



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:44 PM UTC

PDB ID : 7U8Q / pdb_00007u8q
EMDB ID : EMD-26387
Title : Structure of porcine kidney V-ATPase with SidK, Rotary State 2
Authors : Tan, Y.Z.; Keon, K.A.
Deposited on : 2022-03-09
Resolution : 4.10 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

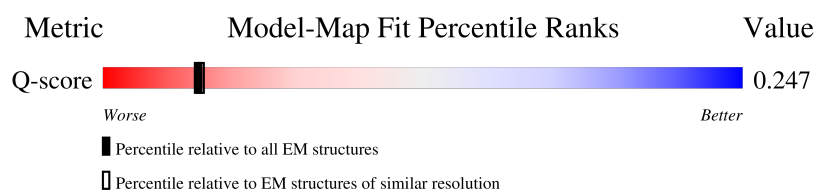
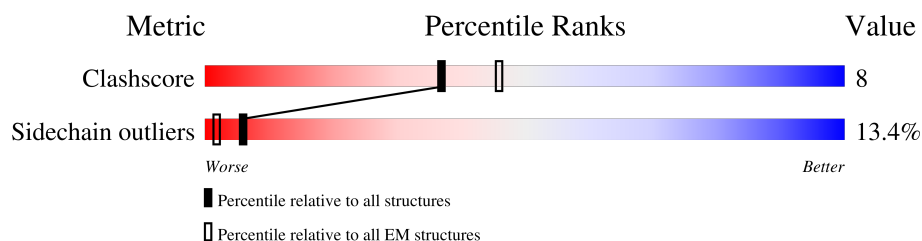
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	
2	E	515	

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Mol	Chain	Length	Quality of chain
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	
16	k	155	

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Mol	Chain	Length	Quality of chain
16	l	155	28% 90% 6%
16	m	155	19% 92% 5%
16	n	155	26% 91% 6%
16	o	155	46% 90% 7%
17	p	351	15% 85%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 62638 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	360	Total	C	N	O	S	0	0
			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	0	0
			3707	2207	750	750		

- 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	0	0
			989	583	203	203		

- 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	0	0
			1016	604	206	206		

- 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	0	0
			394	234	80	80		

- Molecule 15 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	f	84	Total	C	N	O	0	0
			412	244	84	84		

- 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	0	0
			729	429	150	150		
16	h	150	Total	C	N	O	0	0
			729	429	150	150		
16	i	150	Total	C	N	O	0	0
			729	429	150	150		

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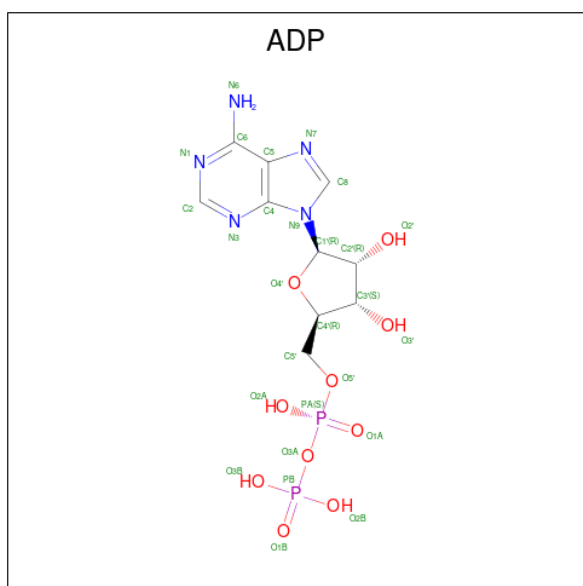
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Mol	Chain	Residues	Atoms				AltConf	Trace
16	j	150	Total	C	N	O	0	0
			729	429	150	150		
16	k	150	Total	C	N	O	0	0
			729	429	150	150		
16	l	150	Total	C	N	O	0	0
			729	429	150	150		
16	m	150	Total	C	N	O	0	0
			729	429	150	150		
16	n	150	Total	C	N	O	0	0
			729	429	150	150		
16	o	150	Total	C	N	O	0	0
			729	429	150	150		

- 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	0	0
			264	158	53	53		

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

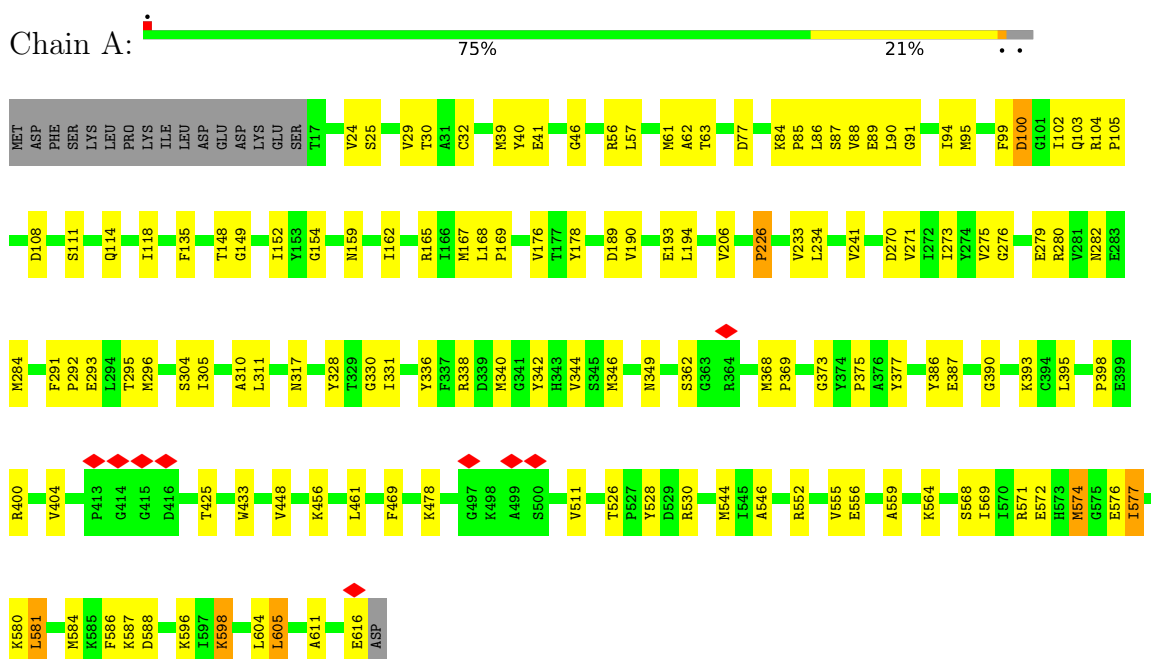


Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

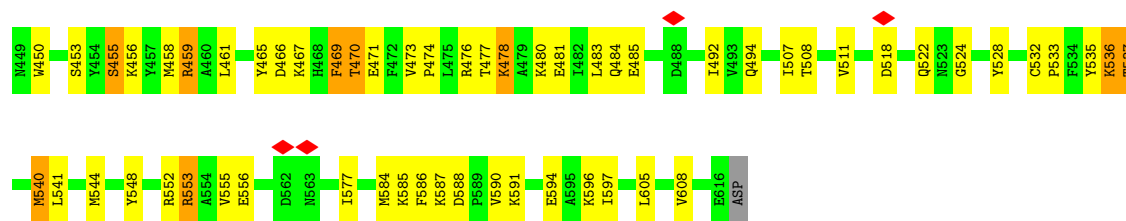
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

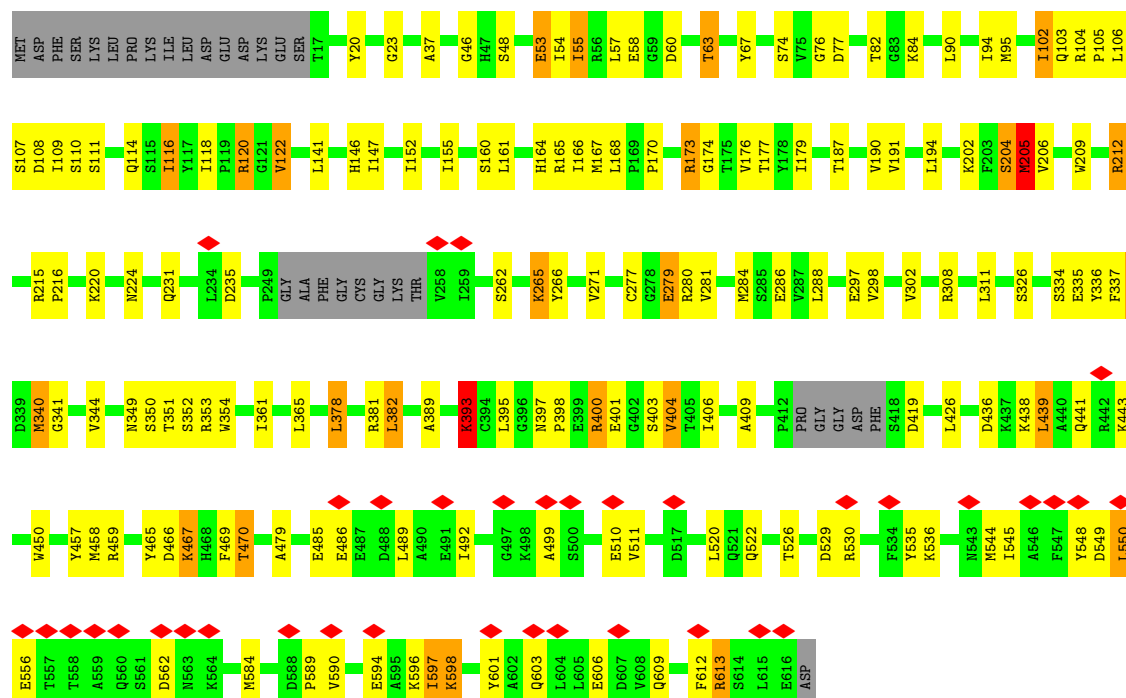


• Molecule 1: V-type proton ATPase catalytic subunit A

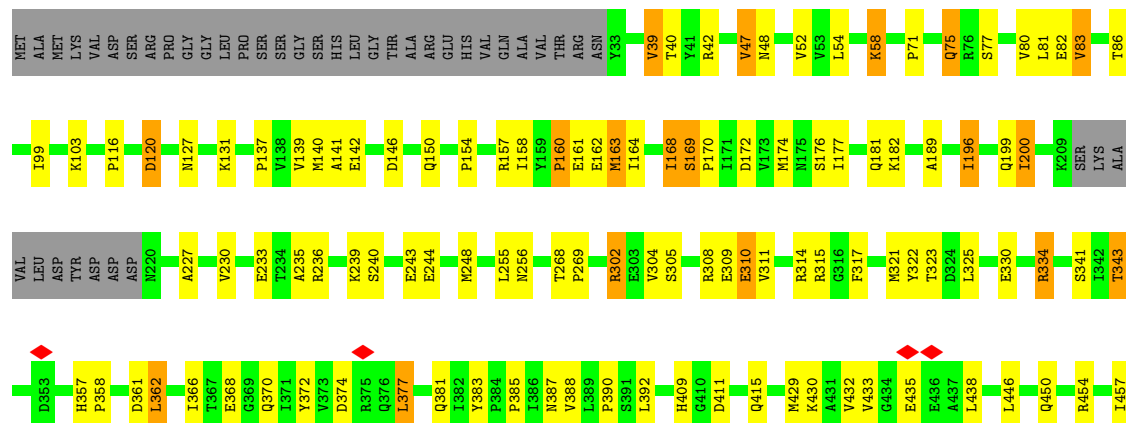




• Molecule 1: V-type proton ATPase catalytic subunit A



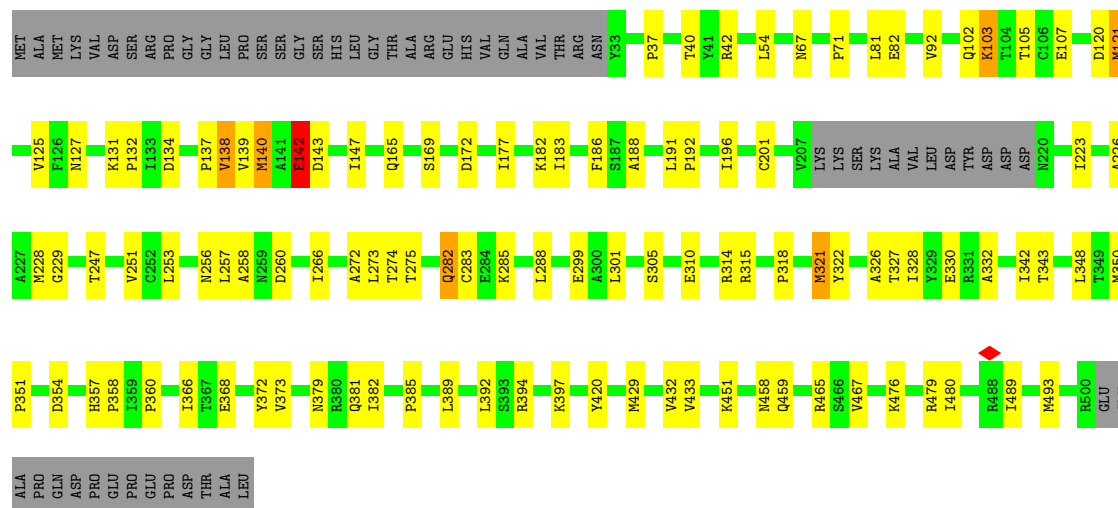
• Molecule 2: Vacuolar proton pump subunit B





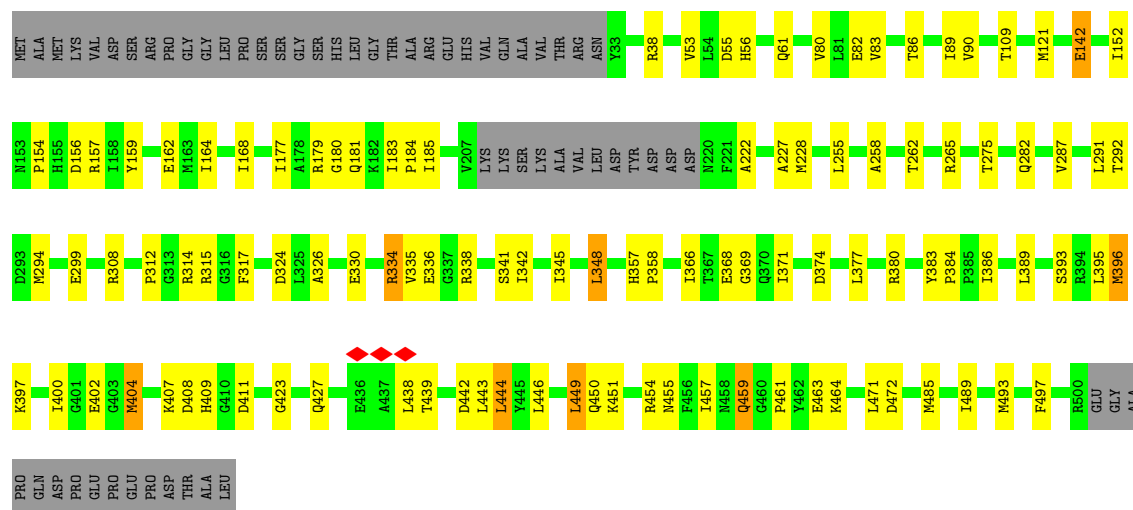
• Molecule 2: Vacuolar proton pump subunit B

Chain E: 68% 20% 11%



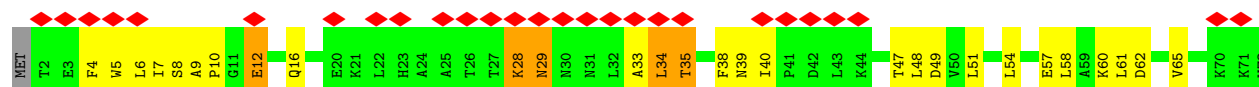
• Molecule 2: Vacuolar proton pump subunit B

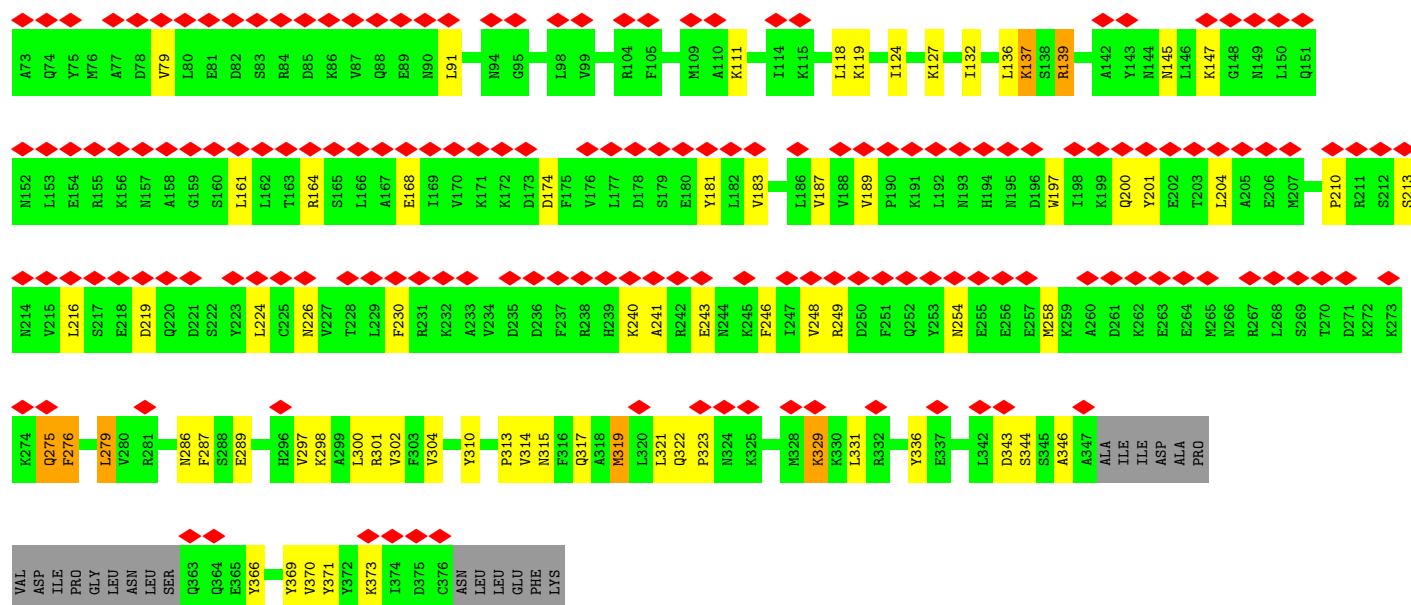
Chain F: 68% 19% 11%



• Molecule 3: V-type proton ATPase subunit C

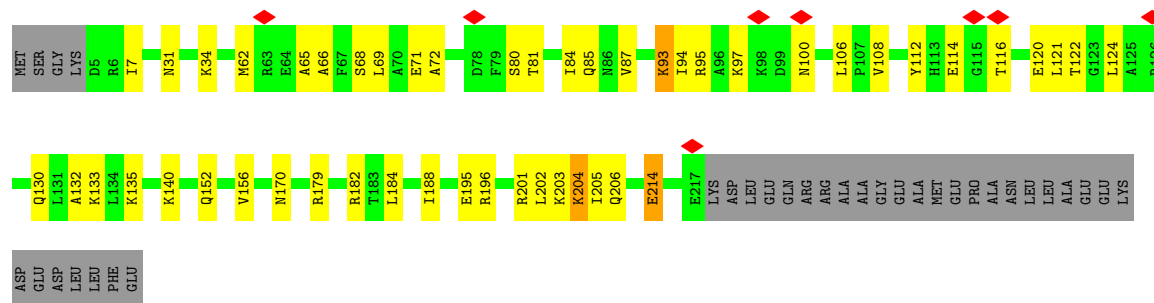
Chain G: 49% 68% 23% 6%





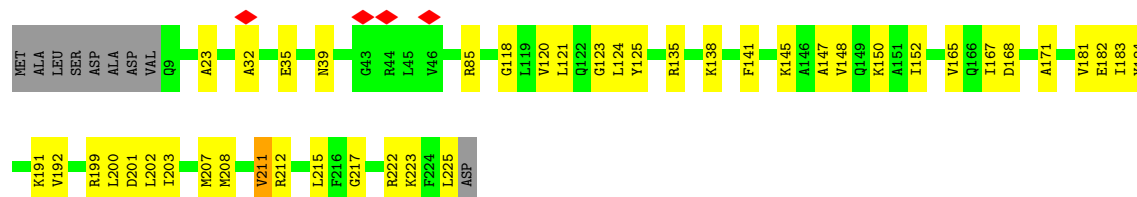
• Molecule 4: V-type proton ATPase subunit D

Chain H: 66% 19% 14%



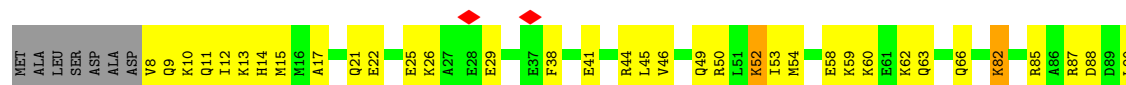
• Molecule 5: V-type proton ATPase subunit E 1

Chain I: 77% 19%



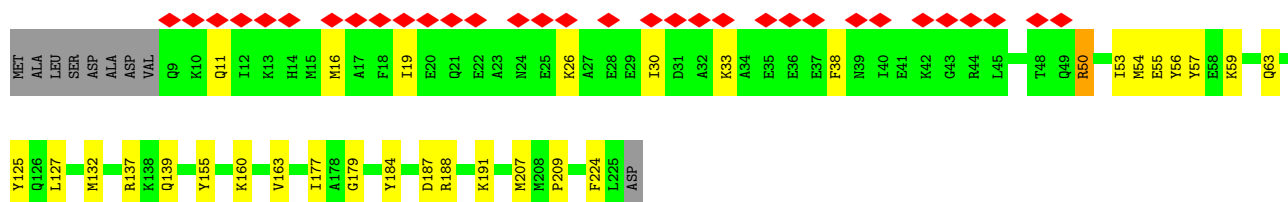
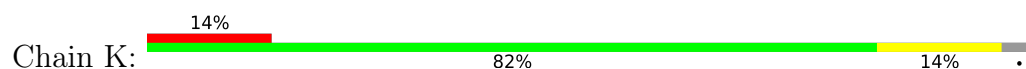
• Molecule 5: V-type proton ATPase subunit E 1

Chain J: 70% 24%

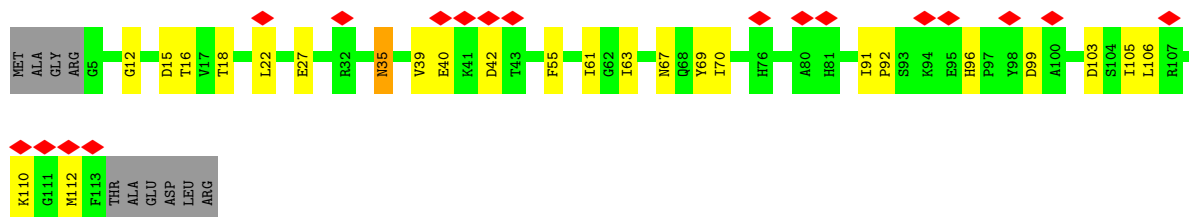




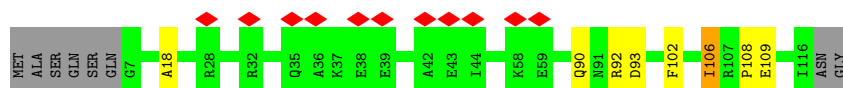
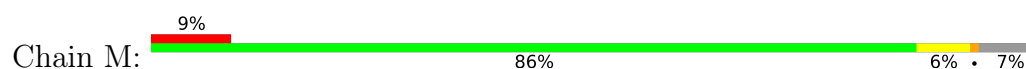
• Molecule 5: V-type proton ATPase subunit E 1



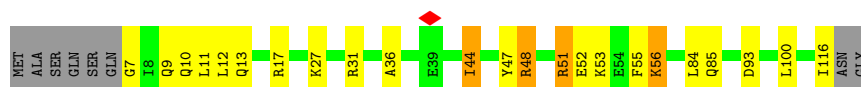
• Molecule 6: V-type proton ATPase subunit F



• Molecule 7: V-type proton ATPase subunit G

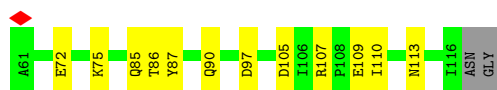


• Molecule 7: V-type proton ATPase subunit G



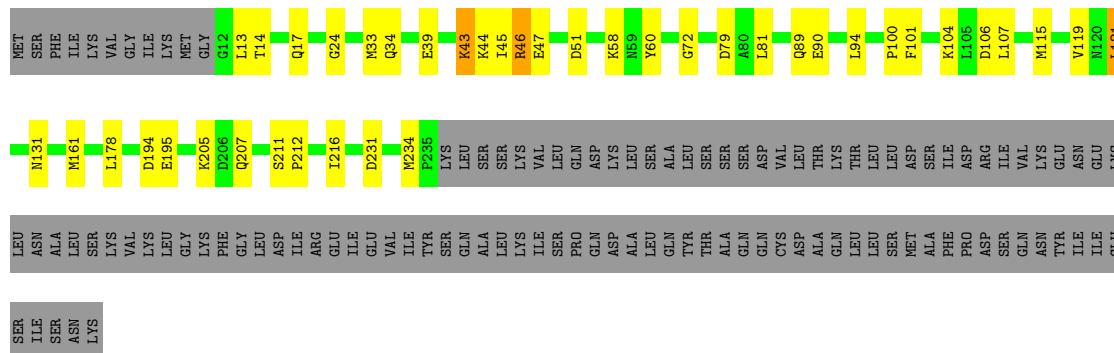
• Molecule 7: V-type proton ATPase subunit G





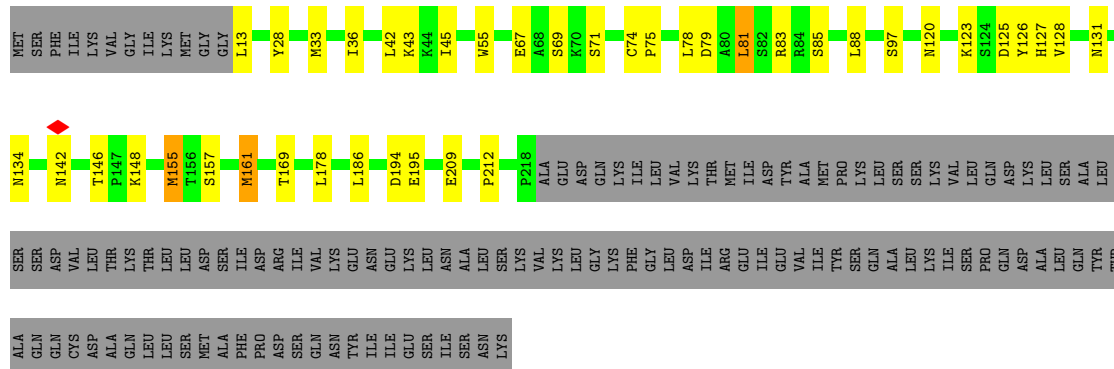
- Molecule 8: Bacterial effector protein SidK

Chain Q: 54% 11% 34%



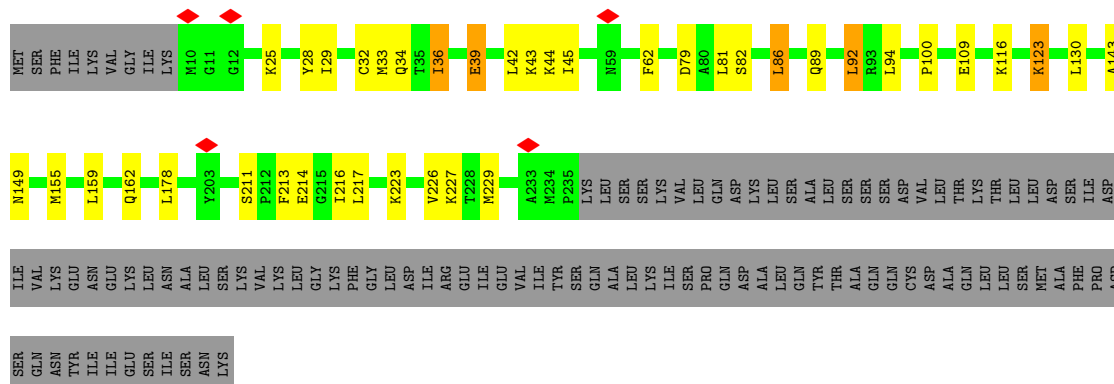
- Molecule 8: Bacterial effector protein SidK

Chain R: 49% 11% 39%

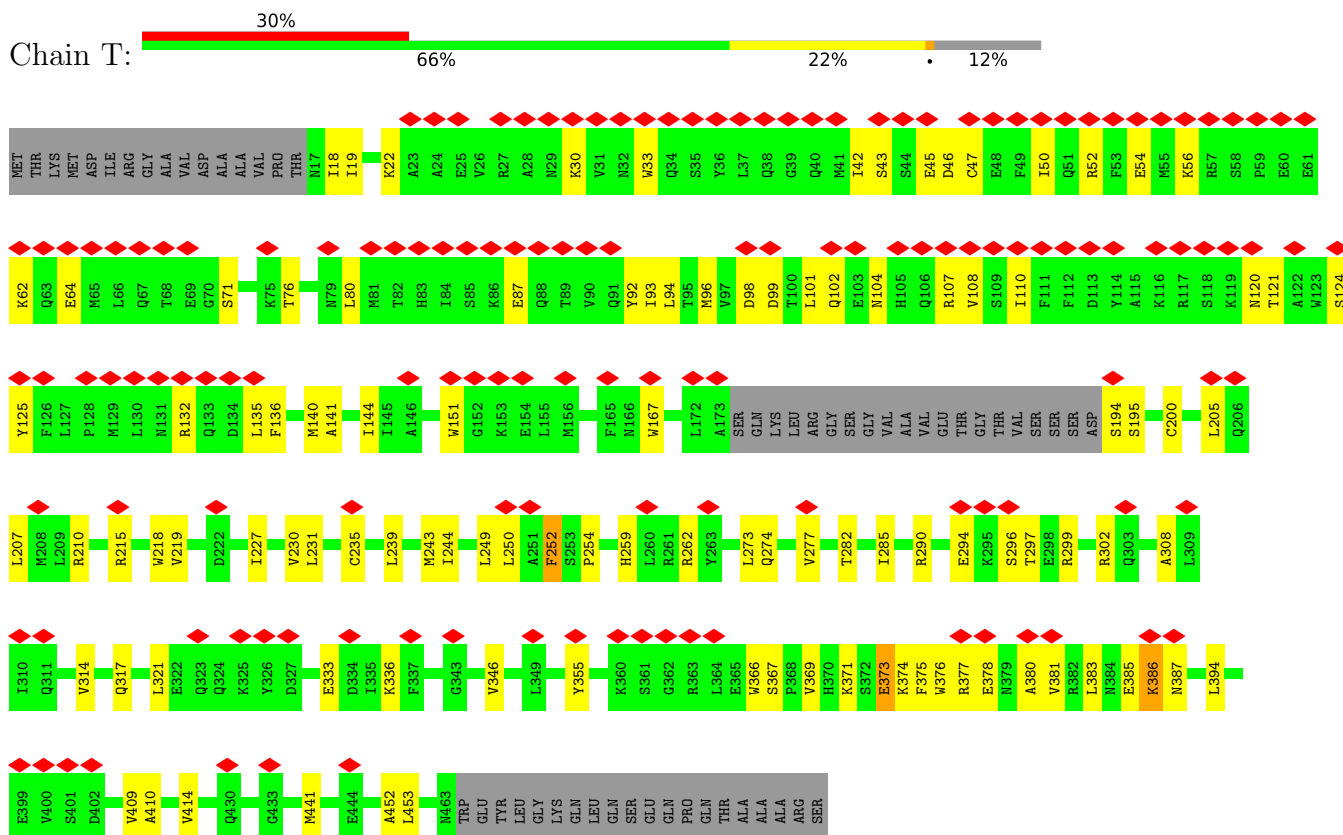


- Molecule 8: Bacterial effector protein SidK

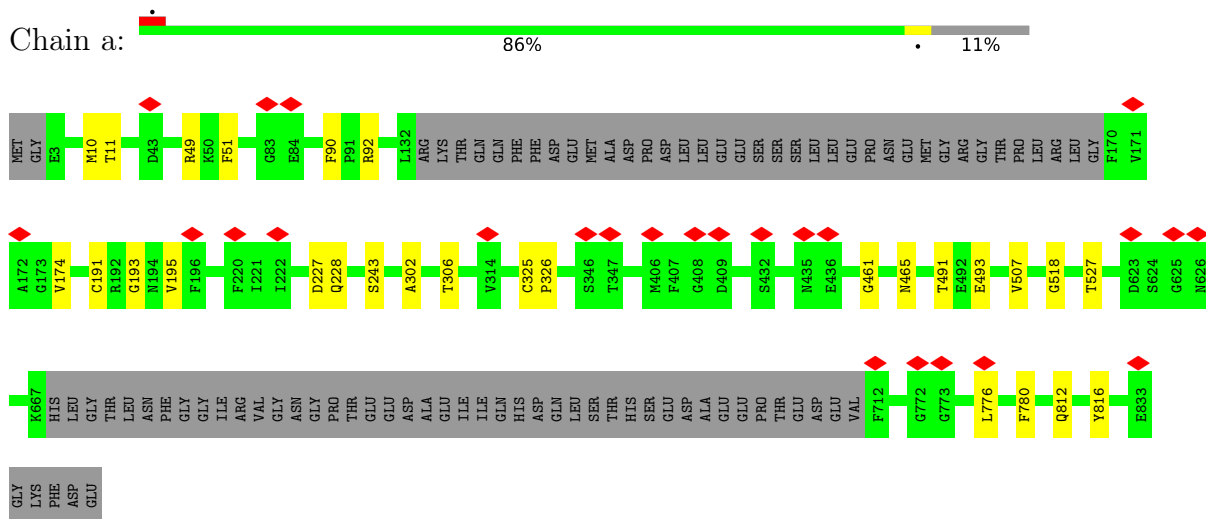
Chain S: 55% 10% 33%



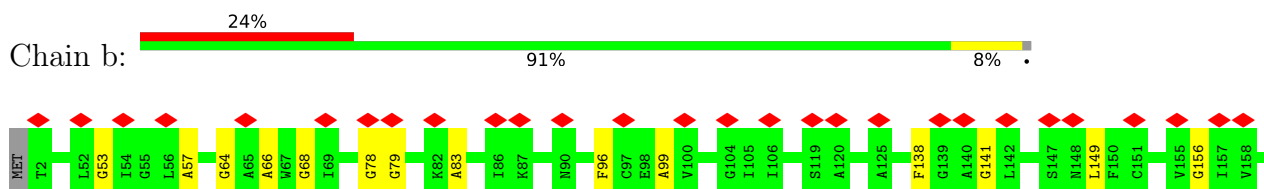
- Molecule 9: V-type proton ATPase subunit H

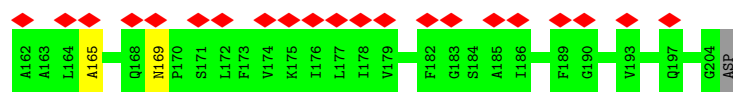


- Molecule 10: V-type proton ATPase subunit a



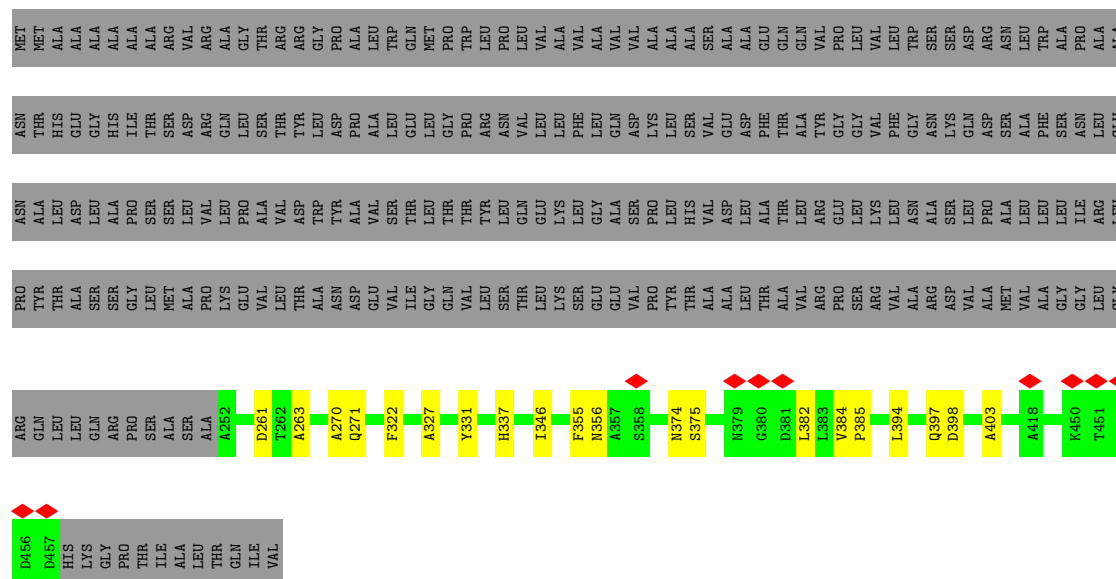
- Molecule 11: V-type proton ATPase 21 kDa proteolipid subunit isoform 1





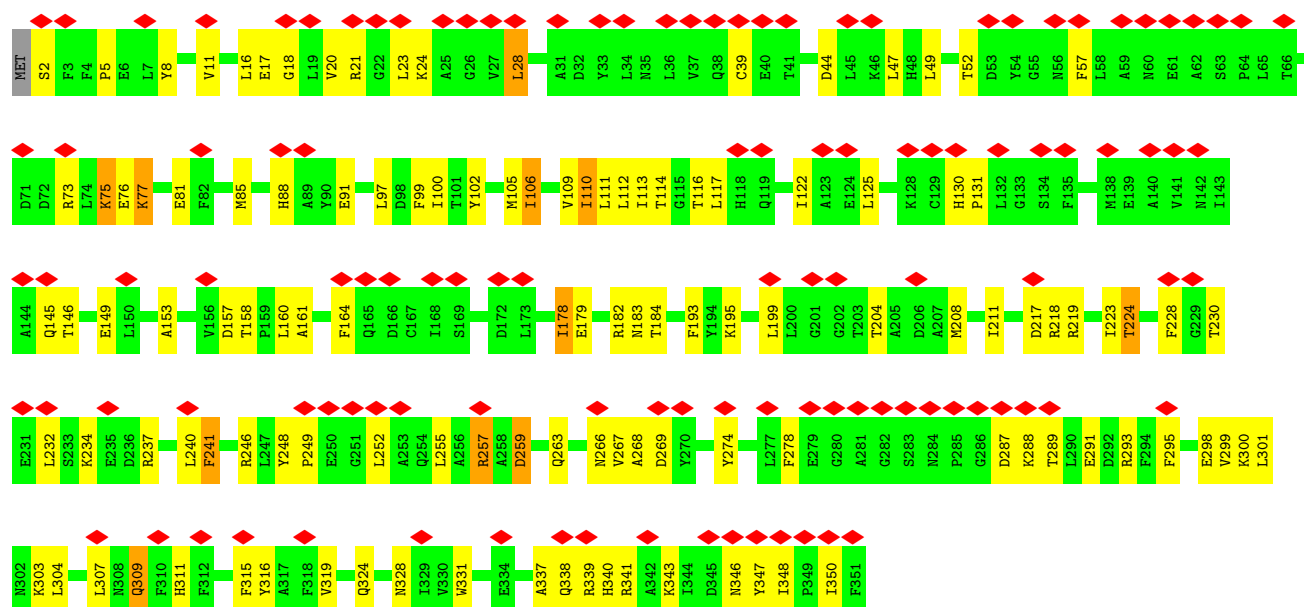
- Molecule 12: ATPase H⁺ transporting accessory protein 1

Chain c: 40% 56%



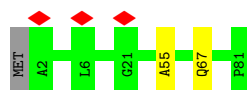
- Molecule 13: V-type proton ATPase subunit

Chain d: 33% 65% 31%

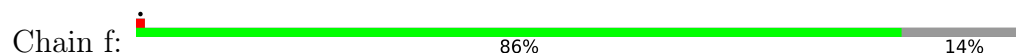


- Molecule 14: V-type proton ATPase subunit

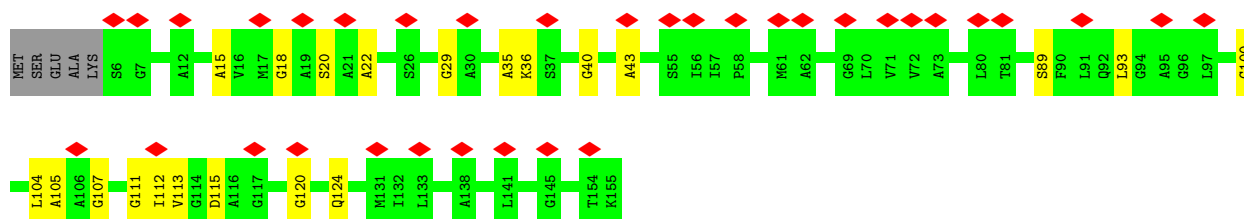
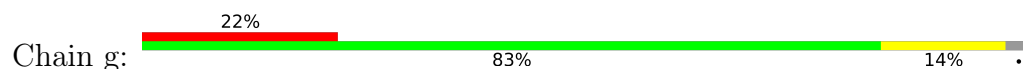
Chain e: 96%



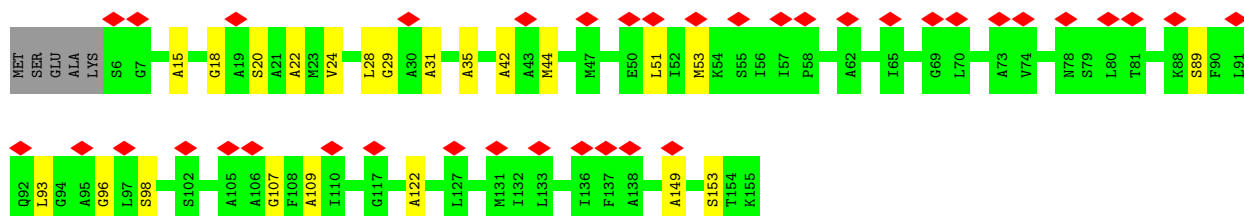
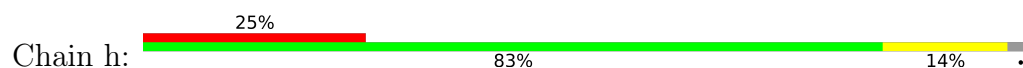
- Molecule 15: Ribonuclease kappa



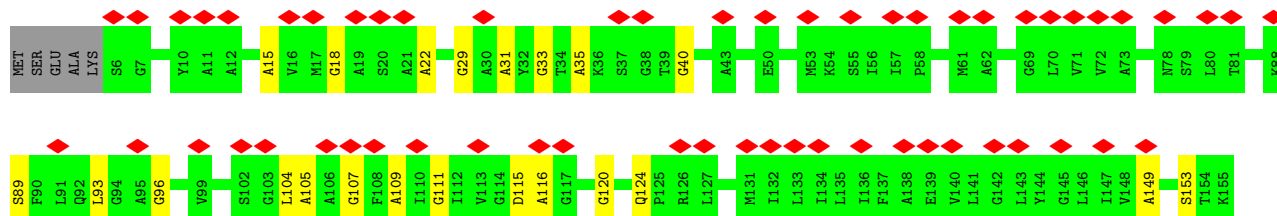
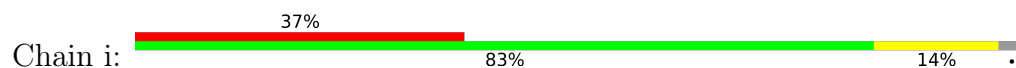
- Molecule 16: V-type proton ATPase proteolipid subunit



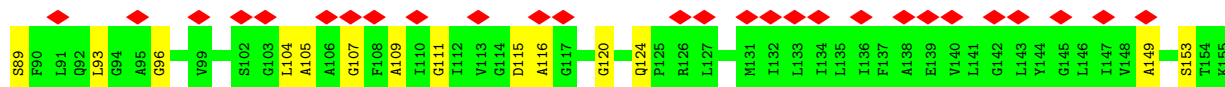
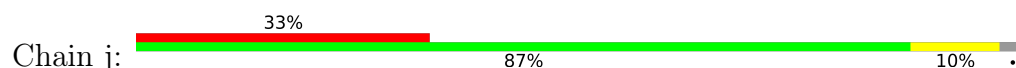
- Molecule 16: V-type proton ATPase proteolipid subunit

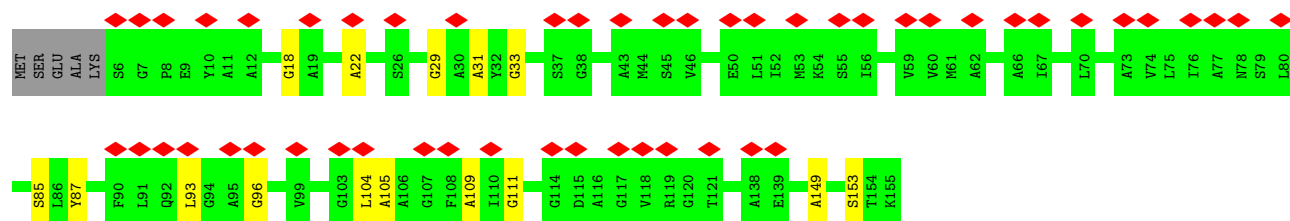


- Molecule 16: V-type proton ATPase proteolipid subunit

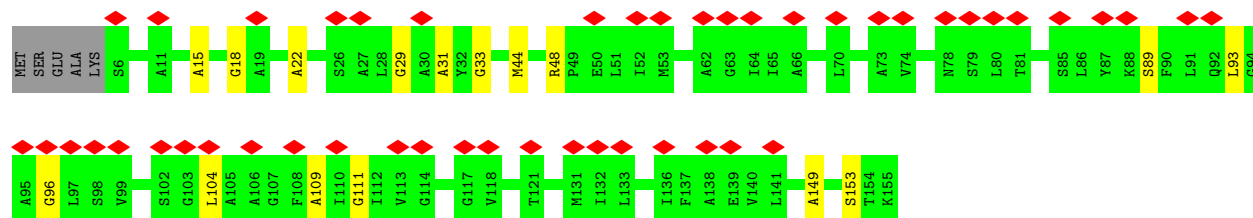
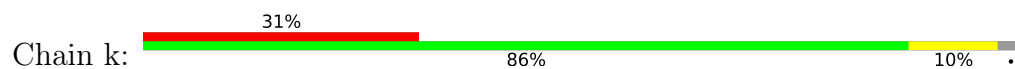


- Molecule 16: V-type proton ATPase proteolipid subunit

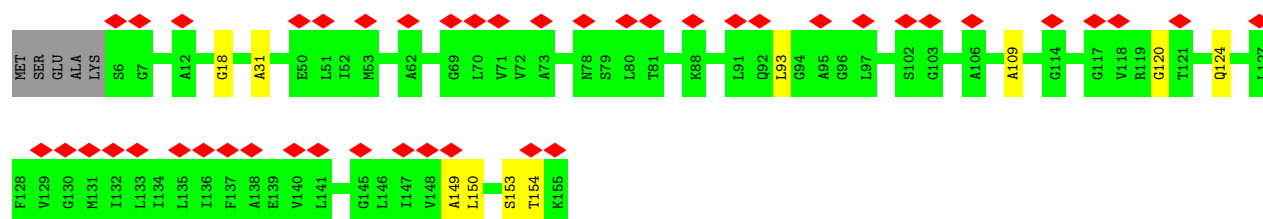
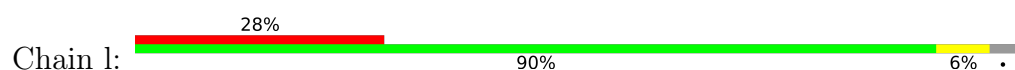




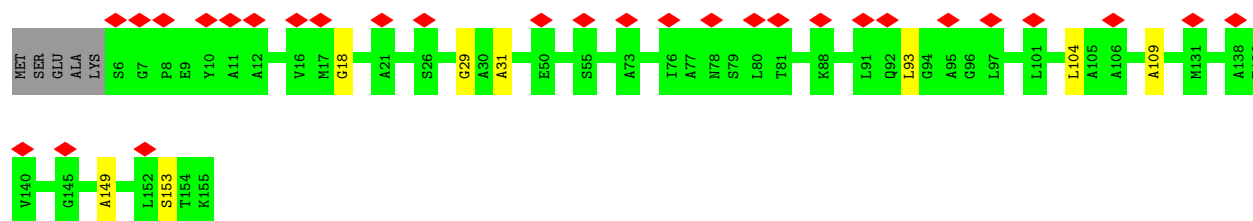
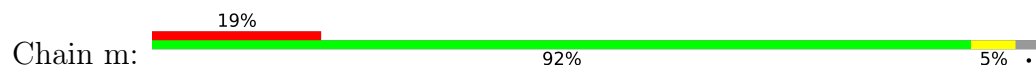
- Molecule 16: V-type proton ATPase proteolipid subunit



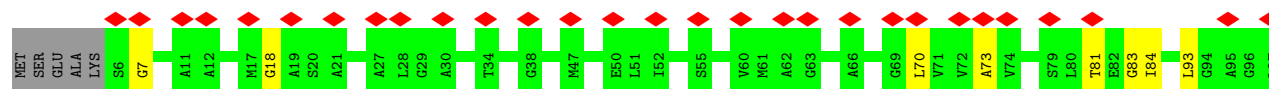
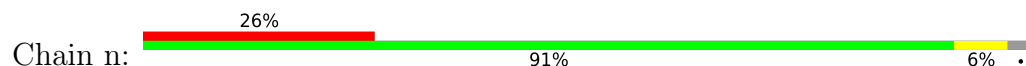
- Molecule 16: V-type proton ATPase proteolipid subunit



- Molecule 16: V-type proton ATPase proteolipid subunit



- Molecule 16: V-type proton ATPase proteolipid subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14746	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	2.390	Depositor
Minimum map value	-0.440	Depositor
Average map value	0.146	Depositor
Map value standard deviation	0.244	Depositor
Recommended contour level	0.6	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	0.67	0/4757	1.16	10/6446 (0.2%)
1	B	0.77	0/4757	1.19	3/6446 (0.0%)
1	C	0.74	0/4668	1.19	5/6324 (0.1%)
2	D	0.76	0/3662	1.20	11/4961 (0.2%)
2	E	0.69	0/3644	1.15	3/4939 (0.1%)
2	F	0.74	0/3644	1.16	5/4939 (0.1%)
3	G	0.59	0/2989	1.03	1/4038 (0.0%)
4	H	0.71	0/1735	1.18	3/2321 (0.1%)
5	I	0.48	0/1427	0.86	1/1948 (0.1%)
5	J	0.68	0/1790	1.14	0/2396
5	K	0.74	0/1783	1.21	3/2386 (0.1%)
6	L	0.72	0/879	1.19	1/1186 (0.1%)
7	M	0.53	0/678	0.74	0/933
7	N	0.50	0/914	1.01	1/1218 (0.1%)
7	O	0.78	0/902	1.28	2/1202 (0.2%)
8	Q	0.68	0/1858	1.17	5/2505 (0.2%)
8	R	0.65	0/1717	1.19	1/2315 (0.0%)
8	S	0.71	0/1870	1.16	1/2520 (0.0%)
9	T	0.51	0/3576	0.91	1/4818 (0.0%)
10	a	0.26	0/3704	0.49	1/5155 (0.0%)
11	b	0.13	0/988	0.33	0/1366
12	c	0.18	0/1015	0.46	0/1411
13	d	0.47	0/2901	0.91	5/3930 (0.1%)
14	e	0.13	0/393	0.39	0/545
15	f	0.16	0/411	0.36	0/569
16	g	0.15	0/728	0.36	0/1005
16	h	0.17	0/728	0.43	0/1005
16	i	0.19	0/728	0.42	0/1005
16	j	0.16	0/728	0.41	0/1005
16	k	0.15	0/728	0.39	0/1005
16	l	0.15	0/728	0.34	0/1005
16	m	0.14	0/728	0.29	0/1005

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	n	0.14	0/728	0.34	0/1005
16	o	0.15	0/728	0.39	0/1005
17	p	0.14	0/263	0.34	0/366
All	All	0.61	0/63477	1.01	63/86228 (0.1%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	142	GLU	N-CA-C	-11.32	99.20	113.23
2	F	142	GLU	N-CA-C	-10.43	98.68	111.40
2	D	142	GLU	N-CA-C	-7.43	103.17	112.90
7	O	33	LEU	N-CA-C	-7.21	102.82	111.69
2	D	196	ILE	N-CA-C	-7.02	104.01	110.82
2	D	160	PRO	CB-CA-C	-6.81	103.06	111.64
1	B	239	PRO	N-CA-C	6.79	120.73	111.22
1	A	226	PRO	CB-CA-C	-6.67	102.85	111.46
9	T	252	PHE	N-CA-C	-6.59	104.98	113.16
4	H	156	VAL	N-CA-C	-6.51	104.51	110.82
1	A	118	ILE	N-CA-C	-6.48	101.66	107.56
2	F	324	ASP	CA-CB-CG	-6.40	106.20	112.60
13	d	259	ASP	N-CA-C	-6.40	106.06	114.31
1	A	340	MET	N-CA-C	-6.28	105.61	113.28
8	R	75	PRO	N-CA-C	-6.22	100.88	110.95
1	A	100	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	396	GLY	CA-C-O	-6.01	117.98	122.37
2	D	343	THR	N-CA-C	-5.96	100.84	110.32
2	E	274	THR	N-CA-C	-5.96	103.45	112.04
2	F	317	PHE	CA-C-O	-5.86	115.27	120.19
8	Q	72	GLY	CA-C-N	5.85	128.04	120.44
8	Q	72	GLY	C-N-CA	5.85	128.04	120.44
13	d	228	PHE	N-CA-C	-5.79	105.31	112.90
4	H	214	GLU	CB-CG-CD	5.67	122.23	112.60
2	D	370	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	C	205	MET	CA-C-N	-5.61	115.64	123.10
1	C	205	MET	C-N-CA	-5.61	115.64	123.10
2	D	317	PHE	CB-CA-C	5.55	116.40	108.68
1	B	537	THR	N-CA-C	-5.54	105.16	111.14
7	O	72	GLU	N-CA-C	-5.54	105.33	111.36
5	K	207	MET	N-CA-C	-5.51	106.46	114.12
1	A	390	GLY	CA-C-O	-5.50	118.43	122.23
1	C	393	LYS	N-CA-C	-5.50	99.76	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	d	241	PHE	CA-C-O	-5.48	115.17	119.66
5	K	179	GLY	N-CA-C	5.46	122.66	112.77
3	G	275	GLN	N-CA-C	-5.41	106.36	113.12
8	Q	34	GLN	N-CA-C	-5.40	105.83	112.90
2	D	478	LEU	N-CA-C	-5.39	106.54	113.01
8	Q	131	ASN	N-CA-C	-5.37	104.85	111.40
2	D	42	ARG	N-CA-C	-5.37	105.03	113.02
2	D	302	ARG	N-CA-C	-5.33	105.51	112.23
8	Q	211	SER	O-C-N	-5.32	116.58	121.37
2	F	404	MET	N-CA-C	-5.29	105.65	112.68
2	D	357	HIS	CB-CG-CD2	-5.28	124.33	131.20
8	S	100	PRO	N-CA-C	-5.26	106.55	113.65
1	A	469	PHE	CA-C-O	-5.25	115.32	121.46
13	d	130	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	A	233	VAL	CA-C-O	-5.18	116.25	121.59
2	E	134	ASP	N-CA-C	-5.17	106.37	113.30
7	N	52	GLU	N-CA-C	-5.15	105.36	111.69
13	d	230	THR	N-CA-C	5.15	116.90	109.07
6	L	35	ASN	N-CA-C	-5.14	105.26	112.25
1	A	456	LYS	N-CA-C	-5.09	106.90	113.01
1	C	465	TYR	N-CA-C	-5.06	105.77	111.28
5	I	217	GLY	CA-C-O	-5.05	118.20	122.29
5	K	50	ARG	N-CA-C	-5.04	105.69	111.14
2	D	200	ILE	N-CA-C	-5.04	105.58	110.42
2	F	472	ASP	N-CA-C	-5.04	105.44	112.45
4	H	87	VAL	N-CA-C	5.03	116.39	111.91
1	A	588	ASP	CA-C-N	5.03	124.69	119.56
1	A	588	ASP	C-N-CA	5.03	124.69	119.56
10	a	507	VAL	N-CA-C	-5.01	108.62	113.53
1	C	114	GLN	N-CA-C	-5.00	106.75	112.86

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	4661	0	4653	83	0
1	B	4661	0	4653	76	0
1	C	4577	0	4577	83	0
2	D	3590	0	3581	55	0
2	E	3572	0	3555	60	0
2	F	3572	0	3555	52	0
3	G	2935	0	2970	82	0
4	H	1717	0	1822	32	0
5	I	1416	0	1167	23	0
5	J	1773	0	1855	29	0
5	K	1766	0	1846	28	0
6	L	865	0	872	22	0
7	M	673	0	476	4	0
7	N	906	0	913	18	0
7	O	894	0	899	16	0
8	Q	1824	0	1835	16	0
8	R	1685	0	1691	21	0
8	S	1836	0	1847	20	0
9	T	3510	0	3493	63	0
10	a	3707	0	1627	16	0
11	b	989	0	489	10	0
12	c	1016	0	457	11	0
13	d	2835	0	2770	75	0
14	e	394	0	167	2	0
15	f	412	0	190	0	0
16	g	729	0	388	15	0
16	h	729	0	388	16	0
16	i	729	0	388	19	0
16	j	729	0	388	10	0
16	k	729	0	388	9	0
16	l	729	0	388	6	0
16	m	729	0	388	5	0
16	n	729	0	388	5	0
16	o	729	0	388	6	0
17	p	264	0	116	0	0
18	B	27	0	12	1	0
All	All	62638	0	55580	896	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (896) 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)
13:d:2:SER:N	13:d:8:TYR:HH	1.53	1.05
1:B:279:GLU:HG3	1:B:284:MET:HE3	1.55	0.88
3:G:343:ASP:HB2	3:G:346:ALA:HB3	1.60	0.82
9:T:43:SER:H	9:T:80:LEU:HD13	1.48	0.79
2:D:168:ILE:HG22	2:D:170:PRO:HD2	1.65	0.78
1:A:91:GLY:HA3	1:A:206:VAL:HG22	1.66	0.77
13:d:88:HIS:CD2	16:g:43:ALA:HB1	2.19	0.77
16:i:18:GLY:HA3	16:i:93:LEU:HA	1.67	0.77
16:j:29:GLY:HA3	16:j:104:LEU:HA	1.67	0.77
16:h:31:ALA:HA	16:i:109:ALA:HB2	1.68	0.76
9:T:92:TYR:HB3	9:T:96:MET:HE1	1.69	0.75
1:C:350:SER:HB3	1:C:353:ARG:HB2	1.69	0.74
2:D:374:ASP:HB2	2:D:387:ASN:HB2	1.70	0.73
9:T:19:ILE:HD12	9:T:200:CYS:HB2	1.69	0.73
4:H:122:THR:HA	13:d:179:GLU:HG2	1.70	0.73
1:C:389:ALA:HA	1:C:404:VAL:HG12	1.70	0.72
1:A:328:TYR:HA	1:A:331:ILE:HG22	1.71	0.72
16:k:29:GLY:HA3	16:k:104:LEU:HA	1.70	0.72
1:C:511:VAL:HG21	1:C:548:TYR:HB2	1.71	0.72
5:I:120:VAL:HG12	5:I:181:VAL:HG21	1.72	0.71
16:n:18:GLY:HA3	16:n:93:LEU:HA	1.72	0.71
1:B:46:GLY:HA2	1:B:77:ASP:HB3	1.71	0.71
3:G:8:SER:HB3	3:G:370:VAL:HB	1.71	0.71
2:E:451:LYS:HD2	2:E:480:ILE:HD11	1.73	0.71
1:C:499:ALA:O	4:H:100:ASN:ND2	2.24	0.70
4:H:31:ASN:OD1	4:H:34:LYS:NZ	2.25	0.70
3:G:28:LYS:HG3	3:G:33:ALA:HB3	1.72	0.70
5:I:118:GLY:HA3	7:M:106:ILE:HD13	1.72	0.69
1:A:56:ARG:NH2	1:A:57:LEU:O	2.25	0.69
11:b:64:GLY:HA3	11:b:149:LEU:HA	1.73	0.69
3:G:276:PHE:HA	3:G:279:LEU:HD23	1.74	0.69
9:T:45:GLU:HB2	9:T:76:THR:HG21	1.74	0.69
9:T:87:GLU:HB3	9:T:135:LEU:HD11	1.73	0.69
16:h:18:GLY:HA3	16:h:93:LEU:HA	1.74	0.69
4:H:93:LYS:HB2	4:H:112:TYR:HD2	1.58	0.68
9:T:373:GLU:HA	9:T:376:TRP:HD1	1.56	0.68
13:d:268:ALA:HB2	13:d:278:PHE:CE2	2.27	0.68
1:A:241:VAL:HG23	1:A:461:LEU:HD21	1.75	0.68
5:I:138:LYS:O	5:I:141:PHE:HB3	1.93	0.68
16:g:18:GLY:HA3	16:g:93:LEU:HA	1.75	0.68
2:D:490:PRO:HG2	2:D:493:MET:HB2	1.74	0.67
2:E:121:MET:HE3	2:E:275:THR:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:m:29:GLY:HA3	16:m:104:LEU:HA	1.77	0.67
1:A:296:MET:HE1	1:A:305:ILE:HG22	1.76	0.67
13:d:241:PHE:HB3	13:d:252:LEU:HD22	1.77	0.67
9:T:99:ASP:OD1	9:T:102:GLN:NE2	2.28	0.66
3:G:111:LYS:NZ	3:G:289:GLU:OE1	2.29	0.66
2:E:188:ALA:H	2:E:191:LEU:HD12	1.58	0.66
2:E:489:ILE:HG23	2:E:493:MET:HE3	1.76	0.66
2:F:185:ILE:HA	2:F:371:ILE:HB	1.77	0.66
2:E:315:ARG:HG3	2:E:358:PRO:HD3	1.78	0.66
4:H:66:ALA:HA	4:H:69:LEU:HD12	1.77	0.66
2:F:282:GLN:HA	5:K:224:PHE:HB3	1.78	0.66
16:i:29:GLY:HA3	16:i:104:LEU:HA	1.78	0.66
16:i:22:ALA:HB2	16:i:96:GLY:HA2	1.77	0.65
3:G:187:VAL:HG22	3:G:248:VAL:HG22	1.78	0.65
1:B:338:ARG:HD3	1:B:404:VAL:HG23	1.78	0.65
3:G:9:ALA:HB3	3:G:317:GLN:HB3	1.79	0.65
1:A:152:ILE:HD13	1:A:167:MET:HB3	1.77	0.65
2:E:321:MET:HA	2:E:321:MET:HE2	1.77	0.65
8:R:97:SER:OG	8:R:134:ASN:ND2	2.29	0.64
1:B:25:SER:HA	2:E:82:GLU:HG2	1.80	0.64
3:G:297:VAL:HG13	3:G:301:ARG:NH1	2.12	0.64
3:G:254:ASN:H	3:G:258:MET:HE1	1.61	0.64
4:H:85:GLN:NE2	13:d:111:LEU:O	2.30	0.64
1:C:522:GLN:HG3	1:C:529:ASP:HB3	1.79	0.64
2:D:47:VAL:HG13	2:D:52:VAL:HG22	1.80	0.64
3:G:139:ARG:HD3	3:G:279:LEU:HB2	1.80	0.64
1:C:165:ARG:HB2	1:C:340:MET:HE3	1.80	0.63
16:m:31:ALA:HB1	16:n:109:ALA:HB2	1.80	0.63
13:d:324:GLN:OE1	13:d:328:ASN:ND2	2.31	0.63
16:k:18:GLY:HA3	16:k:93:LEU:HA	1.80	0.63
12:c:355:PHE:HA	12:c:385:PRO:HA	1.80	0.63
13:d:88:HIS:HD2	16:g:43:ALA:HB1	1.62	0.63
1:C:20:TYR:HB2	1:C:76:GLY:HA2	1.80	0.63
4:H:80:SER:HB2	6:L:18:THR:HG21	1.81	0.63
13:d:211:ILE:HG13	13:d:301:LEU:HG	1.80	0.63
13:d:307:LEU:HD21	16:o:119:ARG:HA	1.81	0.63
16:g:120:GLY:O	16:g:124:GLN:N	2.21	0.62
1:B:215:ARG:HB2	1:B:338:ARG:HH12	1.64	0.62
2:D:172:ASP:O	2:D:176:SER:HB3	1.99	0.62
2:D:430:LYS:HB2	2:D:438:LEU:HD11	1.82	0.62
1:C:284:MET:HE3	1:C:288:LEU:HG	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:297:VAL:O	3:G:301:ARG:HG2	2.00	0.62
1:A:56:ARG:HB3	1:A:63:THR:HB	1.81	0.62
5:K:53:ILE:HD11	7:O:44:ILE:HG23	1.80	0.62
3:G:161:LEU:HG	3:G:219:ASP:HB2	1.82	0.62
6:L:103:ASP:HB3	6:L:106:LEU:HB3	1.80	0.62
13:d:110:ILE:HG13	13:d:182:ARG:HB2	1.82	0.62
8:Q:33:MET:HE1	8:Q:45:ILE:HG22	1.80	0.61
1:A:234:LEU:HD22	1:A:433:TRP:CD1	2.35	0.61
3:G:58:LEU:HD23	3:G:61:LEU:HD12	1.82	0.61
16:h:51:LEU:O	16:h:53:MET:N	2.33	0.61
5:I:182:GLU:OE2	5:I:191:LYS:HB2	2.01	0.61
2:D:227:ALA:HB1	2:D:230:VAL:HG21	1.83	0.61
10:a:11:THR:N	10:a:325:CYS:O	2.27	0.61
2:E:140:MET:HE2	5:J:91:ILE:HD11	1.83	0.61
16:k:15:ALA:HB2	16:k:89:SER:HA	1.82	0.61
11:b:78:GLY:HA3	13:d:18:GLY:HA3	1.82	0.61
3:G:174:ASP:HB3	3:G:216:LEU:HD22	1.82	0.60
6:L:15:ASP:OD1	6:L:16:THR:N	2.33	0.60
9:T:380:ALA:HA	9:T:383:LEU:HD12	1.83	0.60
3:G:216:LEU:HD11	3:G:224:LEU:HD23	1.83	0.60
8:S:213:PHE:HB2	8:S:217:LEU:HD21	1.84	0.60
13:d:340:HIS:HB3	13:d:343:LYS:HE2	1.84	0.60
16:h:44:MET:HA	16:h:122:ALA:HB2	1.82	0.60
3:G:297:VAL:HG13	3:G:301:ARG:CZ	2.32	0.60
13:d:337:ALA:O	13:d:339:ARG:NH2	2.34	0.60
5:J:8:VAL:O	5:J:11:GLN:NE2	2.34	0.60
13:d:113:ILE:O	13:d:114:THR:OG1	2.19	0.59
8:R:125:ASP:HA	8:R:128:VAL:HG12	1.85	0.59
13:d:99:PHE:HA	13:d:102:TYR:CD2	2.37	0.59
16:k:31:ALA:HB1	16:l:109:ALA:HB2	1.84	0.59
13:d:183:ASN:HB2	13:d:240:LEU:HD22	1.85	0.59
1:B:232:ARG:HG2	1:B:537:THR:HG23	1.84	0.59
4:H:31:ASN:HA	4:H:34:LYS:HZ3	1.68	0.59
9:T:46:ASP:HB3	9:T:76:THR:HB	1.85	0.59
4:H:69:LEU:HD13	6:L:15:ASP:HB2	1.85	0.59
13:d:114:THR:HA	13:d:117:LEU:HB2	1.85	0.59
2:D:172:ASP:HB3	2:D:467:VAL:HG23	1.84	0.59
2:F:121:MET:HE2	2:F:275:THR:HG23	1.84	0.59
10:a:10:MET:HA	10:a:326:PRO:HA	1.85	0.59
5:J:10:LYS:O	5:J:14:HIS:ND1	2.33	0.59
3:G:54:LEU:HD11	3:G:119:LYS:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:161:LEU:O	3:G:249:ARG:NH2	2.36	0.58
1:C:297:GLU:HG3	1:C:302:VAL:HG22	1.85	0.58
13:d:300:LYS:HA	13:d:303:LYS:HG2	1.85	0.58
3:G:5:TRP:HZ3	3:G:323:PRO:HG3	1.67	0.58
7:N:7:GLY:N	7:N:9:GLN:OE1	2.36	0.58
13:d:328:ASN:ND2	13:d:348:ILE:O	2.36	0.58
16:l:120:GLY:O	16:l:124:GLN:N	2.32	0.58
11:b:68:GLY:HA2	11:b:156:GLY:HA3	1.85	0.58
8:S:44:LYS:HG3	8:S:109:GLU:HG2	1.85	0.58
9:T:282:THR:HA	9:T:285:ILE:HG22	1.86	0.58
1:B:518:ASP:HA	1:B:585:LYS:HD3	1.86	0.58
1:B:541:LEU:HD12	1:B:544:MET:HE2	1.85	0.58
9:T:56:LYS:O	9:T:62:LYS:NZ	2.27	0.58
1:A:168:LEU:HD12	1:A:169:PRO:HD2	1.85	0.58
1:C:160:SER:O	1:C:161:LEU:HB2	2.02	0.58
16:g:40:GLY:HA3	16:g:115:ASP:HA	1.86	0.58
1:B:232:ARG:HH11	1:B:536:LYS:HE2	1.68	0.57
5:J:90:LEU:HD11	7:N:85:GLN:HG3	1.86	0.57
16:m:18:GLY:HA3	16:m:93:LEU:HA	1.86	0.57
2:E:165:GLN:NE2	2:E:172:ASP:OD2	2.37	0.57
3:G:6:LEU:HD22	3:G:302:VAL:HG21	1.85	0.57
16:o:29:GLY:HA3	16:o:104:LEU:HA	1.86	0.57
5:J:53:ILE:HD11	7:N:44:ILE:HG23	1.87	0.57
13:d:287:ASP:OD1	13:d:293:ARG:NH1	2.35	0.57
1:A:317:ASN:HB3	2:D:330:GLU:HB2	1.87	0.57
1:B:44:ARG:HB2	1:B:80:LEU:HB3	1.86	0.57
16:i:35:ALA:HB2	16:j:109:ALA:HA	1.87	0.57
16:o:18:GLY:HA3	16:o:93:LEU:HA	1.86	0.57
2:E:357:HIS:CG	2:E:358:PRO:HD2	2.39	0.57
1:A:95:MET:HE1	1:A:271:VAL:HG13	1.87	0.57
2:F:489:ILE:HG23	2:F:493:MET:HE3	1.86	0.57
1:A:291:PHE:CD2	1:A:311:LEU:HD11	2.40	0.56
3:G:241:ALA:HB1	3:G:246:PHE:HB2	1.86	0.56
5:J:53:ILE:HG12	7:N:48:ARG:HE	1.70	0.56
12:c:356:ASN:O	12:c:384:VAL:N	2.38	0.56
9:T:167:TRP:HE1	9:T:205:LEU:HD13	1.71	0.56
1:A:526:THR:O	1:A:530:ARG:HG3	2.05	0.56
1:C:397:ASN:HB3	8:S:28:TYR:CG	2.40	0.56
2:D:322:TYR:HD2	2:D:362:LEU:HD12	1.70	0.56
5:I:147:ALA:HA	5:I:150:LYS:HG2	1.87	0.56
5:J:15:MET:HE2	10:a:195:VAL:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:MET:HG3	1:A:40:TYR:CD2	2.41	0.56
1:C:536:LYS:HD2	1:C:589:PRO:HG3	1.87	0.56
3:G:124:ILE:HA	3:G:127:LYS:HE3	1.87	0.56
13:d:146:THR:HG22	13:d:149:GLU:H	1.69	0.56
8:R:33:MET:HA	8:R:36:ILE:HG22	1.88	0.56
16:k:33:GLY:HA2	16:k:111:GLY:HA3	1.88	0.56
2:F:312:PRO:HD2	4:H:205:ILE:HD11	1.88	0.56
5:K:53:ILE:HA	7:O:48:ARG:HH11	1.71	0.56
1:A:398:PRO:HB2	1:A:400:ARG:HD3	1.87	0.56
3:G:5:TRP:CZ3	3:G:323:PRO:HG3	2.41	0.56
16:h:28:LEU:O	16:h:31:ALA:HB3	2.06	0.56
1:A:273:ILE:HG12	1:A:310:ALA:HB3	1.88	0.55
6:L:40:GLU:HG2	6:L:42:ASP:H	1.71	0.55
9:T:132:ARG:HB3	9:T:135:LEU:HD12	1.88	0.55
13:d:193:PHE:HE2	13:d:208:MET:HE2	1.70	0.55
1:C:77:ASP:OD1	7:O:113:ASN:ND2	2.31	0.55
16:j:149:ALA:O	16:j:153:SER:N	2.34	0.55
2:E:71:PRO:HB3	2:E:103:LYS:HB3	1.89	0.55
9:T:33:TRP:HB3	9:T:42:ILE:HG21	1.89	0.55
2:E:392:LEU:HD11	2:E:394:ARG:HE	1.72	0.55
2:F:80:VAL:HG22	2:F:90:VAL:HG22	1.87	0.55
4:H:31:ASN:HA	4:H:34:LYS:NZ	2.20	0.55
9:T:33:TRP:CZ2	9:T:93:ILE:HA	2.42	0.55
9:T:108:VAL:O	9:T:110:ILE:N	2.39	0.55
9:T:441:MET:HE1	9:T:453:LEU:N	2.22	0.55
13:d:204:THR:HA	13:d:311:HIS:HB2	1.89	0.55
5:J:9:GLN:HB3	5:J:13:LYS:HE2	1.87	0.55
4:H:93:LYS:HB2	4:H:112:TYR:CD2	2.41	0.55
13:d:116:THR:HG22	13:d:145:GLN:HA	1.89	0.55
8:Q:194:ASP:OD1	8:Q:195:GLU:N	2.40	0.54
2:F:177:ILE:HG12	2:F:183:ILE:HG13	1.89	0.54
1:C:466:ASP:HA	1:C:470:THR:HA	1.89	0.54
2:D:409:HIS:HA	2:D:471:LEU:HD21	1.89	0.54
2:E:332:ALA:HA	2:E:342:ILE:HB	1.89	0.54
2:E:351:PRO:HG2	2:E:357:HIS:CE1	2.42	0.54
2:F:334:ARG:HB3	2:F:341:SER:HB2	1.90	0.54
13:d:211:ILE:HG21	13:d:316:TYR:HE2	1.70	0.54
2:E:301:LEU:HD13	2:E:321:MET:HE1	1.89	0.54
10:a:491:THR:O	10:a:493:GLU:N	2.41	0.54
3:G:240:LYS:O	3:G:243:GLU:HG3	2.08	0.54
8:S:159:LEU:HA	8:S:178:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:o:33:GLY:HA2	16:o:111:GLY:HA3	1.90	0.54
1:A:279:GLU:HB2	1:A:284:MET:HE3	1.89	0.54
9:T:47:CYS:HA	9:T:50:ILE:HB	1.90	0.54
2:D:235:ALA:HB1	2:D:255:LEU:HD21	1.90	0.54
4:H:114:GLU:HG3	4:H:116:THR:HG23	1.89	0.54
16:h:22:ALA:HB2	16:h:96:GLY:HA2	1.90	0.54
16:h:35:ALA:HB2	16:i:109:ALA:HA	1.89	0.54
1:A:84:LYS:HD2	1:A:87:SER:HB2	1.89	0.54
1:C:271:VAL:HB	1:C:344:VAL:HG22	1.90	0.54
3:G:310:TYR:HB2	3:G:314:VAL:HG11	1.88	0.54
5:J:148:VAL:HG21	5:J:167:ILE:HD11	1.89	0.54
13:d:234:LYS:HA	13:d:237:ARG:HD2	1.89	0.54
16:i:40:GLY:HA3	16:i:115:ASP:HA	1.89	0.54
1:B:508:THR:HG22	1:B:548:TYR:HE1	1.74	0.53
5:J:38:PHE:CD2	7:N:36:ALA:HB2	2.43	0.53
2:F:38:ARG:HD3	2:F:109:THR:HA	1.90	0.53
2:F:384:PRO:HB2	2:F:386:ILE:HG13	1.89	0.53
3:G:298:LYS:NZ	3:G:373:LYS:O	2.34	0.53
1:A:581:LEU:HD12	1:A:584:MET:HE2	1.90	0.53
1:C:389:ALA:HB2	1:C:406:ILE:HG12	1.90	0.53
2:E:169:SER:N	2:E:459:GLN:OE1	2.38	0.53
2:F:294:MET:HB2	2:F:348:LEU:HG	1.90	0.53
9:T:30:LYS:NZ	9:T:54:GLU:OE2	2.41	0.53
2:F:56:HIS:HA	2:F:86:THR:HB	1.90	0.53
5:K:125:TYR:HE1	5:K:155:TYR:HA	1.73	0.53
1:A:100:ASP:HB3	1:A:104:ARG:H	1.73	0.53
1:C:441:GLN:HG2	2:F:389:LEU:HD11	1.91	0.53
1:A:280:ARG:HD3	2:D:368:GLU:HG3	1.91	0.53
1:A:546:ALA:HB3	1:A:605:LEU:HD11	1.91	0.53
2:D:374:ASP:HB3	2:D:377:LEU:HB2	1.91	0.53
2:F:142:GLU:O	5:K:209:PRO:HB3	2.08	0.53
13:d:97:LEU:HD23	13:d:100:ILE:HD12	1.90	0.53
1:C:161:LEU:HD11	1:C:298:VAL:HG11	1.90	0.53
2:D:383:TYR:HE2	2:D:461:PRO:HA	1.73	0.53
13:d:114:THR:HG21	13:d:178:ILE:HG12	1.91	0.53
1:B:220:LYS:NZ	1:B:389:ALA:O	2.42	0.53
16:k:149:ALA:O	16:k:153:SER:N	2.38	0.53
2:F:55:ASP:OD1	2:F:56:HIS:N	2.42	0.53
5:I:121:LEU:HG	5:I:125:TYR:CE2	2.44	0.53
5:I:211:VAL:HG13	5:I:215:LEU:HD12	1.89	0.53
16:g:29:GLY:HA3	16:g:104:LEU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:TYR:HE2	1:B:284:MET:HE1	1.74	0.53
1:C:479:ALA:HB2	1:C:545:ILE:HD11	1.90	0.53
2:D:137:PRO:HG3	5:I:85:ARG:HA	1.91	0.53
2:D:415:GLN:HB2	2:D:488:ARG:HB2	1.91	0.53
5:I:148:VAL:HG21	5:I:167:ILE:HD11	1.91	0.53
16:i:33:GLY:HA2	16:i:111:GLY:CA	2.38	0.53
5:J:88:ASP:HA	5:J:91:ILE:HD12	1.91	0.52
9:T:441:MET:HE2	9:T:441:MET:HA	1.92	0.52
1:C:23:GLY:HA2	2:F:83:VAL:HG12	1.91	0.52
3:G:58:LEU:HB3	3:G:301:ARG:CZ	2.40	0.52
3:G:57:GLU:HA	3:G:60:LYS:HE2	1.92	0.52
9:T:231:LEU:HD13	9:T:243:MET:HB2	1.91	0.52
2:F:168:ILE:HA	2:F:459:GLN:OE1	2.10	0.52
3:G:254:ASN:N	3:G:258:MET:HE1	2.25	0.52
1:B:352:SER:HB2	1:B:411:SER:H	1.73	0.52
2:D:243:GLU:HA	2:D:248:MET:HE1	1.91	0.52
4:H:65:ALA:O	4:H:68:SER:OG	2.24	0.52
1:A:152:ILE:HD12	1:A:165:ARG:HB3	1.92	0.52
9:T:94:LEU:HB3	9:T:140:MET:HE1	1.92	0.52
9:T:230:VAL:HG12	9:T:239:LEU:HD21	1.92	0.52
11:b:53:GLY:HA3	11:b:138:PHE:HA	1.91	0.52
13:d:266:ASN:HA	13:d:269:ASP:OD2	2.10	0.52
1:A:369:PRO:HB2	1:A:373:GLY:HA2	1.92	0.52
1:C:231:GLN:O	1:C:235:ASP:HB2	2.09	0.52
3:G:12:GLU:HG2	3:G:314:VAL:HG23	1.92	0.52
5:I:145:LYS:HD3	5:I:167:ILE:HD12	1.92	0.52
13:d:146:THR:HB	13:d:149:GLU:HB3	1.92	0.52
3:G:58:LEU:O	3:G:301:ARG:NE	2.42	0.52
13:d:158:THR:HG22	13:d:160:LEU:H	1.75	0.52
13:d:263:GLN:O	13:d:267:VAL:HG23	2.10	0.52
1:B:466:ASP:HA	1:B:470:THR:HA	1.92	0.51
2:E:368:GLU:HA	2:E:394:ARG:HD2	1.91	0.51
2:F:450:GLN:HG3	2:F:454:ARG:HH11	1.73	0.51
3:G:28:LYS:HD3	3:G:28:LYS:H	1.75	0.51
3:G:204:LEU:HD22	3:G:240:LYS:HB3	1.91	0.51
1:A:511:VAL:HG13	1:A:544:MET:HE1	1.91	0.51
2:F:164:ILE:HD11	2:F:179:ARG:HA	1.91	0.51
5:K:53:ILE:HG12	7:O:48:ARG:HE	1.75	0.51
2:E:350:MET:SD	2:E:360:PRO:HB3	2.49	0.51
7:N:13:GLN:O	7:N:17:ARG:HG2	2.09	0.51
16:o:22:ALA:HB2	16:o:96:GLY:HA2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:TYR:HE1	1:C:597:ILE:HG12	1.75	0.51
3:G:343:ASP:OD1	3:G:344:SER:N	2.43	0.51
7:O:28:ARG:O	7:O:32:ARG:HG2	2.10	0.51
9:T:52:ARG:HD2	9:T:64:GLU:HG2	1.91	0.51
9:T:218:TRP:HE1	9:T:227:ILE:HD11	1.76	0.51
9:T:274:GLN:HB2	9:T:317:GLN:HE21	1.76	0.51
13:d:208:MET:HE1	13:d:316:TYR:CZ	2.46	0.51
1:B:152:ILE:HD13	1:B:167:MET:HB3	1.93	0.51
1:C:74:SER:HA	2:F:61:GLN:HA	1.93	0.51
9:T:296:SER:HA	9:T:302:ARG:HD2	1.92	0.51
11:b:79:GLY:O	11:b:83:ALA:N	2.38	0.51
1:A:88:VAL:HG12	1:A:103:GLN:HG3	1.93	0.51
1:B:281:VAL:HA	1:B:315:THR:HG21	1.92	0.51
2:F:181:GLN:NE2	2:F:393:SER:OG	2.41	0.51
9:T:273:LEU:HD11	9:T:321:LEU:HD11	1.93	0.51
1:A:24:VAL:HG13	1:A:29:VAL:HG22	1.92	0.51
16:k:44:MET:O	16:k:48:ARG:N	2.30	0.51
1:A:102:ILE:HG13	1:A:104:ARG:HG3	1.92	0.51
1:A:331:ILE:HD12	1:A:346:MET:HE1	1.91	0.51
2:D:432:VAL:HG23	2:D:433:VAL:HG13	1.91	0.51
3:G:216:LEU:HD23	3:G:226:ASN:HB2	1.92	0.51
4:H:120:GLU:HG2	4:H:121:LEU:HG	1.93	0.51
9:T:101:LEU:O	9:T:104:ASN:ND2	2.39	0.51
1:B:165:ARG:HG3	1:B:340:MET:HG2	1.91	0.51
1:C:489:LEU:O	1:C:492:ILE:HG22	2.11	0.51
2:E:165:GLN:OE1	2:E:467:VAL:N	2.43	0.50
3:G:61:LEU:O	3:G:65:VAL:HG23	2.11	0.50
6:L:67:ASN:HB2	6:L:70:ILE:HD12	1.93	0.50
8:R:67:GLU:O	8:R:71:SER:N	2.42	0.50
1:C:284:MET:HE1	1:C:311:LEU:HD11	1.93	0.50
13:d:339:ARG:HG3	13:d:341:ARG:HH12	1.76	0.50
2:D:430:LYS:HE2	2:D:435:GLU:HB3	1.92	0.50
2:F:53:VAL:HG22	2:F:89:ILE:HG12	1.94	0.50
5:I:120:VAL:O	5:I:124:LEU:HG	2.12	0.50
16:n:81:THR:O	16:n:83:GLY:N	2.42	0.50
1:A:178:TYR:HB3	1:A:193:GLU:HB2	1.93	0.50
1:C:350:SER:CB	1:C:353:ARG:HB2	2.41	0.50
1:C:589:PRO:HB3	1:C:597:ILE:HD13	1.92	0.50
2:D:127:ASN:ND2	2:D:131:LYS:HB3	2.26	0.50
4:H:94:ILE:HG21	6:L:63:ILE:HD11	1.93	0.50
8:Q:161:MET:HG3	8:Q:216:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:12:ILE:HD12	7:N:10:GLN:HG3	1.93	0.50
1:B:316:SER:HB3	2:E:322:TYR:HE2	1.77	0.50
3:G:118:LEU:HD13	3:G:304:VAL:HG22	1.94	0.50
8:R:209:GLU:HB2	8:R:212:PRO:HG3	1.94	0.50
16:i:149:ALA:O	16:i:153:SER:N	2.42	0.50
1:A:105:PRO:HB2	1:A:108:ASP:HB2	1.92	0.50
1:A:135:PHE:CE1	1:A:154:GLY:HA3	2.47	0.50
2:E:379:ASN:O	2:E:381:GLN:NE2	2.44	0.50
3:G:5:TRP:CD1	3:G:373:LYS:HA	2.47	0.50
4:H:72:ALA:HA	4:H:130:GLN:HE22	1.76	0.50
8:S:94:LEU:HA	8:S:130:LEU:HD21	1.94	0.50
16:k:22:ALA:HB2	16:k:96:GLY:HA2	1.93	0.50
13:d:224:THR:HG21	13:d:255:LEU:O	2.12	0.50
16:j:18:GLY:HA3	16:j:93:LEU:HA	1.94	0.50
1:A:46:GLY:HA2	1:A:77:ASP:HB3	1.94	0.50
2:E:127:ASN:OD1	2:E:131:LYS:N	2.45	0.50
4:H:135:LYS:HG2	6:L:22:LEU:HB3	1.93	0.50
5:K:132:MET:HA	5:K:132:MET:HE2	1.93	0.50
9:T:235:CYS:SG	9:T:239:LEU:HD22	2.52	0.50
4:H:62:MET:HE2	6:L:92:PRO:HG2	1.95	0.49
2:E:37:PRO:HG2	5:J:126:GLN:HG3	1.93	0.49
2:E:228:MET:HA	2:E:256:ASN:HB3	1.93	0.49
9:T:141:ALA:HA	9:T:144:ILE:HD12	1.94	0.49
12:c:322:PHE:HA	12:c:346:ILE:HA	1.93	0.49
7:N:9:GLN:HA	7:N:12:LEU:HD12	1.94	0.49
1:B:132:LYS:HB3	1:B:184:ASN:HB3	1.94	0.49
2:E:125:VAL:HG13	2:E:253:LEU:HB2	1.95	0.49
2:F:262:THR:O	2:F:265:ARG:HB2	2.12	0.49
6:L:55:PHE:HB3	6:L:61:ILE:HG21	1.94	0.49
6:L:69:TYR:HB3	6:L:96:HIS:CD2	2.48	0.49
1:B:43:VAL:HG11	1:B:64:ILE:HD12	1.93	0.49
3:G:181:TYR:HB3	3:G:230:PHE:CE1	2.47	0.49
3:G:300:LEU:HB2	3:G:301:ARG:NH2	2.28	0.49
1:C:152:ILE:HB	1:C:398:PRO:HG2	1.95	0.49
8:R:120:ASN:HB3	8:R:123:LYS:NZ	2.28	0.49
1:A:39:MET:HG3	1:A:40:TYR:CE2	2.48	0.49
1:B:42:LEU:HD13	1:B:44:ARG:HH12	1.76	0.49
1:B:280:ARG:HB2	1:B:283:GLU:HG2	1.94	0.49
2:F:228:MET:HB3	2:F:265:ARG:HG2	1.94	0.49
2:F:438:LEU:HD13	2:F:446:LEU:HD11	1.94	0.49
3:G:49:ASP:OD2	10:a:227:ASP:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:50:ARG:HG2	5:K:54:MET:HE3	1.93	0.49
1:A:25:SER:HA	2:D:82:GLU:HG2	1.95	0.49
2:E:192:PRO:O	2:E:196:ILE:HG12	2.12	0.49
3:G:164:ARG:NH1	3:G:168:GLU:OE1	2.42	0.49
1:A:61:MET:HA	1:A:61:MET:HE2	1.94	0.49
1:B:150:GLY:HA2	1:B:167:MET:HE2	1.94	0.49
1:B:243:GLY:HA2	1:B:404:VAL:O	2.12	0.49
5:J:223:LYS:H	5:J:223:LYS:HG2	1.46	0.49
8:Q:90:GLU:HG3	8:Q:121:LEU:HG	1.93	0.49
16:l:150:LEU:O	16:l:154:THR:N	2.45	0.49
1:B:511:VAL:HG11	1:B:548:TYR:HB2	1.94	0.48
10:a:812:GLN:O	10:a:816:TYR:N	2.34	0.48
13:d:91:GLU:H	13:d:91:GLU:CD	2.21	0.48
16:l:18:GLY:HA3	16:l:93:LEU:HA	1.94	0.48
7:N:27:LYS:HB3	7:N:31:ARG:HH22	1.78	0.48
1:A:559:ALA:HA	1:A:564:LYS:HB3	1.95	0.48
1:C:37:ALA:HB1	1:C:54:ILE:HD13	1.95	0.48
2:E:389:LEU:HB2	2:E:420:TYR:HE2	1.78	0.48
1:A:30:THR:HA	1:A:62:ALA:O	2.13	0.48
16:i:31:ALA:HA	16:j:109:ALA:HB2	1.95	0.48
1:B:431:VAL:HG13	1:B:455:SER:HB2	1.95	0.48
1:C:116:ILE:HG22	2:F:156:ASP:HB3	1.95	0.48
16:j:31:ALA:HB1	16:k:109:ALA:HB2	1.96	0.48
3:G:58:LEU:HB3	3:G:301:ARG:NE	2.28	0.48
8:Q:207:GLN:HG3	8:Q:212:PRO:HG3	1.95	0.48
9:T:290:ARG:O	9:T:294:GLU:CB	2.61	0.48
1:C:55:ILE:HG13	1:C:63:THR:HB	1.96	0.48
3:G:28:LYS:HE3	3:G:35:THR:HG23	1.96	0.48
3:G:319:MET:HE3	3:G:319:MET:HB3	1.74	0.48
1:A:574:MET:HG2	1:A:611:ALA:HB1	1.96	0.48
8:R:155:MET:HB2	8:R:178:LEU:HD11	1.96	0.48
1:B:540:MET:HG2	1:B:584:MET:HE2	1.95	0.48
3:G:329:LYS:H	3:G:329:LYS:HG3	1.47	0.48
7:N:10:GLN:HA	7:N:13:GLN:CD	2.39	0.48
9:T:94:LEU:HB3	9:T:140:MET:CE	2.44	0.48
9:T:121:THR:HB	9:T:125:TYR:HB3	1.95	0.48
10:a:90:PHE:O	10:a:92:ARG:N	2.44	0.48
1:B:397:ASN:HB3	8:R:28:TYR:CD1	2.49	0.47
1:C:190:VAL:HG21	1:C:202:LYS:HD3	1.95	0.47
2:D:315:ARG:HB2	2:D:358:PRO:HG3	1.94	0.47
6:L:67:ASN:ND2	6:L:91:ILE:HG23	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:69:TYR:HB3	6:L:96:HIS:HD2	1.79	0.47
8:R:43:LYS:HA	8:R:43:LYS:HD3	1.59	0.47
8:R:69:SER:HA	8:R:74:CYS:HB2	1.95	0.47
13:d:161:ALA:HA	13:d:164:PHE:HD2	1.79	0.47
3:G:204:LEU:O	3:G:240:LYS:HG3	2.14	0.47
1:A:148:THR:HG22	8:Q:24:GLY:HA3	1.95	0.47
1:C:102:ILE:H	1:C:102:ILE:HG12	1.39	0.47
4:H:152:GLN:HG2	6:L:105:ILE:HG12	1.95	0.47
5:I:135:ARG:NH2	5:I:184:TYR:OH	2.47	0.47
5:K:184:TYR:HB3	5:K:188:ARG:HA	1.95	0.47
9:T:290:ARG:O	9:T:294:GLU:HB3	2.13	0.47
16:h:29:GLY:C	16:h:107:GLY:HA3	2.39	0.47
16:l:31:ALA:HB1	16:m:109:ALA:HB2	1.96	0.47
1:A:39:MET:HE2	1:A:39:MET:HA	1.96	0.47
3:G:189:VAL:HG13	3:G:246:PHE:CE1	2.49	0.47
16:g:15:ALA:HB2	16:g:89:SER:HA	1.96	0.47
16:i:29:GLY:CA	16:i:104:LEU:HA	2.43	0.47
1:A:395:LEU:HD21	8:Q:13:LEU:HD11	1.96	0.47
1:C:90:LEU:HA	1:C:94:ILE:HD11	1.97	0.47
2:D:170:PRO:O	2:D:174:MET:HB3	2.14	0.47
2:E:132:PRO:HG3	2:E:137:PRO:O	2.13	0.47
2:E:382:ILE:HG23	2:E:458:ASN:HB2	1.96	0.47
5:J:49:GLN:HB2	7:N:44:ILE:HG13	1.97	0.47
13:d:21:ARG:HH11	13:d:309:GLN:HA	1.79	0.47
1:B:263:LEU:HD11	1:B:347:MET:SD	2.54	0.47
2:D:429:MET:O	2:D:433:VAL:HG22	2.14	0.47
9:T:207:LEU:HA	9:T:210:ARG:HE	1.79	0.47
16:m:149:ALA:O	16:m:153:SER:N	2.47	0.47
1:A:226:PRO:HG3	1:A:461:LEU:HD22	1.97	0.47
1:B:383:ALA:HB1	2:F:258:ALA:HB1	1.96	0.47
1:C:147:ILE:HD11	1:C:168:LEU:HD13	1.95	0.47
1:C:164:HIS:CE1	1:C:336:TYR:HE2	2.33	0.47
1:C:174:GLY:HA3	1:C:194:LEU:HB3	1.97	0.47
4:H:179:ARG:HG2	4:H:182:ARG:HH11	1.80	0.47
5:K:57:TYR:CD2	7:O:51:ARG:HB3	2.50	0.47
8:S:36:ILE:HG13	8:S:92:LEU:HA	1.97	0.47
8:S:39:GLU:H	8:S:39:GLU:HG2	1.48	0.47
13:d:16:LEU:HD22	13:d:85:MET:SD	2.55	0.47
16:g:22:ALA:HA	16:g:100:GLY:HA3	1.97	0.47
16:g:29:GLY:C	16:g:107:GLY:HA3	2.40	0.47
1:B:528:TYR:HB3	1:B:586:PHE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ILE:CG2	1:B:608:VAL:HG22	2.44	0.47
2:D:446:LEU:O	2:D:450:GLN:OE1	2.32	0.47
16:h:15:ALA:HB2	16:h:89:SER:HA	1.97	0.47
16:h:18:GLY:O	16:h:96:GLY:HA3	2.15	0.47
2:F:222:ALA:HB3	2:F:287:VAL:HG22	1.97	0.47
3:G:275:GLN:O	3:G:279:LEU:HB3	2.15	0.47
1:C:393:LYS:HB2	1:C:393:LYS:HE3	1.69	0.47
2:E:459:GLN:HG2	2:E:465:ARG:CZ	2.45	0.47
5:K:33:LYS:HB2	5:K:33:LYS:HE3	1.64	0.47
13:d:295:PHE:O	13:d:299:VAL:HG23	2.15	0.47
13:d:315:PHE:O	13:d:319:VAL:HG23	2.15	0.47
1:A:338:ARG:HD3	1:A:404:VAL:HG23	1.96	0.46
2:F:409:HIS:HA	2:F:471:LEU:HD21	1.98	0.46
5:K:16:MET:HE2	5:K:16:MET:HA	1.97	0.46
8:Q:46:ARG:HA	8:Q:46:ARG:HD2	1.68	0.46
8:Q:205:LYS:HA	8:Q:205:LYS:HD3	1.68	0.46
11:b:165:ALA:O	11:b:169:ASN:N	2.35	0.46
8:R:55:TRP:CH2	8:R:74:CYS:HA	2.50	0.46
9:T:151:TRP:HZ2	9:T:210:ARG:HB2	1.79	0.46
13:d:324:GLN:HB3	13:d:350:ILE:HD11	1.97	0.46
5:J:53:ILE:HA	7:N:48:ARG:HH11	1.81	0.46
9:T:333:GLU:O	9:T:336:LYS:HG3	2.14	0.46
2:D:58:LYS:H	2:D:58:LYS:HG2	1.59	0.46
2:E:479:ARG:HA	2:E:479:ARG:HD2	1.71	0.46
12:c:374:ASN:O	12:c:382:LEU:HA	2.15	0.46
1:B:340:MET:HE3	1:B:340:MET:HB2	1.85	0.46
1:B:444:HIS:CE1	1:B:450:TRP:HZ2	2.34	0.46
9:T:394:LEU:HD23	9:T:414:VAL:HG23	1.98	0.46
16:h:42:ALA:HB2	16:i:116:ALA:HB1	1.96	0.46
1:C:164:HIS:HE1	1:C:336:TYR:HE2	1.63	0.46
2:D:169:SER:HB3	2:D:470:SER:HB3	1.97	0.46
2:F:439:THR:HG23	2:F:442:ASP:H	1.81	0.46
9:T:355:TYR:HB2	9:T:369:VAL:HG21	1.97	0.46
1:B:389:ALA:HA	1:B:404:VAL:HB	1.97	0.46
5:K:139:GLN:H	5:K:139:GLN:HG3	1.55	0.46
16:j:22:ALA:HB2	16:j:96:GLY:HA2	1.97	0.46
8:S:211:SER:HB3	8:S:214:GLU:HB3	1.98	0.46
2:E:366:ILE:H	2:E:366:ILE:HG13	1.46	0.46
3:G:79:VAL:CG2	3:G:279:LEU:HD21	2.46	0.46
8:Q:106:ASP:OD1	8:Q:107:LEU:N	2.49	0.46
8:S:223:LYS:HA	8:S:223:LYS:HD3	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLY:HA2	1:A:349:ASN:HB2	1.98	0.46
1:B:356:GLU:HG3	1:B:359:ARG:HH11	1.81	0.46
1:B:507:ILE:HD11	1:B:555:VAL:HG21	1.97	0.46
1:C:104:ARG:HE	1:C:122:VAL:HG12	1.81	0.46
1:C:381:ARG:HD2	1:C:381:ARG:HA	1.71	0.46
13:d:21:ARG:O	13:d:24:LYS:HG3	2.16	0.46
13:d:257:ARG:H	13:d:257:ARG:HG2	1.52	0.46
1:A:86:LEU:HD11	1:A:102:ILE:HG22	1.98	0.45
1:C:173:ARG:HE	1:C:173:ARG:HB3	1.52	0.45
1:C:204:SER:C	1:C:206:VAL:N	2.74	0.45
3:G:7:ILE:HA	3:G:370:VAL:O	2.16	0.45
5:I:125:TYR:HE2	7:M:108:PRO:HB2	1.81	0.45
7:O:31:ARG:HD3	7:O:31:ARG:HA	1.74	0.45
7:O:56:LYS:HE2	7:O:56:LYS:HB2	1.55	0.45
13:d:5:PRO:HA	13:d:8:TYR:CZ	2.52	0.45
13:d:49:LEU:HA	13:d:52:THR:HG22	1.97	0.45
1:A:291:PHE:CE2	1:A:311:LEU:HD11	2.51	0.45
1:C:176:VAL:HA	1:C:194:LEU:HD23	1.98	0.45
3:G:16:GLN:HB3	3:G:317:GLN:HG2	1.97	0.45
1:B:465:TYR:O	1:B:469:PHE:N	2.47	0.45
2:E:229:GLY:N	2:E:256:ASN:O	2.48	0.45
9:T:386:LYS:HE2	9:T:386:LYS:HB2	1.68	0.45
16:h:31:ALA:HB2	16:i:105:ALA:HB1	1.98	0.45
2:D:154:PRO:HA	2:D:157:ARG:HG3	1.98	0.45
8:S:162:GLN:HE21	8:S:162:GLN:HB3	1.60	0.45
9:T:22:LYS:HG2	9:T:136:PHE:CD1	2.51	0.45
12:c:271:GLN:N	12:c:397:GLN:O	2.45	0.45
12:c:356:ASN:N	12:c:384:VAL:O	2.48	0.45
13:d:195:LYS:O	13:d:199:LEU:HG	2.15	0.45
5:I:152:ILE:HD11	5:I:165:VAL:HB	1.97	0.45
5:J:191:LYS:HB2	5:J:191:LYS:HE2	1.53	0.45
2:F:152:ILE:HG21	2:F:157:ARG:HG3	1.98	0.45
3:G:65:VAL:HG21	3:G:297:VAL:HG21	1.98	0.45
4:H:81:THR:HA	4:H:84:ILE:HG12	1.98	0.45
7:N:10:GLN:HA	7:N:13:GLN:NE2	2.32	0.45
8:Q:100:PRO:HG2	8:Q:101:PHE:CE2	2.52	0.45
1:A:292:PRO:HG2	1:A:293:GLU:OE1	2.16	0.45
1:A:317:ASN:HD21	2:D:157:ARG:HH12	1.65	0.45
1:C:212:ARG:H	1:C:212:ARG:HG2	1.67	0.45
1:C:341:GLY:HA3	1:C:400:ARG:HG3	1.99	0.45
2:E:177:ILE:HG12	2:E:183:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:527:THR:N	14:e:67:GLN:O	2.33	0.45
1:A:159:ASN:OD1	1:A:162:ILE:N	2.40	0.45
1:A:393:LYS:HA	1:A:393:LYS:HD3	1.56	0.45
1:B:238:PHE:CZ	1:B:450:TRP:HA	2.52	0.45
2:D:39:VAL:HG13	5:I:192:VAL:HB	1.99	0.45
3:G:187:VAL:HG21	3:G:197:TRP:CZ2	2.52	0.45
5:K:127:LEU:HD13	5:K:132:MET:HE1	1.97	0.45
13:d:17:GLU:HA	13:d:20:VAL:HG12	1.99	0.45
2:D:71:PRO:HG3	2:D:103:LYS:HB2	1.98	0.45
3:G:7:ILE:HD12	3:G:321:LEU:HD22	1.98	0.45
5:J:12:ILE:HD13	5:J:15:MET:HE3	1.99	0.45
8:S:42:LEU:HB3	8:S:45:ILE:HB	1.98	0.45
16:j:33:GLY:HA2	16:j:111:GLY:HA3	1.99	0.45
1:B:218:THR:OG1	1:B:395:LEU:HA	2.16	0.45
1:C:426:LEU:HD13	2:D:189:ALA:HB1	1.99	0.45
2:E:354:ASP:HB3	2:E:357:HIS:HB2	1.99	0.45
3:G:54:LEU:O	3:G:58:LEU:HB2	2.16	0.45
4:H:204:LYS:HD3	4:H:204:LYS:HA	1.57	0.45
13:d:77:LYS:HE2	13:d:77:LYS:HB2	1.75	0.45
13:d:289:THR:O	13:d:293:ARG:HG2	2.18	0.45
1:B:215:ARG:HB2	1:B:338:ARG:NH1	2.32	0.44
1:B:274:TYR:CE2	1:B:284:MET:HE1	2.52	0.44
2:D:476:LYS:HA	2:D:479:ARG:HD2	1.98	0.44
2:F:82:GLU:HB3	2:F:89:ILE:HB	1.99	0.44
2:F:357:HIS:CD2	2:F:358:PRO:HD2	2.52	0.44
3:G:200:GLN:O	3:G:204:LEU:HG	2.16	0.44
5:I:123:GLY:HA3	5:I:183:ILE:HD12	1.99	0.44
7:N:47:TYR:HA	7:N:51:ARG:HH11	1.82	0.44
13:d:8:TYR:O	13:d:11:VAL:HG12	2.17	0.44
1:A:552:ARG:HE	1:A:552:ARG:HB2	1.61	0.44
1:B:217:VAL:O	8:R:13:LEU:HD21	2.17	0.44
1:B:234:LEU:HD22	1:B:433:TRP:CG	2.52	0.44
1:B:540:MET:HB3	1:B:540:MET:HE2	1.73	0.44
1:C:598:LYS:HD2	1:C:598:LYS:HA	1.35	0.44
5:K:155:TYR:CE1	5:K:163:VAL:HB	2.52	0.44
6:L:99:ASP:OD1	6:L:99:ASP:N	2.50	0.44
7:O:17:ARG:HA	7:O:17:ARG:HD3	1.60	0.44
8:R:161:MET:HE3	8:R:161:MET:HB3	1.67	0.44
9:T:102:GLN:CD	9:T:140:MET:HG2	2.43	0.44
12:c:270:ALA:HA	12:c:398:ASP:O	2.18	0.44
1:C:120:ARG:HE	1:C:120:ARG:HB3	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:54:LEU:HD21	3:G:119:LYS:HB2	1.97	0.44
8:R:194:ASP:OD1	8:R:195:GLU:N	2.51	0.44
1:A:149:GLY:HA2	1:A:168:LEU:HB3	1.99	0.44
1:A:295:THR:HG22	1:A:304:SER:HA	2.00	0.44
1:C:105:PRO:HG2	1:C:108:ASP:HB2	1.99	0.44
2:D:199:GLN:HE22	2:D:459:GLN:HG2	1.82	0.44
2:E:103:LYS:HD3	2:E:103:LYS:HA	1.40	0.44
2:E:348:LEU:HG	2:E:350:MET:HE1	1.98	0.44
2:F:228:MET:HE1	2:F:291:LEU:HB3	1.98	0.44
4:H:140:LYS:HD3	4:H:140:LYS:HA	1.67	0.44
8:S:123:LYS:HA	8:S:123:LYS:HD3	1.64	0.44
9:T:94:LEU:O	9:T:98:ASP:HB2	2.17	0.44
8:R:126:TYR:CE1	8:R:169:THR:HA	2.53	0.44
1:C:53:GLU:HB2	1:C:67:TYR:HE1	1.83	0.44
1:C:457:TYR:HE1	2:D:233:GLU:HG3	1.83	0.44
8:Q:43:LYS:HA	8:Q:43:LYS:HD3	1.70	0.44
8:R:125:ASP:OD1	8:R:126:TYR:N	2.50	0.44
13:d:49:LEU:HB3	13:d:57:PHE:HE1	1.82	0.44
13:d:106:ILE:HG13	13:d:160:LEU:HD13	1.98	0.44
13:d:193:PHE:CE2	13:d:208:MET:HE2	2.52	0.44
16:g:36:LYS:CB	16:g:112:ILE:H	2.30	0.44
1:A:271:VAL:HB	1:A:344:VAL:HG22	1.99	0.44
1:A:377:TYR:HA	2:E:299:GLU:OE2	2.18	0.44
1:C:349:ASN:O	1:C:409:ALA:HB3	2.18	0.44
2:D:116:PRO:CB	2:D:141:ALA:HB2	2.48	0.44
4:H:201:ARG:O	4:H:205:ILE:HG13	2.18	0.44
5:K:59:LYS:HG3	5:K:63:GLN:HE22	1.83	0.44
9:T:254:PRO:O	9:T:297:THR:OG1	2.32	0.44
10:a:776:LEU:O	10:a:780:PHE:N	2.39	0.44
16:l:149:ALA:O	16:l:153:SER:N	2.47	0.44
1:B:340:MET:HB3	1:B:342:TYR:HD2	1.83	0.44
1:C:436:ASP:HB3	1:C:439:LEU:HB2	2.00	0.44
1:C:458:MET:SD	1:C:459:ARG:N	2.91	0.44
2:F:181:GLN:NE2	2:F:183:ILE:HD11	2.32	0.44
5:K:38:PHE:HD2	7:O:32:ARG:HB2	1.83	0.44
6:L:27:GLU:H	6:L:35:ASN:HB2	1.83	0.44
7:N:27:LYS:HB3	7:N:31:ARG:NH2	2.33	0.44
8:S:226:VAL:HA	8:S:229:MET:HG2	2.00	0.44
1:B:135:PHE:HB2	1:B:156:VAL:HG22	2.00	0.44
2:F:227:ALA:HA	2:F:292:THR:HG22	2.00	0.44
3:G:201:TYR:CE2	3:G:213:SER:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HB3	1:A:336:TYR:CE2	2.53	0.43
1:A:282:ASN:HD21	2:D:181:GLN:HA	1.83	0.43
1:A:598:LYS:HB2	1:A:598:LYS:HE2	1.51	0.43
1:A:478:LYS:HE3	1:A:478:LYS:HB3	1.66	0.43
1:B:316:SER:HB2	2:E:326:ALA:HB1	2.00	0.43
1:C:467:LYS:HB3	1:C:467:LYS:HE3	1.76	0.43
2:E:432:VAL:HA	4:H:170:ASN:HB3	2.00	0.43
3:G:137:LYS:HE3	3:G:137:LYS:HB3	1.56	0.43
8:S:155:MET:HE3	8:S:155:MET:HB3	1.77	0.43
1:A:111:SER:O	1:A:114:GLN:NE2	2.38	0.43
2:D:163:MET:HE2	2:D:163:MET:HB2	1.81	0.43
2:E:186:PHE:CE1	2:E:348:LEU:HD21	2.53	0.43
3:G:39:ASN:O	3:G:40:ILE:HD13	2.18	0.43
9:T:62:LYS:HG2	9:T:107:ARG:HD2	2.00	0.43
16:g:22:ALA:HA	16:g:100:GLY:CA	2.48	0.43
7:O:55:PHE:HA	7:O:58:LYS:HD2	2.00	0.43
9:T:366:TRP:CE3	9:T:409:VAL:HG22	2.53	0.43
13:d:301:LEU:HD12	13:d:304:LEU:HD21	2.00	0.43
1:A:41:GLU:HA	1:A:85:PRO:HA	2.00	0.43
1:B:465:TYR:O	1:B:466:ASP:C	2.59	0.43
1:B:473:VAL:HB	1:B:474:PRO:HD3	2.01	0.43
1:C:395:LEU:HD23	1:C:395:LEU:HA	1.82	0.43
2:F:227:ALA:HB3	2:F:255:LEU:HA	2.00	0.43
3:G:210:PRO:HD3	5:K:11:GLN:HB2	1.99	0.43
3:G:369:TYR:CE1	3:G:371:TYR:HB2	2.53	0.43
6:L:110:LYS:C	6:L:112:MET:H	2.25	0.43
11:b:68:GLY:CA	11:b:156:GLY:HA3	2.49	0.43
1:A:331:ILE:HA	1:A:346:MET:SD	2.58	0.43
1:B:528:TYR:HD1	1:B:588:ASP:HB2	1.82	0.43
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.74	0.43
2:D:120:ASP:HB2	2:D:139:VAL:HG11	2.00	0.43
2:E:121:MET:HE2	2:E:121:MET:HB2	1.66	0.43
2:E:315:ARG:HG3	2:E:358:PRO:CD	2.46	0.43
2:F:162:GLU:OE1	2:F:162:GLU:N	2.48	0.43
8:R:42:LEU:HB3	8:R:45:ILE:HG13	2.00	0.43
9:T:244:ILE:HD13	9:T:285:ILE:HD12	2.00	0.43
12:c:331:TYR:HA	12:c:337:HIS:HA	2.00	0.43
16:n:7:GLY:HA3	16:n:84:ILE:O	2.18	0.43
1:A:176:VAL:HA	1:A:194:LEU:HD23	1.99	0.43
1:B:350:SER:HB3	1:B:353:ARG:HB2	2.01	0.43
1:B:535:TYR:CZ	1:B:594:GLU:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:THR:HG22	1:C:84:LYS:H	1.82	0.43
1:C:106:LEU:HD13	2:F:154:PRO:HD2	2.00	0.43
1:C:277:CYS:O	1:C:350:SER:HB2	2.19	0.43
2:F:184:PRO:HD2	2:F:369:GLY:O	2.19	0.43
6:L:15:ASP:OD1	6:L:16:THR:HG23	2.19	0.43
13:d:20:VAL:HA	13:d:23:LEU:HG	2.00	0.43
2:F:181:GLN:CD	2:F:395:LEU:HB2	2.44	0.43
2:F:383:TYR:HE2	2:F:461:PRO:HA	1.83	0.43
4:H:7:ILE:HA	4:H:179:ARG:HH11	1.84	0.43
8:S:227:LYS:HD2	8:S:227:LYS:HA	1.35	0.43
9:T:441:MET:HE1	9:T:452:ALA:C	2.44	0.43
13:d:122:ILE:HG12	13:d:145:GLN:NE2	2.34	0.43
2:E:223:ILE:HB	2:E:251:VAL:HG22	2.01	0.43
2:E:357:HIS:CD2	2:E:358:PRO:HD2	2.54	0.43
3:G:6:LEU:HD11	3:G:38:PHE:CD2	2.53	0.43
3:G:47:THR:HG22	5:J:22:GLU:HG2	2.00	0.43
3:G:62:ASP:HA	3:G:297:VAL:HG11	2.01	0.43
3:G:181:TYR:CG	5:K:19:ILE:HG12	2.54	0.43
4:H:132:ALA:HA	4:H:135:LYS:HD3	1.99	0.43
6:L:110:LYS:HA	6:L:110:LYS:HD3	1.80	0.43
8:S:143:ALA:HB1	8:S:149:ASN:ND2	2.34	0.43
10:a:49:ARG:O	10:a:51:PHE:N	2.52	0.43
13:d:217:ASP:HB2	13:d:274:TYR:OH	2.18	0.43
13:d:287:ASP:OD1	13:d:288:LYS:N	2.46	0.43
1:A:284:MET:HE1	1:A:349:ASN:HD22	1.83	0.43
1:A:581:LEU:HD12	1:A:581:LEU:HA	1.80	0.43
1:C:337:PHE:HB3	1:C:344:VAL:HG21	2.00	0.43
1:C:382:LEU:HD13	1:C:382:LEU:HA	1.85	0.43
2:F:396:MET:HE3	2:F:396:MET:HB3	1.91	0.43
5:I:138:LYS:O	5:I:141:PHE:CB	2.64	0.43
1:A:580:LYS:HD2	1:A:604:LEU:HD13	2.01	0.42
1:B:139:LYS:HA	1:B:139:LYS:HD3	1.53	0.42
1:B:247:ALA:HB2	1:B:429:VAL:HG21	2.00	0.42
2:E:429:MET:O	2:E:433:VAL:HG22	2.19	0.42
2:F:444:LEU:HD12	2:F:444:LEU:HA	1.73	0.42
9:T:194:SER:OG	9:T:195:SER:N	2.52	0.42
13:d:75:LYS:HZ3	13:d:131:PRO:HG3	1.84	0.42
13:d:268:ALA:HB2	13:d:278:PHE:CD2	2.53	0.42
2:D:227:ALA:O	2:D:256:ASN:HB3	2.18	0.42
5:J:131:ARG:HE	5:J:131:ARG:HB2	1.58	0.42
8:Q:231:ASP:O	8:Q:234:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:288:LEU:HD23	2:E:343:THR:HB	2.01	0.42
10:a:461:GLY:O	10:a:465:ASN:N	2.53	0.42
13:d:16:LEU:HD11	13:d:88:HIS:O	2.19	0.42
13:d:309:GLN:HE21	13:d:309:GLN:HB2	1.66	0.42
1:A:605:LEU:HD12	1:A:605:LEU:HA	1.70	0.42
1:C:550:LEU:HB3	1:C:612:PHE:CD2	2.53	0.42
2:D:236:ARG:HA	2:D:239:LYS:HG2	2.01	0.42
3:G:34:LEU:HB3	3:G:322:GLN:HB3	2.01	0.42
5:K:160:LYS:HD3	5:K:160:LYS:HA	1.32	0.42
10:a:518:GLY:HA2	14:e:55:ALA:HB1	2.01	0.42
16:i:120:GLY:O	16:i:124:GLN:N	2.38	0.42
1:A:270:ASP:HB2	1:A:342:TYR:HB3	2.01	0.42
3:G:136:LEU:HD21	3:G:286:ASN:HB2	2.00	0.42
5:J:132:MET:HB2	5:J:165:VAL:HG22	2.01	0.42
1:A:89:GLU:HG2	1:A:206:VAL:HG11	2.02	0.42
1:A:386:TYR:HE2	1:A:425:THR:HG22	1.84	0.42
1:C:170:PRO:HG2	1:C:209:TRP:CZ3	2.55	0.42
1:C:262:SER:O	1:C:265:LYS:HG2	2.20	0.42
2:E:397:LYS:H	2:E:397:LYS:HG3	1.43	0.42
4:H:121:LEU:HB3	4:H:124:LEU:HD22	2.01	0.42
9:T:71:SER:O	9:T:76:THR:OG1	2.29	0.42
13:d:331:TRP:CZ2	13:d:346:ASN:HB2	2.55	0.42
1:C:146:HIS:HB3	8:S:62:PHE:CD2	2.55	0.42
1:C:204:SER:C	1:C:206:VAL:H	2.27	0.42
2:D:310:GLU:H	2:D:310:GLU:HG3	1.67	0.42
3:G:336:TYR:OH	3:G:366:TYR:O	2.38	0.42
5:K:38:PHE:HE2	7:O:29:LYS:HG3	1.85	0.42
6:L:12:GLY:HA2	6:L:70:ILE:HD12	2.01	0.42
8:R:155:MET:HB3	8:R:155:MET:HE3	1.81	0.42
16:g:20:SER:HA	16:h:98:SER:CB	2.49	0.42
1:A:90:LEU:O	1:A:206:VAL:HG13	2.19	0.42
1:A:234:LEU:HD21	1:A:448:VAL:HG11	2.02	0.42
1:B:50:LEU:HD12	1:B:50:LEU:H	1.83	0.42
2:E:283:CYS:HB3	2:E:285:LYS:HE2	2.02	0.42
5:I:35:GLU:O	5:I:39:ASN:N	2.38	0.42
8:Q:58:LYS:HB3	8:Q:60:TYR:CE1	2.54	0.42
9:T:18:ILE:HG23	9:T:136:PHE:HE2	1.85	0.42
12:c:261:ASP:C	12:c:263:ALA:H	2.28	0.42
13:d:246:ARG:HH21	13:d:274:TYR:HE2	1.67	0.42
16:i:31:ALA:HB2	16:j:105:ALA:HB1	2.00	0.42
1:B:478:LYS:HD3	1:B:478:LYS:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:ARG:O	1:B:556:GLU:HG3	2.20	0.42
1:C:584:MET:HE3	1:C:601:TYR:CD1	2.55	0.42
1:C:603:GLN:HA	1:C:606:GLU:CD	2.45	0.42
2:D:158:ILE:HB	2:D:334:ARG:HB2	2.01	0.42
2:D:372:TYR:CD2	2:D:390:PRO:HB2	2.54	0.42
2:D:459:GLN:O	2:D:463:GLU:HB2	2.20	0.42
2:D:499:SER:O	2:D:500:ARG:HG2	2.19	0.42
10:a:302:ALA:O	10:a:306:THR:N	2.37	0.42
1:A:362:SER:OG	1:A:375:PRO:HB3	2.20	0.42
1:B:282:ASN:HD22	1:B:282:ASN:HA	1.69	0.42
2:F:326:ALA:HA	2:F:366:ILE:HG21	2.01	0.42
8:S:43:LYS:HB3	8:S:43:LYS:HE3	1.36	0.42
9:T:120:ASN:O	9:T:124:SER:OG	2.37	0.42
13:d:113:ILE:HD11	13:d:178:ILE:HG23	2.02	0.42
16:g:111:GLY:O	16:g:113:VAL:N	2.44	0.42
16:n:70:LEU:HA	16:n:73:ALA:HB3	2.01	0.42
1:A:271:VAL:O	1:A:344:VAL:HA	2.19	0.41
1:B:368:MET:HB2	1:B:368:MET:HE2	1.76	0.41
1:C:215:ARG:HA	1:C:216:PRO:HD3	1.94	0.41
2:E:372:TYR:O	2:E:372:TYR:CD2	2.73	0.41
2:F:443:LEU:HA	2:F:446:LEU:HD12	2.02	0.41
3:G:9:ALA:HB1	3:G:10:PRO:CD	2.49	0.41
5:K:187:ASP:O	5:K:188:ARG:HB2	2.20	0.41
7:N:10:GLN:HG2	7:N:11:LEU:HD12	2.02	0.41
10:a:174:VAL:O	10:a:243:SER:N	2.33	0.41
16:i:18:GLY:O	16:i:96:GLY:HA3	2.20	0.41
1:B:455:SER:O	1:B:458:MET:HG2	2.20	0.41
5:K:137:ARG:HD3	5:K:177:ILE:HG22	2.02	0.41
7:O:75:LYS:HB2	7:O:75:LYS:HE2	1.87	0.41
9:T:394:LEU:HD11	9:T:410:ALA:HA	2.01	0.41
13:d:328:ASN:CG	13:d:347:TYR:HB2	2.46	0.41
16:g:35:ALA:HB2	16:h:109:ALA:HA	2.02	0.41
16:i:33:GLY:HA2	16:i:111:GLY:HA3	2.02	0.41
1:A:368:MET:HE3	1:A:368:MET:HB3	1.67	0.41
1:B:459:ARG:H	1:B:459:ARG:HG3	1.45	0.41
2:D:196:ILE:HD11	2:D:385:PRO:HD2	2.01	0.41
2:D:454:ARG:HA	2:D:458:ASN:HD22	1.85	0.41
11:b:96:PHE:O	11:b:99:ALA:HB3	2.20	0.41
16:h:149:ALA:O	16:h:153:SER:N	2.46	0.41
1:B:231:GLN:HG3	1:B:259:ILE:CD1	2.51	0.41
2:E:257:LEU:N	2:E:260:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:373:VAL:CG2	2:E:385:PRO:HG2	2.50	0.41
2:F:423:GLY:HA3	2:F:449:LEU:HD13	2.03	0.41
5:K:55:GLU:HG3	5:K:56:TYR:N	2.35	0.41
8:Q:104:LYS:NZ	8:Q:106:ASP:H	2.18	0.41
13:d:248:TYR:N	13:d:249:PRO:HD2	2.35	0.41
16:i:29:GLY:C	16:i:107:GLY:HA3	2.45	0.41
1:A:32:CYS:SG	1:A:61:MET:HE1	2.61	0.41
1:C:152:ILE:HD13	1:C:167:MET:HB3	2.03	0.41
1:C:265:LYS:O	1:C:266:TYR:C	2.63	0.41
1:C:335:GLU:HA	1:C:338:ARG:CG	2.50	0.41
3:G:314:VAL:HG13	3:G:315:ASN:O	2.20	0.41
5:I:222:ARG:HB3	5:I:225:LEU:HD21	2.02	0.41
5:J:82:LYS:HB2	5:J:82:LYS:HE2	1.46	0.41
8:R:127:HIS:CD2	8:R:131:ASN:HD21	2.39	0.41
3:G:313:PRO:HD3	5:J:17:ALA:HB1	2.03	0.41
5:I:23:ALA:CB	7:M:18:ALA:HB1	2.50	0.41
5:I:125:TYR:CE2	7:M:108:PRO:HB2	2.55	0.41
5:I:168:ASP:OD2	5:I:171:ALA:HB3	2.20	0.41
7:O:58:LYS:HE3	7:O:58:LYS:HB3	1.48	0.41
9:T:277:VAL:HA	9:T:282:THR:HG21	2.01	0.41
9:T:308:ALA:HB1	9:T:314:VAL:HB	2.03	0.41
16:h:20:SER:O	16:h:24:VAL:N	2.51	0.41
16:o:149:ALA:O	16:o:153:SER:N	2.54	0.41
1:A:387:GLU:HG3	2:E:258:ALA:HB3	2.03	0.41
1:B:142:ARG:HD3	1:B:142:ARG:HA	1.84	0.41
1:B:533:PRO:HB2	1:B:535:TYR:CE2	2.56	0.41
2:F:181:GLN:NE2	2:F:395:LEU:HB2	2.36	0.41
3:G:79:VAL:HG22	3:G:279:LEU:HD21	2.02	0.41
8:R:81:LEU:HD12	8:R:81:LEU:HA	1.74	0.41
13:d:39:CYS:HB2	13:d:44:ASP:CG	2.46	0.41
1:A:577:ILE:HD13	1:A:577:ILE:HA	1.87	0.41
1:B:132:LYS:HD3	1:B:186:ASP:HB3	2.03	0.41
1:B:456:LYS:HA	1:B:456:LYS:HD2	1.76	0.41
1:C:280:ARG:HD3	2:F:368:GLU:HG3	2.01	0.41
2:F:180:GLY:HA2	2:F:342:ILE:O	2.21	0.41
3:G:48:LEU:HA	3:G:51:LEU:HD12	2.03	0.41
3:G:58:LEU:HD22	3:G:301:ARG:NH2	2.36	0.41
5:K:54:MET:HE1	7:O:51:ARG:HE	1.86	0.41
6:L:12:GLY:O	6:L:39:VAL:N	2.54	0.41
8:Q:14:THR:HG23	8:Q:17:GLN:H	1.86	0.41
12:c:327:ALA:HB2	12:c:403:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:i:15:ALA:HB2	16:i:89:SER:HA	2.02	0.41
1:B:238:PHE:HZ	1:B:450:TRP:HA	1.86	0.41
1:B:259:ILE:HD13	1:B:259:ILE:HA	1.94	0.41
1:B:535:TYR:CD1	1:B:536:LYS:N	2.88	0.41
1:C:46:GLY:HA2	1:C:77:ASP:HB3	2.02	0.41
2:D:80:VAL:HG11	2:D:83:VAL:HG13	2.02	0.41
2:D:116:PRO:HB2	2:D:141:ALA:HB2	2.02	0.41
2:D:240:SER:O	2:D:243:GLU:HG3	2.20	0.41
2:E:186:PHE:HB2	2:E:372:TYR:HA	2.02	0.41
2:E:226:ALA:HB2	2:E:272:ALA:HB2	2.03	0.41
4:H:68:SER:HA	4:H:71:GLU:OE1	2.21	0.41
5:K:26:LYS:HE3	5:K:30:ILE:HG13	2.02	0.41
7:N:13:GLN:HB2	7:N:17:ARG:NH2	2.36	0.41
7:O:23:SER:HA	7:O:26:ARG:HG2	2.03	0.41
8:R:88:LEU:HD12	8:R:88:LEU:HA	1.86	0.41
8:S:216:ILE:HD13	8:S:217:LEU:HD23	2.03	0.41
13:d:28:LEU:H	13:d:28:LEU:HD22	1.85	0.41
13:d:112:LEU:HA	13:d:125:LEU:HD13	2.02	0.41
1:A:189:ASP:OD1	1:A:190:VAL:N	2.54	0.41
1:C:279:GLU:HG3	1:C:284:MET:HB2	2.03	0.41
2:D:127:ASN:OD1	2:D:131:LYS:N	2.54	0.41
3:G:201:TYR:CD1	3:G:201:TYR:C	2.99	0.41
4:H:133:LYS:HB2	4:H:133:LYS:HE2	1.69	0.41
5:K:50:ARG:HA	5:K:53:ILE:HD12	2.03	0.41
8:S:86:LEU:HD13	8:S:86:LEU:HA	1.86	0.41
11:b:57:ALA:HB2	11:b:141:GLY:HA2	2.03	0.41
11:b:66:ALA:HB3	16:g:105:ALA:HB1	2.02	0.41
1:B:170:PRO:O	1:B:171:ARG:HB2	2.22	0.40
1:B:471:GLU:O	1:B:474:PRO:HD2	2.20	0.40
1:C:187:THR:HA	1:C:205:MET:HG3	2.03	0.40
2:E:476:LYS:O	2:E:479:ARG:HB2	2.21	0.40
2:F:357:HIS:CG	2:F:358:PRO:HD2	2.56	0.40
5:J:22:GLU:O	5:J:26:LYS:HG2	2.21	0.40
5:J:141:PHE:CE1	5:J:169:GLN:HG3	2.56	0.40
9:T:33:TRP:HZ2	9:T:93:ILE:HA	1.86	0.40
12:c:375:SER:CB	12:c:394:LEU:H	2.35	0.40
1:B:220:LYS:HD2	1:B:392:VAL:HG12	2.03	0.40
1:C:550:LEU:HG	1:C:613:ARG:HH12	1.86	0.40
1:C:553:ARG:O	1:C:556:GLU:HG3	2.21	0.40
2:E:282:GLN:HB3	5:J:222:ARG:HG2	2.03	0.40
2:E:318:PRO:HG2	2:E:321:MET:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:91:LEU:HD12	3:G:287:PHE:CE2	2.56	0.40
13:d:105:MET:O	13:d:109:VAL:HG23	2.21	0.40
1:A:528:TYR:CD1	1:A:586:PHE:HA	2.56	0.40
1:B:232:ARG:HG3	1:B:532:CYS:SG	2.61	0.40
1:C:335:GLU:O	1:C:338:ARG:HG3	2.21	0.40
2:D:75:GLN:HE21	2:D:75:GLN:HB3	1.56	0.40
2:D:268:THR:N	2:D:269:PRO:HD2	2.36	0.40
3:G:8:SER:HA	3:G:317:GLN:O	2.20	0.40
3:G:49:ASP:CG	10:a:228:GLN:H	2.29	0.40
5:J:25:GLU:O	5:J:29:GLU:OE1	2.39	0.40
5:K:191:LYS:HE2	5:K:191:LYS:HB2	1.36	0.40
9:T:299:ARG:O	9:T:299:ARG:NH2	2.48	0.40
13:d:338:GLN:HG3	13:d:340:HIS:ND1	2.37	0.40
16:j:85:SER:C	16:j:87:TYR:H	2.28	0.40
1:A:94:ILE:HD12	1:A:99:PHE:CZ	2.56	0.40
1:B:524:GLY:H	18:B:701:ADP:HN62	1.69	0.40
1:C:286:GLU:HB2	2:F:159:TYR:CE1	2.56	0.40
1:C:351:THR:O	1:C:354:TRP:HB3	2.22	0.40
2:E:138:VAL:O	2:E:139:VAL:C	2.64	0.40
3:G:9:ALA:HB3	3:G:317:GLN:CB	2.50	0.40
3:G:28:LYS:O	3:G:29:ASN:C	2.65	0.40
6:L:12:GLY:HA2	6:L:70:ILE:CD1	2.52	0.40
7:N:56:LYS:HD2	7:N:56:LYS:HA	1.76	0.40
9:T:19:ILE:HG12	9:T:136:PHE:HD2	1.86	0.40
9:T:259:HIS:HB3	9:T:262:ARG:NH1	2.36	0.40
10:a:191:CYS:O	10:a:193:GLY:N	2.53	0.40
13:d:153:ALA:O	13:d:157:ASP:HB2	2.21	0.40
1:A:275:VAL:HG21	1:A:330:GLY:HA3	2.04	0.40
2:E:142:GLU:HG3	5:J:212:ARG:HD3	2.04	0.40
4:H:72:ALA:HA	4:H:130:GLN:NE2	2.36	0.40
5:I:32:ALA:HB1	9:T:249:LEU:HD21	2.03	0.40
5:J:52:LYS:HD3	5:J:52:LYS:HA	1.53	0.40
9:T:249:LEU:HD23	9:T:249:LEU:HA	1.85	0.40
9:T:441:MET:HE2	9:T:441:MET:CA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	56/525 (11%)	41 (73%)	15 (27%)	0	4
1	B	508/525 (97%)	436 (86%)	72 (14%)	3	16
1	C	501/525 (95%)	427 (85%)	74 (15%)	3	15
2	D	392/438 (90%)	331 (84%)	61 (16%)	2	14
2	E	241/438 (55%)	211 (88%)	30 (12%)	4	19
2	F	176/438 (40%)	143 (81%)	33 (19%)	1	10
3	G	271/344 (79%)	254 (94%)	17 (6%)	16	40
4	H	73/211 (35%)	59 (81%)	14 (19%)	1	9
5	I	96/197 (49%)	86 (90%)	10 (10%)	7	24
5	J	167/197 (85%)	137 (82%)	30 (18%)	2	11
7	M	33/101 (33%)	27 (82%)	6 (18%)	2	11
7	N	95/101 (94%)	85 (90%)	10 (10%)	6	24
7	O	71/101 (70%)	49 (69%)	22 (31%)	0	2
8	Q	103/305 (34%)	89 (86%)	14 (14%)	3	17
8	R	94/305 (31%)	82 (87%)	12 (13%)	4	19
8	S	86/305 (28%)	71 (83%)	15 (17%)	2	12
9	T	243/429 (57%)	227 (93%)	16 (7%)	15	39
13	d	305/306 (100%)	284 (93%)	21 (7%)	14	38
All	All	3511/5791 (61%)	3039 (87%)	472 (13%)	6	18

All (472) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	555	VAL
1	A	556	GLU
1	A	568	SER
1	A	569	ILE
1	A	571	ARG
1	A	572	GLU
1	A	574	MET
1	A	576	GLU
1	A	577	ILE
1	A	581	LEU
1	A	587	LYS
1	A	596	LYS
1	A	598	LYS
1	A	605	LEU
1	A	616	GLU
1	B	43	VAL
1	B	53	GLU
1	B	65	GLN
1	B	74	SER
1	B	81	ARG
1	B	82	THR
1	B	84	LYS
1	B	87	SER
1	B	139	LYS
1	B	140	ASN
1	B	141	LEU
1	B	142	ARG
1	B	148	THR
1	B	155	ILE
1	B	167	MET
1	B	173	ARG
1	B	179	ILE
1	B	191	VAL
1	B	192	LEU
1	B	204	SER
1	B	205	MET
1	B	215	ARG
1	B	232	ARG
1	B	233	VAL
1	B	238	PHE
1	B	281	VAL
1	B	316	SER
1	B	344	VAL

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Mol	Chain	Res	Type
1	B	346	MET
1	B	350	SER
1	B	351	THR
1	B	352	SER
1	B	362	SER
1	B	364	ARG
1	B	365	LEU
1	B	368	MET
1	B	371	ASP
1	B	392	VAL
1	B	400	ARG
1	B	426	LEU
1	B	431	VAL
1	B	442	ARG
1	B	443	LYS
1	B	448	VAL
1	B	453	SER
1	B	455	SER
1	B	459	ARG
1	B	461	LEU
1	B	467	LYS
1	B	469	PHE
1	B	470	THR
1	B	476	ARG
1	B	477	THR
1	B	478	LYS
1	B	480	LYS
1	B	481	GLU
1	B	483	LEU
1	B	484	GLN
1	B	485	GLU
1	B	492	ILE
1	B	494	GLN
1	B	522	GLN
1	B	536	LYS
1	B	540	MET
1	B	552	ARG
1	B	553	ARG
1	B	587	LYS
1	B	590	VAL
1	B	591	LYS
1	B	596	LYS

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Mol	Chain	Res	Type
1	B	597	ILE
1	B	605	LEU
1	C	48	SER
1	C	53	GLU
1	C	55	ILE
1	C	57	LEU
1	C	58	GLU
1	C	60	ASP
1	C	63	THR
1	C	95	MET
1	C	102	ILE
1	C	103	GLN
1	C	107	SER
1	C	109	ILE
1	C	110	SER
1	C	111	SER
1	C	116	ILE
1	C	118	ILE
1	C	120	ARG
1	C	122	VAL
1	C	141	LEU
1	C	155	ILE
1	C	166	ILE
1	C	173	ARG
1	C	177	THR
1	C	179	ILE
1	C	191	VAL
1	C	204	SER
1	C	205	MET
1	C	212	ARG
1	C	220	LYS
1	C	224	ASN
1	C	265	LYS
1	C	279	GLU
1	C	281	VAL
1	C	308	ARG
1	C	326	SER
1	C	334	SER
1	C	338	ARG
1	C	340	MET
1	C	352	SER
1	C	361	ILE

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Mol	Chain	Res	Type
1	C	365	LEU
1	C	378	LEU
1	C	382	LEU
1	C	393	LYS
1	C	400	ARG
1	C	401	GLU
1	C	403	SER
1	C	404	VAL
1	C	419	ASP
1	C	438	LYS
1	C	439	LEU
1	C	443	LYS
1	C	450	TRP
1	C	467	LYS
1	C	469	PHE
1	C	470	THR
1	C	485	GLU
1	C	486	GLU
1	C	510	GLU
1	C	520	LEU
1	C	526	THR
1	C	530	ARG
1	C	544	MET
1	C	549	ASP
1	C	550	LEU
1	C	553	ARG
1	C	562	ASP
1	C	590	VAL
1	C	594	GLU
1	C	596	LYS
1	C	597	ILE
1	C	598	LYS
1	C	609	GLN
1	C	613	ARG
2	D	39	VAL
2	D	40	THR
2	D	47	VAL
2	D	48	ASN
2	D	54	LEU
2	D	58	LYS
2	D	75	GLN
2	D	77	SER

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Mol	Chain	Res	Type
2	D	81	LEU
2	D	83	VAL
2	D	86	THR
2	D	99	ILE
2	D	120	ASP
2	D	140	MET
2	D	146	ASP
2	D	150	GLN
2	D	160	PRO
2	D	161	GLU
2	D	162	GLU
2	D	163	MET
2	D	164	ILE
2	D	168	ILE
2	D	169	SER
2	D	177	ILE
2	D	182	LYS
2	D	200	ILE
2	D	244	GLU
2	D	302	ARG
2	D	304	VAL
2	D	305	SER
2	D	308	ARG
2	D	309	GLU
2	D	310	GLU
2	D	311	VAL
2	D	314	ARG
2	D	321	MET
2	D	323	THR
2	D	325	LEU
2	D	334	ARG
2	D	341	SER
2	D	343	THR
2	D	361	ASP
2	D	362	LEU
2	D	366	ILE
2	D	377	LEU
2	D	381	GLN
2	D	388	VAL
2	D	392	LEU
2	D	411	ASP
2	D	457	ILE

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Mol	Chain	Res	Type
2	D	459	GLN
2	D	466	SER
2	D	471	LEU
2	D	473	LEU
2	D	483	LYS
2	D	484	GLU
2	D	485	MET
2	D	488	ARG
2	D	489	ILE
2	D	493	MET
2	D	496	GLU
2	E	40	THR
2	E	42	ARG
2	E	54	LEU
2	E	67	ASN
2	E	81	LEU
2	E	92	VAL
2	E	102	GLN
2	E	103	LYS
2	E	105	THR
2	E	107	GLU
2	E	120	ASP
2	E	121	MET
2	E	138	VAL
2	E	140	MET
2	E	142	GLU
2	E	143	ASP
2	E	147	ILE
2	E	182	LYS
2	E	201	CYS
2	E	247	THR
2	E	266	ILE
2	E	273	LEU
2	E	282	GLN
2	E	305	SER
2	E	310	GLU
2	E	314	ARG
2	E	321	MET
2	E	327	THR
2	E	328	ILE
2	E	330	GLU
2	F	299	GLU

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Mol	Chain	Res	Type
2	F	308	ARG
2	F	314	ARG
2	F	315	ARG
2	F	330	GLU
2	F	334	ARG
2	F	335	VAL
2	F	336	GLU
2	F	338	ARG
2	F	345	ILE
2	F	348	LEU
2	F	374	ASP
2	F	377	LEU
2	F	380	ARG
2	F	396	MET
2	F	397	LYS
2	F	400	ILE
2	F	402	GLU
2	F	404	MET
2	F	407	LYS
2	F	408	ASP
2	F	411	ASP
2	F	427	GLN
2	F	444	LEU
2	F	449	LEU
2	F	451	LYS
2	F	455	ASN
2	F	457	ILE
2	F	459	GLN
2	F	463	GLU
2	F	464	LYS
2	F	485	MET
2	F	497	PHE
3	G	4	PHE
3	G	12	GLU
3	G	28	LYS
3	G	29	ASN
3	G	34	LEU
3	G	35	THR
3	G	132	ILE
3	G	137	LYS
3	G	139	ARG
3	G	145	ASN

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Mol	Chain	Res	Type
3	G	147	LYS
3	G	183	VAL
3	G	276	PHE
3	G	279	LEU
3	G	319	MET
3	G	329	LYS
3	G	331	LEU
4	H	93	LYS
4	H	95	ARG
4	H	97	LYS
4	H	106	LEU
4	H	108	VAL
4	H	184	LEU
4	H	188	ILE
4	H	195	GLU
4	H	196	ARG
4	H	202	LEU
4	H	203	LYS
4	H	204	LYS
4	H	206	GLN
4	H	214	GLU
5	I	199	ARG
5	I	200	LEU
5	I	201	ASP
5	I	202	LEU
5	I	203	ILE
5	I	207	MET
5	I	208	MET
5	I	211	VAL
5	I	212	ARG
5	I	223	LYS
5	J	21	GLN
5	J	41	GLU
5	J	44	ARG
5	J	45	LEU
5	J	46	VAL
5	J	50	ARG
5	J	52	LYS
5	J	54	MET
5	J	58	GLU
5	J	59	LYS
5	J	60	LYS

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Mol	Chain	Res	Type
5	J	62	LYS
5	J	63	GLN
5	J	66	GLN
5	J	82	LYS
5	J	85	ARG
5	J	87	ARG
5	J	99	LYS
5	J	110	THR
5	J	129	GLU
5	J	132	MET
5	J	133	ILE
5	J	135	ARG
5	J	162	ASP
5	J	164	ASP
5	J	168	ASP
5	J	185	ASN
5	J	189	LYS
5	J	191	LYS
5	J	193	SER
7	M	90	GLN
7	M	92	ARG
7	M	93	ASP
7	M	102	PHE
7	M	106	ILE
7	M	109	GLU
7	N	44	ILE
7	N	48	ARG
7	N	51	ARG
7	N	53	LYS
7	N	55	PHE
7	N	56	LYS
7	N	84	LEU
7	N	93	ASP
7	N	100	LEU
7	N	116	ILE
7	O	16	LYS
7	O	17	ARG
7	O	20	GLU
7	O	21	LYS
7	O	27	LYS
7	O	29	LYS
7	O	31	ARG

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Mol	Chain	Res	Type
7	O	33	LEU
7	O	35	GLN
7	O	41	GLN
7	O	45	GLU
7	O	46	GLN
7	O	53	LYS
7	O	85	GLN
7	O	86	THR
7	O	87	TYR
7	O	90	GLN
7	O	97	ASP
7	O	105	ASP
7	O	107	ARG
7	O	109	GLU
7	O	110	ILE
8	Q	39	GLU
8	Q	43	LYS
8	Q	44	LYS
8	Q	46	ARG
8	Q	47	GLU
8	Q	51	ASP
8	Q	79	ASP
8	Q	81	LEU
8	Q	89	GLN
8	Q	94	LEU
8	Q	115	MET
8	Q	119	VAL
8	Q	121	LEU
8	Q	178	LEU
8	R	78	LEU
8	R	79	ASP
8	R	81	LEU
8	R	83	ARG
8	R	85	SER
8	R	142	ASN
8	R	146	THR
8	R	148	LYS
8	R	155	MET
8	R	157	SER
8	R	161	MET
8	R	186	LEU
8	S	25	LYS

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Mol	Chain	Res	Type
8	S	29	ILE
8	S	32	CYS
8	S	33	MET
8	S	34	GLN
8	S	36	ILE
8	S	39	GLU
8	S	79	ASP
8	S	81	LEU
8	S	82	SER
8	S	86	LEU
8	S	89	GLN
8	S	92	LEU
8	S	116	LYS
8	S	123	LYS
9	T	215	ARG
9	T	219	VAL
9	T	250	LEU
9	T	252	PHE
9	T	346	VAL
9	T	367	SER
9	T	371	LYS
9	T	373	GLU
9	T	374	LYS
9	T	375	PHE
9	T	377	ARG
9	T	378	GLU
9	T	381	VAL
9	T	385	GLU
9	T	386	LYS
9	T	387	ASN
13	d	28	LEU
13	d	47	LEU
13	d	73	ARG
13	d	75	LYS
13	d	76	GLU
13	d	77	LYS
13	d	81	GLU
13	d	106	ILE
13	d	110	ILE
13	d	178	ILE
13	d	184	THR
13	d	218	ARG

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Mol	Chain	Res	Type
13	d	219	ARG
13	d	223	ILE
13	d	224	THR
13	d	232	LEU
13	d	257	ARG
13	d	259	ASP
13	d	291	GLU
13	d	298	GLU
13	d	309	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	ASN
1	B	282	ASN
1	B	343	HIS
1	B	349	ASN
1	B	444	HIS
1	B	484	GLN
1	B	521	GLN
1	C	164	HIS
1	C	444	HIS
1	C	609	GLN
2	D	75	GLN
2	D	102	GLN
2	D	199	GLN
2	D	250	ASN
2	D	352	ASN
2	D	376	GLN
2	E	36	HIS
2	E	175	ASN
2	E	199	GLN
2	E	203	GLN
5	I	221	ASN
5	J	47	GLN
5	J	49	GLN
5	J	63	GLN
5	J	71	GLN
5	J	126	GLN
7	M	91	ASN
7	N	41	GLN
7	O	9	GLN

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Mol	Chain	Res	Type
7	O	10	GLN
7	O	35	GLN
7	O	41	GLN
7	O	90	GLN
7	O	91	ASN
8	Q	120	ASN
8	Q	184	HIS
8	R	150	ASN
8	S	89	GLN
9	T	139	HIS
9	T	242	GLN
9	T	255	GLN
9	T	259	HIS
9	T	317	GLN
13	d	88	HIS
13	d	152	ASN
13	d	165	GLN
13	d	309	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	701	-	28,29,29	0.48	0	43,45,45	0.53	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	B	701	-	-	3/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

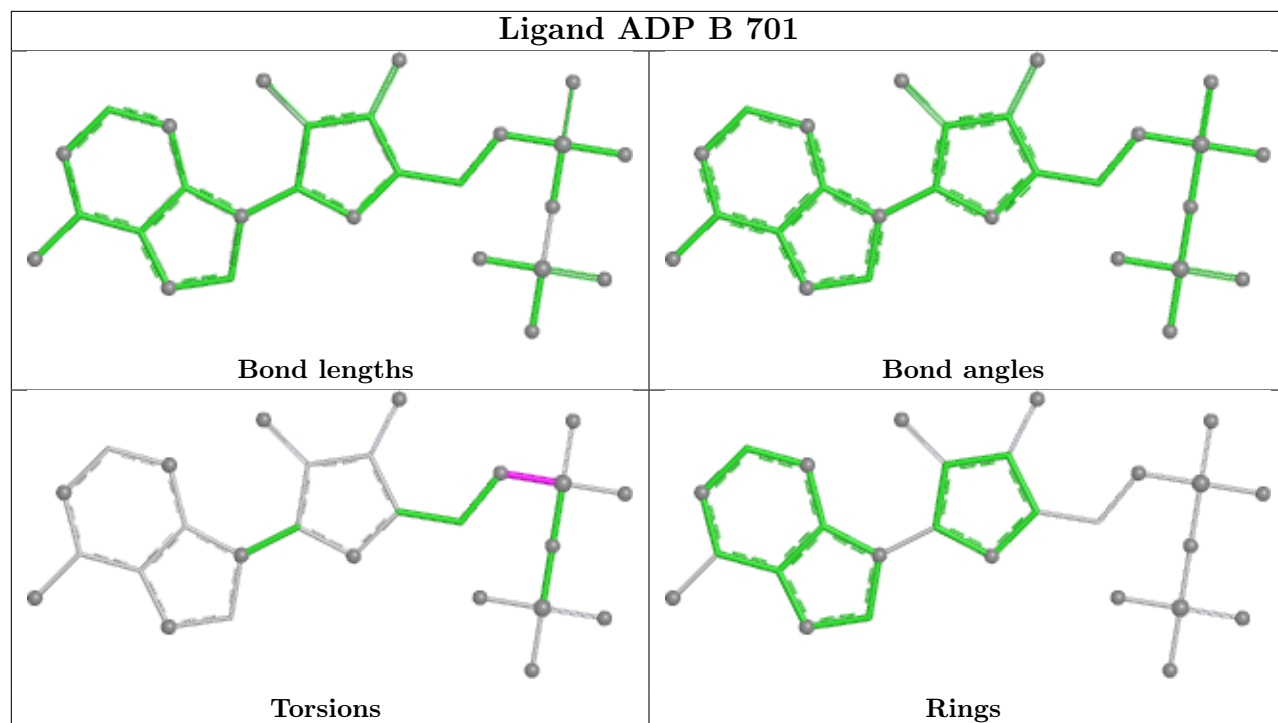
Mol	Chain	Res	Type	Atoms
18	B	701	ADP	C5'-O5'-PA-O2A
18	B	701	ADP	C5'-O5'-PA-O3A
18	B	701	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	701	ADP	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

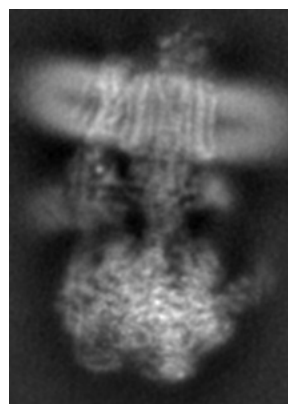
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26387. These allow visual inspection of the internal detail of the map and identification of artifacts.

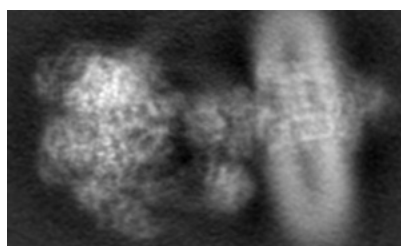
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

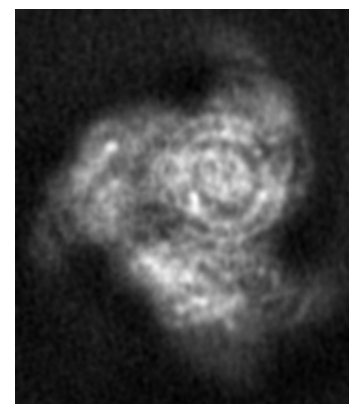
6.1.1 Primary map



X



Y

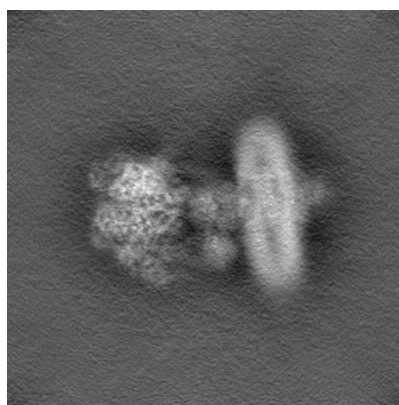


Z

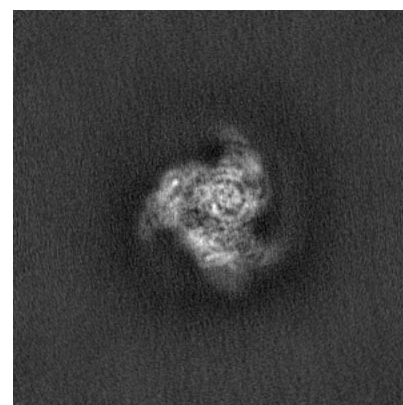
6.1.2 Raw map



X



Y



Z

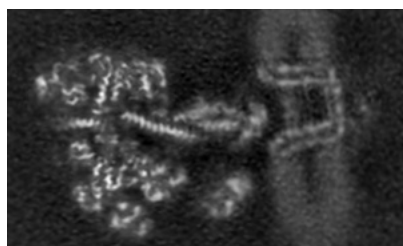
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

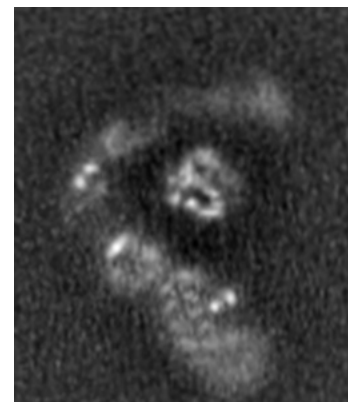
6.2.1 Primary map



X Index: 60

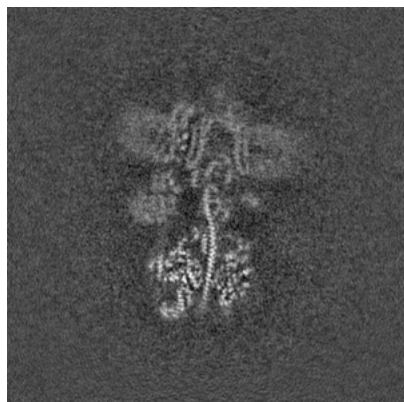


Y Index: 70

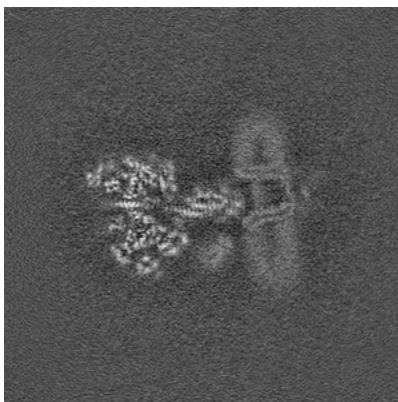


Z Index: 100

6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

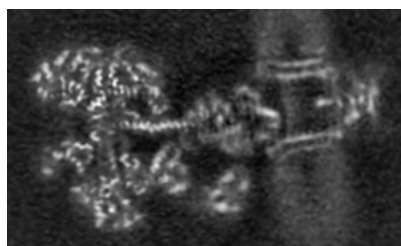
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

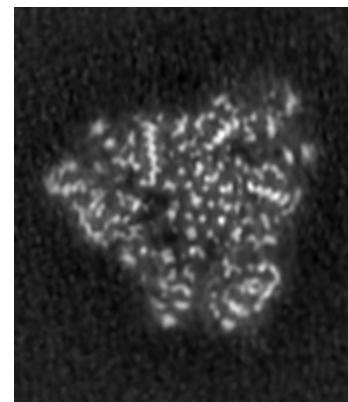
6.3.1 Primary map



X Index: 62

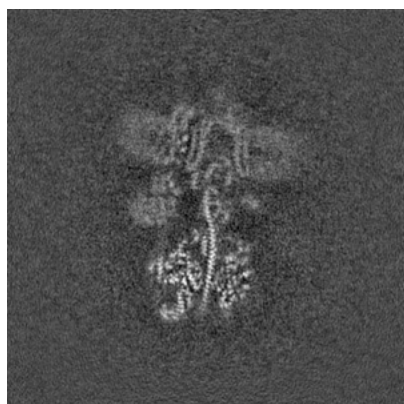


Y Index: 76

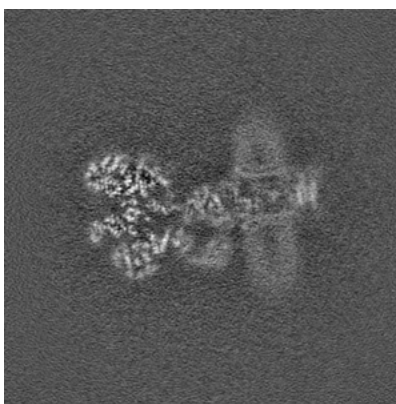


Z Index: 46

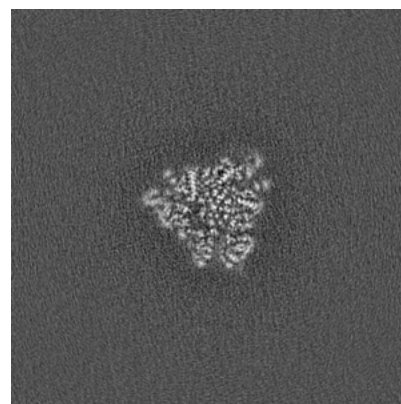
6.3.2 Raw map



X Index: 150



Y Index: 156

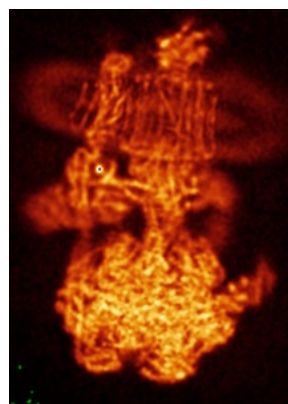


Z Index: 94

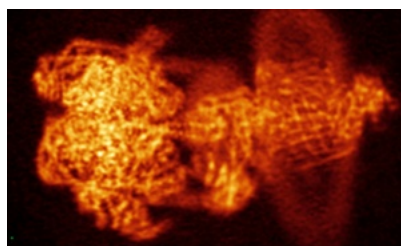
The images above show the largest variance slices of the map in three orthogonal directions.

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

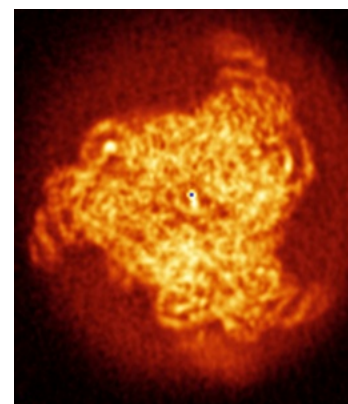
6.4.1 Primary map



X

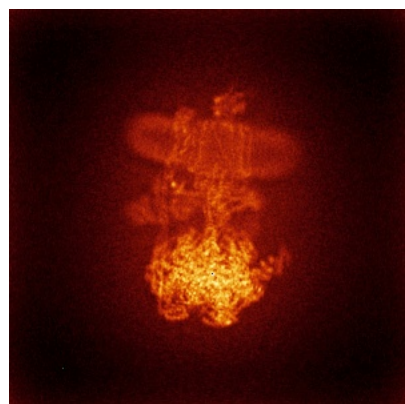


Y

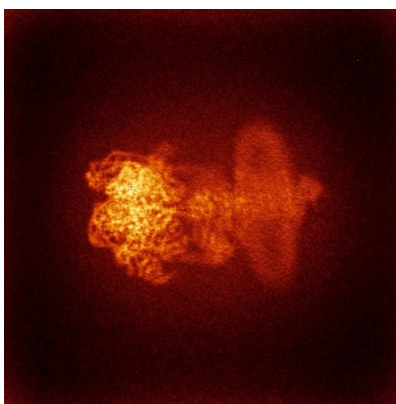


Z

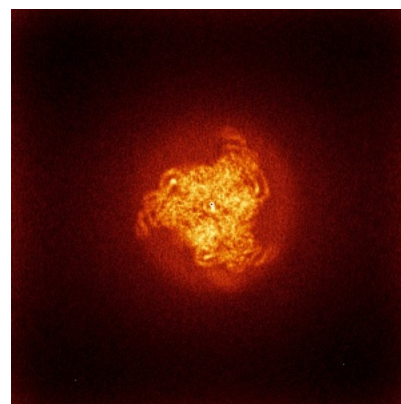
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

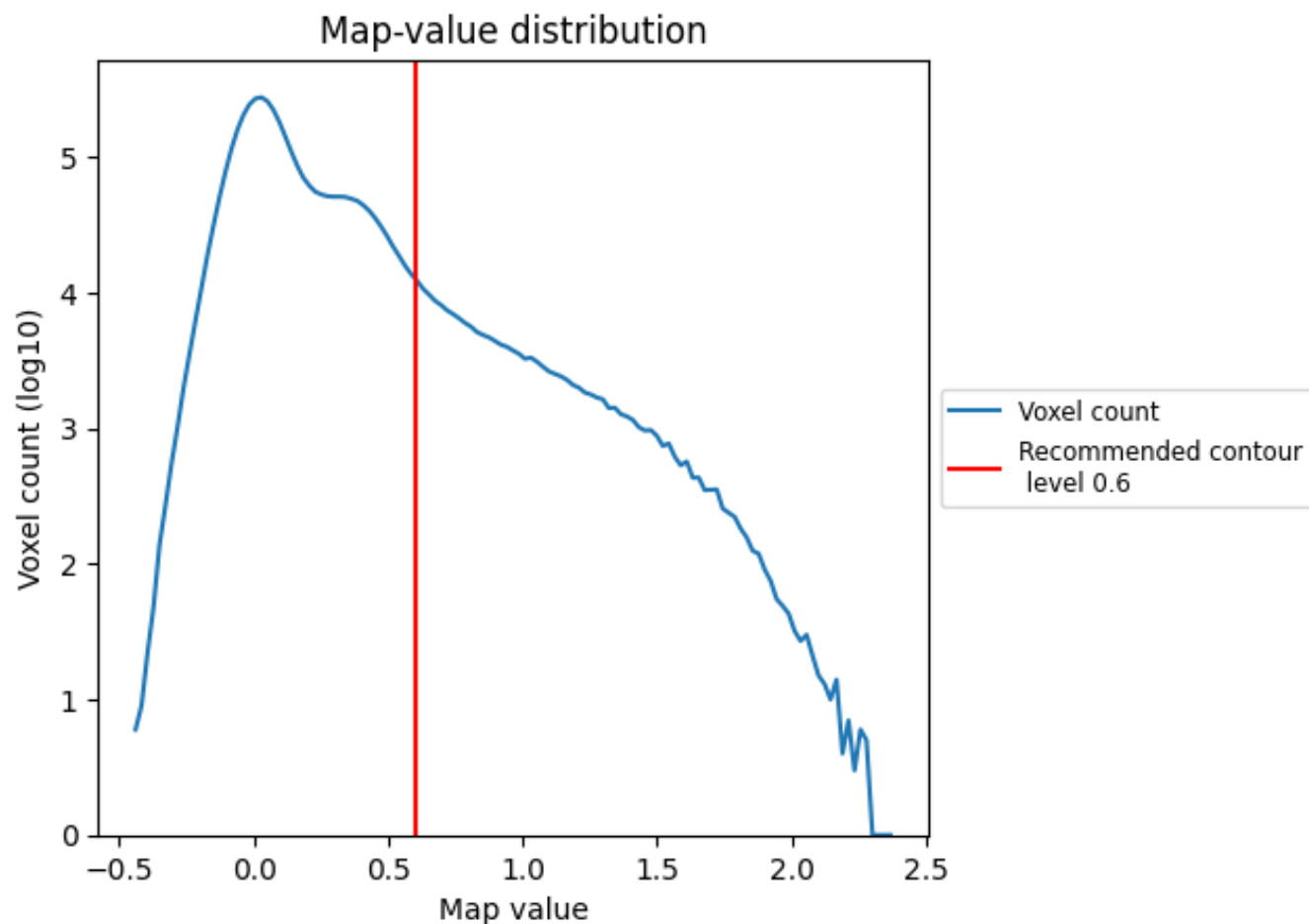
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

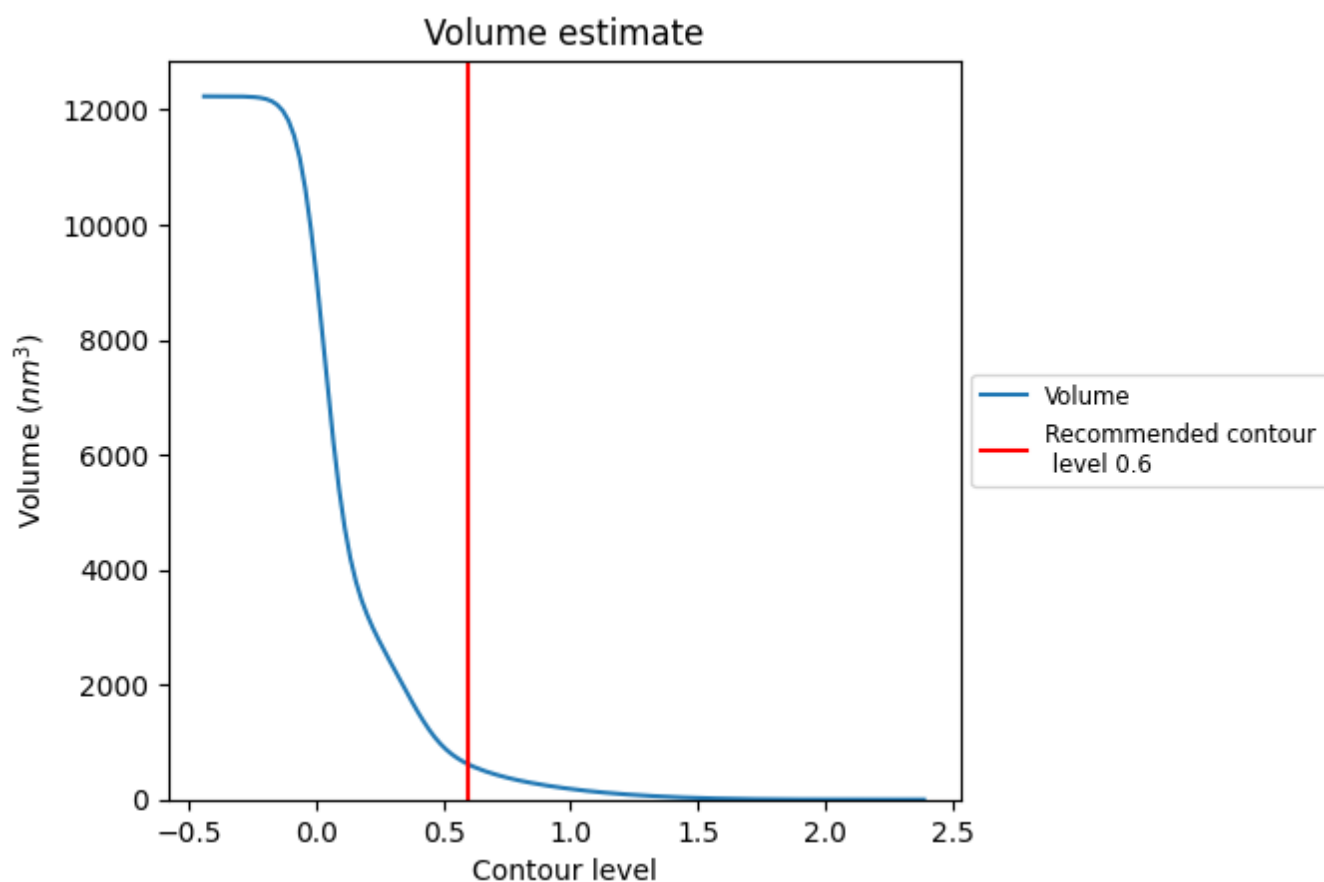
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 611 nm³; this corresponds to an approximate mass of 552 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.

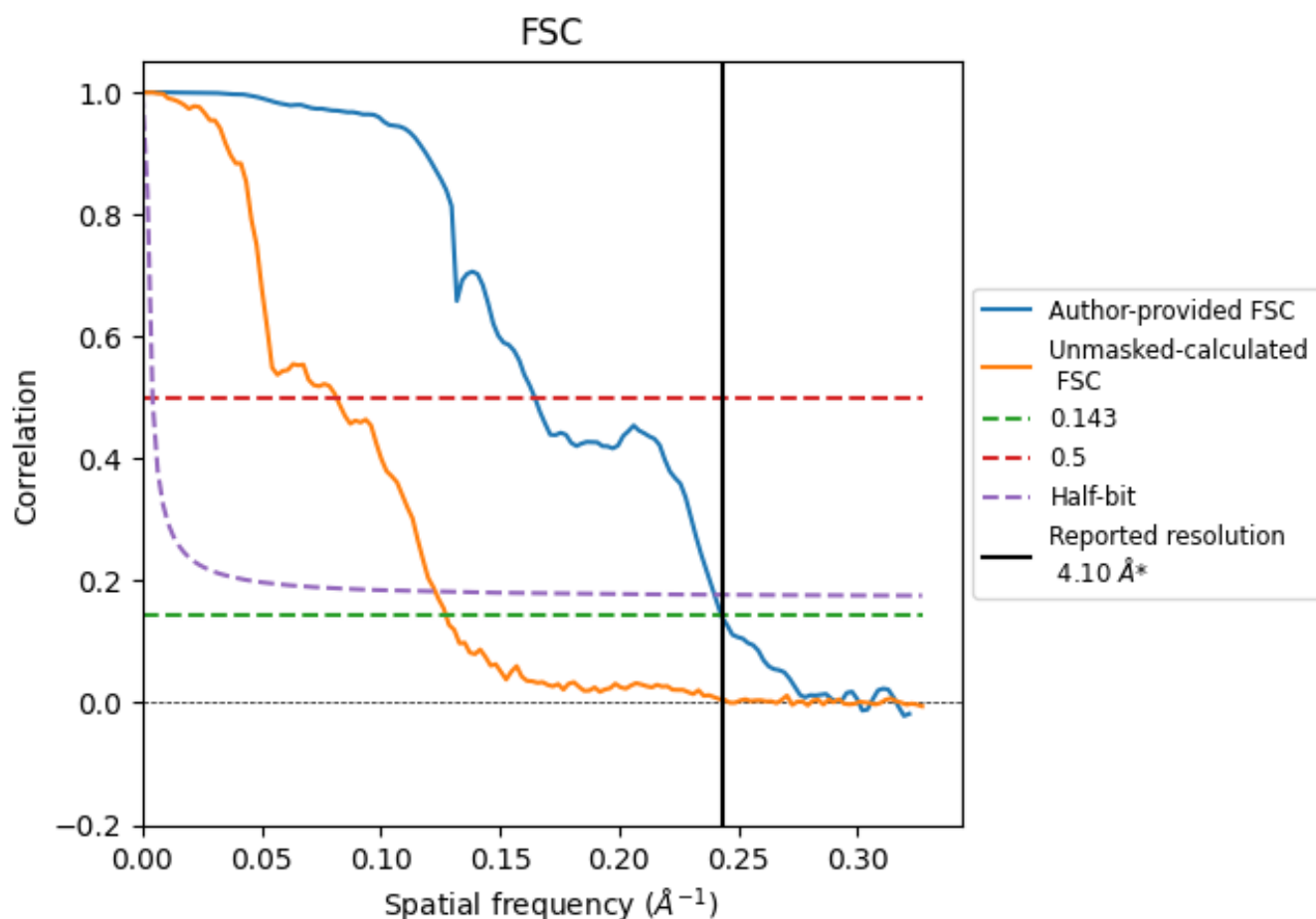
7.3 Rotationally averaged power spectrum [i](#)

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

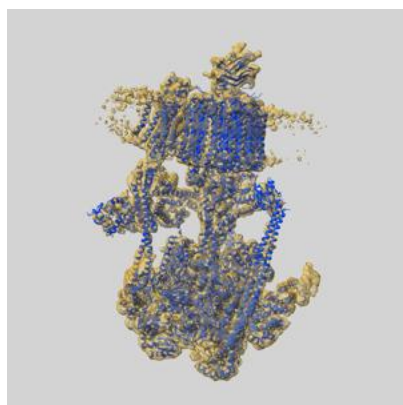
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	6.07	4.17
Unmasked-calculated*	7.84	12.27	8.13

*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 7.84 differs from the reported value 4.1 by more than 10 %

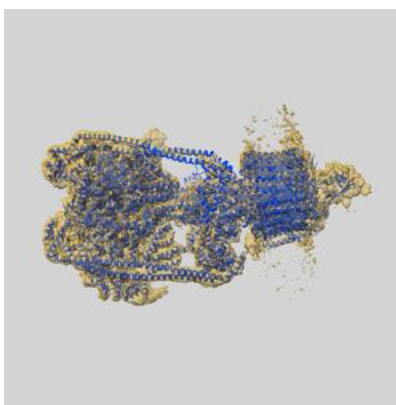
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26387 and PDB model 7U8Q. Per-residue inclusion information can be found in section 3 on page 9.

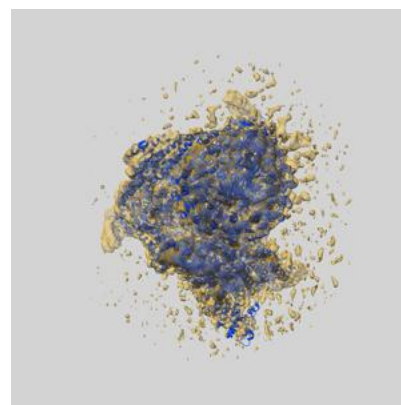
9.1 Map-model overlay [i](#)



X



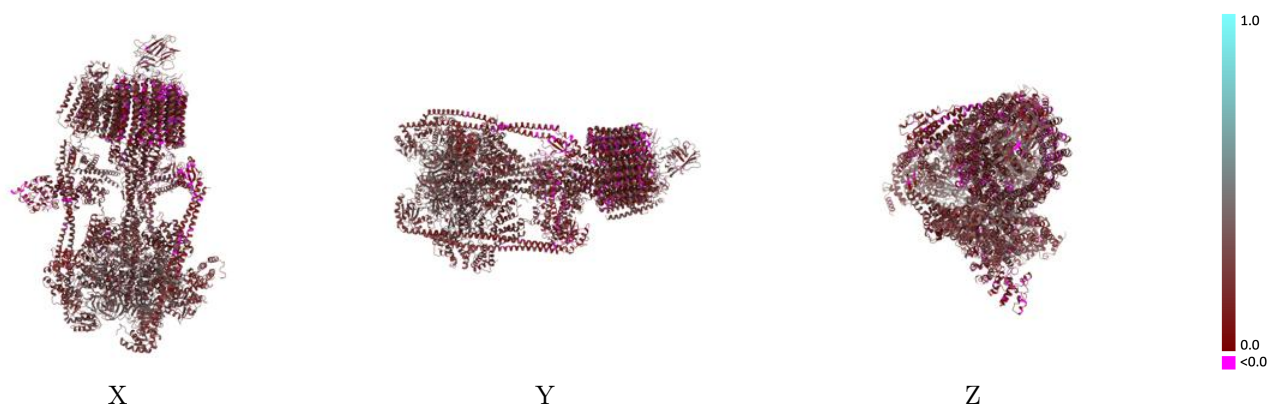
Y



Z

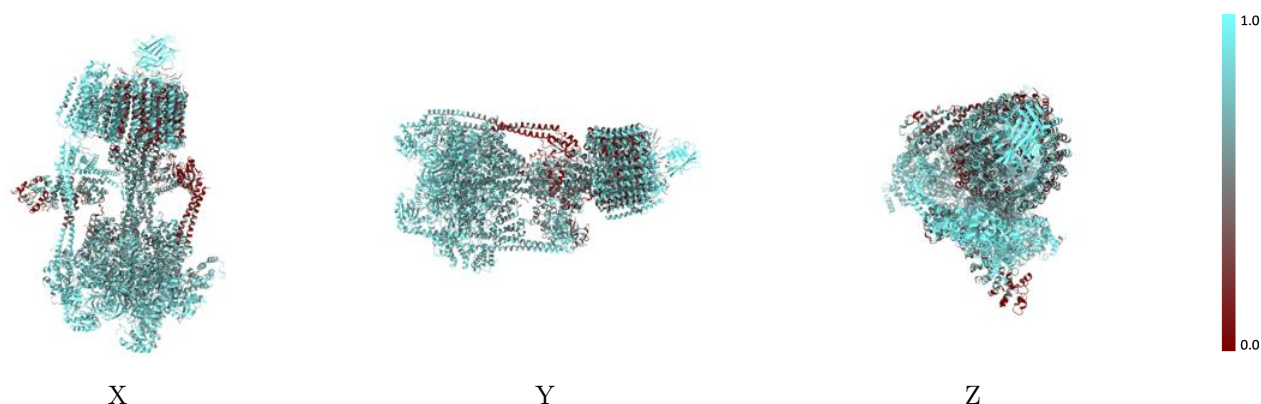
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



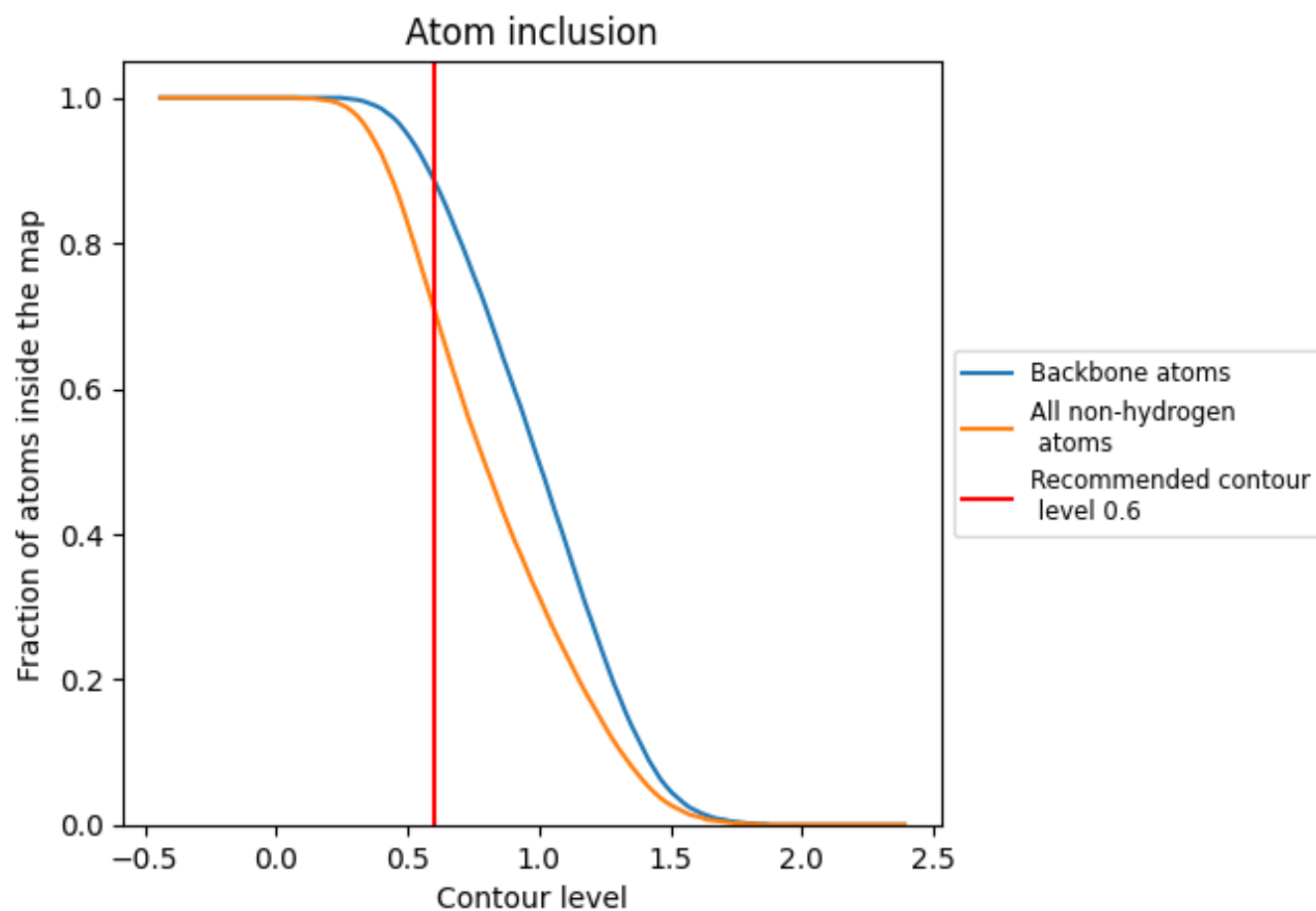
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7100	 0.2470
A	 0.7670	 0.2910
B	 0.7810	 0.3060
C	 0.7420	 0.2960
D	 0.7850	 0.3080
E	 0.7800	 0.3040
F	 0.7780	 0.3130
G	 0.3680	 0.1350
H	 0.6660	 0.2510
I	 0.8640	 0.2900
J	 0.7700	 0.2300
K	 0.6640	 0.2280
L	 0.5950	 0.2440
M	 0.8070	 0.2380
N	 0.7500	 0.2150
O	 0.5340	 0.2000
Q	 0.7610	 0.2360
R	 0.7390	 0.2400
S	 0.7460	 0.2200
T	 0.4870	 0.1410
a	 0.8990	 0.2590
b	 0.6940	 0.2200
c	 0.9030	 0.2650
d	 0.4940	 0.1870
e	 0.8830	 0.2590
f	 0.8910	 0.2590
g	 0.7190	 0.1990
h	 0.6570	 0.1910
i	 0.6090	 0.1520
j	 0.6460	 0.1710
k	 0.6250	 0.1790
l	 0.6540	 0.1980
m	 0.7200	 0.2310
n	 0.6750	 0.2040
o	 0.5290	 0.1570
p	 0.7310	 0.2570

