



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:32 AM UTC

PDB ID : 6XBY / pdb_00006xby
EMDB ID : EMD-22122
Title : Cryo-EM structure of V-ATPase from bovine brain, state 2
Authors : Wang, R.; Li, X.
Deposited on : 2020-06-07
Resolution : 3.79 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

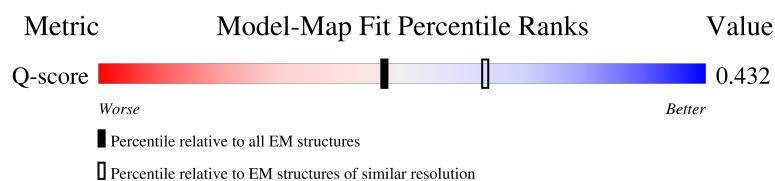
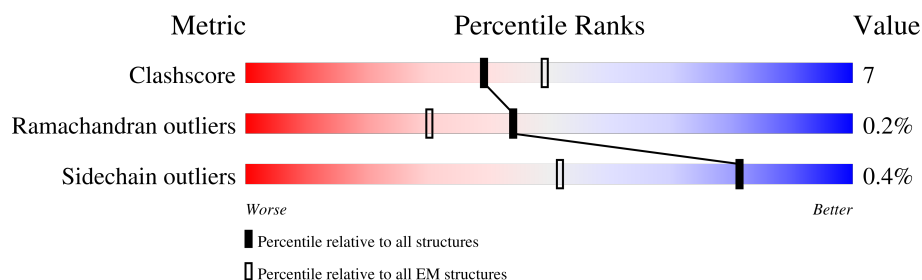
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.79 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.



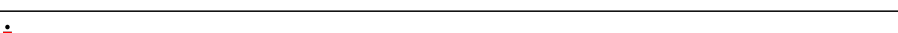
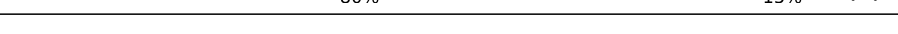
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10018 (3.29 - 4.29)

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

Mol	Chain	Length	Quality of chain
1	A	617	 82% 15% •
1	B	617	 80% 13% 6%
1	C	617	 78% 16% • 6%
2	D	511	 76% 13% •• 11%

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Mol	Chain	Length	Quality of chain
2	E	511	
2	F	511	
3	G	382	
4	H	247	
5	I	226	
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	P	465	
9	a	838	
10	b	205	
11	d	351	
12	c	155	
12	g	155	
12	k	155	
12	l	155	
12	m	155	
12	n	155	
12	o	155	
12	p	155	
12	q	155	
13	s	468	

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Mol	Chain	Length	Quality of chain
14	r	351	 8% . . 88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	NAG	s	507	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 57516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	597	Total	C	N	O	S	0	0
			4628	2935	781	884	28		
1	B	577	Total	C	N	O	S	0	0
			4484	2847	756	853	28		
1	C	583	Total	C	N	O	S	0	0
			4530	2877	763	863	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	457	Total	C	N	O	S	0	0
			3581	2268	615	678	20		
2	E	457	Total	C	N	O	S	0	0
			3576	2268	612	676	20		
2	F	454	Total	C	N	O	S	0	0
			3556	2256	609	671	20		

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	343	Total	C	N	O	S	0	0
			1892	1162	359	369	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	212	Total	C	N	O	S	0	0
			1708	1084	308	311	5		

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	218	Total	C	N	O	S	0	0
			1573	980	293	294	6		
5	J	218	Total	C	N	O	S	0	0
			1577	983	294	294	6		
5	K	220	Total	C	N	O	S	0	0
			1583	986	295	296	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	101	Total	C	N	O	S	0	0
			801	508	138	154	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	108	Total	C	N	O	S	0	0
			665	395	138	129	3		
7	N	108	Total	C	N	O	S	0	0
			661	393	138	127	3		
7	O	108	Total	C	N	O	S	0	0
			665	395	138	129	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	370	Total	C	N	O	0	0
			1837	1097	370	370		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	494	Total	C	N	O	S	0	0
			3917	2507	682	705	23		

- Molecule 10 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

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

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	336	Total	C	N	O	S	0	0
			2740	1771	447	508	14		

- Molecule 12 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		
12	p	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		
12	c	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	g	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	k	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	l	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	m	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	n	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	o	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		

- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	205	Total	C	N	O	S	0	0
			1668	1083	264	312	9		

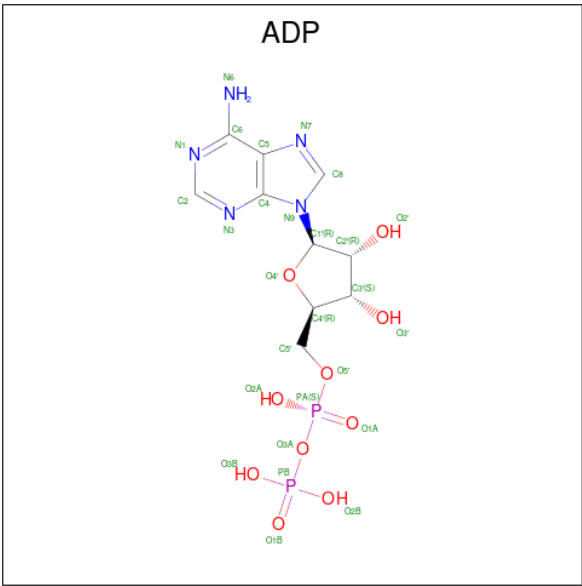
- Molecule 14 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	r	43	Total	C	N	O	S	0	0
			358	245	51	59	3		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

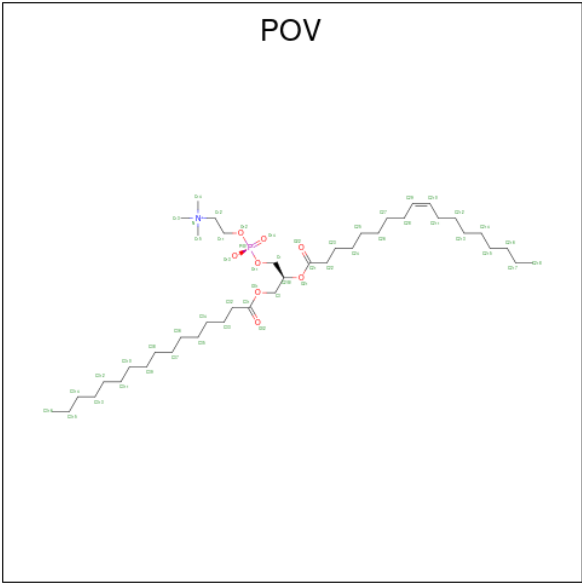
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Mg	0
			1	1	

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

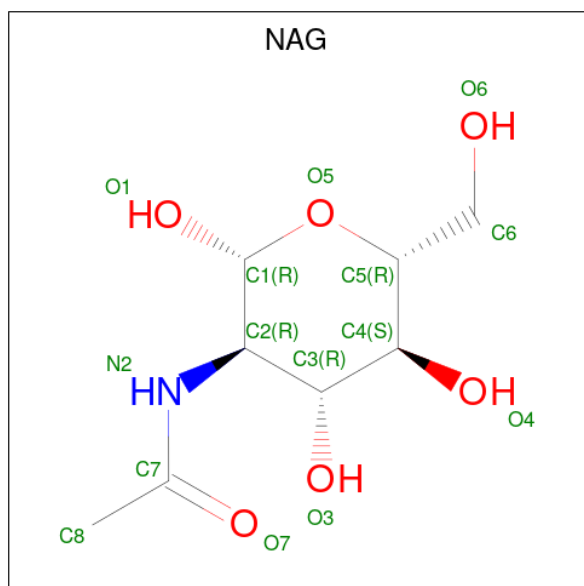
- Molecule 17 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



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Mol	Chain	Residues	Atoms					AltConf
17	l	1	Total	C	N	O	P	0
			42	32	1	8	1	
17	o	1	Total	C	N	O	P	0
			44	34	1	8	1	
17	s	1	Total	C	N	O	P	0
			46	36	1	8	1	
17	r	1	Total	C	N	O	P	0
			43	33	1	8	1	
17	r	1	Total	C	N	O	P	0
			42	32	1	8	1	
17	r	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
18	s	1	Total	C	N	O	0
			14	8	1	5	
18	s	1	Total	C	N	O	0
			14	8	1	5	
18	s	1	Total	C	N	O	0
			14	8	1	5	
18	s	1	Total	C	N	O	0
			14	8	1	5	
18	s	1	Total	C	N	O	0
			14	8	1	5	

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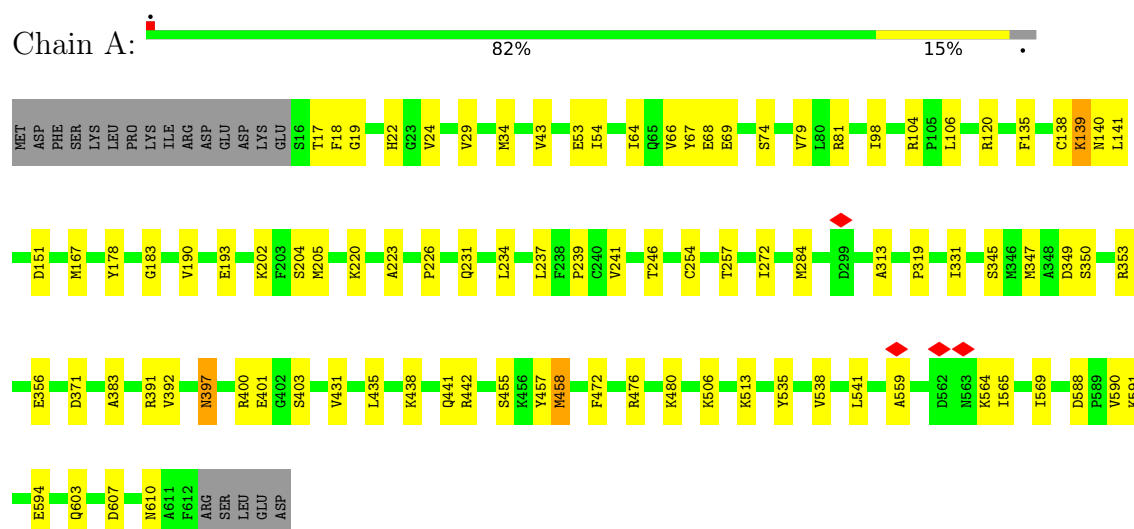
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	s	1	14	8	1	5	0

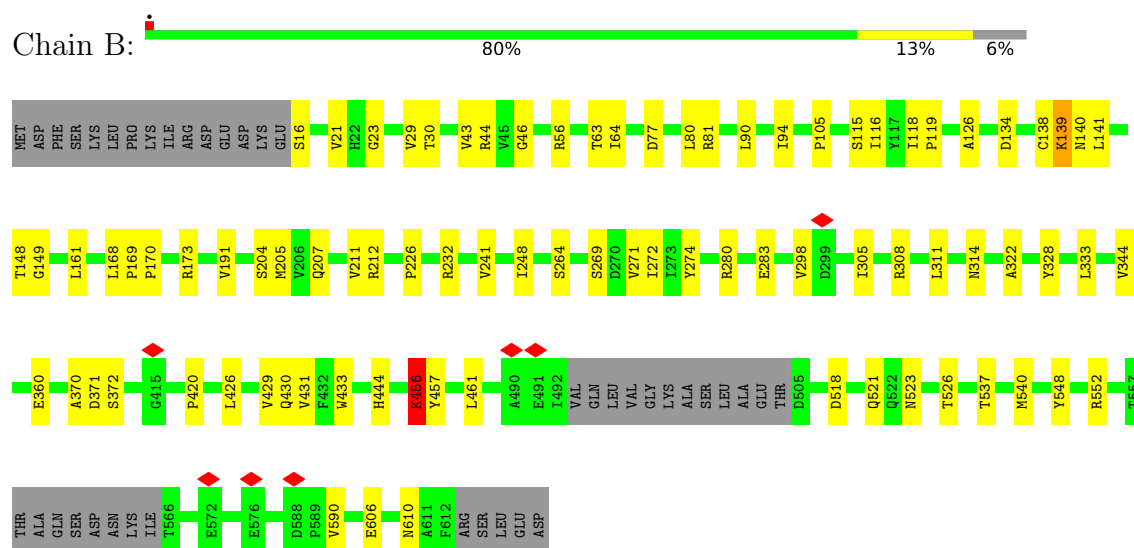
3 Residue-property plots

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

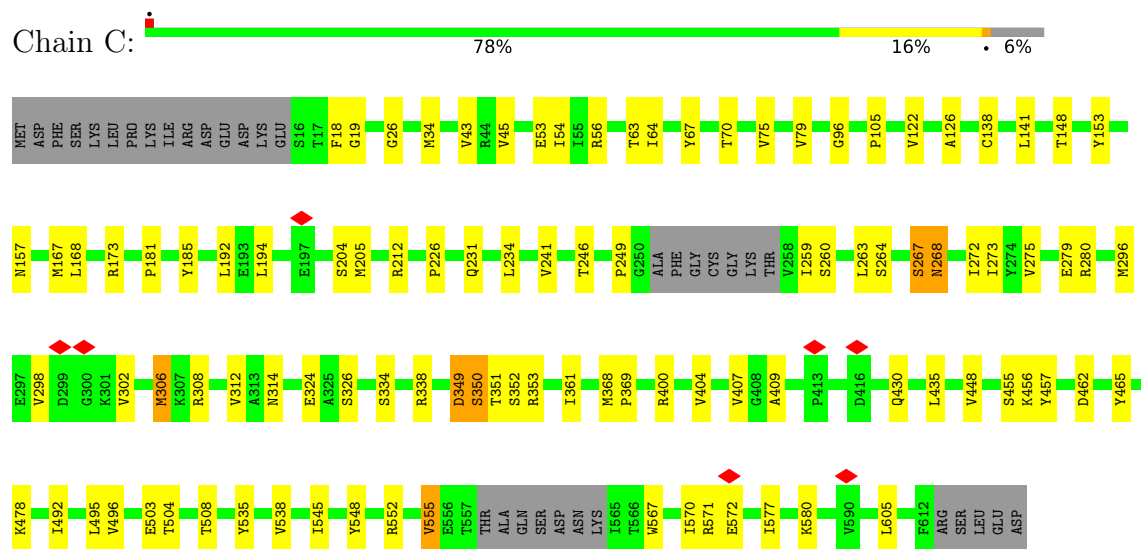
- Molecule 1: V-type proton ATPase catalytic subunit A



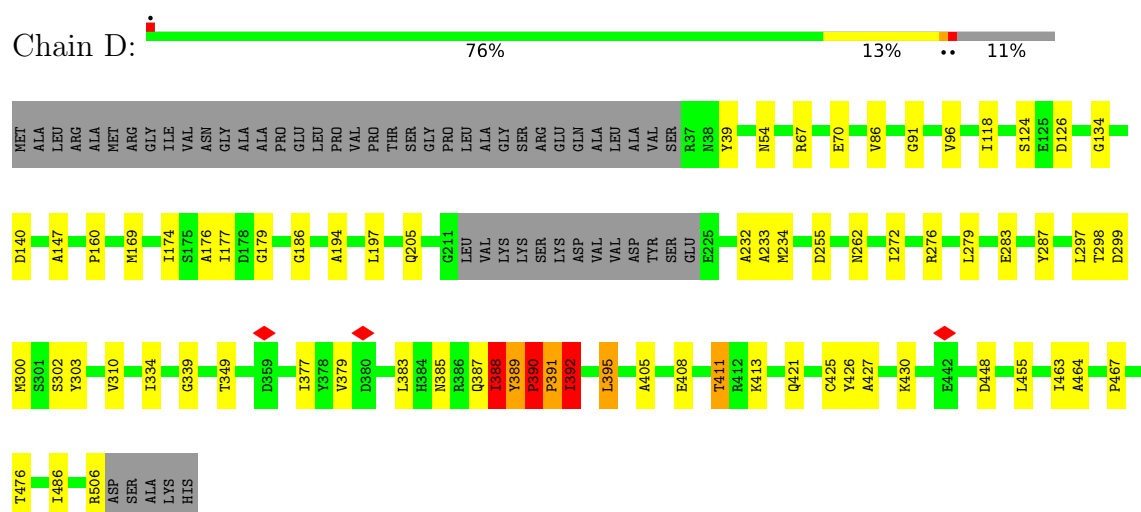
- Molecule 1: V-type proton ATPase catalytic subunit A



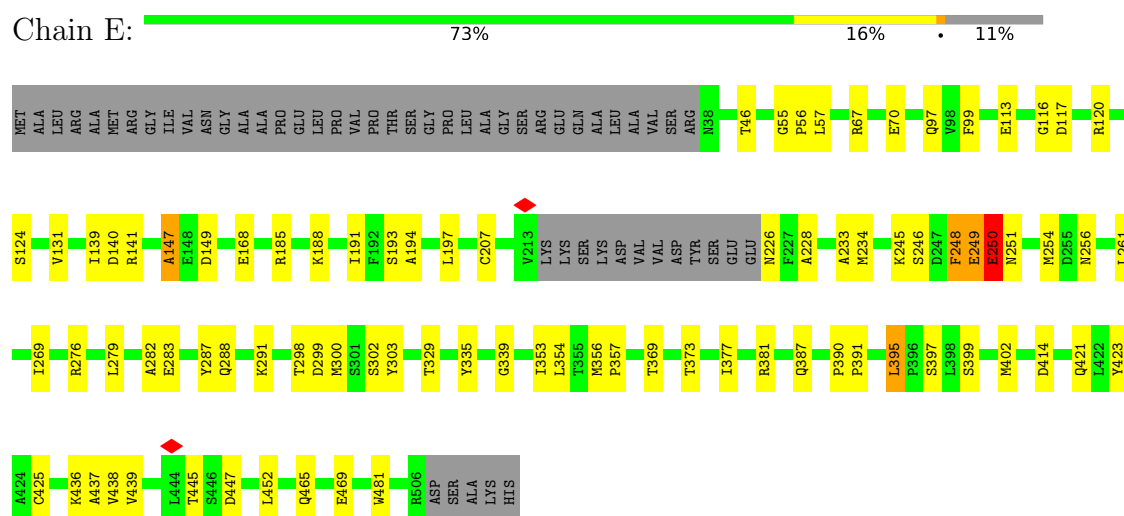
- Molecule 1: V-type proton ATPase catalytic subunit A



- Molecule 2: V-type proton ATPase subunit B, brain isoform

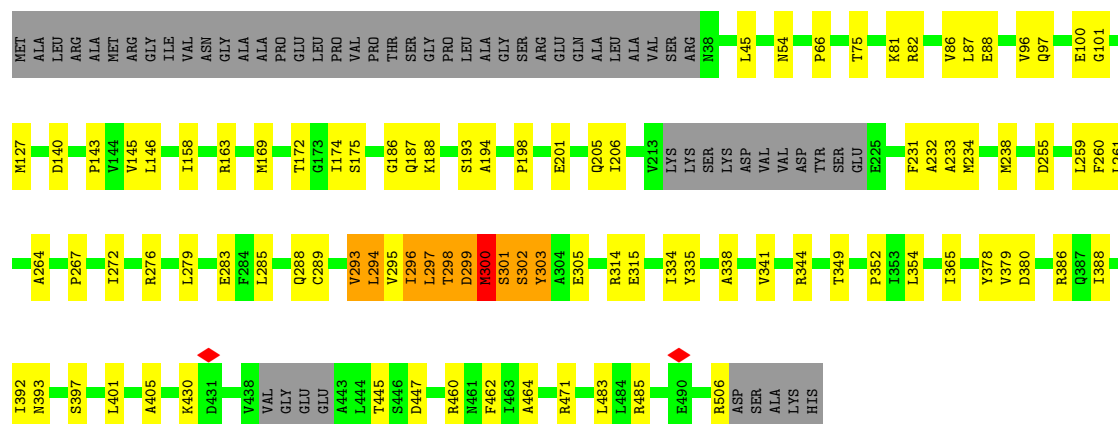


- Molecule 2: V-type proton ATPase subunit B, brain isoform



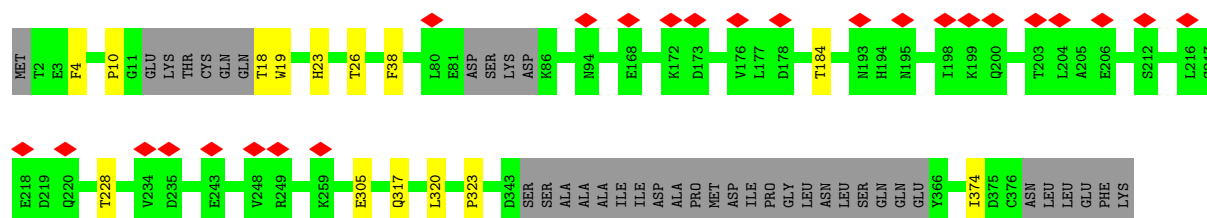
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain F:  70% 16% 11%



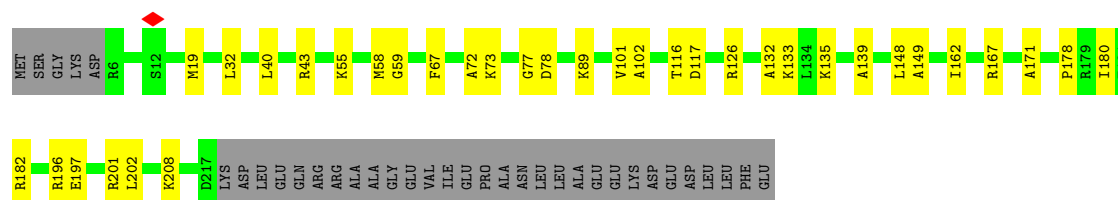
- Molecule 3: V-type proton ATPase subunit C 1

Chain G:  7% 86% 10%



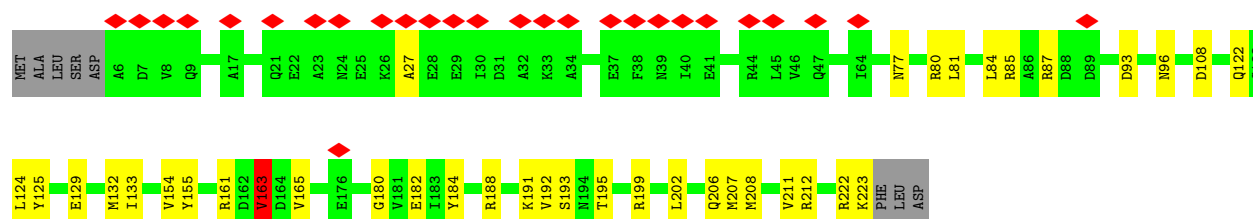
- Molecule 4: V-type proton ATPase subunit D

Chain H:  72% 14% 14%



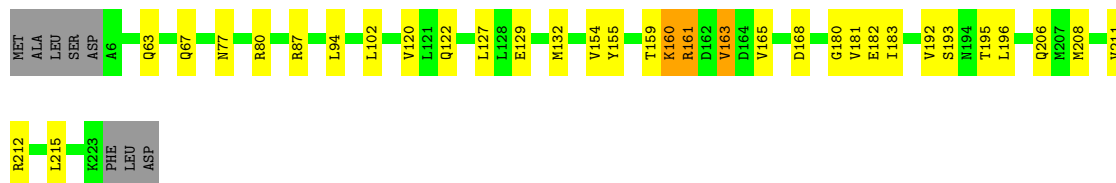
- Molecule 5: V-type proton ATPase subunit E 1

Chain I:  12% 80% 16%

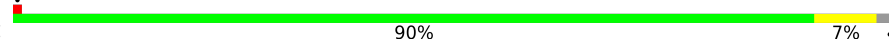


- Molecule 5: V-type proton ATPase subunit E 1

Chain J:  82% 13% ..



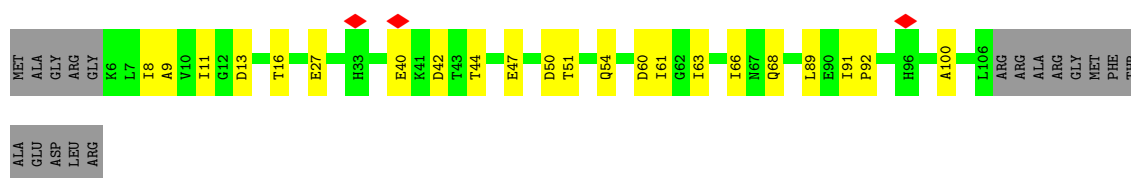
- Molecule 5: V-type proton ATPase subunit E 1

Chain K:  90% 7% .



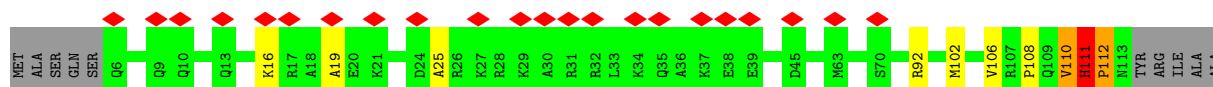
- Molecule 6: V-type proton ATPase subunit F

Chain L:  66% 18% 15%



- Molecule 7: V-type proton ATPase subunit G

Chain M:  19% 83% 6% .. 8%



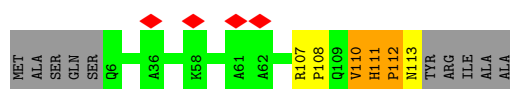
- Molecule 7: V-type proton ATPase subunit G

Chain N:  89% 8% .



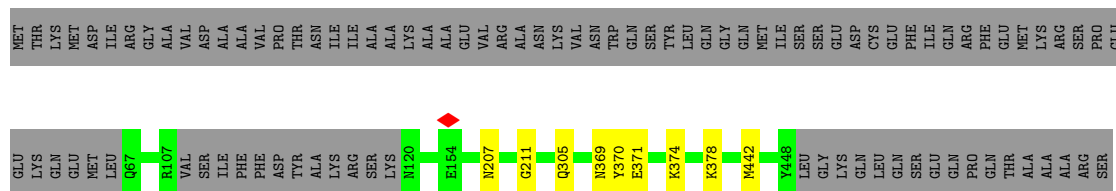
- Molecule 7: V-type proton ATPase subunit G

Chain O:  86% 8% ..

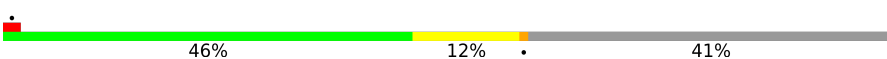


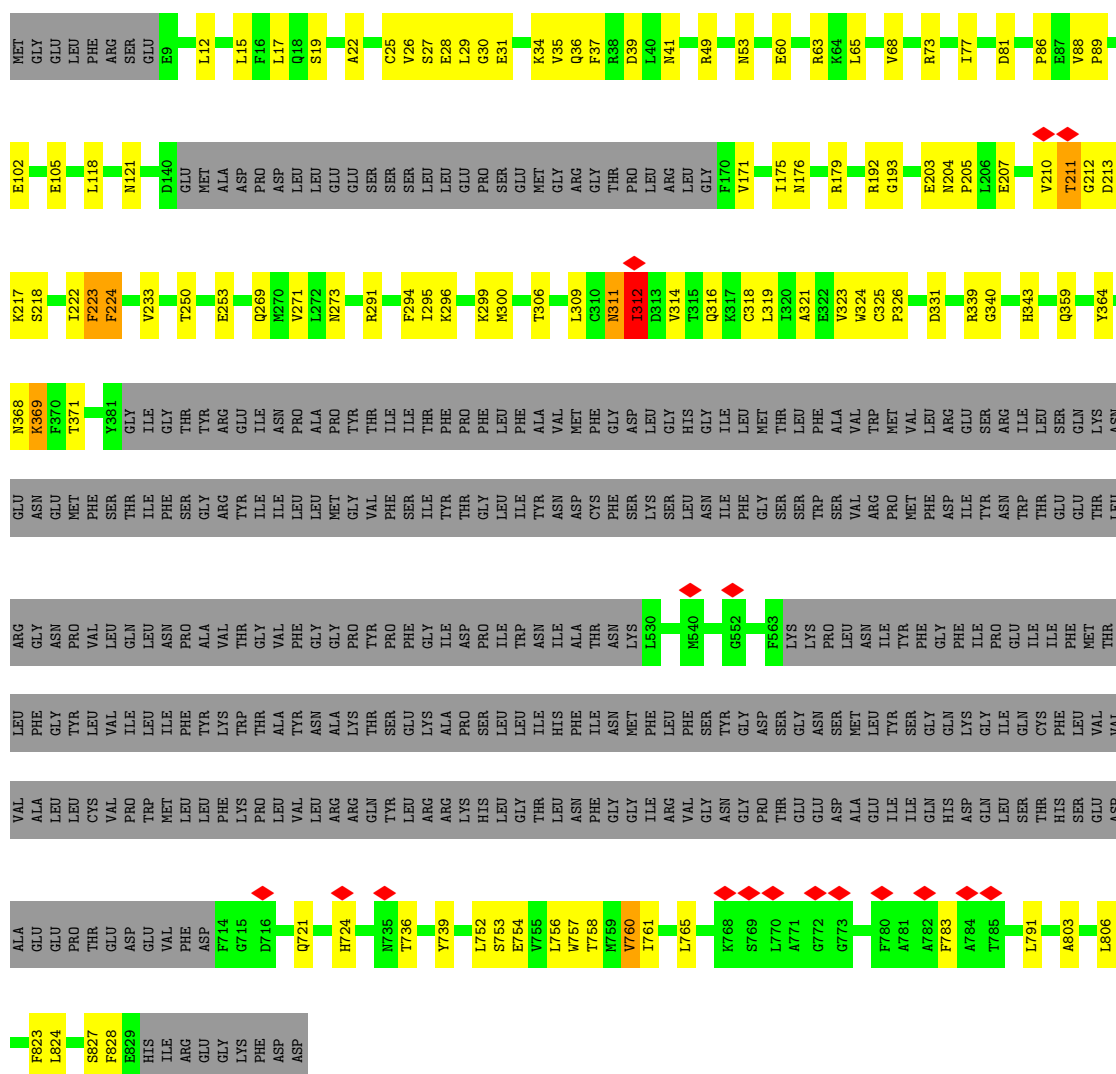
- Molecule 8: V-type proton ATPase subunit H

Chain P:  78% 20%



- Molecule 9: V-type proton ATPase subunit a

Chain a:  46% 12% 41%

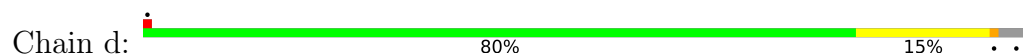


- Molecule 10: V-type proton ATPase 21 kDa proteolipid subunit

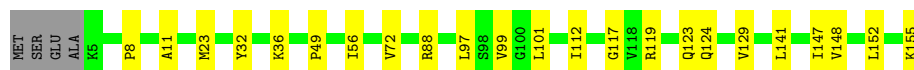
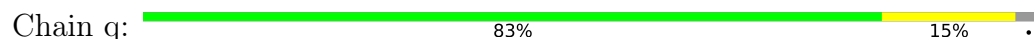
Chain b:  85% 14%



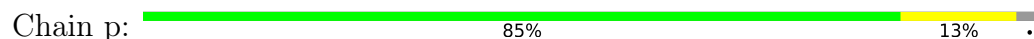
- Molecule 11: V-type proton ATPase subunit d 1



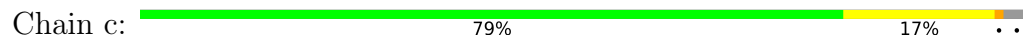
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit



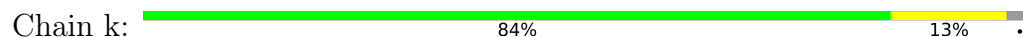
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit



M315	M316	G317	L318	A319	L320	I323	M332	G335	TYR	ASP	SER	TYR	GLY	ILE	TYR	ASN	GLN	LYS	ILE	ARG	MET	ASP
LEU	ILE	ASP	ALA	GLN	LYS	PHE	ASP	ASP	MET	ASP	TYR	GLY	LEU	LEU	ASP	ASN	GLY	VAL	ASP	GLY	ASP	
ASP	LEU	PHE	LEU	SER	GLU	GLN	VAL	ILE	SER	ASP	SER	LEU	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ALA	LEU	VAL	LEU	SER	GLU	LEU	GLN	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
GLN	LEU	VAL	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
LYS	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
PHE	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ILE	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP	ASP	GLY	ASP	GLY	ASP	ASP	
ASP	LEU	GLU	LEU	SER	GLU	GLN	VAL	ASP	SER	ASP	TYR	GLY	LEU	LEU	ASP							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.395	Depositor
Minimum map value	-15.945	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.102	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	424.83002, 424.83002, 424.83002	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.833, 0.833, 0.833	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, POV, 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	3/4724 (0.1%)	0.59	5/6398 (0.1%)
1	B	0.27	0/4578	0.59	5/6197 (0.1%)
1	C	0.36	1/4623 (0.0%)	0.68	8/6260 (0.1%)
2	D	0.39	3/3652 (0.1%)	0.69	6/4949 (0.1%)
2	E	0.43	5/3647 (0.1%)	0.67	3/4944 (0.1%)
2	F	0.66	17/3626 (0.5%)	0.65	7/4914 (0.1%)
3	G	0.16	0/1906	0.50	0/2644
4	H	0.20	0/1726	1.07	4/2309 (0.2%)
5	I	0.40	0/1584	0.65	1/2144 (0.0%)
5	J	0.33	0/1588	0.69	6/2148 (0.3%)
5	K	0.21	0/1594	0.52	0/2158
6	L	0.18	0/814	0.55	0/1103
7	M	0.68	2/667 (0.3%)	0.96	4/912 (0.4%)
7	N	0.17	0/663	0.58	0/907
7	O	0.52	1/667 (0.1%)	1.06	8/912 (0.9%)
8	P	0.16	0/1835	0.57	0/2558
9	a	0.26	0/3995	0.70	5/5401 (0.1%)
10	b	0.44	3/1532 (0.2%)	0.54	0/2083
11	d	0.21	0/2801	0.61	3/3788 (0.1%)
12	c	0.19	0/1079	0.52	0/1459
12	g	0.17	0/1079	0.47	0/1459
12	k	0.17	0/1079	0.48	0/1459
12	l	0.18	0/1079	0.53	2/1459 (0.1%)
12	m	0.20	0/1079	0.51	0/1459
12	n	0.19	0/1079	0.51	0/1459
12	o	0.18	0/1088	0.47	0/1470
12	p	0.18	0/1088	0.49	0/1470
12	q	0.18	0/1088	0.53	1/1470 (0.1%)
13	s	0.43	0/1720	0.77	2/2341 (0.1%)
14	r	1.69	11/370 (3.0%)	1.18	6/508 (1.2%)
All	All	0.37	46/58050 (0.1%)	0.65	76/78742 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
2	D	0	1
2	E	0	1
9	a	0	2
All	All	0	7

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	r	319	ALA	CA-C	-15.42	1.32	1.52
7	M	112	PRO	N-CD	14.11	1.67	1.47
14	r	319	ALA	C-O	-13.69	1.07	1.24
10	b	22	VAL	C-N	11.58	1.50	1.33
14	r	318	LEU	C-O	-11.56	1.09	1.24

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	72	ALA	N-CA-C	38.30	152.72	110.97
4	H	72	ALA	CB-CA-C	-14.30	88.94	110.96
7	M	110	VAL	N-CA-C	12.40	125.13	113.10
2	D	390	PRO	N-CA-C	-11.35	96.85	110.70
7	O	110	VAL	N-CA-C	-10.30	87.92	109.34

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	LYS	Peptide
1	C	267	SER	Peptide
1	C	455	SER	Mainchain
2	D	411	THR	Peptide
2	E	387	GLN	Peptide

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	4628	0	4611	65	0
1	B	4484	0	4458	53	0
1	C	4530	0	4516	70	0
2	D	3581	0	3571	81	0
2	E	3576	0	3574	61	0
2	F	3556	0	3555	64	0
3	G	1892	0	1090	10	0
4	H	1708	0	1816	26	0
5	I	1573	0	1497	45	0
5	J	1577	0	1508	25	0
5	K	1583	0	1501	11	0
6	L	801	0	802	14	0
7	M	665	0	507	13	0
7	N	661	0	503	2	0
7	O	665	0	507	7	0
8	P	1837	0	811	5	0
9	a	3917	0	3829	86	0
10	b	1498	0	1548	28	0
11	d	2740	0	2685	43	0
12	c	1064	0	1132	21	0
12	g	1064	0	1132	13	0
12	k	1064	0	1132	18	0
12	l	1064	0	1132	13	0
12	m	1064	0	1132	14	0
12	n	1064	0	1132	14	0
12	o	1073	0	1145	14	0
12	p	1073	0	1145	13	0
12	q	1073	0	1145	23	0
13	s	1668	0	1554	53	0
14	r	358	0	353	11	0
15	A	1	0	0	0	0
16	D	27	0	12	0	0
17	b	44	0	60	10	0
17	l	42	0	56	0	0
17	o	44	0	60	2	0
17	r	127	0	171	3	0
17	s	46	0	64	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	s	84	0	78	14	0
All	All	57516	0	55524	816	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.

The worst 5 of 816 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)
2:D:383:LEU:CB	2:D:388:ILE:CD1	1.83	1.48
2:D:383:LEU:HB3	2:D:388:ILE:CD1	1.40	1.46
5:I:155:TYR:CE2	5:I:163:VAL:CG1	1.98	1.44
5:I:155:TYR:CE2	5:I:163:VAL:HG11	1.57	1.37
2:D:233:ALA:HA	2:D:298:THR:CG2	1.54	1.37

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	595/617 (96%)	565 (95%)	29 (5%)	1 (0%)	43	73
1	B	571/617 (92%)	533 (93%)	37 (6%)	1 (0%)	43	73
1	C	577/617 (94%)	539 (93%)	37 (6%)	1 (0%)	43	73
2	D	453/511 (89%)	422 (93%)	31 (7%)	0	100	100
2	E	453/511 (89%)	416 (92%)	37 (8%)	0	100	100
2	F	448/511 (88%)	418 (93%)	29 (6%)	1 (0%)	43	73
3	G	335/382 (88%)	315 (94%)	20 (6%)	0	100	100
4	H	210/247 (85%)	199 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	216/226 (96%)	207 (96%)	8 (4%)	1 (0%)	24	57
5	J	216/226 (96%)	209 (97%)	7 (3%)	0	100	100
5	K	218/226 (96%)	209 (96%)	9 (4%)	0	100	100
6	L	99/119 (83%)	89 (90%)	10 (10%)	0	100	100
7	M	106/118 (90%)	102 (96%)	3 (3%)	1 (1%)	14	45
7	N	106/118 (90%)	99 (93%)	7 (7%)	0	100	100
7	O	106/118 (90%)	99 (93%)	6 (6%)	1 (1%)	14	45
8	P	366/465 (79%)	340 (93%)	25 (7%)	1 (0%)	36	67
9	a	486/838 (58%)	444 (91%)	39 (8%)	3 (1%)	21	54
10	b	201/205 (98%)	193 (96%)	8 (4%)	0	100	100
11	d	330/351 (94%)	309 (94%)	20 (6%)	1 (0%)	36	67
12	c	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
12	g	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	k	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
12	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	m	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	n	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	o	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
12	p	149/155 (96%)	148 (99%)	1 (1%)	0	100	100
12	q	149/155 (96%)	148 (99%)	1 (1%)	0	100	100
13	s	203/468 (43%)	172 (85%)	31 (15%)	0	100	100
14	r	41/351 (12%)	39 (95%)	2 (5%)	0	100	100
All	All	7671/9237 (83%)	7240 (94%)	419 (6%)	12 (0%)	44	73

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	ASN
5	I	163	VAL
7	M	111	HIS
2	F	300	MET
7	O	110	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	504/524 (96%)	504 (100%)	0	100	100
1	B	488/524 (93%)	487 (100%)	1 (0%)	87	87
1	C	494/524 (94%)	489 (99%)	5 (1%)	68	74
2	D	390/432 (90%)	384 (98%)	6 (2%)	57	69
2	E	390/432 (90%)	389 (100%)	1 (0%)	86	84
2	F	388/432 (90%)	387 (100%)	1 (0%)	86	84
3	G	52/344 (15%)	52 (100%)	0	100	100
4	H	183/212 (86%)	183 (100%)	0	100	100
5	I	141/198 (71%)	140 (99%)	1 (1%)	76	77
5	J	142/198 (72%)	141 (99%)	1 (1%)	76	77
5	K	141/198 (71%)	141 (100%)	0	100	100
6	L	88/100 (88%)	88 (100%)	0	100	100
7	M	38/97 (39%)	37 (97%)	1 (3%)	40	60
7	N	37/97 (38%)	37 (100%)	0	100	100
7	O	38/97 (39%)	38 (100%)	0	100	100
9	a	410/744 (55%)	407 (99%)	3 (1%)	76	77
10	b	156/158 (99%)	156 (100%)	0	100	100
11	d	294/306 (96%)	293 (100%)	1 (0%)	86	84
12	c	106/110 (96%)	105 (99%)	1 (1%)	70	74
12	g	106/110 (96%)	106 (100%)	0	100	100
12	k	106/110 (96%)	106 (100%)	0	100	100
12	l	106/110 (96%)	106 (100%)	0	100	100
12	m	106/110 (96%)	106 (100%)	0	100	100
12	n	106/110 (96%)	106 (100%)	0	100	100
12	o	107/110 (97%)	107 (100%)	0	100	100
12	p	107/110 (97%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	q	107/110 (97%)	107 (100%)	0	100	100
13	s	184/398 (46%)	184 (100%)	0	100	100
14	r	39/315 (12%)	38 (97%)	1 (3%)	40	60
All	All	5554/7320 (76%)	5531 (100%)	23 (0%)	81	83

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	163	VAL
9	a	211	THR
7	M	111	HIS
9	a	312	ILE
2	D	388	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
6	L	81	HIS
10	b	168	GLN
12	m	78	ASN
7	O	89	GLN
9	a	273	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	POV	r	403	-	41,41,51	1.07	4 (9%)	47,49,59	0.92	2 (4%)
17	POV	o	201	-	43,43,51	1.06	4 (9%)	49,51,59	0.90	2 (4%)
18	NAG	s	504	13	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
17	POV	r	401	-	42,42,51	1.08	4 (9%)	48,50,59	0.96	2 (4%)
18	NAG	s	505	13	14,14,15	0.66	1 (7%)	17,19,21	0.72	1 (5%)
17	POV	b	301	-	43,43,51	2.29	11 (25%)	49,51,59	2.00	17 (34%)
18	NAG	s	506	13	14,14,15	0.41	0	17,19,21	0.35	0
17	POV	l	201	-	41,41,51	1.09	4 (9%)	47,49,59	0.89	2 (4%)
17	POV	s	501	-	45,45,51	1.06	3 (6%)	51,53,59	1.01	2 (3%)
17	POV	r	402	-	41,41,51	1.09	4 (9%)	47,49,59	0.97	2 (4%)
18	NAG	s	507	-	14,14,15	0.27	0	19,19,21	0.33	0
16	ADP	D	601	15	28,29,29	0.91	0	43,45,45	1.82	9 (20%)
18	NAG	s	503	13	14,14,15	0.33	0	17,19,21	0.51	0
18	NAG	s	502	13	14,14,15	0.35	0	17,19,21	0.39	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	POV	r	403	-	-	26/45/45/55	-
17	POV	o	201	-	-	23/47/47/55	-
18	NAG	s	504	13	-	1/6/23/26	0/1/1/1
17	POV	r	401	-	-	25/46/46/55	-
18	NAG	s	505	13	-	0/6/23/26	0/1/1/1
17	POV	b	301	-	-	24/47/47/55	-
18	NAG	s	506	13	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	POV	l	201	-	-	22/45/45/55	-
17	POV	s	501	-	-	26/49/49/55	-
17	POV	r	402	-	-	16/45/45/55	-
18	NAG	s	507	-	-	1/6/22/26	0/1/1/1
16	ADP	D	601	15	-	4/16/32/32	0/3/3/3
18	NAG	s	503	13	-	3/6/23/26	0/1/1/1
18	NAG	s	502	13	-	2/6/23/26	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	301	POV	O21-C2	-6.50	1.31	1.46
17	b	301	POV	O31-C3	-5.96	1.31	1.45
17	b	301	POV	C12-N	-4.86	1.36	1.51
17	b	301	POV	C13-N	-4.58	1.36	1.50
17	b	301	POV	C15-N	-3.61	1.39	1.50

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	601	ADP	C5-C4-N3	-5.65	118.94	126.72
17	b	301	POV	C2-O21-C21	-4.80	106.31	117.80
16	D	601	ADP	N3-C4-N9	4.67	135.11	127.17
17	s	501	POV	O21-C21-C22	4.40	121.00	111.48
17	r	402	POV	O21-C21-C22	4.28	120.74	111.48

There are no chirality outliers.

5 of 174 torsion outliers are listed below:

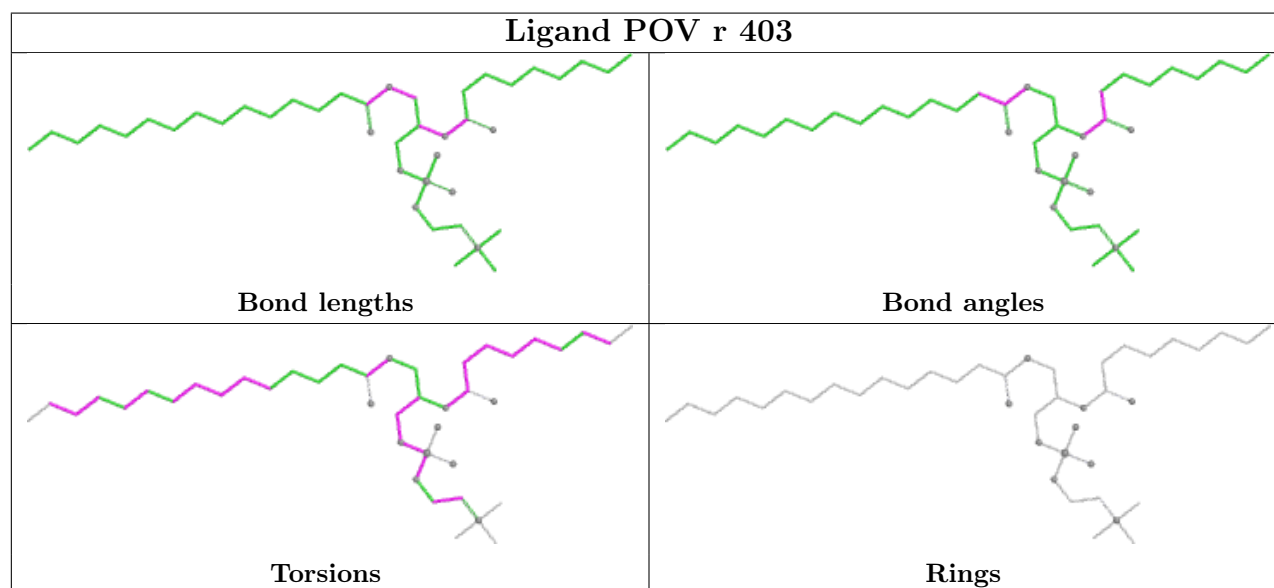
Mol	Chain	Res	Type	Atoms
16	D	601	ADP	C5'-O5'-PA-O2A
16	D	601	ADP	C5'-O5'-PA-O3A
17	b	301	POV	C11-O12-P-O11
17	b	301	POV	C11-O12-P-O14
17	l	201	POV	O12-C11-C12-N

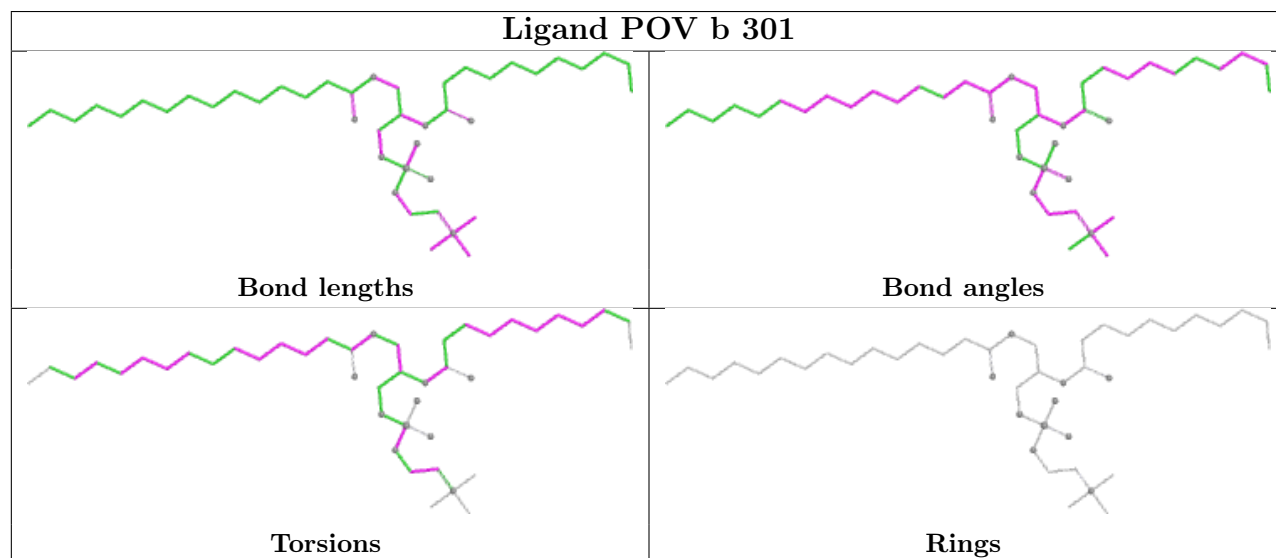
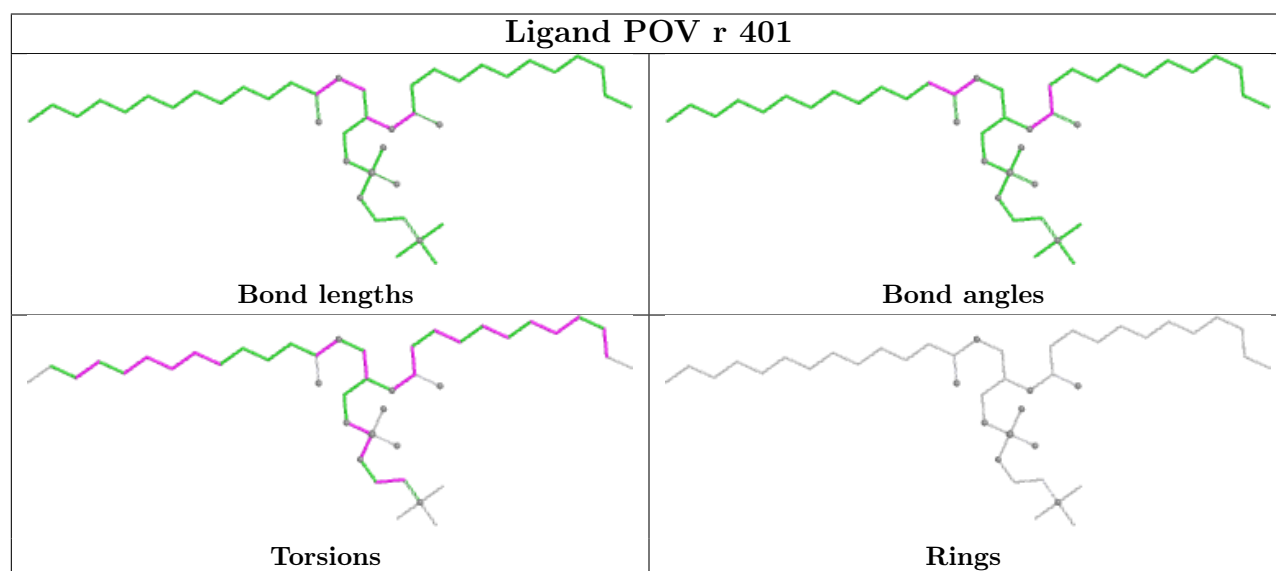
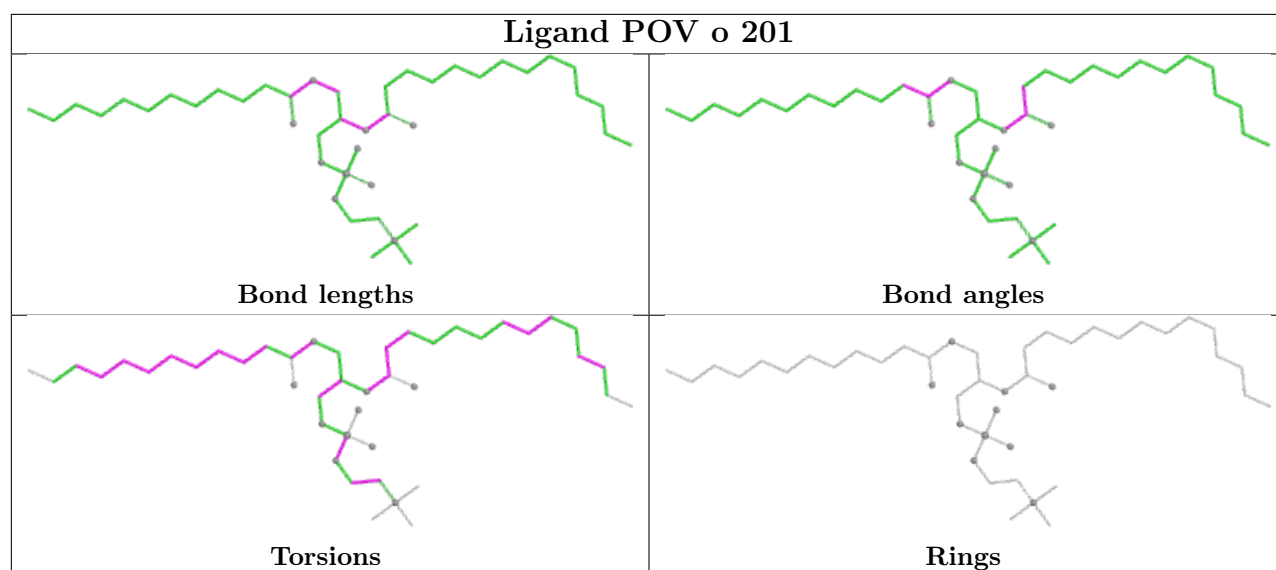
There are no ring outliers.

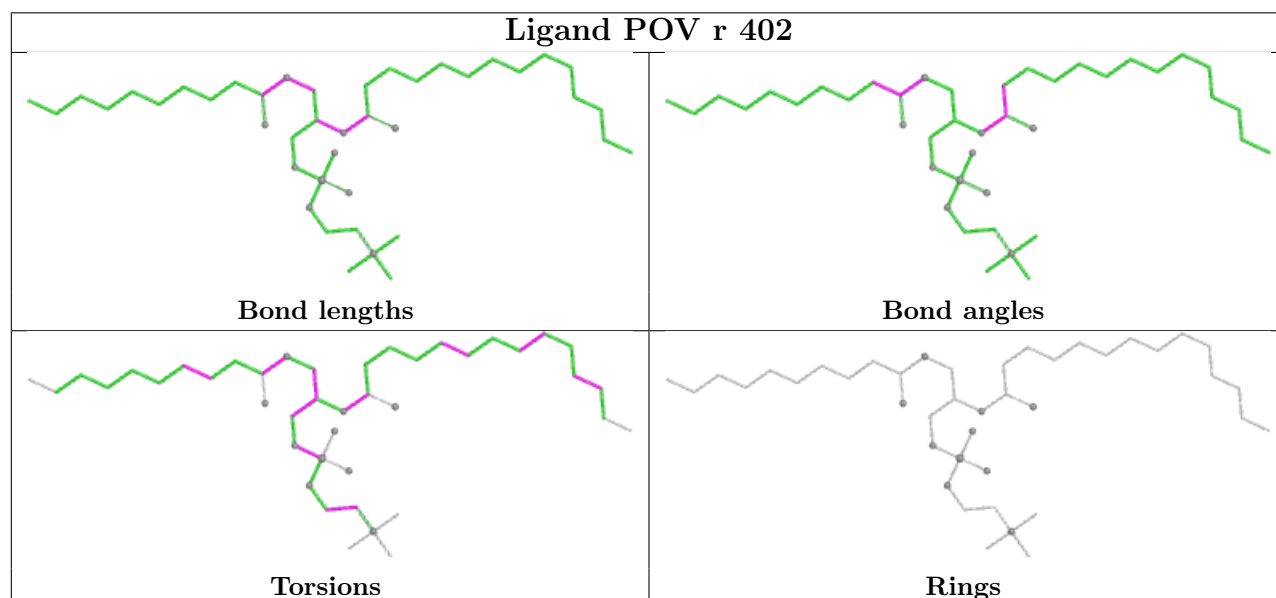
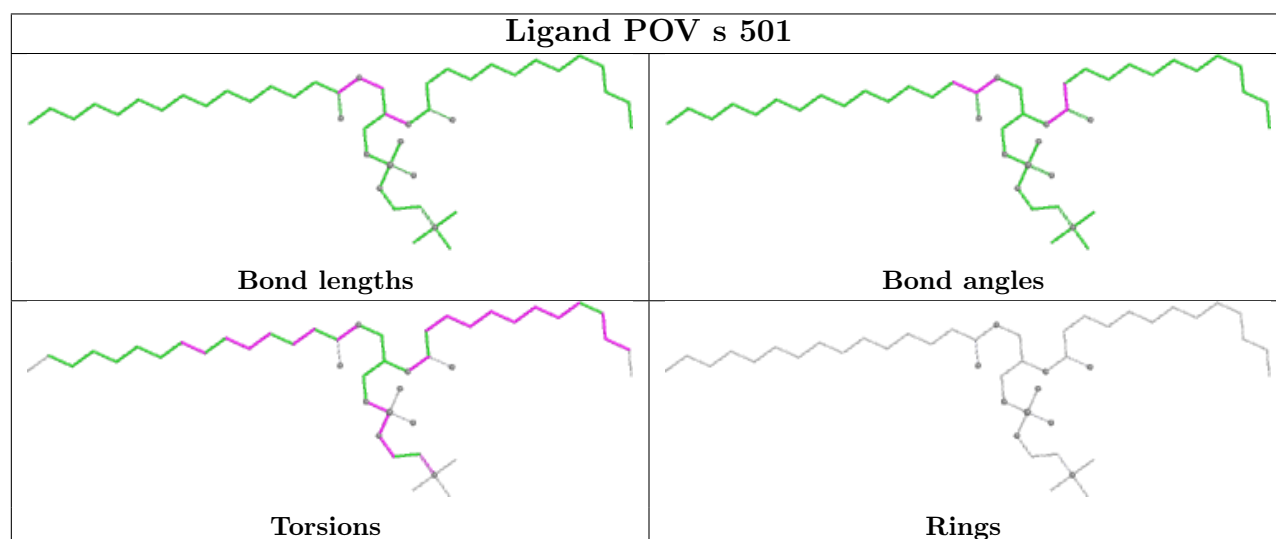
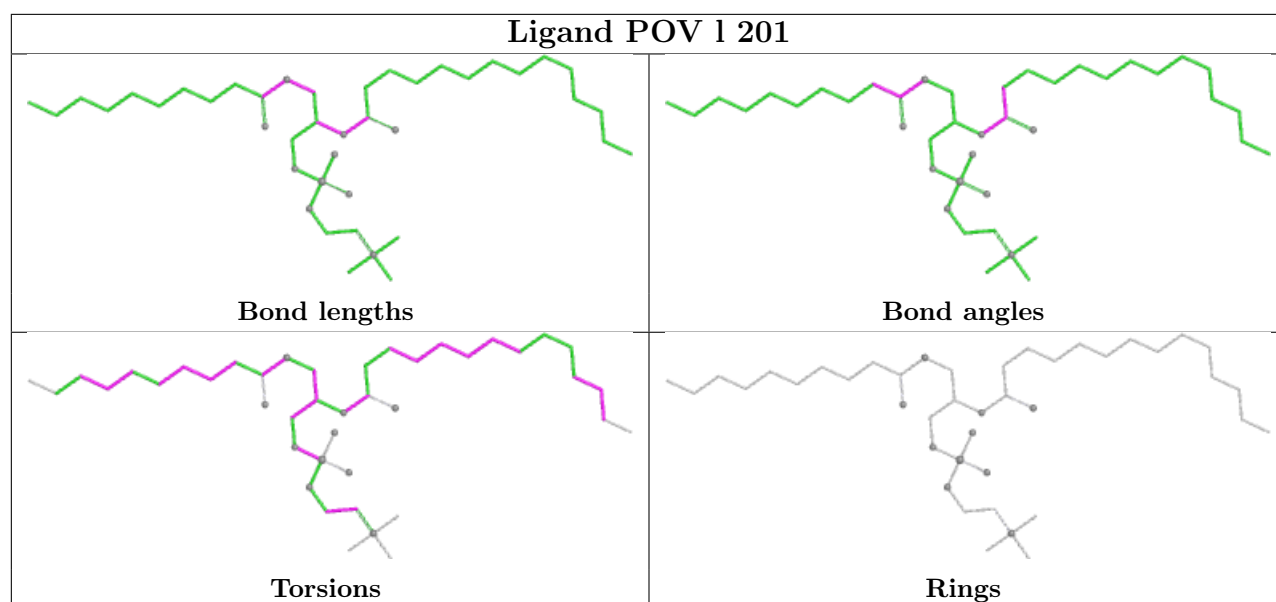
6 monomers are involved in 34 short contacts:

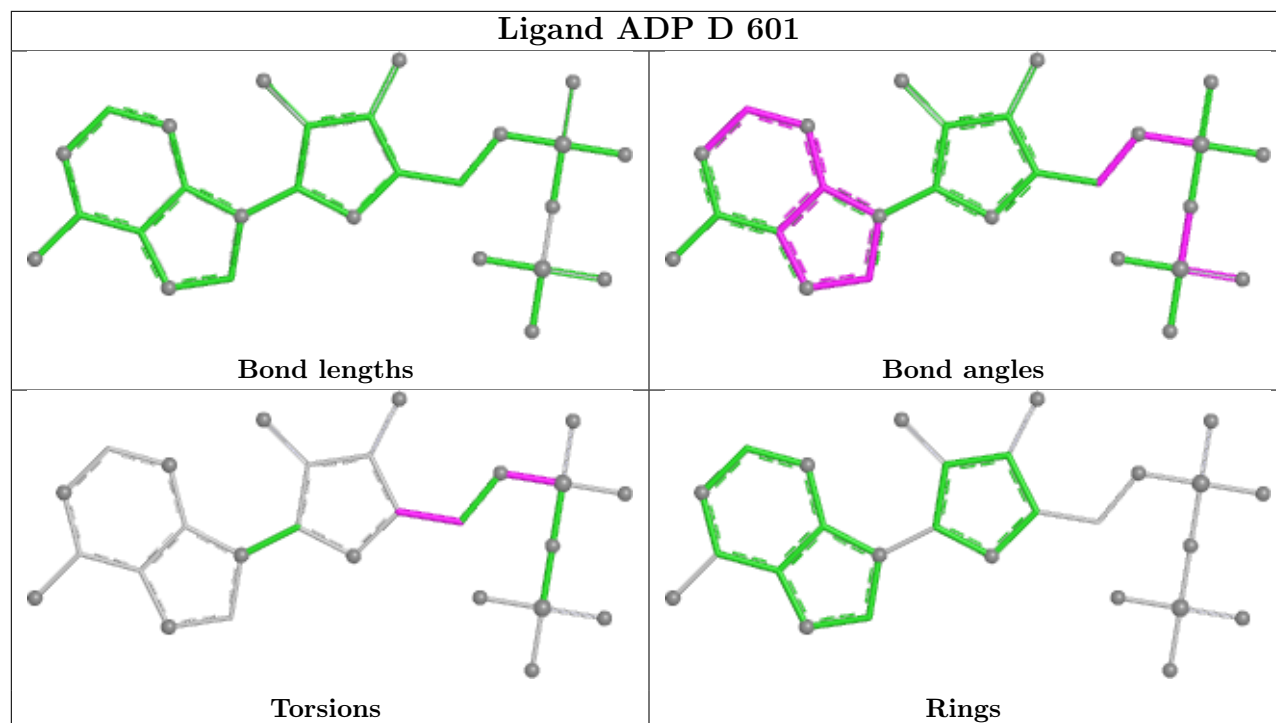
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	r	403	POV	1	0
17	o	201	POV	2	0
17	r	401	POV	2	0
17	b	301	POV	10	0
17	s	501	POV	5	0
18	s	507	NAG	14	0

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.

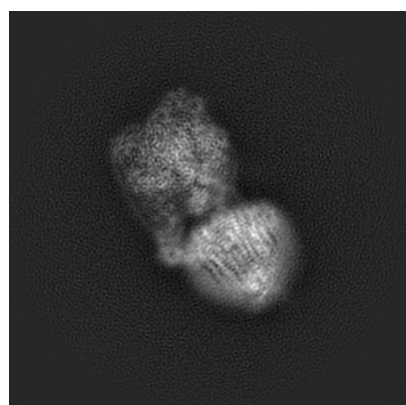
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22122. These allow visual inspection of the internal detail of the map and identification of artifacts.

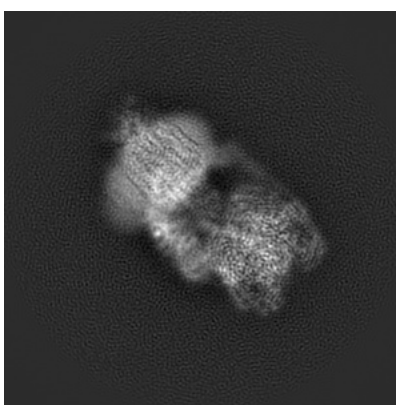
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

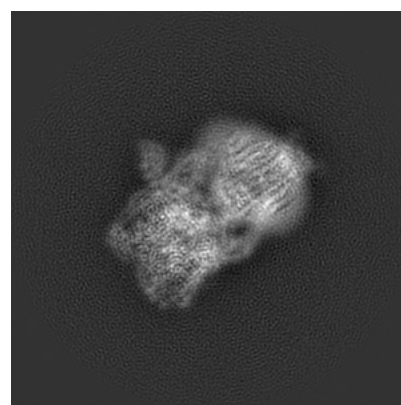
6.1.1 Primary map



X



Y

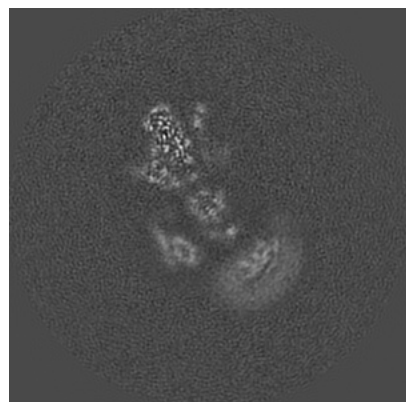


Z

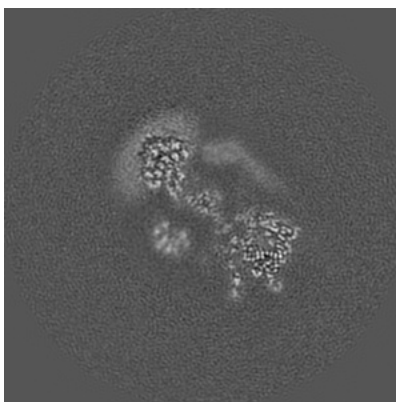
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

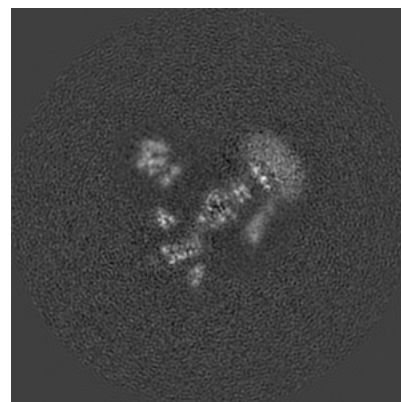
6.2.1 Primary map



X Index: 255



Y Index: 255

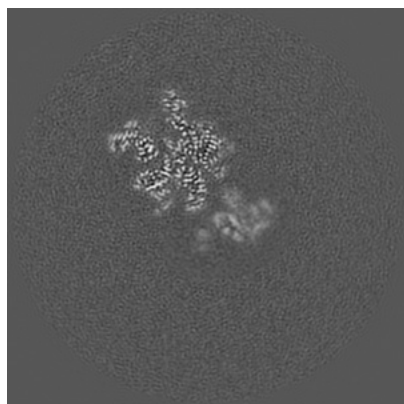


Z Index: 255

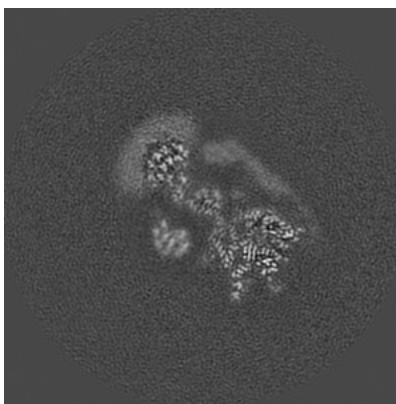
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

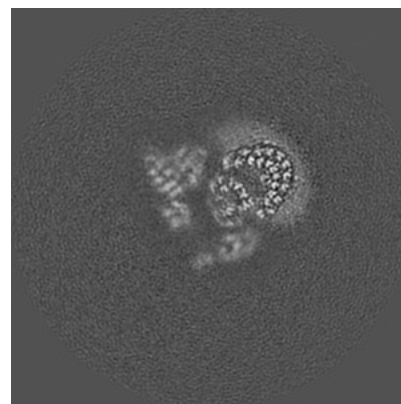
6.3.1 Primary map



X Index: 194



Y Index: 251

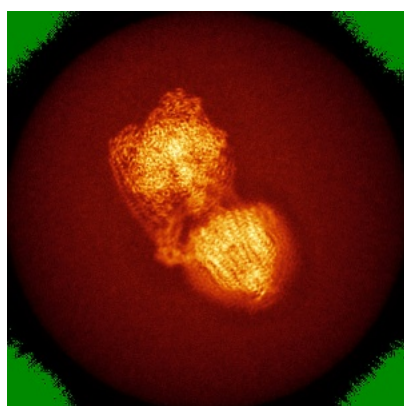


Z Index: 224

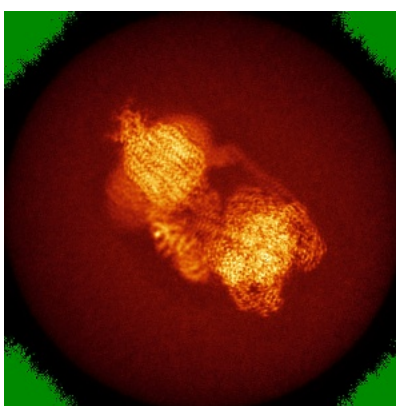
The images above show the largest variance slices of the map in three orthogonal directions.

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

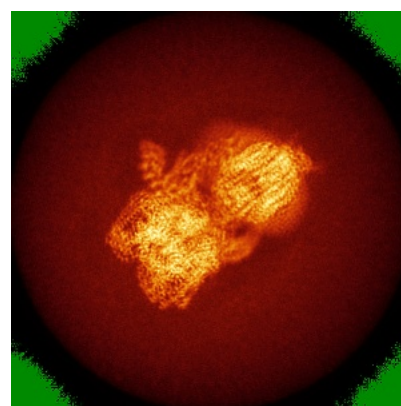
6.4.1 Primary map



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

This section was not generated.

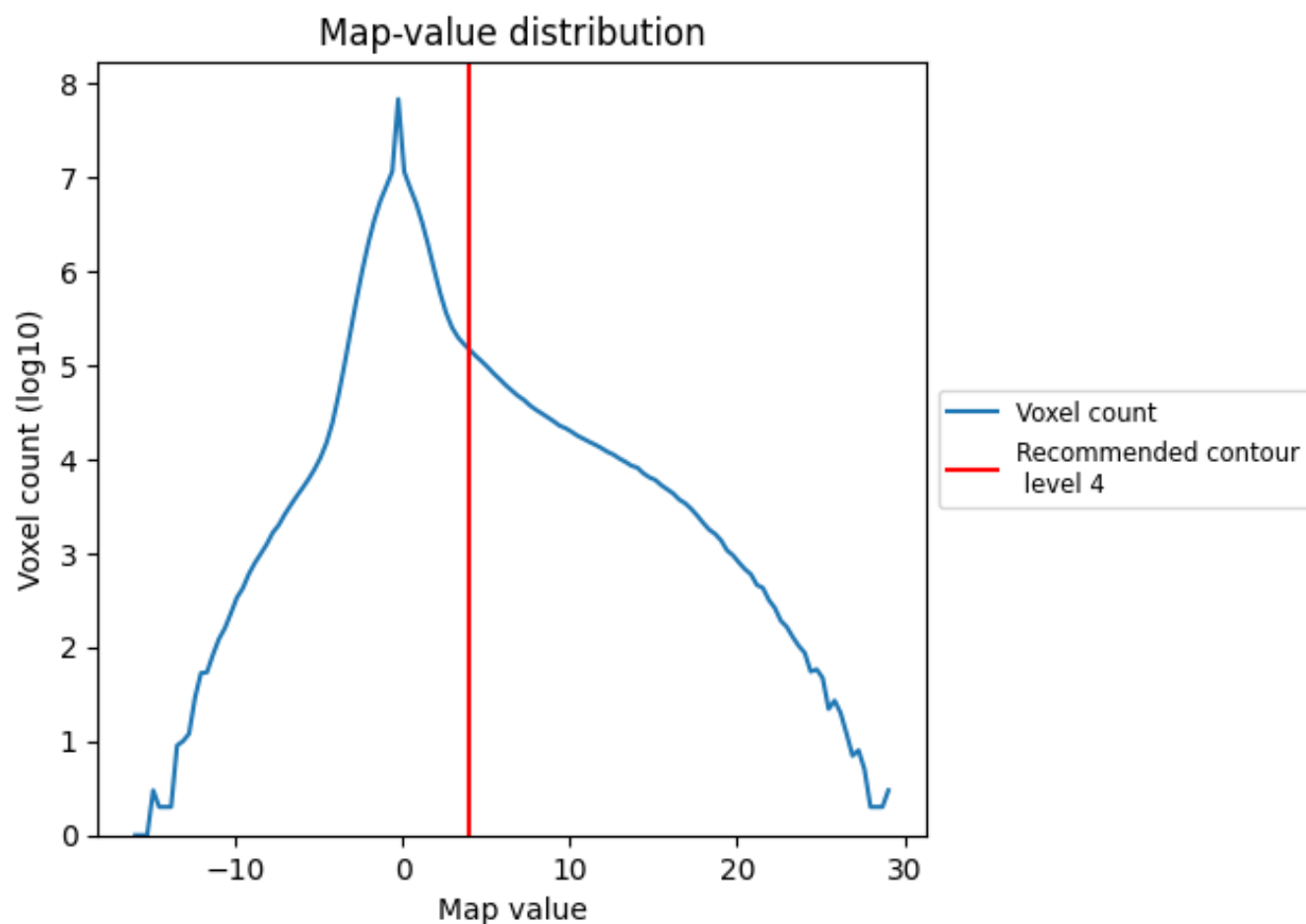
6.6 Mask visualisation

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

7 Map analysis [i](#)

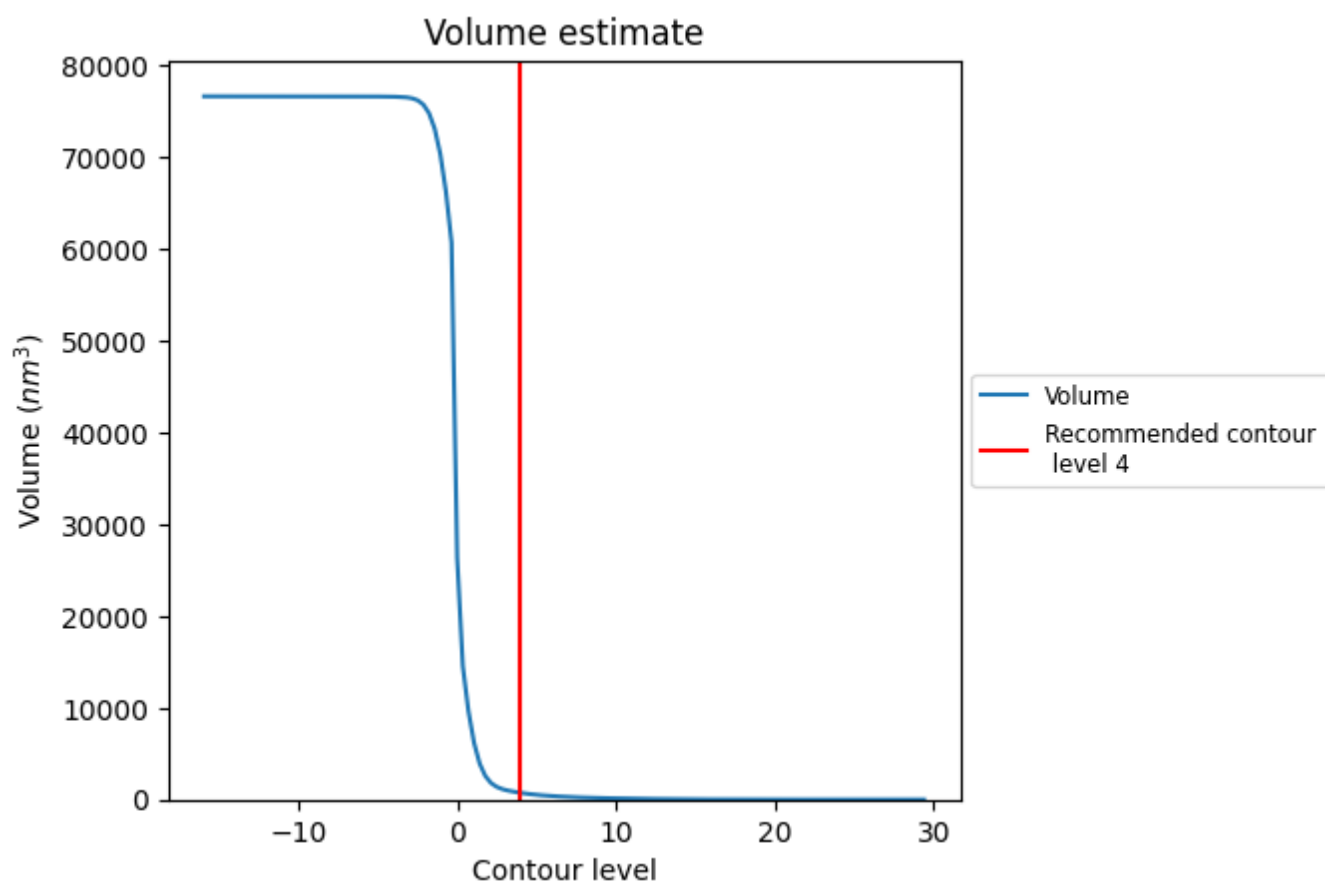
This section contains the results of statistical analysis of the map.

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.

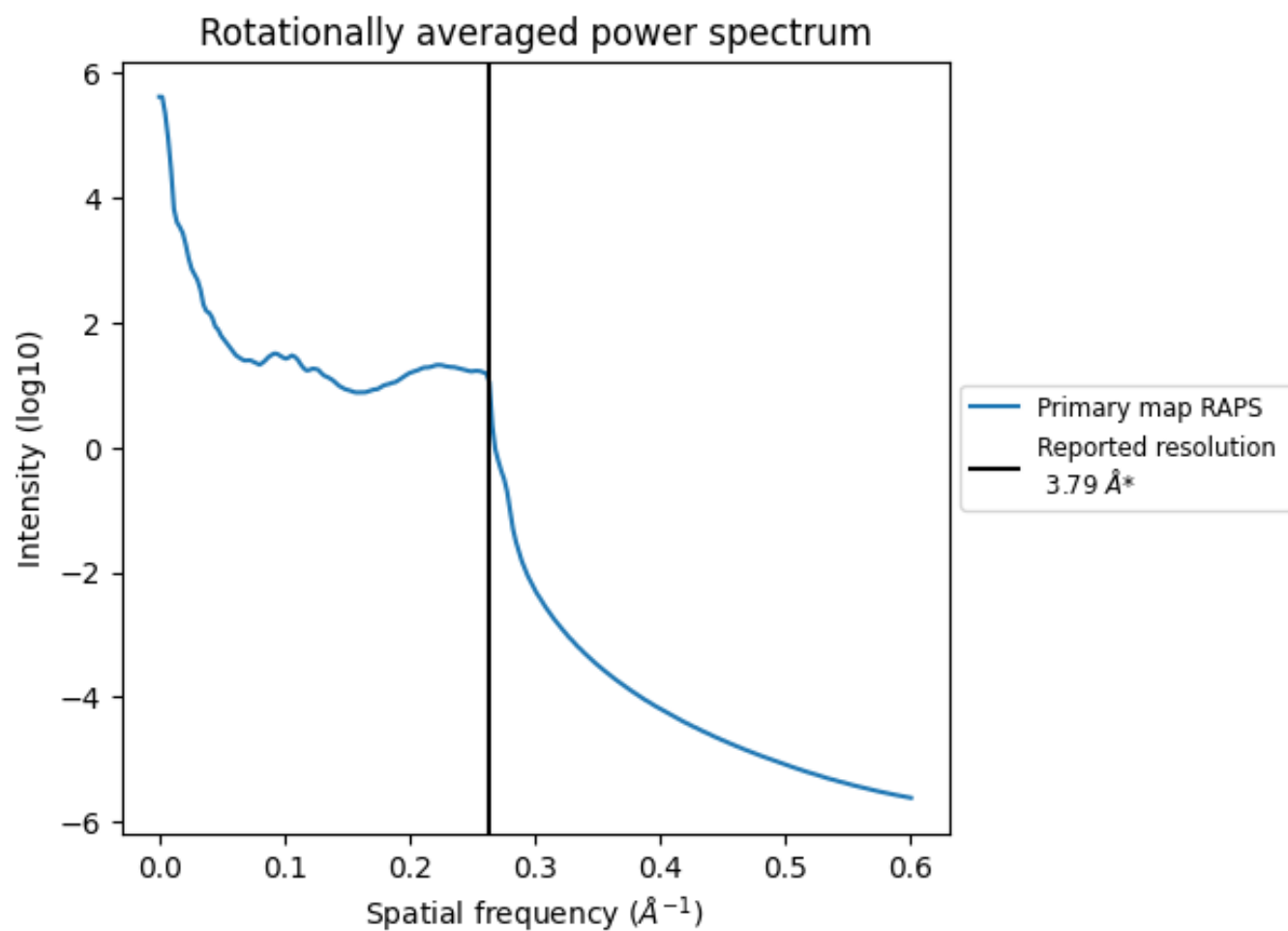
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 729 nm³; this corresponds to an approximate mass of 659 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 0.264 Å⁻¹

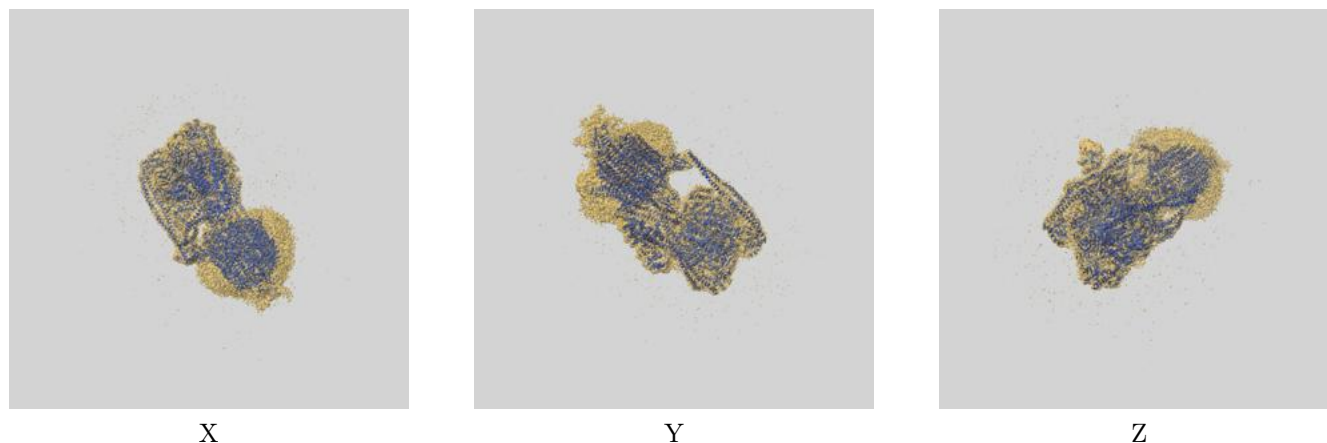
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

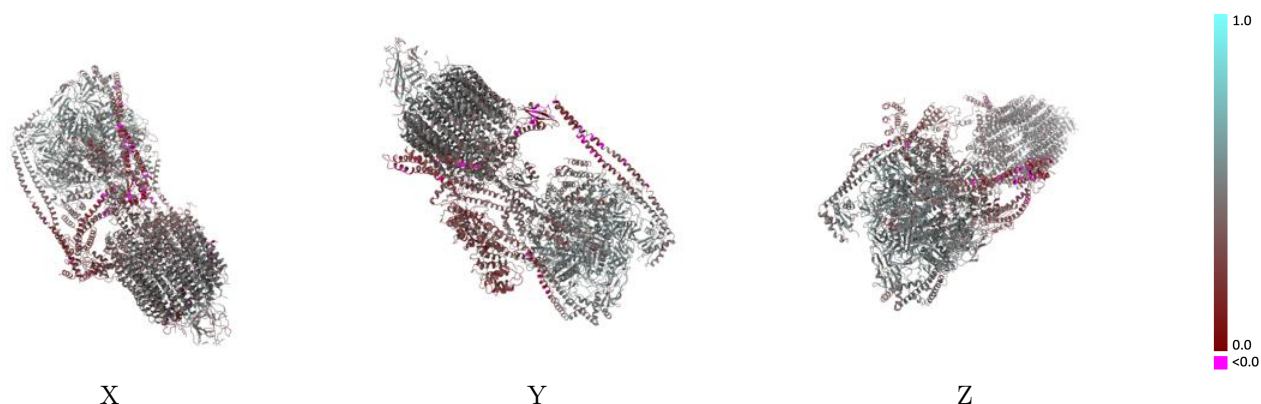
This section contains information regarding the fit between EMDB map EMD-22122 and PDB model 6XBY. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



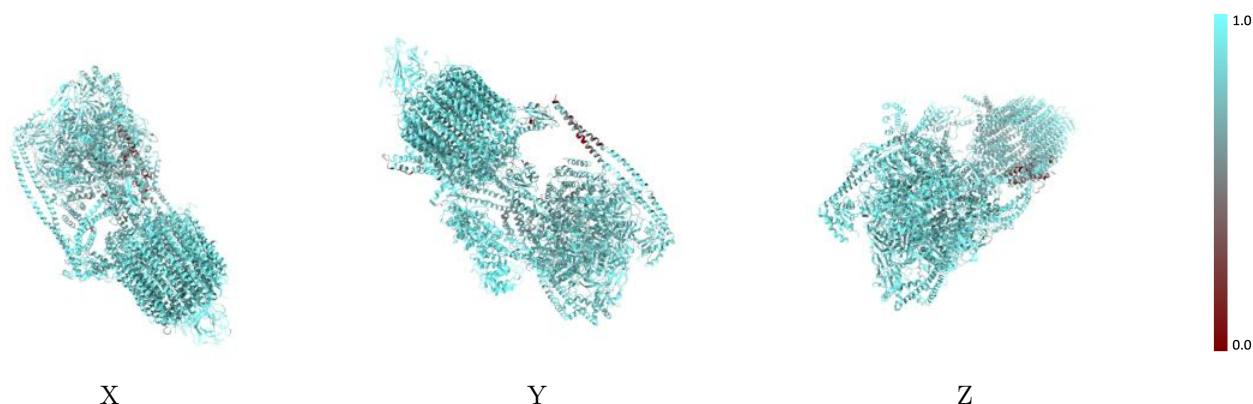
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



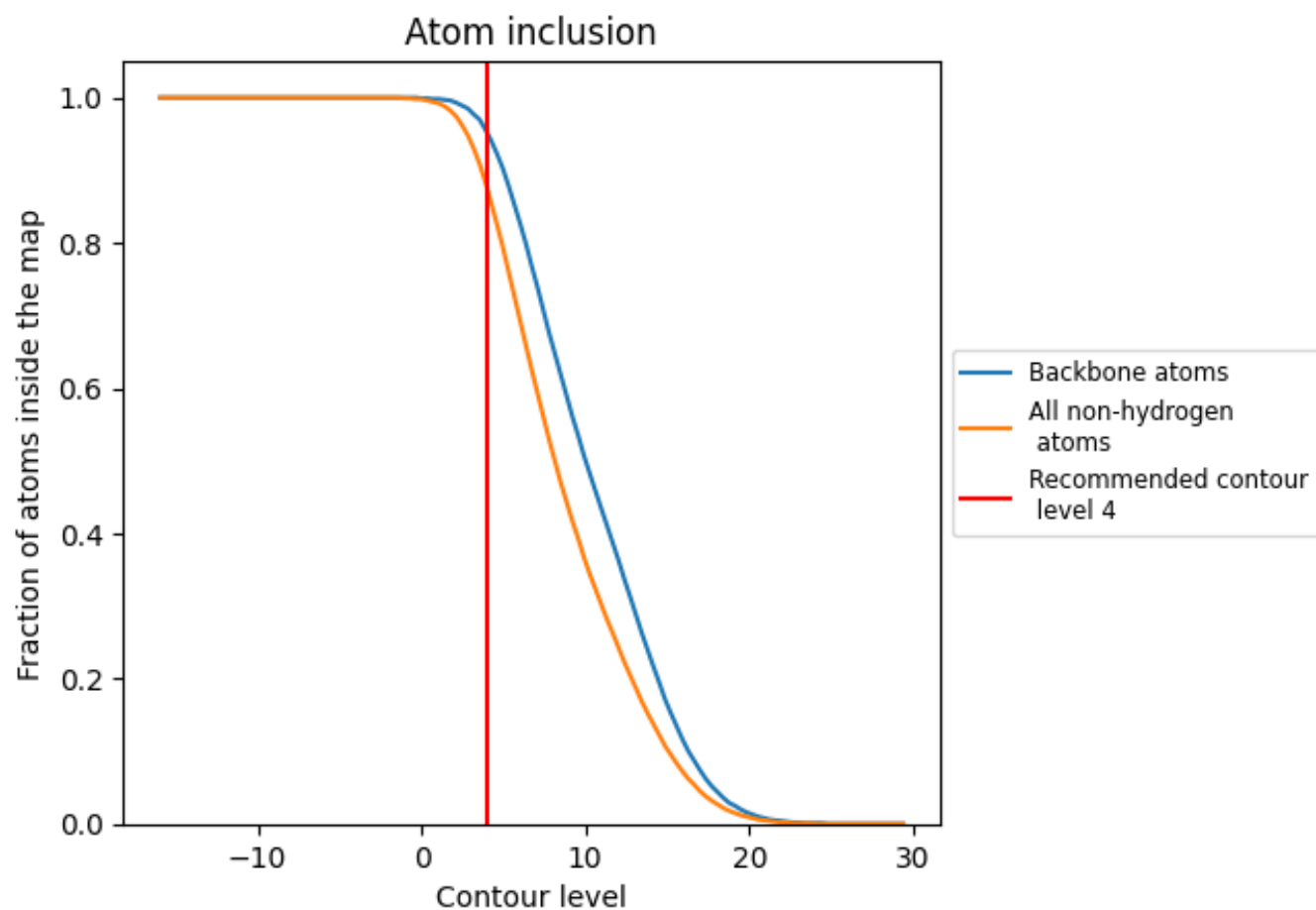
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.4320
A	 0.8690	 0.4800
B	 0.8560	 0.4680
C	 0.8580	 0.4760
D	 0.8700	 0.4910
E	 0.8830	 0.5000
F	 0.8730	 0.4900
G	 0.8660	 0.2370
H	 0.8080	 0.4350
I	 0.8060	 0.3940
J	 0.8760	 0.4280
K	 0.8800	 0.4290
L	 0.7810	 0.3890
M	 0.7460	 0.3150
N	 0.9030	 0.3690
O	 0.8640	 0.3540
P	 0.9880	 0.3010
a	 0.8420	 0.2670
b	 0.9070	 0.4560
c	 0.9110	 0.4460
d	 0.8610	 0.4360
g	 0.9120	 0.4470
k	 0.9100	 0.4430
l	 0.9160	 0.4550
m	 0.9110	 0.4430
n	 0.9210	 0.4560
o	 0.9150	 0.4570
p	 0.9250	 0.4550
q	 0.9220	 0.4640
r	 0.9230	 0.4830
s	 0.9380	 0.4540

