



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:16 AM UTC

PDB ID : 7U8O / pdb_00007u8o
EMDB ID : EMD-26385
Title : Structure of porcine V-ATPase with mEAK7 and SidK, Rotary state 2
Authors : Tan, Y.Z.; Keon, K.A.
Deposited on : 2022-03-09
Resolution : 3.50 Å(reported)

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:

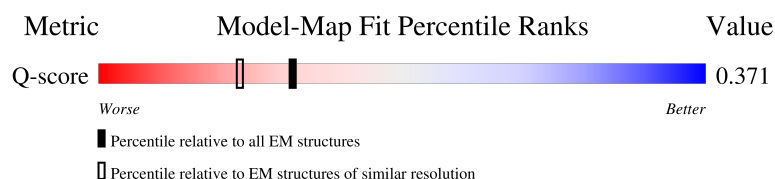
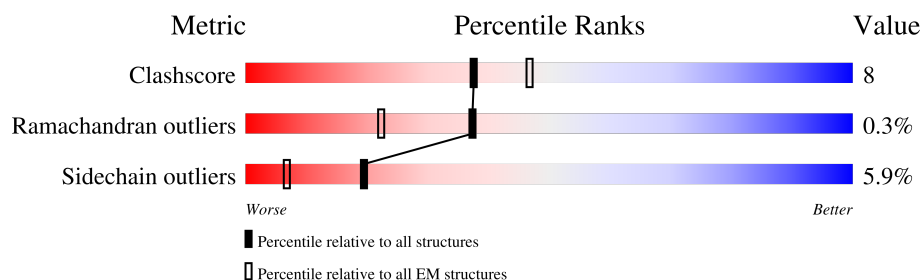
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.50 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	13950 (3.00 - 4.00)

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	617	
1	B	617	
1	C	617	
2	D	515	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	515	
2	F	515	
3	G	382	
4	H	247	
5	I	226	
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	Q	337	
8	R	337	
8	S	337	
9	T	483	
10	U	456	
11	a	838	
12	b	205	
13	c	469	
14	d	351	
15	e	81	
16	f	98	
17	g	155	
17	h	155	
17	i	155	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	j	155	71%26%
17	k	155	80%17%
17	l	155	80%15%
17	m	155	61%30%
17	n	155	72%24%
17	o	155	75%20%
18	p	351	11%85%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 68632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4661	2957	790	889	25		
1	B	588	Total	C	N	O	S	0	0
			4579	2903	777	875	24		
1	C	587	Total	C	N	O	S	0	0
			4577	2904	776	873	24		

- Molecule 2 is a protein called Vacuolar proton pump subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	458	Total	C	N	O	S	0	0
			3590	2278	615	676	21		
2	E	456	Total	C	N	O	S	0	0
			3572	2266	611	674	21		
2	F	456	Total	C	N	O	S	0	0
			3572	2266	611	674	21		

- Molecule 3 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	360	Total	C	N	O	S	0	0
			1791	1070	360	360	1		

- Molecule 4 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	213	Total	C	N	O	S	0	0
			1717	1089	309	314	5		

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	217	Total	C	N	O	S	0	0
			1614	1013	295	300	6		
5	J	218	Total	C	N	O	S	0	0
			1608	1008	296	298	6		
5	K	217	Total	C	N	O	S	0	0
			1707	1073	308	319	7		

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	109	Total	C	N	O	S	0	0
			865	548	153	162	2		

- Molecule 7 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	110	Total	C	N	O	S	0	0
			682	419	130	131	2		
7	N	110	Total	C	N	O	S	0	0
			661	404	128	128	1		
7	O	108	Total	C	N	O	S	0	0
			679	418	130	130	1		

- Molecule 8 is a protein called Bacterial effector protein SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	224	Total	C	N	O	S	0	0
			1824	1162	306	346	10		
8	R	206	Total	C	N	O	S	0	0
			1685	1073	285	319	8		
8	S	226	Total	C	N	O	S	0	0
			1832	1167	308	346	11		

- Molecule 9 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	427	Total	C	N	O	0	0
			2124	1268	428	428		

- Molecule 10 is a protein called TLDc protein mEAK-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	383	Total	C	N	O	S	0	0
			2400	1481	449	459	11		

- Molecule 11 is a protein called V-type proton ATPase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	750	Total	C	N	O	S	0	0
			5635	3662	947	991	35		

- Molecule 12 is a protein called V-type proton ATPase 21 kDa proteolipid subunit isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	203	Total	C	N	O	S	0	0
			1498	993	237	258	10		

- Molecule 13 is a protein called ATPase H⁺ transporting accessory protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	205	Total	C	N	O	S	0	0
			1661	1084	269	301	7		

- Molecule 14 is a protein called V-type proton ATPase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	350	Total	C	N	O	S	0	0
			2835	1829	462	530	14		

- Molecule 15 is a protein called V-type proton ATPase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	80	Total	C	N	O	S	0	0
			652	451	98	98	5		

- Molecule 16 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	84	Total	C	N	O	S	0	0
			653	433	100	114	6		

- Molecule 17 is a protein called V-type proton ATPase proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
17	h	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
17	i	150	Total	C	N	O	S	0	0
			1052	695	164	186	7		
17	j	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
17	k	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
17	l	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
17	m	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
17	n	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
17	o	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		

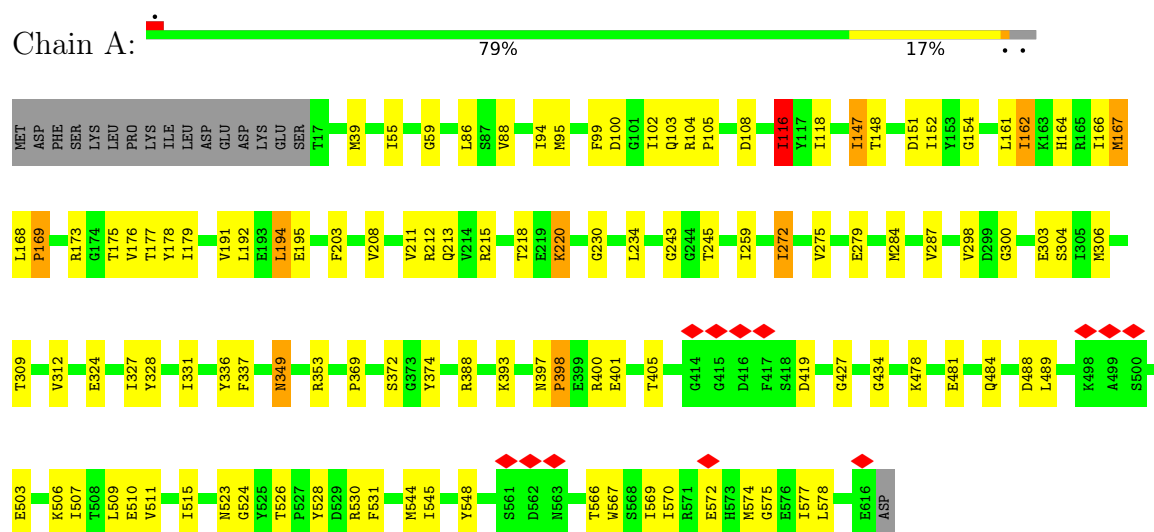
- Molecule 18 is a protein called ATPase H(+)-transporting lysosomal accessory protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	53	Total	C	N	O	S	0	0
			442	297	65	76	4		

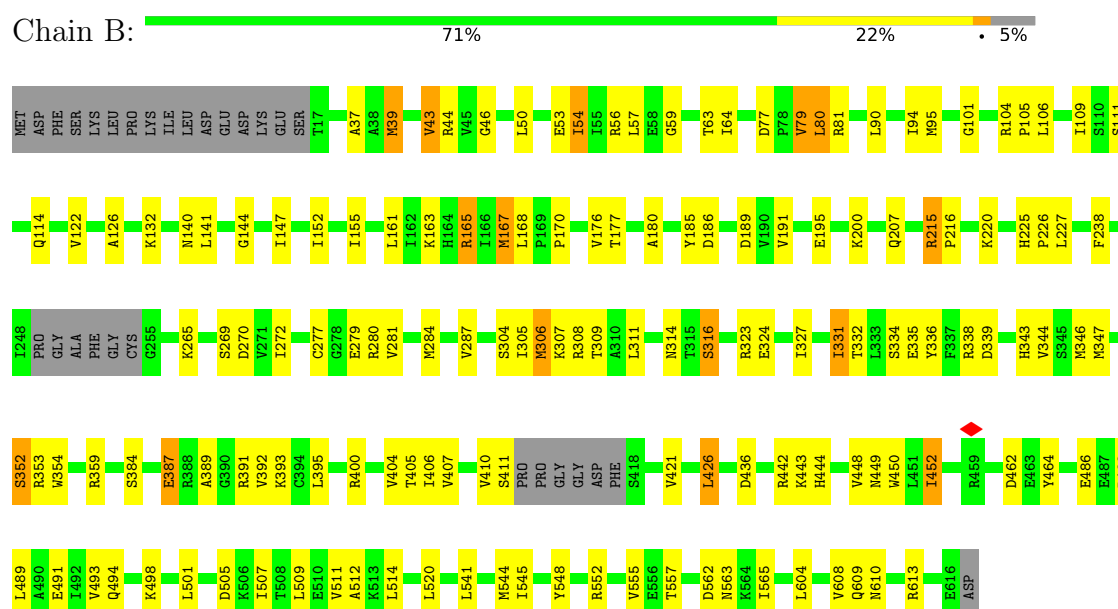
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

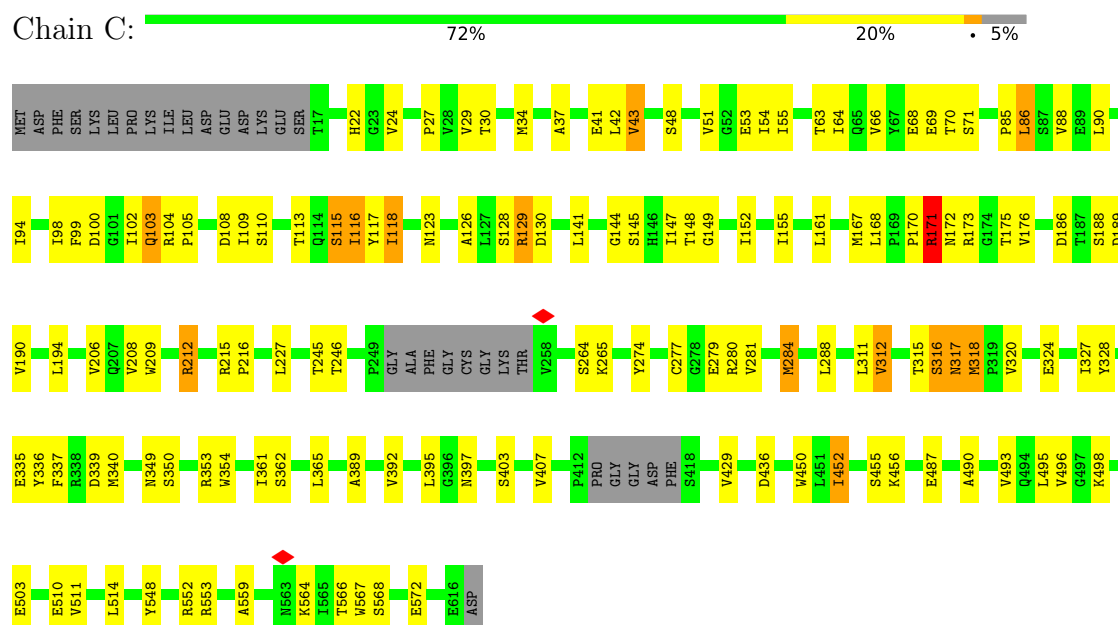
- Molecule 1: V-type proton ATPase catalytic subunit A



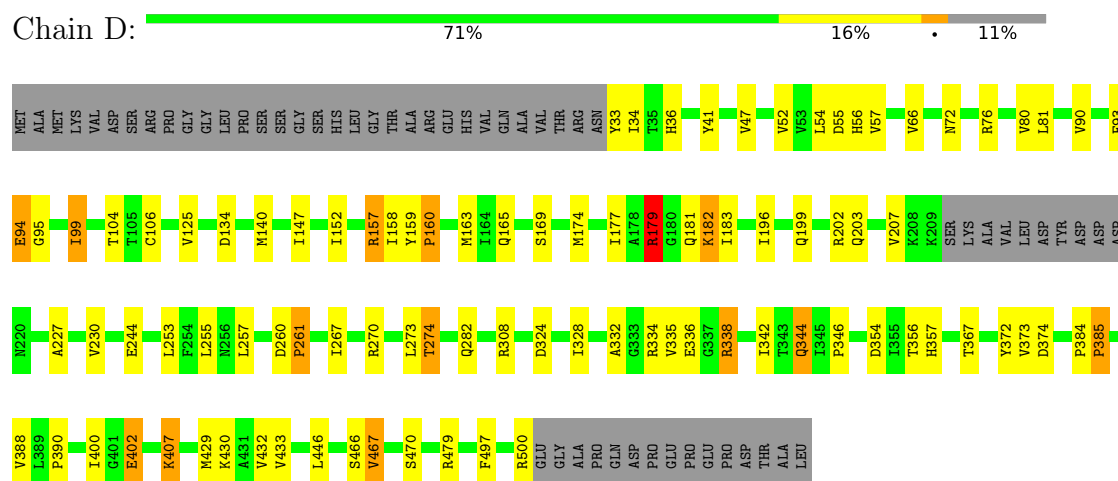
- Molecule 1: V-type proton ATPase catalytic subunit A



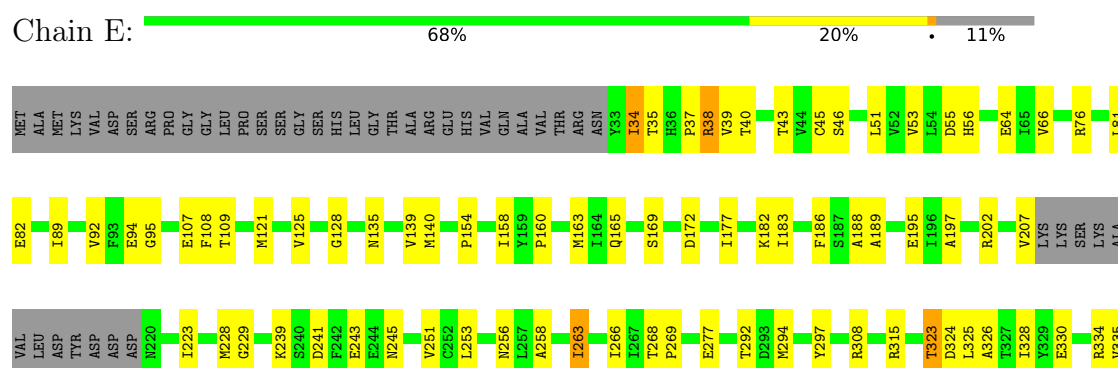
• Molecule 1: V-type proton ATPase catalytic subunit A

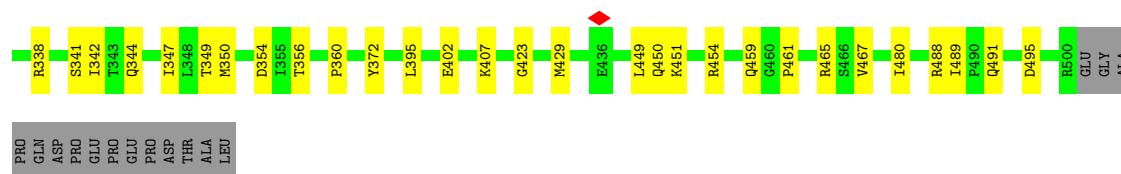


• Molecule 2: Vacuolar proton pump subunit B



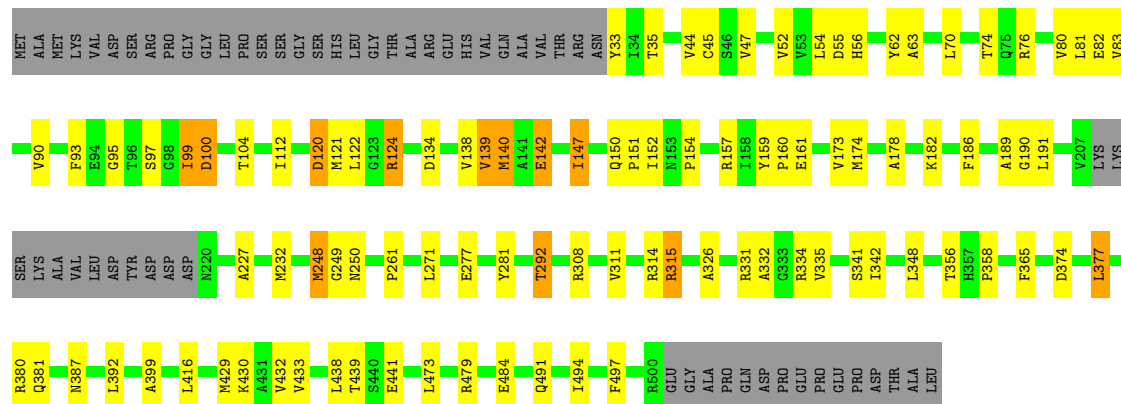
• Molecule 2: Vacuolar proton pump subunit B





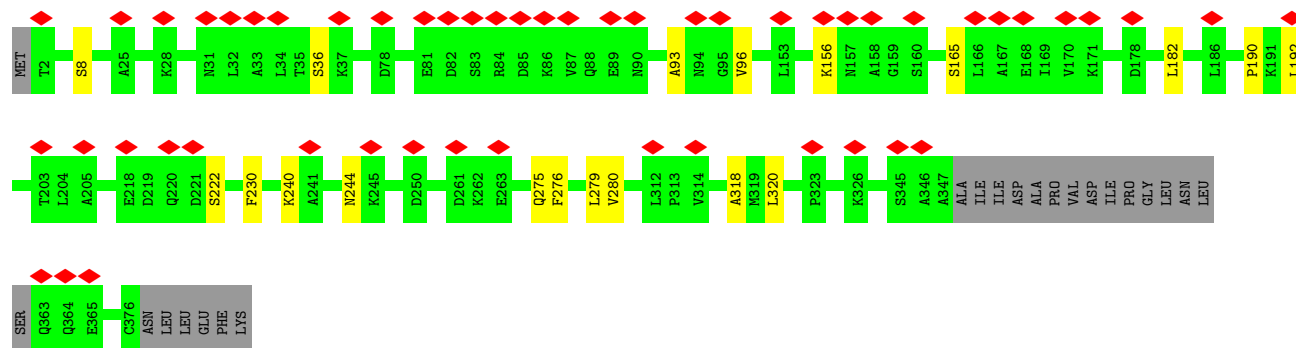
• Molecule 2: Vacuolar proton pump subunit B

Chain F: 70% 17% 11%



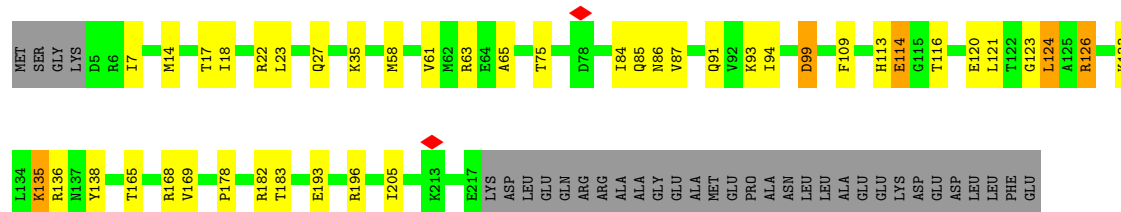
• Molecule 3: V-type proton ATPase subunit C

Chain G: 14% 89% 5% 6%



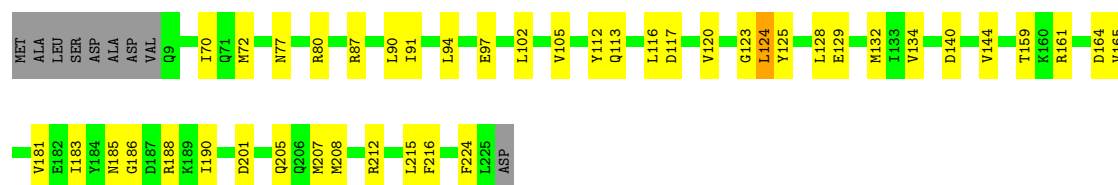
• Molecule 4: V-type proton ATPase subunit D

Chain H: 69% 15% 14%



• Molecule 5: V-type proton ATPase subunit E 1

Chain I:  77% 19% .



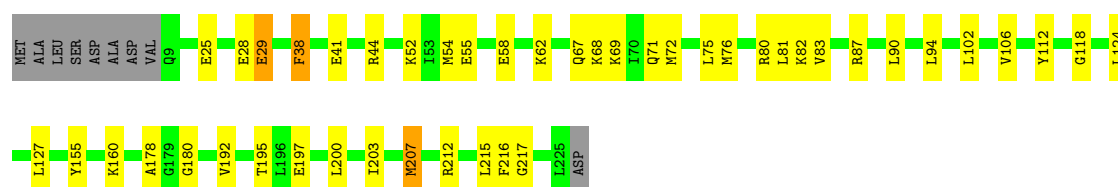
- Molecule 5: V-type proton ATPase subunit E 1

Chain J:  82% 14% . .



- Molecule 5: V-type proton ATPase subunit E 1

Chain K:  76% 19% . .



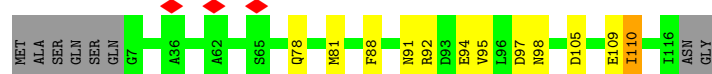
- Molecule 6: V-type proton ATPase subunit F

Chain L:  6% 63% 25% 8% . .



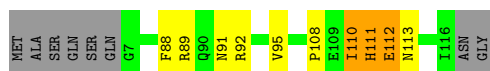
- Molecule 7: V-type proton ATPase subunit G

Chain M:  83% 9% 7% .



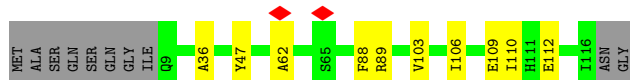
- Molecule 7: V-type proton ATPase subunit G

Chain N:  85% 6% 7%



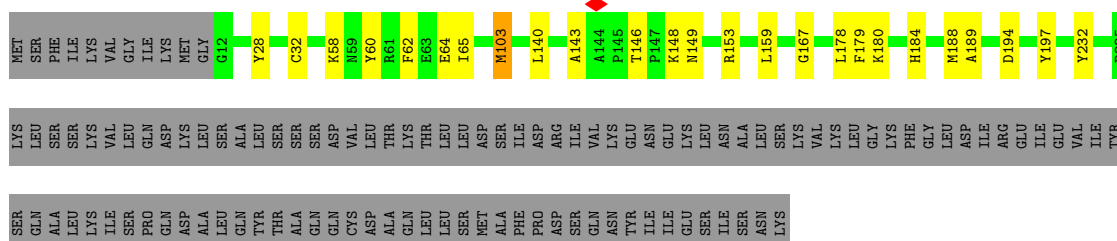
- Molecule 7: V-type proton ATPase subunit G

Chain O:  83% 8% 8%



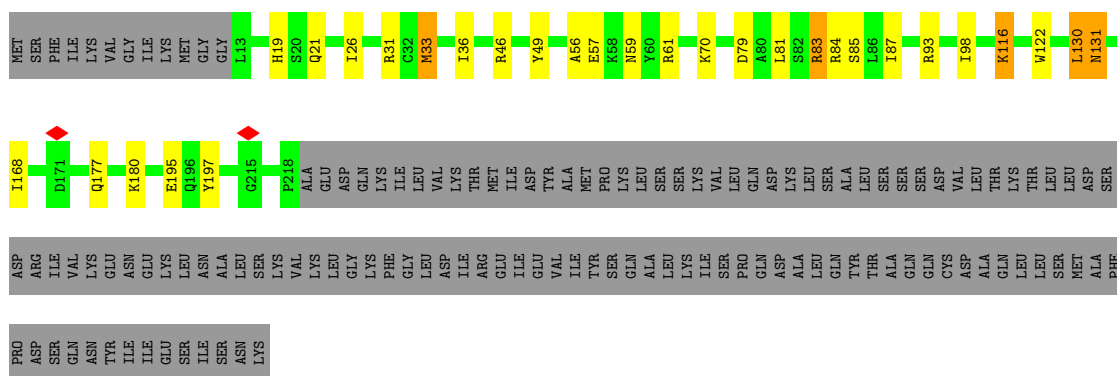
- Molecule 8: Bacterial effector protein SidK

Chain Q:  59% 7% 34%



- Molecule 8: Bacterial effector protein SidK

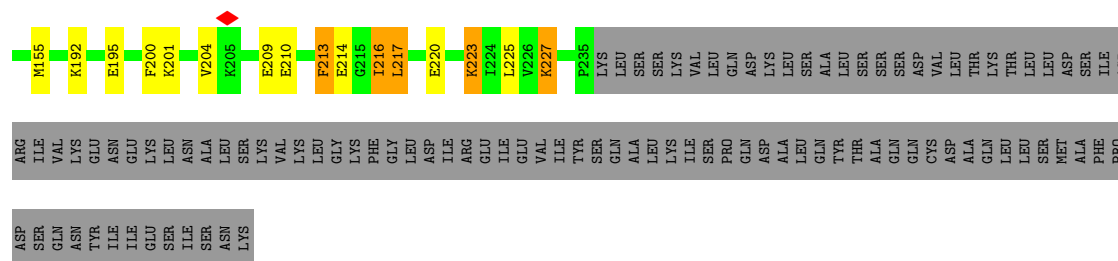
Chain R:  52% 7% 39%



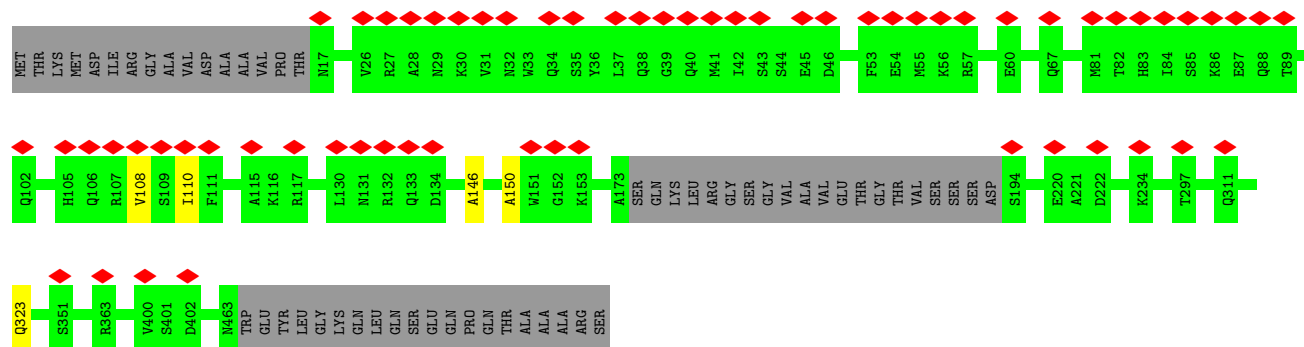
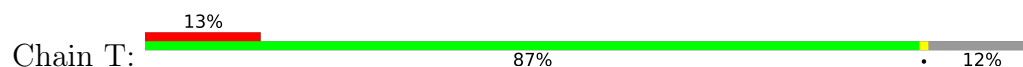
- Molecule 8: Bacterial effector protein SidK

Chain S:  54% 11% 33%

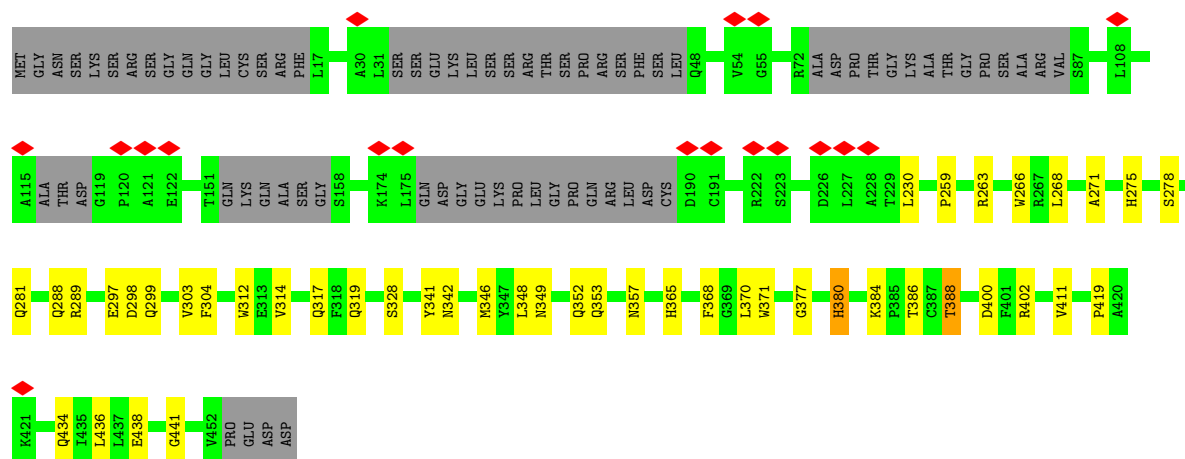




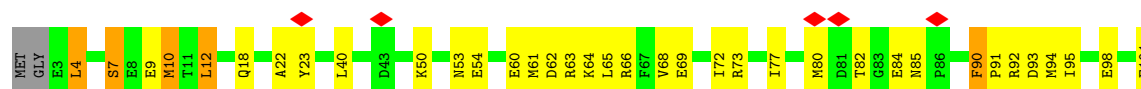
• Molecule 9: V-type proton ATPase subunit H

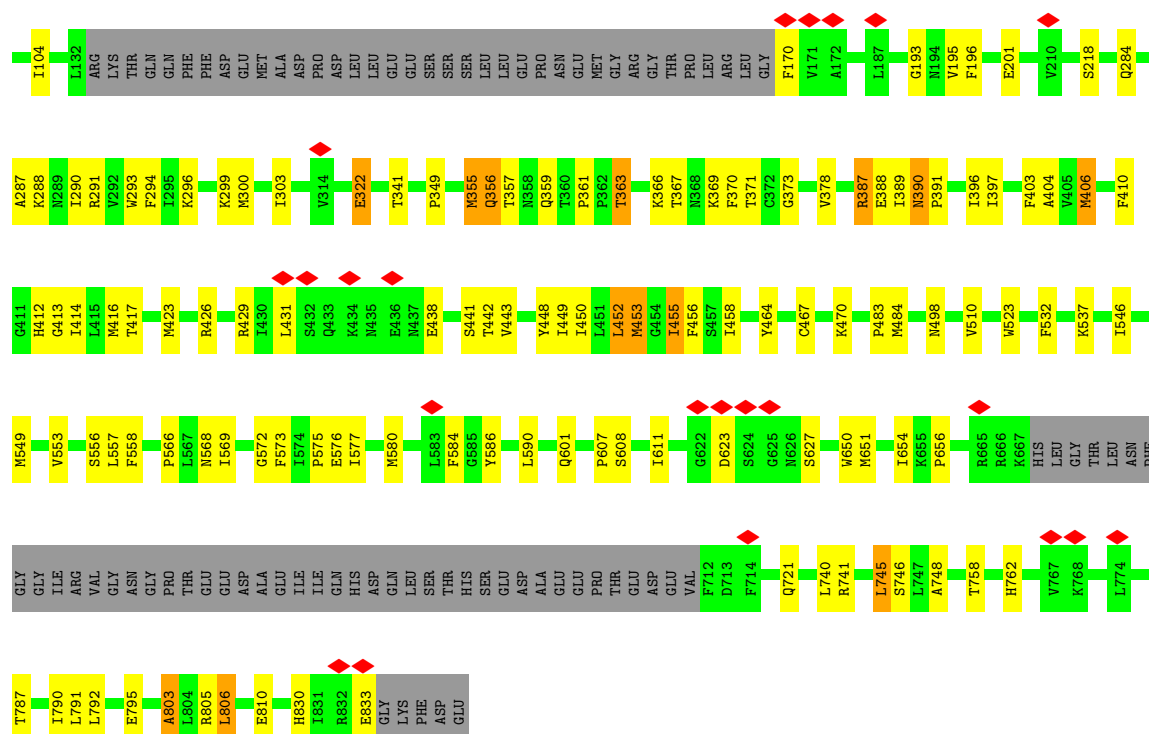


• Molecule 10: TLDC protein mEAK-7



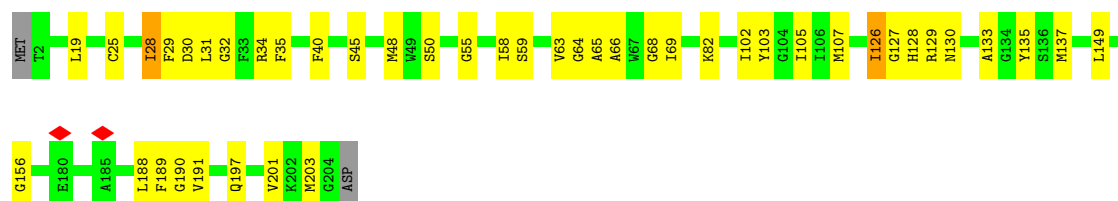
• Molecule 11: V-type proton ATPase subunit a





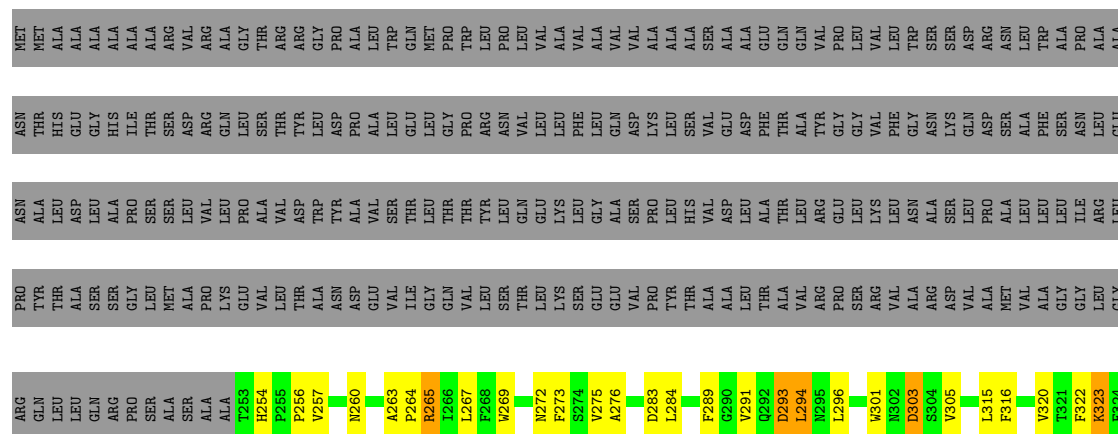
- Molecule 12: V-type proton ATPase 21 kDa proteolipid subunit isoform 1

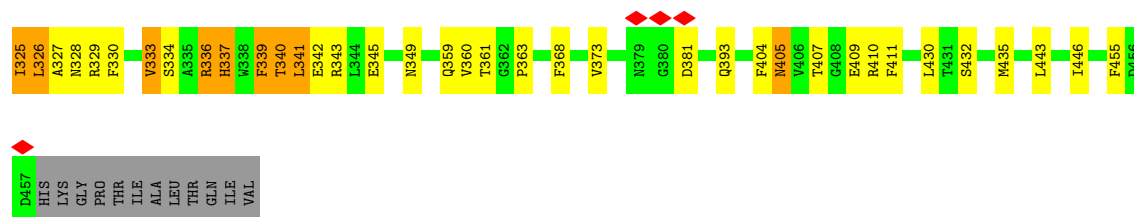
Chain b: 78% 20% ..



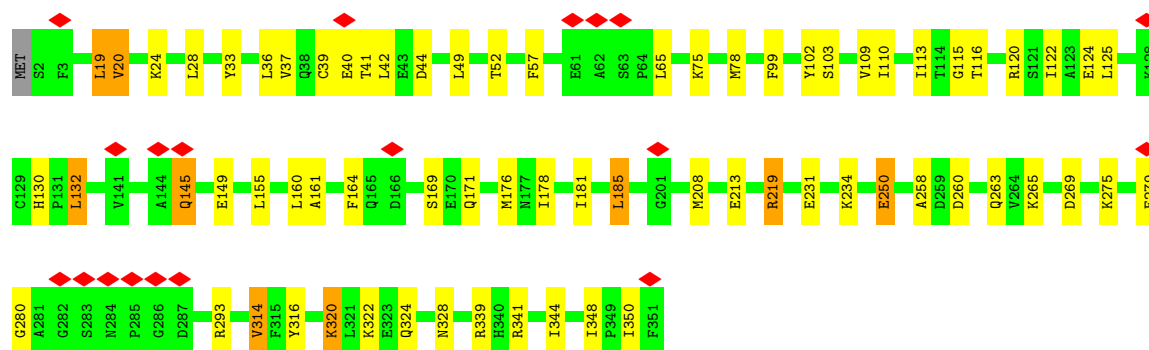
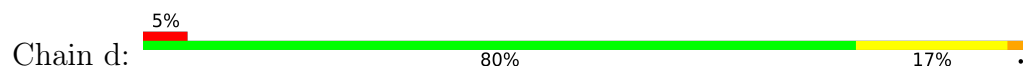
- Molecule 13: ATPase H⁺ transporting accessory protein 1

Chain c: 30% 11% 56%

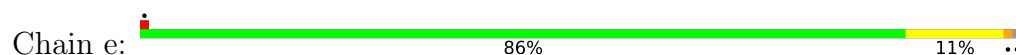




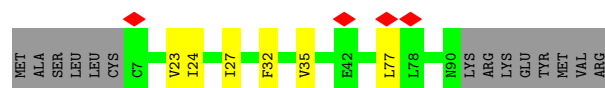
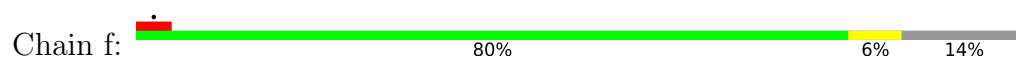
• Molecule 14: V-type proton ATPase subunit



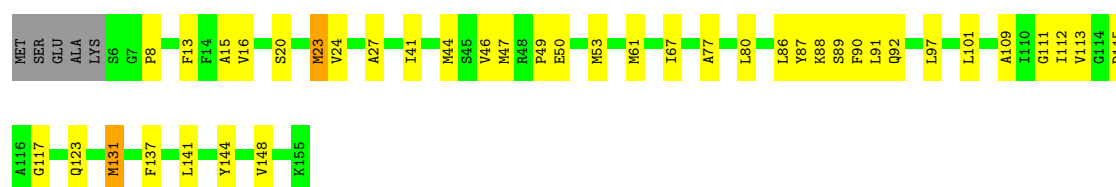
• Molecule 15: V-type proton ATPase subunit



• Molecule 16: Ribonuclease kappa

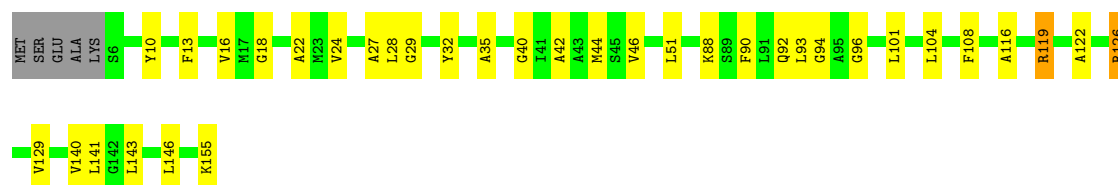


• Molecule 17: V-type proton ATPase proteolipid subunit



• Molecule 17: V-type proton ATPase proteolipid subunit

Chain h: 



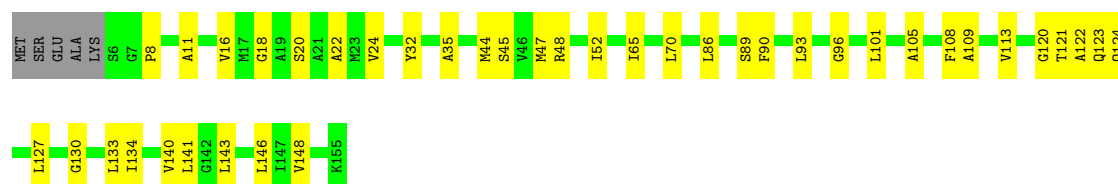
- Molecule 17: V-type proton ATPase proteolipid subunit

Chain i: 



- Molecule 17: V-type proton ATPase proteolipid subunit

Chain j: 



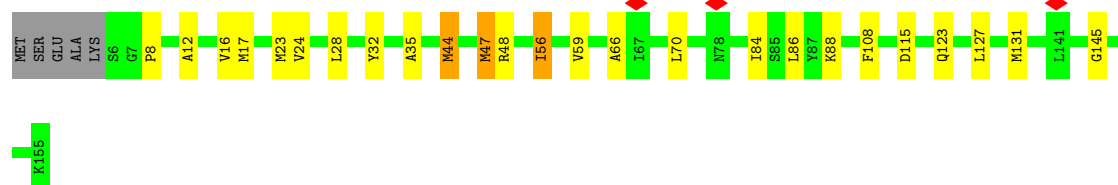
- Molecule 17: V-type proton ATPase proteolipid subunit

Chain k: 



- Molecule 17: V-type proton ATPase proteolipid subunit

Chain l: 



- Molecule 17: V-type proton ATPase proteolipid subunit

Chain m: 

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31814	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	787.921	Depositor
Maximum defocus (nm)	2554.877	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.692	Depositor
Minimum map value	-0.560	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.135	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	476.1, 476.1, 476.1	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3225, 1.3225, 1.3225	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	0.64	1/4757 (0.0%)	1.06	7/6446 (0.1%)
1	B	0.69	0/4668	1.11	8/6322 (0.1%)
1	C	0.68	0/4668	1.11	7/6324 (0.1%)
2	D	0.71	0/3662	1.17	10/4961 (0.2%)
2	E	0.58	1/3644 (0.0%)	0.95	2/4939 (0.0%)
2	F	0.70	0/3644	1.10	7/4939 (0.1%)
3	G	0.09	0/1789	0.23	0/2495
4	H	0.57	0/1735	1.04	1/2321 (0.0%)
5	I	0.31	0/1628	0.64	0/2197
5	J	0.40	0/1621	0.72	0/2188
5	K	0.48	0/1722	0.90	3/2313 (0.1%)
6	L	0.67	0/879	1.26	7/1186 (0.6%)
7	M	0.33	0/687	0.56	0/943
7	N	0.39	0/666	0.59	0/917
7	O	0.54	0/685	0.81	0/942
8	Q	0.47	0/1858	0.87	0/2505
8	R	0.61	0/1717	1.15	3/2315 (0.1%)
8	S	0.60	0/1866	1.07	4/2515 (0.2%)
9	T	0.08	0/2122	0.25	0/2959
10	U	0.36	0/2437	0.60	0/3335
11	a	0.51	0/5767	0.92	5/7838 (0.1%)
12	b	0.47	0/1532	0.90	3/2083 (0.1%)
13	c	0.71	0/1716	1.21	5/2338 (0.2%)
14	d	0.59	0/2901	1.04	2/3930 (0.1%)
15	e	0.57	0/679	1.05	1/934 (0.1%)
16	f	0.56	0/669	1.01	0/907
17	g	0.61	1/1073 (0.1%)	1.04	3/1453 (0.2%)
17	h	0.60	1/1073 (0.1%)	1.03	0/1453
17	i	0.38	0/1067	0.73	1/1446 (0.1%)
17	j	0.48	0/1073	0.95	0/1453
17	k	0.47	0/1073	0.99	0/1453
17	l	0.56	0/1073	1.05	2/1453 (0.1%)
17	m	0.58	0/1073	1.01	2/1453 (0.1%)
17	n	0.65	0/1073	1.14	3/1453 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	o	0.59	0/1073	1.10	3/1453 (0.2%)
18	p	0.56	0/456	0.99	0/625
All	All	0.57	4/69826 (0.0%)	0.98	89/94787 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	323	THR	C-O	-6.95	1.15	1.24
17	h	13	PHE	C-O	-6.50	1.16	1.24
1	A	169	PRO	C-O	-6.39	1.19	1.25
17	g	61	MET	SD-CE	-5.92	1.64	1.79

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	126	ILE	N-CA-C	-8.43	104.80	112.90
2	F	142	GLU	N-CA-C	-8.27	100.96	112.45
1	A	336	TYR	N-CA-C	-8.12	102.97	113.12
17	i	67	ILE	N-CA-C	-7.64	104.34	111.45
2	E	323	THR	CA-C-O	-7.38	112.60	120.42
2	D	373	VAL	N-CA-C	-7.35	99.14	108.84
2	F	134	ASP	N-CA-C	-7.26	102.97	112.41
2	D	196	ILE	N-CA-C	-7.21	103.94	111.58
8	S	216	ILE	N-CA-C	-7.15	105.75	112.83
11	a	803	ALA	N-CA-C	-7.07	104.29	113.12
15	e	61	ASN	CA-CB-CG	6.99	119.59	112.60
2	D	160	PRO	CB-CA-C	-6.92	102.53	111.46
1	A	116	ILE	N-CA-C	-6.88	106.02	112.83
13	c	333	VAL	N-CA-C	-6.85	103.63	110.62
11	a	498	ASN	N-CA-C	-6.83	101.45	110.40
1	A	398	PRO	N-CA-C	-6.78	100.55	111.19
1	B	332	THR	N-CA-C	-6.73	103.75	112.23
1	B	393	LYS	N-CA-C	-6.69	99.02	109.25
11	a	806	LEU	N-CA-C	-6.52	104.09	111.07
6	L	22	LEU	N-CA-C	-6.48	103.72	111.69
1	C	336	TYR	N-CA-C	-6.33	104.51	112.93
1	A	177	THR	N-CA-C	-6.20	106.26	113.88
8	R	131	ASN	N-CA-C	-6.14	104.13	111.69
13	c	373	VAL	N-CA-CB	6.13	117.84	110.31
2	D	95	GLY	CA-C-O	-6.12	118.24	122.22
2	D	179	ARG	CB-CA-C	6.07	119.90	110.67
12	b	29	PHE	N-CA-C	-6.00	100.78	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	99	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	339	ASP	N-CA-C	-5.95	105.52	112.89
13	c	283	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	452	ILE	N-CA-C	-5.93	107.35	113.10
17	n	125	PRO	N-CA-C	-5.88	106.20	113.84
1	B	140	ASN	N-CA-C	-5.83	106.51	113.97
1	C	452	ILE	CA-C-N	5.83	132.16	121.85
1	C	452	ILE	C-N-CA	5.83	132.16	121.85
17	g	67	ILE	N-CA-C	-5.81	105.42	111.58
2	D	274	THR	N-CA-C	-5.79	104.56	111.69
1	A	312	VAL	CA-C-O	-5.76	117.61	122.63
6	L	96	HIS	CA-CB-CG	5.76	119.56	113.80
17	g	50	GLU	N-CA-C	-5.74	106.24	113.18
1	B	225	HIS	CA-C-N	5.69	125.60	119.85
1	B	225	HIS	C-N-CA	5.69	125.60	119.85
1	C	436	ASP	CA-CB-CG	5.68	118.28	112.60
2	D	385	PRO	CB-CA-C	-5.59	105.49	113.09
1	B	391	ARG	N-CA-C	-5.54	102.08	110.28
2	D	470	SER	N-CA-C	-5.51	105.29	112.23
8	S	16	GLU	N-CA-C	-5.48	106.55	113.18
17	n	11	ALA	CA-C-N	5.47	127.87	120.38
17	n	11	ALA	C-N-CA	5.47	127.87	120.38
13	c	363	PRO	N-CA-C	-5.44	102.65	111.14
6	L	95	GLU	CA-C-N	5.42	129.14	121.61
6	L	95	GLU	C-N-CA	5.42	129.14	121.61
5	K	155	TYR	N-CA-C	-5.38	105.50	111.36
17	o	143	LEU	N-CA-C	-5.38	106.40	113.12
1	A	154	GLY	CA-C-O	-5.37	116.34	121.49
1	C	456	LYS	N-CA-C	-5.36	106.59	113.02
17	l	17	MET	CA-C-N	5.30	125.83	119.94
17	l	17	MET	C-N-CA	5.30	125.83	119.94
1	B	336	TYR	N-CA-C	-5.29	103.47	111.56
11	a	746	SER	N-CA-C	-5.24	105.24	111.69
11	a	412	HIS	CB-CG-CD2	-5.21	124.42	131.20
2	F	173	VAL	CB-CA-C	5.21	116.25	110.62
2	F	473	LEU	CA-C-N	5.21	125.72	119.94
2	F	473	LEU	C-N-CA	5.21	125.72	119.94
14	d	219	ARG	N-CA-C	-5.19	105.07	111.40
2	D	324	ASP	CA-CB-CG	-5.19	107.41	112.60
17	m	67	ILE	N-CA-C	-5.18	106.09	111.58
12	b	40	PHE	CA-CB-CG	5.18	118.98	113.80
17	o	56	ILE	CA-C-N	5.17	124.46	120.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	o	56	ILE	C-N-CA	5.17	124.46	120.33
8	S	117	GLN	OE1-CD-NE2	-5.16	117.44	122.60
5	K	217	GLY	CA-C-O	-5.13	118.13	122.29
2	E	325	LEU	N-CA-C	-5.13	105.69	111.28
2	F	190	GLY	N-CA-C	-5.11	108.77	115.47
6	L	21	LEU	N-CA-C	-5.11	106.30	112.54
17	m	56	ILE	N-CA-C	-5.11	106.92	112.80
6	L	77	ALA	CA-C-N	5.11	128.08	120.31
6	L	77	ALA	C-N-CA	5.11	128.08	120.31
5	K	124	LEU	N-CA-C	-5.08	105.74	111.28
1	C	328	TYR	CB-CA-C	5.07	118.92	110.90
14	d	178	ILE	N-CA-C	5.07	115.69	110.36
13	c	293	ASP	O-C-N	-5.06	115.87	122.09
17	g	123	GLN	CB-CA-C	5.06	118.90	111.06
2	F	186	PHE	CA-C-O	-5.04	115.17	120.92
2	D	357	HIS	CB-CG-CD2	-5.03	124.66	131.20
8	R	56	ALA	CA-C-N	5.03	131.14	121.54
8	R	56	ALA	C-N-CA	5.03	131.14	121.54
1	A	162	ILE	CA-C-O	-5.02	118.26	122.63
8	S	87	ILE	N-CA-C	-5.01	105.61	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4661	0	4653	68	0
1	B	4579	0	4575	86	0
1	C	4577	0	4577	73	0
2	D	3590	0	3581	54	0
2	E	3572	0	3555	56	0
2	F	3572	0	3555	66	0
3	G	1791	0	797	10	0
4	H	1717	0	1822	24	0
5	I	1614	0	1567	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	1608	0	1558	23	0
5	K	1707	0	1739	26	0
6	L	865	0	872	12	0
7	M	682	0	499	10	0
7	N	661	0	447	8	0
7	O	679	0	494	6	0
8	Q	1824	0	1835	21	0
8	R	1685	0	1691	13	0
8	S	1832	0	1843	23	0
9	T	2124	0	947	3	0
10	U	2400	0	1768	32	0
11	a	5635	0	5264	99	0
12	b	1498	0	1548	36	0
13	c	1661	0	1566	39	0
14	d	2835	0	2770	40	0
15	e	652	0	668	5	0
16	f	653	0	652	3	0
17	g	1058	0	1136	31	0
17	h	1058	0	1136	30	0
17	i	1052	0	1125	41	0
17	j	1058	0	1136	25	0
17	k	1058	0	1136	22	0
17	l	1058	0	1136	23	0
17	m	1058	0	1136	47	0
17	n	1058	0	1136	30	0
17	o	1058	0	1136	28	0
18	p	442	0	438	11	0
All	All	68632	0	65494	1007	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 8.

All (1007) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:MET:HE1	1:B:308:ARG:C	1.83	1.02
1:A:95:MET:HE2	1:A:337:PHE:CE2	2.06	0.90
1:A:95:MET:CE	1:A:337:PHE:CE2	2.54	0.90
1:B:95:MET:CE	1:B:308:ARG:C	2.49	0.84
1:C:117:TYR:HE1	2:F:152:ILE:CD1	1.92	0.83
17:i:120:GLY:HA2	17:i:123:GLN:HE21	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:40:GLY:HA2	17:i:119:ARG:HH22	1.46	0.80
17:i:120:GLY:HA3	17:i:127:LEU:HD22	1.64	0.80
2:F:374:ASP:HB2	2:F:387:ASN:HB2	1.65	0.78
17:j:44:MET:HG2	17:j:122:ALA:HB2	1.66	0.78
17:m:124:GLN:HB3	17:m:127:LEU:HD13	1.66	0.77
1:C:279:GLU:HB3	1:C:349:ASN:ND2	2.01	0.76
2:E:51:LEU:HB3	2:E:89:ILE:HD11	1.66	0.76
17:o:17:MET:HG3	17:o:93:LEU:HD13	1.68	0.74
17:n:23:MET:HE3	17:o:148:VAL:HG21	1.69	0.74
2:E:223:ILE:HB	2:E:251:VAL:HG22	1.69	0.74
1:A:192:LEU:HD11	1:A:194:LEU:HD21	1.69	0.74
12:b:105:ILE:HD13	17:g:144:TYR:HB3	1.70	0.73
1:B:272:ILE:HB	1:B:309:THR:HG22	1.68	0.72
17:l:28:LEU:HD23	17:m:105:ALA:HB2	1.70	0.72
1:A:95:MET:CE	1:A:337:PHE:HE2	2.00	0.72
1:B:284:MET:HE2	1:B:311:LEU:HD21	1.70	0.72
1:A:194:LEU:HD12	1:A:203:PHE:CE2	2.25	0.72
13:c:305:VAL:HA	13:c:327:ALA:HB3	1.71	0.71
1:A:95:MET:HE1	1:A:337:PHE:CE2	2.25	0.71
2:F:248:MET:C	2:F:250:ASN:H	1.97	0.71
1:C:117:TYR:HE1	2:F:152:ILE:HD11	1.56	0.71
1:B:324:GLU:HA	1:B:354:TRP:CD1	2.26	0.70
1:C:71:SER:HA	2:F:62:TYR:HD2	1.55	0.70
11:a:650:TRP:CD1	11:a:654:ILE:HD12	2.27	0.70
11:a:748:ALA:HB2	17:n:147:ILE:HD11	1.74	0.69
1:A:95:MET:HE2	1:A:337:PHE:HE2	1.53	0.69
17:m:27:ALA:HA	17:n:141:LEU:HD11	1.74	0.69
1:C:43:VAL:HG21	1:C:64:ILE:HG12	1.73	0.69
17:j:120:GLY:O	17:j:124:GLN:N	2.25	0.69
11:a:80:MET:HE2	11:a:291:ARG:HD3	1.75	0.68
17:g:24:VAL:HG22	17:h:101:LEU:HB2	1.74	0.68
1:A:147:ILE:HG12	1:A:168:LEU:HD22	1.74	0.68
17:m:56:ILE:HG12	17:n:133:LEU:HD22	1.76	0.68
1:A:511:VAL:HG11	1:A:548:TYR:HB2	1.76	0.68
1:A:176:VAL:HA	1:A:194:LEU:HD23	1.76	0.68
17:o:124:GLN:NE2	17:o:126:ARG:HD3	2.10	0.67
2:D:163:MET:HE1	2:D:467:VAL:HB	1.75	0.67
17:j:16:VAL:HG12	17:k:94:GLY:HA3	1.77	0.67
1:C:117:TYR:CE1	2:F:152:ILE:CD1	2.77	0.67
3:G:275:GLN:O	3:G:279:LEU:N	2.24	0.66
17:n:84:ILE:HG23	17:n:88:LYS:HE3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:44:MET:HG2	17:i:122:ALA:HB2	1.76	0.66
17:n:18:GLY:HA3	17:n:93:LEU:HA	1.77	0.66
1:C:317:ASN:HD21	2:F:151:PRO:HB3	1.61	0.66
17:i:28:LEU:HD22	17:j:105:ALA:HB2	1.78	0.66
1:C:264:SER:OG	1:C:265:LYS:NZ	2.29	0.66
8:Q:180:LYS:O	8:Q:184:HIS:ND1	2.29	0.65
17:k:48:ARG:NH2	17:k:121:THR:O	2.30	0.65
1:A:95:MET:HE3	1:A:162:ILE:HG21	1.79	0.65
1:C:510:GLU:HG2	1:C:567:TRP:CZ2	2.31	0.65
2:F:47:VAL:HG13	2:F:52:VAL:HG22	1.78	0.64
11:a:830:HIS:HB3	11:a:833:GLU:HB2	1.79	0.64
2:E:188:ALA:HA	2:E:349:THR:HG23	1.78	0.64
1:C:279:GLU:HB3	1:C:349:ASN:HD22	1.61	0.64
1:B:557:THR:O	10:U:317:GLN:NE2	2.30	0.64
2:D:174:MET:HE2	2:D:174:MET:HA	1.80	0.64
17:g:27:ALA:HA	17:h:141:LEU:HD11	1.79	0.64
17:k:120:GLY:O	17:k:124:GLN:N	2.30	0.64
1:C:324:GLU:HG2	1:C:354:TRP:HE1	1.63	0.63
2:F:55:ASP:OD1	2:F:56:HIS:N	2.31	0.63
17:l:70:LEU:HD21	17:m:144:TYR:HB3	1.80	0.63
1:B:494:GLN:HA	2:E:429:MET:HE1	1.81	0.63
1:B:610:ASN:OD1	1:B:613:ARG:NH1	2.30	0.63
17:g:49:PRO:HB2	17:h:126:ARG:HG2	1.80	0.63
2:E:55:ASP:OD1	2:E:56:HIS:N	2.30	0.63
11:a:803:ALA:HA	11:a:806:LEU:HD12	1.81	0.63
11:a:546:ILE:HG12	11:a:584:PHE:HB3	1.81	0.63
1:B:95:MET:HE2	1:B:308:ARG:HA	1.81	0.62
2:E:81:LEU:HD13	2:E:308:ARG:HH21	1.64	0.62
18:p:337:ASP:HB2	18:p:340:ILE:HG12	1.80	0.62
2:D:273:LEU:HD11	2:D:328:ILE:HG23	1.81	0.62
13:c:291:VAL:HG22	13:c:294:LEU:HD13	1.81	0.62
2:E:135:ASN:O	5:J:85:ARG:NH1	2.32	0.62
18:p:325:THR:O	18:p:329:ILE:HG12	1.99	0.62
2:E:76:ARG:NH2	2:E:95:GLY:O	2.32	0.62
2:E:82:GLU:OE2	2:E:308:ARG:NH1	2.32	0.62
11:a:484:MET:HE3	11:a:510:VAL:HG11	1.79	0.62
17:i:40:GLY:O	17:i:119:ARG:NH1	2.29	0.62
17:i:57:ILE:O	17:i:61:MET:HG3	2.00	0.62
1:A:192:LEU:HD21	1:A:194:LEU:HD11	1.80	0.62
17:i:27:ALA:HA	17:j:141:LEU:HD11	1.80	0.62
1:C:117:TYR:CE1	2:F:152:ILE:HG13	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:n:44:MET:HG2	17:n:122:ALA:HB2	1.81	0.62
2:D:163:MET:HE3	2:D:165:GLN:HA	1.82	0.61
17:h:18:GLY:HA3	17:h:93:LEU:HA	1.82	0.61
8:S:13:LEU:HD22	8:S:17:GLN:HG2	1.81	0.61
11:a:557:LEU:HB2	11:a:573:PHE:CG	2.36	0.61
12:b:107:MET:HE3	12:b:107:MET:HA	1.83	0.61
4:H:63:ARG:NH1	14:d:339:ARG:O	2.34	0.60
7:M:78:GLN:HA	7:M:81:MET:HE2	1.83	0.60
5:I:113:GLN:NE2	5:I:117:ASP:OD1	2.34	0.60
1:B:95:MET:HE3	1:B:307:LYS:O	2.02	0.60
11:a:7:SER:HB3	11:a:363:THR:HG23	1.82	0.60
5:I:97:GLU:OE1	7:M:92:ARG:NH2	2.34	0.60
5:J:214:ALA:O	7:N:91:ASN:ND2	2.35	0.60
17:m:99:VAL:HB	17:m:149:ALA:HB2	1.83	0.60
1:B:39:MET:HG2	2:F:97:SER:HA	1.83	0.60
5:I:77:ASN:OD1	5:I:80:ARG:NH2	2.35	0.60
11:a:84:GLU:OE1	11:a:291:ARG:NH2	2.34	0.60
1:B:507:ILE:HD11	1:B:555:VAL:HG21	1.84	0.60
1:C:503:GLU:HG2	1:C:566:THR:HA	1.84	0.59
11:a:483:PRO:HG2	11:a:510:VAL:HG12	1.84	0.59
17:o:91:LEU:HD21	17:o:155:LYS:HB3	1.83	0.59
7:M:97:ASP:OD1	7:M:98:ASN:N	2.35	0.59
17:g:111:GLY:O	17:g:113:VAL:N	2.34	0.59
12:b:64:GLY:HA3	12:b:149:LEU:HA	1.84	0.59
13:c:326:LEU:HB3	13:c:341:LEU:HA	1.84	0.59
2:F:248:MET:C	2:F:250:ASN:N	2.60	0.59
2:D:33:TYR:CZ	5:I:207:MET:HG2	2.37	0.59
5:K:180:GLY:HA3	5:K:195:THR:HA	1.85	0.59
8:R:33:MET:HE2	8:R:46:ARG:HG3	1.83	0.59
11:a:62:ASP:OD2	11:a:66:ARG:NH2	2.36	0.59
1:A:575:GLY:HA2	1:A:578:LEU:HD12	1.85	0.59
1:A:574:MET:HB2	1:A:577:ILE:HD12	1.83	0.59
17:o:124:GLN:HE21	17:o:126:ARG:HD3	1.68	0.59
10:U:299:GLN:HG3	10:U:402:ARG:HB2	1.85	0.59
5:I:94:LEU:HD22	5:I:215:LEU:HD11	1.84	0.58
13:c:328:ASN:HB2	13:c:340:THR:HG22	1.83	0.58
17:i:59:VAL:HG21	17:j:134:ILE:HG12	1.84	0.58
2:E:451:LYS:HD2	2:E:480:ILE:HD11	1.84	0.58
1:B:514:LEU:HG	1:B:544:MET:HE2	1.85	0.58
12:b:58:ILE:HG21	17:g:148:VAL:HG11	1.85	0.58
1:B:227:LEU:HD22	1:B:405:THR:HG21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:72:VAL:HG11	17:i:99:VAL:HG11	1.85	0.58
11:a:92:ARG:HE	11:a:95:ILE:HG13	1.68	0.58
1:B:43:VAL:HG12	1:B:81:ARG:HA	1.86	0.58
2:E:239:LYS:NZ	2:E:243:GLU:OE2	2.36	0.58
13:c:443:LEU:HA	13:c:446:ILE:HG22	1.84	0.58
1:C:490:ALA:HA	1:C:493:VAL:HG12	1.85	0.57
11:a:23:TYR:HB2	11:a:90:PHE:CE2	2.39	0.57
15:e:80:TRP:H	15:e:81:PRO:HD2	1.69	0.57
1:B:104:ARG:HB3	1:B:109:ILE:HD11	1.86	0.57
16:f:24:ILE:HD12	16:f:27:ILE:HD11	1.85	0.57
1:B:389:ALA:HB2	1:B:406:ILE:HD12	1.86	0.57
4:H:168:ARG:HD3	10:U:436:LEU:HD22	1.85	0.57
5:J:215:LEU:HG	7:N:95:VAL:HG11	1.86	0.57
11:a:90:PHE:O	11:a:92:ARG:N	2.34	0.57
5:I:215:LEU:HG	7:M:95:VAL:HG21	1.86	0.57
15:e:28:ILE:HD12	15:e:29:PRO:HD2	1.87	0.57
2:F:432:VAL:HG23	2:F:433:VAL:HG13	1.87	0.57
1:B:486:GLU:HG3	1:B:512:ALA:HB3	1.86	0.57
2:F:356:THR:HB	4:H:14:MET:HE1	1.87	0.57
4:H:135:LYS:HD2	6:L:22:LEU:HG	1.86	0.57
17:n:84:ILE:HG21	17:n:89:SER:HB3	1.85	0.57
10:U:298:ASP:OD1	10:U:299:GLN:N	2.38	0.57
10:U:352:GLN:O	10:U:357:ASN:ND2	2.37	0.57
11:a:72:ILE:HG23	11:a:77:ILE:HB	1.86	0.57
14:d:113:ILE:C	14:d:115:GLY:H	2.12	0.57
17:l:35:ALA:HB2	17:m:109:ALA:HA	1.87	0.57
1:A:566:THR:H	1:A:569:ILE:HD12	1.70	0.57
1:B:111:SER:O	1:B:114:GLN:NE2	2.34	0.57
10:U:319:GLN:HG2	10:U:346:MET:HG3	1.87	0.57
11:a:65:LEU:HD13	11:a:294:PHE:HA	1.86	0.56
12:b:128:HIS:N	17:o:9:GLU:OE1	2.35	0.56
17:n:23:MET:HE1	17:n:70:LEU:HA	1.86	0.56
17:n:41:ILE:HD13	17:o:134:ILE:HD11	1.87	0.56
2:F:277:GLU:HA	2:F:342:ILE:HD11	1.87	0.56
1:B:95:MET:CE	1:B:308:ARG:CA	2.82	0.56
2:D:80:VAL:HG22	2:D:90:VAL:HG22	1.87	0.56
2:D:199:GLN:HE21	2:D:203:GLN:HE22	1.53	0.56
2:E:160:PRO:HB2	2:E:395:LEU:HD23	1.86	0.56
3:G:93:ALA:N	3:G:96:VAL:O	2.36	0.56
12:b:65:ALA:O	12:b:69:ILE:HG12	2.04	0.56
14:d:269:ASP:HA	14:d:275:LYS:HG2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:g:77:ALA:O	17:h:155:LYS:NZ	2.25	0.56
17:l:16:VAL:HG12	17:m:94:GLY:HA3	1.88	0.56
17:l:24:VAL:HG22	17:m:101:LEU:HB2	1.86	0.56
11:a:284:GLN:O	11:a:288:LYS:HG2	2.05	0.56
3:G:276:PHE:O	3:G:280:VAL:N	2.39	0.56
5:K:72:MET:HA	5:K:75:LEU:HD12	1.88	0.56
12:b:48:MET:HE1	13:c:430:LEU:HD11	1.85	0.56
8:R:26:ILE:HG13	8:R:81:LEU:HD21	1.88	0.56
12:b:105:ILE:HD12	17:g:148:VAL:HG23	1.87	0.56
12:b:59:SER:HB2	17:g:101:LEU:HD23	1.88	0.56
17:h:46:VAL:HA	17:i:123:GLN:NE2	2.21	0.56
2:F:140:MET:HE2	5:K:212:ARG:HG3	1.88	0.56
4:H:133:LYS:HG2	4:H:136:ARG:HH12	1.71	0.56
1:B:331:ILE:HD12	1:B:334:SER:HB3	1.88	0.55
2:D:47:VAL:HG13	2:D:52:VAL:HG22	1.88	0.55
13:c:273:PHE:H	13:c:284:LEU:HD13	1.70	0.55
17:j:109:ALA:O	17:j:113:VAL:HG22	2.06	0.55
1:B:132:LYS:NZ	1:B:186:ASP:OD2	2.39	0.55
17:i:53:MET:HA	17:i:53:MET:HE3	1.88	0.55
2:D:432:VAL:HG21	4:H:35:LYS:HB3	1.87	0.55
4:H:17:THR:O	4:H:18:ILE:HB	2.06	0.55
1:C:27:PRO:HA	1:C:70:THR:HG21	1.88	0.55
2:E:37:PRO:HB2	5:J:192:VAL:HG12	1.87	0.55
1:A:397:ASN:HB3	8:Q:28:TYR:CG	2.41	0.55
2:E:121:MET:HE2	2:E:139:VAL:HG11	1.89	0.55
1:B:95:MET:CE	1:B:307:LYS:O	2.55	0.55
17:i:24:VAL:HG22	17:j:101:LEU:HB2	1.89	0.55
1:A:570:ILE:HG22	1:A:578:LEU:HD11	1.89	0.55
8:S:69:SER:O	8:S:76:ASN:ND2	2.40	0.55
14:d:260:ASP:N	14:d:263:GLN:OE1	2.38	0.55
17:i:22:ALA:HB2	17:i:96:GLY:HA2	1.89	0.55
1:C:129:ARG:HH12	1:C:206:VAL:HG21	1.72	0.55
2:E:140:MET:HG2	5:J:212:ARG:HD2	1.89	0.55
10:U:230:LEU:O	10:U:263:ARG:NH1	2.35	0.55
2:D:158:ILE:HD11	2:D:336:GLU:HB3	1.89	0.54
8:R:93:ARG:HH12	8:R:131:ASN:HA	1.72	0.54
8:S:192:LYS:HG3	8:S:195:GLU:HB2	1.88	0.54
17:l:8:PRO:HG3	17:l:86:LEU:HD22	1.88	0.54
3:G:190:PRO:O	3:G:192:LEU:N	2.40	0.54
12:b:68:GLY:HA2	12:b:156:GLY:HA3	1.89	0.54
17:o:110:ILE:HD11	17:o:139:GLU:HG2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:341:THR:HG21	11:a:349:PRO:HA	1.88	0.54
13:c:272:ASN:HA	13:c:284:LEU:HD22	1.88	0.54
2:F:174:MET:HE1	2:F:416:LEU:HB3	1.90	0.54
8:Q:159:LEU:HA	8:Q:178:LEU:HD13	1.89	0.54
11:a:790:ILE:HG13	11:a:791:LEU:HG	1.89	0.54
2:D:253:LEU:HD22	2:D:255:LEU:HD21	1.90	0.54
13:c:327:ALA:HB1	13:c:404:PHE:CZ	2.43	0.54
14:d:20:VAL:HG11	14:d:314:VAL:HG13	1.90	0.54
17:n:40:GLY:HA2	17:n:119:ARG:HE	1.72	0.54
1:A:279:GLU:CD	1:A:349:ASN:HB2	2.33	0.54
11:a:65:LEU:HD23	11:a:101:PHE:CZ	2.43	0.54
17:h:24:VAL:HG11	17:i:101:LEU:HD13	1.90	0.54
1:B:95:MET:HE1	1:B:308:ARG:O	2.04	0.54
5:K:68:LYS:HD3	7:O:62:ALA:HA	1.90	0.54
11:a:90:PHE:H	11:a:91:PRO:HD2	1.73	0.54
12:b:55:GLY:HA3	17:g:97:LEU:HD11	1.89	0.54
1:A:211:VAL:HG12	1:A:328:TYR:HB3	1.89	0.54
11:a:404:ALA:HB2	11:a:456:PHE:HB3	1.89	0.54
14:d:109:VAL:HG21	14:d:160:LEU:HD12	1.89	0.54
1:A:86:LEU:O	1:A:211:VAL:HG23	2.08	0.53
1:A:88:VAL:HG23	1:A:211:VAL:HG22	1.90	0.53
17:l:23:MET:HE2	17:m:145:GLY:HA2	1.90	0.53
1:B:220:LYS:HD2	1:B:392:VAL:HG12	1.90	0.53
5:I:124:LEU:HD23	5:I:183:ILE:HD13	1.89	0.53
2:E:277:GLU:HA	2:E:342:ILE:HD11	1.90	0.53
17:l:66:ALA:O	17:l:70:LEU:HD23	2.08	0.53
1:A:427:GLY:HA3	2:E:189:ALA:HB1	1.91	0.53
1:B:106:LEU:HD13	2:E:154:PRO:HD2	1.90	0.53
2:E:186:PHE:HB3	2:E:350:MET:HE2	1.90	0.53
10:U:434:GLN:NE2	10:U:438:GLU:OE2	2.42	0.53
13:c:410:ARG:HB3	18:p:295:ASN:HB2	1.90	0.53
17:i:99:VAL:HB	17:i:149:ALA:HB2	1.90	0.53
5:K:54:MET:SD	7:O:47:TYR:OH	2.58	0.53
1:A:478:LYS:HB3	1:A:545:ILE:HD13	1.91	0.53
1:A:503:GLU:O	1:A:507:ILE:HG12	2.08	0.53
2:E:64:GLU:OE2	2:E:108:PHE:HB3	2.09	0.53
2:F:81:LEU:HD13	2:F:308:ARG:HD3	1.90	0.53
2:F:430:LYS:HD2	2:F:438:LEU:HD11	1.91	0.53
17:k:23:MET:HE1	17:l:145:GLY:HA2	1.90	0.53
1:B:562:ASP:OD1	1:B:563:ASN:N	2.42	0.53
1:C:27:PRO:HA	1:C:70:THR:CG2	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:54:MET:HE3	5:K:58:GLU:HG2	1.91	0.53
14:d:39:CYS:SG	14:d:40:GLU:N	2.81	0.53
14:d:75:LYS:HE3	14:d:130:HIS:CE1	2.44	0.53
2:F:52:VAL:N	2:F:90:VAL:O	2.38	0.53
17:k:18:GLY:HA3	17:k:93:LEU:HA	1.90	0.53
1:B:37:ALA:HB1	1:B:54:ILE:HD12	1.90	0.52
1:C:170:PRO:O	1:C:171:ARG:HB3	2.09	0.52
1:C:189:ASP:OD1	1:C:190:VAL:N	2.43	0.52
2:D:257:LEU:N	2:D:260:ASP:OD2	2.42	0.52
2:E:491:GLN:NE2	2:E:495:ASP:OD1	2.40	0.52
5:I:134:VAL:HG22	5:I:183:ILE:HG12	1.90	0.52
11:a:403:PHE:CD2	11:a:453:MET:HB2	2.44	0.52
17:n:24:VAL:HG22	17:o:101:LEU:HB2	1.90	0.52
1:C:171:ARG:HH11	1:C:172:ASN:HD22	1.58	0.52
1:B:95:MET:CE	1:B:308:ARG:HA	2.38	0.52
4:H:7:ILE:HG22	4:H:183:THR:HG21	1.91	0.52
12:b:48:MET:HB3	17:g:90:PHE:CZ	2.45	0.52
17:j:8:PRO:HG3	17:j:86:LEU:HD22	1.90	0.52
18:p:319:ALA:O	18:p:323:ILE:HG12	2.09	0.52
1:A:95:MET:HE2	1:A:337:PHE:CZ	2.44	0.52
1:C:24:VAL:HG13	1:C:29:VAL:HG22	1.91	0.52
1:C:99:PHE:HB3	1:C:103:GLN:HA	1.91	0.52
1:C:349:ASN:OD1	1:C:350:SER:N	2.42	0.52
2:D:332:ALA:HA	2:D:342:ILE:HB	1.91	0.52
5:K:178:ALA:N	5:K:197:GLU:OE2	2.33	0.52
10:U:278:SER:HB3	10:U:281:GLN:HG2	1.92	0.52
11:a:290:ILE:HA	11:a:293:TRP:HB2	1.92	0.52
14:d:116:THR:HG23	14:d:122:ILE:HD11	1.91	0.52
1:C:141:LEU:HD11	1:C:147:ILE:HG21	1.91	0.52
17:k:115:ASP:O	17:k:119:ARG:HG2	2.10	0.52
17:n:45:SER:HB2	17:n:52:ILE:HD11	1.91	0.52
1:B:486:GLU:HG2	1:B:509:LEU:HD23	1.91	0.52
5:I:116:LEU:HD21	5:I:144:VAL:HG22	1.92	0.52
9:T:323:GLN:O	11:a:53:ASN:ND2	2.39	0.52
10:U:380:HIS:HB2	10:U:400:ASP:OD1	2.09	0.52
17:k:44:MET:HE1	17:k:51:LEU:HB2	1.92	0.52
17:n:14:PHE:HD2	17:n:93:LEU:HD22	1.74	0.52
2:D:140:MET:HG3	5:I:208:MET:HE3	1.91	0.52
11:a:553:VAL:HG12	11:a:573:PHE:HD1	1.74	0.52
17:m:64:ILE:HG22	17:m:68:TYR:CE2	2.44	0.52
1:A:303:GLU:OE2	1:A:304:SER:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:MET:HE2	1:B:407:VAL:HB	1.92	0.52
2:E:197:ALA:HB2	2:E:347:ILE:HD11	1.90	0.52
7:N:89:ARG:HA	7:N:92:ARG:HD2	1.91	0.52
4:H:65:ALA:HB1	4:H:138:TYR:CE1	2.45	0.51
17:h:46:VAL:HA	17:i:123:GLN:HE22	1.75	0.51
18:p:314:ILE:O	18:p:318:LEU:HD23	2.10	0.51
2:D:207:VAL:HG13	2:D:467:VAL:HG11	1.92	0.51
2:E:163:MET:HE1	2:E:467:VAL:HG21	1.93	0.51
12:b:189:PHE:CE2	17:o:67:ILE:HG12	2.45	0.51
17:h:27:ALA:HA	17:i:141:LEU:HD11	1.93	0.51
1:C:66:VAL:HG12	1:C:68:GLU:H	1.74	0.51
8:R:19:HIS:CE1	8:R:70:LYS:HA	2.45	0.51
11:a:549:MET:N	11:a:549:MET:HE2	2.26	0.51
11:a:623:ASP:N	11:a:623:ASP:OD1	2.42	0.51
12:b:189:PHE:HE2	17:o:67:ILE:HG12	1.75	0.51
11:a:85:ASN:O	11:a:299:LYS:NZ	2.42	0.51
17:l:84:ILE:HA	17:l:88:LYS:HE3	1.92	0.51
1:B:95:MET:HE1	1:B:309:THR:N	2.24	0.51
2:F:479:ARG:NH1	2:F:497:PHE:O	2.39	0.51
1:A:567:TRP:HA	1:A:570:ILE:HD12	1.92	0.51
1:B:216:PRO:HG2	1:B:395:LEU:HD22	1.93	0.51
1:B:511:VAL:HG11	1:B:548:TYR:HB2	1.91	0.51
1:B:552:ARG:NH1	10:U:353:GLN:OE1	2.40	0.51
2:D:140:MET:HE2	5:I:91:ILE:HG13	1.91	0.51
17:k:22:ALA:HB2	17:k:96:GLY:HA2	1.93	0.51
1:B:56:ARG:HB3	1:B:63:THR:HB	1.92	0.51
1:C:66:VAL:HB	1:C:70:THR:HG22	1.93	0.51
5:K:25:GLU:HA	5:K:28:GLU:CD	2.36	0.51
17:h:22:ALA:HB2	17:h:96:GLY:HA2	1.92	0.51
1:C:85:PRO:O	1:C:86:LEU:C	2.54	0.51
2:E:169:SER:N	2:E:459:GLN:OE1	2.43	0.51
11:a:23:TYR:HE2	11:a:91:PRO:HB3	1.76	0.51
17:j:22:ALA:HB2	17:j:96:GLY:HA2	1.93	0.51
1:C:116:ILE:HD12	2:F:335:VAL:HG21	1.93	0.51
5:J:59:LYS:HA	5:J:62:LYS:HE2	1.93	0.51
14:d:41:THR:HG23	14:d:44:ASP:H	1.76	0.51
17:j:11:ALA:O	17:j:89:SER:OG	2.26	0.51
11:a:553:VAL:HG12	11:a:573:PHE:CD1	2.46	0.50
14:d:130:HIS:ND1	14:d:132:LEU:HB2	2.26	0.50
12:b:102:ILE:O	12:b:105:ILE:HG22	2.10	0.50
1:C:274:TYR:HB3	1:C:311:LEU:HD13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:ASP:OD1	2:D:356:THR:OG1	2.23	0.50
10:U:271:ALA:O	10:U:275:HIS:N	2.44	0.50
11:a:406:MET:HB3	11:a:745:LEU:HB3	1.94	0.50
17:o:65:ILE:HD11	17:o:142:GLY:HA3	1.94	0.50
2:E:125:VAL:HG22	2:E:253:LEU:HD12	1.93	0.50
8:Q:197:TYR:CZ	8:Q:232:TYR:HB2	2.46	0.50
11:a:656:PRO:HD3	11:a:721:GLN:HG2	1.93	0.50
17:n:84:ILE:CG2	17:n:89:SER:HB3	2.42	0.50
1:B:604:LEU:O	1:B:608:VAL:HG23	2.12	0.50
2:E:43:THR:HG22	5:J:189:LYS:HB3	1.94	0.50
2:F:174:MET:HE1	2:F:416:LEU:CB	2.42	0.50
15:e:30:LYS:HA	15:e:34:ARG:HD2	1.92	0.50
1:A:272:ILE:HB	1:A:309:THR:HG23	1.94	0.50
5:K:69:LYS:HA	5:K:72:MET:SD	2.52	0.50
13:c:404:PHE:O	13:c:405:ASN:C	2.55	0.50
17:o:121:THR:HA	17:o:124:GLN:O	2.11	0.50
5:J:131:ARG:NH2	5:J:164:ASP:OD2	2.42	0.50
17:h:44:MET:SD	17:h:51:LEU:HB2	2.52	0.50
17:h:44:MET:HG2	17:h:122:ALA:HB2	1.93	0.50
17:k:8:PRO:O	17:k:9:GLU:HG3	2.12	0.50
1:C:215:ARG:HG3	1:C:335:GLU:HB3	1.94	0.49
5:K:41:GLU:OE2	5:K:44:ARG:NH1	2.45	0.49
11:a:371:THR:HG22	11:a:396:ILE:HD11	1.93	0.49
14:d:99:PHE:HA	14:d:102:TYR:CD2	2.47	0.49
17:l:23:MET:HE1	17:l:70:LEU:HD21	1.94	0.49
8:Q:140:LEU:HD13	8:Q:153:ARG:HA	1.92	0.49
8:R:59:ASN:O	8:R:61:ARG:NH2	2.45	0.49
11:a:410:PHE:CZ	11:a:414:ILE:HD11	2.47	0.49
17:g:53:MET:HE2	17:h:126:ARG:HH22	1.78	0.49
17:m:14:PHE:HD2	17:m:93:LEU:HD22	1.77	0.49
1:C:90:LEU:HA	1:C:94:ILE:HD11	1.94	0.49
11:a:12:LEU:HB3	11:a:357:THR:HG22	1.94	0.49
11:a:450:ILE:HA	11:a:453:MET:HG2	1.94	0.49
17:j:123:GLN:NE2	18:p:345:ASN:O	2.39	0.49
1:B:59:GLY:N	2:F:45:CYS:O	2.42	0.49
1:B:144:GLY:N	1:B:176:VAL:O	2.44	0.49
1:C:493:VAL:HA	1:C:496:VAL:HG22	1.93	0.49
2:D:253:LEU:HD22	2:D:255:LEU:CD2	2.42	0.49
8:Q:148:LYS:NZ	8:Q:188:MET:O	2.44	0.49
11:a:94:MET:O	11:a:98:GLU:HG3	2.12	0.49
17:m:137:PHE:O	17:m:141:LEU:HG	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PRO:HB2	1:A:108:ASP:HB2	1.94	0.49
1:C:37:ALA:HB1	1:C:54:ILE:HD13	1.95	0.49
2:E:66:VAL:HG12	2:E:108:PHE:HA	1.93	0.49
2:E:140:MET:HE1	5:J:87:ARG:HB3	1.94	0.49
9:T:146:ALA:O	9:T:150:ALA:N	2.44	0.49
10:U:377:GLY:O	10:U:402:ARG:NE	2.46	0.49
11:a:101:PHE:HA	11:a:104:ILE:HG12	1.94	0.49
11:a:575:PRO:HB2	11:a:651:MET:SD	2.52	0.49
2:D:140:MET:HE1	5:I:87:ARG:HG2	1.93	0.49
13:c:276:ALA:HB3	13:c:393:GLN:HB2	1.93	0.49
17:g:88:LYS:O	17:g:92:GLN:HG2	2.13	0.49
13:c:455:PHE:HB3	17:g:46:VAL:HG21	1.94	0.49
17:k:40:GLY:HA2	17:k:119:ARG:HE	1.76	0.49
17:k:48:ARG:NH1	17:k:122:ALA:O	2.45	0.49
17:n:124:GLN:HG3	17:n:126:ARG:HB2	1.95	0.49
5:I:112:TYR:OH	5:I:140:ASP:OD2	2.28	0.49
5:K:29:GLU:HG3	10:U:341:TYR:CE1	2.48	0.49
5:K:94:LEU:HD11	5:K:215:LEU:HD13	1.95	0.49
6:L:30:LYS:HE2	6:L:30:LYS:HA	1.93	0.49
10:U:288:GLN:HB2	10:U:419:PRO:HD2	1.93	0.49
17:m:65:ILE:HA	17:m:68:TYR:HD2	1.78	0.49
1:B:46:GLY:HA2	1:B:77:ASP:HB3	1.94	0.49
6:L:28:LEU:HG	6:L:32:ARG:HE	1.78	0.49
8:R:19:HIS:CD2	8:R:70:LYS:HG2	2.48	0.49
5:I:132:MET:HB2	5:I:165:VAL:HA	1.94	0.49
5:I:215:LEU:HD23	7:M:91:ASN:HB2	1.95	0.49
10:U:314:VAL:HG13	10:U:349:ASN:HA	1.95	0.49
16:f:23:VAL:HG11	16:f:77:LEU:HD23	1.95	0.49
17:o:18:GLY:HA3	17:o:93:LEU:HA	1.95	0.49
2:D:55:ASP:OD1	2:D:56:HIS:N	2.46	0.48
2:D:66:VAL:HG21	2:D:90:VAL:HG11	1.94	0.48
2:F:227:ALA:HA	2:F:292:THR:HG22	1.94	0.48
3:G:240:LYS:O	3:G:244:ASN:N	2.40	0.48
8:S:227:LYS:HA	8:S:227:LYS:HD2	1.56	0.48
12:b:127:GLY:O	12:b:129:ARG:N	2.44	0.48
17:i:39:THR:HB	18:p:335:GLY:HA3	1.94	0.48
1:A:230:GLY:HA2	1:A:531:PHE:HD1	1.78	0.48
1:C:105:PRO:HG2	1:C:108:ASP:HB2	1.95	0.48
2:D:344:GLN:C	2:D:346:PRO:HD3	2.38	0.48
5:J:108:ASP:OD2	5:J:111:ARG:NE	2.36	0.48
11:a:557:LEU:HB2	11:a:573:PHE:CD1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:787:THR:HG22	11:a:792:LEU:HD23	1.96	0.48
17:g:15:ALA:HB2	17:g:89:SER:HA	1.95	0.48
17:j:130:GLY:O	17:j:133:LEU:HG	2.13	0.48
17:m:76:ILE:HG23	17:m:92:GLN:HB3	1.94	0.48
2:E:402:GLU:HG3	2:E:407:LYS:HG2	1.95	0.48
17:h:32:TYR:CD2	17:h:108:PHE:HA	2.49	0.48
17:l:70:LEU:HG	17:m:144:TYR:CD1	2.48	0.48
11:a:464:TYR:CE1	11:a:537:LYS:HE2	2.49	0.48
11:a:553:VAL:HG11	11:a:577:ILE:HB	1.96	0.48
17:g:47:MET:HE2	17:g:47:MET:HA	1.94	0.48
17:h:32:TYR:CE2	17:h:108:PHE:HA	2.48	0.48
17:l:12:ALA:HB3	17:m:90:PHE:HD2	1.78	0.48
1:B:387:GLU:HG3	2:F:232:MET:HE3	1.96	0.48
3:G:182:LEU:HA	3:G:230:PHE:HA	1.96	0.48
13:c:254:HIS:HB3	13:c:289:PHE:CZ	2.49	0.48
13:c:257:VAL:HG22	13:c:291:VAL:HG21	1.95	0.48
1:B:436:ASP:HA	1:B:449:ASN:HB3	1.96	0.48
1:B:489:LEU:O	1:B:493:VAL:HG23	2.14	0.48
11:a:287:ALA:HA	11:a:290:ILE:HB	1.94	0.48
17:h:44:MET:HE3	17:h:44:MET:HB3	1.80	0.48
1:A:147:ILE:HD11	1:A:168:LEU:HB2	1.95	0.48
2:D:159:TYR:CD1	2:D:160:PRO:HD2	2.49	0.48
2:E:46:SER:HB3	2:E:53:VAL:HB	1.95	0.48
11:a:170:PHE:N	11:a:196:PHE:O	2.47	0.48
17:j:18:GLY:HA3	17:j:93:LEU:HA	1.94	0.48
17:l:56:ILE:O	17:l:59:VAL:HG22	2.14	0.48
11:a:833:GLU:N	11:a:833:GLU:OE1	2.47	0.48
12:b:45:SER:O	12:b:48:MET:HG3	2.13	0.48
13:c:432:SER:HA	13:c:435:MET:HG3	1.96	0.48
17:g:141:LEU:HA	17:g:144:TYR:HD2	1.79	0.48
17:o:99:VAL:HB	17:o:149:ALA:HB2	1.96	0.48
1:C:117:TYR:CE1	2:F:152:ILE:CG1	2.97	0.48
1:C:315:THR:O	1:C:318:MET:HB2	2.14	0.48
2:E:294:MET:HE1	2:E:297:TYR:CD1	2.49	0.48
2:F:248:MET:O	2:F:250:ASN:N	2.47	0.48
5:K:90:LEU:HB2	5:K:216:PHE:HZ	1.78	0.48
5:K:52:LYS:O	5:K:55:GLU:HG3	2.14	0.47
5:I:185:ASN:OD1	5:I:186:GLY:N	2.46	0.47
5:J:137:ARG:NH2	5:J:177:ILE:O	2.47	0.47
8:S:40:ASN:HA	8:S:46:ARG:CZ	2.44	0.47
11:a:54:GLU:OE1	11:a:54:GLU:N	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:g:16:VAL:HG12	17:h:94:GLY:HA3	1.95	0.47
17:h:28:LEU:HD22	17:i:105:ALA:HB2	1.96	0.47
17:i:23:MET:HG2	17:j:148:VAL:HG21	1.96	0.47
2:D:52:VAL:HG21	2:D:99:ILE:HD12	1.95	0.47
2:D:125:VAL:HB	2:D:134:ASP:HB3	1.96	0.47
10:U:268:LEU:HD11	10:U:271:ALA:HB2	1.95	0.47
17:h:24:VAL:HG22	17:i:101:LEU:HB2	1.96	0.47
17:m:44:MET:HG2	17:m:118:VAL:HG13	1.96	0.47
5:J:201:ASP:O	5:J:205:GLN:HG2	2.14	0.47
8:Q:60:TYR:HB3	8:Q:65:ILE:HB	1.96	0.47
10:U:259:PRO:HA	10:U:263:ARG:HG3	1.95	0.47
10:U:297:GLU:HG2	10:U:303:VAL:HG22	1.95	0.47
14:d:341:ARG:HA	14:d:344:ILE:HG13	1.96	0.47
1:B:448:VAL:HG12	1:B:450:TRP:H	1.80	0.47
2:D:177:ILE:HG12	2:D:183:ILE:HD12	1.96	0.47
5:I:72:MET:HE2	5:I:72:MET:HA	1.96	0.47
11:a:576:GLU:O	11:a:580:MET:HG3	2.14	0.47
17:h:22:ALA:HB2	17:h:96:GLY:CA	2.45	0.47
1:B:95:MET:CE	1:B:309:THR:N	2.78	0.47
2:F:159:TYR:CD1	2:F:160:PRO:HD2	2.49	0.47
17:i:40:GLY:HA2	17:i:119:ARG:NH2	2.23	0.47
17:k:8:PRO:HD2	17:k:11:ALA:HB2	1.97	0.47
17:m:67:ILE:HD13	17:m:67:ILE:HA	1.75	0.47
17:o:14:PHE:HA	17:o:17:MET:HE3	1.96	0.47
18:p:293:PRO:HB2	18:p:294:TYR:H	1.53	0.47
1:A:489:LEU:HB2	1:A:509:LEU:HD21	1.96	0.47
1:C:397:ASN:HB3	8:S:28:TYR:CG	2.50	0.47
2:D:54:LEU:HD21	2:D:106:CYS:HB3	1.95	0.47
2:D:244:GLU:HB3	5:I:70:ILE:HG12	1.97	0.47
6:L:17:VAL:O	6:L:21:LEU:HG	2.15	0.47
11:a:69:GLU:OE1	11:a:73:ARG:NH2	2.48	0.47
11:a:413:GLY:O	11:a:417:THR:OG1	2.29	0.47
11:a:467:CYS:N	11:a:470:LYS:O	2.39	0.47
13:c:315:LEU:HB3	13:c:320:VAL:HG21	1.96	0.47
14:d:39:CYS:HB2	14:d:44:ASP:CB	2.45	0.47
14:d:49:LEU:HD13	14:d:57:PHE:CE1	2.50	0.47
14:d:234:LYS:NZ	14:d:258:ALA:O	2.47	0.47
17:n:55:SER:O	17:n:58:PRO:HD2	2.15	0.47
10:U:342:ASN:HD21	10:U:388:THR:HB	1.80	0.47
11:a:296:LYS:O	11:a:300:MET:HG2	2.15	0.47
14:d:49:LEU:HA	14:d:52:THR:HG22	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLN:NE2	1:A:488:ASP:OD1	2.48	0.47
1:C:281:VAL:HG21	2:F:157:ARG:CZ	2.45	0.47
2:D:34:ILE:HG22	2:D:36:HIS:H	1.79	0.47
6:L:15:ASP:OD1	6:L:16:THR:N	2.48	0.47
10:U:368:PHE:HB2	10:U:371:TRP:HB2	1.96	0.47
13:c:328:ASN:HB2	13:c:340:THR:CG2	2.43	0.47
17:i:144:TYR:HA	17:i:147:ILE:HD12	1.97	0.47
2:F:80:VAL:HG22	2:F:90:VAL:HG22	1.97	0.47
4:H:93:LYS:HE2	4:H:114:GLU:HG2	1.96	0.47
17:k:108:PHE:O	17:k:112:ILE:HG22	2.15	0.47
12:b:137:MET:HE1	12:b:203:MET:HE2	1.97	0.46
13:c:275:VAL:HG21	13:c:322:PHE:CZ	2.50	0.46
1:A:168:LEU:HD12	1:A:169:PRO:CD	2.46	0.46
1:C:212:ARG:H	1:C:212:ARG:HG2	1.39	0.46
2:D:41:TYR:CZ	2:D:57:VAL:HA	2.50	0.46
8:Q:58:LYS:NZ	8:Q:64:GLU:OE1	2.37	0.46
11:a:10:MET:HG2	11:a:361:PRO:HB3	1.97	0.46
11:a:397:ILE:HG23	11:a:456:PHE:CZ	2.50	0.46
14:d:39:CYS:HB2	14:d:44:ASP:HB2	1.97	0.46
17:j:32:TYR:CD1	17:j:108:PHE:HA	2.49	0.46
17:m:18:GLY:HA3	17:m:93:LEU:HA	1.97	0.46
17:m:137:PHE:HA	17:m:140:VAL:HG12	1.96	0.46
3:G:156:LYS:O	3:G:165:SER:N	2.47	0.46
11:a:193:GLY:O	11:a:195:VAL:N	2.48	0.46
17:i:136:ILE:O	17:i:140:VAL:HG23	2.15	0.46
1:C:117:TYR:CE1	2:F:152:ILE:HD11	2.42	0.46
2:D:163:MET:HE3	2:D:165:GLN:CA	2.45	0.46
2:E:195:GLU:OE1	2:E:195:GLU:N	2.39	0.46
10:U:312:TRP:HE3	10:U:348:LEU:HB2	1.80	0.46
12:b:28:ILE:HD12	12:b:28:ILE:HA	1.71	0.46
17:h:42:ALA:O	17:h:46:VAL:HG23	2.16	0.46
5:I:216:PHE:HE1	7:M:88:PHE:HB2	1.80	0.46
12:b:59:SER:HB2	17:g:101:LEU:HB3	1.96	0.46
17:l:32:TYR:HE2	17:l:108:PHE:HA	1.80	0.46
1:C:98:ILE:HG21	1:C:288:LEU:HD21	1.98	0.46
5:J:123:GLY:HA3	5:J:183:ILE:HG13	1.98	0.46
8:Q:58:LYS:HB3	8:Q:60:TYR:CE2	2.50	0.46
14:d:42:LEU:HB3	14:d:65:LEU:HD23	1.98	0.46
14:d:265:LYS:NZ	14:d:279:GLU:OE2	2.35	0.46
5:I:102:LEU:HA	5:I:105:VAL:HG12	1.97	0.46
12:b:102:ILE:HA	12:b:105:ILE:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:g:20:SER:O	17:g:24:VAL:HG23	2.15	0.46
17:m:41:ILE:HD11	17:m:55:SER:HB2	1.97	0.46
1:A:300:GLY:HA2	8:Q:189:ALA:HA	1.97	0.46
1:C:144:GLY:N	1:C:176:VAL:O	2.41	0.46
1:C:324:GLU:HA	1:C:354:TRP:CD1	2.50	0.46
2:E:128:GLY:HA3	2:E:256:ASN:HD22	1.81	0.46
11:a:68:VAL:O	11:a:72:ILE:HG12	2.15	0.46
14:d:328:ASN:ND2	14:d:348:ILE:O	2.49	0.46
2:E:229:GLY:HA2	2:E:258:ALA:HA	1.97	0.46
6:L:101:ALA:O	6:L:102:LYS:HG2	2.15	0.46
13:c:305:VAL:HA	13:c:327:ALA:CB	2.45	0.46
12:b:103:TYR:HB3	12:b:191:VAL:HG21	1.98	0.46
13:c:339:PHE:HB2	13:c:404:PHE:CD2	2.51	0.46
17:j:121:THR:HA	17:j:124:GLN:O	2.16	0.46
17:k:22:ALA:HB2	17:k:96:GLY:CA	2.46	0.46
17:n:52:ILE:HD13	17:o:127:LEU:HA	1.98	0.46
17:o:17:MET:CG	17:o:93:LEU:HD13	2.44	0.46
8:Q:140:LEU:HD22	8:Q:153:ARG:HG3	1.98	0.45
8:Q:194:ASP:OD1	8:Q:194:ASP:N	2.49	0.45
13:c:359:GLN:HG3	13:c:381:ASP:HA	1.98	0.45
13:c:316:PHE:HZ	13:c:349:ASN:HB2	1.82	0.45
17:i:61:MET:HE3	17:i:139:GLU:HG3	1.97	0.45
5:I:201:ASP:O	5:I:205:GLN:HG2	2.16	0.45
5:J:174:PRO:O	5:J:177:ILE:HG12	2.16	0.45
2:D:81:LEU:HD13	2:D:308:ARG:HG3	1.99	0.45
11:a:18:GLN:O	11:a:22:ALA:N	2.50	0.45
14:d:320:LYS:HD3	14:d:320:LYS:HA	1.55	0.45
17:m:52:ILE:HG23	17:m:53:MET:HE2	1.99	0.45
1:A:515:ILE:HA	1:A:544:MET:HE1	1.97	0.45
5:J:201:ASP:OD1	5:J:202:LEU:N	2.49	0.45
11:a:60:GLU:O	11:a:64:LYS:HG3	2.16	0.45
12:b:126:ILE:HA	12:b:130:ASN:HD22	1.81	0.45
17:g:16:VAL:HG22	17:g:80:LEU:HD13	1.99	0.45
17:g:117:GLY:HA3	17:g:131:MET:SD	2.56	0.45
17:h:35:ALA:HA	17:i:113:VAL:HG23	1.99	0.45
17:n:144:TYR:HA	17:n:147:ILE:HD12	1.97	0.45
1:C:117:TYR:HB3	2:F:150:GLN:HG3	1.98	0.45
2:E:92:VAL:HG12	2:E:94:GLU:H	1.81	0.45
11:a:90:PHE:CE1	11:a:303:ILE:HG21	2.52	0.45
17:m:44:MET:SD	17:m:122:ALA:HB2	2.56	0.45
1:A:100:ASP:HB2	1:A:104:ARG:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:HG21	1:B:64:ILE:HG12	1.99	0.45
1:B:555:VAL:HG22	1:B:565:ILE:O	2.17	0.45
2:E:34:ILE:HG22	5:J:206:GLN:HE22	1.82	0.45
2:E:241:ASP:O	2:E:245:ASN:ND2	2.45	0.45
2:F:82:GLU:OE1	2:F:308:ARG:NH1	2.48	0.45
2:F:332:ALA:HA	2:F:342:ILE:HB	1.98	0.45
5:I:125:TYR:O	5:I:128:LEU:HG	2.17	0.45
5:I:129:GLU:O	5:I:132:MET:HE2	2.16	0.45
6:L:92:PRO:HB3	6:L:98:TYR:HA	1.99	0.45
14:d:115:GLY:HA3	14:d:125:LEU:HD11	1.99	0.45
12:b:105:ILE:CD1	17:g:148:VAL:HG23	2.46	0.45
14:d:185:LEU:HD12	14:d:185:LEU:HA	1.76	0.45
14:d:280:GLY:O	14:d:293:ARG:NE	2.40	0.45
17:i:42:ALA:HA	17:j:127:LEU:HD21	1.98	0.45
17:m:68:TYR:CD1	17:m:146:LEU:HD22	2.52	0.45
1:A:398:PRO:HD2	1:A:400:ARG:NH2	2.32	0.45
1:A:478:LYS:NZ	1:A:481:GLU:OE2	2.36	0.45
8:Q:159:LEU:HD11	8:Q:179:PHE:CE1	2.51	0.45
9:T:108:VAL:O	9:T:110:ILE:N	2.49	0.45
10:U:289:ARG:NH1	10:U:419:PRO:O	2.50	0.45
13:c:265:ARG:HE	13:c:265:ARG:HB2	1.60	0.45
13:c:327:ALA:HB1	13:c:404:PHE:HZ	1.81	0.45
14:d:33:TYR:HA	14:d:36:LEU:HD12	1.99	0.45
14:d:113:ILE:C	14:d:115:GLY:N	2.74	0.45
17:k:32:TYR:CZ	17:k:36:LYS:HD3	2.52	0.45
1:C:315:THR:HG23	2:F:154:PRO:HG3	1.99	0.45
2:E:165:GLN:NE2	2:E:172:ASP:OD2	2.50	0.45
2:F:99:ILE:HG23	2:F:104:THR:HG21	1.97	0.45
4:H:123:GLY:O	4:H:124:LEU:C	2.60	0.45
5:K:127:LEU:HD23	5:K:127:LEU:HA	1.78	0.45
17:m:41:ILE:HD13	17:m:41:ILE:HA	1.67	0.45
1:A:161:LEU:HD22	1:A:298:VAL:HG11	1.99	0.44
2:E:292:THR:HA	2:E:347:ILE:HB	1.99	0.44
17:o:65:ILE:HD13	17:o:65:ILE:HA	1.73	0.44
1:A:372:SER:C	1:A:374:TYR:H	2.25	0.44
1:B:324:GLU:HA	1:B:354:TRP:HD1	1.77	0.44
1:B:338:ARG:HD3	1:B:404:VAL:HG23	1.99	0.44
2:E:294:MET:CE	2:E:328:ILE:HD11	2.48	0.44
2:F:122:LEU:HD23	2:F:122:LEU:HA	1.87	0.44
3:G:8:SER:HA	3:G:318:ALA:HA	1.98	0.44
7:N:110:ILE:O	7:N:112:GLU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:30:ASP:C	12:b:32:GLY:H	2.24	0.44
13:c:260:ASN:H	13:c:264:PRO:HA	1.82	0.44
14:d:28:LEU:HD21	14:d:52:THR:HG21	1.98	0.44
17:k:121:THR:HA	17:k:124:GLN:O	2.17	0.44
17:o:64:ILE:HA	17:o:67:ILE:HB	1.98	0.44
1:C:216:PRO:HG2	1:C:395:LEU:HD11	1.99	0.44
2:D:402:GLU:HG2	2:D:407:LYS:HB3	1.99	0.44
2:E:165:GLN:HB2	2:E:207:VAL:HG12	2.00	0.44
2:E:228:MET:HB2	2:E:228:MET:HE2	1.83	0.44
6:L:110:LYS:HD3	6:L:110:LYS:HA	1.74	0.44
8:R:83:ARG:O	8:R:87:ILE:HG12	2.17	0.44
11:a:452:LEU:O	11:a:455:ILE:HG13	2.17	0.44
17:l:24:VAL:CG2	17:m:101:LEU:HB2	2.47	0.44
17:l:47:MET:H	17:l:47:MET:HG3	1.43	0.44
17:n:76:ILE:HA	17:n:92:GLN:NE2	2.32	0.44
2:F:44:VAL:HA	2:F:54:LEU:HD23	1.98	0.44
5:I:116:LEU:HD11	5:I:181:VAL:HG13	1.99	0.44
17:i:29:GLY:HA3	17:i:104:LEU:HA	1.99	0.44
1:A:102:ILE:HG13	1:A:104:ARG:HG3	2.00	0.44
1:A:148:THR:C	1:A:168:LEU:HD23	2.43	0.44
1:A:168:LEU:HD12	1:A:169:PRO:HD2	1.99	0.44
1:B:90:LEU:HA	1:B:94:ILE:HD11	1.99	0.44
1:C:149:GLY:HA2	1:C:168:LEU:HB3	1.99	0.44
8:Q:159:LEU:HD13	8:Q:178:LEU:HB2	1.99	0.44
8:R:177:GLN:HA	8:R:180:LYS:HE3	1.98	0.44
8:S:19:HIS:CD2	8:S:70:LYS:HG2	2.52	0.44
11:a:80:MET:HE1	11:a:288:LYS:HA	1.99	0.44
17:m:88:LYS:HA	17:m:91:LEU:HB2	2.00	0.44
1:C:71:SER:HA	2:F:62:TYR:CD2	2.43	0.44
2:D:157:ARG:HE	2:D:157:ARG:HB2	1.42	0.44
4:H:138:TYR:CE2	6:L:19:GLY:HA3	2.53	0.44
5:J:164:ASP:OD1	5:J:166:GLN:NE2	2.49	0.44
17:j:35:ALA:HB1	17:k:112:ILE:HG21	2.00	0.44
17:j:45:SER:HB2	17:j:52:ILE:HD11	1.99	0.44
1:C:88:VAL:HG12	1:C:209:TRP:O	2.18	0.44
5:K:118:GLY:C	7:O:106:ILE:HG21	2.43	0.44
8:S:81:LEU:HD12	8:S:81:LEU:HA	1.77	0.44
1:C:245:THR:HG22	1:C:429:VAL:HG22	2.00	0.44
2:D:338:ARG:NH2	5:I:224:PHE:HB2	2.33	0.44
2:E:202:ARG:NH1	2:E:461:PRO:O	2.51	0.44
5:I:123:GLY:HA3	5:I:183:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:215:LEU:HD11	7:O:88:PHE:CD1	2.53	0.44
10:U:304:PHE:HA	10:U:328:SER:HA	1.99	0.44
11:a:61:MET:HE2	11:a:98:GLU:HA	1.99	0.44
17:m:72:VAL:HG11	17:m:99:VAL:HG11	1.98	0.44
17:n:48:ARG:HE	17:n:122:ALA:HA	1.83	0.44
2:D:182:LYS:O	2:D:367:THR:HB	2.18	0.44
2:D:384:PRO:HA	2:D:385:PRO:HD3	1.82	0.44
5:K:67:GLN:O	5:K:71:GLN:HG2	2.18	0.44
5:K:83:VAL:O	5:K:87:ARG:HG3	2.17	0.44
8:S:10:MET:SD	8:S:10:MET:N	2.91	0.44
10:U:312:TRP:CE3	10:U:348:LEU:HB2	2.53	0.44
11:a:546:ILE:HD13	11:a:584:PHE:O	2.18	0.44
17:g:8:PRO:HD2	17:g:86:LEU:HB2	2.00	0.44
17:g:13:PHE:HB2	17:h:90:PHE:CD2	2.53	0.44
17:g:23:MET:O	17:g:24:VAL:C	2.61	0.44
1:B:316:SER:HB2	2:E:326:ALA:HB1	1.99	0.43
1:C:145:SER:HB2	8:S:31:ARG:NH2	2.33	0.43
1:C:148:THR:HG22	8:S:24:GLY:HA3	2.00	0.43
1:C:337:PHE:HA	1:C:340:MET:HE3	1.99	0.43
5:K:203:ILE:HD13	7:O:103:VAL:HA	1.99	0.43
11:a:607:PRO:HG3	11:a:627:SER:HB2	1.99	0.43
17:k:51:LEU:HD22	17:k:54:LYS:HD3	2.00	0.43
1:A:569:ILE:HA	1:A:572:GLU:HG3	2.00	0.43
1:B:44:ARG:HA	1:B:50:LEU:O	2.18	0.43
4:H:22:ARG:NH2	10:U:441:GLY:HA3	2.34	0.43
4:H:94:ILE:HG23	4:H:109:PHE:HB3	2.00	0.43
11:a:557:LEU:HD13	11:a:573:PHE:CD2	2.53	0.43
17:i:45:SER:HB2	17:i:52:ILE:HD11	2.00	0.43
17:n:54:LYS:HB2	17:n:128:PHE:CZ	2.53	0.43
17:o:95:ALA:HB2	17:o:152:LEU:HB2	2.00	0.43
1:A:243:GLY:H	1:A:405:THR:CG2	2.31	0.43
1:A:523:ASN:O	1:A:526:THR:HG22	2.18	0.43
1:A:524:GLY:HA2	1:A:530:ARG:HA	2.01	0.43
1:C:99:PHE:O	1:C:312:VAL:HA	2.18	0.43
2:D:430:LYS:HD3	2:D:446:LEU:HD11	2.00	0.43
2:F:33:TYR:HE1	5:K:207:MET:HE1	1.82	0.43
2:F:429:MET:O	2:F:433:VAL:HG22	2.18	0.43
8:S:217:LEU:H	8:S:217:LEU:HG	1.44	0.43
11:a:586:TYR:O	11:a:590:LEU:HG	2.18	0.43
11:a:758:THR:HA	11:a:762:HIS:HB3	2.01	0.43
14:d:169:SER:C	14:d:171:GLN:H	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:e:76:LEU:HD12	15:e:80:TRP:CD1	2.54	0.43
17:i:22:ALA:HB2	17:i:96:GLY:CA	2.48	0.43
1:C:316:SER:HB2	2:F:326:ALA:HB1	2.00	0.43
2:D:282:GLN:HA	5:I:224:PHE:HB3	2.01	0.43
2:E:459:GLN:HG2	2:E:465:ARG:CZ	2.48	0.43
2:F:147:ILE:HG13	2:F:271:LEU:HD23	2.00	0.43
7:N:111:HIS:C	7:N:113:ASN:H	2.25	0.43
8:R:49:TYR:HE1	8:R:84:ARG:HB3	1.84	0.43
8:S:63:GLU:OE1	8:S:63:GLU:N	2.45	0.43
11:a:356:GLN:H	11:a:356:GLN:HG2	1.47	0.43
11:a:608:SER:HB3	11:a:611:ILE:HG22	2.00	0.43
13:c:339:PHE:HB2	13:c:404:PHE:HD2	1.83	0.43
17:n:84:ILE:HD12	17:n:84:ILE:H	1.83	0.43
1:B:195:GLU:HB2	1:B:200:LYS:HG2	2.01	0.43
2:E:81:LEU:HD23	2:E:81:LEU:HA	1.91	0.43
2:F:182:LYS:HB2	2:F:182:LYS:HE2	1.73	0.43
6:L:68:GLN:HA	6:L:71:ALA:HB3	1.99	0.43
8:Q:28:TYR:CE1	8:Q:32:CYS:SG	3.11	0.43
11:a:568:ASN:O	11:a:572:GLY:HA3	2.19	0.43
12:b:107:MET:SD	12:b:191:VAL:HG13	2.58	0.43
13:c:325:ILE:H	13:c:325:ILE:HG12	1.62	0.43
17:i:72:VAL:HG21	17:i:99:VAL:HG21	1.99	0.43
17:o:124:GLN:NE2	17:o:126:ARG:HH21	2.16	0.43
1:A:168:LEU:HD13	1:A:194:LEU:HD11	2.00	0.43
1:B:489:LEU:CD2	1:B:505:ASP:HB3	2.49	0.43
2:F:121:MET:HG3	2:F:139:VAL:HG11	2.00	0.43
8:S:195:GLU:OE1	8:S:195:GLU:N	2.51	0.43
1:A:328:TYR:HA	1:A:331:ILE:HG22	2.01	0.43
1:B:284:MET:HE3	1:B:287:VAL:HB	1.99	0.43
1:C:568:SER:O	1:C:572:GLU:HG2	2.19	0.43
2:D:76:ARG:HD3	2:D:94:GLU:HB2	1.99	0.43
2:E:38:ARG:NH2	2:E:109:THR:HA	2.34	0.43
3:G:190:PRO:HA	3:G:222:SER:HA	2.00	0.43
11:a:23:TYR:HD2	11:a:90:PHE:HD2	1.65	0.43
1:A:218:THR:HB	1:A:393:LYS:HB3	2.01	0.43
1:C:105:PRO:HD3	1:C:126:ALA:HA	2.01	0.43
2:F:439:THR:HG23	2:F:441:GLU:H	1.84	0.43
6:L:12:GLY:HA2	6:L:67:ASN:HD22	1.84	0.43
8:S:223:LYS:HA	8:S:223:LYS:HD2	1.36	0.43
10:U:368:PHE:H	10:U:380:HIS:CE1	2.37	0.43
11:a:93:ASP:OD1	11:a:93:ASP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:373:GLY:HA3	11:a:449:ILE:HD11	2.01	0.43
15:e:19:PHE:O	15:e:24:VAL:HG23	2.18	0.43
17:i:99:VAL:HB	17:i:149:ALA:CB	2.49	0.43
2:F:161:GLU:O	2:F:399:ALA:HA	2.19	0.43
2:F:311:VAL:HG22	4:H:205:ILE:HD13	2.01	0.43
14:d:176:MET:SD	14:d:181:ILE:HG12	2.59	0.43
16:f:32:PHE:HA	16:f:35:VAL:HG12	2.00	0.43
17:i:124:GLN:HE22	17:i:126:ARG:HG3	1.84	0.43
17:m:68:TYR:CD1	17:m:146:LEU:HB2	2.54	0.43
17:m:72:VAL:HG21	17:m:99:VAL:HG21	2.00	0.43
2:D:179:ARG:HE	2:D:179:ARG:HB3	1.55	0.43
2:D:227:ALA:HB1	2:D:230:VAL:HG21	2.01	0.43
5:K:106:VAL:HA	5:K:112:TYR:HB2	2.01	0.43
13:c:330:PHE:HA	13:c:337:HIS:HA	2.01	0.43
14:d:19:LEU:HD23	14:d:19:LEU:HA	1.78	0.43
17:n:16:VAL:CG1	17:o:94:GLY:HA3	2.49	0.43
1:A:116:ILE:HD12	2:D:335:VAL:HG21	2.00	0.42
1:B:180:ALA:HB1	1:B:185:TYR:CE2	2.53	0.42
1:B:514:LEU:HG	1:B:544:MET:CE	2.48	0.42
2:D:336:GLU:H	2:D:336:GLU:HG2	1.64	0.42
2:E:268:THR:N	2:E:269:PRO:HD2	2.34	0.42
4:H:165:THR:O	4:H:169:VAL:HG23	2.19	0.42
12:b:19:LEU:HD23	12:b:19:LEU:HA	1.92	0.42
12:b:59:SER:O	12:b:63:VAL:HG23	2.18	0.42
17:g:87:TYR:O	17:g:91:LEU:HG	2.19	0.42
1:B:498:LYS:HA	1:B:501:LEU:HG	2.00	0.42
1:C:559:ALA:HA	1:C:564:LYS:HZ3	1.84	0.42
2:D:93:PHE:O	2:D:261:PRO:HB3	2.20	0.42
2:F:124:ARG:HE	2:F:124:ARG:HB3	1.75	0.42
8:R:130:LEU:HD13	8:R:168:ILE:HD12	2.01	0.42
8:S:152:LEU:HD23	8:S:152:LEU:HA	1.76	0.42
11:a:60:GLU:O	11:a:63:ARG:HG2	2.19	0.42
11:a:416:MET:HE1	11:a:453:MET:HG3	2.01	0.42
14:d:155:LEU:HA	14:d:161:ALA:HB2	2.01	0.42
14:d:250:GLU:HB3	17:m:47:MET:HG3	2.00	0.42
17:h:40:GLY:HA2	17:h:119:ARG:HD3	2.01	0.42
17:m:84:ILE:HG12	17:m:88:LYS:NZ	2.34	0.42
1:B:180:ALA:HB2	1:B:191:VAL:HA	2.01	0.42
2:F:484:GLU:OE1	2:F:484:GLU:N	2.49	0.42
10:U:266:TRP:CD1	10:U:411:VAL:HG12	2.54	0.42
12:b:69:ILE:HG13	17:g:141:LEU:HD11	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:m:50:GLU:H	17:m:50:GLU:HG3	1.53	0.42
1:A:220:LYS:HB3	1:A:220:LYS:HE2	1.41	0.42
1:B:101:GLY:N	1:B:314:ASN:HD21	2.18	0.42
1:B:489:LEU:HD21	1:B:505:ASP:HB3	2.00	0.42
2:F:120:ASP:C	2:F:122:LEU:N	2.74	0.42
5:J:122:GLN:HG3	7:N:108:PRO:HA	2.01	0.42
8:Q:180:LYS:HA	8:Q:180:LYS:HD3	1.75	0.42
5:J:67:GLN:HA	5:J:70:ILE:HG22	2.01	0.42
5:J:125:TYR:O	5:J:128:LEU:HG	2.20	0.42
7:M:94:GLU:HG2	7:M:95:VAL:N	2.35	0.42
8:R:87:ILE:HD12	8:R:116:LYS:HA	2.00	0.42
11:a:387:ARG:HA	11:a:387:ARG:HD2	1.77	0.42
12:b:50:SER:OG	12:b:137:MET:HE3	2.20	0.42
13:c:263:ALA:O	13:c:265:ARG:N	2.52	0.42
13:c:323:LYS:HB3	13:c:323:LYS:HE3	1.82	0.42
17:h:88:LYS:O	17:h:92:GLN:HG2	2.19	0.42
17:m:70:LEU:HA	17:m:70:LEU:HD22	1.80	0.42
1:A:275:VAL:HG11	1:A:327:ILE:HA	2.00	0.42
2:D:429:MET:O	2:D:433:VAL:HG22	2.20	0.42
2:E:38:ARG:HE	5:J:202:LEU:HD13	1.85	0.42
2:E:263:ILE:H	2:E:263:ILE:HG12	1.57	0.42
4:H:23:LEU:HD11	4:H:27:GLN:HE22	1.84	0.42
11:a:378:VAL:HG11	11:a:391:PRO:HD2	2.00	0.42
13:c:293:ASP:OD1	13:c:294:LEU:N	2.53	0.42
13:c:360:VAL:HG13	13:c:368:PHE:CD1	2.54	0.42
17:k:52:ILE:HD13	17:l:127:LEU:HA	2.00	0.42
17:l:44:MET:HE3	17:l:44:MET:HB3	1.74	0.42
1:B:167:MET:HE1	1:B:339:ASP:HB2	2.01	0.42
1:B:170:PRO:HG2	1:B:216:PRO:HD2	2.02	0.42
4:H:65:ALA:HB1	4:H:138:TYR:HE1	1.84	0.42
5:K:81:LEU:HD23	5:K:81:LEU:HA	1.84	0.42
8:Q:146:THR:HG23	8:Q:149:ASN:H	1.85	0.42
8:R:195:GLU:OE1	8:R:195:GLU:N	2.45	0.42
8:S:33:MET:HG3	8:S:53:LEU:HD11	2.01	0.42
11:a:61:MET:HE2	11:a:98:GLU:HG2	2.02	0.42
11:a:450:ILE:HA	11:a:453:MET:CG	2.50	0.42
17:i:13:PHE:O	17:i:17:MET:HG2	2.20	0.42
17:i:128:PHE:O	17:i:132:ILE:HG12	2.19	0.42
17:l:70:LEU:HD11	17:m:144:TYR:HB3	2.01	0.42
1:A:393:LYS:HD2	1:A:393:LYS:HA	1.72	0.42
1:A:397:ASN:ND2	8:Q:28:TYR:HB2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:THR:HG21	1:A:528:TYR:CZ	2.54	0.42
1:B:215:ARG:HG3	1:B:335:GLU:HB3	2.02	0.42
1:C:117:TYR:OH	2:F:281:TYR:HD2	2.03	0.42
8:S:201:LYS:HA	8:S:204:VAL:HG22	2.01	0.42
11:a:389:ILE:HD11	11:a:558:PHE:HB2	2.00	0.42
13:c:265:ARG:HB3	13:c:301:TRP:CE2	2.54	0.42
14:d:37:VAL:HG13	14:d:344:ILE:HG21	2.01	0.42
17:j:47:MET:HB3	18:p:345:ASN:HB3	2.01	0.42
1:A:39:MET:HE1	1:A:55:ILE:O	2.20	0.42
1:B:426:LEU:HD13	1:B:426:LEU:HA	1.91	0.42
1:C:284:MET:HE2	1:C:284:MET:HB3	1.92	0.42
2:D:497:PHE:HA	2:D:500:ARG:HH21	1.85	0.42
5:K:58:GLU:O	5:K:62:LYS:HG2	2.20	0.42
8:R:81:LEU:HD12	8:R:81:LEU:HA	1.84	0.42
12:b:135:TYR:O	17:o:16:VAL:HG11	2.20	0.42
17:m:13:PHE:O	17:m:17:MET:HG2	2.19	0.42
17:m:86:LEU:HG	17:m:90:PHE:CE2	2.55	0.42
1:C:246:THR:HB	1:C:407:VAL:HG22	2.02	0.42
1:C:495:LEU:HD23	1:C:495:LEU:HA	1.86	0.42
2:D:99:ILE:HG23	2:D:104:THR:HG21	2.02	0.42
2:D:497:PHE:HA	2:D:500:ARG:NH2	2.34	0.42
2:F:70:LEU:HD12	2:F:74:THR:HB	2.01	0.42
8:S:200:PHE:HZ	8:S:213:PHE:HZ	1.68	0.42
11:a:390:ASN:HA	11:a:391:PRO:HD3	1.92	0.42
12:b:133:ALA:HA	12:b:201:VAL:HG13	2.00	0.42
17:h:29:GLY:HA3	17:h:104:LEU:HA	2.02	0.42
17:k:8:PRO:C	17:k:9:GLU:HG3	2.45	0.42
17:m:49:PRO:HB2	17:n:126:ARG:HD3	2.01	0.42
1:B:37:ALA:O	2:F:100:ASP:HB2	2.19	0.41
1:B:152:ILE:HG23	1:B:165:ARG:HB3	2.02	0.41
1:B:609:GLN:HB3	1:B:613:ARG:HH22	1.85	0.41
2:F:93:PHE:O	2:F:261:PRO:HB3	2.20	0.41
4:H:22:ARG:HH22	10:U:441:GLY:HA3	1.84	0.41
5:I:120:VAL:HG22	5:I:181:VAL:HG21	2.02	0.41
12:b:197:GLN:NE2	17:o:16:VAL:HG22	2.35	0.41
17:h:104:LEU:HG	17:h:108:PHE:HE2	1.85	0.41
17:i:32:TYR:CE1	17:i:36:LYS:HG3	2.55	0.41
17:m:93:LEU:O	17:m:97:LEU:HD23	2.20	0.41
1:C:277:CYS:H	1:C:349:ASN:CG	2.27	0.41
2:D:181:GLN:NE2	2:D:183:ILE:HD11	2.35	0.41
6:L:49:GLU:HB3	6:L:53:ARG:HH11	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:201:GLU:HA	11:a:218:SER:HA	2.01	0.41
11:a:410:PHE:CE1	11:a:458:ILE:HG23	2.55	0.41
14:d:49:LEU:HD13	14:d:57:PHE:HE1	1.85	0.41
1:B:147:ILE:HG12	1:B:168:LEU:HD22	2.02	0.41
1:B:352:SER:HA	1:B:421:VAL:HG11	2.02	0.41
1:C:22:HIS:N	1:C:30:THR:O	2.46	0.41
1:C:24:VAL:H	2:F:83:VAL:HG23	1.86	0.41
1:C:496:VAL:HG23	1:C:498:LYS:H	1.84	0.41
4:H:126:ARG:HD3	4:H:126:ARG:HA	1.77	0.41
4:H:178:PRO:HB2	4:H:182:ARG:NH2	2.35	0.41
5:I:140:ASP:O	5:I:144:VAL:HG23	2.20	0.41
11:a:557:LEU:HD22	11:a:573:PHE:CE2	2.55	0.41
12:b:103:TYR:CE2	12:b:188:LEU:HD22	2.55	0.41
14:d:78:MET:SD	14:d:322:LYS:HB3	2.60	0.41
17:h:116:ALA:HA	17:h:119:ARG:HH11	1.84	0.41
2:F:374:ASP:HB3	2:F:377:LEU:HB2	2.02	0.41
7:N:88:PHE:O	7:N:92:ARG:HB3	2.20	0.41
11:a:80:MET:HB3	11:a:82:THR:HG23	2.01	0.41
11:a:523:TRP:CH2	11:a:532:PHE:HB3	2.55	0.41
12:b:66:ALA:HB1	17:g:109:ALA:HB2	2.03	0.41
13:c:267:LEU:HG	13:c:411:PHE:CE1	2.55	0.41
13:c:336:ARG:H	13:c:336:ARG:HG2	1.55	0.41
17:j:20:SER:O	17:j:24:VAL:HG23	2.20	0.41
18:p:327:TYR:O	18:p:331:ASN:ND2	2.49	0.41
1:B:226:PRO:HG3	1:B:464:TYR:CD2	2.55	0.41
1:B:541:LEU:HG	1:B:545:ILE:HD12	2.01	0.41
2:F:494:ILE:HD12	2:F:494:ILE:H	1.86	0.41
3:G:36:SER:O	3:G:320:LEU:N	2.52	0.41
8:S:30:ALA:O	8:S:34:GLN:HG2	2.21	0.41
17:m:8:PRO:HG3	17:m:86:LEU:HD22	2.02	0.41
17:m:76:ILE:O	17:m:80:LEU:HG	2.20	0.41
2:D:140:MET:HG3	5:I:208:MET:CE	2.50	0.41
2:D:407:LYS:HB2	2:D:407:LYS:HE2	1.69	0.41
4:H:58:MET:HA	4:H:61:VAL:HG12	2.01	0.41
7:N:110:ILE:C	7:N:112:GLU:H	2.29	0.41
13:c:455:PHE:HE1	17:h:119:ARG:HB3	1.86	0.41
17:l:32:TYR:CE2	17:l:108:PHE:HA	2.56	0.41
17:m:68:TYR:HD1	17:m:146:LEU:HD22	1.85	0.41
1:B:186:ASP:OD1	1:B:189:ASP:N	2.54	0.41
1:C:71:SER:HB2	2:F:63:ALA:CB	2.50	0.41
2:E:354:ASP:OD1	2:E:356:THR:OG1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:103:MET:HE1	8:Q:167:GLY:HA2	2.01	0.41
13:c:256:PRO:HB3	13:c:269:TRP:HB2	2.02	0.41
17:g:41:ILE:HA	17:g:44:MET:HE3	2.03	0.41
17:j:16:VAL:CG1	17:k:94:GLY:HA3	2.47	0.41
17:l:23:MET:SD	17:m:148:VAL:HG21	2.61	0.41
1:A:152:ILE:HD13	1:A:167:MET:HG2	2.03	0.41
1:B:161:LEU:HD12	1:B:307:LYS:HB2	2.03	0.41
1:B:177:THR:HG21	1:B:200:LYS:HE2	2.01	0.41
1:B:331:ILE:HD13	1:B:346:MET:HE3	2.02	0.41
1:C:42:LEU:HD23	1:C:42:LEU:HA	1.90	0.41
2:E:450:GLN:O	2:E:454:ARG:HG2	2.20	0.41
2:F:491:GLN:HA	2:F:494:ILE:HD13	2.02	0.41
17:o:61:MET:O	17:o:64:ILE:HG12	2.20	0.41
1:A:369:PRO:HG2	4:H:196:ARG:HE	1.86	0.41
1:A:506:LYS:O	1:A:510:GLU:HG2	2.20	0.41
1:B:43:VAL:HB	1:B:79:VAL:HG12	2.03	0.41
1:B:343:HIS:H	1:B:343:HIS:CD2	2.38	0.41
1:C:113:THR:HG22	1:C:115:SER:HB3	2.02	0.41
1:C:152:ILE:HD13	1:C:167:MET:HB3	2.03	0.41
2:F:189:ALA:C	2:F:191:LEU:H	2.29	0.41
2:F:334:ARG:HB3	2:F:341:SER:HB3	2.02	0.41
5:I:90:LEU:HD22	7:M:88:PHE:CD2	2.55	0.41
5:I:185:ASN:HB2	5:I:190:ILE:HB	2.03	0.41
5:J:67:GLN:O	5:J:70:ILE:HG22	2.21	0.41
7:M:110:ILE:HA	7:M:110:ILE:HD13	1.81	0.41
10:U:341:TYR:HB2	10:U:388:THR:O	2.21	0.41
10:U:402:ARG:HG3	10:U:402:ARG:HH21	1.86	0.41
12:b:190:GLY:HA2	17:o:23:MET:HG2	2.03	0.41
14:d:122:ILE:HG12	14:d:145:GLN:HG3	2.02	0.41
14:d:132:LEU:HD22	14:d:132:LEU:HA	1.85	0.41
17:i:54:LYS:HB3	17:i:128:PHE:CE1	2.56	0.41
17:j:47:MET:SD	17:j:48:ARG:HG2	2.61	0.41
17:k:23:MET:HE2	17:l:148:VAL:HB	2.02	0.41
17:n:44:MET:SD	17:n:51:LEU:HB2	2.60	0.41
1:A:59:GLY:N	2:E:45:CYS:O	2.54	0.41
1:B:488:ASP:O	1:B:491:GLU:HG3	2.21	0.41
1:C:511:VAL:HG11	1:C:548:TYR:CD1	2.55	0.41
2:E:177:ILE:HG12	2:E:183:ILE:HD12	2.03	0.41
2:F:315:ARG:HB2	2:F:358:PRO:HG2	2.03	0.41
8:Q:143:ALA:HB1	8:Q:149:ASN:ND2	2.36	0.41
11:a:566:PRO:HA	11:a:569:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:208:MET:HE1	14:d:316:TYR:CD1	2.56	0.41
14:d:324:GLN:HB3	14:d:350:ILE:HD11	2.03	0.41
17:m:22:ALA:HB2	17:m:96:GLY:HA2	2.03	0.41
1:A:212:ARG:NH1	1:A:324:GLU:OE1	2.53	0.40
1:B:410:VAL:O	1:B:411:SER:C	2.63	0.40
1:C:109:ILE:HG21	1:C:118:ILE:HG23	2.03	0.40
8:S:192:LYS:HD3	8:S:192:LYS:HA	1.97	0.40
11:a:61:MET:O	11:a:65:LEU:HG	2.21	0.40
11:a:553:VAL:HB	11:a:577:ILE:HD13	2.02	0.40
13:c:303:ASP:O	13:c:404:PHE:HE1	2.04	0.40
17:i:13:PHE:HB2	17:j:90:PHE:CZ	2.56	0.40
17:n:41:ILE:HD11	17:n:52:ILE:HG23	2.02	0.40
17:n:77:ALA:O	17:o:155:LYS:NZ	2.54	0.40
1:A:213:GLN:O	1:A:388:ARG:NH1	2.54	0.40
1:B:105:PRO:HD3	1:B:126:ALA:HA	2.02	0.40
2:F:160:PRO:HB2	2:F:178:ALA:HB1	2.03	0.40
11:a:90:PHE:HD1	11:a:300:MET:HE1	1.85	0.40
11:a:426:ARG:HA	11:a:429:ARG:HH21	1.87	0.40
17:g:137:PHE:O	17:g:141:LEU:HG	2.20	0.40
17:h:10:TYR:CZ	18:p:307:VAL:HG22	2.56	0.40
17:m:13:PHE:HB2	17:n:90:PHE:CE2	2.56	0.40
1:B:238:PHE:CE2	1:B:448:VAL:HG11	2.57	0.40
1:B:443:LYS:O	1:B:444:HIS:C	2.63	0.40
2:E:423:GLY:C	2:E:449:LEU:HD11	2.46	0.40
2:F:76:ARG:NH2	2:F:95:GLY:O	2.55	0.40
5:I:124:LEU:HA	5:I:124:LEU:HD22	1.84	0.40
5:I:188:ARG:C	5:I:190:ILE:H	2.30	0.40
5:J:185:ASN:ND2	5:J:187:ASP:OD1	2.55	0.40
5:K:38:PHE:CD2	7:O:36:ALA:HB2	2.55	0.40
5:K:102:LEU:HD12	5:K:200:LEU:HD22	2.03	0.40
11:a:40:LEU:HD21	11:a:322:GLU:HG3	2.02	0.40
17:m:84:ILE:HG12	17:m:88:LYS:HZ1	1.87	0.40
1:A:88:VAL:HG13	1:A:103:GLN:HG3	2.03	0.40
1:A:94:ILE:HD12	1:A:99:PHE:CZ	2.56	0.40
1:B:80:LEU:H	1:B:80:LEU:HG	1.69	0.40
2:D:140:MET:SD	5:I:212:ARG:HG3	2.61	0.40
2:D:372:TYR:CD2	2:D:390:PRO:HB2	2.56	0.40
5:I:132:MET:N	5:I:164:ASP:O	2.48	0.40
8:S:66:LEU:HA	8:S:66:LEU:HD23	1.75	0.40
10:U:371:TRP:HB3	10:U:380:HIS:O	2.21	0.40
11:a:370:PHE:HB3	11:a:448:TYR:CZ	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:410:PHE:HB3	11:a:467:CYS:HB2	2.03	0.40
11:a:806:LEU:HA	11:a:810:GLU:CD	2.47	0.40
17:n:44:MET:HB3	17:n:44:MET:HE3	1.69	0.40
1:A:397:ASN:HB3	8:Q:28:TYR:HB2	2.04	0.40
1:A:570:ILE:HG23	1:A:574:MET:SD	2.61	0.40
1:B:304:SER:C	1:B:306:MET:N	2.80	0.40
1:B:347:MET:HG3	1:B:407:VAL:O	2.21	0.40
1:C:186:ASP:C	1:C:188:SER:H	2.29	0.40
2:E:350:MET:HG2	2:E:360:PRO:HG3	2.03	0.40
4:H:124:LEU:HD12	4:H:124:LEU:HA	1.78	0.40
5:I:102:LEU:HA	5:I:102:LEU:HD23	1.93	0.40
7:M:105:ASP:OD1	7:M:105:ASP:N	2.55	0.40
8:S:99:SER:OG	8:S:100:PRO:HD3	2.21	0.40
11:a:355:MET:H	11:a:355:MET:HG3	1.79	0.40
11:a:601:GLN:OE1	11:a:601:GLN:N	2.54	0.40
17:i:43:ALA:HB3	17:i:119:ARG:NH1	2.36	0.40
17:i:131:MET:HE3	17:i:131:MET:HB3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/617 (97%)	559 (94%)	37 (6%)	2 (0%)	36	67
1	B	582/617 (94%)	546 (94%)	35 (6%)	1 (0%)	43	74
1	C	581/617 (94%)	539 (93%)	38 (6%)	4 (1%)	18	51
2	D	454/515 (88%)	424 (93%)	28 (6%)	2 (0%)	30	62
2	E	452/515 (88%)	432 (96%)	19 (4%)	1 (0%)	43	74
2	F	452/515 (88%)	418 (92%)	32 (7%)	2 (0%)	30	62
3	G	356/382 (93%)	350 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	211/247 (85%)	203 (96%)	8 (4%)	0	100	100
5	I	215/226 (95%)	204 (95%)	11 (5%)	0	100	100
5	J	216/226 (96%)	212 (98%)	4 (2%)	0	100	100
5	K	215/226 (95%)	213 (99%)	1 (0%)	1 (0%)	24	57
6	L	107/119 (90%)	98 (92%)	6 (6%)	3 (3%)	4	26
7	M	108/118 (92%)	107 (99%)	1 (1%)	0	100	100
7	N	108/118 (92%)	105 (97%)	1 (1%)	2 (2%)	6	33
7	O	106/118 (90%)	106 (100%)	0	0	100	100
8	Q	222/337 (66%)	215 (97%)	7 (3%)	0	100	100
8	R	204/337 (60%)	194 (95%)	8 (4%)	2 (1%)	12	44
8	S	224/337 (66%)	209 (93%)	15 (7%)	0	100	100
9	T	423/483 (88%)	410 (97%)	13 (3%)	0	100	100
10	U	371/456 (81%)	348 (94%)	23 (6%)	0	100	100
11	a	744/838 (89%)	708 (95%)	33 (4%)	3 (0%)	30	62
12	b	201/205 (98%)	192 (96%)	8 (4%)	1 (0%)	24	57
13	c	203/469 (43%)	178 (88%)	22 (11%)	3 (2%)	8	37
14	d	348/351 (99%)	319 (92%)	28 (8%)	1 (0%)	36	67
15	e	78/81 (96%)	76 (97%)	1 (1%)	1 (1%)	9	39
16	f	82/98 (84%)	81 (99%)	1 (1%)	0	100	100
17	g	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	18	51
17	h	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
17	i	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
17	j	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
17	k	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
17	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
17	m	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
17	n	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
17	o	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
18	p	51/351 (14%)	49 (96%)	2 (4%)	0	100	100
All	All	9244/10914 (85%)	8802 (95%)	412 (4%)	30 (0%)	37	67

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	N	111	HIS
7	N	112	GLU
11	a	90	PHE
2	F	331	ARG
12	b	31	LEU
13	c	294	LEU
13	c	405	ASN
14	d	164	PHE
1	C	171	ARG
5	K	160	LYS
6	L	102	LYS
8	R	57	GLU
15	e	80	TRP
1	A	234	LEU
1	B	265	LYS
1	C	86	LEU
1	C	389	ALA
2	D	479	ARG
11	a	4	LEU
11	a	50	LYS
1	A	434	GLY
1	C	161	LEU
2	E	372	TYR
13	c	296	LEU
2	F	249	GLY
2	D	400	ILE
8	R	98	ILE
6	L	26	GLY
17	g	112	ILE
6	L	62	GLY

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	508/525 (97%)	481 (95%)	27 (5%)	20	47
1	B	500/525 (95%)	461 (92%)	39 (8%)	11	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	501/525 (95%)	451 (90%)	50 (10%)	7	28
2	D	392/438 (90%)	369 (94%)	23 (6%)	18	44
2	E	390/438 (89%)	369 (95%)	21 (5%)	20	46
2	F	390/438 (89%)	369 (95%)	21 (5%)	20	46
3	G	1/344 (0%)	1 (100%)	0	100	100
4	H	184/211 (87%)	168 (91%)	16 (9%)	9	33
5	I	150/197 (76%)	147 (98%)	3 (2%)	48	67
5	J	148/197 (75%)	143 (97%)	5 (3%)	32	57
5	K	175/197 (89%)	168 (96%)	7 (4%)	28	54
6	L	93/100 (93%)	81 (87%)	12 (13%)	4	21
7	M	36/101 (36%)	34 (94%)	2 (6%)	19	46
7	N	29/101 (29%)	28 (97%)	1 (3%)	32	57
7	O	36/101 (36%)	32 (89%)	4 (11%)	6	25
8	Q	203/305 (67%)	201 (99%)	2 (1%)	68	75
8	R	188/305 (62%)	177 (94%)	11 (6%)	18	44
8	S	203/305 (67%)	188 (93%)	15 (7%)	13	37
9	T	1/429 (0%)	1 (100%)	0	100	100
10	U	147/382 (38%)	141 (96%)	6 (4%)	27	53
11	a	540/743 (73%)	508 (94%)	32 (6%)	18	44
12	b	156/158 (99%)	151 (97%)	5 (3%)	34	59
13	c	179/387 (46%)	160 (89%)	19 (11%)	6	27
14	d	305/306 (100%)	288 (94%)	17 (6%)	19	46
15	e	71/72 (99%)	71 (100%)	0	100	100
16	f	70/83 (84%)	70 (100%)	0	100	100
17	g	105/109 (96%)	102 (97%)	3 (3%)	37	60
17	h	105/109 (96%)	98 (93%)	7 (7%)	15	41
17	i	104/109 (95%)	103 (99%)	1 (1%)	68	75
17	j	105/109 (96%)	100 (95%)	5 (5%)	23	49
17	k	105/109 (96%)	104 (99%)	1 (1%)	68	75
17	l	105/109 (96%)	98 (93%)	7 (7%)	15	41
17	m	105/109 (96%)	92 (88%)	13 (12%)	4	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	n	105/109 (96%)	99 (94%)	6 (6%)	18	45
17	o	105/109 (96%)	100 (95%)	5 (5%)	23	49
18	p	48/311 (15%)	46 (96%)	2 (4%)	26	52
All	All	6588/9205 (72%)	6200 (94%)	388 (6%)	19	44

All (388) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ILE
1	A	118	ILE
1	A	147	ILE
1	A	151	ASP
1	A	164	HIS
1	A	166	ILE
1	A	167	MET
1	A	173	ARG
1	A	175	THR
1	A	178	TYR
1	A	179	ILE
1	A	191	VAL
1	A	194	LEU
1	A	195	GLU
1	A	208	VAL
1	A	215	ARG
1	A	220	LYS
1	A	245	THR
1	A	259	ILE
1	A	272	ILE
1	A	284	MET
1	A	287	VAL
1	A	306	MET
1	A	349	ASN
1	A	353	ARG
1	A	401	GLU
1	A	419	ASP
1	B	39	MET
1	B	43	VAL
1	B	53	GLU
1	B	54	ILE
1	B	57	LEU
1	B	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	80	LEU
1	B	122	VAL
1	B	141	LEU
1	B	155	ILE
1	B	163	LYS
1	B	165	ARG
1	B	167	MET
1	B	207	GLN
1	B	215	ARG
1	B	269	SER
1	B	270	ASP
1	B	277	CYS
1	B	279	GLU
1	B	280	ARG
1	B	281	VAL
1	B	305	ILE
1	B	306	MET
1	B	316	SER
1	B	323	ARG
1	B	327	ILE
1	B	331	ILE
1	B	344	VAL
1	B	352	SER
1	B	353	ARG
1	B	359	ARG
1	B	384	SER
1	B	387	GLU
1	B	400	ARG
1	B	426	LEU
1	B	442	ARG
1	B	452	ILE
1	B	462	ASP
1	B	520	LEU
1	C	34	MET
1	C	41	GLU
1	C	43	VAL
1	C	48	SER
1	C	51	VAL
1	C	53	GLU
1	C	55	ILE
1	C	63	THR
1	C	69	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	100	ASP
1	C	102	ILE
1	C	103	GLN
1	C	104	ARG
1	C	110	SER
1	C	115	SER
1	C	116	ILE
1	C	118	ILE
1	C	123	ASN
1	C	128	SER
1	C	129	ARG
1	C	130	ASP
1	C	155	ILE
1	C	171	ARG
1	C	173	ARG
1	C	175	THR
1	C	194	LEU
1	C	208	VAL
1	C	212	ARG
1	C	227	LEU
1	C	280	ARG
1	C	284	MET
1	C	312	VAL
1	C	316	SER
1	C	317	ASN
1	C	318	MET
1	C	320	VAL
1	C	327	ILE
1	C	353	ARG
1	C	361	ILE
1	C	362	SER
1	C	365	LEU
1	C	392	VAL
1	C	403	SER
1	C	450	TRP
1	C	452	ILE
1	C	455	SER
1	C	487	GLU
1	C	514	LEU
1	C	552	ARG
1	C	553	ARG
2	D	72	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	94	GLU
2	D	99	ILE
2	D	147	ILE
2	D	152	ILE
2	D	157	ARG
2	D	169	SER
2	D	179	ARG
2	D	182	LYS
2	D	202	ARG
2	D	261	PRO
2	D	267	ILE
2	D	270	ARG
2	D	274	THR
2	D	334	ARG
2	D	338	ARG
2	D	344	GLN
2	D	374	ASP
2	D	388	VAL
2	D	402	GLU
2	D	407	LYS
2	D	466	SER
2	D	467	VAL
2	E	34	ILE
2	E	35	THR
2	E	38	ARG
2	E	39	VAL
2	E	40	THR
2	E	107	GLU
2	E	158	ILE
2	E	182	LYS
2	E	263	ILE
2	E	266	ILE
2	E	315	ARG
2	E	323	THR
2	E	324	ASP
2	E	330	GLU
2	E	334	ARG
2	E	335	VAL
2	E	338	ARG
2	E	341	SER
2	E	344	GLN
2	E	488	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	489	ILE
2	F	35	THR
2	F	99	ILE
2	F	100	ASP
2	F	112	ILE
2	F	120	ASP
2	F	124	ARG
2	F	138	VAL
2	F	139	VAL
2	F	140	MET
2	F	142	GLU
2	F	147	ILE
2	F	248	MET
2	F	292	THR
2	F	314	ARG
2	F	315	ARG
2	F	348	LEU
2	F	365	PHE
2	F	377	LEU
2	F	380	ARG
2	F	381	GLN
2	F	392	LEU
4	H	75	THR
4	H	84	ILE
4	H	85	GLN
4	H	86	ASN
4	H	87	VAL
4	H	91	GLN
4	H	99	ASP
4	H	113	HIS
4	H	114	GLU
4	H	116	THR
4	H	120	GLU
4	H	121	LEU
4	H	124	LEU
4	H	126	ARG
4	H	135	LYS
4	H	193	GLU
5	I	124	LEU
5	I	159	THR
5	I	161	ARG
5	J	121	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	191	LYS
5	J	192	VAL
5	J	202	LEU
5	J	207	MET
5	K	29	GLU
5	K	38	PHE
5	K	76	MET
5	K	80	ARG
5	K	82	LYS
5	K	192	VAL
5	K	207	MET
6	L	13	ASP
6	L	22	LEU
6	L	25	ILE
6	L	38	VAL
6	L	40	GLU
6	L	50	ASP
6	L	56	LEU
6	L	102	LYS
6	L	105	ILE
6	L	107	ARG
6	L	108	ARG
6	L	110	LYS
7	M	109	GLU
7	M	110	ILE
7	N	110	ILE
7	O	89	ARG
7	O	109	GLU
7	O	110	ILE
7	O	112	GLU
8	Q	62	PHE
8	Q	103	MET
8	R	21	GLN
8	R	31	ARG
8	R	33	MET
8	R	36	ILE
8	R	79	ASP
8	R	83	ARG
8	R	85	SER
8	R	116	LYS
8	R	122	TRP
8	R	130	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	R	197	TYR
8	S	16	GLU
8	S	66	LEU
8	S	79	ASP
8	S	83	ARG
8	S	155	MET
8	S	209	GLU
8	S	210	GLU
8	S	213	PHE
8	S	214	GLU
8	S	216	ILE
8	S	217	LEU
8	S	220	GLU
8	S	223	LYS
8	S	225	LEU
8	S	227	LYS
10	U	365	HIS
10	U	370	LEU
10	U	380	HIS
10	U	384	LYS
10	U	386	THR
10	U	388	THR
11	a	4	LEU
11	a	7	SER
11	a	9	GLU
11	a	10	MET
11	a	12	LEU
11	a	322	GLU
11	a	355	MET
11	a	356	GLN
11	a	359	GLN
11	a	363	THR
11	a	366	LYS
11	a	367	THR
11	a	369	LYS
11	a	387	ARG
11	a	388	GLU
11	a	390	ASN
11	a	406	MET
11	a	423	MET
11	a	431	LEU
11	a	438	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	a	441	SER
11	a	442	THR
11	a	443	VAL
11	a	452	LEU
11	a	453	MET
11	a	455	ILE
11	a	556	SER
11	a	740	LEU
11	a	741	ARG
11	a	745	LEU
11	a	795	GLU
11	a	805	ARG
12	b	25	CYS
12	b	28	ILE
12	b	34	ARG
12	b	35	PHE
12	b	82	LYS
13	c	265	ARG
13	c	303	ASP
13	c	323	LYS
13	c	325	ILE
13	c	326	LEU
13	c	329	ARG
13	c	333	VAL
13	c	334	SER
13	c	336	ARG
13	c	337	HIS
13	c	339	PHE
13	c	340	THR
13	c	341	LEU
13	c	342	GLU
13	c	343	ARG
13	c	345	GLU
13	c	361	THR
13	c	407	THR
13	c	409	GLU
14	d	19	LEU
14	d	20	VAL
14	d	24	LYS
14	d	103	SER
14	d	110	ILE
14	d	120	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	d	124	GLU
14	d	132	LEU
14	d	145	GLN
14	d	149	GLU
14	d	185	LEU
14	d	213	GLU
14	d	219	ARG
14	d	231	GLU
14	d	250	GLU
14	d	314	VAL
14	d	320	LYS
17	g	23	MET
17	g	115	ASP
17	g	131	MET
17	h	16	VAL
17	h	119	ARG
17	h	126	ARG
17	h	129	VAL
17	h	140	VAL
17	h	143	LEU
17	h	146	LEU
17	i	67	ILE
17	j	65	ILE
17	j	70	LEU
17	j	140	VAL
17	j	143	LEU
17	j	146	LEU
17	k	110	ILE
17	l	44	MET
17	l	47	MET
17	l	48	ARG
17	l	56	ILE
17	l	115	ASP
17	l	123	GLN
17	l	131	MET
17	m	23	MET
17	m	41	ILE
17	m	45	SER
17	m	46	VAL
17	m	47	MET
17	m	48	ARG
17	m	50	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	m	53	MET
17	m	56	ILE
17	m	67	ILE
17	m	70	LEU
17	m	118	VAL
17	m	133	LEU
17	n	10	TYR
17	n	44	MET
17	n	47	MET
17	n	48	ARG
17	n	123	GLN
17	n	146	LEU
17	o	65	ILE
17	o	67	ILE
17	o	70	LEU
17	o	133	LEU
17	o	146	LEU
18	p	295	ASN
18	p	314	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	184	ASN
1	A	430	GLN
1	A	444	HIS
1	A	523	ASN
1	B	268	ASN
1	B	484	GLN
1	B	494	GLN
1	C	65	GLN
1	C	172	ASN
1	C	224	ASN
1	C	231	GLN
1	C	282	ASN
1	C	317	ASN
2	D	72	ASN
2	D	199	GLN
2	D	427	GLN
2	E	36	HIS
2	E	61	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	67	ASN
2	E	155	HIS
2	E	256	ASN
2	E	286	HIS
2	E	378	HIS
2	F	48	ASN
2	F	155	HIS
2	F	194	ASN
2	F	199	GLN
2	F	203	GLN
2	F	352	ASN
2	F	370	GLN
4	H	86	ASN
5	I	126	GLN
5	I	221	ASN
5	J	67	GLN
5	J	74	ASN
5	J	206	GLN
5	K	122	GLN
5	K	194	ASN
5	K	221	ASN
6	L	54	GLN
6	L	67	ASN
6	L	76	HIS
8	Q	40	ASN
8	Q	41	ASN
8	Q	50	GLN
8	Q	142	ASN
8	Q	162	GLN
8	R	41	ASN
8	R	127	HIS
8	R	134	ASN
8	R	177	GLN
8	S	40	ASN
8	S	41	ASN
8	S	89	GLN
8	S	162	GLN
8	S	176	ASN
10	U	281	GLN
10	U	342	ASN
10	U	380	HIS
11	a	76	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	a	626	ASN
11	a	633	GLN
11	a	751	GLN
11	a	807	HIS
12	b	90	ASN
12	b	128	HIS
12	b	168	GLN
13	c	359	GLN
13	c	405	ASN
14	d	183	ASN
14	d	226	ASN
14	d	311	HIS
16	f	34	ASN
17	g	123	GLN
17	h	123	GLN
17	i	123	GLN
17	j	78	ASN
17	n	78	ASN
17	n	123	GLN
18	p	295	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

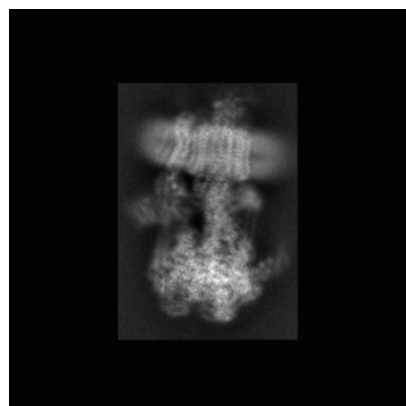
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26385. These allow visual inspection of the internal detail of the map and identification of artifacts.

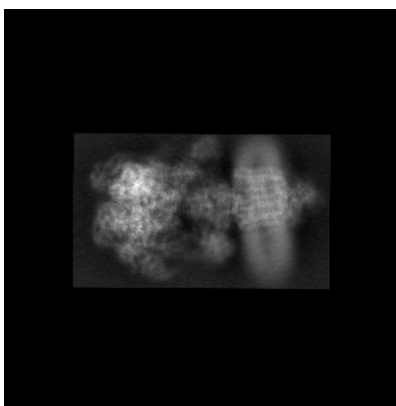
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

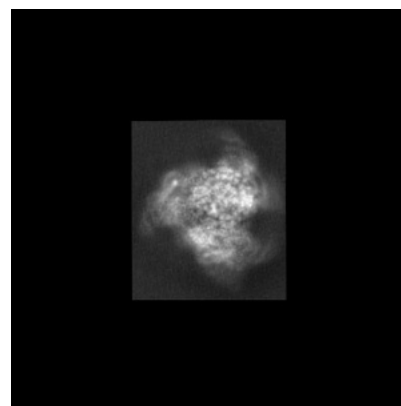
6.1.1 Primary map



X

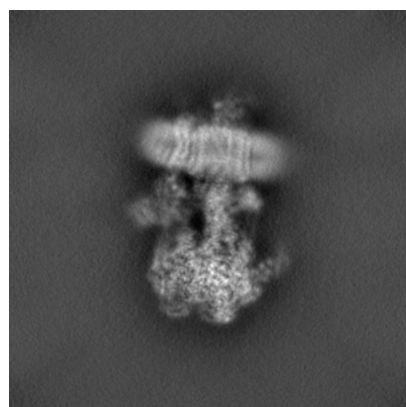


Y

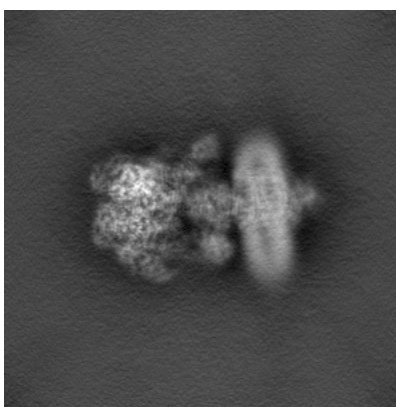


Z

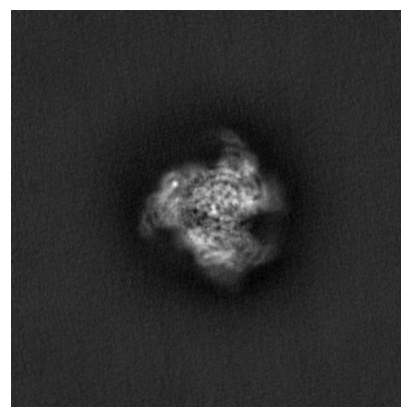
6.1.2 Raw map



X



Y

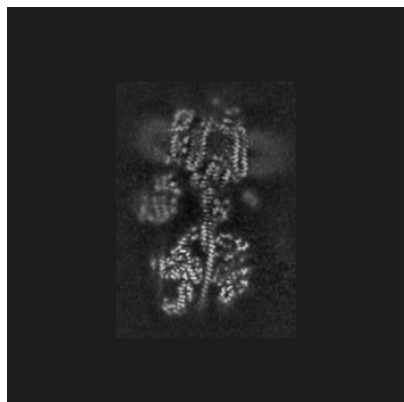


Z

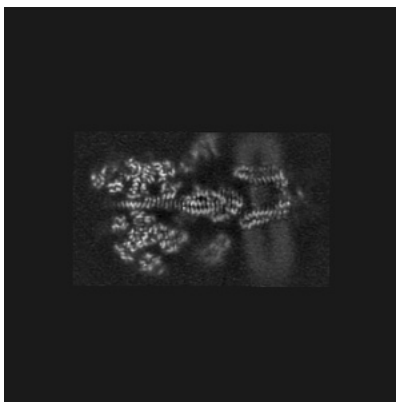
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

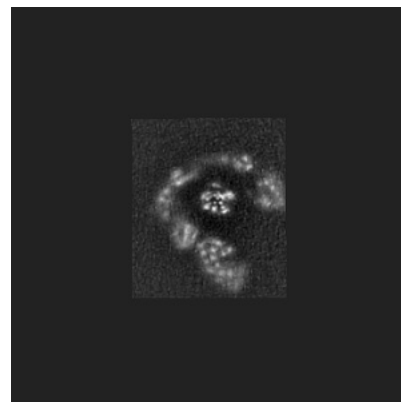
6.2.1 Primary map



X Index: 180

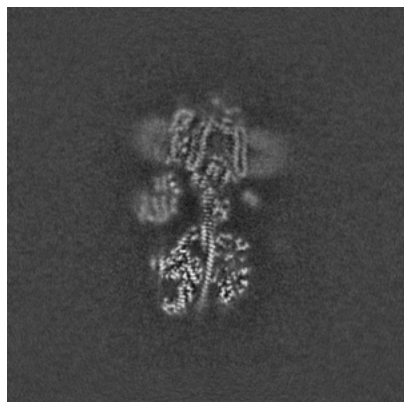


Y Index: 180

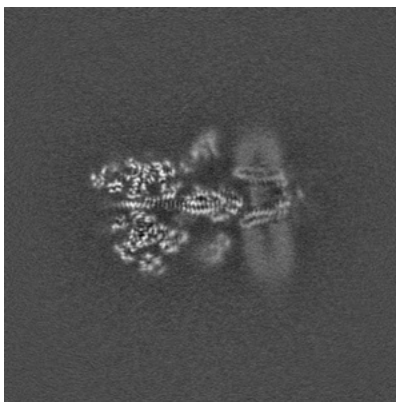


Z Index: 180

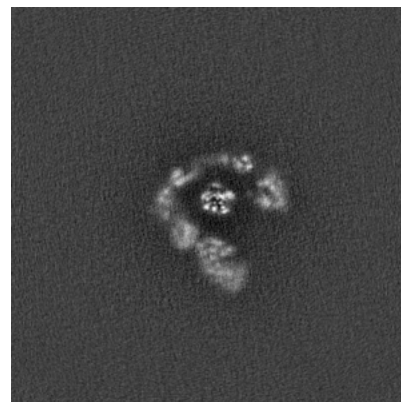
6.2.2 Raw map



X Index: 180



Y Index: 180

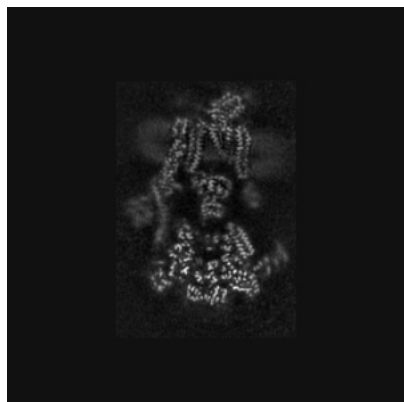


Z Index: 180

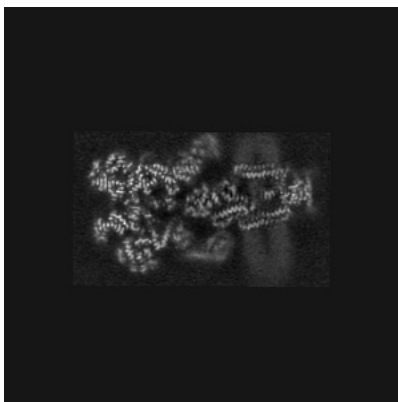
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

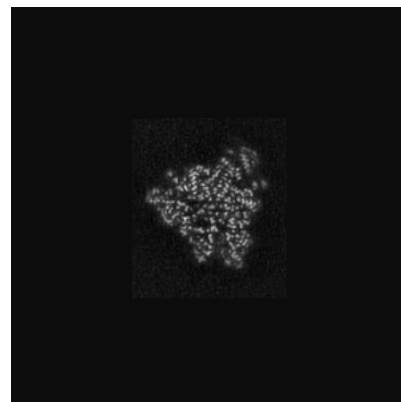
6.3.1 Primary map



X Index: 193

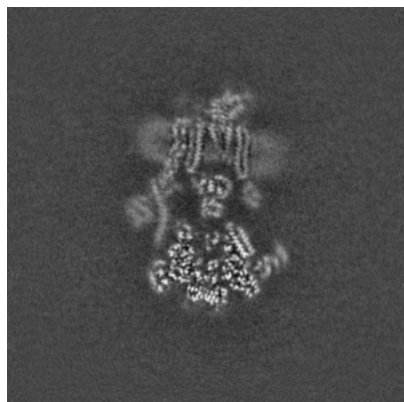


Y Index: 188

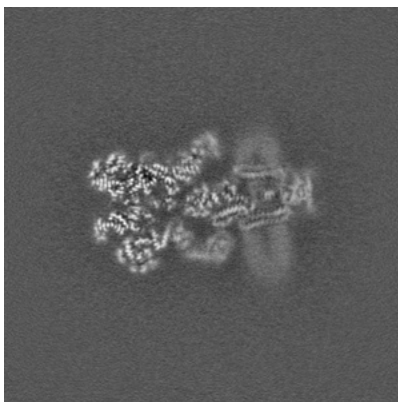


Z Index: 116

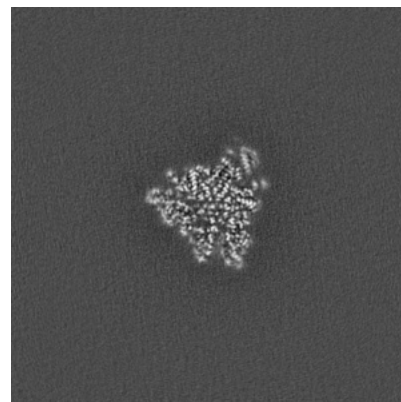
6.3.2 Raw map



X Index: 194



Y Index: 188

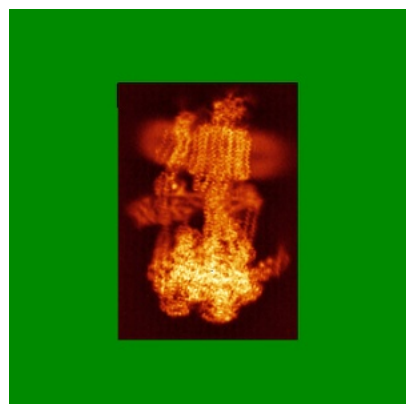


Z Index: 116

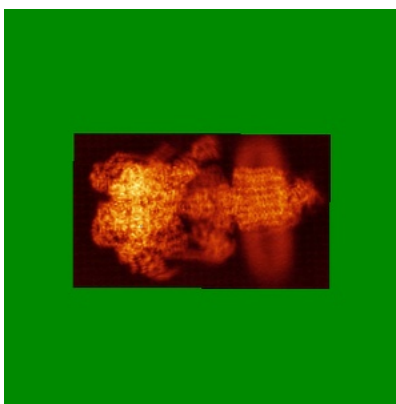
The images above show the largest variance slices of the map in three orthogonal directions.

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

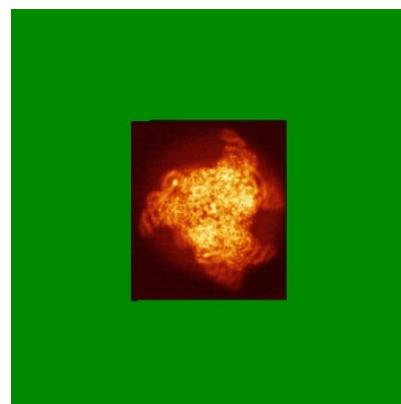
6.4.1 Primary map



X

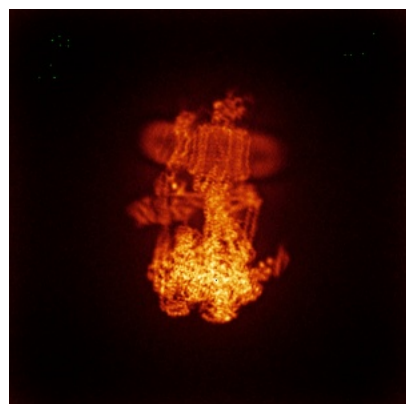


Y

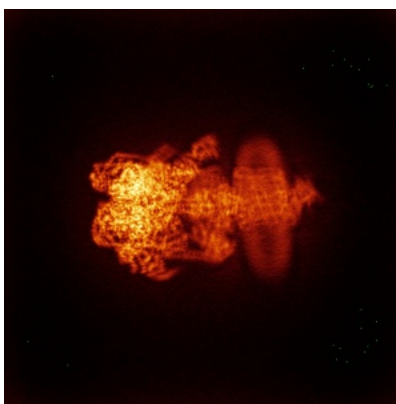


Z

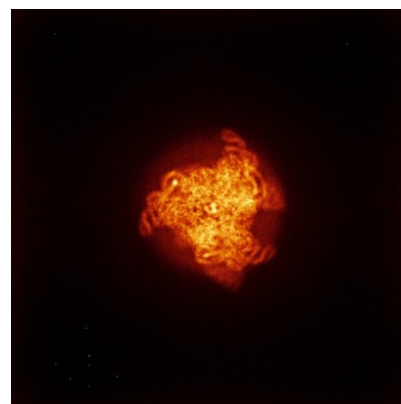
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

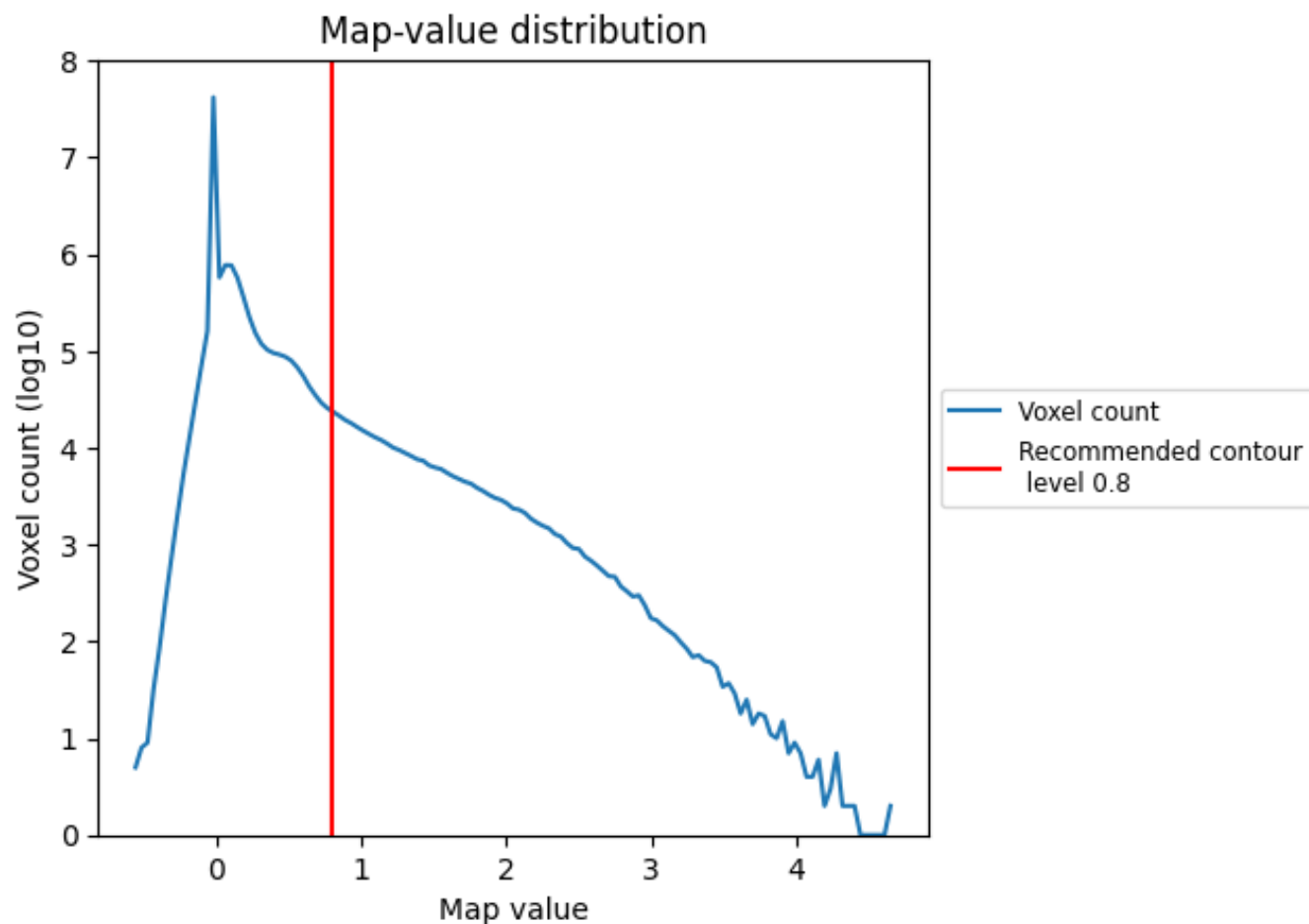
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

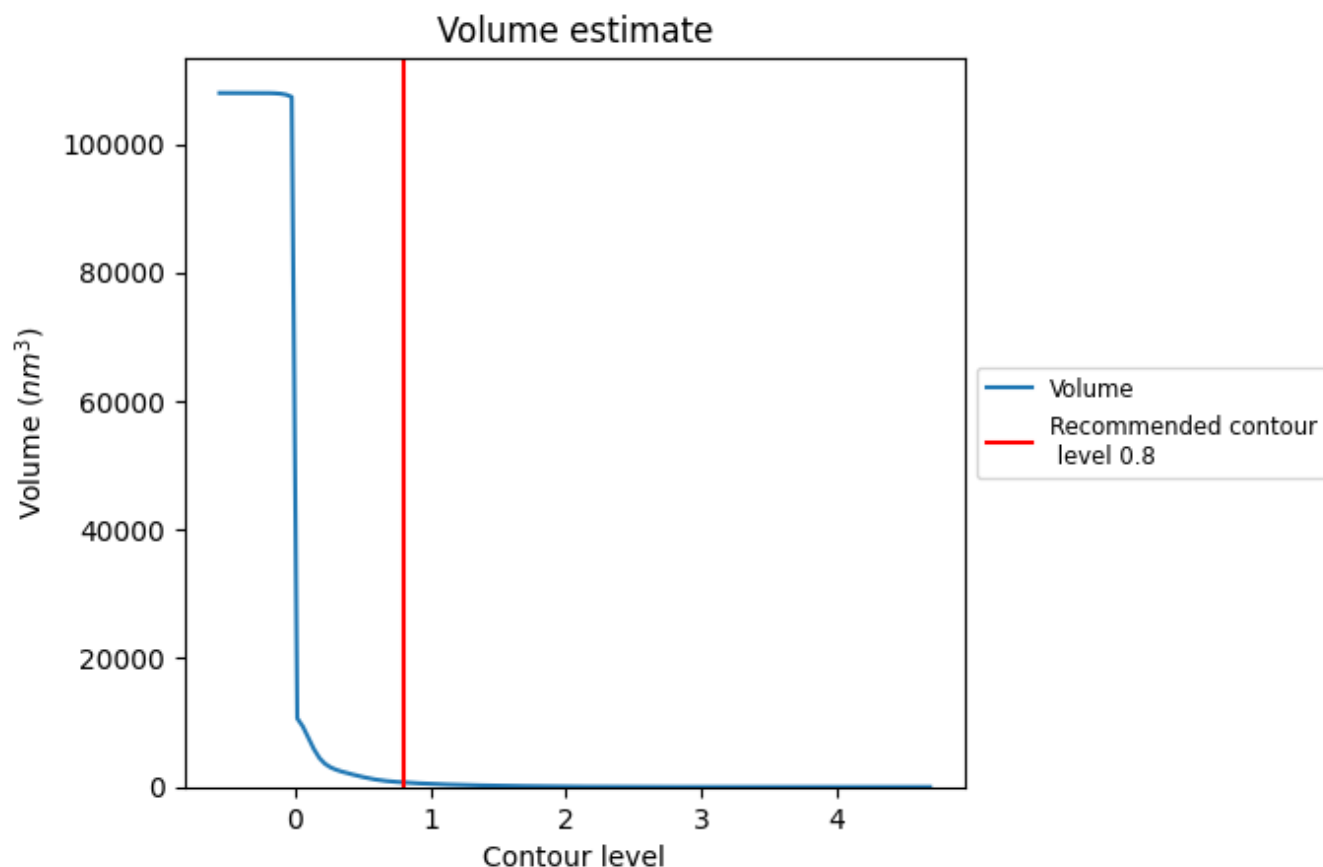
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

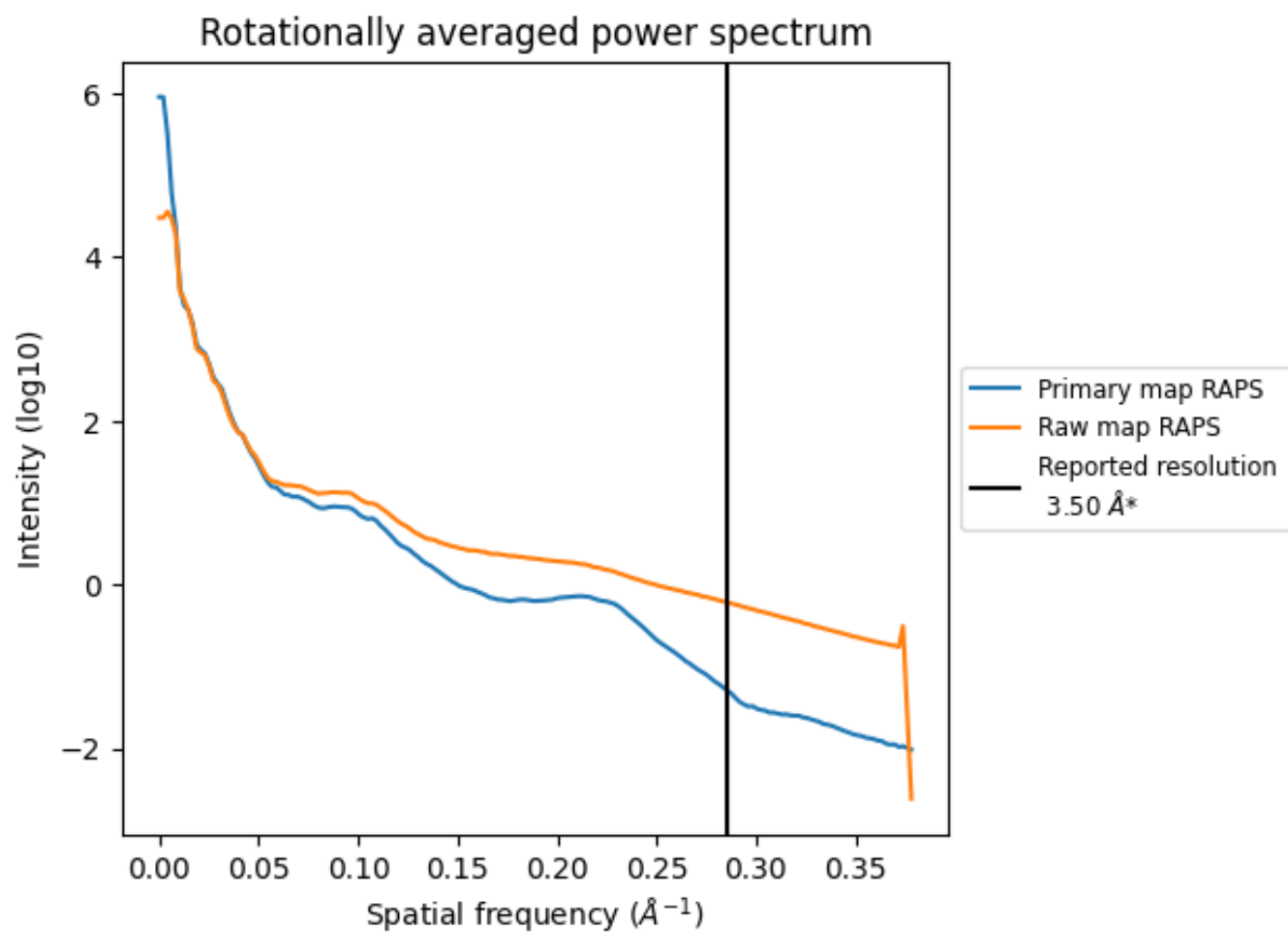
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 707 nm^3 ; this corresponds to an approximate mass of 639 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 ⓘ

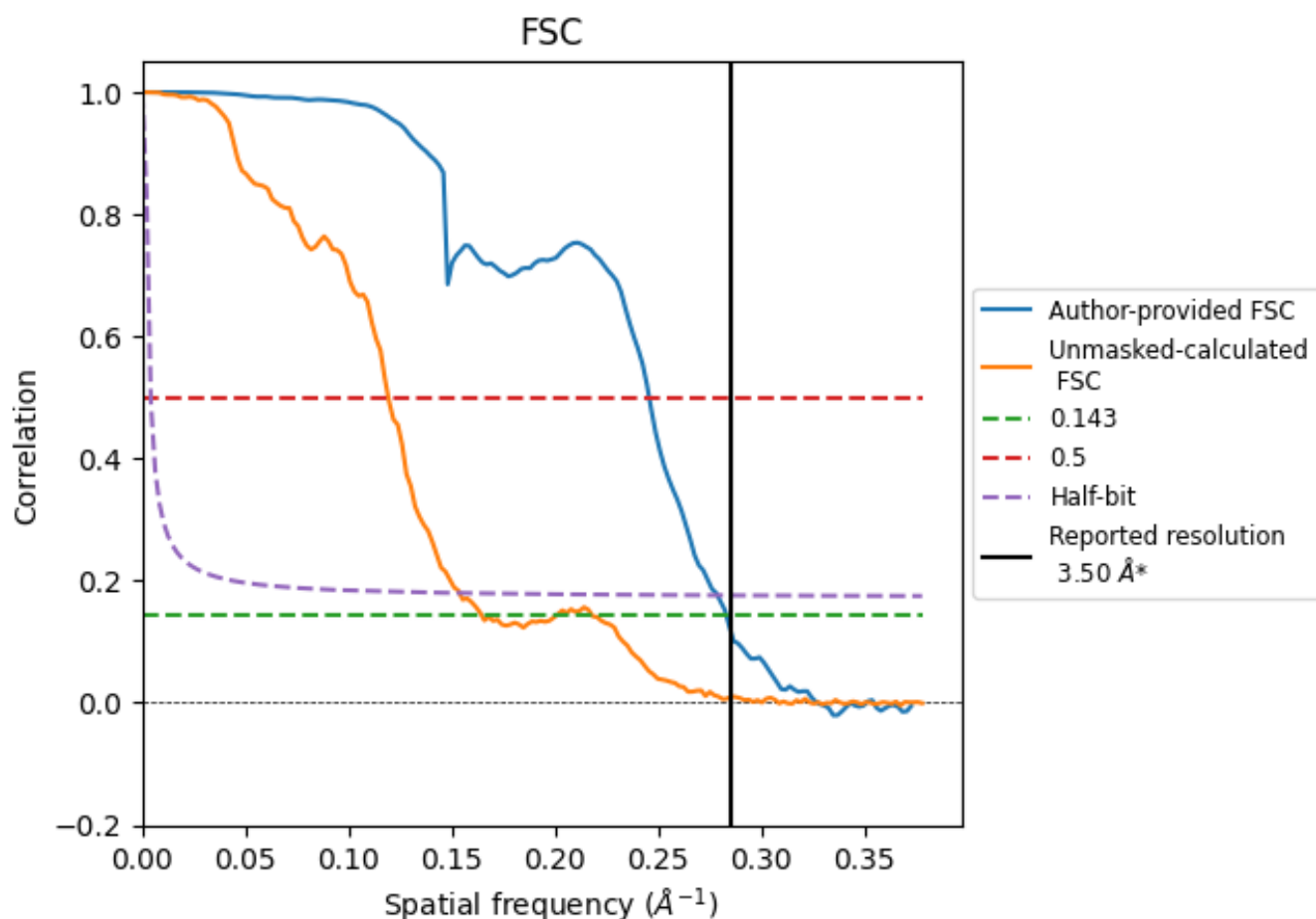


*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

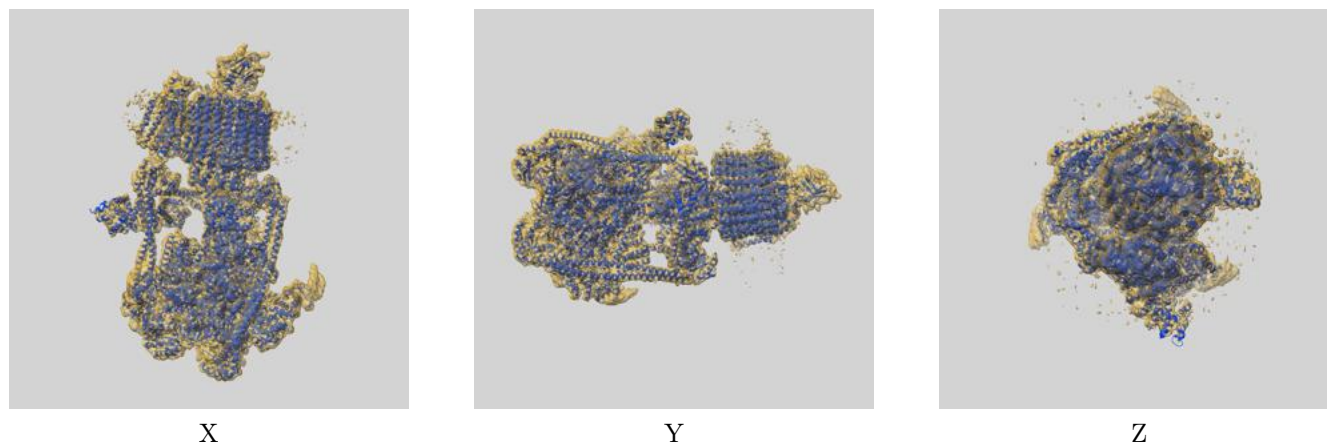
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.53	4.07	3.59
Unmasked-calculated*	6.08	8.38	6.50

*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 6.08 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

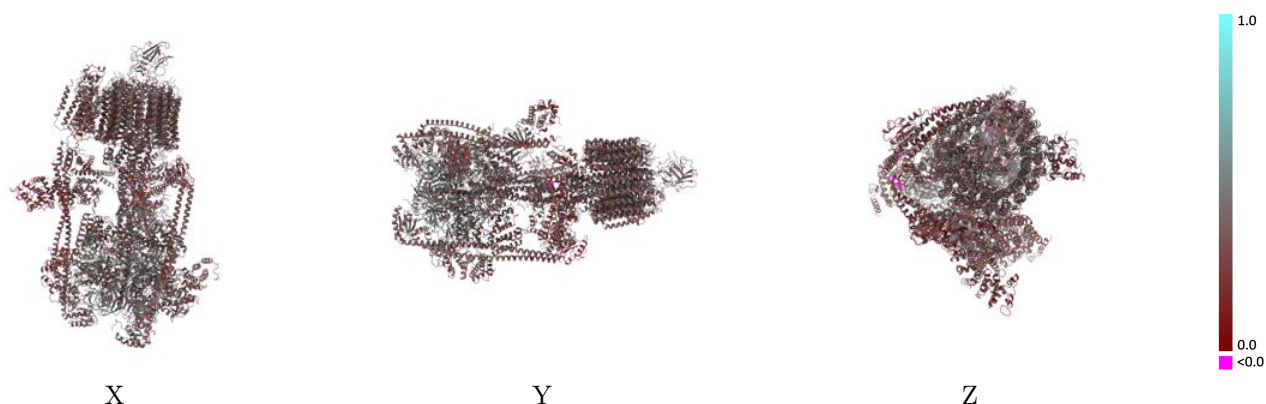
This section contains information regarding the fit between EMDB map EMD-26385 and PDB model 7U8O. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.8 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](#)

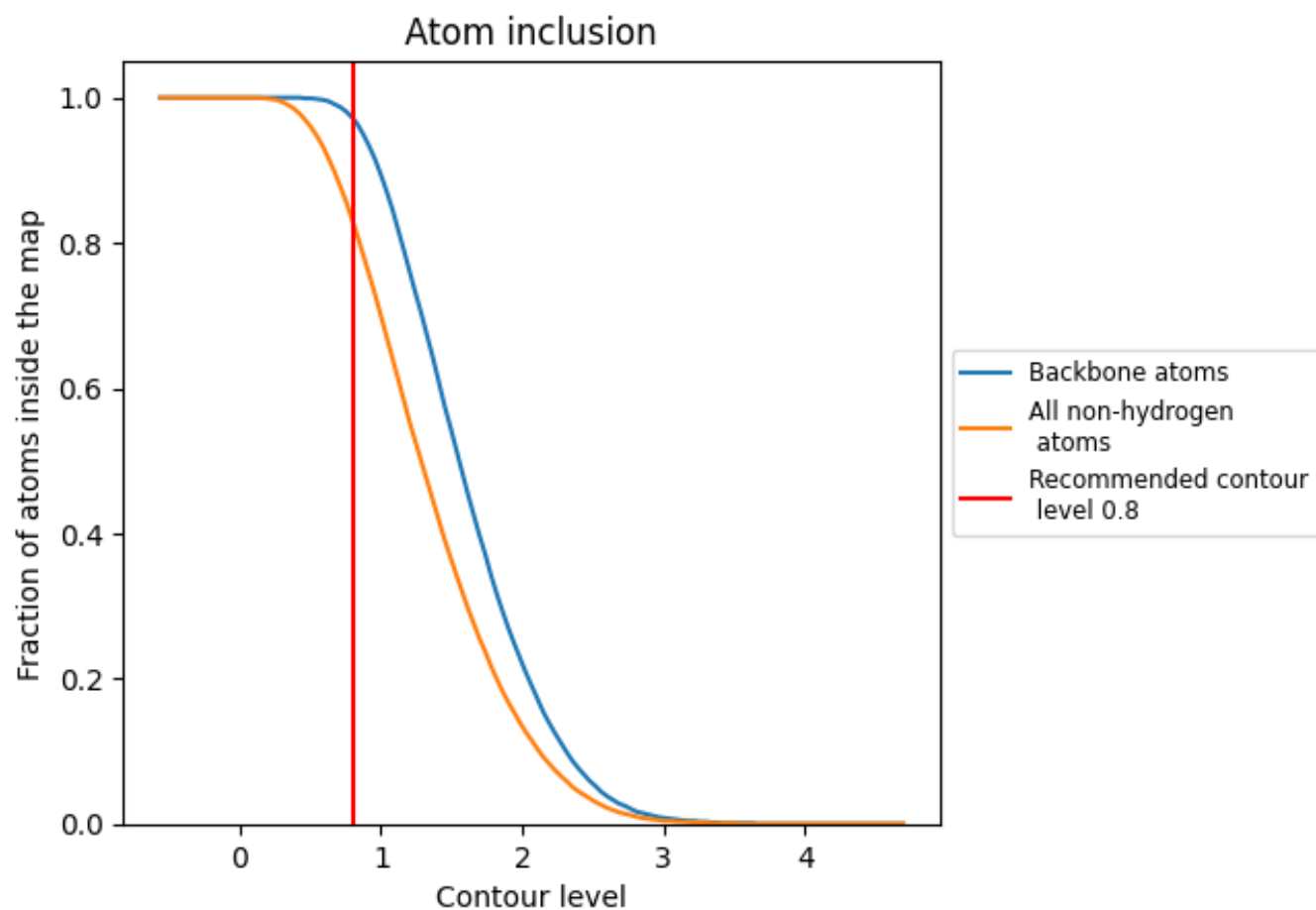


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 83% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8300	 0.3710
A	 0.8480	 0.3930
B	 0.8870	 0.4170
C	 0.8720	 0.4050
D	 0.9060	 0.4360
E	 0.8980	 0.4330
F	 0.9050	 0.4300
G	 0.7740	 0.2760
H	 0.7810	 0.3750
I	 0.8770	 0.3670
J	 0.8900	 0.3740
K	 0.8370	 0.3580
L	 0.7220	 0.3550
M	 0.8810	 0.3390
N	 0.9560	 0.3540
O	 0.9070	 0.3510
Q	 0.8060	 0.3220
R	 0.8110	 0.3220
S	 0.7980	 0.3220
T	 0.7740	 0.2660
U	 0.8920	 0.3760
a	 0.7560	 0.3190
b	 0.7950	 0.3800
c	 0.8550	 0.3750
d	 0.7320	 0.3650
e	 0.7770	 0.3550
f	 0.7380	 0.3090
g	 0.7970	 0.3780
h	 0.8130	 0.3810
i	 0.8190	 0.3640
j	 0.8360	 0.3700
k	 0.7860	 0.3680
l	 0.7530	 0.3530
m	 0.7480	 0.3470
n	 0.7440	 0.3490



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
o	 0.7430	 0.3560
p	 0.7910	 0.3770