



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 01:42 AM EDT

PDB ID : 7KHR
EMDB ID : EMD-22880
Title : Cryo-EM structure of bafilomycin A1-bound intact V-ATPase from bovine brain
Authors : Wang, R.; Li, X.
Deposited on : 2020-10-21
Resolution : 3.62 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

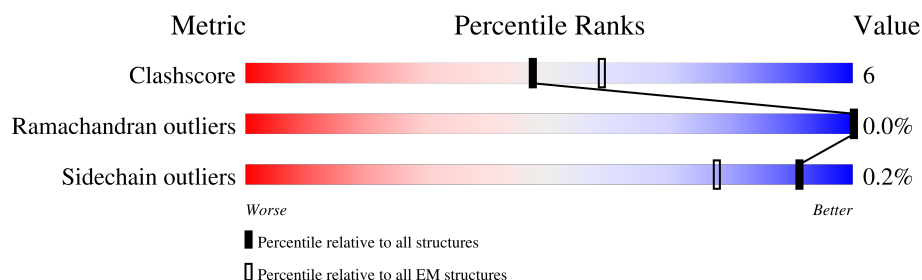
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY









The reported resolution of this entry is 3.62 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.





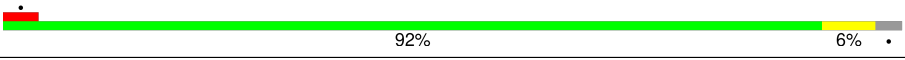

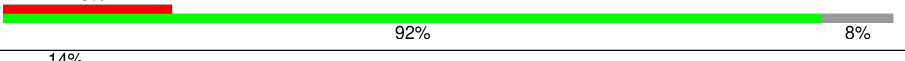
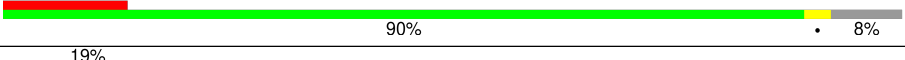

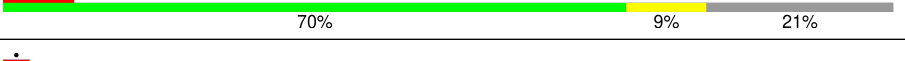

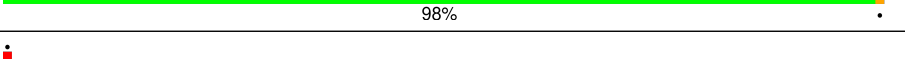
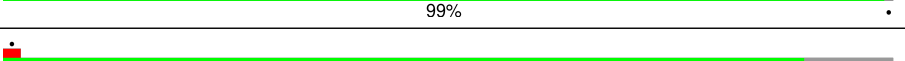


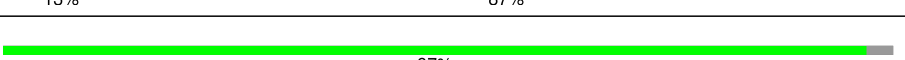
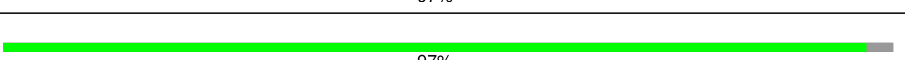
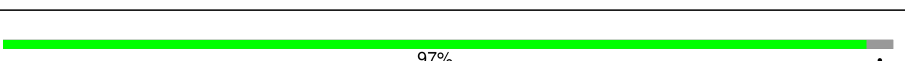
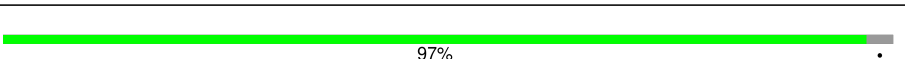
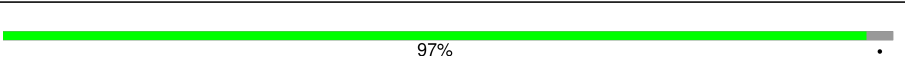
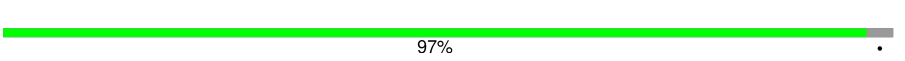
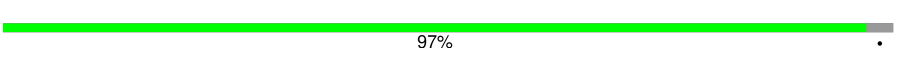
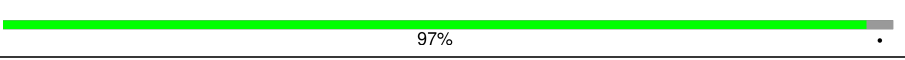
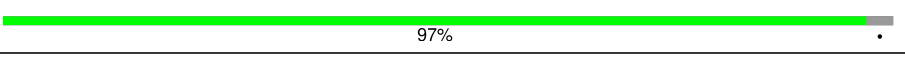
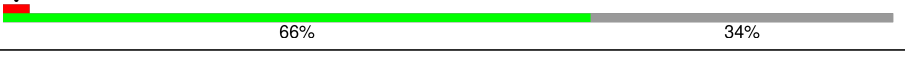
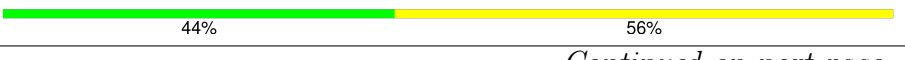

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	


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Mol	Chain	Length	Quality of chain
5	I	226	
5	J	226	
5	K	226	
6	L	119	
7	M	118	
7	N	118	
7	O	118	
8	P	465	
9	a	838	
10	b	205	
11	d	351	
12	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	
17	t	9	

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Mol	Chain	Length	Quality of chain
18	Q	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	WEV	g	202	-	X	-	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 61913 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	591	Total	C	N	O	S	0	0
			4591	2911	774	879	27		
1	C	600	Total	C	N	O	S	0	0
			4654	2950	785	891	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	458	Total	C	N	O	S	0	0
			3585	2273	613	679	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	0	0
			1720	1028	346	346		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	218	Total	C	N	O	S	0	0
			1543	960	288	289	6		
5	J	218	Total	C	N	O	S	0	0
			1636	1024	301	304	7		
5	K	220	Total	C	N	O	S	0	0
			1568	977	293	292	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	109	Total	C	N	O	S	0	0
			663	396	138	126	3		
7	N	109	Total	C	N	O	S	0	0
			684	408	140	133	3		
7	O	109	Total	C	N	O	S	0	0
			677	404	139	131	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
			2499	1558	460	473	8		

- 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
			5827	3788	972	1031	36		

- 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	204	Total	C	N	O	S	0	0
			1660	1078	263	311	8		

- 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		

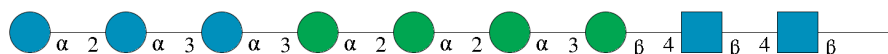
- Molecule 15 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

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	65	Total	C	N	O	S	0	0
			501	336	75	86	4		

- Molecule 17 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
17	t	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 18 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.

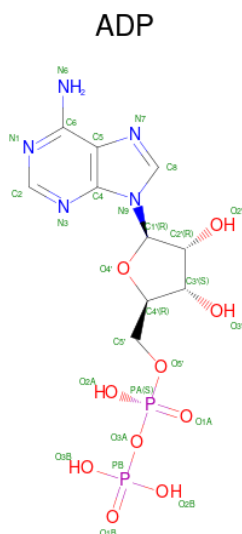


Mol	Chain	Residues	Atoms			AltConf	Trace
18	Q	2	Total	C	O	0	0
			22	12	10		

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

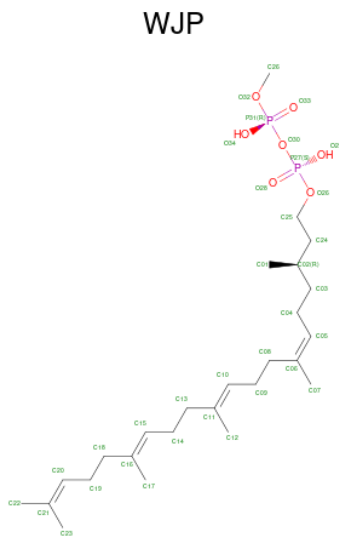
Mol	Chain	Residues	Atoms		AltConf
19	C	1	Total	Mg	0
			1	1	

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



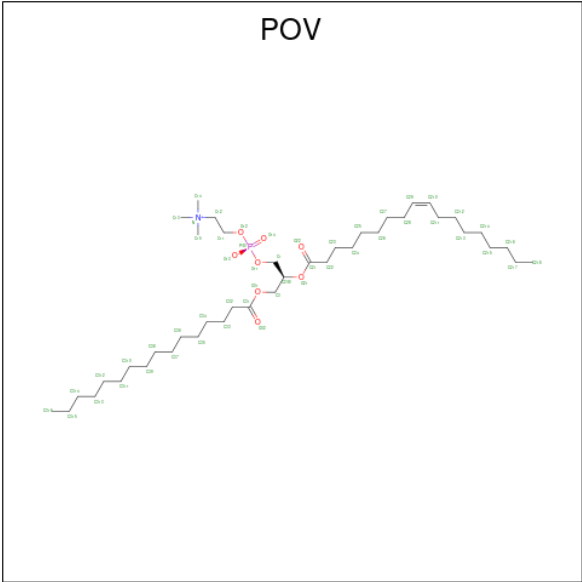
Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 21 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicos-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (three-letter code: WJP) (formula: $C_{26}H_{48}O_7P_2$).



Mol	Chain	Residues	Atoms				AltConf
21	a	1	Total	C	O	P	0
			34	25	7	2	

- Molecule 22 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $\text{C}_{42}\text{H}_{82}\text{NO}_8\text{P}$).



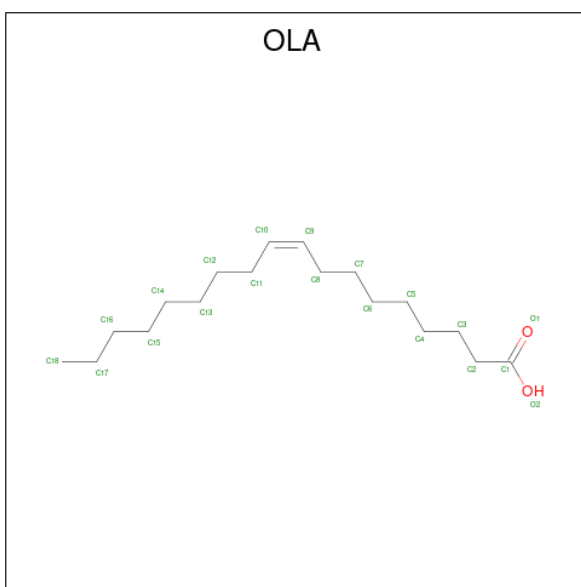
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
22	b	1	Total	C	N	O	P	0
			43	33	1	8	1	
22	s	1	Total	C	N	O	P	0
			40	30	1	8	1	
22	s	1	Total	C	N	O	P	0
			39	29	1	8	1	
22	r	1	Total	C	N	O	P	0
			47	37	1	8	1	
22	r	1	Total	C	N	O	P	0
			45	35	1	8	1	
22	r	1	Total	C	N	O	P	0
			47	37	1	8	1	
22	l	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 23 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



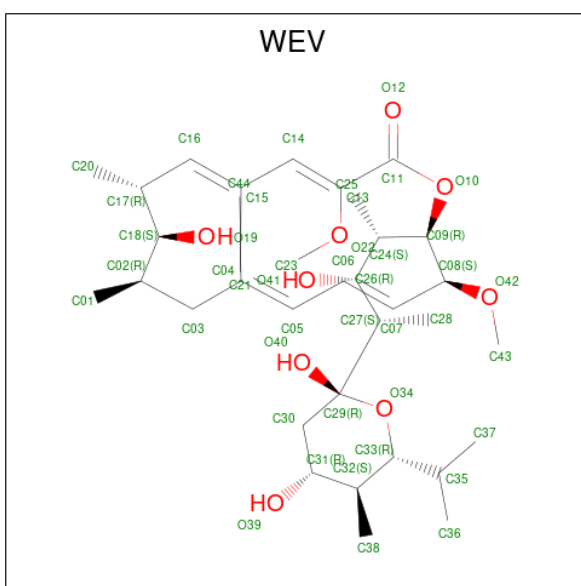
Mol	Chain	Residues	Atoms				AltConf
23	s	1	Total	C	N	O	0
			14	8	1	5	
23	s	1	Total	C	N	O	0
			14	8	1	5	
23	s	1	Total	C	N	O	0
			14	8	1	5	
23	s	1	Total	C	N	O	0
			14	8	1	5	
23	s	1	Total	C	N	O	0
			14	8	1	5	
23	s	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 24 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



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

- Molecule 25 is (5R)-2,4-dideoxy-1-C-[(2S,3R,4S)-3-hydroxy-4-[(2R,3S,4E,6E,9R,10S,11R,12E,14Z)-10-hydroxy-3,15-dimethoxy-7,9,11,13-tetramethyl-16-oxo-1-oxacyclohexadeca-4,6,12,14-tetraen-2-yl]pentan-2-yl]-4-methyl-5-propan-2-yl- α -D-threo-pentopyranose (three-letter code: WEV) (formula: $C_{35}H_{58}O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	g	1	Total	C	O	0
			44	35	9	

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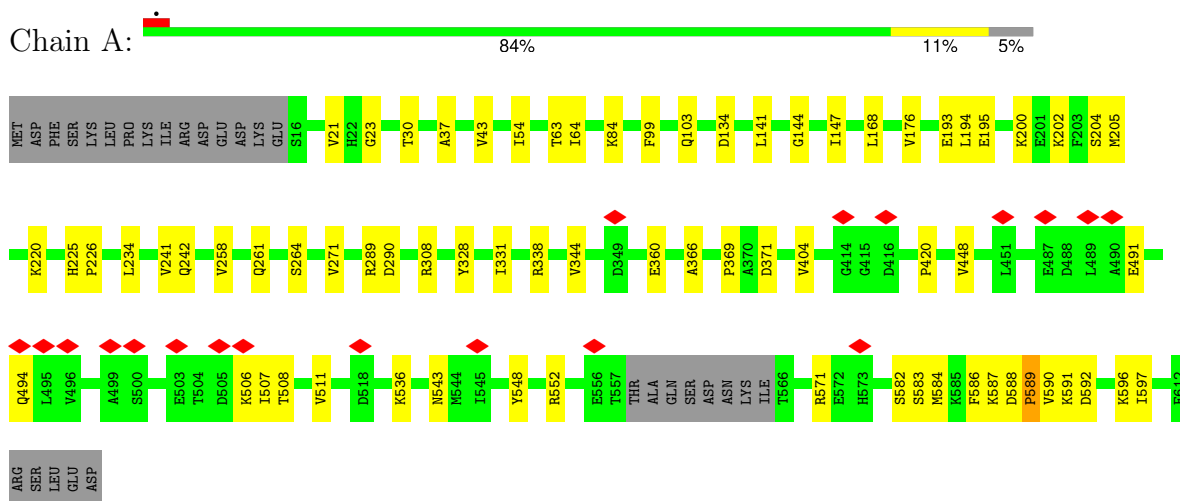
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Mol	Chain	Residues	Atoms			AltConf
25	g	1	Total	C	O	0
			44	35	9	
25	l	1	Total	C	O	0
			44	35	9	
25	m	1	Total	C	O	0
			44	35	9	
25	o	1	Total	C	O	0
			44	35	9	
25	p	1	Total	C	O	0
			44	35	9	

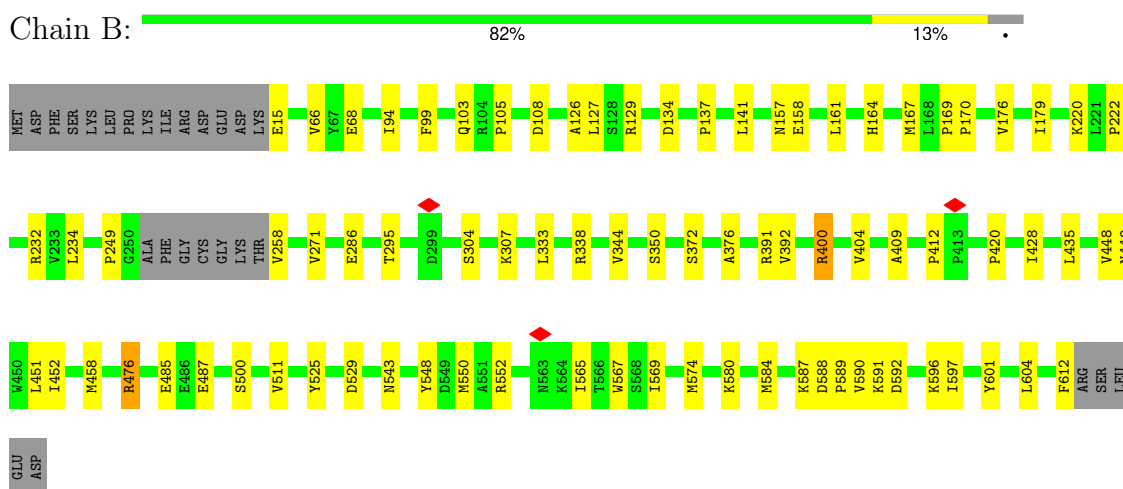
3 Residue-property plots

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

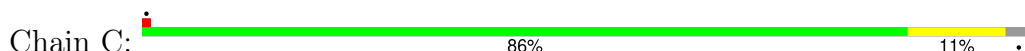
- Molecule 1: V-type proton ATPase catalytic subunit A

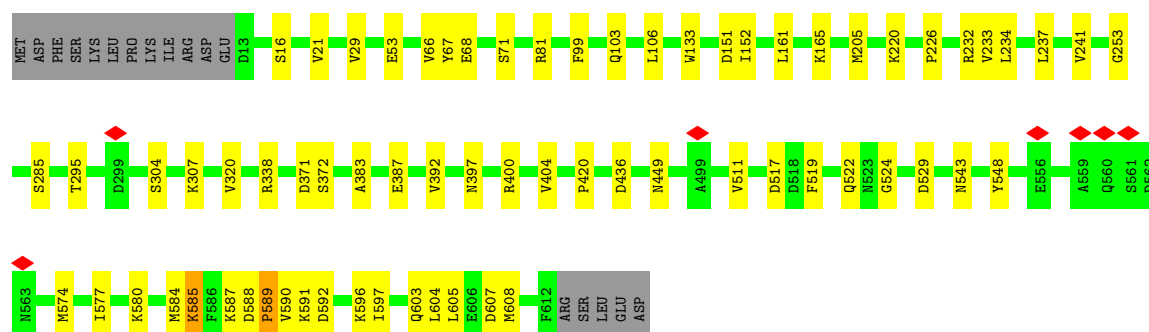


- Molecule 1: V-type proton ATPase catalytic subunit A



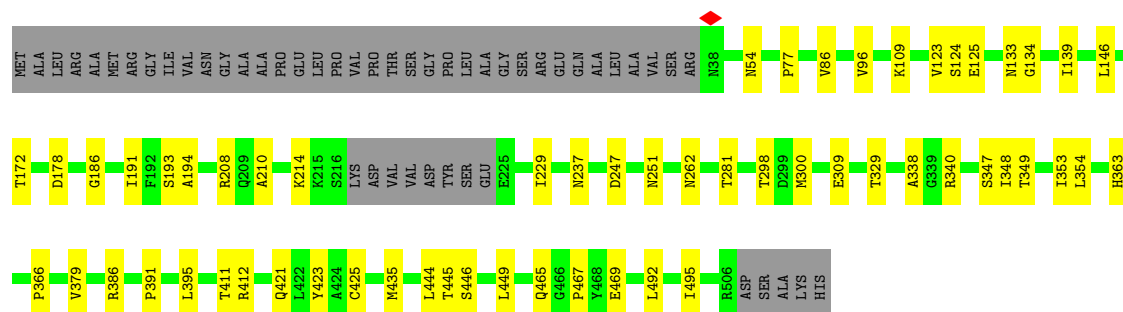
- Molecule 1: V-type proton ATPase catalytic subunit A





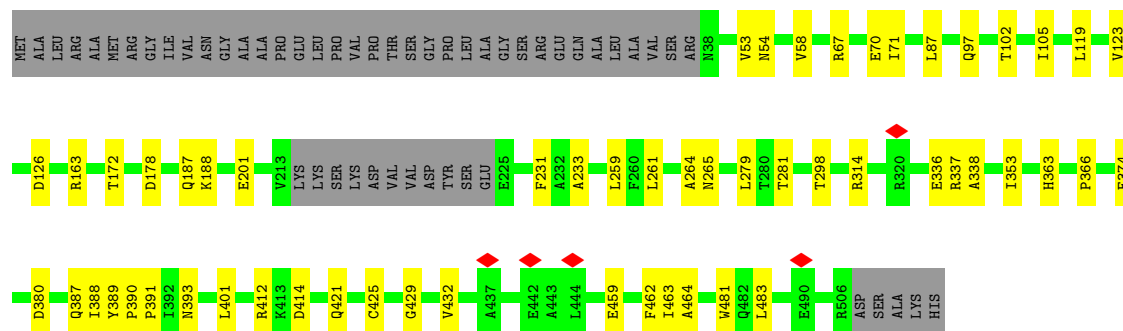
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain D: 79% 12% 10%



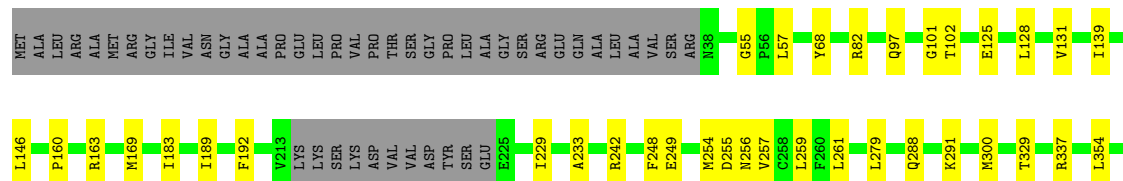
- Molecule 2: V-type proton ATPase subunit B, brain isoform

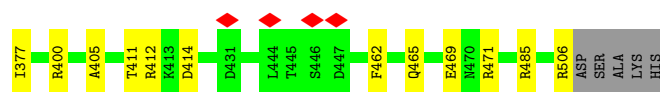
Chain E: 79% 11% 10%



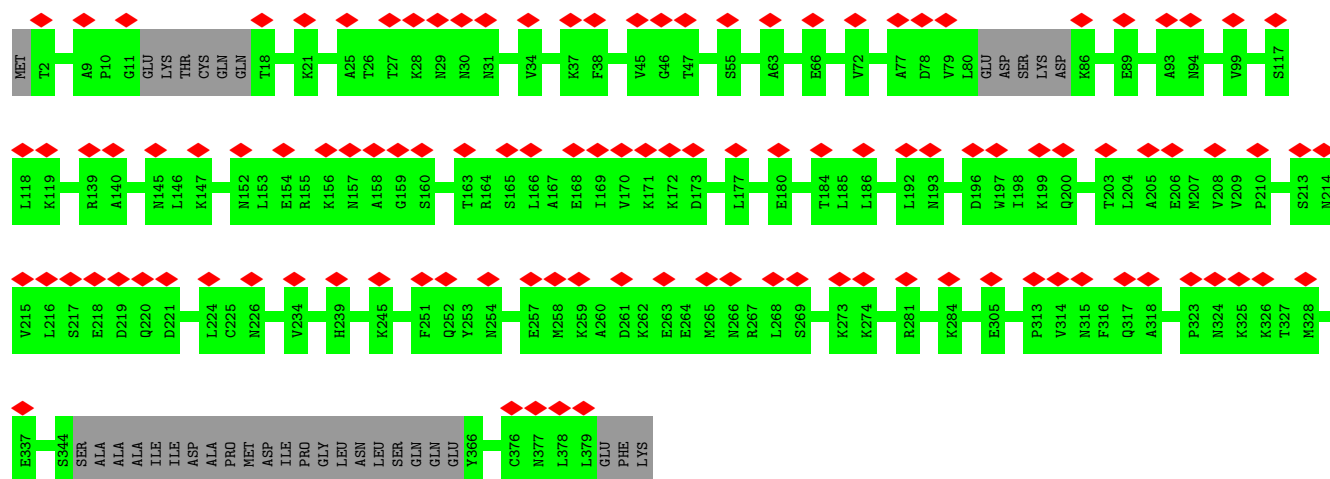
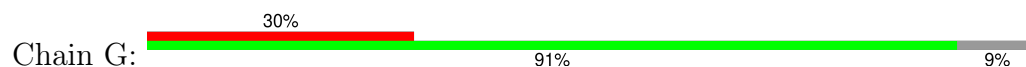
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain F: 80% 9% 10%

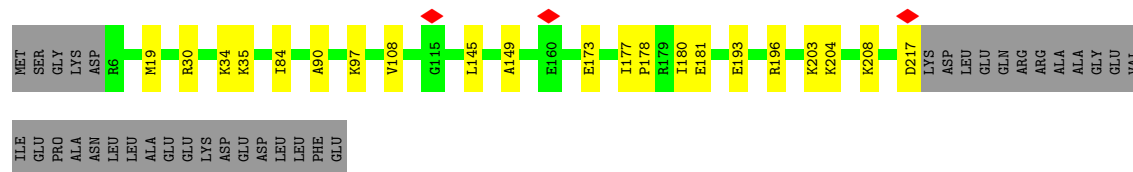
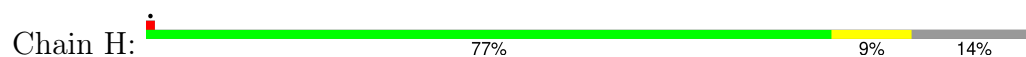




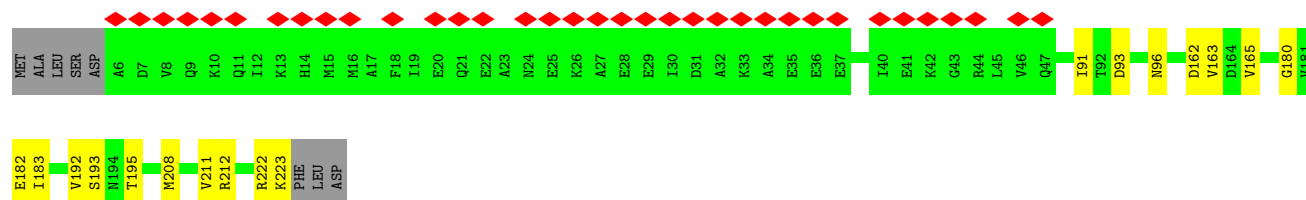
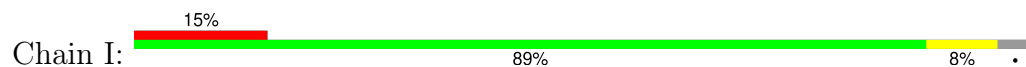
• Molecule 3: V-type proton ATPase subunit C 1



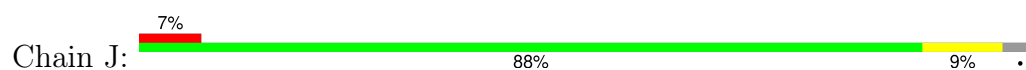
• Molecule 4: V-type proton ATPase subunit D



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



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

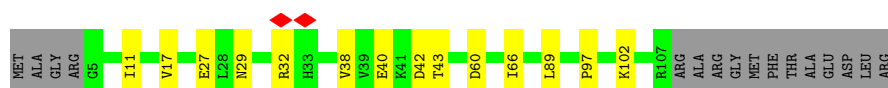




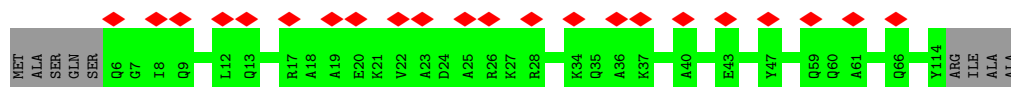
- Molecule 5: V-type proton ATPase subunit E 1



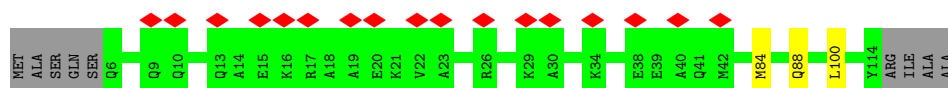
- Molecule 6: V-type proton ATPase subunit F



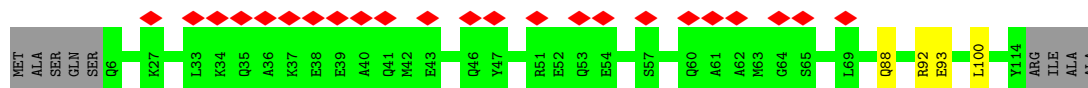
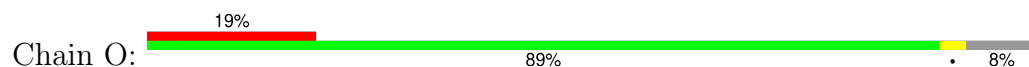
- Molecule 7: V-type proton ATPase subunit G



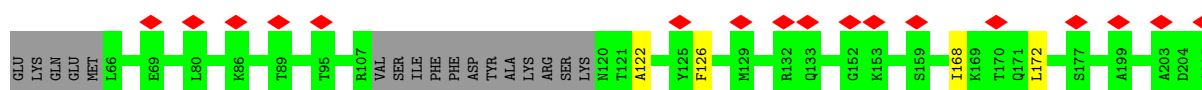
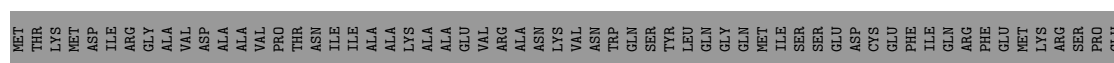
- Molecule 7: V-type proton ATPase subunit G

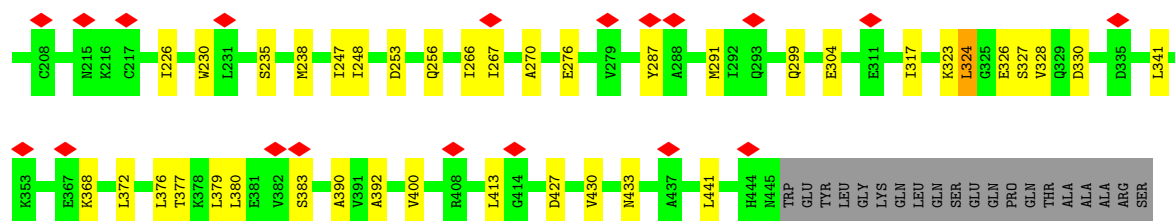


- Molecule 7: V-type proton ATPase subunit G



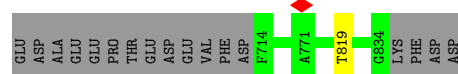
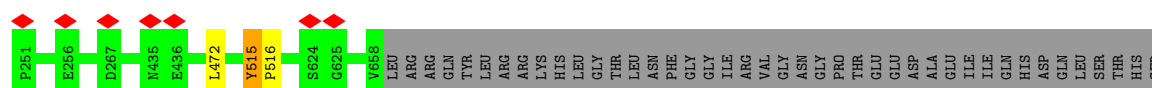
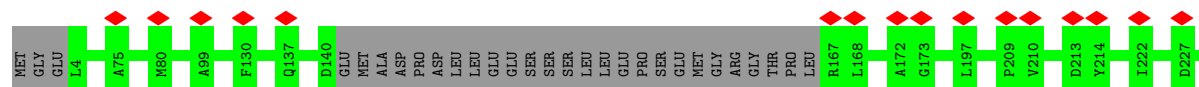
- Molecule 8: V-type proton ATPase subunit H





• Molecule 9: V-type proton ATPase subunit a

Chain a: 89% 11%



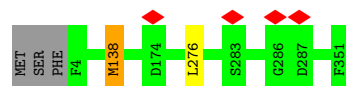
• Molecule 10: V-type proton ATPase 21 kDa proteolipid subunit

Chain b: 98%



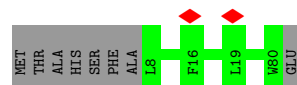
• Molecule 11: V-type proton ATPase subunit d 1

Chain d: 99%



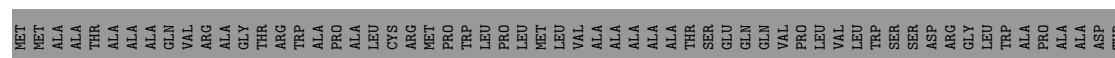
• Molecule 12: V-type proton ATPase subunit e 2

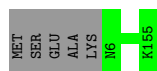
Chain e: 90% 10%



• Molecule 13: V-type proton ATPase subunit S1

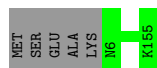
Chain s: 43% 56%





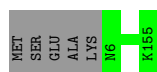
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain l:  97%



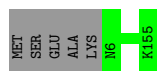
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain m:  97%



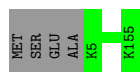
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain n:  97%



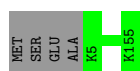
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain o:  97%



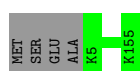
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain p:  97%



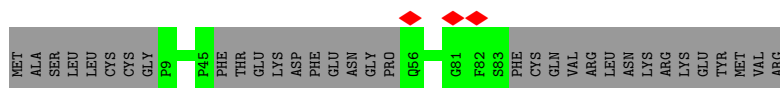
- Molecule 15: V-type proton ATPase 16 kDa proteolipid subunit

Chain q:  97%



- Molecule 16: Ribonuclease kappa

Chain f:  66% 34%



- Molecule 17: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t: 44% 56%



- Molecule 18: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose

Chain Q: 50% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26530	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	28.118	Depositor
Minimum map value	-14.814	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.046	Depositor
Recommended contour level	3.4	Depositor
Map size (\AA)	413.168, 413.168, 413.168	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.833, 0.833, 0.833	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	2/4663 (0.0%)	0.52	0/6314
1	B	0.38	1/4685 (0.0%)	0.53	1/6345 (0.0%)
1	C	0.40	1/4750 (0.0%)	0.55	1/6432 (0.0%)
2	D	0.31	0/3680	0.53	0/4986
2	E	0.33	1/3656 (0.0%)	0.54	2/4956 (0.0%)
2	F	0.30	0/3656	0.50	0/4956
3	G	0.23	0/1716	0.43	0/2390
4	H	0.25	0/1726	0.49	1/2309 (0.0%)
5	I	0.27	0/1554	0.46	0/2108
5	J	0.25	0/1649	0.46	0/2223
5	K	0.26	0/1579	0.46	0/2139
6	L	0.26	0/829	0.50	0/1122
7	M	0.23	0/666	0.39	0/912
7	N	0.24	0/687	0.41	0/939
7	O	0.23	0/680	0.40	0/930
8	P	0.31	0/2526	0.56	1/3439 (0.0%)
9	a	0.33	1/5965 (0.0%)	0.55	2/8090 (0.0%)
10	b	0.47	1/1537 (0.1%)	0.60	3/2090 (0.1%)
11	d	0.29	0/2884	0.54	2/3906 (0.1%)
12	e	0.27	0/613	0.45	0/844
13	s	0.42	0/1712	0.66	3/2331 (0.1%)
14	r	0.28	0/398	0.52	0/547
15	c	0.30	0/1079	0.49	0/1459
15	g	0.29	0/1079	0.49	0/1459
15	k	0.29	0/1079	0.48	0/1459
15	l	0.29	0/1079	0.48	0/1459
15	m	0.29	0/1079	0.46	0/1459
15	n	0.29	0/1079	0.49	0/1459
15	o	0.30	0/1088	0.48	0/1470
15	p	0.30	0/1088	0.50	0/1470
15	q	0.29	0/1088	0.51	0/1470
16	f	0.27	0/512	0.52	0/695

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.33	7/62061 (0.0%)	0.52	16/84167 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	589	PRO	N-CD	-14.12	1.28	1.47
1	B	589	PRO	N-CD	-14.07	1.28	1.47
1	A	589	PRO	N-CD	-14.06	1.28	1.47
2	E	387	GLN	C-N	7.05	1.50	1.34
1	A	582	SER	C-N	5.63	1.47	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	s	448	LEU	CA-CB-CG	8.88	135.73	115.30
9	a	515	TYR	C-N-CD	-8.69	101.48	120.60
9	a	515	TYR	N-CA-C	7.95	132.46	111.00
2	E	391	PRO	O-C-N	-7.91	110.05	122.70
10	b	29	PHE	N-CA-C	-7.56	90.59	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4568	0	4551	61	0
1	B	4591	0	4571	70	0
1	C	4654	0	4630	59	0
2	D	3609	0	3611	38	0
2	E	3585	0	3579	31	0
2	F	3585	0	3580	34	0
3	G	1720	0	758	0	0
4	H	1708	0	1816	15	0
5	I	1543	0	1435	11	0
5	J	1636	0	1614	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	1568	0	1476	9	0
6	L	816	0	818	10	0
7	M	663	0	495	0	0
7	N	684	0	532	2	0
7	O	677	0	516	3	0
8	P	2499	0	2069	33	0
9	a	5827	0	5639	0	0
10	b	1503	0	1550	0	0
11	d	2819	0	2756	0	0
12	e	590	0	613	0	0
13	s	1660	0	1542	0	0
14	r	385	0	373	0	0
15	c	1064	0	1132	0	0
15	g	1064	0	1132	0	0
15	k	1064	0	1132	0	0
15	l	1064	0	1132	0	0
15	m	1064	0	1132	0	0
15	n	1064	0	1132	0	0
15	o	1073	0	1145	0	0
15	p	1073	0	1145	0	0
15	q	1073	0	1145	0	0
16	f	501	0	510	0	0
17	t	105	0	87	0	0
18	Q	22	0	19	0	0
19	C	1	0	0	0	0
20	C	27	0	12	2	0
21	a	34	0	0	0	0
22	b	90	0	125	0	0
22	l	40	0	52	0	0
22	r	139	0	194	0	0
22	s	79	0	103	0	0
23	s	98	0	91	0	0
24	r	20	0	33	0	0
25	g	88	0	0	0	0
25	l	44	0	0	0	0
25	m	44	0	0	0	0
25	o	44	0	0	0	0
25	p	44	0	0	0	0
All	All	61913	0	59977	358	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 6.

The worst 5 of 358 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)
1:A:536:LYS:NZ	1:A:597:ILE:HD13	1.44	1.32
1:C:587:LYS:O	1:C:597:ILE:HD11	1.07	1.24
1:C:587:LYS:O	1:C:597:ILE:CD1	1.86	1.23
8:P:291:MET:CE	8:P:324:LEU:HD21	1.75	1.15
8:P:291:MET:SD	8:P:324:LEU:HD21	1.89	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/617 (95%)	554 (95%)	31 (5%)	0	100	100
1	B	587/617 (95%)	552 (94%)	35 (6%)	0	100	100
1	C	598/617 (97%)	575 (96%)	23 (4%)	0	100	100
2	D	457/511 (89%)	421 (92%)	36 (8%)	0	100	100
2	E	454/511 (89%)	430 (95%)	24 (5%)	0	100	100
2	F	454/511 (89%)	429 (94%)	25 (6%)	0	100	100
3	G	338/382 (88%)	326 (96%)	12 (4%)	0	100	100
4	H	210/247 (85%)	203 (97%)	7 (3%)	0	100	100
5	I	216/226 (96%)	214 (99%)	2 (1%)	0	100	100
5	J	216/226 (96%)	213 (99%)	3 (1%)	0	100	100
5	K	218/226 (96%)	215 (99%)	3 (1%)	0	100	100
6	L	101/119 (85%)	93 (92%)	7 (7%)	1 (1%)	13	46
7	M	107/118 (91%)	106 (99%)	1 (1%)	0	100	100
7	N	107/118 (91%)	107 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	O	107/118 (91%)	103 (96%)	4 (4%)	0	100	100
8	P	364/465 (78%)	342 (94%)	22 (6%)	0	100	100
9	a	744/838 (89%)	678 (91%)	65 (9%)	1 (0%)	48	79
10	b	202/205 (98%)	196 (97%)	5 (2%)	1 (0%)	25	59
11	d	346/351 (99%)	320 (92%)	26 (8%)	0	100	100
12	e	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
13	s	202/468 (43%)	175 (87%)	27 (13%)	0	100	100
14	r	44/351 (12%)	40 (91%)	4 (9%)	0	100	100
15	c	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
15	g	148/155 (96%)	148 (100%)	0	0	100	100
15	k	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	l	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	m	148/155 (96%)	148 (100%)	0	0	100	100
15	n	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
15	o	149/155 (96%)	148 (99%)	1 (1%)	0	100	100
15	p	149/155 (96%)	149 (100%)	0	0	100	100
15	q	149/155 (96%)	149 (100%)	0	0	100	100
16	f	61/98 (62%)	58 (95%)	3 (5%)	0	100	100
All	All	8124/9416 (86%)	7744 (95%)	377 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	a	516	PRO
10	b	30	ASP
6	L	97	PRO

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%)	497 (100%)	0	100	100
1	B	501/524 (96%)	499 (100%)	2 (0%)	89	94
1	C	507/524 (97%)	506 (100%)	1 (0%)	92	96
2	D	394/432 (91%)	394 (100%)	0	100	100
2	E	391/432 (90%)	391 (100%)	0	100	100
2	F	391/432 (90%)	391 (100%)	0	100	100
4	H	183/212 (86%)	183 (100%)	0	100	100
5	I	133/198 (67%)	133 (100%)	0	100	100
5	J	156/198 (79%)	156 (100%)	0	100	100
5	K	137/198 (69%)	136 (99%)	1 (1%)	81	89
6	L	89/100 (89%)	88 (99%)	1 (1%)	70	83
7	M	35/97 (36%)	35 (100%)	0	100	100
7	N	42/97 (43%)	42 (100%)	0	100	100
7	O	39/97 (40%)	39 (100%)	0	100	100
8	P	185/415 (45%)	182 (98%)	3 (2%)	58	76
9	a	597/744 (80%)	594 (100%)	3 (0%)	86	92
10	b	156/158 (99%)	155 (99%)	1 (1%)	84	91
11	d	303/306 (99%)	302 (100%)	1 (0%)	91	96
12	e	62/68 (91%)	62 (100%)	0	100	100
13	s	183/398 (46%)	182 (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	54/84 (64%)	54 (100%)	0	100	100
All	All	6034/7543 (80%)	6020 (100%)	14 (0%)	91	96

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	P	330	ASP
9	a	472	LEU
13	s	396	ARG
10	b	29	PHE
11	d	138	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
9	a	433	GLN
12	e	67	GLN
9	a	524	ASN
11	d	171	GLN
15	c	78	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 monosaccharides 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	$\# Z > 2$
18	MAN	Q	1	18	11,11,12	0.93	1 (9%)	15,15,17	1.10	2 (13%)
18	MAN	Q	2	18	11,11,12	0.85	0	15,15,17	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NAG	t	1	17	14,14,15	0.29	0	17,19,21	0.53	0
17	NAG	t	2	17	14,14,15	0.32	0	17,19,21	1.06	2 (11%)
17	BMA	t	3	17	11,11,12	0.82	0	15,15,17	0.98	1 (6%)
17	MAN	t	4	17	11,11,12	0.87	1 (9%)	15,15,17	1.03	1 (6%)
17	MAN	t	5	17	11,11,12	0.90	0	15,15,17	1.19	2 (13%)
17	MAN	t	6	17	11,11,12	0.82	1 (9%)	15,15,17	0.88	1 (6%)
17	GLC	t	7	17	11,11,12	0.76	0	15,15,17	0.74	0
17	GLC	t	8	17	11,11,12	0.61	0	15,15,17	0.76	0
17	GLC	t	9	17	11,11,12	0.64	0	15,15,17	0.62	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
18	MAN	Q	1	18	-	2/2/19/22	0/1/1/1
18	MAN	Q	2	18	-	1/2/19/22	1/1/1/1
17	NAG	t	1	17	-	4/6/23/26	0/1/1/1
17	NAG	t	2	17	-	2/6/23/26	0/1/1/1
17	BMA	t	3	17	-	0/2/19/22	0/1/1/1
17	MAN	t	4	17	-	2/2/19/22	0/1/1/1
17	MAN	t	5	17	-	2/2/19/22	0/1/1/1
17	MAN	t	6	17	-	2/2/19/22	0/1/1/1
17	GLC	t	7	17	-	1/2/19/22	0/1/1/1
17	GLC	t	8	17	-	0/2/19/22	0/1/1/1
17	GLC	t	9	17	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	t	6	MAN	O5-C1	-2.50	1.39	1.43
17	t	4	MAN	O5-C1	-2.42	1.39	1.43
18	Q	1	MAN	C1-C2	2.15	1.57	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	2	MAN	C1-O5-C5	4.11	117.70	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	t	5	MAN	O2-C2-C3	-2.99	103.96	110.15
17	t	4	MAN	O2-C2-C3	-2.65	104.66	110.15
17	t	3	BMA	O2-C2-C3	-2.60	104.77	110.15
18	Q	1	MAN	C1-O5-C5	2.58	115.64	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

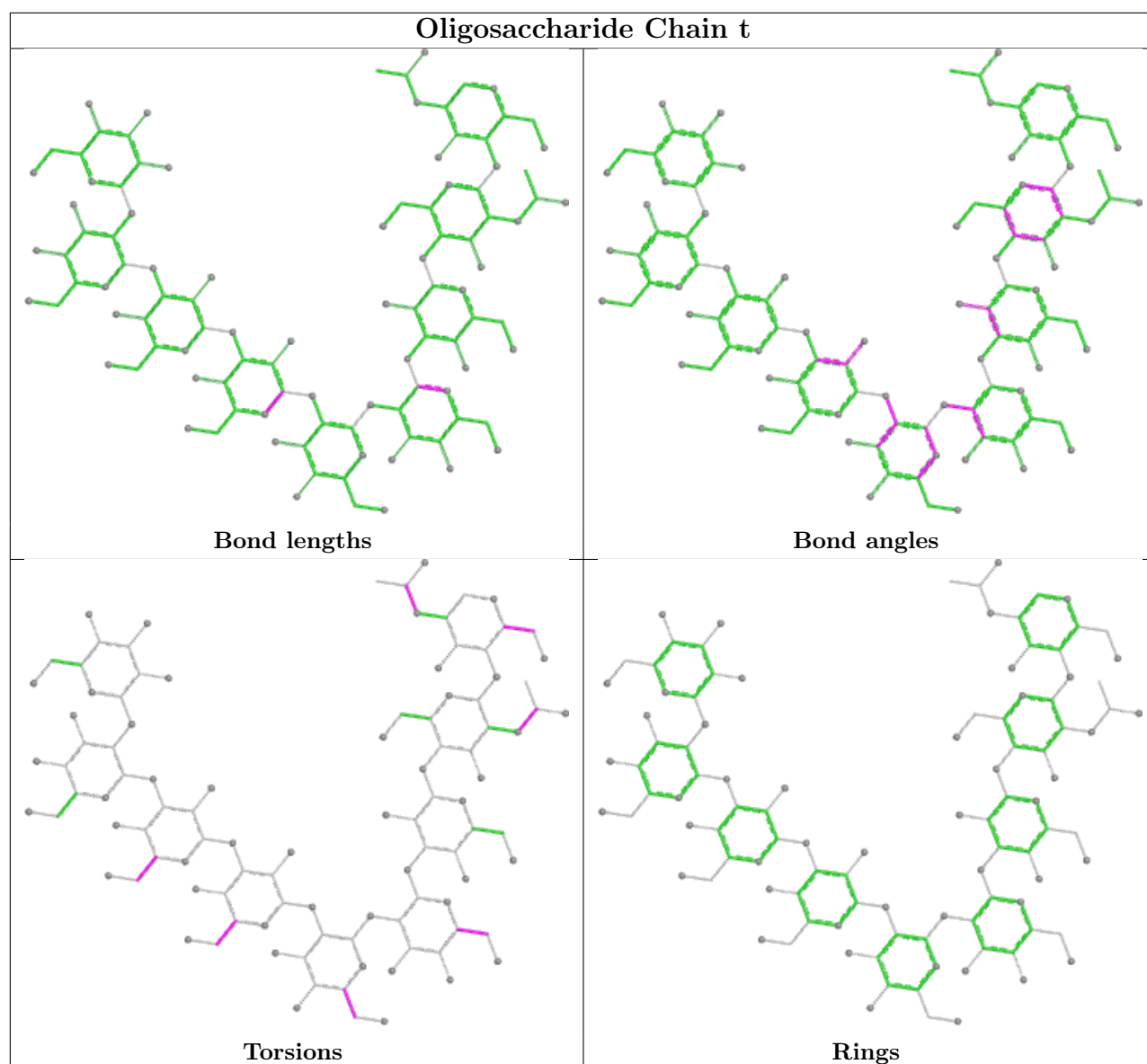
Mol	Chain	Res	Type	Atoms
17	t	1	NAG	C8-C7-N2-C2
17	t	1	NAG	O7-C7-N2-C2
18	Q	1	MAN	O5-C5-C6-O6
17	t	4	MAN	O5-C5-C6-O6
17	t	4	MAN	C4-C5-C6-O6

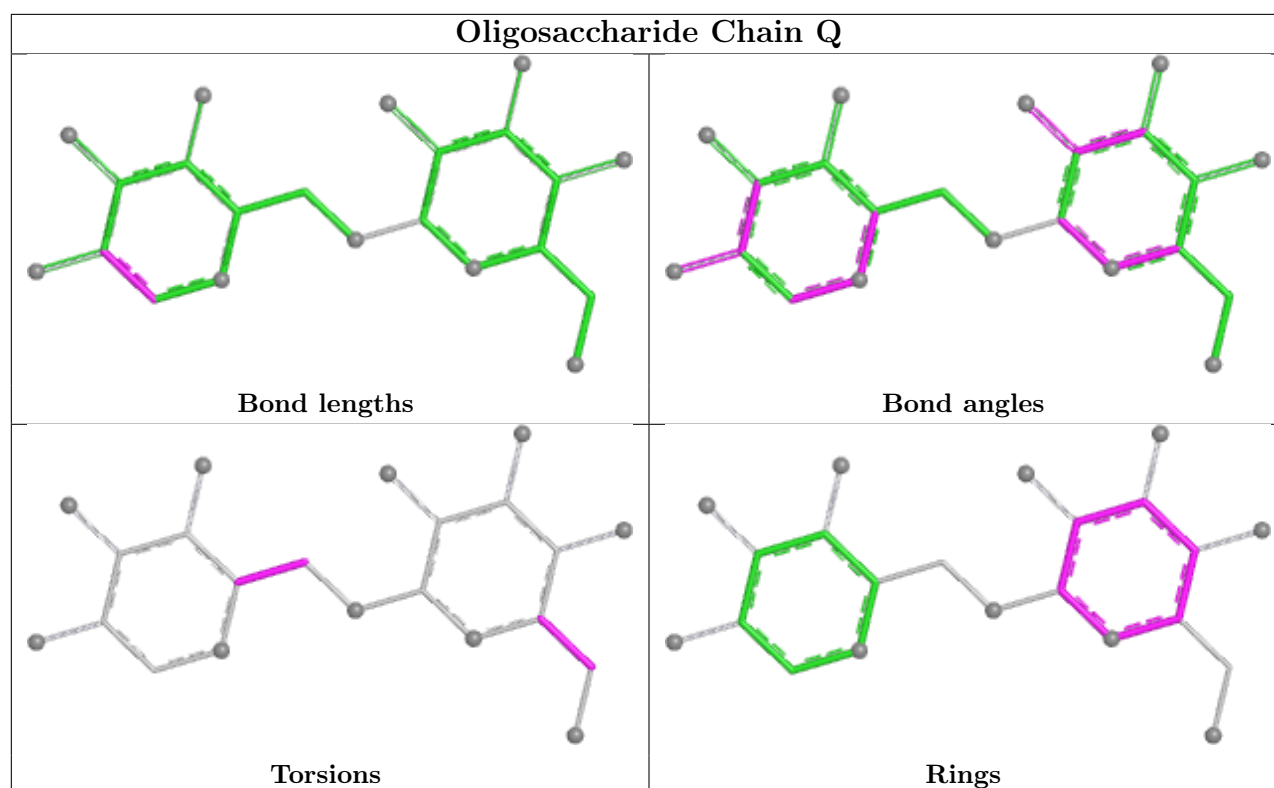
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	Q	2	MAN	C1-C2-C3-C4-C5-O5

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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 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$
23	NAG	s	504	-	14,14,15	0.55	0	17,19,21	0.55	0
20	ADP	C	702	19	24,29,29	1.23	2 (8%)	29,45,45	1.28	3 (10%)
25	WEV	g	202	-	43,45,45	2.06	18 (41%)	47,65,65	4.30	28 (59%)
22	POV	s	502	-	38,38,51	1.14	3 (7%)	44,46,59	1.02	3 (6%)
25	WEV	m	201	-	43,45,45	2.01	15 (34%)	47,65,65	3.22	24 (51%)
23	NAG	s	505	13	14,14,15	0.39	0	17,19,21	0.61	1 (5%)
25	WEV	o	201	-	43,45,45	2.29	18 (41%)	47,65,65	3.85	24 (51%)
23	NAG	s	506	13	14,14,15	0.65	0	17,19,21	0.48	0
25	WEV	l	202	-	43,45,45	2.22	20 (46%)	47,65,65	4.32	26 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	NAG	s	508	-	14,14,15	0.30	0	19,19,21	0.41	0
23	NAG	s	507	13	14,14,15	0.43	0	17,19,21	0.50	0
25	WEV	p	201	-	43,45,45	2.29	16 (37%)	47,65,65	3.93	29 (61%)
22	POV	b	301	-	46,46,51	1.05	4 (8%)	52,54,59	0.96	2 (3%)
25	WEV	g	201	-	43,45,45	2.25	17 (39%)	47,65,65	4.55	26 (55%)
22	POV	r	403	-	46,46,51	1.04	4 (8%)	52,54,59	0.88	3 (5%)
24	OLA	r	404	-	19,19,19	0.47	0	19,19,19	0.78	0
22	POV	b	302	-	42,42,51	1.09	4 (9%)	48,50,59	0.91	2 (4%)
22	POV	l	201	-	39,39,51	1.12	4 (10%)	45,47,59	0.87	2 (4%)
22	POV	r	402	-	44,44,51	1.04	4 (9%)	50,52,59	1.02	2 (4%)
21	WJP	a	901	-	32,33,34	1.02	2 (6%)	39,43,44	1.36	7 (17%)
23	NAG	s	509	13	14,14,15	0.47	0	17,19,21	0.60	0
23	NAG	s	503	13	14,14,15	0.40	0	17,19,21	0.53	0
22	POV	r	401	-	46,46,51	1.01	4 (8%)	52,54,59	0.85	2 (3%)
22	POV	s	501	-	39,39,51	1.12	4 (10%)	45,47,59	0.96	2 (4%)

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
23	NAG	s	504	-	-	1/6/23/26	0/1/1/1
20	ADP	C	702	19	-	3/12/32/32	0/3/3/3
25	WEV	g	202	-	-	39/64/82/82	0/1/2/2
22	POV	s	502	-	-	25/42/42/55	-
25	WEV	m	201	-	-	30/64/82/82	0/1/2/2
23	NAG	s	505	13	-	0/6/23/26	0/1/1/1
25	WEV	o	201	-	-	26/64/82/82	0/1/2/2
23	NAG	s	506	13	-	2/6/23/26	0/1/1/1
25	WEV	l	202	-	-	30/64/82/82	0/1/2/2
23	NAG	s	508	-	-	2/6/22/26	0/1/1/1
23	NAG	s	507	13	-	2/6/23/26	0/1/1/1
25	WEV	p	201	-	-	32/64/82/82	0/1/2/2
22	POV	b	301	-	-	22/50/50/55	-
25	WEV	g	201	-	-	22/64/82/82	0/1/2/2
22	POV	r	403	-	-	25/50/50/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OLA	r	404	-	-	9/17/17/17	-
22	POV	b	302	-	-	24/46/46/55	-
22	POV	l	201	-	-	21/43/43/55	-
22	POV	r	402	-	-	24/48/48/55	-
21	WJP	a	901	-	-	10/37/37/40	-
23	NAG	s	509	13	-	0/6/23/26	0/1/1/1
23	NAG	s	503	13	-	2/6/23/26	0/1/1/1
22	POV	r	401	-	-	26/50/50/55	-
22	POV	s	501	-	-	19/43/43/55	-

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	o	201	WEV	C14-C15	6.73	1.58	1.45
25	p	201	WEV	C09-C08	6.24	1.60	1.52
25	l	202	WEV	C14-C15	5.57	1.56	1.45
25	g	201	WEV	C14-C15	5.55	1.56	1.45
25	g	202	WEV	C14-C15	4.85	1.55	1.45

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	201	WEV	C01-C02-C03	-13.80	90.69	109.92
25	l	202	WEV	O10-C11-C13	12.69	132.39	110.99
25	l	202	WEV	C06-C05-C04	-12.16	110.58	127.69
25	g	202	WEV	C05-C06-C07	-11.36	98.09	124.43
25	p	201	WEV	O10-C11-C13	11.06	129.64	110.99

There are no chirality outliers.

5 of 396 torsion outliers are listed below:

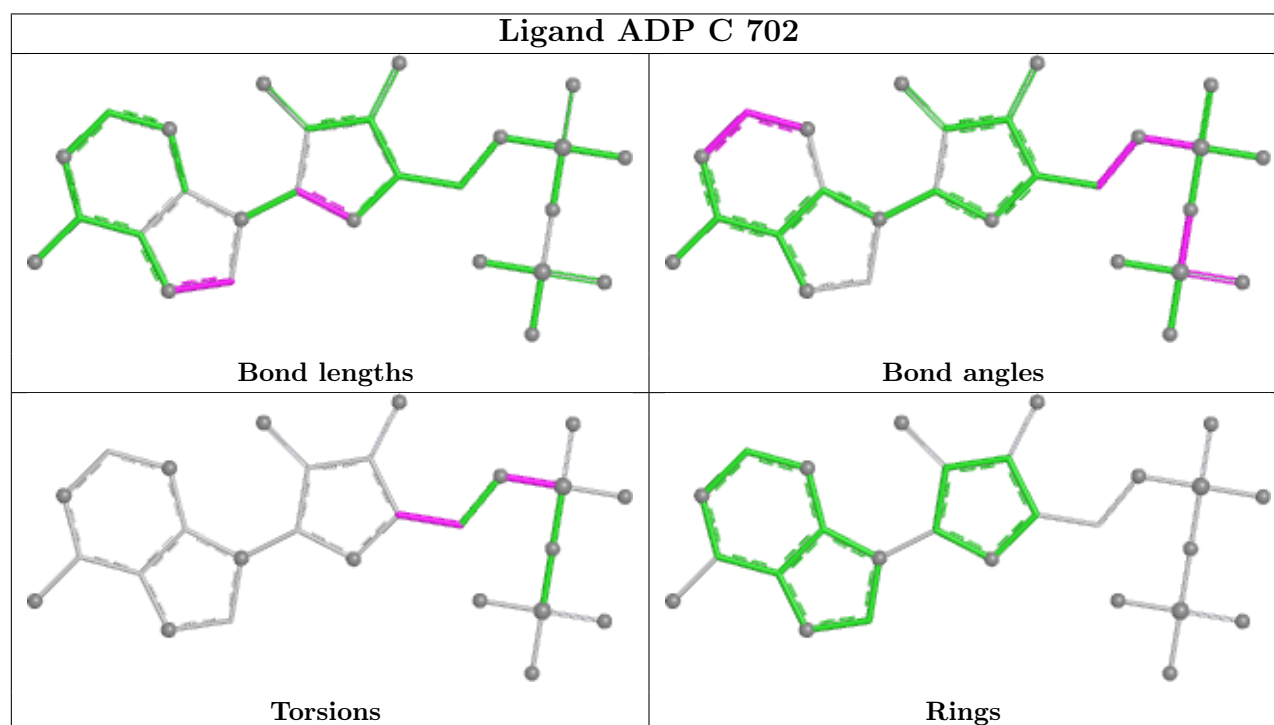
Mol	Chain	Res	Type	Atoms
20	C	702	ADP	C5'-O5'-PA-O1A
21	a	901	WJP	C02-C03-C04-C05
21	a	901	WJP	C02-C24-C25-O26
22	b	301	POV	C1-O11-P-O12
22	b	301	POV	C1-O11-P-O13

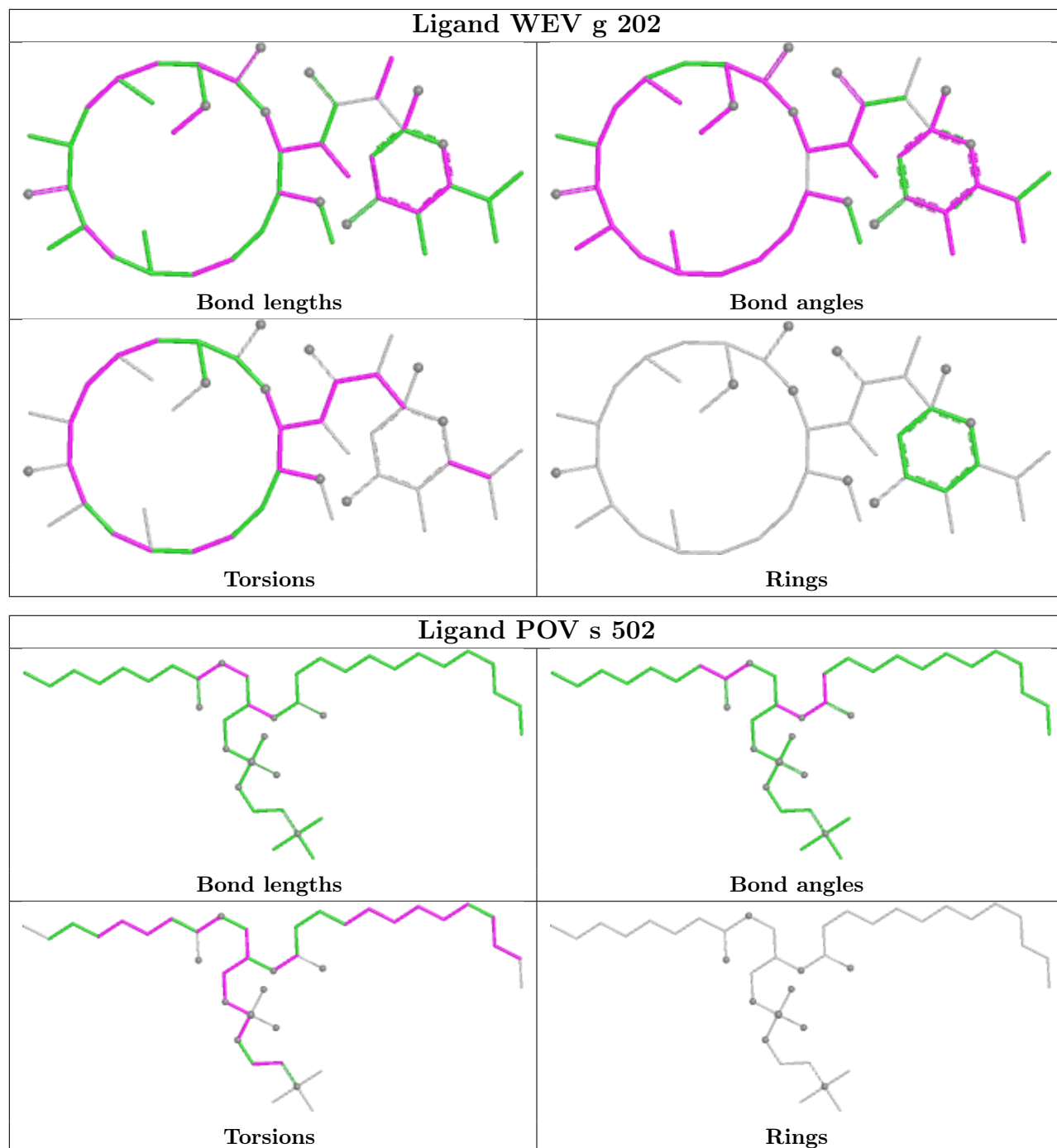
There are no ring outliers.

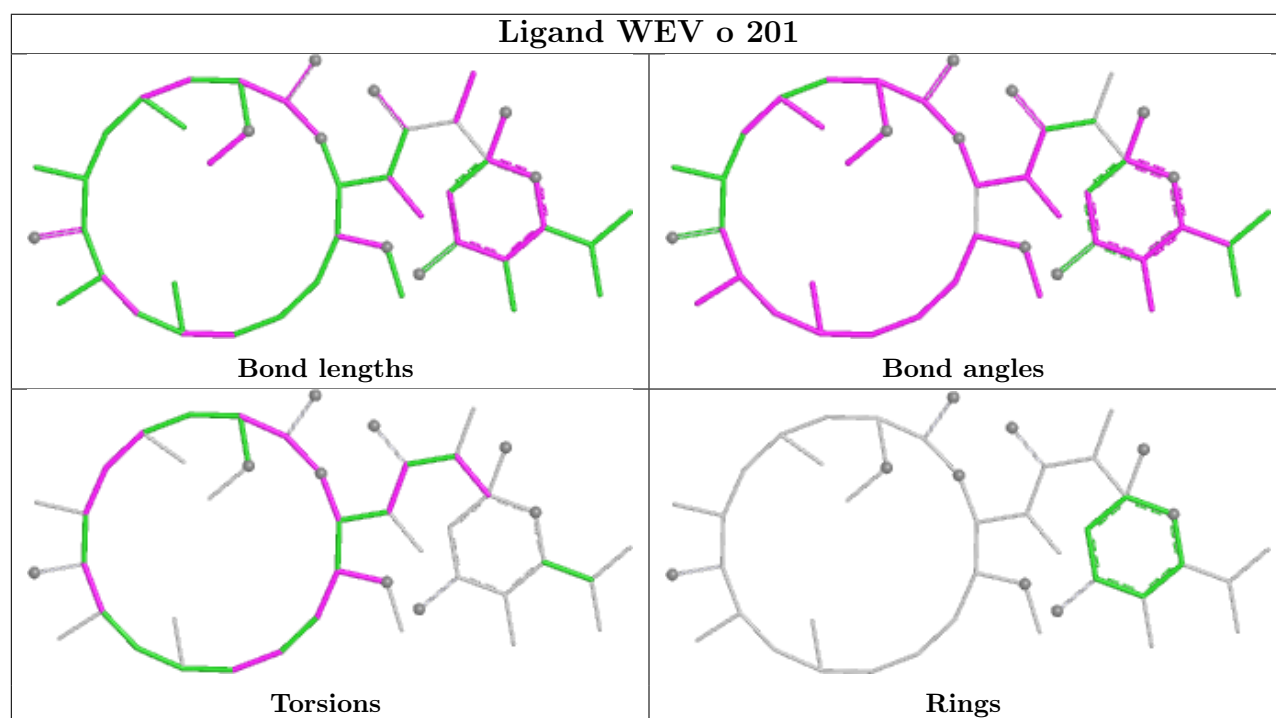
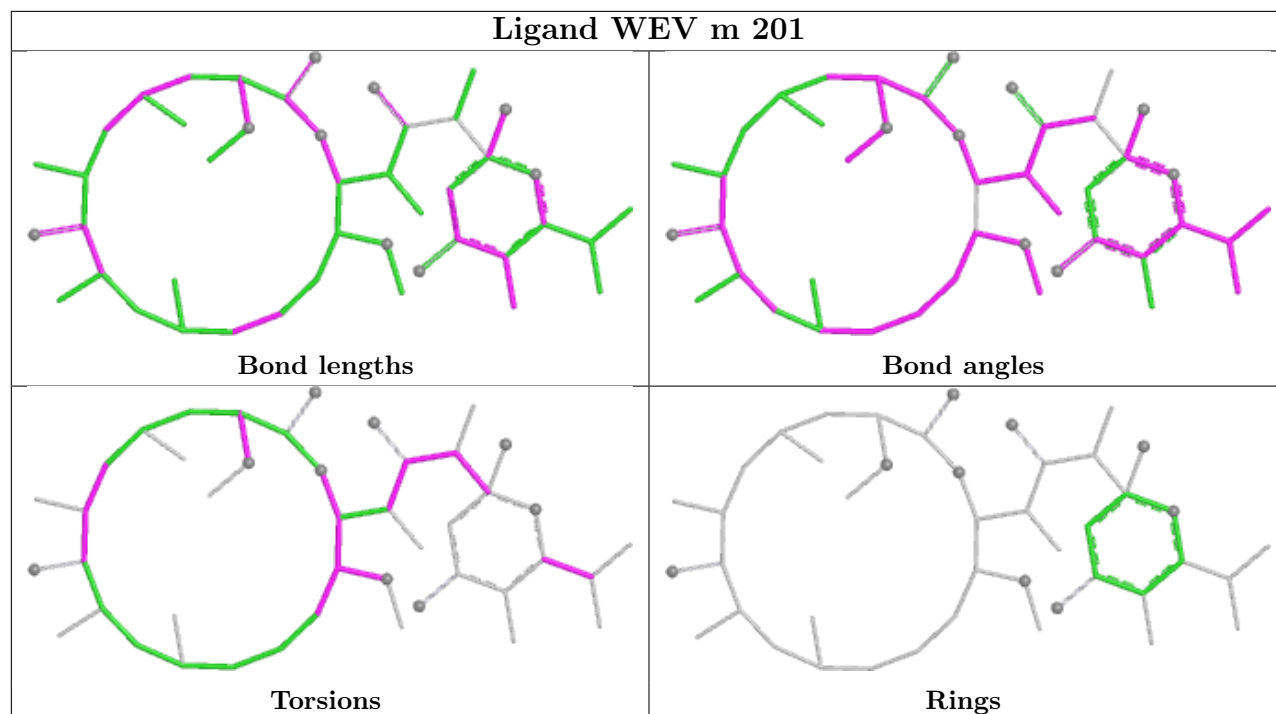
1 monomer is involved in 2 short contacts:

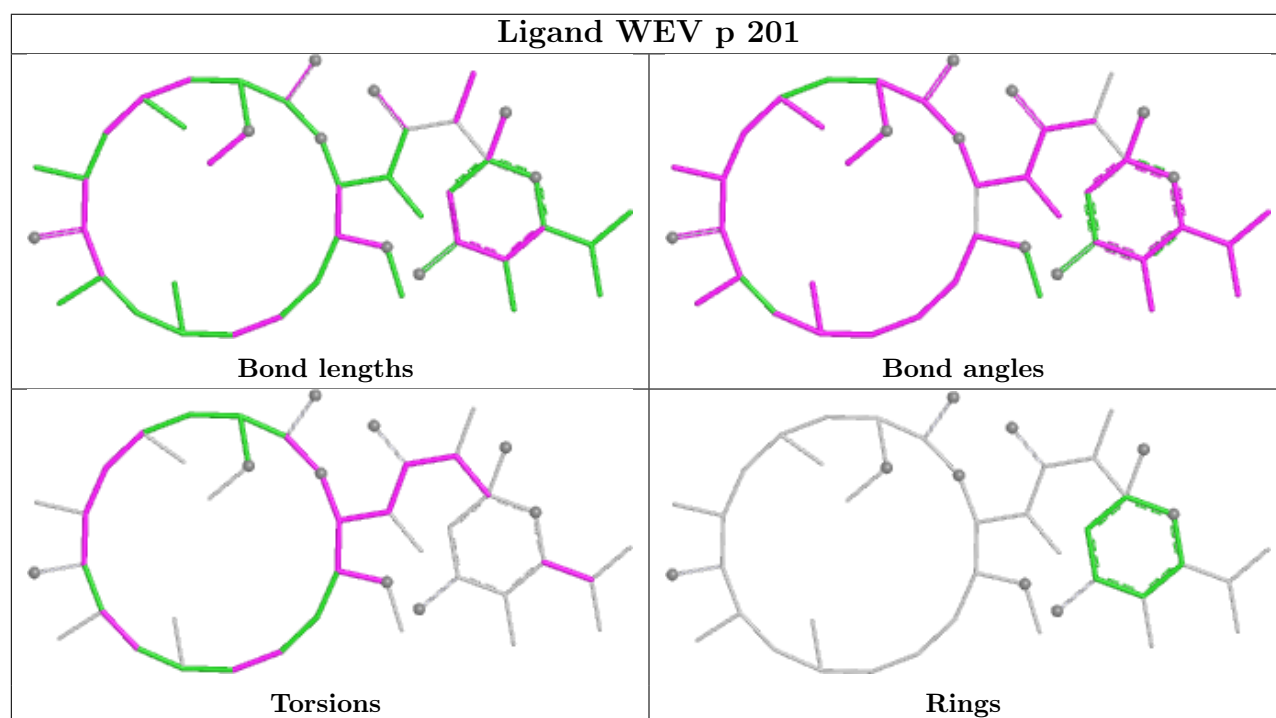
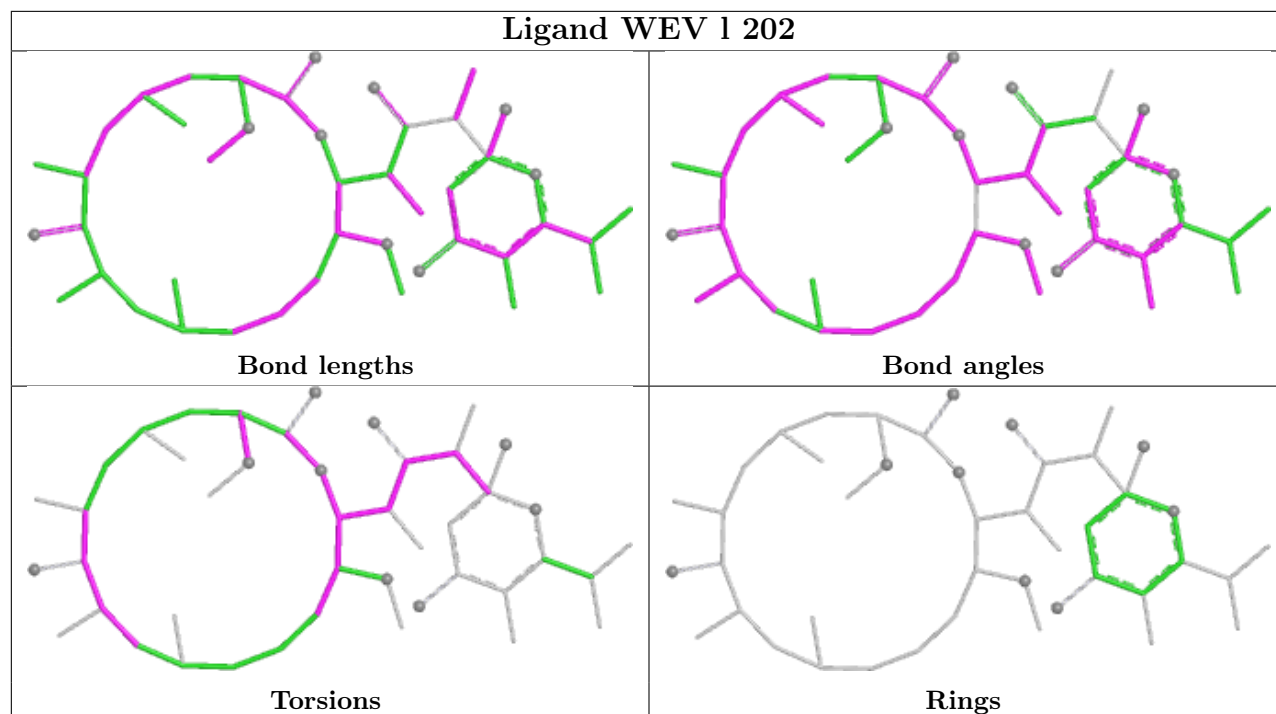
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	702	ADP	2	0

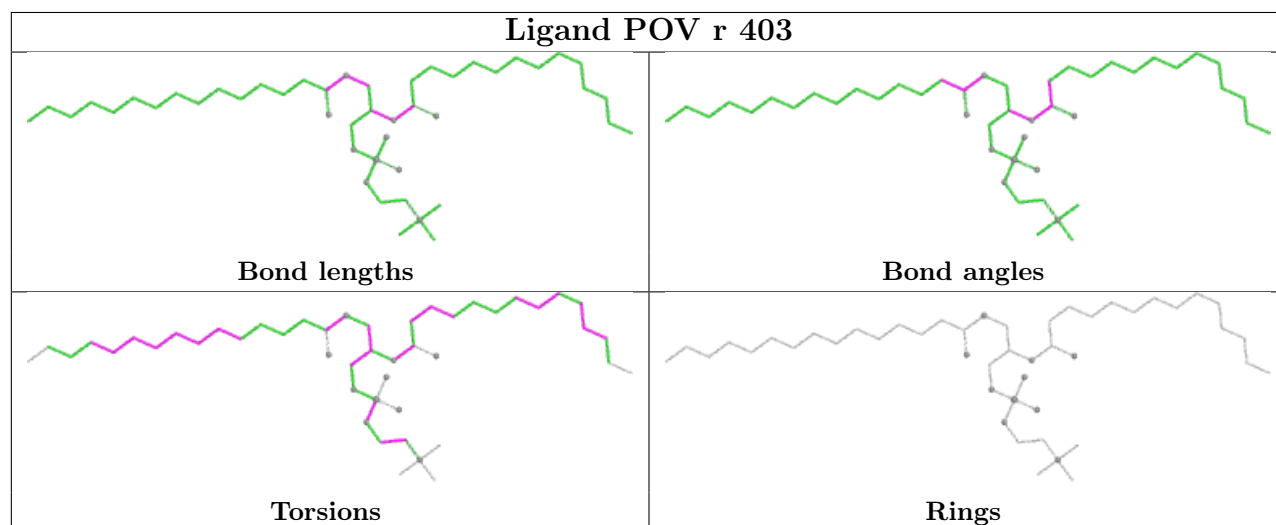
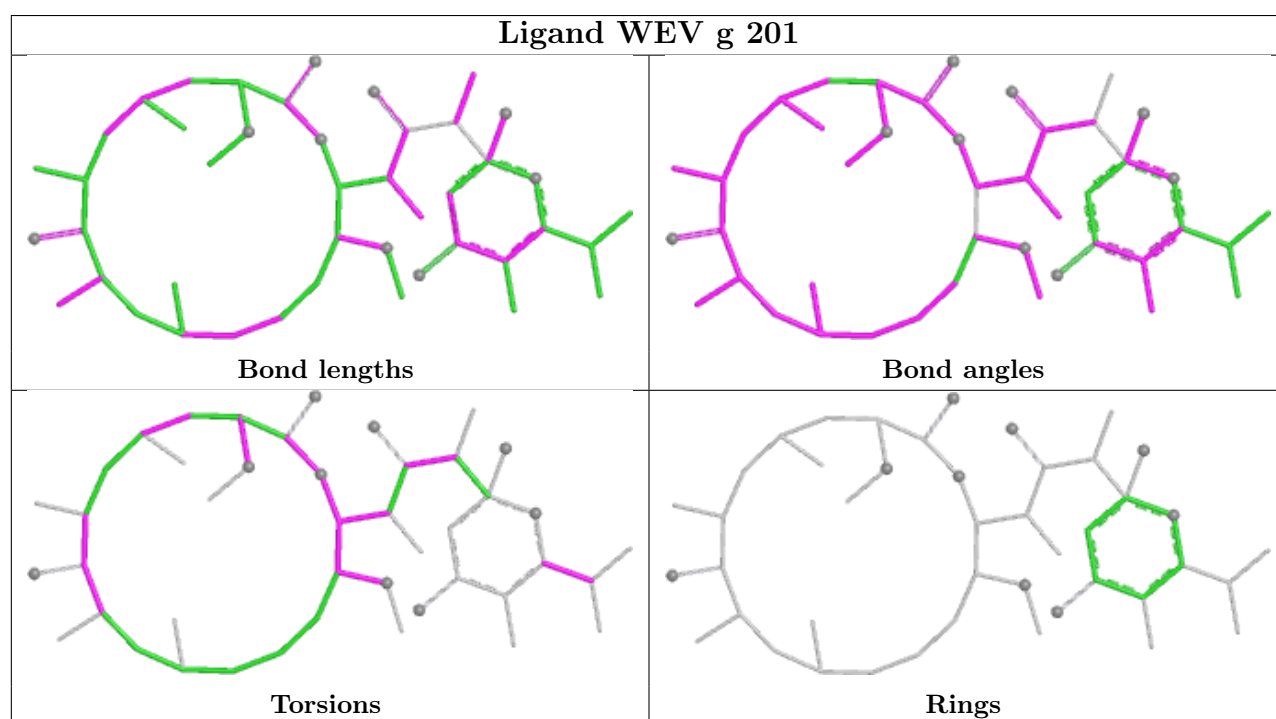
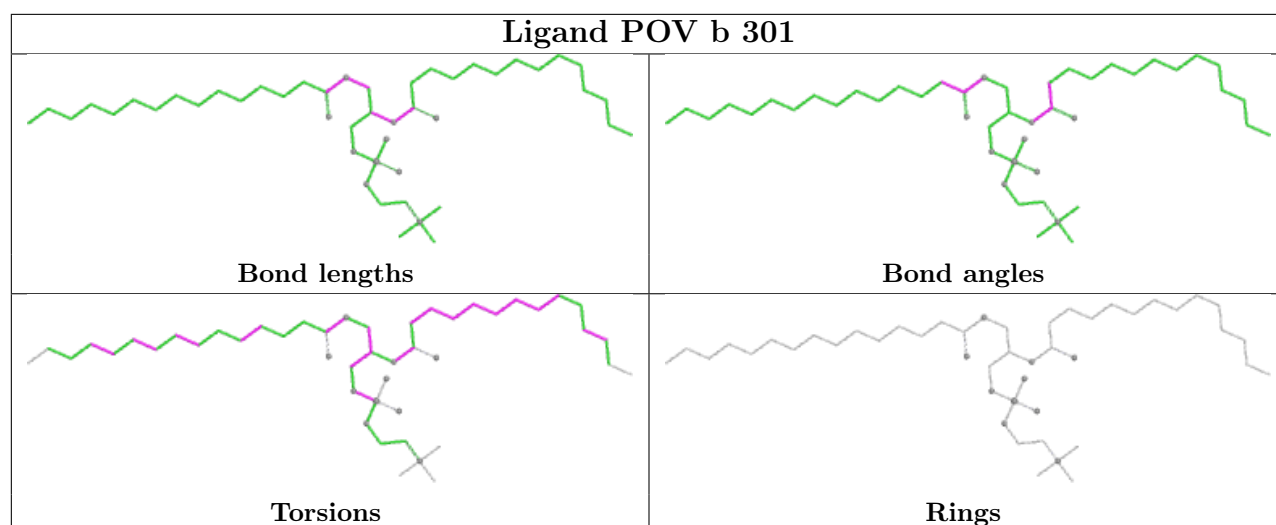
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

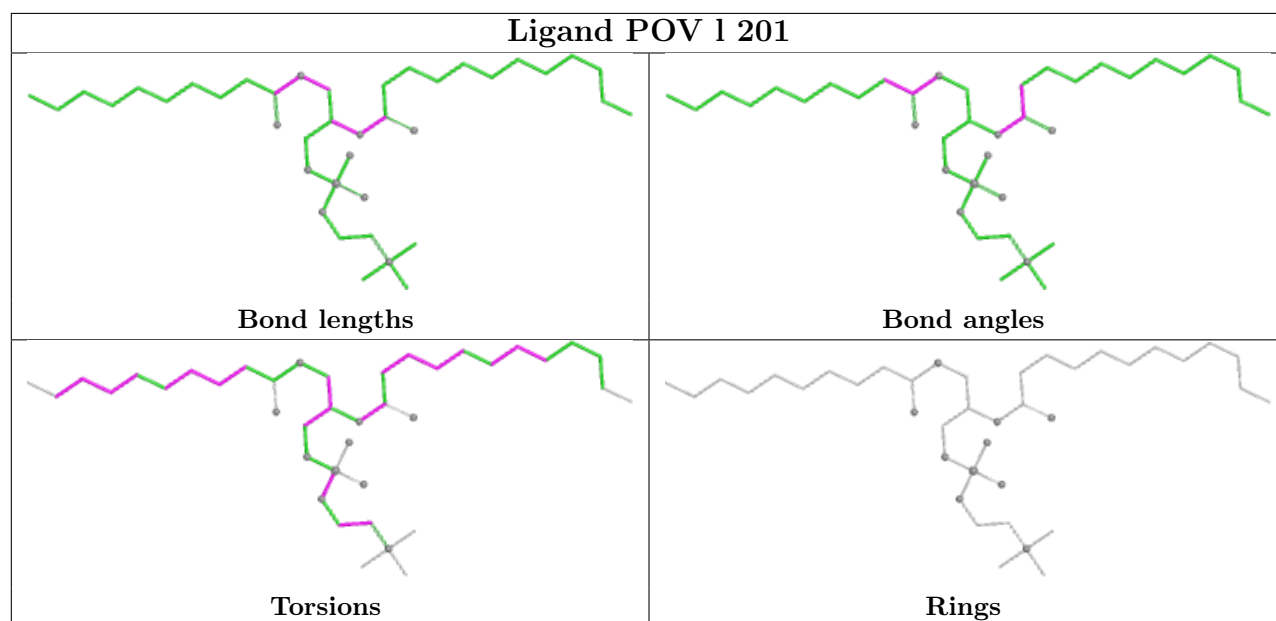
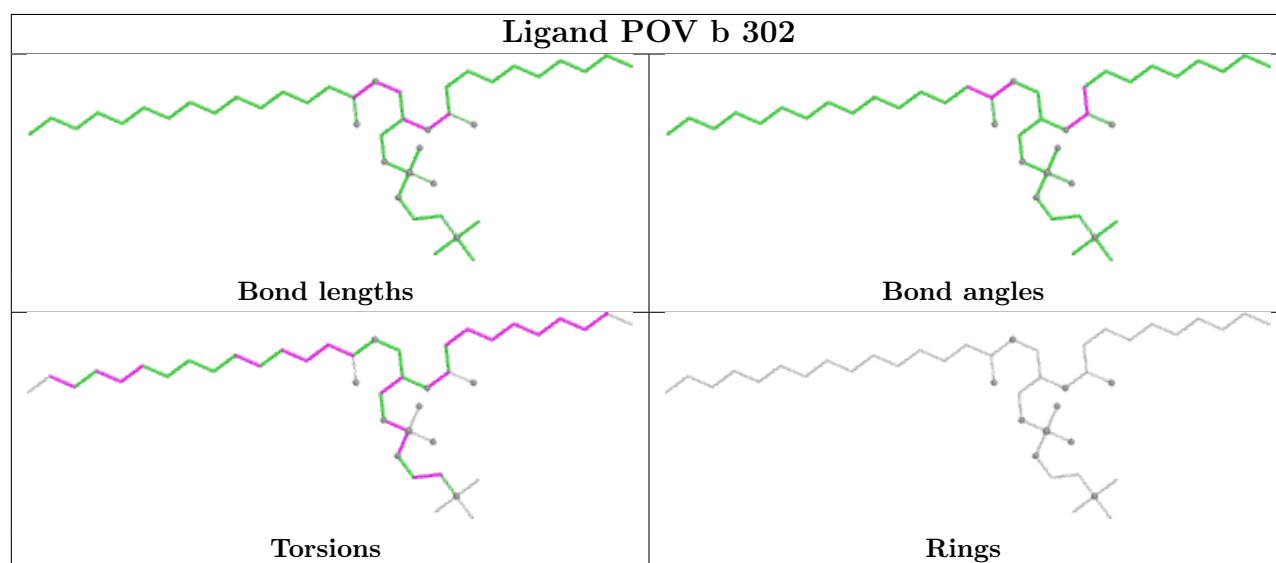
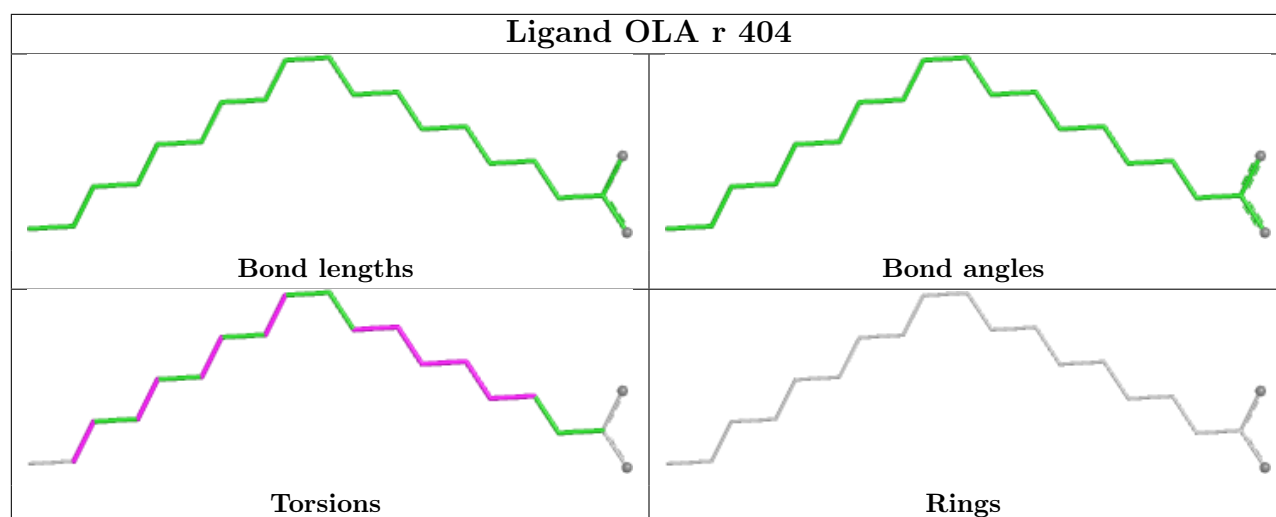


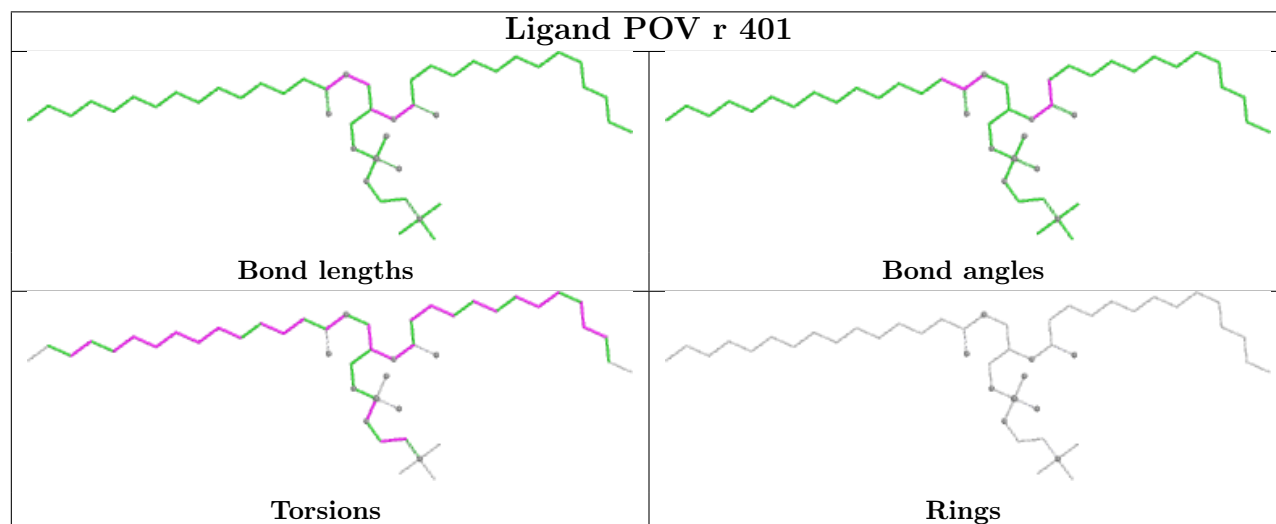
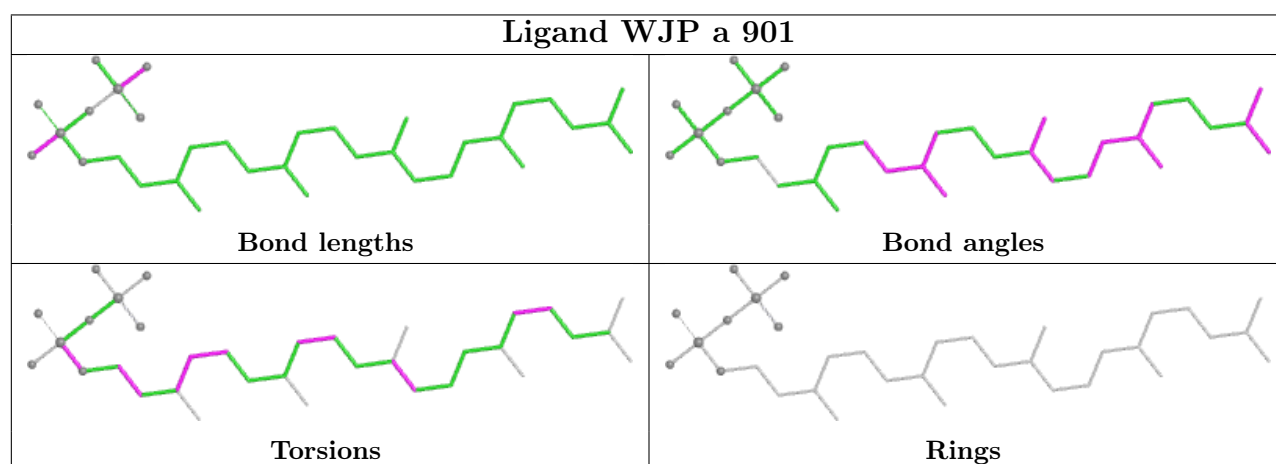
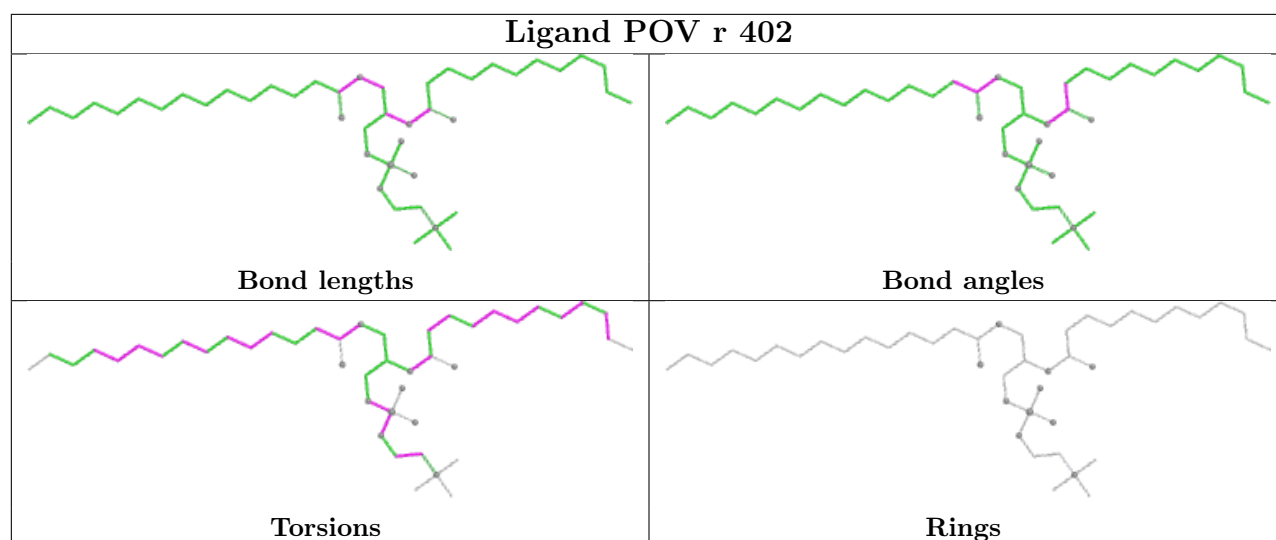


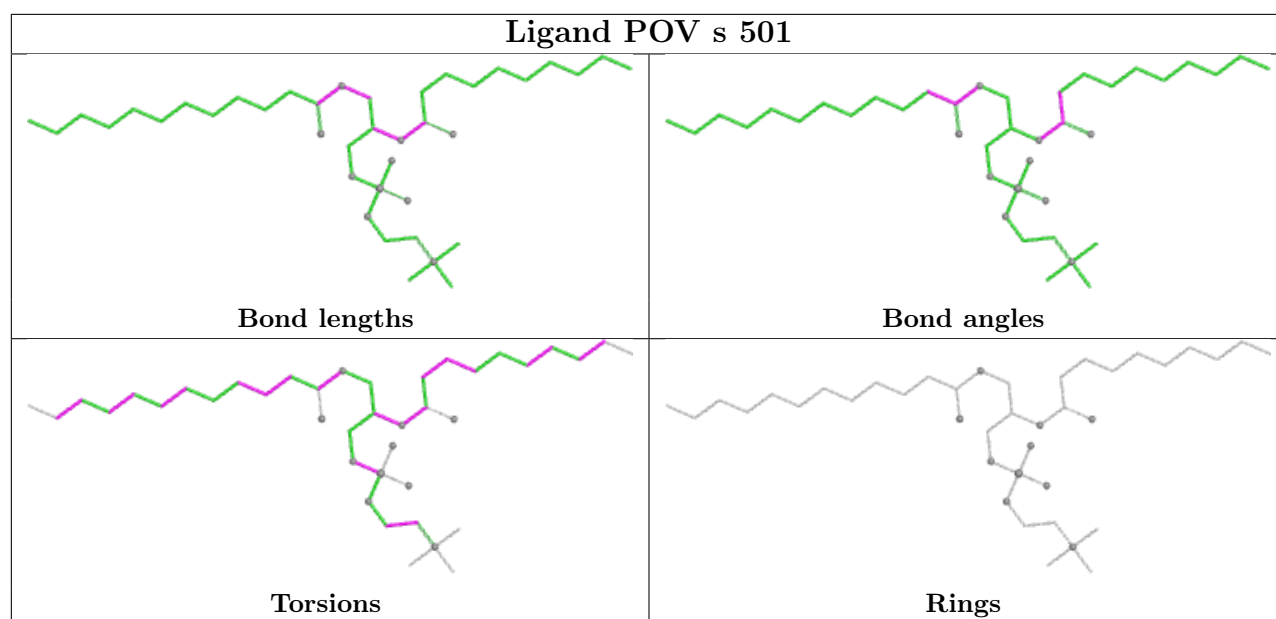












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

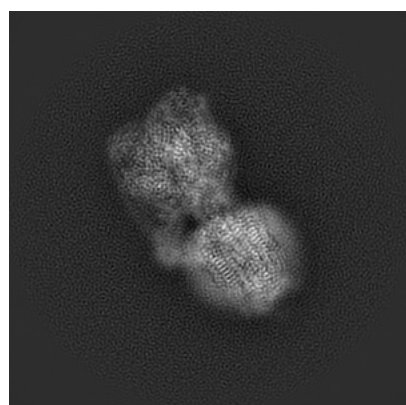
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22880. These allow visual inspection of the internal detail of the map and identification of artifacts.

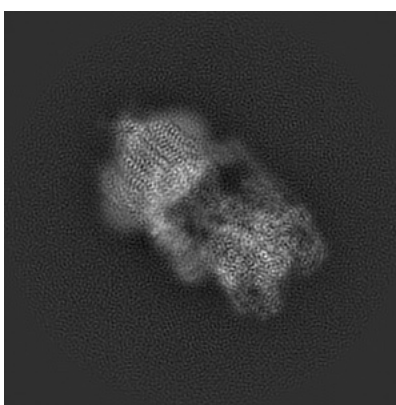
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

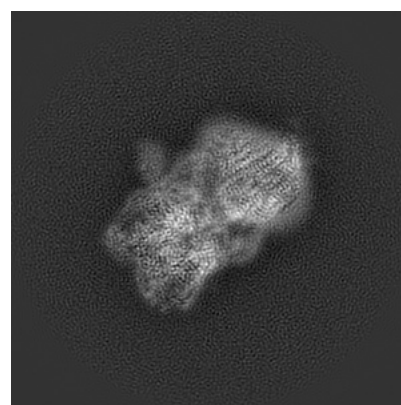
6.1.1 Primary map



X



Y

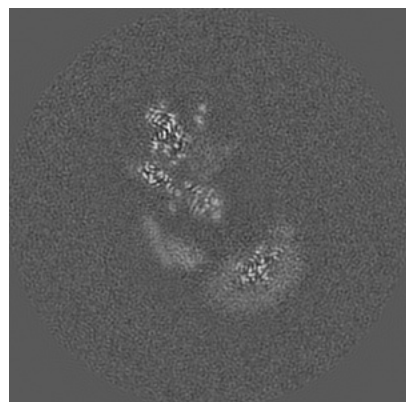


Z

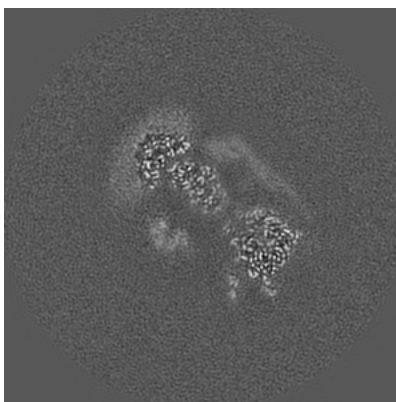
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

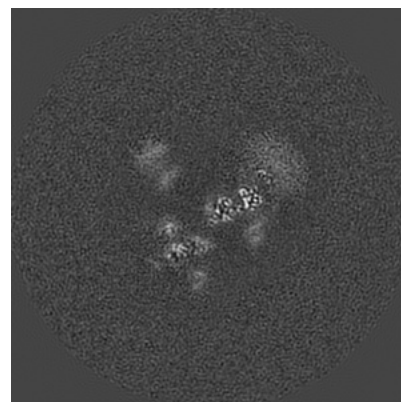
6.2.1 Primary map



X Index: 248



Y Index: 248

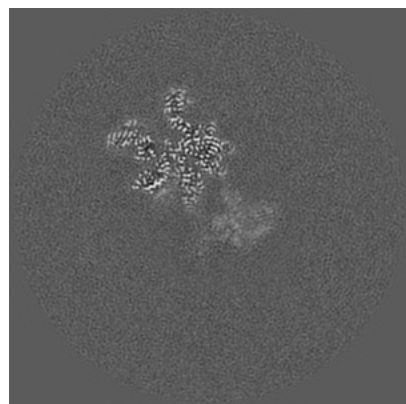


Z Index: 248

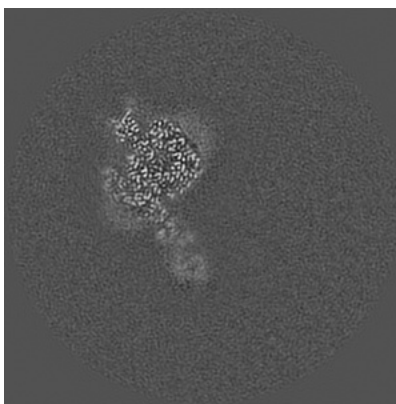
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

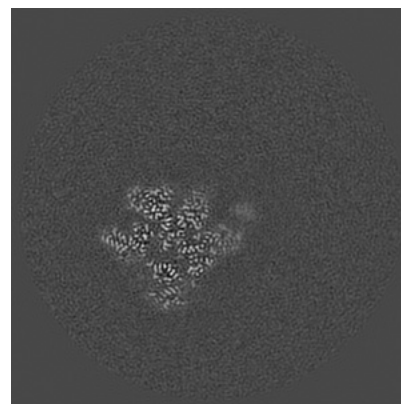
6.3.1 Primary map



X Index: 187



Y Index: 306

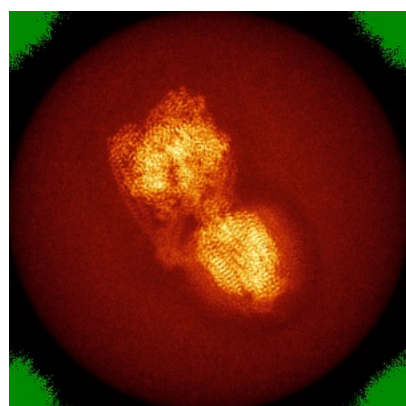


Z Index: 324

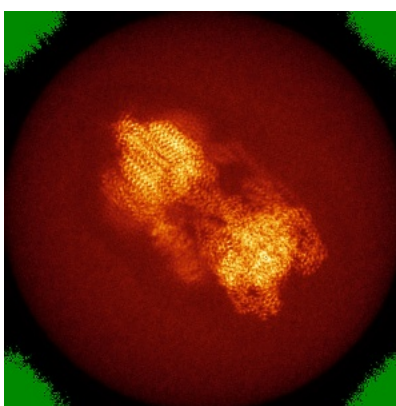
The images above show the largest variance slices of the map in three orthogonal directions.

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

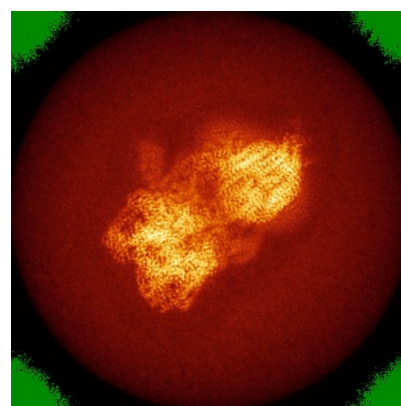
6.4.1 Primary map



X



Y

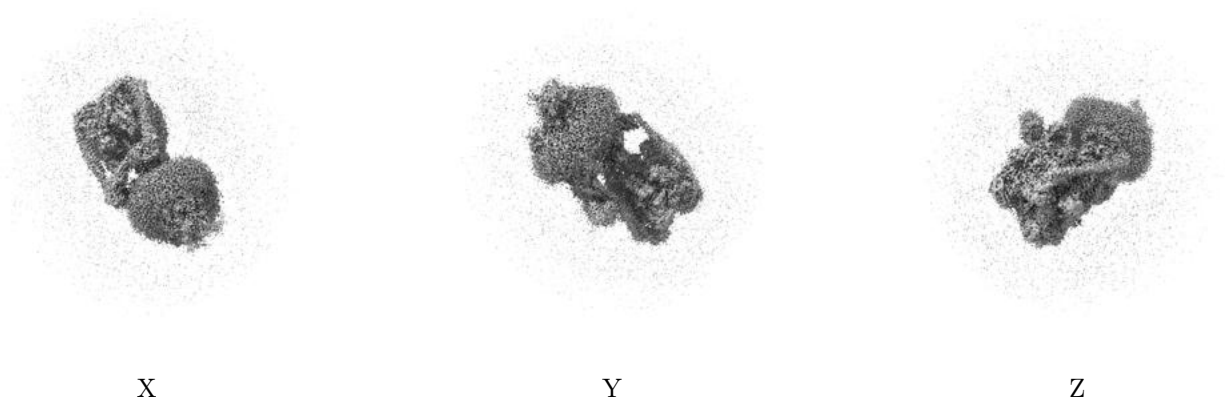


Z

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 3.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

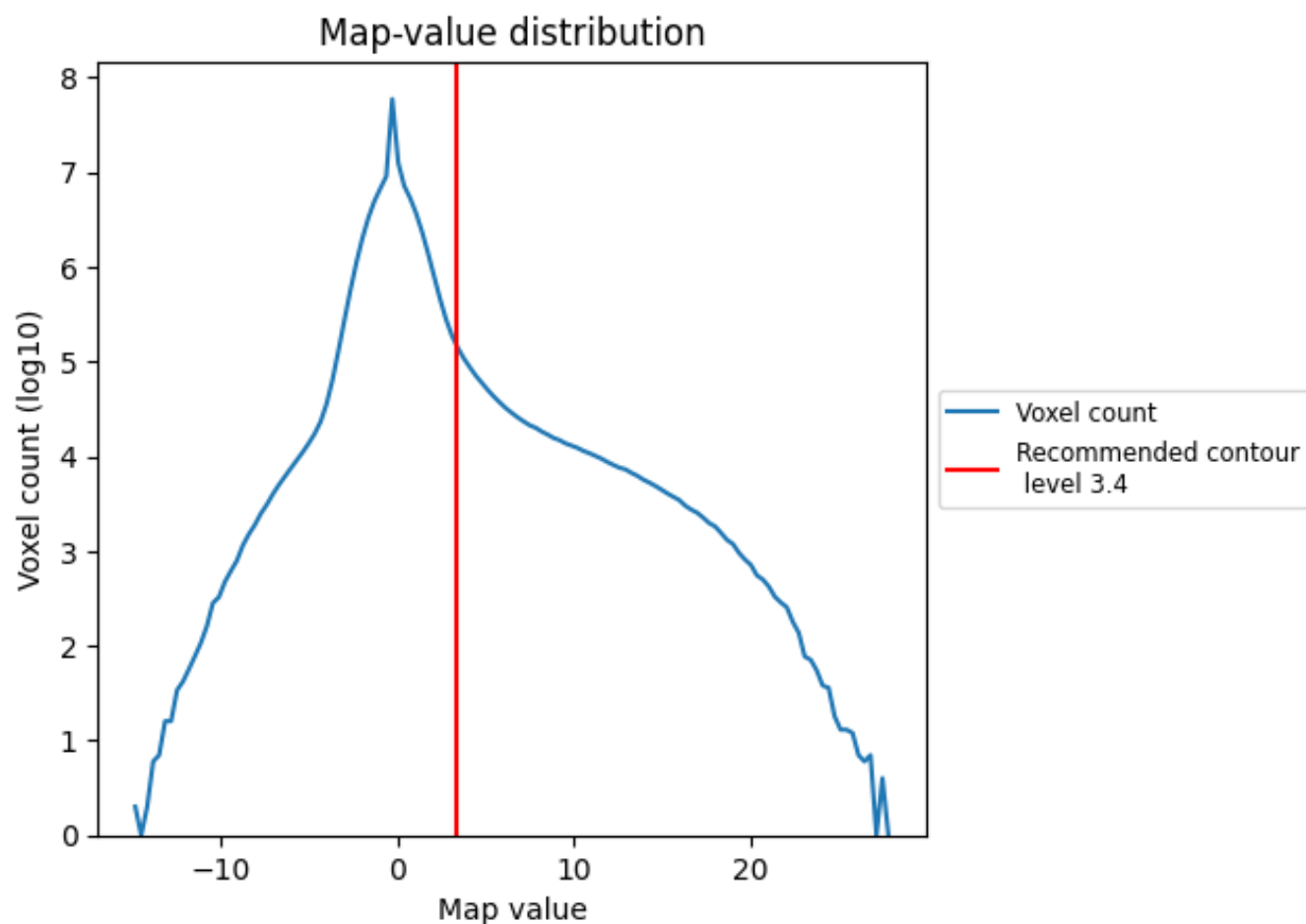
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

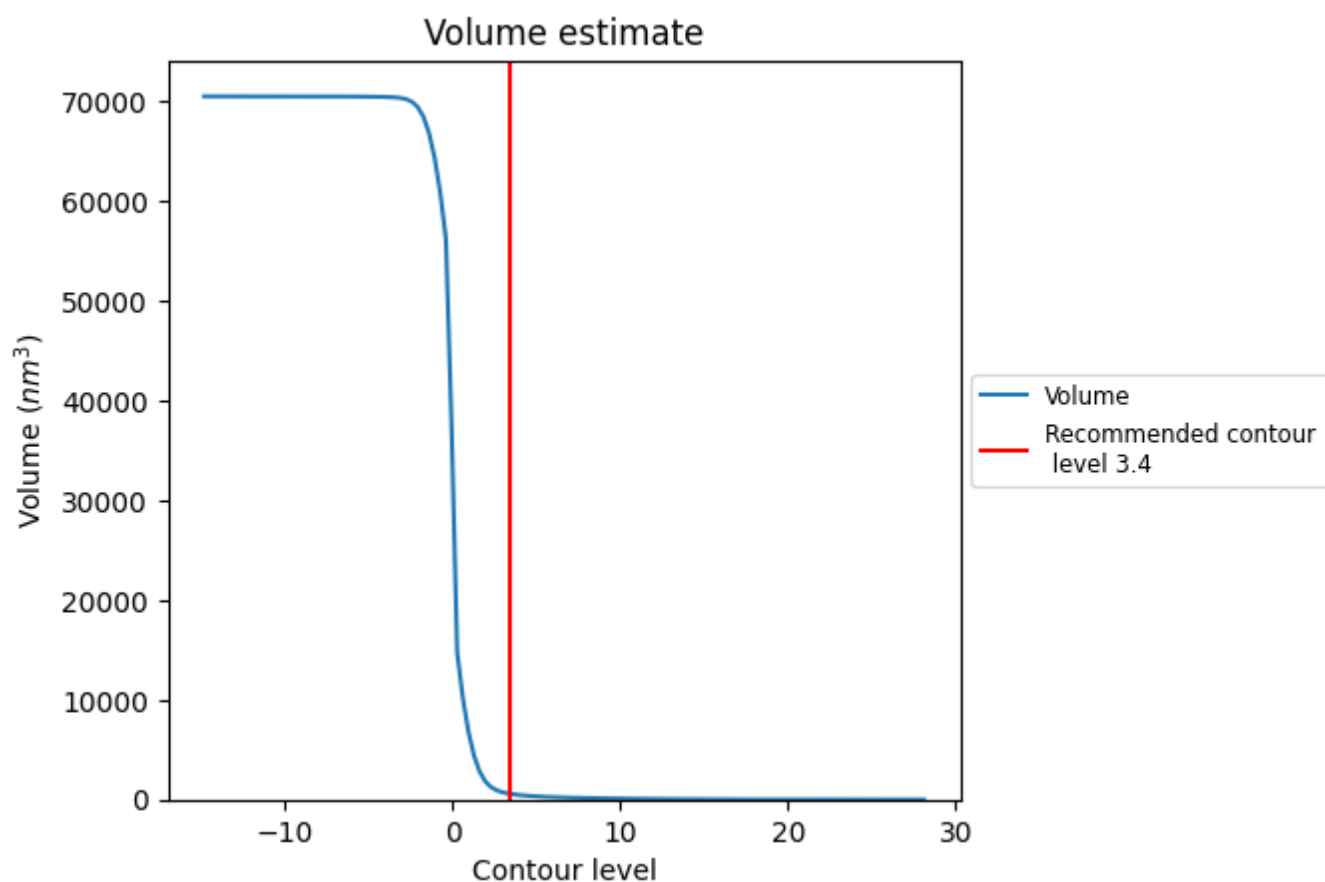
This section contains the results of statistical analysis of the map.

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.

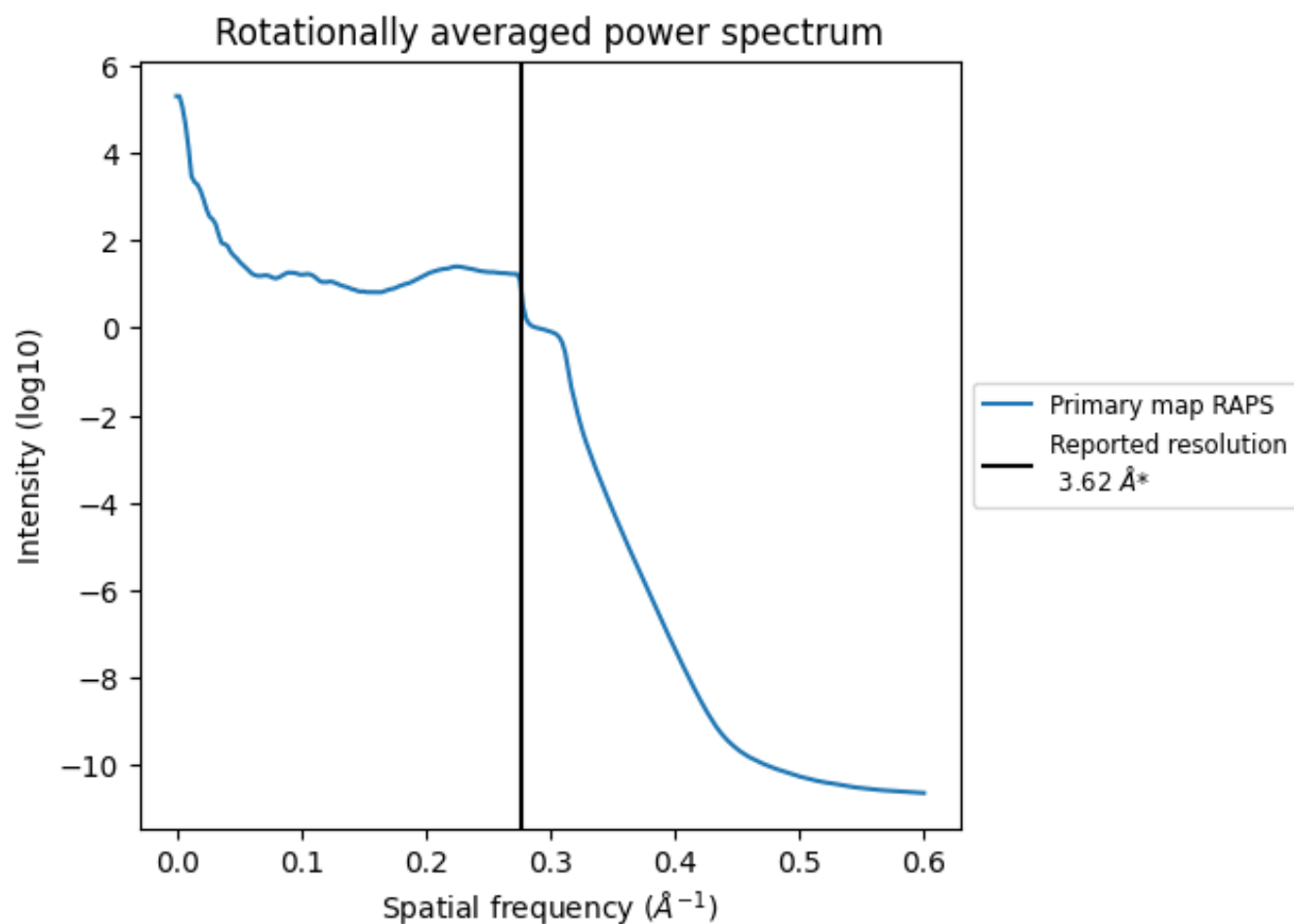
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 585 nm³; this corresponds to an approximate mass of 528 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 0.276 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

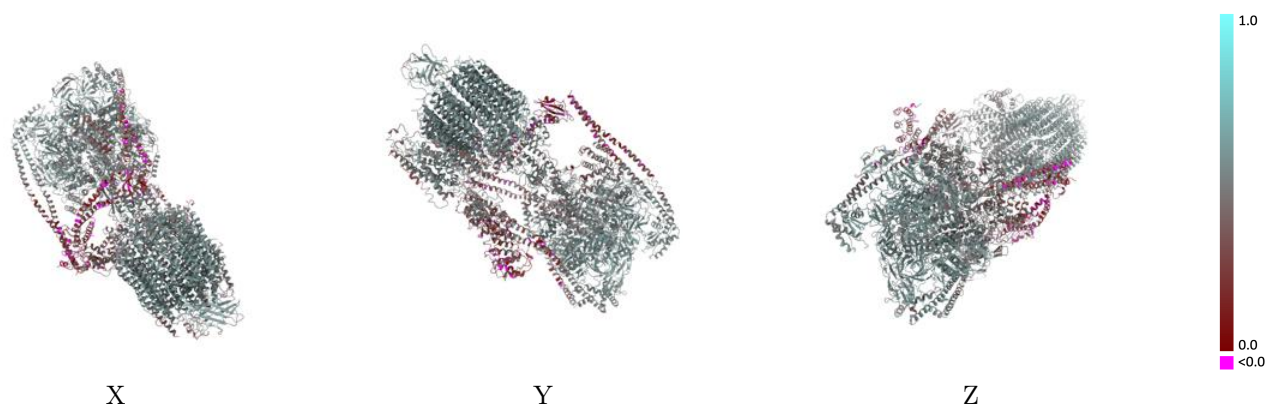
This section contains information regarding the fit between EMDB map EMD-22880 and PDB model 7KHR. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



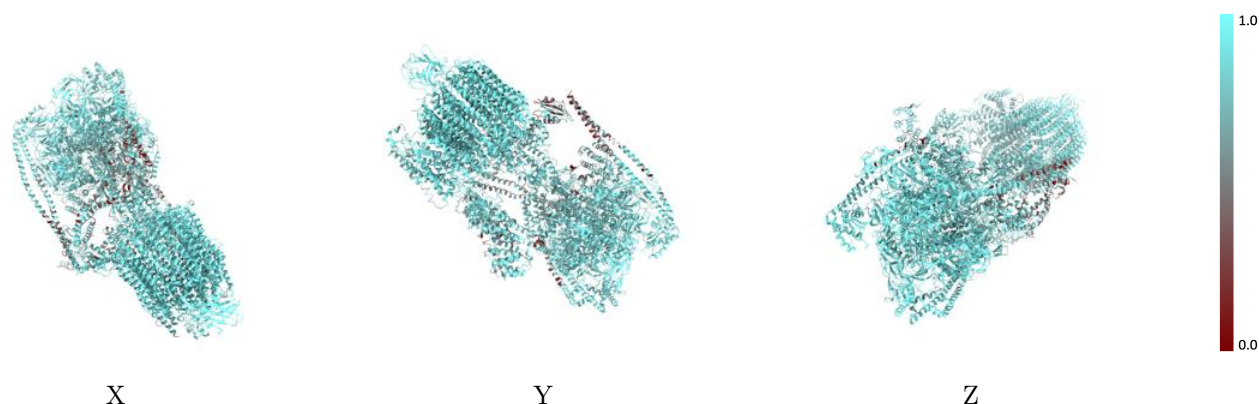
The images above show the 3D surface view of the map at the recommended contour level 3.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



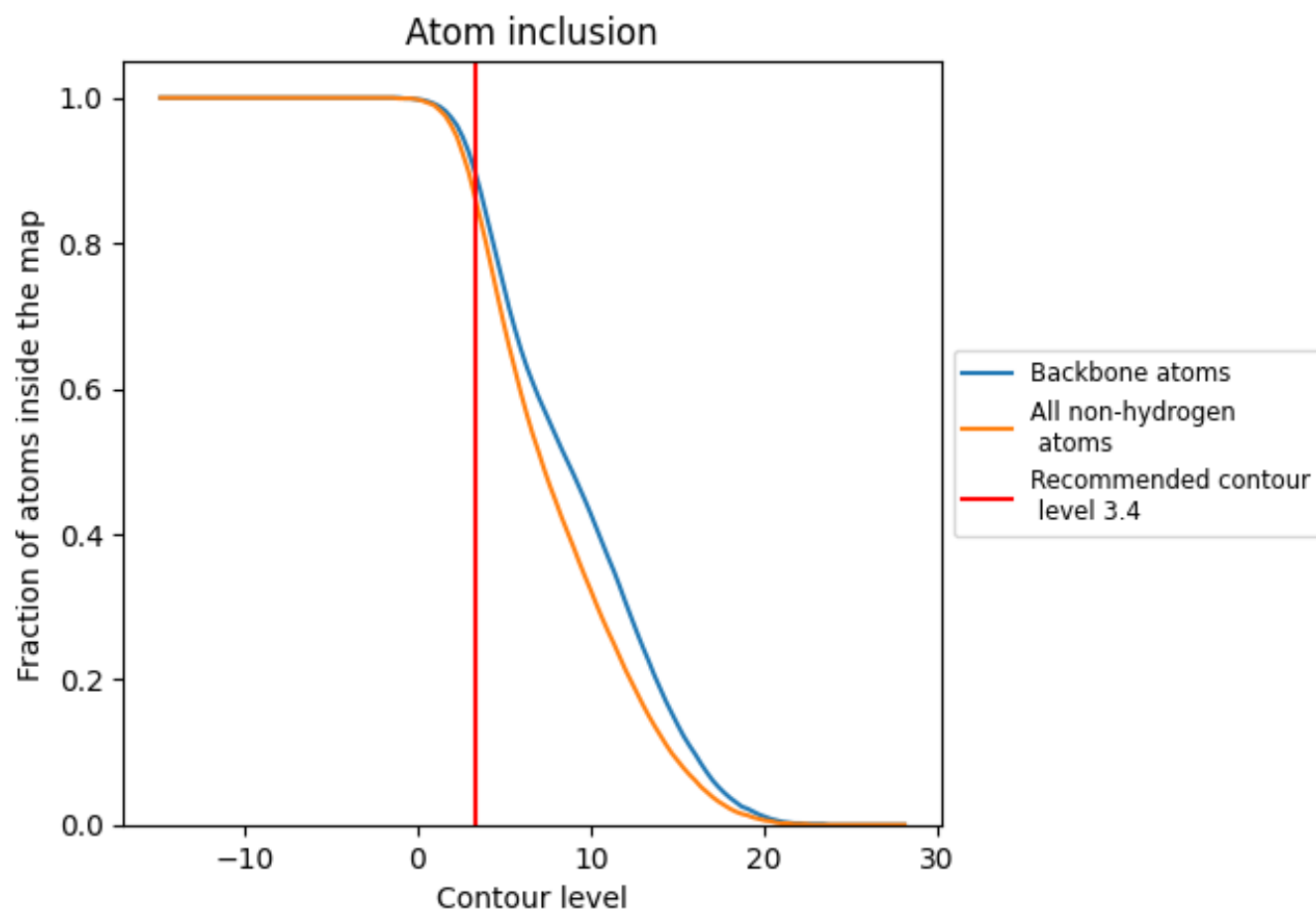
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.4930
A	 0.8310	 0.4920
B	 0.8770	 0.5260
C	 0.8760	 0.5350
D	 0.9050	 0.5510
E	 0.8930	 0.5470
F	 0.8690	 0.5360
G	 0.6190	 0.2050
H	 0.8420	 0.5030
I	 0.8060	 0.4680
J	 0.8290	 0.4860
K	 0.8500	 0.4780
L	 0.8130	 0.4630
M	 0.7340	 0.3860
N	 0.7700	 0.4100
O	 0.7350	 0.4000
P	 0.7360	 0.2810
Q	 0.3640	 0.2250
a	 0.8260	 0.4340
b	 0.9300	 0.5620
c	 0.9290	 0.5530
d	 0.8750	 0.5200
e	 0.7930	 0.4350
f	 0.7640	 0.4370
g	 0.9400	 0.5550
k	 0.9320	 0.5510
l	 0.9280	 0.5530
m	 0.9230	 0.5500
n	 0.9170	 0.5410
o	 0.9290	 0.5500
p	 0.9190	 0.5490
q	 0.9320	 0.5560
r	 0.9230	 0.5530
s	 0.9150	 0.5210
t	 0.7810	 0.4220

