



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 03:49 AM EDT

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 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:

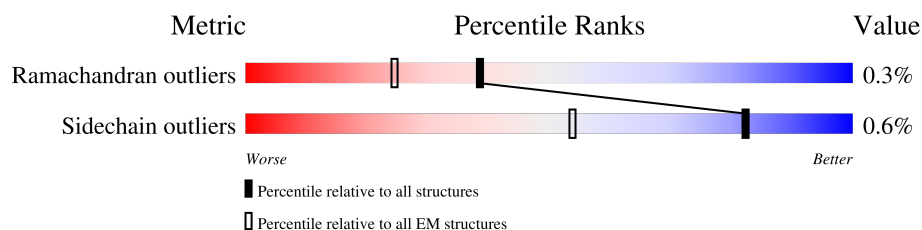
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 3.37 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.



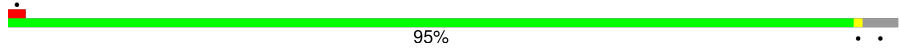
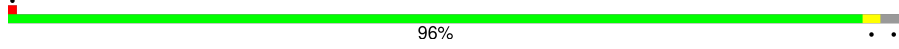
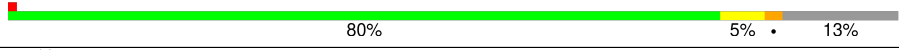



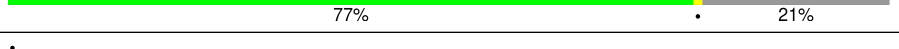
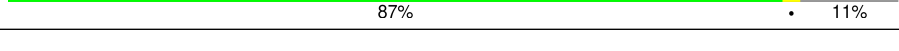
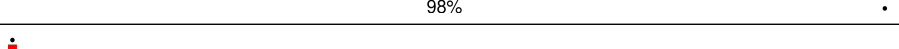
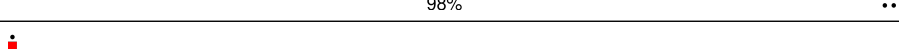



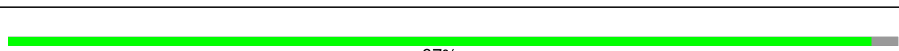
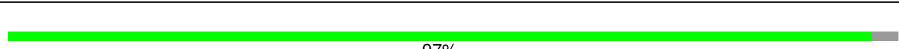
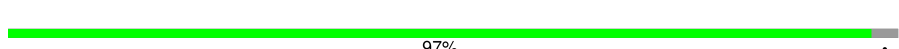
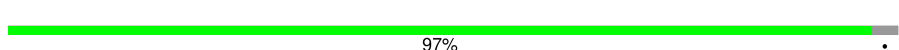
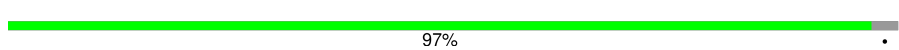
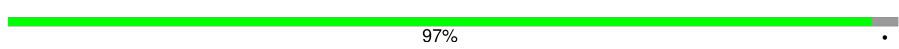
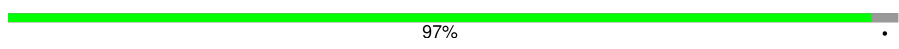
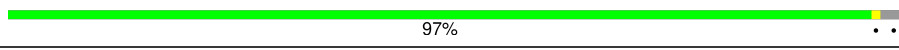


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	e	81	
13	s	468	
14	r	351	
15	c	155	
15	g	155	
15	k	155	
15	l	155	
15	m	155	
15	n	155	
15	o	155	
15	p	155	
15	q	155	
16	f	98	

2 Entry composition

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
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
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
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
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
11	d	348	Total	C	N	O	S	0	0
			2819	1817	460	528	14		

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

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

- 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	46	Total	C	N	O	S	0	0
			385	261	54	67	3		

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

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

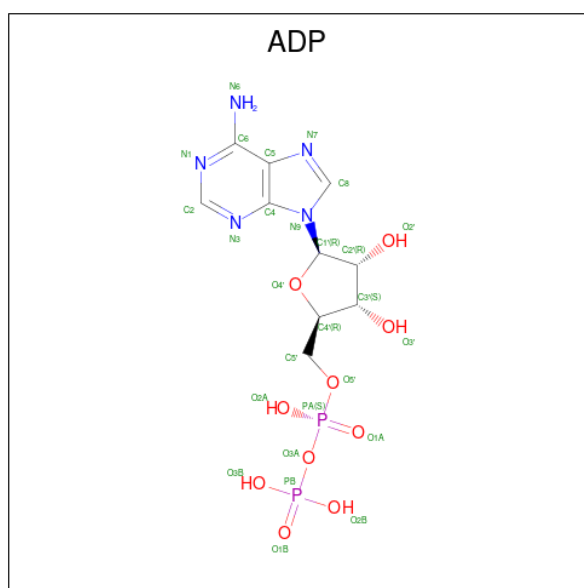
- Molecule 16 is a protein called Ribonuclease kappa.

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

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

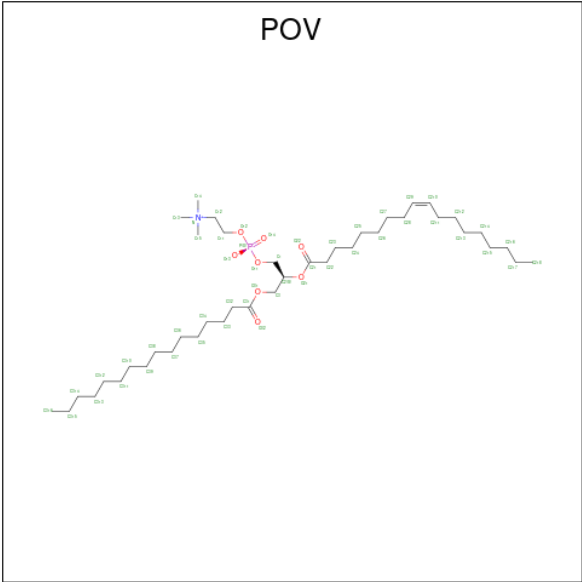
Mol	Chain	Residues	Atoms		AltConf
17	C	1	Total	Mg	0
			1	1	

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



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

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



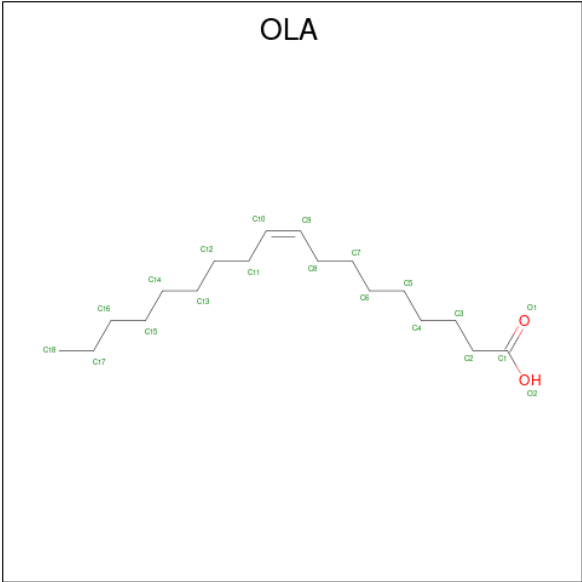
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	b	1	Total	C	N	O	P	0
			41	31	1	8	1	
19	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	b	1	Total	C	N	O	P	0
			31	21	1	8	1	
19	r	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	r	1	Total	C	N	O	P	0
			47	37	1	8	1	
19	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
19	p	1	Total	C	N	O	P	0
			44	34	1	8	1	

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

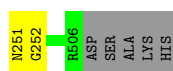


Mol	Chain	Residues	Atoms				AltConf
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	
20	s	1	Total	C	N	O	0
			14	8	1	5	

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

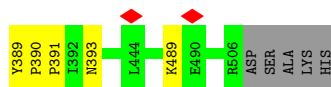
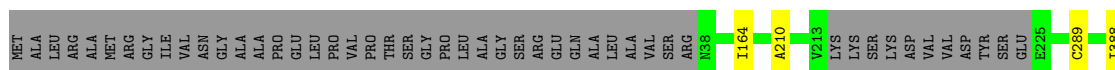


Mol	Chain	Residues	Atoms			AltConf
21	r	1	Total	C	O	0
			20	18	2	



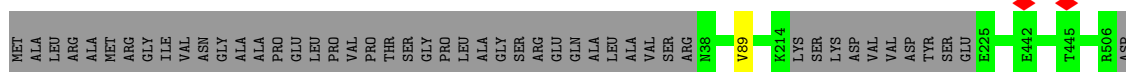
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain E: 88% 10%



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

Chain F: 90% 10%



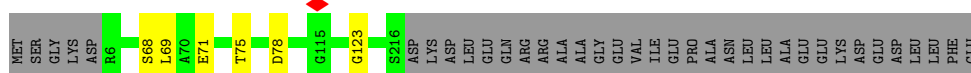
- Molecule 3: V-type proton ATPase subunit C 1

Chain G: 89% 9%



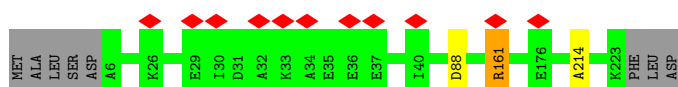
- Molecule 4: V-type proton ATPase subunit D

Chain H: 83% 15%



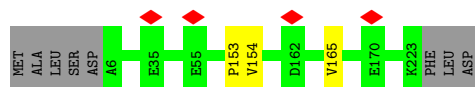
- Molecule 5: V-type proton ATPase subunit E 1

Chain I: 5% 95%



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

Chain J:  95%



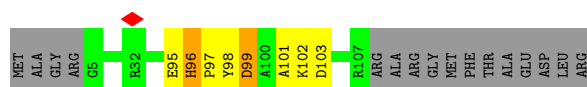
- Molecule 5: V-type proton ATPase subunit E 1

Chain K:  96%




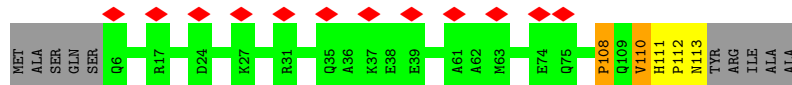
- Molecule 6: V-type proton ATPase subunit F

Chain L:  80% 5% 13%




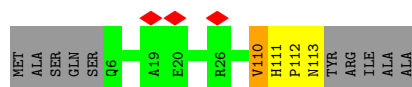
- Molecule 7: V-type proton ATPase subunit G

Chain M:  10% 87% 8%




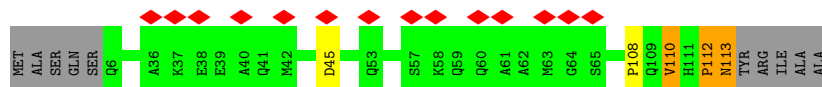
- Molecule 7: V-type proton ATPase subunit G

Chain N:  10% 88% 8%




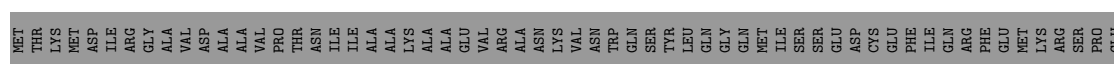
- Molecule 7: V-type proton ATPase subunit G

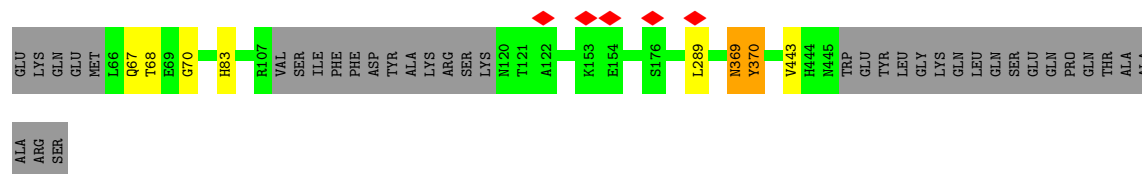
Chain O:  12% 87% 8%



- Molecule 8: V-type proton ATPase subunit H

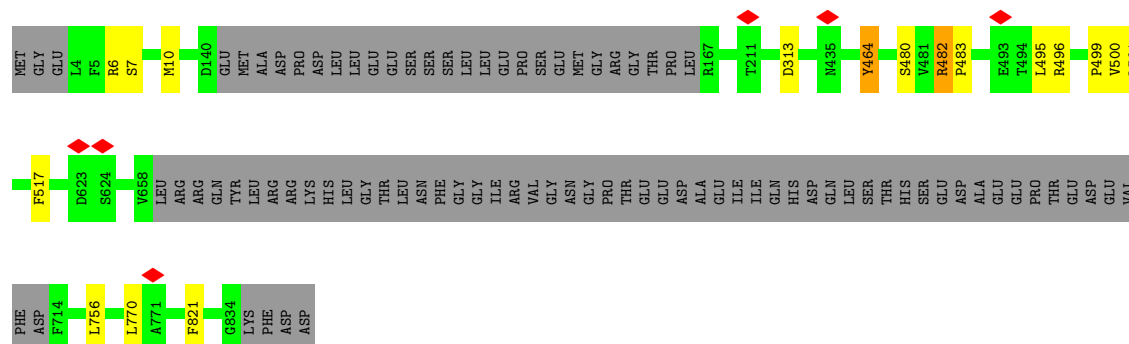
Chain P:  77% 21%





• 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%



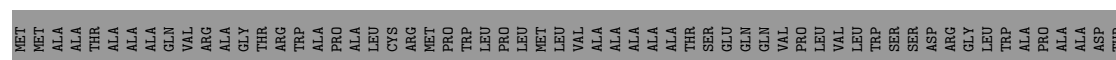
• Molecule 12: V-type proton ATPase subunit e 2

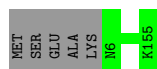
Chain e: 85% 5% 10%



• Molecule 13: V-type proton ATPase subunit S1

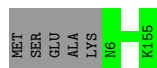
Chain s: 40% 56%





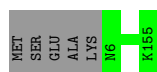
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain l: 97%



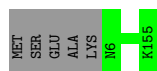
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain m: 97%



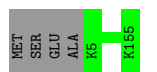
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain n: 97%



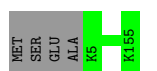
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain o: 97%



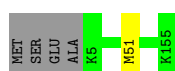
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain p: 97%



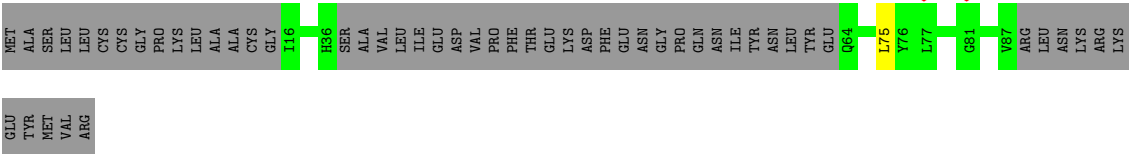
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain q: 97%



- Molecule 16: Ribonuclease kappa

Chain f: 45% 54%



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	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: ADP, OLA, NAG, POV, 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

All (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
5	J	153	PRO	N-CD	-14.46	1.27	1.47
1	B	455	SER	CA-CB	-13.66	1.32	1.52
1	A	534	PHE	CG-CD2	-13.47	1.18	1.38
9	a	483	PRO	N-CD	-13.44	1.29	1.47
1	B	457	TYR	CE1-CZ	-13.20	1.21	1.38
1	B	593	GLY	C-O	-13.13	1.02	1.23
1	B	592	ASP	C-O	-13.07	0.98	1.23
10	b	22	VAL	C-N	12.76	1.56	1.33
1	A	534	PHE	CG-CD1	-12.38	1.20	1.38
1	A	535	TYR	N-CA	-12.13	1.22	1.46
1	B	457	TYR	CB-CG	-11.94	1.33	1.51
1	A	535	TYR	CA-C	-11.62	1.22	1.52
1	C	457	TYR	CE1-CZ	-10.70	1.24	1.38
1	A	535	TYR	CB-CG	-10.41	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	TYR	CD1-CE1	-10.31	1.23	1.39
1	B	592	ASP	CB-CG	-10.28	1.30	1.51
1	B	457	TYR	CZ-OH	-10.28	1.20	1.37
1	A	534	PHE	C-O	-10.20	1.03	1.23
1	C	457	TYR	CB-CG	-10.16	1.36	1.51
13	s	305	ALA	C-N	10.02	1.57	1.34
1	A	457	TYR	CE1-CZ	-9.64	1.26	1.38
1	C	457	TYR	CZ-OH	-9.28	1.22	1.37
1	B	457	TYR	CG-CD1	-9.25	1.27	1.39
7	O	108	PRO	N-CD	-8.96	1.35	1.47
1	B	455	SER	CB-OG	-8.87	1.30	1.42
2	E	388	ILE	C-N	8.81	1.54	1.34
1	B	354	TRP	CB-CG	-8.64	1.34	1.50
1	B	592	ASP	CA-C	-8.62	1.30	1.52
10	b	16	TRP	CB-CG	-8.51	1.34	1.50
9	a	464	TYR	CE1-CZ	-7.86	1.28	1.38
1	A	457	TYR	CB-CG	-7.81	1.40	1.51
1	B	354	TRP	CG-CD1	-7.75	1.25	1.36
1	C	457	TYR	CE2-CZ	-7.15	1.29	1.38
1	A	457	TYR	CG-CD1	-7.08	1.29	1.39
14	r	330	TRP	CB-CG	-7.03	1.37	1.50
1	C	457	TYR	CG-CD2	-7.00	1.30	1.39
1	B	456	LYS	C-O	-6.99	1.10	1.23
1	C	457	TYR	CG-CD1	-6.98	1.30	1.39
1	B	457	TYR	CE2-CZ	-6.73	1.29	1.38
1	A	534	PHE	CD1-CE1	-6.69	1.25	1.39
7	O	112	PRO	C-O	-6.63	1.09	1.23
13	s	365	TYR	CB-CG	-6.61	1.41	1.51
1	B	136	THR	C-N	6.53	1.46	1.34
1	B	356	GLU	CG-CD	-6.39	1.42	1.51
1	B	354	TRP	CD2-CE2	-6.37	1.33	1.41
1	C	143	VAL	C-N	6.32	1.44	1.33
1	B	456	LYS	CA-CB	-6.25	1.40	1.53
13	s	365	TYR	CE1-CZ	-6.23	1.30	1.38
1	C	456	LYS	CA-CB	-6.20	1.40	1.53
7	M	113	ASN	N-CA	-6.18	1.33	1.46
7	N	113	ASN	N-CA	-6.12	1.34	1.46
13	s	365	TYR	CG-CD1	-6.09	1.31	1.39
1	B	457	TYR	CA-CB	-5.98	1.40	1.53
9	a	517	PHE	C-N	5.96	1.43	1.33
1	C	456	LYS	C-O	-5.95	1.12	1.23
1	B	354	TRP	CE3-CZ3	-5.94	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	592	ASP	CG-OD2	-5.94	1.11	1.25
7	O	113	ASN	CG-OD1	-5.84	1.11	1.24
1	A	534	PHE	CE1-CZ	-5.80	1.26	1.37
7	N	111	HIS	CA-C	-5.71	1.38	1.52
7	M	111	HIS	N-CA	-5.69	1.34	1.46
1	B	457	TYR	C-O	-5.67	1.12	1.23
1	C	456	LYS	CA-C	-5.67	1.38	1.52
1	A	535	TYR	CD2-CE2	-5.64	1.30	1.39
1	A	535	TYR	CE2-CZ	-5.58	1.31	1.38
7	O	113	ASN	CG-ND2	-5.56	1.19	1.32
1	B	353	ARG	CA-CB	-5.53	1.41	1.53
1	B	356	GLU	CA-CB	-5.51	1.41	1.53
1	C	195	GLU	CD-OE1	-5.50	1.19	1.25
13	s	365	TYR	CG-CD2	-5.46	1.32	1.39
14	r	330	TRP	C-O	-5.46	1.12	1.23
1	A	534	PHE	CE2-CZ	-5.44	1.27	1.37
13	s	357	SER	C-N	-5.42	1.21	1.34
1	A	457	TYR	CE2-CZ	-5.41	1.31	1.38
7	M	111	HIS	CA-CB	-5.37	1.42	1.53
7	M	113	ASN	CG-ND2	-5.35	1.19	1.32
1	A	457	TYR	CZ-OH	-5.27	1.28	1.37
7	O	112	PRO	CA-CB	-5.27	1.43	1.53
1	B	355	ALA	C-O	-5.25	1.13	1.23
1	B	456	LYS	CA-C	-5.21	1.39	1.52
6	L	98	TYR	CB-CG	-5.17	1.43	1.51
4	H	68	SER	CA-CB	-5.12	1.45	1.52
7	N	111	HIS	N-CA	-5.10	1.36	1.46
2	D	248	PHE	CG-CD2	-5.09	1.31	1.38
7	O	112	PRO	N-CA	-5.09	1.38	1.47
14	r	329	ILE	C-O	-5.07	1.13	1.23
1	A	534	PHE	CB-CG	-5.06	1.42	1.51
7	M	112	PRO	C-O	-5.03	1.13	1.23
13	s	364	ILE	CA-CB	-5.01	1.43	1.54
1	A	534	PHE	CD2-CE2	-5.01	1.29	1.39

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	212	LEU	N-CA-C	-13.86	73.59	111.00
1	B	592	ASP	CB-CG-OD1	11.85	128.97	118.30
8	P	369	ASN	C-N-CA	11.16	149.59	121.70
1	B	259	ILE	N-CA-C	-11.01	81.27	111.00
8	P	370	TYR	CB-CA-C	-10.07	90.25	110.40
13	s	277	GLY	N-CA-C	-10.07	87.93	113.10
5	K	163	VAL	CB-CA-C	-9.94	92.52	111.40
7	M	111	HIS	CB-CA-C	9.81	130.02	110.40
1	C	456	LYS	CD-CE-NZ	-9.49	89.87	111.70
1	B	591	LYS	O-C-N	-9.43	107.62	122.70
1	A	535	TYR	CA-C-O	-9.42	100.31	120.10
11	d	90	TYR	N-CA-C	-9.36	85.74	111.00
1	B	591	LYS	C-N-CA	9.09	144.42	121.70
1	A	535	TYR	CE1-CZ-OH	-9.06	95.62	120.10
1	B	260	SER	N-CA-C	8.98	135.26	111.00
1	B	592	ASP	N-CA-CB	8.92	126.66	110.60
6	L	99	ASP	N-CA-C	8.85	134.91	111.00
1	C	196	PHE	CB-CA-C	-8.69	93.03	110.40
2	D	252	GLY	C-N-CA	8.61	143.21	121.70
13	s	342	ASN	N-CA-C	-8.57	87.87	111.00
9	a	501	LEU	CA-CB-CG	8.49	134.84	115.30
13	s	448	LEU	CA-CB-CG	8.19	134.13	115.30
13	s	312	ASP	CB-CG-OD2	8.11	125.60	118.30
2	E	391	PRO	N-CA-C	-7.97	91.37	112.10
1	A	534	PHE	N-CA-C	7.96	132.49	111.00
13	s	348	ASN	N-CA-C	-7.92	89.63	111.00
1	B	592	ASP	C-N-CA	7.77	138.61	122.30
7	O	110	VAL	N-CA-C	-7.75	90.09	111.00
7	N	112	PRO	N-CA-C	7.74	132.23	112.10
13	s	307	LEU	CB-CG-CD2	-7.70	97.91	111.00
1	B	592	ASP	CB-CA-C	-7.68	95.04	110.40
13	s	421	SER	N-CA-C	-7.61	90.46	111.00
5	K	162	ASP	CB-CG-OD1	-7.54	111.52	118.30
7	M	110	VAL	N-CA-C	-7.46	90.84	111.00
1	C	199	ILE	N-CA-C	-7.32	91.24	111.00
5	I	161	ARG	N-CA-C	-7.30	91.28	111.00
1	B	588	ASP	C-N-CD	-7.25	104.65	120.60
9	a	6	ARG	CB-CA-C	-7.20	96.00	110.40
2	D	252	GLY	N-CA-C	7.16	131.00	113.10
13	s	364	ILE	CB-CA-C	-7.08	97.43	111.60
1	C	143	VAL	O-C-N	7.08	135.24	123.20
1	B	17	THR	N-CA-C	7.06	130.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	164	ILE	C-N-CA	6.96	139.09	121.70
8	P	369	ASN	N-CA-C	6.94	129.75	111.00
9	a	495	LEU	CA-CB-CG	-6.77	99.73	115.30
11	d	276	LEU	CA-CB-CG	6.63	130.55	115.30
9	a	517	PHE	O-C-N	-6.62	111.94	123.20
13	s	417	ALA	N-CA-C	6.58	128.78	111.00
5	J	165	VAL	CB-CA-C	6.56	123.87	111.40
1	A	535	TYR	OH-CZ-CE2	6.50	137.64	120.10
1	A	535	TYR	C-N-CA	-6.47	105.53	121.70
1	B	136	THR	C-N-CD	-6.46	106.38	120.60
5	I	214	ALA	CB-CA-C	6.44	119.77	110.10
7	M	112	PRO	C-N-CA	6.44	137.79	121.70
2	D	212	LEU	CB-CA-C	-6.41	98.03	110.20
1	C	143	VAL	CA-C-N	-6.40	103.41	116.20
1	A	461	LEU	CA-CB-CG	-6.38	100.62	115.30
13	s	305	ALA	O-C-N	-6.38	112.49	122.70
8	P	370	TYR	C-N-CA	6.38	137.65	121.70
13	s	421	SER	C-N-CD	6.35	141.73	128.40
1	A	139	LYS	C-N-CA	6.28	137.41	121.70
9	a	313	ASP	CB-CG-OD1	6.21	123.89	118.30
8	P	70	GLY	N-CA-C	-6.20	97.60	113.10
1	C	198	GLY	N-CA-C	-6.16	97.69	113.10
6	L	103	ASP	CB-CA-C	6.12	122.65	110.40
7	M	113	ASN	N-CA-CB	-6.12	99.58	110.60
2	F	89	VAL	CB-CA-C	-6.11	99.79	111.40
6	L	95	GLU	C-N-CA	6.09	136.92	121.70
2	D	89	VAL	CB-CA-C	-6.08	99.84	111.40
12	e	70	ASN	N-CA-C	6.06	127.36	111.00
7	N	110	VAL	CA-C-N	-6.01	103.97	117.20
7	O	45	ASP	CB-CA-C	5.98	122.36	110.40
1	C	17	THR	CB-CA-C	-5.98	95.45	111.60
1	C	143	VAL	C-N-CA	-5.97	109.77	122.30
2	D	213	VAL	CG1-CB-CG2	-5.94	101.40	110.90
11	d	346	ASN	N-CA-C	-5.90	95.07	111.00
7	M	111	HIS	N-CA-C	-5.89	95.10	111.00
12	e	70	ASN	CB-CA-C	-5.86	98.67	110.40
7	N	112	PRO	C-N-CA	5.86	136.35	121.70
9	a	500	VAL	CB-CA-C	5.85	122.52	111.40
14	r	329	ILE	CG1-CB-CG2	-5.85	98.53	111.40
16	f	75	LEU	CA-CB-CG	5.80	128.64	115.30
6	L	101	ALA	N-CA-C	5.79	126.62	111.00
2	D	249	GLU	N-CA-CB	-5.74	100.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	TYR	CG-CD2-CE2	-5.73	116.72	121.30
4	H	69	LEU	CA-CB-CG	-5.70	102.19	115.30
8	P	443	VAL	CB-CA-C	5.70	122.22	111.40
1	B	588	ASP	N-CA-C	5.69	126.37	111.00
12	e	78	PHE	N-CA-C	5.68	126.34	111.00
1	C	195	GLU	OE1-CD-OE2	-5.67	116.50	123.30
4	H	123	GLY	N-CA-C	-5.65	98.97	113.10
12	e	78	PHE	C-N-CA	5.64	135.81	121.70
13	s	295	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	526	THR	N-CA-CB	-5.58	99.69	110.30
7	O	112	PRO	CA-C-O	-5.58	106.80	120.20
8	P	289	LEU	CB-CA-C	5.58	120.80	110.20
9	a	10	MET	CB-CA-C	-5.58	99.25	110.40
1	B	266	TYR	CB-CA-C	5.57	121.55	110.40
7	M	108	PRO	N-CA-C	5.48	126.36	112.10
9	a	517	PHE	CA-C-N	5.48	127.16	116.20
2	D	212	LEU	C-N-CA	5.45	135.32	121.70
1	A	463	GLU	C-N-CA	5.41	135.23	121.70
7	N	113	ASN	N-CA-CB	-5.35	100.98	110.60
3	G	326	LYS	CB-CA-C	-5.33	99.74	110.40
6	L	102	LYS	CA-C-O	5.32	131.27	120.10
2	E	210	ALA	CB-CA-C	5.30	118.05	110.10
2	E	289	CYS	N-CA-C	-5.29	96.73	111.00
15	q	51	MET	N-CA-C	5.29	125.28	111.00
11	d	172	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	591	LYS	CA-C-N	5.22	128.68	117.20
13	s	342	ASN	C-N-CA	5.22	134.74	121.70
4	H	78	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	535	TYR	O-C-N	5.18	130.99	122.70
2	E	393	ASN	O-C-N	-5.16	114.45	122.70
9	a	6	ARG	N-CA-C	5.12	124.82	111.00
3	G	229	LEU	CA-CB-CG	5.11	127.06	115.30
9	a	821	PHE	CB-CA-C	5.11	120.62	110.40
6	L	98	TYR	N-CA-C	5.11	124.80	111.00
9	a	770	LEU	CA-CB-CG	5.10	127.03	115.30
10	b	22	VAL	O-C-N	-5.10	114.53	123.20
6	L	98	TYR	N-CA-CB	-5.06	101.50	110.60
8	P	83	HIS	N-CA-C	5.05	124.62	111.00
14	r	329	ILE	CB-CA-C	-5.04	101.51	111.60
1	A	461	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	A	535	TYR	CA-C-N	5.02	128.25	117.20
5	K	157	VAL	CB-CA-C	5.02	120.94	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (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
2	D	249	GLU	Mainchain
5	I	161	ARG	Mainchain
7	M	110	VAL	Mainchain
7	N	110	VAL	Mainchain
8	P	369	ASN	Peptide
9	a	480	SER	Mainchain
13	s	366	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%)	44	72
1	B	586/617 (95%)	562 (96%)	19 (3%)	5 (1%)	14	41
1	C	595/617 (96%)	583 (98%)	12 (2%)	0	100	100
2	D	457/511 (89%)	442 (97%)	14 (3%)	1 (0%)	44	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	454/511 (89%)	436 (96%)	17 (4%)	1 (0%)	44	72
2	F	455/511 (89%)	443 (97%)	12 (3%)	0	100	100
3	G	338/382 (88%)	326 (96%)	11 (3%)	1 (0%)	37	66
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%)	3	18
7	M	106/118 (90%)	102 (96%)	3 (3%)	1 (1%)	14	41
7	N	106/118 (90%)	105 (99%)	1 (1%)	0	100	100
7	O	106/118 (90%)	101 (95%)	3 (3%)	2 (2%)	6	26
8	P	364/465 (78%)	342 (94%)	20 (6%)	2 (0%)	25	54
9	a	744/838 (89%)	704 (95%)	37 (5%)	3 (0%)	30	60
10	b	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
11	d	346/351 (99%)	329 (95%)	16 (5%)	1 (0%)	37	66
12	e	71/81 (88%)	63 (89%)	8 (11%)	0	100	100
13	s	203/468 (43%)	177 (87%)	25 (12%)	1 (0%)	25	54
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%)	38	66

All (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
6	L	97	PRO
6	L	99	ASP
8	P	68	THR
8	P	370	TYR
9	a	7	SER
1	A	140	ASN
9	a	499	PRO
13	s	349	GLY
1	B	592	ASP
3	G	179	SER
7	O	110	VAL
7	O	112	PRO
1	B	589	PRO
7	M	108	PRO
2	D	136	GLY
9	a	482	ARG
11	d	91	GLU

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	497/524 (95%)	490 (99%)	7 (1%)	62	78
1	B	500/524 (95%)	495 (99%)	5 (1%)	73	84
1	C	504/524 (96%)	501 (99%)	3 (1%)	84	91
2	D	394/432 (91%)	393 (100%)	1 (0%)	91	95
2	E	391/432 (90%)	390 (100%)	1 (0%)	91	95
2	F	392/432 (91%)	392 (100%)	0	100	100
3	G	313/344 (91%)	310 (99%)	3 (1%)	73	84
4	H	182/212 (86%)	180 (99%)	2 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	150/198 (76%)	149 (99%)	1 (1%)	81	89
5	J	153/198 (77%)	152 (99%)	1 (1%)	81	89
5	K	144/198 (73%)	143 (99%)	1 (1%)	81	89
6	L	89/100 (89%)	88 (99%)	1 (1%)	70	82
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%)	41	65
8	P	275/415 (66%)	274 (100%)	1 (0%)	89	93
9	a	667/744 (90%)	663 (99%)	4 (1%)	84	91
10	b	156/158 (99%)	155 (99%)	1 (1%)	84	91
11	d	303/306 (99%)	303 (100%)	0	100	100
12	e	62/68 (91%)	60 (97%)	2 (3%)	34	60
13	s	184/398 (46%)	183 (100%)	1 (0%)	86	92
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
All	All	6507/7887 (82%)	6471 (99%)	36 (1%)	82	91

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	400	ARG
1	A	462	ASP
1	A	463	GLU
1	A	526	THR

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Mol	Chain	Res	Type
1	A	529	ASP
1	A	534	PHE
1	B	141	LEU
1	B	323	ARG
1	B	400	ARG
1	B	560	GLN
1	B	587	LYS
1	C	400	ARG
1	C	458	MET
1	C	470	THR
2	D	251	ASN
2	E	489	LYS
3	G	109	MET
3	G	199	LYS
3	G	232	LYS
4	H	71	GLU
4	H	75	THR
5	I	88	ASP
5	J	154	VAL
5	K	154	VAL
6	L	96	HIS
7	O	113	ASN
8	P	67	GLN
9	a	464	TYR
9	a	482	ARG
9	a	496	ARG
9	a	756	LEU
10	b	19	LEU
12	e	59	GLN
12	e	74	TRP
13	s	270	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	610	ASN
1	B	314	ASN
1	B	397	ASN
1	B	523	ASN
1	B	610	ASN
1	C	213	GLN

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Mol	Chain	Res	Type
1	C	522	GLN
2	D	209	GLN
2	D	482	GLN
2	E	385	ASN
2	E	482	GLN
2	F	226	ASN
2	F	262	ASN
2	F	385	ASN
2	F	482	GLN
3	G	30	ASN
3	G	39	ASN
3	G	149	ASN
3	G	194	HIS
3	G	239	HIS
3	G	275	GLN
3	G	315	ASN
4	H	113	HIS
4	H	130	GLN
5	I	206	GLN
5	J	149	GLN
5	J	219	ASN
5	K	67	GLN
5	K	100	GLN
6	L	57	ASN
6	L	96	HIS
7	M	98	GLN
7	M	113	ASN
7	N	109	GLN
7	O	88	GLN
7	O	89	GLN
7	O	113	ASN
8	P	222	GLN
8	P	299	GLN
8	P	305	GLN
9	a	53	ASN
9	a	76	ASN
9	a	199	GLN
9	a	365	ASN
9	a	412	HIS
9	a	534	ASN
9	a	612	HIS
9	a	626	ASN

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Mol	Chain	Res	Type
9	a	735	ASN
9	a	751	GLN
10	b	148	ASN
11	d	145	GLN
11	d	152	ASN
11	d	266	ASN
11	d	309	GLN
12	e	67	GLN
12	e	70	ASN
13	s	270	GLN
13	s	358	GLN
13	s	404	ASN
15	c	78	ASN
15	c	124	GLN
15	g	78	ASN
15	g	92	GLN
15	g	124	GLN
15	k	6	ASN
15	k	92	GLN
15	l	78	ASN
15	l	92	GLN
15	m	78	ASN
15	m	92	GLN
15	n	123	GLN
15	o	124	GLN
15	p	78	ASN
15	p	92	GLN
15	q	78	ASN
15	q	81	ASN
15	q	92	GLN
15	q	124	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
21	OLA	r	403	-	19,19,19	0.79	1 (5%)	19,19,19	0.90	0
19	POV	b	301	-	46,46,51	1.02	4 (8%)	52,54,59	0.94	2 (3%)
19	POV	r	401	-	46,46,51	1.01	4 (8%)	52,54,59	0.84	2 (3%)
20	NAG	s	506	-	14,14,15	0.28	0	19,19,21	0.31	0
19	POV	b	303	-	40,40,51	1.10	4 (10%)	46,48,59	0.92	2 (4%)
20	NAG	s	502	13	14,14,15	0.36	0	17,19,21	0.53	0
19	POV	b	304	-	46,46,51	1.03	4 (8%)	52,54,59	0.91	2 (3%)
19	POV	r	402	-	46,46,51	1.03	3 (6%)	52,54,59	0.86	2 (3%)
19	POV	b	305	-	30,30,51	1.27	4 (13%)	36,38,59	0.99	2 (5%)
20	NAG	s	501	13	14,14,15	0.35	0	17,19,21	0.48	0
20	NAG	s	505	13	14,14,15	0.20	0	17,19,21	0.60	0
20	NAG	s	503	13	14,14,15	0.43	0	17,19,21	0.57	0
20	NAG	s	504	13	14,14,15	0.51	0	17,19,21	0.80	1 (5%)
19	POV	g	201	-	42,42,51	1.07	2 (4%)	48,50,59	0.95	2 (4%)
18	ADP	C	702	17	24,29,29	1.24	3 (12%)	29,45,45	1.31	4 (13%)
19	POV	p	201	-	43,43,51	1.07	3 (6%)	49,51,59	0.93	3 (6%)
19	POV	b	302	-	46,46,51	1.03	4 (8%)	52,54,59	0.93	2 (3%)

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
21	OLA	r	403	-	-	9/17/17/17	-
19	POV	b	301	-	-	30/50/50/55	-
19	POV	r	401	-	-	24/50/50/55	-
20	NAG	s	506	-	-	1/6/22/26	0/1/1/1
19	POV	b	303	-	-	23/44/44/55	-
20	NAG	s	502	13	-	2/6/23/26	0/1/1/1
19	POV	b	304	-	-	27/50/50/55	-
19	POV	r	402	-	-	29/50/50/55	-
19	POV	b	305	-	-	19/34/34/55	-
20	NAG	s	501	13	-	0/6/23/26	0/1/1/1
20	NAG	s	505	13	-	1/6/23/26	0/1/1/1
20	NAG	s	503	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	-	-	22/46/46/55	-
18	ADP	C	702	17	-	1/12/32/32	0/3/3/3
19	POV	p	201	-	-	19/47/47/55	-
19	POV	b	302	-	-	24/50/50/55	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	702	ADP	O4'-C1'	3.48	1.45	1.40
19	p	201	POV	O21-C2	-3.10	1.39	1.46
19	b	305	POV	O21-C2	-2.91	1.39	1.46
19	g	201	POV	O21-C2	-2.90	1.39	1.46
19	r	402	POV	O21-C2	-2.89	1.39	1.46
19	b	304	POV	O21-C2	-2.76	1.40	1.46
19	b	303	POV	O21-C2	-2.75	1.40	1.46
21	r	403	OLA	C10-C9	2.74	1.47	1.31
19	b	302	POV	O21-C2	-2.71	1.40	1.46
19	b	304	POV	O31-C3	-2.57	1.39	1.45
19	g	201	POV	O31-C31	2.52	1.40	1.33
19	b	302	POV	O31-C31	2.48	1.40	1.33
19	r	401	POV	O21-C21	2.46	1.41	1.34
19	r	401	POV	O31-C31	2.44	1.40	1.33
19	b	301	POV	O31-C31	2.38	1.40	1.33
19	p	201	POV	O31-C31	2.38	1.40	1.33
19	b	305	POV	O31-C3	-2.37	1.39	1.45
19	b	301	POV	O21-C21	2.36	1.40	1.34
19	b	303	POV	O31-C31	2.35	1.40	1.33
18	C	702	ADP	C8-N7	-2.33	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	r	402	POV	O31-C31	2.31	1.40	1.33
19	b	303	POV	O31-C3	-2.31	1.40	1.45
18	C	702	ADP	PA-O3A	2.28	1.62	1.59
19	r	402	POV	O31-C3	-2.26	1.40	1.45
19	b	304	POV	O31-C31	2.26	1.39	1.33
19	b	305	POV	O31-C31	2.25	1.39	1.33
19	p	201	POV	O31-C3	-2.24	1.40	1.45
19	b	301	POV	O31-C3	-2.22	1.40	1.45
19	r	401	POV	O31-C3	-2.22	1.40	1.45
19	r	401	POV	O21-C2	-2.19	1.41	1.46
19	b	302	POV	O21-C21	2.15	1.40	1.34
19	b	301	POV	O21-C2	-2.13	1.41	1.46
19	b	302	POV	O31-C3	-2.13	1.40	1.45
19	b	304	POV	O21-C21	2.12	1.40	1.34
19	b	305	POV	O21-C21	2.10	1.40	1.34
19	b	303	POV	O21-C21	2.08	1.40	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	702	ADP	N3-C2-N1	-4.84	122.10	128.67
19	b	302	POV	O21-C21-C22	4.55	121.31	111.48
19	b	304	POV	O21-C21-C22	4.13	120.42	111.48
19	b	301	POV	O21-C21-C22	3.95	120.02	111.48
19	g	201	POV	O21-C21-C22	3.88	119.88	111.48
19	b	305	POV	O21-C21-C22	3.72	119.53	111.48
19	b	303	POV	O21-C21-C22	3.71	119.51	111.48
19	r	401	POV	O21-C21-C22	3.71	119.50	111.48
19	r	402	POV	O21-C21-C22	3.61	119.30	111.48
19	p	201	POV	O21-C21-C22	3.60	119.27	111.48
19	g	201	POV	O31-C31-C32	2.96	120.85	111.83
19	b	301	POV	O31-C31-C32	2.93	120.77	111.83
20	s	504	NAG	C1-O5-C5	2.81	115.96	112.19
19	b	302	POV	O31-C31-C32	2.65	119.92	111.83
19	p	201	POV	O31-C31-C32	2.61	119.80	111.83
19	b	303	POV	O31-C31-C32	2.55	119.60	111.83
19	r	402	POV	O31-C31-C32	2.53	119.55	111.83
19	r	401	POV	O31-C31-C32	2.52	119.50	111.83
19	b	305	POV	O31-C31-C32	2.49	119.42	111.83
19	p	201	POV	C2-O21-C21	-2.46	111.90	117.80
18	C	702	ADP	O3B-PB-O3A	2.38	112.62	104.64
19	b	304	POV	O31-C31-C32	2.34	118.98	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	702	ADP	C4-C5-N7	-2.18	107.03	109.34
18	C	702	ADP	PA-O5'-C5'	-2.06	109.53	121.35

There are no chirality outliers.

All (233) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	b	301	POV	C1-O11-P-O12
19	b	301	POV	C1-O11-P-O14
19	b	301	POV	C11-O12-P-O11
19	b	301	POV	C11-O12-P-O13
19	b	301	POV	C3-C2-O21-C21
19	b	301	POV	C22-C21-O21-C2
19	b	302	POV	C1-O11-P-O12
19	b	302	POV	C1-O11-P-O14
19	b	302	POV	C11-O12-P-O11
19	b	302	POV	C11-O12-P-O13
19	b	302	POV	C11-O12-P-O14
19	b	302	POV	O21-C2-C3-O31
19	b	302	POV	C22-C21-O21-C2
19	b	303	POV	C11-O12-P-O14
19	b	304	POV	C1-O11-P-O14
19	b	304	POV	O22-C21-O21-C2
19	b	305	POV	C1-O11-P-O13
19	r	401	POV	C11-O12-P-O11
19	r	401	POV	C11-O12-P-O14
19	r	401	POV	C22-C21-O21-C2
19	r	402	POV	C11-O12-P-O11
19	r	402	POV	C11-O12-P-O13
19	r	402	POV	O12-C11-C12-N
19	g	201	POV	C11-O12-P-O11
19	g	201	POV	O12-C11-C12-N
19	g	201	POV	C22-C21-O21-C2
19	p	201	POV	C1-O11-P-O12
19	p	201	POV	C1-O11-P-O13
19	p	201	POV	C11-O12-P-O11
19	b	301	POV	O32-C31-O31-C3
19	b	301	POV	C32-C31-O31-C3
19	b	301	POV	O22-C21-O21-C2
19	r	401	POV	O22-C21-O21-C2
19	b	304	POV	C22-C21-O21-C2
19	b	302	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
19	g	201	POV	O22-C21-O21-C2
20	s	503	NAG	O5-C5-C6-O6
20	s	502	NAG	O5-C5-C6-O6
21	r	403	OLA	C11-C10-C9-C8
19	p	201	POV	C22-C23-C24-C25
19	r	402	POV	C32-C31-O31-C3
19	r	402	POV	O32-C31-O31-C3
19	b	304	POV	C33-C34-C35-C36
20	s	503	NAG	C4-C5-C6-O6
19	p	201	POV	C22-C21-O21-C2
20	s	502	NAG	C4-C5-C6-O6
19	b	301	POV	C31-C32-C33-C34
19	b	303	POV	C31-C32-C33-C34
19	b	304	POV	C21-C22-C23-C24
19	r	401	POV	C21-C22-C23-C24
21	r	403	OLA	C1-C2-C3-C4
19	g	201	POV	C21-C22-C23-C24
20	s	506	NAG	O5-C5-C6-O6
19	p	201	POV	O22-C21-O21-C2
19	r	402	POV	O21-C2-C3-O31
20	s	505	NAG	O5-C5-C6-O6
19	b	303	POV	C35-C36-C37-C38
21	r	403	OLA	C11-C12-C13-C14
19	b	303	POV	C22-C21-O21-C2
19	b	305	POV	C31-C32-C33-C34
19	b	305	POV	C22-C23-C24-C25
19	r	401	POV	C22-C23-C24-C25
19	b	301	POV	C37-C38-C39-C310
19	p	201	POV	C35-C36-C37-C38
19	p	201	POV	C23-C24-C25-C26
19	b	301	POV	C33-C34-C35-C36
19	b	302	POV	C24-C25-C26-C27
19	b	305	POV	C22-C21-O21-C2
19	r	402	POV	C210-C211-C212-C213
19	b	304	POV	C32-C31-O31-C3
19	r	401	POV	C39-C310-C311-C312
19	r	401	POV	C34-C35-C36-C37
19	b	304	POV	C23-C24-C25-C26
19	b	301	POV	C23-C24-C25-C26
19	r	402	POV	C22-C21-O21-C2
19	b	303	POV	O22-C21-O21-C2
19	b	301	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
19	b	301	POV	C26-C27-C28-C29
19	b	302	POV	C21-C22-C23-C24
19	r	402	POV	C35-C36-C37-C38
19	b	303	POV	C36-C37-C38-C39
19	r	401	POV	C31-C32-C33-C34
19	r	402	POV	C21-C22-C23-C24
19	r	402	POV	O22-C21-O21-C2
19	r	401	POV	C36-C37-C38-C39
19	b	304	POV	O32-C31-O31-C3
19	b	304	POV	C34-C35-C36-C37
19	g	201	POV	C31-C32-C33-C34
19	r	402	POV	C26-C27-C28-C29
19	b	302	POV	C23-C24-C25-C26
19	r	402	POV	C39-C310-C311-C312
19	b	303	POV	C33-C34-C35-C36
19	b	304	POV	C25-C26-C27-C28
19	r	401	POV	C32-C33-C34-C35
19	b	302	POV	C310-C311-C312-C313
19	g	201	POV	C32-C33-C34-C35
19	b	304	POV	C26-C27-C28-C29
19	b	304	POV	O11-C1-C2-C3
19	g	201	POV	O11-C1-C2-C3
19	b	301	POV	C39-C310-C311-C312
19	r	401	POV	C37-C38-C39-C310
19	b	305	POV	O22-C21-O21-C2
19	b	305	POV	C1-C2-C3-O31
19	b	303	POV	C23-C24-C25-C26
19	b	303	POV	C26-C27-C28-C29
19	r	402	POV	C22-C23-C24-C25
19	g	201	POV	C39-C310-C311-C312
19	r	401	POV	C32-C31-O31-C3
19	b	302	POV	C32-C33-C34-C35
19	b	301	POV	C32-C33-C34-C35
19	b	305	POV	C33-C34-C35-C36
19	b	301	POV	C311-C310-C39-C38
19	b	304	POV	C24-C25-C26-C27
19	g	201	POV	C25-C26-C27-C28
19	b	305	POV	C32-C31-O31-C3
19	p	201	POV	C32-C31-O31-C3
19	b	302	POV	C36-C37-C38-C39
19	b	303	POV	O11-C1-C2-C3
19	b	305	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
19	r	402	POV	O11-C1-C2-C3
19	g	201	POV	C310-C311-C312-C313
19	g	201	POV	C33-C34-C35-C36
21	r	403	OLA	C4-C5-C6-C7
19	b	302	POV	C311-C312-C313-C314
19	b	302	POV	C1-C2-C3-O31
19	b	303	POV	C1-C2-C3-O31
19	r	401	POV	C1-C2-C3-O31
19	r	402	POV	C1-C2-C3-O31
21	r	403	OLA	C2-C3-C4-C5
19	p	201	POV	C24-C25-C26-C27
19	b	304	POV	O11-C1-C2-O21
19	g	201	POV	O11-C1-C2-O21
19	r	402	POV	C25-C26-C27-C28
19	g	201	POV	C311-C312-C313-C314
19	b	305	POV	O21-C2-C3-O31
19	r	401	POV	O21-C2-C3-O31
19	b	301	POV	C35-C36-C37-C38
19	r	401	POV	O32-C31-O31-C3
19	r	402	POV	C310-C311-C312-C313
19	g	201	POV	C26-C27-C28-C29
19	b	304	POV	C22-C23-C24-C25
19	b	304	POV	C37-C38-C39-C310
19	b	302	POV	O11-C1-C2-C3
19	p	201	POV	C210-C211-C212-C213
19	b	303	POV	C32-C31-O31-C3
19	p	201	POV	O32-C31-O31-C3
19	b	302	POV	C312-C313-C314-C315
19	b	305	POV	O32-C31-O31-C3
19	p	201	POV	C33-C34-C35-C36
19	r	401	POV	C3-C2-O21-C21
19	b	304	POV	C210-C211-C212-C213
19	b	304	POV	C32-C33-C34-C35
19	r	401	POV	C33-C34-C35-C36
19	b	302	POV	O11-C1-C2-O21
19	p	201	POV	C36-C37-C38-C39
19	g	201	POV	C12-C11-O12-P
19	b	303	POV	O32-C31-O31-C3
19	r	402	POV	C37-C38-C39-C310
19	b	301	POV	O12-C11-C12-N
19	b	302	POV	O12-C11-C12-N
19	b	303	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
19	b	305	POV	O12-C11-C12-N
19	r	401	POV	O12-C11-C12-N
19	p	201	POV	O12-C11-C12-N
19	b	301	POV	C211-C212-C213-C214
19	g	201	POV	C23-C24-C25-C26
19	b	301	POV	C2-C1-O11-P
19	b	303	POV	O11-C1-C2-O21
19	b	305	POV	O11-C1-C2-O21
19	r	402	POV	O11-C1-C2-O21
19	b	301	POV	C29-C210-C211-C212
19	b	301	POV	C27-C28-C29-C210
19	b	301	POV	O21-C2-C3-O31
19	b	303	POV	O21-C2-C3-O31
19	b	304	POV	O21-C2-C3-O31
19	b	301	POV	C1-O11-P-O13
19	b	303	POV	C11-O12-P-O11
19	b	303	POV	C11-O12-P-O13
19	b	305	POV	C1-O11-P-O12
19	b	305	POV	C1-O11-P-O14
19	r	402	POV	C1-O11-P-O12
19	r	402	POV	C1-O11-P-O13
19	r	402	POV	C1-O11-P-O14
19	g	201	POV	C1-O11-P-O14
19	g	201	POV	C11-O12-P-O14
19	p	201	POV	C11-O12-P-O14
19	b	303	POV	C24-C25-C26-C27
19	b	303	POV	C32-C33-C34-C35
19	b	302	POV	C27-C28-C29-C210
21	r	403	OLA	C3-C4-C5-C6
19	r	402	POV	C34-C35-C36-C37
19	g	201	POV	C22-C23-C24-C25
19	r	401	POV	C35-C36-C37-C38
19	b	303	POV	C21-C22-C23-C24
19	b	301	POV	C311-C312-C313-C314
19	b	303	POV	C34-C35-C36-C37
19	g	201	POV	C35-C36-C37-C38
21	r	403	OLA	C6-C7-C8-C9
19	b	304	POV	C310-C311-C312-C313
19	r	401	POV	C29-C210-C211-C212
19	g	201	POV	C27-C28-C29-C210
19	b	304	POV	C29-C210-C211-C212
19	r	402	POV	C27-C28-C29-C210

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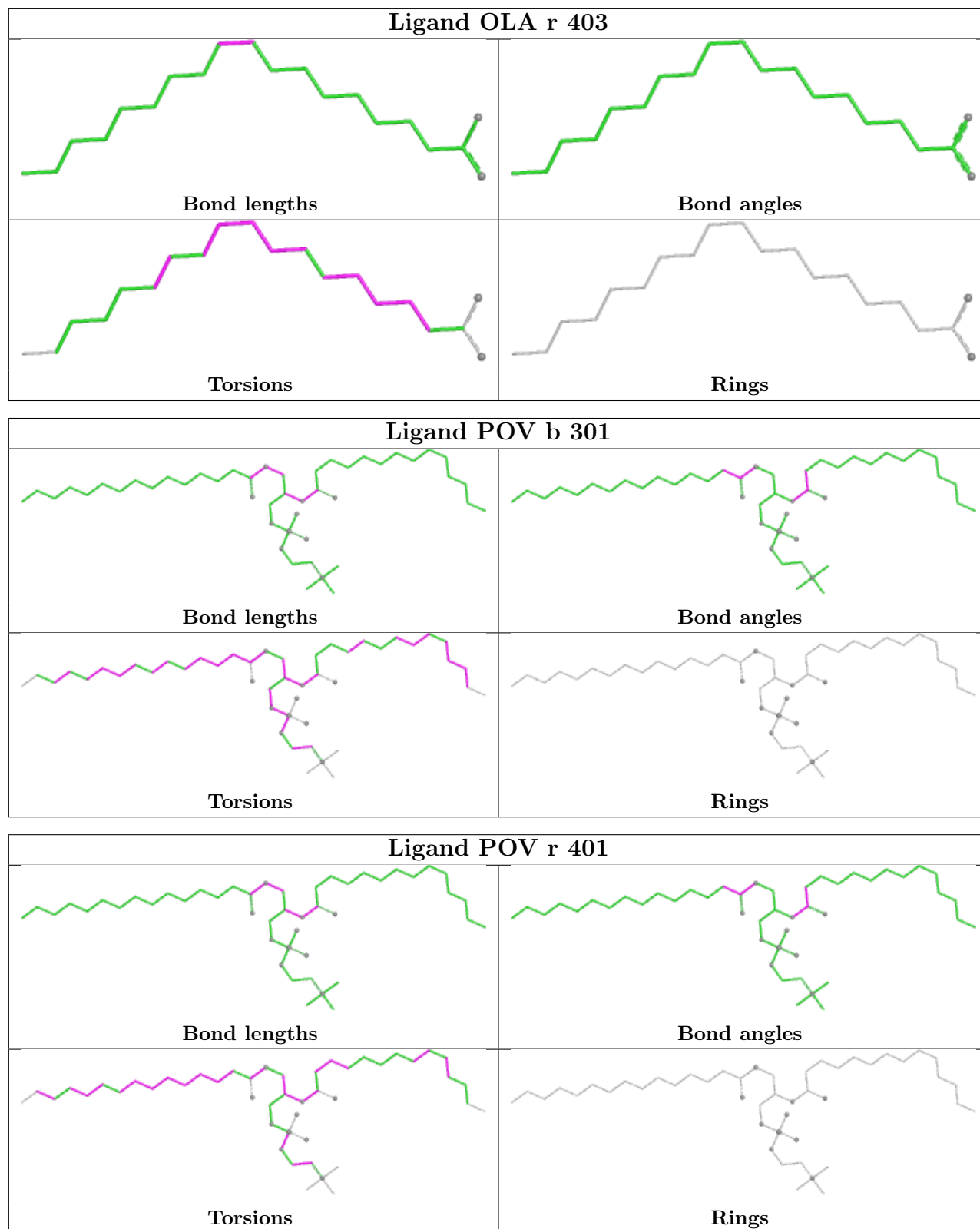
Mol	Chain	Res	Type	Atoms
19	p	201	POV	C29-C210-C211-C212
19	r	402	POV	C33-C34-C35-C36
19	b	302	POV	C39-C310-C311-C312
19	b	304	POV	C27-C28-C29-C210
18	C	702	ADP	PA-O3A-PB-O1B
19	r	401	POV	C312-C313-C314-C315
19	r	401	POV	C27-C28-C29-C210
21	r	403	OLA	C9-C10-C11-C12
19	b	304	POV	C312-C313-C314-C315
19	r	401	POV	C310-C311-C312-C313
19	b	304	POV	C1-C2-C3-O31
21	r	403	OLA	C7-C8-C9-C10
19	b	304	POV	O21-C21-C22-C23
19	b	304	POV	C35-C36-C37-C38
19	b	305	POV	O21-C21-C22-C23
19	b	301	POV	O31-C31-C32-C33
19	b	305	POV	O31-C31-C32-C33
19	r	402	POV	O21-C21-C22-C23
19	b	302	POV	O31-C31-C32-C33
19	b	304	POV	O22-C21-C22-C23
19	b	302	POV	O32-C31-C32-C33
19	r	402	POV	O22-C21-C22-C23
19	b	305	POV	O32-C31-C32-C33
19	b	301	POV	C1-C2-C3-O31
19	p	201	POV	C39-C310-C311-C312
19	b	305	POV	O22-C21-C22-C23
19	r	402	POV	C311-C310-C39-C38
19	b	303	POV	C29-C210-C211-C212
19	p	201	POV	O21-C21-C22-C23
19	b	301	POV	O32-C31-C32-C33

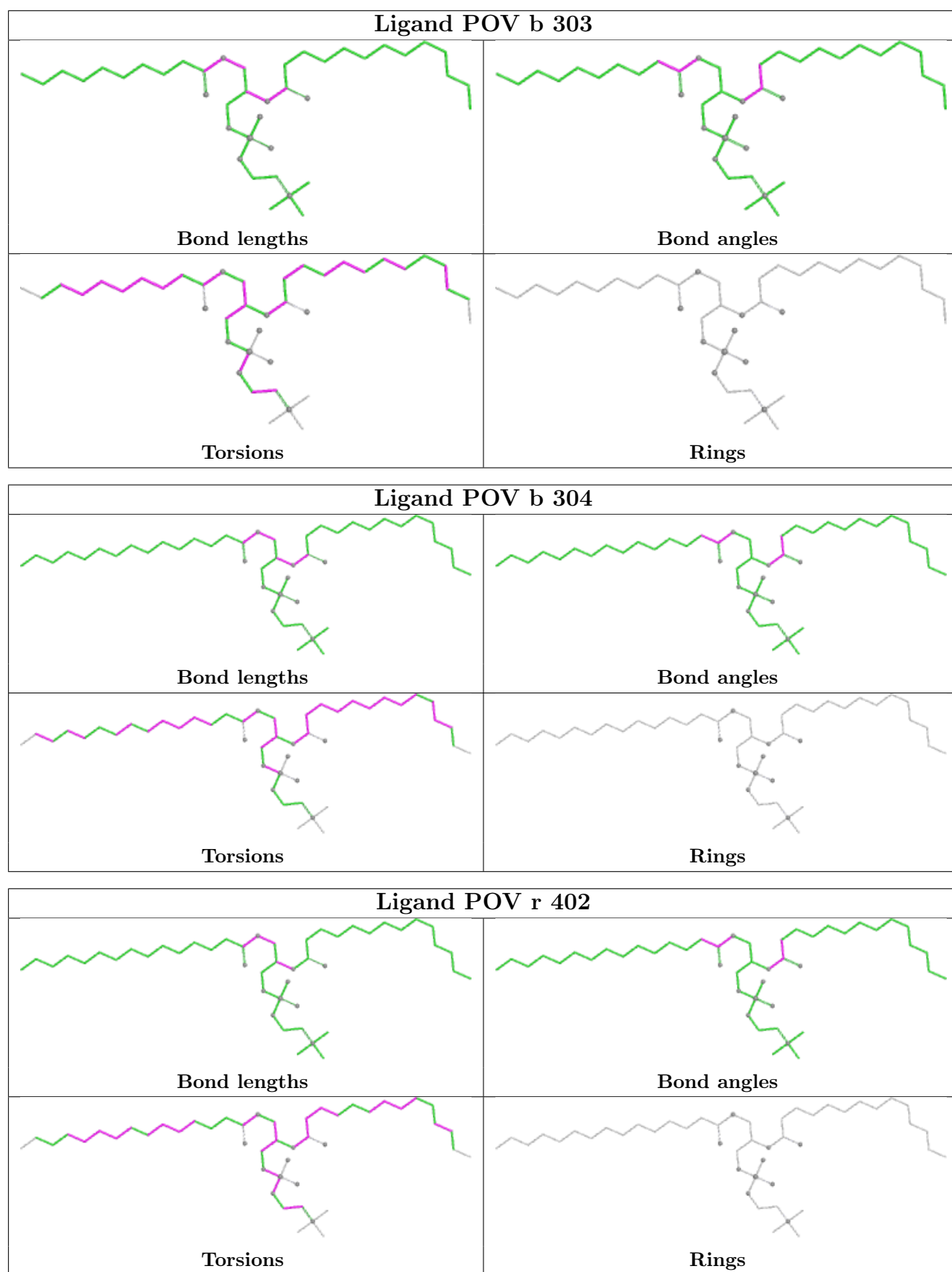
There are no ring outliers.

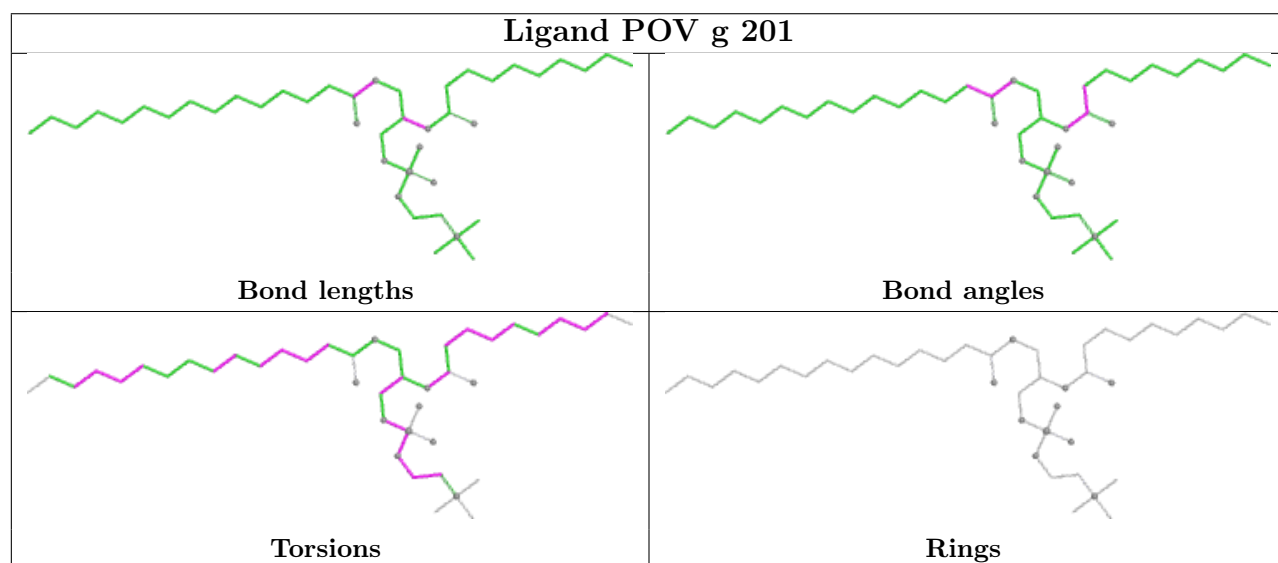
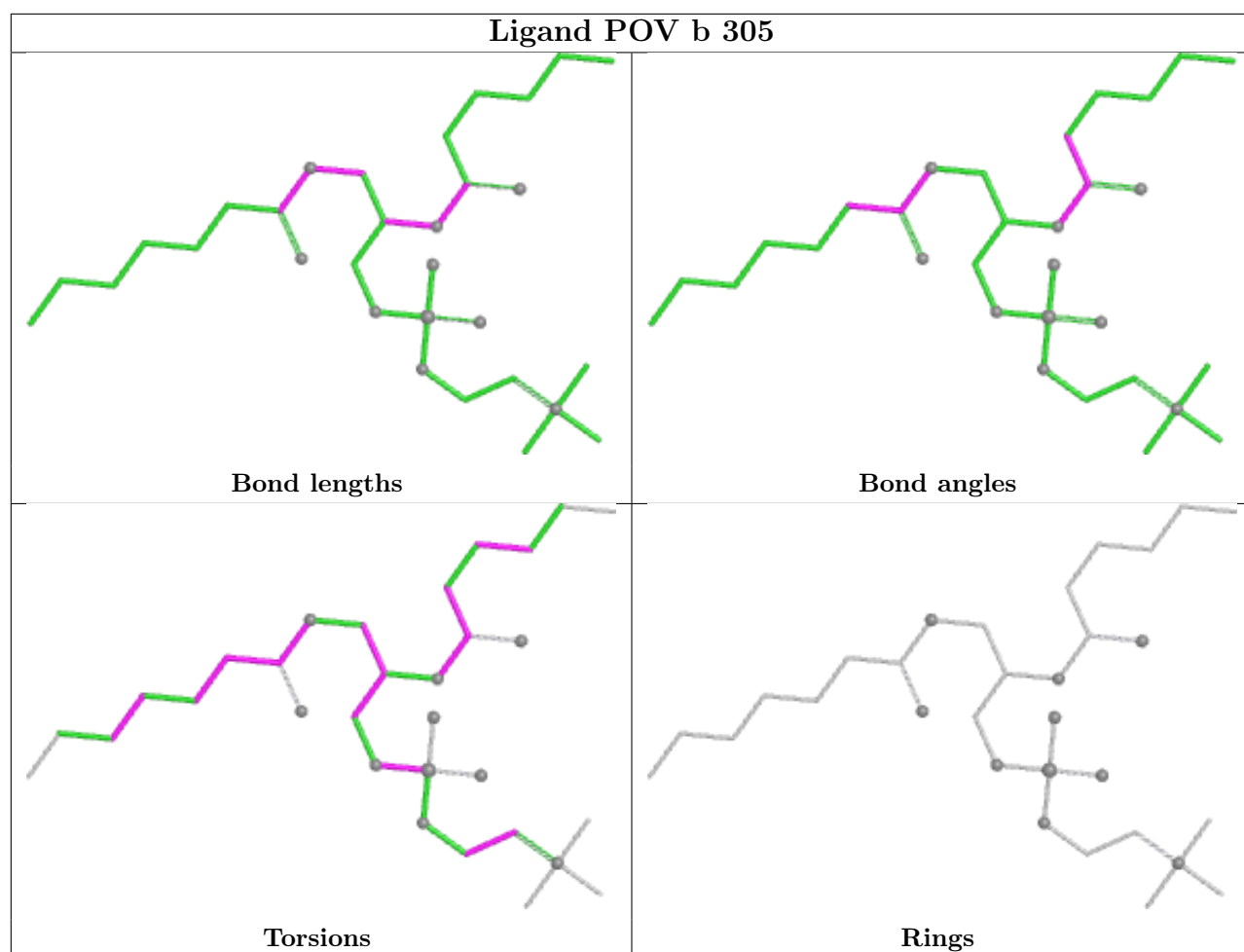
No monomer is involved in short contacts.

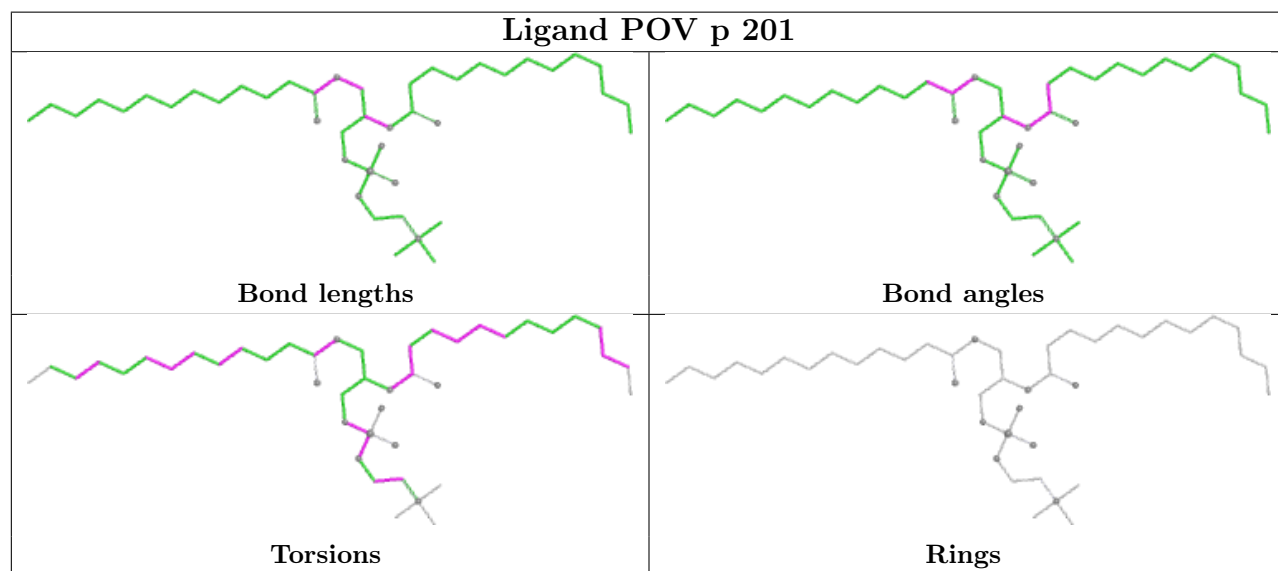
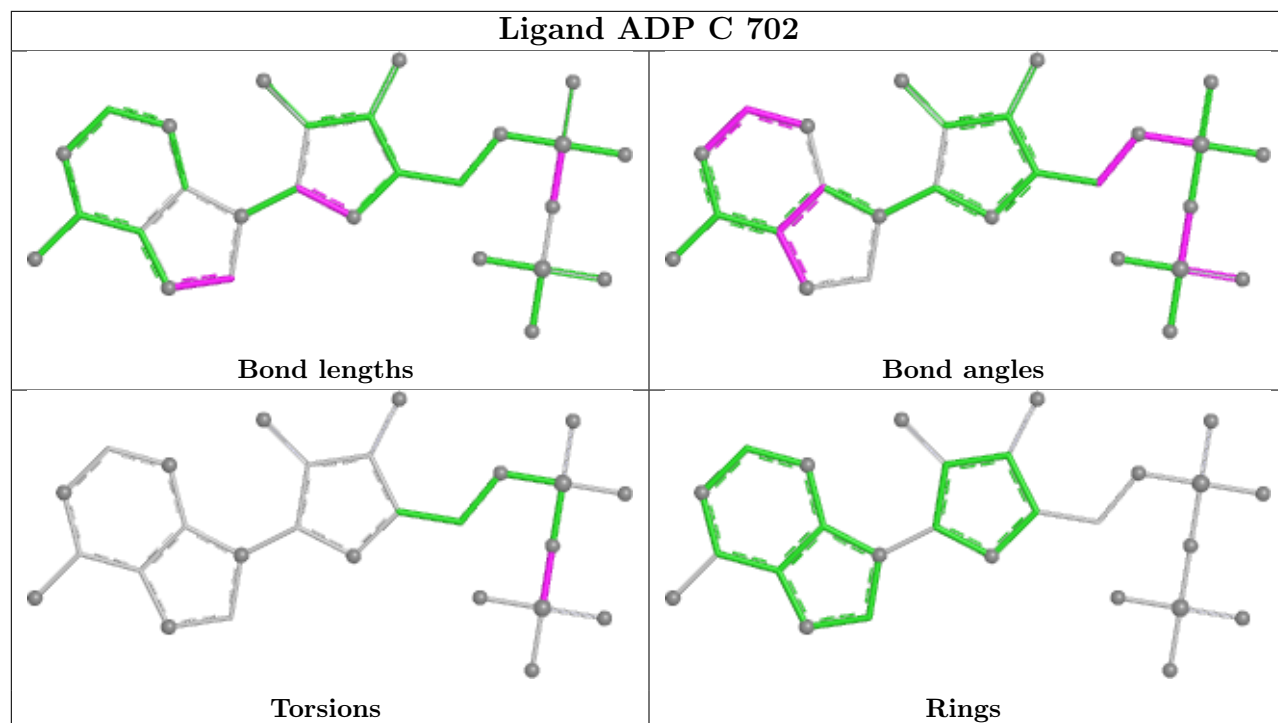
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

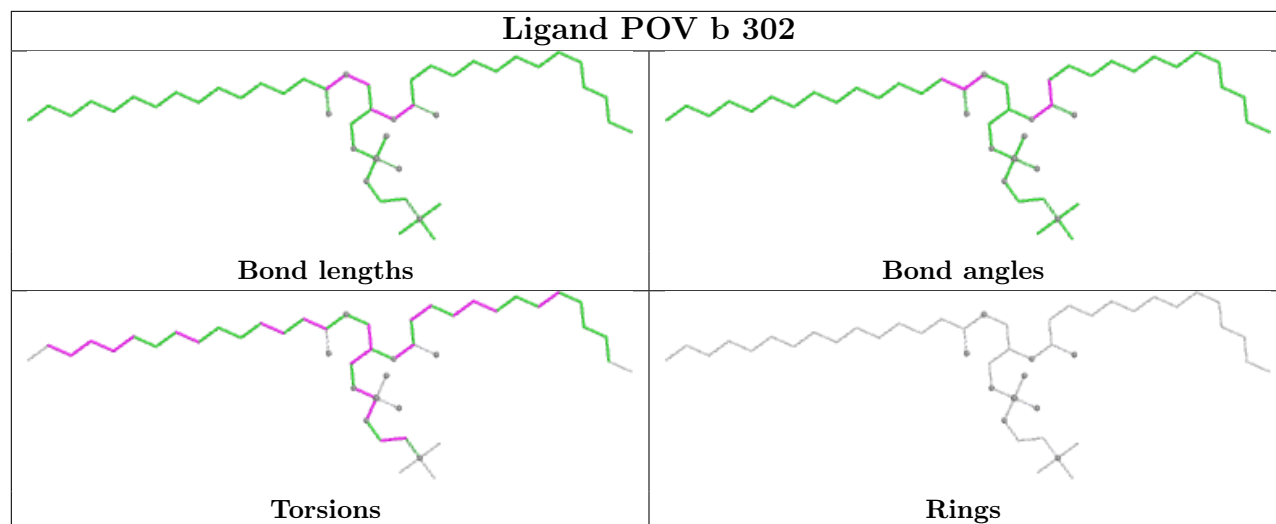
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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.

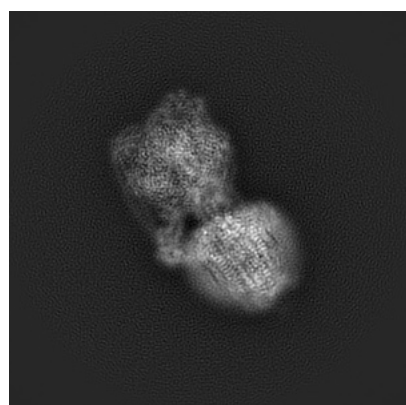
6 Map visualisation [i](#)

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.

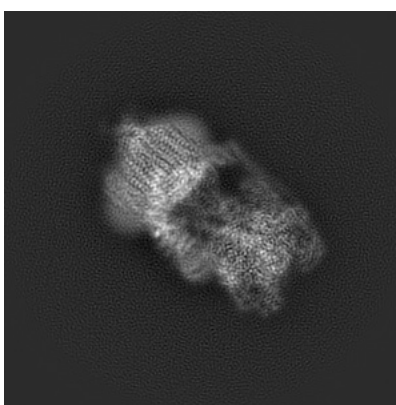
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

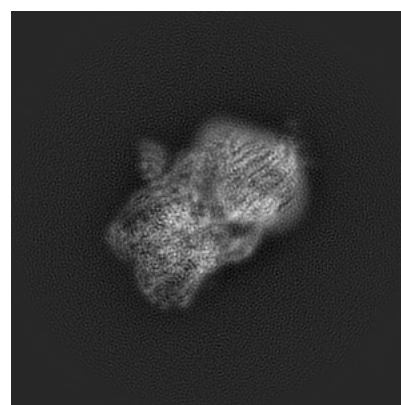
6.1.1 Primary map



X



Y

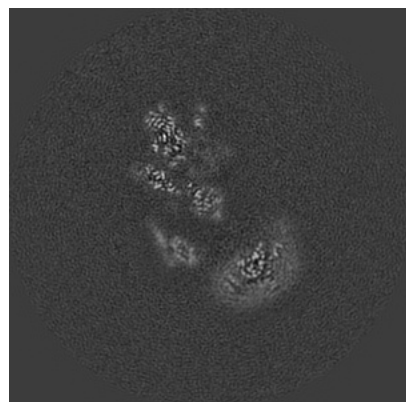


Z

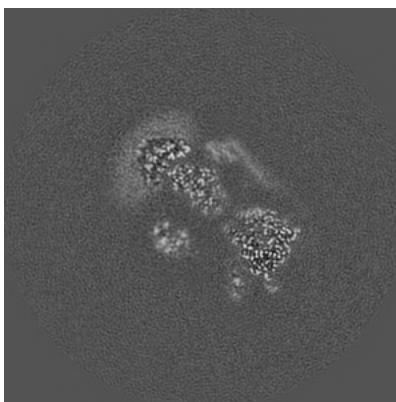
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

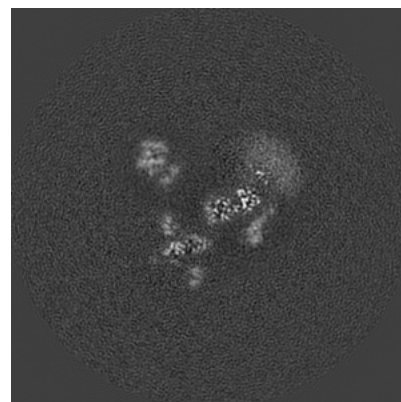
6.2.1 Primary map



X Index: 255



Y Index: 255

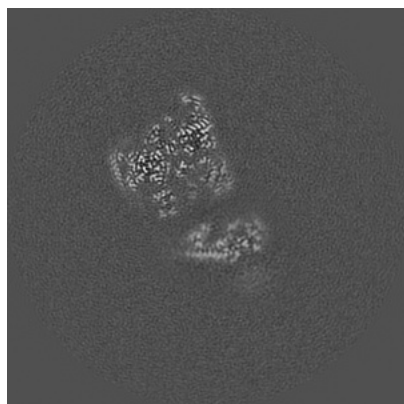


Z Index: 255

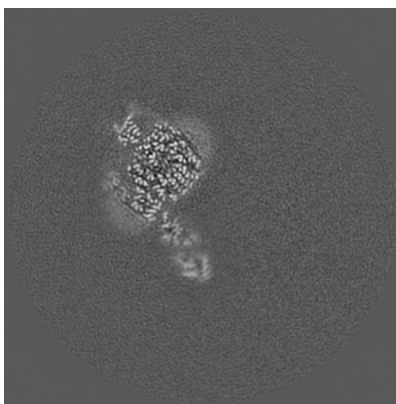
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

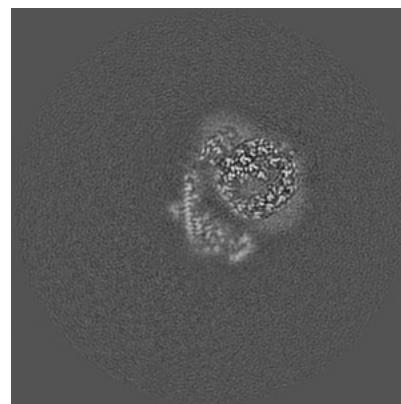
6.3.1 Primary map



X Index: 223



Y Index: 313

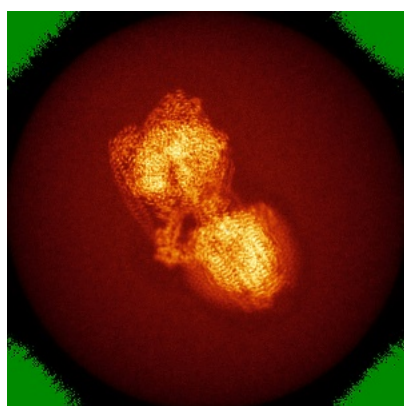


Z Index: 196

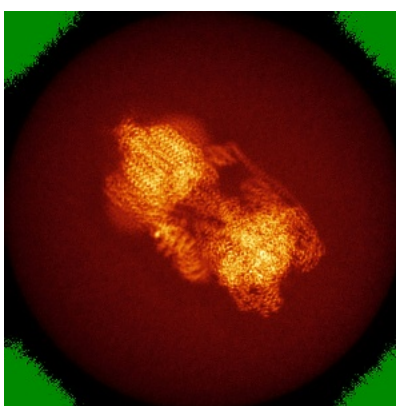
The images above show the largest variance slices of the map in three orthogonal directions.

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

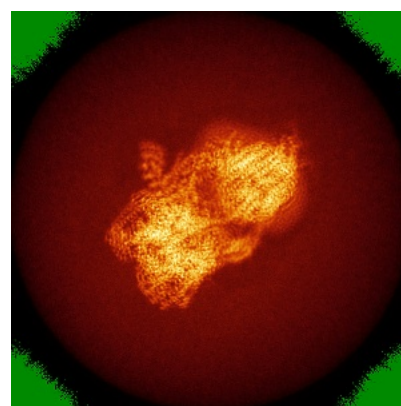
6.4.1 Primary map



X



Y

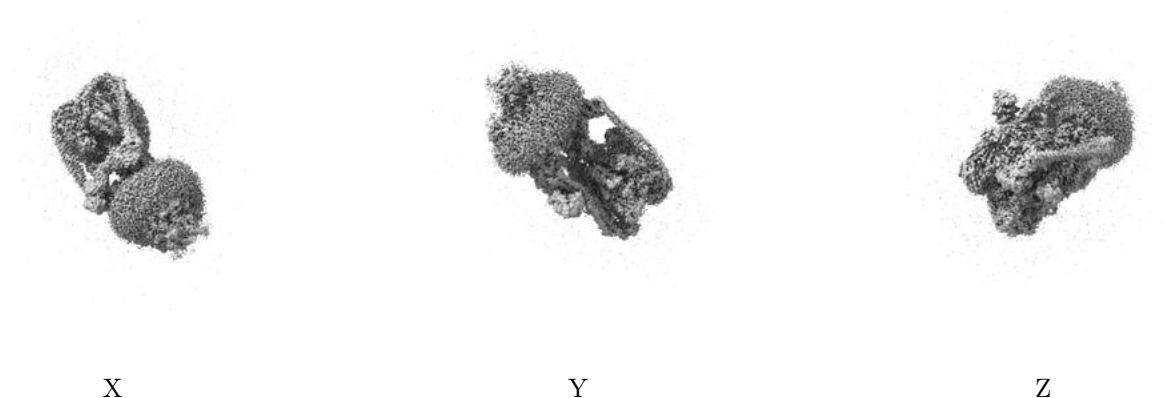


Z

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.

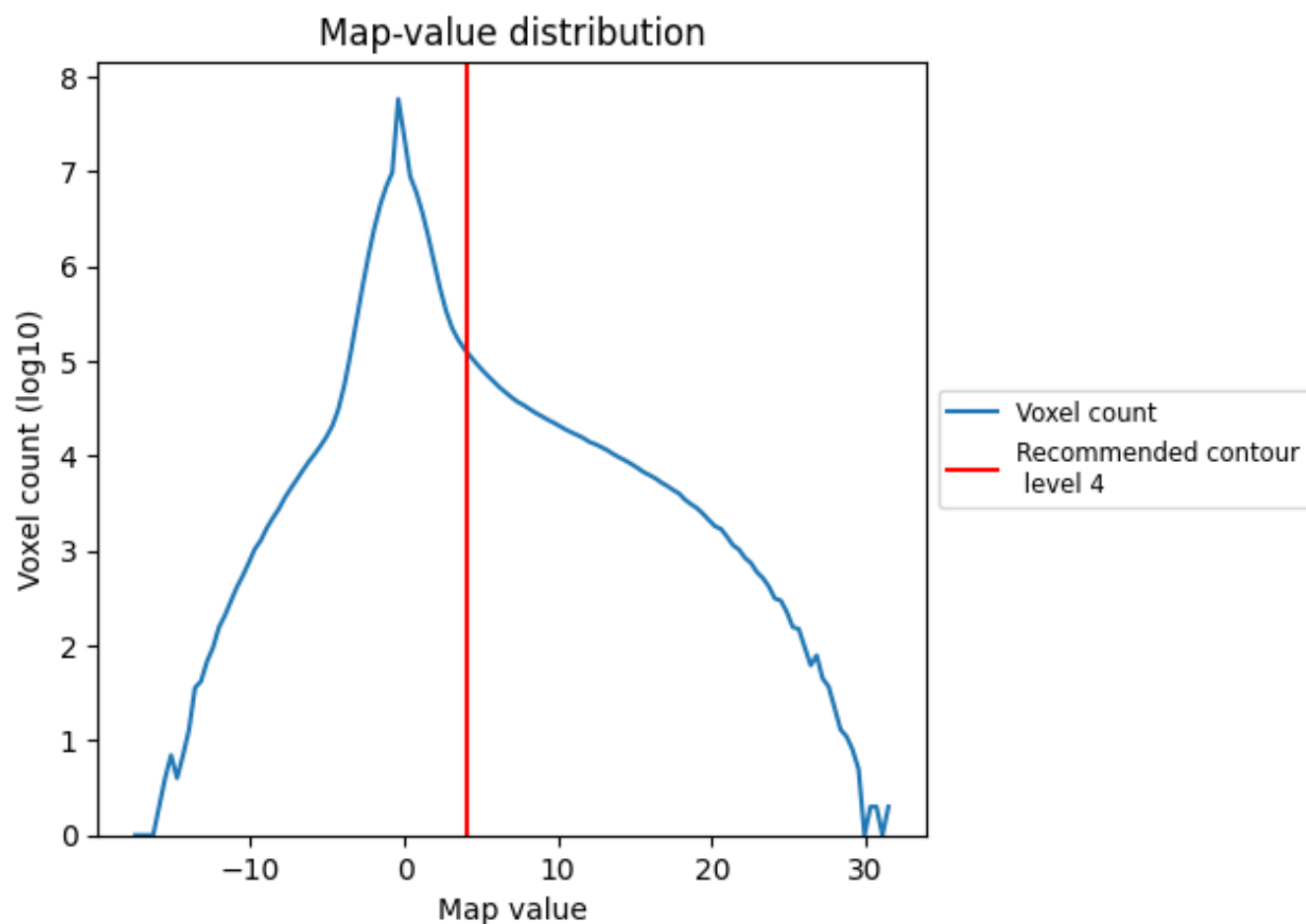
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

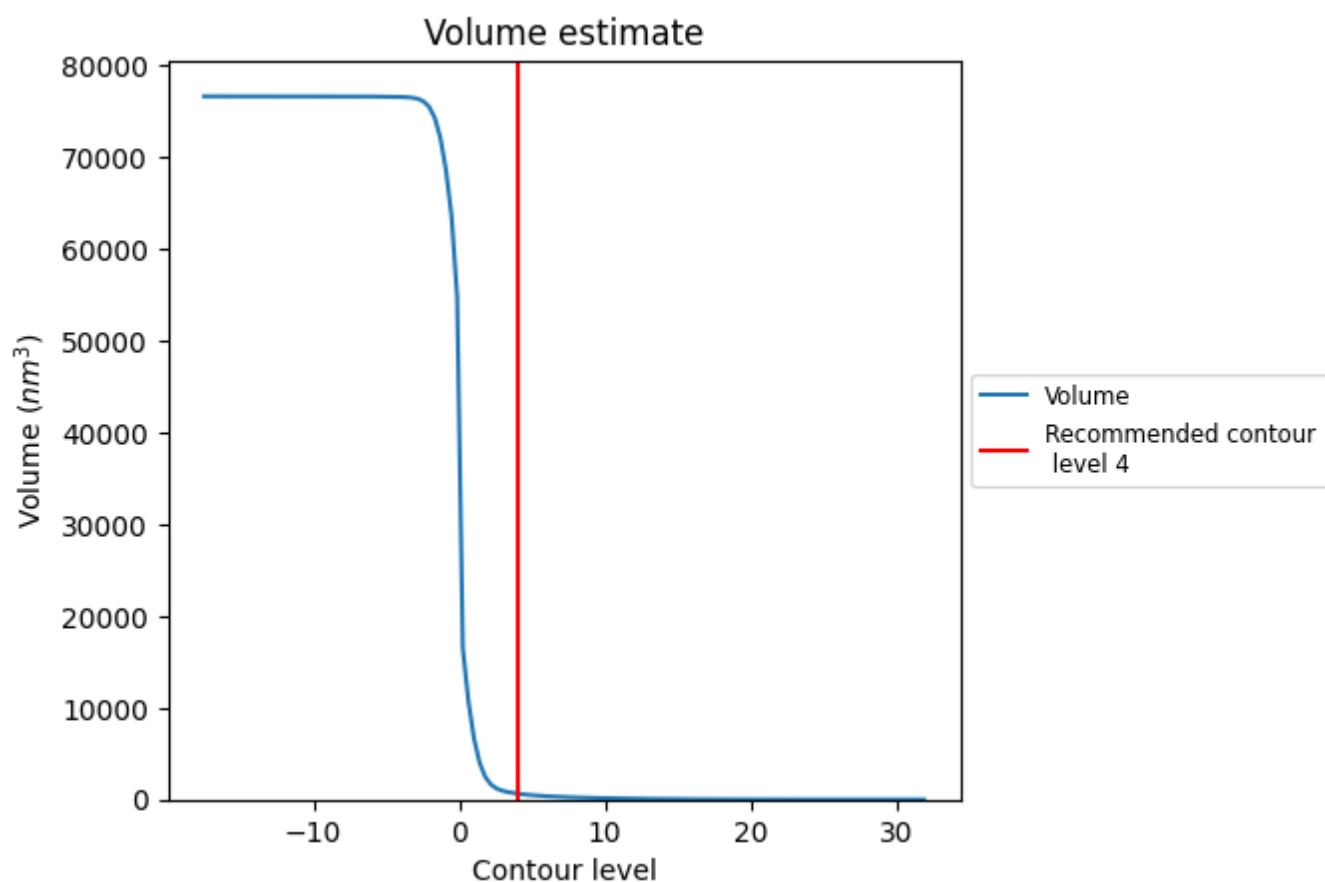
This section contains the results of statistical analysis of the map.

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.

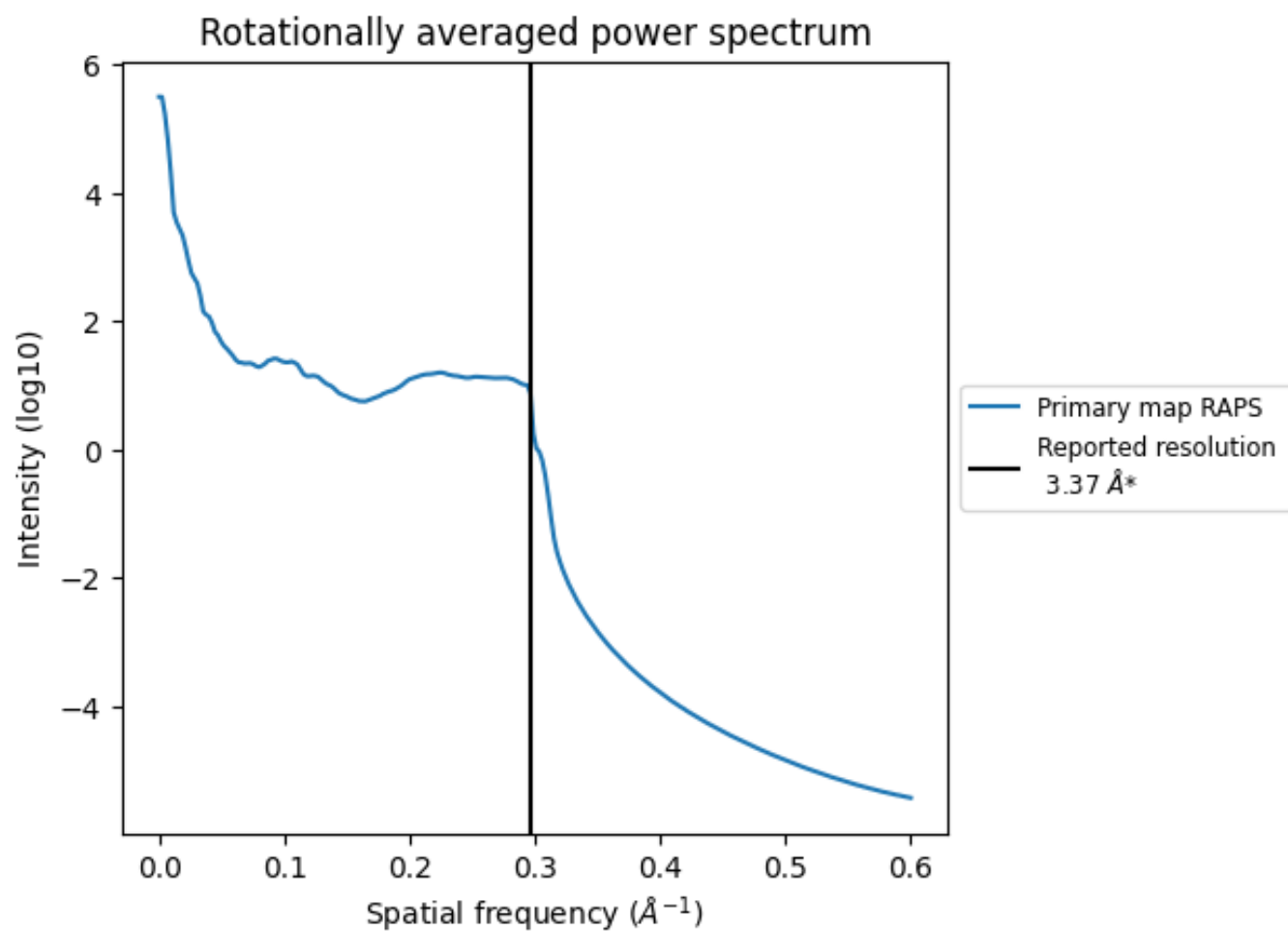
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

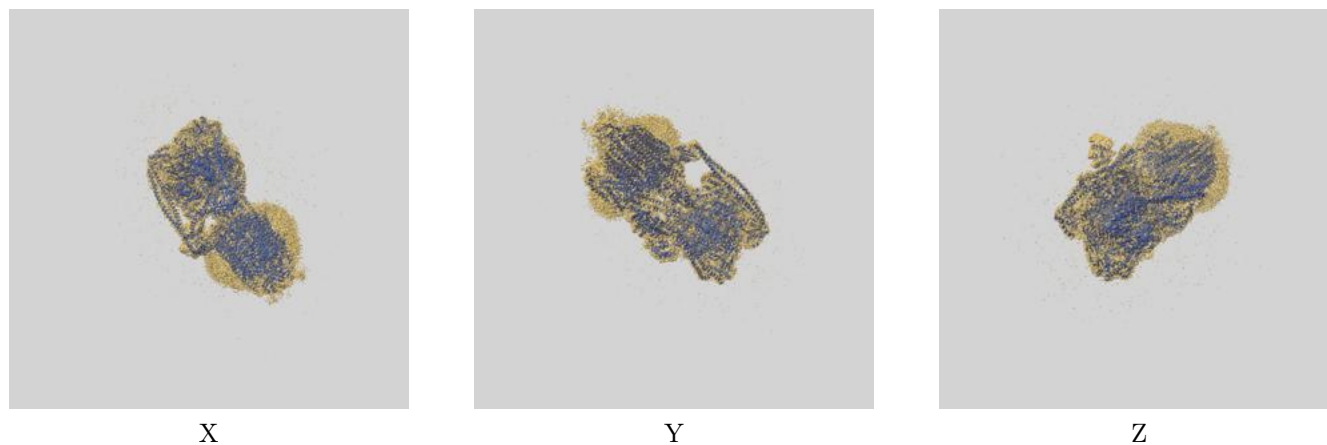
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

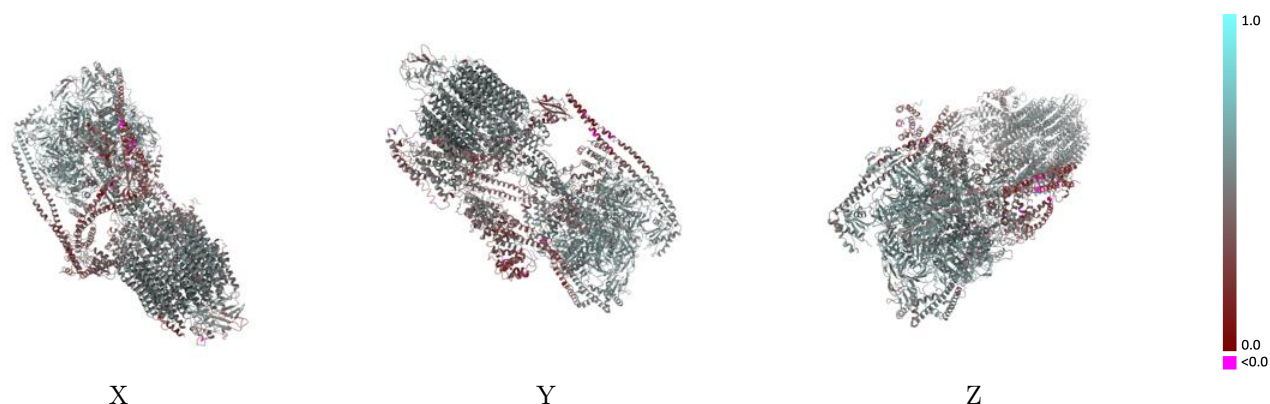
This section contains information regarding the fit between EMDB map EMD-22121 and PDB model 6XBW. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



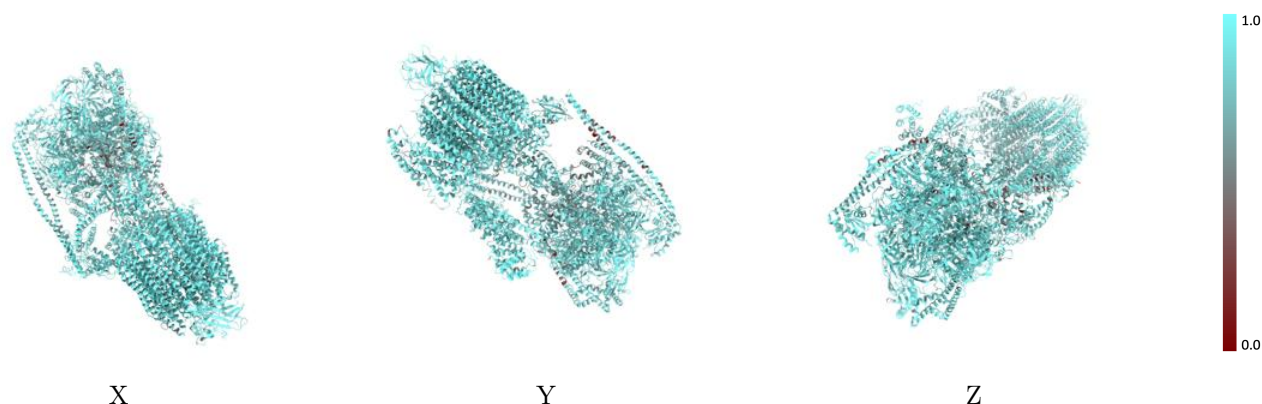
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



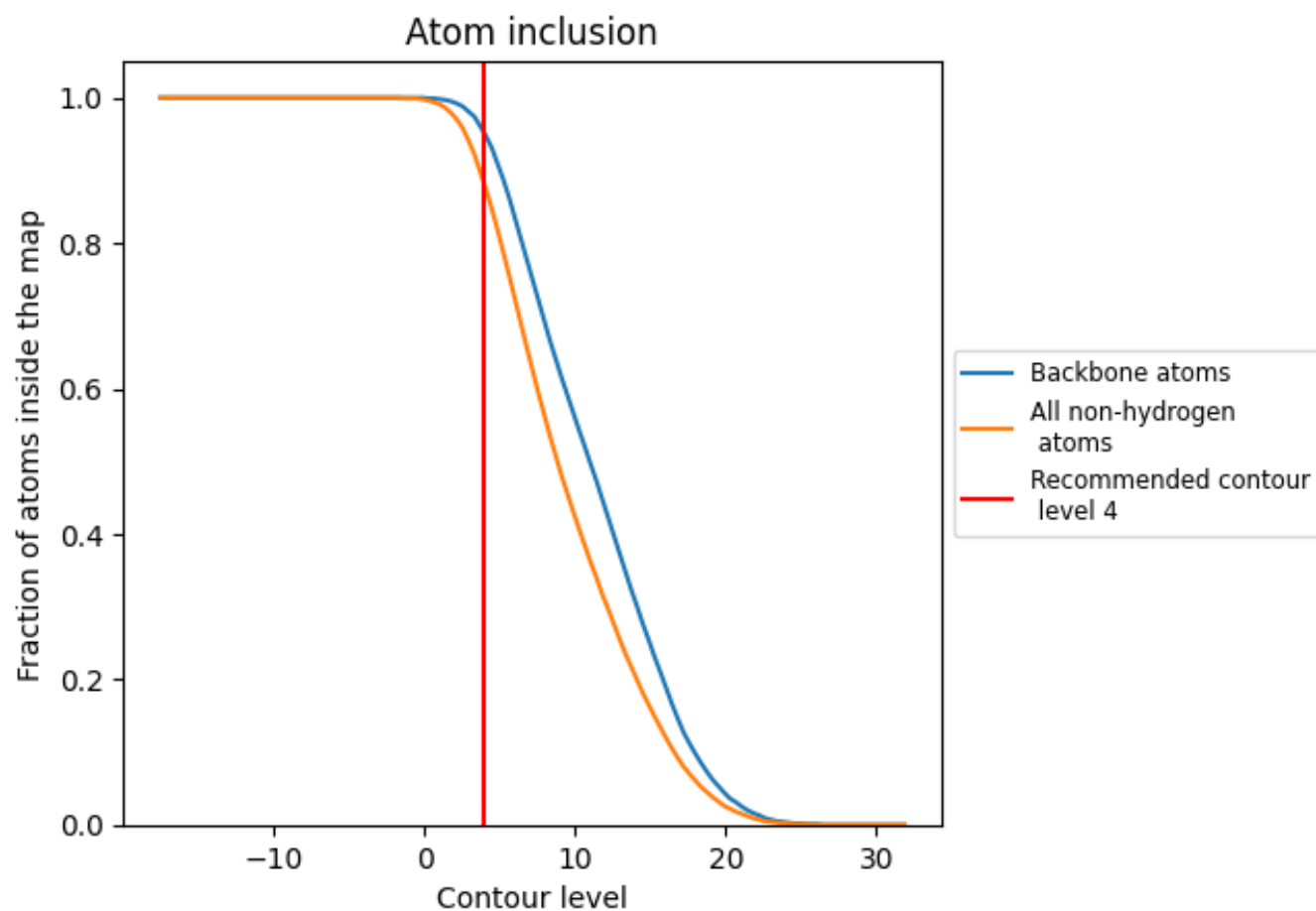
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8800	 0.4790
A	 0.8470	 0.4920
B	 0.8740	 0.5200
C	 0.8850	 0.5290
D	 0.9130	 0.5510
E	 0.9010	 0.5430
F	 0.8910	 0.5350
G	 0.8340	 0.3010
H	 0.8590	 0.5110
I	 0.8220	 0.4430
J	 0.8560	 0.4680
K	 0.8590	 0.4630
L	 0.8300	 0.4760
M	 0.7720	 0.3570
N	 0.8550	 0.4210
O	 0.7760	 0.3890
P	 0.8550	 0.3310
a	 0.8670	 0.4200
b	 0.9340	 0.5250
c	 0.9300	 0.5180
d	 0.8830	 0.4910
e	 0.8270	 0.3950
f	 0.7930	 0.3270
g	 0.9360	 0.5160
k	 0.9260	 0.5090
l	 0.9280	 0.4980
m	 0.9250	 0.5010
n	 0.9230	 0.5110
o	 0.9390	 0.5170
p	 0.9330	 0.5160
q	 0.9350	 0.5170
r	 0.9310	 0.5360
s	 0.9080	 0.4660

