



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:47 AM UTC

PDB ID : 7U8P / pdb_00007u8p
EMDB ID : EMD-26386
Title : Structure of porcine kidney V-ATPase with SidK, Rotary State 1
Authors : Tan, Y.Z.; Keon, K.A.
Deposited on : 2022-03-09
Resolution : 3.70 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:

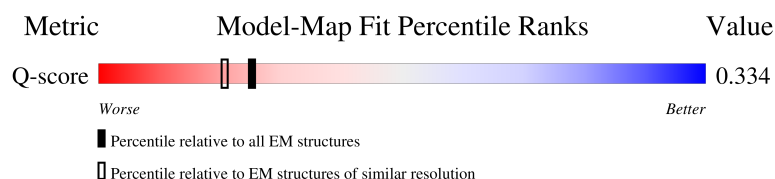
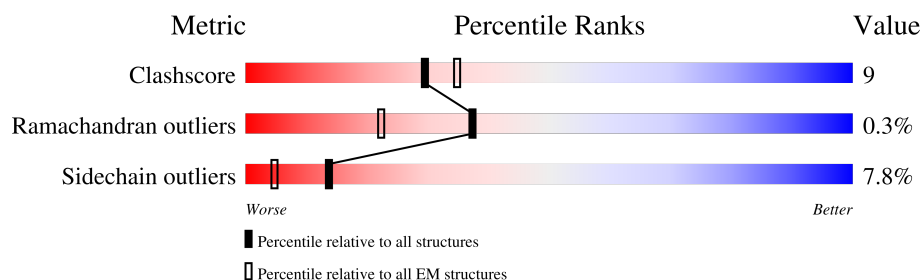
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.70 Å.

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



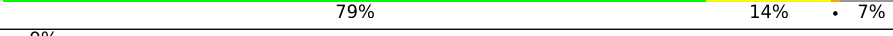
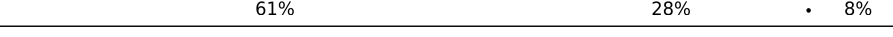
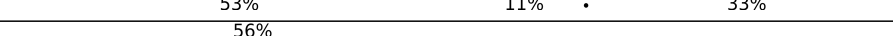
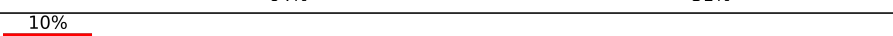
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	

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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	a	838	
11	b	205	
12	c	469	
13	d	351	
14	e	81	
15	f	98	
16	g	155	
16	h	155	
16	i	155	
16	j	155	

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Mol	Chain	Length	Quality of chain
16	k	155	12% 66% 30%
16	l	155	15% 58% 39%
16	m	155	9% 71% 25%
16	n	155	6% 77% 19%
16	o	155	8% 65% 32%
17	p	351	11% 85%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 69827 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	587	Total	C	N	O	S	0	0
			4577	2904	776	873	24		
1	B	600	Total	C	N	O	S	0	0
			4661	2957	790	889	25		
1	C	600	Total	C	N	O	S	0	0
			4661	2957	790	889	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	456	Total	C	N	O	S	0	0
			3572	2266	611	674	21		
2	E	458	Total	C	N	O	S	0	0
			3590	2278	615	676	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
			2935	1880	496	549	10		

- 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
			1416	880	263	269	4		
5	J	218	Total	C	N	O	S	0	0
			1773	1118	317	329	9		
5	K	217	Total	C	N	O	S	0	0
			1766	1113	316	328	9		

- 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
			673	413	129	130	1		
7	N	110	Total	C	N	O	S	0	0
			906	556	172	175	3		
7	O	108	Total	C	N	O	S	0	0
			894	548	170	173	3		

- 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
			1836	1169	308	348	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	S	0	0
			3510	2230	606	651	23		

- Molecule 10 is a protein called V-type proton ATPase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	750	Total	C	N	O	S	0	0
			6099	3978	1017	1063	41		

- Molecule 11 is a protein called V-type proton ATPase 21 kDa proteolipid subunit isoform 1.

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

- Molecule 12 is a protein called ATPase H⁺ transporting accessory protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	c	206	Total	C	N	O	S	0	0
			1666	1087	270	302	7		

- Molecule 13 is a protein called V-type proton ATPase subunit.

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

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

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

- Molecule 15 is a protein called Ribonuclease kappa.

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

- Molecule 16 is a protein called V-type proton ATPase proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	h	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	i	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		

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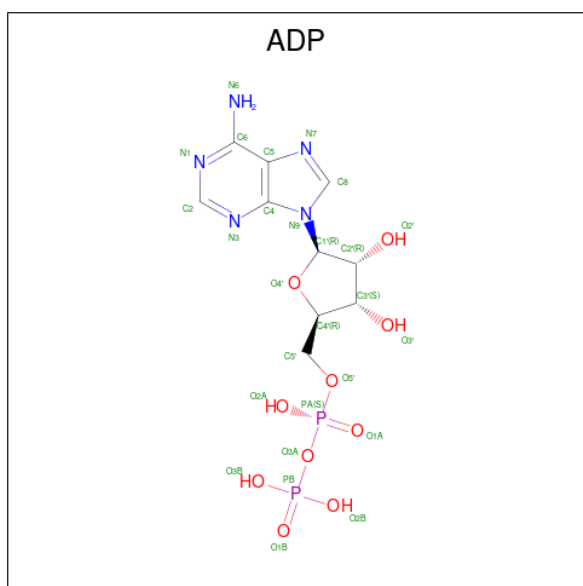
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Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	k	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	l	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	m	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	n	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		
16	o	150	Total	C	N	O	S	0	0
			1058	698	167	186	7		

- Molecule 17 is a protein called ATPase H(+)-transporting lysosomal accessory protein 2.

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

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

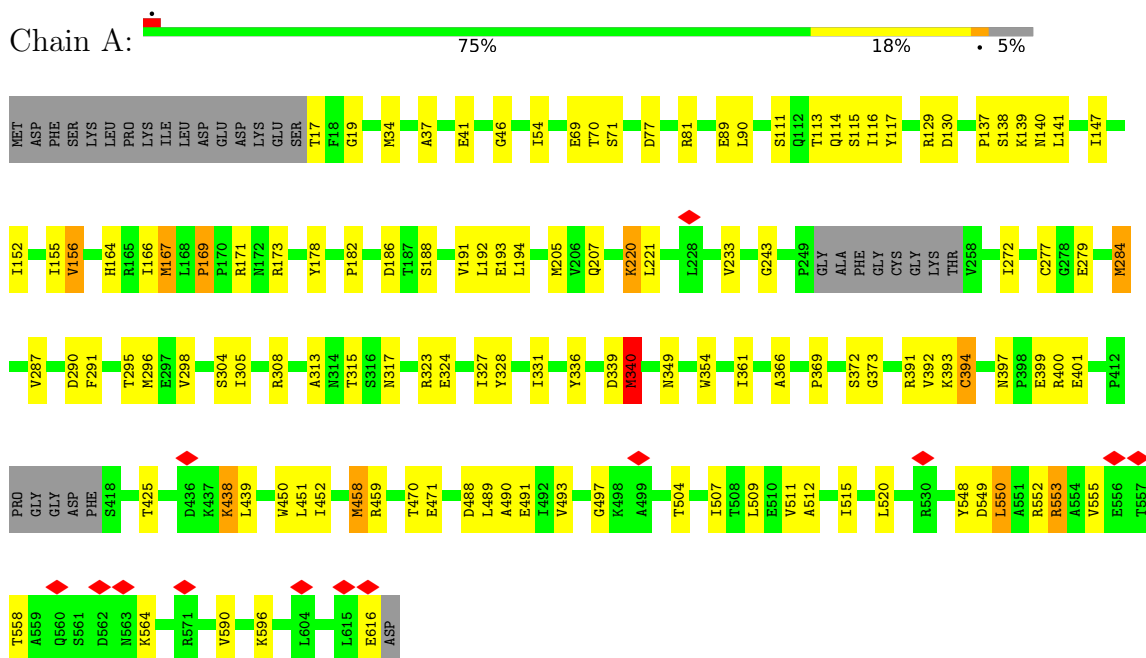


Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

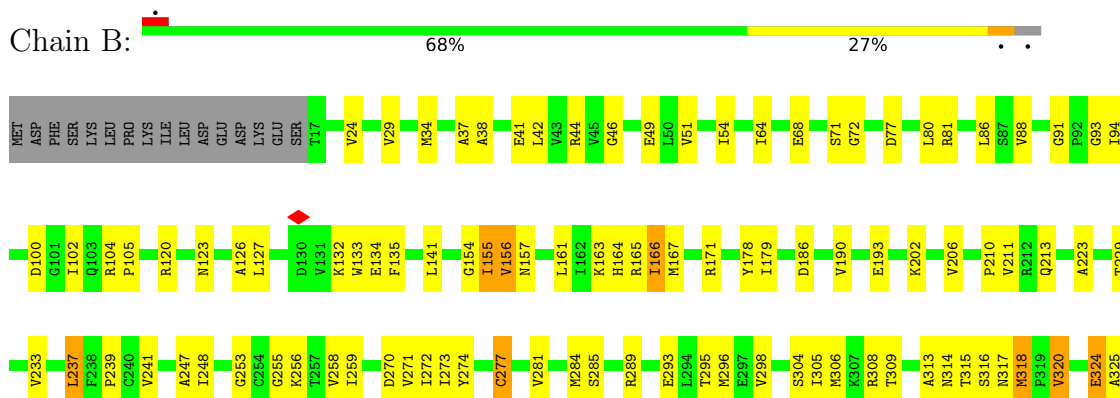
3 Residue-property plots

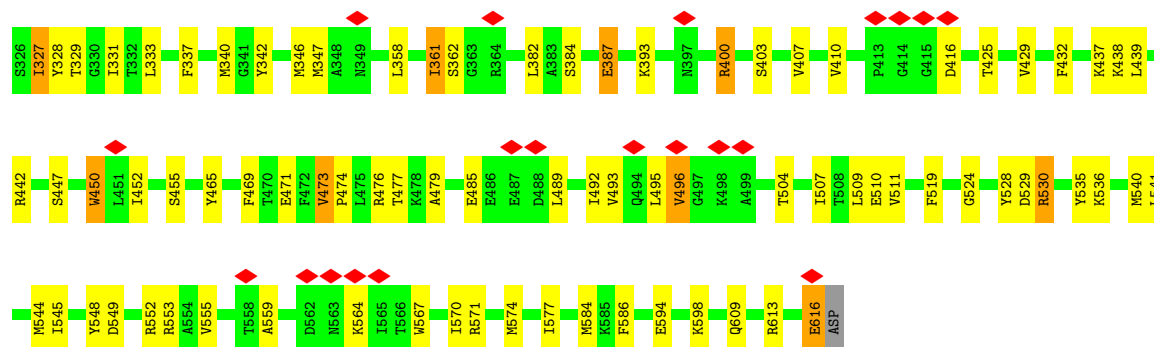
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



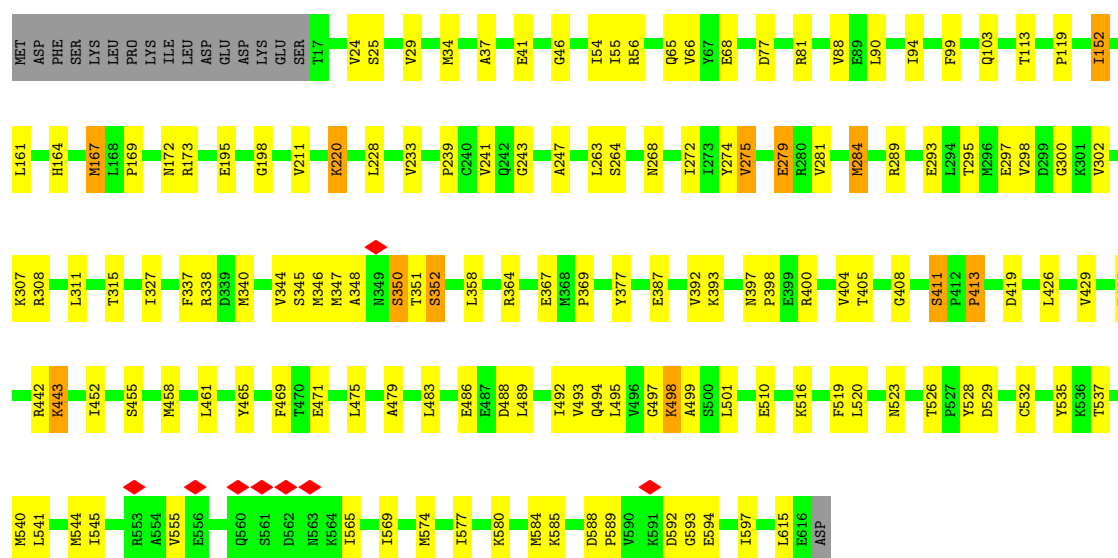
- Molecule 1: V-type proton ATPase catalytic subunit A





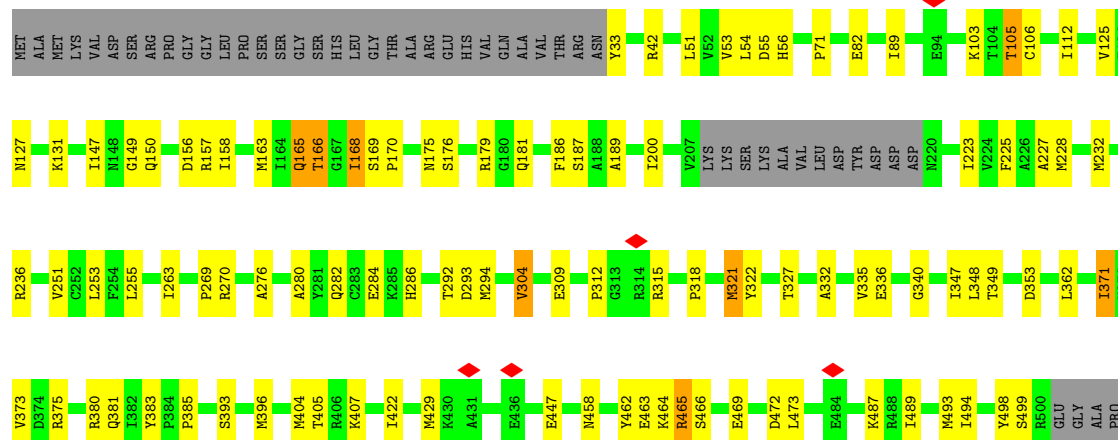
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain C: 74% 21%



• Molecule 2: Vacuolar proton pump subunit B

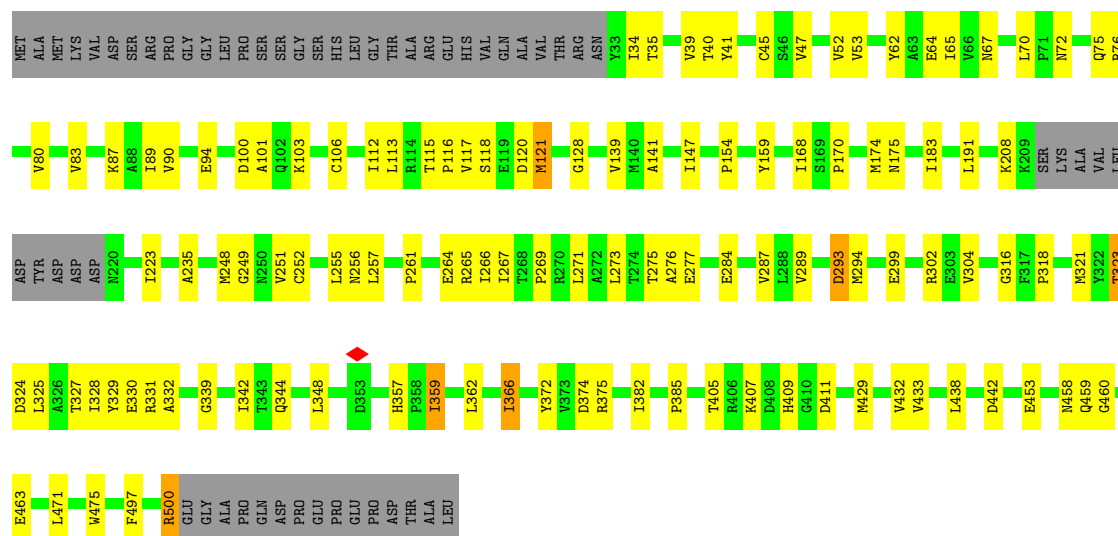
Chain D: 68% 19% 11%



ASP
PRO
GLU
PRO
GLU
PRO
ASP
THR
LEU

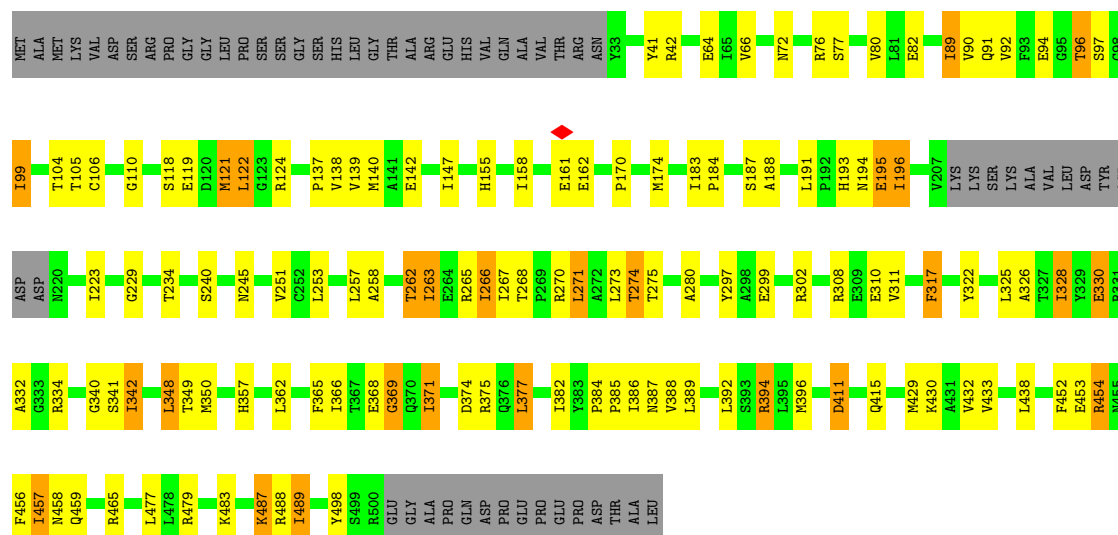
• Molecule 2: Vacuolar proton pump subunit B

Chain E:  66% 22% 11%



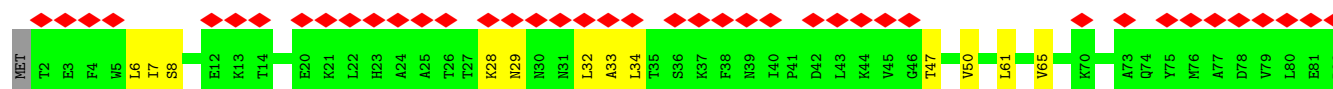
• Molecule 2: Vacuolar proton pump subunit B

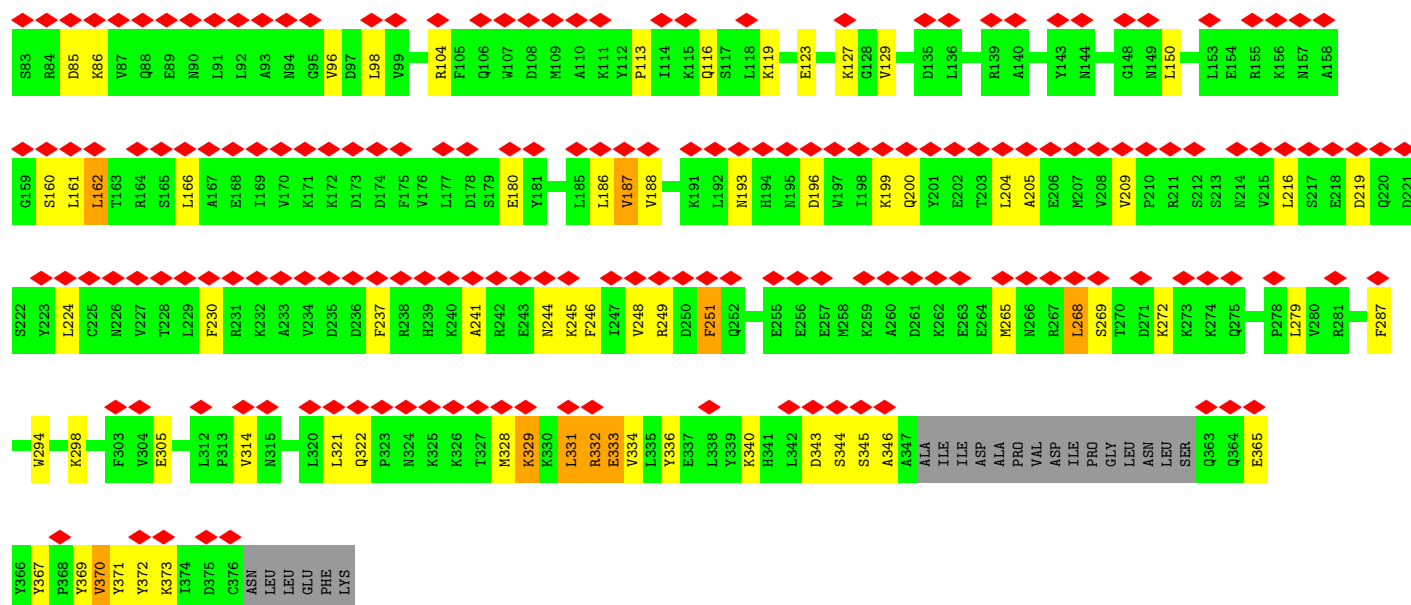
Chain F:  63% 20% 5% 11%



• Molecule 3: V-type proton ATPase subunit C

Chain G:  56% 73% 19% 6%

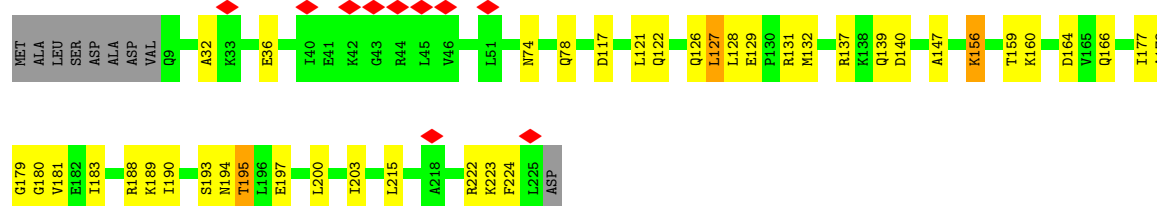
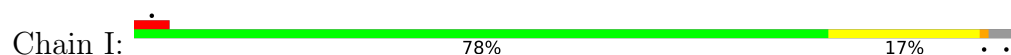




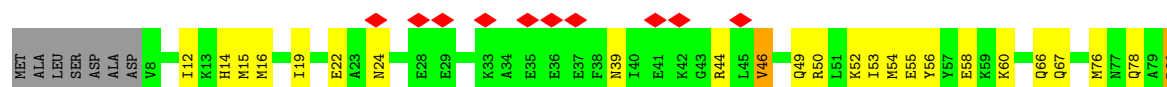
• Molecule 4: V-type proton ATPase subunit D



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

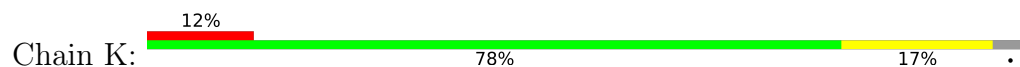


• Molecule 5: V-type proton ATPase subunit E 1

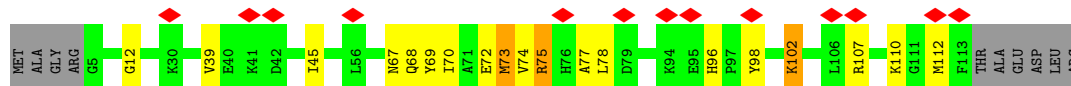
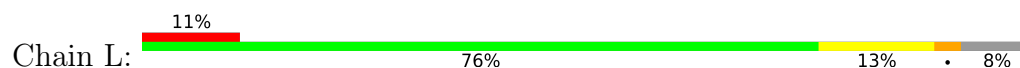




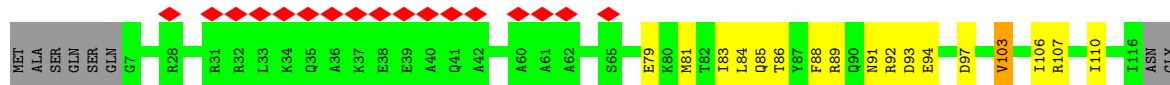
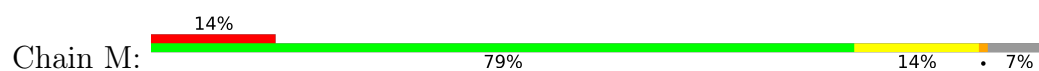
• Molecule 5: V-type proton ATPase subunit E 1



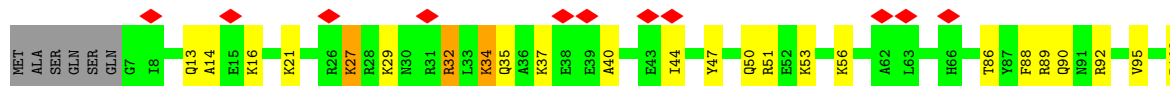
• Molecule 6: V-type proton ATPase subunit F



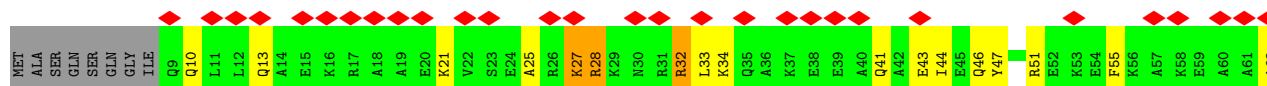
• Molecule 7: V-type proton ATPase subunit G



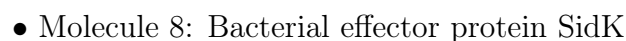
• Molecule 7: V-type proton ATPase subunit G



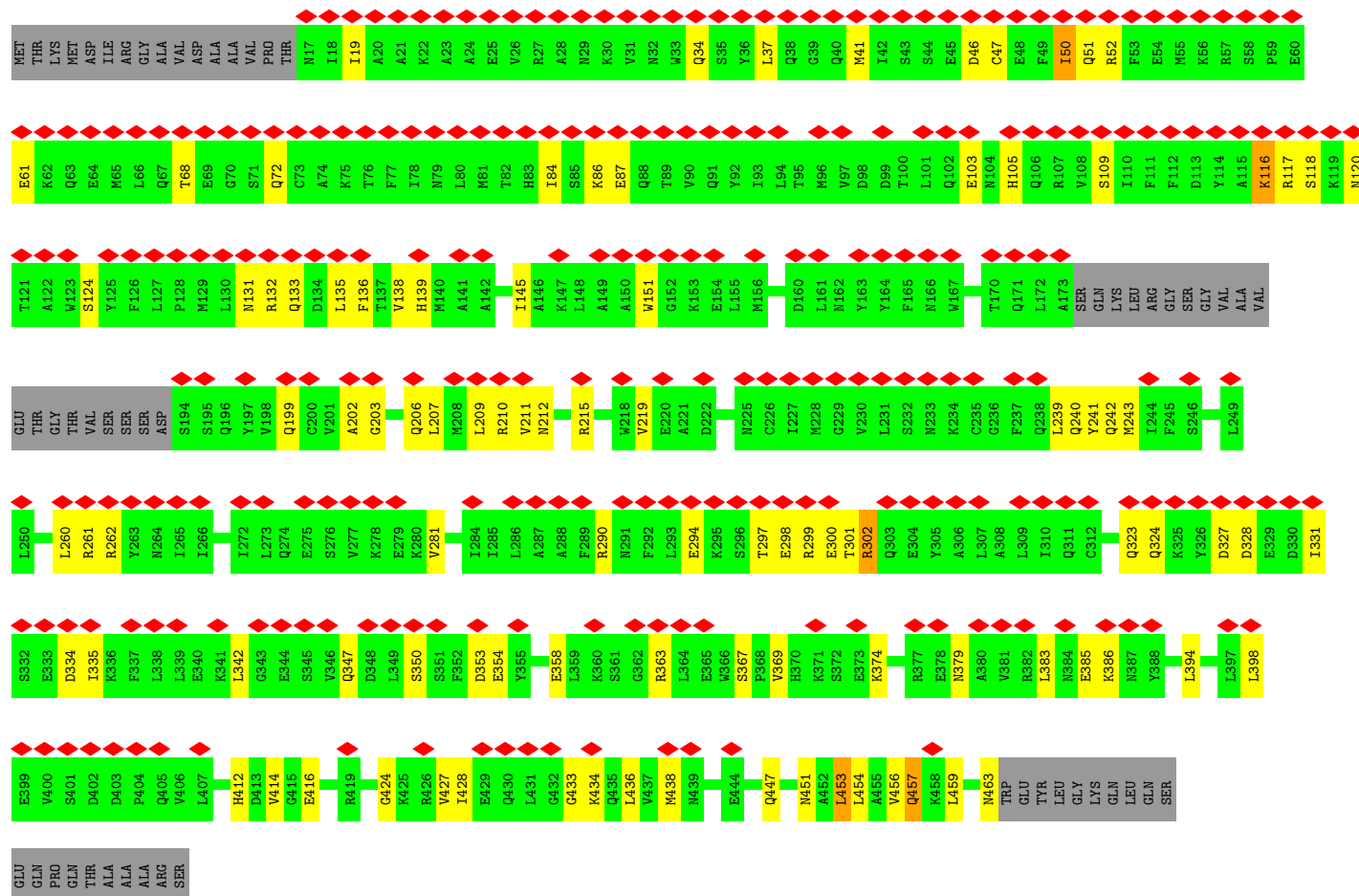
• Molecule 7: V-type proton ATPase subunit G



Chain Q:

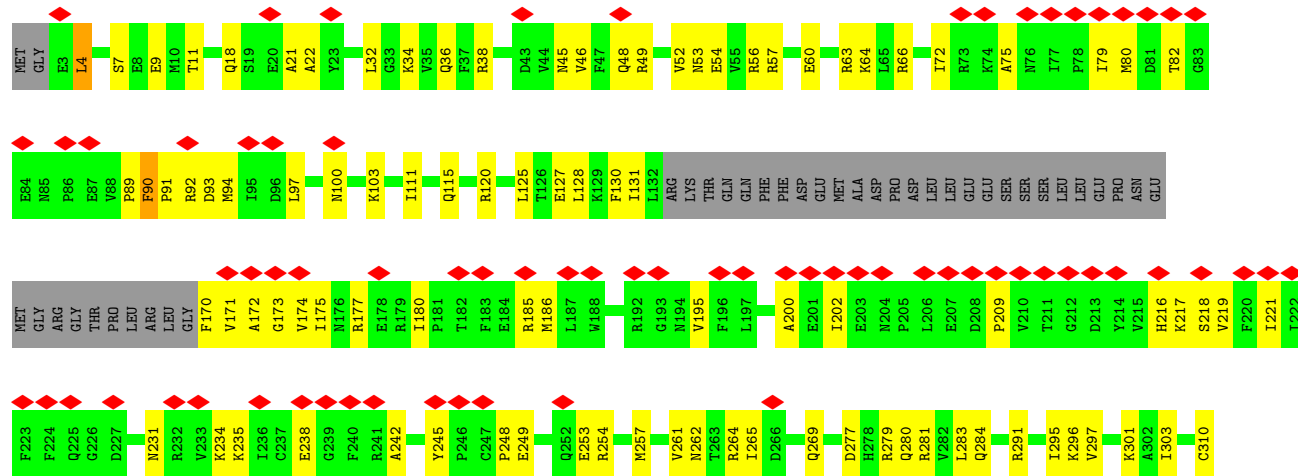


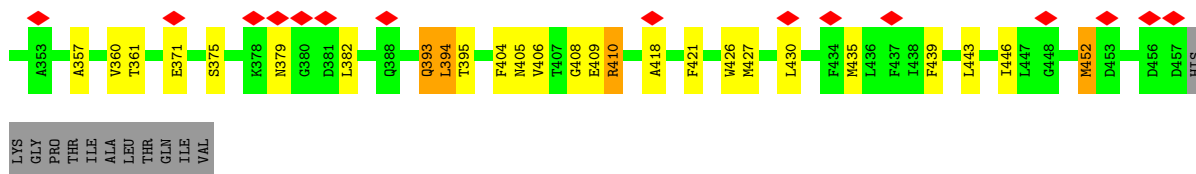
Chain T: 



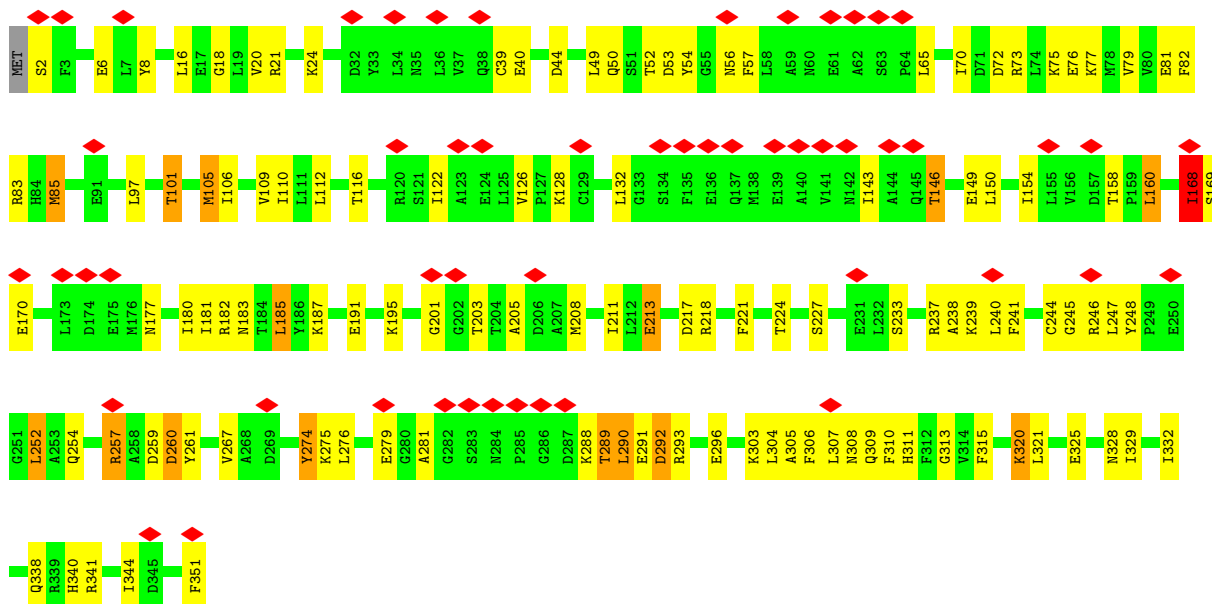
• Molecule 10: V-type proton ATPase subunit a

Chain a: 





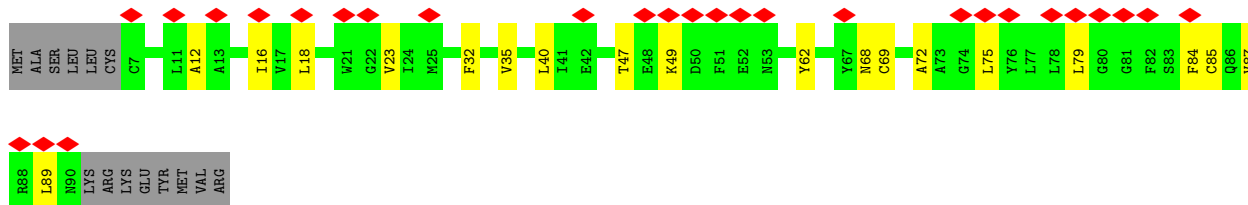
• Molecule 13: V-type proton ATPase subunit



• Molecule 14: V-type proton ATPase subunit

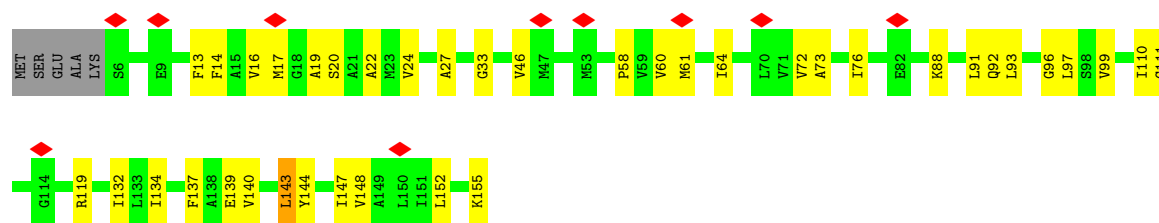


• Molecule 15: Ribonuclease kappa

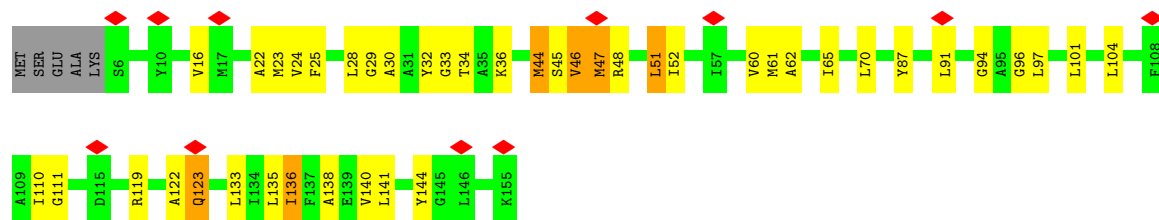


• Molecule 16: V-type proton ATPase proteolipid subunit

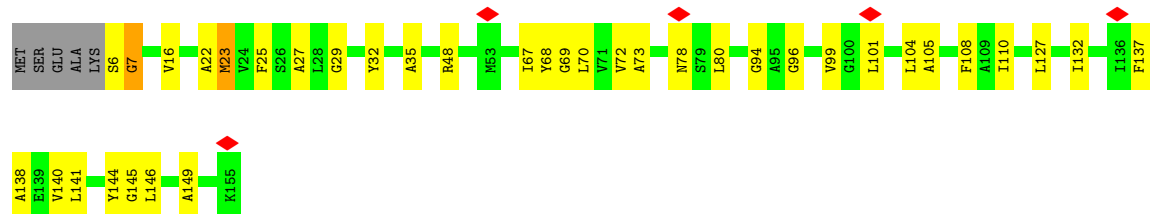




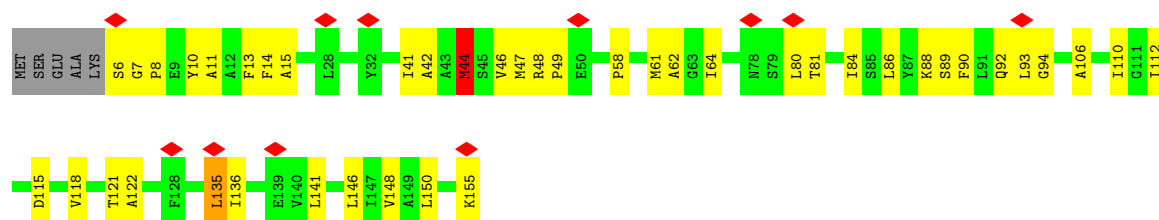
- Molecule 16: V-type proton ATPase proteolipid subunit



- Molecule 16: V-type proton ATPase proteolipid subunit

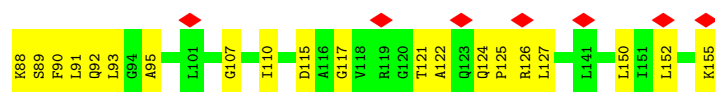


- Molecule 16: V-type proton ATPase proteolipid subunit

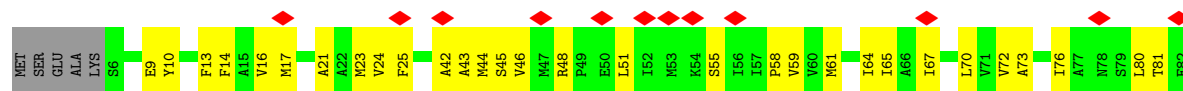


- Molecule 16: V-type proton ATPase proteolipid subunit

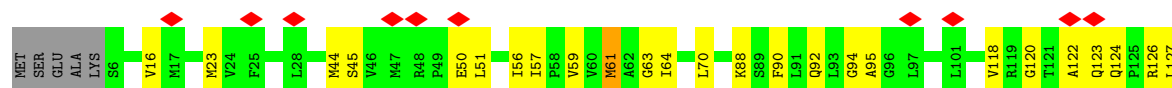




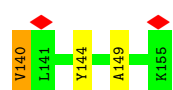
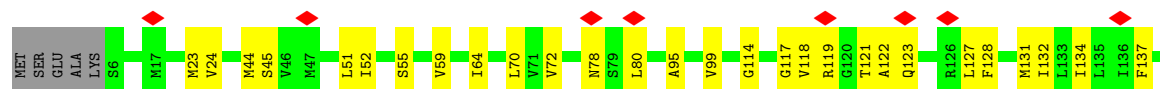
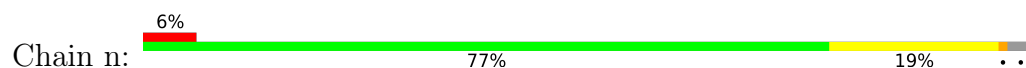
- Molecule 16: V-type proton ATPase proteolipid subunit



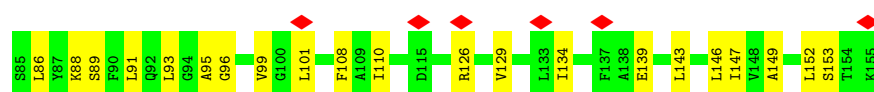
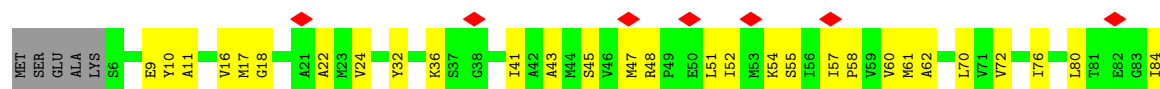
- Molecule 16: V-type proton ATPase proteolipid subunit



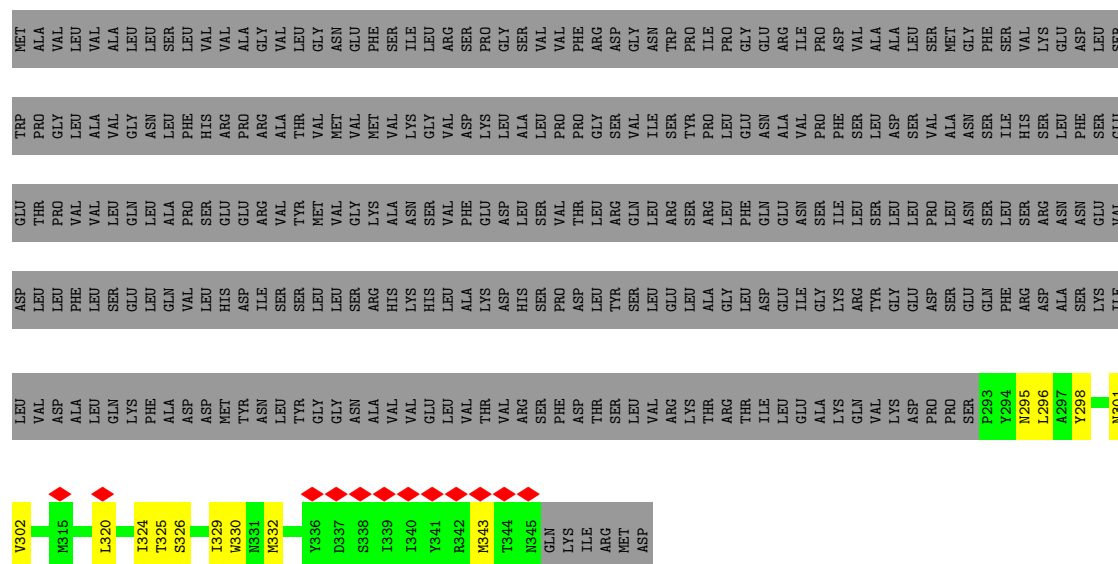
- Molecule 16: V-type proton ATPase proteolipid subunit



- Molecule 16: V-type proton ATPase proteolipid subunit



- Molecule 17: ATPase H(+)-transporting lysosomal accessory protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24327	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	100.00	Depositor
Maximum defocus (nm)	3911.445	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.443	Depositor
Minimum map value	-0.604	Depositor
Average map value	0.168	Depositor
Map value standard deviation	0.283	Depositor
Recommended contour level	0.75	Depositor
Map size ($\text{\AA}$)	184.88861, 215.4487, 307.129	wwPDB
Map dimensions	121, 141, 201	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.528005, 1.528005, 1.528005	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.65	0/4668	1.03	9/6324 (0.1%)
1	B	0.59	0/4757	0.93	2/6446 (0.0%)
1	C	0.60	0/4757	0.97	2/6446 (0.0%)
2	D	0.65	0/3644	1.02	7/4939 (0.1%)
2	E	0.67	0/3662	1.08	7/4961 (0.1%)
2	F	0.74	0/3644	1.16	14/4939 (0.3%)
3	G	0.63	0/2989	1.09	0/4038
4	H	0.64	0/1735	1.16	2/2321 (0.1%)
5	I	0.56	0/1427	0.92	1/1948 (0.1%)
5	J	0.55	0/1790	0.98	1/2396 (0.0%)
5	K	0.44	0/1783	0.87	2/2386 (0.1%)
6	L	0.65	0/879	1.17	0/1186
7	M	0.47	0/678	0.76	1/933 (0.1%)
7	N	0.49	0/914	0.92	0/1218
7	O	0.46	0/902	0.85	0/1202
8	Q	0.54	0/1858	0.97	2/2505 (0.1%)
8	R	0.63	0/1717	1.09	3/2315 (0.1%)
8	S	0.58	0/1870	1.01	2/2520 (0.1%)
9	T	0.56	0/3576	0.98	4/4818 (0.1%)
10	a	0.59	0/6252	1.00	11/8459 (0.1%)
11	b	0.51	0/1532	0.91	0/2083
12	c	0.71	0/1721	1.15	3/2345 (0.1%)
13	d	0.62	0/2901	1.05	3/3930 (0.1%)
14	e	0.47	0/679	0.85	1/934 (0.1%)
15	f	0.59	0/669	1.10	2/907 (0.2%)
16	g	0.52	0/1073	0.93	1/1453 (0.1%)
16	h	0.67	0/1073	1.10	0/1453
16	i	0.58	0/1073	1.08	3/1453 (0.2%)
16	j	0.66	0/1073	1.15	4/1453 (0.3%)
16	k	0.47	0/1073	0.87	0/1453
16	l	0.29	0/1073	0.62	0/1453
16	m	0.55	0/1073	0.99	0/1453

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	n	0.57	0/1073	1.01	2/1453 (0.1%)
16	o	0.42	0/1073	0.79	0/1453
17	p	0.54	0/456	0.95	0/625
All	All	0.60	0/71117	1.01	89/96201 (0.1%)

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	103	VAL	N-CA-C	-9.06	103.90	112.96
10	a	563	PHE	N-CA-C	-8.48	102.48	113.17
1	C	169	PRO	N-CA-CB	7.95	107.35	103.22
2	F	274	THR	N-CA-C	-7.93	102.51	112.90
2	D	422	ILE	N-CA-C	-7.74	102.57	111.00
15	f	23	VAL	N-CA-C	-7.73	104.26	111.45
2	F	369	GLY	CA-C-O	-7.50	117.05	122.23
15	f	68	ASN	CA-CB-CG	7.26	119.86	112.60
2	E	261	PRO	CA-C-O	-7.25	115.95	121.31
8	Q	138	ASP	CA-CB-CG	6.84	119.44	112.60
12	c	289	PHE	CA-CB-CG	6.82	120.62	113.80
8	R	77	ASP	CA-CB-CG	6.66	119.26	112.60
8	R	211	SER	O-C-N	-6.42	115.59	121.37
1	A	243	GLY	N-CA-C	-6.40	106.49	115.32
2	F	196	ILE	N-CA-C	-6.24	104.96	111.58
2	F	454	ARG	CA-C-N	-6.22	111.27	122.46
2	F	454	ARG	C-N-CA	-6.22	111.27	122.46
2	E	261	PRO	N-CA-C	6.20	124.62	113.70
1	A	452	ILE	N-CA-C	-6.16	106.80	112.96
2	E	460	GLY	CA-C-N	6.10	125.99	119.28
2	E	460	GLY	C-N-CA	6.10	125.99	119.28
1	A	298	VAL	O-C-N	-6.06	117.32	121.98
1	B	362	SER	N-CA-C	-6.06	104.24	111.69
13	d	168	ILE	N-CA-C	6.01	116.19	110.42
16	i	132	ILE	CA-C-O	-6.00	114.81	121.17
8	Q	151	PHE	CA-CB-CG	5.81	119.61	113.80
10	a	788	VAL	O-C-N	-5.81	115.85	121.83
2	F	155	HIS	N-CA-C	-5.78	105.49	112.54
10	a	4	LEU	CA-C-N	5.74	127.97	120.28
10	a	4	LEU	C-N-CA	5.74	127.97	120.28
1	A	169	PRO	CB-CA-C	-5.69	106.04	111.39
1	A	470	THR	CA-C-N	5.67	130.19	120.72
1	A	470	THR	C-N-CA	5.67	130.19	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ILE	N-CA-C	-5.66	104.85	110.62
10	a	534	ASN	CA-CB-CG	5.65	118.25	112.60
16	j	44	MET	N-CA-C	-5.62	105.15	111.28
12	c	316	PHE	CA-CB-CG	5.61	119.41	113.80
2	F	96	THR	CA-CB-OG1	-5.57	101.25	109.60
2	E	293	ASP	CA-CB-CG	-5.56	107.04	112.60
2	E	175	ASN	CA-CB-CG	5.55	118.15	112.60
10	a	75	ALA	N-CA-C	-5.53	106.53	113.72
1	A	340	MET	N-CA-C	-5.52	105.42	111.82
5	I	156	LYS	N-CA-C	-5.50	105.30	112.23
16	n	140	VAL	CA-C-N	5.48	127.94	120.54
16	n	140	VAL	C-N-CA	5.48	127.94	120.54
1	C	555	VAL	CA-C-O	-5.47	115.05	120.85
8	S	212	PRO	N-CA-C	-5.47	106.07	113.40
16	j	48	ARG	CB-CA-C	5.44	117.72	110.81
12	c	283	ASP	CA-CB-CG	5.44	118.04	112.60
2	D	472	ASP	N-CA-C	-5.40	104.94	112.45
16	j	106	ALA	CA-C-N	5.38	126.07	119.99
16	j	106	ALA	C-N-CA	5.38	126.07	119.99
2	D	149	GLY	CA-C-O	-5.38	118.52	122.23
9	T	342	LEU	CA-C-N	5.37	125.90	119.94
9	T	342	LEU	C-N-CA	5.37	125.90	119.94
2	F	270	ARG	N-CA-C	-5.34	105.50	112.23
5	K	185	ASN	CA-C-N	5.34	126.81	120.14
5	K	185	ASN	C-N-CA	5.34	126.81	120.14
9	T	151	TRP	CA-C-N	5.33	125.87	120.00
9	T	151	TRP	C-N-CA	5.33	125.87	120.00
13	d	260	ASP	O-C-N	-5.31	116.25	123.15
1	A	138	SER	CA-C-N	5.29	131.65	121.54
1	A	138	SER	C-N-CA	5.29	131.65	121.54
2	F	245	ASN	CA-CB-CG	-5.29	107.31	112.60
4	H	9	ILE	N-CA-C	-5.28	100.81	108.36
10	a	381	TYR	N-CA-C	-5.28	107.02	112.93
2	E	357	HIS	CB-CG-CD2	-5.26	124.36	131.20
2	F	195	GLU	N-CA-C	-5.25	106.39	112.89
8	R	118	HIS	CB-CG-CD2	-5.21	124.43	131.20
5	J	14	HIS	CB-CG-CD2	-5.18	124.47	131.20
8	S	178	LEU	N-CA-C	-5.11	105.40	111.69
2	F	453	GLU	N-CA-C	-5.09	107.61	113.88
14	e	69	LYS	O-C-N	-5.08	117.00	122.79
10	a	391	PRO	CB-CA-C	-5.08	103.13	111.31
10	a	269	GLN	OE1-CD-NE2	-5.07	117.53	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	357	HIS	CB-CG-CD2	-5.07	124.61	131.20
16	g	143	LEU	O-C-N	-5.07	116.29	122.22
2	D	371	ILE	N-CA-C	-5.06	107.87	112.12
2	D	462	TYR	CA-C-N	-5.05	113.70	120.87
2	D	462	TYR	C-N-CA	-5.05	113.70	120.87
13	d	274	TYR	CB-CA-C	5.04	118.76	110.95
16	i	7	GLY	CA-C-N	5.02	125.49	120.52
16	i	7	GLY	C-N-CA	5.02	125.49	120.52
2	F	317	PHE	CB-CA-C	5.02	118.80	109.51
4	H	88	ASN	CA-CB-CG	5.02	117.62	112.60
2	D	165	GLN	N-CA-C	-5.02	101.57	109.25
10	a	812	GLN	N-CA-C	-5.02	106.99	113.01
10	a	431	LEU	N-CA-C	-5.01	105.53	111.69
2	F	415	GLN	N-CA-C	-5.00	105.50	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4577	0	4577	59	0
1	B	4661	0	4653	111	0
1	C	4661	0	4653	84	0
2	D	3572	0	3555	46	0
2	E	3590	0	3581	71	0
2	F	3572	0	3555	62	0
3	G	2935	0	2970	44	0
4	H	1717	0	1822	30	0
5	I	1416	0	1167	18	0
5	J	1773	0	1855	32	0
5	K	1766	0	1846	35	0
6	L	865	0	872	15	0
7	M	673	0	476	14	0
7	N	906	0	913	26	0
7	O	894	0	899	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Q	1824	0	1835	36	0
8	R	1685	0	1691	14	0
8	S	1836	0	1847	27	0
9	T	3510	0	3493	50	0
10	a	6099	0	6128	118	0
11	b	1498	0	1548	49	0
12	c	1666	0	1571	31	0
13	d	2835	0	2770	71	0
14	e	652	0	668	18	0
15	f	653	0	652	6	0
16	g	1058	0	1136	36	0
16	h	1058	0	1136	37	0
16	i	1058	0	1136	31	0
16	j	1058	0	1136	32	0
16	k	1058	0	1136	47	0
16	l	1058	0	1136	62	0
16	m	1058	0	1136	33	0
16	n	1058	0	1136	27	0
16	o	1058	0	1136	40	0
17	p	442	0	438	8	0
18	C	27	0	12	0	0
All	All	69827	0	70271	1283	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 9.

All (1283) 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)
12:c:326:LEU:HB3	12:c:341:LEU:HG	1.32	1.07
16:h:61:MET:HE1	16:h:135:LEU:HB3	1.44	0.98
2:F:64:GLU:O	2:F:80:VAL:HG23	1.80	0.82
10:a:90:PHE:HA	10:a:94:MET:HE1	1.63	0.81
2:E:318:PRO:HG2	2:E:321:MET:HE3	1.63	0.80
13:d:224:THR:HA	13:d:237:ARG:HD2	1.62	0.80
1:B:489:LEU:HD11	1:B:509:LEU:HD21	1.63	0.79
1:A:41:GLU:HB2	1:A:54:ILE:HD12	1.65	0.79
5:J:19:ILE:HG21	7:N:14:ALA:HB1	1.66	0.77
1:B:296:MET:HE2	1:B:308:ARG:HH21	1.50	0.77
16:m:70:LEU:HD22	16:n:144:TYR:HD1	1.49	0.77
12:c:341:LEU:HD22	12:c:357:ALA:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:o:61:MET:HE3	16:o:139:GLU:HB2	1.68	0.75
2:D:51:LEU:HB3	2:D:89:ILE:HD11	1.68	0.75
8:Q:114:LYS:HD3	8:Q:169:THR:HG21	1.67	0.75
16:g:76:ILE:HG12	16:g:92:GLN:OE1	1.88	0.74
12:c:379:ASN:HB2	12:c:382:LEU:HD21	1.69	0.74
10:a:173:GLY:H	10:a:219:VAL:HG11	1.54	0.73
8:S:29:ILE:HG12	8:S:88:LEU:HD21	1.70	0.73
16:l:23:MET:HE1	16:l:70:LEU:HD22	1.70	0.73
8:R:189:ALA:HB3	8:R:192:LYS:HD2	1.71	0.73
16:n:72:VAL:HG11	16:n:99:VAL:HG11	1.69	0.72
12:c:371:GLU:HB3	17:p:302:VAL:HG13	1.72	0.72
6:L:12:GLY:HA2	6:L:70:ILE:HD13	1.71	0.72
16:j:44:MET:HB3	16:j:122:ALA:HB2	1.71	0.72
1:C:337:PHE:HA	1:C:340:MET:HG3	1.72	0.71
1:B:274:TYR:CD1	1:B:347:MET:HG2	2.25	0.71
16:k:28:LEU:HD23	16:l:105:ALA:HB2	1.73	0.71
7:O:25:ALA:HA	7:O:28:ARG:HD2	1.72	0.70
3:G:96:VAL:HG21	3:G:104:ARG:HH22	1.56	0.70
2:E:256:ASN:HD21	2:E:264:GLU:HB3	1.54	0.70
5:K:205:GLN:HA	5:K:208:MET:HG2	1.73	0.70
5:J:49:GLN:HB2	7:N:44:ILE:HG12	1.74	0.70
1:A:369:PRO:HB2	1:A:373:GLY:HA2	1.74	0.69
5:I:180:GLY:HA3	5:I:195:THR:HA	1.74	0.69
12:c:276:ALA:HB3	12:c:393:GLN:HB3	1.74	0.69
2:F:121:MET:HE3	2:F:275:THR:HG23	1.73	0.69
1:C:475:LEU:HD22	1:C:545:ILE:HG21	1.74	0.69
16:l:72:VAL:HG11	16:l:99:VAL:HG11	1.74	0.69
16:l:144:TYR:HA	16:l:147:ILE:HD12	1.75	0.69
10:a:485:PHE:HA	10:a:490:TRP:HB2	1.75	0.69
2:F:174:MET:HE1	2:F:452:PHE:HZ	1.58	0.68
11:b:164:LEU:HD22	13:d:21:ARG:HG3	1.74	0.68
10:a:591:ILE:HG22	10:a:609:LEU:HD13	1.75	0.68
1:C:519:PHE:HB2	1:C:544:MET:HE3	1.76	0.68
13:d:65:LEU:HD21	13:d:70:ILE:HD11	1.76	0.68
16:j:47:MET:SD	16:j:122:ALA:HB1	2.33	0.68
11:b:124:LYS:HE3	11:b:124:LYS:HA	1.76	0.68
10:a:426:ARG:HG3	10:a:429:ARG:HD2	1.76	0.68
10:a:618:LEU:HD13	16:i:78:ASN:HD22	1.57	0.68
10:a:406:MET:HB3	10:a:745:LEU:HB3	1.76	0.67
11:b:7:LEU:HD12	17:p:324:ILE:HD11	1.75	0.67
2:F:432:VAL:HG13	2:F:433:VAL:HG13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:HG11	2:E:62:TYR:HB2	1.75	0.67
16:h:32:TYR:CZ	16:h:36:LYS:HD3	2.29	0.67
16:l:23:MET:HG3	16:m:148:VAL:HG21	1.75	0.67
10:a:420:ALA:HB2	10:a:450:ILE:HG22	1.77	0.67
8:S:216:ILE:HG22	8:S:218:PRO:HD2	1.78	0.66
16:g:72:VAL:HG11	16:g:99:VAL:HG11	1.77	0.66
3:G:65:VAL:HG22	3:G:129:VAL:HG21	1.76	0.66
16:g:22:ALA:HB2	16:g:96:GLY:HA2	1.78	0.66
16:k:72:VAL:O	16:k:76:ILE:HG12	1.96	0.66
16:m:144:TYR:HA	16:m:147:ILE:HD12	1.78	0.66
2:D:158:ILE:HD11	2:D:336:GLU:HA	1.78	0.66
1:C:432:PHE:HE2	1:C:452:ILE:HG22	1.61	0.66
3:G:216:LEU:HD11	3:G:224:LEU:HD23	1.78	0.65
16:l:64:ILE:HA	16:l:67:ILE:HG12	1.78	0.65
16:j:44:MET:HG2	16:j:118:VAL:HG12	1.78	0.65
10:a:611:ILE:HD12	10:a:614:ILE:HD11	1.77	0.65
16:m:63:GLY:HA3	16:n:137:PHE:CZ	2.31	0.65
7:N:50:GLN:HA	7:N:53:LYS:HE2	1.79	0.65
14:e:13:MET:HB2	14:e:52:TRP:CH2	2.31	0.65
2:F:332:ALA:HA	2:F:342:ILE:HB	1.80	0.64
12:c:443:LEU:HA	12:c:446:ILE:HG22	1.79	0.64
16:m:70:LEU:HD22	16:n:144:TYR:CD1	2.30	0.64
5:I:137:ARG:NH1	5:I:140:ASP:OD2	2.30	0.64
16:k:124:GLN:HB3	16:k:127:LEU:HD13	1.77	0.64
16:h:45:SER:HB2	16:h:52:ILE:HD11	1.80	0.64
16:h:65:ILE:HD11	16:h:110:ILE:HG13	1.79	0.64
1:A:152:ILE:HD13	1:A:167:MET:HB3	1.80	0.64
10:a:90:PHE:O	10:a:92:ARG:N	2.31	0.64
10:a:310:CYS:SG	10:a:319:LEU:HD23	2.38	0.64
2:D:223:ILE:HB	2:D:251:VAL:HG22	1.78	0.63
2:F:374:ASP:HB2	2:F:387:ASN:HB2	1.80	0.63
2:F:142:GLU:OE2	5:K:212:ARG:NH2	2.31	0.63
2:D:42:ARG:HG3	2:D:105:THR:HG23	1.80	0.63
5:K:215:LEU:HD23	7:O:91:ASN:HB2	1.80	0.63
1:B:507:ILE:HD11	1:B:555:VAL:HG21	1.80	0.63
6:L:39:VAL:HG11	6:L:70:ILE:HG12	1.81	0.63
1:A:46:GLY:HA2	1:A:77:ASP:HB3	1.79	0.63
1:C:281:VAL:HG22	1:C:315:THR:HG21	1.81	0.63
3:G:123:GLU:HB3	3:G:127:LYS:NZ	2.13	0.63
1:A:156:VAL:HG12	1:A:164:HIS:HB3	1.79	0.63
16:l:72:VAL:HG21	16:l:149:ALA:HB1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:200:ALA:HB3	10:a:219:VAL:HB	1.81	0.63
14:e:19:PHE:HA	14:e:23:LEU:HD12	1.79	0.63
8:Q:158:VAL:HG23	8:Q:178:LEU:HD11	1.80	0.62
16:o:84:ILE:HD12	16:o:88:LYS:HE2	1.81	0.62
8:R:120:ASN:HB3	8:R:123:LYS:HZ2	1.64	0.62
1:C:239:PRO:HD2	1:C:458:MET:HE1	1.81	0.62
14:e:49:TYR:HD1	14:e:50:LEU:HD22	1.64	0.62
2:F:194:ASN:HD22	2:F:234:THR:HG23	1.64	0.62
10:a:127:GLU:HB3	10:a:174:VAL:HG21	1.80	0.62
11:b:94:ILE:HG13	16:g:134:ILE:HD12	1.82	0.62
9:T:239:LEU:HG	9:T:243:MET:HE1	1.82	0.62
16:g:20:SER:HB3	16:h:97:LEU:HD22	1.81	0.62
10:a:249:GLU:HG2	10:a:253:GLU:HB3	1.82	0.62
3:G:150:LEU:HD13	3:G:268:LEU:HB3	1.82	0.62
10:a:80:MET:HB2	10:a:82:THR:HG23	1.81	0.62
13:d:208:MET:HE3	13:d:208:MET:HA	1.81	0.62
13:d:73:ARG:NH2	13:d:76:GLU:OE1	2.33	0.61
1:C:264:SER:HA	1:C:272:ILE:HD13	1.82	0.61
8:S:218:PRO:HB2	8:S:221:ASP:HB3	1.80	0.61
16:n:51:LEU:O	16:n:55:SER:N	2.33	0.61
1:A:147:ILE:HD11	1:A:192:LEU:HD21	1.83	0.61
16:l:48:ARG:NH2	16:l:121:THR:O	2.33	0.61
1:B:549:ASP:O	1:B:553:ARG:HG2	2.01	0.61
2:F:411:ASP:HB2	2:F:489:ILE:HD12	1.81	0.61
16:j:86:LEU:HG	16:j:90:PHE:CE2	2.36	0.61
2:F:99:ILE:HG23	2:F:104:THR:HG21	1.81	0.61
5:J:145:LYS:O	5:J:149:GLN:NE2	2.33	0.61
1:A:291:PHE:HB3	1:A:305:ILE:HD11	1.82	0.61
2:E:332:ALA:HA	2:E:342:ILE:HB	1.83	0.61
8:S:49:TYR:CE2	8:S:88:LEU:HD23	2.36	0.61
1:B:247:ALA:HB2	1:B:429:VAL:HG21	1.81	0.61
2:F:432:VAL:HA	4:H:170:ASN:HB3	1.83	0.61
3:G:34:LEU:HB3	3:G:322:GLN:HB3	1.84	0.60
16:i:138:ALA:O	16:i:141:LEU:HB2	2.01	0.60
1:C:161:LEU:HD13	1:C:308:ARG:HB3	1.83	0.60
9:T:199:GLN:HA	9:T:239:LEU:HD13	1.81	0.60
11:b:196:LEU:O	11:b:200:ARG:NH2	2.34	0.60
13:d:2:SER:N	13:d:8:TYR:OH	2.35	0.60
5:K:35:GLU:HA	7:O:32:ARG:HG3	1.83	0.60
16:m:88:LYS:O	16:m:92:GLN:HG2	2.01	0.60
1:C:161:LEU:HD12	1:C:307:LYS:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:40:GLU:OE1	13:d:341:ARG:NH2	2.35	0.60
16:j:61:MET:HE1	16:j:110:ILE:CG2	2.30	0.60
16:l:42:ALA:HA	16:m:127:LEU:HD11	1.84	0.60
5:J:12:ILE:HG22	5:J:16:MET:HE1	1.84	0.60
5:K:54:MET:SD	7:O:47:TYR:OH	2.59	0.60
7:O:93:ASP:OD1	7:O:94:GLU:N	2.35	0.60
11:b:182:PHE:HE2	16:o:60:VAL:HG23	1.67	0.60
11:b:189:PHE:HB3	16:o:70:LEU:HD21	1.84	0.60
16:g:27:ALA:HA	16:h:141:LEU:HD11	1.84	0.60
16:g:143:LEU:O	16:g:147:ILE:HD12	2.01	0.60
8:S:211:SER:HB2	8:S:214:GLU:HB3	1.83	0.59
2:E:235:ALA:HB1	2:E:255:LEU:HD21	1.84	0.59
16:g:19:ALA:HB2	16:g:76:ILE:HG21	1.85	0.59
5:I:32:ALA:O	9:T:210:ARG:NH1	2.36	0.59
5:K:113:GLN:NE2	5:K:117:ASP:OD1	2.36	0.59
11:b:34:ARG:NH1	12:c:418:ALA:O	2.35	0.59
2:D:53:VAL:HG22	2:D:89:ILE:HD13	1.85	0.59
2:E:294:MET:HE3	2:E:329:TYR:HE1	1.68	0.59
1:B:127:LEU:HD12	1:B:206:VAL:HG22	1.83	0.59
9:T:290:ARG:NH2	9:T:294:GLU:OE1	2.35	0.59
11:b:96:PHE:O	11:b:99:ALA:HB3	2.02	0.59
2:E:284:GLU:OE1	2:E:339:GLY:N	2.35	0.59
16:l:23:MET:HE3	16:l:73:ALA:HB3	1.85	0.59
8:Q:103:MET:SD	8:Q:164:ALA:HA	2.42	0.59
10:a:72:ILE:HD13	10:a:283:LEU:HD22	1.85	0.58
10:a:590:LEU:HD12	10:a:613:PHE:HE1	1.66	0.58
16:k:49:PRO:HB2	16:l:126:ARG:HD3	1.85	0.58
2:F:430:LYS:HB2	2:F:438:LEU:HD11	1.86	0.58
12:c:371:GLU:HB2	17:p:301:ASN:HA	1.85	0.58
16:m:63:GLY:HA3	16:n:137:PHE:HZ	1.68	0.58
1:B:548:TYR:OH	1:B:552:ARG:NH2	2.37	0.58
2:E:432:VAL:HG13	2:E:433:VAL:HG13	1.85	0.58
8:S:148:LYS:NZ	8:S:188:MET:O	2.35	0.58
10:a:479:TRP:CD1	10:a:522:ILE:HG21	2.38	0.58
1:A:166:ILE:HD13	1:A:205:MET:HG2	1.85	0.58
9:T:353:ASP:OD1	9:T:354:GLU:N	2.36	0.58
14:e:43:THR:HA	14:e:46:VAL:HG12	1.84	0.58
10:a:543:ILE:HG22	10:a:588:VAL:HG22	1.85	0.58
16:k:85:SER:H	16:k:88:LYS:HZ1	1.50	0.58
9:T:298:GLU:H	9:T:302:ARG:HH11	1.51	0.58
2:E:432:VAL:HG21	4:H:36:LYS:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:40:PHE:HE1	12:c:430:LEU:HD11	1.68	0.58
1:A:169:PRO:HG3	1:A:207:GLN:HG2	1.86	0.58
16:h:61:MET:HE3	16:h:110:ILE:HD12	1.85	0.58
3:G:29:ASN:HD22	3:G:33:ALA:HB2	1.69	0.57
13:d:281:ALA:HB1	13:d:290:LEU:HA	1.85	0.57
16:l:21:ALA:HA	16:l:24:VAL:HG22	1.86	0.57
1:B:295:THR:HG22	1:B:304:SER:HA	1.85	0.57
10:a:254:ARG:HA	10:a:257:MET:HE2	1.85	0.57
2:D:169:SER:HB2	2:D:465:ARG:HD2	1.86	0.57
2:E:382:ILE:HG23	2:E:458:ASN:HB2	1.85	0.57
16:k:66:ALA:O	16:k:70:LEU:HD23	2.05	0.57
16:k:76:ILE:HA	16:k:92:GLN:NE2	2.20	0.57
5:K:51:LEU:O	5:K:54:MET:HB2	2.05	0.57
8:Q:127:HIS:CD2	8:Q:131:ASN:HD21	2.22	0.57
8:S:79:ASP:OD1	8:S:80:ALA:N	2.37	0.57
1:A:117:TYR:CD1	2:D:150:GLN:HB3	2.39	0.57
16:g:137:PHE:O	16:g:140:VAL:HG22	2.05	0.57
16:k:23:MET:HE1	16:k:70:LEU:HD13	1.86	0.57
16:l:140:VAL:HG12	16:l:144:TYR:CE1	2.40	0.57
1:B:105:PRO:HD3	1:B:126:ALA:HA	1.85	0.57
16:k:11:ALA:HA	16:k:86:LEU:HD13	1.86	0.57
1:C:24:VAL:HG13	1:C:29:VAL:HG22	1.86	0.57
2:D:227:ALA:HB3	2:D:255:LEU:HA	1.87	0.57
5:K:49:GLN:HB2	7:O:44:ILE:HG12	1.86	0.57
7:N:13:GLN:HA	7:N:16:LYS:HG2	1.84	0.57
14:e:9:PRO:HA	14:e:12:VAL:HG12	1.87	0.57
16:g:16:VAL:HG22	16:h:94:GLY:HA3	1.87	0.57
16:n:114:GLY:O	16:n:118:VAL:HG23	2.03	0.57
8:R:127:HIS:CD2	8:R:131:ASN:HD21	2.22	0.57
10:a:63:ARG:HA	10:a:66:ARG:HG2	1.86	0.57
10:a:100:ASN:HA	10:a:103:LYS:NZ	2.20	0.57
10:a:440:PHE:HA	10:a:443:VAL:HG22	1.87	0.57
16:o:17:MET:HA	16:o:17:MET:HE3	1.87	0.57
4:H:31:ASN:HA	4:H:34:LYS:HZ3	1.68	0.57
4:H:43:ARG:HG2	4:H:101:VAL:HG21	1.87	0.57
10:a:60:GLU:O	10:a:63:ARG:HG3	2.04	0.57
10:a:424:VAL:HG21	10:a:451:LEU:HD11	1.86	0.56
13:d:304:LEU:HA	13:d:307:LEU:HD23	1.86	0.56
2:E:70:LEU:HD11	2:E:76:ARG:HE	1.70	0.56
13:d:2:SER:N	13:d:8:TYR:HH	2.02	0.56
1:B:479:ALA:HB2	1:B:545:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:72:ASP:OD1	13:d:75:LYS:NZ	2.38	0.56
13:d:203:THR:HG22	13:d:311:HIS:HB3	1.87	0.56
16:g:17:MET:SD	16:g:93:LEU:HD13	2.46	0.56
16:j:61:MET:HE1	16:j:110:ILE:HG22	1.86	0.56
16:m:44:MET:HG2	16:m:122:ALA:HB2	1.86	0.56
2:E:128:GLY:HA3	2:E:256:ASN:HD22	1.71	0.56
2:E:362:LEU:O	2:E:366:ILE:HG13	2.06	0.56
1:B:24:VAL:HG23	1:B:29:VAL:HG12	1.88	0.56
11:b:173:PHE:O	11:b:177:LEU:HD23	2.06	0.56
16:l:44:MET:HE1	16:l:119:ARG:HA	1.88	0.56
16:h:23:MET:HE1	16:i:144:TYR:HB3	1.87	0.55
1:B:281:VAL:HG23	1:B:315:THR:HG21	1.88	0.55
1:C:46:GLY:HA2	1:C:77:ASP:HB3	1.88	0.55
16:o:143:LEU:O	16:o:147:ILE:HD12	2.06	0.55
5:J:54:MET:HE3	5:J:54:MET:HA	1.87	0.55
8:Q:104:LYS:HE2	8:Q:107:LEU:HB2	1.87	0.55
1:C:540:MET:HE1	1:C:585:LYS:HA	1.88	0.55
9:T:47:CYS:HA	9:T:50:ILE:HB	1.89	0.55
10:a:331:ASP:OD1	10:a:332:SER:N	2.40	0.55
2:E:429:MET:HE3	2:E:429:MET:HA	1.88	0.55
16:o:149:ALA:O	16:o:153:SER:N	2.37	0.55
2:F:137:PRO:HG3	5:K:84:LEU:HB3	1.89	0.55
2:F:223:ILE:HB	2:F:251:VAL:HG22	1.89	0.55
8:S:23:VAL:HG22	8:S:65:ILE:HG22	1.89	0.55
11:b:176:ILE:O	11:b:179:VAL:HG22	2.06	0.55
12:c:340:THR:HG23	12:c:361:THR:HG22	1.88	0.55
14:e:28:ILE:HD12	14:e:29:PRO:HD2	1.89	0.55
16:j:44:MET:HG2	16:j:118:VAL:CG1	2.36	0.55
10:a:484:MET:HE1	10:a:508:LEU:HB2	1.88	0.55
3:G:7:ILE:HA	3:G:370:VAL:O	2.07	0.55
16:h:30:ALA:O	16:h:34:THR:HG23	2.07	0.55
16:k:85:SER:H	16:k:88:LYS:NZ	2.04	0.55
1:C:88:VAL:HG23	1:C:211:VAL:HG12	1.89	0.54
2:D:71:PRO:HG3	2:D:103:LYS:HB2	1.89	0.54
2:E:34:ILE:HG13	2:E:35:THR:H	1.72	0.54
10:a:111:ILE:HG21	10:a:279:ARG:HB2	1.88	0.54
16:l:70:LEU:HG	16:m:144:TYR:HD2	1.71	0.54
1:A:366:ALA:HB1	4:H:209:LYS:HD3	1.88	0.54
9:T:453:LEU:HD12	9:T:457:GLN:HE22	1.71	0.54
2:E:249:GLY:HA2	5:J:80:ARG:HH22	1.72	0.54
5:K:60:LYS:HB3	7:O:55:PHE:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:d:154:ILE:HA	13:d:158:THR:HG23	1.89	0.54
16:o:22:ALA:HB2	16:o:96:GLY:HA2	1.88	0.54
3:G:6:LEU:HB3	3:G:372:TYR:HB2	1.88	0.54
13:d:21:ARG:NH1	13:d:308:ASN:O	2.39	0.54
1:B:190:VAL:HG11	1:B:202:LYS:HD2	1.88	0.54
1:B:273:ILE:HD13	1:B:333:LEU:HB3	1.89	0.54
2:D:189:ALA:O	2:D:375:ARG:NH1	2.39	0.54
5:J:53:ILE:HD11	7:N:47:TYR:HD2	1.73	0.54
16:n:117:GLY:HA3	16:n:131:MET:HG3	1.90	0.54
8:Q:111:GLN:O	8:Q:115:MET:HG3	2.06	0.54
8:Q:126:TYR:HE2	8:Q:169:THR:HG23	1.73	0.54
16:k:18:GLY:HA3	16:k:93:LEU:HA	1.89	0.54
5:I:131:ARG:HH12	5:I:166:GLN:HB2	1.73	0.54
8:Q:50:GLN:HA	8:Q:53:LEU:HB2	1.89	0.54
16:k:15:ALA:HB2	16:k:89:SER:HA	1.89	0.54
16:n:80:LEU:HD22	16:o:91:LEU:HD21	1.89	0.54
1:C:228:LEU:N	1:C:268:ASN:OD1	2.41	0.54
6:L:74:VAL:HG22	6:L:77:ALA:HB3	1.90	0.54
10:a:830:HIS:HB2	10:a:833:GLU:HB2	1.90	0.54
16:h:44:MET:HG2	16:h:122:ALA:HB2	1.90	0.54
1:B:489:LEU:HA	1:B:492:ILE:HD13	1.89	0.54
10:a:18:GLN:O	10:a:22:ALA:N	2.41	0.54
16:j:49:PRO:HB2	16:k:126:ARG:NH2	2.23	0.54
1:A:37:ALA:HB1	1:A:54:ILE:HD13	1.89	0.53
5:K:208:MET:HE3	5:K:208:MET:HA	1.90	0.53
10:a:128:LEU:HD13	10:a:131:ILE:HD12	1.90	0.53
11:b:18:CYS:HA	11:b:21:VAL:HG22	1.89	0.53
16:g:73:ALA:HA	16:g:76:ILE:HD12	1.89	0.53
1:A:272:ILE:HD11	1:A:308:ARG:HH11	1.73	0.53
1:C:56:ARG:NH1	1:C:367:GLU:OE2	2.41	0.53
2:D:228:MET:HE1	2:D:269:PRO:HB3	1.89	0.53
11:b:91:LEU:HD22	16:g:134:ILE:HD11	1.90	0.53
1:C:488:ASP:OD1	1:C:489:LEU:N	2.42	0.53
2:F:479:ARG:NH2	2:F:498:TYR:O	2.42	0.53
9:T:347:GLN:OE1	9:T:374:LYS:NZ	2.42	0.53
11:b:114:MET:SD	11:b:201:VAL:HG12	2.49	0.53
13:d:213:GLU:HG2	13:d:245:GLY:HA2	1.91	0.53
13:d:254:GLN:CD	13:d:267:VAL:HG22	2.34	0.53
16:j:61:MET:HE3	16:j:135:LEU:HG	1.90	0.53
16:k:70:LEU:HD11	16:l:144:TYR:HB3	1.89	0.53
1:B:559:ALA:HA	1:B:564:LYS:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:41:MET:SD	9:T:84:ILE:HG12	2.48	0.53
3:G:8:SER:HB2	3:G:370:VAL:HB	1.90	0.53
10:a:54:GLU:HA	10:a:57:ARG:HE	1.74	0.53
2:E:348:LEU:HD11	2:E:359:ILE:HG22	1.91	0.53
7:M:85:GLN:O	7:M:89:ARG:HG2	2.09	0.53
13:d:72:ASP:HA	13:d:75:LYS:HZ2	1.73	0.53
2:D:396:MET:N	2:D:396:MET:HE2	2.24	0.53
16:i:16:VAL:HG12	16:j:94:GLY:HA3	1.90	0.53
3:G:321:LEU:HD21	3:G:331:LEU:HD13	1.90	0.53
4:H:137:ASN:HA	4:H:140:LYS:HE2	1.91	0.53
13:d:187:LYS:O	13:d:191:GLU:HG2	2.09	0.53
14:e:25:PRO:HB3	14:e:38:ILE:HG23	1.90	0.53
16:l:109:ALA:O	16:l:113:VAL:HG22	2.09	0.53
1:C:164:HIS:CD2	1:C:340:MET:HE1	2.44	0.53
2:E:34:ILE:HG13	2:E:35:THR:N	2.24	0.53
10:a:593:TYR:O	10:a:597:ALA:CB	2.57	0.53
16:h:28:LEU:HD22	16:i:105:ALA:HB2	1.90	0.53
5:J:46:VAL:HA	7:N:44:ILE:HD11	1.91	0.52
11:b:78:GLY:HA3	13:d:18:GLY:HA3	1.90	0.52
16:k:25:PHE:HA	16:k:28:LEU:HD12	1.91	0.52
16:l:80:LEU:HD23	16:l:92:GLN:HE22	1.74	0.52
1:A:471:GLU:CD	1:A:471:GLU:H	2.18	0.52
2:D:54:LEU:HD21	2:D:106:CYS:SG	2.49	0.52
7:O:41:GLN:HA	7:O:44:ILE:HD12	1.91	0.52
11:b:133:ALA:HA	11:b:201:VAL:HG13	1.91	0.52
1:A:296:MET:HE1	1:A:305:ILE:HA	1.91	0.52
1:B:574:MET:HB2	1:B:577:ILE:HB	1.92	0.52
2:F:80:VAL:HG13	2:F:90:VAL:HG22	1.92	0.52
7:M:79:GLU:O	7:M:83:ILE:HD12	2.09	0.52
7:M:83:ILE:O	7:M:86:THR:HG22	2.10	0.52
7:O:92:ARG:HG2	7:O:96:LEU:HD23	1.92	0.52
10:a:806:LEU:O	10:a:810:GLU:HG2	2.08	0.52
15:f:72:ALA:HA	15:f:75:LEU:HD12	1.91	0.52
1:B:161:LEU:HD21	1:B:298:VAL:HG21	1.90	0.52
1:B:178:TYR:HD1	1:B:193:GLU:HG3	1.75	0.52
3:G:209:VAL:HA	5:K:12:ILE:HD11	1.92	0.52
10:a:539:LYS:HE2	10:a:609:LEU:HD12	1.91	0.52
1:A:129:ARG:O	1:A:186:ASP:HB2	2.09	0.52
1:B:256:LYS:O	1:B:259:ILE:HG22	2.09	0.52
8:R:216:ILE:HG22	8:R:217:LEU:HD23	1.92	0.52
9:T:212:ASN:OD1	9:T:215:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:384:GLY:HA2	10:a:818:GLY:HA2	1.90	0.52
13:d:72:ASP:HA	13:d:75:LYS:NZ	2.25	0.52
1:B:317:ASN:HD22	2:E:330:GLU:HB3	1.74	0.52
1:C:243:GLY:N	1:C:405:THR:OG1	2.41	0.52
10:a:231:ASN:HA	10:a:234:LYS:HE2	1.92	0.52
11:b:182:PHE:CE2	16:o:60:VAL:HG23	2.45	0.52
1:B:305:ILE:HG12	1:B:309:THR:HG23	1.92	0.52
8:S:55:TRP:HB3	8:S:65:ILE:HD12	1.92	0.52
10:a:100:ASN:HA	10:a:103:LYS:HZ3	1.74	0.52
3:G:343:ASP:HB2	3:G:346:ALA:HB3	1.92	0.52
8:Q:129:LYS:HE3	8:Q:168:ILE:HG13	1.91	0.52
16:l:141:LEU:HA	16:l:144:TYR:HD1	1.75	0.52
16:o:72:VAL:HG21	16:o:99:VAL:HG11	1.91	0.52
1:B:540:MET:HB2	1:B:584:MET:HE3	1.91	0.52
1:C:34:MET:HE1	1:C:81:ARG:HB2	1.91	0.52
2:F:188:ALA:H	2:F:191:LEU:HD12	1.74	0.52
5:K:68:LYS:HD3	7:O:62:ALA:HB1	1.92	0.52
5:K:205:GLN:N	5:K:205:GLN:OE1	2.39	0.52
8:Q:68:ALA:O	8:Q:72:GLY:N	2.42	0.52
8:S:10:MET:N	8:S:10:MET:HE2	2.25	0.52
16:h:138:ALA:O	16:h:141:LEU:HB3	2.09	0.52
1:C:479:ALA:HB2	1:C:541:LEU:HD11	1.92	0.52
2:E:459:GLN:NE2	2:E:463:GLU:O	2.42	0.52
5:K:48:THR:O	5:K:51:LEU:HG	2.10	0.52
7:N:88:PHE:O	7:N:92:ARG:HG3	2.10	0.52
11:b:105:ILE:HD11	16:g:144:TYR:CG	2.45	0.52
16:j:10:TYR:O	16:j:13:PHE:HB3	2.10	0.52
1:B:132:LYS:HD3	1:B:186:ASP:HB3	1.93	0.51
1:B:510:GLU:HG3	1:B:567:TRP:CE2	2.45	0.51
9:T:209:LEU:HD22	9:T:215:ARG:HA	1.92	0.51
16:o:18:GLY:HA3	16:o:93:LEU:HA	1.92	0.51
1:A:111:SER:O	1:A:114:GLN:NE2	2.41	0.51
1:A:137:PRO:HD2	1:A:182:PRO:HG3	1.91	0.51
1:A:511:VAL:HG11	1:A:548:TYR:HB2	1.91	0.51
2:D:168:ILE:HG22	2:D:170:PRO:HD2	1.92	0.51
2:D:181:GLN:NE2	2:D:393:SER:OG	2.40	0.51
1:B:272:ILE:HB	1:B:309:THR:HG22	1.91	0.51
10:a:45:ASN:OD1	10:a:46:VAL:N	2.44	0.51
1:A:397:ASN:HD22	8:Q:31:ARG:HH22	1.58	0.51
1:B:255:GLY:O	1:B:258:VAL:HG22	2.10	0.51
3:G:161:LEU:HG	3:G:219:ASP:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:194:ASP:OD1	8:S:194:ASP:N	2.42	0.51
10:a:175:ILE:H	10:a:219:VAL:HG22	1.76	0.51
10:a:202:ILE:HD12	10:a:217:LYS:HB2	1.92	0.51
2:F:325:LEU:HD13	2:F:328:ILE:HD11	1.91	0.51
5:J:52:LYS:O	5:J:55:GLU:HG3	2.11	0.51
10:a:180:ILE:HD11	10:a:218:SER:O	2.10	0.51
16:j:42:ALA:O	16:j:46:VAL:HG23	2.10	0.51
1:A:17:THR:HA	1:A:81:ARG:HE	1.75	0.51
1:B:239:PRO:HD2	1:B:455:SER:HB3	1.92	0.51
1:C:426:LEU:HD11	1:C:432:PHE:CG	2.45	0.51
5:J:24:ASN:HA	7:N:21:LYS:HZ3	1.75	0.51
16:g:24:VAL:HG22	16:h:101:LEU:HB2	1.92	0.51
16:o:143:LEU:O	16:o:146:LEU:HB3	2.11	0.51
2:E:168:ILE:HG13	2:E:170:PRO:HD2	1.91	0.51
9:T:327:ASP:OD2	10:a:316:GLN:NE2	2.37	0.51
9:T:424:GLY:O	9:T:427:VAL:HB	2.10	0.51
13:d:24:LYS:HD3	13:d:306:PHE:CD1	2.46	0.51
16:i:72:VAL:HG11	16:i:99:VAL:HG11	1.91	0.51
16:n:99:VAL:HB	16:n:149:ALA:HB2	1.93	0.51
1:A:34:MET:HA	1:A:34:MET:HE2	1.92	0.51
1:A:295:THR:HG22	1:A:304:SER:HA	1.92	0.51
4:H:27:GLN:HA	4:H:30:ARG:HG2	1.92	0.51
5:I:139:GLN:OE1	5:I:139:GLN:N	2.33	0.51
11:b:40:PHE:CE1	12:c:430:LEU:HD11	2.46	0.51
16:m:149:ALA:O	16:m:153:SER:N	2.44	0.51
1:A:178:TYR:HB3	1:A:193:GLU:HB2	1.93	0.51
1:C:493:VAL:HG22	1:C:501:LEU:HD11	1.93	0.51
2:D:55:ASP:OD1	2:D:56:HIS:N	2.43	0.51
2:E:276:ALA:HB1	2:E:342:ILE:HD12	1.93	0.51
10:a:120:ARG:NH1	10:a:209:PRO:O	2.39	0.51
11:b:90:ASN:OD1	11:b:163:ALA:HA	2.11	0.51
11:b:92:VAL:HA	11:b:95:ILE:HD12	1.93	0.51
13:d:54:TYR:O	13:d:77:LYS:NZ	2.43	0.51
1:B:465:TYR:O	1:B:469:PHE:N	2.41	0.51
7:O:94:GLU:HA	7:O:97:ASP:OD2	2.10	0.51
2:E:269:PRO:HB2	2:E:328:ILE:HD12	1.92	0.50
3:G:205:ALA:HB2	3:G:237:PHE:HB2	1.93	0.50
8:Q:158:VAL:HG12	8:Q:216:ILE:HD13	1.93	0.50
12:c:306:ALA:H	12:c:327:ALA:HB3	1.76	0.50
1:A:113:THR:HG22	1:A:115:SER:HB3	1.93	0.50
2:F:262:THR:O	2:F:265:ARG:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:58:GLU:HG3	5:K:61:GLU:OE1	2.11	0.50
16:m:120:GLY:HA3	16:m:127:LEU:HD13	1.93	0.50
1:A:489:LEU:HD13	1:A:509:LEU:HG	1.93	0.50
1:B:314:ASN:HA	1:B:318:MET:HE3	1.93	0.50
2:D:163:MET:HE2	2:D:176:SER:CB	2.41	0.50
10:a:79:ILE:HD11	10:a:291:ARG:HB2	1.92	0.50
11:b:108:ALA:HB1	16:g:148:VAL:HG21	1.93	0.50
16:n:128:PHE:CE1	16:n:132:ILE:HD11	2.46	0.50
1:A:147:ILE:HG13	1:A:194:LEU:HD21	1.92	0.50
1:A:290:ASP:OD1	1:A:291:PHE:N	2.44	0.50
1:B:272:ILE:O	1:B:309:THR:HA	2.11	0.50
5:J:49:GLN:O	5:J:52:LYS:HG3	2.10	0.50
10:a:128:LEU:HA	10:a:131:ILE:HD12	1.93	0.50
16:g:60:VAL:O	16:g:64:ILE:HD12	2.12	0.50
16:l:141:LEU:HA	16:l:144:TYR:CD1	2.46	0.50
1:B:44:ARG:NH2	1:B:51:VAL:HG22	2.27	0.50
1:C:455:SER:HB3	1:C:458:MET:HE3	1.94	0.50
1:B:270:ASP:HB2	1:B:342:TYR:HB3	1.94	0.50
1:B:438:LYS:HG3	1:B:442:ARG:HH11	1.77	0.50
1:C:535:TYR:CE2	1:C:594:GLU:HG3	2.47	0.50
10:a:171:VAL:HG21	10:a:248:PRO:HB3	1.94	0.50
10:a:615:ASN:OD1	16:i:78:ASN:ND2	2.44	0.50
13:d:16:LEU:HB3	13:d:315:PHE:HZ	1.76	0.50
16:g:24:VAL:HG11	16:h:101:LEU:HD12	1.93	0.50
16:h:141:LEU:HA	16:h:144:TYR:CD2	2.47	0.50
16:n:137:PHE:O	16:n:140:VAL:HG12	2.11	0.50
5:K:53:ILE:HG22	7:O:51:ARG:HD3	1.93	0.50
8:S:192:LYS:HG2	8:S:195:GLU:OE1	2.11	0.50
15:f:84:PHE:HA	15:f:87:VAL:HG22	1.94	0.50
9:T:210:ARG:HD3	9:T:211:VAL:HG23	1.92	0.50
11:b:175:LYS:NZ	16:o:52:ILE:HD12	2.27	0.50
1:C:348:ALA:HB3	1:C:408:GLY:HA2	1.93	0.50
1:C:483:LEU:O	1:C:486:GLU:HG3	2.12	0.50
2:F:187:SER:O	2:F:349:THR:HA	2.12	0.50
7:O:71:THR:HB	7:O:75:LYS:NZ	2.27	0.50
9:T:103:GLU:CD	9:T:105:HIS:HB2	2.37	0.50
10:a:18:GLN:HG3	10:a:348:VAL:HB	1.93	0.50
16:k:70:LEU:HD21	16:l:144:TYR:CB	2.42	0.50
10:a:125:LEU:HD22	10:a:261:VAL:HG13	1.93	0.49
10:a:607:PRO:HG3	10:a:627:SER:HB2	1.93	0.49
16:l:16:VAL:HG12	16:m:94:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:280:ALA:O	2:D:340:GLY:HA3	2.12	0.49
5:K:60:LYS:HB3	7:O:55:PHE:CZ	2.47	0.49
16:l:59:VAL:HG21	16:m:134:ILE:HG22	1.94	0.49
1:C:195:GLU:OE2	1:C:198:GLY:N	2.44	0.49
9:T:203:GLY:O	9:T:206:GLN:HG2	2.11	0.49
13:d:325:GLU:O	13:d:329:ILE:HD12	2.12	0.49
1:B:72:GLY:HA2	2:E:112:ILE:HD11	1.94	0.49
1:C:297:GLU:OE2	1:C:300:GLY:N	2.45	0.49
2:F:91:GLN:CD	2:F:263:ILE:HG21	2.38	0.49
7:O:69:CYS:O	7:O:73:VAL:HG23	2.13	0.49
13:d:303:LYS:HD3	13:d:351:PHE:H	1.78	0.49
1:B:511:VAL:HG21	1:B:548:TYR:HB2	1.95	0.49
2:F:174:MET:HE1	2:F:452:PHE:CZ	2.44	0.49
8:Q:100:PRO:HG2	8:Q:101:PHE:CD2	2.47	0.49
8:R:120:ASN:HB3	8:R:123:LYS:NZ	2.28	0.49
1:A:493:VAL:O	1:A:497:GLY:N	2.36	0.49
2:D:312:PRO:HG3	4:H:201:ARG:HB3	1.94	0.49
2:E:327:THR:O	2:E:331:ARG:HG3	2.13	0.49
2:F:82:GLU:HB3	2:F:89:ILE:HB	1.95	0.49
6:L:67:ASN:HB3	6:L:70:ILE:HD12	1.94	0.49
7:M:93:ASP:OD1	7:M:94:GLU:N	2.46	0.49
13:d:50:GLN:NE2	13:d:56:ASN:OD1	2.42	0.49
13:d:211:ILE:HD11	13:d:305:ALA:HB2	1.93	0.49
16:h:24:VAL:HG23	16:h:25:PHE:CD1	2.48	0.49
2:D:294:MET:HB2	2:D:348:LEU:HG	1.94	0.49
2:F:76:ARG:HD3	2:F:94:GLU:HB2	1.94	0.49
11:b:200:ARG:HD3	11:b:200:ARG:H	1.78	0.49
12:c:346:ILE:HD11	12:c:394:LEU:HD21	1.94	0.49
16:h:60:VAL:HG12	16:i:137:PHE:CZ	2.47	0.49
16:l:70:LEU:HG	16:m:144:TYR:CD2	2.48	0.49
8:Q:161:MET:HG3	8:Q:216:ILE:HG12	1.93	0.49
16:g:13:PHE:O	16:g:16:VAL:HG12	2.12	0.49
1:B:49:GLU:OE1	1:B:123:ASN:ND2	2.45	0.49
1:B:519:PHE:HB2	1:B:544:MET:HE1	1.95	0.49
1:C:471:GLU:O	1:C:475:LEU:HG	2.12	0.49
3:G:28:LYS:HB3	3:G:331:LEU:HD22	1.95	0.49
10:a:53:ASN:HA	10:a:56:ARG:HE	1.78	0.49
8:S:94:LEU:HA	8:S:130:LEU:HD21	1.95	0.49
12:c:421:PHE:HB3	12:c:426:TRP:NE1	2.27	0.49
16:i:72:VAL:HG21	16:i:99:VAL:HG21	1.95	0.49
1:C:247:ALA:HB2	1:C:429:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:429:MET:O	2:F:433:VAL:HG22	2.13	0.48
6:L:67:ASN:HB3	6:L:70:ILE:CD1	2.43	0.48
16:g:140:VAL:HA	16:g:143:LEU:HB3	1.93	0.48
1:B:296:MET:HE1	1:B:305:ILE:HG13	1.95	0.48
2:E:438:LEU:HB3	2:E:442:ASP:HB2	1.95	0.48
9:T:379:ASN:O	9:T:383:LEU:HG	2.12	0.48
16:k:21:ALA:HA	16:k:24:VAL:HG22	1.93	0.48
1:C:77:ASP:OD1	7:O:113:ASN:ND2	2.43	0.48
10:a:584:PHE:CZ	10:a:732:CYS:HB3	2.49	0.48
11:b:126:ILE:O	11:b:130:ASN:ND2	2.47	0.48
13:d:191:GLU:HA	13:d:244:CYS:SG	2.54	0.48
17:p:325:THR:O	17:p:329:ILE:HG22	2.13	0.48
1:A:327:ILE:HD12	1:A:327:ILE:H	1.77	0.48
1:B:400:ARG:H	1:B:400:ARG:HD3	1.79	0.48
8:S:26:ILE:HG12	8:S:52:VAL:HG23	1.95	0.48
10:a:202:ILE:HB	10:a:217:LYS:HB2	1.95	0.48
2:D:429:MET:HA	2:D:429:MET:HE2	1.96	0.48
8:Q:33:MET:HE1	8:Q:45:ILE:HG22	1.95	0.48
16:i:25:PHE:HD1	16:i:104:LEU:HD22	1.79	0.48
16:j:13:PHE:HB2	16:k:90:PHE:CE2	2.47	0.48
1:B:54:ILE:HG12	1:B:64:ILE:HG13	1.95	0.48
2:E:289:VAL:HB	2:E:344:GLN:HG2	1.96	0.48
3:G:187:VAL:HG13	3:G:248:VAL:HG22	1.96	0.48
5:K:131:ARG:HD3	5:K:164:ASP:HB3	1.95	0.48
16:h:61:MET:HE3	16:h:110:ILE:CD1	2.43	0.48
16:n:95:ALA:O	16:n:99:VAL:HG12	2.14	0.48
1:C:443:LYS:HB3	2:F:488:ARG:HH22	1.79	0.48
2:D:318:PRO:HD2	2:D:321:MET:HE2	1.95	0.48
9:T:105:HIS:O	9:T:109:SER:N	2.46	0.48
10:a:650:TRP:HA	10:a:654:ILE:HG13	1.96	0.48
13:d:116:THR:HG23	13:d:122:ILE:HD11	1.96	0.48
16:g:72:VAL:O	16:g:76:ILE:HG13	2.13	0.48
1:B:165:ARG:H	1:B:340:MET:HE3	1.78	0.48
1:B:277:CYS:O	1:B:314:ASN:HB3	2.14	0.48
2:D:322:TYR:HD1	2:D:362:LEU:HD22	1.79	0.48
3:G:85:ASP:OD1	3:G:86:LYS:HG2	2.13	0.48
4:H:49:LYS:HB3	4:H:49:LYS:HE3	1.47	0.48
16:o:95:ALA:O	16:o:99:VAL:HG12	2.13	0.48
1:A:512:ALA:HA	1:A:515:ILE:HG22	1.95	0.48
2:D:157:ARG:NH1	2:D:332:ALA:O	2.37	0.48
2:D:186:PHE:O	2:D:373:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:GLN:HA	5:I:224:PHE:HD2	1.79	0.48
1:B:94:ILE:HG23	1:B:127:LEU:HD21	1.95	0.48
2:D:383:TYR:CD1	2:D:383:TYR:C	2.92	0.48
2:F:322:TYR:HE1	2:F:365:PHE:HB2	1.78	0.48
5:J:148:VAL:O	5:J:152:ILE:HG12	2.14	0.48
7:M:107:ARG:HA	7:M:107:ARG:HD3	1.67	0.48
1:A:490:ALA:HA	1:A:493:VAL:HG12	1.96	0.47
2:E:256:ASN:ND2	2:E:264:GLU:HB3	2.27	0.47
3:G:29:ASN:HB3	3:G:32:LEU:HB2	1.96	0.47
11:b:136:SER:HA	16:o:16:VAL:HG21	1.96	0.47
16:i:69:GLY:O	16:i:73:ALA:N	2.37	0.47
2:E:100:ASP:OD2	2:E:103:LYS:NZ	2.35	0.47
4:H:12:SER:H	4:H:15:ALA:HB3	1.79	0.47
10:a:618:LEU:HD23	10:a:618:LEU:O	2.14	0.47
4:H:57:LEU:HA	4:H:60:GLU:HG3	1.96	0.47
5:I:122:GLN:HB3	5:I:194:ASN:HD21	1.79	0.47
13:d:40:GLU:HA	13:d:341:ARG:HH22	1.79	0.47
16:i:27:ALA:HA	16:j:141:LEU:HD11	1.96	0.47
17:p:320:LEU:O	17:p:324:ILE:HG12	2.14	0.47
1:A:504:THR:HA	1:A:507:ILE:HD12	1.96	0.47
2:F:196:ILE:HD11	2:F:385:PRO:HD2	1.95	0.47
10:a:291:ARG:O	10:a:295:ILE:HG12	2.13	0.47
16:m:95:ALA:HB2	16:m:152:LEU:HB2	1.96	0.47
16:o:54:LYS:O	16:o:57:ILE:HG12	2.14	0.47
1:B:325:ALA:HA	1:B:328:TYR:HD2	1.79	0.47
2:E:115:THR:HG22	2:E:147:ILE:HG12	1.97	0.47
2:E:266:ILE:HG13	2:E:304:VAL:HG21	1.96	0.47
10:a:756:LEU:HD22	10:a:791:LEU:HD13	1.95	0.47
12:c:427:MET:HB3	16:g:14:PHE:CZ	2.50	0.47
16:n:44:MET:CE	16:n:119:ARG:HD2	2.45	0.47
4:H:30:ARG:HB3	4:H:172:ILE:HG21	1.96	0.47
11:b:189:PHE:CG	16:o:70:LEU:HD21	2.49	0.47
1:A:277:CYS:SG	1:A:323:ARG:HG3	2.55	0.47
1:C:172:ASN:C	1:C:173:ARG:HD3	2.40	0.47
2:E:64:GLU:O	2:E:80:VAL:HG23	2.15	0.47
2:F:64:GLU:CD	2:F:110:GLY:H	2.23	0.47
3:G:123:GLU:HB3	3:G:127:LYS:HZ1	1.76	0.47
5:J:94:LEU:HD22	5:J:215:LEU:HD11	1.97	0.47
5:K:41:GLU:O	5:K:44:ARG:HG3	2.15	0.47
7:N:88:PHE:CD1	7:N:92:ARG:HG2	2.50	0.47
11:b:200:ARG:HH11	16:o:80:LEU:HB3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:148:VAL:O	16:g:152:LEU:N	2.42	0.47
16:h:33:GLY:HA2	16:h:111:GLY:HA3	1.97	0.47
16:l:44:MET:SD	16:l:122:ALA:HB2	2.54	0.47
2:D:276:ALA:O	2:D:280:ALA:N	2.48	0.47
7:N:27:LYS:HD2	7:N:27:LYS:HA	1.41	0.47
13:d:201:GLY:HA2	13:d:205:ALA:HB2	1.97	0.47
13:d:238:ALA:HA	13:d:241:PHE:CD2	2.50	0.47
16:h:136:ILE:O	16:h:140:VAL:HG23	2.15	0.47
16:k:70:LEU:HD21	16:l:144:TYR:HB3	1.96	0.47
1:B:135:PHE:HE1	1:B:154:GLY:HA3	1.80	0.47
4:H:91:GLN:HA	4:H:114:GLU:HB3	1.96	0.47
5:K:51:LEU:O	5:K:55:GLU:OE1	2.33	0.47
8:S:227:LYS:HA	8:S:227:LYS:HD2	1.66	0.47
9:T:323:GLN:OE1	9:T:324:GLN:NE2	2.48	0.47
11:b:100:VAL:HA	11:b:103:TYR:CD2	2.50	0.47
16:h:36:LYS:HE2	16:h:36:LYS:HB2	1.74	0.47
16:i:78:ASN:O	16:j:155:LYS:NZ	2.48	0.47
16:k:24:VAL:HG23	16:k:25:PHE:H	1.80	0.47
1:A:277:CYS:N	1:A:349:ASN:OD1	2.48	0.47
1:B:347:MET:HA	1:B:407:VAL:O	2.14	0.47
2:E:191:LEU:HD11	2:E:375:ARG:HA	1.97	0.47
2:E:324:ASP:OD1	2:E:325:LEU:N	2.48	0.47
5:I:36:GLU:N	9:T:210:ARG:HH12	2.13	0.47
5:I:222:ARG:C	5:I:223:LYS:HD2	2.41	0.47
8:Q:127:HIS:O	8:Q:131:ASN:ND2	2.48	0.47
10:a:357:THR:HG22	10:a:359:GLN:H	1.80	0.47
16:i:16:VAL:CG1	16:j:94:GLY:HA3	2.44	0.47
1:C:397:ASN:HD22	8:S:31:ARG:HH22	1.61	0.46
5:J:85:ARG:HA	5:J:85:ARG:HD3	1.60	0.46
13:d:289:THR:HG23	13:d:292:ASP:HB2	1.98	0.46
16:i:99:VAL:HB	16:i:149:ALA:HB2	1.97	0.46
16:j:10:TYR:HA	16:k:90:PHE:HE2	1.80	0.46
16:o:48:ARG:HG2	16:o:51:LEU:HG	1.96	0.46
1:B:100:ASP:HB2	1:B:314:ASN:HD22	1.80	0.46
1:B:528:TYR:CE1	1:B:529:ASP:HB2	2.50	0.46
1:C:516:LYS:HA	1:C:520:LEU:HB2	1.97	0.46
2:F:137:PRO:CG	5:K:84:LEU:HB3	2.45	0.46
2:F:371:ILE:HD13	2:F:371:ILE:HA	1.78	0.46
5:J:53:ILE:HD11	7:N:47:TYR:CD2	2.49	0.46
10:a:90:PHE:H	10:a:91:PRO:CD	2.27	0.46
14:e:6:LEU:O	14:e:10:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:k:10:TYR:HA	16:l:90:PHE:HE2	1.80	0.46
16:k:36:LYS:HG3	16:k:115:ASP:HB2	1.96	0.46
16:l:14:PHE:O	16:l:93:LEU:HB2	2.14	0.46
16:l:61:MET:HA	16:l:64:ILE:HG12	1.96	0.46
16:o:95:ALA:HB2	16:o:152:LEU:HB3	1.97	0.46
1:B:91:GLY:O	1:B:94:ILE:HG12	2.15	0.46
9:T:116:LYS:HD2	9:T:116:LYS:HA	1.53	0.46
9:T:463:ASN:HB3	10:a:264:ARG:HE	1.80	0.46
10:a:538:MET:HE2	10:a:740:LEU:HD11	1.98	0.46
11:b:21:VAL:HA	11:b:24:ILE:HG22	1.97	0.46
13:d:54:TYR:HB3	13:d:57:PHE:CE1	2.51	0.46
13:d:191:GLU:O	13:d:195:LYS:HG2	2.16	0.46
1:B:237:LEU:O	1:B:239:PRO:HD3	2.14	0.46
1:B:416:ASP:OD1	1:B:416:ASP:N	2.44	0.46
2:E:118:SER:O	2:E:121:MET:HB3	2.16	0.46
5:K:219:ASN:ND2	5:K:221:ASN:OD1	2.46	0.46
8:S:223:LYS:HA	8:S:223:LYS:HD3	1.71	0.46
10:a:21:ALA:HB2	10:a:346:SER:HB3	1.97	0.46
11:b:133:ALA:O	11:b:137:MET:HG2	2.14	0.46
15:f:85:CYS:O	15:f:89:LEU:HG	2.16	0.46
16:l:72:VAL:O	16:l:76:ILE:HG12	2.15	0.46
1:A:558:THR:HB	1:A:564:LYS:HA	1.96	0.46
2:E:80:VAL:HG22	2:E:90:VAL:HG22	1.97	0.46
2:E:429:MET:O	2:E:433:VAL:HG22	2.15	0.46
2:F:229:GLY:HA2	2:F:258:ALA:HA	1.96	0.46
2:F:280:ALA:O	2:F:340:GLY:HA3	2.15	0.46
3:G:160:SER:C	3:G:162:LEU:H	2.24	0.46
7:M:81:MET:O	7:M:85:GLN:OE1	2.33	0.46
8:Q:62:PHE:O	8:Q:66:LEU:HD23	2.16	0.46
8:S:43:LYS:HA	8:S:43:LYS:HD2	1.36	0.46
10:a:45:ASN:HB3	10:a:48:GLN:OE1	2.15	0.46
11:b:136:SER:HA	16:o:16:VAL:HG11	1.98	0.46
16:h:29:GLY:HA3	16:h:104:LEU:HA	1.97	0.46
16:k:24:VAL:HG23	16:k:25:PHE:N	2.31	0.46
16:k:50:GLU:HA	16:l:126:ARG:HH12	1.80	0.46
1:B:38:ALA:HB3	1:B:41:GLU:HB2	1.96	0.46
1:C:295:THR:HG22	1:C:302:VAL:HB	1.97	0.46
4:H:95:ARG:HB3	4:H:97:LYS:HE3	1.98	0.46
8:S:213:PHE:HB2	8:S:222:GLN:HG2	1.97	0.46
10:a:54:GLU:HG2	10:a:57:ARG:HH11	1.81	0.46
13:d:39:CYS:HB2	13:d:44:ASP:CG	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:i:22:ALA:HB2	16:i:96:GLY:HA2	1.98	0.46
16:i:137:PHE:O	16:i:140:VAL:HB	2.15	0.46
16:j:14:PHE:HD1	16:j:93:LEU:HD22	1.80	0.46
16:l:61:MET:HE1	16:l:136:ILE:HA	1.98	0.46
1:C:465:TYR:O	1:C:469:PHE:N	2.47	0.46
5:K:121:LEU:HD23	7:O:108:PRO:HG2	1.97	0.46
5:K:219:ASN:HD22	5:K:222:ARG:HB2	1.80	0.46
10:a:172:ALA:HA	10:a:221:ILE:HB	1.98	0.46
10:a:629:LEU:HB2	10:a:633:GLN:OE1	2.16	0.46
16:o:55:SER:O	16:o:58:PRO:HD2	2.16	0.46
1:B:473:VAL:HG13	1:B:474:PRO:HD3	1.98	0.46
1:C:90:LEU:HA	1:C:94:ILE:HD11	1.98	0.46
1:C:369:PRO:HG2	4:H:201:ARG:HG2	1.98	0.46
2:D:125:VAL:HG22	2:D:253:LEU:HD12	1.98	0.46
2:F:42:ARG:HG3	2:F:105:THR:HG22	1.97	0.46
3:G:61:LEU:O	3:G:65:VAL:HG23	2.16	0.46
9:T:367:SER:OG	9:T:369:VAL:HG12	2.15	0.46
10:a:649:PRO:HA	10:a:652:LEU:HB3	1.98	0.46
16:j:10:TYR:HA	16:k:90:PHE:CE2	2.51	0.46
16:k:24:VAL:HG23	16:k:25:PHE:CD1	2.50	0.46
16:n:23:MET:HE1	16:n:70:LEU:HA	1.98	0.46
16:o:86:LEU:HA	16:o:89:SER:HB3	1.97	0.46
1:B:34:MET:HE1	1:B:81:ARG:HG2	1.98	0.46
1:B:210:PRO:HB2	1:B:213:GLN:HG2	1.97	0.46
4:H:59:GLY:HA3	6:L:98:TYR:CE1	2.51	0.46
10:a:128:LEU:HD11	10:a:245:TYR:CD2	2.51	0.46
10:a:755:VAL:HG23	16:k:150:LEU:HD21	1.98	0.46
16:i:68:TYR:HD2	16:i:146:LEU:HB2	1.80	0.46
1:B:293:GLU:O	1:B:295:THR:HG23	2.16	0.46
1:B:528:TYR:CD1	1:B:586:PHE:HA	2.50	0.46
1:C:55:ILE:HD13	1:C:65:GLN:HB2	1.97	0.46
1:C:66:VAL:HG12	1:C:68:GLU:H	1.81	0.46
2:E:302:ARG:HD2	2:E:316:GLY:O	2.16	0.46
2:F:42:ARG:NH2	5:K:188:ARG:O	2.49	0.46
3:G:294:TRP:NE1	3:G:298:LYS:HE2	2.31	0.46
3:G:329:LYS:H	3:G:329:LYS:HG3	1.37	0.46
8:S:66:LEU:O	8:S:70:LYS:HG3	2.16	0.46
9:T:46:ASP:HA	9:T:72:GLN:HB3	1.98	0.46
9:T:334:ASP:OD1	9:T:335:ILE:N	2.48	0.46
10:a:646:LEU:HD12	10:a:646:LEU:HA	1.80	0.46
13:d:143:ILE:HD13	13:d:150:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:j:8:PRO:HG2	16:j:11:ALA:HB2	1.96	0.46
16:o:126:ARG:O	16:o:129:VAL:HG12	2.16	0.46
1:C:41:GLU:HB2	1:C:54:ILE:HD12	1.98	0.45
1:C:432:PHE:CE2	1:C:452:ILE:HG22	2.46	0.45
1:C:535:TYR:CZ	1:C:594:GLU:HG3	2.51	0.45
2:E:475:TRP:CE2	2:E:497:PHE:HB2	2.51	0.45
5:K:81:LEU:HB3	5:K:85:ARG:NH2	2.30	0.45
6:L:45:ILE:HD13	6:L:73:MET:HB3	1.98	0.45
6:L:75:ARG:HA	6:L:78:LEU:HD12	1.98	0.45
10:a:613:PHE:O	10:a:616:MET:HB3	2.16	0.45
13:d:21:ARG:NH1	13:d:309:GLN:HA	2.31	0.45
1:C:574:MET:HE1	1:C:615:LEU:HD22	1.98	0.45
2:D:232:MET:HA	2:D:232:MET:HE2	1.98	0.45
16:j:6:SER:OG	16:j:7:GLY:N	2.49	0.45
16:l:24:VAL:HG23	16:l:25:PHE:H	1.81	0.45
1:B:504:THR:HA	1:B:507:ILE:HD12	1.98	0.45
6:L:69:TYR:HB3	6:L:96:HIS:CD2	2.51	0.45
9:T:456:VAL:HA	9:T:459:LEU:HG	1.99	0.45
10:a:249:GLU:HB3	10:a:254:ARG:HB3	1.98	0.45
13:d:49:LEU:HA	13:d:52:THR:HG22	1.98	0.45
16:i:6:SER:OG	16:i:7:GLY:N	2.48	0.45
2:F:374:ASP:HB3	2:F:377:LEU:HB2	1.98	0.45
8:S:201:LYS:HD2	8:S:201:LYS:HA	1.71	0.45
10:a:534:ASN:HD22	10:a:534:ASN:C	2.24	0.45
11:b:51:ASN:OD1	16:g:91:LEU:HA	2.16	0.45
11:b:58:ILE:HG21	16:g:148:VAL:HG11	1.97	0.45
1:B:156:VAL:HB	1:B:166:ILE:HD11	1.99	0.45
2:E:174:MET:HE2	2:E:174:MET:HA	1.98	0.45
5:J:167:ILE:O	5:J:169:GLN:NE2	2.50	0.45
5:K:51:LEU:HA	5:K:54:MET:HB2	1.99	0.45
7:M:81:MET:O	7:M:84:LEU:HB3	2.17	0.45
10:a:262:ASN:O	10:a:265:ILE:HG22	2.17	0.45
11:b:2:THR:HB	11:b:5:VAL:HB	1.99	0.45
11:b:172:LEU:HD22	16:o:45:SER:HB2	1.98	0.45
13:d:248:TYR:HA	13:d:252:LEU:HD23	1.98	0.45
16:g:58:PRO:HA	16:g:61:MET:HB2	1.97	0.45
16:k:88:LYS:O	16:k:92:GLN:HG2	2.16	0.45
16:n:44:MET:HG2	16:n:122:ALA:HB2	1.98	0.45
1:B:271:VAL:HG11	1:B:337:PHE:CG	2.51	0.45
1:B:320:VAL:HG22	1:B:361:ILE:HG12	1.99	0.45
1:C:152:ILE:HG13	1:C:398:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:76:ARG:NH2	2:E:94:GLU:HG2	2.31	0.45
2:F:118:SER:O	2:F:121:MET:HB2	2.17	0.45
4:H:48:LEU:HD11	6:L:112:MET:HB3	1.98	0.45
4:H:139:ALA:HA	4:H:142:VAL:HG12	1.98	0.45
5:I:74:ASN:O	5:I:78:GLN:HG2	2.16	0.45
5:I:127:LEU:HB3	5:I:129:GLU:HG2	1.98	0.45
7:N:32:ARG:HD2	7:N:32:ARG:HA	1.61	0.45
8:Q:177:GLN:O	8:Q:181:LEU:HD23	2.17	0.45
8:S:28:TYR:CZ	8:S:32:CYS:SG	3.10	0.45
10:a:235:LYS:O	10:a:238:GLU:HG2	2.17	0.45
13:d:6:GLU:HA	13:d:310:PHE:CD2	2.51	0.45
13:d:309:GLN:HG3	16:o:43:ALA:HB2	1.99	0.45
16:k:25:PHE:O	16:k:28:LEU:HB2	2.17	0.45
16:n:128:PHE:O	16:n:132:ILE:HG12	2.16	0.45
1:C:220:LYS:HE2	1:C:220:LYS:HB3	1.57	0.45
2:E:100:ASP:OD1	2:E:101:ALA:N	2.50	0.45
4:H:60:GLU:OE2	4:H:61:VAL:HG23	2.16	0.45
7:O:94:GLU:HG2	7:O:95:VAL:N	2.31	0.45
10:a:90:PHE:H	10:a:91:PRO:HD2	1.82	0.45
16:g:19:ALA:HA	16:g:76:ILE:HD13	1.99	0.45
16:j:81:THR:H	16:j:84:ILE:HD11	1.80	0.45
1:A:324:GLU:HG3	1:A:361:ILE:HD12	1.98	0.45
1:C:152:ILE:CG1	1:C:398:PRO:HG2	2.47	0.45
2:E:80:VAL:HA	2:E:90:VAL:HG22	1.99	0.45
3:G:166:LEU:HD12	3:G:251:PHE:HB3	1.99	0.45
10:a:494:THR:O	10:a:498:ASN:HB2	2.16	0.45
12:c:410:ARG:HB3	17:p:295:ASN:HB2	1.97	0.45
15:f:12:ALA:O	15:f:16:ILE:HG12	2.17	0.45
16:g:72:VAL:HG21	16:g:99:VAL:HG21	1.99	0.45
16:h:22:ALA:HB2	16:h:96:GLY:HA2	1.99	0.45
16:l:137:PHE:O	16:l:141:LEU:HG	2.17	0.45
1:B:68:GLU:HG3	1:B:120:ARG:HG3	1.99	0.45
1:B:524:GLY:HA2	1:B:530:ARG:HA	1.99	0.45
1:B:570:ILE:HA	1:B:574:MET:HE3	1.97	0.45
1:C:37:ALA:HB1	1:C:54:ILE:HD13	1.98	0.45
1:C:592:ASP:OD1	1:C:593:GLY:N	2.46	0.45
2:E:67:ASN:OD1	2:E:75:GLN:NE2	2.49	0.45
2:F:271:LEU:HD13	2:F:271:LEU:HA	1.82	0.45
4:H:43:ARG:HA	4:H:43:ARG:HD3	1.66	0.45
10:a:34:LYS:HE2	10:a:326:PRO:HD2	1.99	0.45
10:a:381:TYR:OH	10:a:804:LEU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:729:CYS:O	10:a:733:ILE:HD12	2.17	0.45
16:g:16:VAL:HG21	16:h:91:LEU:HA	1.99	0.45
2:F:266:ILE:HA	2:F:297:TYR:CE2	2.52	0.45
5:J:94:LEU:HB2	7:N:88:PHE:HZ	1.81	0.45
8:Q:234:MET:HE3	8:Q:235:PRO:HD3	1.99	0.45
9:T:358:GLU:HG2	9:T:363:ARG:HH22	1.82	0.45
14:e:53:LEU:HA	14:e:56:ILE:HG22	1.98	0.45
16:l:24:VAL:HG23	16:l:25:PHE:N	2.32	0.45
16:l:48:ARG:CZ	16:l:51:LEU:HD11	2.47	0.45
1:B:248:ILE:HD12	1:B:259:ILE:HG21	1.98	0.44
1:B:274:TYR:CG	1:B:347:MET:HG2	2.52	0.44
1:B:281:VAL:HG23	1:B:315:THR:CG2	2.46	0.44
1:C:297:GLU:OE2	1:C:298:VAL:N	2.50	0.44
2:E:294:MET:HE3	2:E:329:TYR:CE1	2.51	0.44
3:G:193:ASN:O	3:G:196:ASP:HB2	2.17	0.44
5:J:56:TYR:CE2	5:J:60:LYS:HD2	2.52	0.44
10:a:89:PRO:HD2	10:a:296:LYS:HG2	1.99	0.44
10:a:90:PHE:CZ	10:a:303:ILE:HG21	2.53	0.44
1:A:327:ILE:HD13	1:A:354:TRP:CD1	2.53	0.44
8:Q:83:ARG:O	8:Q:87:ILE:HG13	2.17	0.44
13:d:306:PHE:HE2	13:d:321:LEU:HD12	1.82	0.44
16:k:45:SER:HB2	16:l:127:LEU:HD13	1.99	0.44
16:l:9:GLU:HG2	16:l:10:TYR:N	2.32	0.44
16:o:47:MET:HE1	16:o:48:ARG:HH22	1.81	0.44
1:C:99:PHE:HB3	1:C:103:GLN:HA	1.98	0.44
1:C:152:ILE:HD13	1:C:167:MET:HG3	2.00	0.44
2:E:223:ILE:HB	2:E:251:VAL:HG22	2.00	0.44
7:N:53:LYS:HA	7:N:56:LYS:HZ3	1.82	0.44
16:k:36:LYS:O	16:k:39:THR:OG1	2.32	0.44
16:n:45:SER:HB2	16:n:52:ILE:HD11	1.99	0.44
1:B:273:ILE:HD11	1:B:337:PHE:CD2	2.53	0.44
2:E:41:TYR:HB2	2:E:106:CYS:SG	2.57	0.44
3:G:200:GLN:NE2	3:G:244:ASN:OD1	2.51	0.44
5:I:215:LEU:HA	7:M:91:ASN:OD1	2.17	0.44
9:T:241:TYR:HB2	9:T:281:VAL:HG22	1.99	0.44
13:d:293:ARG:O	13:d:296:GLU:HG3	2.17	0.44
16:l:81:THR:O	16:l:84:ILE:HG13	2.18	0.44
16:o:52:ILE:HA	16:o:55:SER:OG	2.18	0.44
17:p:326:SER:O	17:p:330:TRP:HB2	2.18	0.44
1:B:88:VAL:HG22	1:B:329:THR:HG22	2.00	0.44
1:C:113:THR:HG21	1:C:119:PRO:HG2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:TYR:HD1	1:C:284:MET:HE1	1.83	0.44
2:F:302:ARG:HG3	2:F:317:PHE:HA	1.98	0.44
2:F:396:MET:HE2	2:F:396:MET:HB3	1.87	0.44
7:O:43:GLU:O	7:O:46:GLN:HG3	2.17	0.44
8:R:50:GLN:O	8:R:54:ILE:HG23	2.17	0.44
10:a:130:PHE:HB3	10:a:202:ILE:HG12	1.99	0.44
10:a:567:LEU:HD21	10:a:662:GLN:HE22	1.83	0.44
11:b:22:VAL:HA	11:b:25:CYS:SG	2.58	0.44
11:b:106:ILE:O	11:b:110:VAL:N	2.44	0.44
13:d:146:THR:HB	13:d:149:GLU:HB3	2.00	0.44
16:k:59:VAL:HG11	16:l:134:ILE:HG23	2.00	0.44
16:n:117:GLY:O	16:n:121:THR:HG23	2.17	0.44
1:B:387:GLU:HG3	2:F:258:ALA:HB3	1.99	0.44
4:H:15:ALA:O	4:H:19:MET:HB2	2.17	0.44
5:J:101:ARG:O	5:J:105:VAL:HG23	2.18	0.44
8:Q:61:ARG:HH22	8:Q:64:GLU:HB3	1.82	0.44
9:T:323:GLN:HE21	10:a:56:ARG:NH1	2.15	0.44
16:i:23:MET:HG3	16:j:148:VAL:HG21	1.98	0.44
7:M:85:GLN:HB2	7:M:89:ARG:CZ	2.47	0.44
7:M:88:PHE:HB3	7:M:89:ARG:NH2	2.31	0.44
9:T:363:ARG:O	9:T:363:ARG:HG2	2.17	0.44
10:a:599:ASP:OD1	14:e:61:ASN:ND2	2.50	0.44
14:e:37:ILE:HA	14:e:40:MET:HG2	1.99	0.44
16:g:19:ALA:HB2	16:g:76:ILE:CG2	2.48	0.44
1:B:284:MET:SD	1:B:313:ALA:HB1	2.58	0.44
1:C:338:ARG:HD3	1:C:404:VAL:HG23	1.99	0.44
10:a:339:ARG:O	10:a:343:HIS:ND1	2.51	0.44
12:c:452:MET:H	12:c:452:MET:HG3	1.59	0.44
16:l:70:LEU:HD21	16:m:144:TYR:HB3	2.00	0.44
16:n:64:ILE:HD12	16:n:64:ILE:H	1.83	0.44
1:A:438:LYS:HB3	1:A:438:LYS:HE3	1.34	0.44
1:B:331:ILE:HD12	1:B:331:ILE:HA	1.89	0.44
1:C:295:THR:CG2	1:C:302:VAL:HB	2.47	0.44
2:D:166:THR:C	2:D:168:ILE:H	2.26	0.44
5:I:137:ARG:HH11	5:I:179:GLY:HA2	1.83	0.44
10:a:401:PHE:CE2	14:e:47:CYS:HB2	2.53	0.44
16:j:58:PRO:HA	16:j:61:MET:SD	2.58	0.44
16:o:72:VAL:O	16:o:76:ILE:HG12	2.18	0.44
1:B:100:ASP:OD2	1:B:104:ARG:NE	2.47	0.43
2:D:373:VAL:HG13	2:D:385:PRO:HG2	1.99	0.43
2:F:41:TYR:HB2	2:F:106:CYS:SG	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:350:MET:SD	2:F:350:MET:N	2.90	0.43
10:a:170:PHE:CG	10:a:171:VAL:N	2.85	0.43
13:d:328:ASN:O	13:d:332:ILE:HG12	2.18	0.43
16:h:45:SER:HB3	16:i:127:LEU:HD12	2.00	0.43
1:B:541:LEU:HD12	1:B:541:LEU:HA	1.84	0.43
2:D:157:ARG:HA	2:D:335:VAL:HA	2.01	0.43
3:G:336:TYR:O	3:G:340:LYS:HB3	2.18	0.43
4:H:23:LEU:O	4:H:27:GLN:OE1	2.36	0.43
7:M:94:GLU:HA	7:M:97:ASP:OD2	2.17	0.43
9:T:298:GLU:HB2	9:T:301:THR:OG1	2.18	0.43
9:T:433:GLY:HA2	9:T:436:LEU:HD12	1.99	0.43
16:g:46:VAL:HG22	16:h:123:GLN:HB2	2.00	0.43
16:l:70:LEU:CD2	16:m:144:TYR:HD2	2.31	0.43
1:A:339:ASP:HA	1:A:394:CYS:HB3	2.01	0.43
1:B:253:GLY:H	1:B:437:LYS:HZ1	1.66	0.43
10:a:400:PRO:HA	10:a:453:MET:SD	2.58	0.43
10:a:600:ALA:HA	10:a:603:SER:HB2	2.00	0.43
16:j:15:ALA:HA	16:j:92:GLN:HB2	2.00	0.43
16:o:41:ILE:HD12	16:o:55:SER:HB2	1.99	0.43
1:A:220:LYS:HB2	1:A:220:LYS:HE2	1.59	0.43
1:B:93:GLY:HA2	1:B:133:TRP:HH2	1.83	0.43
1:B:135:PHE:CE1	1:B:154:GLY:HA3	2.54	0.43
1:B:361:ILE:HD13	1:B:361:ILE:HA	1.92	0.43
5:J:46:VAL:HG13	5:J:50:ARG:HE	1.83	0.43
5:K:64:ILE:HD11	7:O:55:PHE:CE1	2.53	0.43
7:M:83:ILE:HA	7:M:86:THR:HG22	2.00	0.43
7:O:82:THR:O	7:O:85:GLN:HG3	2.18	0.43
10:a:49:ARG:O	10:a:52:VAL:HG12	2.18	0.43
13:d:85:MET:HE3	13:d:85:MET:HB3	1.71	0.43
13:d:97:LEU:HD21	13:d:315:PHE:CD1	2.54	0.43
14:e:70:ASN:OD1	14:e:71:GLU:N	2.50	0.43
16:k:31:ALA:HB1	16:l:109:ALA:HB2	1.99	0.43
16:l:114:GLY:O	16:l:118:VAL:HG23	2.18	0.43
16:m:136:ILE:HD12	16:m:136:ILE:HA	1.75	0.43
16:o:22:ALA:HB2	16:o:96:GLY:CA	2.48	0.43
1:A:233:VAL:HB	1:A:520:LEU:HG	2.00	0.43
1:B:44:ARG:HB2	1:B:80:LEU:HB3	2.00	0.43
1:C:532:CYS:HG	1:C:537:THR:HG1	1.65	0.43
2:D:284:GLU:OE2	5:I:223:LYS:HB2	2.18	0.43
2:E:287:VAL:HB	2:E:342:ILE:HD13	1.99	0.43
7:N:53:LYS:HA	7:N:56:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:10:GLN:O	7:O:13:GLN:HG3	2.18	0.43
10:a:808:TRP:HA	10:a:812:GLN:HB2	2.01	0.43
1:B:46:GLY:HA2	1:B:77:ASP:HB3	2.00	0.43
1:C:589:PRO:HA	1:C:597:ILE:HD11	2.00	0.43
2:D:163:MET:HE2	2:D:176:SER:HB2	2.01	0.43
2:E:273:LEU:HD11	2:E:328:ILE:HG23	2.00	0.43
2:E:325:LEU:HD23	2:E:325:LEU:HA	1.80	0.43
2:F:456:PHE:HB2	2:F:477:LEU:HD11	2.00	0.43
10:a:63:ARG:HD2	10:a:64:LYS:N	2.33	0.43
12:c:375:SER:OG	12:c:394:LEU:N	2.51	0.43
13:d:177:ASN:O	13:d:181:ILE:HG13	2.18	0.43
14:e:56:ILE:HG23	14:e:57:LEU:HD12	2.00	0.43
16:k:48:ARG:HG3	16:k:122:ALA:HA	2.00	0.43
1:C:243:GLY:N	1:C:405:THR:HG1	2.17	0.43
1:C:497:GLY:C	1:C:499:ALA:N	2.77	0.43
3:G:328:MET:HA	3:G:331:LEU:CD1	2.49	0.43
8:Q:53:LEU:HD22	8:Q:53:LEU:HA	1.92	0.43
8:Q:132:GLN:HB2	8:Q:183:LEU:HD21	1.99	0.43
16:k:95:ALA:HB2	16:k:152:LEU:HB2	2.01	0.43
9:T:434:LYS:O	9:T:438:MET:HG3	2.19	0.43
11:b:19:LEU:HA	11:b:22:VAL:HG12	2.01	0.43
16:l:45:SER:OG	16:m:123:GLN:NE2	2.52	0.43
16:o:11:ALA:HB3	16:o:84:ILE:HG23	2.01	0.43
1:C:495:LEU:HD22	4:H:171:ALA:HB1	2.01	0.43
2:E:409:HIS:HA	2:E:471:LEU:HD21	2.01	0.43
3:G:123:GLU:HB3	3:G:127:LYS:HZ3	1.81	0.43
3:G:328:MET:HA	3:G:331:LEU:HD12	2.01	0.43
6:L:67:ASN:OD1	6:L:68:GLN:N	2.48	0.43
16:i:32:TYR:CD2	16:i:108:PHE:HA	2.54	0.43
16:l:13:PHE:O	16:l:17:MET:HG3	2.19	0.43
16:l:46:VAL:HA	16:m:123:GLN:OE1	2.18	0.43
1:A:277:CYS:SG	1:A:327:ILE:HD11	2.59	0.43
1:A:450:TRP:CD1	1:A:520:LEU:HD11	2.53	0.43
1:B:34:MET:HE3	1:B:37:ALA:HB2	2.00	0.43
1:B:239:PRO:HD2	1:B:455:SER:CB	2.48	0.43
1:B:318:MET:HE2	2:E:154:PRO:HG2	2.00	0.43
1:B:485:GLU:HG3	1:B:489:LEU:HD23	1.99	0.43
1:C:497:GLY:C	1:C:499:ALA:H	2.27	0.43
2:E:117:VAL:HG11	2:E:275:THR:HA	2.01	0.43
5:J:90:LEU:HB3	7:N:88:PHE:CE2	2.54	0.43
5:J:142:PRO:O	5:J:145:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:75:ARG:HA	6:L:75:ARG:HD2	1.72	0.43
8:S:188:MET:HE2	8:S:195:GLU:HB2	2.01	0.43
13:d:257:ARG:HE	13:d:257:ARG:HB3	1.63	0.43
16:n:24:VAL:HG22	16:o:101:LEU:HB2	2.00	0.43
1:A:287:VAL:HG13	1:A:291:PHE:CE2	2.54	0.42
1:B:24:VAL:HG12	2:E:83:VAL:HB	2.00	0.42
1:B:567:TRP:CD1	1:B:571:ARG:HH21	2.37	0.42
1:C:358:LEU:HD22	1:C:377:TYR:HE1	1.84	0.42
1:C:498:LYS:HB2	1:C:501:LEU:HD12	2.01	0.42
1:C:516:LYS:HA	1:C:520:LEU:HD12	2.00	0.42
2:F:119:GLU:C	2:F:121:MET:H	2.26	0.42
4:H:63:ARG:HG2	13:d:340:HIS:HE1	1.84	0.42
5:I:137:ARG:NH1	5:I:178:ALA:O	2.51	0.42
7:N:86:THR:O	7:N:90:GLN:OE1	2.37	0.42
8:Q:123:LYS:HD3	8:Q:123:LYS:HA	1.79	0.42
8:Q:232:TYR:O	8:Q:235:PRO:HD2	2.19	0.42
9:T:19:ILE:HD13	9:T:136:PHE:CE2	2.54	0.42
9:T:34:GLN:HA	9:T:37:LEU:HD23	2.00	0.42
9:T:451:ASN:O	9:T:454:LEU:HG	2.19	0.42
10:a:470:LYS:HE2	10:a:757:TRP:CD2	2.54	0.42
12:c:305:VAL:HA	12:c:327:ALA:O	2.19	0.42
13:d:320:LYS:HD2	13:d:320:LYS:HA	1.58	0.42
16:k:48:ARG:HH12	16:k:125:PRO:HB3	1.84	0.42
1:A:19:GLY:HA3	1:A:34:MET:HE3	2.01	0.42
1:A:164:HIS:HE1	1:A:336:TYR:HE2	1.67	0.42
1:B:134:GLU:HG3	1:B:157:ASN:HD22	1.84	0.42
6:L:102:LYS:HB2	6:L:102:LYS:HE2	1.40	0.42
7:N:13:GLN:HG3	7:N:16:LYS:HZ3	1.84	0.42
7:N:40:ALA:O	7:N:44:ILE:HD12	2.19	0.42
8:Q:223:LYS:HA	8:Q:226:VAL:HG22	2.00	0.42
8:R:148:LYS:HG3	8:R:196:GLN:HG2	2.01	0.42
10:a:804:LEU:HD23	10:a:804:LEU:HA	1.78	0.42
15:f:47:THR:OG1	15:f:49:LYS:HG3	2.19	0.42
16:h:47:MET:H	16:h:47:MET:HG2	1.45	0.42
16:h:48:ARG:HB3	16:h:51:LEU:HB2	2.02	0.42
16:l:72:VAL:HG11	16:l:99:VAL:HG21	2.01	0.42
1:B:102:ILE:HG22	1:B:102:ILE:O	2.19	0.42
1:B:432:PHE:HE2	1:B:452:ILE:HD12	1.85	0.42
2:F:184:PRO:HD2	2:F:369:GLY:O	2.19	0.42
5:I:117:ASP:HA	5:I:147:ALA:HB1	2.01	0.42
9:T:136:PHE:HA	9:T:139:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:412:HIS:HB2	9:T:451:ASN:OD1	2.20	0.42
11:b:41:LEU:HD13	11:b:41:LEU:HA	1.76	0.42
13:d:105:MET:HB3	13:d:160:LEU:HD21	2.01	0.42
13:d:146:THR:HB	13:d:149:GLU:CB	2.50	0.42
13:d:274:TYR:O	13:d:275:LYS:C	2.62	0.42
14:e:52:TRP:CD1	14:e:52:TRP:C	2.97	0.42
16:h:87:TYR:CZ	16:h:91:LEU:HD11	2.55	0.42
16:j:15:ALA:HB2	16:j:89:SER:HA	2.01	0.42
1:A:90:LEU:HB3	1:A:336:TYR:CE2	2.55	0.42
1:A:328:TYR:HA	1:A:331:ILE:HG22	2.02	0.42
1:B:271:VAL:HG21	1:B:337:PHE:CD1	2.54	0.42
1:C:443:LYS:HD2	1:C:443:LYS:HA	1.80	0.42
2:D:263:ILE:HD12	2:D:304:VAL:HG23	2.00	0.42
3:G:98:LEU:HD21	3:G:287:PHE:CE1	2.55	0.42
3:G:241:ALA:HB1	3:G:246:PHE:HB2	2.01	0.42
5:J:215:LEU:HG	7:N:95:VAL:HG11	2.00	0.42
8:R:33:MET:HA	8:R:36:ILE:HG22	2.01	0.42
16:k:14:PHE:O	16:k:93:LEU:HD12	2.19	0.42
1:A:116:ILE:HG22	2:D:156:ASP:HB3	2.00	0.42
1:B:42:LEU:HD11	1:B:86:LEU:HA	2.02	0.42
1:C:528:TYR:HA	1:C:588:ASP:HA	2.01	0.42
2:E:374:ASP:N	2:E:385:PRO:O	2.53	0.42
12:c:341:LEU:HD12	12:c:360:VAL:HG11	2.02	0.42
12:c:406:VAL:HG12	12:c:408:GLY:H	1.83	0.42
12:c:452:MET:HB2	12:c:452:MET:HE2	1.69	0.42
13:d:79:VAL:HG23	13:d:132:LEU:HD23	2.01	0.42
13:d:260:ASP:OD1	13:d:261:TYR:N	2.51	0.42
13:d:332:ILE:HG23	13:d:344:ILE:HD11	2.01	0.42
16:m:61:MET:HE1	16:m:135:LEU:O	2.19	0.42
16:m:128:PHE:O	16:m:132:ILE:HD12	2.20	0.42
1:B:492:ILE:O	1:B:496:VAL:HB	2.19	0.42
1:B:511:VAL:HG11	1:B:548:TYR:CD1	2.55	0.42
16:k:107:GLY:HA2	16:k:110:ILE:HG22	2.00	0.42
16:l:43:ALA:C	16:l:44:MET:HG2	2.42	0.42
2:E:47:VAL:HG22	2:E:52:VAL:HG13	2.02	0.42
2:F:119:GLU:C	2:F:121:MET:N	2.78	0.42
3:G:47:THR:HG22	5:J:22:GLU:HG2	2.00	0.42
3:G:367:TYR:C	3:G:369:TYR:H	2.28	0.42
4:H:17:THR:O	4:H:18:ILE:HB	2.19	0.42
5:J:204:ALA:O	5:J:208:MET:HG2	2.19	0.42
5:K:136:CYS:CB	5:K:144:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:11:THR:HG22	10:a:327:VAL:HG22	2.02	0.42
10:a:93:ASP:O	10:a:97:LEU:HG	2.20	0.42
12:c:435:MET:SD	16:g:97:LEU:HD13	2.59	0.42
13:d:183:ASN:HB2	13:d:240:LEU:HG	2.01	0.42
16:n:24:VAL:HG11	16:o:101:LEU:HD22	2.02	0.42
1:A:284:MET:SD	1:A:313:ALA:HB1	2.59	0.42
1:B:223:ALA:HB1	1:B:241:VAL:CG1	2.50	0.42
2:D:225:PHE:HB3	2:D:253:LEU:HD23	2.01	0.42
2:E:277:GLU:OE2	2:E:331:ARG:HD2	2.20	0.42
3:G:50:VAL:HG11	3:G:119:LYS:HE3	2.01	0.42
7:N:89:ARG:HA	7:N:92:ARG:HD2	2.01	0.42
8:Q:192:LYS:H	8:Q:192:LYS:HG2	1.68	0.42
10:a:470:LYS:CE	10:a:757:TRP:CE2	3.02	0.42
10:a:491:THR:O	10:a:494:THR:OG1	2.37	0.42
11:b:46:PRO:HB2	11:b:203:MET:HE2	2.01	0.42
12:c:404:PHE:O	12:c:405:ASN:C	2.62	0.42
16:h:46:VAL:HB	16:h:47:MET:HE2	2.01	0.42
16:h:62:ALA:HA	16:h:65:ILE:HD12	2.02	0.42
16:i:110:ILE:HG13	16:i:138:ALA:HB1	2.01	0.42
16:l:13:PHE:HB2	16:m:90:PHE:CE2	2.55	0.42
16:l:65:ILE:HG13	16:l:139:GLU:OE2	2.20	0.42
16:m:59:VAL:HG11	16:n:134:ILE:HG23	2.01	0.42
1:A:191:VAL:HG13	1:A:205:MET:HE2	2.02	0.42
1:C:413:PRO:HD2	1:C:419:ASP:OD2	2.20	0.42
2:F:326:ALA:HA	2:F:366:ILE:HG12	2.01	0.42
5:K:75:LEU:HD23	5:K:75:LEU:HA	1.92	0.42
8:R:138:ASP:HA	8:R:141:LYS:HD2	2.01	0.42
10:a:740:LEU:HD13	10:a:740:LEU:HA	1.79	0.42
12:c:307:TRP:HA	12:c:324:PHE:O	2.20	0.42
13:d:82:PHE:CE1	13:d:101:THR:HG22	2.54	0.42
16:g:110:ILE:HD11	16:g:139:GLU:HG3	2.00	0.42
16:i:35:ALA:HB1	16:j:112:ILE:HG21	2.02	0.42
16:m:144:TYR:O	16:m:147:ILE:HB	2.19	0.42
16:o:62:ALA:HB2	16:o:110:ILE:HG21	2.02	0.42
1:A:488:ASP:O	1:A:491:GLU:HG3	2.20	0.42
1:B:305:ILE:HG23	1:B:306:MET:HE2	2.01	0.42
1:B:439:LEU:HB2	1:B:447:SER:HB2	2.01	0.42
1:C:352:SER:HB3	1:C:411:SER:H	1.84	0.42
1:C:364:ARG:HD3	1:C:364:ARG:HA	1.87	0.42
2:D:187:SER:O	2:D:349:THR:HA	2.19	0.42
2:E:47:VAL:HG22	2:E:52:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:PRO:HB3	2:E:141:ALA:HB2	2.02	0.42
2:F:196:ILE:HG12	2:F:384:PRO:HB3	2.01	0.42
5:J:55:GLU:HA	5:J:58:GLU:HG2	2.02	0.42
8:Q:98:ILE:HG23	8:Q:160:GLN:HB3	2.01	0.42
11:b:70:TYR:C	11:b:70:TYR:CD1	2.98	0.42
16:i:29:GLY:HA3	16:i:104:LEU:HA	2.02	0.42
16:i:72:VAL:HG21	16:i:99:VAL:HG11	2.01	0.42
16:j:88:LYS:O	16:j:92:GLN:HG2	2.20	0.42
1:B:324:GLU:HG2	1:B:358:LEU:HD12	2.01	0.41
1:C:565:ILE:HA	1:C:569:ILE:HD11	2.02	0.41
2:E:359:ILE:H	2:E:359:ILE:HG13	1.70	0.41
2:F:121:MET:HB2	2:F:121:MET:HE2	1.73	0.41
2:F:263:ILE:H	2:F:263:ILE:HG12	1.53	0.41
2:F:368:GLU:HA	2:F:394:ARG:HD2	2.02	0.41
5:J:66:GLN:NE2	5:J:67:GLN:HG3	2.34	0.41
7:N:34:LYS:HD2	7:N:34:LYS:HA	1.46	0.41
8:Q:146:THR:HB	8:Q:147:PRO:HD2	2.01	0.41
16:m:124:GLN:OE1	16:m:126:ARG:HG2	2.20	0.41
1:C:497:GLY:O	1:C:499:ALA:N	2.53	0.41
2:E:70:LEU:HD11	2:E:76:ARG:NE	2.35	0.41
2:E:70:LEU:HB2	2:E:72:ASN:OD1	2.19	0.41
2:F:140:MET:HB3	2:F:140:MET:HE3	1.68	0.41
2:F:170:PRO:HB3	2:F:457:ILE:HD13	2.02	0.41
4:H:63:ARG:HH12	6:L:98:TYR:HB2	1.86	0.41
5:I:189:LYS:HA	5:I:189:LYS:HD2	1.83	0.41
7:M:88:PHE:O	7:M:92:ARG:HB2	2.20	0.41
8:Q:128:VAL:HA	8:Q:131:ASN:HD22	1.86	0.41
13:d:112:LEU:HD12	13:d:122:ILE:HD12	2.02	0.41
13:d:128:LYS:HE2	13:d:128:LYS:HA	2.01	0.41
16:k:23:MET:HE1	16:k:70:LEU:CD1	2.50	0.41
16:l:140:VAL:HG12	16:l:144:TYR:CZ	2.55	0.41
16:n:59:VAL:HG21	16:o:134:ILE:HD12	2.02	0.41
1:A:458:MET:HE2	1:A:458:MET:HB3	1.64	0.41
1:B:552:ARG:HB3	1:B:553:ARG:NH1	2.35	0.41
2:D:176:SER:N	2:D:396:MET:HE1	2.35	0.41
2:D:179:ARG:HD2	2:D:286:HIS:ND1	2.35	0.41
2:F:122:LEU:HD12	2:F:122:LEU:HA	1.81	0.41
2:F:377:LEU:HD22	2:F:382:ILE:HD12	2.02	0.41
7:N:47:TYR:O	7:N:51:ARG:HG2	2.20	0.41
7:N:111:HIS:O	7:N:111:HIS:ND1	2.53	0.41
7:O:28:ARG:HE	7:O:28:ARG:HB3	1.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:207:GLN:HG3	8:R:212:PRO:HG3	2.01	0.41
9:T:385:GLU:HG2	9:T:386:LYS:H	1.85	0.41
9:T:428:ILE:HG22	9:T:434:LYS:HB2	2.01	0.41
10:a:80:MET:HG3	10:a:82:THR:H	1.85	0.41
11:b:56:LEU:C	11:b:56:LEU:HD23	2.45	0.41
13:d:52:THR:HG23	13:d:54:TYR:H	1.85	0.41
16:j:146:LEU:O	16:j:150:LEU:HG	2.20	0.41
16:l:148:VAL:HA	16:l:151:ILE:HD12	2.01	0.41
2:D:293:ASP:HA	2:D:347:ILE:O	2.21	0.41
2:E:273:LEU:HD11	2:E:328:ILE:HA	2.02	0.41
2:E:273:LEU:CD1	2:E:328:ILE:HA	2.51	0.41
5:J:125:TYR:CD2	7:N:108:PRO:HB2	2.55	0.41
5:K:215:LEU:HA	7:O:91:ASN:HB2	2.01	0.41
10:a:735:ASN:HB3	10:a:810:GLU:HB3	2.02	0.41
12:c:329:ARG:HB2	12:c:404:PHE:CZ	2.55	0.41
16:h:60:VAL:HG12	16:i:137:PHE:CE2	2.55	0.41
16:m:45:SER:HB3	16:n:127:LEU:HD22	2.03	0.41
1:B:166:ILE:H	1:B:166:ILE:HG12	1.71	0.41
1:C:233:VAL:HG12	1:C:520:LEU:HD22	2.02	0.41
2:E:53:VAL:HG22	2:E:89:ILE:HG13	2.01	0.41
2:E:321:MET:C	2:E:323:THR:H	2.29	0.41
2:F:348:LEU:HD12	2:F:348:LEU:C	2.45	0.41
4:H:217:GLU:H	4:H:217:GLU:HG3	1.66	0.41
5:K:50:ARG:HG3	7:O:47:TYR:CE2	2.56	0.41
8:Q:68:ALA:HB1	8:Q:73:LYS:HB2	2.02	0.41
9:T:202:ALA:HB3	9:T:242:GLN:OE1	2.21	0.41
10:a:297:VAL:O	10:a:301:LYS:HG2	2.20	0.41
13:d:122:ILE:O	13:d:126:VAL:HG23	2.20	0.41
13:d:168:ILE:H	13:d:168:ILE:HG13	1.32	0.41
14:e:12:VAL:HG13	14:e:13:MET:HG3	2.02	0.41
16:l:115:ASP:O	16:l:119:ARG:HG2	2.20	0.41
1:A:287:VAL:HG13	1:A:291:PHE:CD2	2.55	0.41
1:A:340:MET:HE3	1:A:340:MET:HB2	1.76	0.41
1:B:410:VAL:CG2	1:B:425:THR:HG21	2.50	0.41
1:B:535:TYR:HD2	1:B:598:LYS:HE2	1.83	0.41
1:C:263:LEU:C	1:C:263:LEU:HD23	2.46	0.41
1:C:300:GLY:HA3	8:S:148:LYS:HZ3	1.85	0.41
2:D:127:ASN:OD1	2:D:131:LYS:N	2.54	0.41
2:E:256:ASN:OD1	2:E:265:ARG:HG2	2.21	0.41
3:G:160:SER:C	3:G:162:LEU:N	2.76	0.41
3:G:193:ASN:HB2	3:G:245:LYS:HZ1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:196:ASP:O	3:G:199:LYS:HG2	2.21	0.41
3:G:200:GLN:O	3:G:204:LEU:HG	2.20	0.41
5:I:127:LEU:HA	5:I:127:LEU:HD12	1.78	0.41
9:T:331:ILE:HA	9:T:334:ASP:OD2	2.20	0.41
10:a:575:PRO:HA	10:a:578:ILE:HG12	2.03	0.41
10:a:593:TYR:O	10:a:597:ALA:HB2	2.20	0.41
16:k:60:VAL:HG23	16:l:137:PHE:CE1	2.55	0.41
16:n:72:VAL:HG11	16:n:99:VAL:CG1	2.45	0.41
3:G:119:LYS:O	3:G:123:GLU:OE1	2.39	0.41
8:Q:128:VAL:O	8:Q:132:GLN:OE1	2.39	0.41
10:a:177:ARG:HD3	10:a:216:HIS:ND1	2.35	0.41
12:c:439:PHE:O	12:c:443:LEU:HD23	2.20	0.41
13:d:53:ASP:OD1	13:d:54:TYR:N	2.54	0.41
16:j:62:ALA:HA	16:j:110:ILE:CD1	2.50	0.41
16:l:55:SER:O	16:l:58:PRO:HD2	2.20	0.41
16:m:23:MET:HE1	16:n:144:TYR:HB3	2.02	0.41
1:B:155:ILE:CG2	1:B:163:LYS:HB3	2.50	0.41
1:C:426:LEU:HD11	1:C:432:PHE:CD1	2.56	0.41
2:D:232:MET:HG3	2:D:236:ARG:NH2	2.36	0.41
2:F:330:GLU:CG	2:F:366:ILE:HD11	2.51	0.41
3:G:113:PRO:HB2	3:G:116:GLN:HG3	2.02	0.41
3:G:332:ARG:HG3	3:G:333:GLU:N	2.35	0.41
5:K:124:LEU:HD22	5:K:132:MET:HE3	2.02	0.41
7:M:85:GLN:HB2	7:M:89:ARG:NH2	2.36	0.41
8:Q:159:LEU:HD13	8:Q:178:LEU:HD22	2.01	0.41
12:c:288:THR:HG22	12:c:289:PHE:CD1	2.56	0.41
13:d:208:MET:SD	13:d:313:GLY:HA3	2.61	0.41
16:j:80:LEU:O	16:k:155:LYS:HE3	2.20	0.41
1:A:459:ARG:H	1:A:459:ARG:HG2	1.67	0.41
1:B:346:MET:HE2	1:B:346:MET:HB3	1.75	0.41
1:C:275:VAL:HG21	1:C:327:ILE:HA	2.02	0.41
1:C:345:SER:HB3	1:C:347:MET:HE3	2.02	0.41
2:D:494:ILE:O	2:D:498:TYR:HB3	2.20	0.41
2:E:500:ARG:HA	2:E:500:ARG:HD3	1.85	0.41
2:F:193:HIS:HA	2:F:196:ILE:HD12	2.02	0.41
4:H:66:ALA:C	13:d:338:GLN:HE22	2.29	0.41
5:J:50:ARG:O	5:J:54:MET:HG2	2.20	0.41
5:J:201:ASP:O	5:J:202:LEU:C	2.64	0.41
8:R:93:ARG:HH12	8:R:131:ASN:HA	1.85	0.41
8:R:140:LEU:HD22	8:R:153:ARG:HG2	2.02	0.41
8:S:177:GLN:HE21	8:S:178:LEU:HG	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:350:SER:HA	9:T:369:VAL:HG23	2.03	0.41
9:T:394:LEU:O	9:T:398:LEU:N	2.53	0.41
9:T:453:LEU:HD13	9:T:453:LEU:HA	1.84	0.41
10:a:482:ARG:NH1	14:e:77:LYS:O	2.48	0.41
11:b:114:MET:HB3	11:b:114:MET:HE3	1.68	0.41
11:b:131:TYR:HD2	16:o:9:GLU:HG2	1.86	0.41
12:c:302:ASN:N	12:c:305:VAL:O	2.54	0.41
12:c:427:MET:HB3	16:g:14:PHE:HZ	1.84	0.41
16:g:88:LYS:HE3	16:g:88:LYS:HB3	1.96	0.41
16:j:41:ILE:O	16:j:44:MET:HG3	2.20	0.41
16:k:46:VAL:HG12	16:l:123:GLN:HB2	2.02	0.41
16:k:47:MET:HE3	16:k:47:MET:HB3	1.77	0.41
16:k:91:LEU:HB3	16:k:152:LEU:O	2.21	0.41
16:l:87:TYR:CE1	16:l:91:LEU:HD21	2.55	0.41
16:l:136:ILE:O	16:l:140:VAL:HG23	2.21	0.41
16:m:120:GLY:O	16:m:123:GLN:HG3	2.21	0.41
1:B:71:SER:HA	2:E:62:TYR:HD2	1.86	0.41
2:E:45:CYS:SG	2:E:87:LYS:NZ	2.94	0.41
2:F:487:LYS:HB3	2:F:487:LYS:HE3	1.54	0.41
5:J:145:LYS:O	5:J:148:VAL:HG12	2.21	0.41
8:R:154:ALA:O	8:R:158:VAL:HG23	2.21	0.41
9:T:302:ARG:HA	9:T:302:ARG:HD3	1.58	0.41
9:T:323:GLN:NE2	10:a:53:ASN:HB3	2.35	0.41
10:a:283:LEU:HD23	10:a:283:LEU:HA	1.89	0.41
13:d:185:LEU:HD12	13:d:185:LEU:HA	1.73	0.41
14:e:11:ILE:HG13	14:e:12:VAL:N	2.36	0.41
16:k:70:LEU:HG	16:l:144:TYR:CD2	2.56	0.41
16:m:50:GLU:OE2	16:m:51:LEU:HG	2.21	0.41
1:A:458:MET:H	1:A:458:MET:HG2	1.49	0.40
1:B:536:LYS:O	1:B:540:MET:HG2	2.22	0.40
1:C:523:ASN:O	1:C:526:THR:HG22	2.21	0.40
2:F:454:ARG:HA	2:F:458:ASN:HD22	1.85	0.40
5:K:44:ARG:O	5:K:48:THR:HG23	2.21	0.40
8:Q:60:TYR:O	8:Q:61:ARG:HG2	2.21	0.40
8:R:140:LEU:HD13	8:R:153:ARG:HD2	2.03	0.40
10:a:418:LEU:HA	10:a:421:VAL:HG12	2.02	0.40
11:b:91:LEU:O	11:b:95:ILE:HG13	2.21	0.40
16:h:16:VAL:HG13	16:i:94:GLY:HA3	2.03	0.40
16:i:104:LEU:HD21	17:p:325:THR:HG21	2.03	0.40
2:D:292:THR:O	2:D:347:ILE:HB	2.20	0.40
2:E:65:ILE:HD11	2:E:113:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:19:MET:HE3	4:H:180:ILE:HG23	2.03	0.40
6:L:110:LYS:HA	6:L:110:LYS:HE2	2.03	0.40
7:O:32:ARG:HD2	7:O:32:ARG:HA	1.57	0.40
8:Q:69:SER:HA	8:Q:76:ASN:HD21	1.86	0.40
9:T:240:GLN:HA	9:T:243:MET:HE2	2.03	0.40
9:T:328:ASP:O	9:T:331:ILE:HG22	2.21	0.40
10:a:175:ILE:HG12	10:a:242:ALA:HB1	2.04	0.40
10:a:593:TYR:O	10:a:597:ALA:HB3	2.21	0.40
11:b:47:PHE:CZ	11:b:117:PRO:HA	2.57	0.40
16:g:33:GLY:HA2	16:g:111:GLY:HA3	2.03	0.40
16:h:23:MET:HE2	16:i:145:GLY:N	2.36	0.40
16:l:61:MET:HE2	16:l:139:GLU:HB2	2.03	0.40
16:m:44:MET:SD	16:m:118:VAL:HG22	2.61	0.40
1:B:156:VAL:HG12	1:B:164:HIS:HB3	2.03	0.40
1:C:173:ARG:NH1	8:S:16:GLU:OE2	2.54	0.40
1:C:241:VAL:HG12	1:C:461:LEU:HD11	2.03	0.40
4:H:67:PHE:CE1	13:d:340:HIS:HB2	2.56	0.40
5:J:191:LYS:HB2	5:J:191:LYS:HE2	1.91	0.40
7:N:116:ILE:H	7:N:116:ILE:HD12	1.86	0.40
7:O:27:LYS:HZ2	7:O:27:LYS:HG2	1.80	0.40
10:a:807:HIS:O	10:a:811:PHE:HB3	2.21	0.40
15:f:32:PHE:HA	15:f:35:VAL:HG22	2.03	0.40
1:A:550:LEU:HA	1:A:553:ARG:HD3	2.02	0.40
1:B:535:TYR:CE2	1:B:594:GLU:HG3	2.56	0.40
3:G:331:LEU:H	3:G:331:LEU:HG	1.54	0.40
8:Q:42:LEU:HD13	8:Q:45:ILE:HD12	2.03	0.40
10:a:543:ILE:HG21	10:a:591:ILE:HD11	2.03	0.40
11:b:172:LEU:HD13	16:o:45:SER:OG	2.21	0.40
1:B:616:GLU:H	1:B:616:GLU:HG3	1.78	0.40
1:C:279:GLU:H	1:C:279:GLU:HG3	1.63	0.40
1:C:526:THR:HG23	1:C:529:ASP:H	1.87	0.40
8:S:134:ASN:HD22	8:S:134:ASN:HA	1.56	0.40
10:a:36:GLN:HB3	10:a:324:TRP:HB2	2.04	0.40
10:a:254:ARG:HA	10:a:257:MET:HG2	2.03	0.40
12:c:324:PHE:HB3	12:c:326:LEU:HG	2.04	0.40
13:d:187:LYS:HB3	13:d:187:LYS:HE3	1.82	0.40
16:h:24:VAL:CG1	16:i:101:LEU:HB2	2.51	0.40
16:h:44:MET:HE3	16:h:44:MET:HB3	1.86	0.40
16:k:117:GLY:O	16:k:121:THR:HG23	2.22	0.40
16:l:46:VAL:HG12	16:m:123:GLN:CD	2.46	0.40
16:o:32:TYR:CE2	16:o:108:PHE:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/617 (94%)	545 (94%)	35 (6%)	1 (0%)	43	72
1	B	598/617 (97%)	562 (94%)	34 (6%)	2 (0%)	36	65
1	C	598/617 (97%)	577 (96%)	18 (3%)	3 (0%)	24	56
2	D	452/515 (88%)	419 (93%)	33 (7%)	0	100	100
2	E	454/515 (88%)	426 (94%)	25 (6%)	3 (1%)	18	50
2	F	452/515 (88%)	430 (95%)	21 (5%)	1 (0%)	43	72
3	G	356/382 (93%)	337 (95%)	16 (4%)	3 (1%)	16	48
4	H	211/247 (85%)	203 (96%)	8 (4%)	0	100	100
5	I	215/226 (95%)	209 (97%)	6 (3%)	0	100	100
5	J	216/226 (96%)	211 (98%)	5 (2%)	0	100	100
5	K	215/226 (95%)	209 (97%)	6 (3%)	0	100	100
6	L	107/119 (90%)	97 (91%)	10 (9%)	0	100	100
7	M	108/118 (92%)	108 (100%)	0	0	100	100
7	N	108/118 (92%)	107 (99%)	1 (1%)	0	100	100
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%)	196 (96%)	8 (4%)	0	100	100
8	S	224/337 (66%)	215 (96%)	8 (4%)	1 (0%)	30	60
9	T	423/483 (88%)	399 (94%)	22 (5%)	2 (0%)	24	56
10	a	744/838 (89%)	706 (95%)	34 (5%)	4 (0%)	24	56
11	b	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
12	c	204/469 (44%)	181 (89%)	23 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	d	348/351 (99%)	334 (96%)	14 (4%)	0	100	100
14	e	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
15	f	82/98 (84%)	79 (96%)	3 (4%)	0	100	100
16	g	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	18	50
16	h	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
16	i	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
16	j	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
16	k	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
16	l	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
16	m	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	n	148/155 (96%)	138 (93%)	10 (7%)	0	100	100
16	o	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	18	50
17	p	51/351 (14%)	48 (94%)	2 (4%)	1 (2%)	6	32
All	All	8890/10458 (85%)	8472 (95%)	395 (4%)	23 (0%)	37	65

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	a	90	PHE
1	C	498	LYS
2	E	372	TYR
2	F	341	SER
3	G	251	PHE
16	o	10	TYR
1	A	139	LYS
2	E	293	ASP
9	T	120	ASN
10	a	4	LEU
10	a	583	LEU
1	B	171	ARG
1	C	413	PRO
3	G	344	SER
8	S	98	ILE
10	a	432	SER
1	B	450	TRP
1	C	350	SER
2	E	208	LYS

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Mol	Chain	Res	Type
9	T	124	SER
17	p	298	TYR
16	g	132	ILE
3	G	314	VAL

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	501/525 (95%)	460 (92%)	41 (8%)	10	36
1	B	508/525 (97%)	471 (93%)	37 (7%)	13	40
1	C	508/525 (97%)	480 (94%)	28 (6%)	19	46
2	D	390/438 (89%)	355 (91%)	35 (9%)	9	33
2	E	392/438 (90%)	371 (95%)	21 (5%)	20	46
2	F	390/438 (89%)	335 (86%)	55 (14%)	3	18
3	G	325/344 (94%)	302 (93%)	23 (7%)	13	40
4	H	184/211 (87%)	159 (86%)	25 (14%)	3	19
5	I	96/197 (49%)	77 (80%)	19 (20%)	1	9
5	J	191/197 (97%)	173 (91%)	18 (9%)	8	32
5	K	190/197 (96%)	187 (98%)	3 (2%)	55	68
6	L	93/100 (93%)	88 (95%)	5 (5%)	20	46
7	M	33/101 (33%)	30 (91%)	3 (9%)	9	33
7	N	95/101 (94%)	89 (94%)	6 (6%)	16	43
7	O	94/101 (93%)	84 (89%)	10 (11%)	6	27
8	Q	203/305 (67%)	183 (90%)	20 (10%)	7	30
8	R	188/305 (62%)	176 (94%)	12 (6%)	16	43
8	S	204/305 (67%)	186 (91%)	18 (9%)	9	33
9	T	385/429 (90%)	355 (92%)	30 (8%)	11	37
10	a	668/743 (90%)	617 (92%)	51 (8%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	b	156/158 (99%)	149 (96%)	7 (4%)	24	49
12	c	179/387 (46%)	154 (86%)	25 (14%)	3	18
13	d	305/306 (100%)	268 (88%)	37 (12%)	5	22
14	e	71/72 (99%)	70 (99%)	1 (1%)	59	70
15	f	70/83 (84%)	65 (93%)	5 (7%)	13	40
16	g	105/109 (96%)	103 (98%)	2 (2%)	50	65
16	h	105/109 (96%)	96 (91%)	9 (9%)	10	34
16	i	105/109 (96%)	100 (95%)	5 (5%)	23	48
16	j	105/109 (96%)	99 (94%)	6 (6%)	18	45
16	k	105/109 (96%)	102 (97%)	3 (3%)	37	57
16	l	105/109 (96%)	105 (100%)	0	100	100
16	m	105/109 (96%)	95 (90%)	10 (10%)	8	31
16	n	105/109 (96%)	103 (98%)	2 (2%)	50	65
16	o	105/109 (96%)	103 (98%)	2 (2%)	50	65
17	p	48/311 (15%)	45 (94%)	3 (6%)	16	43
All	All	7412/8823 (84%)	6835 (92%)	577 (8%)	14	37

All (577) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLU
1	A	70	THR
1	A	71	SER
1	A	89	GLU
1	A	130	ASP
1	A	140	ASN
1	A	141	LEU
1	A	155	ILE
1	A	156	VAL
1	A	167	MET
1	A	171	ARG
1	A	173	ARG
1	A	188	SER
1	A	220	LYS
1	A	221	LEU
1	A	279	GLU
1	A	284	MET

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Mol	Chain	Res	Type
1	A	315	THR
1	A	317	ASN
1	A	340	MET
1	A	372	SER
1	A	391	ARG
1	A	392	VAL
1	A	393	LYS
1	A	394	CYS
1	A	399	GLU
1	A	400	ARG
1	A	401	GLU
1	A	425	THR
1	A	438	LYS
1	A	439	LEU
1	A	451	LEU
1	A	458	MET
1	A	549	ASP
1	A	550	LEU
1	A	552	ARG
1	A	553	ARG
1	A	555	VAL
1	A	590	VAL
1	A	596	LYS
1	A	616	GLU
1	B	141	LEU
1	B	155	ILE
1	B	156	VAL
1	B	166	ILE
1	B	167	MET
1	B	179	ILE
1	B	211	VAL
1	B	229	THR
1	B	233	VAL
1	B	237	LEU
1	B	277	CYS
1	B	285	SER
1	B	289	ARG
1	B	316	SER
1	B	318	MET
1	B	320	VAL
1	B	324	GLU
1	B	327	ILE

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Mol	Chain	Res	Type
1	B	361	ILE
1	B	382	LEU
1	B	384	SER
1	B	387	GLU
1	B	393	LYS
1	B	400	ARG
1	B	403	SER
1	B	450	TRP
1	B	471	GLU
1	B	473	VAL
1	B	476	ARG
1	B	477	THR
1	B	493	VAL
1	B	495	LEU
1	B	496	VAL
1	B	530	ARG
1	B	609	GLN
1	B	613	ARG
1	B	616	GLU
1	C	25	SER
1	C	152	ILE
1	C	167	MET
1	C	220	LYS
1	C	275	VAL
1	C	279	GLU
1	C	284	MET
1	C	289	ARG
1	C	293	GLU
1	C	311	LEU
1	C	344	VAL
1	C	346	MET
1	C	350	SER
1	C	351	THR
1	C	352	SER
1	C	387	GLU
1	C	392	VAL
1	C	393	LYS
1	C	400	ARG
1	C	411	SER
1	C	442	ARG
1	C	443	LYS
1	C	492	ILE

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Mol	Chain	Res	Type
1	C	494	GLN
1	C	510	GLU
1	C	577	ILE
1	C	580	LYS
1	C	584	MET
2	D	33	TYR
2	D	82	GLU
2	D	105	THR
2	D	112	ILE
2	D	147	ILE
2	D	165	GLN
2	D	166	THR
2	D	168	ILE
2	D	175	ASN
2	D	200	ILE
2	D	270	ARG
2	D	304	VAL
2	D	309	GLU
2	D	315	ARG
2	D	321	MET
2	D	327	THR
2	D	353	ASP
2	D	371	ILE
2	D	380	ARG
2	D	381	GLN
2	D	404	MET
2	D	405	THR
2	D	407	LYS
2	D	447	GLU
2	D	458	ASN
2	D	463	GLU
2	D	464	LYS
2	D	465	ARG
2	D	466	SER
2	D	469	GLU
2	D	473	LEU
2	D	487	LYS
2	D	489	ILE
2	D	493	MET
2	D	499	SER
2	E	39	VAL
2	E	40	THR

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Mol	Chain	Res	Type
2	E	120	ASP
2	E	121	MET
2	E	139	VAL
2	E	159	TYR
2	E	183	ILE
2	E	248	MET
2	E	252	CYS
2	E	257	LEU
2	E	267	ILE
2	E	271	LEU
2	E	299	GLU
2	E	323	THR
2	E	359	ILE
2	E	366	ILE
2	E	405	THR
2	E	407	LYS
2	E	411	ASP
2	E	453	GLU
2	E	500	ARG
2	F	66	VAL
2	F	72	ASN
2	F	77	SER
2	F	89	ILE
2	F	92	VAL
2	F	96	THR
2	F	97	SER
2	F	99	ILE
2	F	121	MET
2	F	122	LEU
2	F	124	ARG
2	F	138	VAL
2	F	139	VAL
2	F	147	ILE
2	F	158	ILE
2	F	161	GLU
2	F	162	GLU
2	F	183	ILE
2	F	195	GLU
2	F	240	SER
2	F	253	LEU
2	F	257	LEU
2	F	262	THR

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Mol	Chain	Res	Type
2	F	263	ILE
2	F	266	ILE
2	F	267	ILE
2	F	268	THR
2	F	271	LEU
2	F	273	LEU
2	F	274	THR
2	F	299	GLU
2	F	308	ARG
2	F	310	GLU
2	F	311	VAL
2	F	328	ILE
2	F	330	GLU
2	F	334	ARG
2	F	342	ILE
2	F	348	LEU
2	F	362	LEU
2	F	371	ILE
2	F	375	ARG
2	F	377	LEU
2	F	386	ILE
2	F	388	VAL
2	F	389	LEU
2	F	392	LEU
2	F	394	ARG
2	F	411	ASP
2	F	457	ILE
2	F	459	GLN
2	F	465	ARG
2	F	483	LYS
2	F	487	LYS
2	F	489	ILE
3	G	162	LEU
3	G	180	GLU
3	G	186	LEU
3	G	187	VAL
3	G	188	VAL
3	G	230	PHE
3	G	249	ARG
3	G	265	MET
3	G	268	LEU
3	G	269	SER

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Mol	Chain	Res	Type
3	G	272	LYS
3	G	279	LEU
3	G	305	GLU
3	G	329	LYS
3	G	331	LEU
3	G	332	ARG
3	G	333	GLU
3	G	334	VAL
3	G	345	SER
3	G	365	GLU
3	G	370	VAL
3	G	371	TYR
3	G	373	LYS
4	H	13	ARG
4	H	17	THR
4	H	19	MET
4	H	20	LYS
4	H	42	LEU
4	H	43	ARG
4	H	45	ARG
4	H	48	LEU
4	H	49	LYS
4	H	50	LYS
4	H	124	LEU
4	H	131	LEU
4	H	167	ARG
4	H	176	ILE
4	H	190	GLU
4	H	195	GLU
4	H	203	LYS
4	H	204	LYS
4	H	209	LYS
4	H	210	LYS
4	H	212	LEU
4	H	213	LYS
4	H	214	GLU
4	H	215	LYS
4	H	217	GLU
5	I	121	LEU
5	I	126	GLN
5	I	127	LEU
5	I	128	LEU

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Mol	Chain	Res	Type
5	I	132	MET
5	I	156	LYS
5	I	159	THR
5	I	160	LYS
5	I	164	ASP
5	I	177	ILE
5	I	181	VAL
5	I	183	ILE
5	I	188	ARG
5	I	190	ILE
5	I	193	SER
5	I	195	THR
5	I	197	GLU
5	I	200	LEU
5	I	203	ILE
5	J	15	MET
5	J	39	ASN
5	J	44	ARG
5	J	46	VAL
5	J	76	MET
5	J	78	GLN
5	J	80	ARG
5	J	81	LEU
5	J	82	LYS
5	J	84	LEU
5	J	85	ARG
5	J	156	LYS
5	J	160	LYS
5	J	162	ASP
5	J	191	LYS
5	J	201	ASP
5	J	202	LEU
5	J	212	ARG
5	K	35	GLU
5	K	70	ILE
5	K	78	GLN
6	L	72	GLU
6	L	73	MET
6	L	75	ARG
6	L	102	LYS
6	L	107	ARG
7	M	103	VAL

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Mol	Chain	Res	Type
7	M	106	ILE
7	M	110	ILE
7	N	27	LYS
7	N	29	LYS
7	N	32	ARG
7	N	34	LYS
7	N	35	GLN
7	N	37	LYS
7	O	21	LYS
7	O	27	LYS
7	O	28	ARG
7	O	32	ARG
7	O	33	LEU
7	O	34	LYS
7	O	81	MET
7	O	84	LEU
7	O	87	TYR
7	O	90	GLN
8	Q	29	ILE
8	Q	36	ILE
8	Q	37	ASP
8	Q	43	LYS
8	Q	46	ARG
8	Q	47	GLU
8	Q	52	VAL
8	Q	53	LEU
8	Q	82	SER
8	Q	83	ARG
8	Q	123	LYS
8	Q	138	ASP
8	Q	188	MET
8	Q	192	LYS
8	Q	193	ILE
8	Q	194	ASP
8	Q	196	GLN
8	Q	199	LEU
8	Q	201	LYS
8	Q	205	LYS
8	R	77	ASP
8	R	89	GLN
8	R	178	LEU
8	R	181	LEU

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Mol	Chain	Res	Type
8	R	193	ILE
8	R	194	ASP
8	R	198	HIS
8	R	199	LEU
8	R	201	LYS
8	R	205	LYS
8	R	206	ASP
8	R	217	LEU
8	S	43	LYS
8	S	92	LEU
8	S	94	LEU
8	S	130	LEU
8	S	134	ASN
8	S	155	MET
8	S	181	LEU
8	S	201	LYS
8	S	203	TYR
8	S	205	LYS
8	S	207	GLN
8	S	211	SER
8	S	214	GLU
8	S	217	LEU
8	S	220	GLU
8	S	221	ASP
8	S	223	LYS
8	S	227	LYS
9	T	50	ILE
9	T	51	GLN
9	T	52	ARG
9	T	61	GLU
9	T	68	THR
9	T	86	LYS
9	T	87	GLU
9	T	116	LYS
9	T	117	ARG
9	T	118	SER
9	T	131	ASN
9	T	132	ARG
9	T	133	GLN
9	T	135	LEU
9	T	138	VAL
9	T	145	ILE

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Mol	Chain	Res	Type
9	T	207	LEU
9	T	219	VAL
9	T	260	LEU
9	T	261	ARG
9	T	262	ARG
9	T	297	THR
9	T	299	ARG
9	T	300	GLU
9	T	302	ARG
9	T	414	VAL
9	T	416	GLU
9	T	447	GLN
9	T	453	LEU
9	T	457	GLN
10	a	7	SER
10	a	9	GLU
10	a	32	LEU
10	a	38	ARG
10	a	115	GLN
10	a	185	ARG
10	a	186	MET
10	a	195	VAL
10	a	277	ASP
10	a	280	GLN
10	a	281	ARG
10	a	284	GLN
10	a	322	GLU
10	a	323	VAL
10	a	378	VAL
10	a	383	ILE
10	a	385	THR
10	a	388	GLU
10	a	394	TYR
10	a	439	MET
10	a	445	SER
10	a	528	ASN
10	a	530	LEU
10	a	534	ASN
10	a	538	MET
10	a	546	ILE
10	a	549	MET
10	a	550	MET

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Mol	Chain	Res	Type
10	a	553	VAL
10	a	554	SER
10	a	583	LEU
10	a	587	LEU
10	a	643	VAL
10	a	646	LEU
10	a	653	LEU
10	a	654	ILE
10	a	659	LEU
10	a	660	ARG
10	a	721	GLN
10	a	738	SER
10	a	740	LEU
10	a	742	LEU
10	a	745	LEU
10	a	776	LEU
10	a	810	GLU
10	a	812	GLN
10	a	814	LYS
10	a	829	GLU
10	a	830	HIS
10	a	831	ILE
10	a	832	ARG
11	b	37	VAL
11	b	41	LEU
11	b	43	GLU
11	b	76	ILE
11	b	112	SER
11	b	114	MET
11	b	184	SER
12	c	266	ILE
12	c	274	SER
12	c	282	GLU
12	c	284	LEU
12	c	288	THR
12	c	289	PHE
12	c	303	ASP
12	c	305	VAL
12	c	323	LYS
12	c	325	ILE
12	c	326	LEU
12	c	332	GLN

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Mol	Chain	Res	Type
12	c	333	VAL
12	c	334	SER
12	c	337	HIS
12	c	338	TRP
12	c	339	PHE
12	c	343	ARG
12	c	344	LEU
12	c	393	GLN
12	c	394	LEU
12	c	395	THR
12	c	409	GLU
12	c	410	ARG
12	c	452	MET
13	d	20	VAL
13	d	81	GLU
13	d	83	ARG
13	d	85	MET
13	d	101	THR
13	d	105	MET
13	d	106	ILE
13	d	109	VAL
13	d	110	ILE
13	d	146	THR
13	d	160	LEU
13	d	168	ILE
13	d	169	SER
13	d	170	GLU
13	d	180	ILE
13	d	182	ARG
13	d	185	LEU
13	d	213	GLU
13	d	217	ASP
13	d	218	ARG
13	d	221	PHE
13	d	227	SER
13	d	233	SER
13	d	239	LYS
13	d	246	ARG
13	d	247	LEU
13	d	252	LEU
13	d	257	ARG
13	d	259	ASP

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Mol	Chain	Res	Type
13	d	276	LEU
13	d	279	GLU
13	d	288	LYS
13	d	289	THR
13	d	290	LEU
13	d	291	GLU
13	d	292	ASP
13	d	320	LYS
14	e	68	LEU
15	f	18	LEU
15	f	40	LEU
15	f	62	TYR
15	f	69	CYS
15	f	79	LEU
16	g	119	ARG
16	g	155	LYS
16	h	44	MET
16	h	46	VAL
16	h	47	MET
16	h	51	LEU
16	h	70	LEU
16	h	119	ARG
16	h	123	GLN
16	h	133	LEU
16	h	136	ILE
16	i	23	MET
16	i	48	ARG
16	i	67	ILE
16	i	70	LEU
16	i	80	LEU
16	j	44	MET
16	j	64	ILE
16	j	115	ASP
16	j	121	THR
16	j	135	LEU
16	j	136	ILE
16	k	44	MET
16	k	46	VAL
16	k	47	MET
16	m	16	VAL
16	m	56	ILE
16	m	57	ILE

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Mol	Chain	Res	Type
16	m	61	MET
16	m	64	ILE
16	m	136	ILE
16	m	139	GLU
16	m	140	VAL
16	m	141	LEU
16	m	143	LEU
16	n	78	ASN
16	n	123	GLN
16	o	24	VAL
16	o	36	LYS
17	p	296	LEU
17	p	332	MET
17	p	343	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	164	HIS
1	A	242	GLN
1	A	317	ASN
1	A	441	GLN
1	A	543	ASN
1	B	146	HIS
1	B	157	ASN
1	B	164	HIS
1	B	184	ASN
1	B	317	ASN
1	B	397	ASN
1	C	184	ASN
1	C	213	GLN
1	C	242	GLN
1	C	397	ASN
2	D	175	ASN
2	D	344	GLN
2	D	450	GLN
2	E	148	ASN
2	E	256	ASN
2	E	352	ASN
2	E	379	ASN
2	E	381	GLN

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Mol	Chain	Res	Type
2	E	414	ASN
2	F	61	GLN
2	F	75	GLN
2	F	79	GLN
2	F	155	HIS
2	F	256	ASN
2	F	259	ASN
2	F	414	ASN
2	F	458	ASN
2	F	459	GLN
3	G	200	GLN
3	G	286	ASN
4	H	46	GLN
4	H	86	ASN
4	H	206	GLN
5	I	122	GLN
5	I	126	GLN
5	I	205	GLN
5	J	39	ASN
5	J	47	GLN
5	J	71	GLN
5	J	126	GLN
5	J	169	GLN
5	J	206	GLN
5	J	221	ASN
5	K	166	GLN
6	L	96	HIS
7	N	9	GLN
7	N	30	ASN
7	N	66	HIS
7	N	85	GLN
7	O	9	GLN
7	O	30	ASN
7	O	50	GLN
7	O	66	HIS
7	O	91	ASN
8	Q	127	HIS
8	Q	131	ASN
8	Q	134	ASN
8	R	40	ASN
8	R	127	HIS
8	R	131	ASN

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Mol	Chain	Res	Type
8	R	198	HIS
8	S	17	GLN
8	S	177	GLN
8	S	196	GLN
8	S	207	GLN
8	S	222	GLN
9	T	104	ASN
9	T	320	ASN
9	T	379	ASN
9	T	412	HIS
9	T	420	HIS
9	T	447	GLN
9	T	457	GLN
10	a	18	GLN
10	a	115	GLN
10	a	273	ASN
10	a	359	GLN
10	a	498	ASN
10	a	534	ASN
10	a	626	ASN
10	a	751	GLN
11	b	90	ASN
11	b	130	ASN
12	c	271	GLN
12	c	332	GLN
12	c	337	HIS
12	c	379	ASN
13	d	88	HIS
13	d	183	ASN
13	d	243	HIS
13	d	297	HIS
14	e	67	GLN
15	f	53	ASN
16	h	123	GLN
16	i	78	ASN
16	j	78	ASN
16	m	78	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	ADP	C	701	-	28,29,29	0.47	0	43,45,45	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ADP	C	701	-	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	701	ADP	O4'-C4'-C5'-O5'
18	C	701	ADP	C3'-C4'-C5'-O5'
18	C	701	ADP	C5'-O5'-PA-O1A
18	C	701	ADP	C5'-O5'-PA-O2A

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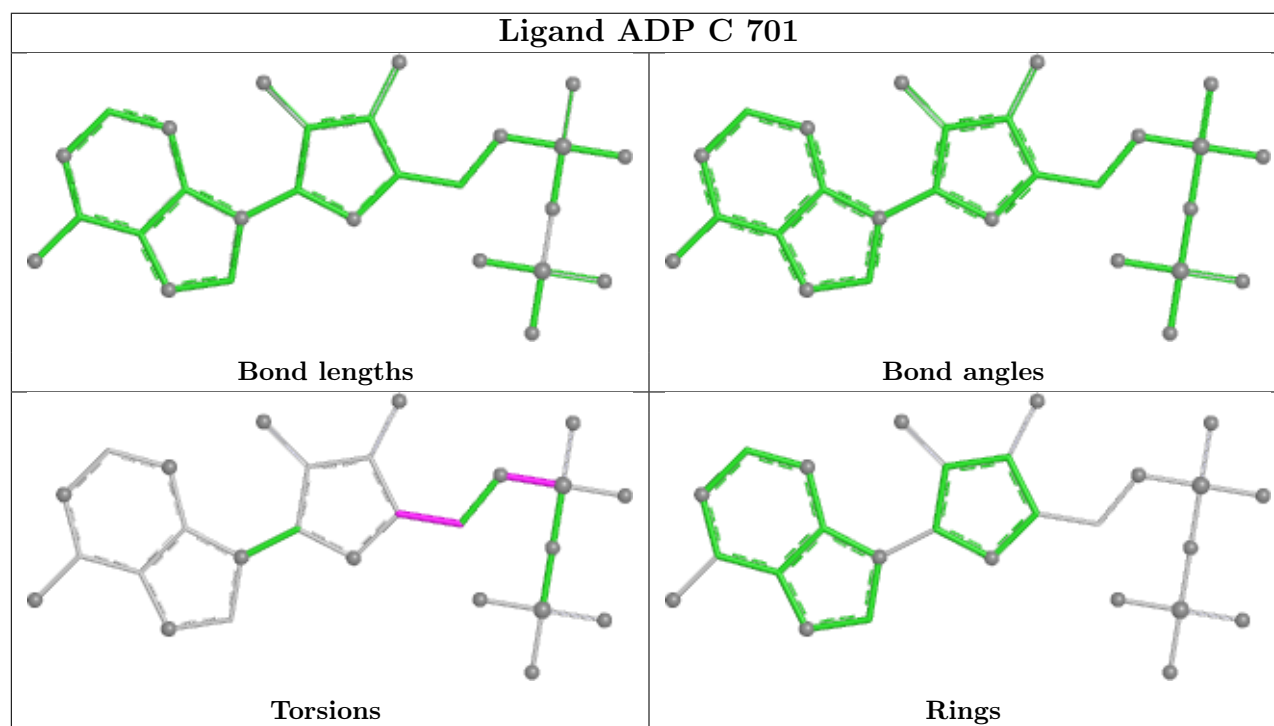
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Mol	Chain	Res	Type	Atoms
18	C	701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

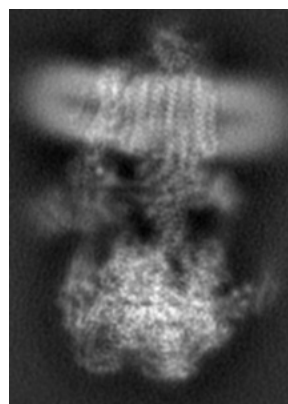
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26386. These allow visual inspection of the internal detail of the map and identification of artifacts.

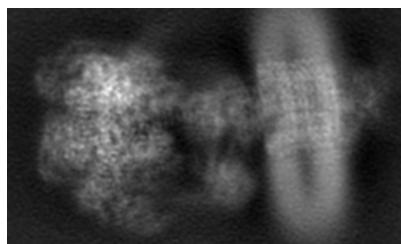
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

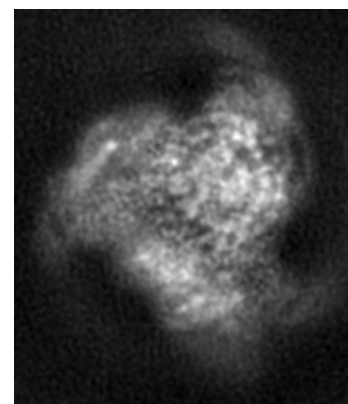
6.1.1 Primary map



X



Y

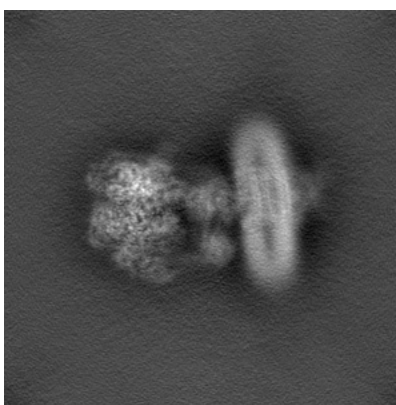


Z

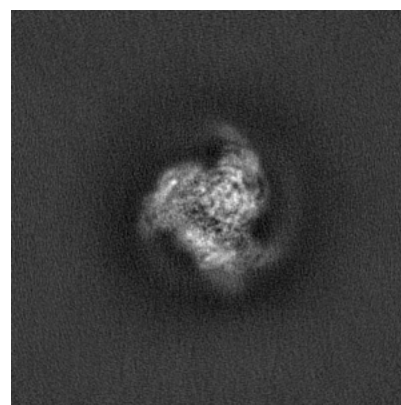
6.1.2 Raw map



X



Y



Z

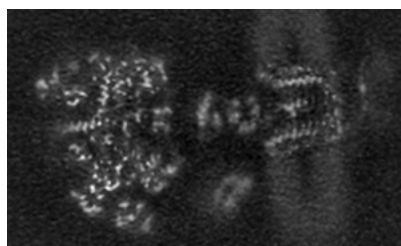
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

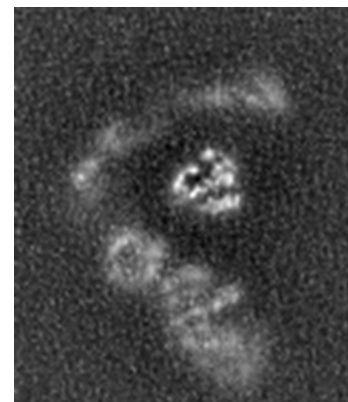
6.2.1 Primary map



X Index: 60

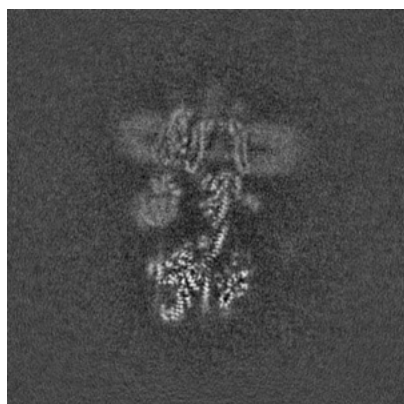


Y Index: 70

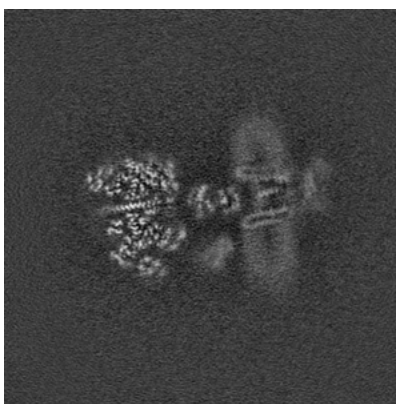


Z Index: 100

6.2.2 Raw map



X Index: 150



Y Index: 150

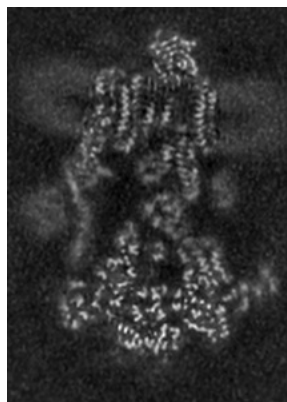


Z Index: 150

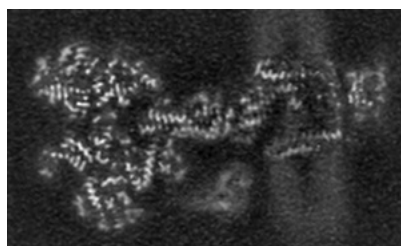
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

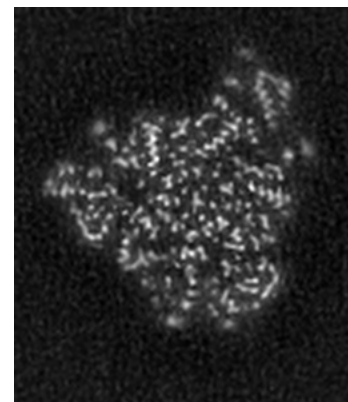
6.3.1 Primary map



X Index: 73

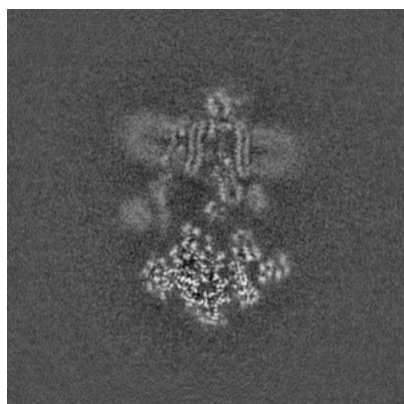


Y Index: 78

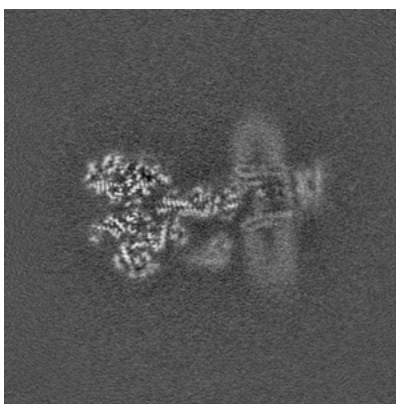


Z Index: 47

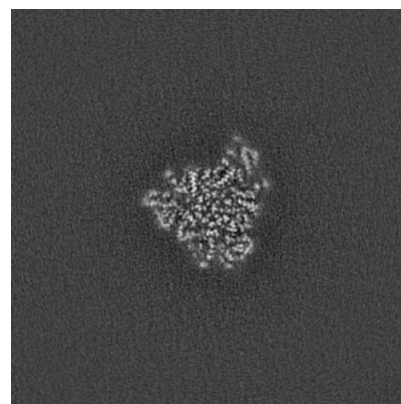
6.3.2 Raw map



X Index: 166



Y Index: 156

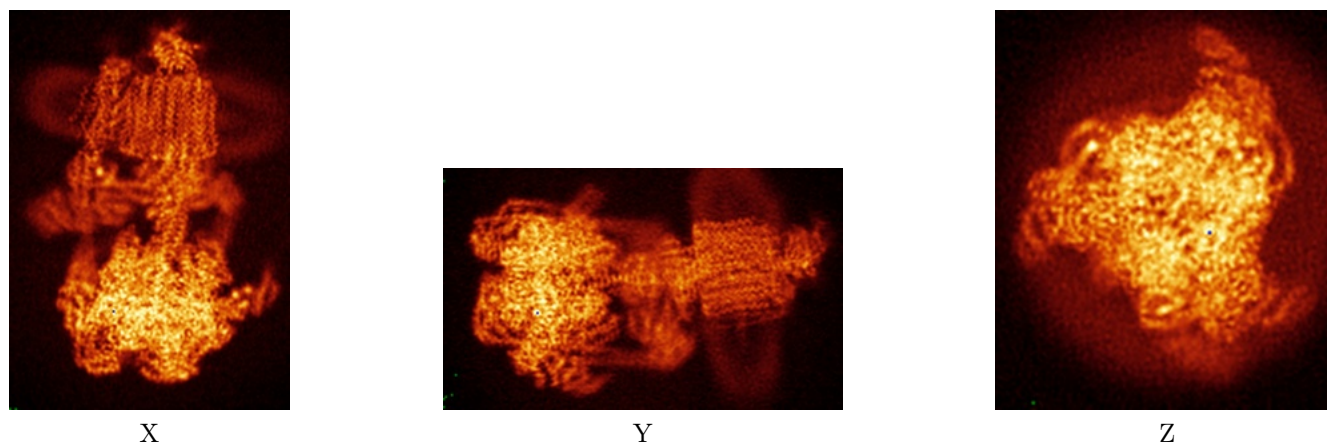


Z Index: 95

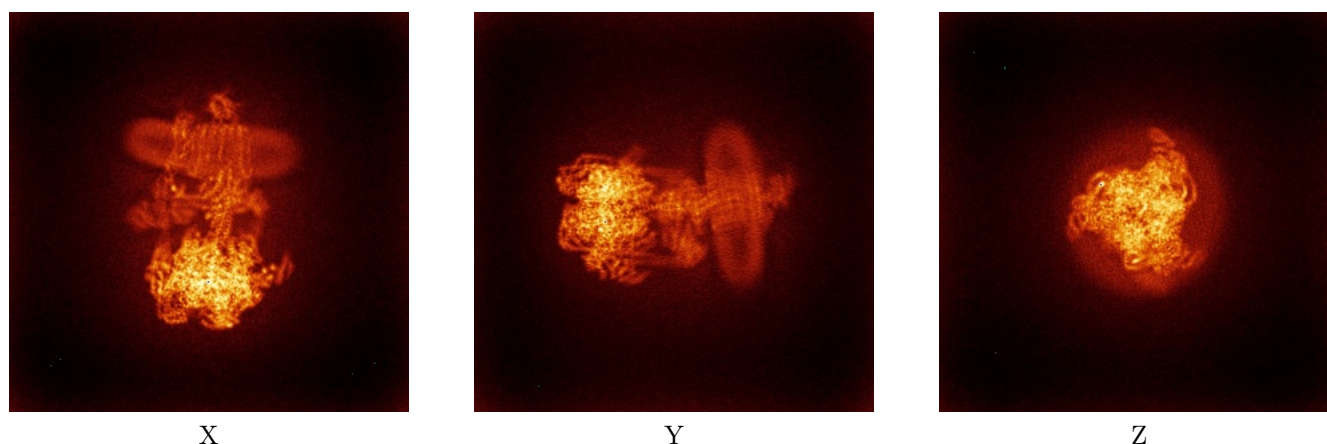
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

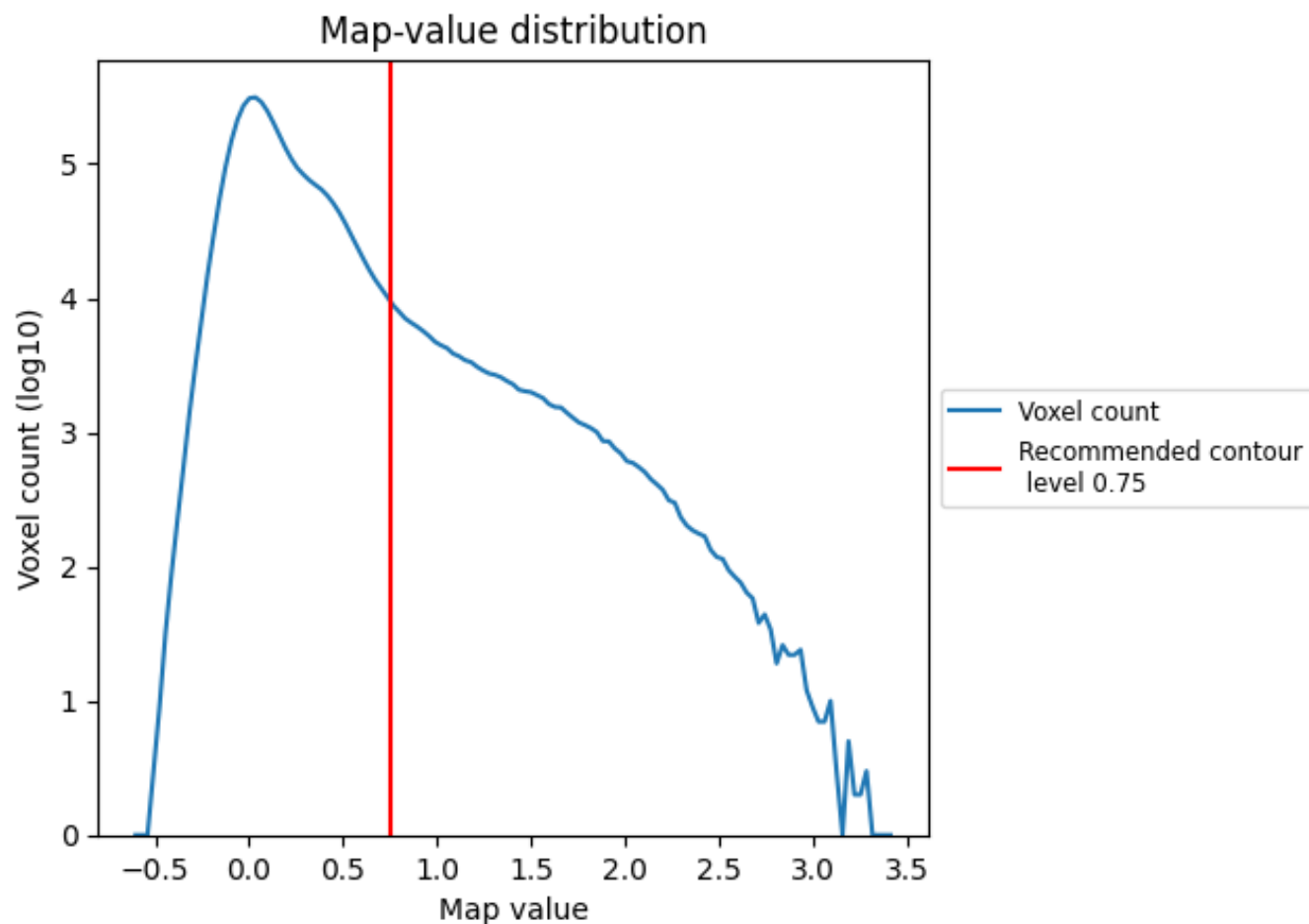
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

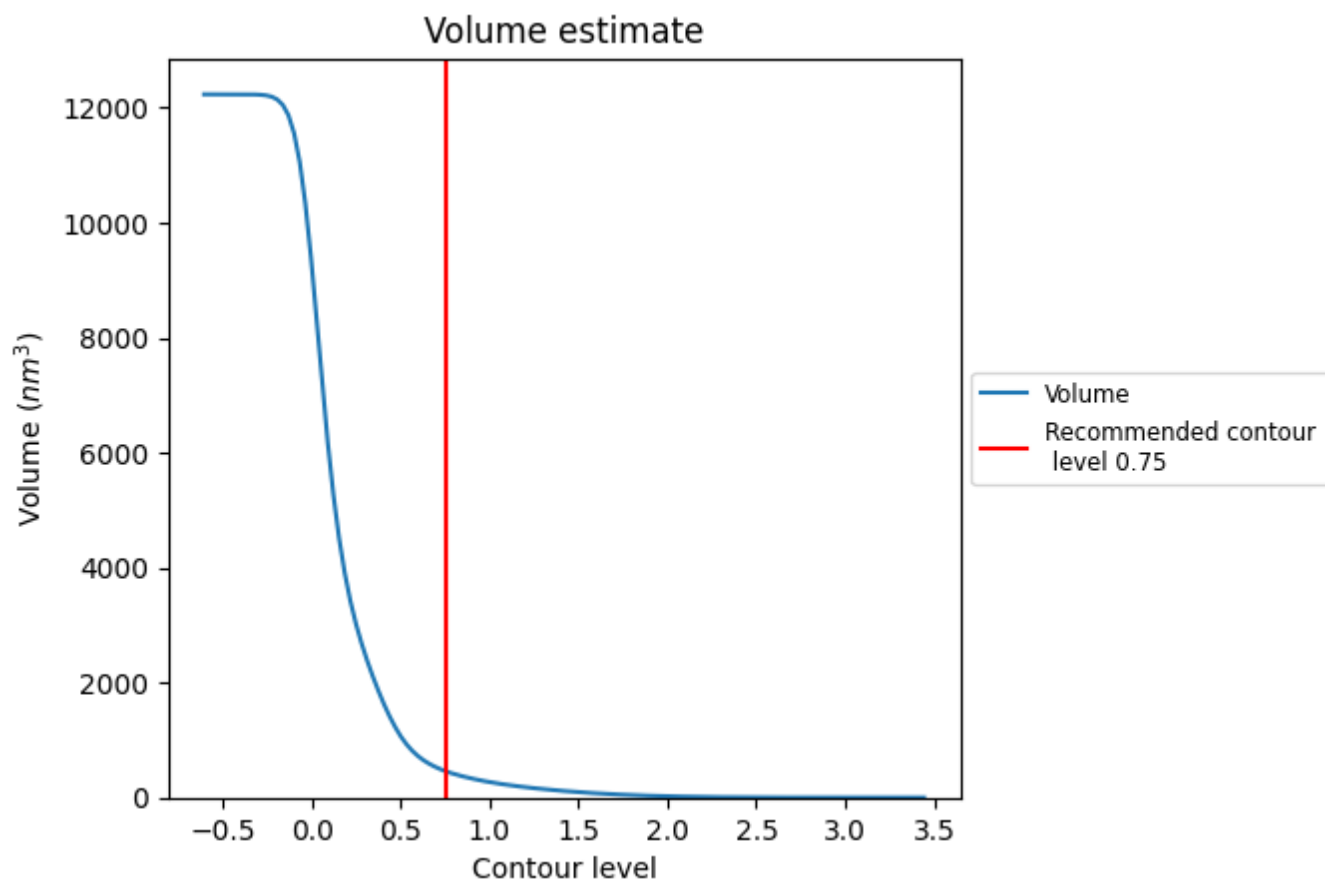
This section contains the results of statistical analysis of the map.

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 463 nm³; this corresponds to an approximate mass of 418 kDa.

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

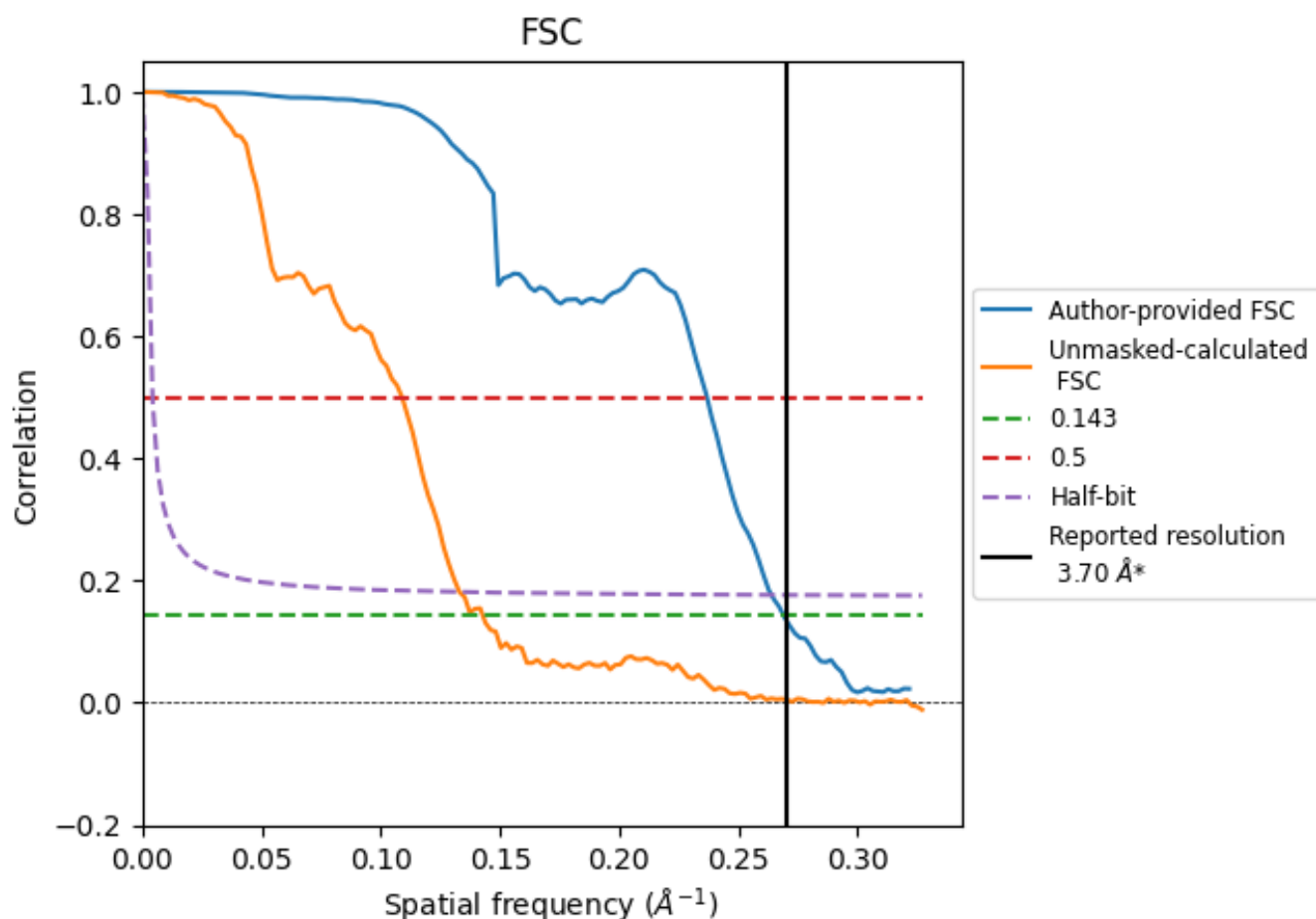
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

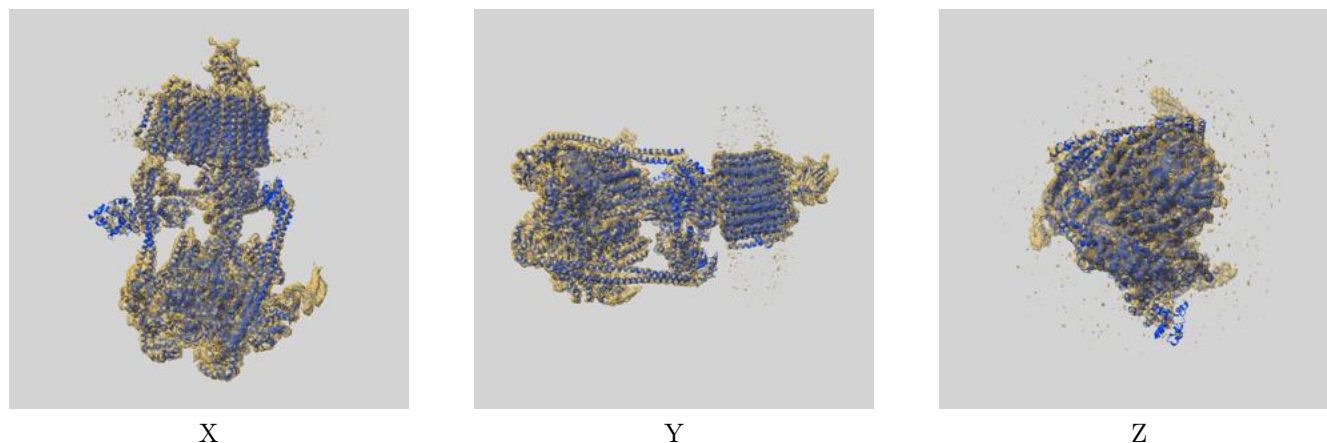
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.22	3.79
Unmasked-calculated*	7.00	9.17	7.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

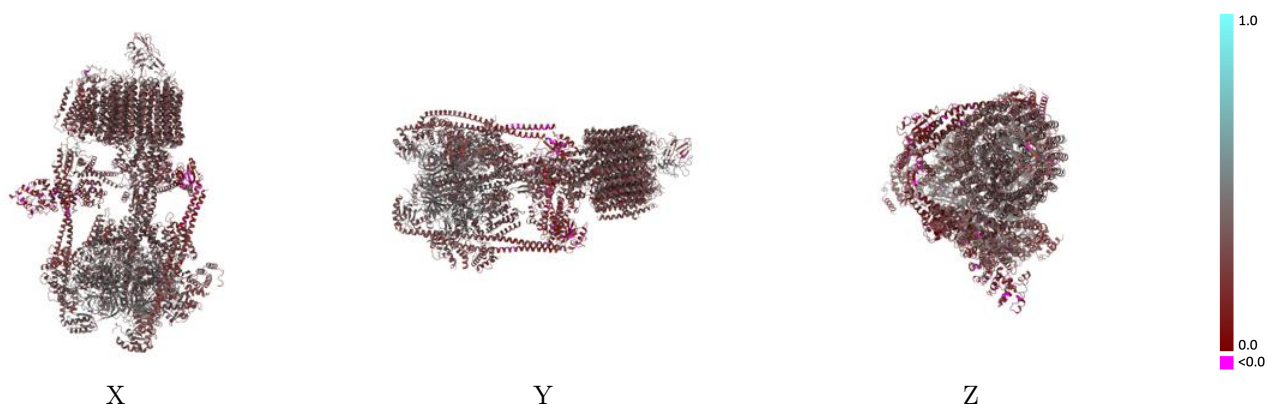
This section contains information regarding the fit between EMDB map EMD-26386 and PDB model 7U8P. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



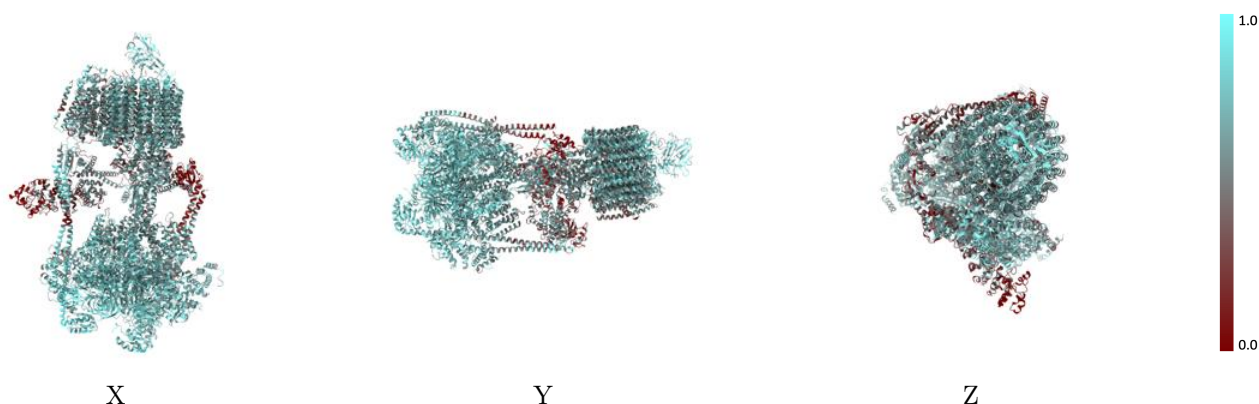
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



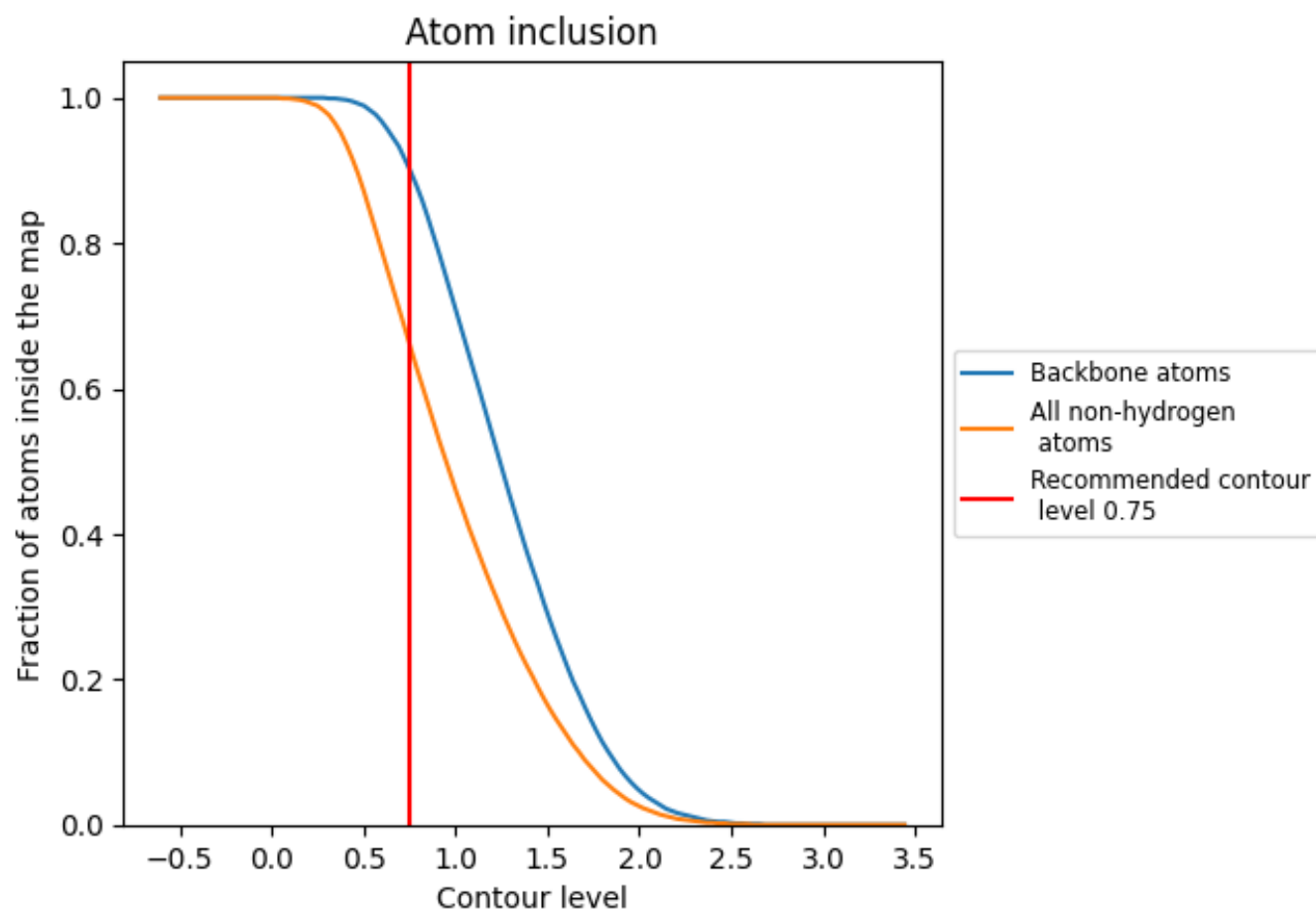
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 66% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6600	 0.3340
A	 0.7600	 0.3950
B	 0.7490	 0.3800
C	 0.7820	 0.3980
D	 0.7920	 0.4110
E	 0.7990	 0.4150
F	 0.7810	 0.4040
G	 0.3100	 0.1650
H	 0.7000	 0.3600
I	 0.8090	 0.3470
J	 0.7240	 0.3200
K	 0.6440	 0.3020
L	 0.6410	 0.3400
M	 0.7480	 0.3000
N	 0.6530	 0.2740
O	 0.5740	 0.2610
Q	 0.7150	 0.3110
R	 0.7220	 0.3170
S	 0.6880	 0.3090
T	 0.3030	 0.1780
a	 0.5600	 0.2840
b	 0.6650	 0.3380
c	 0.7250	 0.3530
d	 0.5880	 0.3320
e	 0.6330	 0.3410
f	 0.4970	 0.2690
g	 0.6570	 0.3510
h	 0.6210	 0.3280
i	 0.6590	 0.3390
j	 0.6400	 0.3400
k	 0.5930	 0.3340
l	 0.5930	 0.3190
m	 0.6140	 0.3260
n	 0.6460	 0.3260
o	 0.6590	 0.3300
p	 0.5870	 0.3650

