



Full wwPDB EM Validation Report ⓘ

Sep 2, 2026 – 03:31 PM EDT

PDB ID : 36QU / pdb_000036qu
EMDB ID : EMD-77786
Title : Arabidopsis thaliana V-type ATPase, State 1
Authors : Khamina, M.; Rubinstein, J.L.
Deposited on : 2026-06-26
Resolution : 3.00 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:

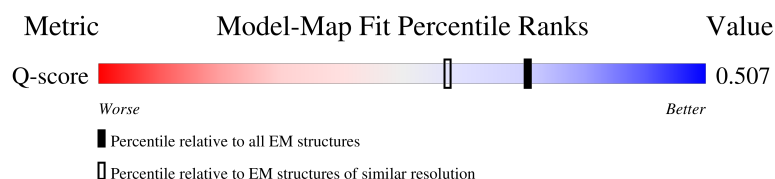
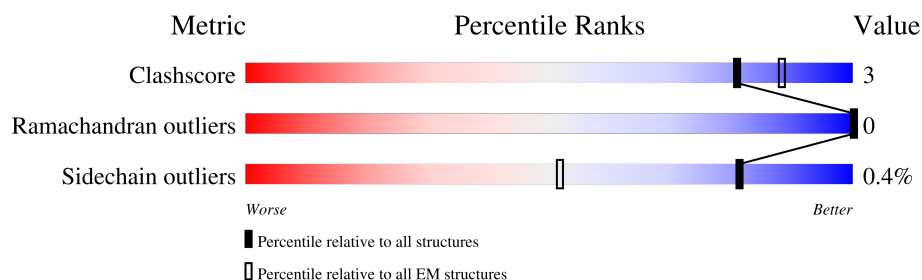
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.00 Å.

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



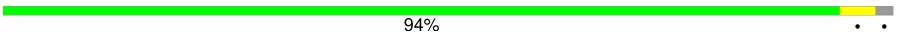
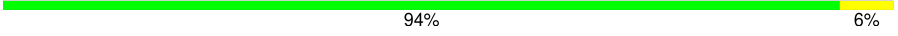
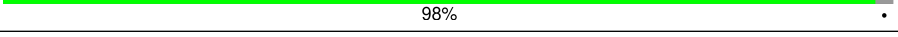
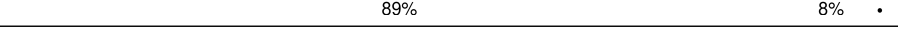
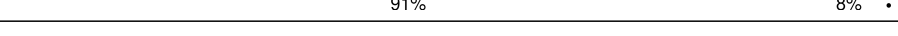
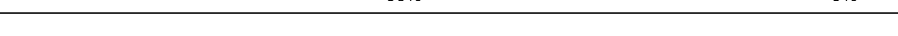
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	486	 87% 7% 6%
1	D	486	 89% 6% 5%
1	F	486	 85% 9% 6%
2	G	230	 91% 7% 2% 1%

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Mol	Chain	Length	Quality of chain
2	I	230	
2	K	230	
3	H	110	
3	J	110	
3	L	110	
4	M	261	
5	N	128	
6	P	441	
7	b	321	
8	c	180	
9	d	351	
10	e	70	
11	g	164	
11	h	164	
11	i	164	
11	j	164	
11	k	164	
11	l	164	
11	m	164	
11	n	164	
11	o	164	
12	r	364	
13	A	623	
13	C	623	
13	E	623	

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Mol	Chain	Length	Quality of chain
14	O	375	6% 94% • 5%
15	a	821	86% • 11%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 54320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called V-type proton ATPase subunit B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	456	Total	C	N	O	S	0	0
			3401	2171	589	628	13		
1	D	462	Total	C	N	O	S	0	0
			3391	2169	600	608	14		
1	B	458	Total	C	N	O	S	0	0
			3391	2168	591	616	16		

- Molecule 2 is a protein called V-type proton ATPase subunit E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	213	Total	C	N	O	S	0	0
			1432	904	262	259	7		
2	I	226	Total	C	N	O	S	0	0
			1489	931	277	274	7		
2	K	224	Total	C	N	O	S	0	0
			1511	949	274	282	6		

- Molecule 3 is a protein called V-type proton ATPase subunit G1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	105	Total	C	N	O	S	0	0
			585	357	112	115	1		
3	J	110	Total	C	N	O	S	0	0
			613	371	119	122	1		
3	L	107	Total	C	N	O	S	0	0
			636	391	124	120	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	218	Total	C	N	O	S	0	0
			1415	885	273	255	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	101	Total	C	N	O	0	0
			502	300	101	101		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	433	Total	C	N	O	0	0
			2149	1283	433	433		

- Molecule 7 is a protein called V-type proton ATPase subunit AP1 fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	44	Total	C	N	O	S	0	0
			313	207	45	57	4		

- Molecule 8 is a protein called V-type proton ATPase subunit c"1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	171	Total	C	N	O	S	0	0
			1206	795	188	217	6		

- Molecule 9 is a protein called V-type proton ATPase subunit d1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	342	Total	C	N	O	S	0	0
			2394	1548	413	418	15		

- Molecule 10 is a protein called V-type proton ATPase subunit e2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	e	66	Total	C	N	O	S	0	0
			472	318	73	76	5		

- Molecule 11 is a protein called V-type proton ATPase subunit c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	162	Total	C	N	O	S	0	0
			1115	730	181	197	7		
11	h	162	Total	C	N	O	S	0	0
			1133	741	186	198	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	161	Total	C	N	O	S	0	0
			1117	732	182	195	8		
11	j	161	Total	C	N	O	S	0	0
			1102	722	184	190	6		
11	k	161	Total	C	N	O	S	0	0
			1087	712	181	188	6		
11	l	161	Total	C	N	O	S	0	0
			1070	702	177	185	6		
11	m	162	Total	C	N	O	S	0	0
			1101	724	181	189	7		
11	n	162	Total	C	N	O	S	0	0
			1088	713	180	187	8		
11	o	159	Total	C	N	O	S	0	0
			1061	697	174	184	6		

- Molecule 12 is a protein called V-type proton ATPase subunit AP2 fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	r	48	Total	C	N	O	S	0	0
			334	224	53	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	610	Total	C	N	O	S	0	0
			4354	2796	756	785	17		
13	E	616	Total	C	N	O	S	0	0
			4422	2839	761	801	21		
13	A	577	Total	C	N	O	S	0	0
			3926	2507	697	706	16		

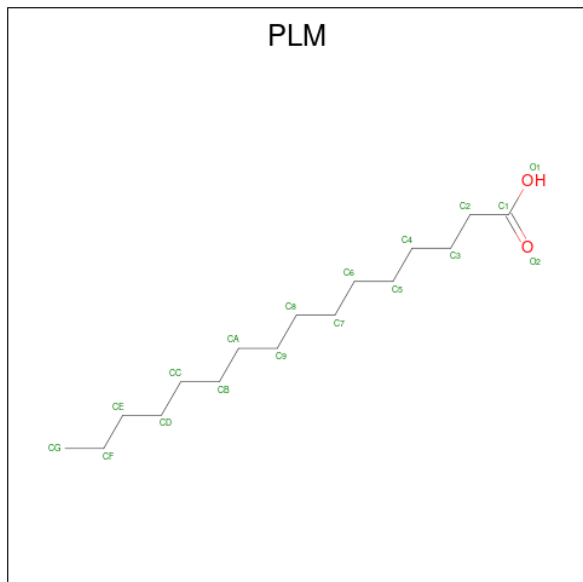
- Molecule 14 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	356	Total	C	N	O	0	0
			1770	1058	356	356		

- Molecule 15 is a protein called V-type proton ATPase subunit a3.

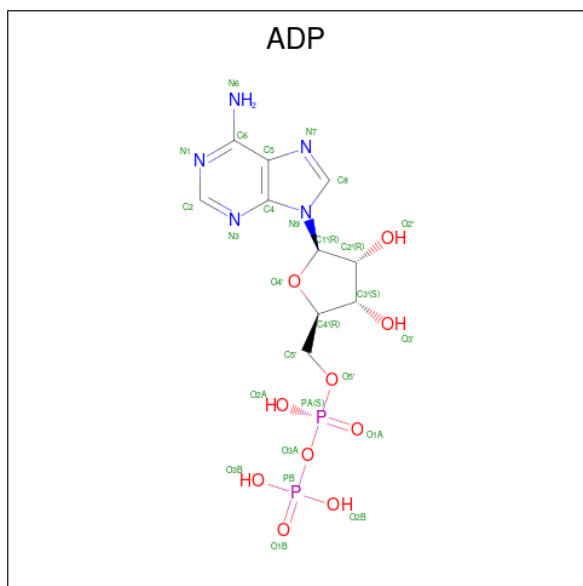
Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	734	Total	C	N	O	S	0	0
			4687	3029	820	821	17		

- Molecule 16 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	b	1	Total	C	O	0
			17	16	1	
16	b	1	Total	C	O	0
			8	7	1	

- Molecule 17 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
17	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

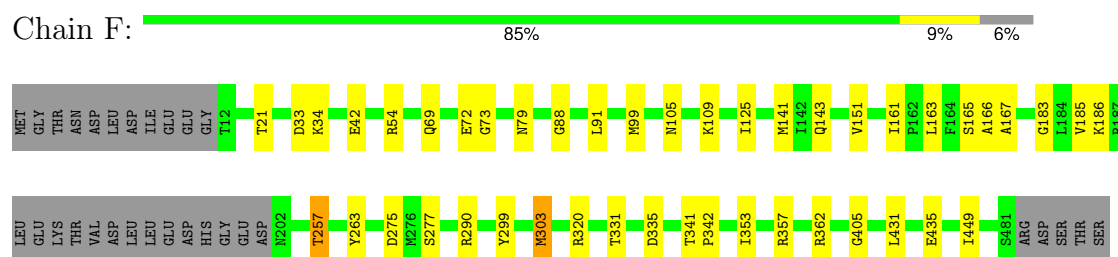
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	E	1	Total	Mg	0
			1	1	

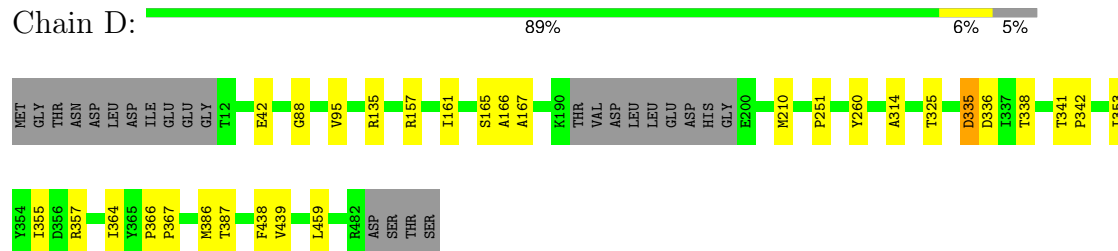
3 Residue-property plots

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

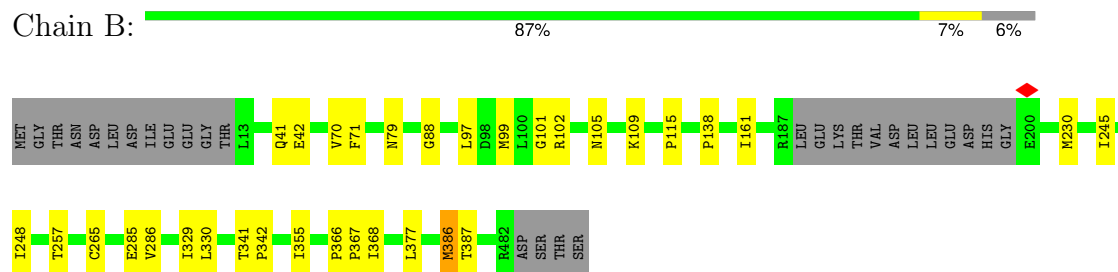
- Molecule 1: V-type proton ATPase subunit B1



- Molecule 1: V-type proton ATPase subunit B1

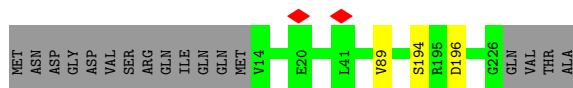


- Molecule 1: V-type proton ATPase subunit B1



- Molecule 2: V-type proton ATPase subunit E1





- Molecule 2: V-type proton ATPase subunit E1

Chain I: 94%



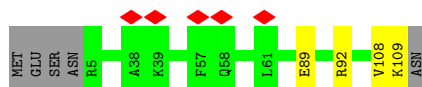
- Molecule 2: V-type proton ATPase subunit E1

Chain K: 93%



- Molecule 3: V-type proton ATPase subunit G1

Chain H: 92% 5%



- Molecule 3: V-type proton ATPase subunit G1

Chain J: 94% 6%



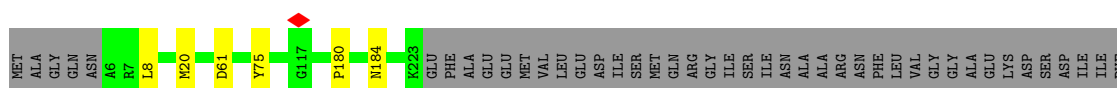
- Molecule 3: V-type proton ATPase subunit G1

Chain L: 93% 5%



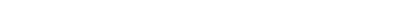
- Molecule 4: V-type proton ATPase subunit D

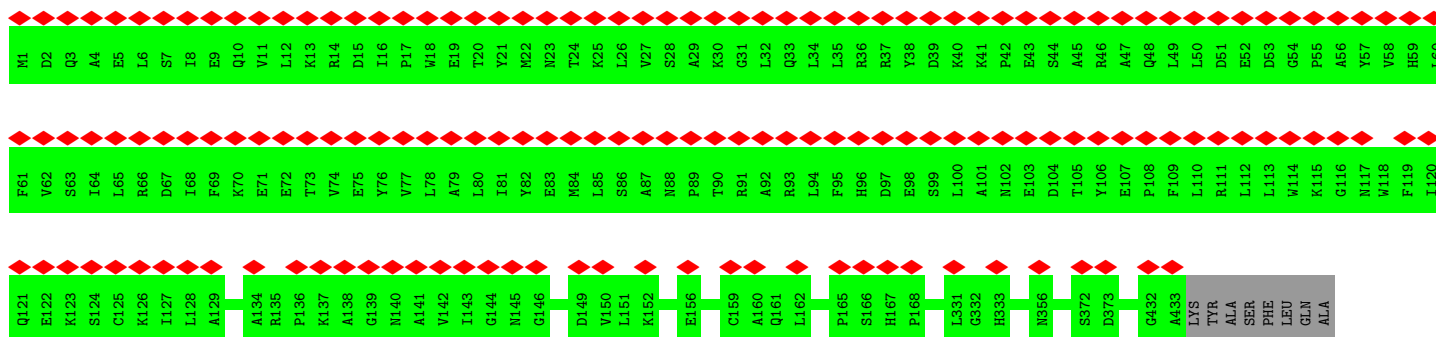
Chain M: 81% 16%



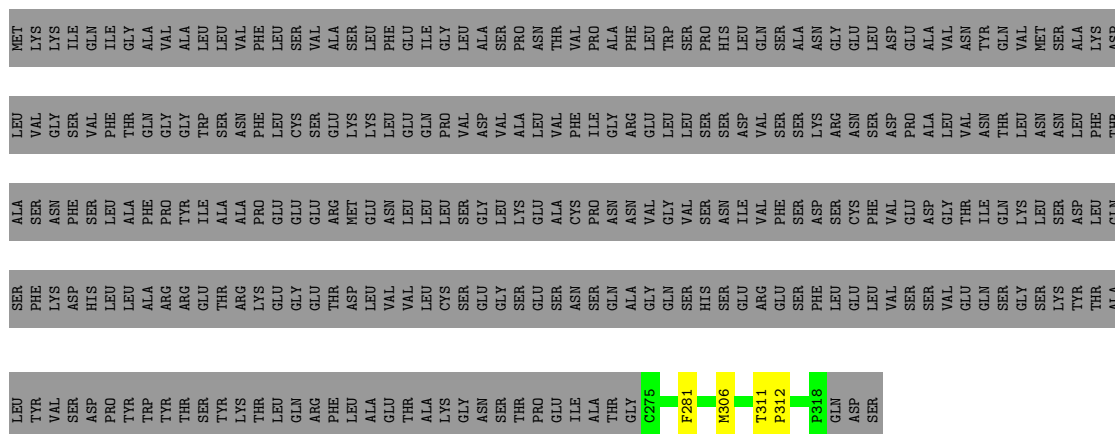
- Molecule 5: V-type proton ATPase subunit F

MET	GLY	ARG	THR	ILE	PRO	ALA	ARG	ASN	SER	L14	R38	R39	A108	S114	ARG	VAL	LVS	TYR	LEU	PHE	SER	SER	ALA	GLU	SER	VAL	SER	GLN	ARG
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- Chain P:  36% 98%

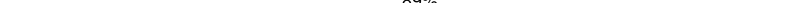


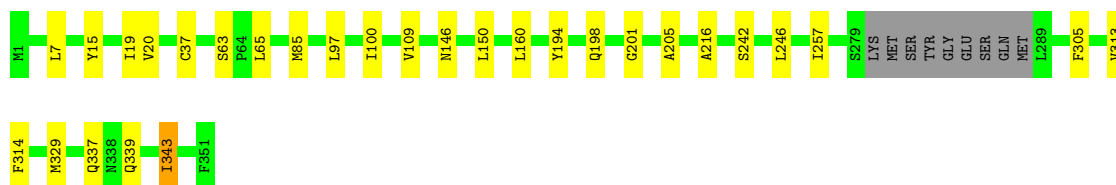
- Chain b:  12% . 86%



- Chain c: 83% 11% • 5%



- Chain d:  89% 8% .



- Molecule 10: V-type proton ATPase subunit e2

Chain e: 76% 19% 6%



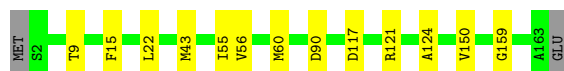
- Molecule 11: V-type proton ATPase subunit c1

Chain g: 92% 7% .



- Molecule 11: V-type proton ATPase subunit c1

Chain h: 91% 8% .



- Molecule 11: V-type proton ATPase subunit c1

Chain i: 91% 7% .



- Molecule 11: V-type proton ATPase subunit c1

Chain j: 88% 10% .



- Molecule 11: V-type proton ATPase subunit c1

Chain k: 90% 8% .



- Molecule 11: V-type proton ATPase subunit c1

MET	SER	T3	A10	P11	L22	S36	V40	M43	A93	A124	G147	V150	A158	A163	GLU
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-
- | Model | Percentage |
|-------|------------|
| MET | 0% |
| S2 | 100% |
| F15 | 100% |
| A21 | 100% |
| L22 | 100% |
| M43 | 100% |
| G44 | 100% |
| L50 | 100% |
| I55 | 100% |
| M60 | 100% |
| L69 | 100% |
| S76 | 100% |
| G98 | 100% |
| L137 | 100% |
| G147 | 100% |
| V150 | 100% |
| A163 | 100% |
| GLU | 100% |

-
- | Category | Count |
|----------|-------|
| MET | 1 |
| S2 | 1 |
| A10 | 1 |
| P11 | 1 |
| L22 | 1 |
| M43 | 1 |
| S54 | 1 |
| I55 | 1 |
| V56 | 1 |
| P57 | 1 |
| M60 | 1 |
| S96 | 1 |
| A124 | 1 |
| L137 | 1 |
| G147 | 1 |
| R157 | 1 |
| A163 | 1 |
| GLU | 1 |

- | MET | SER | THR | PHE | SE | G14 | L22 | M27 | T33 | S54 | P67 | V58 | I79 | A100 | G116 | V120 | G147 | V150 | A163 | GLU |
|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|
|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|

- | |
|-----|
| MET | LYS | ALA | ALA | PHE | TYR | VAL | PHE | VAL | VAL | ALA | ALA | LEU | LEU | LEU | THR | LEU | LEU | ASN | TYR | ARG | GLY | GLU | ALA | ALA | SER | SER | PHE | PHE | ILE | ILE | ASP | GLY | SER | SER | ASN | ASN | GLN | TYR | LEU | ARG | ARG | PRO | PRO | ARG | ARG | SER | SER | SER | SER | GLU | ALA | ALA | LEU | PRO | PRO | MET | MET | SER | SER | PRO | PRO | VAL | VAL | GLU | GLU | ILE | ILE | SER | ALA | ALA | ALA | VAL | VAL | SER | SER | ALA | ALA | LEU | LEU |
|-----|

GLY	PHE	ALA	PRO	SER	SER	ASP	THR	LEU	LEU	ALA	ALA	GLY	SER	SER	LYS	LEU	ASN	LYS	ILE	LEU	LEU	LYS	PRO	PRO	ASN	PHE	PHE	VAL	ARG	PRO	ARG	ALA	ALA	ALA	PHE	GLY	GLY	ILE	ILE	ALA	GLY	GLY	ASP	ASP	MET	LEU	LEU	LEU	GLU	THR	SER	PRO	SER	HIS	SER	SER	PHE	PHE	LEU	GLY	GLY	ASN	ALA	ALA	ILE	ILE	ARG	SER
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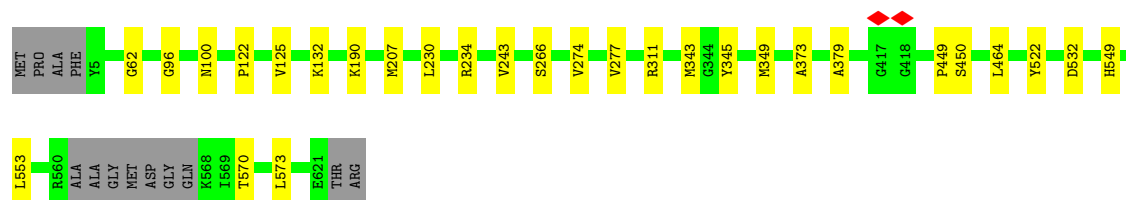
ILE	LYS	SER	ASP	SER	TYR	LYS	ALA	ALA	ASP	THR	GLU	LEU	PRO	PRO	ASN	ASN	GLU	PRO	SER	SER	SER	ASP	VAL	THR	ASP	LYS	ILE	ILE	ASN	ASP	PHE	THR	LEU	TRP	SER	GLY	GLY	SER	TYR	VAL	ALA	GLY	ALA	GLU	PRO	SER	SER	GLY	LEU	ILE	ILE	PRO
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ALA	GLY	GLY	ALA	ASN	VAL	GLU	PHE	ASN	LEU	GLU	LYS	GLY	LEU	TYR	GLN	ASN	ILE	ARG	GLN	ALA	VAL	SER	SER	VAL	THR	ASP	ASP	LEU	SER	HIS	GLY	ILE	ASP	ARG	THR	ALA	GLU	LEU	THR	VAL	GLY	ARG	PHE	GLY	ILE	ASP	ALA	LEU
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ALA	GLN	GLU	TYR	GLN	GLY	MET	ALA	LYS	GLN	GLY	MET	ASP	VAL	LEU	LEU	SER	THR	LEU	SER	LYS	PHE	ASN	LEU	GLU	THR	SER	HIS	LYS	GLY	GLN	ILE	VAL	GLY	LEU	VAL	VAL	ASP	GLU	ARG	VAL	ASN	GLN	GLU	SER	GLU	ASN	LEU	LEU	ASN	PHE	GLY	SER	SER	ARG	SER
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SER	ALA	ARG	SER	MET	VAL	GLU	VAL	GLU	GLY	ILE	PRO	S314	V324	L328	T353	N361	VAL	LYS	LEU	ASP
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- Chain C: 93% 5%



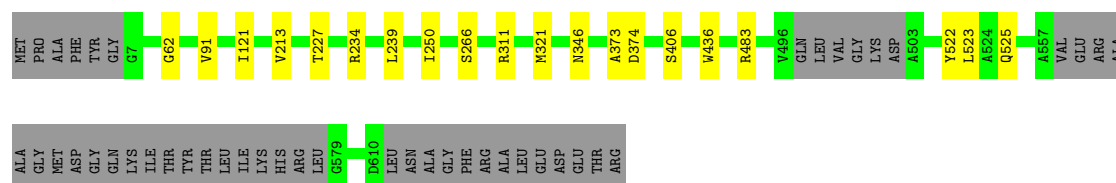
- Molecule 13: V-type proton ATPase catalytic subunit A

Chain E: 95%



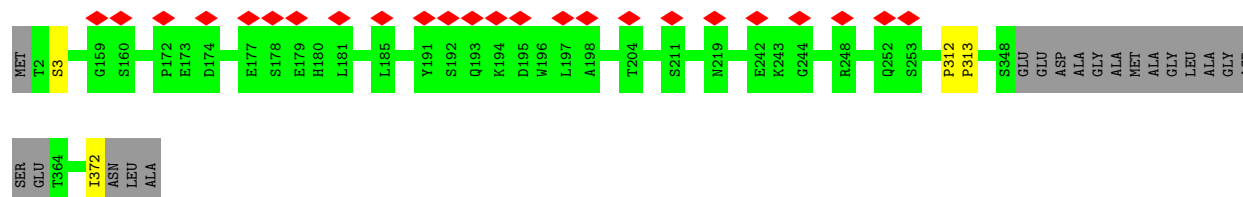
- Molecule 13: V-type proton ATPase catalytic subunit A

Chain A: 89%



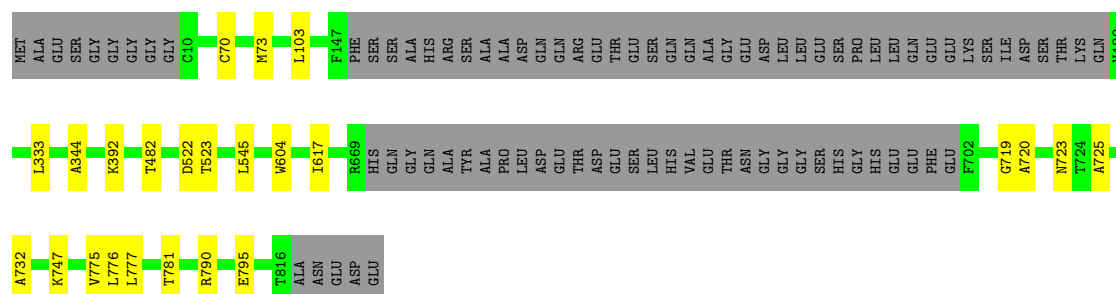
- Molecule 14: V-type proton ATPase subunit C

Chain O: 6%



- Molecule 15: V-type proton ATPase subunit a3

Chain a: 86%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54020	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.836	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	476.16, 476.16, 476.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93, 0.93, 0.93	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, PLM, 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	B	0.20	0/3457	0.29	0/4708
1	D	0.19	0/3457	0.29	0/4709
1	F	0.17	0/3467	0.26	0/4716
2	G	0.15	0/1448	0.26	0/1979
2	I	0.19	0/1504	0.31	0/2057
2	K	0.16	0/1527	0.29	0/2085
3	H	0.16	0/584	0.31	0/805
3	J	0.18	0/613	0.31	0/843
3	L	0.15	0/637	0.32	0/874
4	M	0.15	0/1427	0.32	0/1946
5	N	0.12	0/501	0.35	0/698
6	P	0.12	0/2148	0.29	0/2996
7	b	0.19	0/317	0.27	0/430
8	c	0.22	0/1227	0.31	0/1675
9	d	0.20	0/2449	0.34	0/3352
10	e	0.17	0/482	0.37	0/667
11	g	0.24	0/1134	0.29	0/1541
11	h	0.23	0/1152	0.29	0/1560
11	i	0.23	0/1136	0.27	0/1539
11	j	0.23	0/1121	0.29	0/1521
11	k	0.22	0/1106	0.30	0/1504
11	l	0.23	0/1089	0.28	0/1484
11	m	0.23	0/1120	0.30	0/1522
11	n	0.22	0/1107	0.30	0/1505
11	o	0.23	0/1079	0.30	0/1472
12	r	0.16	0/339	0.25	0/467
13	A	0.16	0/4012	0.30	0/5507
13	C	0.17	0/4445	0.29	0/6075
13	E	0.19	0/4521	0.28	0/6177
14	O	0.14	0/1768	0.33	0/2466
15	a	0.15	0/4789	0.31	0/6588
All	All	0.18	0/55163	0.30	0/75468

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	B	3391	0	3287	19	0
1	D	3391	0	3261	18	0
1	F	3401	0	3299	26	0
2	G	1432	0	1286	1	0
2	I	1489	0	1287	10	0
2	K	1511	0	1336	7	0
3	H	585	0	408	3	0
3	J	613	0	415	4	0
3	L	636	0	495	3	0
4	M	1415	0	1215	3	0
5	N	502	0	226	0	0
6	P	2149	0	960	0	0
7	b	313	0	314	3	0
8	c	1206	0	1238	17	0
9	d	2394	0	2009	20	0
10	e	472	0	474	8	0
11	g	1115	0	1133	8	0
11	h	1133	0	1176	13	0
11	i	1117	0	1163	12	0
11	j	1102	0	1116	18	0
11	k	1087	0	1079	14	0
11	l	1070	0	1048	11	0
11	m	1101	0	1112	13	0
11	n	1088	0	1079	12	0
11	o	1061	0	1052	13	0
12	r	334	0	324	3	0
13	A	3926	0	3420	11	0
13	C	4354	0	4053	17	0
13	E	4422	0	4091	14	0
14	O	1770	0	770	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	a	4687	0	3586	17	0
16	b	25	0	41	1	0
17	E	27	0	12	0	0
18	E	1	0	0	0	0
All	All	54320	0	47765	267	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 3.

All (267) 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)
8:c:127:LEU:HD11	9:d:7:LEU:HD22	1.64	0.79
1:D:157:ARG:O	1:D:325:THR:OG1	2.02	0.78
11:i:77:THR:HG21	15:a:617:ILE:HG21	1.67	0.77
8:c:117:ILE:HG23	11:o:22:LEU:HD23	1.66	0.76
13:E:234:ARG:NH1	13:E:535:CYS:SG	2.64	0.70
1:F:54:ARG:NH1	1:F:73:GLY:O	2.25	0.70
13:A:91:VAL:HG23	13:A:213:VAL:HG12	1.75	0.68
11:n:43:MET:HG3	11:n:124:ALA:HB2	1.76	0.66
1:D:386:MET:O	1:D:387:THR:OG1	2.09	0.65
15:a:723:ASN:ND2	15:a:795:GLU:OE1	2.29	0.65
11:n:22:LEU:HD23	11:o:100:ALA:HB1	1.77	0.65
9:d:20:VAL:HG21	9:d:314:PHE:CD1	2.31	0.64
11:h:117:ASP:OD1	11:h:121:ARG:NH1	2.31	0.64
3:L:10:ILE:HD12	3:L:11:GLN:N	2.13	0.64
1:B:386:MET:O	1:B:387:THR:OG1	2.15	0.63
16:b:401:PLM:H52	8:c:39:LEU:HD22	1.81	0.62
11:o:33:THR:HG23	11:o:58:VAL:HG13	1.82	0.62
1:B:71:PHE:CD1	1:B:245:ILE:HG21	2.35	0.62
1:D:364:ILE:HG22	1:D:366:PRO:HD2	1.81	0.61
11:l:22:LEU:HD22	11:m:150:VAL:HG21	1.82	0.61
11:h:43:MET:HG3	11:h:124:ALA:HB2	1.83	0.60
11:n:22:LEU:HD21	11:o:147:GLY:HA2	1.82	0.60
13:C:266:SER:O	13:C:311:ARG:NH2	2.34	0.60
3:J:89:GLU:OE2	3:J:92:ARG:NH2	2.32	0.59
1:F:335:ASP:OD2	1:F:357:ARG:NH1	2.35	0.59
1:F:362:ARG:NH2	1:F:435:GLU:OE1	2.36	0.59
1:B:248:ILE:HD12	1:B:286:VAL:HG21	1.84	0.59
11:i:22:LEU:HD21	11:j:147:GLY:HA2	1.85	0.59
8:c:164:GLY:HA2	11:o:22:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:34:ILE:HD12	11:g:150:VAL:HG21	1.84	0.58
1:F:33:ASP:OD1	1:F:34:LYS:N	2.37	0.58
11:l:22:LEU:HD21	11:m:147:GLY:HA2	1.86	0.57
15:a:73:MET:HE1	15:a:103:LEU:HD11	1.84	0.57
8:c:83:VAL:HG11	8:c:118:VAL:HG21	1.88	0.56
11:j:22:LEU:HD21	11:k:147:GLY:HA2	1.87	0.56
13:C:570:THR:HG23	13:C:573:LEU:H	1.70	0.56
2:K:85:GLN:HG2	3:L:86:LEU:HD21	1.88	0.56
9:d:15:TYR:CZ	9:d:19:ILE:HD11	2.40	0.56
13:C:96:GLY:O	13:C:100:ASN:ND2	2.36	0.56
15:a:719:GLY:O	15:a:720:ALA:C	2.48	0.55
11:k:22:LEU:HD22	11:l:150:VAL:HG21	1.87	0.55
1:F:42:GLU:OE2	1:F:88:GLY:N	2.40	0.55
9:d:246:LEU:HD13	9:d:246:LEU:O	2.06	0.55
1:B:42:GLU:OE2	1:B:88:GLY:N	2.38	0.55
13:E:447:HIS:O	13:E:447:HIS:ND1	2.39	0.55
1:D:167:ALA:O	1:D:357:ARG:NH2	2.38	0.55
11:n:43:MET:CG	11:n:124:ALA:HB2	2.36	0.55
1:F:72:GLU:N	1:F:72:GLU:OE1	2.40	0.54
8:c:124:VAL:HG11	11:o:27:MET:HG2	1.90	0.54
11:h:22:LEU:HD22	11:i:150:VAL:HG21	1.89	0.54
11:j:43:MET:HG3	11:j:124:ALA:HB2	1.89	0.54
1:F:263:TYR:O	1:F:320:ARG:NH1	2.41	0.54
9:d:146:ASN:O	9:d:150:LEU:N	2.39	0.54
7:b:306:MET:HE1	11:g:30:ALA:HB3	1.90	0.54
11:i:79:ILE:O	11:j:157:ARG:NH2	2.37	0.54
1:F:341:THR:HB	1:F:342:PRO:HD3	1.90	0.53
13:C:266:SER:HA	13:C:274:VAL:HG21	1.88	0.53
13:C:379:ALA:HB1	1:B:285:GLU:HA	1.88	0.53
11:l:93:ALA:HB3	11:l:158:ALA:HB2	1.90	0.53
11:m:22:LEU:HD21	11:n:147:GLY:HA2	1.90	0.53
13:C:62:GLY:O	1:B:79:ASN:ND2	2.41	0.53
11:j:43:MET:CG	11:j:124:ALA:HB2	2.38	0.53
9:d:20:VAL:HG22	9:d:85:MET:SD	2.49	0.53
11:j:56:VAL:HG11	11:j:134:ILE:HD12	1.90	0.52
1:F:275:ASP:OD1	1:F:277:SER:OG	2.28	0.52
2:I:132:LEU:HD13	2:I:192:LEU:CD2	2.40	0.52
1:D:42:GLU:OE2	1:D:88:GLY:N	2.42	0.52
11:h:22:LEU:HD21	11:i:147:GLY:HA2	1.92	0.52
11:j:69:LEU:C	11:j:69:LEU:HD23	2.35	0.52
15:a:333:LEU:HD22	15:a:344:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:ASN:ND2	13:A:62:GLY:O	2.43	0.51
3:H:89:GLU:OE2	3:H:92:ARG:NH2	2.43	0.51
11:k:22:LEU:HD21	11:l:147:GLY:HA2	1.93	0.51
12:r:353:THR:HG23	12:r:353:THR:O	2.09	0.51
4:M:8:LEU:HD12	4:M:20:MET:HE1	1.91	0.51
1:D:135:ARG:NH2	1:D:314:ALA:O	2.41	0.51
13:A:346:ASN:OD1	13:A:406:SER:OG	2.24	0.51
8:c:101:ASP:OD1	8:c:102:ALA:N	2.44	0.51
15:a:545:LEU:C	15:a:545:LEU:HD23	2.35	0.51
1:D:364:ILE:O	1:D:367:PRO:HB3	2.10	0.51
3:J:40:GLU:O	3:J:44:LYS:N	2.44	0.51
8:c:117:ILE:CG2	11:o:22:LEU:HD23	2.38	0.51
2:I:121:CYS:HB3	2:I:192:LEU:HD12	1.91	0.50
13:A:234:ARG:NH1	13:A:522:TYR:O	2.41	0.50
2:I:29:SER:O	2:I:33:GLU:CB	2.60	0.50
11:h:90:ASP:OD1	11:h:159:GLY:N	2.40	0.50
14:O:312:PRO:N	14:O:313:PRO:HA	2.27	0.50
1:B:341:THR:HB	1:B:342:PRO:HD3	1.93	0.50
2:I:28:ILE:O	2:I:29:SER:C	2.54	0.50
2:I:121:CYS:CB	2:I:192:LEU:HD12	2.42	0.50
9:d:257:ILE:C	9:d:257:ILE:HD12	2.37	0.50
1:F:21:THR:OG1	1:F:33:ASP:O	2.20	0.49
1:D:161:ILE:HD11	1:D:353:ILE:CD1	2.42	0.49
1:B:138:PRO:HG2	1:B:377:LEU:HD13	1.94	0.49
2:K:89:VAL:HG12	2:K:213:PHE:HZ	1.77	0.49
11:l:22:LEU:HD22	11:m:150:VAL:CG2	2.42	0.49
1:F:277:SER:OG	1:F:331:THR:OG1	2.30	0.49
1:D:341:THR:HB	1:D:342:PRO:HD3	1.93	0.49
11:h:9:THR:HG23	12:r:328:LEU:HD11	1.94	0.49
11:m:43:MET:SD	11:m:44:GLY:N	2.85	0.49
13:A:266:SER:O	13:A:311:ARG:NH2	2.45	0.49
1:B:161:ILE:O	1:B:161:ILE:HG23	2.12	0.49
13:C:549:HIS:NE2	13:C:553:LEU:HD11	2.28	0.49
15:a:333:LEU:HD22	15:a:344:ALA:CB	2.43	0.49
13:E:71:GLU:OE2	13:E:107:ARG:NH1	2.47	0.48
13:C:132:LYS:O	13:C:190:LYS:NZ	2.42	0.48
11:h:9:THR:HG22	11:h:9:THR:O	2.13	0.48
10:e:12:VAL:O	10:e:16:ILE:HG23	2.14	0.48
15:a:70:CYS:HA	15:a:73:MET:HE3	1.95	0.47
15:a:777:LEU:O	15:a:781:THR:OG1	2.29	0.47
1:F:141:MET:HE1	1:F:449:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:d:37:CYS:SG	9:d:343:ILE:HD12	2.53	0.47
11:j:70:ILE:HD11	15:a:732:ALA:HA	1.97	0.47
11:m:21:ALA:HB2	11:m:98:GLY:HA2	1.96	0.47
13:E:137:GLU:OE2	13:E:186:GLN:NE2	2.41	0.47
1:D:438:PHE:HB2	1:D:459:LEU:HD11	1.95	0.47
13:E:449:PRO:O	13:E:450:SER:OG	2.32	0.47
2:G:194:SER:OG	2:G:196:ASP:OD1	2.31	0.47
11:j:22:LEU:HD22	11:k:150:VAL:HG21	1.97	0.47
11:m:69:LEU:C	11:m:69:LEU:HD23	2.39	0.47
1:D:161:ILE:HG23	1:D:161:ILE:O	2.14	0.47
7:b:281:PHE:CE1	12:r:324:VAL:HG22	2.50	0.47
14:O:3:SER:N	14:O:372:ILE:O	2.47	0.47
2:K:21:ALA:HB2	3:L:20:ALA:HB1	1.96	0.46
13:E:69:VAL:HG12	13:E:71:GLU:H	1.80	0.46
2:K:132:LEU:C	2:K:132:LEU:HD23	2.40	0.46
11:g:22:LEU:HD13	11:h:150:VAL:HG21	1.98	0.46
1:F:161:ILE:HG23	1:F:161:ILE:O	2.16	0.46
2:I:28:ILE:O	2:I:32:ALA:HB3	2.15	0.46
4:M:180:PRO:O	4:M:184:ASN:ND2	2.49	0.46
11:g:22:LEU:CD1	11:h:150:VAL:HG21	2.45	0.46
13:C:373:ALA:HB2	13:C:379:ALA:HB2	1.97	0.46
15:a:790:ARG:NH1	15:a:795:GLU:OE2	2.43	0.46
1:D:165:SER:OG	1:D:166:ALA:N	2.49	0.46
1:B:97:LEU:HD21	1:B:265:CYS:SG	2.55	0.46
9:d:109:VAL:HG21	9:d:160:LEU:HD12	1.97	0.46
10:e:36:LEU:HD22	10:e:40:ILE:HD13	1.98	0.46
11:l:10:ALA:N	11:l:11:PRO:CD	2.79	0.46
1:D:336:ASP:OD1	1:D:338:THR:OG1	2.29	0.46
1:B:329:ILE:C	1:B:330:LEU:HD12	2.41	0.46
2:K:75:ASN:OD1	2:K:75:ASN:C	2.59	0.46
9:d:20:VAL:HG21	9:d:314:PHE:CE1	2.50	0.46
11:j:134:ILE:O	11:j:138:ILE:HG12	2.16	0.46
13:A:91:VAL:CG2	13:A:213:VAL:HG12	2.45	0.46
11:n:55:ILE:O	11:n:55:ILE:HG22	2.16	0.45
2:K:211:VAL:O	2:K:215:MET:HG2	2.16	0.45
11:m:43:MET:HE1	11:m:50:LEU:HB2	1.99	0.45
1:B:70:VAL:HG12	1:B:71:PHE:O	2.17	0.45
1:B:105:ASN:OD1	1:B:109:LYS:N	2.41	0.45
8:c:113:ALA:HB3	8:c:171:MET:HE1	1.99	0.45
13:E:352:ASP:O	13:E:412:ALA:HB3	2.17	0.45
10:e:20:CYS:O	10:e:21:THR:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:GLN:N	1:F:183:GLY:O	2.45	0.45
3:H:89:GLU:OE1	3:H:92:ARG:NH1	2.46	0.44
11:o:54:SER:O	11:o:57:PRO:HD2	2.16	0.44
13:A:121:ILE:HD12	13:A:321:MET:HE1	1.98	0.44
11:j:60:MET:O	11:j:63:VAL:HG12	2.17	0.44
11:m:60:MET:HE3	11:m:137:LEU:HB3	1.98	0.44
15:a:522:ASP:O	15:a:523:THR:OG1	2.31	0.44
1:F:69:GLN:OE1	1:F:290:ARG:NH2	2.43	0.44
9:d:15:TYR:CE2	9:d:19:ILE:HD11	2.52	0.44
11:l:22:LEU:HD22	11:m:150:VAL:CB	2.48	0.44
9:d:337:GLN:O	9:d:339:GLN:N	2.48	0.44
1:B:366:PRO:O	1:B:368:ILE:N	2.48	0.44
1:F:405:GLY:C	1:F:431:LEU:HD11	2.42	0.44
1:F:163:LEU:HD23	1:F:353:ILE:HB	1.99	0.44
13:E:37:MET:HE1	13:E:84:ARG:HG3	1.98	0.44
1:B:355:ILE:HG23	1:B:367:PRO:HG2	1.99	0.44
11:k:43:MET:HG3	11:k:124:ALA:HB2	2.00	0.44
8:c:88:GLN:O	11:g:157:ARG:NH1	2.50	0.44
11:k:22:LEU:HD22	11:l:150:VAL:CG2	2.48	0.44
1:D:335:ASP:OD1	1:D:335:ASP:N	2.49	0.44
2:I:132:LEU:HD13	2:I:192:LEU:HD21	1.99	0.43
1:F:185:VAL:HG12	1:F:186:LYS:N	2.33	0.43
13:C:234:ARG:NH2	13:C:532:ASP:OD1	2.51	0.43
11:j:149:ILE:HD11	15:a:725:ALA:HB1	1.99	0.43
1:D:95:VAL:HG11	1:D:260:TYR:CB	2.48	0.43
11:n:10:ALA:N	11:n:11:PRO:CD	2.81	0.43
1:F:167:ALA:O	1:F:357:ARG:NH2	2.51	0.43
11:k:54:SER:O	11:k:57:PRO:HD2	2.18	0.43
13:A:250:ILE:HG22	13:A:436:TRP:HB2	2.00	0.43
1:F:151:VAL:O	1:F:151:VAL:HG12	2.17	0.43
4:M:75:TYR:HB2	9:d:329:MET:HE1	1.99	0.43
15:a:777:LEU:O	15:a:781:THR:CB	2.67	0.43
1:F:99:MET:HE1	1:F:257:THR:OG1	2.19	0.43
1:F:299:TYR:CD1	1:F:303:MET:HE2	2.54	0.43
13:E:353:SER:OG	13:E:356:ARG:HG2	2.18	0.43
9:d:305:PHE:CE1	9:d:313:VAL:HG13	2.54	0.43
10:e:55:ILE:CG2	15:a:604:TRP:HB3	2.48	0.43
11:j:76:SER:O	11:k:157:ARG:NH1	2.52	0.43
11:h:22:LEU:HD22	11:i:150:VAL:CG2	2.48	0.43
11:m:76:SER:O	11:n:157:ARG:NH1	2.52	0.43
13:C:449:PRO:O	13:C:450:SER:OG	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:91:VAL:HG23	13:E:213:VAL:HG12	2.01	0.43
8:c:25:PHE:HB3	8:c:112:PHE:HB2	2.01	0.43
11:k:51:VAL:O	11:k:55:ILE:HG12	2.19	0.43
13:C:234:ARG:NH1	13:C:522:TYR:O	2.46	0.43
11:k:10:ALA:N	11:k:11:PRO:CD	2.83	0.42
11:n:54:SER:O	11:n:57:PRO:HD2	2.19	0.42
13:C:122:PRO:HD2	13:C:125:VAL:HG11	2.02	0.42
1:B:71:PHE:CD1	1:B:71:PHE:N	2.86	0.42
11:i:10:ALA:N	11:i:11:PRO:CD	2.82	0.42
13:C:230:LEU:N	13:C:230:LEU:HD22	2.35	0.42
13:C:343:MET:HE2	13:C:345:TYR:CE2	2.54	0.42
8:c:46:TYR:CD1	8:c:46:TYR:C	2.97	0.42
8:c:167:VAL:HB	11:o:22:LEU:HD22	2.01	0.42
11:h:15:PHE:HB3	11:i:96:SER:OG	2.20	0.42
11:m:55:ILE:HG22	11:m:55:ILE:O	2.18	0.42
10:e:38:LEU:O	10:e:41:THR:HG22	2.20	0.42
8:c:44:GLY:O	8:c:48:THR:HG22	2.20	0.42
10:e:5:VAL:HG13	10:e:6:THR:N	2.35	0.42
13:C:277:VAL:HG21	13:C:349:MET:HE3	2.02	0.42
13:E:321:MET:O	13:E:322:PRO:C	2.62	0.42
13:A:239:LEU:HD11	13:A:483:ARG:HG2	2.02	0.42
2:I:208:ARG:NH1	3:J:105:VAL:O	2.53	0.42
9:d:97:LEU:HA	9:d:100:ILE:HD12	2.02	0.42
9:d:194:TYR:O	9:d:198:GLN:HG2	2.20	0.42
11:g:54:SER:O	11:g:57:PRO:HD2	2.20	0.42
9:d:20:VAL:HG21	9:d:314:PHE:HD1	1.78	0.42
3:H:108:VAL:HG12	3:H:109:LYS:N	2.35	0.41
11:j:22:LEU:HD22	11:k:150:VAL:CB	2.50	0.41
11:k:55:ILE:HG22	11:k:55:ILE:O	2.19	0.41
13:C:243:VAL:HG12	13:C:464:LEU:HD21	2.02	0.41
13:E:91:VAL:HG23	13:E:213:VAL:CG1	2.50	0.41
2:I:132:LEU:HD13	2:I:192:LEU:HD23	2.02	0.41
11:o:14:GLY:HA3	11:o:79:ILE:HD11	2.01	0.41
13:A:373:ALA:O	13:A:374:ASP:C	2.62	0.41
11:j:22:LEU:HD22	11:k:150:VAL:HB	2.02	0.41
2:I:132:LEU:HD12	2:I:133:ARG:N	2.36	0.41
7:b:311:THR:HG22	7:b:312:PRO:HD2	2.01	0.41
8:c:112:PHE:CZ	8:c:116:ILE:HD11	2.56	0.41
10:e:49:MET:HE1	15:a:482:THR:HG23	2.02	0.41
10:e:6:THR:HA	10:e:9:ILE:HG12	2.02	0.41
11:h:56:VAL:HG12	11:h:60:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:43:MET:HG3	11:l:124:ALA:HB2	2.02	0.41
2:K:189:GLY:HA3	2:K:204:THR:HA	2.03	0.41
9:d:216:ALA:HB1	9:d:242:SER:CB	2.50	0.41
11:l:36:SER:O	11:l:40:VAL:HG23	2.20	0.41
11:i:3:THR:OG1	11:j:162:ARG:NH1	2.52	0.41
11:k:16:LEU:HD23	11:k:16:LEU:HA	1.97	0.41
9:d:201:GLY:O	9:d:205:ALA:HB2	2.20	0.41
11:n:22:LEU:HD22	11:o:150:VAL:HB	2.01	0.41
1:F:165:SER:OG	1:F:166:ALA:N	2.53	0.41
3:J:93:ILE:O	3:J:94:SER:C	2.64	0.41
11:i:59:VAL:HG22	11:j:139:PHE:CZ	2.56	0.41
13:E:222:LYS:NZ	13:E:390:GLU:O	2.52	0.41
1:B:102:ARG:NH1	1:B:115:PRO:O	2.47	0.41
11:i:22:LEU:HD22	11:j:150:VAL:HB	2.03	0.40
11:o:116:GLY:O	11:o:120:VAL:HG23	2.21	0.40
8:c:167:VAL:CB	11:o:22:LEU:HD22	2.51	0.40
11:n:60:MET:HE1	11:n:137:LEU:HB2	2.04	0.40
13:E:338:GLU:OE2	13:E:391:ARG:NE	2.39	0.40
9:d:63:SER:O	9:d:65:LEU:N	2.51	0.40
11:i:16:LEU:HD23	11:i:16:LEU:HA	1.95	0.40
1:D:210:MET:SD	1:D:251:PRO:HG3	2.62	0.40
1:D:355:ILE:HG23	1:D:367:PRO:HD2	2.03	0.40
1:B:101:GLY:HA2	1:B:230:MET:O	2.21	0.40
1:F:91:LEU:HD21	1:F:125:ILE:HD11	2.03	0.40
1:F:105:ASN:OD1	1:F:109:LYS:N	2.53	0.40
11:g:21:ALA:HB2	11:g:98:GLY:HA2	2.03	0.40
11:g:36:SER:O	11:g:40:VAL:HG23	2.21	0.40
11:h:55:ILE:O	11:h:55:ILE:HG22	2.21	0.40
11:m:15:PHE:HB3	11:n:96:SER:OG	2.22	0.40
1:D:366:PRO:HG2	1:D:439:VAL:HG12	2.04	0.40
15:a:775:VAL:HG23	15:a:776:LEU:N	2.36	0.40
1:B:99:MET:HE1	1:B:257:THR:OG1	2.21	0.40
13:A:523:LEU:O	13:A:525:GLN:N	2.54	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	B	454/486 (93%)	439 (97%)	15 (3%)	0	100	100
1	D	458/486 (94%)	447 (98%)	11 (2%)	0	100	100
1	F	452/486 (93%)	445 (98%)	7 (2%)	0	100	100
2	G	211/230 (92%)	206 (98%)	5 (2%)	0	100	100
2	I	224/230 (97%)	219 (98%)	5 (2%)	0	100	100
2	K	222/230 (96%)	220 (99%)	2 (1%)	0	100	100
3	H	103/110 (94%)	103 (100%)	0	0	100	100
3	J	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
3	L	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
4	M	216/261 (83%)	206 (95%)	10 (5%)	0	100	100
5	N	99/128 (77%)	91 (92%)	8 (8%)	0	100	100
6	P	431/441 (98%)	422 (98%)	9 (2%)	0	100	100
7	b	42/321 (13%)	42 (100%)	0	0	100	100
8	c	169/180 (94%)	168 (99%)	1 (1%)	0	100	100
9	d	338/351 (96%)	326 (96%)	12 (4%)	0	100	100
10	e	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
11	g	160/164 (98%)	157 (98%)	3 (2%)	0	100	100
11	h	160/164 (98%)	159 (99%)	1 (1%)	0	100	100
11	i	159/164 (97%)	158 (99%)	1 (1%)	0	100	100
11	j	159/164 (97%)	157 (99%)	2 (1%)	0	100	100
11	k	159/164 (97%)	156 (98%)	3 (2%)	0	100	100
11	l	159/164 (97%)	156 (98%)	3 (2%)	0	100	100
11	m	160/164 (98%)	157 (98%)	3 (2%)	0	100	100
11	n	160/164 (98%)	158 (99%)	2 (1%)	0	100	100
11	o	157/164 (96%)	155 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	r	46/364 (13%)	46 (100%)	0	0	100	100
13	A	571/623 (92%)	555 (97%)	16 (3%)	0	100	100
13	C	606/623 (97%)	588 (97%)	18 (3%)	0	100	100
13	E	612/623 (98%)	592 (97%)	20 (3%)	0	100	100
14	O	352/375 (94%)	337 (96%)	15 (4%)	0	100	100
15	a	728/821 (89%)	693 (95%)	35 (5%)	0	100	100
All	All	8044/9135 (88%)	7829 (97%)	215 (3%)	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	B	333/415 (80%)	331 (99%)	2 (1%)	78	88
1	D	323/415 (78%)	322 (100%)	1 (0%)	86	91
1	F	337/415 (81%)	335 (99%)	2 (1%)	78	88
2	G	114/201 (57%)	113 (99%)	1 (1%)	70	85
2	I	112/201 (56%)	112 (100%)	0	100	100
2	K	122/201 (61%)	122 (100%)	0	100	100
3	H	22/93 (24%)	22 (100%)	0	100	100
3	J	22/93 (24%)	22 (100%)	0	100	100
3	L	33/93 (36%)	32 (97%)	1 (3%)	36	69
4	M	96/219 (44%)	95 (99%)	1 (1%)	68	84
7	b	34/279 (12%)	34 (100%)	0	100	100
8	c	120/136 (88%)	117 (98%)	3 (2%)	42	72
9	d	182/312 (58%)	181 (100%)	1 (0%)	81	89
10	e	47/62 (76%)	47 (100%)	0	100	100
11	g	103/115 (90%)	102 (99%)	1 (1%)	68	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	h	108/115 (94%)	108 (100%)	0	100	100
11	i	107/115 (93%)	107 (100%)	0	100	100
11	j	98/115 (85%)	98 (100%)	0	100	100
11	k	93/115 (81%)	93 (100%)	0	100	100
11	l	89/115 (77%)	89 (100%)	0	100	100
11	m	97/115 (84%)	97 (100%)	0	100	100
11	n	93/115 (81%)	93 (100%)	0	100	100
11	o	90/115 (78%)	90 (100%)	0	100	100
12	r	28/303 (9%)	28 (100%)	0	100	100
13	A	309/517 (60%)	308 (100%)	1 (0%)	86	91
13	C	388/517 (75%)	387 (100%)	1 (0%)	86	91
13	E	397/517 (77%)	396 (100%)	1 (0%)	86	91
15	a	282/713 (40%)	280 (99%)	2 (1%)	76	86
All	All	4179/6737 (62%)	4161 (100%)	18 (0%)	81	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	257	THR
1	F	303	MET
2	G	89	VAL
3	L	100	MET
4	M	61	ASP
8	c	46	TYR
8	c	66	ASN
8	c	171	MET
9	d	343	ILE
11	g	117	ASP
13	C	207	MET
13	E	37	MET
1	D	335	ASP
15	a	392	LYS
15	a	747	LYS
1	B	41	GLN
1	B	386	MET
13	A	227	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	409	GLN
3	J	110	ASN
2	K	102	ASN
8	c	66	ASN
9	d	48	HIS
11	n	123	ASN
13	C	546	ASN
13	E	487	GLN
15	a	23	GLN
15	a	410	GLN
1	B	153	ASN
13	A	433	GLN
13	A	447	HIS

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, 1 is monoatomic - leaving 3 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
17	ADP	E	701	18	28,29,29	1.37	5 (17%)	43,45,45	1.81	8 (18%)
16	PLM	b	402	7	6,7,17	0.43	0	5,6,17	0.54	0
16	PLM	b	401	7	15,16,17	0.35	0	14,15,17	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	E	701	18	-	5/16/32/32	0/3/3/3
16	PLM	b	402	7	-	3/5/5/15	-
16	PLM	b	401	7	-	7/14/14/15	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	701	ADP	C5-C4	4.40	1.46	1.39
17	E	701	ADP	C5-N7	-2.55	1.34	1.39
17	E	701	ADP	C5-C6	2.37	1.47	1.41
17	E	701	ADP	C8-N7	2.29	1.36	1.31
17	E	701	ADP	C4-N9	-2.05	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	701	ADP	C5-C4-N3	-5.74	118.81	126.72
17	E	701	ADP	N3-C4-N9	4.69	135.15	127.17
17	E	701	ADP	C2-N3-C4	3.75	120.99	111.83
17	E	701	ADP	N3-C2-N1	-3.53	123.23	128.58
17	E	701	ADP	C4-C5-N7	-3.13	107.00	110.58
17	E	701	ADP	C4-N9-C8	2.93	108.81	105.74
17	E	701	ADP	C5-N7-C8	2.51	107.39	103.45
17	E	701	ADP	N9-C8-N7	-2.24	110.75	113.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	b	401	PLM	C1-C2-C3-C4

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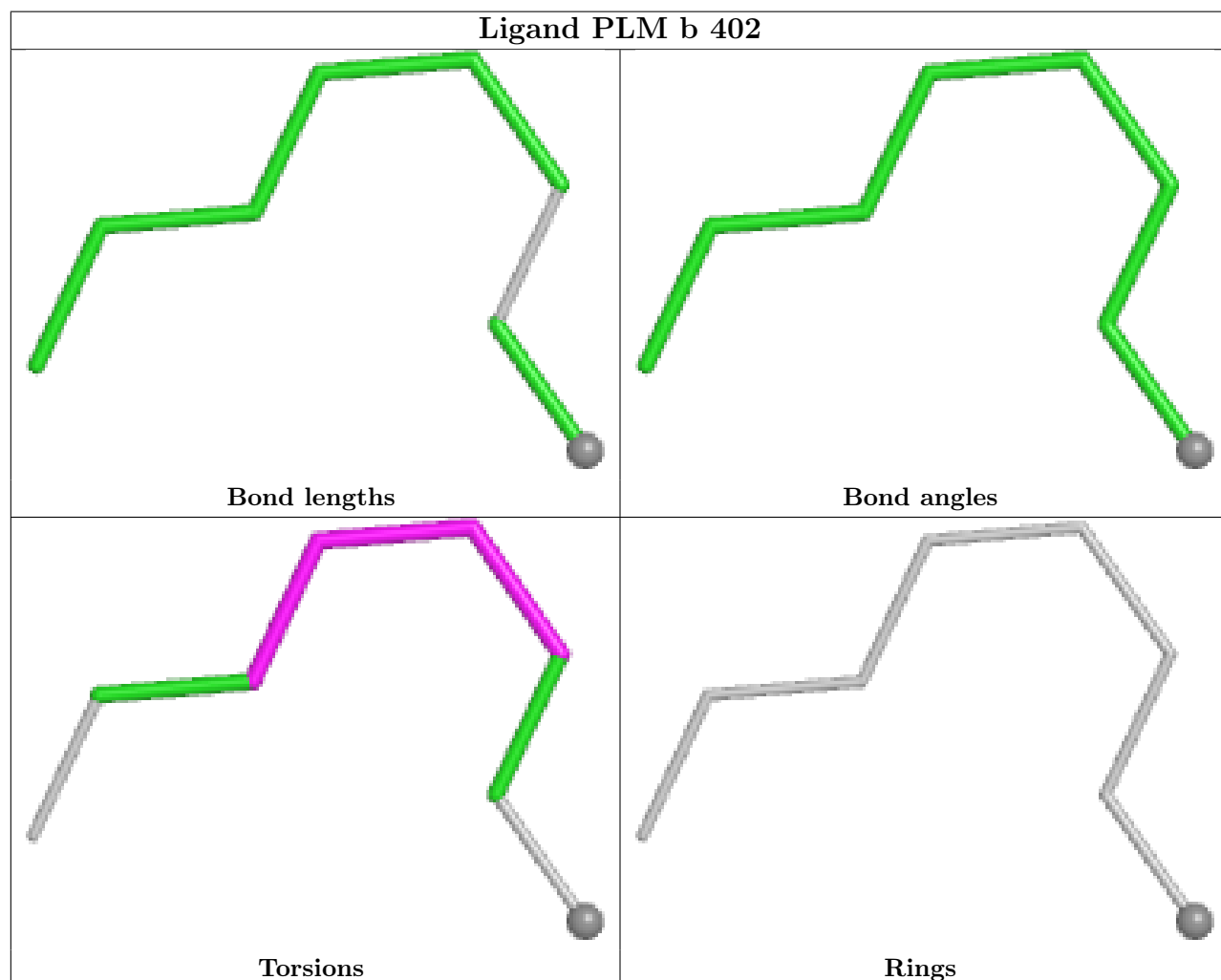
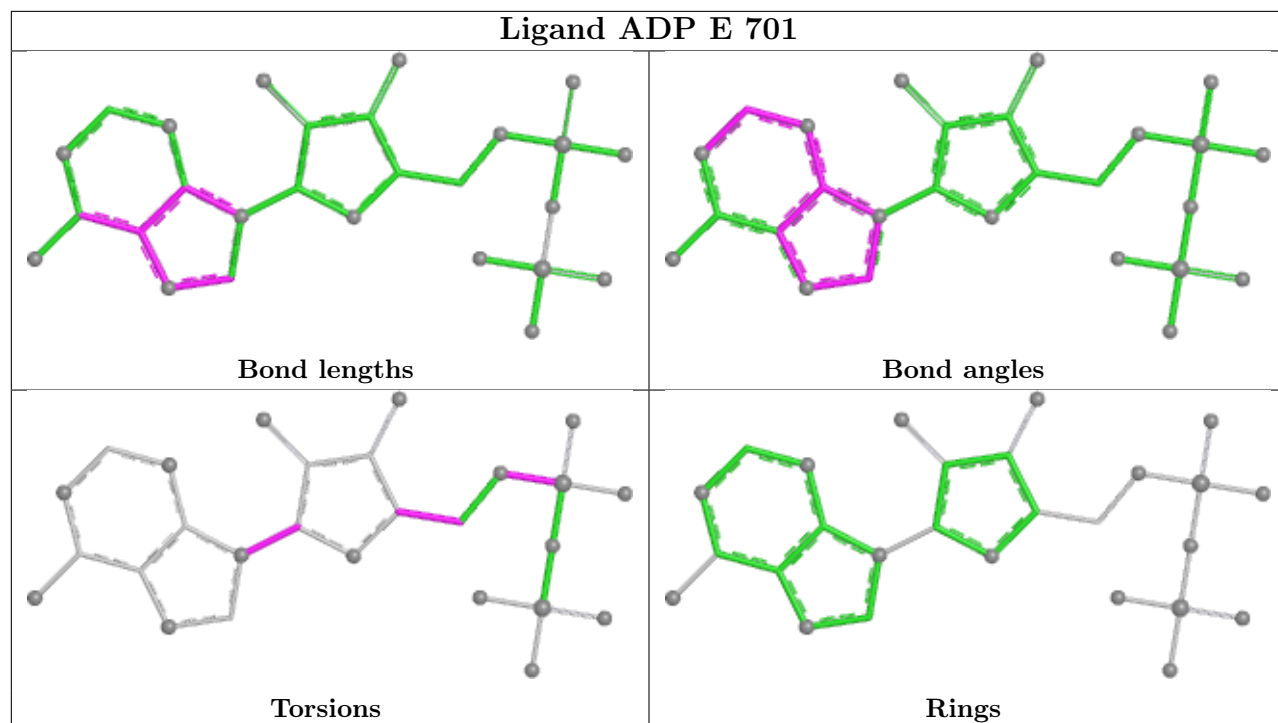
Mol	Chain	Res	Type	Atoms
17	E	701	ADP	C5'-O5'-PA-O2A
17	E	701	ADP	C5'-O5'-PA-O3A
17	E	701	ADP	O4'-C1'-N9-C4
16	b	401	PLM	C7-C8-C9-CA
16	b	401	PLM	C8-C9-CA-CB
16	b	402	PLM	C2-C3-C4-C5
17	E	701	ADP	O4'-C1'-N9-C8
16	b	401	PLM	C2-C3-C4-C5
16	b	401	PLM	C9-CA-CB-CC
16	b	402	PLM	C3-C4-C5-C6
16	b	401	PLM	C6-C7-C8-C9
16	b	401	PLM	CD-CE-CF-CG
16	b	402	PLM	C1-C2-C3-C4
17	E	701	ADP	O4'-C4'-C5'-O5'

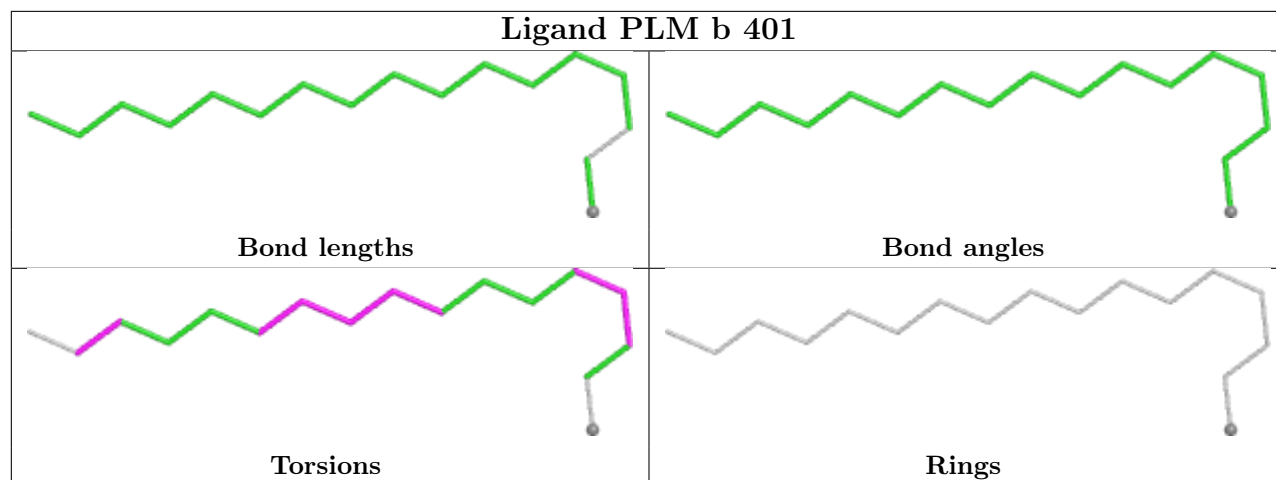
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	401	PLM	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

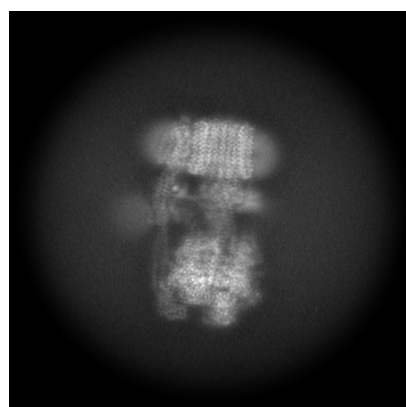
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77786. These allow visual inspection of the internal detail of the map and identification of artifacts.

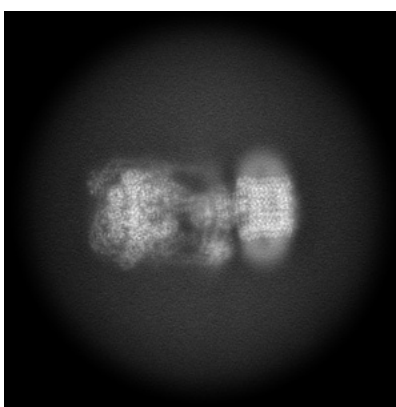
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

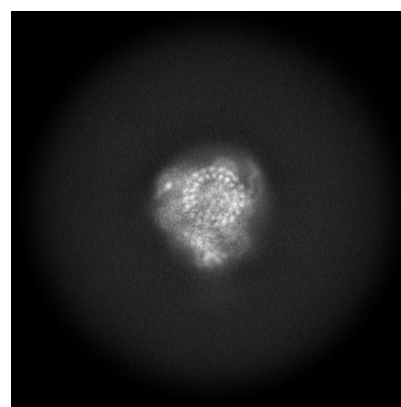
6.1.1 Primary map



X



Y

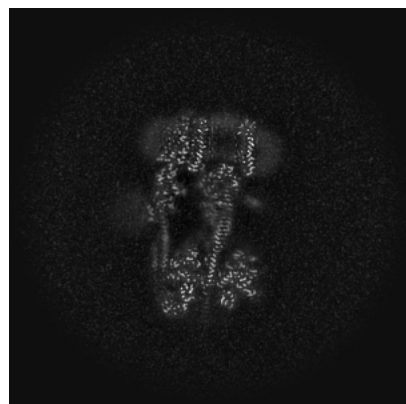


Z

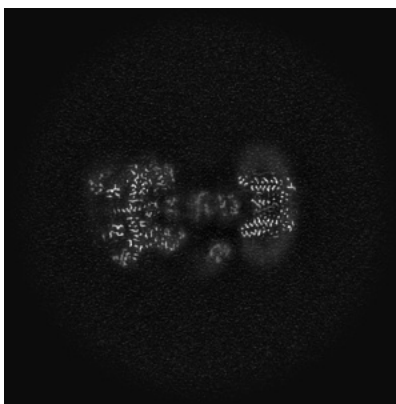
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

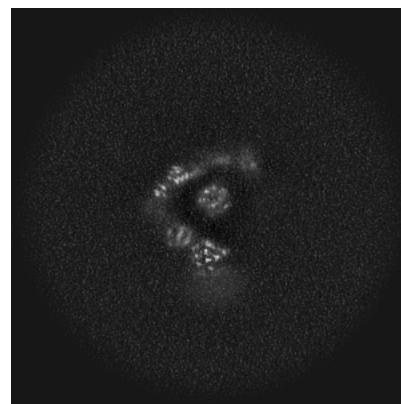
6.2.1 Primary map



X Index: 256



Y Index: 256

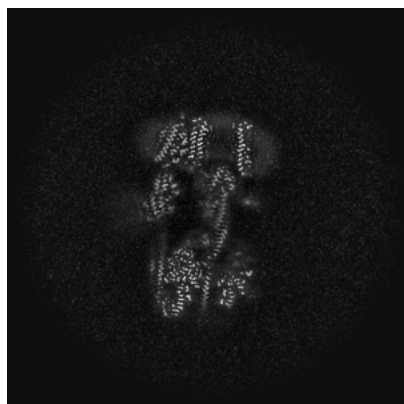


Z Index: 256

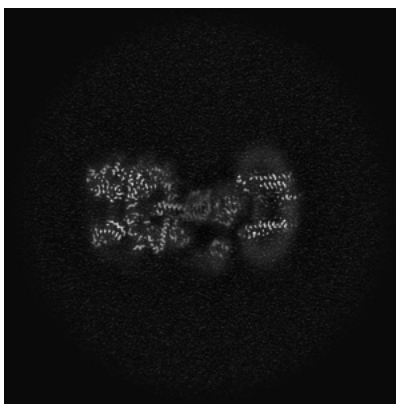
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

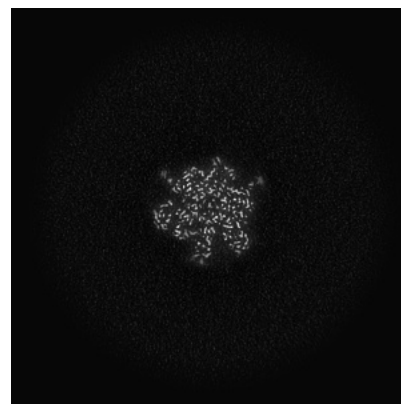
6.3.1 Primary map



X Index: 252



Y Index: 266

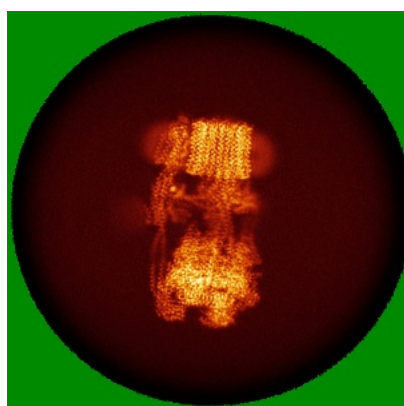


Z Index: 164

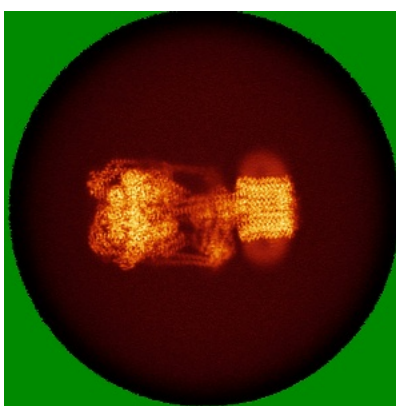
The images above show the largest variance slices of the map in three orthogonal directions.

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

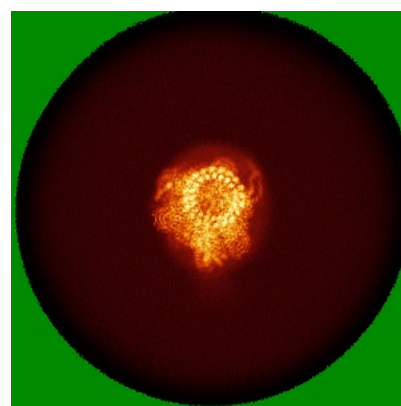
6.4.1 Primary map



X



Y



Z

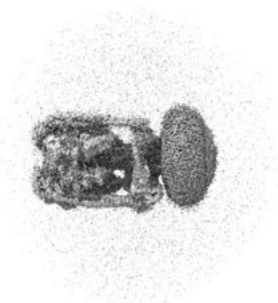
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

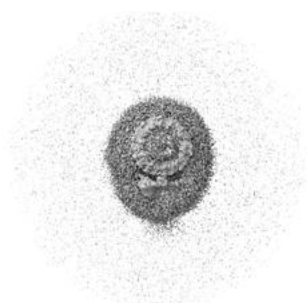
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

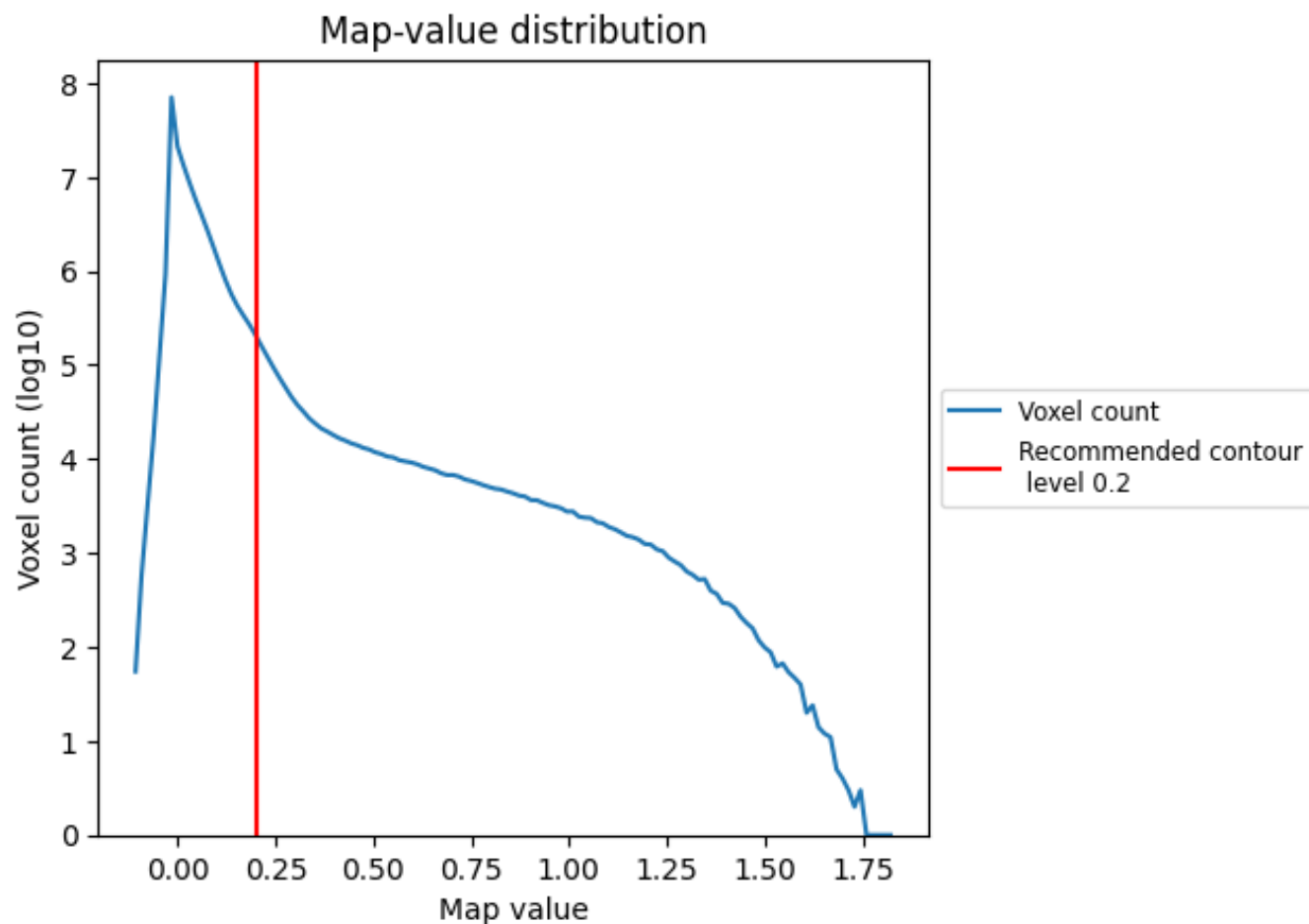
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

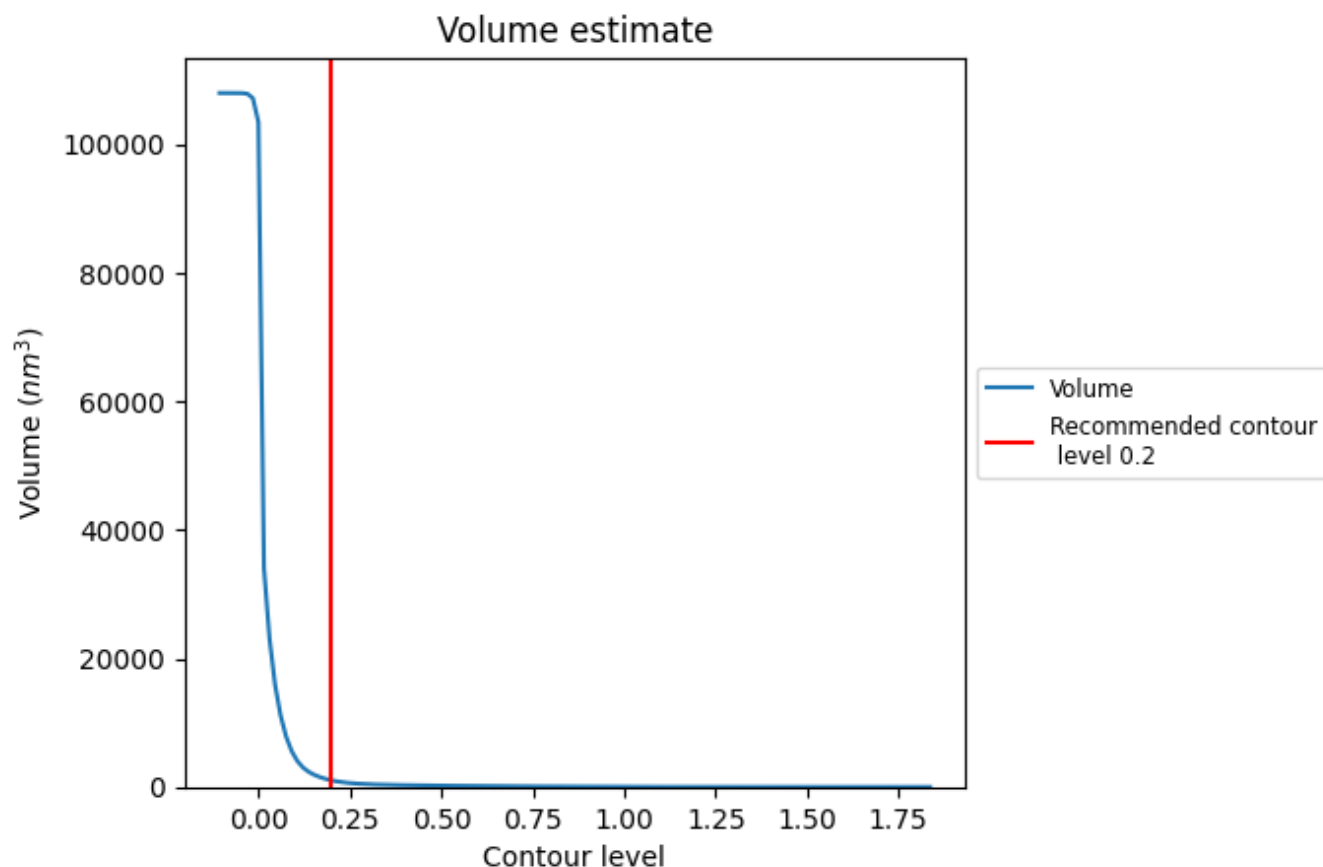
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

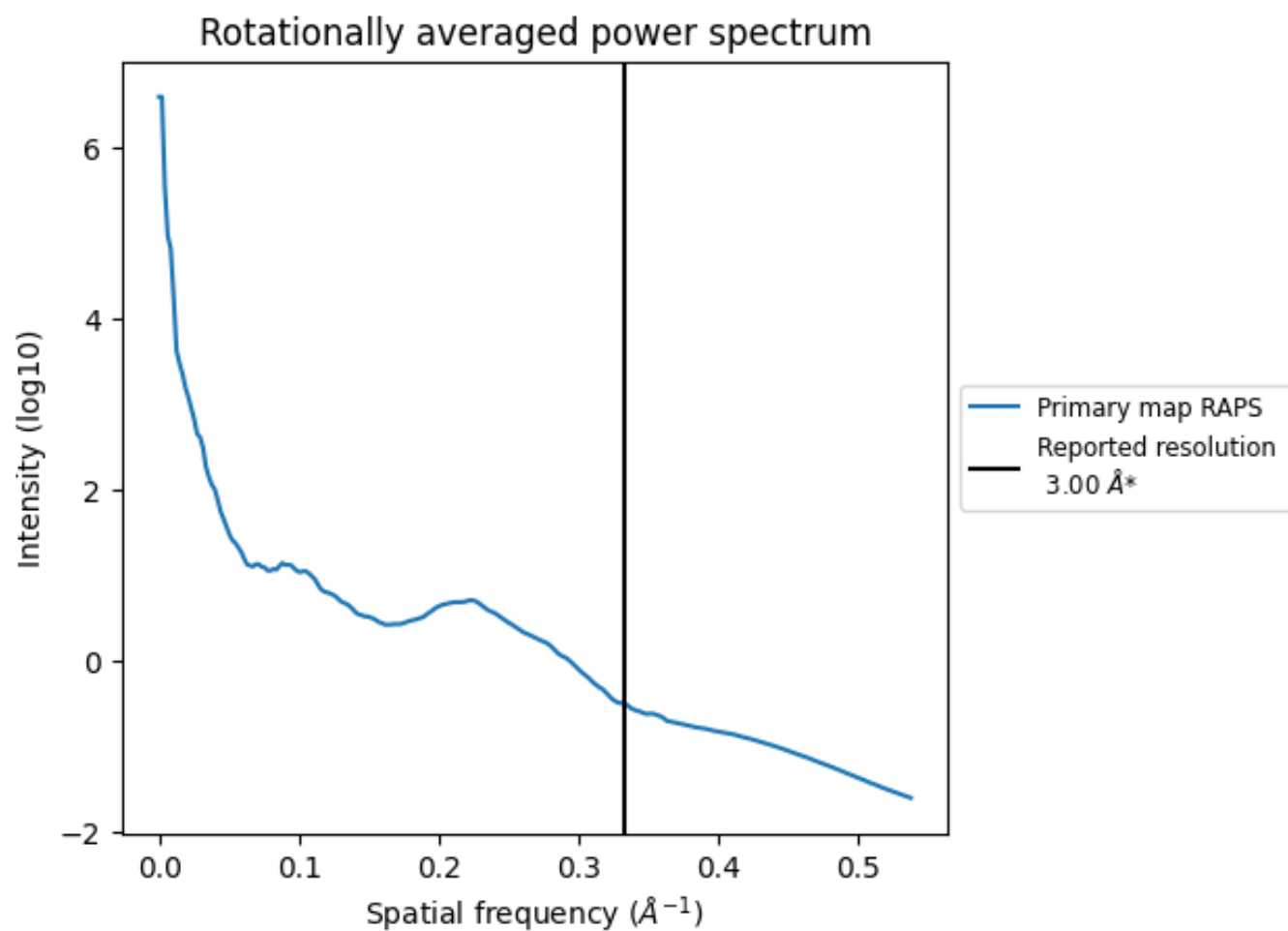
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1022 nm^3 ; this corresponds to an approximate mass of 923 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 0.333 Å⁻¹

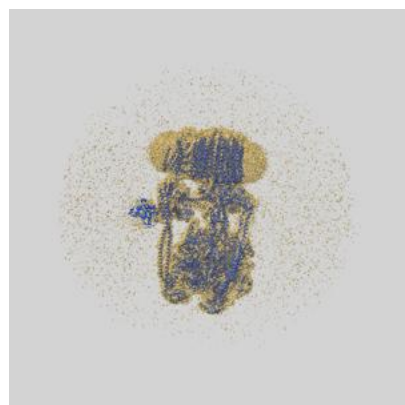
8 Fourier-Shell correlation ⓘ

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

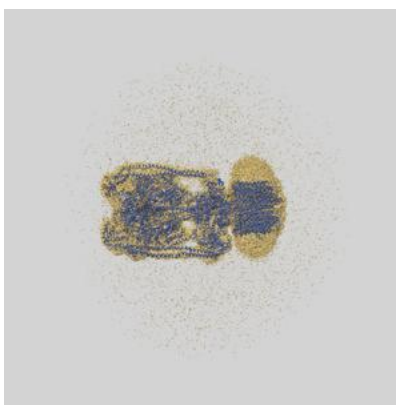
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77786 and PDB model 36QU. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

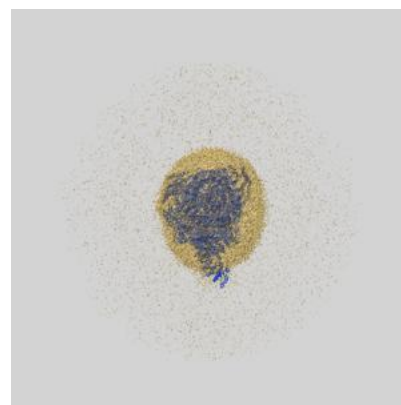
9.1 Map-model overlay [i](#)



X



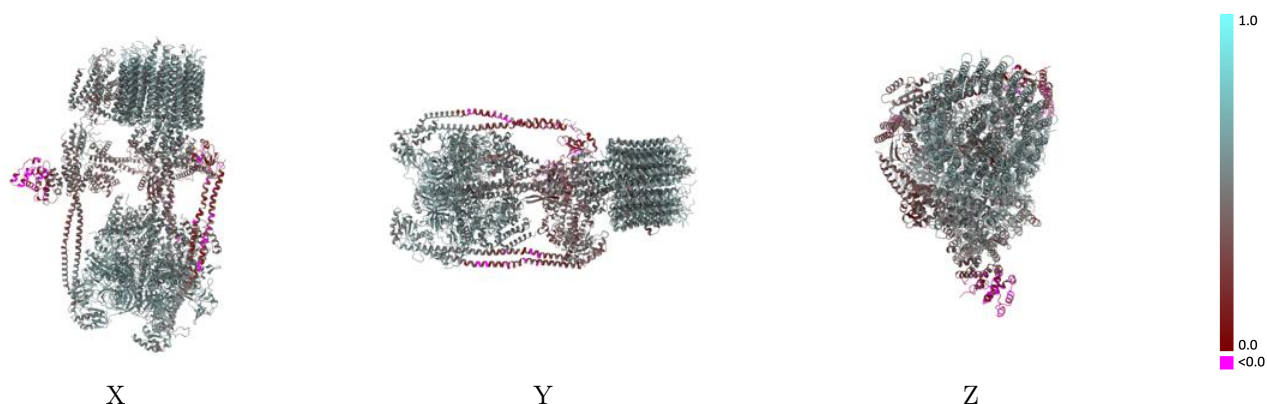
Y



Z

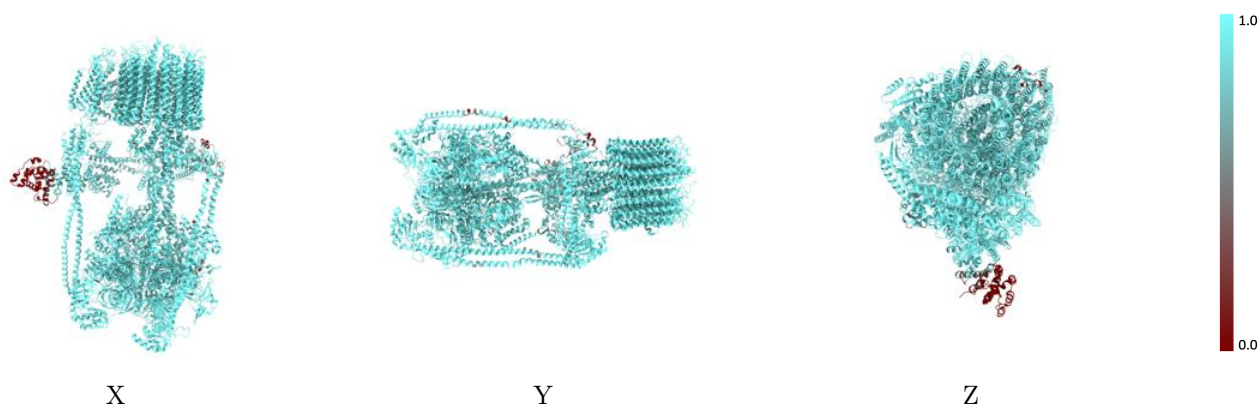
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



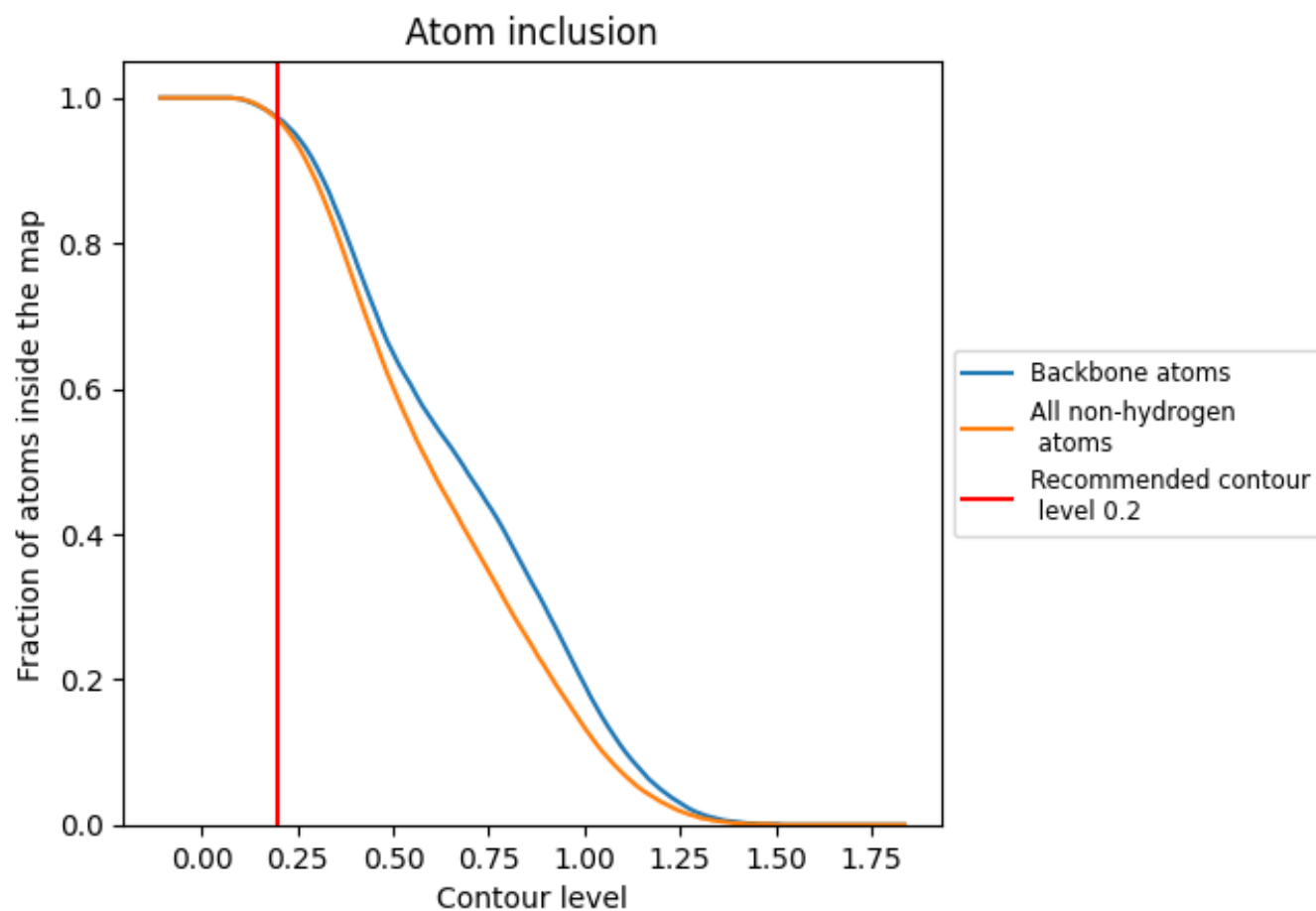
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9700	 0.5070
A	 0.9920	 0.5290
B	 0.9930	 0.5640
C	 0.9890	 0.5410
D	 0.9960	 0.5660
E	 0.9960	 0.5680
F	 0.9870	 0.5500
G	 0.9700	 0.4720
H	 0.8920	 0.3070
I	 0.9820	 0.4740
J	 0.9480	 0.3390
K	 0.9800	 0.4930
L	 0.9530	 0.4040
M	 0.9680	 0.4670
N	 0.9580	 0.3540
O	 0.9000	 0.3460
P	 0.6200	 0.2650
a	 0.9890	 0.4650
b	 0.9790	 0.5380
c	 0.9960	 0.5410
d	 0.9780	 0.5030
e	 0.9890	 0.4740
g	 0.9980	 0.5490
h	 0.9960	 0.5570
i	 0.9960	 0.5590
j	 0.9960	 0.5530
k	 0.9950	 0.5580
l	 0.9980	 0.5590
m	 0.9970	 0.5560
n	 0.9940	 0.5510
o	 0.9950	 0.5510
r	 0.9760	 0.5270

