



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 03:53 AM EST

PDB ID : 7TMM  
EMDB ID : EMD-25996  
Title : Complete V1 Complex from *Saccharomyces cerevisiae*  
Authors : Vasanthakumar, T.; Keon, K.A.; Bueler, S.A.; Jaskolka, M.C.; Rubinstein, J.L.  
Deposited on : 2022-01-19  
Resolution : 3.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

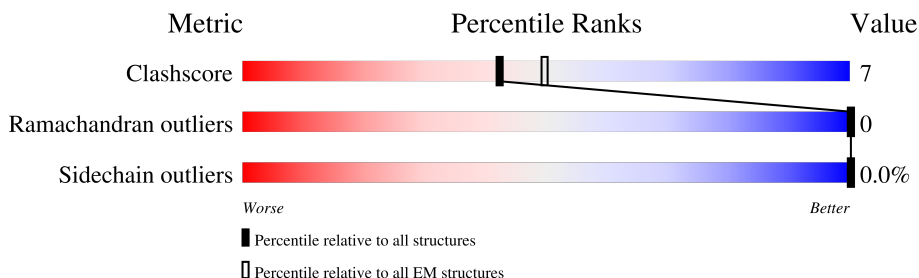
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	639	76% 17% 7%
1	C	639	78% 15% 7%
1	E	639	72% 18% 10%
2	B	517	73% 17% 10%
2	D	517	71% 18% 11%
2	F	517	72% 17% 11%
3	G	233	88% 7% 6%
3	I	233	84% 10% 6%

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Mol	Chain	Length	Quality of chain
3	K	233	 77%14%9%
4	H	114	 89%6%5%
4	J	114	 90%5%5%
4	L	114	 82%13%5%
5	M	256	 77%6%16%
6	N	118	 86%8%6%
7	O	392	 89%8%8%
8	P	478	 91%8%8%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33713 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 H(+)-transporting two-sector ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	593	Total	C	N	O	S	0	0
			4150	2690	720	722	18		
1	C	592	Total	C	N	O	S	0	0
			3985	2578	704	687	16		
1	E	576	Total	C	N	O	S	0	0
			4006	2595	703	693	15		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	ASP	-	expression tag	UNP A0A6L0YX77
A	618	TYR	-	expression tag	UNP A0A6L0YX77
A	619	LYS	-	expression tag	UNP A0A6L0YX77
A	620	ASP	-	expression tag	UNP A0A6L0YX77
A	621	HIS	-	expression tag	UNP A0A6L0YX77
A	622	ASP	-	expression tag	UNP A0A6L0YX77
A	623	GLY	-	expression tag	UNP A0A6L0YX77
A	624	ASP	-	expression tag	UNP A0A6L0YX77
A	625	TYR	-	expression tag	UNP A0A6L0YX77
A	626	LYS	-	expression tag	UNP A0A6L0YX77
A	627	ASP	-	expression tag	UNP A0A6L0YX77
A	628	HIS	-	expression tag	UNP A0A6L0YX77
A	629	ASP	-	expression tag	UNP A0A6L0YX77
A	630	ILE	-	expression tag	UNP A0A6L0YX77
A	631	ASP	-	expression tag	UNP A0A6L0YX77
A	632	TYR	-	expression tag	UNP A0A6L0YX77
A	633	LYS	-	expression tag	UNP A0A6L0YX77
A	634	ASP	-	expression tag	UNP A0A6L0YX77
A	635	ASP	-	expression tag	UNP A0A6L0YX77
A	636	ASP	-	expression tag	UNP A0A6L0YX77
A	637	ASP	-	expression tag	UNP A0A6L0YX77
A	638	LYS	-	expression tag	UNP A0A6L0YX77
C	617	ASP	-	expression tag	UNP A0A6L0YX77
C	618	TYR	-	expression tag	UNP A0A6L0YX77

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Chain	Residue	Modelled	Actual	Comment	Reference
C	619	LYS	-	expression tag	UNP A0A6L0YX77
C	620	ASP	-	expression tag	UNP A0A6L0YX77
C	621	HIS	-	expression tag	UNP A0A6L0YX77
C	622	ASP	-	expression tag	UNP A0A6L0YX77
C	623	GLY	-	expression tag	UNP A0A6L0YX77
C	624	ASP	-	expression tag	UNP A0A6L0YX77
C	625	TYR	-	expression tag	UNP A0A6L0YX77
C	626	LYS	-	expression tag	UNP A0A6L0YX77
C	627	ASP	-	expression tag	UNP A0A6L0YX77
C	628	HIS	-	expression tag	UNP A0A6L0YX77
C	629	ASP	-	expression tag	UNP A0A6L0YX77
C	630	ILE	-	expression tag	UNP A0A6L0YX77
C	631	ASP	-	expression tag	UNP A0A6L0YX77
C	632	TYR	-	expression tag	UNP A0A6L0YX77
C	633	LYS	-	expression tag	UNP A0A6L0YX77
C	634	ASP	-	expression tag	UNP A0A6L0YX77
C	635	ASP	-	expression tag	UNP A0A6L0YX77
C	636	ASP	-	expression tag	UNP A0A6L0YX77
C	637	ASP	-	expression tag	UNP A0A6L0YX77
C	638	LYS	-	expression tag	UNP A0A6L0YX77
E	617	ASP	-	expression tag	UNP A0A6L0YX77
E	618	TYR	-	expression tag	UNP A0A6L0YX77
E	619	LYS	-	expression tag	UNP A0A6L0YX77
E	620	ASP	-	expression tag	UNP A0A6L0YX77
E	621	HIS	-	expression tag	UNP A0A6L0YX77
E	622	ASP	-	expression tag	UNP A0A6L0YX77
E	623	GLY	-	expression tag	UNP A0A6L0YX77
E	624	ASP	-	expression tag	UNP A0A6L0YX77
E	625	TYR	-	expression tag	UNP A0A6L0YX77
E	626	LYS	-	expression tag	UNP A0A6L0YX77
E	627	ASP	-	expression tag	UNP A0A6L0YX77
E	628	HIS	-	expression tag	UNP A0A6L0YX77
E	629	ASP	-	expression tag	UNP A0A6L0YX77
E	630	ILE	-	expression tag	UNP A0A6L0YX77
E	631	ASP	-	expression tag	UNP A0A6L0YX77
E	632	TYR	-	expression tag	UNP A0A6L0YX77
E	633	LYS	-	expression tag	UNP A0A6L0YX77
E	634	ASP	-	expression tag	UNP A0A6L0YX77
E	635	ASP	-	expression tag	UNP A0A6L0YX77
E	636	ASP	-	expression tag	UNP A0A6L0YX77
E	637	ASP	-	expression tag	UNP A0A6L0YX77
E	638	LYS	-	expression tag	UNP A0A6L0YX77

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	464	Total	C	N	O	S	0	0
			3375	2175	599	591	10		
2	D	459	Total	C	N	O	S	0	0
			3266	2123	583	549	11		
2	F	459	Total	C	N	O	S	0	0
			3276	2116	584	567	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	220	Total	C	N	O	S	0	0
			1322	844	239	238	1		
3	I	220	Total	C	N	O	S	0	0
			1313	834	241	237	1		
3	K	212	Total	C	N	O	S	0	0
			1288	829	236	222	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	109	Total	C	N	O		0	0
			578	353	113	112			
4	J	108	Total	C	N	O		0	0
			570	350	111	109			
4	L	99	Total	C	N	O		0	0
			522	321	101	100			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	214	Total	C	N	O	S	0	0
			1341	852	252	234	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	111	Total	C	N	O		0	0
			610	384	114	112			

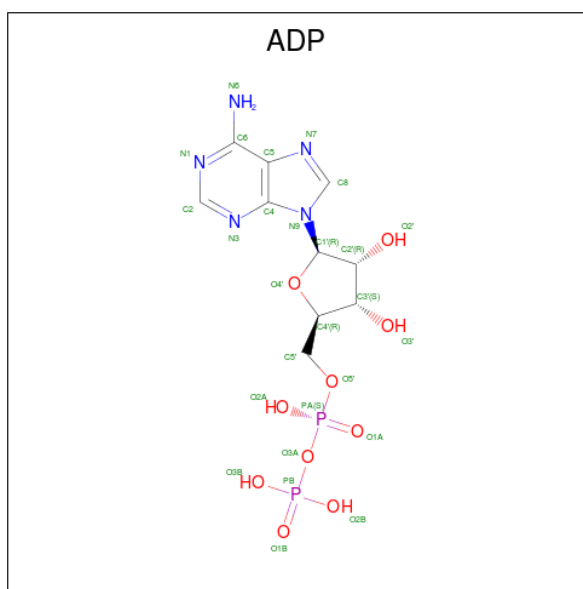
- Molecule 7 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	359	Total	C	N	O	0	0
			1873	1147	362	364		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	441	Total	C	N	O	0	0
			2211	1329	441	441		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

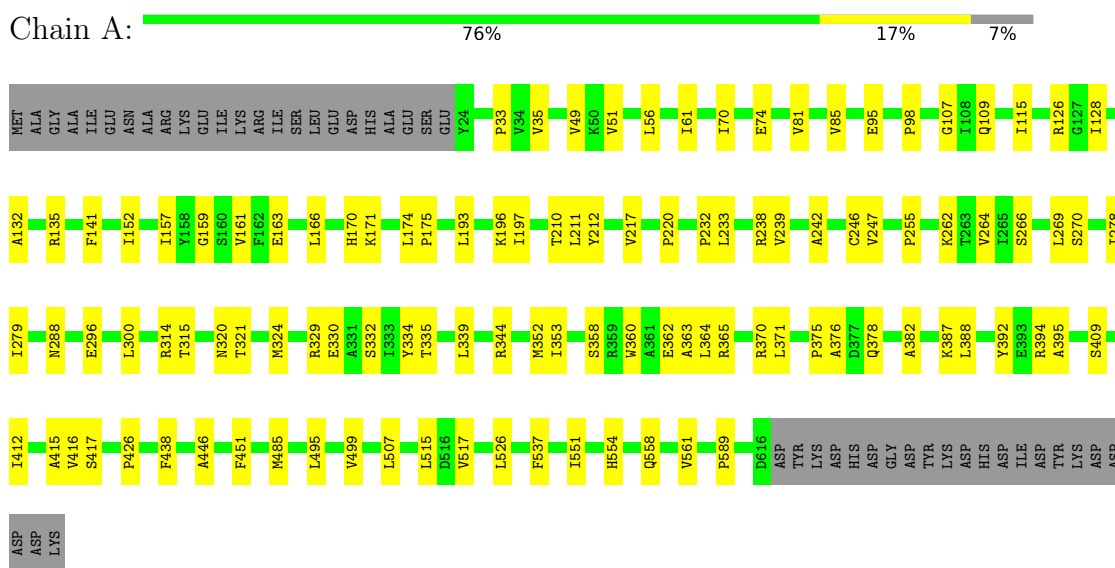


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

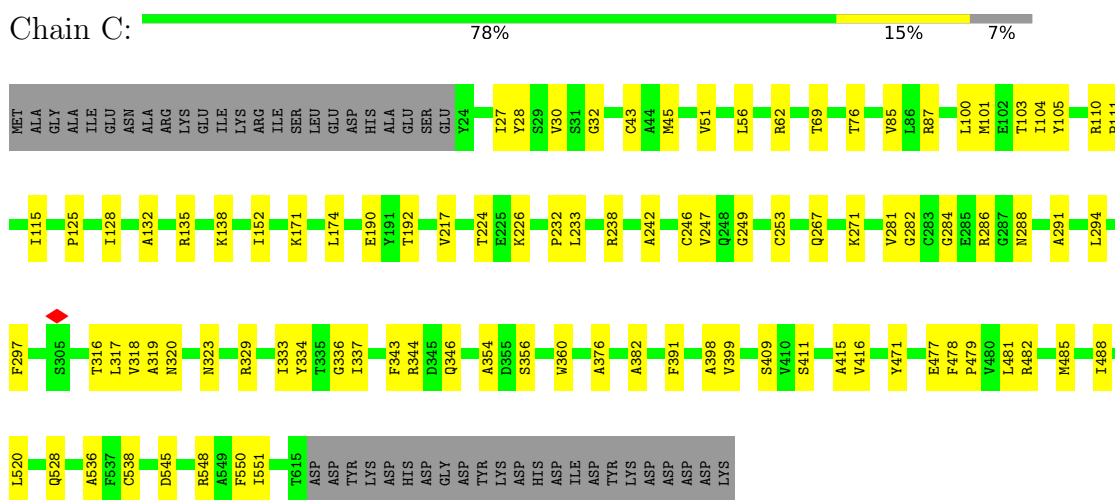
### 3 Residue-property plots

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: H(+)-transporting two-sector ATPase



- Molecule 1: H(+)-transporting two-sector ATPase



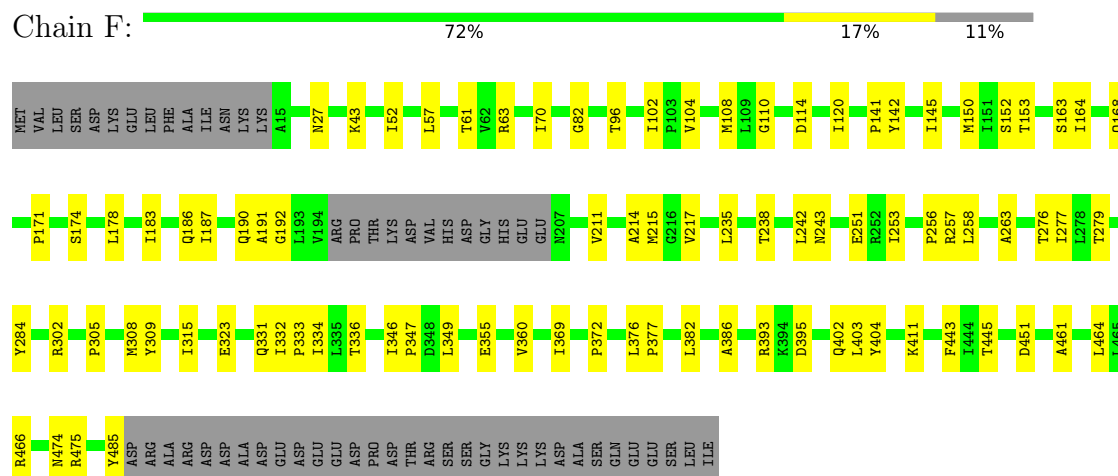
- Molecule 1: H(+)-transporting two-sector ATPase

V399	GLY	V85	MET
T407	CYS	L86	ALA
V410	LYS	R87	GLY
A415	THR	L92	ALA
V416	V264	P98	ILE
S417	I265	G99	GLU
PRO	S266	L100	ASN
ALA	C283	I104	ALA
GLY	R286	I104	ARG
TYR	G287	P111	LYS
LYS	N288	L112	LYS
PHE	E289	K116	ILE
HIS	M290	R126	SER
S424	L294	R126	LEU
D425	P298	A132	GLU
P426	T302	W139	ASP
	P310	S160	ALA
T429	I311	V161	GLY
V437	M312	H170	SER
F438	K313	K171	GLY
W439	R314	P176	SER
L445	N320	G32	ASP
K449	R329	I182	ASP
H450	S332	L193	LYS
I454	I333	T210	ASP
L467	Y334	L211	ASP
F470	I337	W215	LYS
E477	T338	P216	ASP
L481	L339	W217	ASP
R484	A340	V223	ASP
M485	E341	I161	ASP
I488	R344	P232	ASP
V499	D345	L233	ASP
K504	Q346	P239	ASP
V517	I353	L240	ASP
F525	S356	I70	ASP
L526	R365	L243	ASP
M546	Q378	C246	ASP
M547		T252	ASP
F550	P381	P255	ASP
V554	A382	GLY	ASP
	R394	ALA	ASP
		PRO	ASP

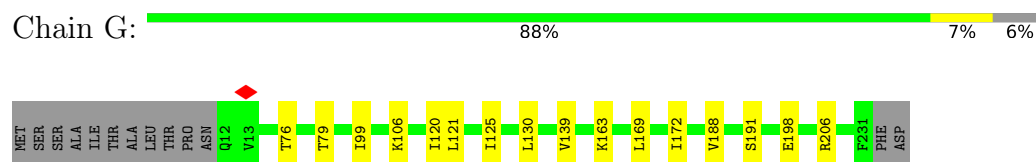
[illegible]

M416	L266	R111
V419	P124	
V420	T270	F127
F439	E271	
	R272	L132
A461	L278	R144
L464	T279	
	A287	P147
Y485	L288	E148
ASP	R289	E149
ARG	E290	M150
ALA		
ARG	A293	T153
ASP		E154
ASP	E296	V155
ALA		
ASP	L315	T160
GLU	V316	M161
ASP	E317	
GLU	R318	F173
GLU	A319	S174
ASP	G320	A175
PRO	R321	
ASP		L178
THR	Q331	
ARG		L187
SER	L334	
SER	L335	A191
GLY		
LVS	H344	V194
LVS	P345	ARG
LVS	T346	PRO
ASP	P347	THR
ALA		LYS
SER	E355	ASP
GLN		VAL
GLU	L358	HIS
GLU		ASP
SER	R362	GLY
LEU		HIS
ILE	L376	GLU
	A386	H207
	R391	A213
		A214
	D395	M215
	H396	
		T250
	V399	
		L253
	Q402	
	L403	P256
	Y404	R257
	A405	L258
	K406	
		T263

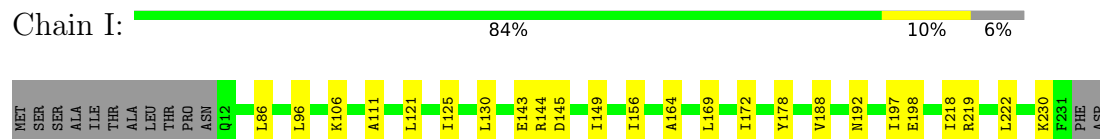
- Molecule 2: Vacuolar proton pump subunit B



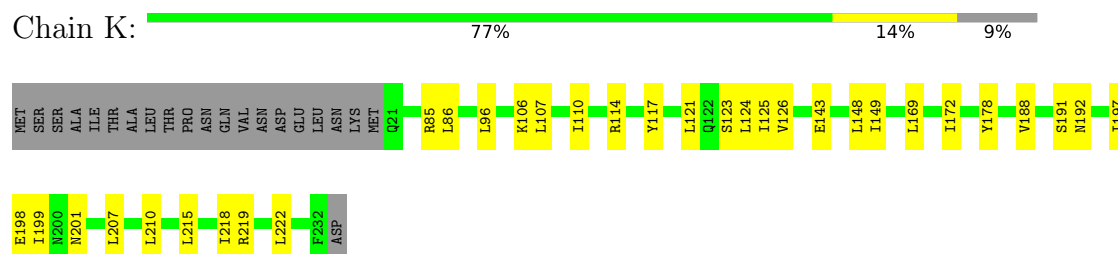
- Molecule 3: V-ATPase subunit E



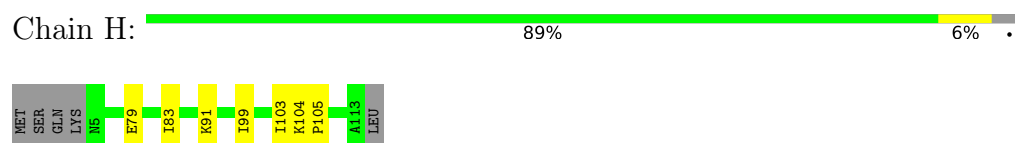
- Molecule 3: V-ATPase subunit E




- Molecule 3: V-ATPase subunit E

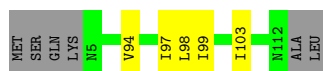


- Molecule 4: V-type proton ATPase subunit G




- Molecule 4: V-type proton ATPase subunit G

Chain J:  90% • 5%




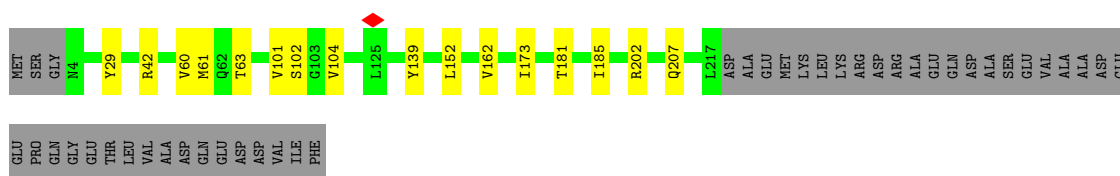
- Molecule 4: V-type proton ATPase subunit G

Chain L:  82% • 13%




- Molecule 5: V-type proton ATPase subunit D

Chain M:  77% 6% 16%




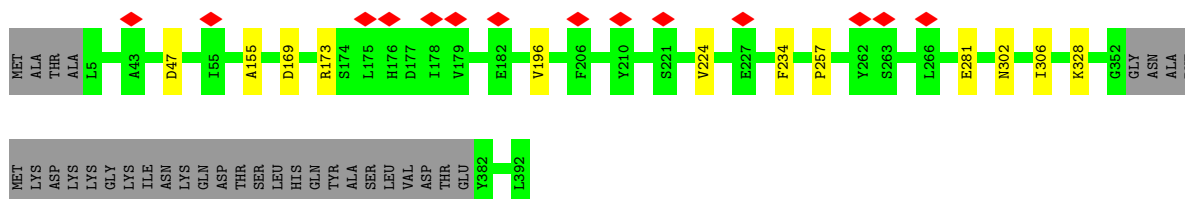
- Molecule 6: V-type proton ATPase subunit F

Chain N:  86% 8% 6%



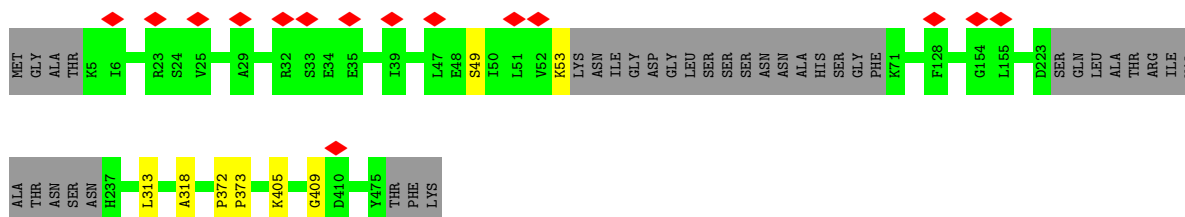
- Molecule 7: V-type proton ATPase subunit C

Chain O:  89% • 8%



- Molecule 8: V-type proton ATPase subunit H

Chain P:  91% • 8%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105017	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	43	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.078	Depositor
Minimum map value	-3.634	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	412.0, 412.0, 412.0	wwPDB
Map dimensions	400, 400, 400	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

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	0/4247	0.49	0/5812
1	C	0.31	0/4072	0.48	0/5586
1	E	0.32	0/4096	0.48	0/5609
2	B	0.35	0/3444	0.52	0/4700
2	D	0.33	0/3334	0.52	0/4559
2	F	0.34	0/3343	0.51	0/4571
3	G	0.26	0/1331	0.43	0/1838
3	I	0.26	0/1322	0.43	0/1827
3	K	0.26	0/1299	0.44	0/1790
4	H	0.24	0/579	0.34	0/802
4	J	0.25	0/571	0.34	0/793
4	L	0.24	0/523	0.36	0/728
5	M	0.26	0/1355	0.44	0/1857
6	N	0.24	0/617	0.42	0/859
7	O	0.24	0/1895	0.38	0/2653
8	P	0.22	0/2217	0.34	0/3099
All	All	0.30	0/34245	0.47	0/47083

There are no bond length outliers.

There are no bond angle outliers.

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	4150	0	3839	67	0
1	C	3985	0	3554	59	0
1	E	4006	0	3652	76	0
2	B	3375	0	3240	65	0
2	D	3266	0	3094	68	0
2	F	3276	0	3089	60	0
3	G	1322	0	1061	13	0
3	I	1313	0	1014	20	0
3	K	1288	0	1034	22	0
4	H	578	0	363	6	0
4	J	570	0	359	6	0
4	L	522	0	323	4	0
5	M	1341	0	1077	12	0
6	N	610	0	381	6	0
7	O	1873	0	961	6	0
8	P	2211	0	993	4	0
9	A	27	0	12	3	0
All	All	33713	0	28046	446	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 7.

All (446) 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:344:ARG:HG2	1:E:410:VAL:HG23	1.58	0.83
2:F:187:ILE:O	2:F:191:ALA:HB2	1.79	0.81
2:D:40:ILE:HG13	2:D:76:ILE:HG23	1.64	0.78
1:A:51:VAL:HA	1:A:85:VAL:HG12	1.65	0.78
3:K:125:ILE:HG13	3:K:188:VAL:HG21	1.65	0.77
2:B:150:MET:HB2	2:B:386:ALA:HB1	1.66	0.76
5:M:61:MET:HG3	6:N:95:PRO:HD2	1.67	0.76
1:E:27:ILE:HD12	1:E:83:ASP:HB2	1.68	0.75
2:B:210:ILE:HB	2:B:238:THR:HG22	1.68	0.75
1:E:51:VAL:HA	1:E:85:VAL:HG12	1.69	0.74
1:A:262:LYS:NZ	9:A:701:ADP:O1B	2.21	0.74
2:D:296:GLU:O	5:M:207:GLN:NE2	2.22	0.71
1:E:223:VAL:HG12	1:E:344:ARG:HH12	1.55	0.71
1:E:239:VAL:HG22	1:E:526:LEU:HG	1.73	0.71
1:E:283:CYS:SG	1:E:332:SER:OG	2.49	0.71
2:D:144:ARG:NH2	2:D:317:GLU:O	2.25	0.70
1:E:356:SER:H	1:E:415:ALA:HB3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:MET:HE2	2:D:403:LEU:HB3	1.75	0.68
2:F:360:VAL:HG13	2:F:372:PRO:HG2	1.77	0.67
2:D:178:LEU:HD21	2:D:362:ARG:HD3	1.75	0.67
1:E:341:GLU:OE2	1:E:394:ARG:NE	2.28	0.66
2:F:63:ARG:NH1	2:F:82:GLY:O	2.29	0.66
1:C:485:MET:HA	1:C:488:ILE:HG22	1.78	0.65
2:F:376:LEU:HA	2:F:404:TYR:HE1	1.59	0.65
2:F:214:ALA:HB3	2:F:242:LEU:HA	1.80	0.64
2:D:290:GLU:HA	1:E:382:ALA:HB1	1.79	0.64
1:C:232:PRO:HA	1:C:247:VAL:HA	1.79	0.63
2:D:55:LEU:HD22	2:D:93:VAL:HG22	1.80	0.63
1:C:51:VAL:N	1:C:56:LEU:O	2.29	0.63
2:D:109:LEU:O	3:K:85:ARG:NH2	2.31	0.63
1:E:77:ALA:O	1:E:126:ARG:NH1	2.32	0.63
2:F:211:VAL:HG21	2:F:263:ALA:HB2	1.81	0.63
2:B:155:VAL:HG23	2:B:158:ILE:HB	1.82	0.62
1:A:157:ILE:HD13	1:A:171:LYS:HD2	1.81	0.62
1:C:545:ASP:OD1	1:C:548:ARG:NH2	2.33	0.61
2:F:443:PHE:HB2	2:F:464:LEU:HD11	1.80	0.61
2:B:308:MET:HE3	2:B:349:LEU:HD12	1.83	0.61
1:C:152:ILE:HG12	1:C:174:LEU:HD22	1.82	0.60
3:G:125:ILE:HG12	3:G:188:VAL:HG21	1.84	0.60
2:F:376:LEU:HD11	2:F:411:LYS:HG3	1.82	0.60
1:E:449:LYS:HG2	2:F:404:TYR:HD2	1.67	0.60
2:B:55:LEU:HG	2:B:93:VAL:HG22	1.83	0.60
2:B:403:LEU:HD11	2:B:461:ALA:HB1	1.84	0.60
1:A:163:GLU:OE1	1:A:170:HIS:ND1	2.34	0.60
1:E:116:LYS:HD3	2:F:142:TYR:HD2	1.67	0.60
1:A:61:ILE:HD12	1:A:371:LEU:HD11	1.84	0.59
1:C:376:ALA:HB2	1:C:382:ALA:HA	1.83	0.59
2:B:160:THR:HG21	2:B:443:PHE:HZ	1.67	0.59
2:B:160:THR:HG23	2:B:161:MET:HG3	1.83	0.59
2:B:34:VAL:HG13	1:C:45:MET:HE3	1.84	0.59
1:C:51:VAL:HA	1:C:85:VAL:HG13	1.84	0.59
1:C:242:ALA:HA	1:C:478:PHE:HZ	1.68	0.59
1:E:298:PRO:HA	1:E:312:MET:HG2	1.83	0.59
5:M:139:TYR:HB3	6:N:23:ALA:HB2	1.85	0.59
2:D:47:PRO:HG2	2:D:70:ILE:HD11	1.84	0.58
2:F:279:THR:HB	2:F:334:ILE:HD12	1.84	0.58
2:D:215:MET:SD	2:D:256:PRO:HG3	2.43	0.58
1:E:252:THR:HA	1:E:437:VAL:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:MET:HG2	1:C:551:ILE:HD11	1.85	0.58
2:D:147:PRO:HA	2:D:321:ARG:HD3	1.84	0.58
3:K:222:LEU:HD13	4:L:94:VAL:HG21	1.85	0.58
2:B:240:LEU:HD23	2:B:242:LEU:HD21	1.85	0.58
1:C:471:TYR:HE2	1:C:482:ARG:HH12	1.51	0.58
2:D:270:THR:HG21	2:D:272:ARG:HH21	1.68	0.58
1:E:286:ARG:HB2	1:E:289:GLU:HG2	1.86	0.58
1:E:210:THR:HG22	1:E:211:LEU:H	1.67	0.58
2:F:102:ILE:HD12	2:F:258:LEU:HD22	1.86	0.58
1:C:217:VAL:HG12	1:C:334:TYR:HB3	1.86	0.58
2:F:235:LEU:HA	2:F:238:THR:HG22	1.85	0.58
1:A:376:ALA:HB2	1:A:382:ALA:HA	1.86	0.57
1:A:81:VAL:HG23	2:B:70:ILE:HD12	1.87	0.57
1:A:152:ILE:HG12	1:A:174:LEU:HD22	1.86	0.57
1:A:517:VAL:HG11	1:A:554:HIS:HB2	1.85	0.57
2:B:183:ILE:HD11	2:B:372:PRO:HD2	1.85	0.57
3:K:114:ARG:HA	3:K:117:TYR:HB3	1.86	0.57
1:C:226:LYS:HD2	1:C:398:ALA:HB2	1.86	0.57
2:F:376:LEU:HB2	2:F:377:PRO:HD3	1.87	0.57
2:D:319:ALA:HB2	2:D:331:GLN:HE21	1.70	0.57
1:E:139:TRP:HB3	1:E:161:VAL:HG21	1.87	0.56
1:E:426:PRO:HA	1:E:429:THR:HG22	1.88	0.56
1:C:111:PRO:HD3	1:C:132:ALA:HA	1.88	0.56
1:E:81:VAL:HG23	2:F:70:ILE:HD12	1.87	0.56
2:B:153:THR:HG23	2:B:187:ILE:HG23	1.87	0.56
1:C:125:PRO:HG2	1:C:128:ILE:HB	1.86	0.56
7:O:47:ASP:HA	7:O:328:LYS:HA	1.88	0.56
2:F:308:MET:HE3	2:F:349:LEU:HD12	1.87	0.56
2:D:402:GLN:HE21	2:D:406:LYS:HG2	1.71	0.56
2:D:344:HIS:HB3	2:D:347:PRO:HD2	1.88	0.56
1:A:446:ALA:HA	1:A:451:PHE:HE2	1.71	0.56
1:A:49:VAL:HG21	1:A:70:ILE:HD13	1.87	0.56
2:B:212:PHE:HE2	2:B:214:ALA:HB2	1.71	0.55
2:F:376:LEU:HA	2:F:404:TYR:CE1	2.41	0.55
2:B:264:GLU:HA	2:B:329:ILE:HD11	1.88	0.55
1:A:239:VAL:HG23	1:A:526:LEU:HD22	1.88	0.55
1:E:243:LEU:HD11	1:E:485:MET:HE2	1.89	0.55
4:J:99:ILE:O	4:J:103:ILE:HG12	2.05	0.55
1:C:520:LEU:HG	1:C:550:PHE:HE1	1.72	0.55
2:D:149:GLU:HA	2:D:391:MET:HG2	1.89	0.55
3:I:222:LEU:HD13	4:J:94:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASN:HB2	2:B:355:GLU:OE1	2.07	0.55
2:B:53:VAL:N	2:B:65:GLY:O	2.37	0.55
1:E:104:ILE:HG12	1:E:294:LEU:HD22	1.88	0.55
2:B:147:PRO:HB3	2:B:167:GLY:H	1.72	0.55
2:B:129:GLU:OE1	2:B:265:TYR:OH	2.22	0.55
2:F:243:ASN:ND2	2:F:251:GLU:OE1	2.39	0.55
2:D:419:VAL:HG13	2:D:420:VAL:HG13	1.89	0.55
3:I:125:ILE:HG12	3:I:188:VAL:HG21	1.88	0.54
7:O:224:VAL:HA	7:O:234:PHE:HA	1.90	0.54
7:O:155:ALA:HB1	7:O:281:GLU:HA	1.90	0.54
1:E:517:VAL:HG11	1:E:554:HIS:HB2	1.89	0.54
3:K:121:LEU:HD22	3:K:148:LEU:HD22	1.89	0.54
1:C:249:GLY:H	1:C:411:SER:HB3	1.72	0.54
2:D:279:THR:HA	2:D:334:ILE:HB	1.89	0.54
2:F:186:GLN:O	2:F:190:GLN:HG2	2.08	0.54
2:F:466:ARG:HA	2:F:485:TYR:HE1	1.73	0.54
2:B:20:PHE:HE2	4:J:97:ILE:HG12	1.73	0.54
2:B:160:THR:HG21	2:B:443:PHE:CZ	2.43	0.54
2:B:41:LEU:HD11	2:B:93:VAL:HG11	1.91	0.53
2:F:153:THR:HG21	2:F:164:ILE:HD12	1.90	0.53
1:C:294:LEU:HD21	1:C:319:ALA:HB2	1.91	0.53
5:M:42:ARG:NH1	5:M:101:VAL:HG22	2.23	0.53
2:B:161:MET:HE1	2:B:375:VAL:HG11	1.90	0.53
6:N:95:PRO:HG3	6:N:101:TYR:HB3	1.90	0.53
1:A:98:PRO:HB3	1:A:161:VAL:HG21	1.90	0.53
3:K:121:LEU:HD21	3:K:149:ILE:HG12	1.89	0.53
2:B:111:ARG:HH11	2:B:111:ARG:HG2	1.74	0.53
2:B:319:ALA:HB2	2:B:331:GLN:HG3	1.91	0.53
1:E:170:HIS:CE1	1:E:346:GLN:HE22	2.26	0.53
1:E:217:VAL:HB	1:E:334:TYR:HB3	1.90	0.53
2:D:214:ALA:HA	2:D:279:THR:HB	1.91	0.53
2:D:153:THR:HG22	2:D:155:VAL:H	1.75	0.52
2:B:387:ILE:HG23	2:B:396:HIS:HB3	1.90	0.52
2:D:253:ILE:HG13	2:D:287:ALA:HB1	1.91	0.52
2:F:346:ILE:HB	2:F:347:PRO:HD3	1.90	0.52
1:A:232:PRO:HA	1:A:247:VAL:HA	1.92	0.52
2:D:105:SER:O	2:D:108:MET:HG2	2.09	0.52
2:D:439:PHE:HA	2:D:464:LEU:HD21	1.92	0.52
2:B:302:ARG:HB3	2:B:345:PRO:HG2	1.92	0.52
2:B:417:LYS:HB2	2:B:425:LEU:HD11	1.91	0.52
2:D:278:LEU:O	2:D:334:ILE:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:SER:O	2:B:238:THR:HG23	2.09	0.52
3:I:121:LEU:HD11	3:I:188:VAL:HG13	1.90	0.52
1:C:43:CYS:HB3	1:C:87:ARG:HD3	1.92	0.51
2:B:105:SER:O	2:B:108:MET:HG3	2.10	0.51
2:F:309:TYR:HB2	2:F:349:LEU:HD13	1.91	0.51
2:B:263:ALA:HB1	2:B:274:VAL:HG11	1.93	0.51
2:D:266:LEU:O	2:D:272:ARG:HG2	2.11	0.51
2:B:20:PHE:CE2	4:J:97:ILE:HG12	2.46	0.51
3:G:76:THR:HA	3:G:79:THR:HG22	1.93	0.51
1:A:358:SER:HB2	1:A:417:SER:H	1.75	0.51
2:B:275:LEU:HD11	2:B:332:ILE:HD11	1.93	0.51
2:B:156:SER:OG	2:B:452:ARG:NE	2.32	0.51
1:C:233:LEU:N	1:C:246:CYS:O	2.37	0.51
2:B:111:ARG:HH12	3:I:86:LEU:HD11	1.75	0.51
1:C:281:VAL:HG23	1:C:354:ALA:HA	1.93	0.51
2:D:346:ILE:HB	2:D:347:PRO:HD3	1.94	0.50
2:F:183:ILE:HD11	2:F:372:PRO:HD2	1.93	0.50
5:M:181:THR:O	5:M:185:ILE:HG12	2.11	0.50
1:E:223:VAL:HG12	1:E:344:ARG:NH1	2.22	0.50
1:E:310:PRO:HD2	1:E:313:LYS:HD2	1.92	0.50
3:I:111:ALA:O	3:I:144:ARG:NH2	2.43	0.50
2:D:35:ASN:HA	1:E:62:ARG:HG3	1.92	0.50
2:B:438:LYS:NZ	2:B:467:ILE:HD11	2.27	0.50
1:E:111:PRO:HD3	1:E:132:ALA:HA	1.94	0.50
3:I:192:ASN:HB2	3:I:197:ILE:HB	1.93	0.50
2:B:127:PHE:HE1	3:I:96:LEU:HD22	1.75	0.50
1:A:375:PRO:HD2	5:M:202:ARG:HG2	1.94	0.50
2:B:175:ALA:HB3	2:B:178:LEU:HG	1.92	0.50
1:E:62:ARG:O	1:E:69:THR:N	2.41	0.50
2:F:150:MET:HB2	2:F:386:ALA:HB1	1.93	0.50
1:A:365:ARG:HD3	2:B:306:GLY:HA3	1.93	0.50
1:E:112:LEU:HD13	2:F:141:PRO:HD2	1.94	0.50
3:G:121:LEU:HD11	3:G:188:VAL:HG13	1.93	0.50
2:D:187:ILE:O	2:D:191:ALA:HB2	2.11	0.49
1:E:288:ASN:HD22	2:F:355:GLU:CD	2.15	0.49
2:D:175:ALA:HB3	2:D:178:LEU:HG	1.94	0.49
1:E:344:ARG:NH1	1:E:345:ASP:OD1	2.44	0.49
1:C:282:GLY:O	1:C:284:GLY:N	2.45	0.49
2:D:253:ILE:O	2:D:256:PRO:HD2	2.11	0.49
2:D:316:TYR:O	2:D:331:GLN:NE2	2.45	0.49
1:C:27:ILE:HD11	1:C:51:VAL:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:125:ILE:HG21	3:I:156:ILE:HD13	1.93	0.49
1:C:356:SER:H	1:C:415:ALA:HB3	1.78	0.49
1:E:217:VAL:HG12	1:E:338:THR:HG21	1.94	0.49
1:E:365:ARG:HA	1:E:381:PRO:HD3	1.95	0.49
3:G:99:ILE:HD13	4:H:91:LYS:HZ3	1.78	0.49
5:M:42:ARG:HH11	5:M:101:VAL:HG22	1.76	0.49
1:A:321:THR:OG1	1:A:324:MET:HG3	2.13	0.49
1:E:52:GLY:HA2	1:E:83:ASP:HB3	1.95	0.49
1:A:166:LEU:HD23	1:A:314:ARG:HB3	1.94	0.49
1:A:485:MET:HG3	1:A:551:ILE:HD11	1.95	0.49
2:B:443:PHE:HB2	2:B:464:LEU:HD11	1.95	0.49
1:E:72:VAL:HG21	1:E:76:THR:HB	1.95	0.49
1:A:266:SER:HB3	1:A:353:ILE:HG21	1.95	0.48
2:D:150:MET:HB2	2:D:386:ALA:HB1	1.94	0.48
3:G:191:SER:HA	3:G:198:GLU:HA	1.95	0.48
2:D:52:ILE:O	2:D:96:THR:OG1	2.20	0.48
5:M:29:TYR:HB2	5:M:173:ILE:HG21	1.94	0.48
1:A:270:SER:HA	1:A:278:ILE:HD13	1.94	0.48
2:B:81:GLU:HG3	2:B:248:PRO:HG2	1.95	0.48
1:E:30:VAL:HG13	1:E:35:VAL:HG22	1.94	0.48
1:C:103:THR:HG23	1:C:105:TYR:CE2	2.49	0.48
1:C:28:TYR:OH	2:D:71:ARG:NH2	2.46	0.48
1:A:330:GLU:HG3	1:A:360:TRP:NE1	2.28	0.48
3:I:145:ASP:O	3:I:149:ILE:HG12	2.13	0.48
3:G:206:ARG:NH2	4:H:105:PRO:HB3	2.28	0.48
2:F:305:PRO:HG2	2:F:308:MET:HB2	1.96	0.48
1:E:399:VAL:HG22	1:E:407:THR:HG22	1.96	0.47
1:C:344:ARG:HG3	1:C:409:SER:N	2.28	0.47
1:E:581:VAL:HG12	1:E:603:LEU:HD21	1.96	0.47
3:K:191:SER:HA	3:K:198:GLU:HA	1.95	0.47
1:A:270:SER:HB3	1:A:353:ILE:HD12	1.96	0.47
2:D:173:PHE:N	2:D:358:ILE:O	2.47	0.47
1:E:485:MET:SD	1:E:547:MET:HG3	2.53	0.47
1:E:525:PHE:HD2	1:E:526:LEU:HD12	1.78	0.47
3:I:192:ASN:N	3:I:197:ILE:O	2.41	0.47
7:O:169:ASP:O	7:O:173:ARG:N	2.45	0.47
1:C:171:LYS:HB2	1:C:346:GLN:HG2	1.95	0.47
1:E:477:GLU:O	1:E:481:LEU:HD13	2.14	0.47
1:C:333:ILE:HG12	1:C:360:TRP:CD1	2.50	0.47
2:D:127:PHE:HE1	3:K:96:LEU:HD22	1.79	0.47
2:F:211:VAL:HG23	2:F:276:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:VAL:HG12	1:C:318:VAL:HB	1.96	0.47
2:F:178:LEU:HD13	2:F:360:VAL:HG12	1.97	0.47
2:F:402:GLN:OE1	2:F:475:ARG:HB2	2.15	0.47
3:G:120:ILE:HD12	4:H:104:LYS:H	1.79	0.47
1:A:269:LEU:HD22	1:A:353:ILE:HD11	1.97	0.47
1:C:297:PHE:HD2	1:C:317:LEU:HD11	1.79	0.47
1:A:278:ILE:HB	1:A:315:THR:HG22	1.97	0.47
1:E:233:LEU:N	1:E:246:CYS:O	2.41	0.46
1:A:33:PRO:HD2	1:A:370:ARG:HG3	1.97	0.46
2:D:403:LEU:HD11	2:D:461:ALA:HB1	1.96	0.46
1:E:232:PRO:HG3	1:E:470:PHE:CE2	2.50	0.46
1:A:193:LEU:HD23	1:A:212:TYR:HB3	1.97	0.46
1:A:264:VAL:HG11	9:A:701:ADP:C5	2.50	0.46
2:B:34:VAL:HG22	1:C:45:MET:CE	2.45	0.46
2:D:213:ALA:HB3	2:D:278:LEU:HD23	1.97	0.46
1:E:320:ASN:ND2	1:E:329:ARG:HA	2.30	0.46
8:P:49:SER:HA	8:P:53:LYS:HA	1.96	0.46
2:B:335:LEU:HD11	2:B:346:ILE:HG22	1.97	0.46
1:C:288:ASN:HD22	2:D:147:PRO:HD3	1.81	0.46
3:K:215:LEU:HA	3:K:218:ILE:HG22	1.97	0.46
1:A:107:GLY:HA2	1:A:332:SER:HB3	1.97	0.46
1:E:63:ILE:HA	1:E:68:ALA:HA	1.98	0.46
2:F:114:ASP:HA	2:F:120:ILE:HD11	1.98	0.46
1:A:56:LEU:HD21	1:A:126:ARG:HB3	1.98	0.46
2:F:171:PRO:HB3	2:F:333:PRO:HG2	1.97	0.46
1:C:284:GLY:HA2	1:C:329:ARG:HD2	1.97	0.46
1:E:43:CYS:SG	1:E:60:VAL:HG21	2.56	0.46
1:C:101:MET:HA	1:C:316:THR:HG22	1.97	0.46
2:F:174:SER:O	2:F:336:THR:HA	2.16	0.46
2:F:215:MET:CE	2:F:256:PRO:HB3	2.46	0.46
1:C:32:GLY:O	1:C:76:THR:HG21	2.16	0.45
1:E:49:VAL:HG12	1:E:87:ARG:HA	1.96	0.45
3:I:106:LYS:HD3	4:J:99:ILE:HG13	1.97	0.45
4:L:103:ILE:O	4:L:105:PRO:HD3	2.16	0.45
1:A:344:ARG:HG3	1:A:409:SER:N	2.31	0.45
2:B:34:VAL:HG22	1:C:45:MET:HE3	1.97	0.45
2:B:110:GLY:HA2	2:B:235:LEU:O	2.16	0.45
1:C:281:VAL:HG11	1:C:336:GLY:HA3	1.98	0.45
7:O:196:VAL:HA	7:O:257:PRO:HA	1.97	0.45
2:B:269:GLN:O	3:I:230:LYS:N	2.49	0.45
2:F:257:ARG:NH1	2:F:315:ILE:HD11	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:80:LEU:O	4:L:83:ILE:HG22	2.16	0.45
1:A:395:ALA:HB2	1:A:412:ILE:HG13	1.98	0.45
2:D:416:MET:O	2:D:420:VAL:HG22	2.17	0.45
2:B:58:PRO:HD3	2:B:91:THR:HG22	1.98	0.45
2:D:53:VAL:N	2:D:65:GLY:O	2.37	0.45
3:K:124:LEU:HD23	4:L:105:PRO:HG3	1.98	0.45
2:F:57:LEU:HD12	2:F:61:THR:OG1	2.17	0.45
2:F:168:GLN:HB2	2:F:382:LEU:HD12	1.98	0.45
1:A:109:GLN:HG2	1:A:132:ALA:HB1	1.99	0.45
2:B:127:PHE:HD2	3:I:219:ARG:HD2	1.82	0.45
2:B:178:LEU:HD13	2:B:360:VAL:HG12	1.99	0.45
3:G:139:VAL:HG21	3:G:172:ILE:HD11	1.99	0.45
1:C:291:ALA:HB2	2:D:144:ARG:HB3	1.98	0.45
2:F:403:LEU:HD11	2:F:461:ALA:HB1	1.97	0.45
1:A:330:GLU:HG3	1:A:360:TRP:HE1	1.81	0.45
1:A:446:ALA:HA	1:A:451:PHE:CE2	2.50	0.45
1:C:238:ARG:NH1	1:C:538:CYS:SG	2.90	0.45
2:D:111:ARG:NH2	2:D:124:PRO:O	2.44	0.45
1:A:141:PHE:CE1	1:A:159:GLY:HA3	2.52	0.44
3:K:107:LEU:HD12	3:K:207:LEU:HD22	1.99	0.44
5:M:60:VAL:HA	5:M:63:THR:HG22	1.98	0.44
2:F:27:ASN:HB2	3:G:198:GLU:HG2	2.00	0.44
2:B:168:GLN:NE2	2:B:382:LEU:HB2	2.33	0.44
1:C:267:GLN:O	1:C:271:LYS:HG2	2.18	0.44
1:E:43:CYS:HB3	1:E:63:ILE:HD12	1.99	0.44
2:D:127:PHE:CE2	3:K:219:ARG:HG3	2.52	0.44
1:A:378:GLN:HB3	1:A:426:PRO:HG2	2.00	0.44
1:C:477:GLU:O	1:C:481:LEU:HD23	2.17	0.44
1:A:197:ILE:HG13	1:A:211:LEU:HG	2.00	0.44
1:C:62:ARG:HG2	1:C:69:THR:HB	1.99	0.44
1:A:495:LEU:HB3	1:A:515:LEU:HD21	1.99	0.44
1:E:232:PRO:HB3	1:E:467:LEU:HD21	2.00	0.44
1:A:358:SER:O	1:A:362:GLU:HG3	2.18	0.44
1:E:288:ASN:ND2	2:F:355:GLU:OE2	2.50	0.44
3:G:106:LYS:HE2	3:G:106:LYS:HB2	1.79	0.44
1:E:378:GLN:HB3	1:E:426:PRO:HG3	2.00	0.43
3:I:130:LEU:HD22	3:I:164:ALA:HB2	1.99	0.43
5:M:104:VAL:HG21	5:M:162:VAL:HG21	1.99	0.43
2:B:281:MET:HG2	2:B:316:TYR:OH	2.17	0.43
1:C:224:THR:HB	1:C:399:VAL:HG13	1.98	0.43
2:B:156:SER:O	2:B:160:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:LEU:HD21	2:B:362:ARG:HE	1.82	0.43
1:E:266:SER:HA	1:E:353:ILE:HD13	2.01	0.43
1:A:56:LEU:HD22	1:A:74:GLU:CB	2.48	0.43
2:B:51:GLU:O	2:B:53:VAL:HG23	2.18	0.43
2:D:55:LEU:CD2	2:D:93:VAL:HG22	2.47	0.43
2:D:253:ILE:HD11	2:D:288:LEU:HA	2.01	0.43
1:C:297:PHE:CD2	1:C:317:LEU:HD21	2.53	0.43
2:D:293:ALA:HB3	1:E:382:ALA:HB2	2.00	0.43
1:A:238:ARG:O	1:A:242:ALA:HB3	2.18	0.43
2:B:209:SER:O	2:B:274:VAL:HA	2.18	0.43
3:K:215:LEU:O	3:K:218:ILE:HG22	2.19	0.43
1:A:220:PRO:HB3	1:A:394:ARG:HD2	2.00	0.43
2:D:22:VAL:CG2	3:K:210:LEU:HD12	2.49	0.43
2:D:67:VAL:HA	2:D:77:VAL:HA	2.01	0.43
1:E:302:THR:HG21	1:E:314:ARG:NH1	2.33	0.43
2:F:277:ILE:HD13	2:F:332:ILE:HB	2.01	0.43
3:I:143:GLU:HA	3:I:178:TYR:CD2	2.53	0.43
2:D:108:MET:HE3	2:D:262:THR:HG23	2.00	0.43
2:D:250:ILE:HD12	2:D:250:ILE:H	1.83	0.43
1:E:484:ARG:O	1:E:488:ILE:HG12	2.19	0.43
3:K:192:ASN:N	3:K:197:ILE:O	2.48	0.43
2:B:212:PHE:CE2	2:B:214:ALA:HB2	2.52	0.43
1:C:100:LEU:HD12	1:C:316:THR:HG21	2.00	0.43
1:C:471:TYR:CD2	1:C:479:PRO:HG3	2.54	0.43
2:D:28:TYR:CE1	2:D:44:VAL:HA	2.53	0.43
2:D:160:THR:O	2:D:396:HIS:NE2	2.48	0.43
2:D:335:LEU:HD11	2:D:346:ILE:HG22	2.01	0.43
1:E:160:SER:HA	1:E:171:LYS:HA	2.00	0.43
1:E:290:MET:O	1:E:294:LEU:HG	2.19	0.43
1:C:337:ILE:HB	1:C:391:PHE:HE1	1.84	0.43
1:C:528:GLN:HE21	1:C:536:ALA:HA	1.83	0.43
1:E:176:PRO:HG2	1:E:215:TRP:CZ3	2.53	0.43
2:F:302:ARG:HH11	2:F:302:ARG:HG2	1.84	0.42
1:A:115:ILE:HG12	1:A:128:ILE:HG21	2.01	0.42
2:B:127:PHE:CD2	3:I:219:ARG:HD2	2.55	0.42
2:D:102:ILE:CG2	2:D:258:LEU:HD22	2.49	0.42
4:H:79:GLU:O	4:H:83:ILE:HG12	2.19	0.42
3:I:218:ILE:HD11	4:J:98:LEU:HD21	2.01	0.42
2:B:163:SER:O	2:B:380:SER:OG	2.21	0.42
1:C:138:LYS:HB3	1:C:190:GLU:CG	2.49	0.42
1:E:439:TRP:HB3	1:E:454:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:405:LYS:O	8:P:409:GLY:N	2.52	0.42
1:A:388:LEU:O	1:A:392:TYR:HD2	2.03	0.42
1:A:364:LEU:HD11	1:A:387:LYS:HD3	2.01	0.42
2:D:38:LEU:HD23	2:D:76:ILE:CG2	2.49	0.42
2:F:253:ILE:HA	2:F:284:TYR:HE1	1.85	0.42
3:G:99:ILE:HD13	4:H:91:LYS:NZ	2.34	0.42
3:K:106:LYS:O	3:K:110:ILE:N	2.48	0.42
5:M:42:ARG:HH12	5:M:102:SER:CB	2.32	0.42
1:A:233:LEU:N	1:A:246:CYS:O	2.48	0.42
2:D:64:GLN:HB3	2:D:80:PHE:CD2	2.55	0.42
1:E:302:THR:HG21	1:E:314:ARG:HH12	1.85	0.42
2:F:215:MET:HB2	2:F:279:THR:O	2.20	0.42
1:A:95:GLU:OE1	1:A:135:ARG:NH2	2.51	0.42
1:E:92:LEU:HD23	1:E:217:VAL:HG21	2.01	0.42
1:E:445:LEU:HD12	1:E:450:HIS:ND1	2.34	0.42
6:N:10:VAL:HA	6:N:68:LEU:HB2	2.02	0.42
1:A:35:VAL:N	1:A:70:ILE:O	2.47	0.42
1:A:485:MET:HB3	1:A:485:MET:HE2	1.71	0.42
1:C:135:ARG:O	1:C:192:THR:OG1	2.37	0.42
1:C:320:ASN:HD21	1:C:329:ARG:HA	1.83	0.42
1:E:35:VAL:N	1:E:70:ILE:O	2.51	0.42
3:I:169:LEU:HD23	3:I:172:ILE:HB	2.01	0.42
3:K:143:GLU:HA	3:K:178:TYR:CE1	2.55	0.42
1:A:196:LYS:HA	1:A:210:THR:HG22	2.01	0.42
2:D:102:ILE:HG21	2:D:258:LEU:HD22	2.01	0.42
1:E:98:PRO:HG2	1:E:193:LEU:HD21	2.02	0.42
1:E:283:CYS:SG	1:E:333:ILE:HG12	2.60	0.42
8:P:372:PRO:N	8:P:373:PRO:HD2	2.35	0.42
1:A:255:PRO:HG2	1:A:438:PHE:HE1	1.84	0.42
2:B:193:LEU:HD23	2:B:196:PRO:HA	2.00	0.42
1:C:320:ASN:ND2	1:C:329:ARG:HA	2.35	0.41
1:E:32:GLY:O	1:E:76:THR:HG21	2.20	0.41
1:E:182:ILE:O	1:E:182:ILE:HG13	2.20	0.41
2:F:43:LYS:HB3	2:F:43:LYS:HE3	1.84	0.41
3:G:130:LEU:HD11	3:G:163:LYS:HD2	2.02	0.41
5:M:152:LEU:HD23	5:M:152:LEU:HA	1.90	0.41
7:O:302:ASN:O	7:O:306:ILE:HG12	2.20	0.41
1:A:329:ARG:HD2	1:A:363:ALA:HB2	2.02	0.41
1:A:451:PHE:CD1	9:A:701:ADP:C4	3.08	0.41
1:E:485:MET:HE2	1:E:485:MET:HB3	1.93	0.41
2:F:152:SER:N	2:F:192:GLY:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PHE:O	1:A:589:PRO:HG3	2.20	0.41
2:F:150:MET:SD	2:F:163:SER:HB2	2.61	0.41
2:F:214:ALA:HB1	2:F:217:VAL:HG22	2.03	0.41
1:A:320:ASN:HA	1:A:324:MET:HE3	2.03	0.41
1:A:335:THR:O	1:A:339:LEU:HG	2.21	0.41
2:B:27:ASN:HB2	3:I:198:GLU:HG2	2.01	0.41
2:D:127:PHE:CE1	3:K:96:LEU:HD22	2.55	0.41
1:E:334:TYR:HA	1:E:337:ILE:HG22	2.02	0.41
1:E:499:VAL:HG13	1:E:504:LYS:CB	2.51	0.41
1:E:546:MET:HG3	1:E:600:PHE:CZ	2.56	0.41
2:F:334:ILE:H	2:F:334:ILE:HG13	1.74	0.41
1:C:104:ILE:HD12	1:C:294:LEU:HD22	2.02	0.41
2:D:376:LEU:HA	2:D:404:TYR:CE2	2.55	0.41
2:F:331:GLN:HG2	2:F:333:PRO:HD3	2.02	0.41
6:N:5:ARG:O	6:N:65:ALA:HB2	2.19	0.41
2:B:111:ARG:NH1	3:I:86:LEU:HD11	2.36	0.41
1:E:240:LEU:HD21	1:E:454:ILE:HG13	2.02	0.41
2:F:279:THR:HA	2:F:334:ILE:HB	2.02	0.41
3:K:169:LEU:HD23	3:K:172:ILE:HB	2.02	0.41
8:P:313:LEU:HA	8:P:318:ALA:HB3	2.03	0.41
1:A:255:PRO:HA	1:A:416:VAL:O	2.20	0.41
2:B:416:MET:O	2:B:420:VAL:HG22	2.21	0.41
1:C:110:ARG:HB2	1:C:115:ILE:HD11	2.03	0.41
2:D:153:THR:HG23	2:D:187:ILE:HG12	2.03	0.41
2:D:161:MET:CE	2:D:403:LEU:HB3	2.47	0.41
2:F:145:ILE:HD11	2:F:323:GLU:HA	2.02	0.41
1:A:174:LEU:HG	1:A:175:PRO:HD2	2.02	0.41
2:B:156:SER:HB2	2:B:452:ARG:HH21	1.86	0.41
2:B:401:ASN:HB3	2:B:475:ARG:HH11	1.84	0.41
1:C:100:LEU:HD11	1:C:343:PHE:CZ	2.56	0.41
1:E:100:LEU:HD13	1:E:339:LEU:HD22	2.03	0.41
1:E:525:PHE:HB2	1:E:550:PHE:CE2	2.56	0.41
2:F:393:ARG:HG3	2:F:395:ASP:H	1.86	0.41
3:G:169:LEU:HD23	3:G:172:ILE:HB	2.03	0.41
4:H:99:ILE:O	4:H:103:ILE:HG12	2.20	0.41
3:K:86:LEU:HD23	3:K:86:LEU:HA	1.89	0.41
2:D:104:VAL:HG21	2:D:132:LEU:HD13	2.03	0.41
2:F:52:ILE:O	2:F:96:THR:OG1	2.23	0.41
2:F:104:VAL:HA	2:F:108:MET:HE3	2.03	0.41
6:N:20:LEU:HD12	6:N:25:ILE:HG21	2.02	0.41
1:C:30:VAL:O	2:D:70:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:CYS:SG	1:C:416:VAL:HB	2.61	0.40
1:C:286:ARG:HD3	2:D:355:GLU:HG2	2.03	0.40
2:F:190:GLN:OE1	2:F:451:ASP:HA	2.21	0.40
2:F:474:ASN:OD1	2:F:474:ASN:N	2.55	0.40
3:K:199:ILE:HG22	3:K:201:ASN:HB2	2.03	0.40
1:A:279:ILE:HB	1:A:352:MET:HG2	2.01	0.40
1:A:499:VAL:HG21	1:A:507:LEU:HD11	2.03	0.40
1:A:558:GLN:O	1:A:561:VAL:HG12	2.21	0.40
2:D:315:ILE:HD13	2:D:315:ILE:HA	1.94	0.40
2:D:395:ASP:O	2:D:399:VAL:HG23	2.22	0.40
2:F:110:GLY:HA2	2:F:235:LEU:O	2.21	0.40
1:A:217:VAL:HB	1:A:334:TYR:HB3	2.03	0.40
1:A:262:LYS:HB3	1:A:415:ALA:HB1	2.04	0.40
2:B:81:GLU:HA	2:B:248:PRO:HB3	2.04	0.40
2:D:257:ARG:NH1	2:D:315:ILE:HD11	2.37	0.40
2:F:369:ILE:HG23	2:F:445:THR:OG1	2.22	0.40
1:A:296:GLU:O	1:A:300:LEU:HG	2.21	0.40
1:E:33:PRO:O	1:E:72:VAL:HG22	2.20	0.40
3:K:123:SER:HA	3:K:126:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	591/639 (92%)	561 (95%)	30 (5%)	0	100	100
1	C	590/639 (92%)	559 (95%)	31 (5%)	0	100	100
1	E	570/639 (89%)	542 (95%)	28 (5%)	0	100	100
2	B	460/517 (89%)	434 (94%)	26 (6%)	0	100	100
2	D	455/517 (88%)	429 (94%)	26 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	455/517 (88%)	439 (96%)	16 (4%)	0	100	100
3	G	218/233 (94%)	215 (99%)	3 (1%)	0	100	100
3	I	218/233 (94%)	215 (99%)	3 (1%)	0	100	100
3	K	210/233 (90%)	205 (98%)	5 (2%)	0	100	100
4	H	107/114 (94%)	104 (97%)	3 (3%)	0	100	100
4	J	106/114 (93%)	104 (98%)	2 (2%)	0	100	100
4	L	97/114 (85%)	97 (100%)	0	0	100	100
5	M	212/256 (83%)	208 (98%)	4 (2%)	0	100	100
6	N	109/118 (92%)	105 (96%)	4 (4%)	0	100	100
7	O	355/392 (91%)	345 (97%)	10 (3%)	0	100	100
8	P	435/478 (91%)	430 (99%)	5 (1%)	0	100	100
All	All	5188/5753 (90%)	4992 (96%)	196 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	356/537 (66%)	356 (100%)	0	100	100
1	C	306/537 (57%)	305 (100%)	1 (0%)	92	97
1	E	331/537 (62%)	331 (100%)	0	100	100
2	B	313/444 (70%)	313 (100%)	0	100	100
2	D	282/444 (64%)	282 (100%)	0	100	100
2	F	289/444 (65%)	289 (100%)	0	100	100
3	G	74/208 (36%)	74 (100%)	0	100	100
3	I	67/208 (32%)	67 (100%)	0	100	100
3	K	68/208 (33%)	68 (100%)	0	100	100
4	H	13/94 (14%)	13 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	13/94 (14%)	13 (100%)	0	100	100
4	L	12/94 (13%)	12 (100%)	0	100	100
5	M	76/221 (34%)	76 (100%)	0	100	100
6	N	17/104 (16%)	17 (100%)	0	100	100
7	O	26/348 (8%)	26 (100%)	0	100	100
8	P	9/439 (2%)	9 (100%)	0	100	100
All	All	2252/4961 (45%)	2251 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	323	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	344	HIS
2	D	331	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 monosaccharides 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
9	ADP	A	701	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)

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
9	ADP	A	701	-	-	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)
9	A	701	ADP	C5-C4	2.36	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	701	ADP	PA-O3A-PB	-3.92	119.37	132.83
9	A	701	ADP	N3-C2-N1	-3.03	123.95	128.68
9	A	701	ADP	C3'-C2'-C1'	2.72	105.07	100.98
9	A	701	ADP	C4-C5-N7	-2.51	106.78	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

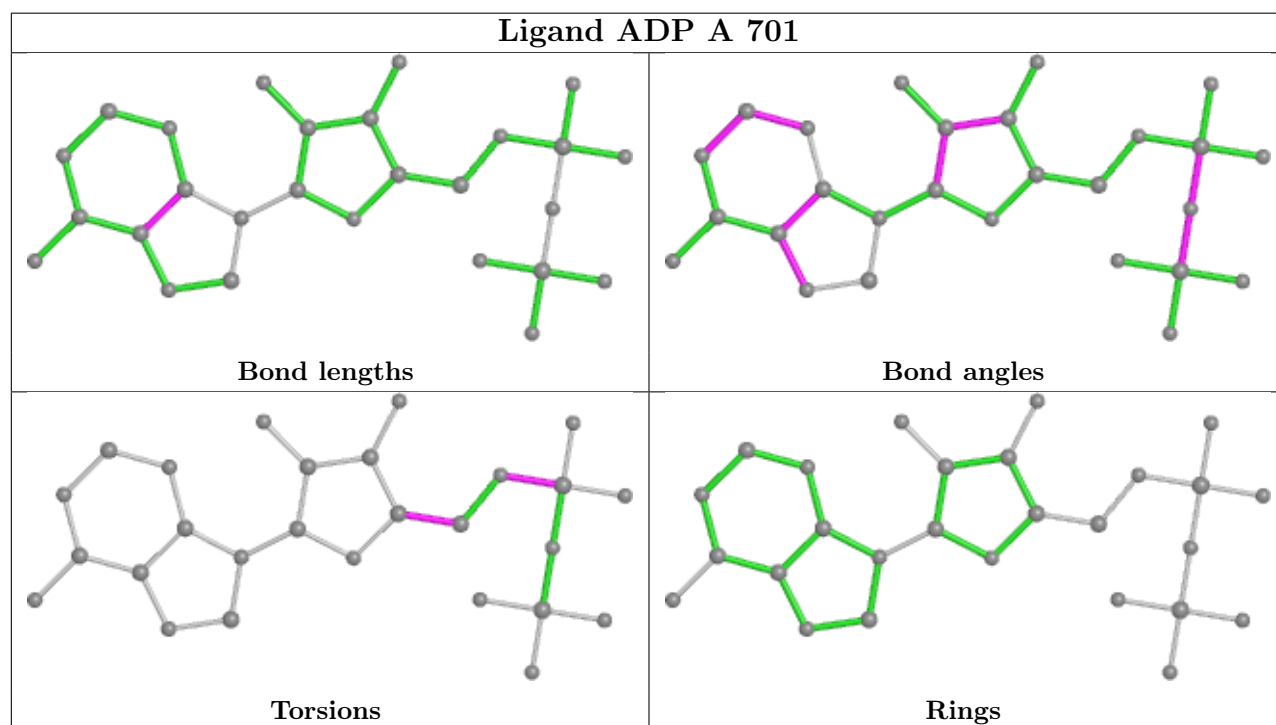
Mol	Chain	Res	Type	Atoms
9	A	701	ADP	C5'-O5'-PA-O3A
9	A	701	ADP	C5'-O5'-PA-O1A
9	A	701	ADP	C3'-C4'-C5'-O5'
9	A	701	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	701	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 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.

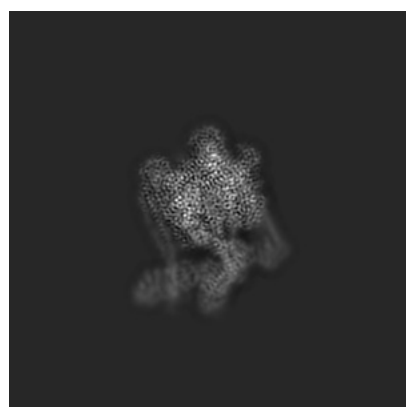
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25996. These allow visual inspection of the internal detail of the map and identification of artifacts.

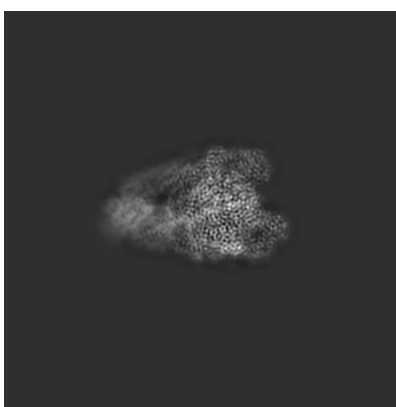
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

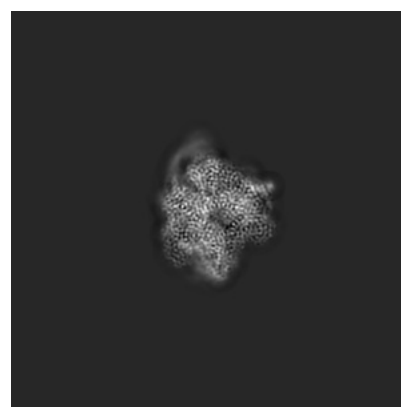
#### 6.1.1 Primary map



X



Y

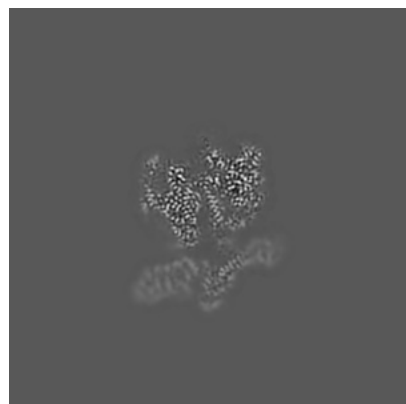


Z

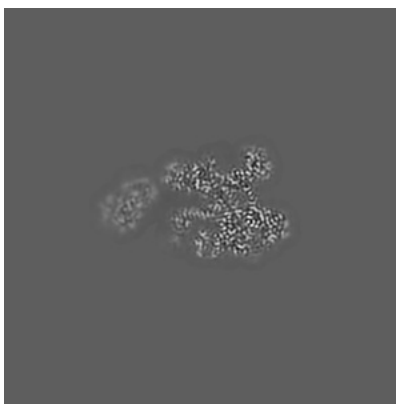
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

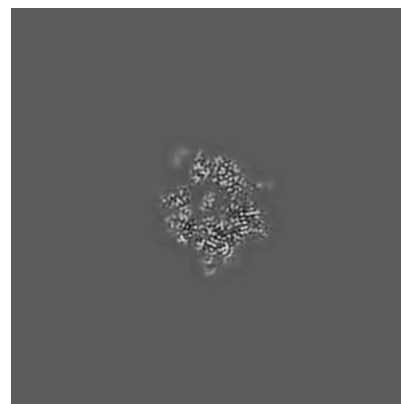
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

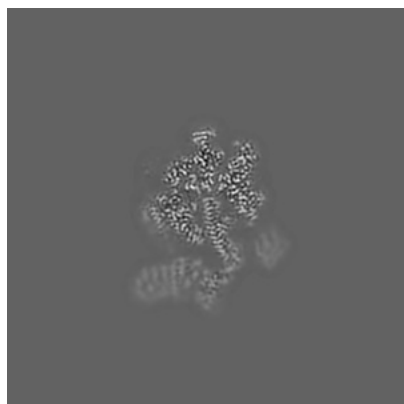


Z Index: 200

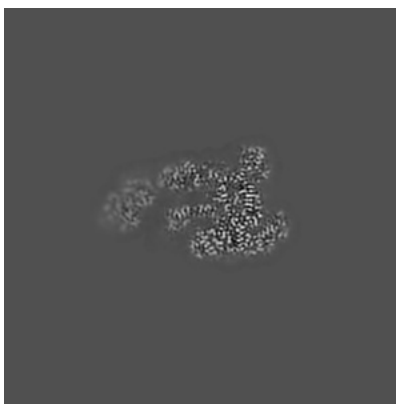
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

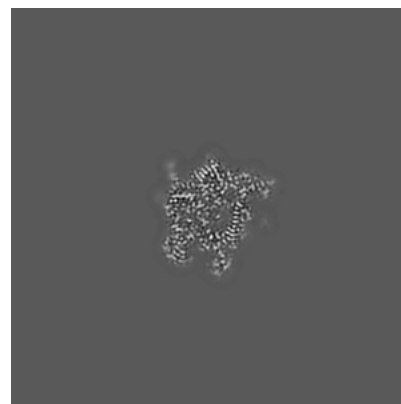
### 6.3.1 Primary map



X Index: 193



Y Index: 205

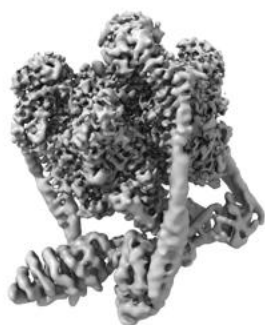


Z Index: 231

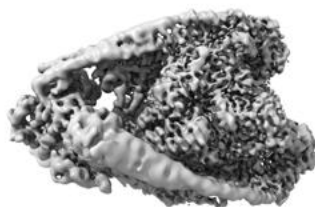
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

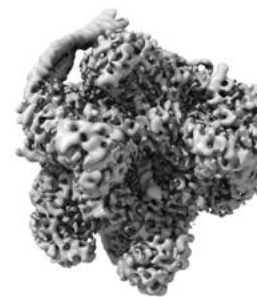
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

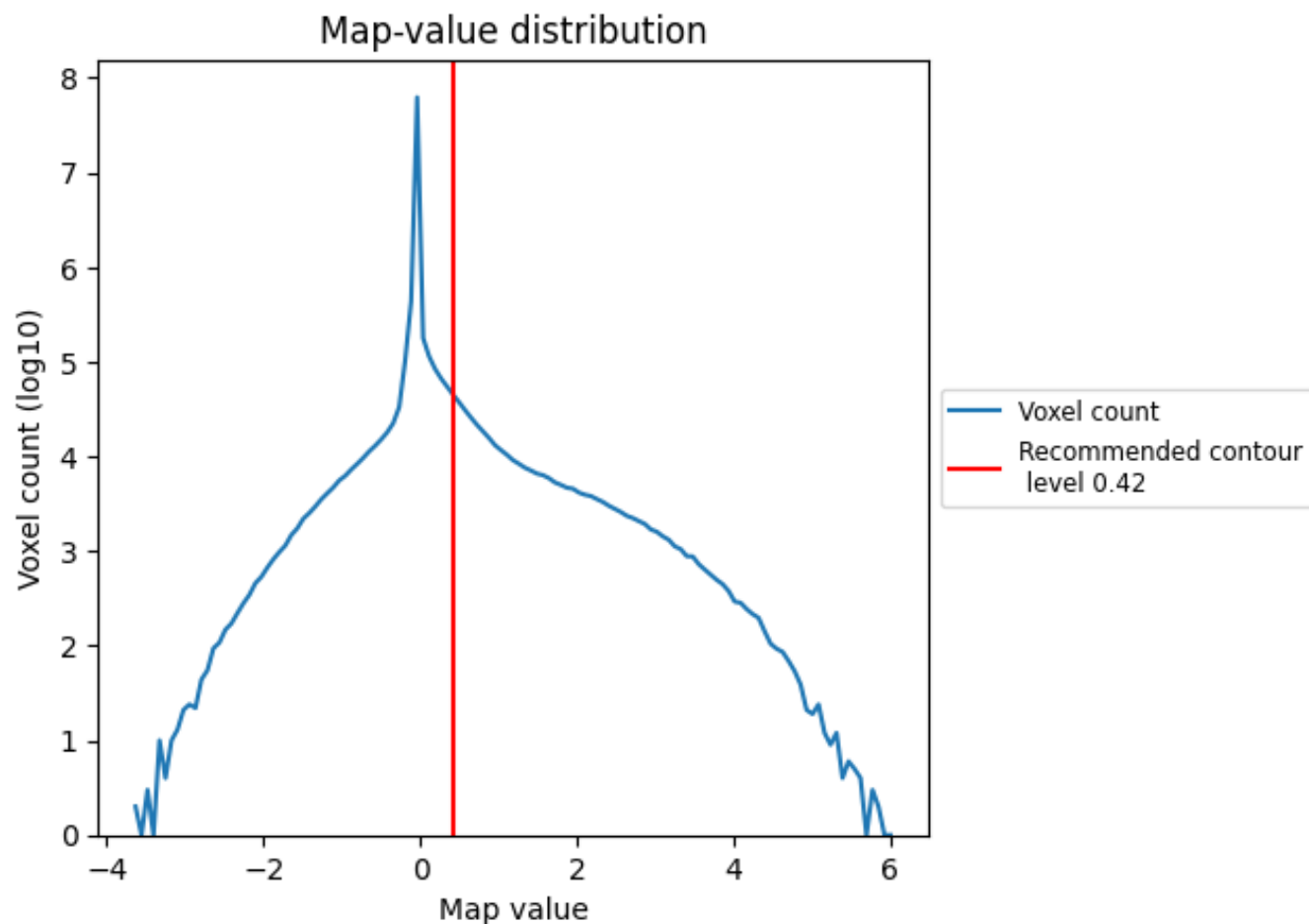
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

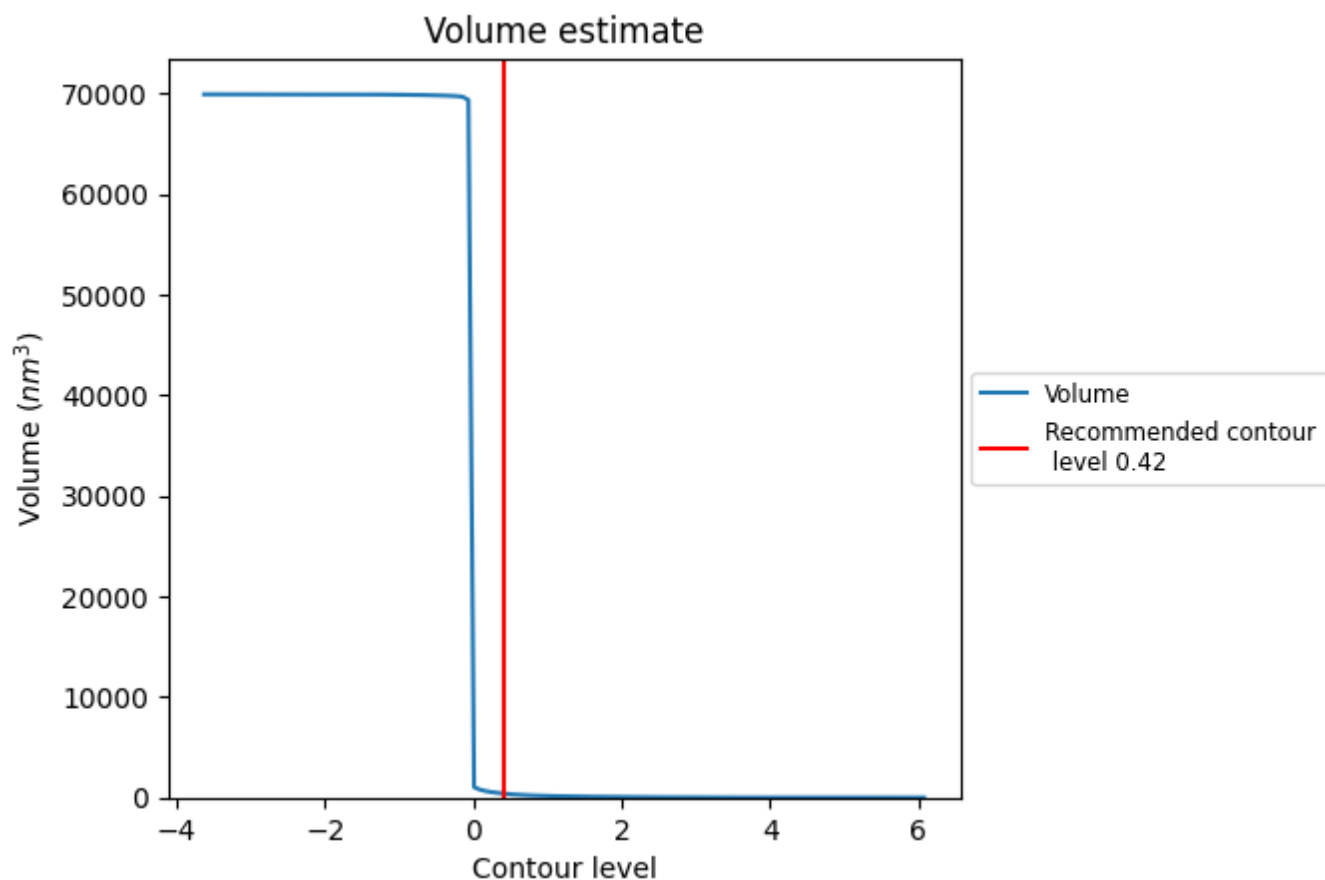
This section contains the results of statistical analysis of the map.

### 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.

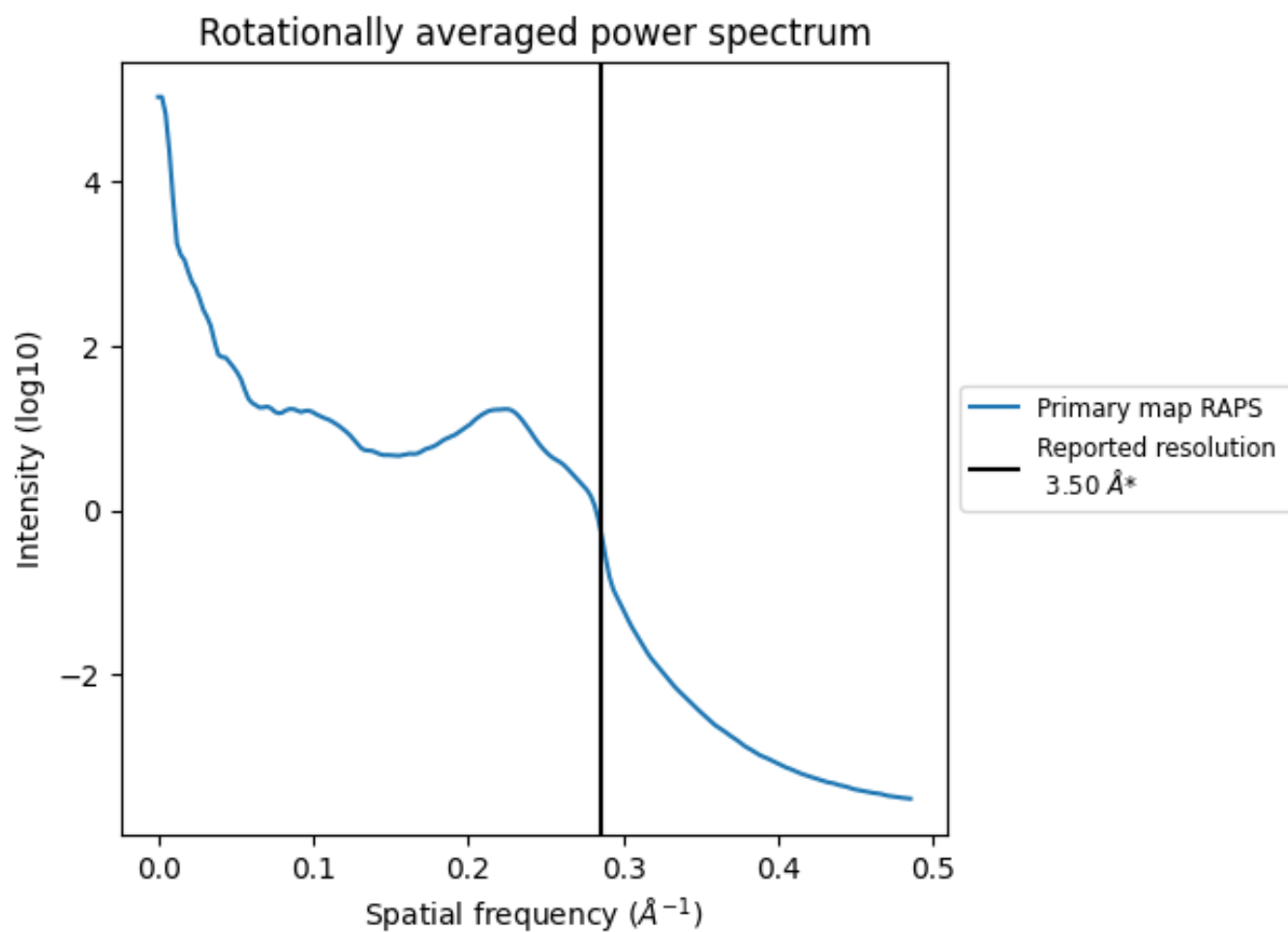
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 385 nm<sup>3</sup>; this corresponds to an approximate mass of 347 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

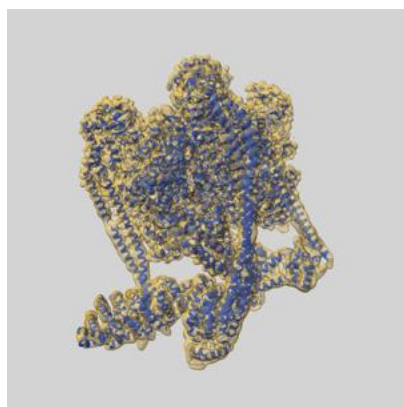
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

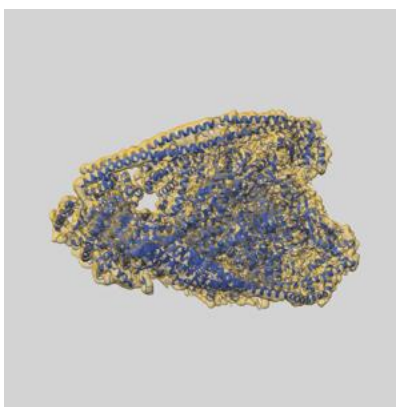
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25996 and PDB model 7TMM. Per-residue inclusion information can be found in section 3 on page 8.

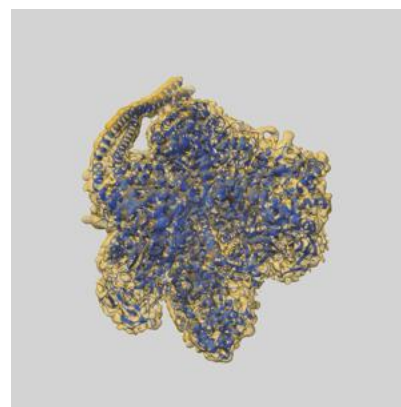
### 9.1 Map-model overlay [i](#)



X



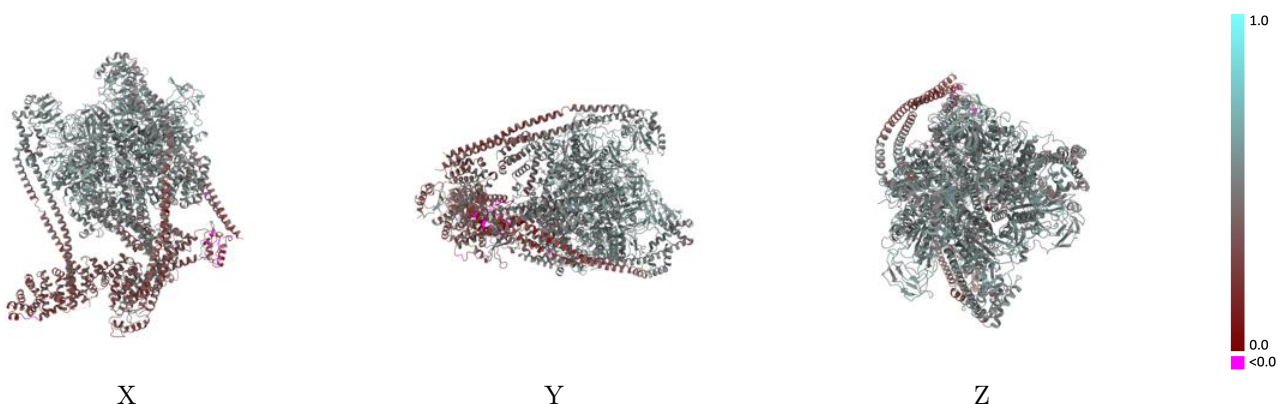
Y



Z

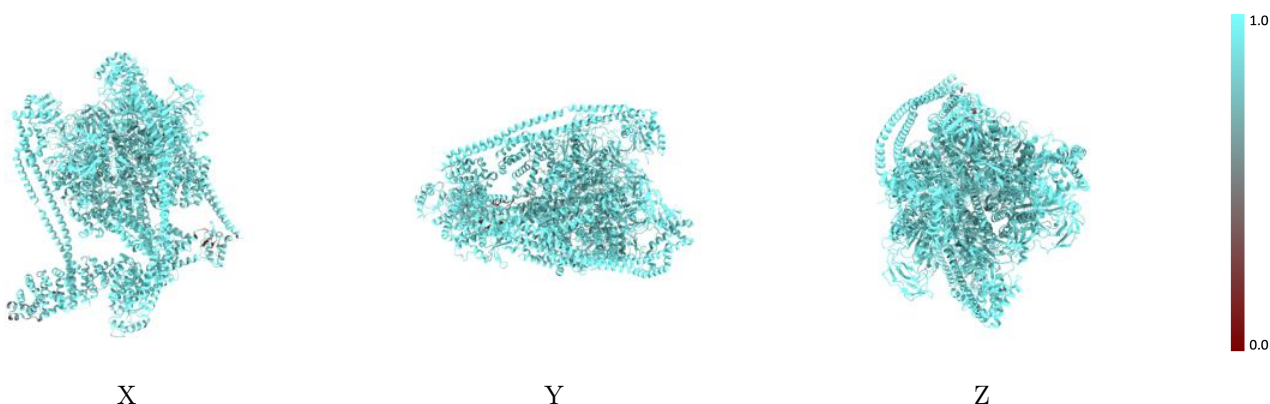
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



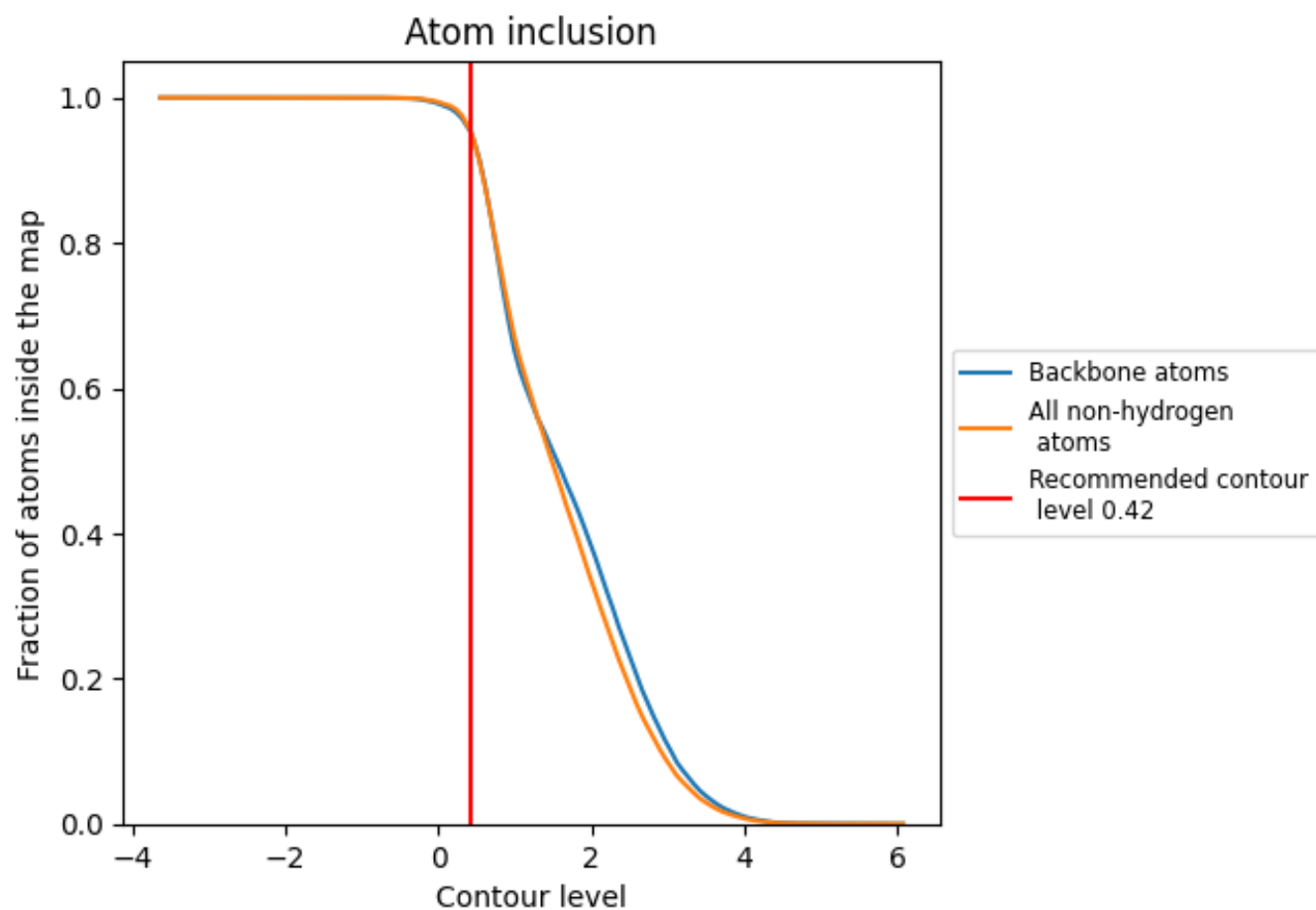
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.42).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9547	 0.4850
A	 0.9554	 0.5370
B	 0.9527	 0.5390
C	 0.9615	 0.5160
D	 0.9545	 0.5350
E	 0.9601	 0.5260
F	 0.9557	 0.5420
G	 0.9763	 0.4600
H	 0.9775	 0.3520
I	 0.9815	 0.4720
J	 0.9789	 0.3730
K	 0.9835	 0.4770
L	 0.9808	 0.3770
M	 0.9432	 0.4640
N	 0.9654	 0.4160
O	 0.9042	 0.3300
P	 0.9172	 0.2970

