Full wwPDB EM Validation Report

May 26, 2025 – 06:10 AM EDT

PDB ID	:	9COP / pdb_00009cop
EMDB ID	:	EMD-45788
Title	:	Yeast RAVE bound to V-ATPase V1 complex
Authors	:	Wang, H.; Rubinstein, J.L.
Deposited on	:	2024-07-17
Resolution	:	2.70 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:

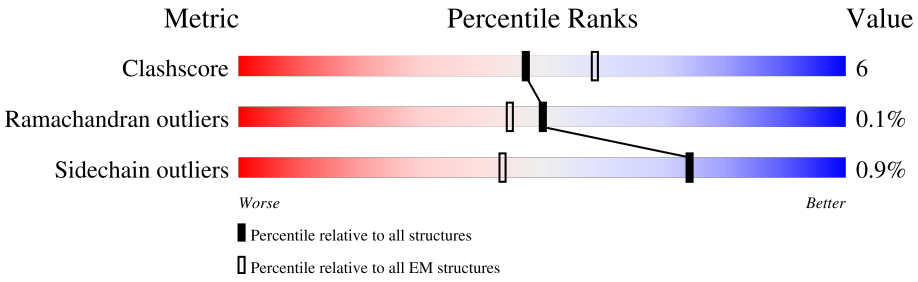
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	1071	49% 7% 44%
1	E	1071	45% 9% 45%
2	B	517	80% 10% • 9%
2	F	517	74% 15% • 10%
3	I	233	78% 12% • 9%
3	K	233	73% 12% 15%
4	J	114	72% 16% 12%
4	L	114	66% 10% 25%

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Mol	Chain	Length	Quality of chain
5	M	256	
6	N	117	
7	P	478	
8	x	1357	
9	y	351	
10	z	194	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 70017 atoms, of which 33522 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	596	Total	C	H	N	O	S	0	0
			9129	2916	4530	763	900	20		
1	E	587	Total	C	H	N	O	S	0	0
			8981	2869	4461	751	882	18		

- Molecule 2 is a protein called V-type proton ATPase subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	471	Total	C	H	N	O	S	0	0
			7396	2340	3698	634	712	12		
2	F	467	Total	C	H	N	O	S	0	0
			7313	2318	3649	627	707	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	212	Total	C	H	N	O	S	0	0
			3435	1058	1748	289	336	4		
3	K	197	Total	C	H	N	O	S	0	0
			3056	953	1537	263	299	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	100	Total	C	H	N	O	0	0
			1483	461	748	130	144		
4	L	86	Total	C	H	N	O	0	0
			1026	341	475	97	113		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	M	213	Total	C	H	N	O	S	0	0
			2896	939	1386	280	287	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	115	Total	C	H	N	O	0	0
			1466	499	671	148	148		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	436	Total	C	H	N	O	0	0
			3168	1315	981	436	436		

- Molecule 8 is a protein called Regulator of V-ATPase in vacuolar membrane protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	x	1192	Total	C	H	N	O	S	0	0
			17086	5701	8239	1540	1571	35		

- Molecule 9 is a protein called Regulator of V-ATPase in vacuolar membrane protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	y	242	Total	C	H	N	O	0	0
			1779	735	560	242	242		

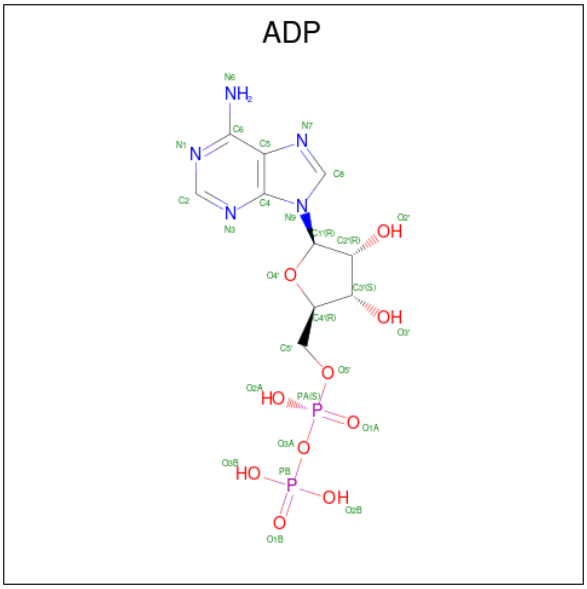
- Molecule 10 is a protein called Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	z	127	Total	C	H	N	O	S	0	0
			1723	571	815	168	166	3		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	
11	E	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



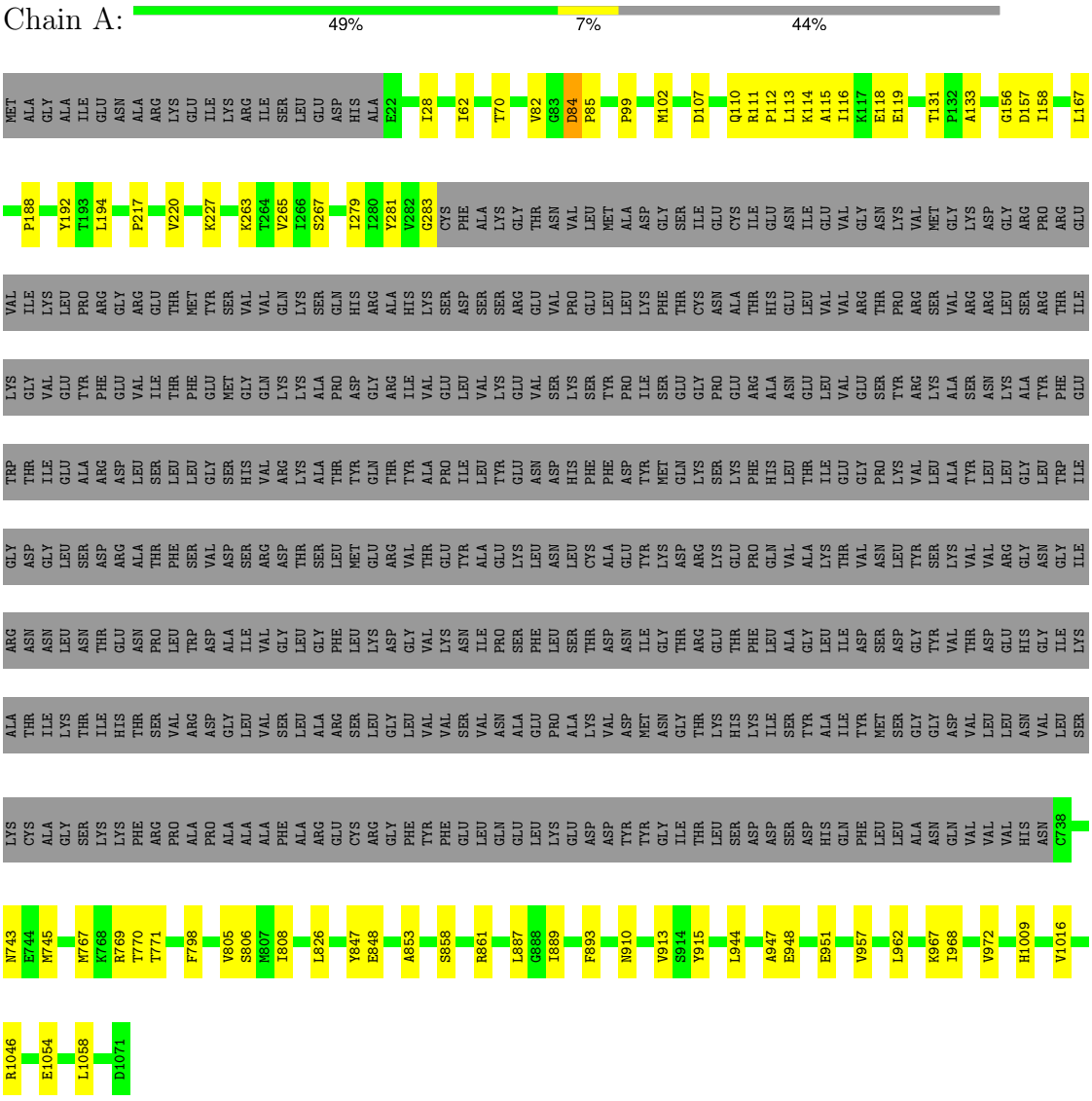
Mol	Chain	Residues	Atoms						AltConf
12	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
12	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

3 Residue-property plots (i)

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

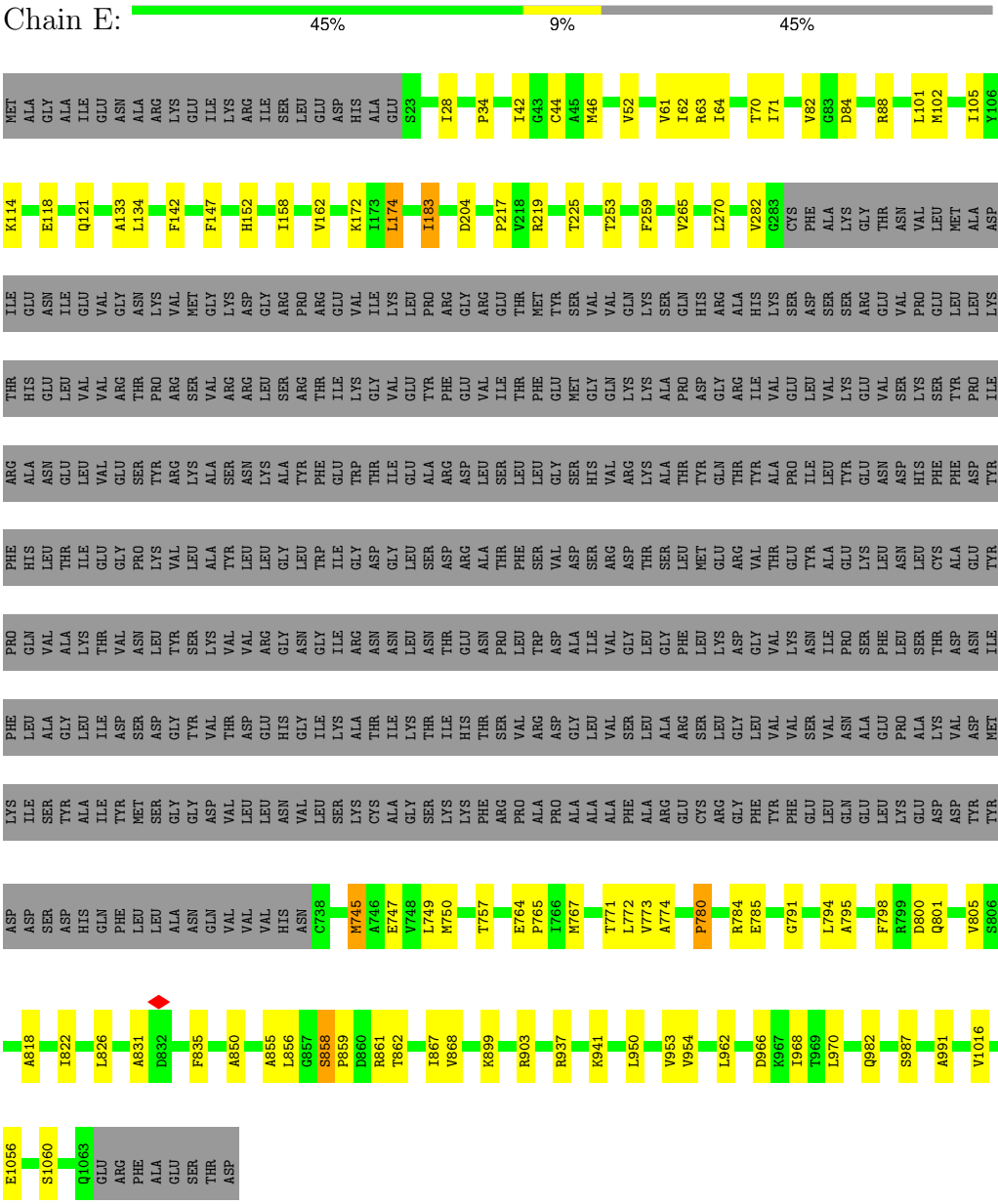
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain A:



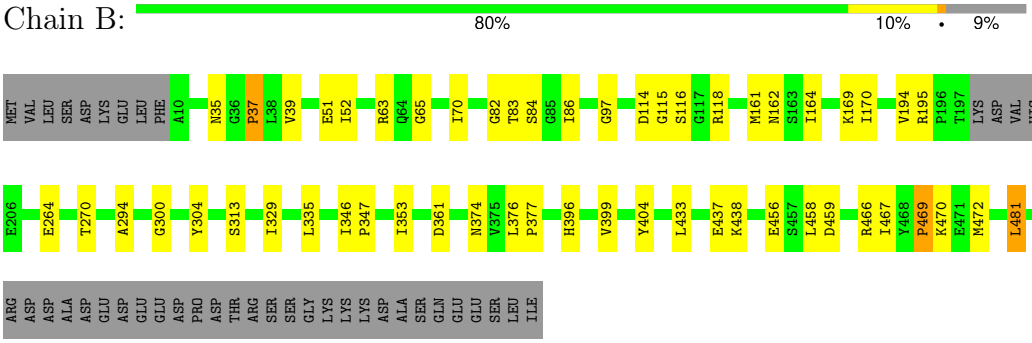
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain E:



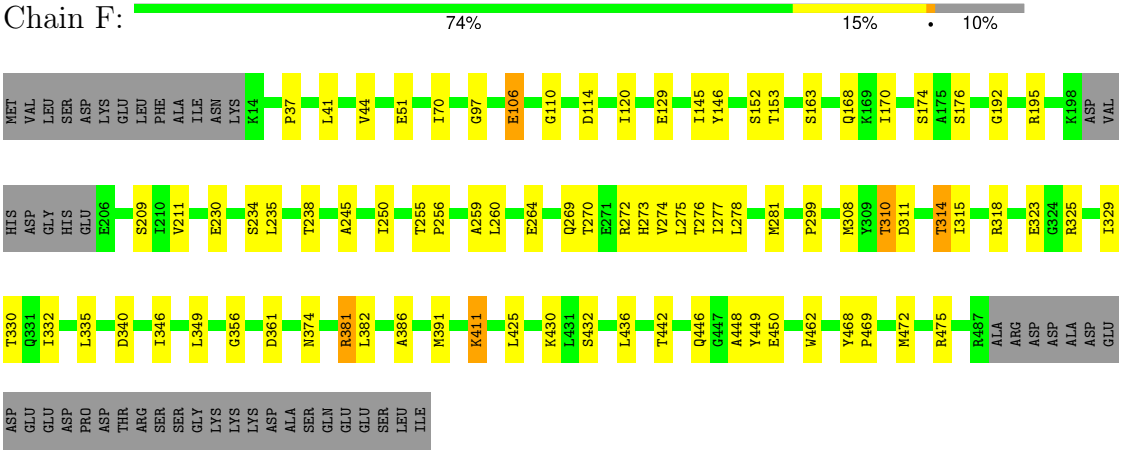
• Molecule 2: V-type proton ATPase subunit B

Chain B:



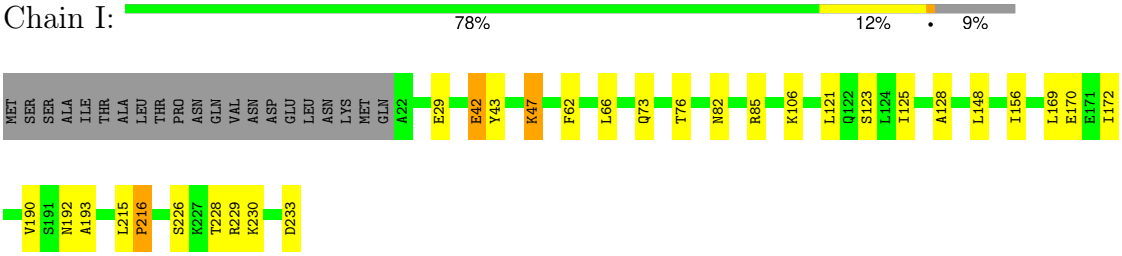
• Molecule 2: V-type proton ATPase subunit B

Chain F:



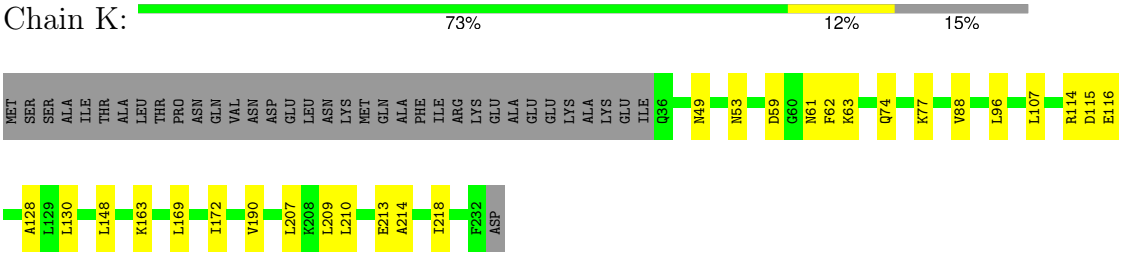
• Molecule 3: V-type proton ATPase subunit E

Chain I:



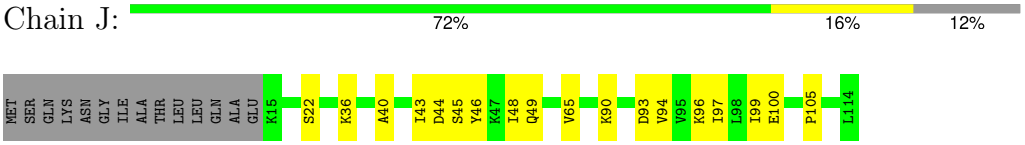
• Molecule 3: V-type proton ATPase subunit E

Chain K:



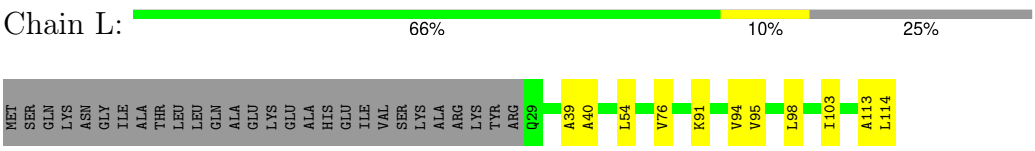
• Molecule 4: V-type proton ATPase subunit G

Chain J:



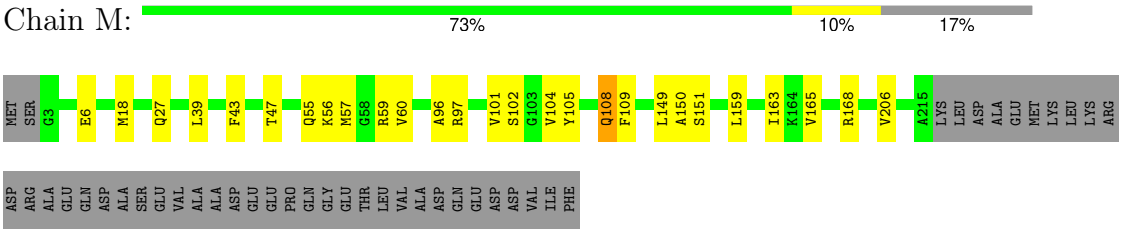
• Molecule 4: V-type proton ATPase subunit G

Chain L:



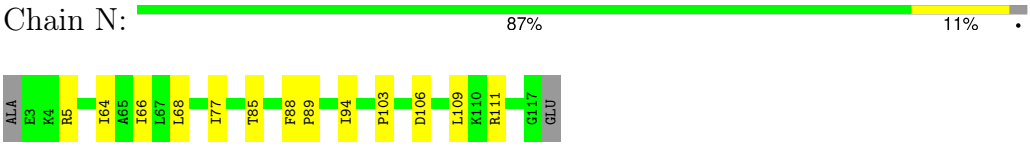
• Molecule 5: V-type proton ATPase subunit D

Chain M:



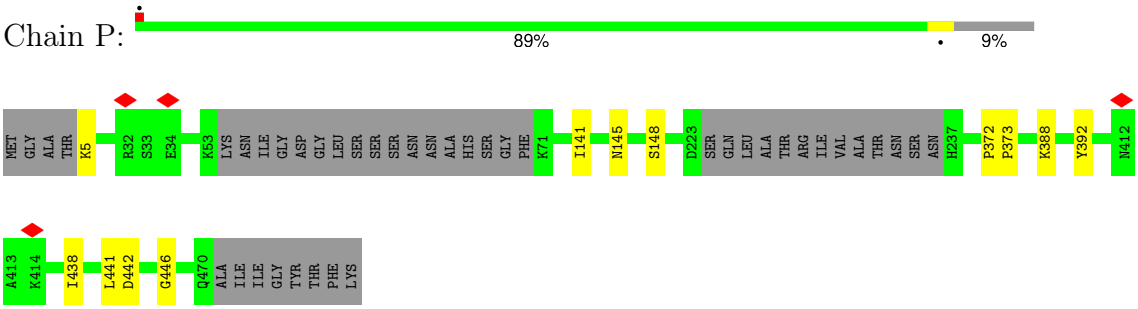
• Molecule 6: V-type proton ATPase subunit F

Chain N:



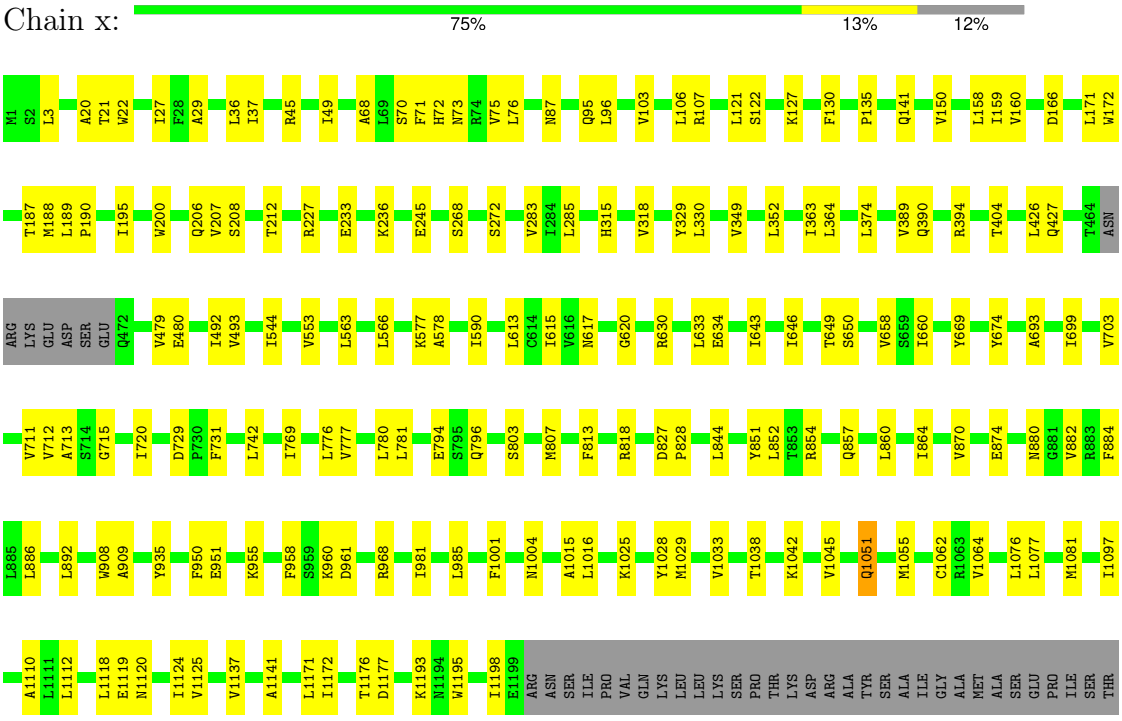
• Molecule 7: V-type proton ATPase subunit H

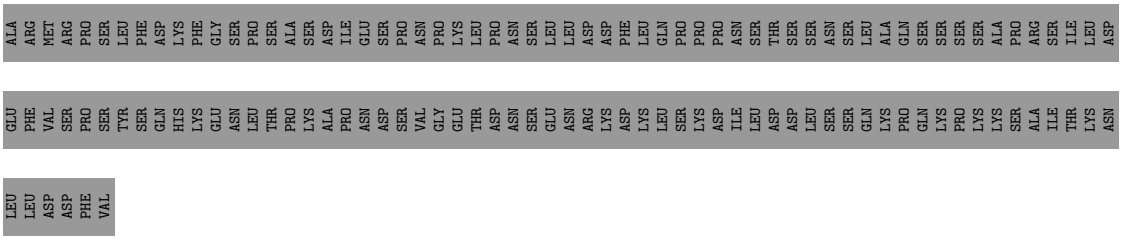
Chain P:



• Molecule 8: Regulator of V-ATPase in vacuolar membrane protein 1

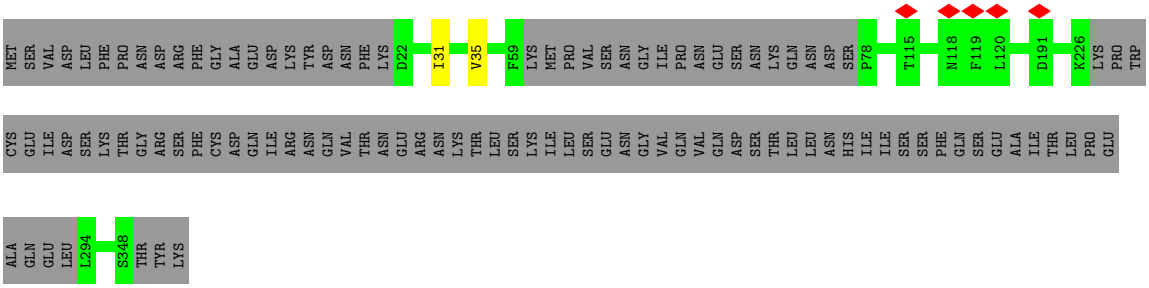
Chain x:





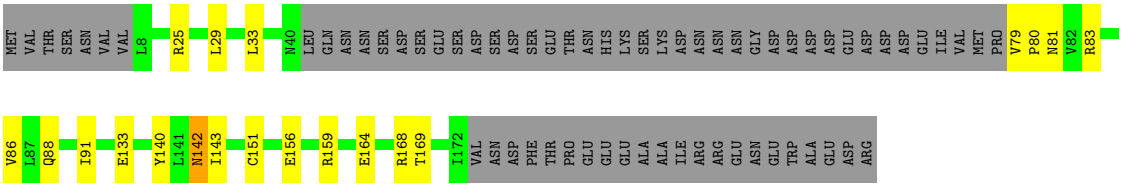
• Molecule 9: Regulator of V-ATPase in vacuolar membrane protein 2

Chain y:



• Molecule 10: Suppressor of kinetochore protein 1

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71341	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.183	Depositor
Minimum map value	-2.780	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	401.69998, 401.69998, 401.69998	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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, MG

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	0.33	2/4698 (0.0%)	0.49	4/6368 (0.1%)
1	E	0.62	5/4618 (0.1%)	0.85	5/6263 (0.1%)
2	B	0.54	3/3767 (0.1%)	0.77	7/5103 (0.1%)
2	F	0.67	1/3733 (0.0%)	0.97	11/5059 (0.2%)
3	I	0.35	1/1700 (0.1%)	0.58	2/2279 (0.1%)
3	K	0.15	0/1531	0.35	0/2058
4	J	0.26	0/737	0.51	0/983
4	L	0.30	0/552	0.47	0/750
5	M	0.30	0/1523	0.52	1/2058 (0.0%)
6	N	0.16	0/808	0.41	0/1103
7	P	0.10	0/2193	0.27	0/3066
8	x	0.30	0/9048	0.50	5/12364 (0.0%)
9	y	0.12	0/1224	0.32	0/1710
10	z	0.19	0/921	0.41	0/1253
All	All	0.42	12/37053 (0.0%)	0.63	35/50417 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	PRO	C-O	-7.66	1.15	1.23
1	E	217	PRO	C-O	-6.24	1.15	1.23
1	E	807	MET	C-O	-6.09	1.16	1.24
1	E	34	PRO	C-O	-5.76	1.17	1.24
1	A	915	TYR	C-O	-5.73	1.16	1.23
2	B	37	PRO	C-O	-5.46	1.17	1.24
2	B	469	PRO	C-O	-5.44	1.17	1.23
2	B	39	VAL	C-O	-5.38	1.18	1.24
2	F	174	SER	CA-CB	-5.27	1.45	1.53
3	I	216	PRO	C-O	-5.25	1.17	1.24
1	E	71	ILE	C-O	-5.15	1.18	1.24
1	E	800	ASP	C-O	-5.05	1.17	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	x	880	ASN	N-CA-C	-9.32	102.03	113.50
2	F	129	GLU	N-CA-C	-8.27	102.96	113.72
1	E	784	ARG	N-CA-C	-7.18	103.99	112.89
2	B	82	GLY	CA-C-O	-6.93	117.05	122.52
2	F	106	GLU	N-CA-C	-6.39	105.45	113.18
1	A	85	PRO	N-CA-CB	-6.32	97.47	103.34
2	F	356	GLY	CA-C-O	-6.11	117.15	122.16
2	B	396	HIS	CA-C-O	-6.02	113.97	121.02
2	F	325	ARG	CB-CA-C	6.00	120.11	109.72
2	F	273	HIS	N-CA-C	-5.85	101.39	110.10
1	E	745	MET	N-CA-C	-5.84	105.99	113.23
5	M	108	GLN	CA-C-O	-5.63	115.58	121.99
2	B	459	ASP	N-CA-C	-5.62	105.53	112.90
2	B	194	VAL	N-CA-C	-5.61	105.06	110.72
8	x	1025	LYS	N-CA-C	-5.58	106.50	113.15
2	B	162	ASN	N-CA-C	-5.58	103.73	110.88
2	F	153	THR	N-CA-C	-5.47	106.11	112.89
8	x	20	ALA	CA-C-O	-5.44	114.89	120.99
2	F	318	ARG	N-CA-C	-5.41	107.24	112.97
1	A	85	PRO	CA-C-O	-5.35	114.89	121.31
2	F	462	TRP	N-CA-C	-5.31	105.57	111.36
2	B	458	LEU	N-CA-C	-5.30	106.81	113.28
1	E	259	PHE	CA-CB-CG	5.30	119.10	113.80
8	x	130	PHE	N-CA-C	-5.26	106.72	112.72
2	F	315	ILE	N-CA-C	-5.25	107.04	111.56
2	F	314	THR	N-CA-C	-5.25	106.65	113.16
2	B	399	VAL	CA-C-O	-5.24	115.30	120.85
3	I	42	GLU	N-CA-C	-5.20	105.53	111.14
1	A	263	LYS	N-CA-C	-5.16	105.34	111.69
1	E	780	PRO	N-CA-CB	-5.15	97.85	103.25
1	A	84	ASP	CA-CB-CG	5.08	117.67	112.60
1	E	152	HIS	CB-CA-C	-5.07	101.48	109.80
3	I	47	LYS	N-CA-C	-5.05	107.10	114.12
8	x	158	LEU	CB-CA-C	-5.01	110.42	117.23
2	F	281	MET	N-CA-C	-5.00	105.95	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4599	4530	4531	48	0
1	E	4520	4461	4461	73	0
2	B	3698	3698	3697	31	0
2	F	3664	3649	3648	51	0
3	I	1687	1748	1748	20	0
3	K	1519	1537	1537	16	0
4	J	735	748	748	19	0
4	L	551	475	475	10	0
5	M	1510	1386	1386	20	0
6	N	795	671	671	10	0
7	P	2187	981	979	6	0
8	x	8847	8239	8238	112	0
9	y	1219	560	559	1	0
10	z	908	815	814	16	0
11	A	1	0	0	0	0
11	E	1	0	0	0	0
12	A	27	12	12	1	0
12	E	27	12	12	3	0
All	All	36495	33522	33516	405	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (405) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:CYS:SG	1:E:61:VAL:HG21	2.15	0.86
1:E:102:MET:HE3	1:E:798:PHE:CE2	2.15	0.81
1:E:70:THR:HG21	1:E:826:LEU:CD1	2.12	0.79
1:A:968:ILE:HD11	1:A:1016:VAL:HG21	1.64	0.78
1:E:102:MET:HE3	1:E:798:PHE:CZ	2.25	0.71
1:A:1046:ARG:NH2	1:A:1054:GLU:OE1	2.24	0.71
2:F:275:LEU:HD12	2:F:330:THR:HB	1.74	0.70
1:E:225:THR:HG22	1:E:856:LEU:HD23	1.75	0.69
4:J:93:ASP:O	4:J:97:ILE:HD12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:z:142:ASN:O	10:z:142:ASN:ND2	2.22	0.69
1:E:265:VAL:HG23	12:E:1102:ADP:O1A	1.93	0.68
3:K:49:ASN:O	3:K:53:ASN:ND2	2.26	0.68
2:F:277:ILE:HG23	2:F:332:ILE:O	1.96	0.66
10:z:86:VAL:HG11	10:z:133:GLU:HG3	1.77	0.66
1:E:950:LEU:HD21	1:E:966:ASP:HB3	1.77	0.65
8:x:21:THR:O	8:x:21:THR:HG22	1.97	0.64
5:M:57:MET:HE2	6:N:94:ILE:HG22	1.79	0.64
3:I:121:LEU:HD23	3:I:148:LEU:HD22	1.78	0.64
1:A:102:MET:HE2	1:A:771:THR:OG1	1.98	0.63
1:E:855:ALA:HB3	1:E:861:ARG:HG2	1.79	0.63
4:L:113:ALA:O	4:L:114:LEU:C	2.42	0.63
8:x:844:LEU:O	8:x:857:GLN:NE2	2.32	0.62
6:N:77:ILE:O	6:N:77:ILE:HG22	1.99	0.62
8:x:188:MET:HE2	8:x:188:MET:HA	1.82	0.61
1:E:105:ILE:HD11	1:E:774:ALA:HB2	1.81	0.61
1:E:118:GLU:O	1:E:121:GLN:NE2	2.32	0.61
2:F:209:SER:HB2	2:F:274:VAL:HG22	1.83	0.61
8:x:1124:ILE:HG22	8:x:1125:VAL:HG13	1.83	0.60
1:A:962:LEU:O	1:A:967:LYS:NZ	2.34	0.60
8:x:389:VAL:HG21	8:x:713:ALA:HB1	1.84	0.60
8:x:807:MET:O	10:z:159:ARG:NH2	2.35	0.60
8:x:981:ILE:O	8:x:985:LEU:HD23	2.02	0.60
1:E:950:LEU:HD23	1:E:970:LEU:HG	1.83	0.60
8:x:870:VAL:O	8:x:874:GLU:N	2.35	0.60
1:A:70:THR:HG21	1:A:826:LEU:HD21	1.84	0.60
7:P:388:LYS:O	7:P:392:TYR:N	2.34	0.60
1:E:70:THR:HG21	1:E:826:LEU:HD13	1.82	0.59
1:E:105:ILE:CD1	1:E:749:LEU:HD11	2.32	0.59
2:F:264:GLU:HA	2:F:329:ILE:HD11	1.85	0.59
2:F:469:PRO:HD2	2:F:472:MET:HE3	1.85	0.59
2:F:168:GLN:HB2	2:F:382:LEU:HD12	1.85	0.59
8:x:617:ASN:OD1	8:x:620:GLY:N	2.35	0.59
1:E:46:MET:HE1	1:E:62:ILE:O	2.03	0.59
1:E:82:VAL:HG23	2:F:70:ILE:HD12	1.84	0.59
2:B:481:LEU:HD23	2:B:485:TYR:HB2	1.85	0.58
2:B:114:ASP:OD1	2:B:115:GLY:N	2.36	0.58
8:x:71:PHE:CZ	8:x:76:LEU:HD13	2.38	0.58
8:x:958:PHE:O	8:x:968:ARG:NH2	2.35	0.58
1:A:217:PRO:HB2	1:A:220:VAL:HG12	1.86	0.58
8:x:318:VAL:CB	8:x:374:LEU:CB	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:HG23	12:A:1102:ADP:O1A	2.04	0.57
1:E:270:LEU:HD22	1:E:808:ILE:CD1	2.34	0.57
5:M:57:MET:HA	5:M:60:VAL:HG12	1.87	0.57
2:B:433:LEU:O	2:B:437:GLU:OE1	2.23	0.57
8:x:233:GLU:O	8:x:236:LYS:N	2.37	0.57
10:z:143:ILE:HG23	10:z:143:ILE:O	2.05	0.57
1:E:270:LEU:HD22	1:E:808:ILE:HD11	1.85	0.57
1:E:750:MET:HE1	2:F:146:TYR:CD2	2.40	0.57
3:I:62:PHE:O	3:I:66:LEU:HD23	2.03	0.57
1:A:283:GLY:HA3	1:A:745:MET:HE3	1.86	0.56
10:z:142:ASN:HD22	10:z:142:ASN:C	2.12	0.56
6:N:5:ARG:NE	6:N:64:ILE:O	2.31	0.56
5:M:6:GLU:OE1	5:M:18:MET:HE1	2.05	0.56
5:M:101:VAL:HG13	5:M:102:SER:H	1.70	0.56
1:A:887:LEU:HD21	1:A:893:PHE:CD1	2.41	0.56
3:K:115:ASP:OD1	3:K:116:GLU:N	2.39	0.55
8:x:781:LEU:HD22	8:x:864:ILE:CD1	2.35	0.55
1:A:114:LYS:O	1:A:118:GLU:OE1	2.24	0.55
1:E:968:ILE:HD11	1:E:1016:VAL:HG21	1.89	0.55
8:x:1081:MET:HG2	8:x:1097:ILE:HD11	1.87	0.55
1:E:28:ILE:HD12	1:E:84:ASP:HB2	1.89	0.55
2:F:469:PRO:HG3	2:F:472:MET:HE2	1.88	0.55
3:K:128:ALA:HB3	3:K:190:VAL:HG21	1.88	0.55
8:x:1198:ILE:HG23	8:x:1198:ILE:O	2.06	0.55
2:B:270:THR:O	2:B:270:THR:HG22	2.05	0.54
3:I:29:GLU:OE1	4:J:22:SER:OG	2.20	0.54
3:I:73:GLN:OE1	4:J:65:VAL:HG13	2.07	0.54
4:J:45:SER:O	4:J:48:ILE:HG22	2.06	0.54
1:E:1056:GLU:OE1	1:E:1056:GLU:N	2.40	0.54
2:F:211:VAL:HB	2:F:276:THR:HG23	1.89	0.54
5:M:150:ALA:HB2	6:N:66:ILE:HD12	1.90	0.54
1:A:267:SER:HB3	1:A:808:ILE:HG21	1.89	0.54
8:x:96:LEU:HD23	8:x:135:PRO:HG2	1.89	0.54
1:E:105:ILE:HD13	1:E:749:LEU:HD11	1.90	0.54
2:F:469:PRO:CD	2:F:472:MET:HE3	2.37	0.54
1:A:115:ALA:O	1:A:119:GLU:OE1	2.25	0.54
6:N:103:PRO:O	6:N:109:LEU:HD23	2.06	0.54
8:x:950:PHE:CD2	8:x:1064:VAL:HG21	2.43	0.54
2:F:106:GLU:HG2	2:F:272:ARG:HH12	1.73	0.54
8:x:330:LEU:HD23	8:x:349:VAL:HG13	1.90	0.53
5:M:149:LEU:HD23	5:M:149:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:125:ILE:HG21	3:I:156:ILE:HD13	1.90	0.53
4:L:103:ILE:O	4:L:103:ILE:HG22	2.08	0.53
5:M:101:VAL:HG13	5:M:102:SER:N	2.23	0.53
1:A:107:ASP:HB3	1:A:113:LEU:HD21	1.90	0.53
8:x:908:TRP:HZ2	8:x:1141:ALA:HB1	1.73	0.53
2:B:116:SER:OG	2:B:118:ARG:NE	2.41	0.53
8:x:1045:VAL:HG11	8:x:1062:CYS:SG	2.49	0.53
1:E:265:VAL:HG11	12:E:1102:ADP:C5	2.43	0.53
1:E:850:ALA:HB2	1:E:867:ILE:HD12	1.90	0.52
1:E:142:PHE:HA	1:E:162:VAL:HG12	1.90	0.52
2:F:335:LEU:HD11	2:F:346:ILE:HG22	1.91	0.52
12:E:1102:ADP:H5'2	2:F:381:ARG:HD2	1.91	0.52
1:E:70:THR:HG21	1:E:826:LEU:HD11	1.89	0.52
1:E:767:MET:HE1	1:E:772:LEU:HD13	1.90	0.52
2:F:152:SER:N	2:F:192:GLY:O	2.43	0.52
8:x:45:ARG:NH2	8:x:693:ALA:O	2.43	0.52
2:B:470:LYS:HG3	2:B:481:LEU:HD22	1.91	0.52
1:E:225:THR:HG22	1:E:856:LEU:HA	1.91	0.52
8:x:1055:MET:HE1	8:x:1076:LEU:HG	1.90	0.52
2:F:299:PRO:HD3	5:M:206:VAL:HG21	1.92	0.52
2:F:195:ARG:O	2:F:195:ARG:HG2	2.10	0.51
3:I:47:LYS:HB2	4:J:36:LYS:CE	2.40	0.51
8:x:769:ILE:HG13	8:x:777:VAL:HG21	1.92	0.51
2:F:41:LEU:HD22	2:F:44:VAL:HG22	1.92	0.51
3:I:106:LYS:CB	4:J:99:ILE:HD11	2.40	0.51
1:E:953:VAL:HG22	5:M:27:GLN:HG3	1.92	0.51
3:K:96:LEU:HD11	3:K:218:ILE:HG21	1.93	0.51
8:x:141:GLN:HG3	8:x:172:TRP:CH2	2.46	0.51
8:x:363:ILE:HG23	8:x:364:LEU:HD12	1.93	0.51
1:A:158:ILE:HD11	1:A:861:ARG:CD	2.41	0.50
2:B:51:GLU:OE2	2:B:97:GLY:N	2.42	0.50
8:x:1015:ALA:HB3	8:x:1038:THR:CG2	2.41	0.50
8:x:1176:THR:O	8:x:1177:ASP:HB3	2.11	0.50
4:L:94:VAL:O	4:L:98:LEU:HD13	2.11	0.50
5:M:96:ALA:HA	5:M:109:PHE:HA	1.93	0.50
1:E:147:PHE:HB3	1:E:183:ILE:CD1	2.42	0.50
3:I:192:ASN:OD1	3:I:193:ALA:N	2.45	0.50
5:M:159:LEU:O	5:M:163:ILE:HG13	2.11	0.50
7:P:372:PRO:N	7:P:373:PRO:HD2	2.27	0.50
8:x:1119:GLU:O	8:x:1120:ASN:OD1	2.29	0.50
2:F:446:GLN:NE2	2:F:450:GLU:O	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:x:166:ASP:O	8:x:195:ILE:HD12	2.11	0.50
1:E:818:ALA:O	1:E:822:ILE:HD12	2.11	0.50
2:F:277:ILE:N	2:F:277:ILE:HD12	2.27	0.50
8:x:121:LEU:HD21	8:x:159:ILE:HG21	1.93	0.50
4:J:45:SER:O	4:J:49:GLN:OE1	2.29	0.50
2:F:211:VAL:HG11	2:F:259:ALA:O	2.12	0.49
1:E:107:ASP:O	1:E:109:ILE:N	2.45	0.49
8:x:852:LEU:O	8:x:854:ARG:NH2	2.44	0.49
1:A:847:TYR:HB2	1:A:889:ILE:HG21	1.92	0.49
4:L:91:LYS:O	4:L:95:VAL:HG23	2.11	0.49
8:x:630:ARG:NH2	8:x:634:GLU:OE2	2.43	0.49
1:E:204:ASP:OD1	8:x:1016:LEU:CD1	2.61	0.49
1:A:968:ILE:HD11	1:A:1016:VAL:CG2	2.38	0.49
1:E:795:ALA:HA	1:E:805:VAL:HG11	1.93	0.49
1:A:972:VAL:HG21	1:A:1009:HIS:HB2	1.95	0.49
1:E:114:LYS:NZ	1:E:118:GLU:OE2	2.33	0.49
3:K:209:LEU:O	3:K:213:GLU:OE1	2.31	0.49
8:x:776:LEU:O	8:x:780:LEU:HD13	2.13	0.49
1:E:858:SER:HA	1:E:859:PRO:C	2.38	0.49
8:x:426:LEU:HD23	8:x:427:GLN:N	2.28	0.49
8:x:729:ASP:OD1	8:x:731:PHE:N	2.40	0.49
1:A:957:VAL:HG12	1:A:957:VAL:O	2.13	0.48
2:F:308:MET:HE2	2:F:349:LEU:HD12	1.93	0.48
2:F:110:GLY:N	2:F:238:THR:O	2.43	0.48
8:x:674:TYR:CZ	8:x:1137:VAL:HG11	2.48	0.48
8:x:1193:LYS:HG3	10:z:151:CYS:SG	2.53	0.48
1:A:102:MET:HE3	1:A:798:PHE:CE2	2.48	0.48
1:E:822:ILE:O	1:E:826:LEU:HB2	2.14	0.48
4:L:39:ALA:CA	4:L:40:ALA:HB3	2.44	0.48
8:x:71:PHE:CE2	8:x:76:LEU:HD13	2.48	0.48
2:B:487:ARG:O	2:B:488:ALA:HB3	2.13	0.48
8:x:613:LEU:CD2	8:x:615:ILE:HG23	2.44	0.48
8:x:36:LEU:HD23	8:x:49:ILE:HD12	1.96	0.48
10:z:168:ARG:NH1	10:z:169:THR:HG22	2.29	0.48
8:x:389:VAL:HG22	8:x:715:GLY:O	2.13	0.48
8:x:329:TYR:O	8:x:352:LEU:HD12	2.14	0.47
8:x:1110:ALA:HA	8:x:1118:LEU:HD11	1.96	0.47
8:x:1081:MET:CG	8:x:1097:ILE:HD11	2.44	0.47
2:F:386:ALA:O	2:F:391:MET:HE2	2.15	0.47
3:K:114:ARG:NE	3:K:148:LEU:HD21	2.29	0.47
4:L:39:ALA:HA	4:L:40:ALA:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:THR:CG2	1:E:868:VAL:HG22	2.45	0.47
2:B:335:LEU:HD11	2:B:346:ILE:HG22	1.96	0.47
2:F:386:ALA:C	2:F:391:MET:HE2	2.40	0.47
3:K:74:GLN:O	3:K:77:LYS:HG2	2.14	0.47
3:K:210:LEU:O	3:K:214:ALA:HB3	2.15	0.47
6:N:68:LEU:HD21	6:N:94:ILE:HD13	1.96	0.47
8:x:187:THR:C	8:x:188:MET:HE2	2.40	0.47
8:x:187:THR:O	8:x:188:MET:HE2	2.14	0.47
8:x:643:ILE:HG21	8:x:646:ILE:HD11	1.96	0.47
1:A:848:GLU:HG3	2:F:245:ALA:HB3	1.96	0.47
10:z:86:VAL:HG11	10:z:133:GLU:CG	2.45	0.47
1:A:102:MET:HE3	1:A:798:PHE:CZ	2.49	0.47
1:A:107:ASP:OD2	1:A:111:ARG:NH2	2.48	0.47
3:I:62:PHE:CE2	3:I:66:LEU:HD21	2.50	0.47
5:M:43:PHE:O	5:M:47:THR:HG23	2.15	0.47
1:E:101:LEU:HD13	1:E:134:LEU:HD21	1.97	0.47
8:x:1028:TYR:CD1	8:x:1051:GLN:HB3	2.50	0.47
1:A:115:ALA:O	1:A:116:ILE:C	2.57	0.46
10:z:29:LEU:HD12	10:z:33:LEU:CB	2.44	0.46
4:J:45:SER:O	4:J:46:TYR:C	2.58	0.46
3:K:169:LEU:HD23	3:K:172:ILE:CG1	2.46	0.46
8:x:45:ARG:NH1	8:x:45:ARG:HB3	2.30	0.46
1:A:156:GLY:O	1:A:861:ARG:NH2	2.48	0.46
2:B:469:PRO:HG2	2:B:472:MET:HE3	1.97	0.46
1:E:1046:ARG:HG3	1:E:1051:VAL:HG23	1.98	0.46
2:F:411:LYS:HD3	2:F:436:LEU:HD11	1.98	0.46
3:K:59:ASP:O	3:K:62:PHE:HB3	2.16	0.46
5:M:39:LEU:HD22	5:M:159:LEU:CD1	2.45	0.46
8:x:394:ARG:HB2	8:x:703:VAL:HG21	1.98	0.46
8:x:854:ARG:NH1	8:x:857:GLN:OE1	2.49	0.46
1:A:82:VAL:HG23	2:B:70:ILE:HD12	1.97	0.46
2:B:470:LYS:HG3	2:B:481:LEU:HD13	1.97	0.46
8:x:544:ILE:HD12	8:x:566:LEU:HD23	1.97	0.46
8:x:769:ILE:HG21	8:x:886:LEU:HD13	1.98	0.46
8:x:892:LEU:HD21	8:x:935:TYR:OH	2.15	0.46
2:F:51:GLU:OE2	2:F:97:GLY:N	2.47	0.46
1:A:28:ILE:HD12	1:A:84:ASP:HB2	1.97	0.46
1:E:105:ILE:HG13	1:E:772:LEU:HB3	1.98	0.46
1:A:70:THR:HG21	1:A:826:LEU:CD2	2.43	0.46
6:N:85:THR:HG22	6:N:111:ARG:NH2	2.30	0.46
1:A:848:GLU:CG	2:F:245:ALA:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:954:VAL:CG2	1:E:962:LEU:HD11	2.45	0.45
2:F:145:ILE:HD11	2:F:323:GLU:HA	1.98	0.45
1:E:105:ILE:HD12	1:E:749:LEU:HD11	1.97	0.45
2:F:170:ILE:O	2:F:170:ILE:HG23	2.16	0.45
1:A:767:MET:HA	1:A:770:THR:HG22	1.98	0.45
1:E:42:ILE:O	1:E:88:ARG:NH2	2.49	0.45
2:F:469:PRO:CG	2:F:472:MET:HE2	2.46	0.45
8:x:649:THR:O	8:x:650:SER:OG	2.28	0.45
3:I:82:ASN:OD1	3:I:85:ARG:NH2	2.49	0.45
4:J:40:ALA:HA	4:J:43:ILE:HG22	1.98	0.45
1:A:281:TYR:CD2	1:A:745:MET:HE1	2.52	0.45
1:A:167:LEU:HD21	1:A:769:ARG:HG2	1.98	0.45
1:E:282:VAL:HG22	1:E:773:VAL:HG21	1.97	0.45
1:E:101:LEU:HD21	1:E:794:LEU:CD2	2.47	0.45
10:z:88:GLN:OE1	10:z:91:ILE:HD11	2.17	0.45
1:E:987:SER:O	1:E:991:ALA:HB2	2.16	0.45
8:x:711:VAL:HG22	8:x:720:ILE:CG1	2.47	0.45
2:B:264:GLU:HA	2:B:329:ILE:HD11	1.98	0.45
1:E:158:ILE:HG21	1:E:172:LYS:HD2	1.98	0.45
2:F:234:SER:O	2:F:238:THR:OG1	2.28	0.45
8:x:633:LEU:HD23	8:x:633:LEU:O	2.17	0.45
1:E:899:LYS:O	1:E:903:ARG:HG3	2.17	0.45
8:x:22:TRP:CE3	8:x:27:ILE:HD11	2.52	0.45
8:x:283:VAL:HG12	8:x:285:LEU:CD1	2.47	0.44
2:B:313:SER:HA	2:B:353:ILE:HG21	1.99	0.44
8:x:171:LEU:C	8:x:171:LEU:HD23	2.42	0.44
2:B:376:LEU:HB2	2:B:377:PRO:HD3	1.98	0.44
3:I:106:LYS:HB2	4:J:99:ILE:HD11	2.00	0.44
8:x:207:VAL:CB	8:x:208:SER:HA	2.48	0.44
10:z:81:ASN:ND2	10:z:140:TYR:CE2	2.83	0.44
10:z:83:ARG:HB3	10:z:86:VAL:HG22	1.98	0.44
1:A:157:ASP:OD1	1:A:858:SER:N	2.47	0.44
2:F:272:ARG:O	2:F:274:VAL:HG23	2.16	0.44
2:F:277:ILE:HG13	2:F:332:ILE:HB	2.00	0.44
2:B:195:ARG:HH11	2:B:195:ARG:HG2	1.82	0.44
3:I:170:GLU:OE1	3:I:170:GLU:N	2.50	0.44
8:x:329:TYR:C	8:x:330:LEU:HD12	2.42	0.44
2:B:486:ASP:O	2:B:487:ARG:C	2.60	0.44
1:E:968:ILE:HD11	1:E:1016:VAL:CG2	2.47	0.44
8:x:803:SER:OG	10:z:164:GLU:OE1	2.32	0.44
8:x:950:PHE:CE2	8:x:1064:VAL:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:ILE:C	1:E:63:ARG:HD2	2.43	0.44
6:N:106:ASP:OD1	6:N:109:LEU:HB3	2.17	0.44
8:x:794:GLU:OE1	8:x:796:GLN:NE2	2.45	0.44
1:E:745:MET:HE3	1:E:774:ALA:HA	1.98	0.44
1:E:937:ARG:O	1:E:941:LYS:HG2	2.18	0.44
7:P:141:ILE:O	7:P:145:ASN:N	2.51	0.44
8:x:70:SER:OG	8:x:103:VAL:HB	2.17	0.44
1:A:110:GLN:O	1:A:110:GLN:HG3	2.18	0.44
3:I:215:LEU:N	3:I:216:PRO:HD2	2.33	0.44
8:x:159:ILE:HG22	8:x:160:VAL:N	2.32	0.44
10:z:79:VAL:HB	10:z:80:PRO:HD3	2.00	0.44
2:B:37:PRO:HD2	2:B:294:ALA:HB2	1.99	0.43
2:B:486:ASP:O	2:B:488:ALA:N	2.50	0.43
8:x:107:ARG:NH1	8:x:150:VAL:O	2.51	0.43
8:x:1055:MET:HE2	8:x:1077:LEU:HD23	2.00	0.43
2:B:52:ILE:HD12	2:B:65:GLY:O	2.18	0.43
2:F:114:ASP:OD1	2:F:120:ILE:HG21	2.17	0.43
2:F:310:THR:O	2:F:314:THR:HG23	2.18	0.43
3:K:62:PHE:O	3:K:63:LYS:C	2.61	0.43
2:B:361:ASP:HB2	2:B:374:ASN:HB2	2.01	0.43
2:B:346:ILE:HB	2:B:347:PRO:CD	2.48	0.43
2:F:260:LEU:HD11	2:F:278:LEU:HD11	1.99	0.43
9:y:31:ILE:O	9:y:35:VAL:N	2.50	0.43
2:B:300:GLY:N	2:B:304:TYR:O	2.45	0.43
1:E:747:GLU:HG3	1:E:750:MET:HE2	2.01	0.43
8:x:1001:PHE:O	8:x:1004:ASN:ND2	2.46	0.43
1:E:174:LEU:HD11	1:E:801:GLN:HG2	2.01	0.43
1:E:764:GLU:O	1:E:765:PRO:C	2.60	0.43
1:E:831:ALA:HB3	1:E:835:PHE:O	2.19	0.43
8:x:577:LYS:N	8:x:590:ILE:O	2.48	0.43
8:x:813:PHE:N	8:x:813:PHE:CD1	2.84	0.43
2:B:63:ARG:NH2	2:B:84:SER:O	2.47	0.43
5:M:104:VAL:HG22	5:M:105:TYR:N	2.34	0.43
8:x:1172:ILE:HD11	8:x:1195:TRP:CE2	2.53	0.43
1:E:28:ILE:HD11	1:E:52:VAL:CG1	2.49	0.43
1:E:110:GLN:HG3	1:E:133:ALA:CB	2.48	0.43
3:K:107:LEU:HD12	3:K:207:LEU:HD22	2.00	0.43
8:x:227:ARG:NE	8:x:245:GLU:OE2	2.47	0.43
8:x:699:ILE:HG23	8:x:712:VAL:HG13	2.01	0.43
1:E:63:ARG:NH1	1:E:826:LEU:CD2	2.82	0.43
2:F:37:PRO:HB3	2:F:250:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:45:SER:C	4:J:49:GLN:OE1	2.61	0.43
8:x:394:ARG:HD2	8:x:553:VAL:HG12	2.01	0.43
1:A:99:PRO:HG2	1:A:194:LEU:HD21	2.01	0.43
2:F:230:GLU:OE2	2:F:235:LEU:CD2	2.67	0.43
8:x:75:VAL:HB	8:x:96:LEU:HB2	2.01	0.43
7:P:441:LEU:O	7:P:446:GLY:N	2.49	0.42
8:x:870:VAL:HG13	8:x:882:VAL:HG22	2.01	0.42
2:B:164:ILE:HG12	2:B:170:ILE:HG21	1.99	0.42
1:E:282:VAL:HG22	1:E:773:VAL:CG2	2.49	0.42
2:F:275:LEU:CD2	2:F:277:ILE:HD11	2.48	0.42
3:I:42:GLU:O	3:I:43:TYR:C	2.61	0.42
3:K:130:LEU:HD21	3:K:163:LYS:HB2	2.01	0.42
8:x:390:GLN:N	8:x:404:THR:O	2.48	0.42
8:x:1029:MET:O	8:x:1033:VAL:HG23	2.20	0.42
10:z:156:GLU:OE1	10:z:156:GLU:HA	2.18	0.42
4:J:96:LYS:O	4:J:100:GLU:HG2	2.19	0.42
4:L:39:ALA:N	4:L:40:ALA:HB3	2.35	0.42
1:A:158:ILE:HD11	1:A:861:ARG:NE	2.35	0.42
2:F:255:THR:N	2:F:256:PRO:HD2	2.34	0.42
3:I:47:LYS:HB2	4:J:36:LYS:HD2	2.01	0.42
8:x:3:LEU:C	8:x:3:LEU:HD23	2.44	0.42
8:x:781:LEU:HD22	8:x:864:ILE:HD12	2.00	0.42
8:x:860:LEU:O	8:x:864:ILE:HG12	2.19	0.42
1:A:279:ILE:HD13	1:A:806:SER:HB2	2.01	0.42
2:B:83:THR:HA	2:B:86:ILE:HD12	2.02	0.42
1:E:1056:GLU:O	1:E:1060:SER:HB2	2.20	0.42
2:F:106:GLU:HG2	3:I:228:THR:HG21	2.00	0.42
4:J:44:ASP:OD1	4:J:44:ASP:C	2.63	0.42
8:x:492:ILE:O	8:x:493:VAL:HG13	2.20	0.42
1:A:111:ARG:HB3	1:A:116:ILE:HD11	2.02	0.42
1:A:798:PHE:HB2	1:A:805:VAL:HG21	2.01	0.42
2:B:161:MET:HE2	2:B:404:TYR:CD2	2.55	0.42
2:F:361:ASP:HB2	2:F:374:ASN:HB2	2.02	0.42
8:x:958:PHE:CE2	8:x:985:LEU:CD1	3.02	0.42
2:F:448:ALA:O	2:F:449:TYR:HB2	2.20	0.42
8:x:479:VAL:HG12	8:x:480:GLU:N	2.35	0.42
2:B:35:ASN:CG	2:B:35:ASN:O	2.62	0.42
4:J:90:LYS:O	4:J:94:VAL:HG23	2.20	0.42
8:x:1112:LEU:HD12	8:x:1171:LEU:HG	2.00	0.42
1:E:105:ILE:HB	1:E:749:LEU:HD21	2.01	0.41
1:E:785:GLU:HA	1:E:815:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:850:ALA:HB2	1:E:867:ILE:CD1	2.50	0.41
7:P:5:LYS:N	7:P:148:SER:O	2.52	0.41
8:x:87:ASN:OD1	8:x:87:ASN:O	2.38	0.41
8:x:643:ILE:HG23	8:x:660:ILE:HG23	2.02	0.41
8:x:827:ASP:N	8:x:828:PRO:HD2	2.35	0.41
1:A:62:ILE:HD12	1:A:826:LEU:HD11	2.01	0.41
1:A:112:PRO:HD2	1:A:131:THR:HG23	2.02	0.41
2:F:110:GLY:HA2	2:F:235:LEU:O	2.20	0.41
2:F:432:SER:HA	2:F:468:TYR:OH	2.20	0.41
3:K:88:VAL:HG22	4:L:76:VAL:HG13	2.02	0.41
2:B:161:MET:HE2	2:B:404:TYR:CE2	2.55	0.41
3:K:61:ASN:O	3:K:62:PHE:C	2.62	0.41
1:A:910:ASN:HB3	1:A:913:VAL:HG22	2.03	0.41
3:I:169:LEU:HD23	3:I:172:ILE:CG1	2.50	0.41
8:x:68:ALA:HB1	8:x:106:LEU:HD21	2.01	0.41
8:x:951:GLU:O	8:x:955:LYS:HG2	2.20	0.41
1:A:1058:LEU:C	1:A:1058:LEU:HD23	2.45	0.41
2:F:425:LEU:O	2:F:430:LYS:NZ	2.53	0.41
3:I:76:THR:HG21	4:J:65:VAL:HB	2.02	0.41
5:M:150:ALA:CB	6:N:66:ILE:HD12	2.49	0.41
6:N:88:PHE:HB2	6:N:89:PRO:HD3	2.01	0.41
8:x:76:LEU:HD11	8:x:95:GLN:HE22	1.85	0.41
8:x:189:LEU:N	8:x:190:PRO:CD	2.83	0.41
8:x:742:LEU:HD13	8:x:851:TYR:OH	2.20	0.41
5:M:97:ARG:N	5:M:108:GLN:O	2.53	0.41
1:E:982:GLN:HE22	2:F:475:ARG:CZ	2.34	0.41
2:F:299:PRO:CD	5:M:206:VAL:HG21	2.51	0.41
4:J:36:LYS:O	4:J:36:LYS:HD3	2.21	0.41
8:x:160:VAL:HG23	8:x:200:TRP:HZ2	1.86	0.41
1:A:110:GLN:HG3	1:A:133:ALA:HB1	2.03	0.41
1:A:944:LEU:O	1:A:948:GLU:HG3	2.20	0.41
1:E:1046:ARG:HD3	1:E:1050:GLU:HG2	2.03	0.41
3:K:62:PHE:CE1	4:L:54:LEU:CB	3.04	0.41
5:M:55:GLN:NE2	5:M:59:ARG:HD3	2.36	0.41
8:x:29:ALA:HA	8:x:37:ILE:O	2.21	0.41
8:x:658:VAL:HG13	8:x:669:TYR:HB2	2.03	0.41
8:x:711:VAL:HG22	8:x:720:ILE:HG12	2.03	0.41
10:z:25:ARG:HG3	10:z:143:ILE:HD11	2.03	0.41
1:E:253:THR:HG23	1:E:868:VAL:HA	2.01	0.41
2:F:468:TYR:HB3	2:F:469:PRO:HD2	2.03	0.41
7:P:438:ILE:O	7:P:442:ASP:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:x:72:HIS:HB3	8:x:73:ASN:H	1.75	0.41
8:x:818:ARG:HG3	8:x:818:ARG:HH11	1.86	0.41
1:A:227:LYS:HD2	1:A:853:ALA:HB2	2.03	0.40
1:A:947:ALA:O	1:A:951:GLU:HG3	2.21	0.40
1:E:282:VAL:HG21	1:E:791:GLY:HA3	2.02	0.40
1:E:771:THR:O	1:E:772:LEU:HD12	2.21	0.40
1:E:1046:ARG:HG3	1:E:1046:ARG:O	2.21	0.40
5:M:56:LYS:O	5:M:60:VAL:HG12	2.21	0.40
8:x:544:ILE:CD1	8:x:566:LEU:HD23	2.51	0.40
8:x:563:LEU:HD12	8:x:578:ALA:HB2	2.03	0.40
8:x:1118:LEU:O	8:x:1119:GLU:C	2.64	0.40
2:B:438:LYS:HD3	2:B:467:ILE:HD11	2.04	0.40
1:E:61:VAL:HG11	1:E:64:ILE:HD11	2.04	0.40
3:I:123:SER:HB3	4:J:105:PRO:CB	2.51	0.40
5:M:165:VAL:HG22	5:M:168:ARG:NH2	2.35	0.40
8:x:206:GLN:CB	8:x:212:THR:HG21	2.52	0.40
8:x:658:VAL:HG13	8:x:658:VAL:O	2.21	0.40
1:A:115:ALA:C	1:A:119:GLU:OE1	2.65	0.40
1:A:188:PRO:O	1:A:192:TYR:OH	2.35	0.40
2:B:270:THR:O	2:B:270:THR:CG2	2.69	0.40
1:E:204:ASP:OD1	8:x:1016:LEU:HD12	2.21	0.40
3:I:128:ALA:HB3	3:I:190:VAL:HG21	2.03	0.40
8:x:884:PHE:CD1	8:x:909:ALA:HB2	2.57	0.40
4:L:103:ILE:O	4:L:103:ILE:CG2	2.69	0.40
4:J:93:ASP:O	4:J:97:ILE:CD1	2.67	0.40
8:x:268:SER:O	8:x:272:SER:N	2.49	0.40
8:x:960:LYS:HG3	8:x:961:ASP:H	1.87	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	594/1071 (56%)	577 (97%)	17 (3%)	0	100	100
1	E	585/1071 (55%)	558 (95%)	26 (4%)	1 (0%)	44	68
2	B	467/517 (90%)	453 (97%)	13 (3%)	1 (0%)	44	68
2	F	463/517 (90%)	444 (96%)	19 (4%)	0	100	100
3	I	210/233 (90%)	204 (97%)	6 (3%)	0	100	100
3	K	195/233 (84%)	189 (97%)	6 (3%)	0	100	100
4	J	98/114 (86%)	93 (95%)	5 (5%)	0	100	100
4	L	84/114 (74%)	81 (96%)	3 (4%)	0	100	100
5	M	211/256 (82%)	202 (96%)	9 (4%)	0	100	100
6	N	113/117 (97%)	103 (91%)	10 (9%)	0	100	100
7	P	430/478 (90%)	413 (96%)	17 (4%)	0	100	100
8	x	1188/1357 (88%)	1097 (92%)	90 (8%)	1 (0%)	48	73
9	y	236/351 (67%)	234 (99%)	2 (1%)	0	100	100
10	z	123/194 (63%)	112 (91%)	11 (9%)	0	100	100
All	All	4997/6623 (75%)	4760 (95%)	234 (5%)	3 (0%)	50	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	487	ARG
8	x	127	LYS
1	E	183	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/908 (55%)	498 (100%)	1 (0%)	92	98
1	E	490/908 (54%)	483 (99%)	7 (1%)	62	84
2	B	402/444 (90%)	398 (99%)	4 (1%)	73	89
2	F	398/444 (90%)	388 (98%)	10 (2%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	187/208 (90%)	183 (98%)	4 (2%)	48 76
3	K	162/208 (78%)	162 (100%)	0	100 100
4	J	69/94 (73%)	69 (100%)	0	100 100
4	L	40/94 (43%)	40 (100%)	0	100 100
5	M	129/221 (58%)	128 (99%)	1 (1%)	79 91
6	N	61/103 (59%)	61 (100%)	0	100 100
7	P	9/439 (2%)	9 (100%)	0	100 100
8	x	839/1244 (67%)	835 (100%)	4 (0%)	86 95
9	y	8/327 (2%)	8 (100%)	0	100 100
10	z	79/179 (44%)	78 (99%)	1 (1%)	65 85
All	All	3372/5821 (58%)	3340 (99%)	32 (1%)	74 90

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	743	ASN
2	B	169	LYS
2	B	456	GLU
2	B	466	ARG
2	B	481	LEU
1	E	174	LEU
1	E	219	ARG
1	E	757	THR
1	E	780	PRO
1	E	814	ARG
1	E	858	SER
1	E	862	THR
2	F	163	SER
2	F	176	SER
2	F	269	GLN
2	F	270	THR
2	F	310	THR
2	F	311	ASP
2	F	340	ASP
2	F	381	ARG
2	F	411	LYS
2	F	442	THR
3	I	226	SER

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Mol	Chain	Res	Type
3	I	229	ARG
3	I	230	LYS
3	I	233	ASP
5	M	151	SER
8	x	122	SER
8	x	315	HIS
8	x	1042	LYS
8	x	1051	GLN
10	z	142	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	249	GLN
1	A	743	ASN
1	A	905	HIS
1	A	929	ASN
1	A	982	GLN
2	B	64	GLN
2	B	122	ASN
2	B	460	GLN
2	B	474	ASN
1	E	40	ASN
1	E	249	GLN
1	E	804	ASN
1	E	982	GLN
2	F	35	ASN
2	F	66	GLN
2	F	186	GLN
2	F	232	ASN
2	F	326	ASN
2	F	374	ASN
4	L	77	GLN
8	x	19	GLN
8	x	24	ASN
8	x	63	GLN
8	x	72	HIS
8	x	496	ASN
8	x	641	ASN
8	x	748	HIS
8	x	775	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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
12	ADP	A	1102	11	24,29,29	0.85	1 (4%)	29,45,45	0.77	1 (3%)
12	ADP	E	1102	11	24,29,29	0.78	0	29,45,45	0.81	1 (3%)

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
12	ADP	A	1102	11	-	0/12/32/32	0/3/3/3
12	ADP	E	1102	11	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1102	ADP	C8-N7	-2.00	1.31	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	1102	ADP	C5-C6-N6	2.48	124.10	120.31
12	E	1102	ADP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	1102	ADP	C5'-O5'-PA-O1A
12	E	1102	ADP	C5'-O5'-PA-O2A
12	E	1102	ADP	C5'-O5'-PA-O3A
12	E	1102	ADP	C4'-C5'-O5'-PA

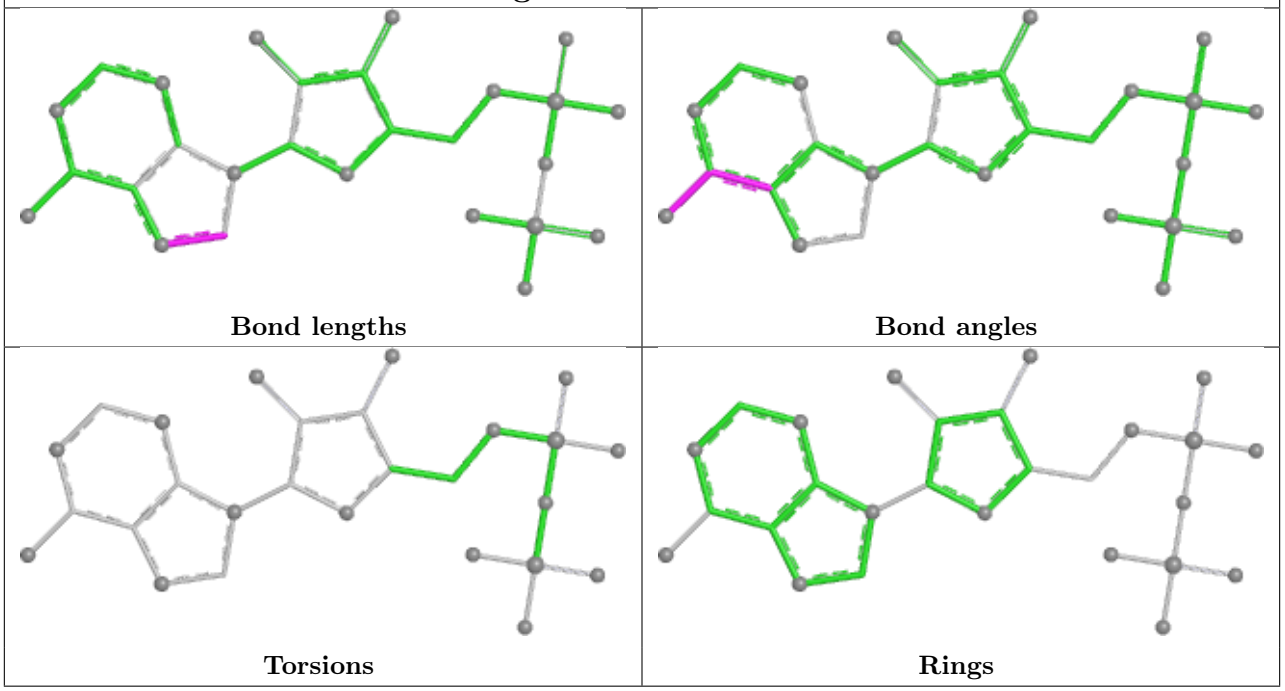
There are no ring outliers.

2 monomers are involved in 4 short contacts:

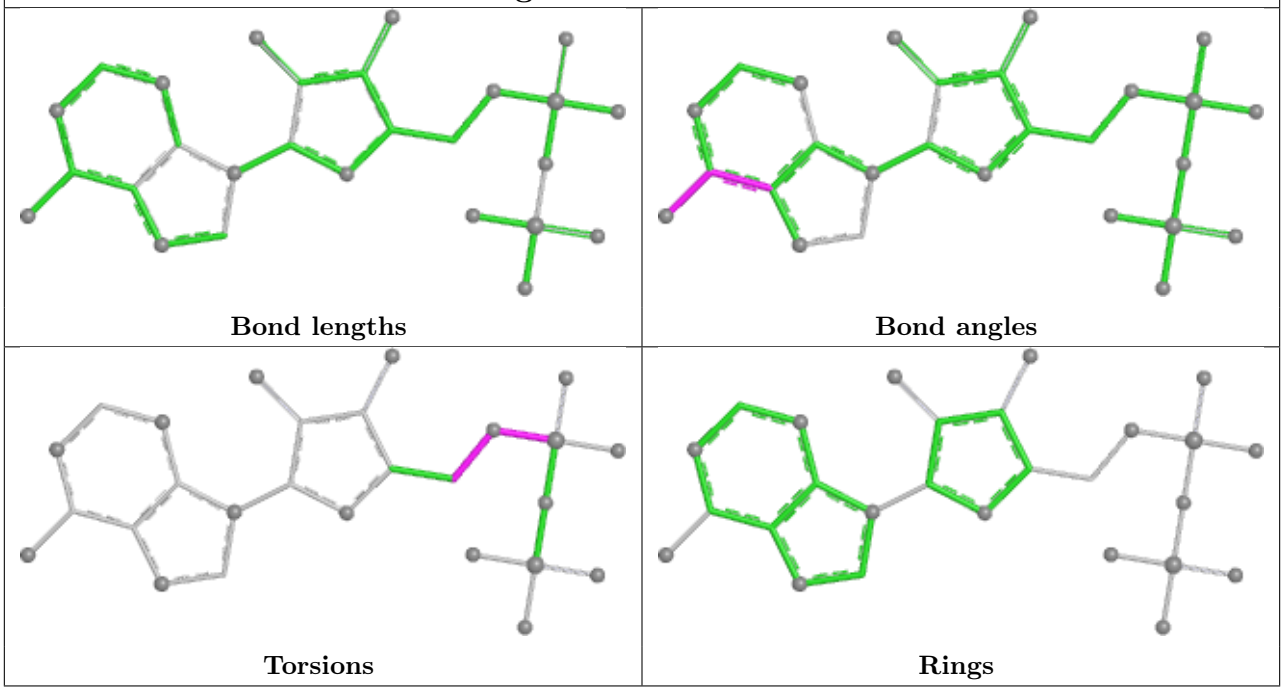
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1102	ADP	1	0
12	E	1102	ADP	3	0

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 then 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.

Ligand ADP A 1102



Ligand ADP E 1102



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.

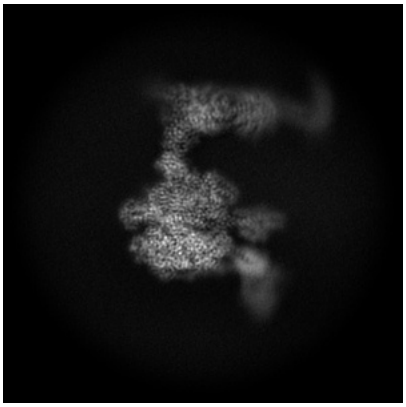
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45788. These allow visual inspection of the internal detail of the map and identification of artifacts.

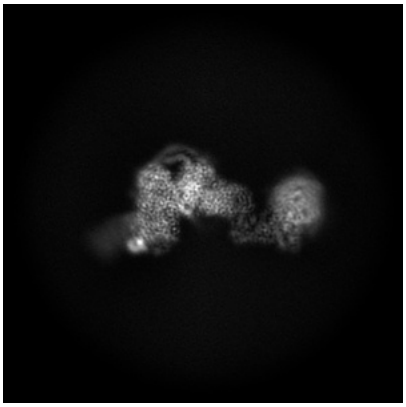
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

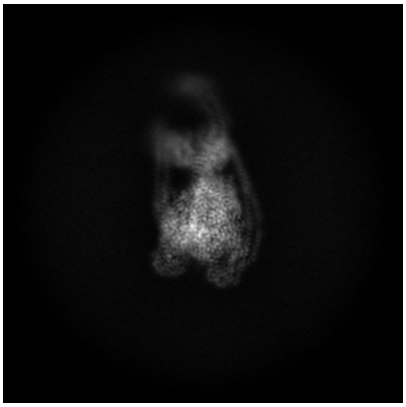
6.1.1 Primary map



X



Y

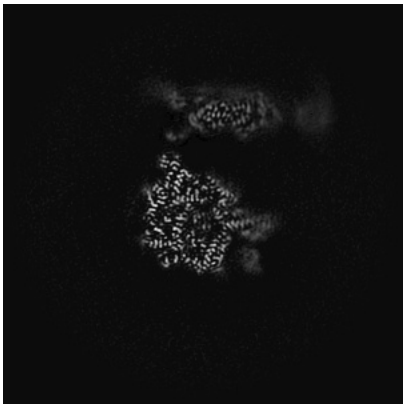


Z

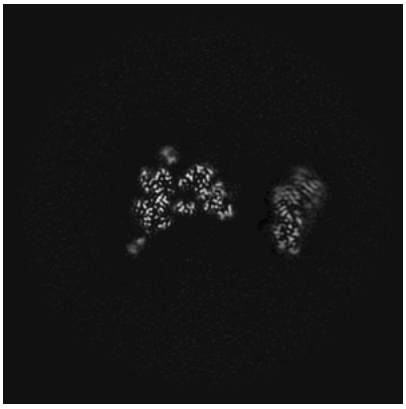
The images above show the map projected in three orthogonal directions.

6.2 Central slices

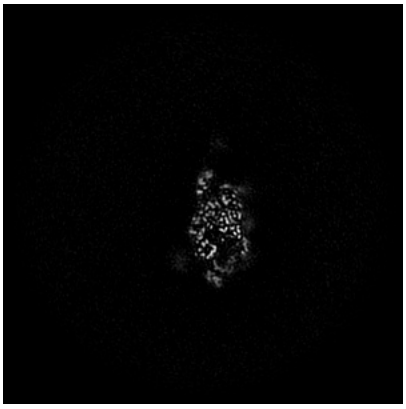
6.2.1 Primary map



X Index: 195



Y Index: 195

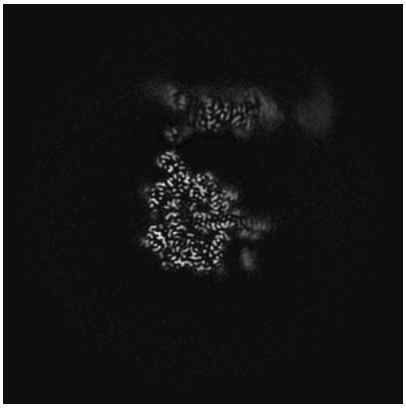


Z Index: 195

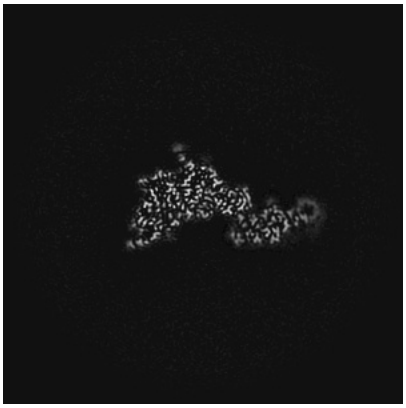
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 192



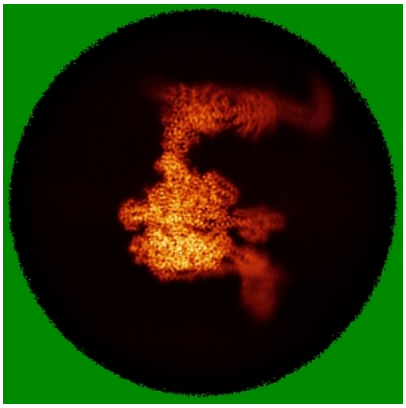
Y Index: 168

Z Index: 151

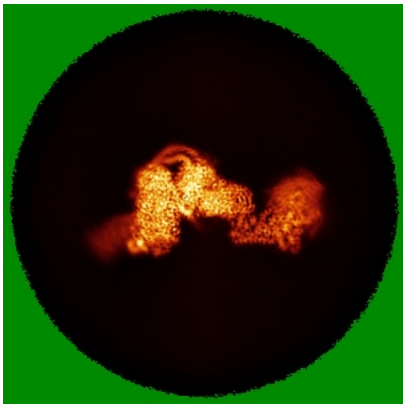
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

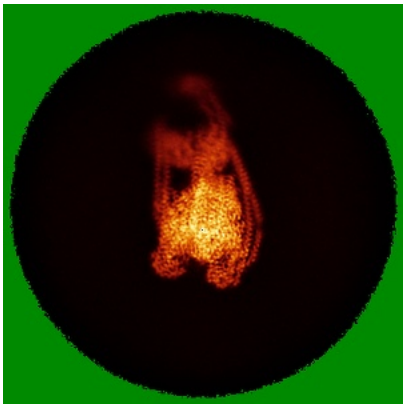
6.4.1 Primary map



X



Y

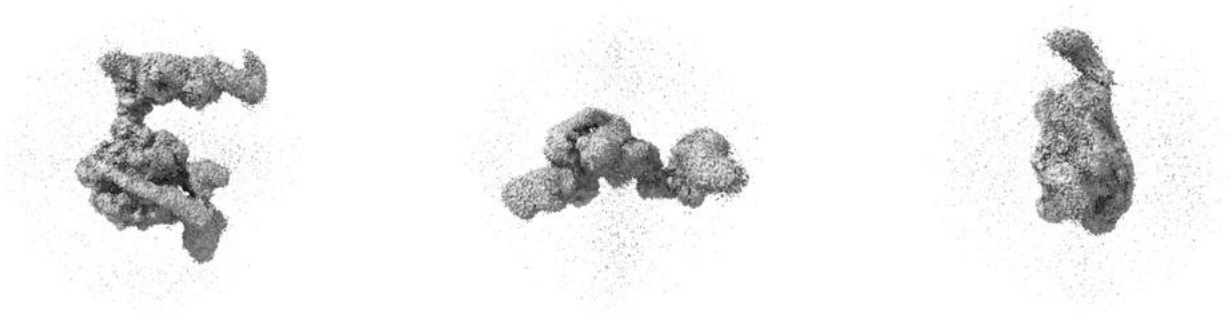


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

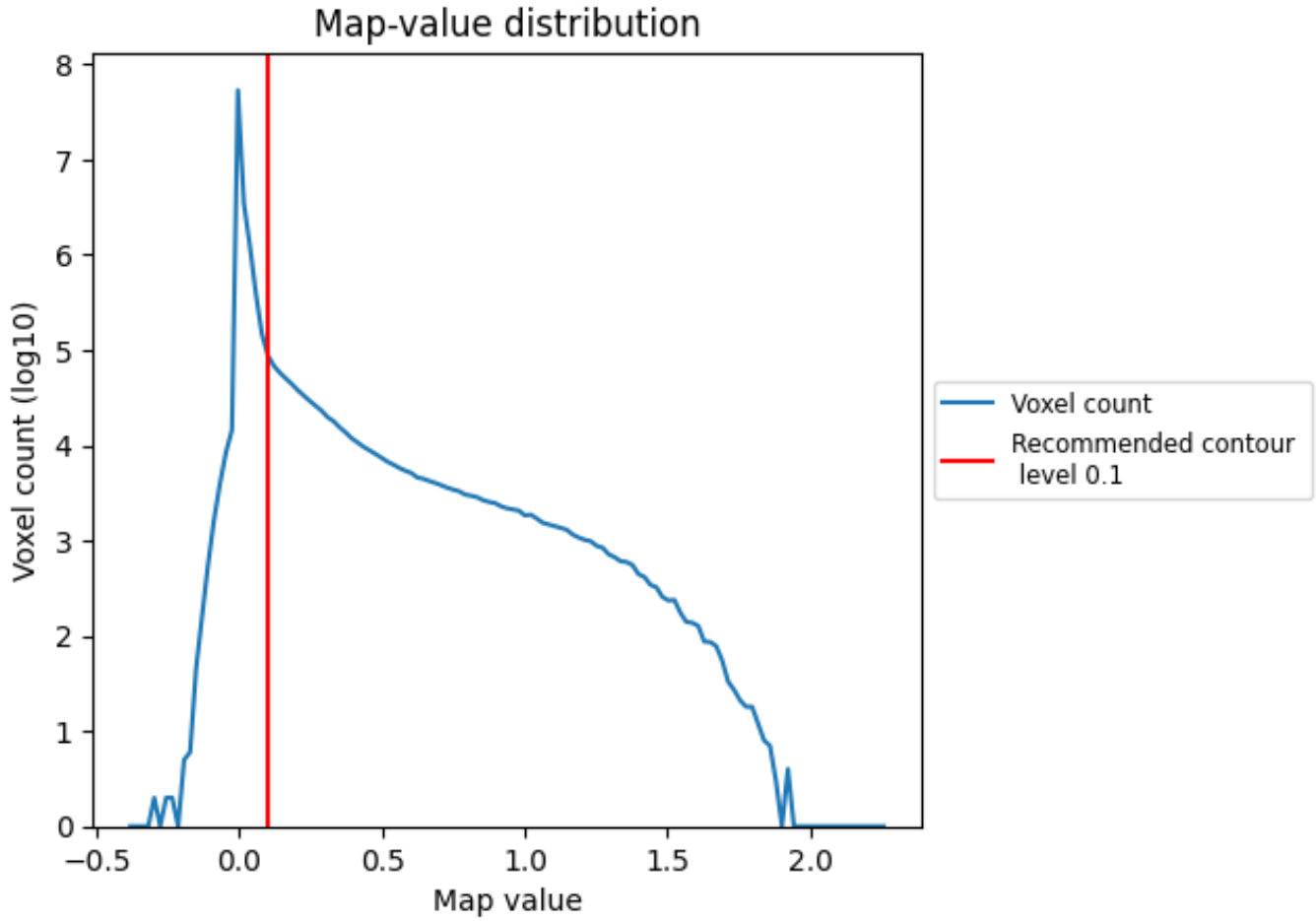
6.6 Mask visualisation (i)

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

7 Map analysis

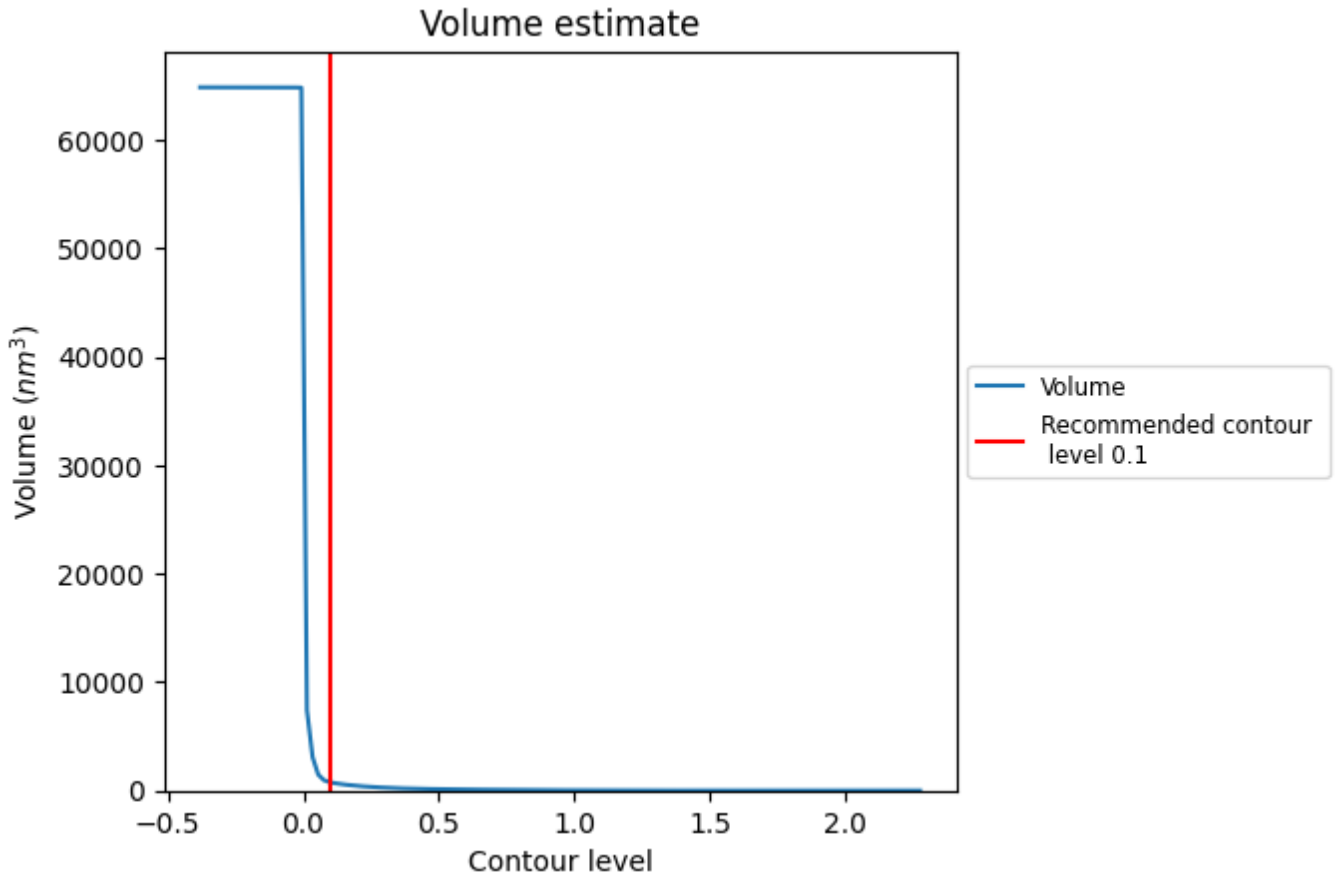
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

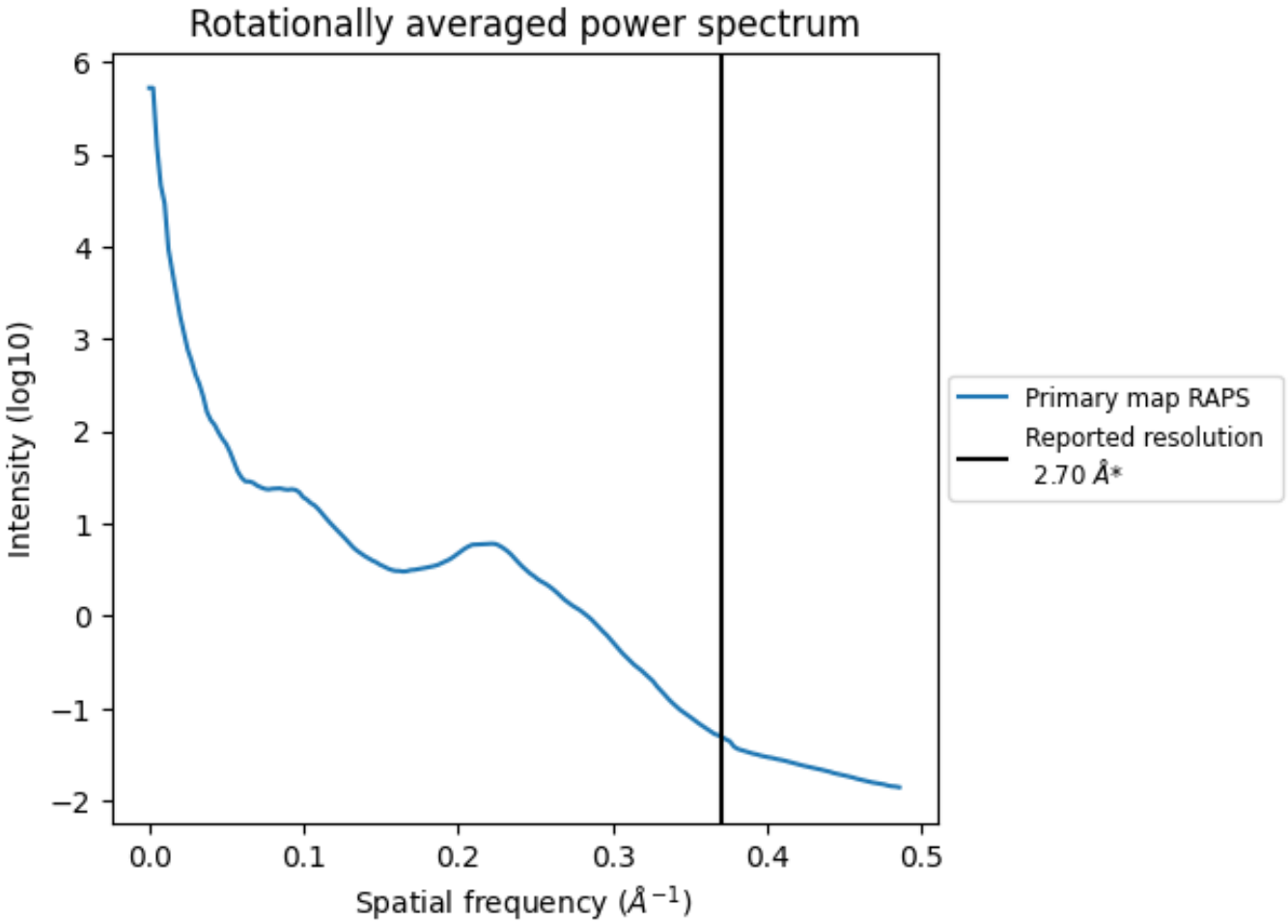
7.2 Volume estimate



The volume at the recommended contour level is 759 nm^3; this corresponds to an approximate mass of 686 kDa.

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

7.3 Rotationally averaged power spectrum (i)

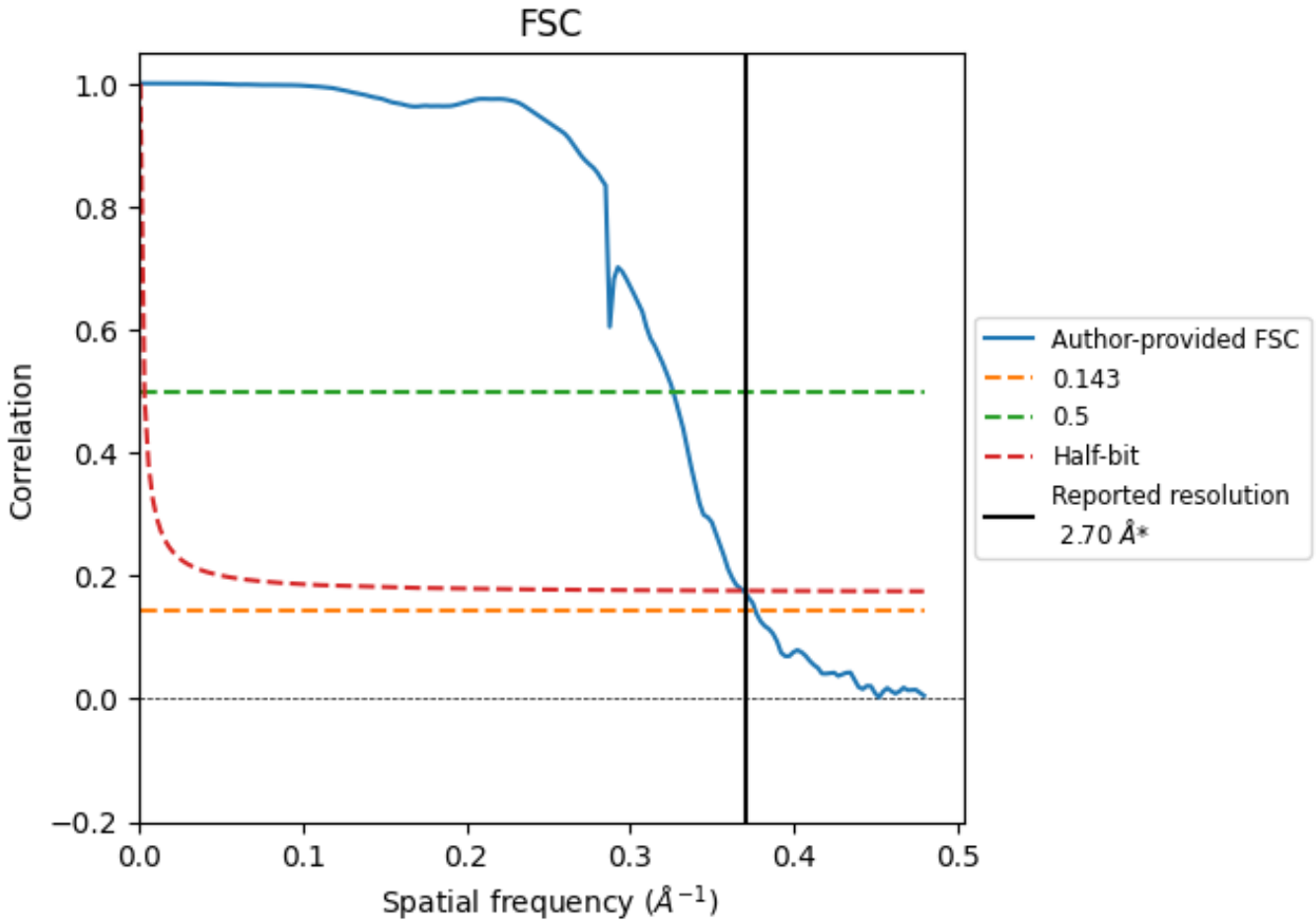


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8.2 Resolution estimates (i)

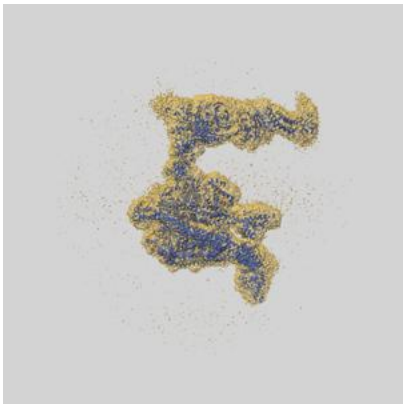
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.66	3.07	2.71
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

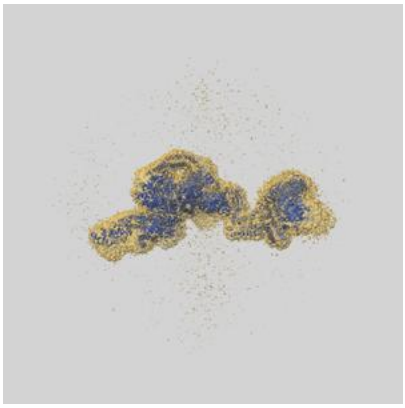
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45788 and PDB model 9COP. Per-residue inclusion information can be found in section 3 on page 7.

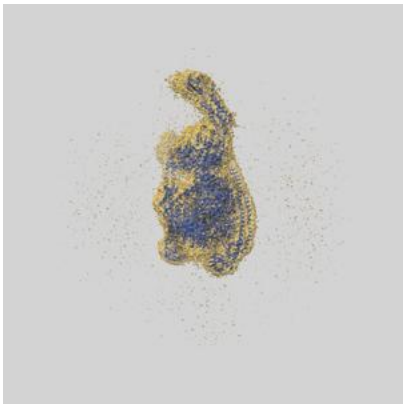
9.1 Map-model overlay



X



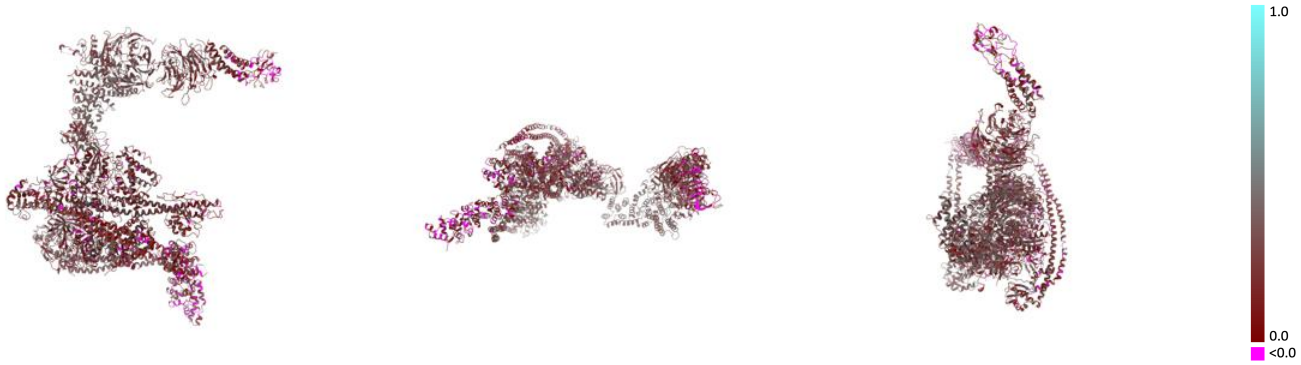
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

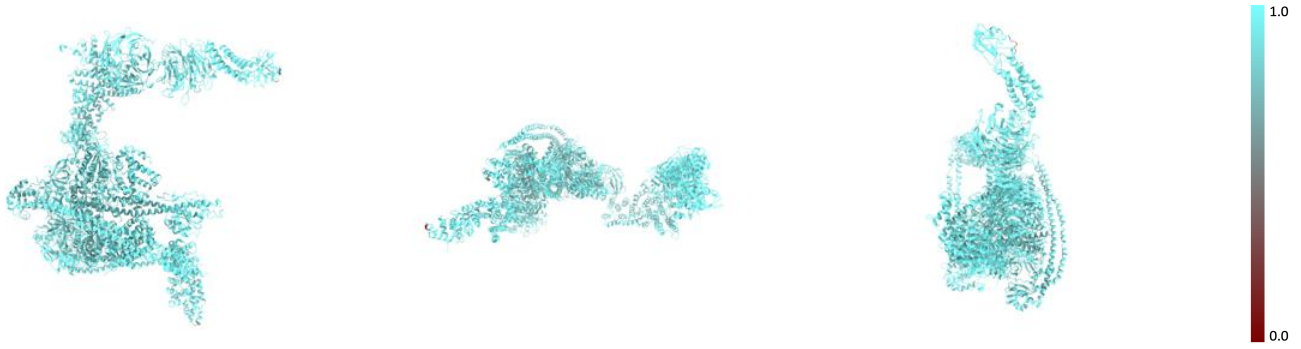
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

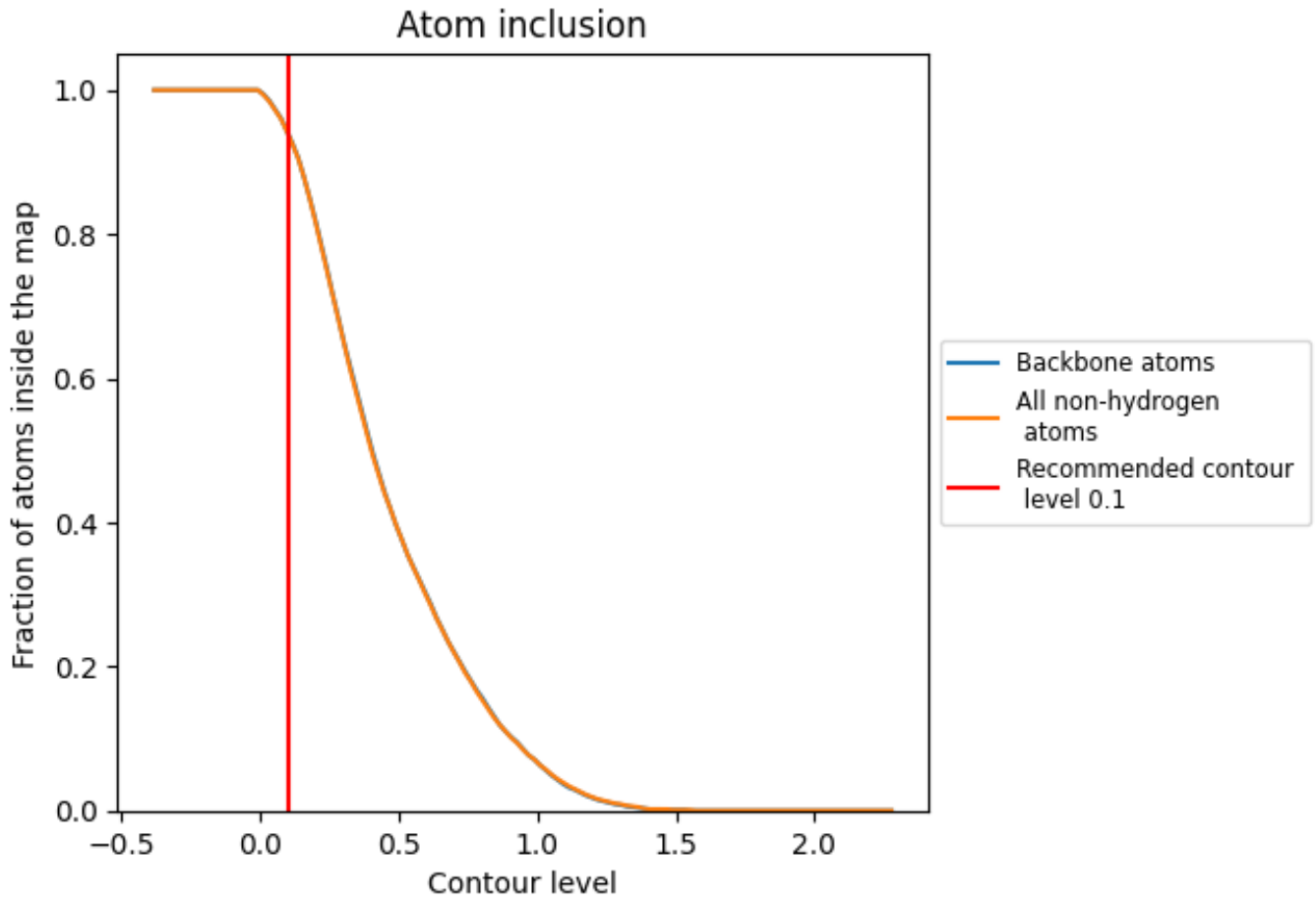
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.2520
A	0.9140	0.2320
B	0.9400	0.2790
E	0.9360	0.2500
F	0.9070	0.2220
I	0.9220	0.2110
J	0.9140	0.1660
K	0.9680	0.3100
L	0.9600	0.2850
M	0.9560	0.2230
N	0.9640	0.2210
P	0.9850	0.1390
x	0.9570	0.3140
y	0.9680	0.1450
z	0.9510	0.2890