



Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 04:42 AM EDT

PDB ID : 6XBY
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

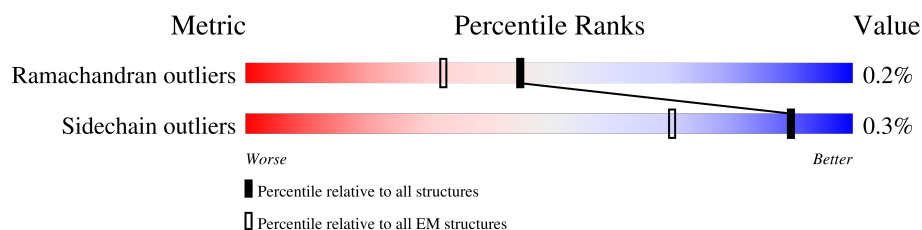
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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.



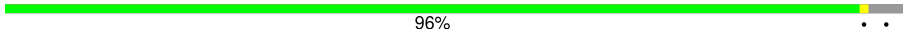
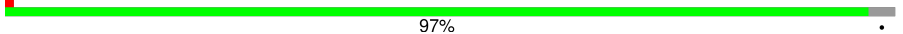












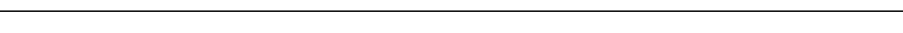
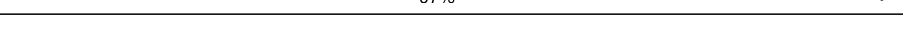
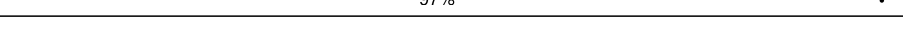
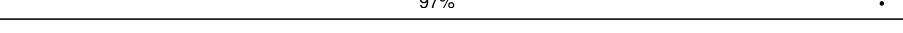
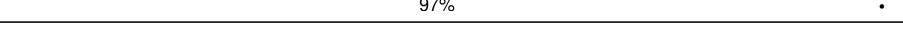
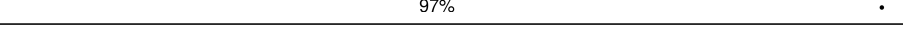

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	617	
1	C	617	
2	D	511	
2	E	511	
2	F	511	
3	G	382	
4	H	247	
5	I	226	

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Mol	Chain	Length	Quality of chain
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	
14	r	351	

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		

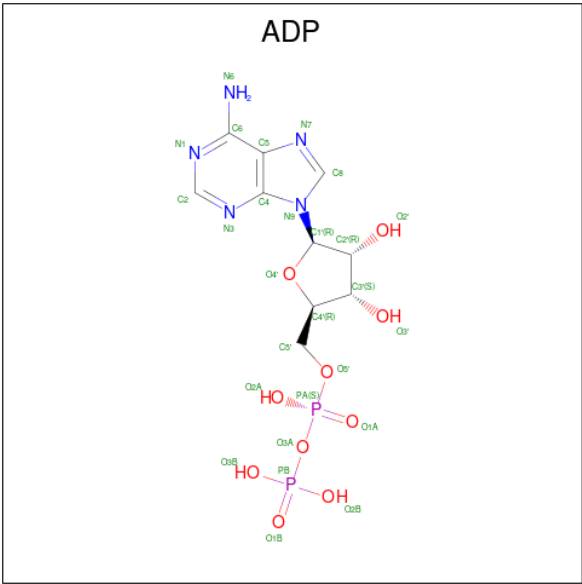
- Molecule 14 is a protein called Renin receptor.

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 (three-letter code: MG) (formula: Mg).

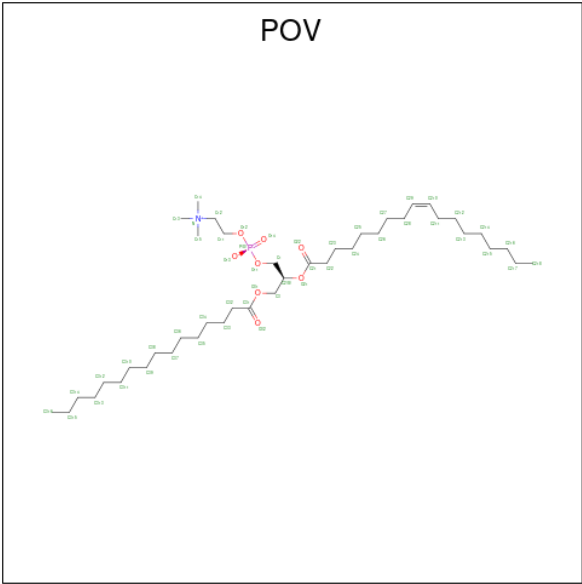
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Mg	0
			1	1	

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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



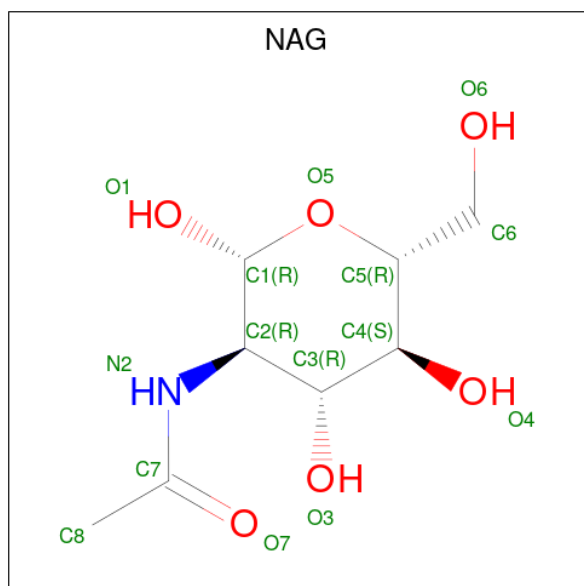
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	b	1	44	34	1	8	1	0

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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 (three-letter code: 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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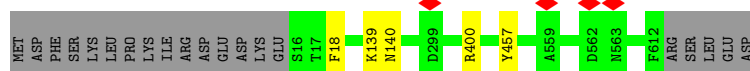
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	s	1	14	8	1	5	0

3 Residue-property plots [i](#)

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

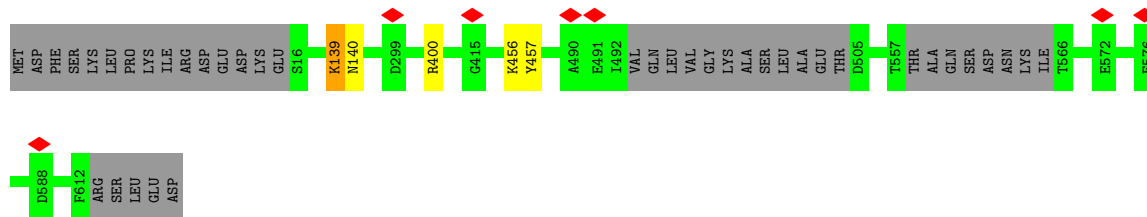
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain A:  96%



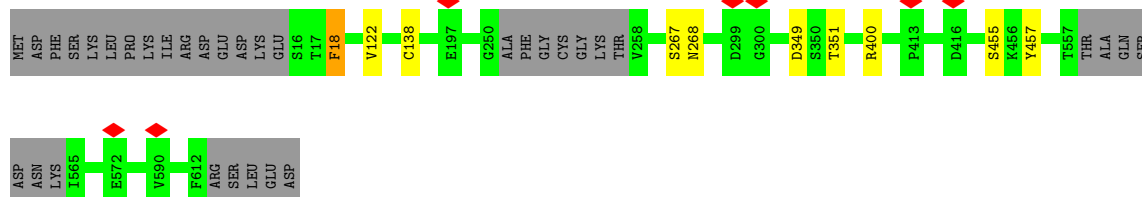
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain B:  93% 6%




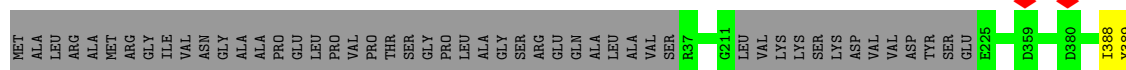
- Molecule 1: V-type proton ATPase catalytic subunit A

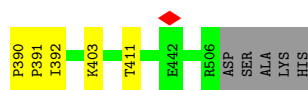
Chain C:  93% 6%



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

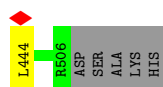
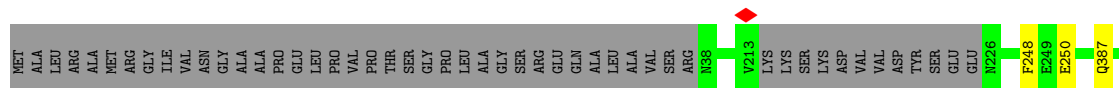
Chain D:  88% 11%





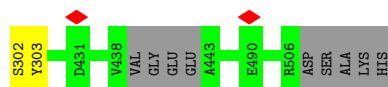
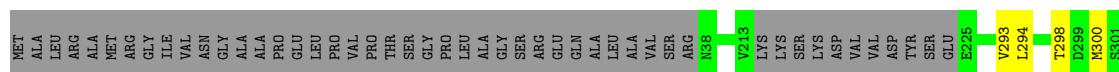
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain E: 89% 11%



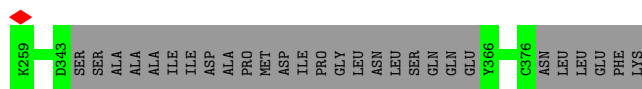
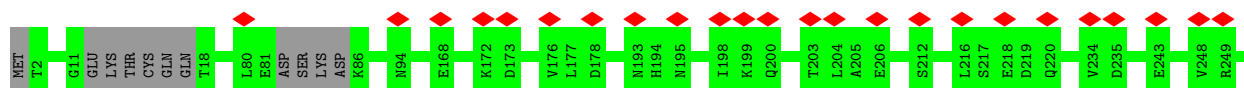
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain F: 88% 11%



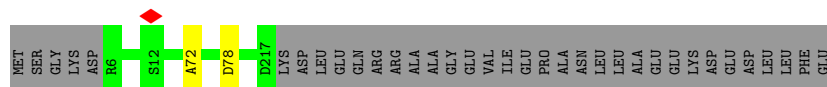
- Molecule 3: V-type proton ATPase subunit C 1

Chain G: 7% 90% 10%



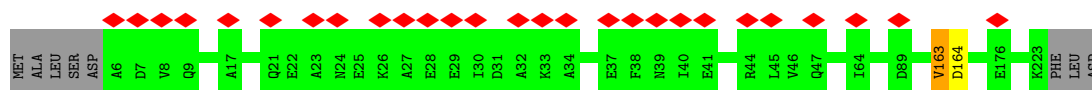
- Molecule 4: V-type proton ATPase subunit D

Chain H: 85% 14%



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

Chain I: 12% 96%



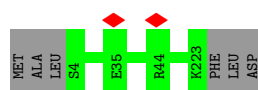
- Molecule 5: V-type proton ATPase subunit E 1

Chain J: 96%



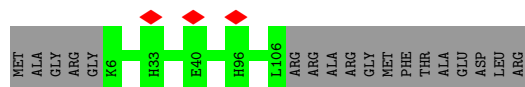
- Molecule 5: V-type proton ATPase subunit E 1

Chain K: 97%



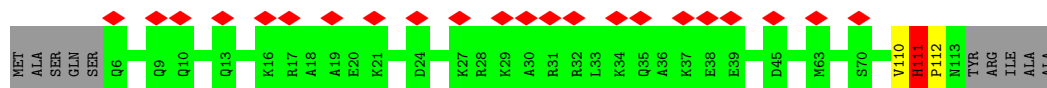
- Molecule 6: V-type proton ATPase subunit F

Chain L: 85%



- Molecule 7: V-type proton ATPase subunit G

Chain M: 19% 89% 8%



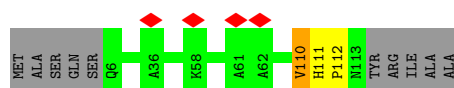
- Molecule 7: V-type proton ATPase subunit G

Chain N: 92% 8%




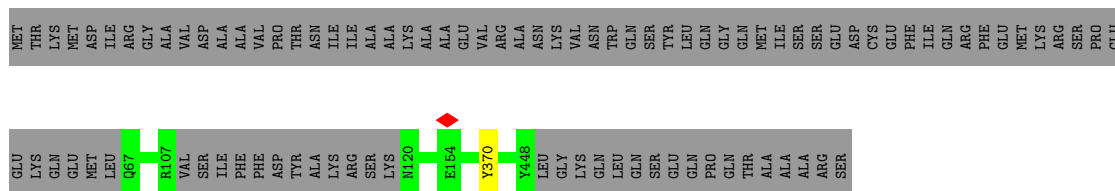
- Molecule 7: V-type proton ATPase subunit G

Chain O: 89% 8%



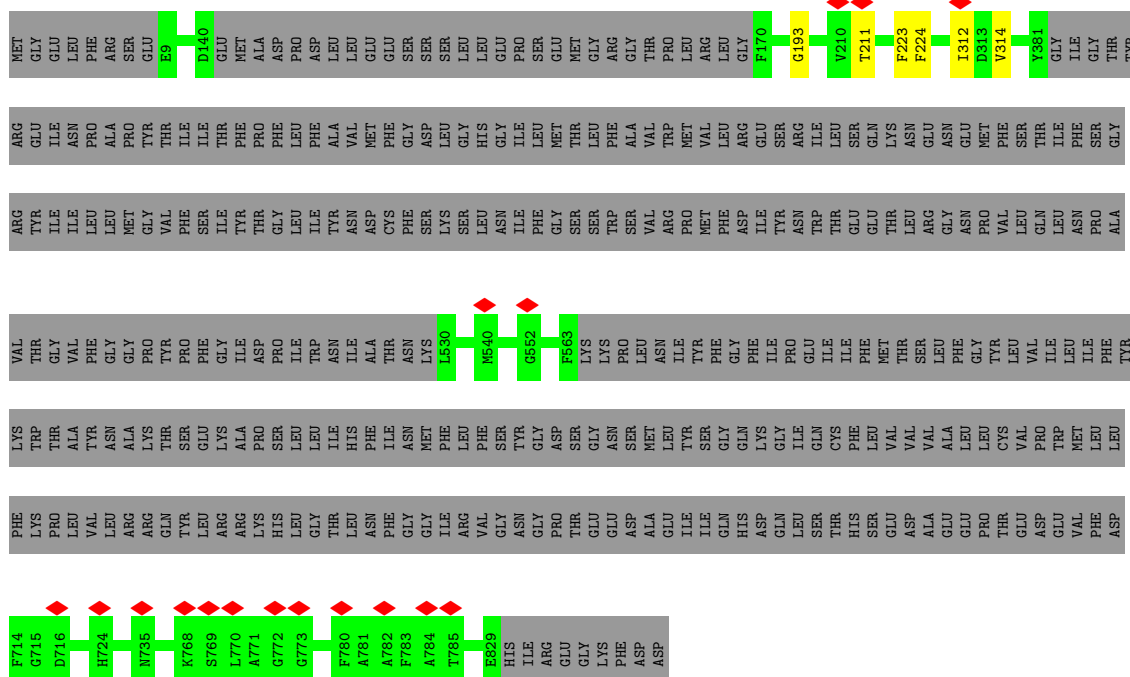
- Molecule 8: V-type proton ATPase subunit H

Chain P:  79% 20%



- Molecule 9: V-type proton ATPase subunit a

Chain a:  58% 41%



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

Chain b:  99%



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

Chain d:  95%



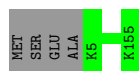
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain q:  97% .



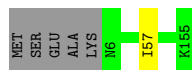
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain p:  97% .



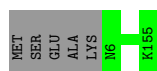
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain c:  96% . .



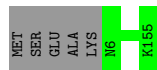
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain g:  97% .



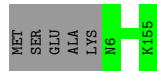
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain k:  97% .



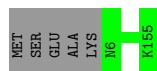
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain l:  97% .



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

Chain m:  97% .



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

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 (\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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, POV, 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	0.37	2/4724 (0.0%)	0.53	1/6398 (0.0%)
1	B	0.34	1/4578 (0.0%)	0.51	1/6197 (0.0%)
1	C	0.41	4/4623 (0.1%)	0.57	3/6260 (0.0%)
2	D	0.36	0/3652	0.58	3/4949 (0.1%)
2	E	0.41	2/3647 (0.1%)	0.58	2/4944 (0.0%)
2	F	0.54	6/3626 (0.2%)	0.60	2/4914 (0.0%)
3	G	0.23	0/1906	0.43	0/2644
4	H	0.25	0/1726	0.69	3/2309 (0.1%)
5	I	0.34	0/1584	0.58	1/2144 (0.0%)
5	J	0.30	0/1588	0.54	1/2148 (0.0%)
5	K	0.26	0/1594	0.45	0/2158
6	L	0.25	0/814	0.50	0/1103
7	M	0.65	1/667 (0.1%)	0.63	3/912 (0.3%)
7	N	0.23	0/663	0.45	0/907
7	O	0.37	0/667	0.75	5/912 (0.5%)
8	P	0.23	0/1835	0.40	0/2558
9	a	0.28	0/3995	0.55	0/5401
10	b	0.43	1/1532 (0.1%)	0.52	0/2083
11	d	0.28	0/2801	0.54	1/3788 (0.0%)
12	c	0.28	0/1079	0.49	0/1459
12	g	0.26	0/1079	0.45	0/1459
12	k	0.26	0/1079	0.44	0/1459
12	l	0.26	0/1079	0.45	0/1459
12	m	0.28	0/1079	0.47	0/1459
12	n	0.27	0/1079	0.45	0/1459
12	o	0.27	0/1088	0.47	0/1470
12	p	0.28	0/1088	0.46	0/1470
12	q	0.26	0/1088	0.45	0/1470
13	s	0.46	0/1720	0.69	3/2341 (0.1%)
14	r	1.07	3/370 (0.8%)	1.04	3/508 (0.6%)
All	All	0.36	20/58050 (0.0%)	0.54	32/78742 (0.0%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	112	PRO	N-CD	14.04	1.67	1.47
10	b	22	VAL	C-N	9.64	1.50	1.33
1	C	457	TYR	CB-CG	-8.18	1.39	1.51
14	r	319	ALA	C-O	-8.17	1.07	1.23
14	r	319	ALA	CA-C	-7.71	1.32	1.52
14	r	318	LEU	C-O	-7.28	1.09	1.23
2	F	303	TYR	CE1-CZ	-6.70	1.29	1.38
2	F	303	TYR	CG-CD1	-6.45	1.30	1.39
1	A	457	TYR	CE1-CZ	-6.14	1.30	1.38
2	E	248	PHE	CB-CG	-6.09	1.41	1.51
1	C	457	TYR	CE2-CZ	-6.06	1.30	1.38
2	F	303	TYR	C-O	-5.70	1.12	1.23
1	B	457	TYR	CE1-CZ	-5.65	1.31	1.38
1	C	457	TYR	CG-CD1	-5.62	1.31	1.39
2	F	303	TYR	CB-CG	-5.56	1.43	1.51
2	F	303	TYR	CG-CD2	-5.53	1.31	1.39
2	E	248	PHE	CG-CD1	-5.50	1.30	1.38
2	F	302	SER	CA-CB	-5.25	1.45	1.52
1	A	18	PHE	CB-CG	-5.09	1.42	1.51
1	C	18	PHE	CB-CG	-5.01	1.42	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	72	ALA	N-CA-C	15.45	152.72	111.00
4	H	72	ALA	CB-CA-C	-14.11	88.94	110.10
2	F	294	LEU	CB-CG-CD2	-10.12	93.81	111.00
14	r	320	LEU	CB-CG-CD2	9.52	127.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	r	318	LEU	CB-CG-CD2	-8.99	95.71	111.00
7	O	110	VAL	N-CA-C	-8.55	87.92	111.00
5	I	164	ASP	CB-CG-OD2	8.50	125.95	118.30
13	s	448	LEU	CA-CB-CG	7.75	133.12	115.30
7	O	111	HIS	CB-CA-C	-7.44	95.52	110.40
7	O	112	PRO	N-CA-C	-7.42	92.80	112.10
1	C	268	ASN	N-CA-C	-7.35	91.16	111.00
5	J	163	VAL	CB-CA-C	-7.17	97.78	111.40
2	E	444	LEU	CA-CB-CG	7.12	131.68	115.30
13	s	312	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	139	LYS	C-N-CA	6.50	137.96	121.70
1	A	139	LYS	C-N-CA	6.14	137.04	121.70
2	D	392	ILE	CB-CA-C	-6.05	99.51	111.60
2	D	389	TYR	N-CA-C	6.03	127.27	111.00
2	E	248	PHE	CB-CA-C	-6.01	98.38	110.40
2	F	293	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	C	349	ASP	CB-CA-C	-5.86	98.67	110.40
2	D	390	PRO	N-CA-C	-5.86	96.85	112.10
7	M	110	VAL	CB-CA-C	-5.83	100.32	111.40
11	d	276	LEU	CA-CB-CG	5.77	128.56	115.30
7	O	112	PRO	C-N-CA	5.70	135.94	121.70
1	C	268	ASN	CB-CA-C	5.34	121.08	110.40
7	O	112	PRO	CB-CA-C	5.32	125.31	112.00
7	M	110	VAL	N-CA-C	5.23	125.13	111.00
7	M	111	HIS	N-CA-C	5.20	125.04	111.00
13	s	375	GLU	CA-CB-CG	5.18	124.80	113.40
4	H	78	ASP	CB-CG-OD2	5.16	122.94	118.30
14	r	316	ILE	N-CA-CB	5.07	122.45	110.80

There are no chirality outliers.

All (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
9	a	193	GLY	Peptide
9	a	314	VAL	Peptide

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	595/617 (96%)	565 (95%)	29 (5%)	1 (0%)	44	74
1	B	571/617 (92%)	533 (93%)	37 (6%)	1 (0%)	44	74
1	C	577/617 (94%)	539 (93%)	37 (6%)	1 (0%)	44	74
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%)	44	74
3	G	335/382 (88%)	315 (94%)	20 (6%)	0	100	100
4	H	210/247 (85%)	199 (95%)	11 (5%)	0	100	100
5	I	216/226 (96%)	207 (96%)	8 (4%)	1 (0%)	25	58
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%)	37	69
9	a	486/838 (58%)	444 (91%)	39 (8%)	3 (1%)	22	55
10	b	201/205 (98%)	193 (96%)	8 (4%)	0	100	100
11	d	330/351 (94%)	309 (94%)	20 (6%)	1 (0%)	37	69
12	c	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
12	g	148/155 (96%)	147 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	45	74

All (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
8	P	370	TYR
11	d	91	GLU
1	A	140	ASN
9	a	223	PHE
9	a	312	ILE
1	C	351	THR
9	a	224	PHE

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%)	503 (100%)	1 (0%)	92	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	488/524 (93%)	486 (100%)	2 (0%)	89	91
1	C	494/524 (94%)	490 (99%)	4 (1%)	79	84
2	D	390/432 (90%)	387 (99%)	3 (1%)	79	84
2	E	390/432 (90%)	389 (100%)	1 (0%)	91	92
2	F	388/432 (90%)	387 (100%)	1 (0%)	91	92
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%)	81	86
5	J	142/198 (72%)	141 (99%)	1 (1%)	81	86
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%)	41	61
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%)	409 (100%)	1 (0%)	92	94
10	b	156/158 (99%)	156 (100%)	0	100	100
11	d	294/306 (96%)	293 (100%)	1 (0%)	91	92
12	c	106/110 (96%)	105 (99%)	1 (1%)	75	82
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
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%)	41	61
All	All	5554/7320 (76%)	5535 (100%)	19 (0%)	90	92

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	ARG
1	B	400	ARG
1	B	456	LYS
1	C	18	PHE
1	C	122	VAL
1	C	138	CYS
1	C	400	ARG
2	D	388	ILE
2	D	391	PRO
2	D	403	LYS
2	E	250	GLU
2	F	298	THR
5	I	163	VAL
5	J	161	ARG
7	M	111	HIS
9	a	211	THR
11	d	276	LEU
12	c	57	ILE
14	r	304	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	GLN
1	B	159	ASN
1	B	225	HIS
1	B	282	ASN
1	B	523	ASN
1	C	314	ASN
1	C	521	GLN
2	D	171	GLN
2	D	181	ASN
2	D	262	ASN
2	D	387	GLN
2	E	181	ASN
2	E	482	GLN
2	F	42	GLN
2	F	205	GLN
2	F	385	ASN
2	F	420	ASN
2	F	482	GLN
4	H	137	ASN
4	H	152	GLN

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Mol	Chain	Res	Type
5	I	74	ASN
5	I	78	GLN
5	I	206	GLN
5	J	77	ASN
5	J	149	GLN
5	K	67	GLN
5	K	96	ASN
5	K	122	GLN
6	L	57	ASN
7	M	111	HIS
7	O	89	GLN
7	O	111	HIS
9	a	106	ASN
9	a	316	GLN
9	a	375	GLN
9	a	762	HIS
10	b	132	HIS
10	b	168	GLN
11	d	338	GLN
12	q	78	ASN
12	q	92	GLN
12	q	123	GLN
12	q	124	GLN
12	p	78	ASN
12	p	92	GLN
12	c	92	GLN
12	c	124	GLN
12	g	6	ASN
12	g	78	ASN
12	g	92	GLN
12	k	78	ASN
12	k	124	GLN
12	l	6	ASN
12	l	78	ASN
12	l	92	GLN
12	m	6	ASN
12	m	78	ASN
12	m	92	GLN
12	n	6	ASN
12	n	78	ASN
12	n	92	GLN
12	o	78	ASN

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Mol	Chain	Res	Type
13	s	270	GLN
13	s	342	ASN
13	s	404	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
18	NAG	s	507	-	14,14,15	0.27	0	19,19,21	0.33	0
17	POV	r	401	-	42,42,51	1.08	4 (9%)	48,50,59	0.96	2 (4%)
17	POV	s	501	-	45,45,51	1.06	3 (6%)	51,53,59	1.01	2 (3%)
18	NAG	s	503	13	14,14,15	0.33	0	17,19,21	0.51	0
16	ADP	D	601	15	24,29,29	1.22	2 (8%)	29,45,45	1.26	3 (10%)
17	POV	o	201	-	43,43,51	1.06	4 (9%)	49,51,59	0.90	2 (4%)
17	POV	b	301	-	43,43,51	2.29	11 (25%)	49,51,59	2.00	17 (34%)
17	POV	l	201	-	41,41,51	1.09	4 (9%)	47,49,59	0.89	2 (4%)
18	NAG	s	506	13	14,14,15	0.41	0	17,19,21	0.35	0

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%)
18	NAG	s	504	13	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
17	POV	r	402	-	41,41,51	1.09	4 (9%)	47,49,59	0.97	2 (4%)
18	NAG	s	502	13	14,14,15	0.35	0	17,19,21	0.39	0
18	NAG	s	505	13	14,14,15	0.66	1 (7%)	17,19,21	0.72	1 (5%)

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
18	NAG	s	507	-	-	1/6/22/26	0/1/1/1
17	POV	r	401	-	-	25/46/46/55	-
17	POV	s	501	-	-	26/49/49/55	-
18	NAG	s	503	13	-	3/6/23/26	0/1/1/1
16	ADP	D	601	15	-	4/12/32/32	0/3/3/3
17	POV	o	201	-	-	23/47/47/55	-
17	POV	b	301	-	-	24/47/47/55	-
17	POV	l	201	-	-	22/45/45/55	-
18	NAG	s	506	13	-	1/6/23/26	0/1/1/1
17	POV	r	403	-	-	26/45/45/55	-
18	NAG	s	504	13	-	1/6/23/26	0/1/1/1
17	POV	r	402	-	-	16/45/45/55	-
18	NAG	s	502	13	-	2/6/23/26	0/1/1/1
18	NAG	s	505	13	-	0/6/23/26	0/1/1/1

All (37) 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
17	b	301	POV	C14-N	-3.53	1.39	1.50
16	D	601	ADP	O4'-C1'	3.44	1.45	1.40
17	b	301	POV	O12-C11	-3.29	1.31	1.44
17	b	301	POV	O32-C31	-3.09	1.13	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	301	POV	P-O13	-3.07	1.41	1.55
17	r	401	POV	O21-C2	-2.85	1.39	1.46
17	r	403	POV	O21-C2	-2.82	1.40	1.46
17	l	201	POV	O21-C2	-2.81	1.40	1.46
17	b	301	POV	O22-C21	-2.77	1.14	1.22
17	r	402	POV	O21-C2	-2.70	1.40	1.46
17	s	501	POV	O21-C2	-2.69	1.40	1.46
17	o	201	POV	O21-C2	-2.65	1.40	1.46
17	b	301	POV	O11-C1	-2.55	1.34	1.44
17	r	402	POV	O31-C31	2.47	1.40	1.33
17	s	501	POV	O31-C31	2.44	1.40	1.33
17	l	201	POV	O31-C31	2.37	1.40	1.33
17	o	201	POV	O31-C31	2.37	1.40	1.33
17	s	501	POV	O31-C3	-2.37	1.39	1.45
16	D	601	ADP	C8-N7	-2.34	1.30	1.34
17	r	401	POV	O31-C31	2.31	1.40	1.33
17	r	401	POV	O31-C3	-2.28	1.40	1.45
17	r	403	POV	O31-C31	2.27	1.40	1.33
17	o	201	POV	O31-C3	-2.25	1.40	1.45
17	r	403	POV	O31-C3	-2.23	1.40	1.45
17	l	201	POV	O31-C3	-2.21	1.40	1.45
17	r	402	POV	O21-C21	2.18	1.40	1.34
17	o	201	POV	O21-C21	2.13	1.40	1.34
17	l	201	POV	O21-C21	2.08	1.40	1.34
17	r	401	POV	O21-C21	2.07	1.40	1.34
18	s	505	NAG	C1-C2	2.06	1.55	1.52
17	r	403	POV	O21-C21	2.06	1.40	1.34
17	r	402	POV	O31-C3	-2.01	1.40	1.45

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	601	ADP	N3-C2-N1	-4.80	122.15	128.67
17	b	301	POV	C2-O21-C21	-4.80	106.31	117.80
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
17	r	401	POV	O21-C21-C22	4.01	120.16	111.48
17	b	301	POV	O31-C3-C2	-3.99	96.89	108.40
17	o	201	POV	O21-C21-C22	3.97	120.07	111.48
17	b	301	POV	P-O12-C11	-3.92	102.58	121.26
17	b	301	POV	O12-C11-C12	-3.91	90.83	109.65
17	r	403	POV	O21-C21-C22	3.86	119.83	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	l	201	POV	O21-C21-C22	3.80	119.69	111.48
17	b	301	POV	O31-C31-O32	-3.64	114.51	123.63
17	b	301	POV	C11-C12-N	-3.64	104.14	115.82
17	b	301	POV	O12-P-O14	3.18	121.55	108.94
17	s	501	POV	O31-C31-C32	3.08	121.23	111.83
17	r	402	POV	O31-C31-C32	2.72	120.14	111.83
17	r	403	POV	O31-C31-C32	2.71	120.09	111.83
17	b	301	POV	C33-C32-C31	-2.65	104.00	113.69
17	b	301	POV	C26-C25-C24	-2.61	101.16	114.37
17	l	201	POV	O31-C31-C32	2.58	119.71	111.83
17	o	201	POV	O31-C31-C32	2.56	119.63	111.83
17	b	301	POV	C25-C24-C23	-2.55	101.47	114.37
17	r	401	POV	O31-C31-C32	2.52	119.53	111.83
17	b	301	POV	C36-C35-C34	-2.50	101.75	114.37
17	b	301	POV	C37-C36-C35	-2.48	101.85	114.37
17	b	301	POV	C14-N-C13	-2.41	102.63	108.98
18	s	504	NAG	C1-O5-C5	2.36	115.35	112.19
18	s	505	NAG	C1-O5-C5	2.28	115.24	112.19
17	b	301	POV	C28-C29-C210	-2.27	113.27	130.48
17	b	301	POV	C38-C37-C36	-2.16	103.46	114.37
17	b	301	POV	C38-C39-C310	-2.13	103.61	114.37
16	D	601	ADP	O3B-PB-O3A	2.11	111.73	104.64
17	b	301	POV	O31-C31-C32	2.09	118.21	111.83
16	D	601	ADP	PA-O5'-C5'	-2.00	109.89	121.35

There are no chirality outliers.

All (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
17	o	201	POV	C11-O12-P-O11
17	o	201	POV	C11-O12-P-O13
17	o	201	POV	C11-O12-P-O14
17	o	201	POV	O12-C11-C12-N
17	o	201	POV	O22-C21-O21-C2
17	s	501	POV	C1-O11-P-O12
17	s	501	POV	C1-O11-P-O13
17	s	501	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
17	s	501	POV	C210-C211-C212-C213
17	s	501	POV	O22-C21-O21-C2
17	r	401	POV	C1-O11-P-O12
17	r	401	POV	C1-O11-P-O13
17	r	401	POV	C1-O11-P-O14
17	r	401	POV	C11-O12-P-O11
17	r	401	POV	C11-O12-P-O13
17	r	401	POV	O21-C2-C3-O31
17	r	401	POV	O12-C11-C12-N
17	r	401	POV	C22-C21-O21-C2
17	r	402	POV	C1-O11-P-O12
17	r	402	POV	C1-O11-P-O13
17	r	402	POV	C1-O11-P-O14
17	r	402	POV	O12-C11-C12-N
17	r	402	POV	O22-C21-O21-C2
17	r	403	POV	C1-O11-P-O12
17	r	403	POV	C1-O11-P-O13
17	r	403	POV	C1-O11-P-O14
17	r	403	POV	C11-O12-P-O11
17	r	403	POV	C11-O12-P-O13
17	b	301	POV	O32-C31-O31-C3
17	b	301	POV	O22-C21-O21-C2
17	r	401	POV	O22-C21-O21-C2
17	r	401	POV	C32-C31-O31-C3
17	r	403	POV	C32-C31-O31-C3
17	o	201	POV	C22-C21-O21-C2
17	s	501	POV	C22-C21-O21-C2
17	r	402	POV	C22-C21-O21-C2
17	r	401	POV	O32-C31-O31-C3
17	r	403	POV	O32-C31-O31-C3
17	b	301	POV	C22-C21-O21-C2
16	D	601	ADP	O4'-C4'-C5'-O5'
16	D	601	ADP	C3'-C4'-C5'-O5'
17	b	301	POV	C32-C31-O31-C3
18	s	503	NAG	O5-C5-C6-O6
17	s	501	POV	C32-C31-O31-C3
18	s	502	NAG	O5-C5-C6-O6
18	s	502	NAG	C4-C5-C6-O6
17	r	401	POV	C22-C23-C24-C25
17	o	201	POV	C31-C32-C33-C34
17	l	201	POV	C31-C32-C33-C34
17	s	501	POV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	s	501	POV	O32-C31-O31-C3
17	o	201	POV	C21-C22-C23-C24
17	l	201	POV	C22-C21-O21-C2
17	r	403	POV	C21-C22-C23-C24
17	o	201	POV	C32-C31-O31-C3
17	b	301	POV	C34-C35-C36-C37
17	l	201	POV	C1-C2-C3-O31
17	r	403	POV	C22-C21-O21-C2
17	o	201	POV	O32-C31-O31-C3
17	l	201	POV	O22-C21-O21-C2
18	s	506	NAG	O5-C5-C6-O6
17	b	301	POV	C24-C25-C26-C27
17	s	501	POV	C33-C34-C35-C36
17	l	201	POV	C210-C211-C212-C213
17	b	301	POV	C22-C23-C24-C25
17	l	201	POV	C25-C26-C27-C28
17	s	501	POV	C31-C32-C33-C34
17	r	402	POV	O11-C1-C2-O21
17	r	401	POV	C26-C27-C28-C29
17	r	403	POV	C22-C23-C24-C25
17	o	201	POV	C33-C34-C35-C36
17	l	201	POV	C35-C36-C37-C38
17	s	501	POV	C34-C35-C36-C37
17	r	403	POV	C24-C25-C26-C27
17	s	501	POV	C22-C23-C24-C25
17	l	201	POV	O11-C1-C2-C3
17	r	403	POV	O11-C1-C2-C3
17	r	402	POV	C32-C33-C34-C35
17	r	403	POV	O22-C21-O21-C2
17	o	201	POV	C36-C37-C38-C39
17	o	201	POV	C26-C27-C28-C29
18	s	504	NAG	O5-C5-C6-O6
17	b	301	POV	C39-C310-C311-C312
17	s	501	POV	C25-C26-C27-C28
17	s	501	POV	C24-C25-C26-C27
17	b	301	POV	C37-C38-C39-C310
17	b	301	POV	C26-C27-C28-C29
17	r	402	POV	C210-C211-C212-C213
17	b	301	POV	C33-C34-C35-C36
17	r	403	POV	O11-C1-C2-O21
17	r	402	POV	C32-C31-O31-C3
17	o	201	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
17	l	201	POV	C211-C212-C213-C214
17	r	403	POV	C37-C38-C39-C310
17	r	402	POV	O11-C1-C2-C3
18	s	503	NAG	C4-C5-C6-O6
17	r	403	POV	C23-C24-C25-C26
17	b	301	POV	C1-C2-C3-O31
17	r	401	POV	C1-C2-C3-O31
17	r	402	POV	C1-C2-C3-O31
17	b	301	POV	C23-C24-C25-C26
17	s	501	POV	C23-C24-C25-C26
17	o	201	POV	C35-C36-C37-C38
17	r	402	POV	O21-C2-C3-O31
17	b	301	POV	C311-C310-C39-C38
17	l	201	POV	C32-C33-C34-C35
17	o	201	POV	C32-C33-C34-C35
17	r	403	POV	C36-C37-C38-C39
17	r	402	POV	O32-C31-O31-C3
17	b	301	POV	C311-C312-C313-C314
17	l	201	POV	C36-C37-C38-C39
17	r	401	POV	C34-C35-C36-C37
17	l	201	POV	C33-C34-C35-C36
17	r	401	POV	C36-C37-C38-C39
17	l	201	POV	C26-C27-C28-C29
17	s	501	POV	C26-C27-C28-C29
17	r	403	POV	C39-C310-C311-C312
17	r	403	POV	C26-C27-C28-C29
17	l	201	POV	O11-C1-C2-O21
17	s	501	POV	C12-C11-O12-P
17	o	201	POV	C311-C310-C39-C38
17	l	201	POV	C24-C25-C26-C27
17	r	403	POV	O12-C11-C12-N
17	r	403	POV	C35-C36-C37-C38
17	r	403	POV	C34-C35-C36-C37
17	l	201	POV	C22-C23-C24-C25
17	o	201	POV	O11-C1-C2-C3
17	s	501	POV	C29-C210-C211-C212
17	o	201	POV	O11-C1-C2-O21
17	r	403	POV	C311-C312-C313-C314
17	b	301	POV	O21-C2-C3-O31
17	l	201	POV	O21-C2-C3-O31
17	l	201	POV	C23-C24-C25-C26
17	b	301	POV	C11-O12-P-O13

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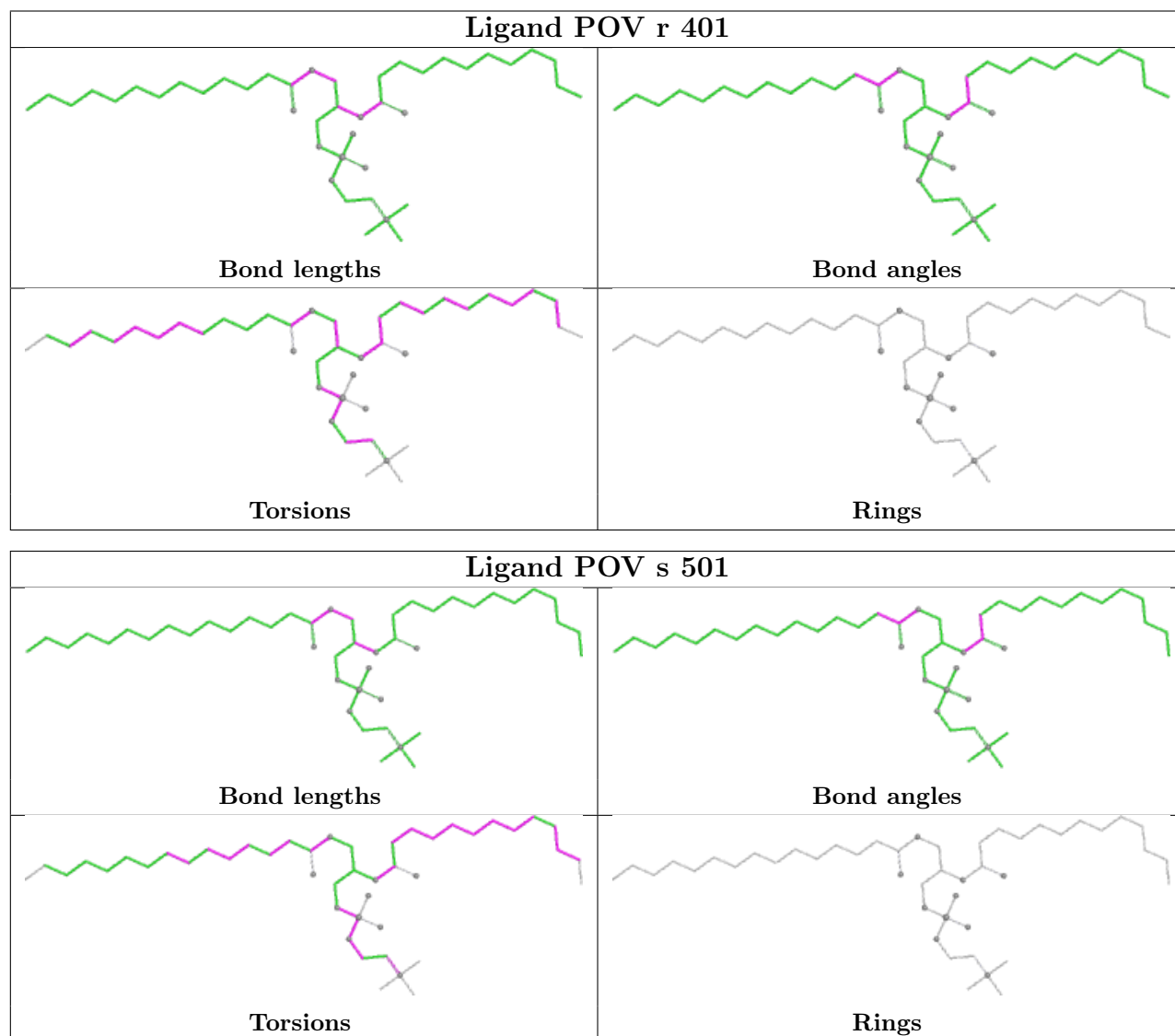
Mol	Chain	Res	Type	Atoms
17	l	201	POV	C1-O11-P-O14
17	s	501	POV	C11-O12-P-O11
17	s	501	POV	C11-O12-P-O13
17	s	501	POV	C11-O12-P-O14
17	r	401	POV	C11-O12-P-O14
17	o	201	POV	C37-C38-C39-C310
17	l	201	POV	O32-C31-O31-C3
17	r	401	POV	C29-C210-C211-C212
17	r	401	POV	C39-C310-C311-C312
17	l	201	POV	C32-C31-O31-C3
17	o	201	POV	C27-C28-C29-C210
17	o	201	POV	C210-C211-C212-C213
18	s	503	NAG	C1-C2-N2-C7
17	r	403	POV	C312-C313-C314-C315
17	r	401	POV	C24-C25-C26-C27
17	r	401	POV	C35-C36-C37-C38
17	r	403	POV	C2-C1-O11-P
17	s	501	POV	C36-C37-C38-C39
17	r	402	POV	C24-C25-C26-C27
17	r	401	POV	C37-C38-C39-C310
17	s	501	POV	C27-C28-C29-C210
17	r	401	POV	C27-C28-C29-C210
17	b	301	POV	C31-C32-C33-C34
17	b	301	POV	C27-C28-C29-C210
17	r	402	POV	C27-C28-C29-C210
17	b	301	POV	O12-C11-C12-N
17	r	401	POV	O21-C21-C22-C23
18	s	507	NAG	C4-C5-C6-O6
17	s	501	POV	C11-C12-N-C13
17	r	401	POV	O22-C21-C22-C23
17	b	301	POV	C32-C33-C34-C35
17	b	301	POV	C25-C26-C27-C28
17	r	403	POV	O21-C21-C22-C23
17	s	501	POV	C11-C12-N-C14
17	o	201	POV	O21-C21-C22-C23

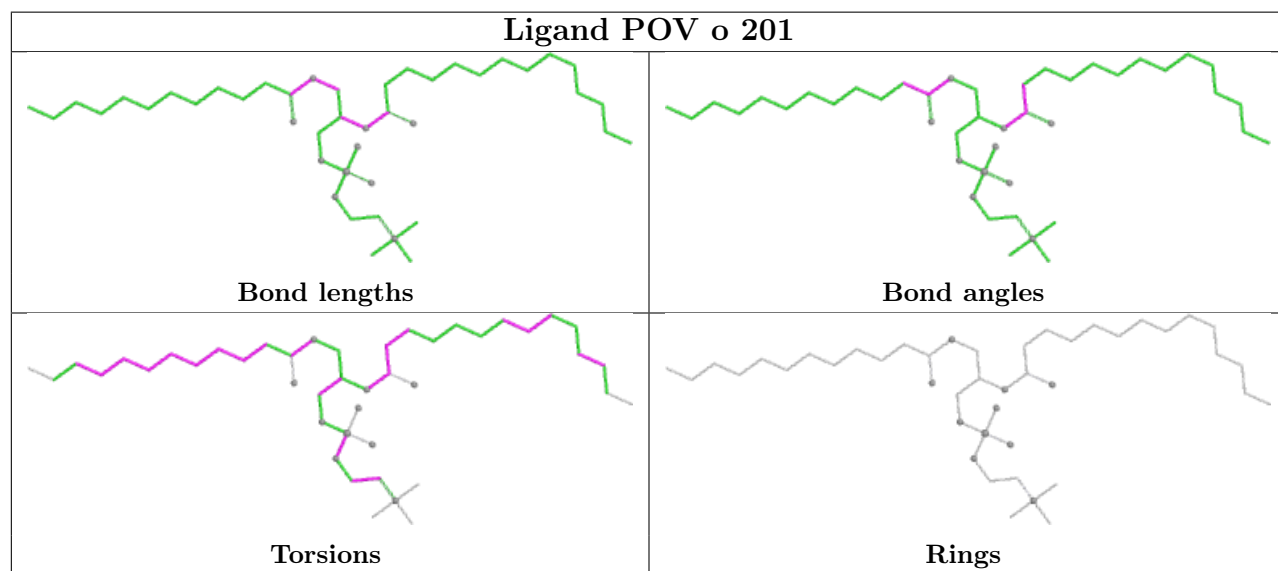
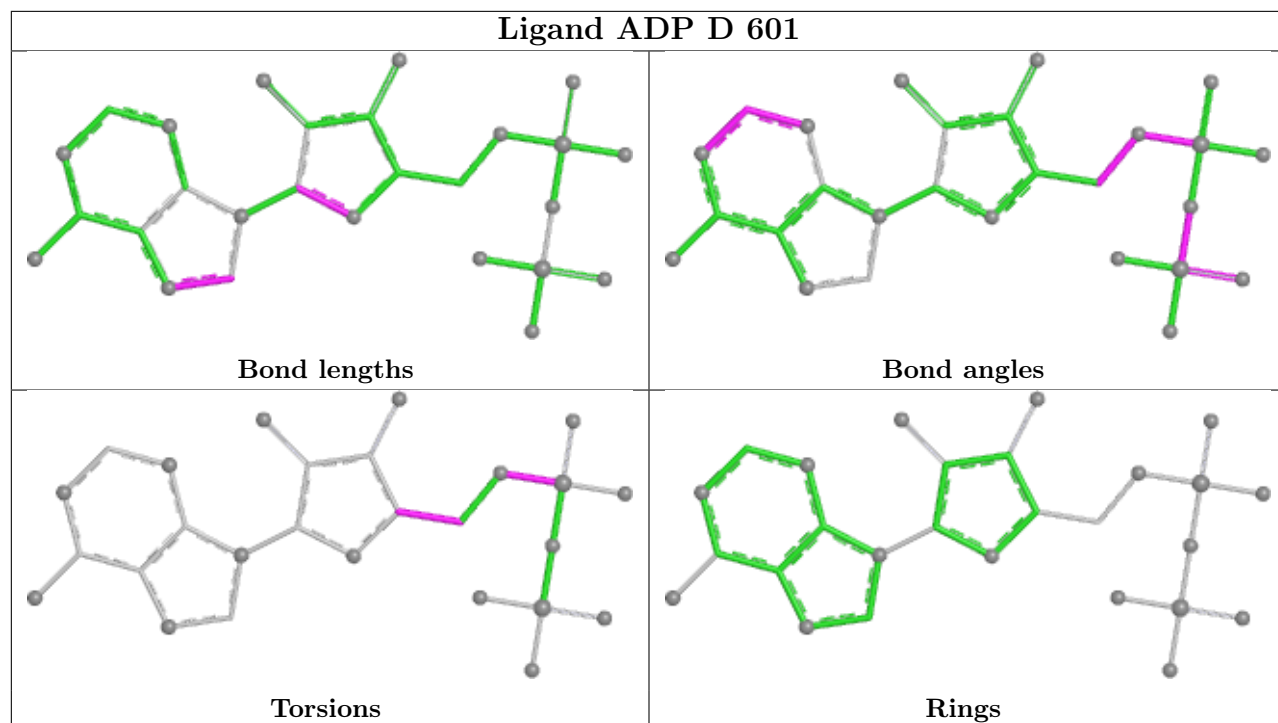
There are no ring outliers.

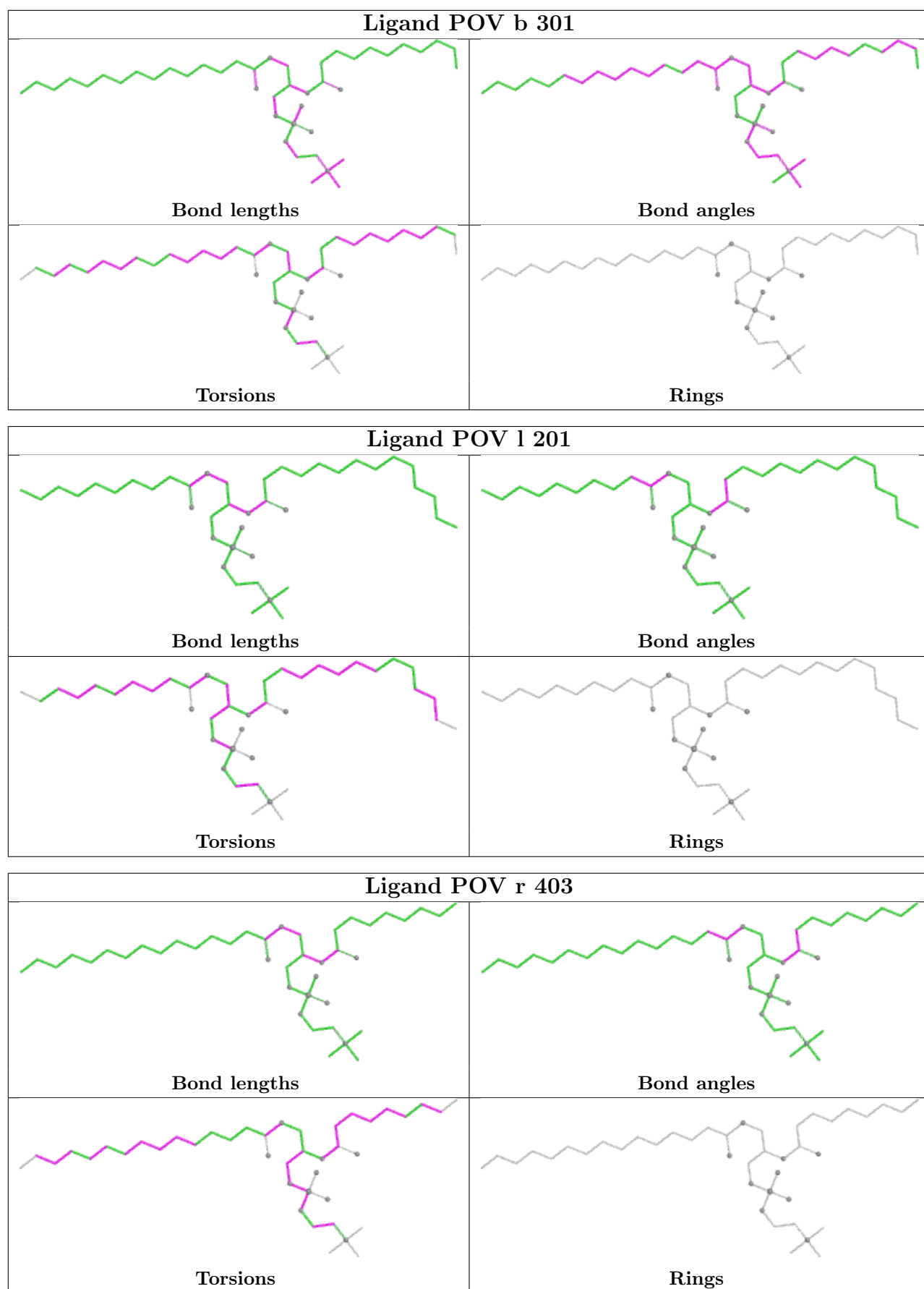
No monomer is involved in short contacts.

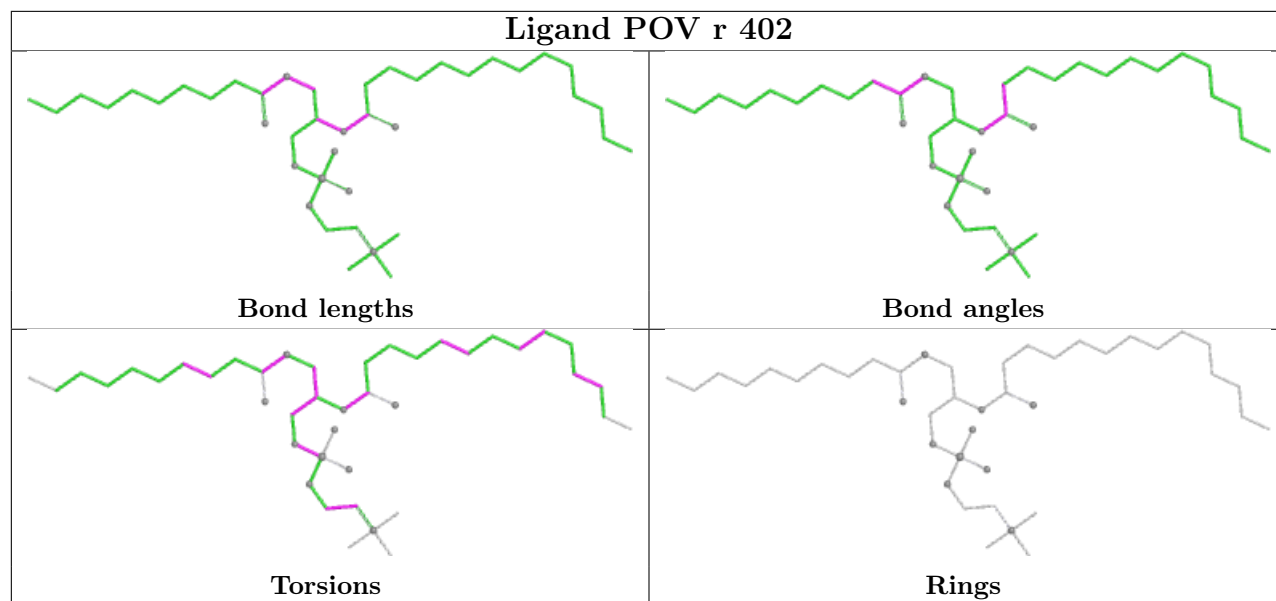
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

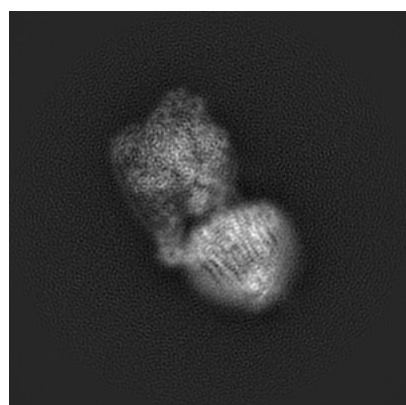
6 Map visualisation [i](#)

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

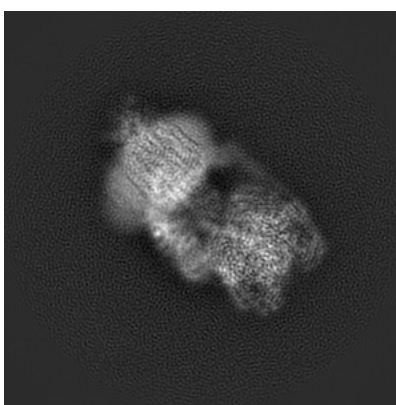
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

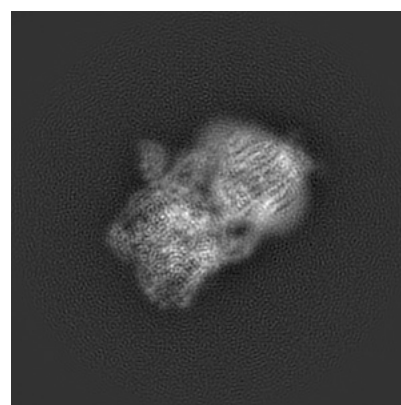
6.1.1 Primary map



X



Y

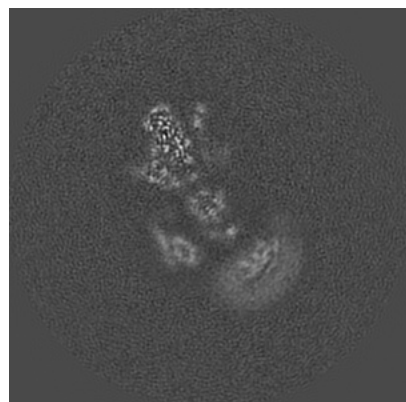


Z

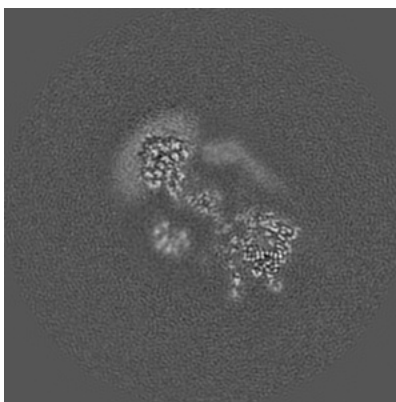
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

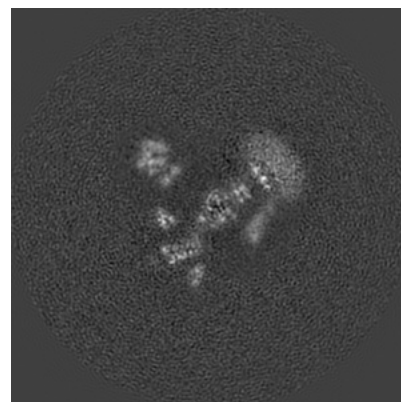
6.2.1 Primary map



X Index: 255



Y Index: 255

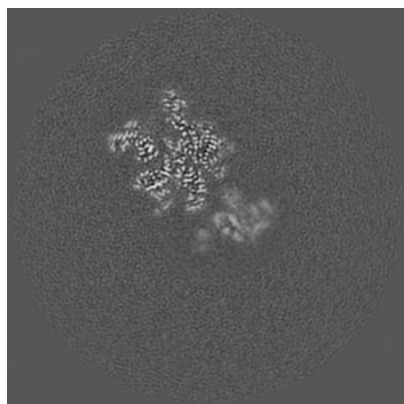


Z Index: 255

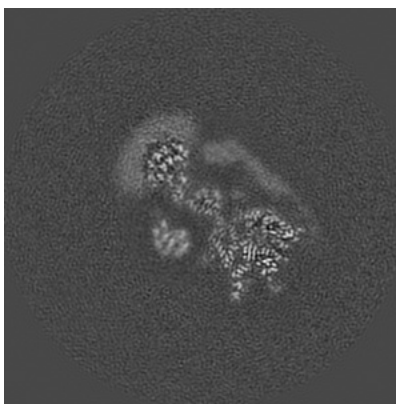
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

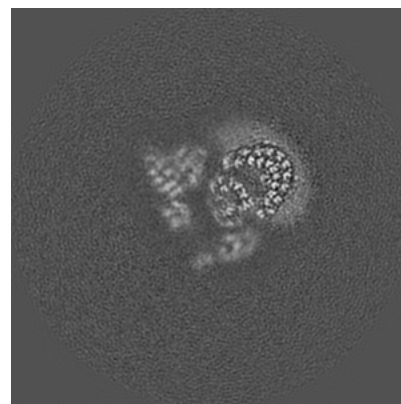
6.3.1 Primary map



X Index: 194



Y Index: 251

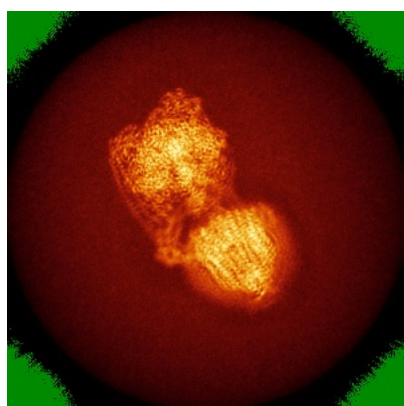


Z Index: 224

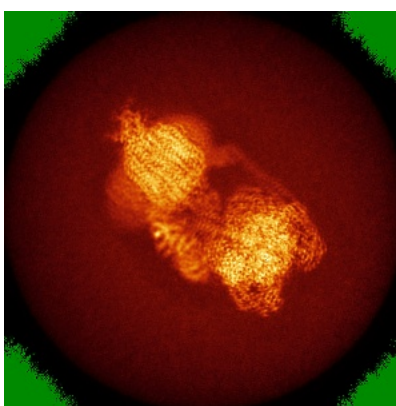
The images above show the largest variance slices of the map in three orthogonal directions.

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

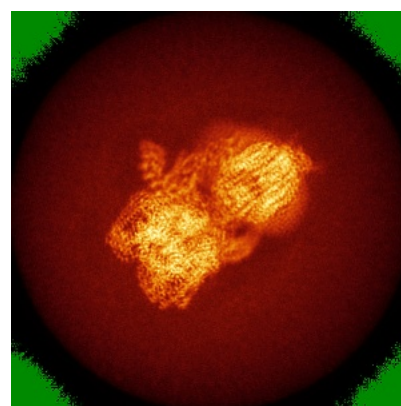
6.4.1 Primary map



X



Y

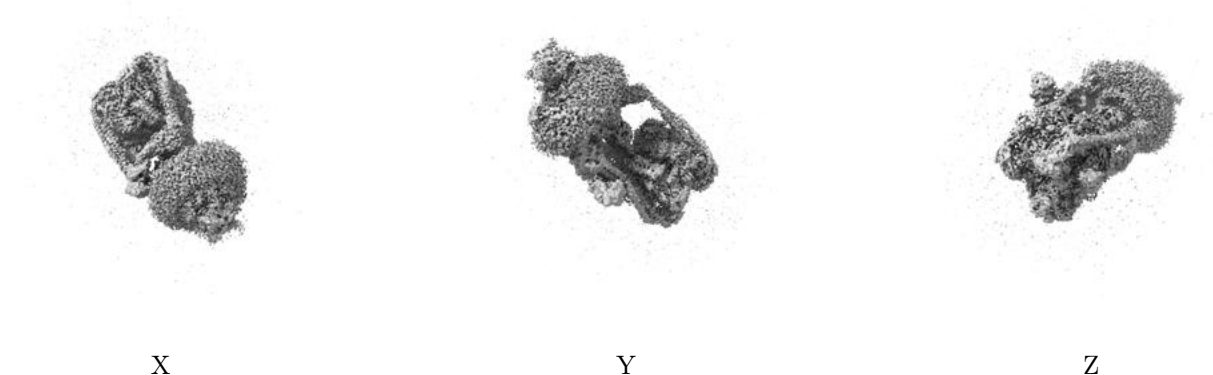


Z

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 [i](#)

6.5.1 Primary map



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.

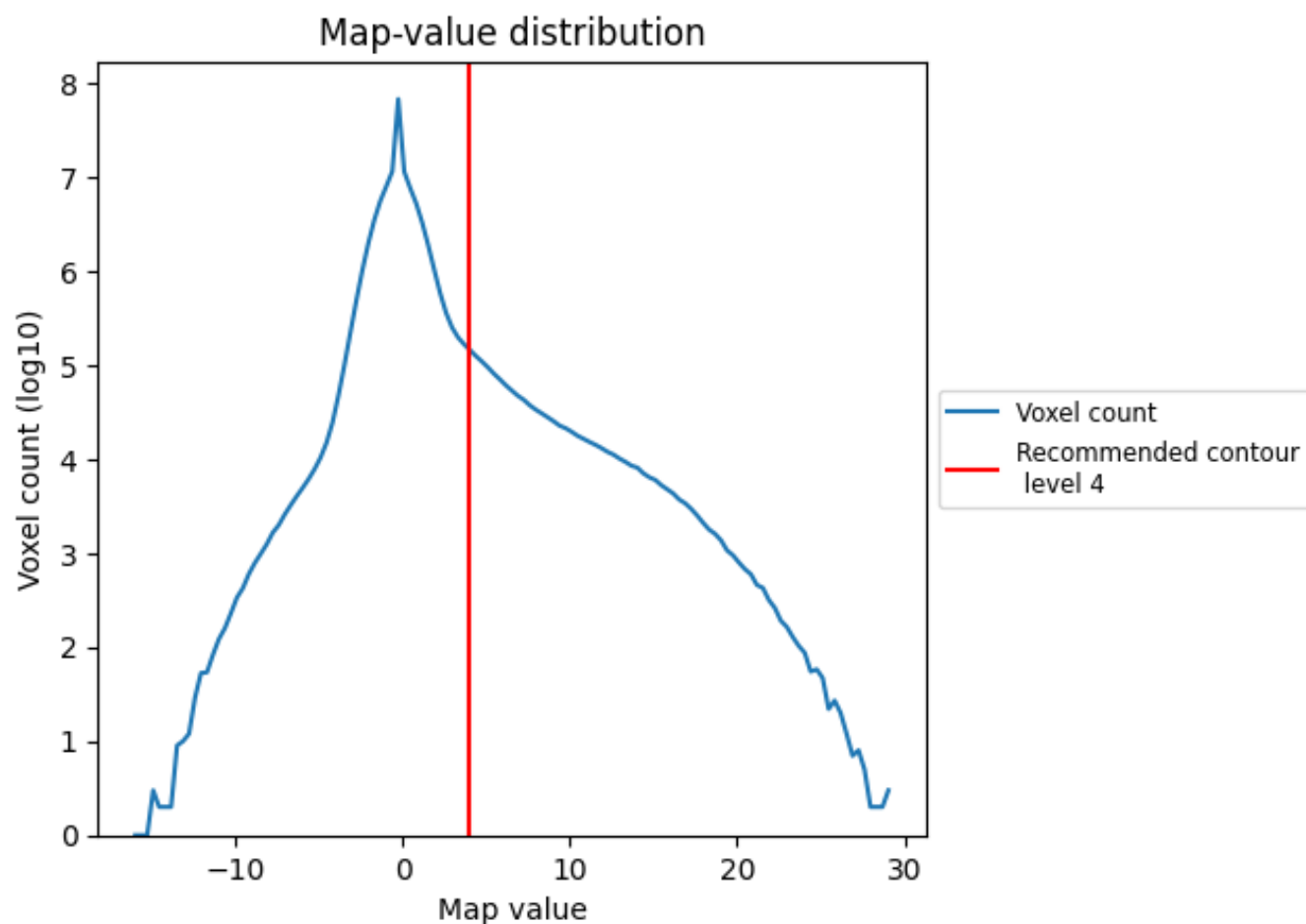
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

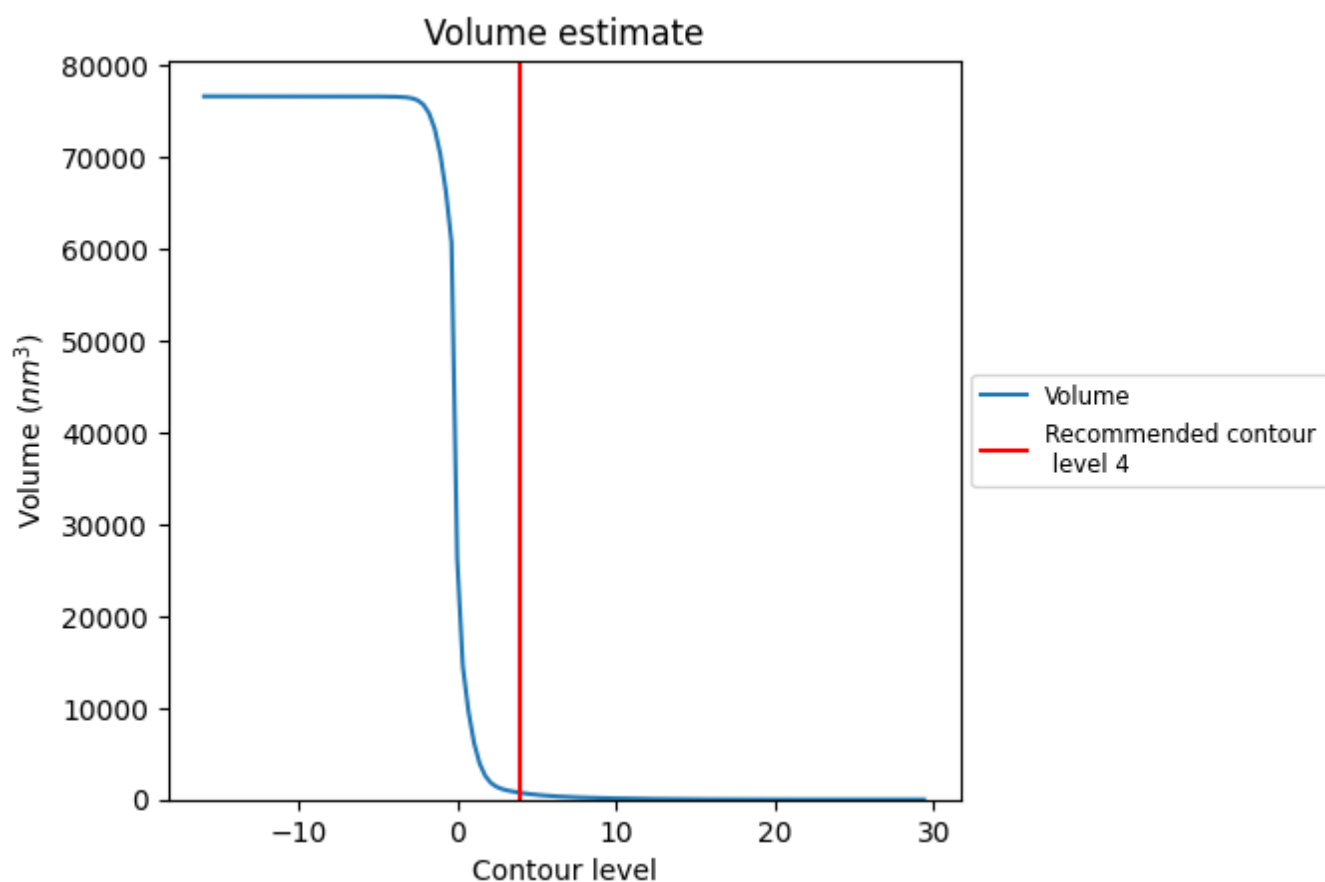
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

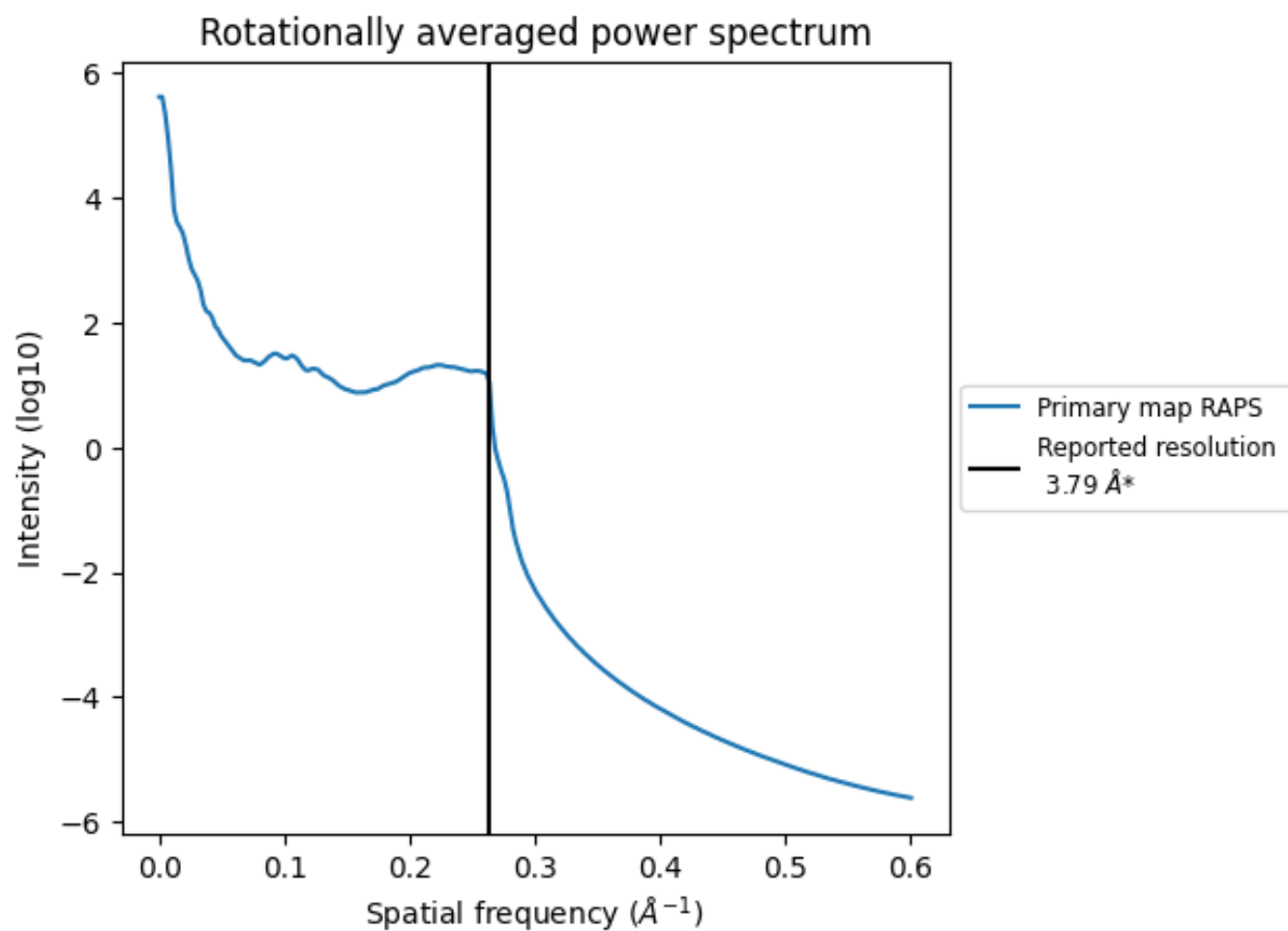
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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

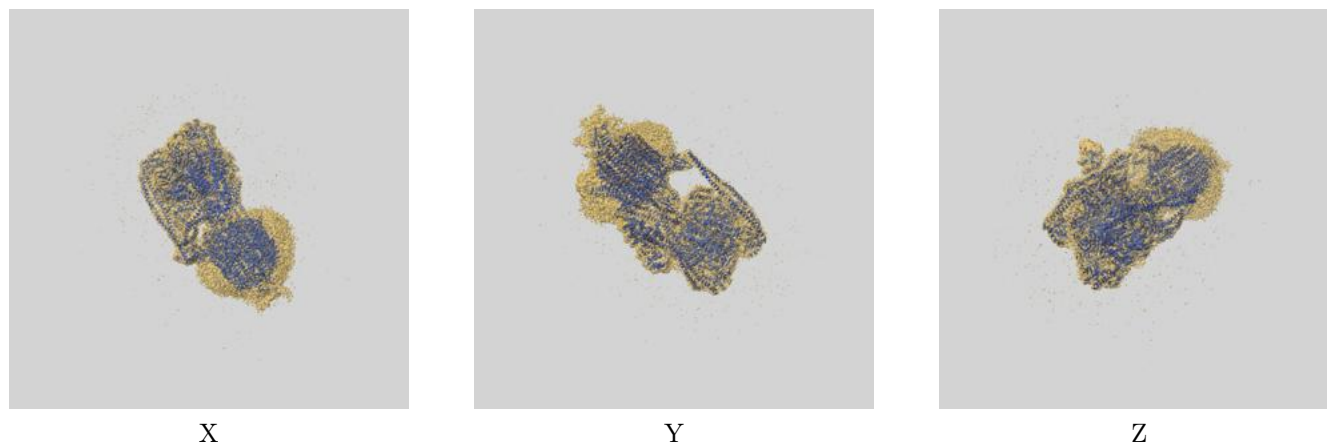
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

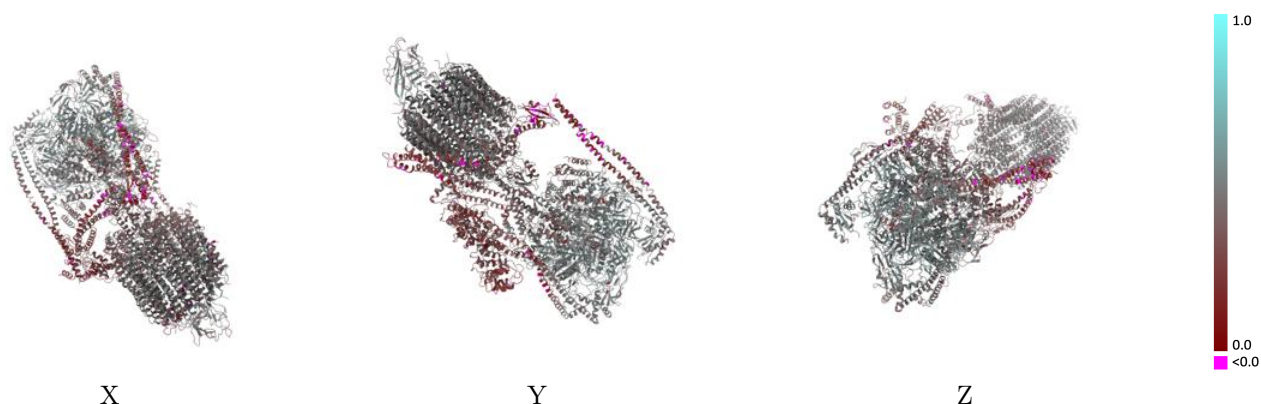
This section contains information regarding the fit between EMDB map EMD-22122 and PDB model 6XBY. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



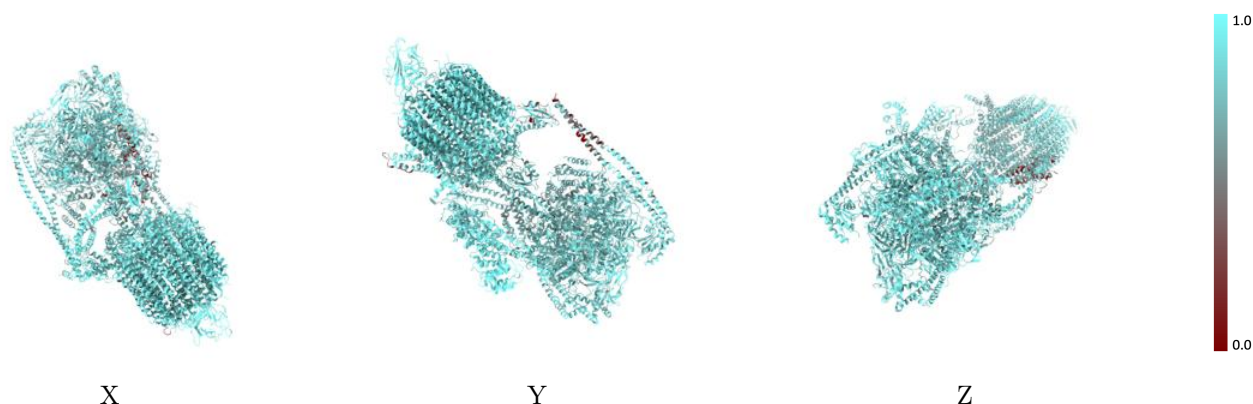
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



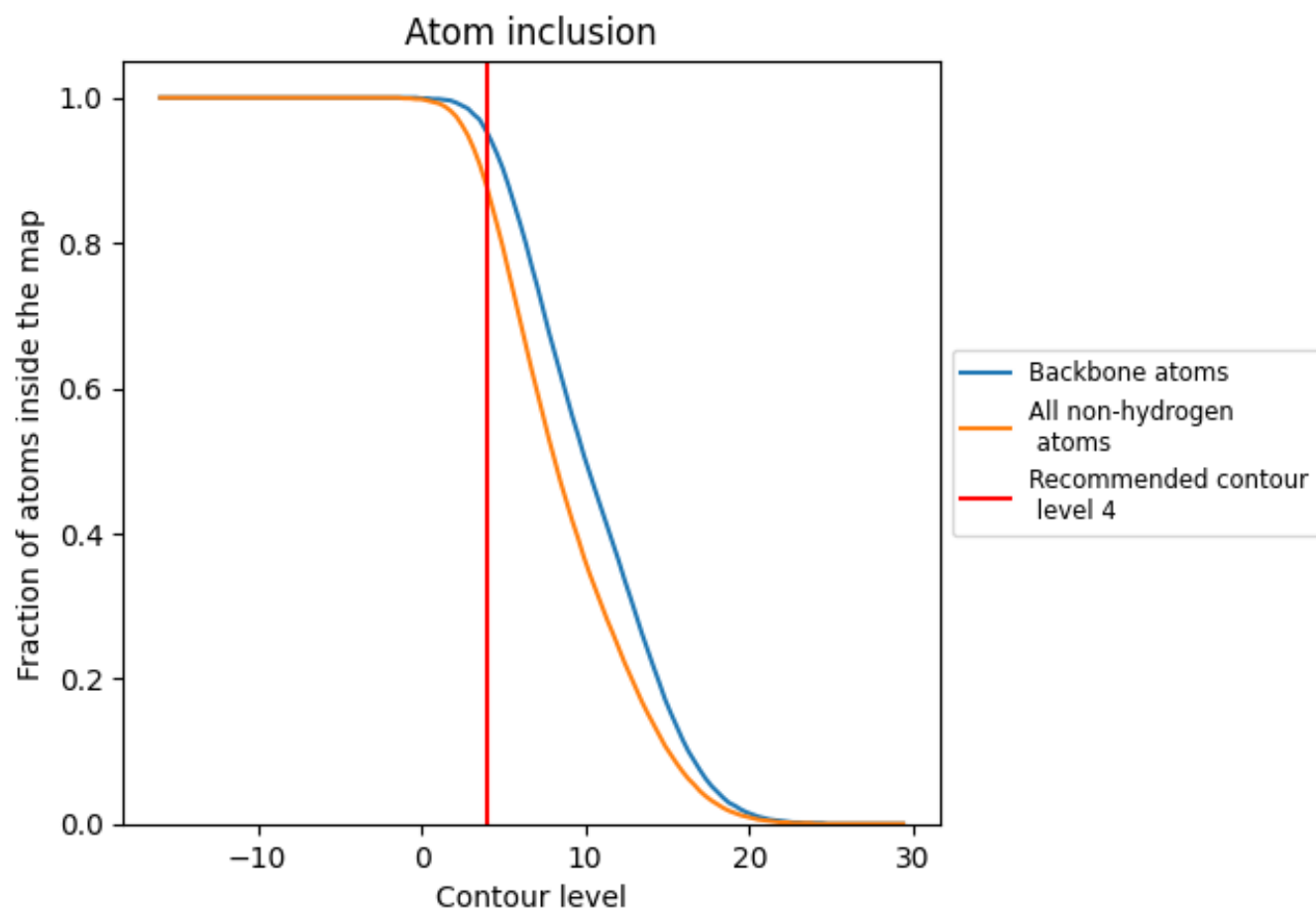
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

