



## Full wwPDB EM Validation Report ⓘ

Sep 2, 2025 – 10:18 AM EDT

PDB ID : 9DET / pdb\_00009det  
EMDB ID : EMD-46798  
Title : Human V-ATPase Vo subcomplex (containing subunit isoform a4) bound to nanobody and inhibitor  
Authors : Oot, R.A.; Park, J.B.; Roh, S.-H.; Wilkens, S.  
Deposited on : 2024-08-29  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

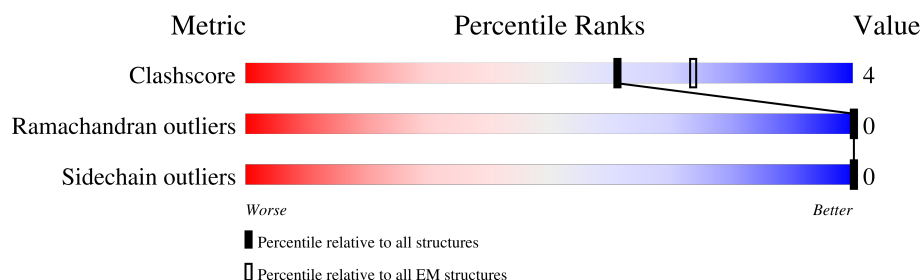
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



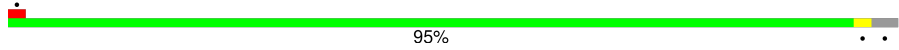
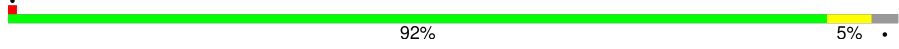
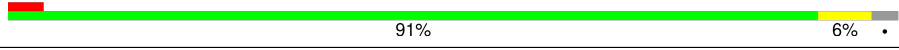


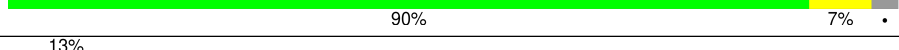
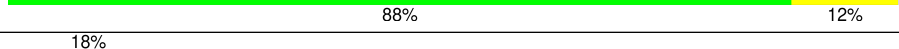
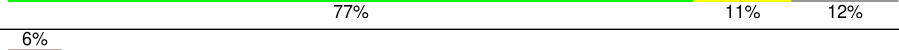
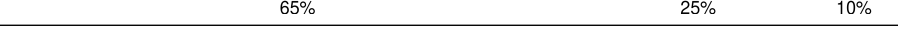
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	e	81	<div> <div>16%</div> <div>80%</div> <div>12%</div> <div>7%</div> </div>
2	f	137	<div> <div>25%</div> <div>53%</div> <div>8%</div> <div>39%</div> </div>
3	o	470	<div> <div>43%</div> <div>56%</div> </div>
4	p	350	<div> <div>14%</div> <div>85%</div> </div>
5	b	205	<div> <div>95%</div> <div>5%</div> </div>
6	c	155	<div> <div>86%</div> <div>10%</div> <div>•</div> </div>
6	g	155	<div> <div>91%</div> <div>6%</div> <div>•</div> </div>
6	h	155	<div> <div>90%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
6	i	155	
6	j	155	
6	k	155	
6	l	155	
6	m	155	
6	n	155	
7	d	351	
8	a	863	
9	q	139	

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 50652 atoms, of which 25567 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	e	75	Total	C	H	N	O	S	0	0
			1256	428	639	93	91	5		

- Molecule 2 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	f	84	Total	C	H	N	O	S	0	0
			1299	431	647	101	114	6		

- Molecule 3 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	o	209	Total	C	H	N	O	S	0	0
			3320	1109	1621	275	305	10		

- Molecule 4 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	p	52	Total	C	H	N	O	S	0	0
			867	295	430	63	75	4		

- Molecule 5 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	b	204	Total	C	H	N	O	S	0	0
			3042	990	1544	238	259	11		

- Molecule 6 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	c	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	g	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		
6	h	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		
6	i	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		
6	j	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		
6	k	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		
6	l	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		
6	m	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		
6	n	150	Total	C	H	N	O	S	0	0
			2196	698	1131	169	191	7		

- Molecule 7 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	d	351	Total	C	H	N	O	S	0	0
			5626	1834	2782	463	532	15		

- Molecule 8 is a protein called V-type proton ATPase 116 kDa subunit a 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	a	759	Total	C	H	N	O	S	0	0
			12389	4036	6212	1020	1076	45		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	841	GLY	-	expression tag	UNP Q9HBG4
a	842	ASP	-	expression tag	UNP Q9HBG4
a	843	LEU	-	expression tag	UNP Q9HBG4
a	844	ASP	-	expression tag	UNP Q9HBG4
a	845	TYR	-	expression tag	UNP Q9HBG4
a	846	LYS	-	expression tag	UNP Q9HBG4
a	847	ASP	-	expression tag	UNP Q9HBG4
a	848	ASP	-	expression tag	UNP Q9HBG4
a	849	ASP	-	expression tag	UNP Q9HBG4
a	850	ASP	-	expression tag	UNP Q9HBG4

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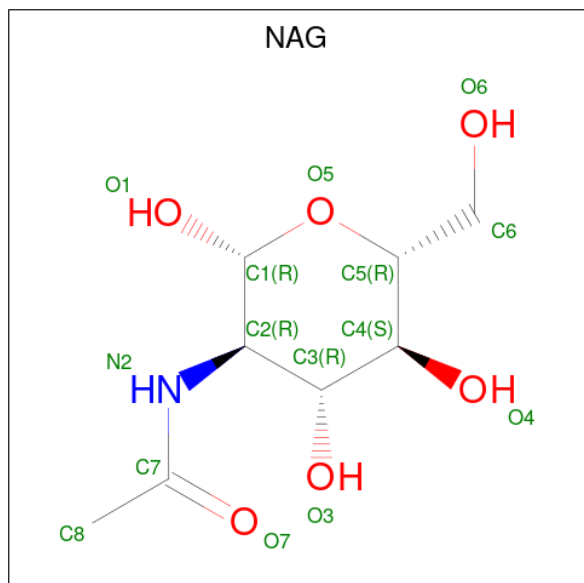
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Chain	Residue	Modelled	Actual	Comment	Reference
a	851	LYS	-	expression tag	UNP Q9HBG4
a	852	LEU	-	expression tag	UNP Q9HBG4
a	853	ASP	-	expression tag	UNP Q9HBG4
a	854	TYR	-	expression tag	UNP Q9HBG4
a	855	LYS	-	expression tag	UNP Q9HBG4
a	856	ASP	-	expression tag	UNP Q9HBG4
a	857	ASP	-	expression tag	UNP Q9HBG4
a	858	ASP	-	expression tag	UNP Q9HBG4
a	859	ASP	-	expression tag	UNP Q9HBG4
a	860	LYS	-	expression tag	UNP Q9HBG4
a	861	ALA	-	expression tag	UNP Q9HBG4
a	862	ASP	-	expression tag	UNP Q9HBG4
a	863	LEU	-	expression tag	UNP Q9HBG4

- Molecule 9 is a protein called Anti V-ATPase Nanobody 2CAS66.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	q	125	Total	C	H	N	O	S	0	0
			1881	598	919	167	191	6		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



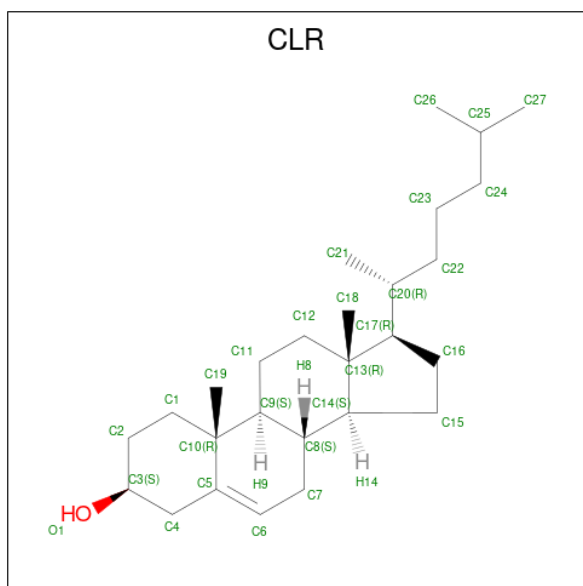
Mol	Chain	Residues	Atoms					AltConf
10	o	1	Total	C	H	N	O	0
			30	8	15	1	6	

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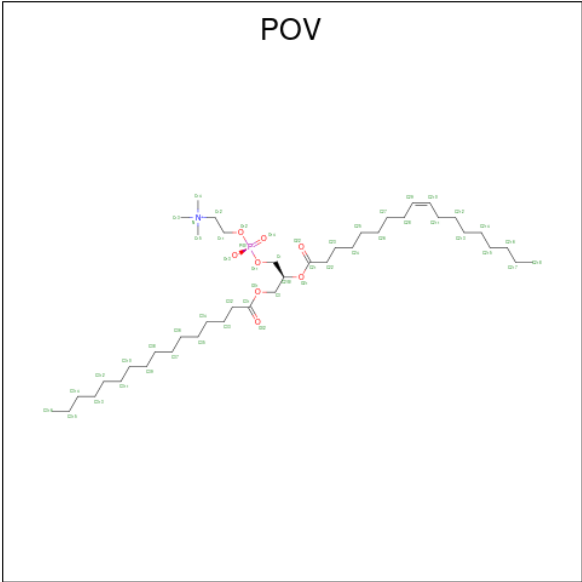
Mol	Chain	Residues	Atoms					AltConf
10	o	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	o	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	o	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	o	1	Total	C	H	N	O	0
			27	8	13	1	5	
10	a	1	Total	C	H	N	O	0
			30	8	15	1	6	
10	a	1	Total	C	H	N	O	0
			30	8	15	1	6	
10	a	1	Total	C	H	N	O	0
			30	8	15	1	6	

- Molecule 11 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ).



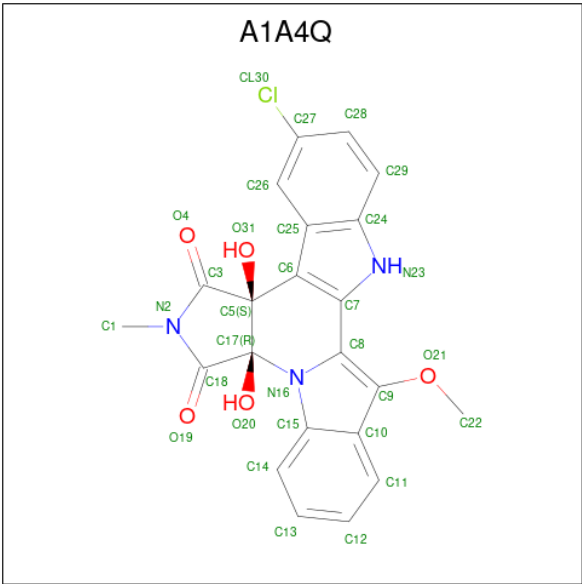
Mol	Chain	Residues	Atoms				AltConf
11	p	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 12 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula:  $C_{42}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms						AltConf
12	p	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
12	b	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
12	b	1	Total 134	C 42	H 82	N 1	O 8	P 1	0

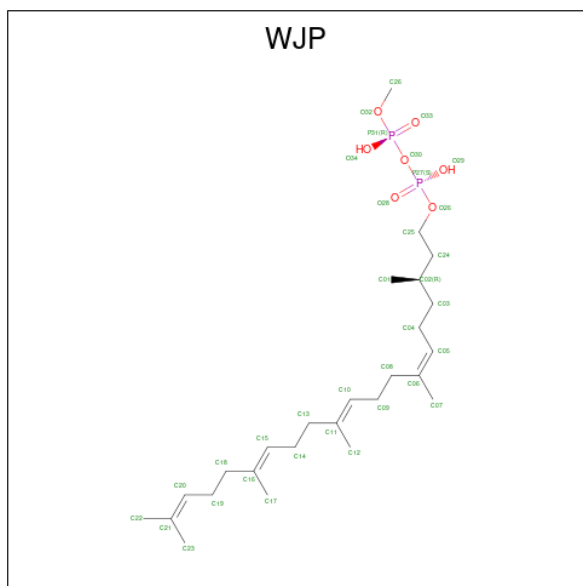
- Molecule 13 is Cladoniamide A (CCD ID: A1A4Q) (formula: C<sub>22</sub>H<sub>16</sub>ClN<sub>3</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms						AltConf
13	c	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	
13	g	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	
13	h	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	
13	i	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	
13	j	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	
13	k	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	
13	l	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	
13	m	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	
13	n	1	Total	C	Cl	H	N	O	0
			47	22	1	16	3	5	

- Molecule 14 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (CCD ID: WJP) (formula:  $C_{26}H_{48}O_7P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	H	O	P	0
			81	26	46	7	2	



- Molecule 5: V-type proton ATPase 21 kDa proteolipid subunit

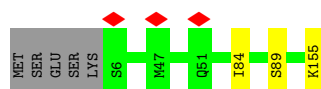
- Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit

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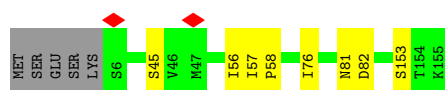
- Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit

Chain i:  95%



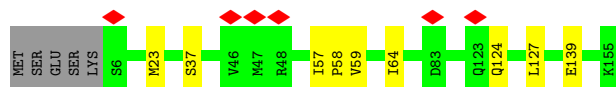
- Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit

Chain j:  92%




- Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit

Chain k:  91%




- Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit

Chain l:  88%




- Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit

Chain m:  89%




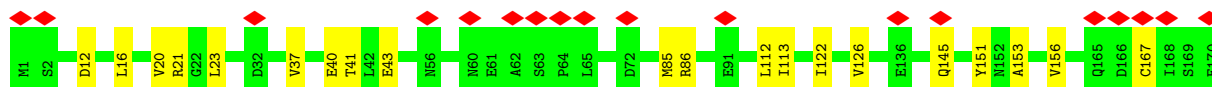
- Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit

Chain n:  90%



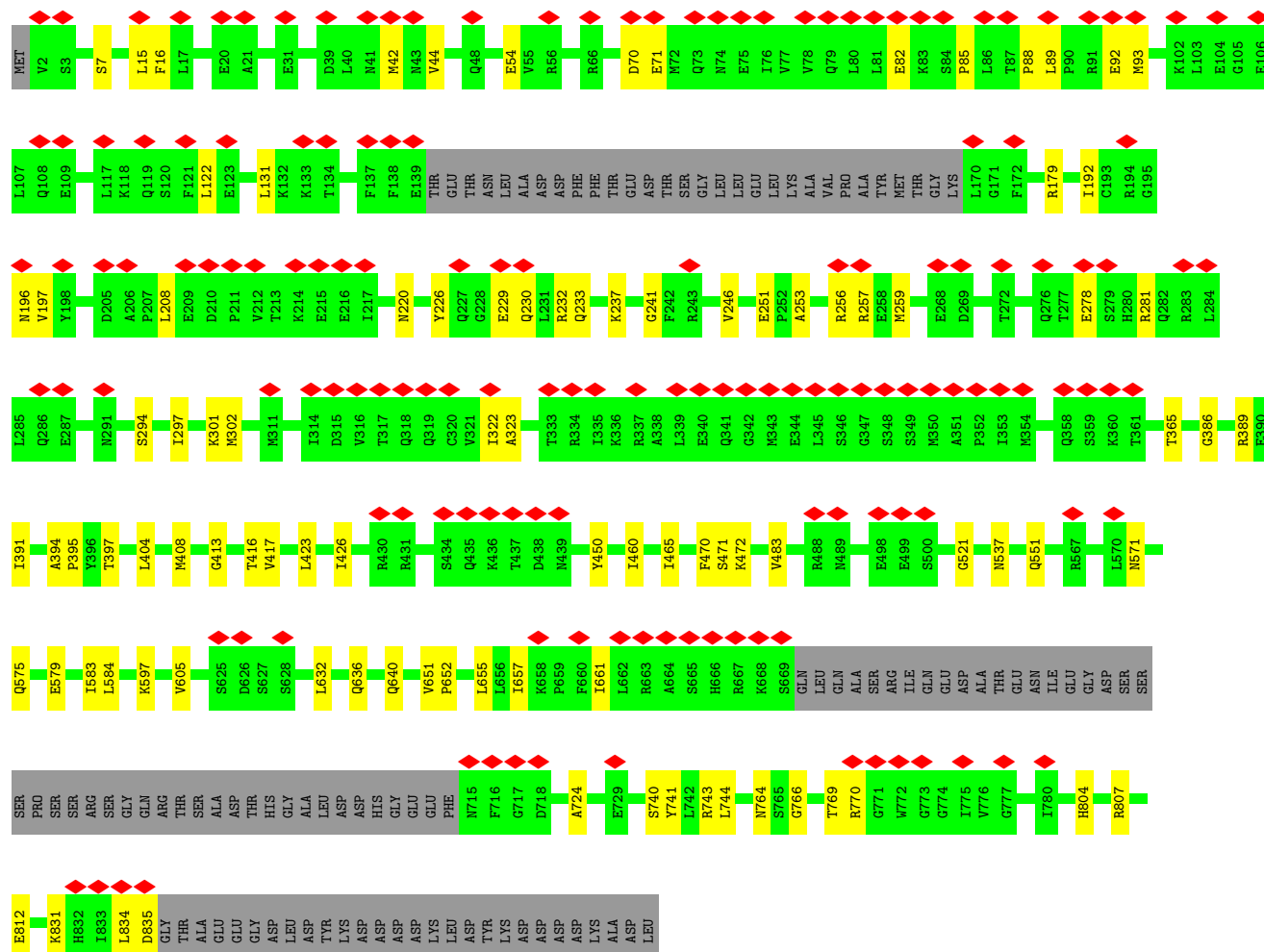
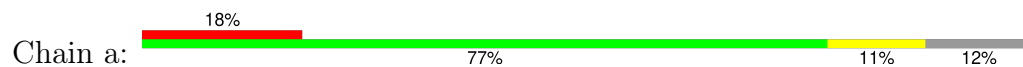
- Molecule 7: V-type proton ATPase subunit d 1

Chain d:  13% 88% 12%

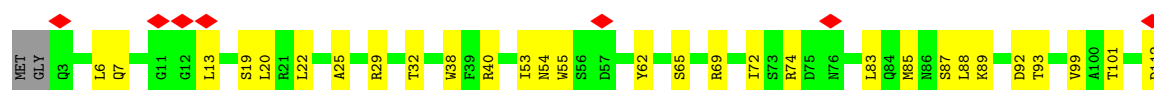




• Molecule 8: V-type proton ATPase 116 kDa subunit a 4



• Molecule 9: Anti V-ATPase Nanobody 2CAS66



N113	V114	D115	Y116	W117	G118	Q119	T124	S127	ALA	ALA	ALA	ALA	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PRO	LYS
------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	39.96	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	30.665	Depositor
Minimum map value	-18.650	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.996	Depositor
Recommended contour level	5	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: WJP, POV, NAG, CLR, A1A4Q

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	e	0.12	0/642	0.24	0/882
2	f	0.09	0/668	0.26	0/907
3	o	0.15	0/1755	0.29	0/2386
4	p	0.15	0/451	0.22	0/616
5	b	0.16	0/1532	0.24	0/2082
6	c	0.17	0/1080	0.25	0/1461
6	g	0.16	0/1080	0.24	0/1461
6	h	0.17	0/1080	0.27	0/1461
6	i	0.16	0/1080	0.24	0/1461
6	j	0.15	0/1080	0.24	0/1461
6	k	0.15	0/1080	0.24	0/1461
6	l	0.14	0/1080	0.24	0/1461
6	m	0.16	0/1080	0.27	0/1461
6	n	0.16	0/1080	0.23	0/1461
7	d	0.12	0/2910	0.22	0/3940
8	a	0.11	0/6331	0.21	0/8574
9	q	0.10	0/981	0.24	0/1330
All	All	0.14	0/24990	0.24	0/33866

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	617	639	637	9	0
2	f	652	647	647	8	0
3	o	1699	1621	1622	11	0
4	p	437	430	430	2	0
5	b	1498	1544	1544	9	0
6	c	1065	1131	1131	14	0
6	g	1065	1131	1131	8	0
6	h	1065	1131	1131	9	0
6	i	1065	1131	1131	2	0
6	j	1065	1131	1131	6	0
6	k	1065	1131	1131	7	0
6	l	1065	1131	1131	9	0
6	m	1065	1131	1131	7	0
6	n	1065	1131	1131	11	0
7	d	2844	2782	2782	31	0
8	a	6177	6212	6212	66	0
9	q	962	919	919	25	0
10	a	45	45	45	4	0
10	o	71	67	67	3	0
11	p	28	46	46	0	0
12	b	104	164	164	1	0
12	p	52	82	82	2	0
13	c	31	16	0	0	0
13	g	31	16	0	0	0
13	h	31	16	0	0	0
13	i	31	16	0	0	0
13	j	31	16	0	0	0
13	k	31	16	0	1	0
13	l	31	16	0	1	0
13	m	31	16	0	0	0
13	n	31	16	0	2	0
14	a	35	46	0	0	0
All	All	25085	25567	25376	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:246:ARG:NH1	7:d:273:GLU:OE1	2.16	0.79
8:a:251:GLU:O	8:a:256:ARG:NH2	2.16	0.78
6:m:72:VAL:HG21	6:m:99:VAL:HG21	1.66	0.77
5:b:151:CYS:SG	5:b:187:GLY:N	2.58	0.77
8:a:551:GLN:OE1	8:a:741:TYR:OH	2.02	0.76
8:a:597:LYS:NZ	10:a:903:NAG:O6	2.17	0.74
2:f:82:ASP:OD1	8:a:764:ASN:ND2	2.20	0.73
6:g:48:ARG:NH1	6:g:122:ALA:O	2.22	0.73
8:a:230:GLN:N	8:a:230:GLN:OE1	2.21	0.73
2:f:81:GLU:OE2	8:a:472:LYS:NZ	2.21	0.73
8:a:82:GLU:N	8:a:82:GLU:OE1	2.21	0.73
1:e:59:GLN:NE2	8:a:521:GLY:O	2.21	0.73
1:e:79:HIS:NE2	2:f:75:HIS:O	2.22	0.72
9:q:40:ARG:NH2	9:q:92:ASP:OD1	2.23	0.71
9:q:69:ARG:NE	9:q:87:SER:OG	2.24	0.70
1:e:64:PHE:CE1	10:a:903:NAG:H83	2.27	0.70
7:d:208:MET:HE1	7:d:316:TYR:CG	2.28	0.69
8:a:179:ARG:NH1	8:a:220:ASN:OD1	2.25	0.68
6:k:64:ILE:HD11	6:k:139:GLU:OE2	1.93	0.68
6:j:45:SER:O	6:k:124:GLN:NE2	2.27	0.68
7:d:324:GLN:O	7:d:324:GLN:NE2	2.27	0.67
7:d:324:GLN:NE2	7:d:328:ASN:OD1	2.27	0.67
1:e:70:ASN:OD1	1:e:71:GLU:N	2.29	0.65
7:d:167:CYS:SG	7:d:184:THR:HG21	2.36	0.65
8:a:54:GLU:N	8:a:54:GLU:OE1	2.29	0.64
7:d:20:VAL:HG22	7:d:85:MET:SD	2.37	0.64
9:q:32:THR:O	9:q:74:ARG:NH2	2.31	0.64
8:a:70:ASP:OD1	8:a:71:GLU:N	2.32	0.63
7:d:174:ASP:OD1	7:d:177:ASN:ND2	2.30	0.63
9:q:65:SER:O	9:q:89:LYS:NZ	2.32	0.63
7:d:151:TYR:O	7:d:156:VAL:HG23	1.99	0.63
9:q:53:ILE:HD11	9:q:72:ILE:HG13	1.81	0.62
6:h:80:LEU:O	6:i:155:LYS:NZ	2.32	0.62
8:a:85:PRO:O	8:a:301:LYS:NZ	2.32	0.62
3:o:450:LEU:HD11	6:g:112:ILE:HD13	1.82	0.62
8:a:229:GLU:N	8:a:229:GLU:OE1	2.32	0.62
7:d:260:ASP:OD1	7:d:261:TYR:N	2.33	0.62
8:a:246:VAL:O	9:q:29:ARG:NH2	2.32	0.61
6:c:140:VAL:HG21	8:a:804:HIS:CE1	2.35	0.61
9:q:13:LEU:HD22	9:q:124:THR:HG22	1.83	0.60
6:c:136:ILE:O	6:c:140:VAL:HG23	2.01	0.60
8:a:408:MET:HE2	8:a:744:LEU:CD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:21:ARG:NH2	7:d:308:ASN:O	2.34	0.60
7:d:20:VAL:HG21	7:d:315:PHE:CE2	2.36	0.60
9:q:101:THR:OG1	9:q:113:ASN:O	2.12	0.60
1:e:64:PHE:CZ	10:a:903:NAG:H83	2.37	0.59
8:a:196:ASN:OD1	8:a:197:VAL:HG13	2.02	0.59
9:q:38:TRP:CE2	9:q:83:LEU:HD23	2.38	0.59
6:h:56:ILE:O	6:h:56:ILE:HG22	2.03	0.58
6:k:57:ILE:HD11	13:k:201:A1A4Q:O20	2.04	0.58
10:o:503:NAG:O7	10:o:503:NAG:O3	2.19	0.57
8:a:807:ARG:NH1	8:a:812:GLU:OE2	2.37	0.57
9:q:53:ILE:HG22	9:q:54:ASN:H	1.70	0.56
9:q:7:GLN:O	9:q:25:ALA:N	2.38	0.56
6:k:59:VAL:HG21	6:l:134:ILE:HD12	1.87	0.56
9:q:53:ILE:HD11	9:q:72:ILE:CG1	2.35	0.56
6:c:6:SER:OG	6:c:7:GLY:N	2.40	0.55
6:i:84:ILE:HG21	6:i:89:SER:OG	2.06	0.55
8:a:15:LEU:N	8:a:323:ALA:O	2.37	0.55
6:n:48:ARG:NH1	6:n:122:ALA:O	2.40	0.55
7:d:112:LEU:HD12	7:d:122:ILE:HD11	1.89	0.54
8:a:423:LEU:HA	8:a:426:ILE:HG22	1.90	0.54
8:a:408:MET:HE2	8:a:744:LEU:HD23	1.89	0.54
5:b:48:MET:O	5:b:52:LEU:HD13	2.08	0.54
5:b:59:SER:OG	6:c:101:LEU:HD23	2.07	0.54
9:q:114:VAL:HG11	9:q:117:TRP:CE2	2.43	0.54
3:o:450:LEU:HD12	3:o:450:LEU:O	2.08	0.54
6:l:11:ALA:O	6:l:89:SER:OG	2.20	0.54
10:a:901:NAG:O7	10:a:901:NAG:O1	2.25	0.54
6:l:6:SER:OG	6:l:7:GLY:N	2.40	0.53
6:m:48:ARG:NH2	6:m:122:ALA:O	2.41	0.53
3:o:303:ASN:OD1	10:o:503:NAG:N2	2.41	0.53
6:m:37:SER:O	6:m:41:ILE:HD12	2.08	0.53
6:j:76:ILE:HG22	6:j:153:SER:OG	2.09	0.53
6:n:56:ILE:HD11	13:n:201:A1A4Q:C27	2.39	0.53
8:a:131:LEU:HD21	8:a:259:MET:HB3	1.92	0.52
8:a:416:THR:HA	8:a:460:ILE:HD11	1.92	0.52
6:j:56:ILE:HG22	6:j:56:ILE:O	2.09	0.52
7:d:43:GLU:OE1	7:d:43:GLU:N	2.41	0.52
2:f:89:ASP:OD1	2:f:96:ASN:ND2	2.42	0.52
6:c:56:ILE:O	6:c:56:ILE:HG22	2.10	0.51
6:l:45:SER:OG	6:l:52:ILE:HD11	2.10	0.51
8:a:365:THR:HG21	8:a:386:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:q:93:THR:HG23	9:q:124:THR:HB	1.92	0.51
9:q:29:ARG:NH1	9:q:116:TYR:OH	2.43	0.51
1:e:73:ILE:HG23	8:a:483:VAL:HG21	1.92	0.51
8:a:575:GLN:NE2	8:a:579:GLU:OE2	2.44	0.51
6:l:57:ILE:HD11	13:l:201:A1A4Q:O20	2.11	0.51
7:d:86:ARG:O	7:d:86:ARG:NH1	2.40	0.51
8:a:89:LEU:N	8:a:92:GLU:OE1	2.38	0.50
6:c:140:VAL:HG21	8:a:804:HIS:NE2	2.27	0.50
10:o:504:NAG:O7	10:o:504:NAG:O3	2.18	0.50
7:d:40:GLU:O	7:d:41:THR:HG23	2.12	0.50
7:d:16:LEU:O	7:d:20:VAL:HG23	2.11	0.50
9:q:53:ILE:HG22	9:q:54:ASN:N	2.26	0.50
6:c:115:ASP:OD1	6:c:119:ARG:NH1	2.45	0.50
7:d:324:GLN:HG3	7:d:350:ILE:HD11	1.94	0.49
6:j:81:ASN:OD1	6:j:82:ASP:N	2.45	0.49
8:a:426:ILE:HD11	8:a:450:TYR:CE2	2.47	0.49
7:d:153:ALA:HB1	8:a:192:ILE:HD11	1.93	0.49
8:a:655:LEU:HD13	8:a:724:ALA:HA	1.95	0.49
7:d:20:VAL:HG21	7:d:315:PHE:CD2	2.48	0.48
6:g:77:ALA:O	6:h:155:LYS:NZ	2.46	0.48
5:b:200:ARG:NH2	6:n:80:LEU:O	2.47	0.48
9:q:19:SER:O	9:q:20:LEU:HD22	2.14	0.48
1:e:19:PHE:CE1	1:e:23:LEU:HD11	2.49	0.48
8:a:636:GLN:NE2	8:a:640:GLN:OE1	2.43	0.48
8:a:82:GLU:OE2	8:a:294:SER:N	2.47	0.47
6:h:15:ALA:HB1	6:h:80:LEU:HD21	1.97	0.47
3:o:450:LEU:HD12	3:o:450:LEU:C	2.39	0.47
5:b:31:LEU:HD13	12:b:302:POV:H1A	1.97	0.47
6:l:24:VAL:HG13	6:m:101:LEU:HB3	1.96	0.47
6:n:56:ILE:HD11	13:n:201:A1A4Q:C26	2.44	0.47
6:h:45:SER:OG	6:h:52:ILE:HD11	2.15	0.47
7:d:208:MET:HE3	7:d:212:LEU:CD2	2.45	0.47
7:d:122:ILE:O	7:d:126:VAL:HG23	2.16	0.46
8:a:42:MET:O	8:a:44:VAL:HG23	2.15	0.46
6:l:32:TYR:OH	6:l:36:LYS:NZ	2.39	0.46
8:a:237:LYS:O	8:a:241:GLY:N	2.45	0.46
7:d:113:ILE:HG21	7:d:178:ILE:HD12	1.98	0.46
7:d:145:GLN:C	7:d:173:LEU:HD23	2.39	0.46
5:b:82:LYS:HZ2	7:d:23:LEU:HD23	1.80	0.46
3:o:432:THR:OG1	6:c:93:LEU:HD21	2.16	0.46
6:m:99:VAL:HG23	6:m:149:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:88:PRO:HB2	8:a:302:MET:HE2	1.96	0.46
8:a:253:ALA:O	8:a:257:ARG:N	2.41	0.46
5:b:82:LYS:NZ	7:d:23:LEU:HD23	2.31	0.46
6:h:9:GLU:O	6:h:10:TYR:CG	2.69	0.46
7:d:180:ILE:O	7:d:184:THR:HG22	2.16	0.46
8:a:766:GLY:O	8:a:769:THR:HG22	2.16	0.46
8:a:397:THR:O	8:a:397:THR:HG22	2.14	0.46
8:a:831:LYS:O	8:a:835:ASP:N	2.45	0.46
3:o:450:LEU:HD11	6:g:112:ILE:CD1	2.46	0.45
8:a:259:MET:HE3	9:q:55:TRP:CD1	2.51	0.45
5:b:177:LEU:HD23	5:b:177:LEU:O	2.16	0.45
8:a:413:GLY:O	8:a:417:VAL:HG23	2.15	0.45
6:n:121:THR:HG22	6:n:121:THR:O	2.16	0.45
8:a:233:GLN:NE2	9:q:112:ASP:O	2.44	0.45
8:a:404:LEU:O	8:a:408:MET:HE3	2.17	0.45
8:a:651:VAL:HB	8:a:652:PRO:HD3	1.99	0.45
5:b:62:VAL:HG13	6:c:141:LEU:HB3	1.97	0.45
12:p:402:POV:O12	12:p:402:POV:H14A	2.17	0.45
6:k:23:MET:HE3	6:k:23:MET:O	2.16	0.45
3:o:428:MET:O	3:o:432:THR:HG22	2.17	0.45
6:g:56:ILE:O	6:g:56:ILE:CG2	2.65	0.45
8:a:122:LEU:HD11	8:a:208:LEU:HD13	1.99	0.45
4:p:334:GLY:O	4:p:337:SER:OG	2.27	0.45
6:h:146:LEU:O	6:h:150:LEU:HD13	2.17	0.44
6:n:113:VAL:HG21	6:n:134:ILE:HG22	1.98	0.44
9:q:99:VAL:HB	9:q:114:VAL:HG13	1.99	0.44
6:g:83:ASP:OD1	6:g:83:ASP:N	2.50	0.44
6:n:113:VAL:HG21	6:n:134:ILE:CG2	2.48	0.44
9:q:38:TRP:CD2	9:q:83:LEU:HD23	2.51	0.44
8:a:16:PHE:HD1	8:a:322:ILE:HG22	1.81	0.44
9:q:62:TYR:OH	9:q:72:ILE:HG22	2.17	0.44
6:c:56:ILE:O	6:c:56:ILE:CG2	2.65	0.44
6:j:45:SER:CB	6:k:127:LEU:HD12	2.47	0.44
6:n:109:ALA:O	6:n:113:VAL:HG12	2.18	0.43
9:q:6:LEU:O	9:q:119:GLN:NE2	2.50	0.43
2:f:80:ILE:O	2:f:83:VAL:HG22	2.19	0.43
8:a:226:TYR:OH	8:a:232:ARG:NE	2.52	0.43
2:f:84:PRO:O	8:a:770:ARG:NH2	2.52	0.43
6:h:56:ILE:O	6:h:56:ILE:CG2	2.67	0.43
6:l:121:THR:O	6:l:121:THR:HG22	2.18	0.43
6:c:148:VAL:O	6:c:152:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:12:ASP:OD1	7:d:12:ASP:N	2.50	0.43
2:f:74:VAL:HG12	2:f:75:HIS:N	2.34	0.42
6:j:57:ILE:HG22	6:j:58:PRO:HD3	2.01	0.42
12:p:402:POV:H316	6:h:101:LEU:HD11	2.00	0.42
1:e:37:ILE:O	1:e:37:ILE:HG22	2.20	0.42
6:c:10:TYR:O	6:c:10:TYR:CD1	2.73	0.42
6:g:84:ILE:HG22	6:g:85:SER:H	1.85	0.42
9:q:22:LEU:HD23	9:q:85:MET:HE1	2.02	0.42
7:d:37:VAL:O	7:d:341:ARG:NH2	2.53	0.42
6:g:80:LEU:HD23	6:g:84:ILE:HD11	2.02	0.42
8:a:7:SER:O	8:a:389:ARG:NH1	2.45	0.42
2:f:58:SER:O	2:f:62:VAL:HG22	2.20	0.42
6:k:37:SER:HB3	6:k:58:PRO:HB2	2.01	0.42
6:n:127:LEU:HD23	6:n:127:LEU:O	2.20	0.42
8:a:394:ALA:N	8:a:395:PRO:HD2	2.34	0.42
6:l:9:GLU:O	6:l:10:TYR:CG	2.73	0.42
8:a:470:PHE:O	8:a:471:SER:HB3	2.20	0.42
8:a:93:MET:CB	8:a:302:MET:HE1	2.49	0.42
8:a:259:MET:HE2	8:a:259:MET:HA	2.01	0.42
7:d:204:THR:O	7:d:204:THR:HG22	2.20	0.41
8:a:657:ILE:O	8:a:661:ILE:HD12	2.20	0.41
9:q:87:SER:O	9:q:88:LEU:C	2.64	0.41
6:n:136:ILE:O	6:n:140:VAL:HG23	2.21	0.41
7:d:206:ASP:OD1	7:d:207:ALA:N	2.53	0.41
8:a:297:ILE:HG23	8:a:834:LEU:HD13	2.02	0.41
8:a:740:SER:O	8:a:743:ARG:NH1	2.54	0.41
1:e:36:VAL:HG12	1:e:36:VAL:O	2.21	0.41
8:a:632:LEU:N	8:a:636:GLN:OE1	2.47	0.41
6:m:118:VAL:HA	6:m:121:THR:HG22	2.01	0.41
3:o:334:VAL:HG12	3:o:334:VAL:O	2.20	0.41
3:o:461:GLY:N	3:o:462:PRO:CD	2.84	0.41
8:a:583:ILE:HG23	8:a:584:LEU:N	2.35	0.41
6:n:140:VAL:O	6:n:140:VAL:HG12	2.20	0.41
7:d:181:ILE:HA	7:d:184:THR:HG22	2.02	0.41
8:a:278:GLU:O	8:a:281:ARG:HG2	2.20	0.41
8:a:391:ILE:O	8:a:391:ILE:HG23	2.21	0.41
3:o:296:ASN:OD1	3:o:296:ASN:N	2.44	0.40
6:m:34:THR:HG23	6:m:59:VAL:HG13	2.03	0.40
6:c:151:ILE:HG22	8:a:537:ASN:ND2	2.35	0.40
8:a:465:ILE:H	8:a:465:ILE:HD12	1.87	0.40
8:a:571:ASN:O	8:a:575:GLN:N	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:605:VAL:HG12	8:a:605:VAL:O	2.21	0.40
4:p:320:ALA:O	4:p:324:THR:HG22	2.21	0.40
3:o:407:VAL:O	3:o:407:VAL:HG13	2.22	0.40
8:a:16:PHE:CD1	8:a:322:ILE:HG22	2.55	0.40
6:c:57:ILE:N	6:c:58:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	73/81 (90%)	69 (94%)	4 (6%)	0	100	100
2	f	82/137 (60%)	79 (96%)	3 (4%)	0	100	100
3	o	207/470 (44%)	193 (93%)	14 (7%)	0	100	100
4	p	50/350 (14%)	47 (94%)	3 (6%)	0	100	100
5	b	202/205 (98%)	198 (98%)	4 (2%)	0	100	100
6	c	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
6	g	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
6	h	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
6	i	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
6	j	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
6	k	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
6	l	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
6	m	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
6	n	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
7	d	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
8	a	753/863 (87%)	725 (96%)	28 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	q	123/139 (88%)	112 (91%)	11 (9%)	0	100	100
All	All	3171/3991 (80%)	3065 (97%)	106 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	68/72 (94%)	68 (100%)	0	100	100
2	f	70/116 (60%)	70 (100%)	0	100	100
3	o	186/397 (47%)	186 (100%)	0	100	100
4	p	47/308 (15%)	47 (100%)	0	100	100
5	b	154/155 (99%)	154 (100%)	0	100	100
6	c	107/112 (96%)	107 (100%)	0	100	100
6	g	107/112 (96%)	107 (100%)	0	100	100
6	h	107/112 (96%)	107 (100%)	0	100	100
6	i	107/112 (96%)	107 (100%)	0	100	100
6	j	107/112 (96%)	107 (100%)	0	100	100
6	k	107/112 (96%)	107 (100%)	0	100	100
6	l	107/112 (96%)	107 (100%)	0	100	100
6	m	107/112 (96%)	107 (100%)	0	100	100
6	n	107/112 (96%)	107 (100%)	0	100	100
7	d	306/306 (100%)	306 (100%)	0	100	100
8	a	680/767 (89%)	680 (100%)	0	100	100
9	q	103/112 (92%)	103 (100%)	0	100	100
All	All	2577/3241 (80%)	2577 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	f	75	HIS
3	o	255	HIS
5	b	197	GLN
7	d	165	GLN
7	d	308	ASN
7	d	324	GLN
8	a	571	ASN
8	a	575	GLN
8	a	723	GLN
8	a	832	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

22 ligands are modelled in this entry.

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	$\# Z  > 2$
13	A1A4Q	c	201	-	31,36,36	1.29	3 (9%)	30,60,60	0.98	2 (6%)
13	A1A4Q	g	201	-	31,36,36	1.31	3 (9%)	30,60,60	0.95	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	a	904	-	15,15,15	0.61	0	21,21,21	0.76	0
13	A1A4Q	k	201	-	31,36,36	1.37	3 (9%)	30,60,60	0.96	2 (6%)
13	A1A4Q	i	201	-	31,36,36	1.33	3 (9%)	30,60,60	0.95	1 (3%)
10	NAG	o	504	3	14,14,15	0.67	0	17,19,21	1.28	1 (5%)
10	NAG	o	505	3	14,14,15	0.73	0	17,19,21	0.81	0
10	NAG	a	901	-	15,15,15	0.60	0	21,21,21	0.77	0
14	WJP	a	902	-	34,34,34	3.23	6 (17%)	39,44,44	2.76	14 (35%)
10	NAG	o	502	3	14,14,15	0.74	0	17,19,21	1.06	1 (5%)
10	NAG	o	501	-	15,15,15	0.55	0	21,21,21	0.83	0
13	A1A4Q	l	201	-	31,36,36	1.38	3 (9%)	30,60,60	0.94	1 (3%)
12	POV	b	302	-	51,51,51	0.52	0	57,59,59	0.48	0
11	CLR	p	401	-	31,31,31	0.39	0	48,48,48	0.48	0
13	A1A4Q	n	201	-	31,36,36	1.34	3 (9%)	30,60,60	0.95	2 (6%)
13	A1A4Q	j	201	-	31,36,36	1.33	3 (9%)	30,60,60	0.94	2 (6%)
13	A1A4Q	m	201	-	31,36,36	1.31	3 (9%)	30,60,60	0.95	1 (3%)
12	POV	b	301	-	51,51,51	0.51	0	57,59,59	0.47	0
12	POV	p	402	-	51,51,51	0.50	0	57,59,59	0.48	0
10	NAG	a	903	-	15,15,15	0.60	0	21,21,21	0.87	0
13	A1A4Q	h	201	-	31,36,36	1.35	3 (9%)	30,60,60	1.02	3 (10%)
10	NAG	o	503	3	14,14,15	0.76	0	17,19,21	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	A1A4Q	c	201	-	-	0/0/47/47	0/6/6/6
13	A1A4Q	g	201	-	-	0/0/47/47	0/6/6/6
10	NAG	a	904	-	-	0/6/26/26	0/1/1/1
13	A1A4Q	k	201	-	-	0/0/47/47	0/6/6/6
13	A1A4Q	i	201	-	-	0/0/47/47	0/6/6/6
10	NAG	o	504	3	-	1/6/23/26	0/1/1/1
10	NAG	o	505	3	-	1/6/23/26	0/1/1/1
10	NAG	a	901	-	-	2/6/26/26	0/1/1/1
14	WJP	a	902	-	-	19/40/40/40	-
10	NAG	o	502	3	-	1/6/23/26	0/1/1/1
10	NAG	o	501	-	-	2/6/26/26	0/1/1/1
13	A1A4Q	l	201	-	-	0/0/47/47	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	POV	b	302	-	-	18/55/55/55	-
11	CLR	p	401	-	-	3/10/68/68	0/4/4/4
13	A1A4Q	n	201	-	-	0/0/47/47	0/6/6/6
13	A1A4Q	j	201	-	-	0/0/47/47	0/6/6/6
13	A1A4Q	m	201	-	-	0/0/47/47	0/6/6/6
12	POV	b	301	-	-	17/55/55/55	-
12	POV	p	402	-	-	16/55/55/55	-
10	NAG	a	903	-	-	0/6/26/26	0/1/1/1
13	A1A4Q	h	201	-	-	0/0/47/47	0/6/6/6
10	NAG	o	503	3	-	3/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	902	WJP	C15-C16	8.73	1.53	1.33
14	a	902	WJP	C10-C11	8.68	1.53	1.33
14	a	902	WJP	C05-C06	8.64	1.52	1.33
14	a	902	WJP	C20-C21	6.93	1.53	1.32
14	a	902	WJP	P31-O30	5.12	1.65	1.59
14	a	902	WJP	P27-O30	4.92	1.64	1.59
13	l	201	A1A4Q	C5-C6	-4.46	1.45	1.53
13	k	201	A1A4Q	C5-C6	-4.41	1.45	1.53
13	n	201	A1A4Q	C5-C6	-4.17	1.46	1.53
13	h	201	A1A4Q	C5-C6	-4.12	1.46	1.53
13	j	201	A1A4Q	C5-C6	-4.04	1.46	1.53
13	i	201	A1A4Q	C5-C6	-3.96	1.46	1.53
13	m	201	A1A4Q	C5-C6	-3.71	1.47	1.53
13	g	201	A1A4Q	C5-C6	-3.60	1.47	1.53
13	c	201	A1A4Q	C6-C25	3.55	1.46	1.40
13	m	201	A1A4Q	C6-C25	3.54	1.46	1.40
13	g	201	A1A4Q	C6-C25	3.51	1.46	1.40
13	i	201	A1A4Q	C6-C25	3.50	1.46	1.40
13	c	201	A1A4Q	C5-C6	-3.48	1.47	1.53
13	h	201	A1A4Q	C6-C25	3.46	1.45	1.40
13	n	201	A1A4Q	C6-C25	3.39	1.45	1.40
13	j	201	A1A4Q	C6-C25	3.37	1.45	1.40
13	l	201	A1A4Q	C9-C10	3.36	1.44	1.40
13	i	201	A1A4Q	C9-C10	3.33	1.44	1.40
13	k	201	A1A4Q	C9-C10	3.30	1.44	1.40
13	g	201	A1A4Q	C9-C10	3.30	1.44	1.40
13	k	201	A1A4Q	C6-C25	3.28	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	h	201	A1A4Q	C9-C10	3.26	1.44	1.40
13	l	201	A1A4Q	C6-C25	3.26	1.45	1.40
13	n	201	A1A4Q	C9-C10	3.25	1.44	1.40
13	m	201	A1A4Q	C9-C10	3.25	1.44	1.40
13	j	201	A1A4Q	C9-C10	3.20	1.44	1.40
13	c	201	A1A4Q	C9-C10	3.10	1.44	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	902	WJP	C14-C15-C16	-6.55	112.62	127.62
14	a	902	WJP	C09-C10-C11	-6.41	112.96	127.62
14	a	902	WJP	C04-C05-C06	-6.25	113.31	127.62
14	a	902	WJP	C12-C11-C10	-4.58	111.88	123.63
14	a	902	WJP	C19-C20-C21	-4.39	113.01	127.64
14	a	902	WJP	C13-C11-C10	-4.28	111.56	121.17
14	a	902	WJP	C17-C16-C15	-4.20	112.85	123.63
14	a	902	WJP	C08-C06-C05	-4.11	111.95	121.17
14	a	902	WJP	C07-C06-C05	-4.07	113.18	123.63
14	a	902	WJP	C18-C16-C15	-3.62	113.05	121.17
10	o	504	NAG	C2-N2-C7	3.54	127.64	122.90
14	a	902	WJP	C23-C21-C20	-3.26	112.88	122.66
10	o	502	NAG	C1-O5-C5	3.20	116.47	112.19
14	a	902	WJP	C22-C21-C20	-3.17	113.13	122.66
14	a	902	WJP	O29-P27-O28	-2.50	100.83	112.44
13	m	201	A1A4Q	C7-N23-C24	2.48	108.99	103.90
13	n	201	A1A4Q	C7-N23-C24	2.48	108.99	103.90
13	c	201	A1A4Q	C7-N23-C24	2.48	108.99	103.90
13	g	201	A1A4Q	C7-N23-C24	2.47	108.98	103.90
13	i	201	A1A4Q	C7-N23-C24	2.47	108.98	103.90
13	h	201	A1A4Q	C7-N23-C24	2.47	108.97	103.90
13	j	201	A1A4Q	C7-N23-C24	2.46	108.96	103.90
13	k	201	A1A4Q	C7-N23-C24	2.43	108.90	103.90
13	l	201	A1A4Q	C7-N23-C24	2.43	108.88	103.90
13	h	201	A1A4Q	O20-C17-C5	-2.42	109.92	114.90
14	a	902	WJP	O34-P31-O33	-2.33	101.62	112.44
13	c	201	A1A4Q	O20-C17-C5	-2.20	110.36	114.90
13	n	201	A1A4Q	O20-C17-C5	-2.11	110.56	114.90
13	j	201	A1A4Q	O20-C17-C5	-2.09	110.60	114.90
13	h	201	A1A4Q	O31-C5-C6	-2.05	107.97	111.37
13	k	201	A1A4Q	O31-C5-C6	-2.03	108.00	111.37

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	o	504	NAG	C3-C2-N2-C7
12	p	402	POV	C1-O11-P-O12
12	p	402	POV	C1-O11-P-O14
12	p	402	POV	C11-O12-P-O11
12	p	402	POV	C11-O12-P-O14
12	p	402	POV	C22-C21-O21-C2
12	b	301	POV	C1-O11-P-O12
12	b	301	POV	C1-O11-P-O13
12	b	301	POV	C1-O11-P-O14
12	b	302	POV	C1-O11-P-O12
12	b	302	POV	C1-O11-P-O13
12	b	302	POV	C11-O12-P-O13
14	a	902	WJP	C09-C10-C11-C13
14	a	902	WJP	C14-C15-C16-C17
14	a	902	WJP	C02-C24-C25-O26
14	a	902	WJP	C19-C20-C21-C23
12	b	301	POV	O32-C31-O31-C3
12	p	402	POV	O22-C21-O21-C2
12	b	301	POV	C32-C31-O31-C3
14	a	902	WJP	C04-C05-C06-C07
14	a	902	WJP	C14-C15-C16-C18
14	a	902	WJP	C10-C11-C13-C14
14	a	902	WJP	C16-C18-C19-C20
11	p	401	CLR	C17-C20-C22-C23
11	p	401	CLR	C21-C20-C22-C23
12	b	302	POV	C22-C21-O21-C2
10	o	501	NAG	C8-C7-N2-C2
10	o	501	NAG	O7-C7-N2-C2
14	a	902	WJP	C06-C08-C09-C10
12	b	302	POV	O22-C21-O21-C2
10	a	901	NAG	C3-C2-N2-C7
12	p	402	POV	C25-C26-C27-C28
12	p	402	POV	C214-C215-C216-C217
12	b	301	POV	C32-C33-C34-C35
11	p	401	CLR	C22-C23-C24-C25
12	b	302	POV	C32-C31-O31-C3
12	p	402	POV	C212-C213-C214-C215
12	b	301	POV	C23-C24-C25-C26
12	b	302	POV	O32-C31-O31-C3
12	b	302	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
10	o	502	NAG	O5-C5-C6-O6
10	o	505	NAG	O5-C5-C6-O6
12	b	301	POV	C1-C2-C3-O31
10	o	503	NAG	O5-C5-C6-O6
12	b	302	POV	C33-C34-C35-C36
14	a	902	WJP	C09-C10-C11-C12
14	a	902	WJP	C07-C06-C08-C09
14	a	902	WJP	C17-C16-C18-C19
12	b	302	POV	C211-C212-C213-C214
12	p	402	POV	C21-C22-C23-C24
14	a	902	WJP	P31-O30-P27-O26
12	p	402	POV	C312-C313-C314-C315
12	b	302	POV	C35-C36-C37-C38
14	a	902	WJP	C26-O32-P31-O33
12	p	402	POV	C36-C37-C38-C39
12	b	301	POV	C22-C23-C24-C25
12	b	302	POV	C22-C23-C24-C25
12	b	301	POV	C25-C26-C27-C28
12	b	301	POV	O21-C2-C3-O31
10	o	503	NAG	C3-C2-N2-C7
12	b	301	POV	C11-O12-P-O13
10	a	901	NAG	C1-C2-N2-C7
14	a	902	WJP	C13-C14-C15-C16
12	p	402	POV	C27-C28-C29-C210
12	p	402	POV	C29-C210-C211-C212
12	p	402	POV	C24-C25-C26-C27
12	b	301	POV	C212-C213-C214-C215
12	b	301	POV	C311-C310-C39-C38
10	o	503	NAG	C1-C2-N2-C7
12	b	302	POV	C29-C210-C211-C212
12	b	302	POV	C31-C32-C33-C34
14	a	902	WJP	C19-C20-C21-C22
14	a	902	WJP	P31-O30-P27-O29
14	a	902	WJP	P27-O30-P31-O34
12	b	301	POV	C35-C36-C37-C38
12	p	402	POV	O31-C31-C32-C33
12	b	301	POV	C39-C310-C311-C312
12	b	301	POV	C24-C25-C26-C27
12	b	302	POV	O21-C21-C22-C23
12	b	302	POV	O31-C31-C32-C33
14	a	902	WJP	P31-O30-P27-O28
12	b	302	POV	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
12	b	302	POV	O32-C31-C32-C33

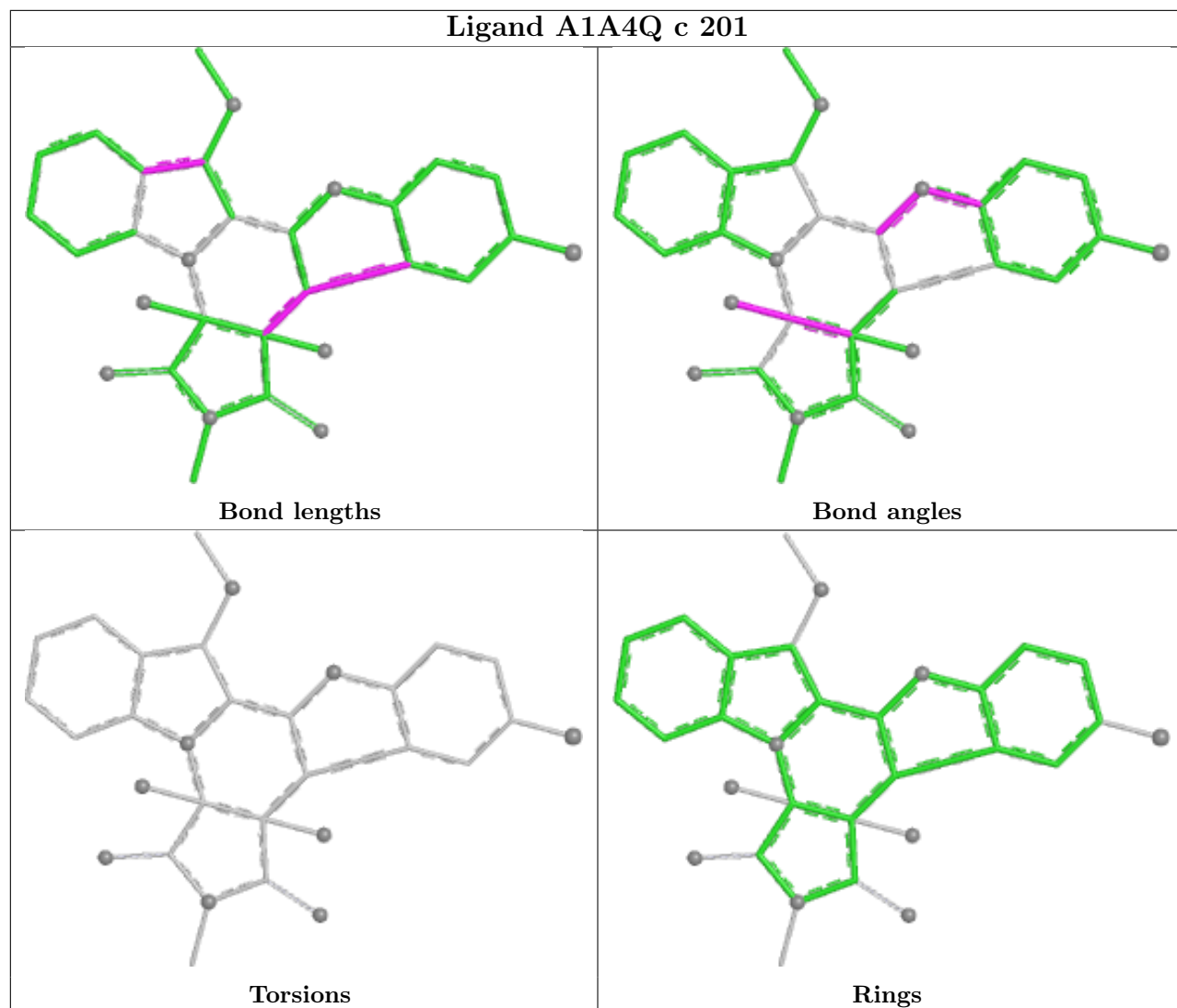
There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	k	201	A1A4Q	1	0
10	o	504	NAG	1	0
10	a	901	NAG	1	0
13	l	201	A1A4Q	1	0
12	b	302	POV	1	0
13	n	201	A1A4Q	2	0
12	p	402	POV	2	0
10	a	903	NAG	3	0
10	o	503	NAG	2	0

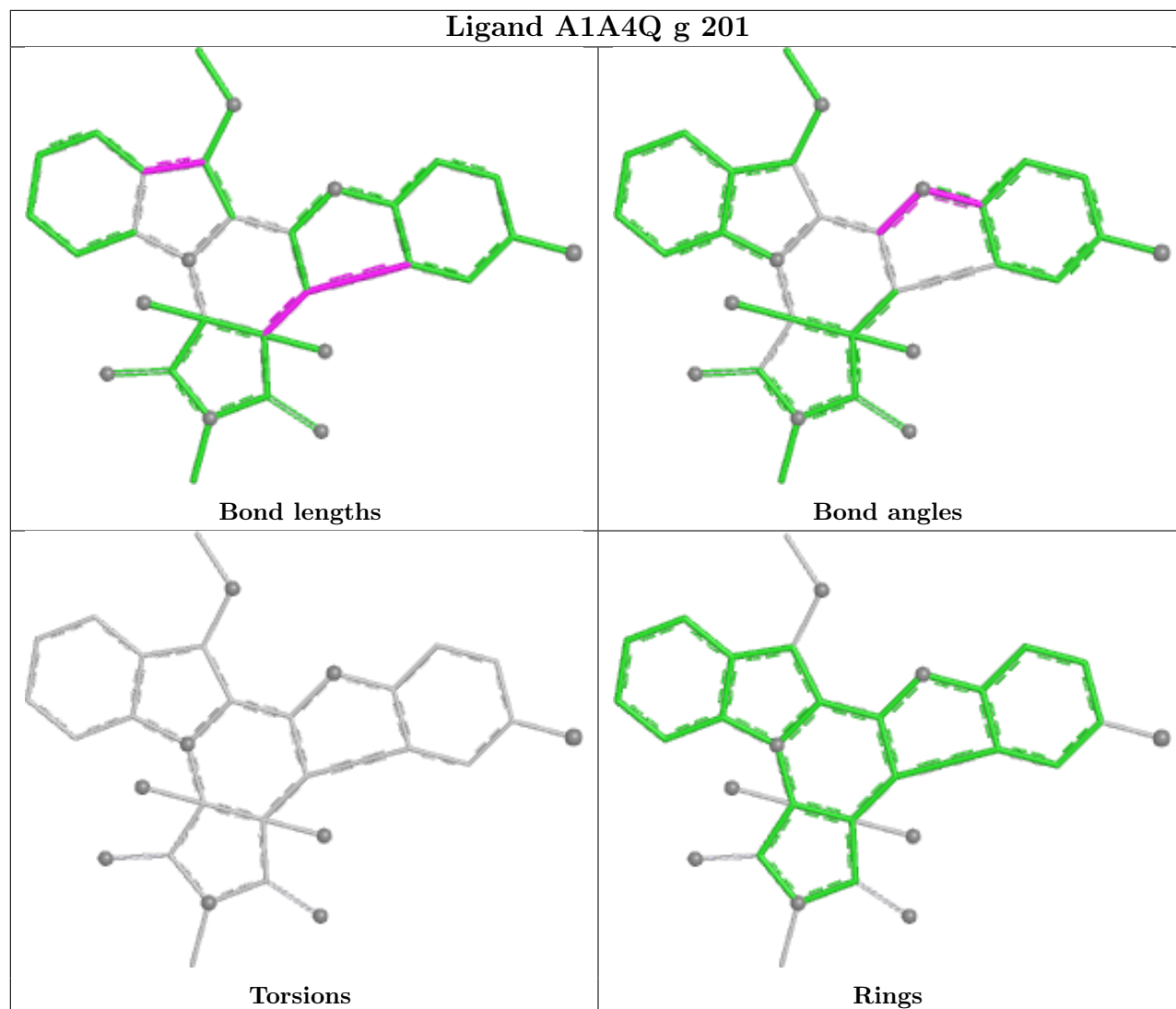
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand A1A4Q c 201

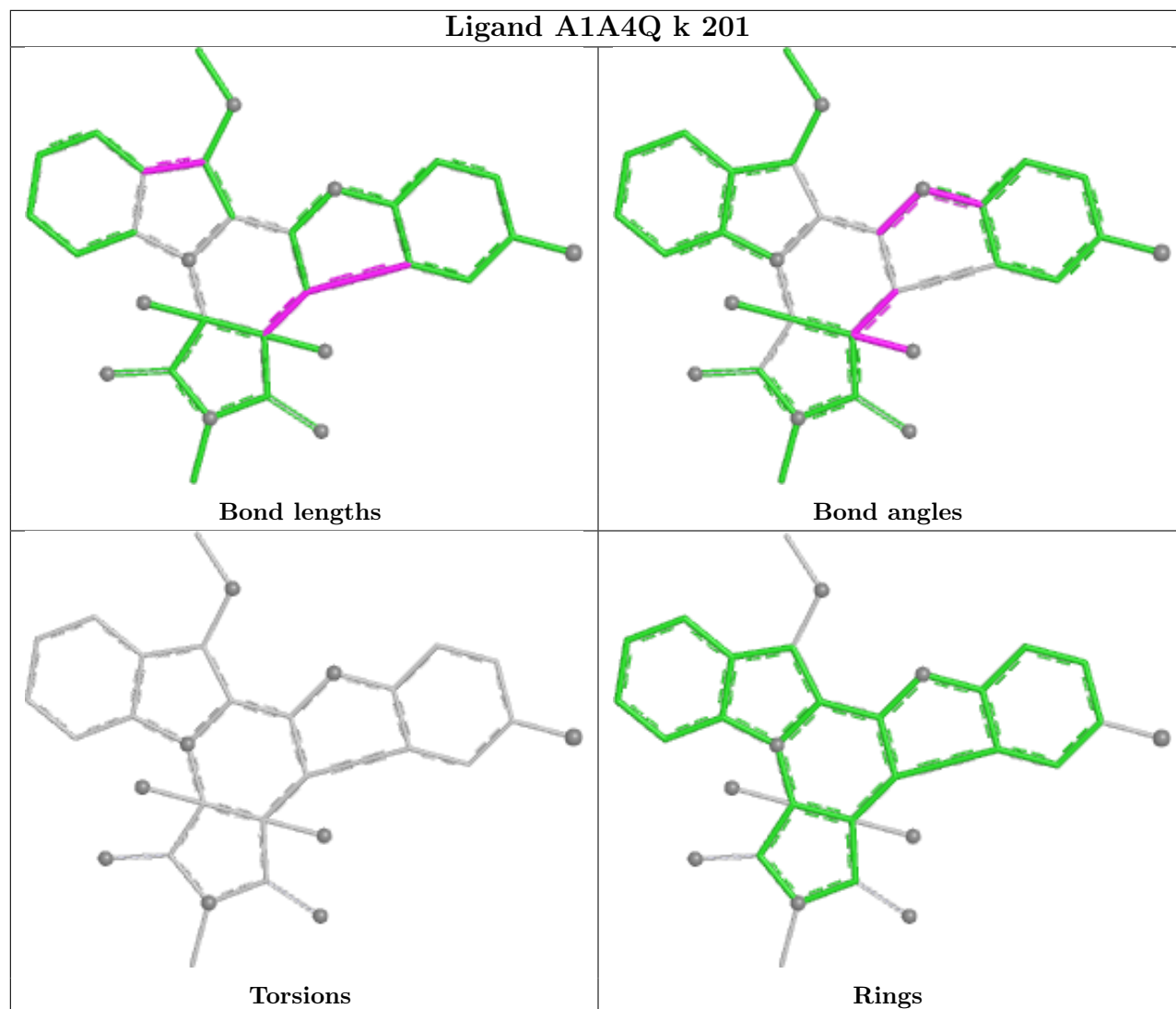




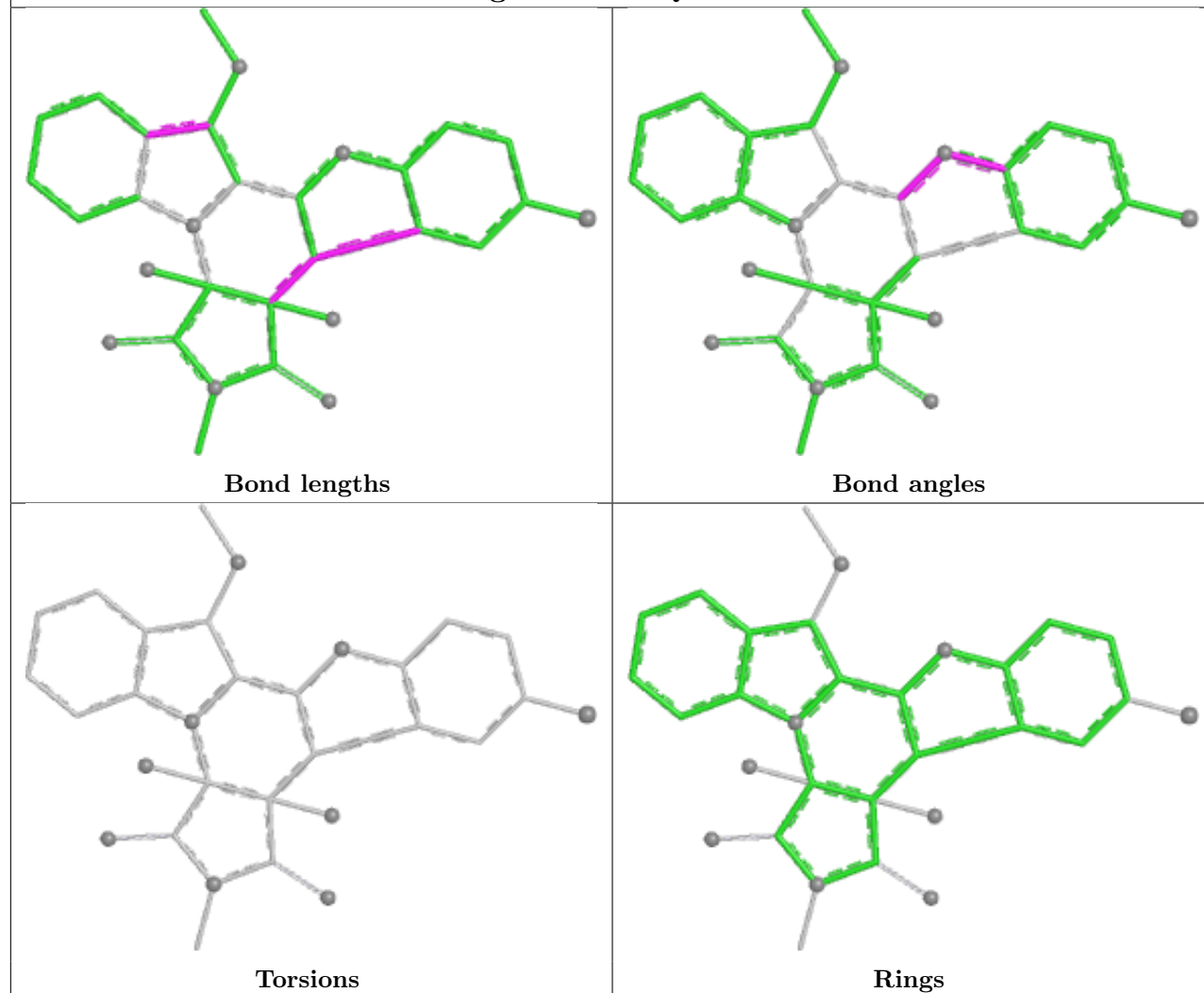
## Ligand A1A4Q g 201



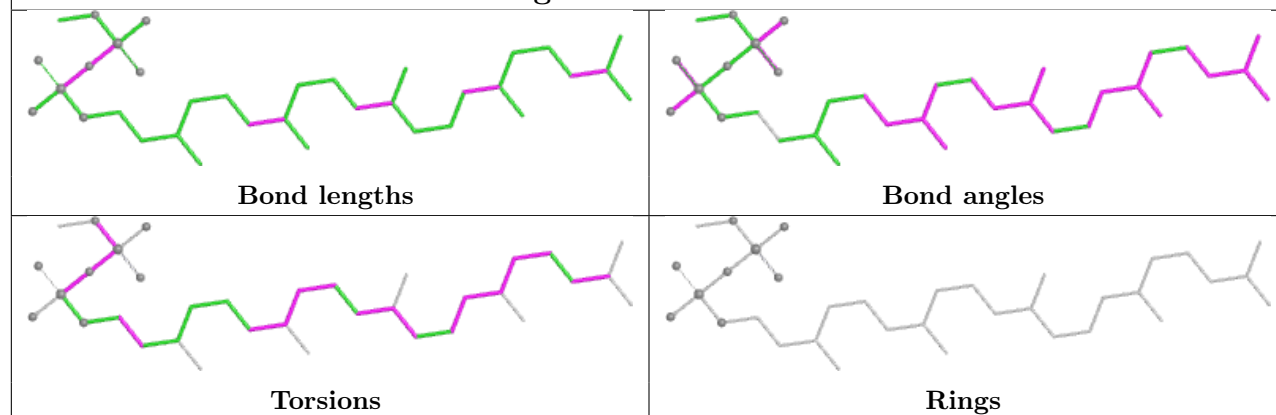
## Ligand A1A4Q k 201



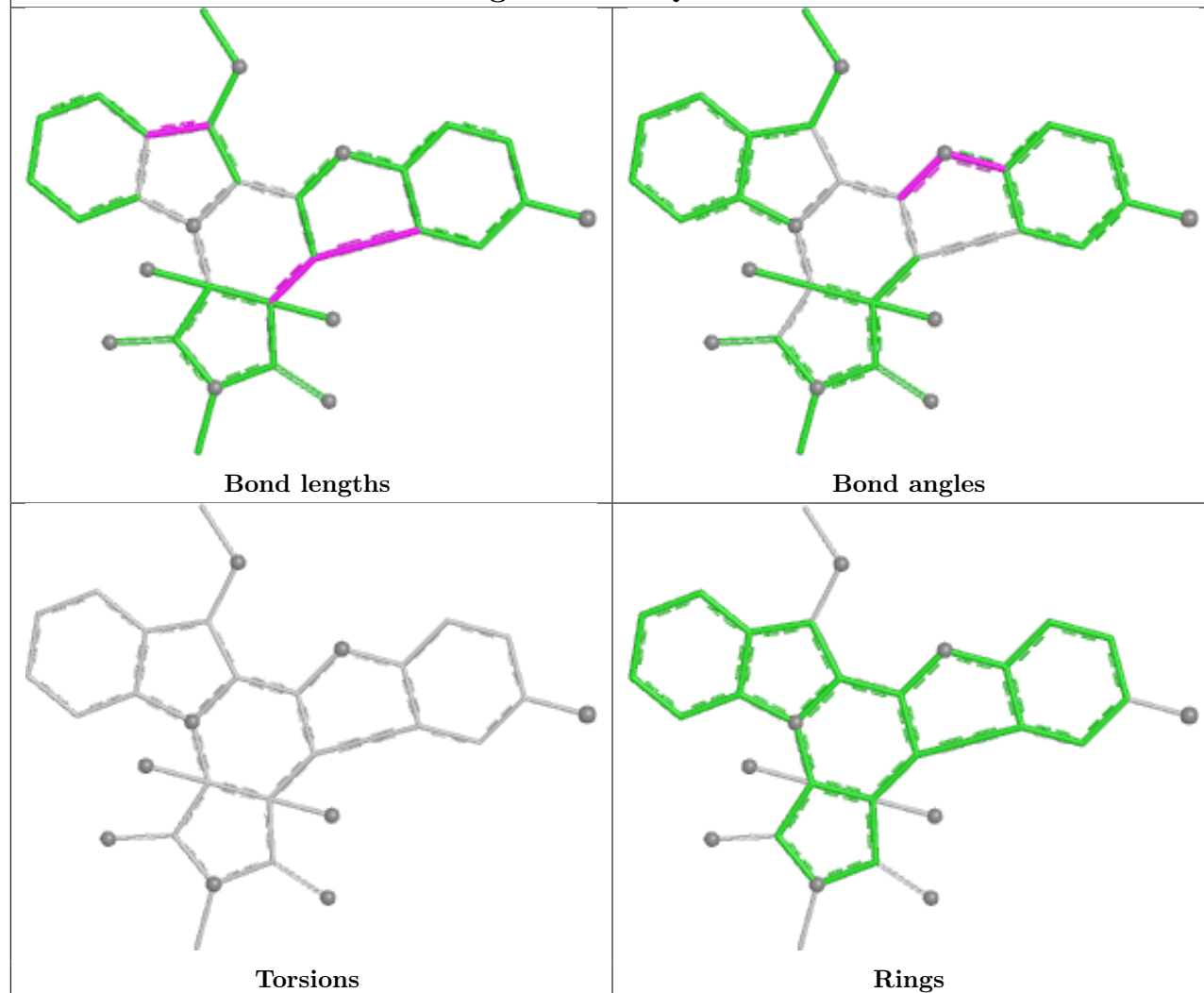
## Ligand A1A4Q i 201



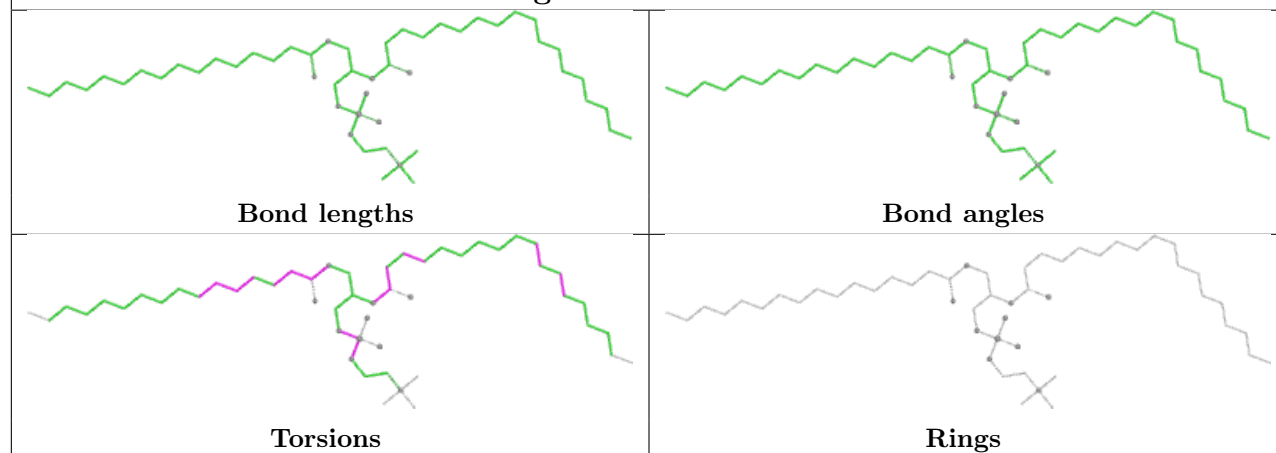
## Ligand WJP a 902

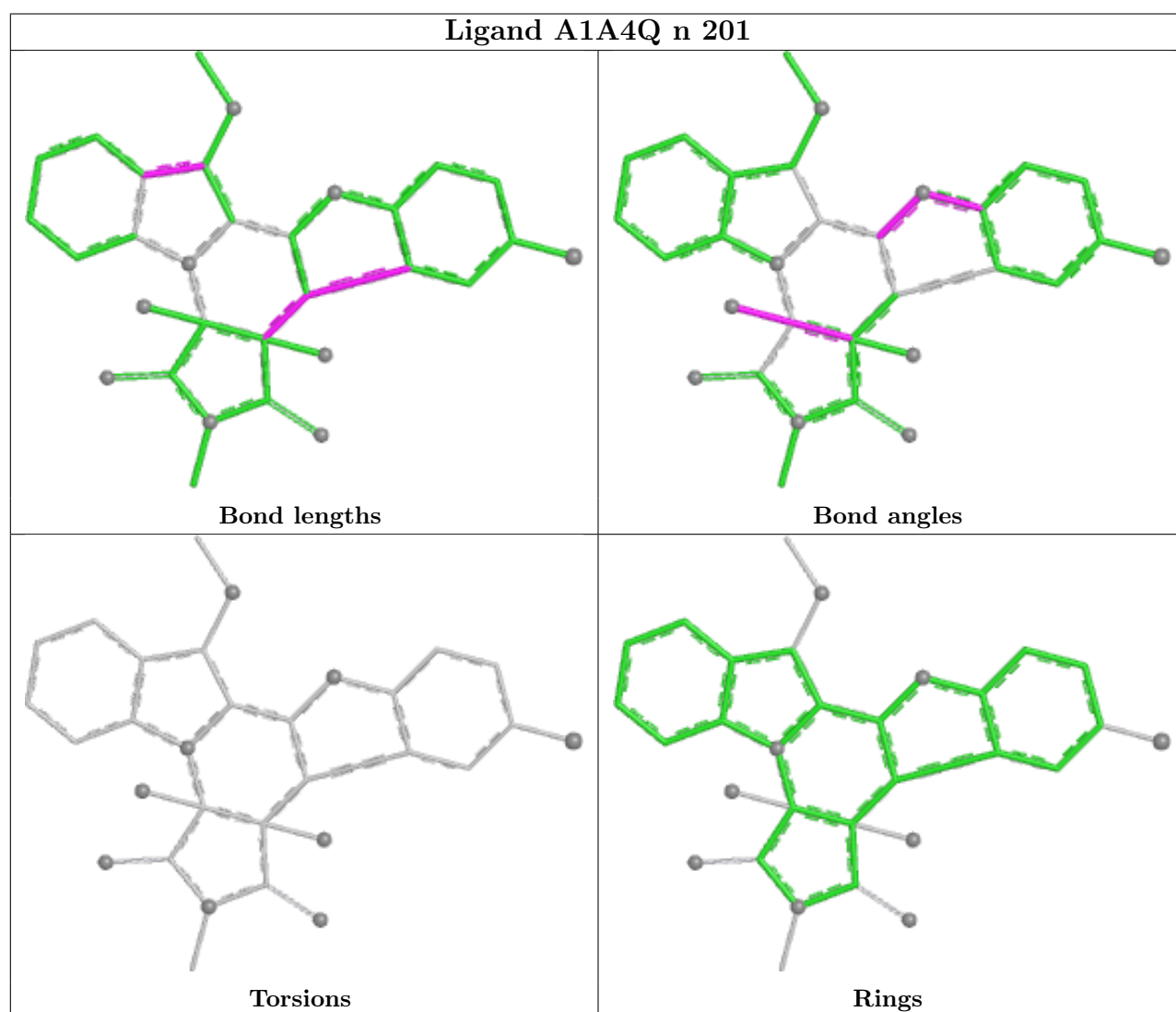
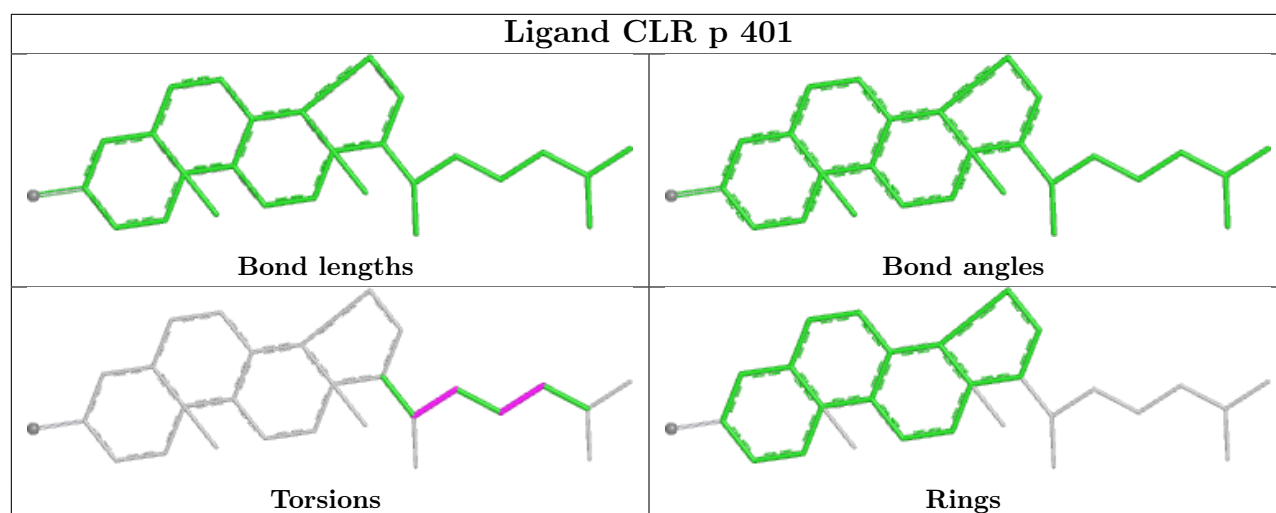


## Ligand A1A4Q 1 201

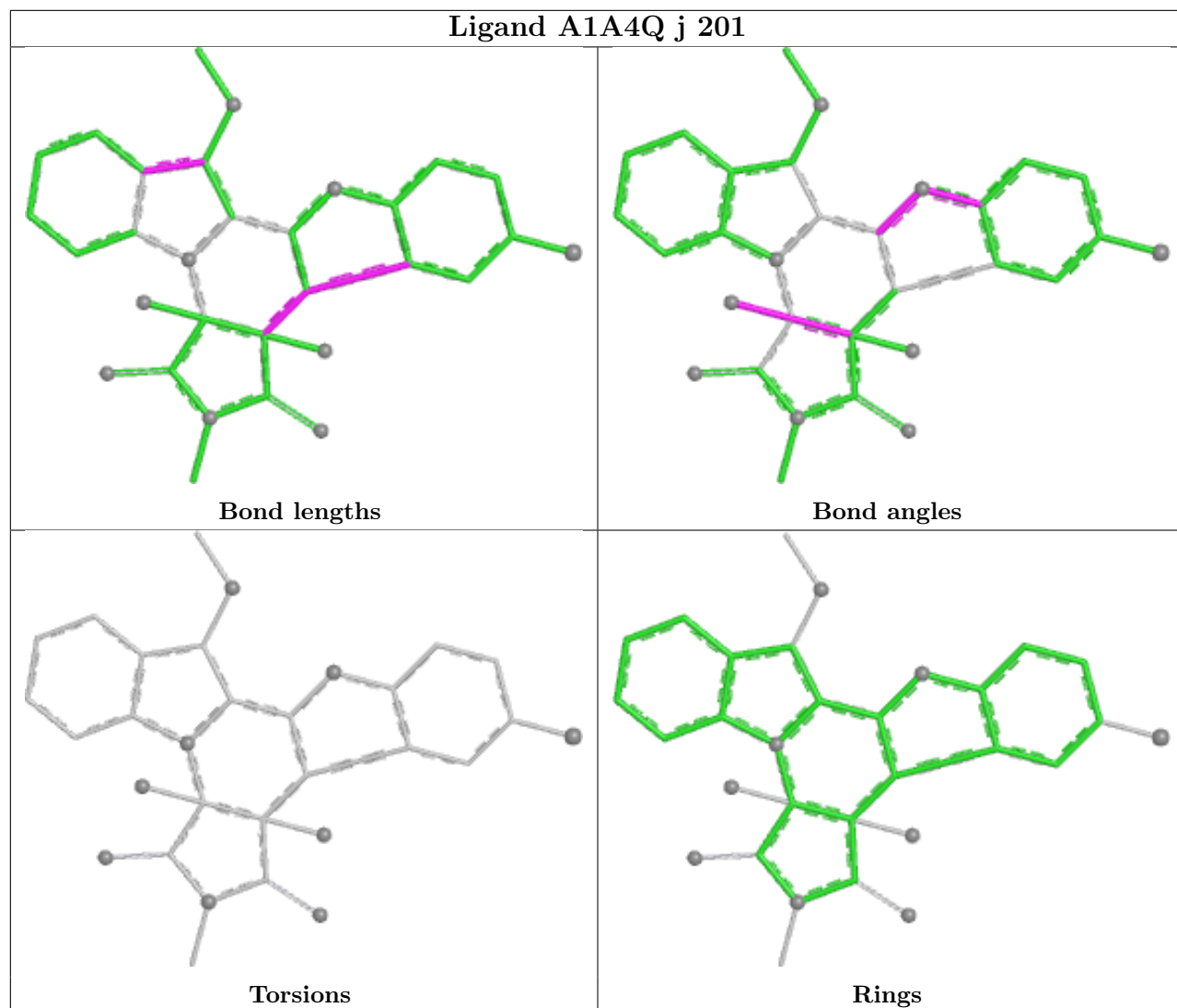


## Ligand POV b 302

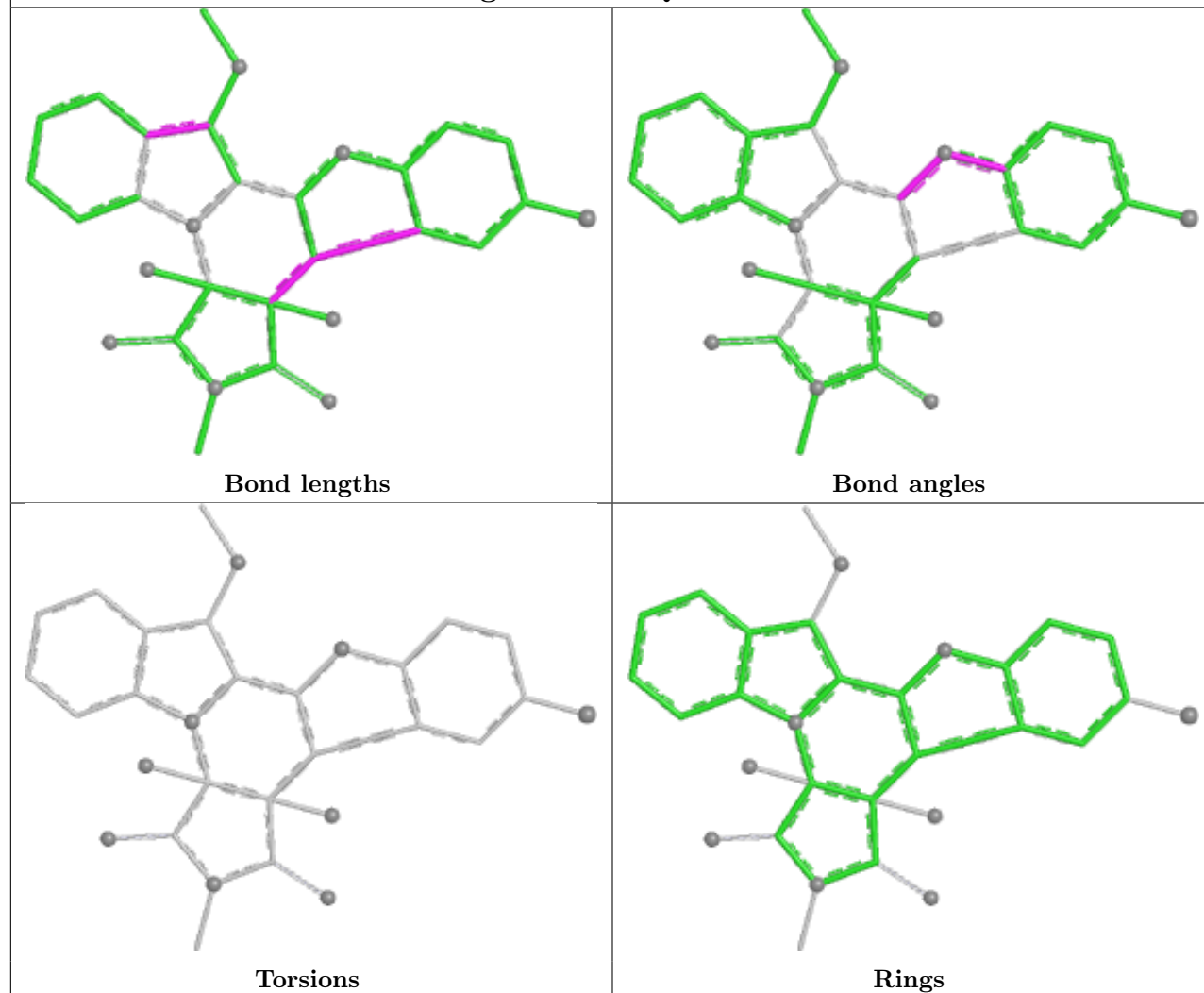




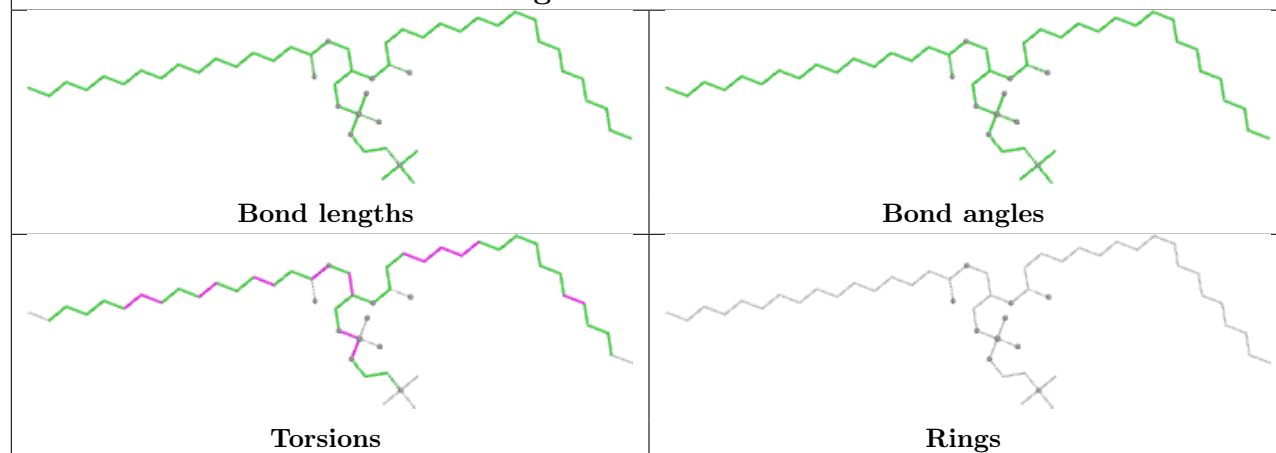
## Ligand A1A4Q j 201

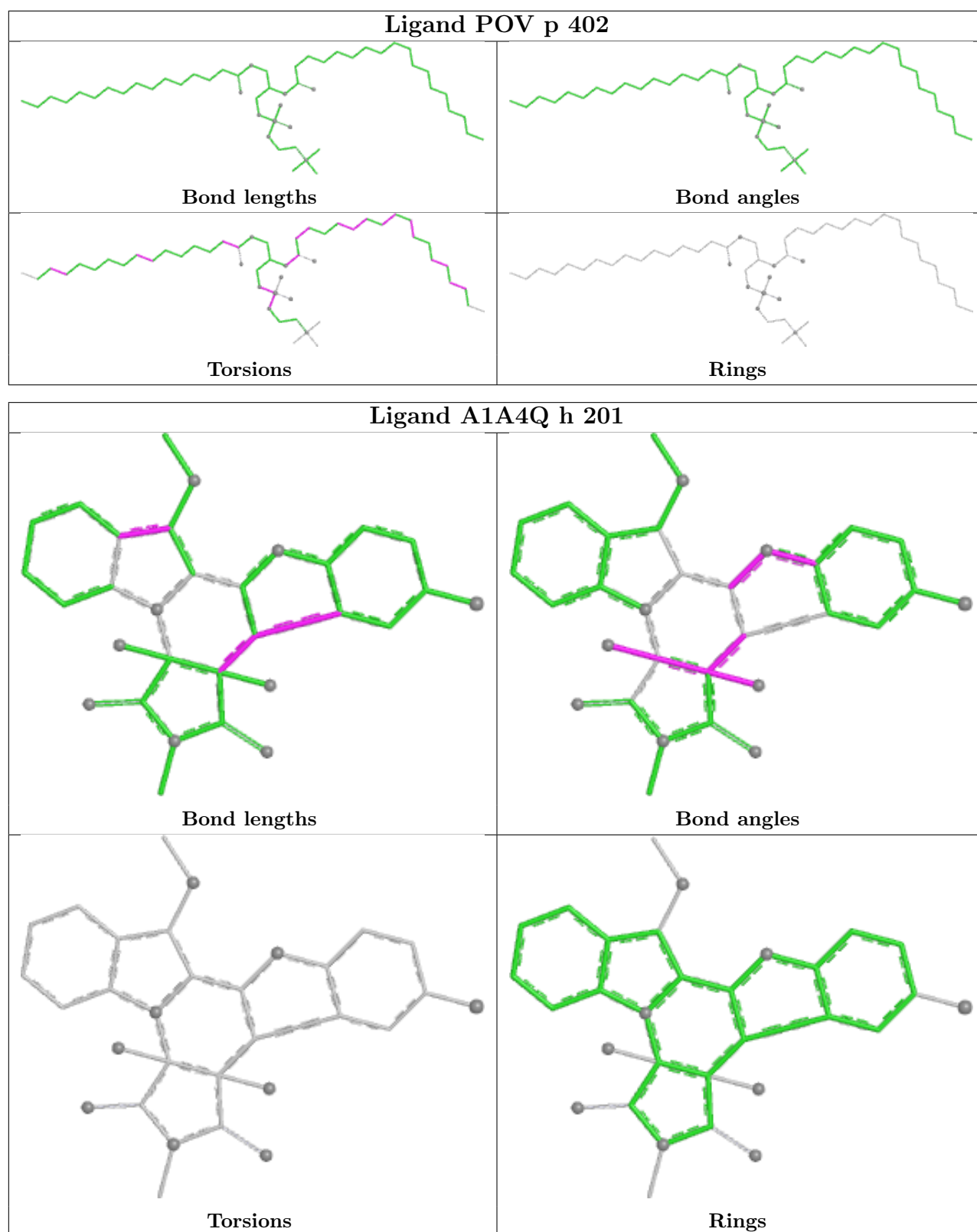


## Ligand A1A4Q m 201



## Ligand POV b 301





## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

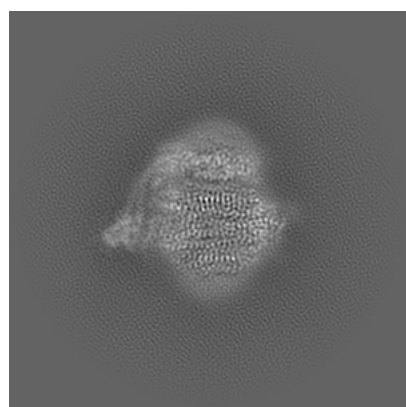
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46798. These allow visual inspection of the internal detail of the map and identification of artifacts.

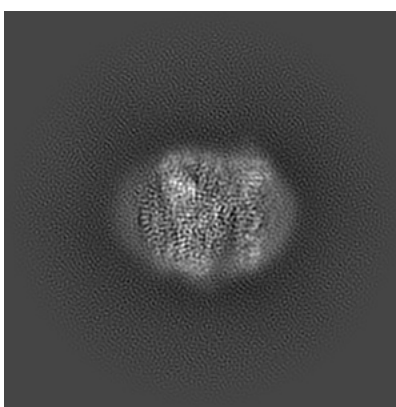
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

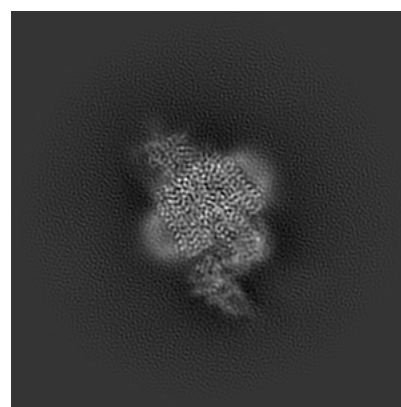
#### 6.1.1 Primary map



X



Y

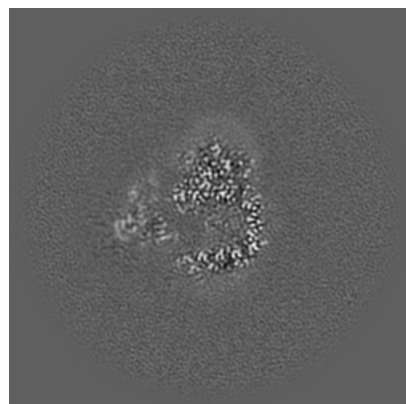


Z

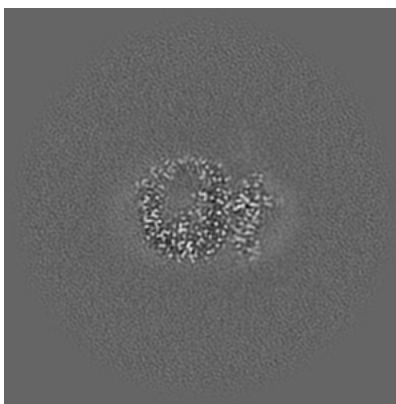
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

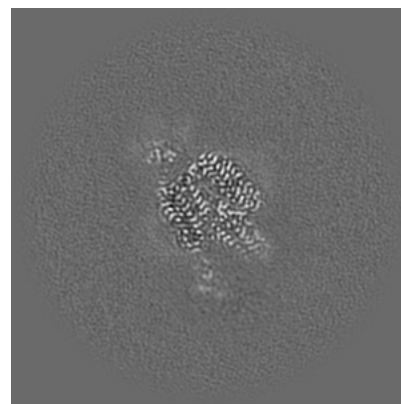
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

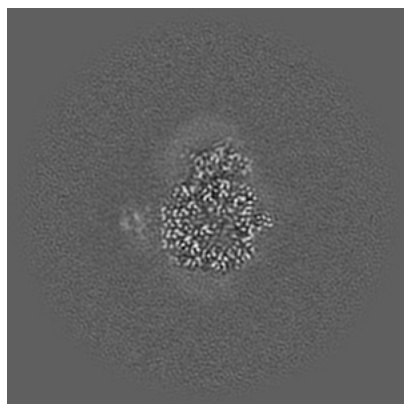


Z Index: 150

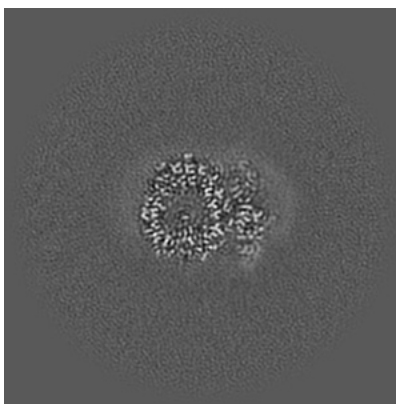
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

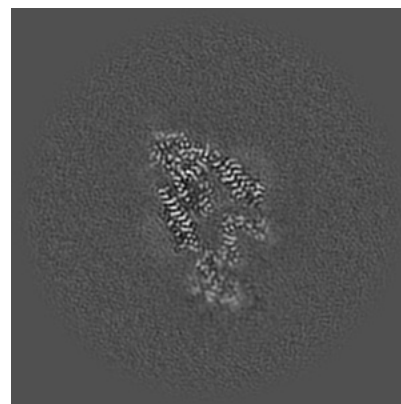
### 6.3.1 Primary map



X Index: 137



Y Index: 164

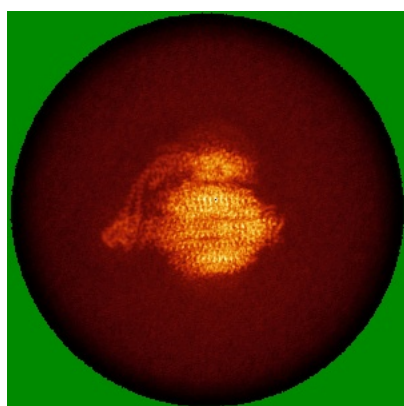


Z Index: 138

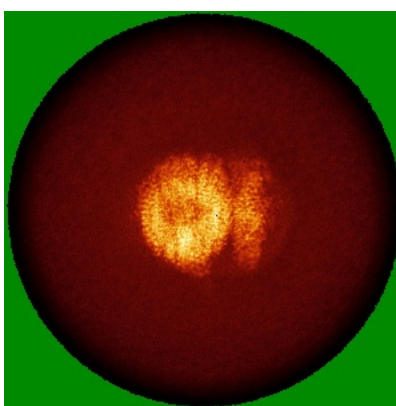
The images above show the largest variance slices of the map in three orthogonal directions.

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

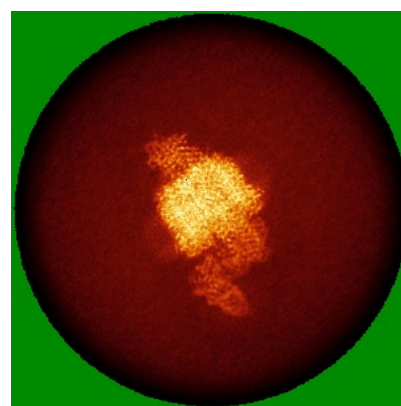
### 6.4.1 Primary map



X



Y

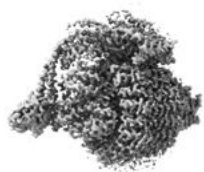


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

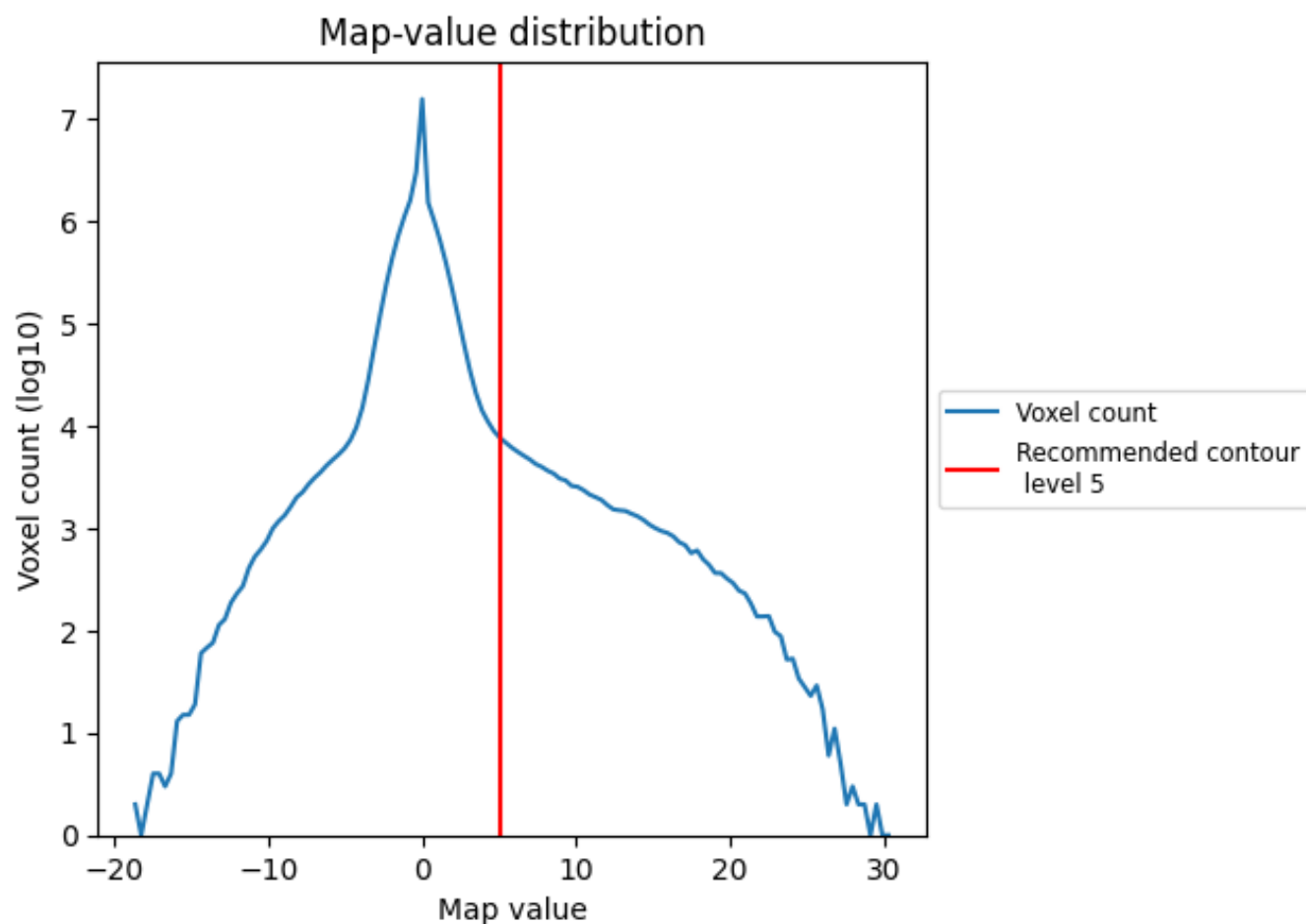
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

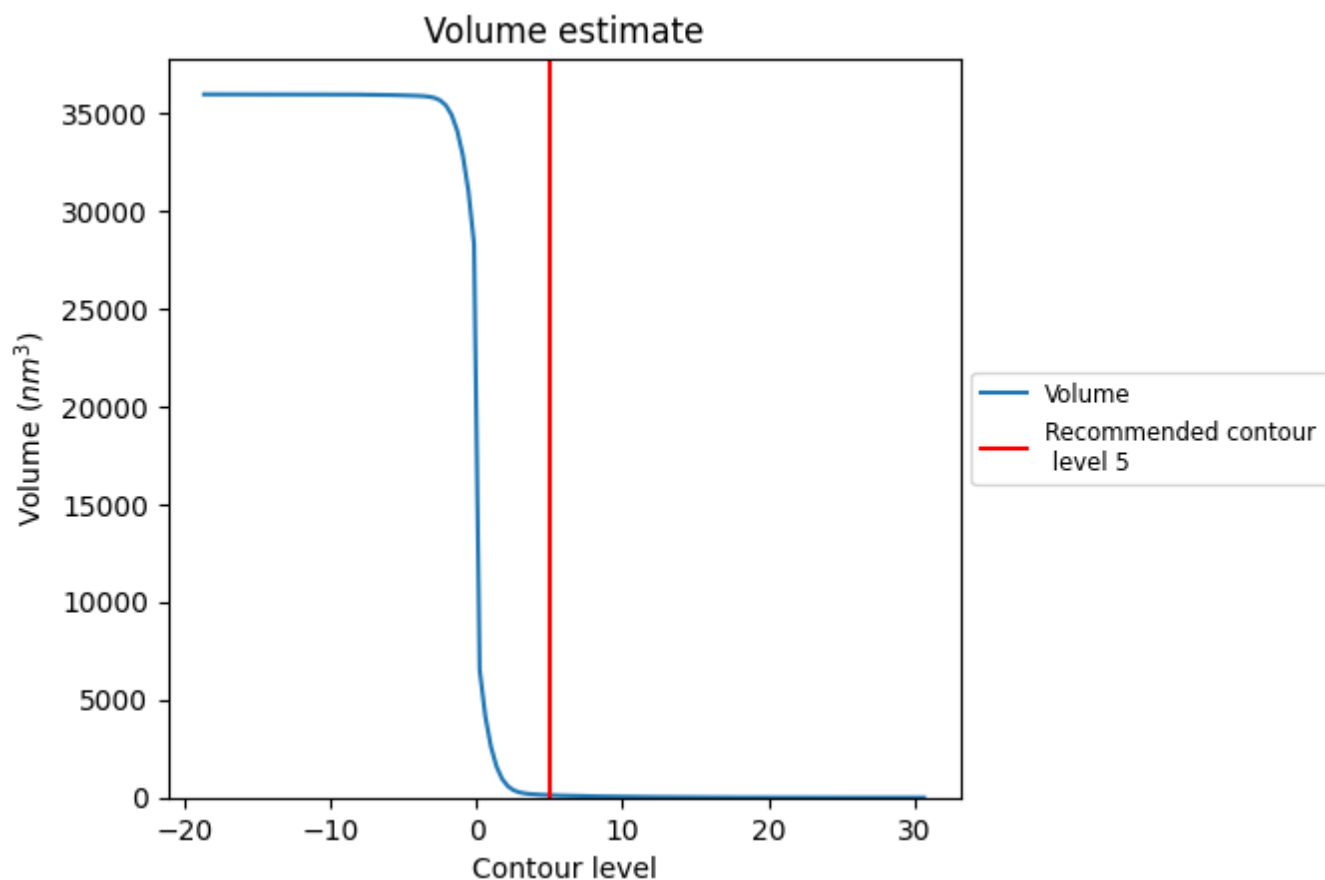
This section contains the results of statistical analysis of the map.

### 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.

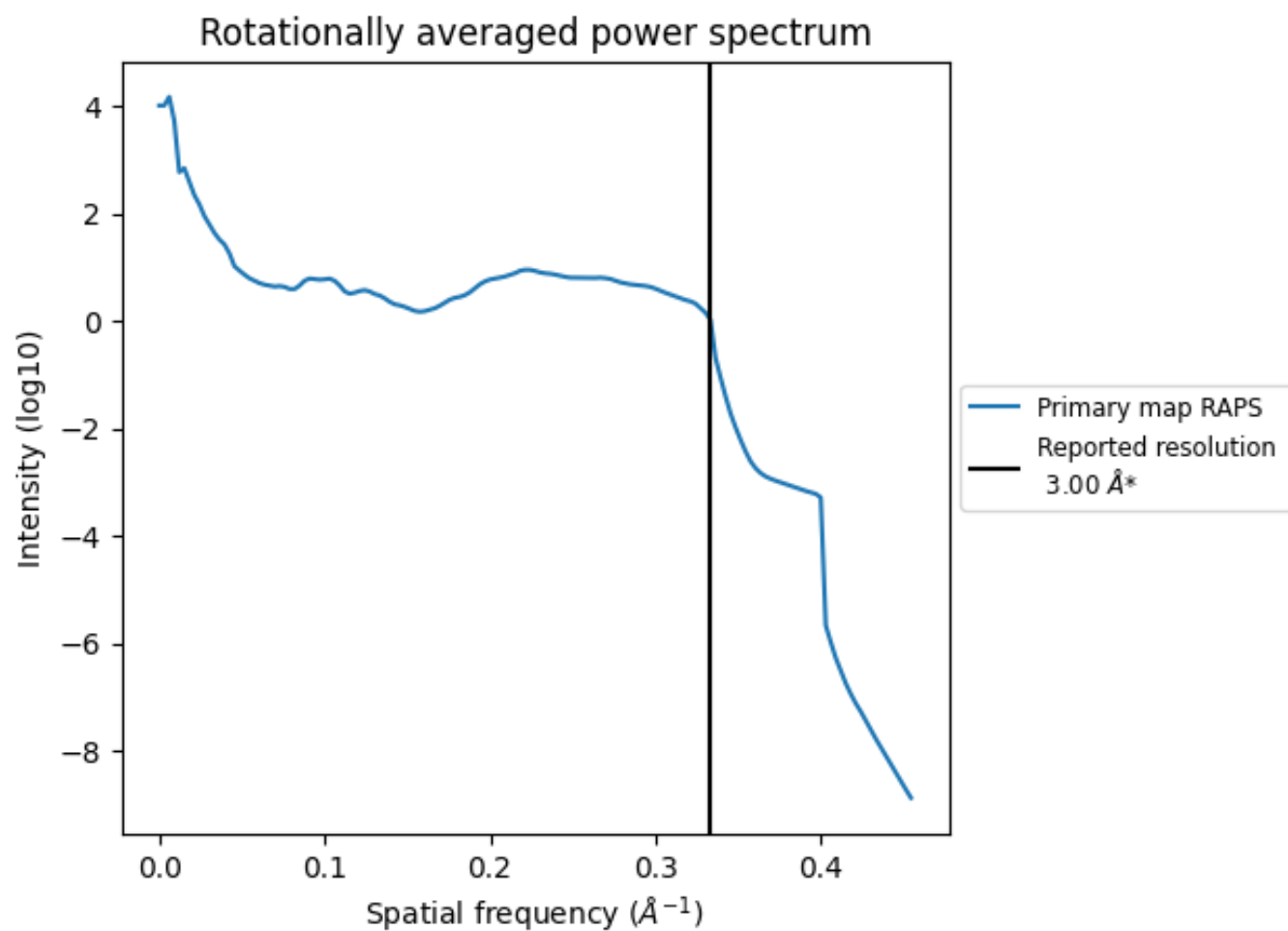
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 123 nm<sup>3</sup>; this corresponds to an approximate mass of 111 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

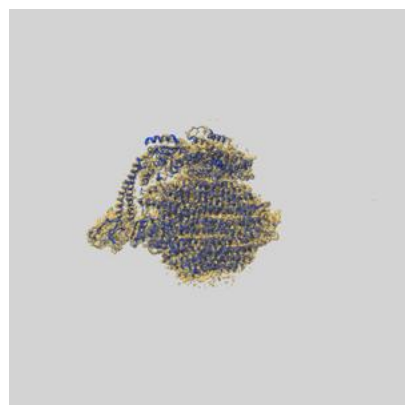
This section was not generated. No FSC curve or half-maps provided.



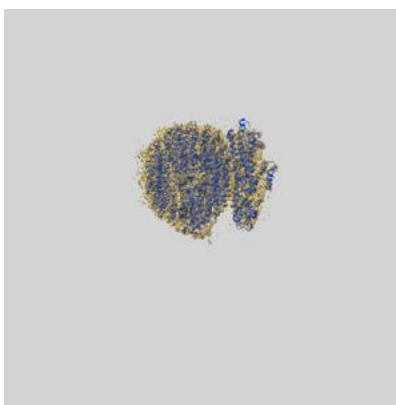
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46798 and PDB model 9DET. Per-residue inclusion information can be found in section 3 on page 10.

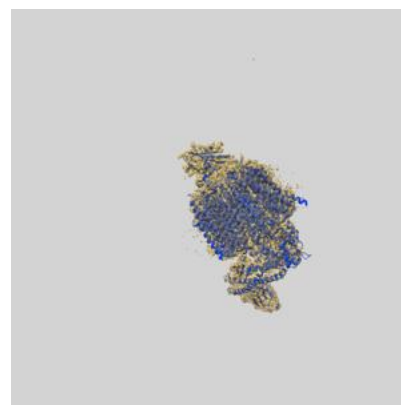
### 9.1 Map-model overlay [i](#)



X



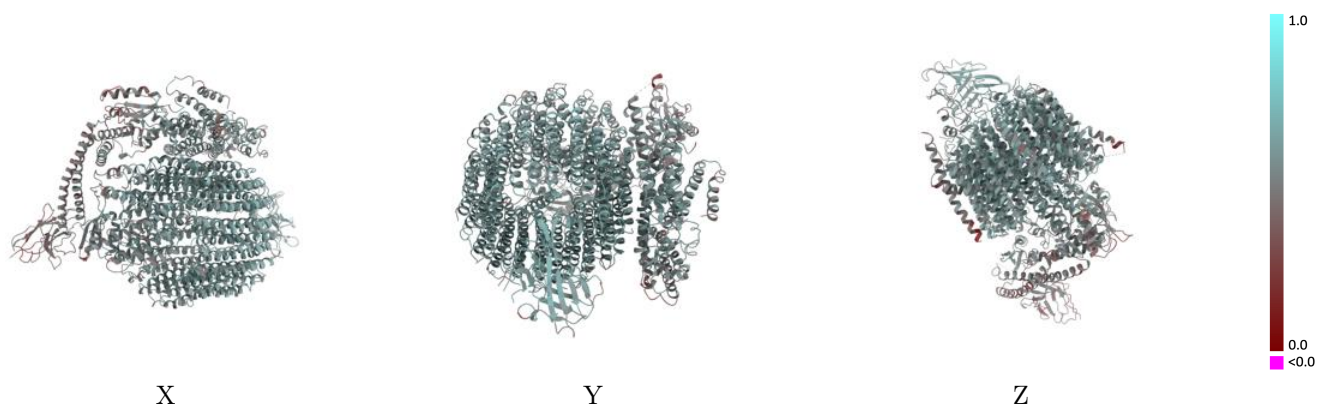
Y



Z

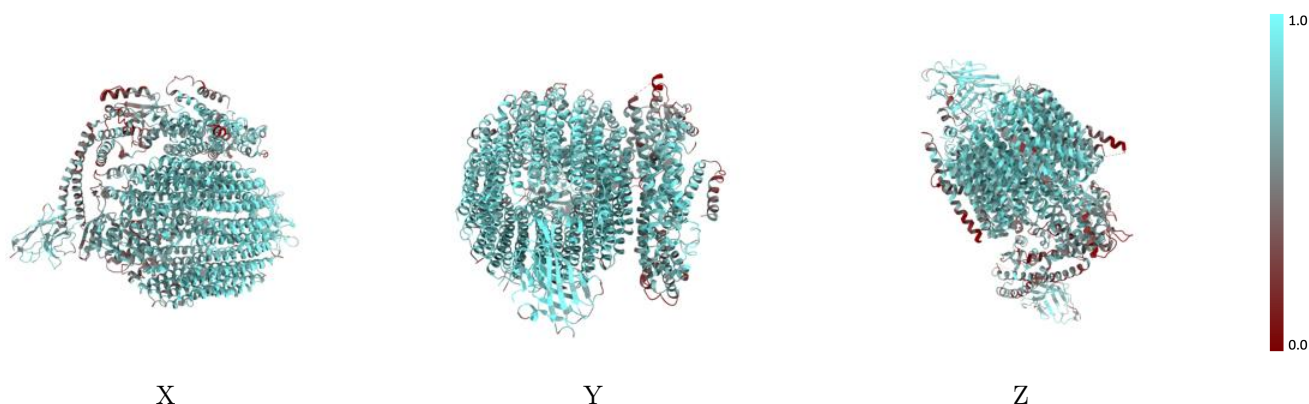
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



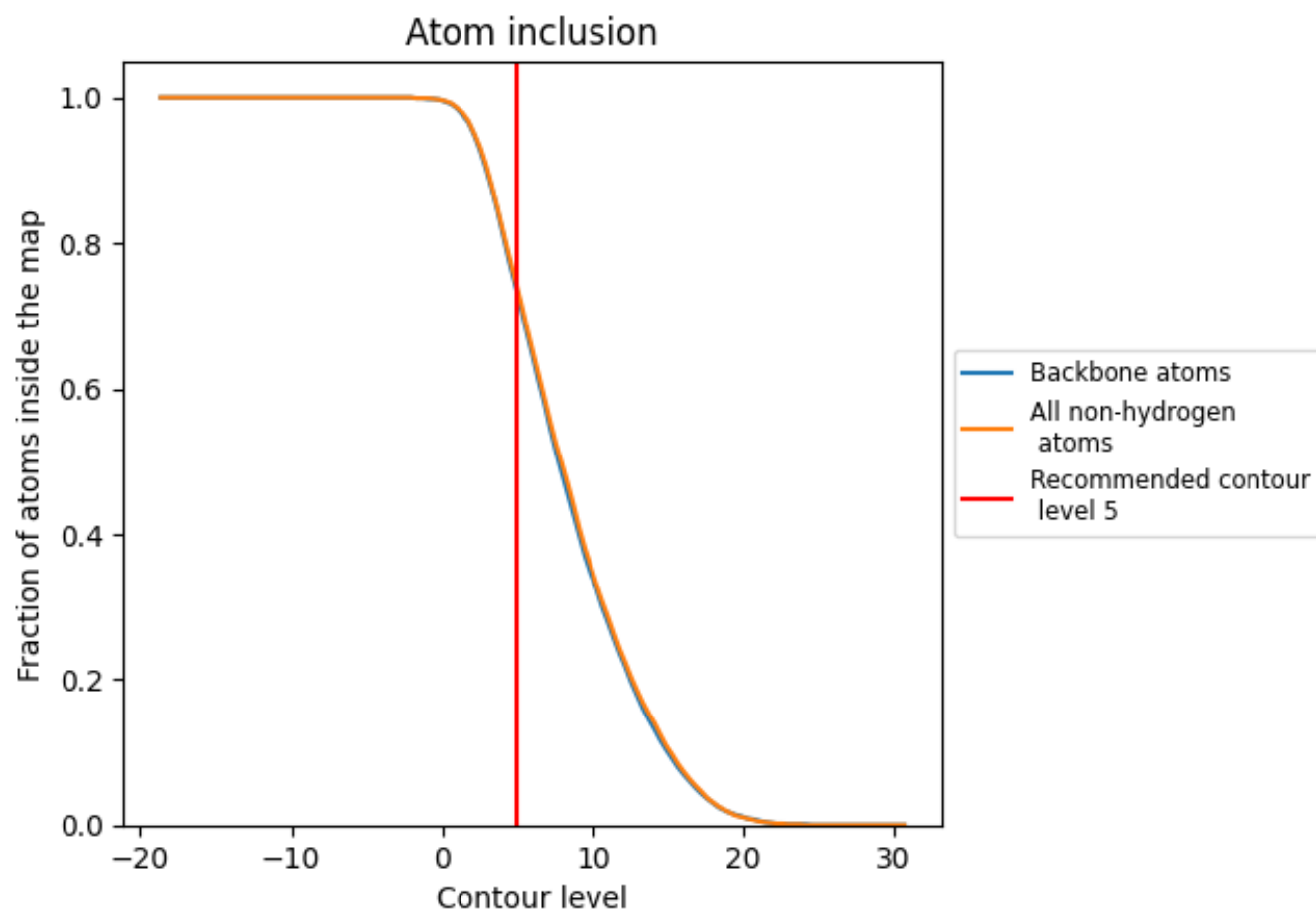
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 74% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7380	<div></div> 0.5480
a	<div></div> 0.6170	<div></div> 0.5070
b	<div></div> 0.8610	<div></div> 0.5950
c	<div></div> 0.8480	<div></div> 0.5860
d	<div></div> 0.6750	<div></div> 0.5350
e	<div></div> 0.6590	<div></div> 0.5230
f	<div></div> 0.4740	<div></div> 0.4580
g	<div></div> 0.8460	<div></div> 0.5940
h	<div></div> 0.8490	<div></div> 0.5920
i	<div></div> 0.8310	<div></div> 0.5870
j	<div></div> 0.8010	<div></div> 0.5780
k	<div></div> 0.8040	<div></div> 0.5720
l	<div></div> 0.8040	<div></div> 0.5750
m	<div></div> 0.8420	<div></div> 0.5870
n	<div></div> 0.8640	<div></div> 0.5920
o	<div></div> 0.7980	<div></div> 0.5680
p	<div></div> 0.8180	<div></div> 0.5910
q	<div></div> 0.7040	<div></div> 0.4210

1.0

0.0

<0.0