



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 10:24 AM EST

PDB ID : 6XBW
EMDB ID : EMD-22121
Title : Cryo-EM structure of V-ATPase from bovine brain, state 1
Authors : Wang, R.; Li, X.
Deposited on : 2020-06-07
Resolution : 3.37 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:

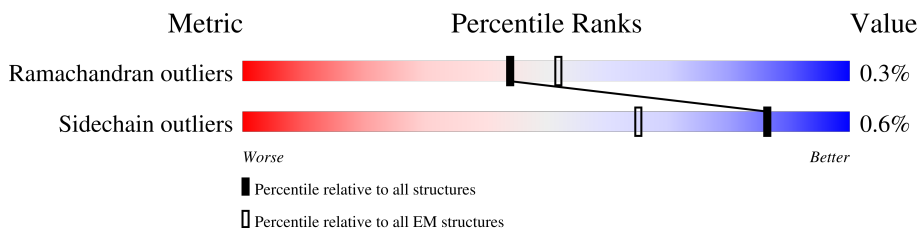
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.37 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.



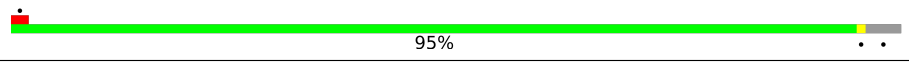
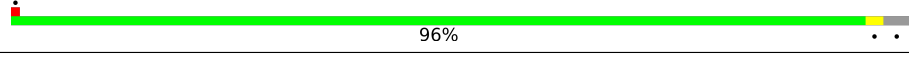
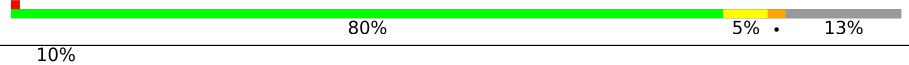

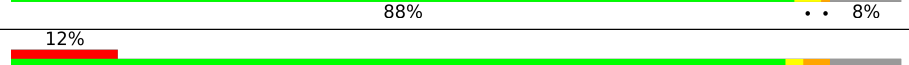
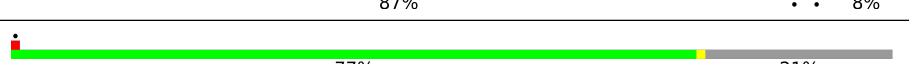
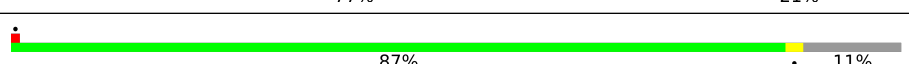
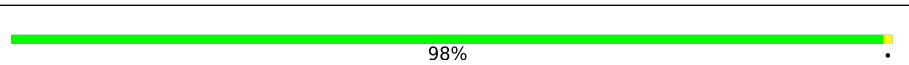
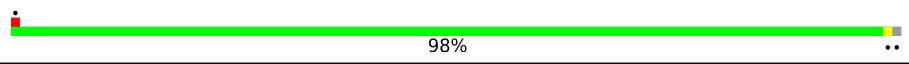
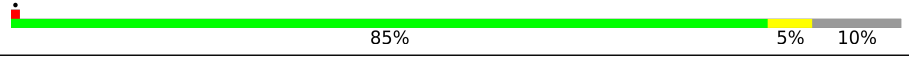
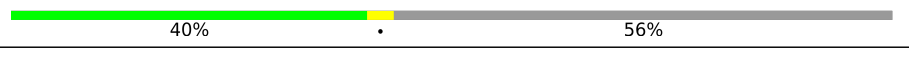

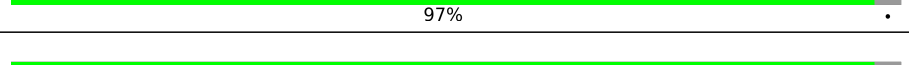
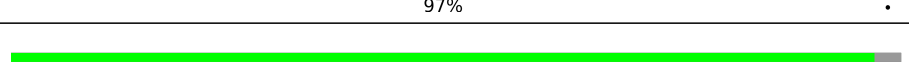
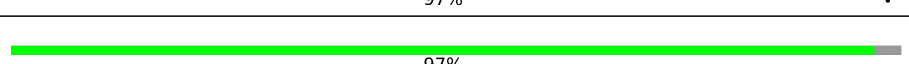
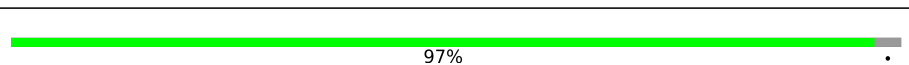
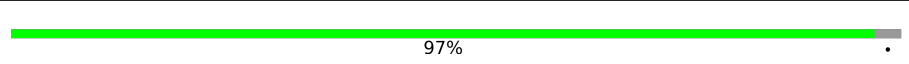
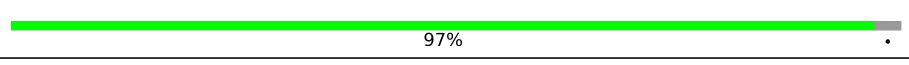
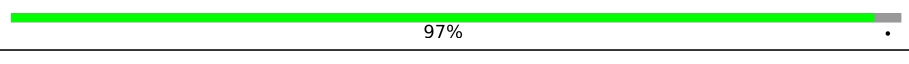
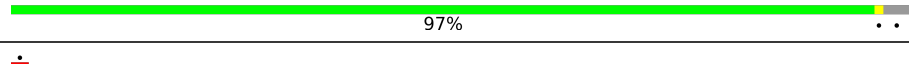



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	93% .. 5%
1	B	617	92% ...
1	C	617	95% ..
2	D	511	89% . 10%
2	E	511	88% . 10%
2	F	511	90% 10%
3	G	382	89% . 9%
4	H	247	83% . 15%
5	I	226	5% 95% ..

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Mol	Chain	Length	Quality of chain
5	J	226	 95%
5	K	226	 96%
6	L	119	 80% 5% 13%
7	M	118	 10% 87% 8%
7	N	118	 88% 8%
7	O	118	 12% 87% 8%
8	P	465	 77% 21%
9	a	838	 87% 11%
10	b	205	 98%
11	d	351	 98%
12	e	81	 85% 5% 10%
13	s	468	 40% 56%
14	r	351	 13% 87%
15	c	155	 97%
15	g	155	 97%
15	k	155	 97%
15	l	155	 97%
15	m	155	 97%
15	n	155	 97%
15	o	155	 97%
15	p	155	 97%
15	q	155	 97%
16	f	98	 45% 54%

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 63090 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
			Total	C	N	O	S		
1	A	589	Total	C	N	O	S	0	0
			4568	2900	770	870	28		
1	B	590	Total	C	N	O	S	0	0
			4582	2906	773	876	27		
1	C	597	Total	C	N	O	S	0	0
			4628	2935	781	884	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	461	Total	C	N	O	S	0	0
			3609	2288	618	683	20		
2	E	458	Total	C	N	O	S	0	0
			3585	2273	613	679	20		
2	F	459	Total	C	N	O	S	0	0
			3594	2279	615	680	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	346	Total	C	N	O	S	0	0
			2823	1820	475	519	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	211	Total	C	N	O	S	0	0
			1700	1080	307	308	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
			1614	1009	296	302	7		
5	J	218	Total	C	N	O	S	0	0
			1624	1018	297	302	7		
5	K	220	Total	C	N	O	S	0	0
			1595	994	297	298	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	103	Total	C	N	O	S	0	0
			816	516	143	156	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
			665	395	138	129	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	368	Total	C	N	O	S	0	0
			2819	1783	498	522	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	750	Total	C	N	O	S	0	0
			6093	3979	1013	1062	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	204	Total	C	N	O	S	0	0
			1503	996	238	259	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	d	348	2819	1817	460	528	14	0	0

- Molecule 12 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	e	73	590	409	91	87	3	0	0

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

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

- Molecule 14 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	r	46	385	261	54	67	3	0	0

- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

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

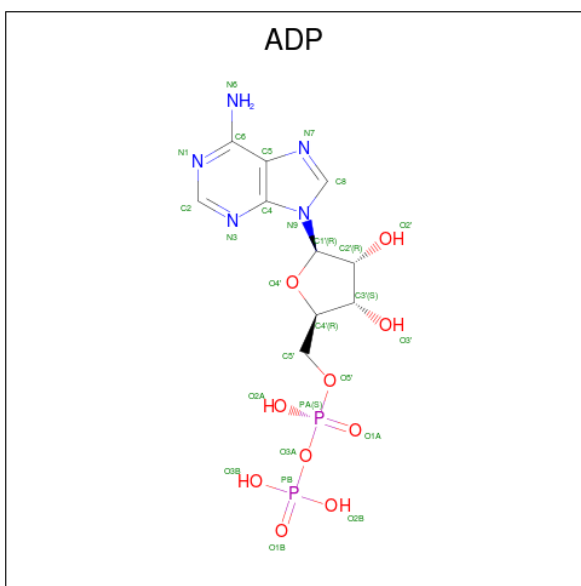
- Molecule 16 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	f	45	351	240	52	55	4	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

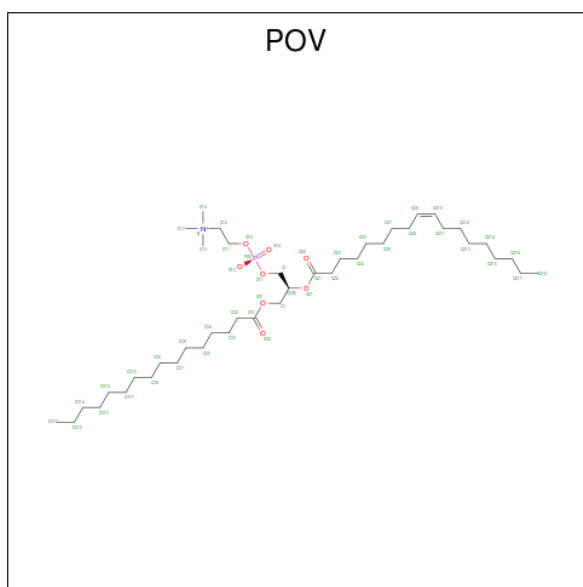
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
17	C	1	1	1	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



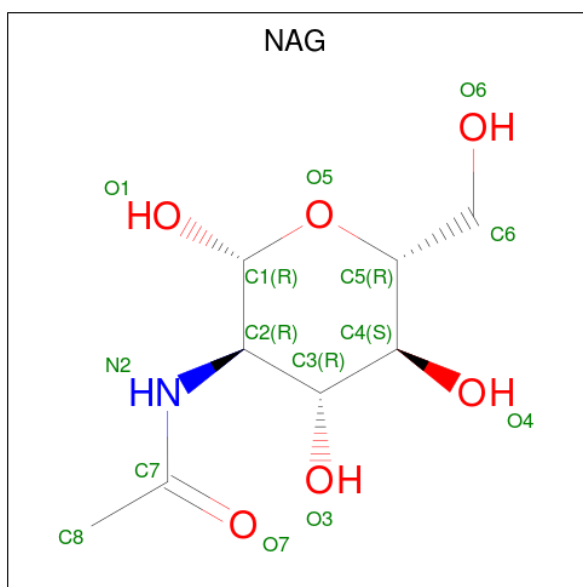
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	C	1	27	10	5	10	2	0

- Molecule 19 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



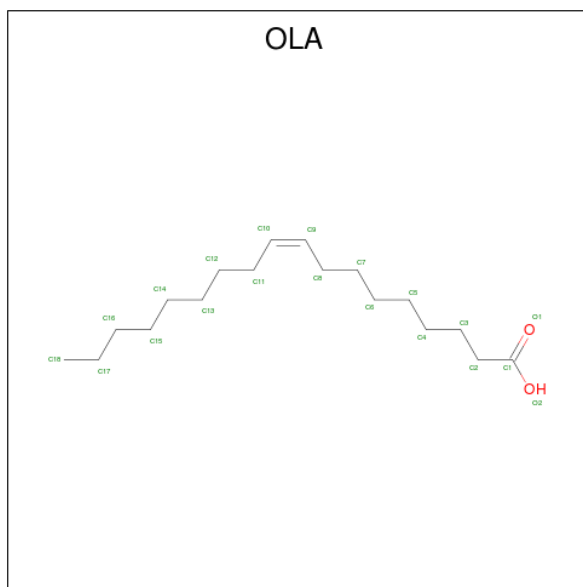
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	b	1	Total 213	163	5	40	5	0
19	b	1	Total 213	163	5	40	5	0
19	b	1	Total 213	163	5	40	5	0
19	b	1	Total 213	163	5	40	5	0
19	b	1	Total 213	163	5	40	5	0
19	r	1	Total 94	74	2	16	2	0
19	r	1	Total 94	74	2	16	2	0
19	g	1	Total 43	33	1	8	1	0
19	p	1	Total 44	34	1	8	1	0

- Molecule 20 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
20	s	1	Total	C	N	O	0
			84	48	6	30	
20	s	1	Total	C	N	O	0
			84	48	6	30	
20	s	1	Total	C	N	O	0
			84	48	6	30	
20	s	1	Total	C	N	O	0
			84	48	6	30	
20	s	1	Total	C	N	O	0
			84	48	6	30	
20	s	1	Total	C	N	O	0
			84	48	6	30	

- Molecule 21 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).

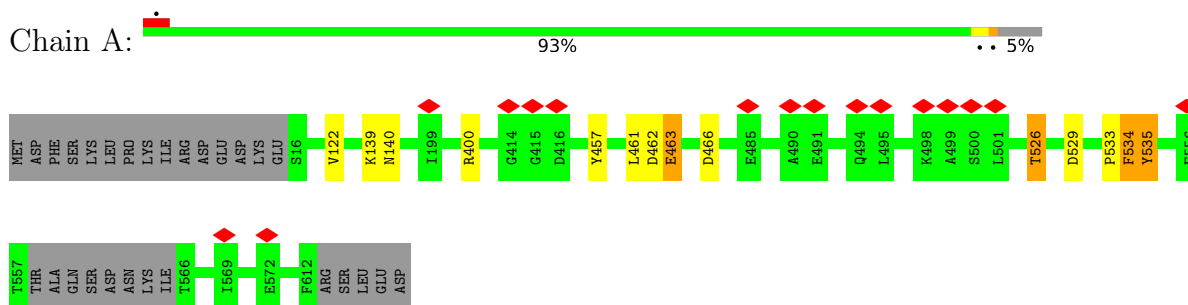


Mol	Chain	Residues	Atoms			AltConf
21	r	1	Total	C	O	0
			20	18	2	

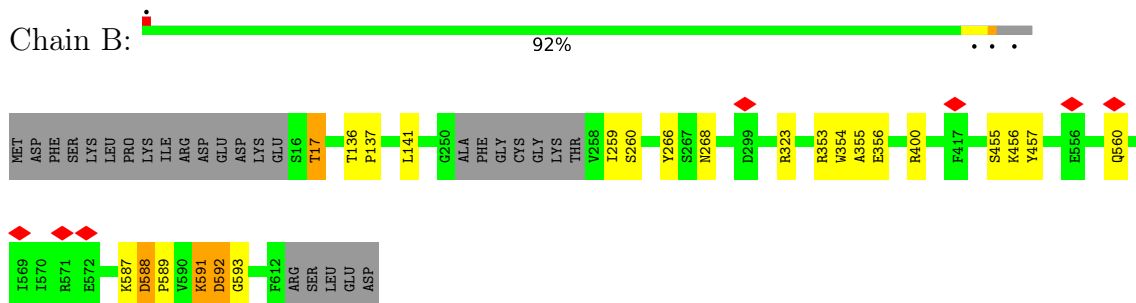
3 Residue-property plots [i](#)

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

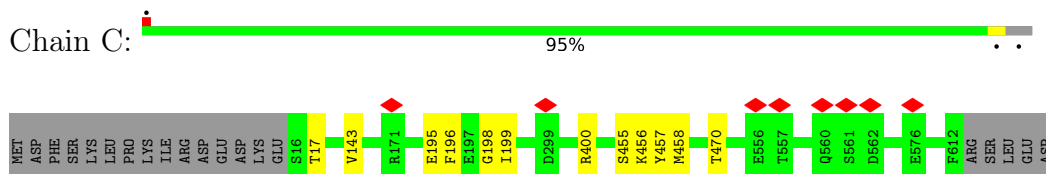
- Molecule 1: V-type proton ATPase catalytic subunit A



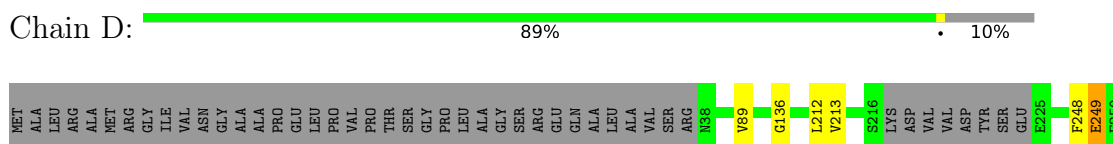
- Molecule 1: V-type proton ATPase catalytic subunit A



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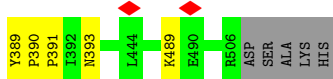
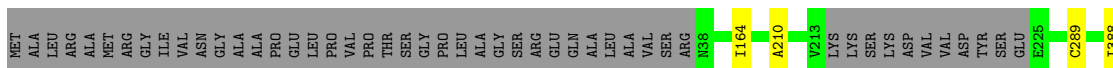
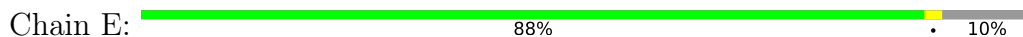


- Molecule 2: V-type proton ATPase subunit B, brain isoform

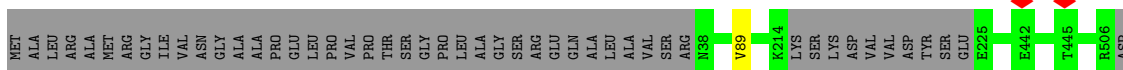




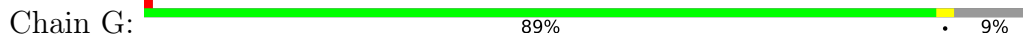
- Molecule 2: V-type proton ATPase subunit B, brain isoform



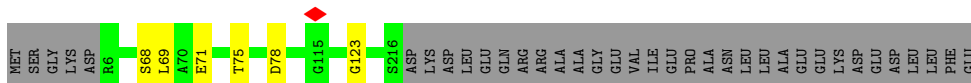
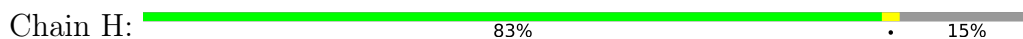
- Molecule 2: V-type proton ATPase subunit B, brain isoform



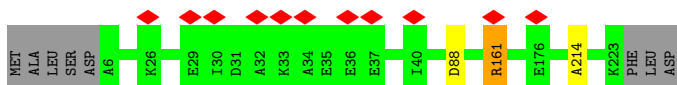
- Molecule 3: V-type proton ATPase subunit C 1



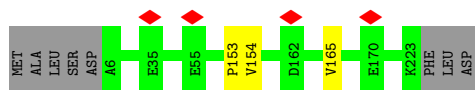
- Molecule 4: V-type proton ATPase subunit D



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



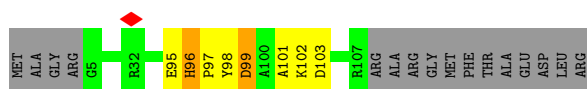
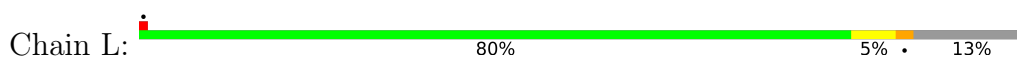
- Molecule 5: V-type proton ATPase subunit E 1



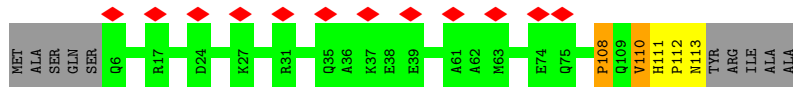
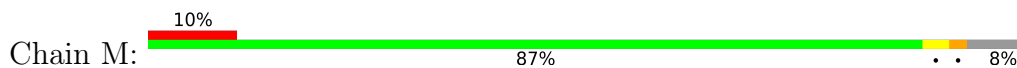
• Molecule 5: V-type proton ATPase subunit E 1



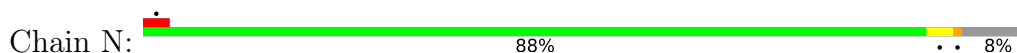
• Molecule 6: V-type proton ATPase subunit F



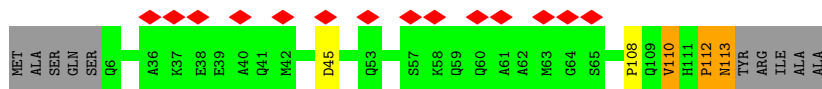
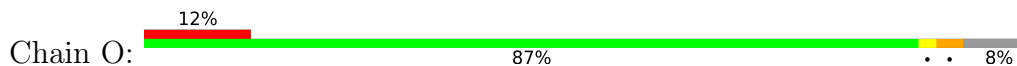
• Molecule 7: V-type proton ATPase subunit G



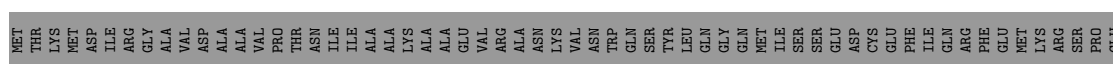
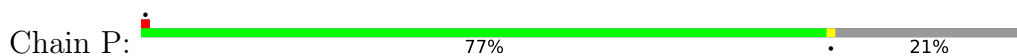
• Molecule 7: V-type proton ATPase subunit G

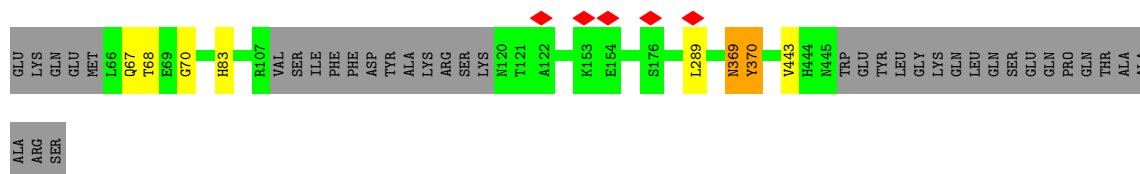


• Molecule 7: V-type proton ATPase subunit G



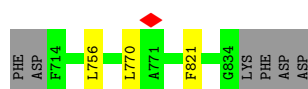
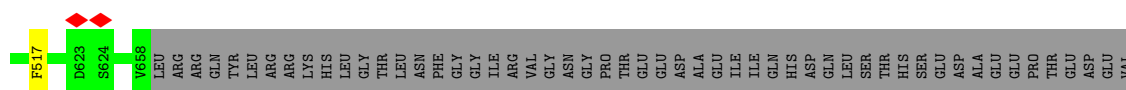
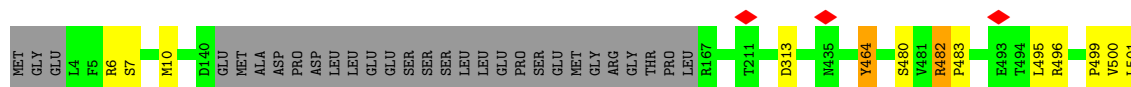
• Molecule 8: V-type proton ATPase subunit H





- Molecule 9: V-type proton ATPase subunit a

Chain a: 87% 11%



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

Chain b: 98%



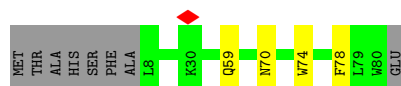
- Molecule 11: V-type proton ATPase subunit d 1

Chain d: 98%



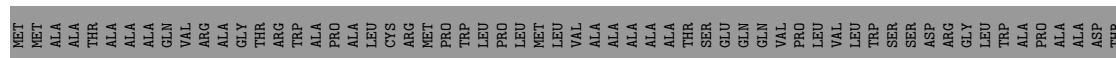
- Molecule 12: V-type proton ATPase subunit e 2

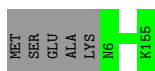
Chain e: 85% 5% 10%



- Molecule 13: V-type proton ATPase subunit S1

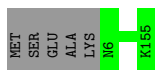
Chain s: 40% 56%





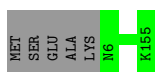
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain l: 97%



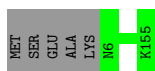
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain m: 97%



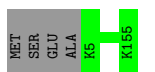
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain n: 97%



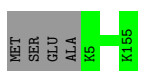
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain o: 97%



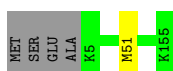
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain p: 97%



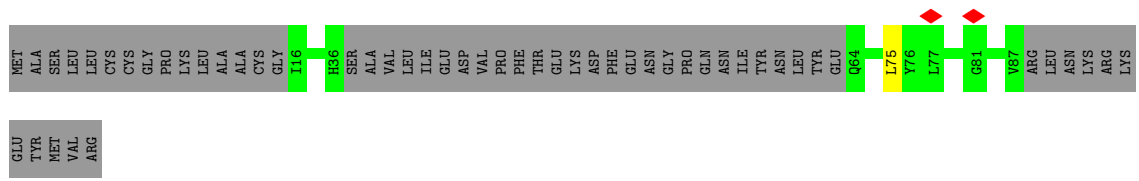
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain q: 97%



- Molecule 16: Ribonuclease kappa

Chain f: 45%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84345	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	31.875	Depositor
Minimum map value	-17.506	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.129	Depositor
Recommended contour level	4.0	Depositor
Map size (\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 (\AA)	0.833, 0.833, 0.833	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, POV, OLA, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.96	23/4663 (0.5%)	0.66	13/6314 (0.2%)
1	B	0.88	27/4676 (0.6%)	0.79	16/6333 (0.3%)
1	C	0.57	11/4724 (0.2%)	0.64	9/6398 (0.1%)
2	D	0.44	1/3680 (0.0%)	0.67	8/4986 (0.2%)
2	E	0.38	1/3656 (0.0%)	0.63	6/4956 (0.1%)
2	F	0.28	0/3665	0.53	1/4967 (0.0%)
3	G	0.26	0/2875	0.57	2/3883 (0.1%)
4	H	0.45	1/1718 (0.1%)	0.61	3/2298 (0.1%)
5	I	0.35	0/1627	0.69	3/2196 (0.1%)
5	J	0.53	1/1637 (0.1%)	0.57	1/2208 (0.0%)
5	K	0.38	0/1606	0.63	3/2171 (0.1%)
6	L	0.72	1/829 (0.1%)	0.95	7/1122 (0.6%)
7	M	0.71	5/667 (0.7%)	0.85	6/912 (0.7%)
7	N	0.70	3/667 (0.4%)	0.70	4/912 (0.4%)
7	O	0.78	6/667 (0.9%)	0.72	3/912 (0.3%)
8	P	0.29	0/2865	0.70	8/3877 (0.2%)
9	a	0.39	3/6246 (0.0%)	0.64	11/8451 (0.1%)
10	b	0.68	2/1537 (0.1%)	0.59	1/2090 (0.0%)
11	d	0.28	0/2884	0.60	4/3906 (0.1%)
12	e	0.68	0/613	0.91	4/844 (0.5%)
13	s	0.75	7/1720 (0.4%)	0.98	14/2341 (0.6%)
14	r	1.07	3/398 (0.8%)	0.78	2/547 (0.4%)
15	c	0.27	0/1079	0.46	0/1459
15	g	0.26	0/1079	0.43	0/1459
15	k	0.26	0/1079	0.43	0/1459
15	l	0.26	0/1079	0.44	0/1459
15	m	0.27	0/1079	0.45	0/1459
15	n	0.26	0/1079	0.44	0/1459
15	o	0.27	0/1088	0.44	0/1470
15	p	0.26	0/1088	0.43	0/1470
15	q	0.26	0/1088	0.49	1/1470 (0.1%)
16	f	0.28	0/359	0.55	1/485 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.54	95/63717 (0.1%)	0.65	131/86273 (0.2%)

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	A	0	3
1	B	0	1
1	C	0	1
2	D	0	1
5	I	0	1
7	M	0	1
7	N	0	1
8	P	0	1
9	a	0	1
13	s	0	1
All	All	0	12

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	TYR	CE1-CZ	-33.58	0.94	1.38
1	A	535	TYR	CZ-OH	-20.45	1.03	1.37
1	A	535	TYR	CG-CD2	-16.71	1.17	1.39
1	B	137	PRO	N-CD	-15.78	1.25	1.47
1	A	535	TYR	C-O	-15.72	0.93	1.23

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	161	ARG	CB-CA-C	18.29	146.97	110.40
1	B	259	ILE	CB-CA-C	14.98	141.56	111.60
13	s	417	ALA	CB-CA-C	-14.87	87.79	110.10
2	E	389	TYR	C-N-CD	-14.09	89.60	120.60
2	D	212	LEU	N-CA-C	-13.86	73.59	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466	ASP	Mainchain
1	A	533	PRO	Mainchain
1	A	535	TYR	Sidechain
1	B	591	LYS	Mainchain
1	C	455	SER	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	585/617 (95%)	566 (97%)	18 (3%)	1 (0%)	47	78
1	B	586/617 (95%)	562 (96%)	19 (3%)	5 (1%)	17	51
1	C	595/617 (96%)	583 (98%)	12 (2%)	0	100	100
2	D	457/511 (89%)	442 (97%)	14 (3%)	1 (0%)	47	78
2	E	454/511 (89%)	436 (96%)	17 (4%)	1 (0%)	47	78
2	F	455/511 (89%)	443 (97%)	12 (3%)	0	100	100
3	G	338/382 (88%)	326 (96%)	11 (3%)	1 (0%)	41	73
4	H	209/247 (85%)	204 (98%)	5 (2%)	0	100	100
5	I	216/226 (96%)	211 (98%)	5 (2%)	0	100	100
5	J	216/226 (96%)	212 (98%)	4 (2%)	0	100	100
5	K	218/226 (96%)	212 (97%)	6 (3%)	0	100	100
6	L	101/119 (85%)	92 (91%)	6 (6%)	3 (3%)	4	26
7	M	106/118 (90%)	102 (96%)	3 (3%)	1 (1%)	17	51
7	N	106/118 (90%)	105 (99%)	1 (1%)	0	100	100
7	O	106/118 (90%)	101 (95%)	3 (3%)	2 (2%)	8	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	P	364/465 (78%)	342 (94%)	20 (6%)	2 (0%)	29	63
9	a	744/838 (89%)	704 (95%)	37 (5%)	3 (0%)	34	68
10	b	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
11	d	346/351 (99%)	329 (95%)	16 (5%)	1 (0%)	41	73
12	e	71/81 (88%)	63 (89%)	8 (11%)	0	100	100
13	s	203/468 (43%)	177 (87%)	25 (12%)	1 (0%)	29	63
14	r	44/351 (12%)	39 (89%)	5 (11%)	0	100	100
15	c	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	g	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	k	148/155 (96%)	148 (100%)	0	0	100	100
15	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	m	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	n	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
15	o	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
15	p	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
15	q	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
16	f	41/98 (42%)	40 (98%)	1 (2%)	0	100	100
All	All	8098/9416 (86%)	7811 (96%)	265 (3%)	22 (0%)	44	73

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	B	268	ASN
1	B	588	ASP
2	E	390	PRO
6	L	96	HIS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	497/524 (95%)	490 (99%)	7 (1%)	67	83
1	B	500/524 (95%)	495 (99%)	5 (1%)	76	87
1	C	504/524 (96%)	501 (99%)	3 (1%)	86	93
2	D	394/432 (91%)	393 (100%)	1 (0%)	92	96
2	E	391/432 (90%)	390 (100%)	1 (0%)	92	96
2	F	392/432 (91%)	392 (100%)	0	100	100
3	G	313/344 (91%)	310 (99%)	3 (1%)	76	87
4	H	182/212 (86%)	180 (99%)	2 (1%)	73	86
5	I	150/198 (76%)	149 (99%)	1 (1%)	84	92
5	J	153/198 (77%)	152 (99%)	1 (1%)	84	92
5	K	144/198 (73%)	143 (99%)	1 (1%)	84	92
6	L	89/100 (89%)	88 (99%)	1 (1%)	73	86
7	M	38/97 (39%)	38 (100%)	0	100	100
7	N	38/97 (39%)	38 (100%)	0	100	100
7	O	38/97 (39%)	37 (97%)	1 (3%)	46	72
8	P	275/415 (66%)	274 (100%)	1 (0%)	91	95
9	a	667/744 (90%)	663 (99%)	4 (1%)	86	93
10	b	156/158 (99%)	155 (99%)	1 (1%)	86	93
11	d	303/306 (99%)	303 (100%)	0	100	100
12	e	62/68 (91%)	60 (97%)	2 (3%)	39	68
13	s	184/398 (46%)	183 (100%)	1 (0%)	88	94
14	r	42/315 (13%)	42 (100%)	0	100	100
15	c	106/110 (96%)	106 (100%)	0	100	100
15	g	106/110 (96%)	106 (100%)	0	100	100
15	k	106/110 (96%)	106 (100%)	0	100	100
15	l	106/110 (96%)	106 (100%)	0	100	100
15	m	106/110 (96%)	106 (100%)	0	100	100
15	n	106/110 (96%)	106 (100%)	0	100	100
15	o	107/110 (97%)	107 (100%)	0	100	100
15	p	107/110 (97%)	107 (100%)	0	100	100
15	q	107/110 (97%)	107 (100%)	0	100	100
16	f	38/84 (45%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6507/7887 (82%)	6471 (99%)	36 (1%)	86	93

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	a	464	TYR
13	s	270	GLN
9	a	482	ARG
10	b	19	LEU
1	C	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
12	e	70	ASN
15	m	92	GLN
13	s	358	GLN
15	g	124	GLN
15	p	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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
20	NAG	s	501	13	14,14,15	0.33	0	17,19,21	0.46	0
19	POV	r	402	-	46,46,51	1.01	3 (6%)	52,54,59	0.85	2 (3%)
19	POV	b	302	-	46,46,51	1.01	4 (8%)	52,54,59	0.92	2 (3%)
19	POV	b	304	-	46,46,51	1.01	4 (8%)	52,54,59	0.90	2 (3%)
20	NAG	s	503	13	14,14,15	0.41	0	17,19,21	0.56	0
20	NAG	s	502	13	14,14,15	0.35	0	17,19,21	0.51	0
20	NAG	s	504	13	14,14,15	0.49	0	17,19,21	0.78	1 (5%)
19	POV	g	201	-	42,42,51	1.05	2 (4%)	48,50,59	0.94	2 (4%)
19	POV	p	201	-	43,43,51	1.04	3 (6%)	49,51,59	0.91	3 (6%)
19	POV	r	401	-	46,46,51	1.00	4 (8%)	52,54,59	0.83	2 (3%)
19	POV	b	301	-	46,46,51	1.01	4 (8%)	52,54,59	0.93	2 (3%)
18	ADP	C	702	17	24,29,29	1.09	2 (8%)	29,45,45	1.70	5 (17%)
20	NAG	s	506	-	14,14,15	0.28	0	19,19,21	0.29	0
20	NAG	s	505	13	14,14,15	0.20	0	17,19,21	0.59	0
19	POV	b	305	-	30,30,51	1.25	4 (13%)	36,38,59	0.97	2 (5%)
19	POV	b	303	-	40,40,51	1.08	4 (10%)	46,48,59	0.90	2 (4%)
21	OLA	r	403	-	19,19,19	0.77	1 (5%)	19,19,19	0.90	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
20	NAG	s	501	13	-	0/6/23/26	0/1/1/1
19	POV	r	402	-	-	29/50/50/55	-
19	POV	b	302	-	-	24/50/50/55	-
19	POV	b	304	-	-	28/50/50/55	-
20	NAG	s	503	13	-	2/6/23/26	0/1/1/1
20	NAG	s	502	13	-	2/6/23/26	0/1/1/1
20	NAG	s	504	13	-	0/6/23/26	0/1/1/1
19	POV	g	201	-	-	23/46/46/55	-
19	POV	p	201	-	-	20/47/47/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	POV	r	401	-	-	25/50/50/55	-
19	POV	b	301	-	-	31/50/50/55	-
18	ADP	C	702	17	-	1/12/32/32	0/3/3/3
20	NAG	s	506	-	-	1/6/22/26	0/1/1/1
20	NAG	s	505	13	-	1/6/23/26	0/1/1/1
19	POV	b	305	-	-	21/34/34/55	-
19	POV	b	303	-	-	24/44/44/55	-
21	OLA	r	403	-	-	9/17/17/17	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	702	ADP	O4'-C1'	3.14	1.45	1.41
19	p	201	POV	O21-C2	-2.91	1.39	1.46
19	b	305	POV	O21-C2	-2.74	1.39	1.46
19	g	201	POV	O21-C2	-2.73	1.39	1.46
19	r	402	POV	O21-C2	-2.72	1.39	1.46

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	702	ADP	PA-O3A-PB	-6.06	112.02	132.83
19	b	302	POV	O21-C21-C22	4.55	121.31	111.50
18	C	702	ADP	N3-C2-N1	-4.21	122.10	128.68
19	b	304	POV	O21-C21-C22	4.14	120.42	111.50
19	b	301	POV	O21-C21-C22	3.95	120.02	111.50

There are no chirality outliers.

5 of 241 torsion outliers are listed below:

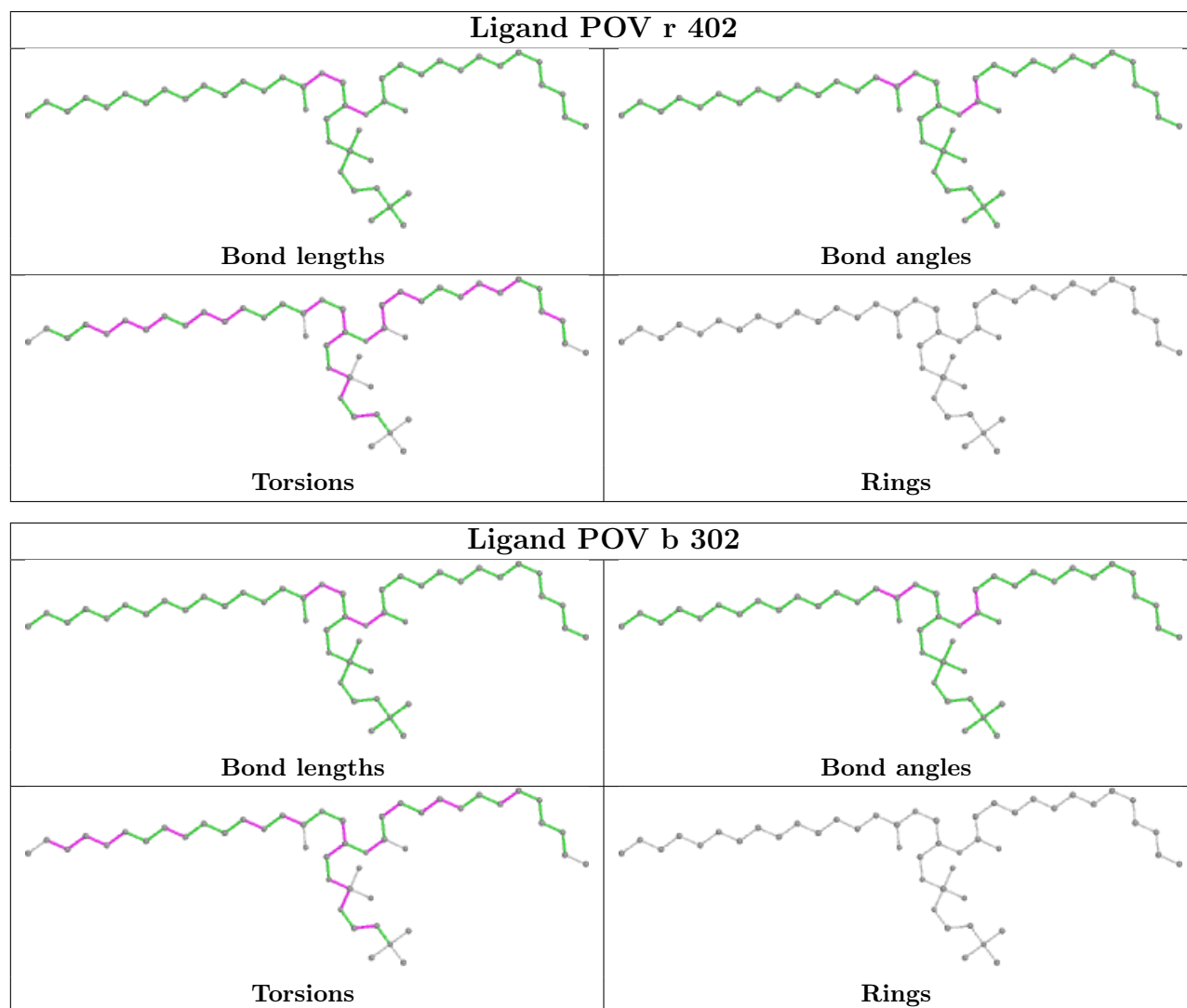
Mol	Chain	Res	Type	Atoms
19	b	301	POV	C1-O11-P-O14
19	b	301	POV	C3-C2-O21-C21
19	b	301	POV	C22-C21-O21-C2
19	b	302	POV	C1-O11-P-O14
19	b	302	POV	C11-O12-P-O13

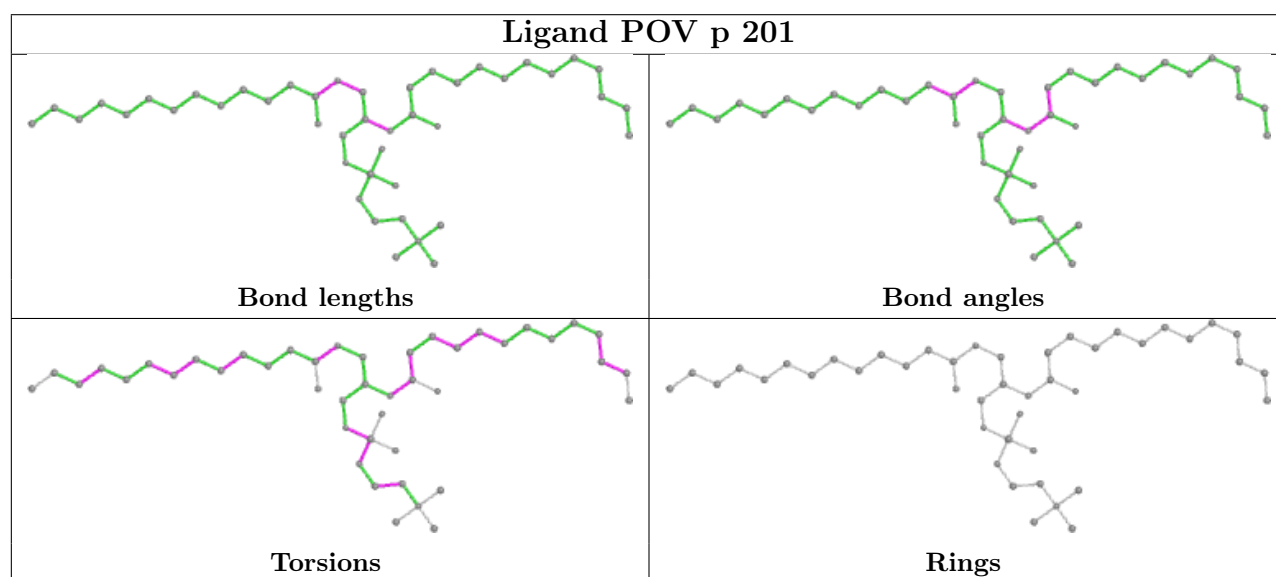
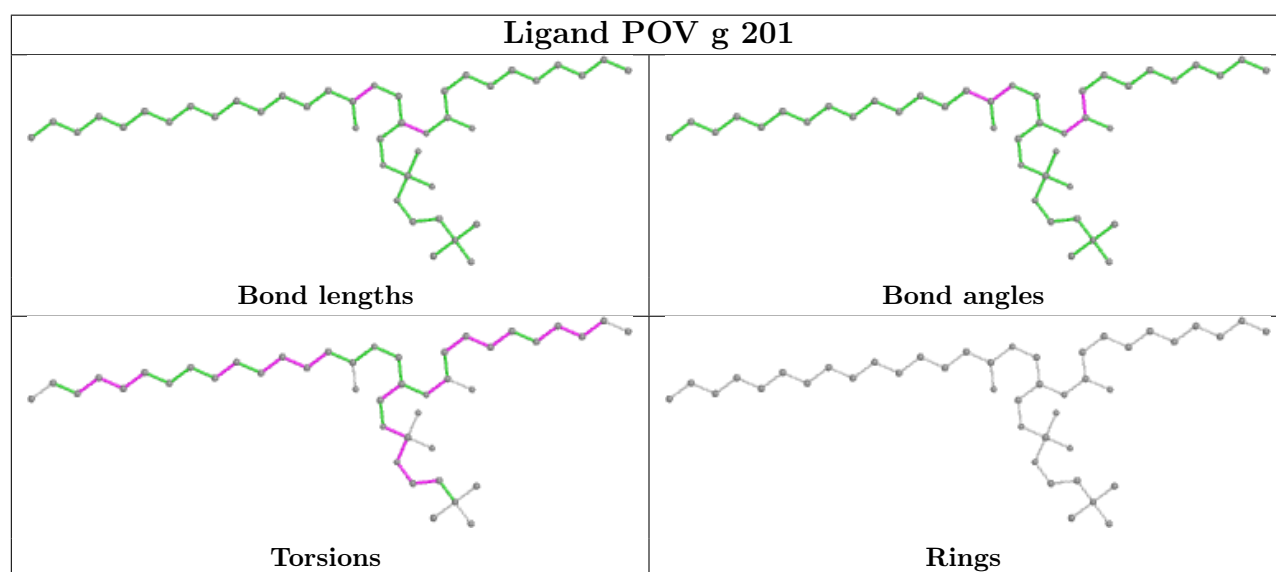
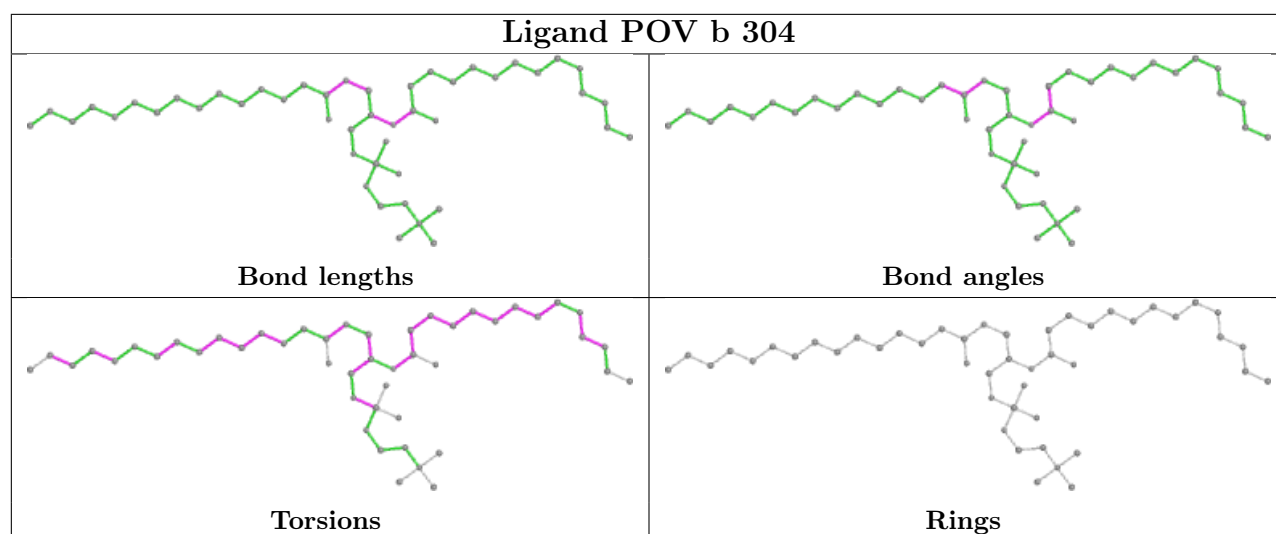
There are no ring outliers.

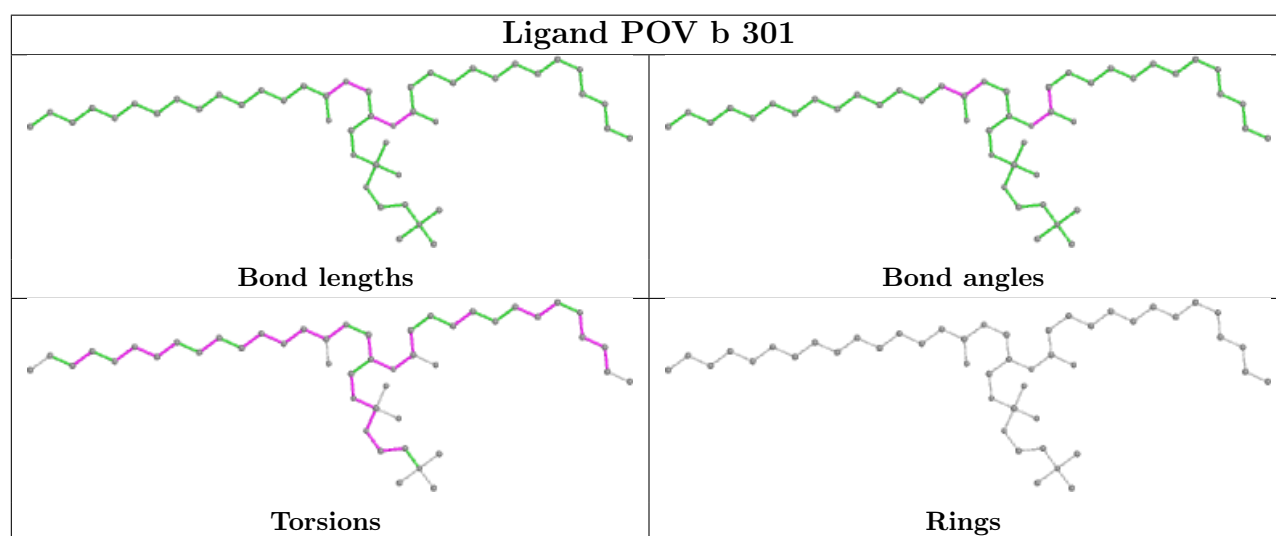
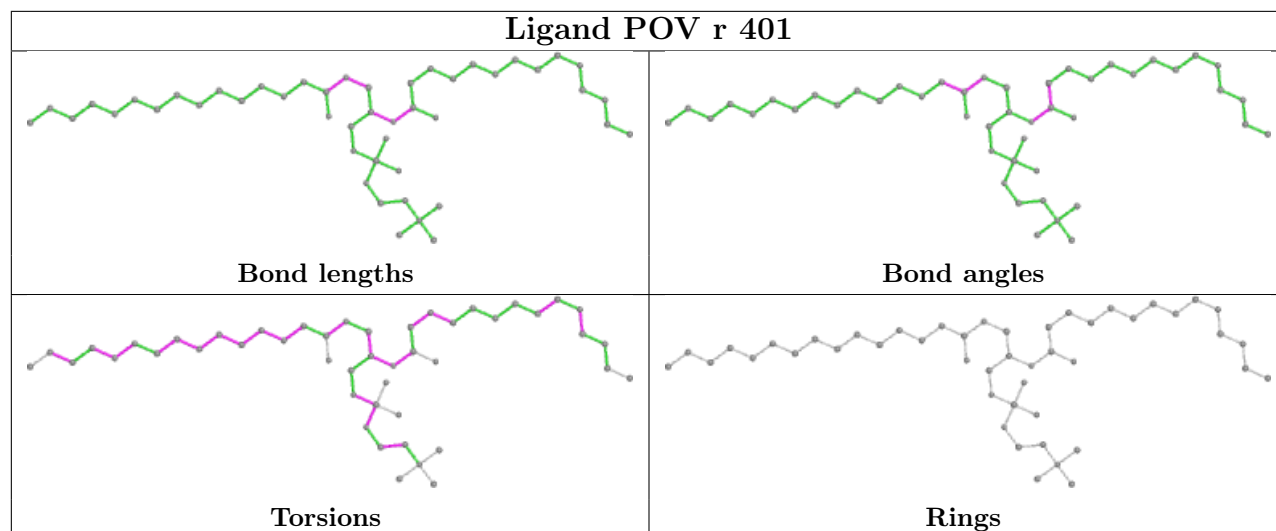
No monomer is involved in short contacts.

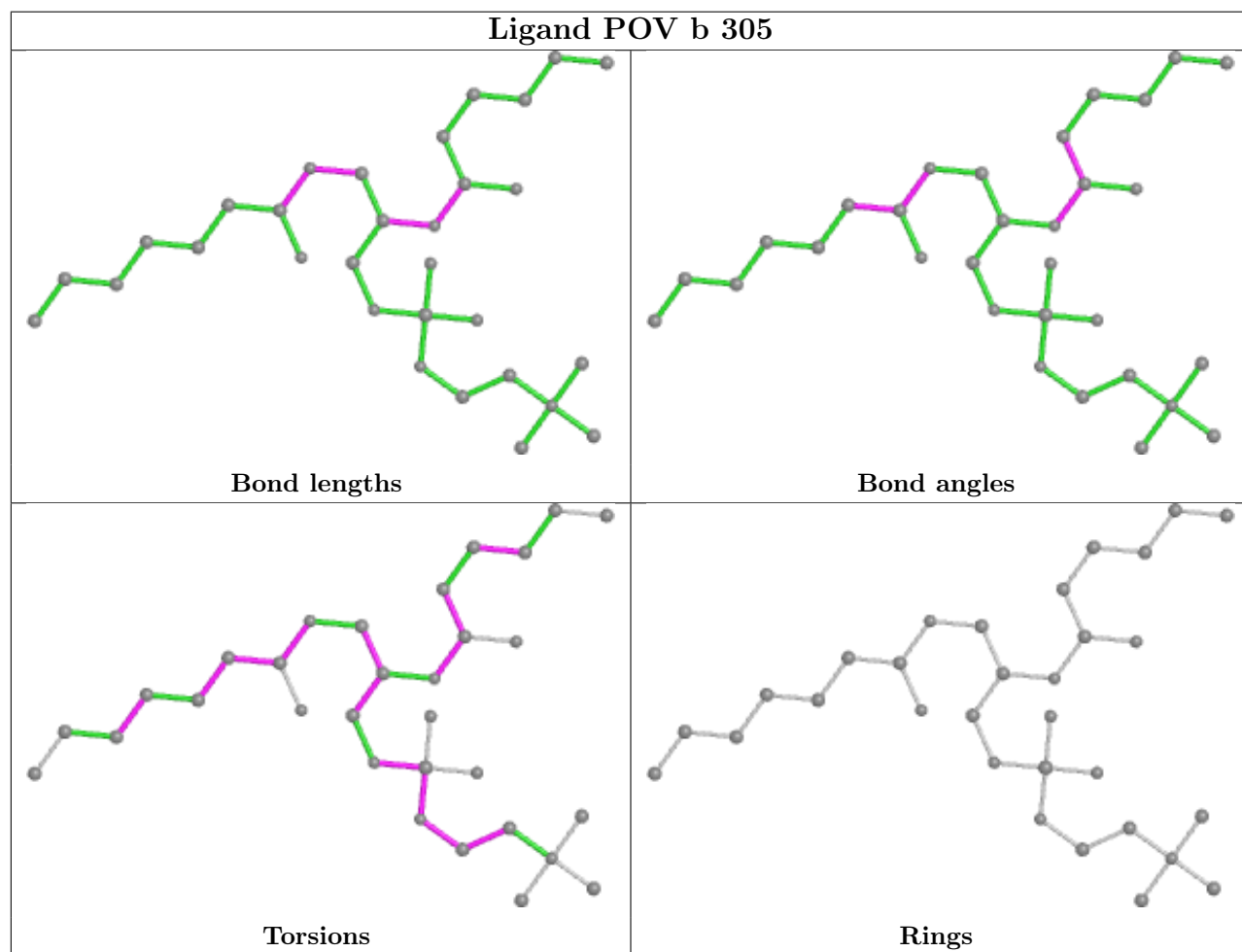
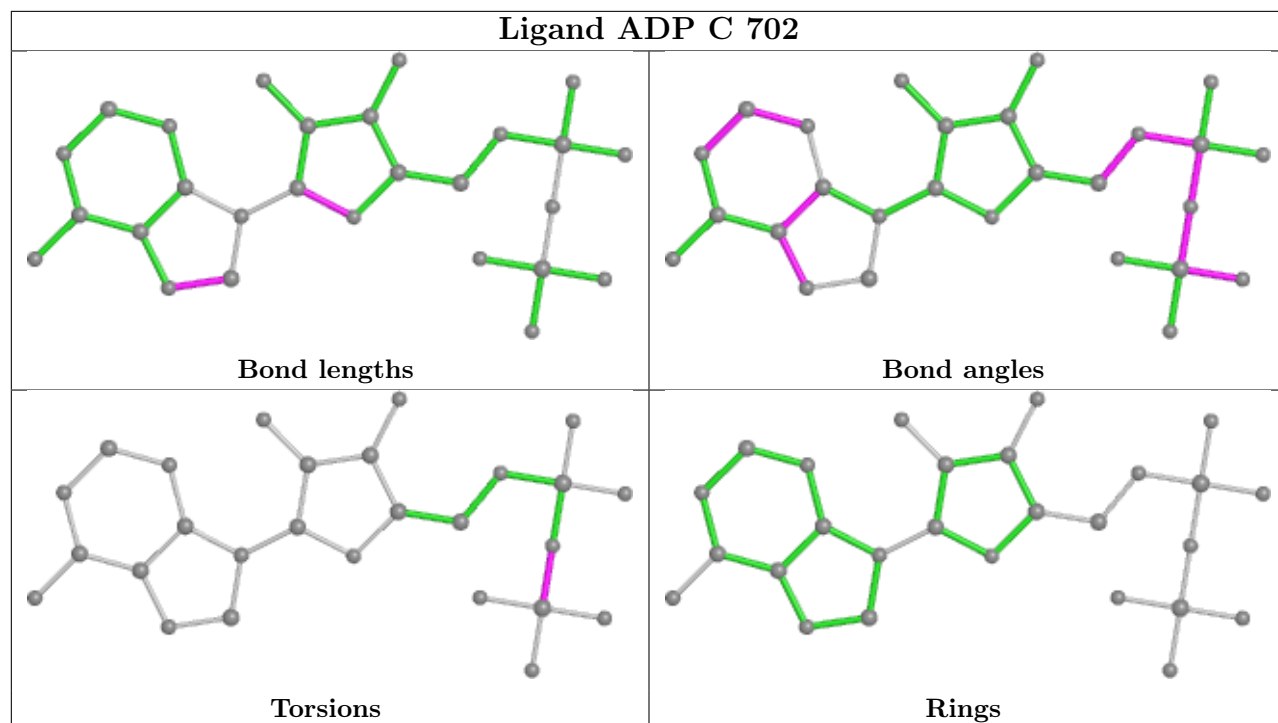
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

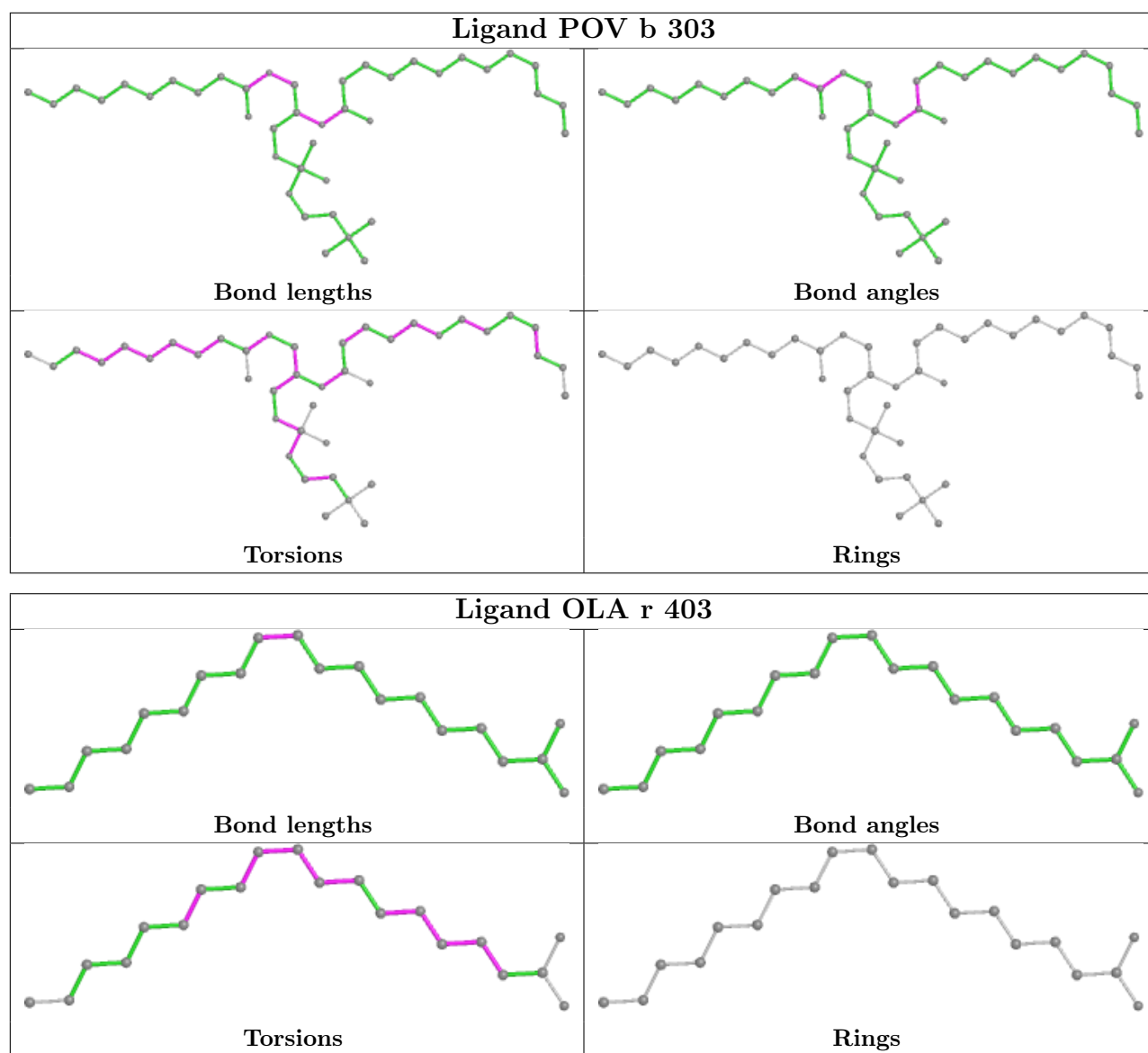
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

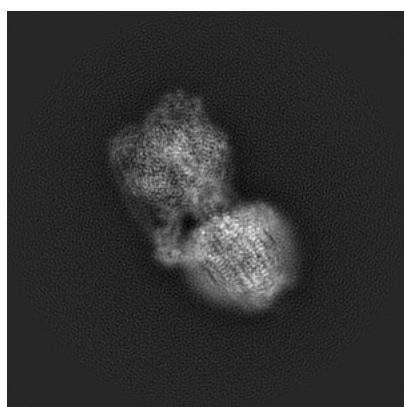
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22121. These allow visual inspection of the internal detail of the map and identification of artifacts.

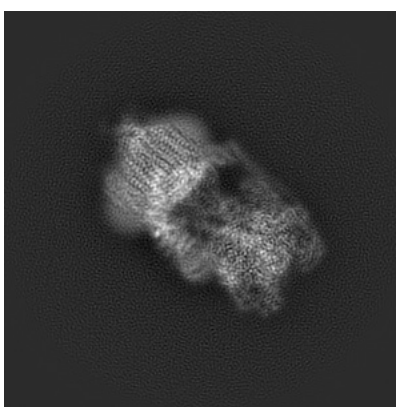
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

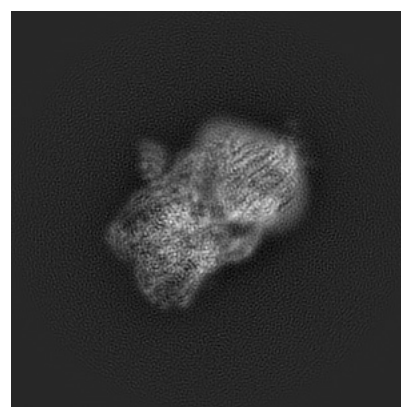
6.1.1 Primary map



X



Y

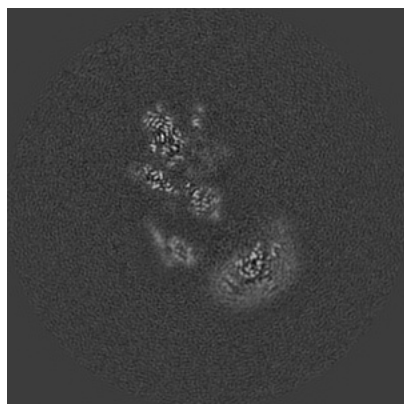


Z

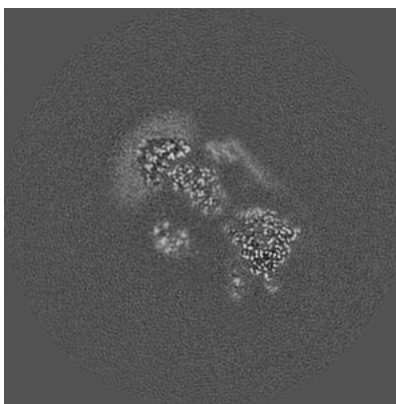
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

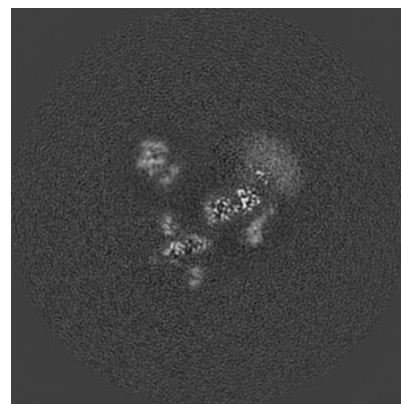
6.2.1 Primary map



X Index: 255



Y Index: 255

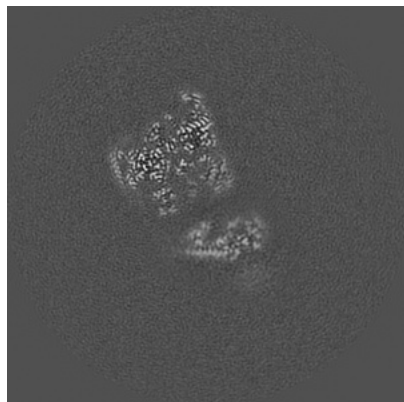


Z Index: 255

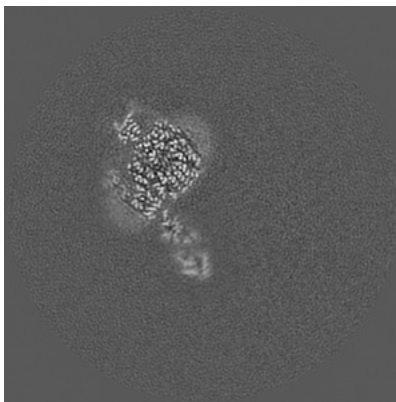
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

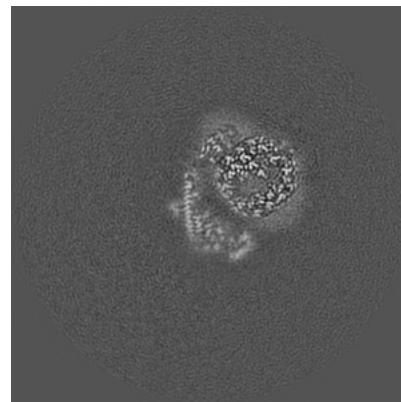
6.3.1 Primary map



X Index: 223



Y Index: 313



Z Index: 196

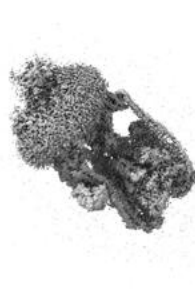
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

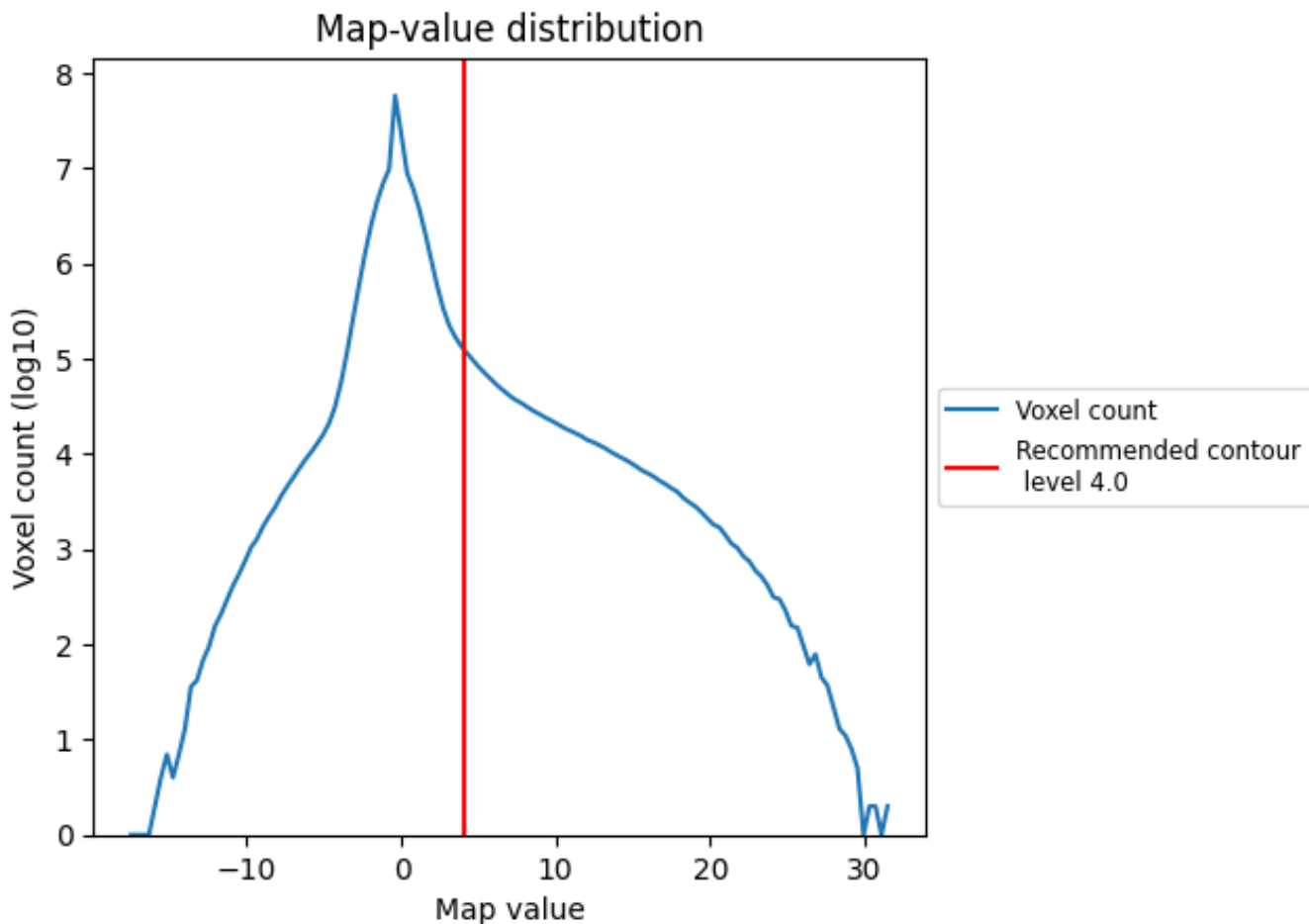
6.5 Mask visualisation

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

7 Map analysis [i](#)

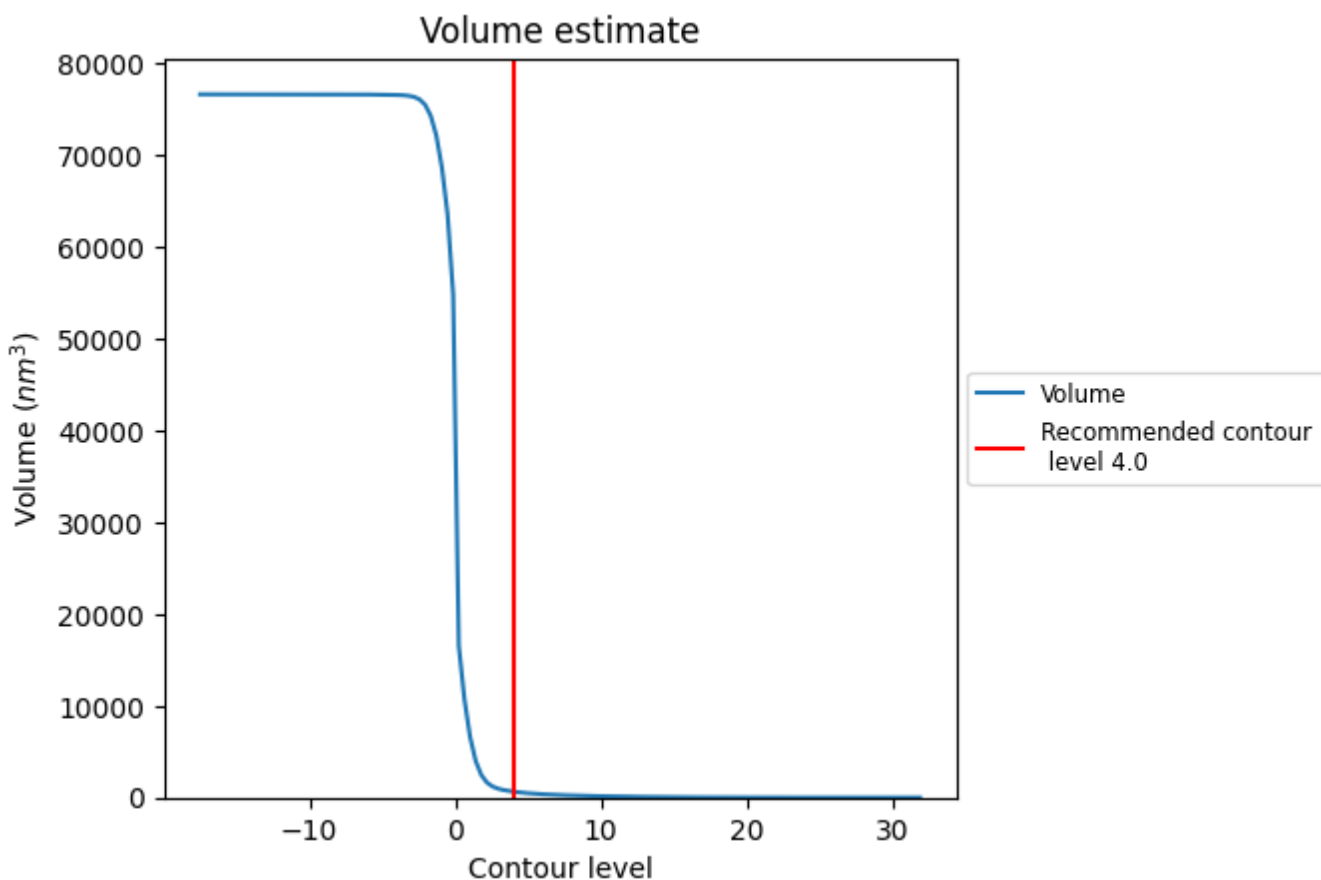
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

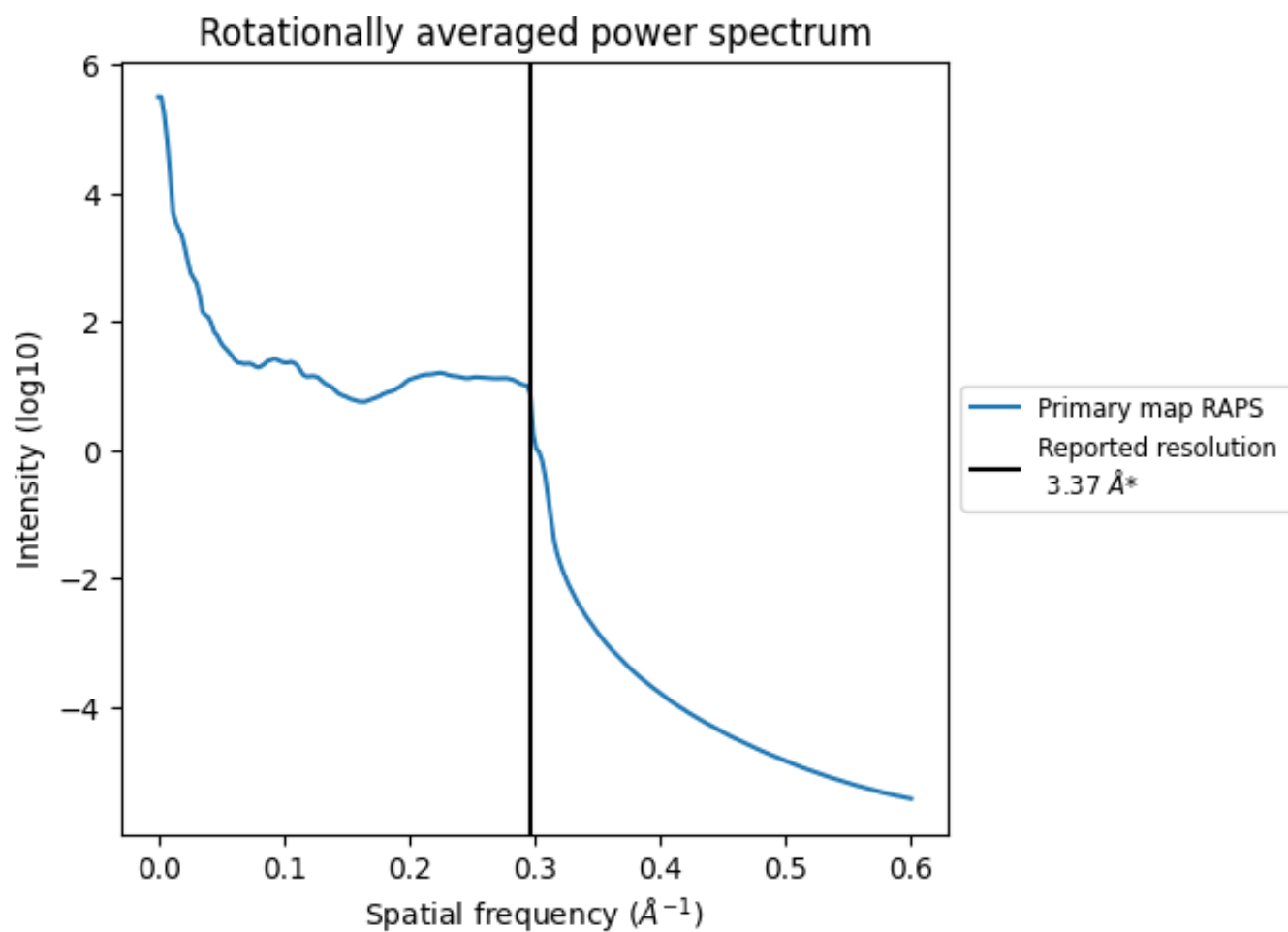
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 642 nm³; this corresponds to an approximate mass of 580 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.297\AA^{-1}

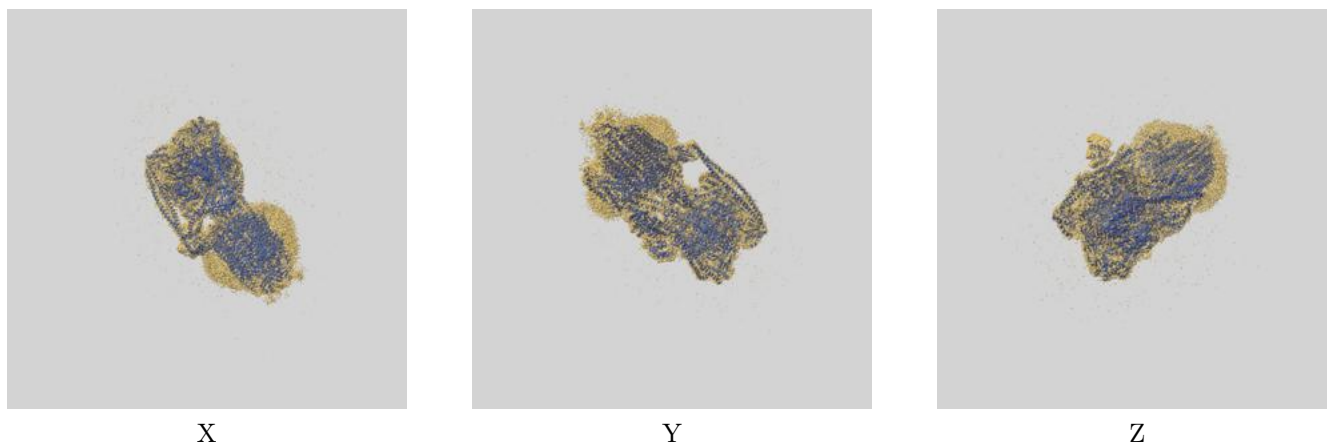
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

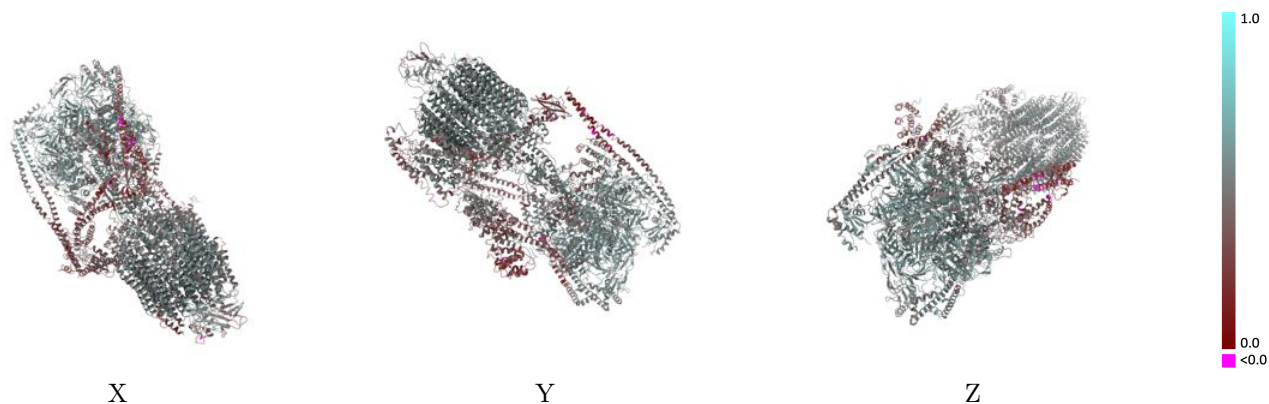
This section contains information regarding the fit between EMDB map EMD-22121 and PDB model 6XBW. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



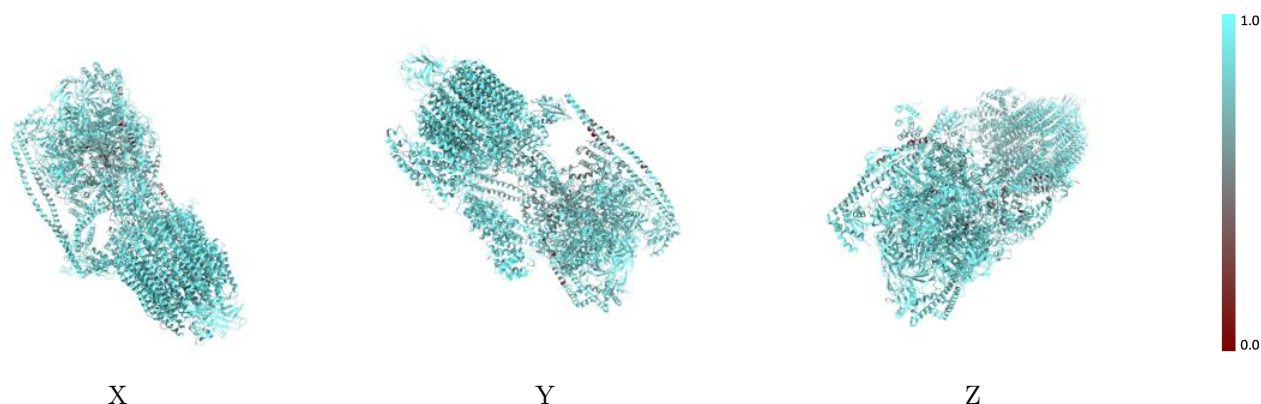
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



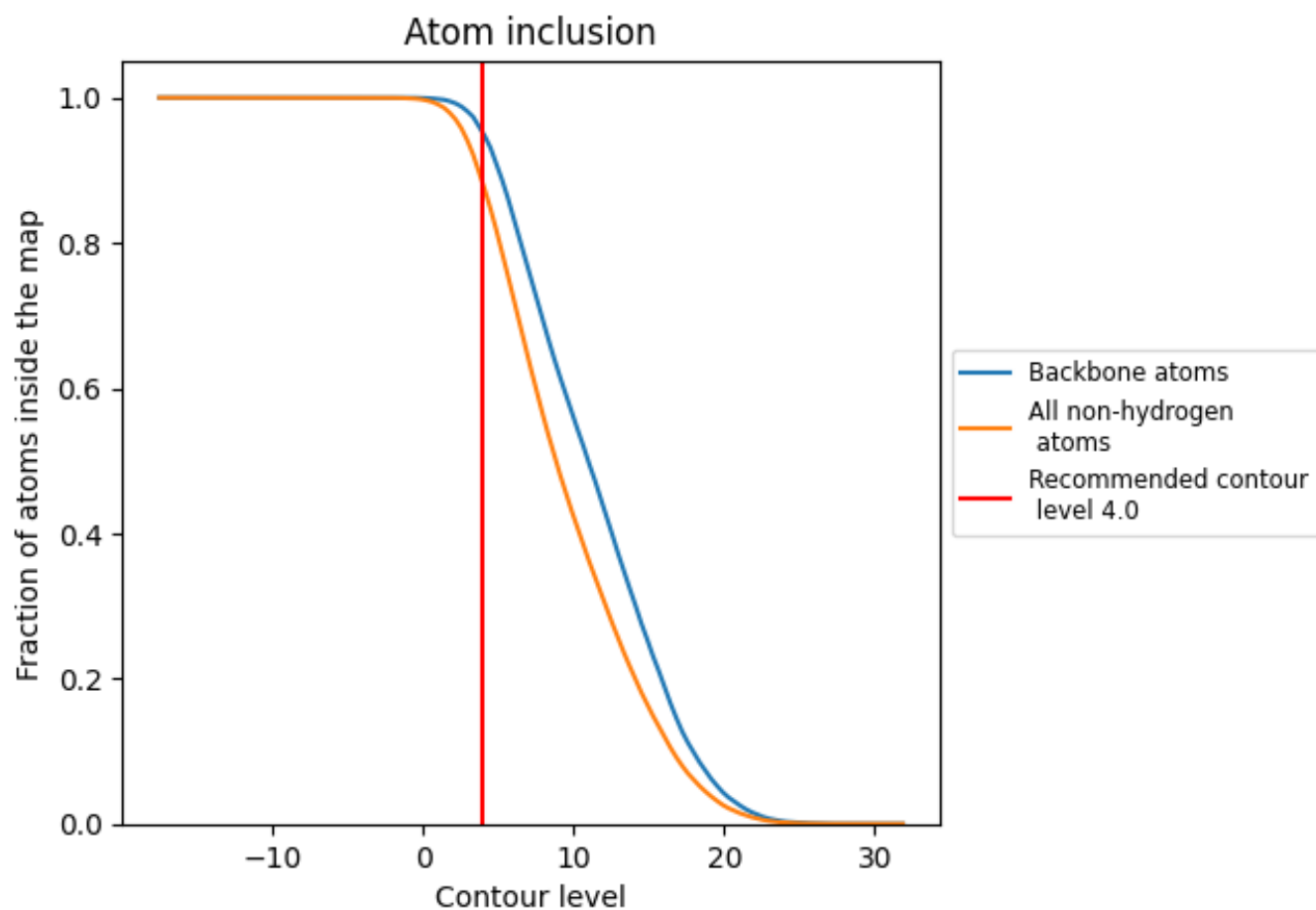
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).



































































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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8801	 0.4790
A	 0.8472	 0.4920
B	 0.8735	 0.5200
C	 0.8854	 0.5290
D	 0.9134	 0.5510
E	 0.9009	 0.5430
F	 0.8914	 0.5350
G	 0.8338	 0.3020
H	 0.8585	 0.5110
I	 0.8216	 0.4430
J	 0.8561	 0.4680
K	 0.8587	 0.4630
L	 0.8304	 0.4760
M	 0.7718	 0.3570
N	 0.8545	 0.4210
O	 0.7764	 0.3890
P	 0.8552	 0.3310
a	 0.8671	 0.4200
b	 0.9340	 0.5250
c	 0.9305	 0.5180
d	 0.8830	 0.4910
e	 0.8273	 0.3950
f	 0.7931	 0.3270
g	 0.9360	 0.5160
k	 0.9258	 0.5090
l	 0.9277	 0.4980
m	 0.9248	 0.5010
n	 0.9229	 0.5110
o	 0.9387	 0.5170
p	 0.9330	 0.5160
q	 0.9349	 0.5170
r	 0.9308	 0.5360
s	 0.9078	 0.4660

