357509	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 ($e^-/\text{\AA}^2$)	46.276	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	588.0422, 588.0422, 588.0422	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36754, 1.36754, 1.36754	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	0.31	1/3460 (0.0%)	0.55	0/4686
1	b	0.29	0/3460	0.57	0/4686
1	c	0.30	0/3460	0.57	0/4686
1	d	0.30	0/3460	0.59	0/4686
1	e	0.34	0/3460	0.65	2/4686 (0.0%)
1	f	0.34	0/3454	0.63	0/4679
1	g	0.31	0/3460	0.61	1/4686 (0.0%)
1	h	0.32	0/3454	0.61	0/4679
1	i	0.31	0/3460	0.59	0/4686
1	j	0.30	0/3460	0.59	3/4686 (0.1%)
1	k	0.29	0/3460	0.57	0/4686
1	l	0.30	0/3460	0.57	0/4686
1	m	0.31	0/3460	0.59	2/4686 (0.0%)
1	n	0.31	0/3460	0.59	0/4686
2	J	0.29	0/4890	0.60	0/6625
3	I	0.33	0/4319	0.65	2/5849 (0.0%)
3	K	0.32	0/4606	0.63	5/6234 (0.1%)
4	B	0.32	0/5119	0.64	0/6912
4	D	0.37	0/4897	0.70	3/6610 (0.0%)
4	F	0.32	0/5036	0.66	0/6798
4	H	0.33	0/4935	0.67	0/6659
4	N	0.29	0/5001	0.59	0/6750
5	A	0.32	0/5038	0.65	1/6801 (0.0%)
5	C	0.31	0/5145	0.63	0/6948
5	E	0.35	0/5311	0.70	3/7169 (0.0%)
5	G	0.34	1/5295 (0.0%)	0.68	1/7147 (0.0%)
5	M	0.27	0/5295	0.58	1/7147 (0.0%)
6	L	0.34	0/5051	0.66	1/6860 (0.0%)
All	All	0.32	2/118366 (0.0%)	0.62	25/160099 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	70	GLU	C-O	-6.36	1.21	1.23
5	G	684	GLN	C-O	-5.85	1.17	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	88	PRO	N-CA-C	-9.52	101.08	114.98
1	e	88	PRO	N-CA-C	-9.20	103.97	114.92
3	I	166	PRO	N-CA-C	7.16	119.43	110.70
3	K	332	ILE	N-CA-C	-6.67	103.98	110.72
3	K	331	ARG	N-CA-C	-6.66	103.95	111.07
6	L	574	VAL	N-CA-C	-6.39	102.99	110.21
5	E	423	TYR	N-CA-C	-5.93	106.37	113.97
1	e	408	PHE	N-CA-C	-5.90	102.70	110.43
5	G	425	ASP	N-CA-C	-5.79	103.41	111.52
3	K	334	SER	N-CA-C	-5.76	106.38	113.41
4	D	882	PHE	CA-C-O	-5.66	113.30	120.20
5	M	418	ARG	CB-CG-CD	5.45	123.84	111.30
1	j	408	PHE	CA-C-O	-5.40	115.83	121.55
5	E	422	ASP	CA-CB-CG	5.35	117.95	112.60
5	E	499	LEU	N-CA-CB	5.31	118.02	110.16
4	D	786	GLN	OE1-CD-NE2	-5.26	117.34	122.60
3	K	199	GLN	CA-C-N	5.24	131.55	121.54
3	K	199	GLN	C-N-CA	5.24	131.55	121.54
1	g	408	PHE	CA-C-O	-5.16	116.08	121.55
4	D	669	ARG	N-CA-CB	5.15	117.47	110.01
1	m	409	ARG	N-CA-C	-5.13	105.77	111.36
1	j	269	LEU	CA-C-N	5.12	129.89	121.39
1	j	269	LEU	C-N-CA	5.12	129.89	121.39
5	A	518	ARG	CA-CB-CG	5.11	124.33	114.10
3	I	474	LYS	N-CA-C	-5.09	105.73	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3380	3327	3317	33	0
1	b	3380	3327	3317	30	0
1	c	3380	3327	3317	43	0
1	d	3380	3327	3317	42	0
1	e	3380	3305	3317	60	0
1	f	3374	3316	3306	38	0
1	g	3380	3327	3317	38	0
1	h	3374	3305	3306	35	0
1	i	3380	3327	3317	36	0
1	j	3380	3327	3317	30	0
1	k	3380	3327	3317	28	0
1	l	3380	3316	3317	32	0
1	m	3380	3316	3317	31	0
1	n	3380	3327	3317	45	0
2	J	4789	4769	4769	48	0
3	I	4222	4250	4250	52	0
3	K	4503	4507	4518	51	0
4	B	5015	4969	4991	83	0
4	D	4796	4764	4775	89	0
4	F	4933	4919	4919	68	0
4	H	4835	4820	4820	75	0
4	N	4899	4880	4880	44	0
5	A	4934	4956	4956	57	0
5	C	5038	5070	5070	74	0
5	E	5202	5241	5241	88	0
5	G	5186	5208	5219	99	0
5	M	5186	5219	5219	51	0
6	L	4918	4951	4951	55	0
All	All	115764	115024	114994	1368	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 (1368) 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:B:287:LEU:CD1	4:B:366:ARG:NH2	2.15	1.10
1:e:295:ARG:CD	1:e:345:LEU:HD11	1.84	1.06
1:e:295:ARG:HD2	1:e:345:LEU:CD1	1.87	1.05
3:K:329:VAL:O	3:K:333:ARG:HB3	1.69	0.91
6:L:1507:PHE:CZ	6:L:1614:ILE:CG2	2.52	0.91
6:L:1507:PHE:HZ	6:L:1614:ILE:CG2	1.82	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:287:LEU:HD12	4:B:366:ARG:NH2	1.88	0.88
1:a:17:ILE:HD12	1:a:236:MET:HE1	1.55	0.88
4:H:717:GLN:OE1	4:H:879:ARG:HB3	1.74	0.87
1:e:271:THR:HG22	1:e:378:MET:HE1	1.55	0.87
1:a:411:GLU:OE2	1:a:415:LYS:NZ	2.07	0.86
6:L:1507:PHE:HZ	6:L:1614:ILE:HG21	1.39	0.85
1:n:235:ILE:HD13	1:n:304:MET:HE1	1.56	0.85
4:B:287:LEU:HD11	4:B:366:ARG:HH22	1.44	0.83
4:B:287:LEU:HD12	4:B:366:ARG:HH21	1.44	0.82
1:d:322:ASN:ND2	1:d:357:GLN:O	2.13	0.81
2:J:883:MET:HE3	2:J:980:ILE:HD11	1.62	0.81
3:K:330:ASP:HA	3:K:333:ARG:HG2	1.62	0.80
6:L:1513:LEU:HD11	6:L:1615:VAL:HG11	1.61	0.80
1:j:376:LEU:HD21	1:j:378:MET:HE3	1.64	0.80
4:H:457:ASP:OD2	4:H:654:ARG:NE	2.15	0.79
5:A:459:VAL:HG23	5:A:460:VAL:HG13	1.64	0.79
1:i:376:LEU:HD21	1:i:378:MET:HE3	1.64	0.79
5:E:432:TYR:OH	5:E:458:ASN:ND2	2.17	0.78
4:H:883:ASN:ND2	1:h:348:PHE:O	2.17	0.78
1:e:295:ARG:HD2	1:e:345:LEU:HD11	1.50	0.78
5:E:658:VAL:HG22	5:E:762:MET:HE3	1.64	0.78
5:E:719:ILE:HD13	5:E:722:VAL:HG21	1.65	0.78
5:A:221:LEU:HD21	5:A:263:ILE:HD13	1.64	0.78
4:B:287:LEU:HD11	4:B:366:ARG:NH2	1.95	0.77
4:B:287:LEU:CD1	4:B:366:ARG:HH22	1.94	0.77
4:D:774:GLN:NE2	4:D:860:GLN:OE1	2.18	0.77
4:H:377:ARG:NH1	4:H:410:TYR:OH	2.18	0.77
3:K:333:ARG:O	3:K:337:ALA:HB3	1.85	0.77
1:d:260:LEU:O	1:d:380:ASN:ND2	2.18	0.77
1:l:340:ILE:HG12	1:l:343:ARG:HH21	1.50	0.77
5:C:614:GLU:O	5:C:643:ARG:NH2	2.18	0.76
4:B:287:LEU:CD1	4:B:366:ARG:HH21	1.91	0.76
4:D:855:GLN:OE1	4:D:886:TYR:OH	2.03	0.76
4:B:250:LEU:HD13	4:B:287:LEU:HD21	1.68	0.76
5:G:313:LEU:HD23	5:G:319:LEU:HD12	1.67	0.76
4:N:564:ARG:O	4:N:570:GLN:N	2.19	0.75
5:E:201:THR:O	5:E:231:ARG:NE	2.19	0.75
3:K:646:LEU:HD13	3:K:649:LEU:HD23	1.69	0.74
5:M:557:LEU:HD11	5:M:561:MET:HE3	1.68	0.74
5:A:468:THR:O	5:A:494:TYR:OH	2.04	0.74
5:E:201:THR:N	4:F:282:ASN:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:271:THR:OG1	4:B:272:GLU:OE1	2.04	0.74
5:G:628:LEU:HD11	5:G:723:LEU:HD11	1.69	0.74
5:C:164:LYS:NZ	5:C:284:GLU:O	2.20	0.73
6:L:611:ARG:NH1	6:L:1510:GLU:OE1	2.21	0.73
4:B:425:PRO:O	4:B:428:SER:OG	2.06	0.73
4:D:578:MET:HE1	4:D:671:LYS:HG3	1.71	0.73
4:D:738:VAL:HG13	4:D:747:ILE:HD12	1.70	0.73
1:d:320:ILE:O	1:d:357:GLN:NE2	2.21	0.73
5:E:509:LEU:HD13	5:E:626:LEU:HD22	1.71	0.73
1:m:63:ARG:NH1	1:m:125:GLU:OE1	2.22	0.73
1:g:260:LEU:O	1:g:380:ASN:ND2	2.21	0.72
1:c:338:GLN:OE1	1:c:341:ARG:NH1	2.22	0.72
5:E:424:ASN:HD22	5:E:430:GLN:HB3	1.55	0.72
5:C:532:MET:SD	5:C:653:ARG:NH2	2.63	0.72
5:M:837:LEU:HD12	5:M:856:ILE:HG23	1.70	0.72
2:J:710:LEU:O	2:J:716:LEU:N	2.22	0.72
4:D:660:TYR:OH	4:D:751:HIS:NE2	2.20	0.72
1:g:172:PHE:CD2	1:g:204:VAL:HG23	2.25	0.72
1:c:172:PHE:CD2	1:c:204:VAL:HG23	2.23	0.72
5:G:851:GLY:N	5:G:854:SER:HG	1.88	0.71
4:H:493:LEU:HD13	4:H:548:VAL:HG11	1.73	0.71
4:F:670:ALA:O	4:F:719:GLN:NE2	2.24	0.70
5:A:555:LEU:HD22	5:A:575:ILE:HD11	1.71	0.70
5:G:397:ARG:NH1	5:G:467:VAL:O	2.23	0.70
1:h:248:TYR:O	1:h:249:MET:HE2	1.92	0.70
5:E:698:MET:HE2	5:E:699:PHE:CZ	2.27	0.70
1:m:186:TYR:HD1	1:m:421:MET:HE2	1.57	0.70
3:K:543:GLN:NE2	3:K:547:GLN:OE1	2.24	0.70
2:J:429:ASN:ND2	2:J:489:ALA:O	2.25	0.70
4:B:531:GLN:NE2	4:B:535:ASP:OD2	2.24	0.70
5:G:421:GLU:O	5:G:627:SER:OG	2.09	0.70
1:c:230:GLN:O	1:c:234:THR:HG23	1.93	0.69
6:L:1791:VAL:O	6:L:1795:VAL:HG13	1.93	0.69
5:C:499:LEU:O	5:C:502:PHE:N	2.24	0.69
5:E:427:TYR:CE1	5:E:628:LEU:HD13	2.28	0.69
4:F:320:VAL:HG23	4:F:425:PRO:HG2	1.74	0.69
3:I:363:LEU:HD12	3:I:482:LEU:HG	1.73	0.69
5:E:364:PHE:CE1	5:E:479:LEU:HD11	2.27	0.69
1:e:295:ARG:CD	1:e:345:LEU:CD1	2.55	0.69
4:H:365:ARG:HG3	4:H:368:LEU:HD22	1.75	0.68
3:K:332:ILE:O	3:K:336:VAL:HG12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:637:ARG:NH2	5:A:731:ASP:OD1	2.26	0.68
1:g:294:MET:SD	1:g:322:ASN:ND2	2.67	0.68
4:H:584:GLU:OE2	4:H:596:ASN:ND2	2.25	0.68
4:H:555:LEU:HD12	4:H:648:ILE:HG23	1.74	0.68
3:K:275:LYS:HD2	3:K:333:ARG:HD2	1.75	0.68
4:N:331:GLU:OE2	4:N:377:ARG:NH1	2.27	0.68
2:J:473:LEU:HD12	2:J:638:LEU:HD22	1.76	0.67
4:H:395:GLU:O	4:H:398:SER:OG	2.10	0.67
5:A:236:GLN:O	5:A:244:ARG:NH2	2.27	0.67
4:B:546:LEU:HD13	4:B:747:ILE:HD12	1.75	0.67
5:E:698:MET:HE3	1:e:248:TYR:HB2	1.75	0.67
4:H:364:LEU:HD22	4:H:370:TRP:HE1	1.58	0.67
5:C:169:ASN:O	5:C:172:GLN:NE2	2.27	0.67
3:I:502:ARG:O	3:I:508:ASN:ND2	2.28	0.67
5:G:428:TRP:CZ2	5:G:459:VAL:HG21	2.29	0.67
3:K:333:ARG:O	3:K:333:ARG:HG3	1.93	0.67
4:B:287:LEU:CG	4:B:366:ARG:NH2	2.56	0.67
3:I:49:GLY:O	3:I:53:ILE:HD12	1.94	0.67
2:J:895:ASN:ND2	1:j:357:GLN:OE1	2.27	0.67
1:a:172:PHE:CD1	1:a:204:VAL:HG23	2.30	0.67
5:E:296:MET:O	5:E:300:VAL:HG23	1.93	0.67
5:E:691:GLN:HG3	1:e:249:MET:HE2	1.77	0.67
3:K:475:TYR:HE1	3:K:565:LEU:HD21	1.60	0.66
4:F:257:VAL:HG21	4:F:266:ILE:HG21	1.77	0.66
5:G:862:ASN:ND2	1:g:348:PHE:O	2.28	0.66
3:K:191:MET:HE2	3:K:192:LEU:HD22	1.78	0.66
4:B:486:ILE:HD11	4:B:541:THR:HB	1.75	0.66
1:i:235:ILE:HG12	1:i:304:MET:HE1	1.77	0.66
4:D:649:ALA:O	4:D:652:PHE:C	2.37	0.66
5:A:221:LEU:HD11	5:A:263:ILE:HG21	1.78	0.66
1:n:294:MET:HE3	1:n:358:VAL:HG12	1.76	0.66
3:I:540:GLN:OE1	3:I:543:GLN:NE2	2.29	0.66
4:D:726:VAL:HG11	4:D:762:CYS:SG	2.35	0.66
5:E:698:MET:HE2	5:E:699:PHE:CE2	2.29	0.66
1:l:297:LEU:HD21	1:l:377:MET:HB2	1.77	0.66
1:n:322:ASN:ND2	1:n:357:GLN:O	2.28	0.66
3:K:540:GLN:OE1	3:K:567:ASN:ND2	2.28	0.66
4:B:394:GLY:N	4:B:470:MET:SD	2.69	0.66
5:C:225:LEU:HD23	5:C:307:VAL:HG22	1.77	0.66
4:B:247:GLU:O	4:B:251:VAL:HG23	1.95	0.66
5:G:425:ASP:OD1	5:G:628:LEU:HD12	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:840:LEU:HB2	5:G:856:ILE:HD11	1.77	0.66
5:C:499:LEU:O	5:C:501:ASP:N	2.29	0.65
4:F:738:VAL:HG13	4:F:747:ILE:HD12	1.77	0.65
5:A:534:LEU:HG	5:A:554:LEU:HD22	1.77	0.65
4:B:287:LEU:HG	4:B:366:ARG:NH2	2.11	0.65
5:C:517:LYS:NZ	5:C:523:ASP:OD2	2.19	0.65
6:L:1513:LEU:CD1	6:L:1615:VAL:HG11	2.26	0.65
5:A:314:HIS:CD2	5:A:319:LEU:HD23	2.32	0.65
1:k:47:ARG:HE	1:k:50:VAL:HG23	1.61	0.65
4:D:763:LEU:HD11	4:D:873:LEU:HD21	1.77	0.65
5:E:422:ASP:HB2	5:E:631:ASN:HB2	1.79	0.65
2:J:939:ASP:OD2	2:J:944:ARG:NH2	2.29	0.65
6:L:1507:PHE:CZ	6:L:1614:ILE:HG21	2.25	0.65
5:M:495:ALA:O	5:M:499:LEU:HD23	1.97	0.64
4:N:718:MET:HE1	4:N:876:LEU:HD11	1.78	0.64
1:k:297:LEU:HD21	1:k:377:MET:HB3	1.79	0.64
1:e:295:ARG:HD3	1:e:343:ARG:HD3	1.80	0.64
4:D:561:ALA:HB3	4:D:617:ILE:HD11	1.80	0.64
4:H:457:ASP:HA	4:H:649:ALA:HB1	1.79	0.64
5:M:507:LYS:HD2	5:M:626:LEU:HD12	1.80	0.64
1:b:299:GLN:HE22	1:b:301:LYS:HG2	1.63	0.64
1:d:172:PHE:CD1	1:d:204:VAL:HG23	2.33	0.64
5:A:654:GLN:O	5:A:657:SER:OG	2.13	0.64
4:D:427:LEU:O	4:D:431:TYR:N	2.30	0.64
4:B:493:LEU:HD21	4:B:545:LEU:HD12	1.79	0.64
4:D:734:LEU:HD22	4:D:754:PHE:CG	2.32	0.63
1:g:223:PRO:O	1:g:227:GLN:NE2	2.32	0.63
4:H:659:HIS:HB2	4:H:755:LEU:HD21	1.80	0.63
2:J:710:LEU:HD23	2:J:716:LEU:HD12	1.80	0.63
5:G:641:LEU:HD12	5:G:734:LEU:HD12	1.80	0.63
4:D:297:LEU:HD12	4:D:378:LEU:HD23	1.79	0.63
1:e:124:ARG:NH2	1:e:125:GLU:OE2	2.31	0.63
3:K:7:LEU:O	3:K:10:SER:OG	2.14	0.63
3:K:337:ALA:HA	3:K:340:LEU:HD12	1.81	0.63
4:F:367:LEU:O	4:F:371:THR:HG23	1.99	0.63
5:E:637:ARG:NH1	5:E:731:ASP:OD1	2.32	0.63
5:G:658:VAL:HG13	5:G:762:MET:HE2	1.81	0.63
4:H:718:MET:HE1	4:H:775:LEU:HD13	1.81	0.63
3:I:397:GLN:OE1	3:I:401:HIS:NE2	2.29	0.63
4:N:310:GLN:OE1	4:N:311:ARG:NH1	2.31	0.63
4:H:365:ARG:CG	4:H:368:LEU:HD22	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:503:SER:O	6:L:507:GLN:NE2	2.32	0.63
6:L:359:VAL:HG22	6:L:366:ALA:HB3	1.81	0.63
5:E:517:LYS:HG3	5:E:521:LEU:HD12	1.80	0.62
5:A:641:LEU:HD11	5:A:702:MET:HE1	1.80	0.62
5:C:263:ILE:HG23	5:C:328:ILE:HD13	1.81	0.62
5:C:550:ARG:NH1	4:D:871:GLU:OE1	2.31	0.62
4:N:649:ALA:O	4:N:653:THR:HA	1.99	0.62
5:A:765:PHE:CD2	5:A:766:THR:HG23	2.34	0.62
1:e:295:ARG:NE	1:e:345:LEU:HD11	2.15	0.62
4:D:882:PHE:HB2	1:d:355:SER:HB3	1.81	0.62
4:H:315:ARG:NH2	3:I:159:LYS:O	2.32	0.62
4:D:676:ILE:HG21	4:D:786:GLN:CD	2.25	0.62
1:f:158:ASN:OD1	1:f:159:ASP:N	2.32	0.62
5:C:536:GLU:OE2	5:C:540:ARG:NE	2.32	0.62
4:H:600:ILE:HD12	4:H:603:THR:OG1	1.99	0.62
1:c:241:THR:OG1	1:c:244:ARG:NH2	2.32	0.62
1:i:290:VAL:HA	1:i:293:VAL:HG22	1.82	0.62
4:B:734:LEU:HD22	4:B:754:PHE:CG	2.34	0.62
4:F:700:VAL:HB	4:F:843:MET:HE1	1.82	0.62
1:b:235:ILE:HG12	1:b:304:MET:HE1	1.82	0.62
3:I:532:LEU:C	3:I:532:LEU:HD12	2.25	0.61
4:B:342:LEU:HD22	4:B:367:LEU:HD23	1.83	0.61
3:I:530:TYR:O	3:I:534:VAL:HG23	2.00	0.61
1:g:290:VAL:HA	1:g:293:VAL:HG22	1.81	0.61
5:A:333:ARG:O	5:A:337:ILE:HD12	1.99	0.61
4:B:665:ASN:OD1	4:B:666:PHE:N	2.33	0.61
4:D:497:CYS:HB2	4:D:553:TYR:CE1	2.35	0.61
3:I:117:LEU:HD11	3:I:121:HIS:HB2	1.81	0.61
6:L:1792:THR:O	6:L:1796:ASN:ND2	2.33	0.61
3:K:646:LEU:CD1	3:K:649:LEU:HD23	2.31	0.61
4:N:573:PHE:HA	4:N:608:THR:HG21	1.82	0.61
5:A:443:LEU:O	5:A:447:ALA:N	2.34	0.61
1:f:127:ASP:OD1	1:g:295:ARG:NH1	2.33	0.61
1:k:342:GLU:OE1	2:J:747:ARG:NH2	2.33	0.61
5:A:457:LEU:H	5:A:459:VAL:HG22	1.66	0.61
4:B:538:TYR:O	4:B:542:SER:OG	2.19	0.61
4:D:649:ALA:O	4:D:652:PHE:O	2.19	0.61
5:C:221:LEU:HD22	5:C:324:LEU:HD21	1.82	0.60
5:G:546:ILE:HD11	5:G:611:SER:OG	2.01	0.60
3:K:185:LYS:O	3:K:188:SER:OG	2.16	0.60
5:C:713:LEU:HD22	5:C:722:VAL:HG13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:397:ARG:NH1	5:E:469:CYS:SG	2.74	0.60
5:G:475:ILE:HG22	5:G:487:GLN:OE1	2.01	0.60
1:e:338:GLN:OE1	1:e:341:ARG:NE	2.34	0.60
6:L:1748:ARG:HH12	6:L:1773:MET:HE3	1.67	0.60
4:F:438:GLU:OE1	4:F:439:LEU:N	2.35	0.60
1:j:355:SER:OG	1:j:356:ILE:N	2.34	0.60
4:F:660:TYR:OH	4:F:751:HIS:NE2	2.33	0.60
4:H:485:LEU:HD23	4:H:538:TYR:HE1	1.65	0.60
1:b:241:THR:OG1	1:b:244:ARG:NH2	2.35	0.60
1:f:274:THR:HG21	1:f:293:VAL:HG13	1.83	0.60
5:C:499:LEU:C	5:C:501:ASP:N	2.58	0.60
3:I:477:VAL:HG12	3:I:574:ILE:HD11	1.84	0.60
5:M:840:LEU:HD21	5:M:855:VAL:HG11	1.84	0.60
2:J:480:ILE:HD13	2:J:562:ALA:HB3	1.84	0.59
4:N:486:ILE:HG23	4:N:541:THR:HG23	1.82	0.59
1:h:158:ASN:OD1	1:h:159:ASP:N	2.34	0.59
5:E:638:TYR:OH	5:E:726:HIS:NE2	2.33	0.59
5:M:174:LEU:HD12	5:M:175:PRO:HD2	1.84	0.59
4:B:271:THR:HG1	4:B:272:GLU:CD	2.10	0.59
5:A:660:ILE:HG13	1:a:165:LEU:HD11	1.84	0.59
4:B:743:ASP:OD1	4:B:746:HIS:N	2.35	0.59
5:E:638:TYR:HH	5:E:726:HIS:HE2	1.42	0.59
4:H:562:MET:HE1	4:H:566:LEU:HD13	1.85	0.59
5:A:360:HIS:O	5:A:363:SER:OG	2.21	0.59
1:c:204:VAL:HG21	1:c:384:ILE:HD11	1.84	0.59
5:G:540:ARG:HA	5:G:613:LEU:HD11	1.84	0.59
3:I:117:LEU:HD11	3:I:121:HIS:CB	2.32	0.59
1:b:289:THR:OG1	1:b:332:GLN:OE1	2.21	0.59
3:K:278:PHE:HB2	3:K:333:ARG:HH22	1.67	0.59
4:D:554:SER:O	4:D:558:HIS:ND1	2.34	0.59
4:D:542:SER:OG	4:D:742:GLN:O	2.20	0.59
5:E:273:VAL:HG13	5:E:296:MET:SD	2.43	0.59
1:h:291:LEU:HD12	1:h:336:SER:HB2	1.84	0.59
3:K:59:ILE:O	3:K:63:THR:HG22	2.03	0.59
5:C:414:LEU:HD11	5:C:430:GLN:OE1	2.03	0.59
5:M:757:MET:HE2	5:M:825:PHE:CZ	2.38	0.59
1:a:232:VAL:HA	1:a:235:ILE:HD12	1.85	0.59
1:c:158:ASN:OD1	1:c:159:ASP:N	2.36	0.59
1:e:235:ILE:HG12	1:e:304:MET:HE1	1.85	0.59
1:h:24:GLN:HE22	1:h:233:SER:C	2.11	0.59
4:H:717:GLN:HE22	1:h:355:SER:HB3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:426:GLU:OE2	1:d:430:GLN:NE2	2.35	0.59
5:G:507:LYS:HB3	5:G:626:LEU:HD11	1.83	0.58
1:i:297:LEU:HD12	1:i:377:MET:HG2	1.85	0.58
1:j:235:ILE:HG12	1:j:304:MET:HE1	1.85	0.58
4:F:863:VAL:O	4:F:866:THR:HG23	2.03	0.58
5:C:460:VAL:HG13	5:C:467:VAL:HG12	1.85	0.58
5:E:658:VAL:CG2	5:E:762:MET:HE3	2.32	0.58
4:F:632:ASP:OD1	4:F:633:THR:N	2.36	0.58
3:K:450:TRP:O	3:K:480:LYS:NZ	2.36	0.58
4:B:632:ASP:OD2	4:B:637:VAL:HG23	2.02	0.58
5:M:273:VAL:HG13	5:M:296:MET:HE2	1.83	0.58
5:A:682:LEU:HD22	5:A:758:PHE:CZ	2.38	0.58
4:D:700:VAL:HG21	4:D:843:MET:HE2	1.86	0.58
1:i:274:THR:OG1	1:i:293:VAL:O	2.21	0.58
6:L:1539:LEU:HD12	6:L:1552:LEU:HD21	1.86	0.58
1:a:158:ASN:OD1	1:a:159:ASP:N	2.37	0.58
5:C:731:ASP:OD1	5:C:735:LYS:NZ	2.31	0.58
4:D:448:VAL:HG22	4:D:484:LEU:HD12	1.84	0.58
4:H:326:ALA:HB2	3:I:165:LEU:HD23	1.86	0.58
4:N:434:ILE:HG23	4:N:486:ILE:HG21	1.86	0.58
5:G:458:ASN:OD1	5:G:461:ARG:NH2	2.36	0.58
4:F:319:LEU:N	4:F:445:GLU:OE2	2.37	0.58
4:F:452:PRO:O	4:F:453:THR:OG1	2.19	0.58
1:d:56:ASP:OD2	1:e:372:ARG:NH2	2.37	0.58
1:g:204:VAL:HG21	1:g:384:ILE:HD11	1.85	0.58
1:m:297:LEU:HD21	1:m:377:MET:HB3	1.86	0.58
1:m:406:GLU:HB2	1:m:411:GLU:HG2	1.86	0.58
1:n:235:ILE:CD1	1:n:304:MET:HE1	2.29	0.58
4:B:689:LYS:O	4:B:692:ARG:NH1	2.35	0.58
5:E:613:LEU:HD13	5:E:650:HIS:ND1	2.19	0.58
4:F:459:LEU:HD23	4:F:496:VAL:HG21	1.84	0.58
4:H:573:PHE:HA	4:H:608:THR:HG21	1.85	0.58
3:I:498:LEU:HD12	3:I:502:ARG:HB2	1.86	0.58
3:I:541:PHE:CZ	3:I:545:LEU:HD11	2.39	0.58
4:H:855:GLN:NE2	4:H:886:TYR:OH	2.37	0.57
4:N:553:TYR:O	4:N:558:HIS:NE2	2.37	0.57
5:A:455:LYS:HB3	5:A:719:ILE:HD13	1.86	0.57
1:g:158:ASN:OD1	1:g:159:ASP:N	2.37	0.57
2:J:558:GLN:NE2	2:J:696:ASP:OD1	2.37	0.57
4:B:362:LEU:HG	4:B:367:LEU:HD11	1.86	0.57
1:n:274:THR:O	1:n:302:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:245:ILE:HD11	4:F:287:LEU:CD1	2.34	0.57
5:A:555:LEU:HD22	5:A:575:ILE:CD1	2.34	0.57
4:N:681:ARG:NH1	1:n:262:PRO:O	2.37	0.57
2:J:429:ASN:OD1	2:J:430:VAL:N	2.38	0.57
2:J:903:THR:HG21	1:j:249:MET:HE2	1.87	0.57
4:D:764:LEU:HA	4:D:772:LEU:HD11	1.86	0.57
1:d:158:ASN:OD1	1:d:159:ASP:N	2.38	0.57
1:m:290:VAL:HA	1:m:293:VAL:HG22	1.86	0.57
1:k:270:MET:HE3	1:k:305:VAL:HB	1.86	0.57
5:G:762:MET:HE3	5:G:763:GLN:N	2.20	0.57
1:a:340:ILE:HD13	1:a:343:ARG:HD2	1.87	0.57
1:c:399:ARG:NH1	1:c:402:GLU:OE1	2.37	0.57
1:h:290:VAL:HA	1:h:293:VAL:HG22	1.85	0.57
1:m:158:ASN:OD1	1:m:159:ASP:N	2.37	0.57
3:K:180:HIS:NE2	3:K:267:TYR:OH	2.28	0.57
4:F:734:LEU:HD22	4:F:754:PHE:CG	2.39	0.57
1:e:158:ASN:OD1	1:e:159:ASP:N	2.38	0.57
1:e:378:MET:HE3	1:e:378:MET:HA	1.84	0.57
4:H:553:TYR:O	4:H:558:HIS:NE2	2.37	0.57
4:N:718:MET:CE	4:N:876:LEU:HD11	2.35	0.57
3:I:493:GLN:CD	1:i:254:ILE:HD12	2.30	0.56
1:a:6:ILE:HG22	1:a:132:LEU:HD11	1.87	0.56
5:G:843:TYR:O	5:G:844:SER:C	2.48	0.56
4:F:305:ARG:HA	4:F:308:THR:HG22	1.87	0.56
5:G:694:GLN:NE2	1:g:249:MET:HE3	2.19	0.56
5:M:686:MET:HE2	5:M:755:CYS:SG	2.46	0.56
1:b:158:ASN:OD1	1:b:159:ASP:N	2.38	0.56
1:e:297:LEU:HD21	1:e:377:MET:HB3	1.86	0.56
5:E:703:GLU:HB3	5:E:704:PRO:HD3	1.86	0.56
5:A:645:MET:HE3	5:A:698:MET:SD	2.45	0.56
1:n:297:LEU:HD21	1:n:377:MET:HB3	1.87	0.56
4:N:597:LEU:HD12	4:N:625:LEU:HD11	1.87	0.56
1:d:174:ASN:O	1:d:208:THR:OG1	2.11	0.56
4:D:490:ILE:HD12	4:D:493:LEU:HD23	1.87	0.56
5:A:456:TYR:HB2	5:A:719:ILE:HG22	1.88	0.56
4:B:731:TRP:CZ3	4:B:734:LEU:HD23	2.41	0.56
4:F:497:CYS:O	4:F:553:TYR:OH	2.09	0.56
1:n:158:ASN:OD1	1:n:159:ASP:N	2.39	0.56
3:K:131:LEU:HD21	3:K:165:LEU:HD12	1.87	0.56
1:h:4:GLU:OE1	1:h:63:ARG:NH1	2.39	0.56
5:G:205:ILE:HD13	5:G:232:TYR:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:1506:TYR:OH	6:L:1706:LEU:HD21	2.05	0.56
4:F:411:MET:O	4:F:415:VAL:HG22	2.05	0.56
6:L:1641:LEU:HD12	6:L:1677:VAL:HG21	1.88	0.56
5:E:325:TRP:CZ3	5:E:332:MET:HE2	2.41	0.55
1:j:158:ASN:OD1	1:j:159:ASP:N	2.39	0.55
4:F:342:LEU:HD22	4:F:367:LEU:HD22	1.87	0.55
4:F:459:LEU:HD11	4:F:492:PHE:CD1	2.42	0.55
4:H:646:GLY:O	4:H:649:ALA:HB3	2.06	0.55
1:a:77:ILE:O	1:a:86:TYR:OH	2.23	0.55
1:k:158:ASN:OD1	1:k:159:ASP:N	2.39	0.55
5:M:397:ARG:HD2	5:M:399:ILE:HD12	1.87	0.55
1:c:235:ILE:HG12	1:c:304:MET:HE1	1.88	0.55
1:j:297:LEU:HD21	1:j:377:MET:HB3	1.88	0.55
3:K:336:VAL:O	3:K:340:LEU:N	2.39	0.55
3:K:363:LEU:HD12	3:K:482:LEU:HB3	1.87	0.55
5:E:388:PHE:O	5:E:391:LEU:N	2.40	0.55
5:A:400:ILE:HD11	5:A:432:TYR:HE1	1.70	0.55
5:A:400:ILE:HD11	5:A:432:TYR:CE1	2.42	0.55
1:i:290:VAL:HG11	1:i:328:VAL:HG13	1.88	0.55
4:B:457:ASP:HB3	4:B:653:THR:HA	1.88	0.55
4:B:559:MET:HG2	4:B:651:VAL:HG21	1.88	0.55
5:C:256:ILE:HD12	5:C:321:LEU:HD13	1.89	0.55
5:C:500:LEU:HD11	5:C:719:ILE:HD11	1.88	0.55
5:E:509:LEU:HD11	5:E:630:ILE:CD1	2.36	0.55
4:F:578:MET:HE1	4:F:675:TYR:HB2	1.89	0.55
4:N:604:ALA:O	4:N:608:THR:HG22	2.06	0.55
1:l:158:ASN:OD1	1:l:159:ASP:N	2.39	0.55
4:B:304:ILE:HG23	4:B:328:LEU:HD11	1.88	0.55
5:E:728:GLY:O	5:E:732:THR:HG23	2.07	0.55
4:N:608:THR:HG23	4:N:610:ALA:H	1.72	0.55
5:C:448:ASP:OD1	5:C:449:LYS:N	2.40	0.55
5:E:682:LEU:HD13	5:E:826:ASP:HA	1.89	0.55
1:h:340:ILE:HD13	1:h:343:ARG:HD2	1.87	0.55
5:C:246:PHE:CD1	5:C:264:LEU:HD21	2.42	0.55
4:H:681:ARG:NH1	1:h:262:PRO:O	2.40	0.55
1:a:4:GLU:O	1:a:132:LEU:HD12	2.07	0.55
1:e:294:MET:HE1	1:e:358:VAL:HG12	1.88	0.55
4:F:719:GLN:HG3	1:f:249:MET:HE3	1.89	0.54
6:L:1688:ILE:HG23	6:L:1692:THR:HG21	1.88	0.54
5:E:719:ILE:HD13	5:E:722:VAL:CG2	2.37	0.54
3:I:493:GLN:OE1	1:i:254:ILE:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:459:VAL:HG11	5:M:628:LEU:HD11	1.88	0.54
1:e:172:PHE:CD1	1:e:204:VAL:HG23	2.42	0.54
2:J:392:THR:HG21	3:I:112:LEU:HD13	1.89	0.54
1:h:320:ILE:HG21	1:h:356:ILE:HD12	1.89	0.54
4:F:719:GLN:CG	1:f:249:MET:HE3	2.38	0.54
1:f:376:LEU:HD21	1:f:378:MET:HE2	1.89	0.54
1:j:270:MET:HE1	1:j:384:ILE:HD13	1.89	0.54
2:J:729:MET:HE1	2:J:824:VAL:CG1	2.38	0.54
3:I:153:ILE:HG23	3:I:154:LEU:HD12	1.90	0.54
1:c:238:ALA:HB1	1:c:376:LEU:HD23	1.89	0.54
1:m:89:GLU:OE1	1:n:215:THR:HG22	2.07	0.54
3:K:314:LEU:HD21	3:K:328:VAL:HG11	1.88	0.54
4:D:780:ASP:HA	4:D:783:ILE:HG22	1.90	0.54
5:C:682:LEU:HD22	5:C:758:PHE:CZ	2.42	0.54
5:E:217:VAL:HG23	5:E:321:LEU:HD21	1.89	0.54
5:E:325:TRP:HZ3	5:E:332:MET:HE2	1.73	0.54
5:G:160:MET:HE1	5:G:285:TYR:CE2	2.42	0.54
5:G:628:LEU:CD1	5:G:723:LEU:HD21	2.38	0.54
1:f:188:SER:O	1:f:192:LEU:HD23	2.07	0.54
4:B:377:ARG:NH2	4:B:410:TYR:OH	2.39	0.54
5:E:658:VAL:HG22	5:E:762:MET:CE	2.35	0.54
4:B:266:ILE:CD1	4:B:277:VAL:HG13	2.37	0.54
4:B:493:LEU:HB3	4:B:549:LEU:HD13	1.88	0.54
1:b:153:LEU:O	1:b:157:LEU:HD23	2.08	0.54
2:J:556:LEU:O	2:J:560:ILE:HD12	2.07	0.53
5:A:397:ARG:HH21	5:A:399:ILE:HD11	1.74	0.53
1:c:204:VAL:O	1:c:205:LEU:HD22	2.07	0.53
1:e:295:ARG:HD3	1:e:345:LEU:HD11	1.85	0.53
1:h:235:ILE:HD11	1:h:304:MET:SD	2.48	0.53
1:k:294:MET:HA	1:k:294:MET:HE3	1.88	0.53
5:C:229:ASP:OD1	5:C:230:GLY:N	2.40	0.53
5:C:638:TYR:CD1	5:C:730:LEU:HD13	2.42	0.53
5:E:364:PHE:HE1	5:E:479:LEU:HD11	1.70	0.53
3:I:589:LEU:HD21	3:I:619:PHE:HB2	1.90	0.53
5:A:818:PHE:O	5:A:821:THR:OG1	2.22	0.53
4:B:287:LEU:CG	4:B:366:ARG:HH21	2.18	0.53
4:B:490:ILE:HD11	4:B:541:THR:HG22	1.90	0.53
4:F:726:VAL:HG11	4:F:762:CYS:SG	2.48	0.53
4:H:456:THR:O	4:H:649:ALA:HB1	2.09	0.53
3:I:136:VAL:HG22	3:I:172:LEU:HD11	1.90	0.53
1:a:34:GLU:O	1:a:84:LYS:NZ	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:392:THR:HG21	3:I:112:LEU:CD1	2.39	0.53
4:D:490:ILE:HD12	4:D:493:LEU:CD2	2.39	0.53
5:G:222:LEU:O	4:H:365:ARG:NH1	2.42	0.53
5:M:448:ASP:OD1	5:M:449:LYS:N	2.41	0.53
5:A:448:ASP:OD1	5:A:449:LYS:N	2.42	0.53
5:C:334:THR:OG1	5:C:371:GLN:NE2	2.39	0.53
5:A:541:LYS:CE	5:A:546:ILE:HA	2.39	0.53
1:b:188:SER:O	1:b:192:LEU:HD23	2.09	0.53
1:i:154:LEU:HD12	1:i:166:VAL:HG11	1.91	0.53
2:J:267:GLU:HB2	2:J:302:VAL:HG11	1.90	0.53
4:B:495:GLN:HG3	4:B:496:VAL:HG23	1.90	0.53
5:C:532:MET:HE1	5:C:646:PHE:CZ	2.43	0.53
5:M:503:LEU:CD2	5:M:719:ILE:HD12	2.39	0.53
4:N:542:SER:C	4:N:544:TYR:H	2.17	0.53
1:d:297:LEU:HD21	1:d:377:MET:HB2	1.90	0.53
1:i:238:ALA:HB3	1:i:376:LEU:HD13	1.91	0.53
1:m:297:LEU:HD11	1:m:377:MET:HG3	1.90	0.53
4:B:367:LEU:HD12	4:B:367:LEU:N	2.23	0.53
5:E:446:MET:HE3	5:E:485:VAL:HG22	1.90	0.53
1:e:252:ASP:OD1	1:e:252:ASP:N	2.42	0.53
3:K:282:SER:HB3	3:K:340:LEU:HD13	1.90	0.53
1:c:290:VAL:HA	1:c:293:VAL:HG22	1.90	0.53
1:l:174:ASN:O	1:l:208:THR:OG1	2.26	0.53
4:F:694:MET:HE3	4:F:800:LEU:HD22	1.92	0.52
5:A:486:GLU:N	5:A:486:GLU:OE1	2.42	0.52
1:b:297:LEU:HD21	1:b:377:MET:HB3	1.89	0.52
1:m:190:LEU:HD21	1:m:421:MET:SD	2.49	0.52
1:m:406:GLU:HB3	1:m:408:PHE:CZ	2.43	0.52
1:k:341:ARG:HD3	3:K:646:LEU:HD12	1.91	0.52
4:D:251:VAL:HA	4:D:254:ILE:HG22	1.91	0.52
4:N:461:HIS:NE2	4:N:748:ILE:HD11	2.25	0.52
1:e:69:LEU:HD21	1:e:110:GLN:OE1	2.08	0.52
1:f:174:ASN:O	1:f:208:THR:OG1	2.22	0.52
2:J:762:LEU:HD22	2:J:763:GLN:HE22	1.75	0.52
3:K:199:GLN:O	3:K:200:HIS:ND1	2.42	0.52
5:E:427:TYR:CZ	5:E:628:LEU:HD13	2.44	0.52
5:G:493:ASN:OD1	5:G:494:TYR:N	2.42	0.52
5:M:205:ILE:HD12	5:M:208:LEU:HD12	1.91	0.52
1:d:249:MET:HE3	1:d:250:ASN:H	1.74	0.52
1:g:77:ILE:O	1:g:86:TYR:OH	2.27	0.52
1:i:158:ASN:OD1	1:i:159:ASP:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:563:ARG:NE	1:d:248:TYR:OH	2.40	0.52
4:F:765:ASP:OD1	4:F:766:SER:N	2.43	0.52
6:L:1525:LEU:HD22	6:L:1627:VAL:HG21	1.91	0.52
1:j:270:MET:HE1	1:j:305:VAL:HG11	1.91	0.52
4:B:460:TRP:CD1	4:B:650:THR:O	2.62	0.52
4:F:709:SER:O	4:F:712:VAL:HG12	2.10	0.52
5:G:355:THR:HG22	5:G:355:THR:O	2.10	0.52
1:a:204:VAL:HG21	1:a:384:ILE:HD11	1.90	0.52
1:c:406:GLU:HB3	1:c:408:PHE:CE2	2.45	0.52
2:J:891:MET:HE1	1:j:258:ALA:O	2.09	0.52
4:B:266:ILE:HD13	4:B:277:VAL:HG13	1.90	0.52
4:F:377:ARG:HD3	4:F:414:LEU:HD22	1.91	0.52
6:L:1608:VAL:HG23	6:L:1613:ASN:OD1	2.08	0.52
5:M:413:GLU:OE2	5:M:413:GLU:N	2.42	0.52
1:b:290:VAL:HA	1:b:293:VAL:HG22	1.92	0.52
1:c:132:LEU:HD21	1:c:135:PHE:HE1	1.75	0.52
1:m:189:LEU:HD23	1:m:421:MET:HE3	1.91	0.52
2:J:699:TYR:OH	2:J:922:ASP:OD1	2.24	0.52
4:D:324:PHE:HB2	4:D:422:VAL:HG22	1.92	0.52
5:E:658:VAL:HG23	5:E:763:GLN:OE1	2.09	0.52
5:A:517:LYS:HZ3	5:A:706:TRP:CD1	2.27	0.52
1:j:206:ASP:OD2	1:j:305:VAL:HG13	2.10	0.52
2:J:473:LEU:HD12	2:J:638:LEU:CD2	2.40	0.52
4:D:692:ARG:NH2	1:d:197:GLN:O	2.43	0.52
5:E:419:ILE:HG22	5:E:420:GLN:O	2.10	0.52
5:G:428:TRP:CZ3	5:G:628:LEU:HD22	2.43	0.52
5:G:837:LEU:HD13	5:G:856:ILE:HG23	1.91	0.52
4:H:274:CYS:SG	4:H:275:TYR:N	2.83	0.52
1:e:405:LEU:O	1:e:407:GLN:N	2.41	0.52
1:n:294:MET:HE1	1:n:322:ASN:OD1	2.10	0.52
5:C:412:HIS:ND1	5:C:430:GLN:O	2.43	0.52
4:D:342:LEU:HD22	4:D:367:LEU:HD22	1.91	0.52
4:D:496:VAL:O	4:D:553:TYR:CE2	2.63	0.52
4:D:707:LEU:HD11	4:D:711:MET:HE2	1.91	0.52
5:E:424:ASN:HB2	5:E:430:GLN:OE1	2.10	0.52
1:b:261:ILE:HD12	1:b:267:HIS:HA	1.90	0.52
1:n:294:MET:CE	1:n:358:VAL:HG12	2.40	0.52
5:E:419:ILE:HD13	5:E:423:TYR:CD1	2.45	0.52
1:b:252:ASP:OD1	1:b:252:ASP:N	2.42	0.52
1:l:343:ARG:HB3	1:l:345:LEU:HG	1.92	0.52
5:E:434:ILE:HB	5:E:451:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:69:LEU:HD23	1:f:70:GLU:HG3	1.92	0.51
1:k:112:GLU:O	1:k:115:HIS:ND1	2.40	0.51
3:K:475:TYR:CE1	3:K:565:LEU:HD21	2.42	0.51
5:G:338:LEU:CD2	5:G:379:LEU:HD21	2.41	0.51
5:G:357:SER:OG	5:G:440:PRO:O	2.29	0.51
5:M:503:LEU:HD23	5:M:719:ILE:HD12	1.92	0.51
1:f:108:PHE:HE2	1:f:194:ARG:HH12	1.57	0.51
1:m:87:ASN:ND2	1:n:219:HIS:HA	2.25	0.51
5:C:412:HIS:O	5:C:431:ARG:NE	2.43	0.51
4:D:865:LEU:CD2	4:D:873:LEU:HD23	2.40	0.51
4:N:721:TYR:CD2	4:N:876:LEU:HD13	2.45	0.51
1:d:16:GLN:HE21	1:d:73:VAL:HG11	1.75	0.51
1:f:297:LEU:HD21	1:f:377:MET:HB3	1.92	0.51
1:i:174:ASN:O	1:i:208:THR:HG23	2.09	0.51
4:F:245:ILE:HD11	4:F:287:LEU:HD13	1.91	0.51
4:F:562:MET:HE1	4:F:657:MET:HE1	1.91	0.51
5:A:840:LEU:HD21	5:A:855:VAL:CG2	2.40	0.51
1:d:290:VAL:HA	1:d:293:VAL:HG22	1.92	0.51
1:k:77:ILE:O	1:k:86:TYR:OH	2.29	0.51
3:K:328:VAL:HA	3:K:331:ARG:CD	2.41	0.51
4:D:726:VAL:HG13	4:D:761:ARG:HB3	1.91	0.51
5:E:359:LEU:HB3	5:E:380:THR:HG22	1.92	0.51
5:G:705:THR:HA	5:G:708:ILE:HD12	1.92	0.51
4:H:584:GLU:CD	4:H:596:ASN:HD22	2.19	0.51
4:N:446:PHE:CD2	4:N:448:VAL:HG12	2.45	0.51
1:i:377:MET:O	1:i:378:MET:HE2	2.10	0.51
4:B:364:LEU:HD12	4:B:364:LEU:H	1.76	0.51
4:D:609:ASN:ND2	1:d:46:ASP:O	2.42	0.51
4:H:564:ARG:O	4:H:570:GLN:N	2.35	0.51
1:k:290:VAL:HA	1:k:293:VAL:HG22	1.93	0.51
5:G:654:GLN:O	5:G:658:VAL:HG23	2.11	0.51
6:L:1795:VAL:HG12	6:L:1803:LEU:HB2	1.92	0.51
4:B:319:LEU:N	4:B:445:GLU:OE2	2.42	0.51
5:C:507:LYS:HA	5:C:507:LYS:HE3	1.92	0.51
4:D:438:GLU:OE2	4:D:491:ASN:ND2	2.43	0.51
5:E:213:GLN:O	5:E:217:VAL:HG22	2.11	0.51
1:a:406:GLU:HB3	1:a:408:PHE:CE2	2.46	0.51
1:g:295:ARG:HD3	1:g:343:ARG:HD3	1.92	0.51
4:F:492:PHE:HE2	4:F:549:LEU:HD21	1.76	0.51
5:M:550:ARG:O	5:M:554:LEU:HD23	2.11	0.51
5:M:682:LEU:HD22	5:M:758:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:252:ASP:OD1	1:c:252:ASP:N	2.43	0.51
1:e:115:HIS:NE2	1:e:116:GLU:OE2	2.44	0.51
1:m:252:ASP:OD1	1:m:252:ASP:N	2.44	0.51
1:n:8:LEU:HD23	1:n:65:VAL:HB	1.92	0.51
5:A:448:ASP:O	5:A:452:SER:OG	2.22	0.51
1:n:66:LEU:HD22	1:n:91:ILE:HD13	1.92	0.51
1:k:252:ASP:N	1:k:252:ASP:OD1	2.44	0.50
5:C:638:TYR:CE1	5:C:730:LEU:HD13	2.47	0.50
5:G:174:LEU:HD13	5:G:404:TYR:HE1	1.76	0.50
5:G:460:VAL:HG23	5:G:502:PHE:CD1	2.45	0.50
3:I:532:LEU:HD12	3:I:532:LEU:O	2.11	0.50
5:M:373:GLN:O	5:M:377:LEU:HD12	2.11	0.50
5:A:409:VAL:HG22	5:A:451:LEU:HD13	1.92	0.50
1:f:69:LEU:HD21	1:f:110:GLN:OE1	2.10	0.50
5:G:541:LYS:HE3	5:G:546:ILE:HG22	1.92	0.50
5:G:685:ARG:NH1	5:G:830:SER:OG	2.45	0.50
5:M:394:TRP:HE1	5:M:450:ILE:HG22	1.76	0.50
1:m:183:VAL:HG22	1:m:186:TYR:HB2	1.93	0.50
1:n:77:ILE:O	1:n:86:TYR:OH	2.28	0.50
2:J:810:ASP:OD1	2:J:811:ILE:N	2.44	0.50
4:H:485:LEU:HD23	4:H:538:TYR:CE1	2.47	0.50
4:N:734:LEU:HD12	4:N:754:PHE:HB2	1.93	0.50
1:f:156:ARG:O	1:f:160:ARG:NE	2.41	0.50
1:i:127:ASP:OD1	1:j:295:ARG:HD3	2.11	0.50
5:C:455:LYS:O	5:C:459:VAL:HG23	2.11	0.50
4:D:574:ILE:HG22	4:D:578:MET:HE3	1.93	0.50
4:F:882:PHE:HB3	1:f:355:SER:HB2	1.94	0.50
4:H:744:LEU:HA	4:H:747:ILE:HG22	1.92	0.50
5:A:388:PHE:CD1	5:A:475:ILE:HD12	2.45	0.50
1:d:257:ILE:HG23	1:d:261:ILE:HD13	1.94	0.50
1:l:405:LEU:HD11	1:l:418:PHE:CD1	2.47	0.50
2:J:752:TRP:HH2	2:J:799:LEU:HD21	1.76	0.50
5:G:762:MET:HA	5:G:765:PHE:CE2	2.46	0.50
1:j:252:ASP:OD1	1:j:252:ASP:N	2.45	0.50
1:j:406:GLU:HB3	1:j:408:PHE:CE2	2.46	0.50
4:D:691:LEU:HD23	4:D:691:LEU:O	2.11	0.50
5:E:575:ILE:HD12	5:E:616:PHE:CZ	2.46	0.50
5:G:428:TRP:CE3	5:G:628:LEU:HD13	2.46	0.50
6:L:1688:ILE:HG22	6:L:1689:LEU:H	1.76	0.50
5:M:282:SER:O	5:M:290:HIS:NE2	2.45	0.50
1:d:77:ILE:O	1:d:86:TYR:OH	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:260:LEU:HD21	1:f:321:LEU:HB3	1.94	0.50
5:C:701:VAL:HG11	5:C:737:CYS:SG	2.52	0.50
4:D:697:PHE:CE2	4:D:796:ALA:HB1	2.46	0.50
4:H:717:GLN:NE2	1:h:355:SER:HB3	2.27	0.50
5:M:221:LEU:HD11	5:M:260:VAL:HG13	1.94	0.50
1:d:204:VAL:HG21	1:d:384:ILE:HD11	1.94	0.50
5:G:313:LEU:HD21	5:G:323:LYS:HE3	1.94	0.50
5:A:705:THR:HG22	5:A:729:PHE:HD1	1.77	0.50
1:g:297:LEU:HD21	1:g:377:MET:HB3	1.93	0.50
1:n:206:ASP:HB2	1:n:209:ALA:HB3	1.94	0.50
1:a:290:VAL:HG11	1:a:328:VAL:HG13	1.92	0.50
1:l:190:LEU:HD11	1:l:421:MET:HE2	1.94	0.50
4:F:579:ASP:OD1	1:f:3:ARG:NH2	2.45	0.49
5:G:214:GLU:O	5:G:218:VAL:HG23	2.11	0.49
5:G:408:MET:HE1	5:G:450:ILE:CD1	2.41	0.49
3:I:158:TYR:HD1	3:I:176:LEU:HD11	1.77	0.49
1:g:231:LEU:O	1:g:234:THR:OG1	2.27	0.49
1:h:290:VAL:HG11	1:h:333:VAL:HG22	1.94	0.49
1:i:252:ASP:N	1:i:252:ASP:OD1	2.43	0.49
4:H:396:LEU:O	4:H:400:VAL:HG23	2.12	0.49
1:h:183:VAL:HG22	1:h:186:TYR:HB2	1.95	0.49
4:B:663:VAL:HG22	4:B:667:LEU:HD23	1.93	0.49
5:C:429:ASP:OD1	5:C:430:GLN:N	2.45	0.49
4:D:568:LEU:HD11	4:D:664:PHE:CD1	2.48	0.49
1:a:186:TYR:HD1	1:a:421:MET:HE3	1.78	0.49
1:c:260:LEU:HD13	1:c:269:LEU:HD23	1.93	0.49
4:B:840:ILE:HD13	4:B:843:MET:CE	2.42	0.49
5:C:647:TYR:O	5:C:651:VAL:HG13	2.12	0.49
4:D:723:THR:HG23	1:d:248:TYR:CB	2.42	0.49
4:F:385:VAL:HG12	4:F:385:VAL:O	2.11	0.49
4:F:689:LYS:NZ	1:f:162:PRO:O	2.42	0.49
5:M:414:LEU:HD23	5:M:426:LYS:HB2	1.94	0.49
1:h:231:LEU:O	1:h:234:THR:OG1	2.25	0.49
1:i:406:GLU:HB3	1:i:408:PHE:CE2	2.47	0.49
2:J:498:LYS:O	2:J:502:VAL:HG13	2.13	0.49
5:C:409:VAL:HG22	5:C:451:LEU:HD12	1.93	0.49
4:H:584:GLU:CD	4:H:596:ASN:ND2	2.69	0.49
1:e:77:ILE:O	1:e:86:TYR:OH	2.30	0.49
1:e:231:LEU:O	1:e:234:THR:OG1	2.29	0.49
1:h:252:ASP:OD1	1:h:252:ASP:N	2.45	0.49
1:m:87:ASN:HD22	1:n:219:HIS:HA	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:714:PHE:CE1	4:D:778:VAL:HG11	2.46	0.49
5:E:263:ILE:HG23	5:E:328:ILE:CD1	2.42	0.49
5:G:693:ILE:HD13	5:G:855:VAL:HG21	1.94	0.49
4:N:486:ILE:HG12	4:N:542:SER:HB2	1.95	0.49
5:M:557:LEU:CD1	5:M:561:MET:HE3	2.42	0.49
1:d:256:LEU:HD21	1:d:378:MET:SD	2.53	0.49
1:l:406:GLU:HB3	1:l:408:PHE:CZ	2.48	0.49
4:B:550:ASN:HD21	4:B:556:LEU:HD12	1.78	0.49
4:B:651:VAL:HG13	4:B:652:PHE:CD1	2.48	0.49
4:D:367:LEU:O	4:D:371:THR:HG23	2.12	0.49
5:M:440:PRO:O	5:M:441:SER:OG	2.18	0.49
1:a:290:VAL:HA	1:a:293:VAL:HG22	1.94	0.49
1:g:252:ASP:OD1	1:g:252:ASP:N	2.45	0.49
5:C:263:ILE:HG23	5:C:328:ILE:CD1	2.43	0.49
5:E:409:VAL:HG22	5:E:451:LEU:HD13	1.95	0.49
5:E:619:ASP:OD1	5:E:620:TYR:N	2.46	0.49
5:G:252:LEU:O	5:G:257:ARG:NH2	2.46	0.49
4:N:341:VAL:HG12	4:N:345:GLN:OE1	2.13	0.49
4:B:492:PHE:CE2	4:B:650:THR:HB	2.47	0.49
5:G:351:LEU:N	5:G:354:SER:OG	2.44	0.49
5:G:532:MET:HE1	5:G:539:LEU:HD12	1.95	0.49
5:M:414:LEU:HD11	5:M:418:ARG:NH2	2.28	0.49
1:h:204:VAL:C	1:h:205:LEU:HD12	2.38	0.49
1:l:77:ILE:O	1:l:86:TYR:OH	2.30	0.49
1:l:252:ASP:OD1	1:l:252:ASP:N	2.45	0.49
5:C:225:LEU:CD2	5:C:307:VAL:HG22	2.41	0.48
4:D:544:TYR:O	4:D:548:VAL:HG12	2.14	0.48
6:L:1507:PHE:CZ	6:L:1614:ILE:HG22	2.44	0.48
5:M:408:MET:HE1	5:M:450:ILE:HD12	1.94	0.48
5:A:765:PHE:HD2	5:A:766:THR:HG23	1.76	0.48
1:d:235:ILE:HD11	1:d:304:MET:SD	2.52	0.48
1:e:204:VAL:HG21	1:e:384:ILE:HD11	1.95	0.48
4:B:458:ARG:H	4:B:653:THR:HA	1.78	0.48
4:F:315:ARG:NH1	5:G:366:TYR:OH	2.43	0.48
4:F:788:ALA:O	4:F:792:ILE:HD12	2.13	0.48
5:G:844:SER:C	5:G:852:MET:SD	2.96	0.48
3:I:532:LEU:HG	3:I:533:GLN:N	2.28	0.48
6:L:601:THR:HG23	6:L:1506:TYR:CD1	2.47	0.48
1:b:407:GLN:O	1:b:408:PHE:C	2.56	0.48
1:l:290:VAL:HG11	1:l:328:VAL:HG13	1.95	0.48
4:B:747:ILE:HG22	4:B:747:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:270:MET:HE3	1:d:305:VAL:HB	1.95	0.48
1:e:139:HIS:HE1	1:e:141:ILE:HD13	1.78	0.48
1:f:77:ILE:O	1:f:86:TYR:OH	2.30	0.48
1:n:252:ASP:N	1:n:252:ASP:OD1	2.46	0.48
2:J:951:LYS:HD2	2:J:955:MET:HE3	1.94	0.48
1:f:405:LEU:HD23	1:f:407:GLN:HG2	1.95	0.48
1:g:249:MET:HE2	1:g:249:MET:HA	1.94	0.48
4:D:738:VAL:HG13	4:D:747:ILE:CD1	2.41	0.48
5:M:446:MET:HE3	5:M:485:VAL:HG13	1.95	0.48
1:c:260:LEU:HD13	1:c:269:LEU:CD2	2.43	0.48
1:j:290:VAL:HA	1:j:293:VAL:HG22	1.95	0.48
1:l:290:VAL:HA	1:l:293:VAL:HG22	1.95	0.48
1:m:290:VAL:HG23	1:m:336:SER:HB2	1.96	0.48
2:J:267:GLU:O	2:J:271:ILE:HD12	2.14	0.48
4:B:541:THR:HA	4:B:545:LEU:HD23	1.94	0.48
4:F:734:LEU:HD22	4:F:754:PHE:CD2	2.48	0.48
5:M:160:MET:HE2	5:M:349:GLU:OE2	2.13	0.48
4:B:342:LEU:HD13	4:B:367:LEU:HD23	1.96	0.48
5:G:747:VAL:HG23	5:G:836:LEU:HD12	1.95	0.48
3:I:475:TYR:CZ	3:I:565:LEU:HD21	2.48	0.48
6:L:605:LEU:HD12	6:L:606:LYS:N	2.29	0.48
6:L:1609:ASP:O	6:L:1612:LEU:N	2.47	0.48
5:A:310:LEU:HD12	5:A:324:LEU:HD13	1.96	0.48
1:b:290:VAL:HG11	1:b:328:VAL:HG13	1.94	0.48
1:e:338:GLN:O	1:e:341:ARG:HG2	2.14	0.48
1:i:56:ASP:OD1	1:i:57:ASP:N	2.46	0.48
1:m:340:ILE:HD13	1:m:343:ARG:HD2	1.94	0.48
2:J:265:VAL:HG12	2:J:300:ILE:HG23	1.96	0.48
5:C:565:ASN:OD1	5:C:566:THR:N	2.45	0.48
5:E:221:LEU:HA	5:E:224:VAL:HG12	1.95	0.48
3:I:500:MET:SD	1:i:165:LEU:HD11	2.53	0.48
3:I:533:GLN:O	3:I:537:LEU:HD23	2.14	0.48
1:b:321:LEU:HD13	1:b:357:GLN:HE21	1.77	0.48
1:f:137:LEU:HD13	1:f:166:VAL:HG13	1.96	0.48
2:J:955:MET:HE2	2:J:955:MET:N	2.29	0.48
4:B:304:ILE:CG2	4:B:328:LEU:HD11	2.43	0.48
5:G:428:TRP:HZ2	5:G:459:VAL:HG21	1.76	0.48
5:A:260:VAL:O	5:A:264:LEU:HD23	2.14	0.48
1:b:329:ASP:OD1	1:b:331:THR:HG22	2.13	0.48
1:g:323:ILE:HD13	1:g:376:LEU:HD11	1.96	0.48
5:E:655:LEU:HB3	5:E:687:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:365:ARG:HB3	4:H:368:LEU:HB2	1.96	0.48
1:a:8:LEU:HD12	1:a:137:LEU:HD11	1.96	0.48
4:F:486:ILE:HA	4:F:541:THR:HG21	1.96	0.47
3:I:85:TYR:HB3	3:I:153:ILE:HG21	1.95	0.47
5:M:188:ILE:HG22	5:M:278:GLU:HG3	1.95	0.47
1:b:77:ILE:O	1:b:86:TYR:OH	2.31	0.47
1:c:417:ASN:OD1	1:c:418:PHE:N	2.47	0.47
1:e:201:CYS:SG	1:e:202:VAL:N	2.87	0.47
1:f:21:PHE:HB2	1:f:236:MET:HE3	1.96	0.47
1:h:238:ALA:HB3	1:h:376:LEU:HD13	1.96	0.47
1:j:295:ARG:HG3	1:j:345:LEU:HD11	1.94	0.47
2:J:888:VAL:HA	2:J:891:MET:HG2	1.96	0.47
4:B:884:GLU:CG	4:B:888:ALA:HB2	2.44	0.47
5:G:174:LEU:HD13	5:G:404:TYR:CE1	2.49	0.47
4:H:675:TYR:HA	4:H:678:THR:HG22	1.96	0.47
1:b:8:LEU:HD23	1:b:65:VAL:HB	1.94	0.47
1:c:172:PHE:HD2	1:c:204:VAL:HG23	1.76	0.47
1:e:69:LEU:HD23	1:e:70:GLU:HG3	1.95	0.47
4:D:456:THR:HG21	4:D:654:ARG:HH22	1.79	0.47
5:E:446:MET:SD	5:E:446:MET:N	2.87	0.47
4:H:364:LEU:HD22	4:H:370:TRP:NE1	2.28	0.47
5:M:174:LEU:HD11	5:M:404:TYR:CE2	2.49	0.47
1:g:201:CYS:SG	1:g:202:VAL:N	2.87	0.47
1:i:66:LEU:HD22	1:i:91:ILE:HD13	1.96	0.47
3:K:192:LEU:HD12	3:K:304:GLU:OE1	2.14	0.47
4:D:245:ILE:HD12	4:D:250:LEU:HD21	1.96	0.47
2:J:902:MET:HE3	1:j:248:TYR:CD1	2.49	0.47
5:C:839:ARG:HA	5:C:842:ILE:HG22	1.96	0.47
5:E:396:TYR:OH	5:E:487:GLN:OE1	2.33	0.47
5:G:512:HIS:CD2	5:G:626:LEU:HD21	2.49	0.47
5:G:628:LEU:HD11	5:G:723:LEU:HD21	1.95	0.47
6:L:1795:VAL:HG12	6:L:1803:LEU:CB	2.44	0.47
5:A:503:LEU:HG	5:A:509:LEU:HD13	1.96	0.47
1:c:188:SER:O	1:c:192:LEU:HD23	2.15	0.47
1:e:406:GLU:HB3	1:e:408:PHE:CE2	2.50	0.47
1:j:257:ILE:HG23	1:j:261:ILE:HD13	1.95	0.47
5:C:717:SER:OG	5:C:718:ASN:OD1	2.23	0.47
4:D:734:LEU:HD22	4:D:754:PHE:CD2	2.48	0.47
5:E:496:SER:O	5:E:499:LEU:HD23	2.15	0.47
5:M:408:MET:HE1	5:M:450:ILE:CD1	2.45	0.47
4:N:714:PHE:CE2	4:N:778:VAL:HG11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:274:THR:O	1:a:302:ASN:ND2	2.48	0.47
1:e:295:ARG:NH1	1:e:345:LEU:HD13	2.30	0.47
1:k:183:VAL:HG22	1:k:186:TYR:HB2	1.95	0.47
3:K:143:ILE:HA	3:K:148:ILE:HD12	1.97	0.47
3:K:190:TRP:CE3	3:K:205:ILE:HD13	2.49	0.47
4:B:460:TRP:HB3	4:B:650:THR:HG23	1.97	0.47
5:E:855:VAL:HG22	5:E:859:LEU:HD13	1.96	0.47
4:F:286:SER:OG	4:F:366:ARG:NH1	2.48	0.47
4:F:459:LEU:CD2	4:F:496:VAL:HG21	2.43	0.47
4:F:685:MET:CE	1:f:165:LEU:HD21	2.44	0.47
5:G:473:LYS:HE3	5:G:473:LYS:HA	1.97	0.47
5:G:719:ILE:O	5:G:719:ILE:HG22	2.15	0.47
4:H:454:VAL:HG12	4:H:456:THR:HG23	1.97	0.47
4:H:608:THR:HG23	4:H:610:ALA:H	1.79	0.47
4:N:391:ARG:HH11	4:N:399:ALA:HB2	1.80	0.47
4:N:446:PHE:HD2	4:N:448:VAL:HG12	1.79	0.47
1:d:321:LEU:HD12	1:d:357:GLN:HB2	1.96	0.47
1:e:12:GLN:OE1	1:e:16:GLN:NE2	2.45	0.47
1:e:340:ILE:HD13	1:e:343:ARG:HE	1.79	0.47
1:h:245:TYR:OH	1:h:364:SER:OG	2.21	0.47
1:n:406:GLU:HB3	1:n:408:PHE:CE2	2.49	0.47
4:D:882:PHE:O	4:D:883:ASN:CG	2.58	0.47
5:E:300:VAL:HG12	5:E:304:LEU:HD23	1.96	0.47
5:G:263:ILE:HG23	5:G:328:ILE:CD1	2.45	0.47
5:G:855:VAL:O	5:G:859:LEU:HD13	2.15	0.47
4:H:734:LEU:HD12	4:H:754:PHE:HB2	1.96	0.47
1:b:274:THR:HB	1:b:275:PRO:HD3	1.96	0.47
1:c:321:LEU:HD12	1:c:322:ASN:N	2.30	0.47
1:d:172:PHE:CE1	1:d:204:VAL:HG23	2.50	0.47
4:F:377:ARG:CD	4:F:414:LEU:HD22	2.45	0.47
6:L:1687:GLN:HB2	6:L:1688:ILE:HD12	1.97	0.47
1:k:190:LEU:HD11	1:k:421:MET:HE2	1.96	0.47
3:K:592:SER:O	3:K:595:SER:OG	2.22	0.47
4:D:868:SER:OG	4:D:870:ASP:OD1	2.20	0.47
4:F:319:LEU:HD11	5:G:367:THR:HG22	1.97	0.47
1:g:406:GLU:HB3	1:g:408:PHE:CE2	2.49	0.47
4:B:254:ILE:HA	4:B:257:VAL:HG12	1.97	0.46
4:B:549:LEU:HG	4:B:555:LEU:CD1	2.44	0.46
4:D:882:PHE:HB2	1:d:355:SER:CB	2.45	0.46
5:E:613:LEU:HD13	5:E:650:HIS:CE1	2.50	0.46
5:E:701:VAL:HG12	5:E:702:MET:HE2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:600:ILE:O	4:H:603:THR:OG1	2.24	0.46
6:L:1624:TYR:CE1	6:L:1717:LEU:HD11	2.50	0.46
5:M:855:VAL:HG13	5:M:856:ILE:HG13	1.96	0.46
1:m:329:ASP:OD1	1:m:331:THR:HG22	2.15	0.46
4:D:255:LEU:HD12	4:D:339:LEU:CD2	2.46	0.46
1:l:186:TYR:HB3	1:l:421:MET:HE1	1.96	0.46
3:K:307:PHE:CD1	3:K:332:ILE:HG12	2.50	0.46
5:C:709:LEU:HD21	5:C:713:LEU:HD11	1.97	0.46
4:D:568:LEU:HD13	4:D:667:LEU:HB3	1.98	0.46
5:E:546:ILE:HD11	5:E:551:LEU:HD11	1.96	0.46
5:M:214:GLU:O	5:M:218:VAL:HG23	2.15	0.46
1:f:231:LEU:O	1:f:234:THR:OG1	2.32	0.46
1:g:153:LEU:O	1:g:157:LEU:HD23	2.15	0.46
1:l:183:VAL:HG22	1:l:186:TYR:HB2	1.96	0.46
5:E:414:LEU:O	5:E:419:ILE:HG21	2.15	0.46
5:G:494:TYR:O	5:G:498:VAL:HG23	2.15	0.46
5:G:684:GLN:O	5:G:685:ARG:C	2.58	0.46
3:I:275:LYS:NZ	3:I:326:GLU:OE1	2.44	0.46
4:B:651:VAL:HG23	4:B:751:HIS:CE1	2.50	0.46
5:G:679:ALA:O	5:G:683:ARG:HD2	2.16	0.46
4:H:659:HIS:HB3	4:H:755:LEU:HD11	1.98	0.46
4:H:682:LYS:HG3	1:h:165:LEU:HD11	1.97	0.46
4:H:718:MET:HE1	4:H:775:LEU:CD1	2.46	0.46
3:I:627:PHE:HA	3:I:630:LEU:HD13	1.98	0.46
6:L:1685:ALA:HA	6:L:1689:LEU:CD1	2.46	0.46
4:N:545:LEU:HD12	4:N:546:LEU:HG	1.98	0.46
1:e:295:ARG:HD2	1:e:345:LEU:HD12	1.89	0.46
1:m:153:LEU:O	1:m:157:LEU:HD23	2.16	0.46
1:n:212:ARG:HA	1:n:215:THR:HG23	1.97	0.46
1:n:217:ARG:CZ	1:n:231:LEU:HD21	2.45	0.46
4:D:754:PHE:CZ	4:D:758:ILE:HD11	2.51	0.46
5:G:843:TYR:CD1	5:G:843:TYR:C	2.93	0.46
5:M:456:TYR:HB3	5:M:499:LEU:HD21	1.97	0.46
1:e:165:LEU:HD12	1:e:254:ILE:HG22	1.97	0.46
1:f:376:LEU:HD23	1:f:377:MET:N	2.30	0.46
1:n:288:THR:OG1	1:n:371:HIS:NE2	2.44	0.46
1:k:290:VAL:HG23	1:k:336:SER:HB2	1.98	0.46
4:F:245:ILE:HG12	4:F:281:ALA:HB2	1.98	0.46
4:H:464:TYR:OH	4:H:491:ASN:OD1	2.30	0.46
4:H:537:ALA:O	4:H:541:THR:OG1	2.31	0.46
4:H:691:LEU:HD11	4:H:797:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:274:THR:HG23	1:c:296:ARG:HB2	1.98	0.46
1:e:341:ARG:NH1	1:e:342:GLU:OE2	2.49	0.46
5:C:513:LEU:HD21	5:C:726:HIS:HE1	1.81	0.46
4:D:498:HIS:O	4:D:499:ASP:C	2.56	0.46
5:E:468:THR:HG22	5:E:468:THR:O	2.16	0.46
5:G:428:TRP:CH2	5:G:628:LEU:HD22	2.51	0.46
6:L:1507:PHE:CZ	6:L:1614:ILE:HG23	2.45	0.46
1:a:183:VAL:HG22	1:a:186:TYR:HB2	1.98	0.46
1:c:154:LEU:HD12	1:c:166:VAL:HG11	1.98	0.46
1:l:153:LEU:O	1:l:157:LEU:HD23	2.16	0.46
2:J:902:MET:HE3	1:j:248:TYR:HD1	1.79	0.46
5:C:703:GLU:OE1	1:c:248:TYR:OH	2.30	0.46
5:E:395:ILE:CD1	5:E:450:ILE:HG23	2.45	0.46
4:F:726:VAL:HG13	4:F:761:ARG:HB2	1.97	0.46
4:H:367:LEU:O	4:H:368:LEU:C	2.58	0.46
4:H:617:ILE:HG22	4:H:642:TYR:OH	2.16	0.46
4:N:714:PHE:CE1	4:N:718:MET:HE3	2.51	0.46
1:n:153:LEU:O	1:n:157:LEU:HD23	2.16	0.46
2:J:334:VAL:HG23	2:J:365:MET:HG2	1.98	0.46
4:B:694:MET:HE3	4:B:800:LEU:HD13	1.98	0.46
4:D:606:ARG:O	4:D:611:GLN:NE2	2.49	0.46
1:b:183:VAL:HG22	1:b:186:TYR:HB2	1.98	0.46
4:D:297:LEU:HD12	4:D:378:LEU:CD2	2.44	0.45
4:D:496:VAL:O	4:D:553:TYR:CZ	2.69	0.45
5:E:679:ALA:HA	5:E:822:ILE:HD12	1.98	0.45
5:M:700:GLU:OE2	1:m:334:HIS:ND1	2.49	0.45
1:j:290:VAL:HG11	1:j:328:VAL:HG13	1.99	0.45
4:B:364:LEU:HD22	4:B:370:TRP:CD1	2.51	0.45
4:B:376:ILE:HG22	4:B:411:MET:HE2	1.99	0.45
4:D:317:PHE:CZ	4:D:321:GLY:HA3	2.51	0.45
4:F:648:ILE:H	4:F:648:ILE:HD12	1.81	0.45
4:H:457:ASP:HB3	4:H:653:THR:HA	1.99	0.45
5:M:156:LEU:HD23	5:M:159:LYS:HZ2	1.80	0.45
1:e:153:LEU:O	1:e:157:LEU:HD23	2.16	0.45
1:g:183:VAL:HG22	1:g:186:TYR:HB2	1.99	0.45
1:i:298:LEU:HD22	1:i:346:ALA:HB2	1.97	0.45
1:l:186:TYR:CZ	1:l:405:LEU:HA	2.50	0.45
3:K:282:SER:CB	3:K:340:LEU:HD13	2.46	0.45
4:B:252:ARG:CZ	5:C:210:LEU:HD21	2.47	0.45
5:E:459:VAL:HG11	5:E:499:LEU:HD12	1.99	0.45
5:G:702:MET:HE3	5:G:737:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:499:LEU:HD12	5:M:719:ILE:HG12	1.98	0.45
5:A:641:LEU:HD11	5:A:702:MET:CE	2.47	0.45
1:f:406:GLU:HB3	1:f:408:PHE:CE2	2.52	0.45
1:m:186:TYR:CD1	1:m:421:MET:HE2	2.44	0.45
1:m:238:ALA:HB3	1:m:376:LEU:HD13	1.98	0.45
4:F:434:ILE:HG22	4:F:435:TYR:CD1	2.52	0.45
5:G:174:LEU:HD22	5:G:404:TYR:CE1	2.51	0.45
3:I:132:LEU:O	3:I:136:VAL:HG23	2.16	0.45
3:I:403:VAL:HG13	3:I:403:VAL:O	2.16	0.45
6:L:611:ARG:NH1	6:L:1502:ALA:O	2.49	0.45
6:L:613:TYR:OH	6:L:1498:LEU:HD12	2.17	0.45
5:M:698:MET:HE3	1:m:249:MET:SD	2.56	0.45
4:N:728:GLU:HG3	1:n:330:PRO:HB3	1.99	0.45
1:h:329:ASP:O	1:h:333:VAL:HG23	2.16	0.45
1:j:238:ALA:HB3	1:j:376:LEU:HD13	1.98	0.45
3:K:105:LEU:HD22	6:L:458:THR:HG22	1.98	0.45
4:D:617:ILE:HD12	4:D:642:TYR:OH	2.16	0.45
4:F:253:ASP:OD2	4:F:266:ILE:HG22	2.17	0.45
4:H:328:LEU:HD21	4:H:385:VAL:HG12	1.98	0.45
1:a:153:LEU:O	1:a:157:LEU:HD23	2.16	0.45
1:c:132:LEU:HD21	1:c:135:PHE:CE1	2.51	0.45
1:e:238:ALA:HB1	1:e:376:LEU:HD23	1.97	0.45
1:g:204:VAL:HG21	1:g:384:ILE:CD1	2.46	0.45
1:m:257:ILE:HG23	1:m:261:ILE:HD13	1.99	0.45
1:n:274:THR:HB	1:n:275:PRO:HD3	1.98	0.45
5:E:306:LEU:O	5:E:310:LEU:HD23	2.17	0.45
4:N:496:VAL:HG11	4:N:647:PRO:HG3	1.97	0.45
1:a:201:CYS:SG	1:a:202:VAL:N	2.90	0.45
1:e:165:LEU:CD1	1:e:254:ILE:HG22	2.46	0.45
1:e:296:ARG:O	1:e:302:ASN:ND2	2.50	0.45
1:f:252:ASP:N	1:f:252:ASP:OD1	2.49	0.45
1:g:139:HIS:CD2	1:g:141:ILE:HD13	2.51	0.45
1:g:238:ALA:HB1	1:g:376:LEU:HD23	1.98	0.45
1:n:290:VAL:HA	1:n:293:VAL:HG22	1.98	0.45
5:E:660:ILE:HG22	1:e:165:LEU:HD21	1.98	0.45
6:L:1673:MET:SD	6:L:1748:ARG:NH2	2.90	0.45
2:J:742:ILE:HD12	2:J:752:TRP:CH2	2.51	0.45
3:K:78:GLN:O	3:K:81:LEU:N	2.50	0.45
5:C:687:LEU:O	5:C:690:VAL:HG22	2.17	0.45
4:F:391:ARG:NH2	4:F:395:GLU:O	2.49	0.45
4:H:400:VAL:HG21	4:H:422:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:254:ILE:HA	4:N:257:VAL:HG22	1.99	0.45
1:c:349:ILE:HG23	1:c:349:ILE:O	2.17	0.45
4:B:868:SER:HB3	4:B:873:LEU:HD23	1.99	0.45
5:E:499:LEU:HD23	5:E:500:LEU:N	2.32	0.45
5:E:640:MET:HE3	5:E:640:MET:O	2.16	0.45
4:F:447:PHE:HZ	4:F:483:VAL:HG11	1.82	0.45
6:L:1641:LEU:CD1	6:L:1677:VAL:HG21	2.46	0.45
1:c:205:LEU:HD11	1:c:235:ILE:HD13	1.99	0.45
1:f:183:VAL:HG22	1:f:186:TYR:HB2	1.98	0.45
1:n:154:LEU:HD12	1:n:166:VAL:HG11	1.98	0.45
1:k:296:ARG:O	1:k:302:ASN:ND2	2.50	0.45
2:J:410:LYS:NZ	3:I:60:GLU:OE2	2.48	0.45
5:C:855:VAL:HG23	5:C:858:ARG:HD3	1.98	0.45
5:E:738:MET:HB3	5:E:745:LEU:HD12	1.98	0.45
5:G:423:TYR:HB2	5:G:632:ARG:CB	2.47	0.45
6:L:576:ILE:HG23	6:L:592:ALA:HB3	1.98	0.45
5:M:220:ASP:O	5:M:224:VAL:HG23	2.16	0.45
1:k:162:PRO:O	3:K:501:GLN:NE2	2.50	0.44
4:B:757:THR:HG22	4:B:761:ARG:HE	1.82	0.44
5:C:214:GLU:HG2	5:C:321:LEU:HD12	1.98	0.44
5:C:402:ASP:OD1	5:C:406:GLU:N	2.50	0.44
4:D:430:LEU:O	4:D:430:LEU:HD23	2.17	0.44
4:D:495:GLN:CB	4:D:647:PRO:CD	2.94	0.44
5:G:843:TYR:CD2	5:G:852:MET:HB2	2.52	0.44
4:H:685:MET:HE2	1:h:200:ASP:HB3	1.99	0.44
3:I:136:VAL:HG22	3:I:172:LEU:CD1	2.46	0.44
5:A:682:LEU:HD22	5:A:758:PHE:CE2	2.52	0.44
1:d:183:VAL:HG22	1:d:186:TYR:HB2	1.99	0.44
1:h:290:VAL:HG11	1:h:328:VAL:HG13	2.00	0.44
2:J:382:ILE:HD11	2:J:401:LYS:HD2	2.00	0.44
3:K:254:LEU:HD22	3:K:465:ILE:HA	1.99	0.44
5:C:507:LYS:O	5:C:626:LEU:HD21	2.17	0.44
5:G:442:PHE:O	5:G:484:TYR:OH	2.27	0.44
4:H:555:LEU:HD11	4:H:651:VAL:CG2	2.47	0.44
3:I:333:ARG:O	3:I:337:ALA:HB3	2.17	0.44
1:a:25:LEU:HD21	1:a:244:ARG:HD3	1.98	0.44
1:f:130:ASP:OD1	1:f:131:SER:N	2.50	0.44
1:f:153:LEU:O	1:f:157:LEU:HD23	2.17	0.44
1:f:329:ASP:OD1	1:f:331:THR:HG22	2.18	0.44
2:J:281:VAL:HG22	3:K:41:VAL:HG22	2.00	0.44
4:B:287:LEU:HG	4:B:366:ARG:HH21	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:191:PHE:CZ	4:D:293:ARG:HD3	2.52	0.44
5:C:292:LEU:HD23	5:C:383:ALA:HB2	2.00	0.44
5:C:491:ALA:O	5:C:495:ALA:HB3	2.17	0.44
5:C:684:GLN:CG	1:c:354:ALA:HB2	2.47	0.44
4:F:802:ARG:NH2	4:F:828:GLU:OE2	2.51	0.44
4:H:338:LEU:HD23	4:H:342:LEU:HD13	1.99	0.44
4:H:680:ILE:HD11	4:H:786:GLN:HA	1.99	0.44
5:A:332:MET:SD	5:A:333:ARG:N	2.90	0.44
5:A:655:LEU:HD22	5:A:687:LEU:HD13	1.98	0.44
5:A:689:PHE:HZ	5:A:836:LEU:HD23	1.82	0.44
1:b:296:ARG:O	1:b:302:ASN:ND2	2.51	0.44
1:c:270:MET:SD	1:c:379:ALA:HB3	2.57	0.44
1:d:228:ILE:HD13	1:d:231:LEU:HD12	1.99	0.44
1:k:21:PHE:CD2	1:k:236:MET:HE2	2.52	0.44
5:E:655:LEU:HD12	5:E:759:THR:HG21	2.00	0.44
3:I:477:VAL:HG12	3:I:574:ILE:CD1	2.45	0.44
5:A:218:VAL:HG22	5:A:314:HIS:CE1	2.53	0.44
1:n:293:VAL:HG11	1:n:373:VAL:HG12	1.98	0.44
2:J:479:TRP:CE2	2:J:563:GLY:HA3	2.53	0.44
2:J:836:TYR:O	2:J:840:VAL:HG23	2.17	0.44
4:B:432:ARG:NH1	4:B:438:GLU:O	2.51	0.44
4:B:762:CYS:C	4:B:763:LEU:HD12	2.43	0.44
5:C:701:VAL:HG13	5:C:736:ASP:HB3	1.98	0.44
1:c:204:VAL:HG21	1:c:384:ILE:CD1	2.47	0.44
1:c:321:LEU:HD12	1:c:322:ASN:H	1.82	0.44
1:j:153:LEU:O	1:j:157:LEU:HD23	2.17	0.44
1:m:189:LEU:O	1:m:424:SER:OG	2.35	0.44
3:K:548:ILE:CD1	3:K:557:ILE:HG23	2.48	0.44
5:G:341:LEU:HD11	5:G:359:LEU:HD21	1.98	0.44
3:I:504:HIS:NE2	1:i:200:ASP:OD1	2.51	0.44
4:N:682:LYS:HG2	1:n:165:LEU:HD11	2.00	0.44
5:A:719:ILE:HG13	5:A:720:ASP:N	2.32	0.44
1:h:8:LEU:HD21	1:h:122:ILE:HD12	2.00	0.44
1:k:186:TYR:HB3	1:k:421:MET:HE1	1.99	0.44
4:F:301:HIS:HA	4:F:304:ILE:HG22	2.00	0.44
5:G:364:PHE:CD1	5:G:479:LEU:HD11	2.53	0.44
4:H:559:MET:HE1	4:H:651:VAL:HG11	2.00	0.44
3:I:259:LEU:HB2	3:I:277:LEU:HD11	1.99	0.44
1:n:174:ASN:O	1:n:208:THR:N	2.51	0.44
3:K:649:LEU:HD12	3:K:649:LEU:HA	1.88	0.44
5:C:682:LEU:O	5:C:682:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:376:CYS:O	5:E:380:THR:HG23	2.18	0.44
4:F:854:TYR:O	4:F:858:VAL:HG12	2.18	0.44
5:G:341:LEU:HD11	5:G:359:LEU:CD2	2.47	0.44
5:G:408:MET:HE1	5:G:450:ILE:HD12	1.99	0.44
6:L:1648:LEU:HD23	6:L:1667:GLN:OE1	2.17	0.44
1:d:203:VAL:HG22	1:d:269:LEU:HD23	2.00	0.44
1:g:260:LEU:HD21	1:g:321:LEU:HB3	1.98	0.44
1:h:294:MET:SD	1:h:322:ASN:ND2	2.91	0.44
2:J:423:VAL:HG13	2:J:423:VAL:O	2.18	0.44
3:K:328:VAL:HA	3:K:331:ARG:HD3	2.00	0.44
5:E:391:LEU:O	5:E:394:TRP:N	2.50	0.44
6:L:1795:VAL:HG11	6:L:1807:LEU:HD23	2.00	0.44
5:M:854:SER:O	1:m:334:HIS:NE2	2.51	0.44
4:N:567:LEU:HD13	4:N:727:LEU:HD11	2.00	0.44
1:c:189:LEU:O	1:c:424:SER:OG	2.34	0.44
1:e:47:ARG:NH1	1:e:251:ASN:O	2.51	0.44
1:i:274:THR:HB	1:i:275:PRO:HD3	1.98	0.44
1:j:77:ILE:O	1:j:86:TYR:OH	2.34	0.44
1:j:377:MET:O	1:j:378:MET:HE2	2.18	0.44
4:D:670:ALA:O	4:D:719:GLN:NE2	2.51	0.43
4:H:456:THR:OG1	4:H:457:ASP:N	2.51	0.43
6:L:1494:ALA:O	6:L:1498:LEU:HD23	2.18	0.43
6:L:1743:LEU:HD11	6:L:1779:THR:HG22	2.01	0.43
4:N:461:HIS:HE2	4:N:748:ILE:HD11	1.81	0.43
1:c:77:ILE:O	1:c:86:TYR:OH	2.36	0.43
1:c:201:CYS:SG	1:c:202:VAL:N	2.91	0.43
1:g:206:ASP:OD2	1:g:305:VAL:HG13	2.18	0.43
1:h:77:ILE:O	1:h:86:TYR:OH	2.33	0.43
1:i:183:VAL:HG22	1:i:186:TYR:HB2	1.99	0.43
1:l:114:ILE:HG22	1:l:114:ILE:O	2.18	0.43
1:l:238:ALA:HB3	1:l:376:LEU:HD13	2.00	0.43
1:n:201:CYS:SG	1:n:202:VAL:N	2.91	0.43
5:C:266:VAL:HG22	5:C:332:MET:HA	2.00	0.43
5:E:499:LEU:HD23	5:E:500:LEU:H	1.82	0.43
4:F:381:LEU:HD21	4:F:418:ILE:HD11	1.99	0.43
3:I:343:LEU:O	3:I:348:SER:N	2.51	0.43
3:I:354:LEU:HD21	3:I:561:HIS:HE1	1.83	0.43
4:N:624:ARG:C	4:N:625:LEU:HD12	2.43	0.43
5:A:518:ARG:NE	5:A:524:GLN:HG3	2.32	0.43
1:j:183:VAL:HG22	1:j:186:TYR:HB2	2.01	0.43
1:n:208:THR:HB	1:n:212:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:550:ASN:O	4:B:554:SER:HA	2.19	0.43
5:E:682:LEU:HD23	5:E:758:PHE:CE1	2.54	0.43
4:F:364:LEU:HD22	4:F:370:TRP:NE1	2.33	0.43
3:I:601:LEU:HG	3:I:602:GLY:H	1.83	0.43
6:L:1513:LEU:HD13	6:L:1612:LEU:HD13	1.99	0.43
6:L:1812:PHE:CE2	1:l:356:ILE:HG22	2.54	0.43
1:g:25:LEU:HD21	1:g:244:ARG:HD3	2.00	0.43
1:i:293:VAL:HG21	1:i:324:ILE:HD12	1.99	0.43
4:D:249:ALA:O	4:D:252:ARG:HG2	2.18	0.43
4:D:765:ASP:OD1	4:D:766:SER:N	2.48	0.43
6:L:576:ILE:HG23	6:L:592:ALA:CB	2.48	0.43
4:N:694:MET:SD	4:N:803:ARG:NH1	2.91	0.43
1:i:417:ASN:OD1	1:i:418:PHE:N	2.52	0.43
1:l:174:ASN:O	1:l:208:THR:N	2.52	0.43
5:C:840:LEU:HB2	5:C:856:ILE:HD11	2.01	0.43
5:E:702:MET:HE1	5:E:733:CYS:HB3	2.01	0.43
5:G:418:ARG:HB3	5:G:422:ASP:HA	2.00	0.43
5:G:428:TRP:CE3	5:G:628:LEU:HD22	2.52	0.43
4:H:365:ARG:HG2	4:H:368:LEU:HD22	2.00	0.43
4:H:673:MET:O	4:H:677:LEU:HD23	2.19	0.43
6:L:1621:VAL:HG12	6:L:1624:TYR:CE2	2.53	0.43
1:k:399:ARG:NH1	1:k:402:GLU:OE1	2.52	0.43
5:C:458:ASN:C	5:C:458:ASN:HD22	2.26	0.43
4:D:377:ARG:HG2	4:D:414:LEU:HD13	2.01	0.43
4:D:489:SER:HB2	4:D:545:LEU:HD22	2.01	0.43
4:F:569:GLY:HA2	1:f:248:TYR:CE1	2.53	0.43
3:I:505:LEU:HD11	1:i:158:ASN:ND2	2.32	0.43
6:L:1660:SER:O	6:L:1663:PHE:HB3	2.18	0.43
1:d:274:THR:HB	1:d:275:PRO:HD3	2.00	0.43
1:e:324:ILE:HD12	1:e:328:VAL:HG21	1.99	0.43
1:e:409:ARG:H	1:e:409:ARG:HD2	1.83	0.43
1:l:257:ILE:HG23	1:l:261:ILE:HD13	1.99	0.43
1:k:153:LEU:O	1:k:157:LEU:HD23	2.18	0.43
1:k:232:VAL:HA	1:k:235:ILE:HD12	2.01	0.43
3:K:310:GLU:O	3:K:314:LEU:HD23	2.19	0.43
5:G:843:TYR:CE2	5:G:852:MET:CB	3.01	0.43
1:b:293:VAL:HG21	1:b:324:ILE:CD1	2.48	0.43
1:c:260:LEU:HD21	1:c:321:LEU:HB3	1.99	0.43
5:C:753:SER:O	5:C:756:VAL:HG12	2.19	0.43
4:D:624:ARG:NH1	4:D:625:LEU:O	2.52	0.43
4:D:763:LEU:HB2	4:D:772:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:660:ILE:HG22	1:e:165:LEU:HD11	2.00	0.43
5:E:679:ALA:HB2	5:E:818:PHE:HZ	1.84	0.43
5:G:837:LEU:HD21	5:G:859:LEU:CD2	2.49	0.43
3:I:341:TRP:CE2	3:I:345:VAL:HG21	2.54	0.43
6:L:559:GLU:HB3	6:L:567:LEU:HB3	1.99	0.43
5:A:507:LYS:HG2	5:A:626:LEU:HD11	2.00	0.43
1:f:349:ILE:HG23	1:f:349:ILE:O	2.19	0.43
2:J:938:HIS:CD2	2:J:943:LEU:HD23	2.53	0.43
4:D:882:PHE:CB	1:d:355:SER:HB3	2.49	0.43
5:E:858:ARG:NE	1:e:337:LEU:HD13	2.34	0.43
5:M:467:VAL:O	5:M:467:VAL:HG13	2.19	0.43
4:N:734:LEU:HD12	4:N:754:PHE:CB	2.48	0.43
4:D:247:GLU:O	4:D:366:ARG:NH1	2.46	0.43
4:F:365:ARG:HA	4:F:365:ARG:NE	2.33	0.43
1:a:329:ASP:OD1	1:a:331:THR:HG22	2.19	0.43
1:b:297:LEU:HD11	1:b:377:MET:HG3	2.00	0.43
1:i:329:ASP:OD1	1:i:331:THR:HG22	2.19	0.43
1:j:190:LEU:HD21	1:j:421:MET:SD	2.59	0.43
1:l:241:THR:OG1	1:l:244:ARG:NH2	2.52	0.43
1:l:408:PHE:CD1	1:l:408:PHE:N	2.85	0.43
1:n:257:ILE:HG23	1:n:261:ILE:HD13	2.01	0.43
4:B:878:PHE:HB2	1:b:338:GLN:HE22	1.84	0.42
4:D:404:THR:HG22	4:D:404:THR:O	2.19	0.42
5:G:337:ILE:HG21	5:G:375:LEU:HD22	2.00	0.42
5:G:427:TYR:HB2	5:G:428:TRP:CE3	2.54	0.42
4:H:324:PHE:O	4:H:328:LEU:HD13	2.18	0.42
1:n:437:ALA:HA	1:n:440:ARG:HE	1.84	0.42
4:B:549:LEU:HG	4:B:555:LEU:HD13	2.00	0.42
4:B:884:GLU:HG2	4:B:888:ALA:HB2	2.01	0.42
5:G:221:LEU:HD23	5:G:263:ILE:HG21	2.01	0.42
6:L:373:PRO:HA	6:L:377:PHE:HB3	2.00	0.42
1:d:8:LEU:HD23	1:d:65:VAL:HB	2.01	0.42
1:j:413:MET:SD	1:j:414:PHE:N	2.92	0.42
4:D:438:GLU:O	4:D:440:GLU:N	2.53	0.42
4:D:447:PHE:CE1	4:D:448:VAL:HG23	2.54	0.42
5:E:507:LYS:O	5:E:626:LEU:HD11	2.19	0.42
4:H:308:THR:O	4:H:312:SER:OG	2.31	0.42
4:H:605:VAL:HG11	4:H:618:LEU:HD22	2.01	0.42
4:N:727:LEU:HD23	1:n:248:TYR:CE1	2.53	0.42
1:e:257:ILE:HG23	1:e:261:ILE:HD13	1.99	0.42
1:g:165:LEU:HD22	1:g:254:ILE:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:189:LEU:O	1:g:424:SER:OG	2.34	0.42
1:i:77:ILE:O	1:i:86:TYR:OH	2.36	0.42
1:i:257:ILE:HG23	1:i:261:ILE:HD13	2.02	0.42
1:i:415:LYS:NZ	1:i:420:GLU:HB2	2.34	0.42
1:j:246:PRO:HD2	1:j:362:ARG:NH2	2.34	0.42
2:J:721:GLN:NE2	2:J:914:GLN:OE1	2.52	0.42
4:D:862:LEU:HD21	4:D:880:LEU:HB2	2.00	0.42
4:H:493:LEU:CD1	4:H:548:VAL:HG11	2.46	0.42
1:e:294:MET:HE1	1:e:358:VAL:CG1	2.48	0.42
1:f:290:VAL:HG11	1:f:328:VAL:HG13	2.01	0.42
1:j:201:CYS:SG	1:j:202:VAL:N	2.92	0.42
1:l:25:LEU:HD21	1:l:244:ARG:HD3	2.02	0.42
1:m:171:VAL:HG23	1:m:171:VAL:O	2.20	0.42
2:J:752:TRP:CH2	2:J:799:LEU:HD21	2.54	0.42
5:C:509:LEU:HD21	5:C:629:ILE:HG21	2.00	0.42
5:E:543:VAL:HG12	5:E:609:ALA:HA	2.01	0.42
5:G:572:ASP:OD1	5:G:572:ASP:N	2.53	0.42
4:H:660:TYR:CE1	4:H:755:LEU:HD13	2.54	0.42
5:M:156:LEU:HD23	5:M:159:LYS:NZ	2.35	0.42
1:b:114:ILE:HG22	1:b:118:ILE:HG23	2.00	0.42
1:c:384:ILE:HD12	1:c:387:LEU:HB2	2.01	0.42
1:l:398:LEU:HD22	1:l:404:PHE:CD2	2.54	0.42
1:m:87:ASN:ND2	1:n:218:LEU:O	2.53	0.42
4:B:376:ILE:HG22	4:B:411:MET:CE	2.49	0.42
5:C:451:LEU:HD23	5:C:455:LYS:HE2	2.00	0.42
3:I:354:LEU:HD21	3:I:561:HIS:CE1	2.55	0.42
6:L:371:CYS:HB3	6:L:376:ALA:HB3	2.02	0.42
5:M:205:ILE:HD13	5:M:232:TYR:CE2	2.54	0.42
5:A:515:SER:OG	5:A:567:ASP:OD2	2.32	0.42
1:c:270:MET:HE2	1:c:303:VAL:HG13	2.02	0.42
1:d:3:ARG:HB2	1:d:133:GLU:HB2	2.02	0.42
1:g:235:ILE:HD11	1:g:304:MET:SD	2.59	0.42
3:K:260:ARG:HB2	3:K:263:ILE:HG22	2.02	0.42
5:E:658:VAL:HA	5:E:763:GLN:OE1	2.20	0.42
4:F:477:MET:HE3	4:F:477:MET:HA	2.00	0.42
4:F:574:ILE:HG23	4:F:668:TRP:HZ3	1.85	0.42
4:N:581:LEU:HD13	4:N:600:ILE:HG21	2.02	0.42
1:b:133:GLU:OE2	1:b:254:ILE:HG21	2.20	0.42
1:e:399:ARG:NH1	1:e:402:GLU:OE1	2.52	0.42
1:i:171:VAL:O	1:i:171:VAL:HG23	2.20	0.42
1:n:224:SER:O	1:n:228:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:171:VAL:HG23	1:k:171:VAL:O	2.20	0.42
5:C:857:SER:OG	1:c:338:GLN:NE2	2.47	0.42
5:E:246:PHE:HB2	5:E:264:LEU:HD13	2.02	0.42
5:G:426:LYS:O	5:G:431:ARG:N	2.49	0.42
5:G:843:TYR:CE2	5:G:852:MET:HB2	2.55	0.42
5:A:543:VAL:HA	5:A:546:ILE:HD12	2.01	0.42
1:d:68:ASP:HB3	1:d:74:ILE:HG12	2.02	0.42
1:f:25:LEU:HD21	1:f:244:ARG:HD3	2.01	0.42
1:i:367:LEU:HB2	1:i:368:PRO:HD2	2.01	0.42
1:n:275:PRO:HB3	1:n:371:HIS:ND1	2.35	0.42
1:k:132:LEU:HD21	1:k:135:PHE:HE1	1.84	0.42
5:C:499:LEU:C	5:C:501:ASP:H	2.27	0.42
5:E:837:LEU:HD21	5:E:859:LEU:HD22	2.01	0.42
5:G:684:GLN:NE2	5:G:687:LEU:HD23	2.35	0.42
5:A:631:ASN:OD1	5:A:632:ARG:N	2.53	0.42
1:c:291:LEU:HD23	1:c:336:SER:HA	2.01	0.42
1:m:408:PHE:CD2	1:m:411:GLU:HB2	2.55	0.42
2:J:810:ASP:OD1	2:J:811:ILE:HD12	2.19	0.42
5:C:224:VAL:HG21	5:C:233:VAL:HG13	2.01	0.42
5:C:277:ILE:HA	5:C:293:ALA:HB1	2.01	0.42
4:D:495:GLN:CB	4:D:647:PRO:HD3	2.49	0.42
5:E:699:PHE:CE2	1:e:360:LEU:HB3	2.54	0.42
5:E:713:LEU:HD22	5:E:722:VAL:HG13	2.00	0.42
5:G:658:VAL:CG1	5:G:762:MET:HE2	2.49	0.42
5:G:762:MET:SD	5:G:762:MET:C	3.03	0.42
4:H:562:MET:HE3	4:H:660:TYR:HD2	1.84	0.42
1:b:291:LEU:HD12	1:b:336:SER:HB2	2.02	0.42
1:e:337:LEU:HD12	1:e:358:VAL:HG13	2.01	0.42
1:h:292:ASP:HB3	1:h:296:ARG:CZ	2.50	0.42
5:C:659:TRP:CE3	1:c:254:ILE:HD11	2.55	0.41
4:D:568:LEU:HD11	4:D:664:PHE:CE1	2.54	0.41
4:D:694:MET:HG2	4:D:800:LEU:HD11	2.01	0.41
5:G:351:LEU:O	5:G:438:GLN:NE2	2.49	0.41
6:L:1498:LEU:HD13	6:L:1501:LYS:HD2	2.02	0.41
1:a:232:VAL:CG1	1:a:236:MET:HE3	2.50	0.41
1:a:232:VAL:HG13	1:a:236:MET:HE3	2.02	0.41
1:a:290:VAL:CG1	1:a:328:VAL:HG13	2.50	0.41
1:b:174:ASN:O	1:b:208:THR:N	2.53	0.41
1:h:317:TYR:CD2	1:h:320:ILE:HD11	2.55	0.41
1:m:290:VAL:HG11	1:m:328:VAL:HG13	2.01	0.41
4:B:485:LEU:HD12	4:B:745:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:546:LEU:HD13	4:B:747:ILE:CD1	2.48	0.41
4:B:862:LEU:HD21	4:B:880:LEU:HD22	2.00	0.41
5:G:684:GLN:NE2	5:G:684:GLN:HA	2.35	0.41
5:G:684:GLN:HA	5:G:684:GLN:HE21	1.85	0.41
4:H:365:ARG:O	4:H:368:LEU:HD13	2.19	0.41
3:I:504:HIS:NE2	1:i:198:ASN:O	2.52	0.41
1:b:171:VAL:O	1:b:171:VAL:HG23	2.19	0.41
1:e:68:ASP:HB3	1:e:74:ILE:HG12	2.01	0.41
4:D:754:PHE:CE2	4:D:758:ILE:HD11	2.54	0.41
5:G:414:LEU:HD11	5:G:418:ARG:HE	1.86	0.41
5:G:638:TYR:OH	5:G:726:HIS:NE2	2.50	0.41
4:H:707:LEU:HD13	4:H:851:THR:HG23	2.02	0.41
1:e:183:VAL:HG22	1:e:186:TYR:HB2	2.01	0.41
1:g:263:THR:HG21	1:g:266:LEU:HD13	2.02	0.41
1:h:406:GLU:HB3	1:h:408:PHE:CE2	2.55	0.41
1:i:141:ILE:HB	1:i:173:PRO:HD3	2.02	0.41
1:l:270:MET:HG3	1:l:305:VAL:HG21	2.01	0.41
4:B:490:ILE:HD11	4:B:541:THR:CG2	2.51	0.41
4:D:392:LYS:O	4:D:470:MET:HE1	2.20	0.41
4:F:304:ILE:HD12	4:F:381:LEU:HB3	2.01	0.41
4:F:553:TYR:HB3	4:F:648:ILE:HD11	2.01	0.41
5:G:351:LEU:HD12	5:G:406:GLU:OE2	2.21	0.41
6:L:1520:LEU:HD21	6:L:1624:TYR:HE2	1.85	0.41
1:d:442:ASP:OD1	1:d:442:ASP:N	2.53	0.41
1:g:349:ILE:HG23	1:g:349:ILE:O	2.20	0.41
3:K:387:VAL:HG12	3:K:387:VAL:O	2.20	0.41
4:F:430:LEU:O	4:F:434:ILE:HD12	2.21	0.41
3:I:541:PHE:CE2	3:I:545:LEU:HD11	2.56	0.41
5:M:532:MET:HE1	5:M:649:LYS:HG3	2.01	0.41
4:N:555:LEU:HD13	4:N:648:ILE:HG13	2.03	0.41
5:A:259:LEU:HD22	5:A:262:ARG:HH21	1.86	0.41
1:g:274:THR:HB	1:g:275:PRO:HD3	2.03	0.41
1:h:205:LEU:CD2	1:h:232:VAL:HG23	2.50	0.41
1:h:406:GLU:HB3	1:h:408:PHE:CD2	2.56	0.41
1:l:293:VAL:HG21	1:l:324:ILE:CD1	2.51	0.41
1:k:290:VAL:HG11	1:k:328:VAL:HG13	2.03	0.41
2:J:494:ILE:O	2:J:494:ILE:HG13	2.20	0.41
2:J:707:MET:HE1	2:J:926:LEU:CD2	2.50	0.41
5:C:499:LEU:O	5:C:500:LEU:C	2.63	0.41
4:D:879:ARG:HA	4:D:882:PHE:CE2	2.55	0.41
3:I:505:LEU:HD11	1:i:158:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:697:MET:CE	5:A:738:MET:HE1	2.50	0.41
1:a:274:THR:HB	1:a:275:PRO:HD3	2.02	0.41
1:c:260:LEU:HB3	1:c:269:LEU:HD21	2.02	0.41
5:E:457:LEU:O	5:E:460:VAL:HG22	2.20	0.41
4:F:365:ARG:HG3	4:F:368:LEU:HD12	2.03	0.41
4:F:616:GLU:OE2	4:F:620:ARG:NH1	2.53	0.41
5:G:423:TYR:CD2	5:G:424:ASN:N	2.89	0.41
4:H:597:LEU:CD1	4:H:625:LEU:HD21	2.51	0.41
4:N:616:GLU:OE1	4:N:616:GLU:N	2.53	0.41
1:b:201:CYS:SG	1:b:202:VAL:N	2.93	0.41
1:e:114:ILE:HG22	1:e:118:ILE:HG23	2.03	0.41
1:l:171:VAL:HG23	1:l:171:VAL:O	2.20	0.41
2:J:275:LEU:HD23	2:J:379:LEU:HD22	2.00	0.41
4:B:651:VAL:HG13	4:B:652:PHE:CG	2.56	0.41
4:D:865:LEU:HD22	4:D:873:LEU:HD23	2.03	0.41
5:E:276:PHE:HZ	5:E:292:LEU:HD23	1.86	0.41
4:H:775:LEU:HA	4:H:778:VAL:HG12	2.02	0.41
1:d:384:ILE:HD12	1:d:387:LEU:HB2	2.02	0.41
1:e:329:ASP:OD1	1:e:331:THR:HG22	2.20	0.41
1:g:293:VAL:HG21	1:g:324:ILE:CD1	2.51	0.41
1:l:273:TYR:HB2	1:l:304:MET:HE1	2.02	0.41
3:K:30:ASP:OD1	3:K:30:ASP:N	2.54	0.41
3:K:105:LEU:HD21	6:L:461:PHE:HB2	2.03	0.41
3:K:272:VAL:CG2	3:K:329:VAL:HG11	2.51	0.41
3:K:329:VAL:O	3:K:333:ARG:N	2.48	0.41
3:K:571:GLN:OE1	3:K:638:ILE:HG21	2.20	0.41
4:B:284:SER:HA	4:B:288:ARG:HB3	2.02	0.41
5:C:471:VAL:O	5:C:471:VAL:HG13	2.21	0.41
5:C:659:TRP:HE3	1:c:254:ILE:HD11	1.86	0.41
4:D:447:PHE:CD1	4:D:448:VAL:HG23	2.56	0.41
4:D:723:THR:HG23	1:d:248:TYR:HB2	2.03	0.41
5:E:446:MET:CE	5:E:485:VAL:HG22	2.51	0.41
4:F:685:MET:HE1	1:f:165:LEU:HD21	2.03	0.41
3:I:93:LEU:HA	3:I:96:VAL:HG22	2.02	0.41
3:I:361:TYR:CD2	3:I:455:LEU:HD22	2.56	0.41
6:L:1476:GLU:O	6:L:1477:LEU:HB2	2.21	0.41
5:M:223:TYR:OH	4:N:366:ARG:NH1	2.54	0.41
5:M:555:LEU:HB2	5:M:575:ILE:HD11	2.03	0.41
4:N:503:THR:O	4:N:503:THR:HG22	2.21	0.41
5:A:452:SER:HA	5:A:719:ILE:CD1	2.51	0.41
1:a:6:ILE:CG2	1:a:132:LEU:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:171:VAL:O	1:a:171:VAL:HG23	2.21	0.41
1:d:238:ALA:HB1	1:d:376:LEU:CD2	2.50	0.41
1:f:114:ILE:O	1:f:114:ILE:HG22	2.20	0.41
1:f:274:THR:HB	1:f:275:PRO:HD3	2.02	0.41
1:g:3:ARG:HB2	1:g:133:GLU:HB2	2.03	0.41
1:g:172:PHE:CE2	1:g:204:VAL:HG23	2.56	0.41
1:h:206:ASP:OD2	1:h:305:VAL:HG13	2.21	0.41
1:l:37:VAL:HG12	1:l:58:GLU:OE2	2.21	0.41
1:n:217:ARG:HH12	1:n:218:LEU:HD12	1.85	0.41
1:k:274:THR:HB	1:k:275:PRO:HD3	2.02	0.41
4:B:547:ASP:HA	4:B:550:ASN:HB3	2.03	0.41
4:D:608:THR:HG23	4:D:610:ALA:H	1.86	0.41
5:E:685:ARG:HG2	1:e:353:PRO:HG3	2.03	0.41
5:G:418:ARG:HG3	5:G:424:ASN:HB3	2.02	0.41
5:G:709:LEU:CD1	5:G:713:LEU:HD13	2.51	0.41
5:G:843:TYR:CE2	5:G:852:MET:HB3	2.56	0.41
6:L:1542:LYS:CB	6:L:1552:LEU:HD13	2.52	0.41
5:M:153:SER:OG	5:M:157:LYS:NZ	2.54	0.41
5:M:747:VAL:HG23	5:M:836:LEU:HD12	2.02	0.41
4:N:541:THR:O	4:N:542:SER:CB	2.68	0.41
1:c:171:VAL:HG23	1:c:171:VAL:O	2.21	0.41
1:c:274:THR:HB	1:c:275:PRO:HD3	2.03	0.41
1:f:201:CYS:SG	1:f:202:VAL:N	2.94	0.41
1:g:154:LEU:HD12	1:g:166:VAL:HG11	2.03	0.41
1:g:241:THR:OG1	1:g:244:ARG:NH2	2.54	0.41
1:h:21:PHE:HB2	1:h:236:MET:HE3	2.03	0.41
1:j:171:VAL:HG23	1:j:171:VAL:O	2.21	0.41
1:n:217:ARG:NH1	1:n:231:LEU:HD21	2.35	0.41
1:n:290:VAL:HG13	1:n:336:SER:HB2	2.01	0.41
1:n:367:LEU:HB2	1:n:368:PRO:HD2	2.03	0.41
2:J:428:ARG:O	2:J:432:ARG:NH1	2.54	0.40
4:B:562:MET:SD	4:B:566:LEU:HD23	2.62	0.40
4:B:880:LEU:HD23	4:B:880:LEU:O	2.21	0.40
5:C:586:LEU:H	5:C:586:LEU:HD23	1.86	0.40
5:C:613:LEU:HD22	5:C:650:HIS:HE2	1.86	0.40
4:D:740:GLN:O	4:D:742:GLN:NE2	2.54	0.40
4:D:882:PHE:CB	1:d:355:SER:CB	2.99	0.40
5:G:762:MET:HE3	5:G:762:MET:C	2.46	0.40
4:H:545:LEU:O	4:H:548:VAL:HG12	2.22	0.40
1:a:169:TYR:HB3	1:a:236:MET:HE2	2.03	0.40
1:b:402:GLU:OE2	1:b:405:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:274:THR:HB	1:l:275:PRO:HD3	2.03	0.40
1:l:290:VAL:CG1	1:l:328:VAL:HG13	2.51	0.40
3:K:333:ARG:HE	3:K:333:ARG:HB2	1.58	0.40
5:C:277:ILE:HD11	5:C:296:MET:HB3	2.03	0.40
5:C:504:MET:HE3	5:C:505:GLU:OE2	2.22	0.40
3:I:1:MET:HA	3:I:1:MET:HE2	2.04	0.40
5:M:765:PHE:CZ	5:M:821:THR:HG21	2.56	0.40
1:d:65:VAL:HG12	1:d:67:LEU:HD21	2.03	0.40
1:k:8:LEU:HD23	1:k:65:VAL:HB	2.03	0.40
1:k:201:CYS:SG	1:k:202:VAL:N	2.94	0.40
2:J:729:MET:HE3	2:J:821:TYR:HD1	1.86	0.40
4:B:691:LEU:HD12	4:B:691:LEU:O	2.22	0.40
5:E:698:MET:HB2	1:e:248:TYR:HB2	2.03	0.40
4:F:546:LEU:HD12	4:F:742:GLN:O	2.22	0.40
5:G:516:ILE:HG21	5:G:638:TYR:CE2	2.56	0.40
4:H:555:LEU:HD11	4:H:651:VAL:HG21	2.03	0.40
4:H:597:LEU:HA	4:H:600:ILE:HG22	2.03	0.40
4:H:715:ILE:HD11	4:H:782:ILE:HD11	2.02	0.40
6:L:1524:LEU:HD22	6:L:1624:TYR:HB3	2.02	0.40
6:L:1688:ILE:HD12	6:L:1688:ILE:N	2.36	0.40
1:a:68:ASP:HB3	1:a:74:ILE:HG12	2.04	0.40
1:a:189:LEU:O	1:a:424:SER:OG	2.38	0.40
1:d:12:GLN:HG2	1:d:73:VAL:HG12	2.04	0.40
1:e:88:PRO:O	1:e:89:GLU:C	2.65	0.40
1:e:274:THR:HB	1:e:275:PRO:HD3	2.04	0.40
1:n:139:HIS:CE1	1:n:150:GLY:HA3	2.56	0.40
5:C:718:ASN:O	5:C:721:ASP:N	2.49	0.40
5:G:837:LEU:HD22	5:G:856:ILE:HG13	2.03	0.40
3:I:361:TYR:CE1	3:I:475:TYR:HB3	2.56	0.40
4:N:496:VAL:HG11	4:N:647:PRO:CG	2.51	0.40
5:A:400:ILE:HD12	5:A:400:ILE:H	1.86	0.40
1:a:297:LEU:HD21	1:a:377:MET:HB3	2.04	0.40
1:d:205:LEU:HD23	1:d:232:VAL:HG12	2.04	0.40
1:m:406:GLU:HB3	1:m:408:PHE:CE2	2.56	0.40
1:k:139:HIS:CE1	1:k:150:GLY:HA3	2.56	0.40
4:B:269:ASN:ND2	4:B:272:GLU:OE1	2.54	0.40
4:B:790:ASP:OD1	4:B:791:ALA:N	2.54	0.40
4:D:380:THR:O	4:D:384:LEU:HD23	2.21	0.40
5:G:156:LEU:HG	5:G:160:MET:HE2	2.04	0.40
5:G:467:VAL:HG21	5:G:498:VAL:HG11	2.04	0.40
5:G:610:LEU:HD22	5:G:613:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:403:VAL:HG21	1:i:49:ASP:HB2	2.04	0.40
6:L:1526:MET:HE2	6:L:1631:LEU:HB3	2.04	0.40
5:M:512:HIS:CE1	5:M:516:ILE:HD11	2.56	0.40
4:N:542:SER:C	4:N:544:TYR:N	2.79	0.40
5:A:470:PRO:HD3	5:A:494:TYR:CZ	2.56	0.40
5:A:693:ILE:HD13	5:A:859:LEU:HD21	2.02	0.40
1:h:171:VAL:O	1:h:171:VAL:HG23	2.22	0.40
1:n:204:VAL:C	1:n:205:LEU:HD22	2.46	0.40
1:n:406:GLU:HB3	1:n:408:PHE:CD2	2.56	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	a	410/451 (91%)	394 (96%)	16 (4%)	0	100	100
1	b	410/451 (91%)	397 (97%)	12 (3%)	1 (0%)	43	71
1	c	410/451 (91%)	394 (96%)	16 (4%)	0	100	100
1	d	410/451 (91%)	395 (96%)	14 (3%)	1 (0%)	43	71
1	e	410/451 (91%)	394 (96%)	16 (4%)	0	100	100
1	f	410/451 (91%)	393 (96%)	17 (4%)	0	100	100
1	g	410/451 (91%)	390 (95%)	20 (5%)	0	100	100
1	h	410/451 (91%)	396 (97%)	14 (3%)	0	100	100
1	i	410/451 (91%)	396 (97%)	14 (3%)	0	100	100
1	j	410/451 (91%)	391 (95%)	19 (5%)	0	100	100
1	k	410/451 (91%)	395 (96%)	15 (4%)	0	100	100
1	l	410/451 (91%)	397 (97%)	12 (3%)	1 (0%)	43	71
1	m	410/451 (91%)	394 (96%)	14 (3%)	2 (0%)	24	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	410/451 (91%)	394 (96%)	16 (4%)	0	100	100
2	J	580/1024 (57%)	545 (94%)	35 (6%)	0	100	100
3	I	511/667 (77%)	488 (96%)	23 (4%)	0	100	100
3	K	539/667 (81%)	521 (97%)	18 (3%)	0	100	100
4	B	602/907 (66%)	573 (95%)	29 (5%)	0	100	100
4	D	571/907 (63%)	542 (95%)	27 (5%)	2 (0%)	30	60
4	F	591/907 (65%)	554 (94%)	37 (6%)	0	100	100
4	H	576/907 (64%)	549 (95%)	27 (5%)	0	100	100
4	N	584/907 (64%)	562 (96%)	21 (4%)	1 (0%)	43	71
5	A	595/902 (66%)	570 (96%)	25 (4%)	0	100	100
5	C	606/902 (67%)	575 (95%)	30 (5%)	1 (0%)	43	71
5	E	626/902 (69%)	599 (96%)	27 (4%)	0	100	100
5	G	624/902 (69%)	593 (95%)	31 (5%)	0	100	100
5	M	624/902 (69%)	595 (95%)	29 (5%)	0	100	100
6	L	610/1819 (34%)	575 (94%)	34 (6%)	1 (0%)	43	71
All	All	13979/19536 (72%)	13361 (96%)	608 (4%)	10 (0%)	49	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	500	LEU
4	D	495	GLN
4	N	542	SER
1	b	408	PHE
4	D	497	CYS
1	m	408	PHE
1	l	406	GLU
1	m	407	GLN
1	d	407	GLN
6	L	1688	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	377/400 (94%)	376 (100%)	1 (0%)	86	83
1	b	377/400 (94%)	377 (100%)	0	100	100
1	c	377/400 (94%)	377 (100%)	0	100	100
1	d	377/400 (94%)	377 (100%)	0	100	100
1	e	377/400 (94%)	377 (100%)	0	100	100
1	f	376/400 (94%)	376 (100%)	0	100	100
1	g	377/400 (94%)	377 (100%)	0	100	100
1	h	376/400 (94%)	375 (100%)	1 (0%)	86	83
1	i	377/400 (94%)	377 (100%)	0	100	100
1	j	377/400 (94%)	377 (100%)	0	100	100
1	k	377/400 (94%)	377 (100%)	0	100	100
1	l	377/400 (94%)	375 (100%)	2 (0%)	81	80
1	m	377/400 (94%)	375 (100%)	2 (0%)	81	80
1	n	377/400 (94%)	377 (100%)	0	100	100
2	J	525/933 (56%)	525 (100%)	0	100	100
3	I	471/594 (79%)	470 (100%)	1 (0%)	87	86
3	K	500/594 (84%)	497 (99%)	3 (1%)	78	79
4	B	547/798 (68%)	547 (100%)	0	100	100
4	D	525/798 (66%)	523 (100%)	2 (0%)	84	81
4	F	539/798 (68%)	539 (100%)	0	100	100
4	H	528/798 (66%)	528 (100%)	0	100	100
4	N	536/798 (67%)	535 (100%)	1 (0%)	87	86
5	A	544/791 (69%)	544 (100%)	0	100	100
5	C	555/791 (70%)	554 (100%)	1 (0%)	87	86
5	E	574/791 (73%)	573 (100%)	1 (0%)	87	86
5	G	572/791 (72%)	571 (100%)	1 (0%)	87	86
5	M	572/791 (72%)	572 (100%)	0	100	100
6	L	539/1546 (35%)	539 (100%)	0	100	100
All	All	12803/17212 (74%)	12787 (100%)	16 (0%)	87	88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	333	ARG
3	K	336	VAL
3	K	340	LEU
5	C	458	ASN
4	D	495	GLN
4	D	496	VAL
5	E	423	TYR
5	G	423	TYR
3	I	532	LEU
4	N	543	LYS
1	a	407	GLN
1	h	407	GLN
1	l	404	PHE
1	l	408	PHE
1	m	406	GLU
1	m	407	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	9	GLN
1	k	54	GLN
1	k	75	HIS
1	k	139	HIS
1	k	174	ASN
1	k	198	ASN
2	J	482	HIS
2	J	495	GLN
2	J	642	HIS
2	J	721	GLN
2	J	898	HIS
3	K	29	GLN
3	K	61	GLN
3	K	67	GLN
3	K	284	GLN
3	K	397	GLN
4	B	401	HIS
4	B	461	HIS
4	B	609	ASN
4	B	801	GLN
4	B	830	ASN
4	B	852	HIS
5	C	287	GLN

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Mol	Chain	Res	Type
5	C	289	ASN
5	C	458	ASN
5	C	487	GLN
5	C	639	GLN
4	D	269	ASN
4	D	343	HIS
4	D	345	GLN
4	D	424	HIS
4	D	461	HIS
4	D	531	GLN
4	D	705	HIS
4	D	774	GLN
5	E	401	HIS
5	E	424	ASN
5	E	458	ASN
5	E	580	HIS
5	E	585	GLN
5	E	654	GLN
5	E	725	HIS
4	F	329	HIS
4	F	389	GLN
4	F	560	GLN
4	F	576	HIS
4	F	703	GLN
4	F	885	HIS
5	G	329	GLN
5	G	512	HIS
5	G	650	HIS
5	G	691	GLN
5	G	763	GLN
5	G	832	HIS
4	H	479	GLN
4	H	550	ASN
4	H	596	ASN
4	H	609	ASN
4	H	716	HIS
4	H	717	GLN
4	H	801	GLN
3	I	82	HIS
3	I	152	GLN
3	I	377	GLN
3	I	393	ASN

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Mol	Chain	Res	Type
3	I	415	HIS
6	L	507	GLN
6	L	1522	HIS
5	M	289	ASN
5	M	373	GLN
5	M	424	ASN
5	M	436	GLN
4	N	479	GLN
4	N	609	ASN
4	N	719	GLN
5	A	309	GLN
5	A	412	HIS
5	A	692	ASN
5	A	707	HIS
1	a	9	GLN
1	a	75	HIS
1	a	174	ASN
1	a	198	ASN
1	a	211	ASN
1	a	407	GLN
1	b	9	GLN
1	b	54	GLN
1	b	75	HIS
1	b	174	ASN
1	b	198	ASN
1	b	334	HIS
1	c	9	GLN
1	c	54	GLN
1	c	59	HIS
1	c	174	ASN
1	c	198	ASN
1	d	16	GLN
1	d	54	GLN
1	d	75	HIS
1	d	322	ASN
1	e	54	GLN
1	e	75	HIS
1	e	139	HIS
1	e	174	ASN
1	e	198	ASN
1	e	299	GLN
1	e	371	HIS

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Mol	Chain	Res	Type
1	f	198	ASN
1	f	357	GLN
1	f	407	GLN
1	g	9	GLN
1	g	54	GLN
1	g	198	ASN
1	g	347	ASN
1	g	371	HIS
1	g	436	HIS
1	h	9	GLN
1	h	29	HIS
1	h	54	GLN
1	h	75	HIS
1	h	139	HIS
1	h	198	ASN
1	h	207	ASN
1	h	334	HIS
1	h	407	GLN
1	i	9	GLN
1	i	54	GLN
1	i	75	HIS
1	i	230	GLN
1	j	9	GLN
1	j	54	GLN
1	j	198	ASN
1	l	9	GLN
1	l	54	GLN
1	l	139	HIS
1	l	198	ASN
1	l	314	ASN
1	m	9	GLN
1	m	75	HIS
1	m	139	HIS
1	m	174	ASN
1	m	198	ASN
1	m	338	GLN
1	m	407	GLN
1	n	9	GLN
1	n	75	HIS
1	n	139	HIS
1	n	198	ASN
1	n	219	HIS

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Mol	Chain	Res	Type
1	n	221	GLN
1	n	229	ASN

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](#)

There are no chain breaks in this entry.

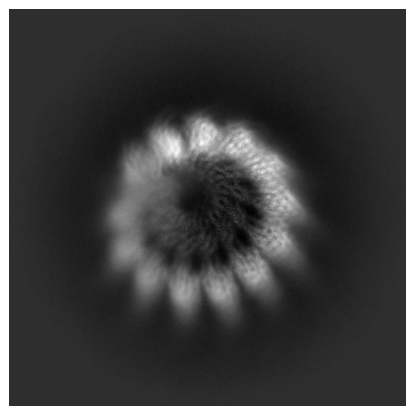
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18181. These allow visual inspection of the internal detail of the map and identification of artifacts.

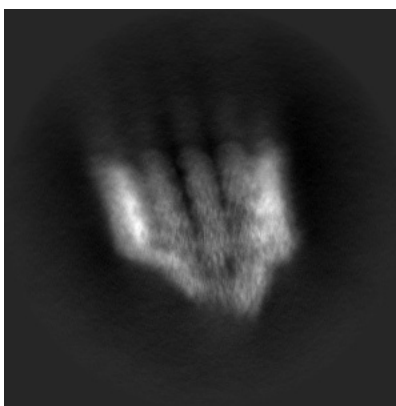
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

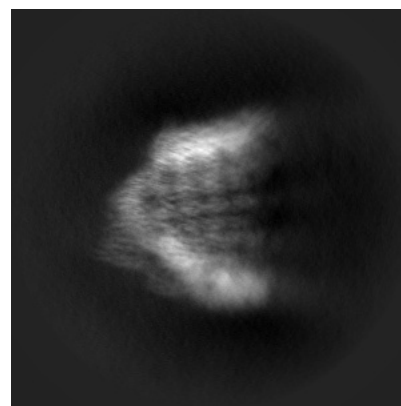
6.1.1 Primary map



X

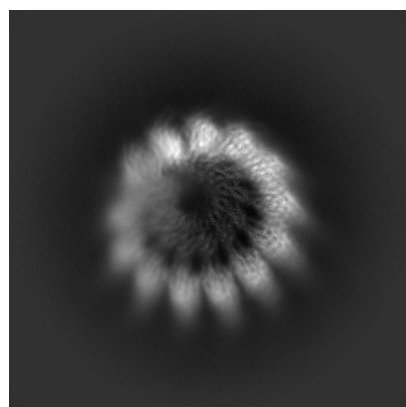


Y

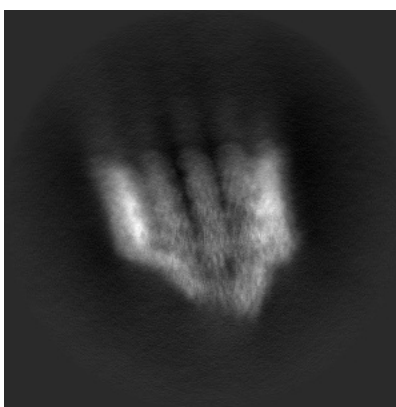


Z

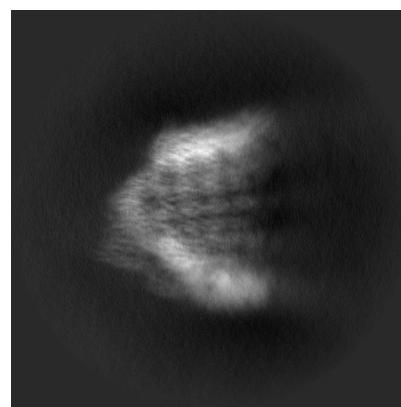
6.1.2 Raw map



X



Y

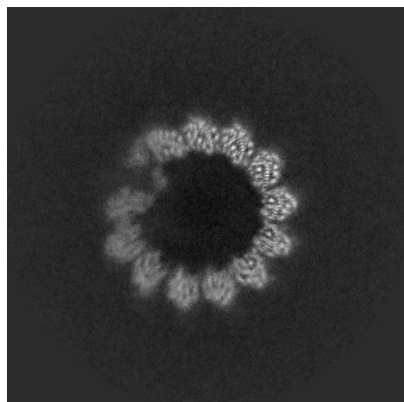


Z

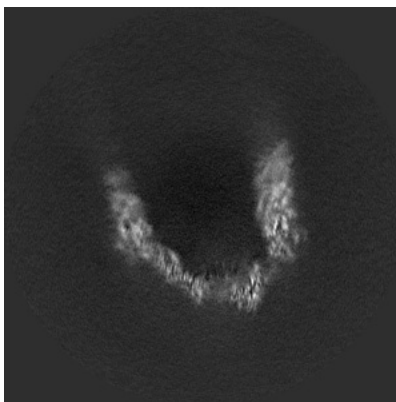
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

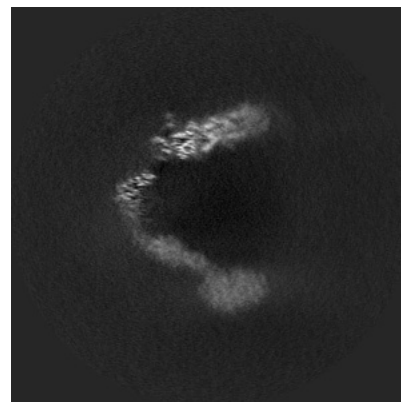
6.2.1 Primary map



X Index: 215

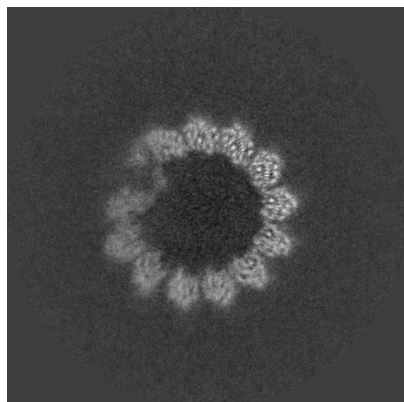


Y Index: 215

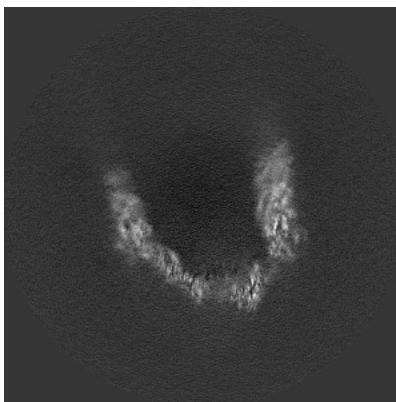


Z Index: 215

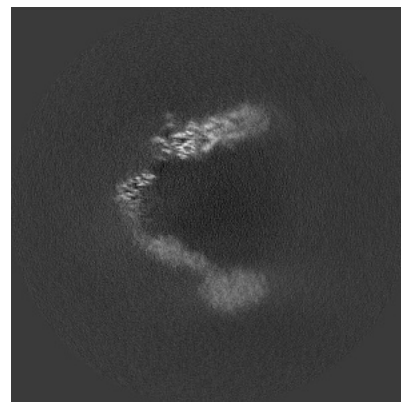
6.2.2 Raw map



X Index: 215



Y Index: 215

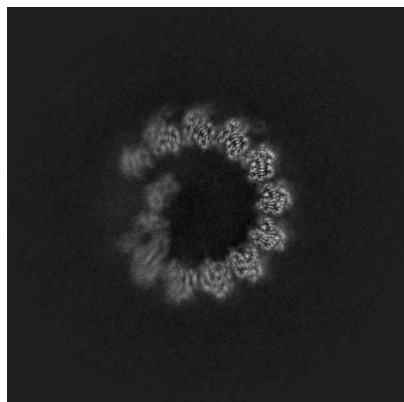


Z Index: 215

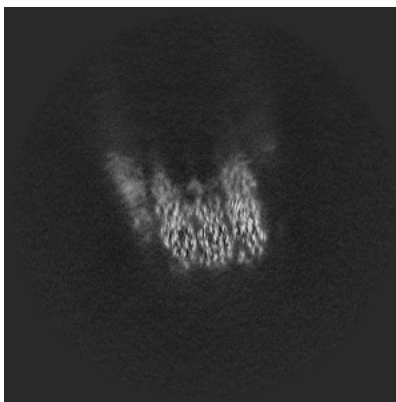
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

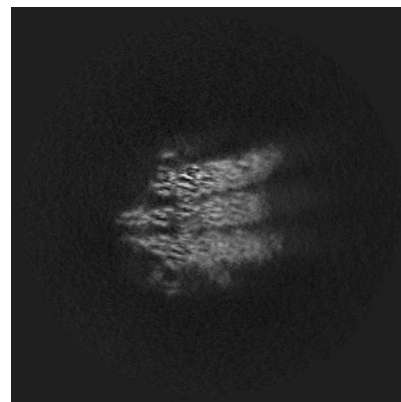
6.3.1 Primary map



X Index: 189

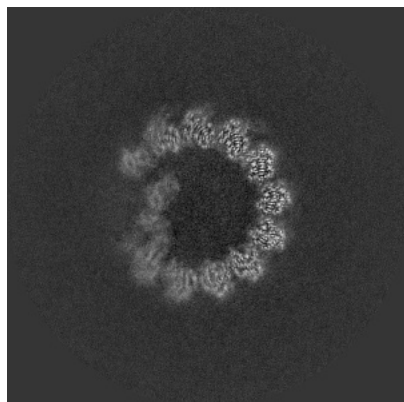


Y Index: 280

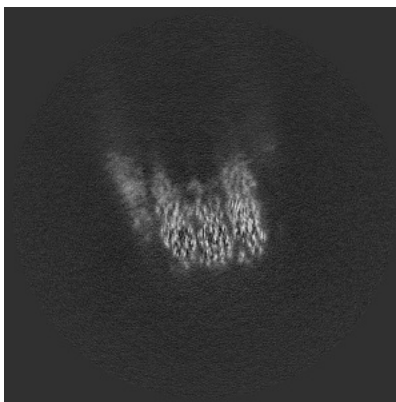


Z Index: 284

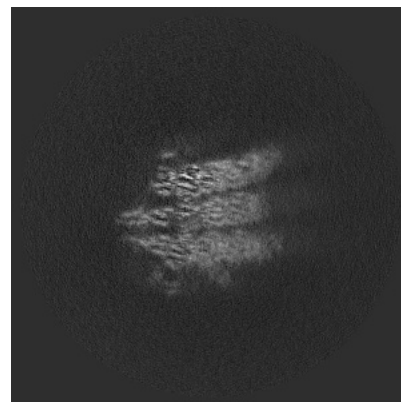
6.3.2 Raw map



X Index: 188



Y Index: 280



Z Index: 284

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

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

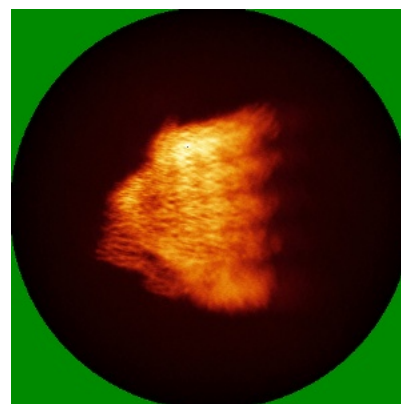
6.4.1 Primary map



X

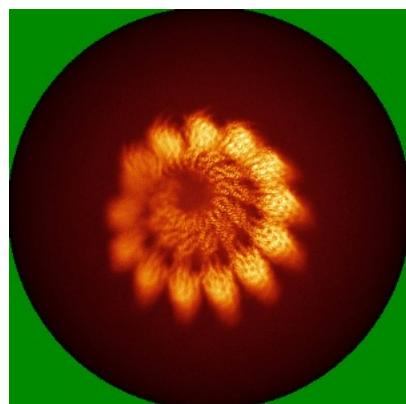


Y

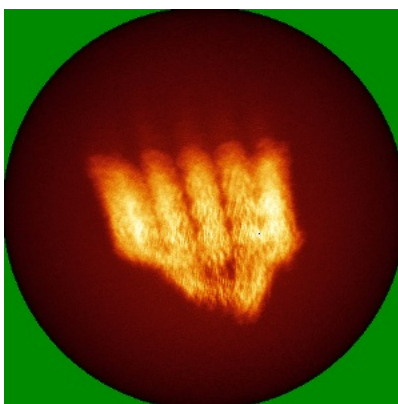


Z

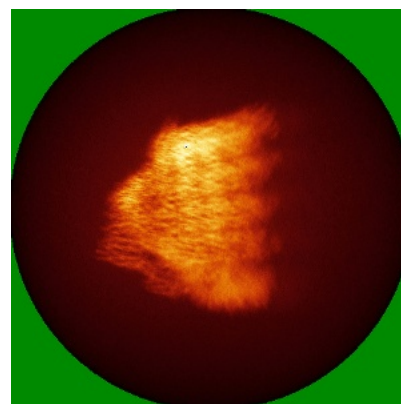
6.4.2 Raw map



X



Y

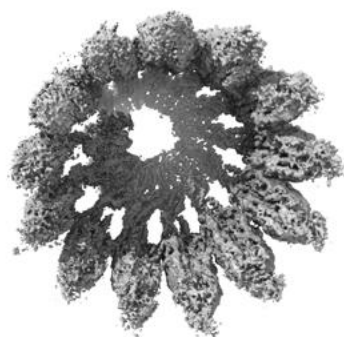


Z

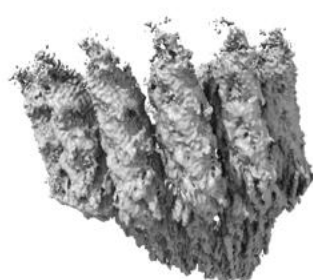
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



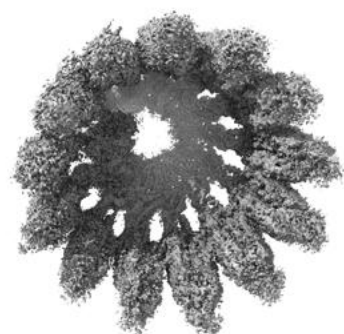
Y



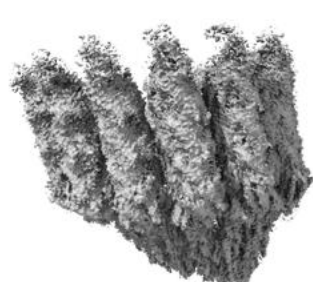
Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. 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



X



Y



Z

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

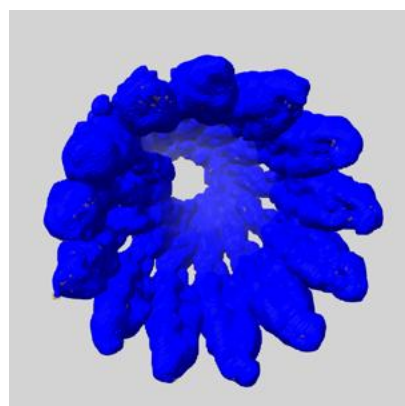
6.6 Mask visualisation [i](#)

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

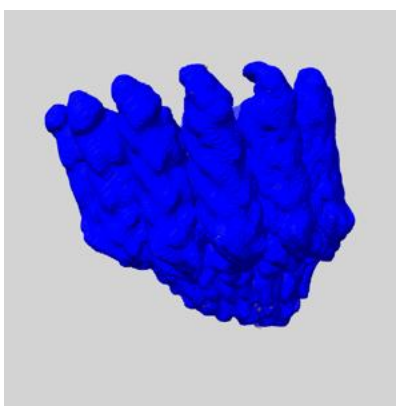
A mask typically either:

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

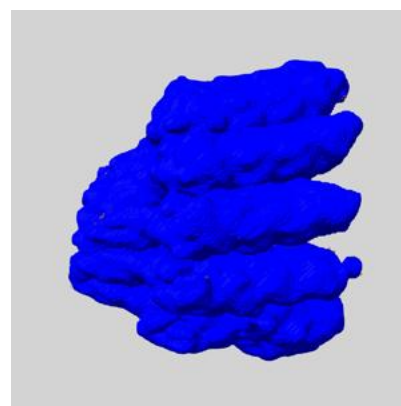
6.6.1 emd_18181_msk_1.map [i](#)



X



Y

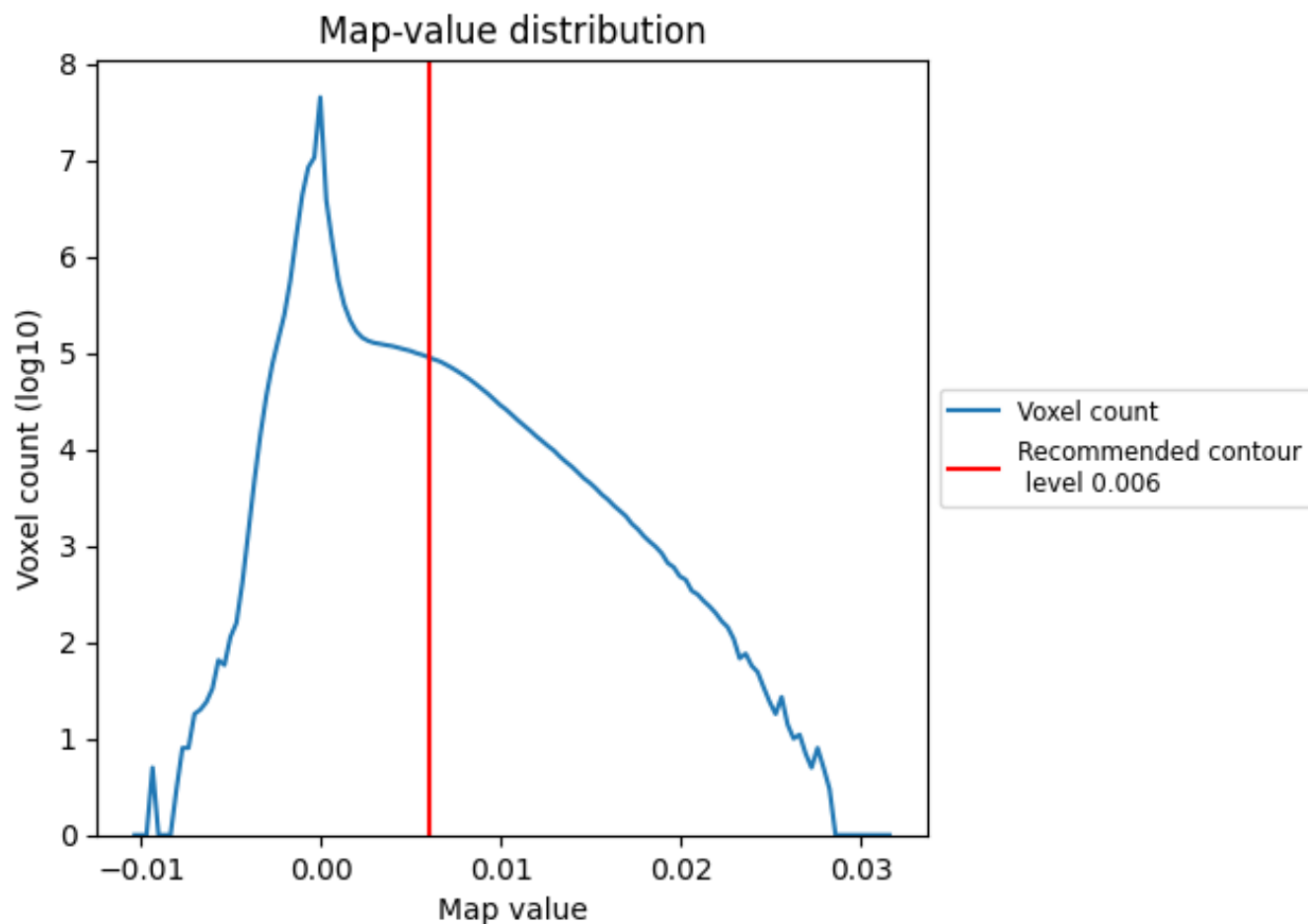


Z

7 Map analysis [i](#)

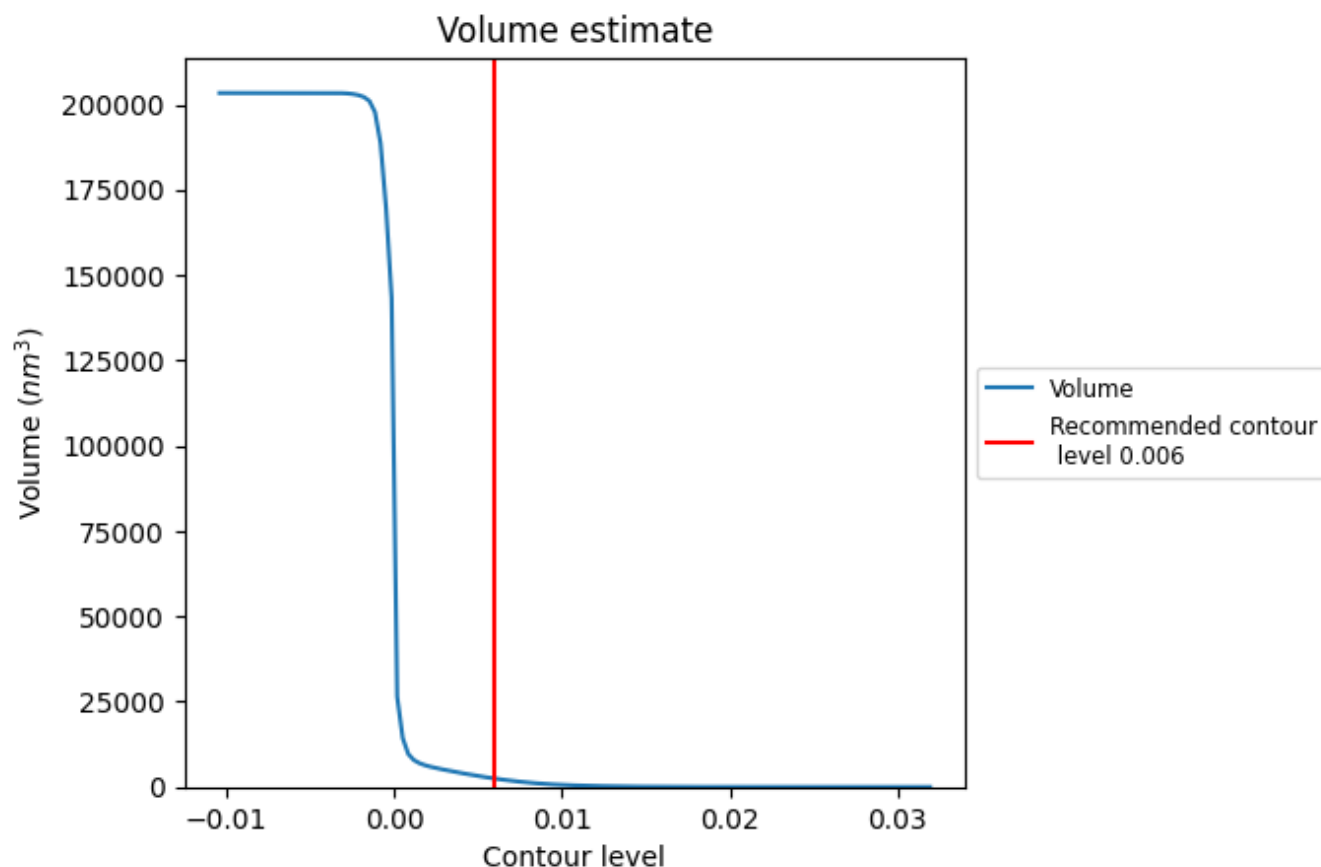
This section contains the results of statistical analysis of the map.

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.

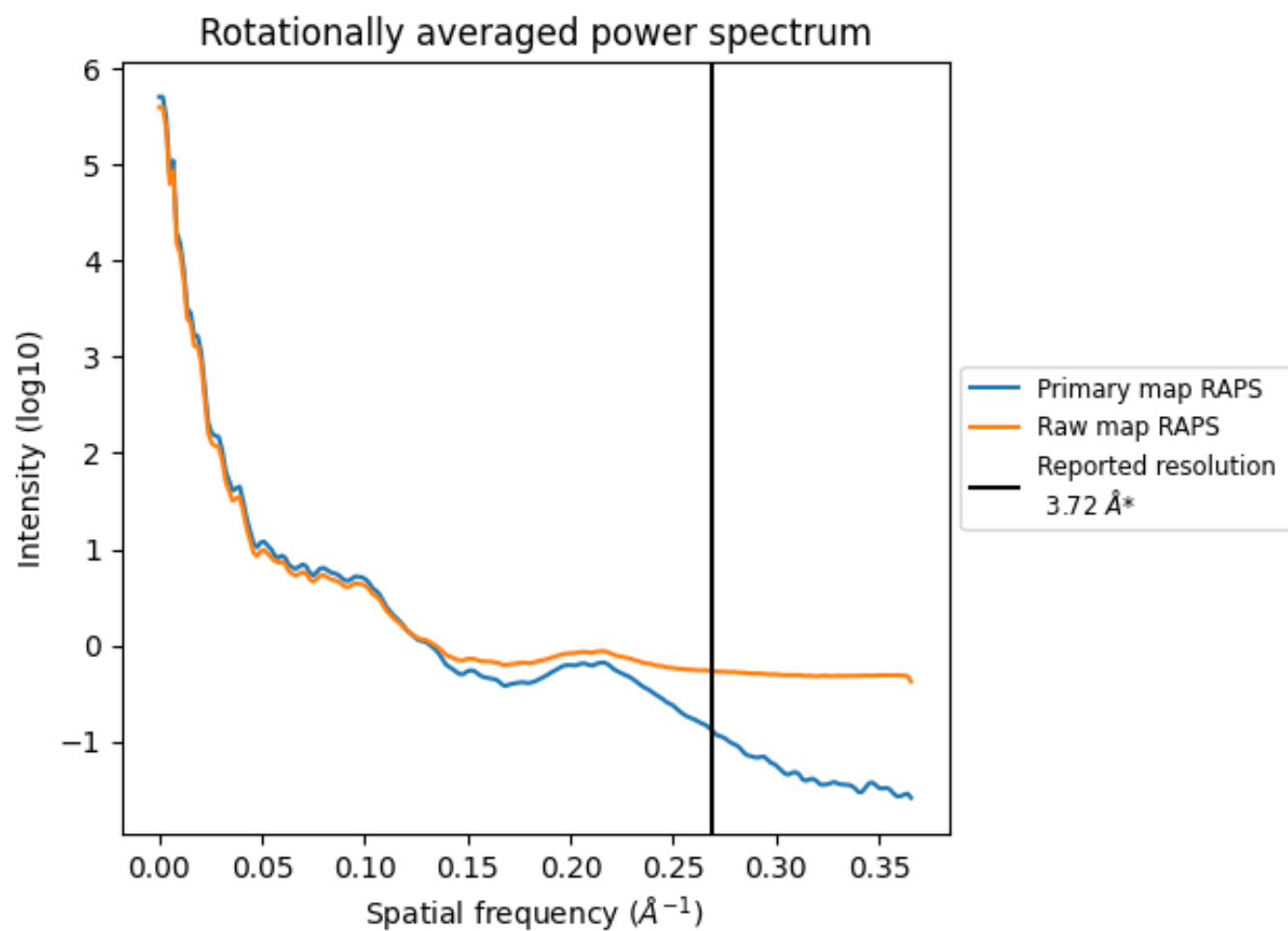
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2467 nm^3 ; this corresponds to an approximate mass of 2228 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

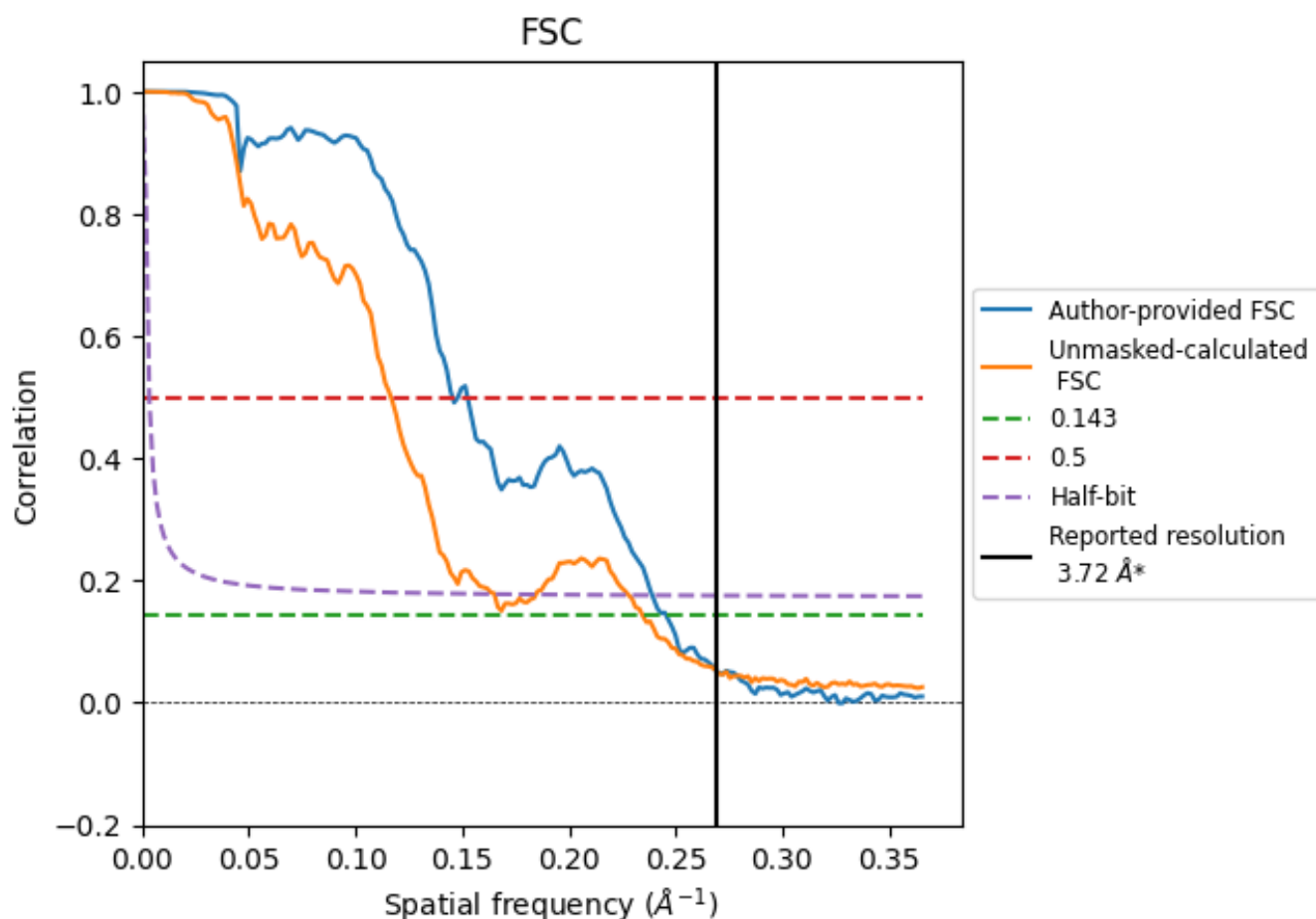


*Reported resolution corresponds to spatial frequency of 0.269 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.269 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

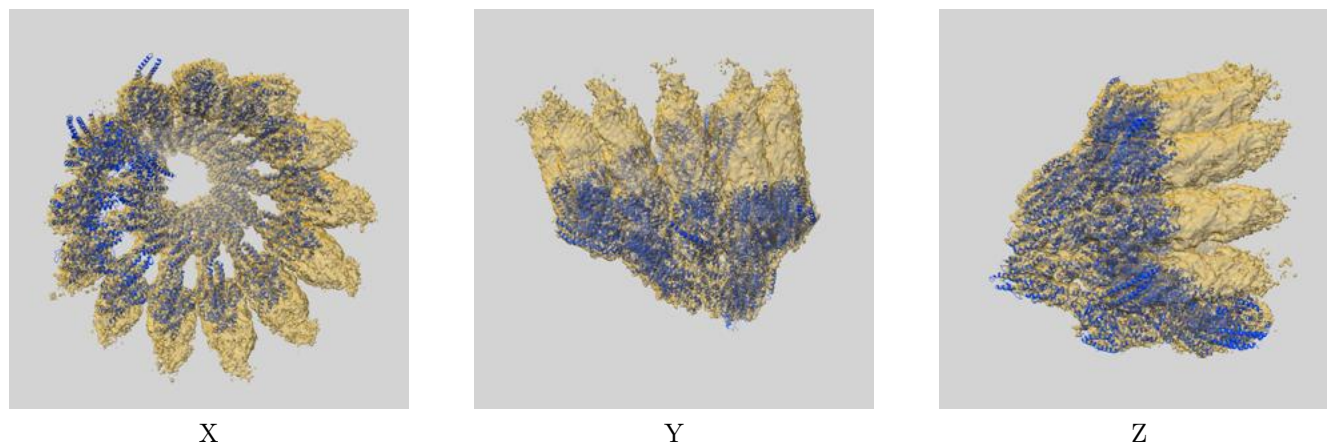
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	4.07	6.87	4.18
Unmasked-calculated*	4.26	8.58	6.06

*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 4.26 differs from the reported value 3.72 by more than 10 %

9 Map-model fit [i](#)

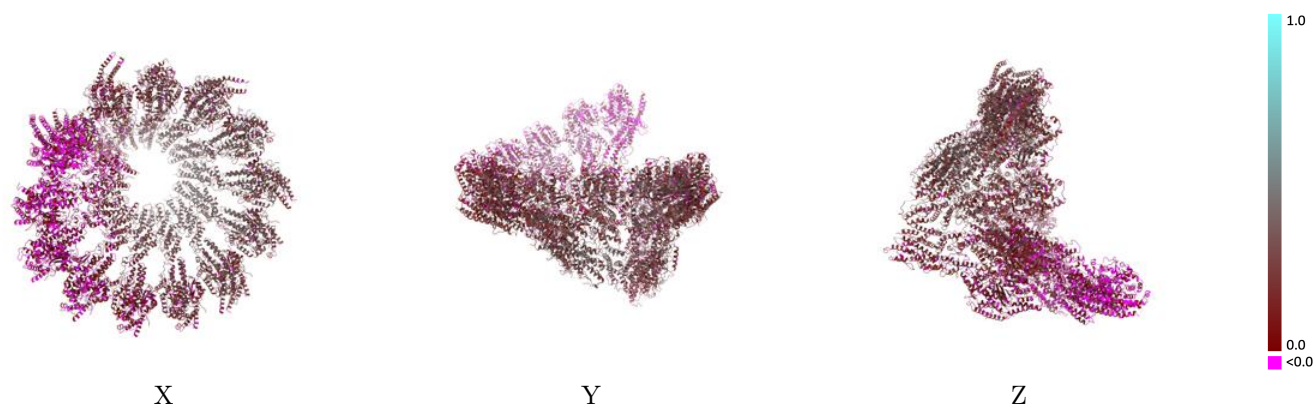
This section contains information regarding the fit between EMDB map EMD-18181 and PDB model 8Q62. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



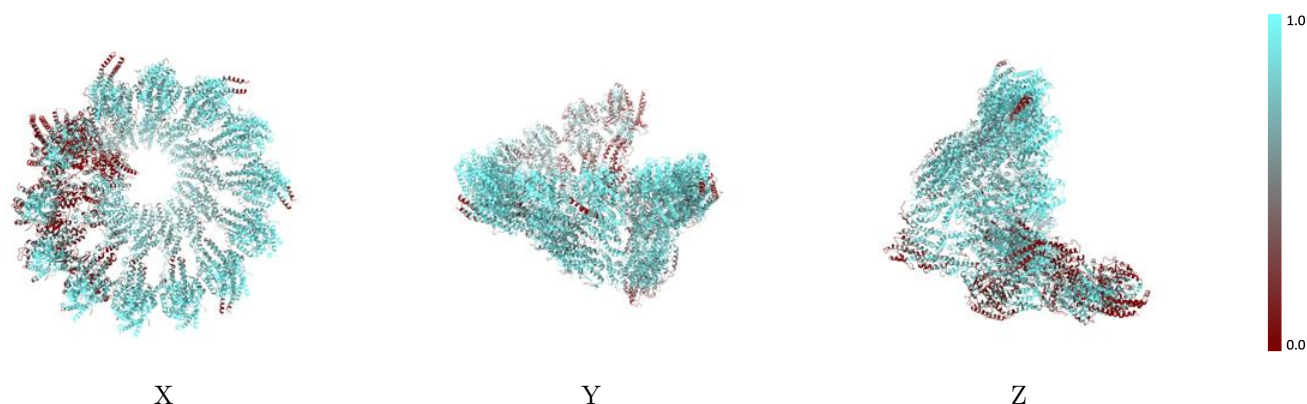
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



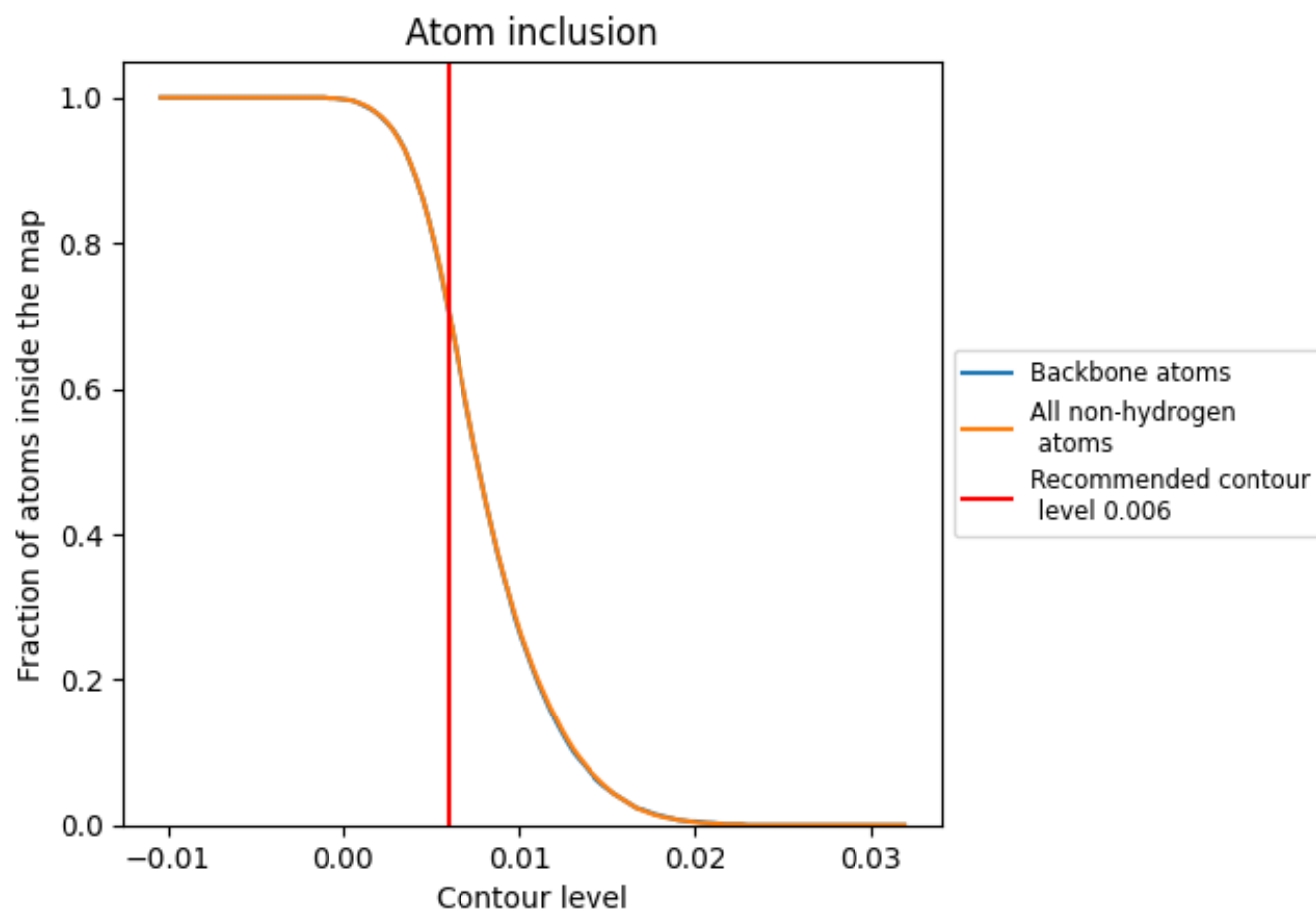
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7070	 0.1770
A	 0.4680	 0.1320
B	 0.6230	 0.1790
C	 0.7620	 0.2330
D	 0.7560	 0.2680
E	 0.7890	 0.2940
F	 0.7840	 0.3040
G	 0.7700	 0.2970
H	 0.7740	 0.2800
I	 0.7560	 0.2340
J	 0.7860	 0.1890
K	 0.7270	 0.1210
L	 0.6040	 0.0830
M	 0.5480	 0.0630
N	 0.3180	 0.0450
a	 0.4800	 0.0950
b	 0.7720	 0.1630
c	 0.8480	 0.2190
d	 0.8830	 0.2490
e	 0.9100	 0.2680
f	 0.8890	 0.2630
g	 0.9070	 0.2570
h	 0.8810	 0.2240
i	 0.8840	 0.1740
j	 0.8490	 0.0990
k	 0.7360	 0.0480
l	 0.6620	 0.0250
m	 0.5100	 0.0220
n	 0.3960	 0.0060

