



Full wwPDB EM Validation Report ⓘ

Oct 20, 2024 – 10:35 PM EDT

PDB ID : 7UNF
EMDB ID : EMD-26623
Title : CryoEM structure of a mEAK7 bound human V-ATPase complex
Authors : Wang, R.; Li, X.
Deposited on : 2022-04-10
Resolution : 4.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

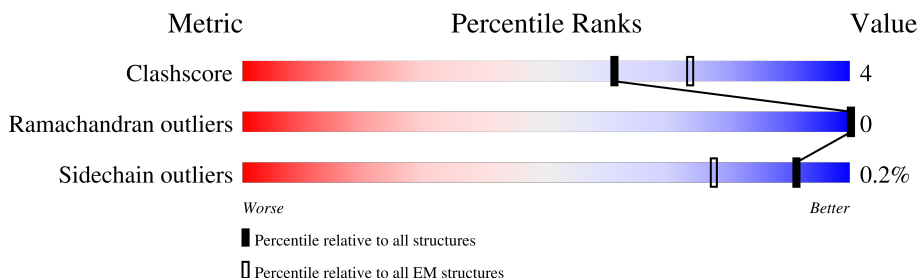
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.08 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.




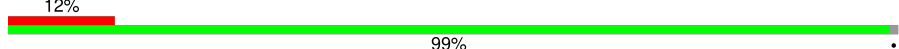
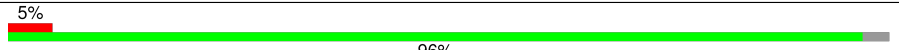
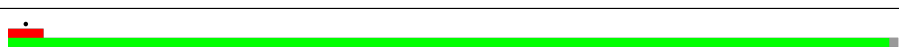
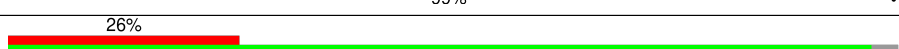
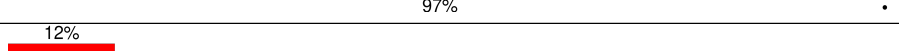
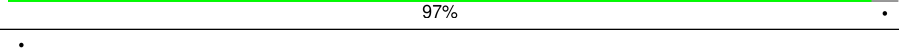
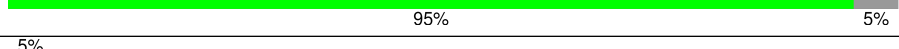

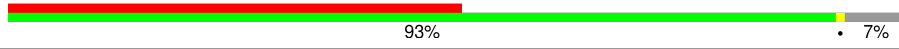

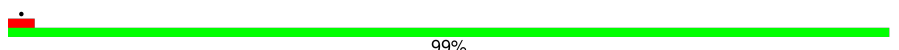
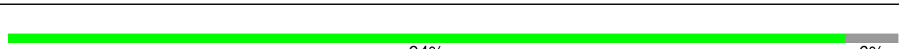


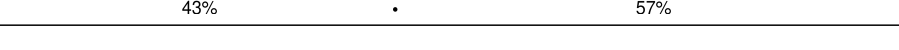

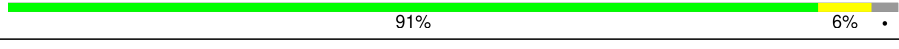
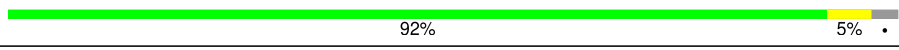
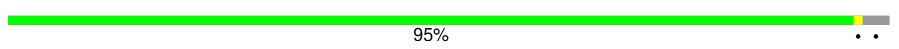



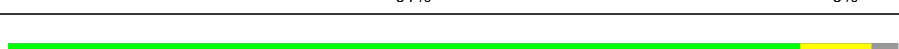
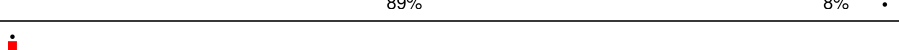
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	856	 5% 88% 12%
2	U	456	 15% 79% 15% 6%
3	L	617	 88% 9%
3	M	617	 84% 13%
3	N	617	 89% 8%
4	O	511	 84% 8% 8%
4	P	511	 82% 9% 8%
4	Q	511	 79% 12% 8%


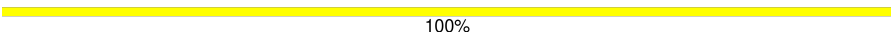
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Mol	Chain	Length	Quality of chain
5	D	247	
6	b	226	
6	c	226	
6	d	226	
7	e	118	
7	f	118	
7	g	118	
8	F	119	
9	C	382	
10	H	483	
11	k	351	
12	m	81	
13	n	137	
14	s	470	
15	r	345	
16	0	155	
16	2	155	
16	3	155	
16	4	155	
16	5	155	
16	6	155	
16	7	155	
16	8	155	
16	9	155	
17	1	205	

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Mol	Chain	Length	Quality of chain
18	t	8	 <div>25% 75%</div>
19	w	2	 <div>100%</div>

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
20	ADP	M	701	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 66971 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 116 kDa subunit a 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	752	Total	C	N	O	S	0	0
			6127	4000	1016	1066	45		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	252	ARG	PRO	conflict	UNP Q9HBG4
a	841	ASP	-	expression tag	UNP Q9HBG4
a	842	TYR	-	expression tag	UNP Q9HBG4
a	843	LYS	-	expression tag	UNP Q9HBG4
a	844	ASP	-	expression tag	UNP Q9HBG4
a	845	ASP	-	expression tag	UNP Q9HBG4
a	846	ASP	-	expression tag	UNP Q9HBG4
a	847	ASP	-	expression tag	UNP Q9HBG4
a	848	LYS	-	expression tag	UNP Q9HBG4
a	849	ASP	-	expression tag	UNP Q9HBG4
a	850	TYR	-	expression tag	UNP Q9HBG4
a	851	LYS	-	expression tag	UNP Q9HBG4
a	852	ASP	-	expression tag	UNP Q9HBG4
a	853	ASP	-	expression tag	UNP Q9HBG4
a	854	ASP	-	expression tag	UNP Q9HBG4
a	855	ASP	-	expression tag	UNP Q9HBG4
a	856	LYS	-	expression tag	UNP Q9HBG4

- Molecule 2 is a protein called KIAA1609 protein, isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	427	Total	C	N	O	S	0	0
			3365	2119	594	631	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
3	M	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		
3	N	600	Total	C	N	O	S	0	0
			4656	2952	786	890	28		

- Molecule 4 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		
4	P	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		
4	Q	468	Total	C	N	O	S	0	0
			3666	2325	625	696	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	213	Total	C	N	O	S	0	0
			1717	1090	310	312	5		

- Molecule 6 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	223	Total	C	N	O	S	0	0
			1809	1134	320	345	10		
6	c	219	Total	C	N	O	S	0	0
			1782	1120	316	336	10		
6	d	224	Total	C	N	O	S	0	0
			1817	1140	321	346	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
7	f	114	Total	C	N	O	S	0	0
			938	573	179	183	3		
7	g	112	Total	C	N	O	S	0	0
			923	565	176	179	3		

- Molecule 8 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	108	Total	C	N	O	S	0	0
			856	538	155	162	1		

- Molecule 9 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	C	356	Total	C	N	O	0	0
			1770	1058	356	356		

- Molecule 10 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	H	425	Total	C	N	O	0	0
			2111	1261	425	425		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	350	Total	C	N	O	S	0	0
			2836	1829	462	531	14		

- Molecule 12 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	76	Total	C	N	O	S	0	0
			621	430	94	92	5		

- Molecule 13 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	85	Total	C	N	O	S	0	0
			658	434	102	115	7		

- Molecule 14 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	s	204	Total	C	N	O	S	0	0
			1662	1086	267	299	10		

- Molecule 15 is a protein called ATPase H(+)-transporting lysosomal accessory protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	45	Total	C	N	O	S	0	0
			377	256	53	65	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
16	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
16	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
16	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
16	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
16	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
16	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
16	7	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
16	0	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

- Molecule 17 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1	204	Total	C	N	O	S	0	0
			1498	990	238	259	11		

- Molecule 18 is an oligosaccharide called 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.



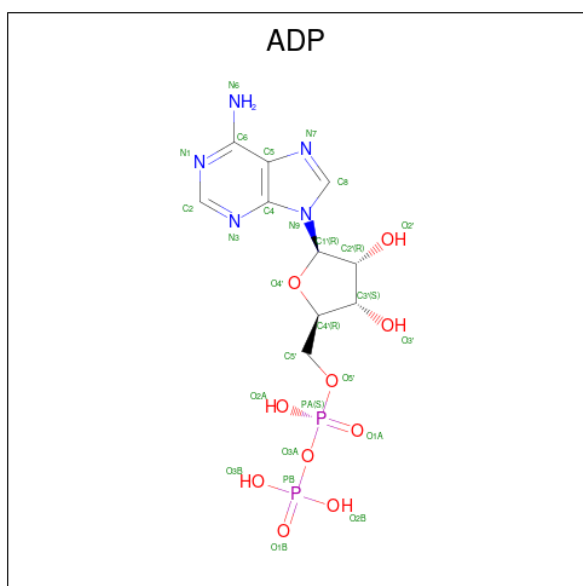
Mol	Chain	Residues	Atoms				AltConf	Trace
18	t	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 19 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
19	w	2	Total	C	O	0	0
			22	12	10		

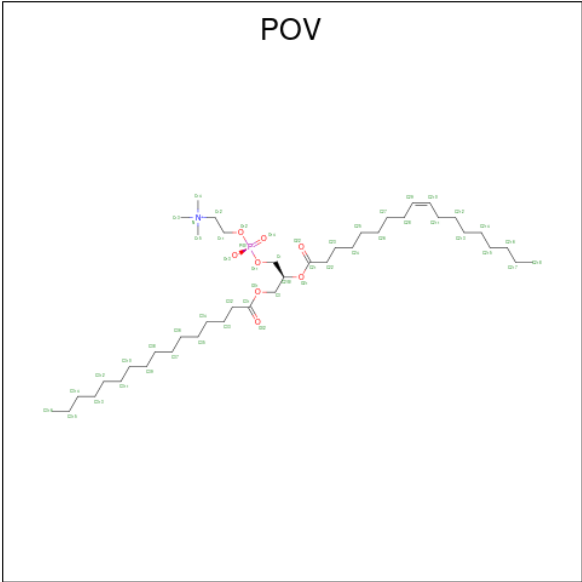
- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





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

- Molecule 22 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).

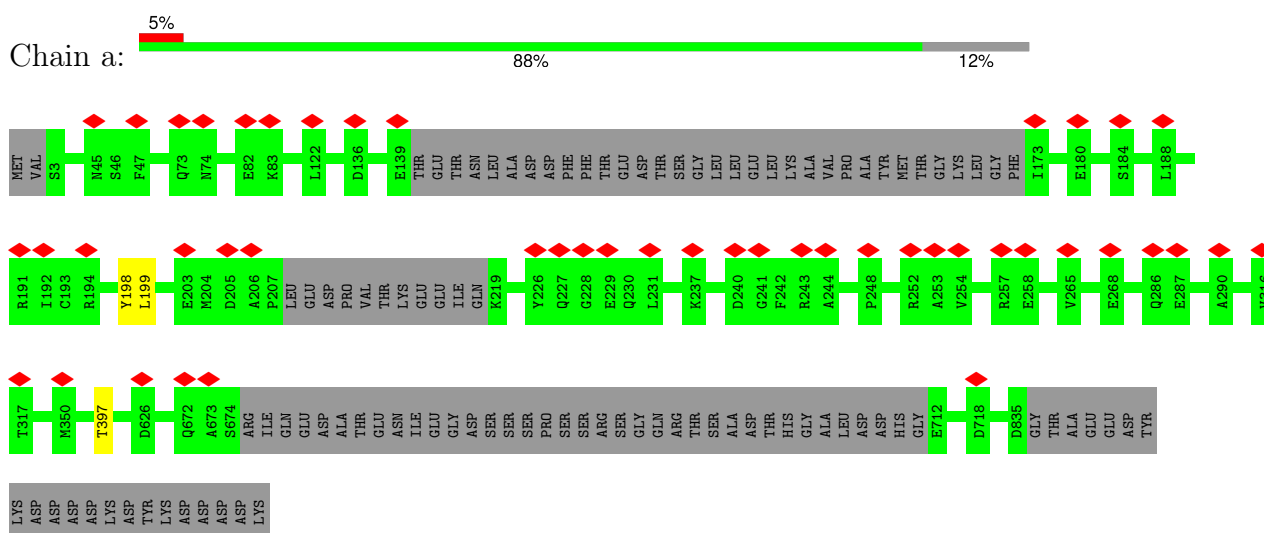


Mol	Chain	Residues	Atoms					AltConf
22	s	1	Total	C	N	O	P	0
			43	33	1	8	1	
22	s	1	Total	C	N	O	P	0
			46	36	1	8	1	
22	r	1	Total	C	N	O	P	0
			49	39	1	8	1	
22	r	1	Total	C	N	O	P	0
			44	34	1	8	1	
22	r	1	Total	C	N	O	P	0
			49	39	1	8	1	
22	8	1	Total	C	N	O	P	0
			34	24	1	8	1	
22	1	1	Total	C	N	O	P	0
			45	35	1	8	1	
22	1	1	Total	C	N	O	P	0
			38	28	1	8	1	
22	1	1	Total	C	N	O	P	0
			40	30	1	8	1	

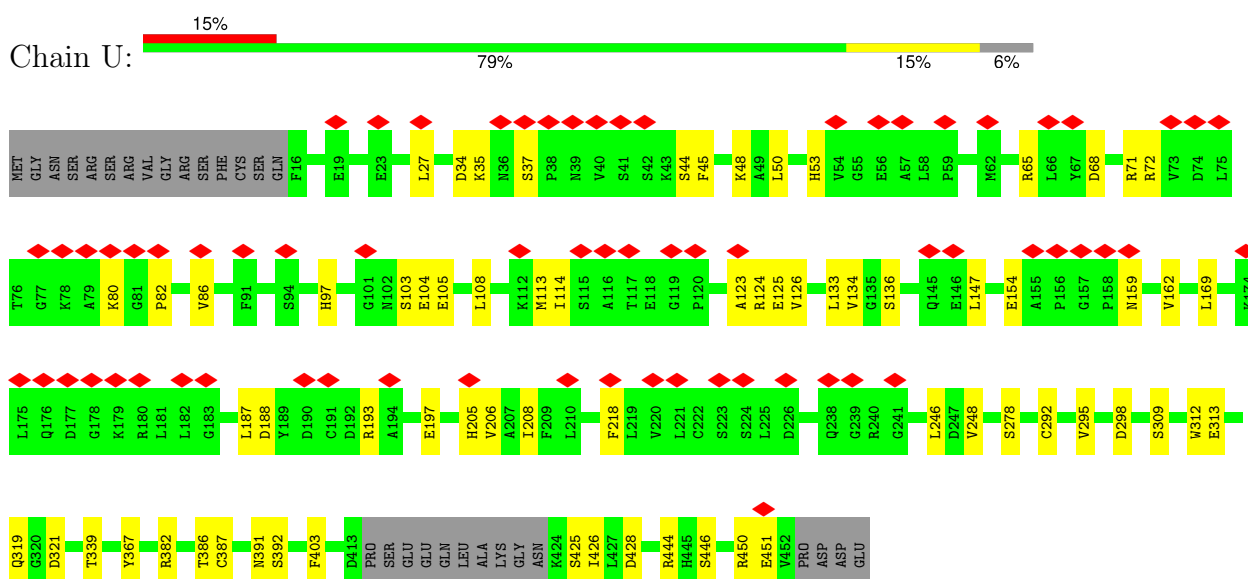
3 Residue-property plots

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 116 kDa subunit a 4

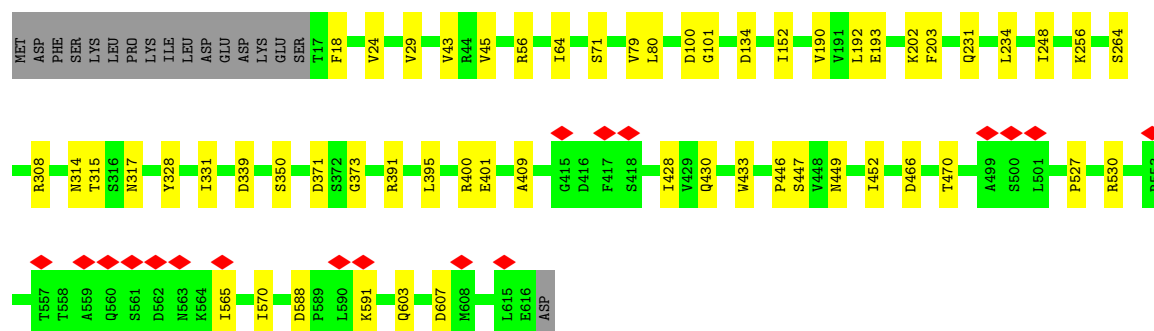


- Molecule 2: KIAA1609 protein, isoform CRA_a




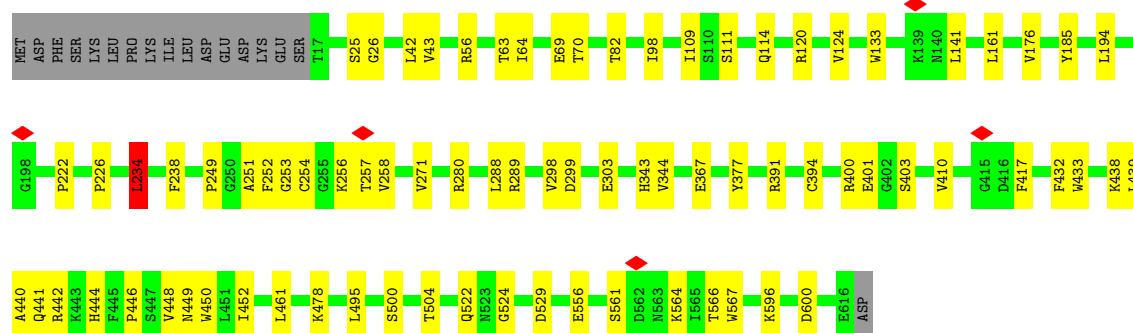
- Molecule 3: V-type proton ATPase catalytic subunit A

Chain L:  88% 9%




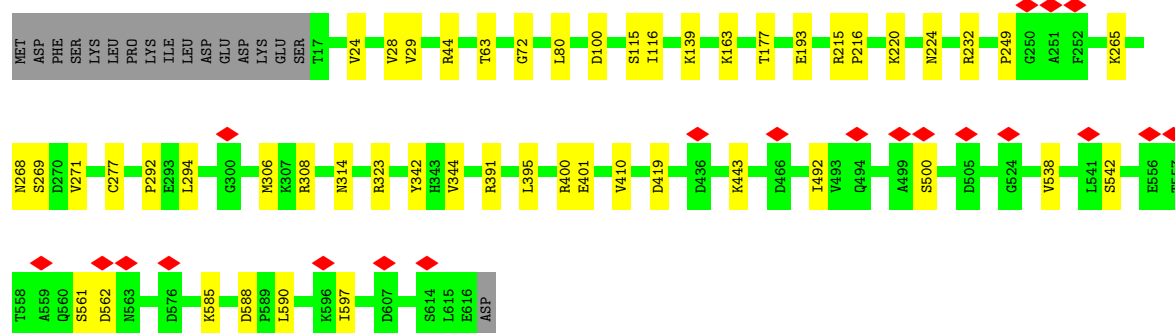
- Molecule 3: V-type proton ATPase catalytic subunit A

Chain M:  84% 13%




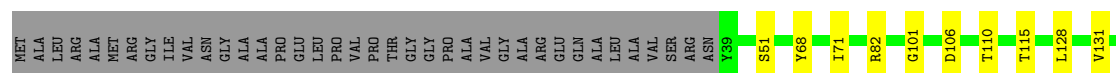
- Molecule 3: V-type proton ATPase catalytic subunit A

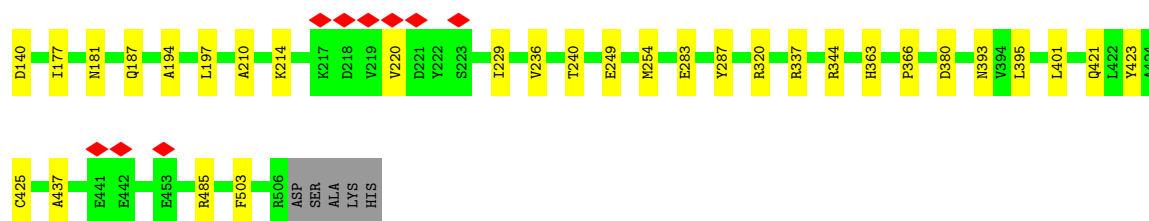
Chain N:  89% 8%



- Molecule 4: V-type proton ATPase subunit B, brain isoform

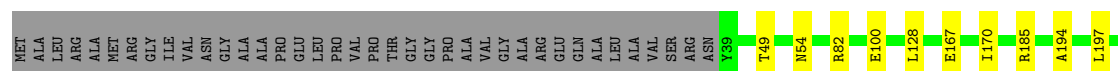
Chain O:  84% 8% 8%





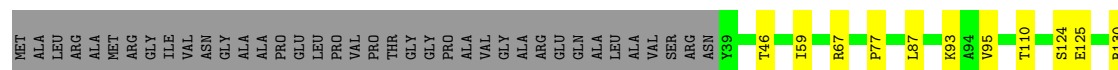
- Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain P: 82% 9% 8%



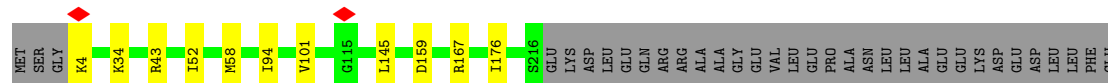
- Molecule 4: V-type proton ATPase subunit B, brain isoform

Chain Q: 79% 12% 8%



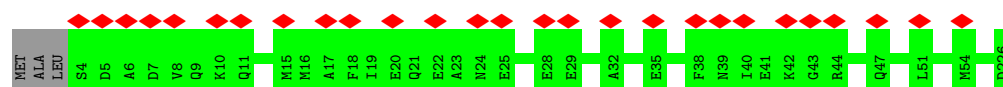
- Molecule 5: V-type proton ATPase subunit D

Chain D: 82% 14% 4%

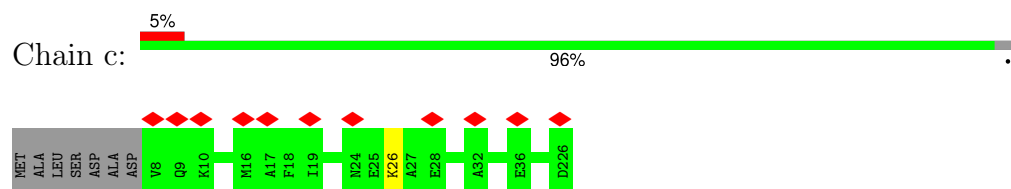


- Molecule 6: V-type proton ATPase subunit E 1

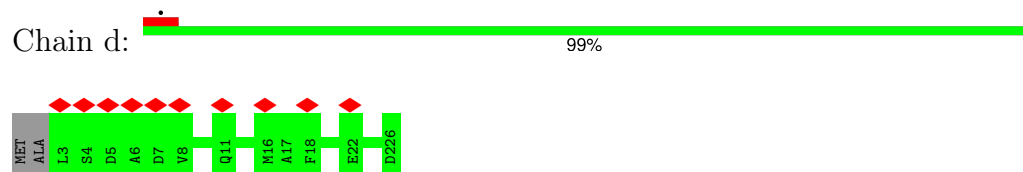
Chain b: 12% 99% 1%



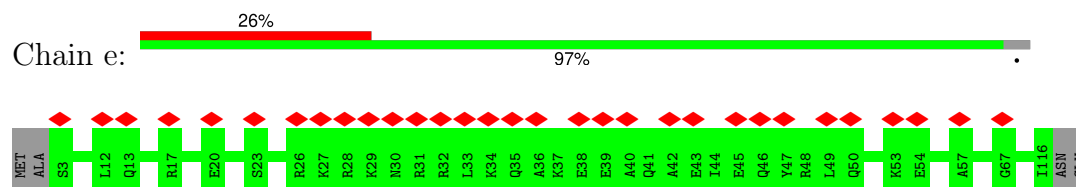
- Molecule 6: V-type proton ATPase subunit E 1



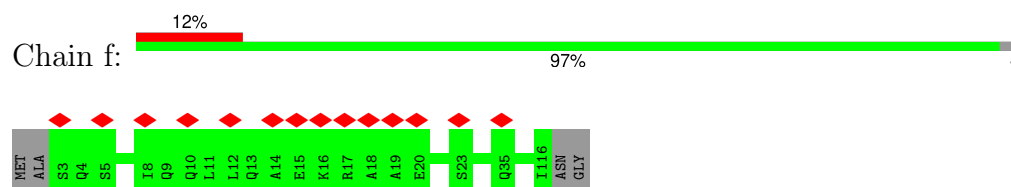
- Molecule 6: V-type proton ATPase subunit E 1



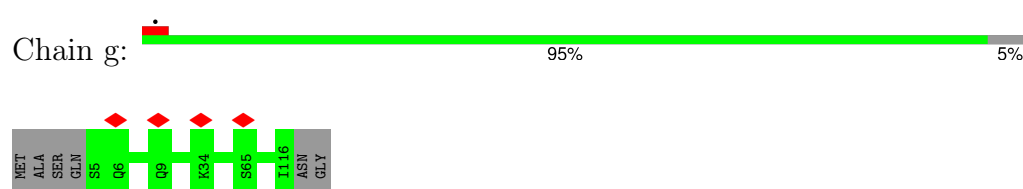
- Molecule 7: V-type proton ATPase subunit G 1



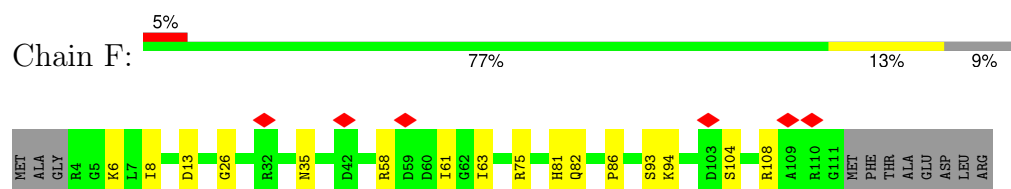
- Molecule 7: V-type proton ATPase subunit G 1



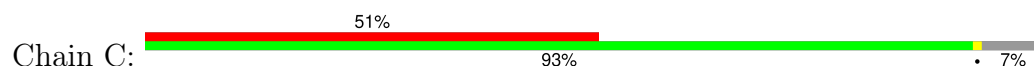
- Molecule 7: V-type proton ATPase subunit G 1

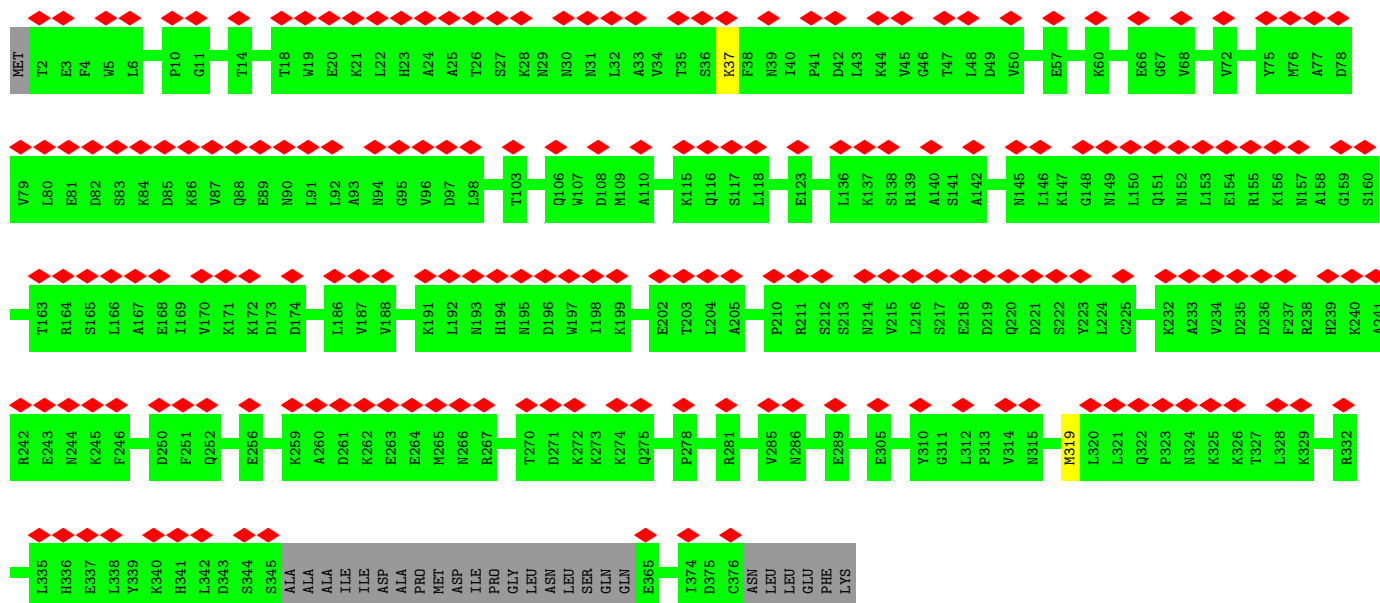


- Molecule 8: V-type proton ATPase subunit F




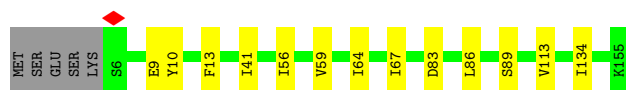
- Molecule 9: V-type proton ATPase subunit C 1






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

Chain 8:  88% 8% .



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

Chain 9:  89% 8% .



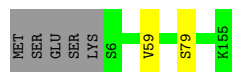
- Molecule 16: V-type proton ATPase 16 kDa proteolipid subunit

Chain 2:  92% 5% .




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

Chain 3:  95% . .




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

Chain 4:  88% 9% .



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

Chain 5:  89% 8% .




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

Chain 6:  91% 6% .



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

Chain 7:  89% 8%



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

Chain 0:  91% 6%



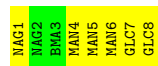
- Molecule 17: V-type proton ATPase 21 kDa proteolipid subunit

Chain 1:  94% 5%



- Molecule 18: 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:  25% 75%



- Molecule 19: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose

Chain w:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24984	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	23.543	Depositor
Minimum map value	-13.098	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.021	Depositor
Recommended contour level	2.95	Depositor
Map size (\AA)	404.16, 404.16, 404.16	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.842, 0.842, 0.842	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.32	0/6278	0.51	0/8497
2	U	0.38	0/3445	0.53	0/4660
3	L	0.35	0/4752	0.53	1/6435 (0.0%)
3	M	0.39	0/4752	0.54	2/6435 (0.0%)
3	N	0.34	0/4752	0.53	0/6435
4	O	0.38	0/3739	0.51	0/5067
4	P	0.39	0/3739	0.53	0/5067
4	Q	0.42	0/3739	0.55	0/5067
5	D	0.29	0/1735	0.49	0/2320
6	b	0.31	0/1826	0.51	0/2444
6	c	0.32	0/1799	0.50	0/2407
6	d	0.31	0/1834	0.51	0/2455
7	e	0.29	0/945	0.49	0/1258
7	f	0.30	0/945	0.44	0/1258
7	g	0.29	0/930	0.46	0/1238
8	F	0.30	0/869	0.52	0/1174
9	C	0.24	0/1768	0.44	0/2466
10	H	0.23	0/2109	0.43	0/2941
11	k	0.34	0/2902	0.53	0/3930
12	m	0.34	0/646	0.54	0/887
13	n	0.33	0/674	0.61	1/915 (0.1%)
14	s	0.53	0/1716	0.65	1/2333 (0.0%)
15	r	0.36	0/390	0.51	0/534
16	0	0.35	0/1080	0.54	0/1461
16	2	0.35	0/1080	0.54	0/1461
16	3	0.34	0/1080	0.56	0/1461
16	4	0.35	0/1080	0.52	0/1461
16	5	0.36	0/1080	0.53	0/1461
16	6	0.34	0/1080	0.52	0/1461
16	7	0.37	0/1080	0.54	0/1461
16	8	0.36	0/1080	0.56	0/1461
16	9	0.37	0/1080	0.57	0/1461

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1	0.36	0/1532	0.52	0/2082
All	All	0.35	0/67536	0.52	5/91454 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	s	387	ARG	NE-CZ-NH2	-7.28	116.66	120.30
13	n	79	LEU	CA-CB-CG	7.13	131.69	115.30
3	L	234	LEU	CA-CB-CG	6.39	130.00	115.30
3	M	234	LEU	CA-CB-CG	5.88	128.83	115.30
3	M	194	LEU	CA-CB-CG	5.01	126.82	115.30

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	a	6127	0	6155	0	0
2	U	3365	0	3271	44	0
3	L	4656	0	4642	33	0
3	M	4656	0	4642	70	0
3	N	4656	0	4642	33	0
4	O	3666	0	3665	24	0
4	P	3666	0	3665	44	0
4	Q	3666	0	3665	42	0
5	D	1717	0	1829	10	0
6	b	1809	0	1870	0	0
6	c	1782	0	1852	0	0
6	d	1817	0	1881	0	0
7	e	938	0	947	0	0
7	f	938	0	947	0	0
7	g	923	0	934	0	0
8	F	856	0	860	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	1770	0	780	1	0
10	H	2111	0	937	1	0
11	k	2836	0	2770	0	0
12	m	621	0	640	0	0
13	n	658	0	652	0	0
14	s	1662	0	1582	0	0
15	r	377	0	365	0	0
16	0	1065	0	1131	6	0
16	2	1065	0	1131	6	0
16	3	1065	0	1131	2	0
16	4	1065	0	1131	12	0
16	5	1065	0	1131	10	0
16	6	1065	0	1131	7	0
16	7	1065	0	1131	8	0
16	8	1065	0	1131	12	0
16	9	1065	0	1131	8	0
17	1	1498	0	1544	13	0
18	t	94	0	79	0	0
19	w	22	0	19	0	0
20	M	27	0	12	12	0
21	s	84	0	78	0	0
22	1	123	0	162	4	0
22	8	34	0	42	8	0
22	r	142	0	207	0	0
22	s	89	0	125	0	0
All	All	66971	0	65640	357	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 (357) 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)
3:M:234:LEU:HD21	3:M:433:TRP:CZ2	1.84	1.13
2:U:367:TYR:HE1	2:U:382:ARG:O	1.34	1.09
22:8:201:POV:H22	17:1:27:THR:HG22	1.33	1.07
3:M:234:LEU:HD21	3:M:433:TRP:CE2	1.90	1.05
20:M:701:ADP:O1B	4:P:400:ARG:NE	1.90	1.05
3:M:234:LEU:CD2	3:M:433:TRP:CE2	2.44	1.00
20:M:701:ADP:O1B	4:P:400:ARG:CZ	2.14	0.94
20:M:701:ADP:O1B	4:P:400:ARG:NH2	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:375:GLY:H	4:P:400:ARG:NH1	1.70	0.89
3:M:504:THR:HG21	3:M:556:GLU:OE2	1.75	0.87
4:Q:500:LEU:O	4:Q:500:LEU:HD23	1.78	0.84
2:U:367:TYR:CE1	2:U:382:ARG:O	2.26	0.83
3:M:442:ARG:HD3	4:P:395:LEU:O	1.81	0.81
3:M:234:LEU:HD22	3:M:433:TRP:NE1	1.95	0.81
3:M:442:ARG:HH22	4:P:423:TYR:HB3	1.44	0.79
4:P:375:GLY:H	4:P:400:ARG:HH11	1.30	0.77
3:M:504:THR:CG2	3:M:556:GLU:OE2	2.37	0.73
3:M:234:LEU:HD22	3:M:433:TRP:CE2	2.21	0.73
16:8:9:GLU:HG3	22:8:201:POV:H13A	1.71	0.72
2:U:451:GLU:HB2	4:Q:493:LYS:NZ	2.05	0.72
3:N:443:LYS:NZ	4:Q:494:ARG:HH22	1.88	0.71
3:M:442:ARG:HH22	4:P:423:TYR:CB	2.03	0.71
2:U:292:CYS:HG	2:U:312:TRP:HE1	1.39	0.70
4:P:375:GLY:N	4:P:400:ARG:HH11	1.91	0.69
3:M:442:ARG:NH2	4:P:423:TYR:CD1	2.62	0.68
4:P:375:GLY:N	4:P:400:ARG:NH1	2.42	0.67
4:Q:489:LYS:HE2	4:Q:500:LEU:HD22	1.76	0.66
22:8:201:POV:H32A	17:1:27:THR:HG21	1.77	0.66
3:M:254:CYS:SG	3:M:440:ALA:O	2.55	0.65
3:M:524:GLY:H	20:M:701:ADP:HN62	1.45	0.65
4:Q:500:LEU:HD23	4:Q:500:LEU:C	2.18	0.64
3:N:314:ASN:HD21	3:N:323:ARG:HG2	1.62	0.64
3:M:252:PHE:HE1	3:M:441:GLN:HE22	1.46	0.64
16:7:72:VAL:HG11	16:7:99:VAL:HG11	1.80	0.64
20:M:701:ADP:PB	4:P:400:ARG:HE	2.20	0.63
2:U:428:ASP:OD1	2:U:450:ARG:NH1	2.32	0.62
3:L:391:ARG:NH1	3:L:401:GLU:OE2	2.32	0.62
17:1:3:GLY:HA3	22:1:303:POV:H1	1.80	0.62
3:N:492:ILE:HD13	4:O:437:ALA:HB1	1.81	0.62
4:O:187:GLN:HG3	4:O:401:LEU:HD12	1.82	0.61
2:U:50:LEU:HD12	2:U:53:HIS:HE1	1.66	0.61
3:M:449:ASN:HD22	3:M:452:ILE:HG12	1.66	0.61
3:M:234:LEU:CD2	3:M:433:TRP:NE1	2.58	0.61
3:N:249:PRO:HB3	3:N:410:VAL:HB	1.83	0.61
4:P:205:GLN:HE21	4:P:209:GLN:HE22	1.47	0.61
3:M:449:ASN:ND2	3:M:452:ILE:HG12	2.16	0.60
3:M:249:PRO:HG3	3:M:432:PHE:CZ	2.38	0.59
3:M:251:ALA:O	3:M:256:LYS:NZ	2.35	0.59
3:N:72:GLY:O	4:Q:67:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:170:ILE:HG12	4:Q:185:ARG:HG2	1.85	0.59
4:O:421:GLN:NE2	4:O:425:CYS:SG	2.76	0.59
4:Q:193:SER:OG	4:Q:194:ALA:N	2.36	0.59
4:Q:187:GLN:HG3	4:Q:401:LEU:HD12	1.85	0.58
3:M:252:PHE:CE1	3:M:441:GLN:NE2	2.72	0.58
16:0:81:ASN:H	16:0:84:ILE:HD11	1.67	0.58
4:O:214:LYS:HB2	4:O:220:VAL:HG12	1.84	0.58
3:M:391:ARG:NH1	3:M:401:GLU:OE2	2.37	0.58
3:L:231:GLN:HG2	3:L:446:PRO:HG3	1.87	0.57
2:U:387:CYS:O	2:U:391:ASN:HA	2.03	0.57
3:L:449:ASN:HD22	3:L:452:ILE:HG12	1.69	0.57
4:Q:216:SER:OG	4:Q:217:LYS:N	2.37	0.57
4:Q:77:PRO:HD3	4:Q:110:THR:HG22	1.87	0.57
16:5:48:ARG:NH1	16:5:121:THR:O	2.37	0.57
16:7:115:ASP:OD1	16:7:119:ARG:NH1	2.38	0.57
3:M:56:ARG:HB3	3:M:63:THR:HB	1.87	0.57
8:F:82:GLN:OE1	8:F:108:ARG:NH1	2.38	0.57
2:U:124:ARG:NH2	2:U:188:ASP:OD1	2.38	0.56
2:U:339:THR:HG21	2:U:391:ASN:HB2	1.87	0.56
3:N:395:LEU:O	3:N:400:ARG:NH2	2.38	0.56
3:N:443:LYS:NZ	4:Q:494:ARG:NH2	2.54	0.56
4:P:216:SER:OG	4:P:217:LYS:N	2.38	0.56
5:D:94:ILE:HB	8:F:6:LYS:HB2	1.88	0.56
20:M:701:ADP:H4'	4:P:400:ARG:HG2	1.87	0.56
4:Q:158:ILE:HB	4:Q:163:ARG:HH21	1.70	0.56
3:M:438:LYS:HD2	5:D:4:LYS:HB3	1.88	0.56
3:N:265:LYS:HD2	3:N:294:LEU:HD22	1.88	0.56
4:P:200:ASN:HD22	4:P:240:THR:HG23	1.71	0.56
3:M:234:LEU:HD22	3:M:433:TRP:CD1	2.39	0.55
4:P:197:LEU:HD21	4:P:381:ARG:HG3	1.88	0.55
3:N:419:ASP:OD1	3:N:419:ASP:N	2.39	0.55
16:5:113:VAL:HG21	16:5:134:ILE:HG21	1.89	0.55
2:U:451:GLU:HB2	4:Q:493:LYS:HZ2	1.72	0.55
4:P:380:ASP:HB2	4:P:393:ASN:HB2	1.88	0.54
16:9:83:ASP:OD1	16:9:83:ASP:N	2.39	0.54
3:M:448:VAL:HG21	3:M:450:TRP:CE2	2.43	0.54
3:L:45:VAL:HA	3:L:79:VAL:HG12	1.89	0.54
17:1:36:ASP:OD1	22:1:302:POV:H2	2.08	0.54
16:6:113:VAL:HG21	16:6:134:ILE:HG21	1.88	0.54
3:M:111:SER:O	3:M:114:GLN:NE2	2.41	0.54
16:4:91:LEU:HD13	16:4:155:LYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:238:PHE:HZ	3:M:448:VAL:HG23	1.72	0.54
3:M:442:ARG:NH2	4:P:423:TYR:CG	2.75	0.54
2:U:313:GLU:H	2:U:319:GLN:HE22	1.57	0.53
3:N:443:LYS:HZ2	4:Q:494:ARG:HH22	1.54	0.53
16:9:34:THR:HG21	16:0:138:ALA:HB2	1.91	0.53
3:M:141:LEU:HD21	3:M:176:VAL:HG21	1.90	0.53
3:M:289:ARG:NH1	4:P:167:GLU:OE2	2.42	0.53
3:M:561:SER:O	3:M:564:LYS:NZ	2.41	0.53
4:Q:305:GLU:OE1	4:Q:308:ARG:NH2	2.41	0.53
16:5:44:MET:HG3	16:5:122:ALA:HB2	1.90	0.53
3:M:433:TRP:CH2	3:M:446:PRO:HB3	2.44	0.53
3:N:391:ARG:NH1	3:N:401:GLU:OE2	2.42	0.53
4:Q:380:ASP:HB2	4:Q:393:ASN:HB2	1.91	0.53
16:8:113:VAL:HG21	16:8:134:ILE:HG21	1.91	0.53
4:O:380:ASP:OD1	4:O:393:ASN:ND2	2.42	0.53
2:U:103:SER:OG	2:U:197:GLU:O	2.27	0.53
3:N:271:VAL:HB	3:N:344:VAL:HG22	1.91	0.52
2:U:425:SER:OG	2:U:426:ILE:N	2.41	0.52
3:L:373:GLY:HA3	4:O:320:ARG:HD2	1.91	0.52
3:M:439:LEU:HD13	3:M:444:HIS:HB3	1.90	0.52
2:U:27:LEU:HD11	2:U:218:PHE:HB3	1.92	0.52
3:M:258:VAL:HG11	20:M:701:ADP:H3'	1.91	0.52
2:U:205:HIS:HA	2:U:208:ILE:HB	1.92	0.52
3:M:448:VAL:HG21	3:M:450:TRP:CZ2	2.44	0.51
16:9:59:VAL:HG21	16:0:134:ILE:HD12	1.91	0.51
3:L:264:SER:O	3:L:308:ARG:NH2	2.42	0.51
4:Q:124:SER:OG	4:Q:125:GLU:N	2.44	0.51
3:L:395:LEU:O	3:L:400:ARG:NH2	2.43	0.51
4:Q:205:GLN:HE21	4:Q:209:GLN:HE22	1.57	0.51
2:U:134:VAL:HG23	2:U:162:VAL:HG13	1.93	0.51
4:O:485:ARG:NH2	4:O:503:PHE:O	2.43	0.51
17:1:77:ILE:HG21	16:2:117:GLY:HA2	1.93	0.51
3:L:588:ASP:OD2	3:L:591:LYS:NZ	2.41	0.50
4:P:400:ARG:O	4:P:403:LYS:NZ	2.44	0.50
8:F:8:ILE:HG23	8:F:63:ILE:HB	1.94	0.50
16:8:10:TYR:HB3	22:8:201:POV:H1	1.93	0.50
3:M:343:HIS:ND1	3:M:403:SER:OG	2.42	0.49
4:O:283:GLU:OE2	4:O:337:ARG:NH2	2.45	0.49
4:O:194:ALA:H	4:O:197:LEU:HD12	1.77	0.49
17:1:171:SER:O	17:1:175:LYS:NZ	2.45	0.49
3:M:438:LYS:HD2	5:D:4:LYS:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:82:ARG:NH1	4:O:101:GLY:O	2.44	0.49
4:Q:335:TYR:HA	4:Q:350:GLN:HE22	1.77	0.49
2:U:124:ARG:HB3	2:U:187:LEU:HB3	1.95	0.49
4:P:379:VAL:HG13	4:P:391:PRO:HG2	1.93	0.49
4:Q:87:LEU:HD13	4:Q:314:ARG:HD2	1.94	0.49
16:4:34:THR:HG23	16:4:59:VAL:HG13	1.94	0.49
2:U:71:ARG:HB3	2:U:86:VAL:HG22	1.94	0.49
3:M:253:GLY:N	20:M:701:ADP:O2B	2.42	0.49
3:M:394:CYS:HB2	3:M:400:ARG:HB2	1.94	0.49
3:N:115:SER:OG	3:N:116:ILE:N	2.46	0.49
8:F:13:ASP:OD1	8:F:13:ASP:N	2.45	0.49
3:L:56:ARG:HH11	4:P:54:ASN:HD22	1.61	0.49
20:M:701:ADP:PB	4:P:400:ARG:HH21	2.36	0.49
17:1:87:LYS:HG3	17:1:88:THR:HG23	1.95	0.49
3:M:222:PRO:O	3:M:391:ARG:NH2	2.46	0.48
3:N:538:VAL:O	3:N:542:SER:OG	2.31	0.48
17:1:175:LYS:HD2	16:0:52:ILE:HD12	1.94	0.48
3:M:257:THR:HB	20:M:701:ADP:O2A	2.13	0.48
4:Q:497:GLN:O	4:Q:497:GLN:HG3	2.13	0.48
16:9:8:PRO:HG2	16:9:86:LEU:HD22	1.94	0.48
5:D:159:ASP:HB3	8:F:108:ARG:HH21	1.78	0.48
4:P:216:SER:HB3	4:P:219:VAL:HG22	1.94	0.48
3:L:527:PRO:HA	3:L:530:ARG:HD2	1.95	0.48
4:P:320:ARG:NH2	4:P:362:THR:O	2.47	0.48
3:L:339:ASP:O	3:L:400:ARG:NE	2.47	0.48
3:L:565:ILE:HD12	3:L:570:ILE:HD11	1.94	0.48
17:1:36:ASP:OD1	22:1:302:POV:O22	2.32	0.48
3:L:43:VAL:HG21	3:L:64:ILE:HD13	1.95	0.47
3:M:69:GLU:OE1	3:M:120:ARG:NH2	2.47	0.47
5:D:58:MET:HG3	5:D:145:LEU:HD21	1.95	0.47
16:3:79:SER:O	16:3:79:SER:OG	2.31	0.47
16:6:81:ASN:H	16:6:84:ILE:HD11	1.78	0.47
4:Q:59:ILE:HB	4:Q:95:VAL:HG12	1.96	0.47
2:U:298:ASP:HA	2:U:403:PHE:HA	1.97	0.47
3:N:28:VAL:HG13	3:N:63:THR:HG23	1.97	0.47
3:L:350:SER:H	3:L:409:ALA:HB3	1.79	0.47
3:M:271:VAL:HB	3:M:344:VAL:HG12	1.96	0.47
3:N:269:SER:O	3:N:308:ARG:NH1	2.48	0.47
3:M:43:VAL:HG21	3:M:64:ILE:HD13	1.96	0.47
3:M:442:ARG:NH2	4:P:423:TYR:CB	2.74	0.47
9:C:37:LYS:HA	9:C:319:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:117:GLY:O	16:4:121:THR:OG1	2.29	0.47
16:6:59:VAL:HG21	16:7:134:ILE:HD12	1.97	0.47
4:O:249:GLU:HA	4:O:254:MET:HB2	1.96	0.47
8:F:26:GLY:HA2	8:F:35:ASN:HD21	1.80	0.47
16:8:83:ASP:N	16:8:83:ASP:OD1	2.48	0.47
2:U:387:CYS:N	2:U:392:SER:O	2.47	0.46
4:Q:404:SER:OG	4:Q:404:SER:O	2.32	0.46
3:N:44:ARG:HB2	3:N:80:LEU:HB2	1.97	0.46
4:O:210:ALA:HB3	4:O:229:ILE:HD11	1.97	0.46
4:O:395:LEU:HA	4:O:423:TYR:HE2	1.80	0.46
16:4:28:LEU:HD12	16:5:105:ALA:HB2	1.96	0.46
16:8:13:PHE:CD2	22:8:201:POV:H32	2.50	0.46
16:8:86:LEU:HA	16:8:89:SER:HB3	1.96	0.46
3:L:18:PHE:HE1	3:L:80:LEU:HD12	1.79	0.46
16:8:64:ILE:HD12	16:8:67:ILE:HD12	1.97	0.46
2:U:451:GLU:HB2	4:Q:493:LYS:HZ3	1.78	0.46
16:6:77:ALA:O	16:7:155:LYS:NZ	2.41	0.46
3:L:192:LEU:HB3	3:L:203:PHE:HB2	1.98	0.46
4:Q:363:HIS:HB3	4:Q:366:PRO:HD2	1.98	0.46
22:8:201:POV:H11	22:8:201:POV:H15A	1.57	0.46
3:N:232:ARG:HH22	3:N:585:LYS:HE3	1.81	0.46
16:8:13:PHE:CE2	22:8:201:POV:H32	2.51	0.46
16:7:83:ASP:OD1	16:7:83:ASP:N	2.45	0.46
4:O:71:ILE:O	4:O:115:THR:OG1	2.26	0.46
8:F:75:ARG:HH12	8:F:104:SER:HB2	1.80	0.46
16:8:9:GLU:CG	22:8:201:POV:H13A	2.41	0.46
4:O:236:VAL:HB	4:O:240:THR:HG23	1.97	0.45
2:U:246:LEU:HD21	2:U:295:VAL:HG21	1.98	0.45
3:L:248:ILE:HG22	3:L:433:TRP:HB2	1.98	0.45
2:U:72:ARG:HG2	2:U:82:PRO:HB3	1.99	0.45
16:8:59:VAL:HG21	16:9:134:ILE:HD12	1.99	0.45
3:L:134:ASP:OD1	3:L:134:ASP:N	2.46	0.45
3:L:603:GLN:NE2	3:L:607:ASP:OD2	2.49	0.45
16:4:59:VAL:HG21	16:5:134:ILE:HD12	1.97	0.45
16:4:83:ASP:OD1	16:4:83:ASP:N	2.50	0.45
2:U:35:LYS:HB2	2:U:35:LYS:HE2	1.66	0.45
2:U:68:ASP:HA	2:U:71:ARG:HG2	1.98	0.45
3:M:495:LEU:HD21	5:D:176:ILE:HD11	1.99	0.45
3:N:268:ASN:OD1	3:N:268:ASN:N	2.41	0.45
4:O:177:ILE:HA	4:O:181:ASN:HB2	1.98	0.45
3:L:71:SER:HA	4:O:68:TYR:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:51:SER:O	4:O:51:SER:OG	2.32	0.45
4:O:287:TYR:O	4:O:344:ARG:NH1	2.41	0.45
4:P:359:ASP:OD2	4:P:381:ARG:NH2	2.50	0.45
16:4:58:PRO:HG3	16:4:135:LEU:HD11	1.98	0.45
3:M:252:PHE:HE1	3:M:441:GLN:NE2	2.09	0.45
4:Q:421:GLN:HG2	4:Q:495:ILE:HD11	1.99	0.45
3:M:433:TRP:HH2	3:M:446:PRO:HB3	1.82	0.45
4:P:421:GLN:HE22	4:P:494:ARG:H	1.65	0.45
3:M:25:SER:O	3:M:25:SER:OG	2.33	0.45
4:Q:137:LYS:HD3	4:Q:138:PRO:HD2	1.99	0.45
8:F:93:SER:OG	8:F:94:LYS:N	2.50	0.45
22:1:303:POV:H14B	22:1:303:POV:H11A	1.81	0.45
3:L:190:VAL:HG11	3:L:202:LYS:HD2	1.98	0.44
3:M:226:PRO:HG3	3:M:461:LEU:HD22	1.99	0.44
16:4:23:MET:HG2	16:5:148:VAL:HG11	2.00	0.44
16:7:34:THR:HG23	16:7:59:VAL:HG13	1.99	0.44
3:M:596:LYS:NZ	3:M:600:ASP:OD2	2.41	0.44
3:N:24:VAL:HG12	3:N:29:VAL:HG22	1.99	0.44
3:N:561:SER:OG	3:N:562:ASP:N	2.50	0.44
2:U:147:LEU:HD22	2:U:248:VAL:HG21	1.99	0.44
4:Q:130:ARG:NH2	4:Q:143:PRO:O	2.46	0.44
2:U:104:GLU:O	2:U:193:ARG:NH2	2.50	0.44
4:P:82:ARG:HD3	4:P:100:GLU:HB2	2.00	0.44
16:9:58:PRO:HG3	16:9:135:LEU:HD11	1.99	0.44
2:U:169:LEU:HD13	2:U:206:VAL:HG22	1.99	0.44
4:P:464:ALA:O	4:P:471:ARG:NH2	2.51	0.44
2:U:44:SER:OG	2:U:45:PHE:N	2.51	0.44
3:N:277:CYS:O	3:N:314:ASN:ND2	2.38	0.44
3:M:298:VAL:HG12	3:M:299:ASP:H	1.82	0.44
4:O:131:VAL:HB	4:O:140:ASP:HB3	2.00	0.44
16:5:59:VAL:HG21	16:6:134:ILE:HD12	2.00	0.44
3:M:109:ILE:HG12	3:M:124:VAL:HG21	2.00	0.44
4:P:311:SER:HA	4:P:314:ARG:HB3	2.00	0.44
3:N:588:ASP:HB3	3:N:590:LEU:HD23	2.00	0.44
4:P:444:LEU:HD12	4:P:448:ASP:HB3	1.99	0.44
5:D:52:ILE:HD12	5:D:52:ILE:HA	1.90	0.44
16:2:86:LEU:HA	16:2:89:SER:HB3	2.00	0.44
4:Q:255:ASP:OD1	4:Q:255:ASP:N	2.48	0.43
16:0:34:THR:HG23	16:0:59:VAL:HG13	2.00	0.43
2:U:34:ASP:OD1	2:U:34:ASP:N	2.45	0.43
4:O:380:ASP:HB2	4:O:393:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:566:THR:OG1	3:M:567:TRP:N	2.51	0.43
4:O:106:ASP:OD1	4:O:110:THR:OG1	2.36	0.43
17:1:26:TYR:HD1	17:1:26:TYR:HA	1.73	0.43
3:L:315:THR:HG23	3:L:317:ASN:H	1.84	0.43
2:U:108:LEU:HD23	2:U:108:LEU:HA	1.84	0.43
3:L:371:ASP:N	3:L:371:ASP:OD1	2.52	0.43
16:9:57:ILE:HA	16:9:60:VAL:HG12	1.99	0.43
3:N:163:LYS:O	3:N:342:TYR:OH	2.37	0.43
16:0:22:ALA:HB2	16:0:96:GLY:HA2	2.01	0.43
2:U:37:SER:HB2	2:U:48:LYS:HD2	2.01	0.43
3:M:249:PRO:HB3	3:M:410:VAL:HB	2.01	0.43
3:L:466:ASP:HA	3:L:470:THR:HA	2.01	0.43
3:M:280:ARG:NH2	4:P:370:GLY:O	2.52	0.43
2:U:446:SER:O	2:U:446:SER:OG	2.36	0.42
2:U:309:SER:OG	2:U:321:ASP:OD1	2.31	0.42
3:M:449:ASN:ND2	3:M:449:ASN:O	2.52	0.42
4:P:255:ASP:N	4:P:255:ASP:OD1	2.52	0.42
16:3:59:VAL:HG21	16:4:134:ILE:HD12	2.00	0.42
2:U:321:ASP:OD1	2:U:321:ASP:N	2.52	0.42
4:P:194:ALA:H	4:P:197:LEU:HD12	1.84	0.42
3:L:24:VAL:HG12	3:L:29:VAL:HG22	2.01	0.42
3:L:152:ILE:HD11	3:L:400:ARG:HD3	2.00	0.42
3:N:292:PRO:HA	3:N:306:MET:HG2	2.01	0.42
4:Q:197:LEU:HD21	4:Q:381:ARG:HA	2.02	0.42
4:Q:213:VAL:HG11	4:Q:411:THR:HG22	2.00	0.42
4:Q:232:ALA:HB3	4:Q:297:LEU:HD23	2.01	0.42
3:L:101:GLY:N	3:L:314:ASN:HD21	2.17	0.42
3:L:428:ILE:O	3:L:430:GLN:NE2	2.52	0.42
3:M:522:GLN:HG2	3:M:529:ASP:HB3	2.01	0.42
2:U:278:SER:OG	4:Q:453:GLU:OE1	2.37	0.42
3:N:100:ASP:OD1	3:N:100:ASP:N	2.49	0.42
5:D:34:LYS:HD2	5:D:34:LYS:HA	1.88	0.42
3:L:193:GLU:HG3	3:L:202:LYS:HD3	2.00	0.42
3:M:42:LEU:O	3:M:82:THR:OG1	2.34	0.42
4:Q:500:LEU:C	4:Q:500:LEU:CD2	2.87	0.42
4:P:439:VAL:HA	5:D:167:ARG:HG3	2.01	0.42
3:L:256:LYS:HE3	3:L:256:LYS:HB2	1.88	0.42
3:L:447:SER:O	3:L:447:SER:OG	2.34	0.42
4:O:128:LEU:HD23	4:O:128:LEU:HA	1.90	0.42
4:Q:369:THR:O	4:Q:373:THR:OG1	2.29	0.42
10:H:93:ILE:O	10:H:98:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:97:HIS:CD2	2:U:105:GLU:HB3	2.55	0.42
3:M:133:TRP:N	3:M:185:TYR:O	2.51	0.42
3:N:215:ARG:HA	3:N:216:PRO:HD3	1.94	0.42
4:P:128:LEU:HD23	4:P:128:LEU:HA	1.89	0.42
4:Q:93:LYS:HE2	4:Q:93:LYS:HB2	1.88	0.42
8:F:81:HIS:CE1	8:F:86:PRO:HG2	2.55	0.42
16:4:80:LEU:HD23	16:4:80:LEU:HA	1.84	0.42
4:P:411:THR:OG1	4:P:412:ARG:N	2.52	0.41
2:U:133:LEU:O	2:U:136:SER:OG	2.38	0.41
4:Q:46:THR:O	4:Q:46:THR:OG1	2.37	0.41
16:7:22:ALA:O	16:7:26:SER:OG	2.28	0.41
3:M:258:VAL:HG21	20:M:701:ADP:N7	2.34	0.41
4:O:363:HIS:HB3	4:O:366:PRO:HD2	2.01	0.41
4:P:170:ILE:HD11	4:P:185:ARG:HG2	2.02	0.41
4:P:506:ARG:HD2	4:P:506:ARG:HA	1.78	0.41
16:6:7:GLY:HA3	16:6:85:SER:HA	2.02	0.41
3:M:253:GLY:HA2	4:P:398:LEU:HD22	2.03	0.41
4:Q:317:VAL:HA	4:Q:318:PRO:HD3	1.90	0.41
16:6:77:ALA:HA	16:6:80:LEU:HD23	2.01	0.41
2:U:45:PHE:HE2	2:U:50:LEU:HD22	1.85	0.41
3:M:417:PHE:HE2	3:M:452:ILE:HD11	1.85	0.41
5:D:43:ARG:HG2	5:D:101:VAL:HG11	2.02	0.41
16:8:64:ILE:HD12	16:8:64:ILE:HA	1.91	0.41
16:4:75:LEU:HD12	16:4:75:LEU:HA	1.93	0.41
4:Q:185:ARG:HH11	4:Q:212:LEU:HD22	1.86	0.41
16:4:155:LYS:HD2	16:4:155:LYS:HA	1.91	0.41
3:N:597:ILE:HD12	3:N:597:ILE:HA	1.91	0.41
4:Q:229:ILE:HB	4:Q:257:VAL:HG22	2.03	0.41
2:U:65:ARG:HB3	2:U:113:MET:HG2	2.03	0.41
2:U:444:ARG:HD2	2:U:444:ARG:HA	1.69	0.41
3:L:328:TYR:HA	3:L:331:ILE:HG22	2.03	0.41
3:M:478:LYS:HA	3:M:478:LYS:HD3	1.91	0.41
3:N:224:ASN:OD1	3:N:224:ASN:N	2.52	0.41
3:N:500:SER:O	3:N:500:SER:OG	2.34	0.41
17:1:52:LEU:HD23	17:1:52:LEU:HA	1.95	0.41
17:1:59:SER:HB2	16:2:101:LEU:HB3	2.02	0.41
2:U:123:ALA:HA	2:U:126:VAL:HG22	2.02	0.41
2:U:154:GLU:HB3	2:U:159:ASN:HD21	1.85	0.41
3:M:26:GLY:O	3:M:70:THR:OG1	2.36	0.41
3:N:585:LYS:HE3	3:N:585:LYS:HB2	1.82	0.41
16:8:41:ILE:HD13	16:8:56:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:12:SER:O	16:5:12:SER:OG	2.37	0.41
3:L:100:ASP:N	3:L:100:ASP:OD1	2.54	0.40
3:M:98:ILE:HD12	3:M:288:LEU:HD21	2.02	0.40
3:M:367:GLU:OE1	3:M:377:TYR:OH	2.32	0.40
4:P:219:VAL:HA	4:P:222:TYR:HD2	1.86	0.40
16:5:80:LEU:HD12	16:5:80:LEU:HA	1.85	0.40
16:7:91:LEU:HD13	16:7:155:LYS:HB3	2.02	0.40
4:Q:270:GLU:O	4:Q:274:THR:OG1	2.35	0.40
17:1:63:VAL:HG22	16:2:105:ALA:HB2	2.03	0.40
3:M:161:LEU:HD11	3:M:303:GLU:HG3	2.04	0.40
8:F:58:ARG:HD2	8:F:61:ILE:HD11	2.03	0.40
16:9:117:GLY:HA3	16:9:131:MET:HG3	2.03	0.40
3:M:500:SER:O	3:M:500:SER:OG	2.38	0.40
3:M:524:GLY:H	20:M:701:ADP:N6	2.16	0.40
3:N:177:THR:OG1	3:N:193:GLU:O	2.37	0.40
3:N:220:LYS:HB3	3:N:220:LYS:HE3	1.91	0.40
16:2:34:THR:HG23	16:2:59:VAL:HG13	2.03	0.40
16:2:81:ASN:OD1	16:2:81:ASN:N	2.55	0.40
2:U:114:ILE:HD11	2:U:125:GLU:HB3	2.03	0.40
4:P:214:LYS:HD2	4:P:214:LYS:HA	1.82	0.40
16:5:121:THR:HG22	16:5:127:LEU:HB3	2.03	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	a	744/856 (87%)	722 (97%)	22 (3%)	0	100	100
2	U	423/456 (93%)	407 (96%)	16 (4%)	0	100	100
3	L	598/617 (97%)	569 (95%)	29 (5%)	0	100	100
3	M	598/617 (97%)	551 (92%)	47 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	598/617 (97%)	561 (94%)	37 (6%)	0	100	100
4	O	466/511 (91%)	445 (96%)	21 (4%)	0	100	100
4	P	466/511 (91%)	449 (96%)	17 (4%)	0	100	100
4	Q	466/511 (91%)	445 (96%)	21 (4%)	0	100	100
5	D	211/247 (85%)	204 (97%)	7 (3%)	0	100	100
6	b	221/226 (98%)	218 (99%)	3 (1%)	0	100	100
6	c	217/226 (96%)	207 (95%)	10 (5%)	0	100	100
6	d	222/226 (98%)	218 (98%)	4 (2%)	0	100	100
7	e	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
7	f	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
7	g	110/118 (93%)	109 (99%)	1 (1%)	0	100	100
8	F	106/119 (89%)	100 (94%)	6 (6%)	0	100	100
9	C	352/382 (92%)	337 (96%)	15 (4%)	0	100	100
10	H	421/483 (87%)	368 (87%)	53 (13%)	0	100	100
11	k	348/351 (99%)	329 (94%)	19 (6%)	0	100	100
12	m	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
13	n	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
14	s	202/470 (43%)	175 (87%)	27 (13%)	0	100	100
15	r	43/345 (12%)	38 (88%)	5 (12%)	0	100	100
16	0	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
16	2	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	3	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
16	4	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
16	5	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
16	6	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
16	7	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	8	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
16	9	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
17	1	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
All	All	8727/9943 (88%)	8308 (95%)	419 (5%)	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	a	673/762 (88%)	670 (100%)	3 (0%)	89	91
2	U	371/396 (94%)	369 (100%)	2 (0%)	86	90
3	L	508/525 (97%)	508 (100%)	0	100	100
3	M	508/525 (97%)	507 (100%)	1 (0%)	92	94
3	N	508/525 (97%)	507 (100%)	1 (0%)	92	94
4	O	401/430 (93%)	401 (100%)	0	100	100
4	P	401/430 (93%)	400 (100%)	1 (0%)	92	94
4	Q	401/430 (93%)	398 (99%)	3 (1%)	81	87
5	D	184/212 (87%)	184 (100%)	0	100	100
6	b	197/199 (99%)	197 (100%)	0	100	100
6	c	194/199 (98%)	193 (100%)	1 (0%)	86	90
6	d	198/199 (100%)	198 (100%)	0	100	100
7	e	99/101 (98%)	99 (100%)	0	100	100
7	f	99/101 (98%)	99 (100%)	0	100	100
7	g	97/101 (96%)	97 (100%)	0	100	100
8	F	92/100 (92%)	92 (100%)	0	100	100
11	k	305/306 (100%)	304 (100%)	1 (0%)	91	92
12	m	68/72 (94%)	68 (100%)	0	100	100
13	n	71/116 (61%)	71 (100%)	0	100	100
14	s	182/397 (46%)	180 (99%)	2 (1%)	70	80
15	r	40/303 (13%)	40 (100%)	0	100	100
16	0	107/112 (96%)	107 (100%)	0	100	100
16	2	107/112 (96%)	107 (100%)	0	100	100
16	3	107/112 (96%)	107 (100%)	0	100	100
16	4	107/112 (96%)	107 (100%)	0	100	100
16	5	107/112 (96%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	6	107/112 (96%)	107 (100%)	0	100	100
16	7	107/112 (96%)	107 (100%)	0	100	100
16	8	107/112 (96%)	107 (100%)	0	100	100
16	9	107/112 (96%)	107 (100%)	0	100	100
17	1	154/155 (99%)	153 (99%)	1 (1%)	84	88
All	All	6714/7592 (88%)	6698 (100%)	16 (0%)	91	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	198	TYR
1	a	199	LEU
1	a	397	THR
2	U	80	LYS
2	U	386	THR
3	M	234	LEU
3	N	139	LYS
4	P	49	THR
4	Q	214	LYS
4	Q	495	ILE
4	Q	499	THR
6	c	26	LYS
11	k	41	THR
14	s	344	ARG
14	s	416	SER
17	1	26	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	220	ASN
1	a	282	GLN
1	a	293	HIS
1	a	300	GLN
1	a	318	GLN
1	a	435	GLN
1	a	443	ASN
1	a	495	HIS
1	a	516	ASN

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Mol	Chain	Res	Type
1	a	640	GLN
1	a	764	ASN
1	a	768	GLN
2	U	97	HIS
2	U	159	ASN
2	U	366	ASN
3	L	146	HIS
3	L	314	ASN
3	L	449	ASN
3	M	261	GLN
3	M	397	ASN
3	M	449	ASN
3	N	231	GLN
4	O	205	GLN
4	O	292	HIS
4	O	382	GLN
4	P	42	GLN
4	P	54	ASN
4	P	205	GLN
4	P	421	GLN
4	Q	181	ASN
4	Q	199	HIS
4	Q	205	GLN
4	Q	256	ASN
4	Q	292	HIS
4	Q	350	GLN
4	Q	421	GLN
6	b	9	GLN
6	b	39	ASN
6	b	77	ASN
6	b	78	GLN
6	c	67	GLN
6	c	71	GLN
6	c	77	ASN
6	c	113	GLN
6	c	122	GLN
6	c	161	ASN
6	d	24	ASN
6	d	77	ASN
6	d	206	GLN
6	d	221	ASN
7	f	35	GLN

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Mol	Chain	Res	Type
7	f	98	ASN
7	f	111	HIS
7	f	113	ASN
7	g	85	GLN
7	g	91	ASN
8	F	81	HIS
11	k	50	GLN
11	k	84	HIS
11	k	177	ASN
11	k	183	ASN
13	n	99	ASN
14	s	255	HIS
14	s	348	HIS
14	s	398	GLN
14	s	403	GLN
17	1	128	HIS
17	1	148	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

10 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	NAG	t	1	18	14,14,15	0.25	0	17,19,21	0.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	NAG	t	2	18	14,14,15	0.28	0	17,19,21	0.55	0
18	BMA	t	3	18	11,11,12	0.63	0	15,15,17	0.82	0
18	MAN	t	4	18	11,11,12	0.73	0	15,15,17	1.18	2 (13%)
18	MAN	t	5	18	11,11,12	0.72	0	15,15,17	1.37	2 (13%)
18	MAN	t	6	18	11,11,12	1.00	1 (9%)	15,15,17	0.88	1 (6%)
18	GLC	t	7	18	11,11,12	0.60	0	15,15,17	0.85	1 (6%)
18	GLC	t	8	18	11,11,12	0.56	0	15,15,17	0.90	1 (6%)
19	MAN	w	1	19	11,11,12	0.82	0	15,15,17	1.30	2 (13%)
19	MAN	w	2	19	11,11,12	1.14	1 (9%)	15,15,17	1.64	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	NAG	t	1	18	-	2/6/23/26	0/1/1/1
18	NAG	t	2	18	-	0/6/23/26	0/1/1/1
18	BMA	t	3	18	-	2/2/19/22	0/1/1/1
18	MAN	t	4	18	-	2/2/19/22	0/1/1/1
18	MAN	t	5	18	-	2/2/19/22	0/1/1/1
18	MAN	t	6	18	-	0/2/19/22	0/1/1/1
18	GLC	t	7	18	-	2/2/19/22	0/1/1/1
18	GLC	t	8	18	-	0/2/19/22	0/1/1/1
19	MAN	w	1	19	-	1/2/19/22	0/1/1/1
19	MAN	w	2	19	-	0/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	w	2	MAN	O5-C5	2.90	1.49	1.43
18	t	6	MAN	O5-C1	-2.28	1.39	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	w	2	MAN	C1-O5-C5	5.18	119.13	112.19
18	t	5	MAN	O2-C2-C3	-3.65	102.60	110.15
19	w	1	MAN	C1-O5-C5	3.31	116.63	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	t	5	MAN	C1-O5-C5	3.27	116.57	112.19
18	t	4	MAN	C1-O5-C5	2.89	116.06	112.19
18	t	4	MAN	O2-C2-C3	-2.81	104.32	110.15
19	w	2	MAN	O2-C2-C3	-2.53	104.90	110.15
18	t	8	GLC	C1-O5-C5	2.28	115.24	112.19
19	w	1	MAN	O2-C2-C3	-2.26	105.48	110.15
18	t	7	GLC	C1-O5-C5	2.26	115.21	112.19
18	t	6	MAN	O2-C2-C3	-2.16	105.68	110.15
18	t	1	NAG	C1-O5-C5	2.09	114.98	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

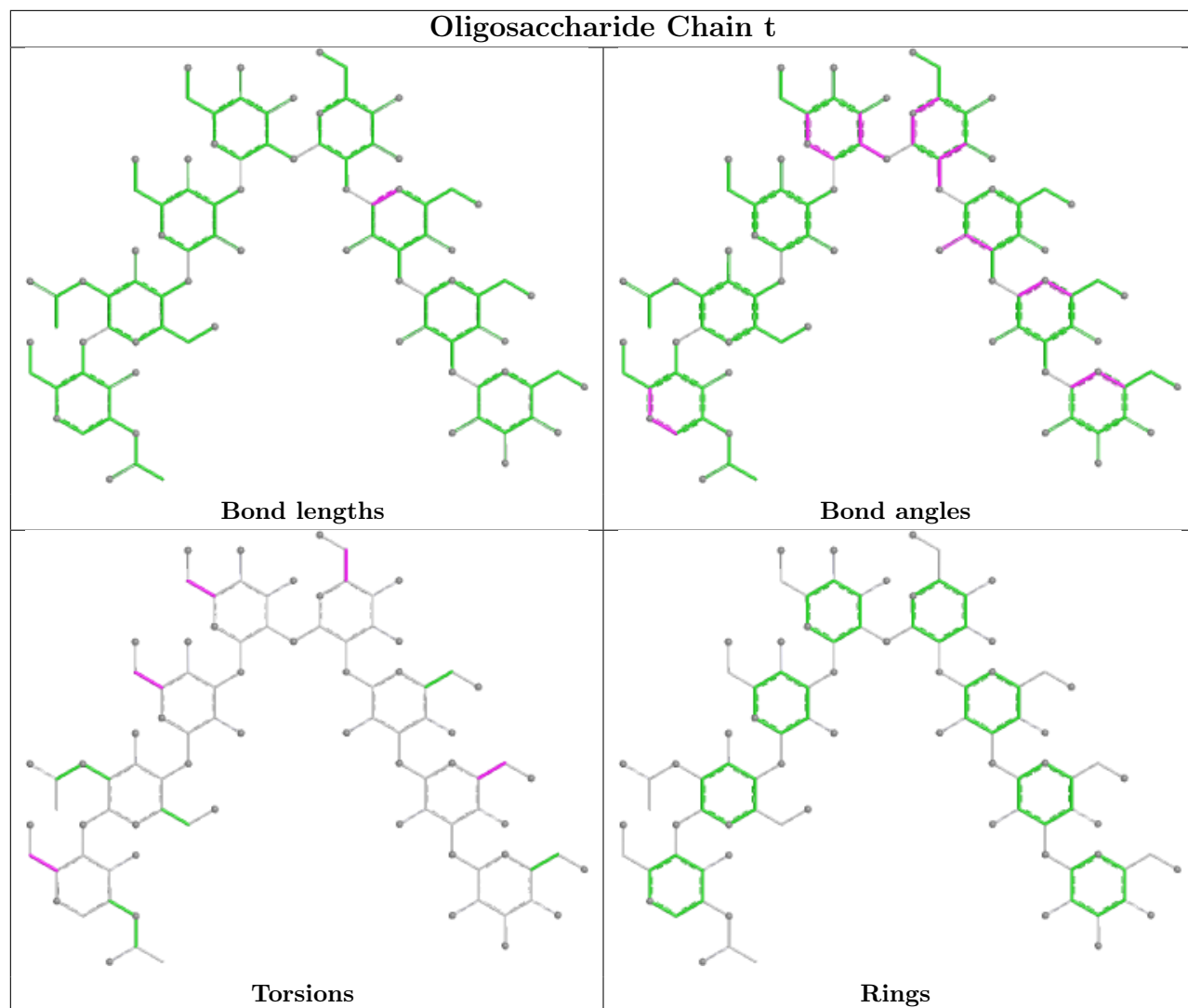
Mol	Chain	Res	Type	Atoms
18	t	5	MAN	O5-C5-C6-O6
18	t	5	MAN	C4-C5-C6-O6
18	t	3	BMA	O5-C5-C6-O6
18	t	4	MAN	O5-C5-C6-O6
18	t	1	NAG	O5-C5-C6-O6
18	t	4	MAN	C4-C5-C6-O6
18	t	1	NAG	C4-C5-C6-O6
18	t	3	BMA	C4-C5-C6-O6
18	t	7	GLC	O5-C5-C6-O6
18	t	7	GLC	C4-C5-C6-O6
19	w	1	MAN	C4-C5-C6-O6

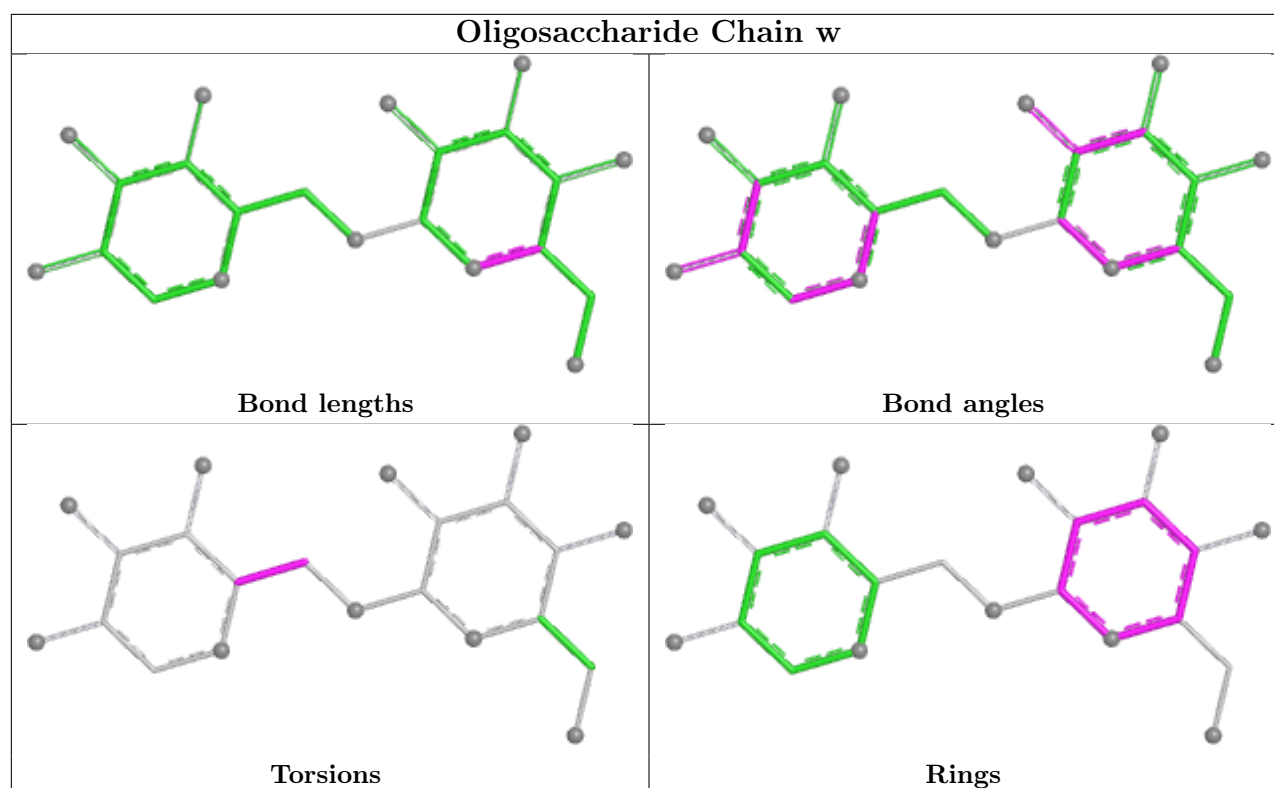
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	w	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](#)

16 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	$\# Z > 2$
21	NAG	s	504	-	14,14,15	0.50	0	17,19,21	0.48	0
22	POV	s	507	-	42,42,51	1.71	11 (26%)	48,50,59	1.50	8 (16%)
22	POV	r	401	-	48,48,51	1.18	5 (10%)	54,56,59	1.13	3 (5%)
21	NAG	s	506	14	14,14,15	0.38	0	17,19,21	0.45	0
21	NAG	s	501	14	14,14,15	0.39	0	17,19,21	0.57	0
22	POV	r	403	-	48,48,51	1.11	7 (14%)	54,56,59	1.12	4 (7%)
22	POV	1	303	-	39,39,51	1.31	5 (12%)	45,47,59	1.23	4 (8%)
22	POV	8	201	-	33,33,51	1.44	8 (24%)	39,41,59	1.51	7 (17%)
20	ADP	M	701	-	24,29,29	1.24	2 (8%)	29,45,45	1.31	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	NAG	s	503	14	14,14,15	0.20	0	17,19,21	0.47	0
22	POV	1	301	-	44,44,51	1.24	5 (11%)	50,52,59	1.21	4 (8%)
22	POV	1	302	-	37,37,51	1.37	6 (16%)	43,45,59	1.29	4 (9%)
22	POV	r	402	-	43,43,51	1.22	5 (11%)	49,51,59	1.17	3 (6%)
21	NAG	s	505	14	14,14,15	0.34	0	17,19,21	0.50	0
22	POV	s	508	-	45,45,51	1.21	5 (11%)	51,53,59	1.22	4 (7%)
21	NAG	s	502	14	14,14,15	0.52	0	17,19,21	0.82	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	NAG	s	504	-	-	0/6/23/26	0/1/1/1
22	POV	s	507	-	-	26/46/46/55	-
22	POV	r	401	-	-	19/52/52/55	-
21	NAG	s	506	14	-	2/6/23/26	0/1/1/1
21	NAG	s	501	14	-	2/6/23/26	0/1/1/1
22	POV	r	403	-	-	27/52/52/55	-
22	POV	1	303	-	-	28/43/43/55	-
22	POV	8	201	-	-	10/37/37/55	-
20	ADP	M	701	-	-	2/12/32/32	0/3/3/3
21	NAG	s	503	14	-	2/6/23/26	0/1/1/1
22	POV	1	301	-	-	18/48/48/55	-
22	POV	1	302	-	-	20/41/41/55	-
22	POV	r	402	-	-	24/47/47/55	-
21	NAG	s	505	14	-	2/6/23/26	0/1/1/1
22	POV	s	508	-	-	28/49/49/55	-
21	NAG	s	502	14	-	3/6/23/26	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	507	POV	O21-C2	-4.61	1.35	1.46
22	1	301	POV	C29-C210	3.86	1.53	1.31
22	1	303	POV	C29-C210	3.83	1.53	1.31
22	r	401	POV	C29-C210	3.79	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	302	POV	C29-C210	3.78	1.53	1.31
22	s	508	POV	C29-C210	3.74	1.53	1.31
22	r	402	POV	C210-C29	3.72	1.53	1.29
22	s	507	POV	C29-C210	3.71	1.52	1.31
22	8	201	POV	O21-C2	-3.58	1.38	1.46
20	M	701	ADP	O4'-C1'	3.37	1.45	1.40
22	s	507	POV	C12-N	-3.33	1.41	1.51
22	r	403	POV	O21-C2	-3.15	1.39	1.46
22	s	507	POV	C14-N	-3.14	1.40	1.50
22	s	507	POV	O31-C3	-3.12	1.38	1.45
22	s	507	POV	C13-N	-3.07	1.41	1.50
22	s	507	POV	C15-N	-3.03	1.41	1.50
22	s	507	POV	P-O13	-2.92	1.41	1.55
22	s	507	POV	O22-C21	-2.82	1.14	1.22
22	1	302	POV	O21-C2	-2.71	1.40	1.46
22	r	401	POV	O21-C2	-2.70	1.40	1.46
22	8	201	POV	C12-N	-2.67	1.43	1.51
22	1	303	POV	O21-C2	-2.67	1.40	1.46
22	1	301	POV	O21-C2	-2.66	1.40	1.46
22	8	201	POV	C15-N	-2.66	1.42	1.50
20	M	701	ADP	C8-N7	-2.63	1.29	1.34
22	1	302	POV	O31-C3	-2.55	1.39	1.45
22	8	201	POV	O22-C21	-2.54	1.14	1.22
22	s	507	POV	P-O14	-2.44	1.42	1.50
22	r	403	POV	O32-C31	-2.44	1.15	1.22
22	1	301	POV	O31-C3	-2.42	1.39	1.45
22	s	508	POV	O31-C3	-2.42	1.39	1.45
22	8	201	POV	C13-N	-2.42	1.43	1.50
22	8	201	POV	C14-N	-2.38	1.43	1.50
22	1	303	POV	O31-C3	-2.36	1.39	1.45
22	r	401	POV	O31-C31	2.36	1.40	1.33
22	r	402	POV	O31-C3	-2.35	1.39	1.45
22	s	508	POV	O21-C21	2.31	1.40	1.34
22	1	303	POV	O31-C31	2.29	1.40	1.33
22	s	508	POV	O31-C31	2.27	1.40	1.33
22	r	403	POV	C13-N	-2.25	1.43	1.50
22	8	201	POV	O31-C3	-2.25	1.40	1.45
22	r	401	POV	O31-C3	-2.24	1.40	1.45
22	1	302	POV	O31-C31	2.24	1.39	1.33
22	r	402	POV	O31-C31	2.24	1.39	1.33
22	s	507	POV	O32-C31	-2.23	1.15	1.22
22	r	402	POV	O21-C2	-2.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	402	POV	O21-C21	2.22	1.40	1.34
22	s	508	POV	O21-C2	-2.20	1.41	1.46
22	l	301	POV	O31-C31	2.19	1.39	1.33
22	r	403	POV	O31-C31	2.16	1.39	1.33
22	r	403	POV	O31-C3	-2.15	1.40	1.45
22	r	403	POV	C15-N	-2.15	1.43	1.50
22	l	302	POV	O21-C21	2.12	1.40	1.34
22	l	303	POV	O21-C21	2.10	1.40	1.34
22	l	301	POV	O21-C21	2.06	1.40	1.34
22	r	401	POV	O21-C21	2.05	1.40	1.34
22	8	201	POV	O32-C31	-2.05	1.16	1.22
22	r	403	POV	C12-N	-2.02	1.45	1.51
22	l	302	POV	P-O13	-2.02	1.46	1.55

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	403	POV	O21-C21-C22	5.24	122.82	111.48
20	M	701	ADP	N3-C2-N1	-5.07	121.79	128.67
22	8	201	POV	O21-C21-C22	4.92	122.12	111.48
22	s	507	POV	O21-C21-C22	4.85	121.97	111.48
22	l	301	POV	O21-C21-C22	4.40	121.00	111.48
22	l	302	POV	O21-C21-C22	4.27	120.73	111.48
22	l	303	POV	O21-C21-C22	4.27	120.72	111.48
22	s	508	POV	O21-C21-C22	4.24	120.64	111.48
22	r	401	POV	O21-C21-C22	3.94	120.00	111.48
22	r	402	POV	O21-C21-C22	3.83	119.77	111.48
22	8	201	POV	C11-C12-N	-3.76	103.74	115.82
22	r	403	POV	O31-C31-C32	3.41	122.24	111.83
22	l	303	POV	O31-C31-C32	3.12	121.35	111.83
21	s	502	NAG	C1-O5-C5	3.00	116.20	112.19
22	s	507	POV	C34-C33-C32	-2.91	102.44	113.13
22	l	302	POV	O31-C31-C32	2.84	120.50	111.83
22	s	507	POV	O31-C31-C32	2.80	120.38	111.83
22	8	201	POV	O31-C31-C32	2.80	120.38	111.83
22	r	401	POV	O31-C31-C32	2.79	120.33	111.83
22	l	301	POV	O31-C31-C32	2.77	120.28	111.83
22	s	507	POV	O21-C21-O22	-2.71	117.37	123.70
22	r	402	POV	O31-C31-C32	2.70	120.06	111.83
20	M	701	ADP	PA-O5'-C5'	-2.63	106.27	121.35
22	8	201	POV	O31-C3-C2	2.60	115.90	108.40
22	s	508	POV	O31-C31-C32	2.60	119.77	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	401	POV	O13-P-O14	-2.53	100.70	112.44
22	1	302	POV	O13-P-O14	-2.51	100.78	112.44
22	8	201	POV	O13-P-O11	2.49	118.83	107.57
22	s	508	POV	O13-P-O14	-2.47	100.96	112.44
22	8	201	POV	O13-P-O14	-2.43	101.12	112.44
22	s	508	POV	C211-C210-C29	-2.41	111.95	126.42
22	s	507	POV	P-O12-C11	-2.36	110.05	121.26
22	r	403	POV	O21-C21-O22	-2.35	118.21	123.70
22	s	507	POV	C15-N-C14	2.33	115.10	108.98
22	1	301	POV	O13-P-O14	-2.28	101.82	112.44
22	1	303	POV	O13-P-O14	-2.26	101.91	112.44
22	r	402	POV	O13-P-O14	-2.21	102.16	112.44
22	s	507	POV	C3-C2-C1	-2.21	106.64	111.78
22	8	201	POV	C25-C24-C23	-2.17	103.40	114.37
22	r	403	POV	O31-C31-O32	-2.14	118.28	123.63
22	1	302	POV	C211-C210-C29	-2.12	113.64	126.42
22	1	303	POV	C211-C210-C29	-2.12	113.69	126.42
22	s	507	POV	O21-C2-C3	-2.07	100.90	108.34
22	1	301	POV	C3-C2-C1	-2.05	107.01	111.78

There are no chirality outliers.

All (213) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	M	701	ADP	C5'-O5'-PA-O2A
22	s	507	POV	C1-O11-P-O12
22	s	507	POV	C1-O11-P-O13
22	s	507	POV	C1-O11-P-O14
22	s	507	POV	C11-O12-P-O11
22	s	507	POV	C11-O12-P-O13
22	s	507	POV	C11-O12-P-O14
22	s	507	POV	O11-C1-C2-O21
22	s	507	POV	O12-C11-C12-N
22	s	508	POV	C11-O12-P-O11
22	s	508	POV	C11-O12-P-O13
22	s	508	POV	C11-O12-P-O14
22	s	508	POV	C22-C21-O21-C2
22	r	401	POV	C22-C21-O21-C2
22	r	402	POV	C11-O12-P-O11
22	r	402	POV	C11-O12-P-O13
22	r	402	POV	C11-O12-P-O14
22	r	402	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
22	r	403	POV	O12-C11-C12-N
22	r	403	POV	C22-C21-O21-C2
22	r	403	POV	O22-C21-O21-C2
22	8	201	POV	O21-C2-C3-O31
22	1	301	POV	C11-O12-P-O11
22	1	301	POV	C11-O12-P-O13
22	1	301	POV	C22-C21-O21-C2
22	1	302	POV	C1-O11-P-O12
22	1	302	POV	C11-O12-P-O13
22	1	302	POV	O12-C11-C12-N
22	1	303	POV	C1-O11-P-O12
22	1	303	POV	C1-O11-P-O13
22	1	303	POV	C1-O11-P-O14
22	1	303	POV	C11-O12-P-O11
22	1	303	POV	C11-O12-P-O13
22	1	303	POV	O12-C11-C12-N
22	1	303	POV	C22-C21-O21-C2
22	s	508	POV	O22-C21-O21-C2
22	r	401	POV	O22-C21-O21-C2
22	r	402	POV	O22-C21-O21-C2
22	1	301	POV	O22-C21-O21-C2
22	1	303	POV	O22-C21-O21-C2
22	r	402	POV	C32-C31-O31-C3
22	r	402	POV	C22-C21-O21-C2
21	s	501	NAG	O5-C5-C6-O6
22	1	301	POV	C32-C31-O31-C3
22	r	402	POV	O32-C31-O31-C3
21	s	502	NAG	C4-C5-C6-O6
22	r	403	POV	C32-C31-O31-C3
21	s	505	NAG	O5-C5-C6-O6
21	s	503	NAG	C4-C5-C6-O6
22	1	301	POV	O32-C31-O31-C3
21	s	501	NAG	C4-C5-C6-O6
22	r	403	POV	O32-C31-O31-C3
21	s	502	NAG	O5-C5-C6-O6
21	s	506	NAG	O5-C5-C6-O6
22	1	302	POV	C211-C210-C29-C28
21	s	503	NAG	O5-C5-C6-O6
22	1	302	POV	C32-C31-O31-C3
22	s	507	POV	C11-C12-N-C13
22	s	507	POV	C11-C12-N-C14
22	s	507	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
22	l	302	POV	O32-C31-O31-C3
22	s	508	POV	O21-C2-C3-O31
22	s	507	POV	C211-C210-C29-C28
22	r	401	POV	C21-C22-C23-C24
22	s	507	POV	C21-C22-C23-C24
22	r	403	POV	C21-C22-C23-C24
22	l	303	POV	C32-C31-O31-C3
21	s	505	NAG	C4-C5-C6-O6
22	l	303	POV	C31-C32-C33-C34
22	s	507	POV	C32-C31-O31-C3
22	l	302	POV	C21-C22-C23-C24
22	s	508	POV	C1-C2-O21-C21
22	s	507	POV	O32-C31-O31-C3
22	l	303	POV	O32-C31-O31-C3
22	r	403	POV	C23-C24-C25-C26
22	r	401	POV	C37-C38-C39-C310
22	r	401	POV	C311-C312-C313-C314
22	s	508	POV	C311-C312-C313-C314
22	r	403	POV	C35-C36-C37-C38
22	s	508	POV	C24-C25-C26-C27
22	l	301	POV	C22-C23-C24-C25
22	s	507	POV	C11-C12-N-C15
22	r	403	POV	C22-C23-C24-C25
22	l	303	POV	C26-C27-C28-C29
22	s	508	POV	C310-C311-C312-C313
22	8	201	POV	C22-C23-C24-C25
22	r	401	POV	C23-C24-C25-C26
22	l	303	POV	C25-C26-C27-C28
22	l	303	POV	C33-C34-C35-C36
22	l	302	POV	C29-C210-C211-C212
22	r	402	POV	C311-C312-C313-C314
22	l	303	POV	C34-C35-C36-C37
22	l	303	POV	C32-C33-C34-C35
22	s	507	POV	C22-C21-O21-C2
22	s	507	POV	O22-C21-O21-C2
22	s	508	POV	C26-C27-C28-C29
22	l	301	POV	C21-C22-C23-C24
22	s	507	POV	C25-C26-C27-C28
22	8	201	POV	C23-C24-C25-C26
22	r	402	POV	C23-C24-C25-C26
22	r	403	POV	C211-C212-C213-C214
22	r	401	POV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	1	303	POV	C22-C23-C24-C25
22	r	402	POV	C34-C35-C36-C37
22	s	507	POV	O11-C1-C2-C3
22	s	508	POV	O11-C1-C2-C3
22	1	303	POV	O11-C1-C2-C3
22	s	507	POV	C35-C36-C37-C38
22	r	402	POV	C32-C33-C34-C35
22	1	301	POV	C31-C32-C33-C34
22	s	508	POV	C1-C2-C3-O31
22	8	201	POV	C1-C2-C3-O31
22	1	303	POV	C23-C24-C25-C26
22	1	301	POV	C24-C25-C26-C27
22	s	507	POV	C22-C23-C24-C25
22	s	508	POV	C22-C23-C24-C25
22	r	402	POV	C3-C2-O21-C21
22	r	403	POV	C39-C310-C311-C312
22	1	301	POV	C39-C310-C311-C312
22	s	508	POV	C34-C35-C36-C37
22	8	201	POV	C25-C26-C27-C28
22	r	403	POV	C312-C313-C314-C315
22	1	302	POV	C32-C33-C34-C35
22	1	301	POV	C211-C210-C29-C28
22	1	303	POV	C211-C210-C29-C28
22	r	403	POV	C34-C35-C36-C37
22	s	508	POV	C32-C31-O31-C3
22	r	403	POV	C37-C38-C39-C310
22	1	302	POV	O11-C1-C2-C3
22	r	403	POV	C1-C2-C3-O31
22	r	401	POV	C33-C34-C35-C36
22	1	302	POV	C35-C36-C37-C38
22	1	302	POV	O11-C1-C2-O21
22	r	403	POV	O21-C2-C3-O31
22	1	302	POV	O21-C2-C3-O31
22	1	303	POV	O21-C2-C3-O31
22	r	401	POV	C35-C36-C37-C38
21	s	506	NAG	C4-C5-C6-O6
22	r	401	POV	C36-C37-C38-C39
22	r	403	POV	C212-C213-C214-C215
22	r	403	POV	C24-C25-C26-C27
22	s	508	POV	O32-C31-O31-C3
22	1	303	POV	C1-C2-C3-O31
22	s	507	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
22	1	303	POV	C12-C11-O12-P
22	s	508	POV	O12-C11-C12-N
22	8	201	POV	O12-C11-C12-N
22	1	301	POV	O12-C11-C12-N
22	8	201	POV	C34-C35-C36-C37
22	1	303	POV	C24-C25-C26-C27
22	s	507	POV	C23-C24-C25-C26
22	8	201	POV	C26-C27-C28-C29
22	r	403	POV	C26-C27-C28-C29
22	1	301	POV	C32-C33-C34-C35
22	1	302	POV	C22-C23-C24-C25
22	1	303	POV	O11-C1-C2-O21
22	s	507	POV	C34-C35-C36-C37
22	1	301	POV	O21-C2-C3-O31
20	M	701	ADP	C5'-O5'-PA-O3A
22	s	508	POV	C1-O11-P-O12
22	s	508	POV	C1-O11-P-O14
22	r	401	POV	C1-O11-P-O12
22	r	401	POV	C1-O11-P-O14
22	r	402	POV	C1-O11-P-O12
22	r	402	POV	C1-O11-P-O13
22	r	402	POV	C1-O11-P-O14
22	r	403	POV	C1-O11-P-O14
22	r	403	POV	C11-O12-P-O14
22	1	301	POV	C1-O11-P-O12
22	1	302	POV	C11-O12-P-O11
22	1	302	POV	C11-O12-P-O14
22	1	303	POV	C11-O12-P-O14
22	r	402	POV	C2-C1-O11-P
22	8	201	POV	C2-C1-O11-P
22	r	401	POV	C32-C33-C34-C35
22	1	302	POV	C33-C34-C35-C36
22	s	508	POV	O11-C1-C2-O21
22	r	403	POV	O11-C1-C2-O21
22	r	401	POV	C25-C26-C27-C28
22	1	302	POV	O21-C21-C22-C23
22	s	508	POV	C35-C36-C37-C38
22	s	508	POV	C29-C210-C211-C212
22	r	401	POV	C311-C310-C39-C38
22	1	303	POV	O21-C21-C22-C23
22	s	508	POV	C312-C313-C314-C315
22	1	301	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
22	8	201	POV	C32-C33-C34-C35
22	s	508	POV	C27-C28-C29-C210
22	1	302	POV	C27-C28-C29-C210
22	s	508	POV	C39-C310-C311-C312
21	s	502	NAG	C1-C2-N2-C7
22	s	507	POV	C37-C38-C39-C310
22	r	402	POV	C27-C28-C29-C210
22	r	403	POV	C11-C12-N-C15
22	r	402	POV	O11-C1-C2-C3
22	r	403	POV	C11-C12-N-C13
22	r	401	POV	C27-C28-C29-C210
22	1	301	POV	C29-C210-C211-C212
22	1	302	POV	C1-C2-C3-O31
22	r	401	POV	C29-C210-C211-C212
22	r	401	POV	C12-C11-O12-P
22	r	403	POV	C29-C210-C211-C212
22	1	303	POV	C27-C28-C29-C210
22	s	508	POV	C33-C34-C35-C36
22	r	401	POV	C24-C25-C26-C27
22	r	403	POV	C311-C310-C39-C38
22	s	508	POV	C31-C32-C33-C34
22	r	402	POV	O21-C21-C22-C23
22	r	402	POV	O31-C31-C32-C33
22	r	403	POV	O11-C1-C2-C3
22	r	402	POV	C310-C311-C312-C313
22	r	402	POV	O32-C31-C32-C33
22	r	402	POV	O22-C21-C22-C23

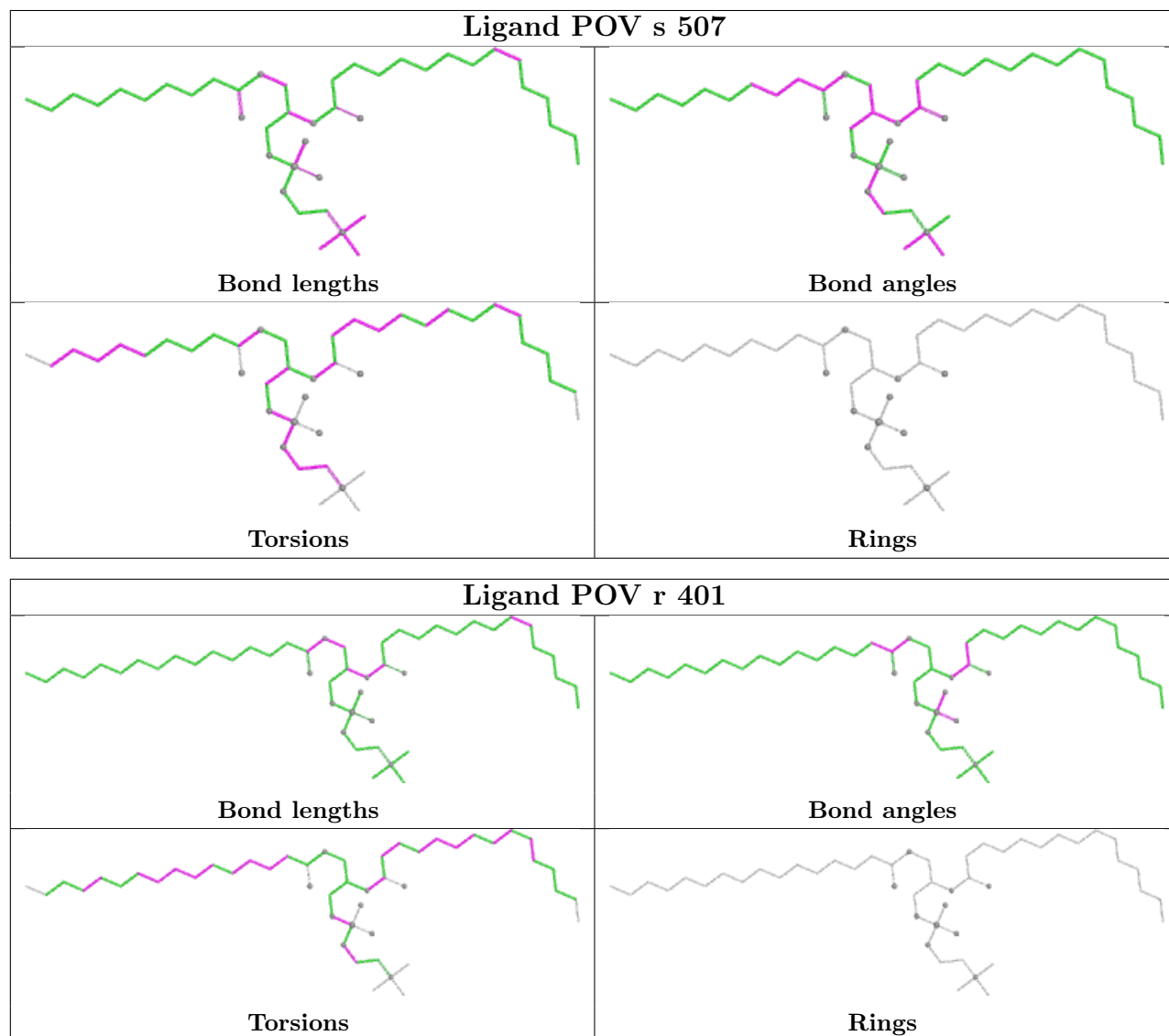
There are no ring outliers.

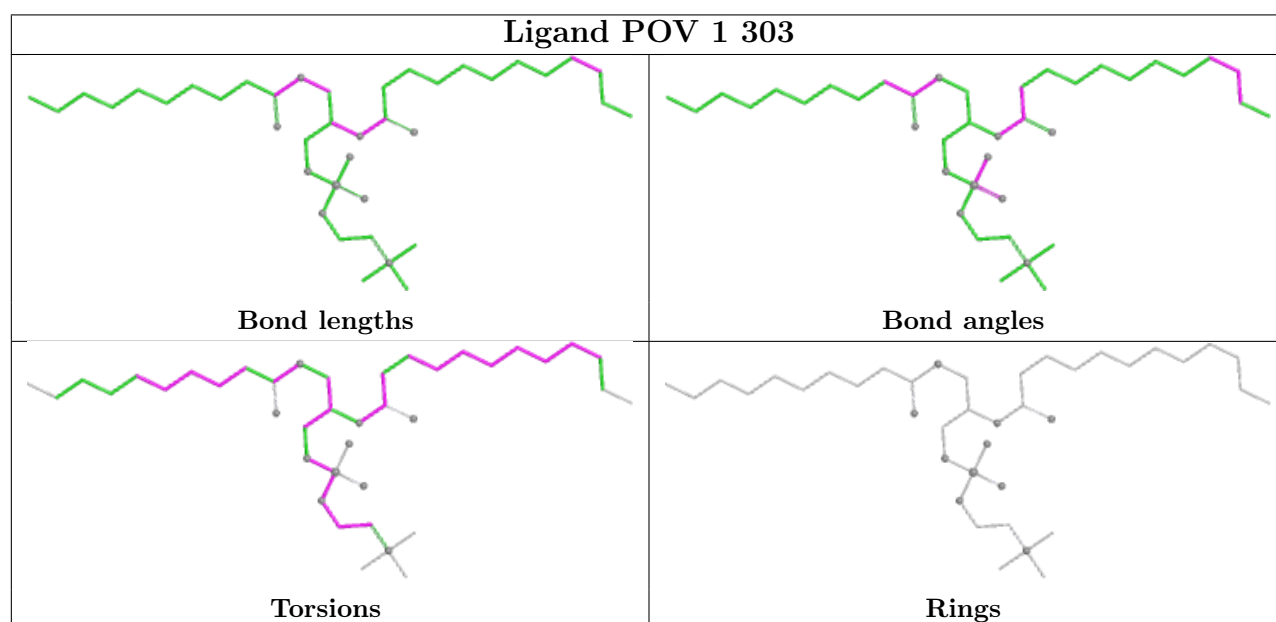
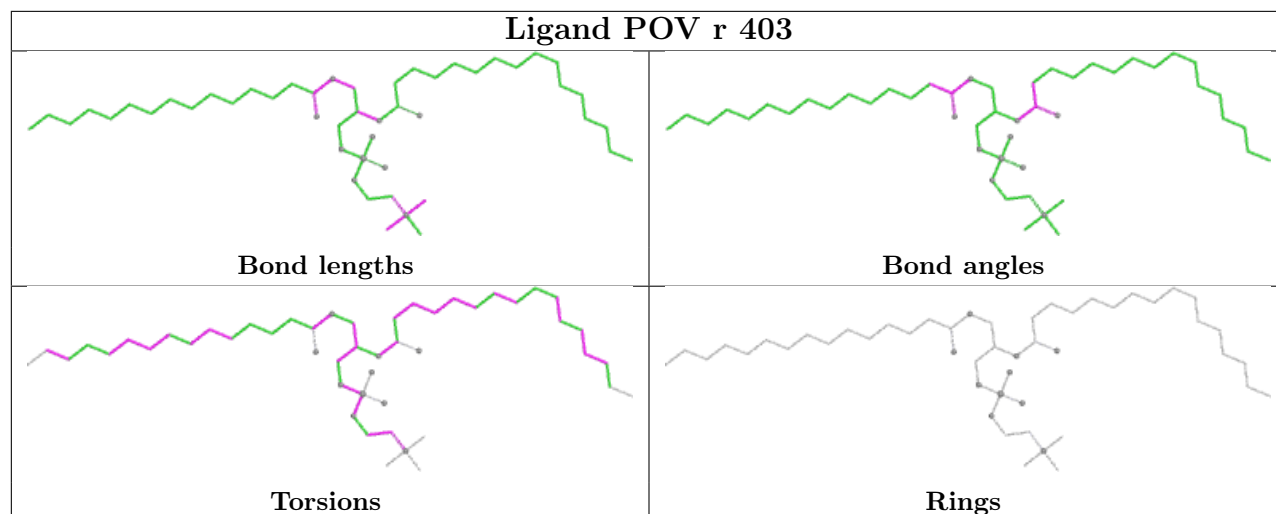
4 monomers are involved in 24 short contacts:

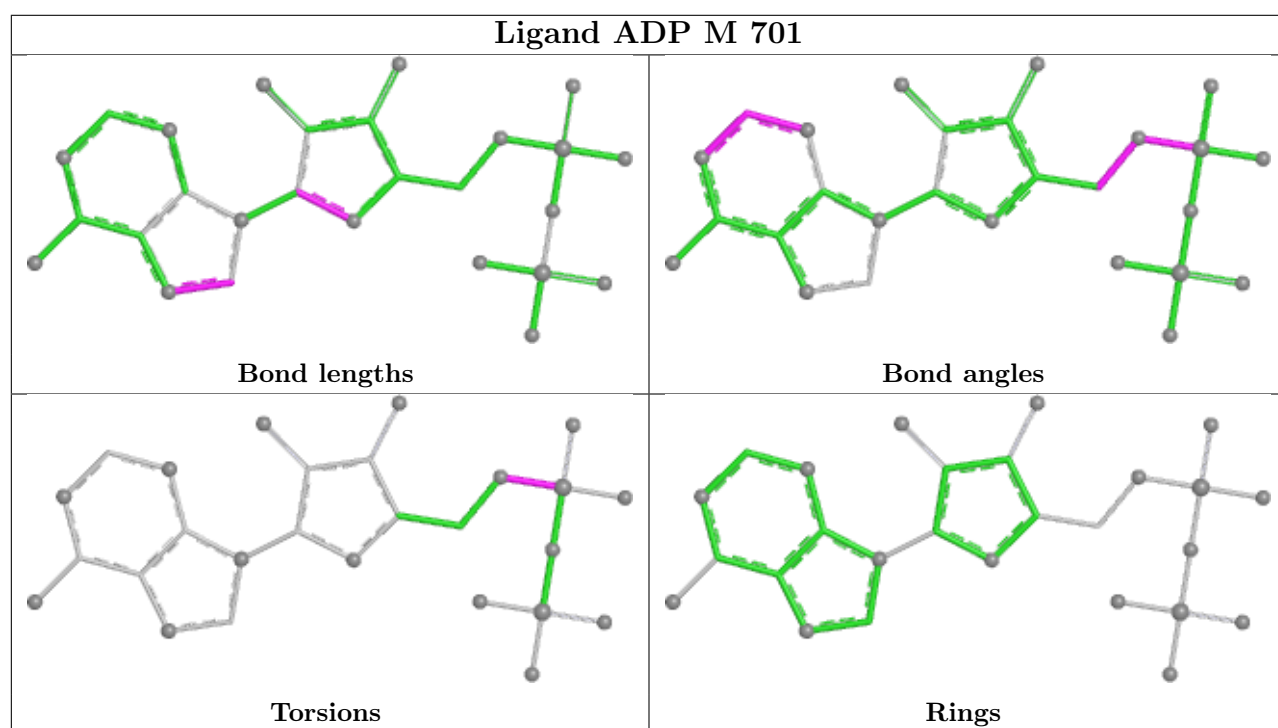
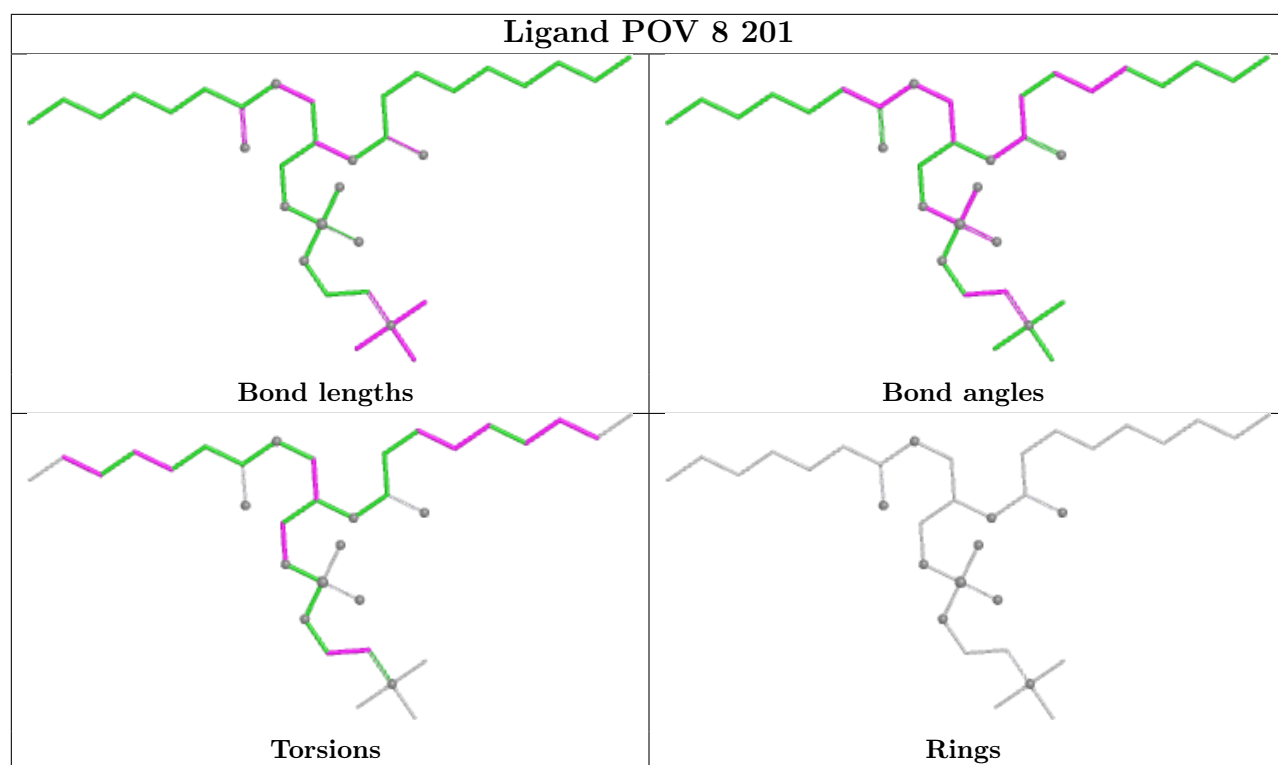
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	303	POV	2	0
22	8	201	POV	8	0
20	M	701	ADP	12	0
22	1	302	POV	2	0

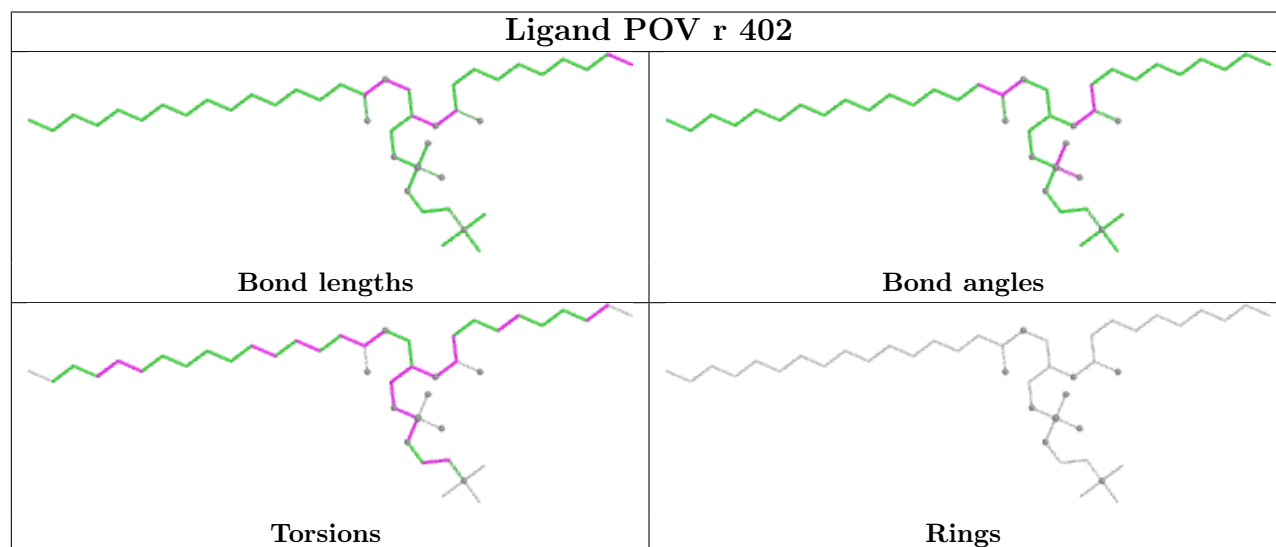
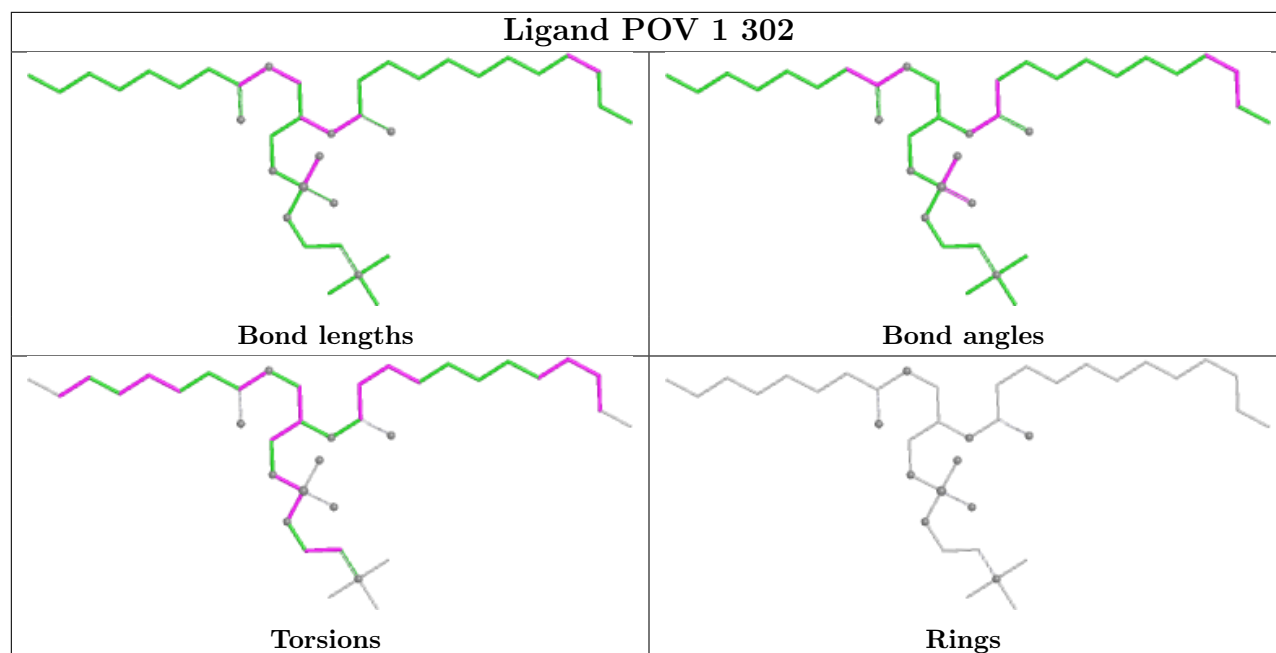
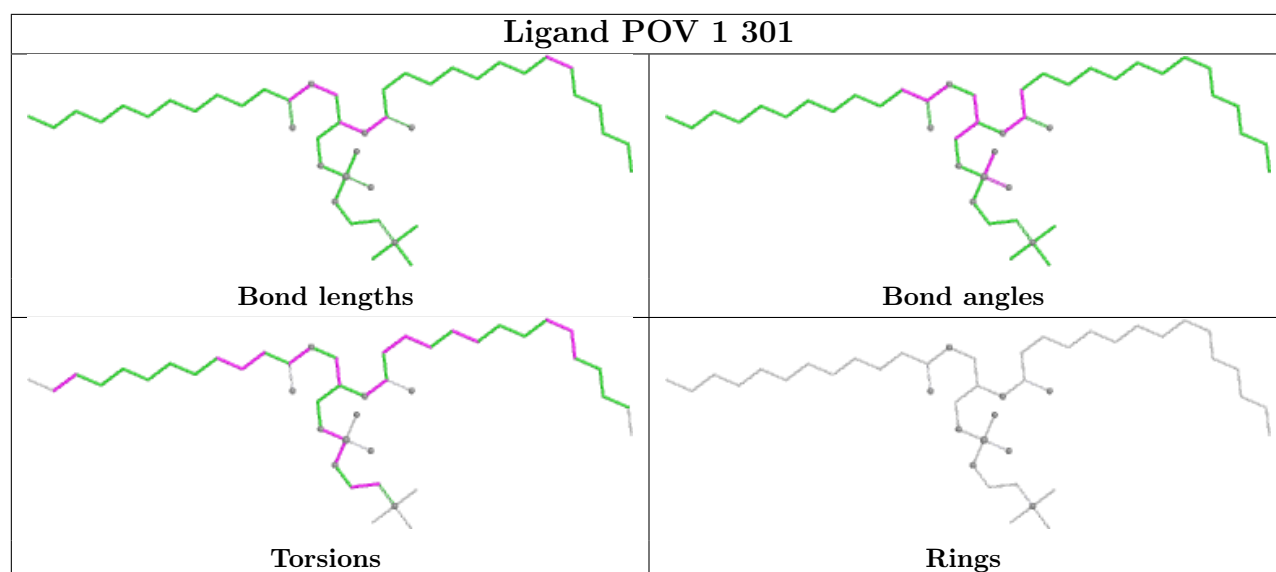
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

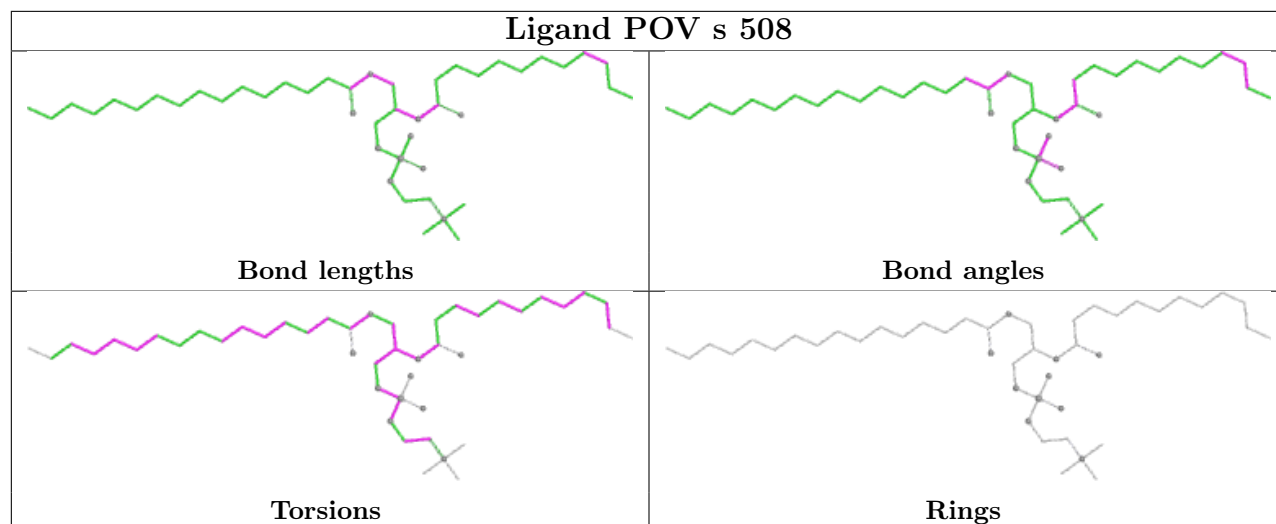
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

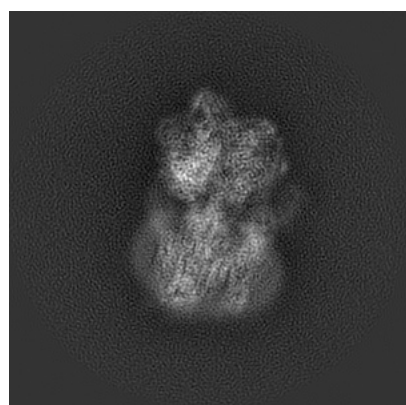
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26623. These allow visual inspection of the internal detail of the map and identification of artifacts.

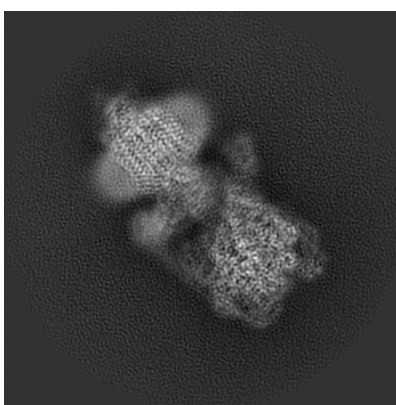
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

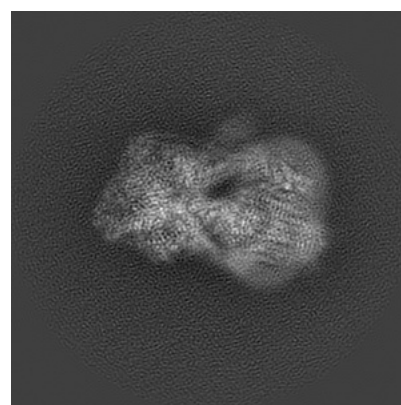
6.1.1 Primary map



X



Y

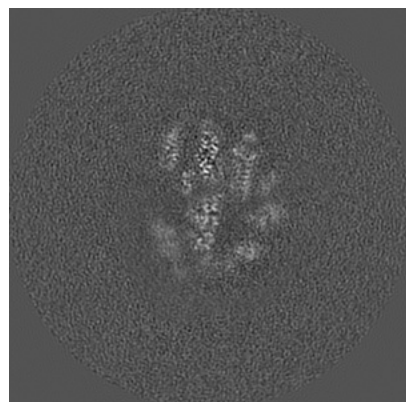


Z

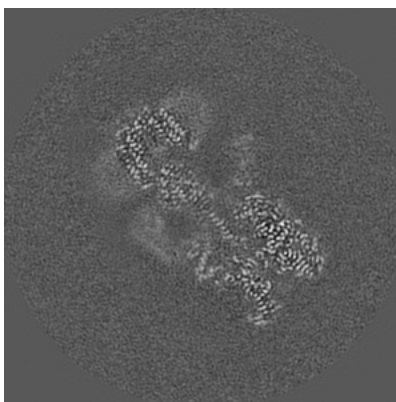
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

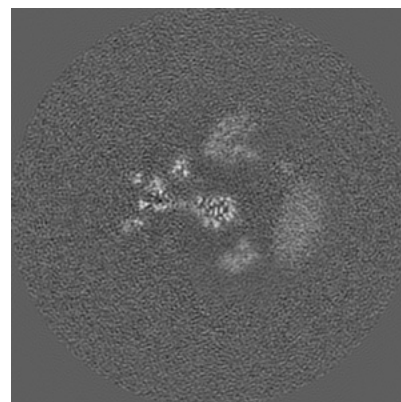
6.2.1 Primary map



X Index: 240



Y Index: 240

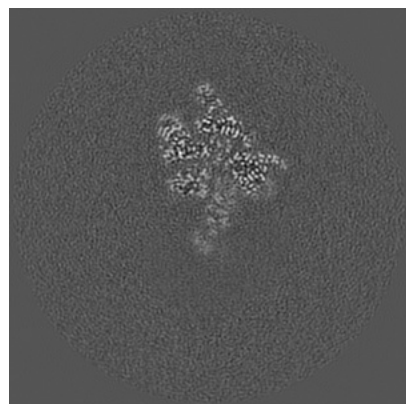


Z Index: 240

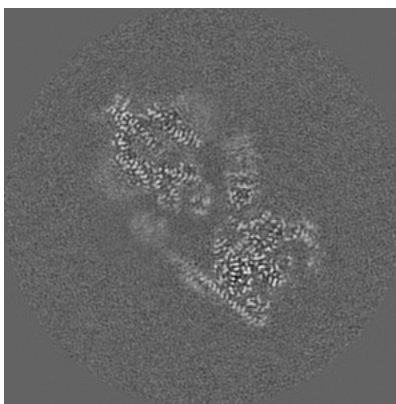
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

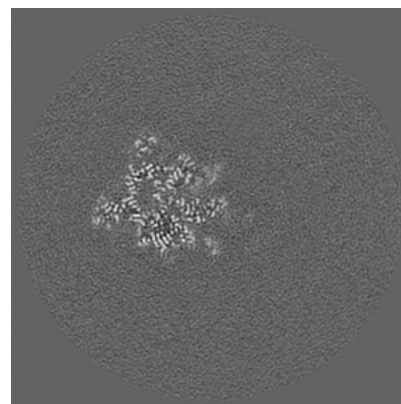
6.3.1 Primary map



X Index: 182



Y Index: 222

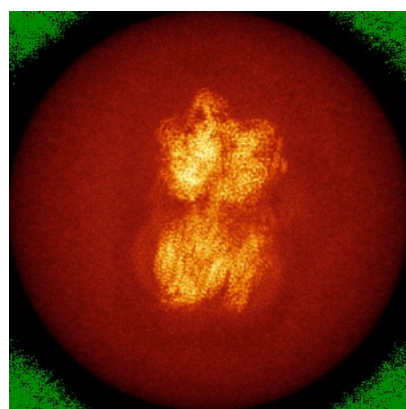


Z Index: 308

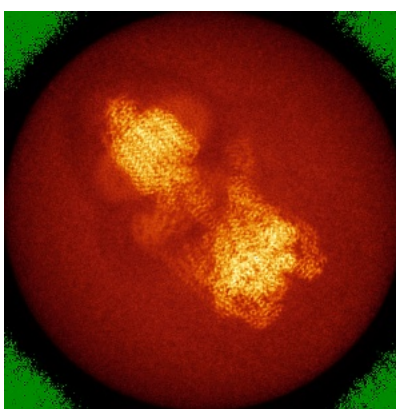
The images above show the largest variance slices of the map in three orthogonal directions.

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

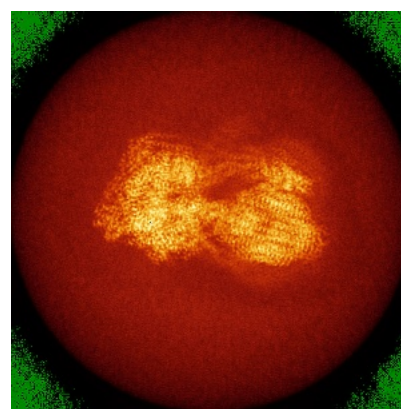
6.4.1 Primary map



X



Y

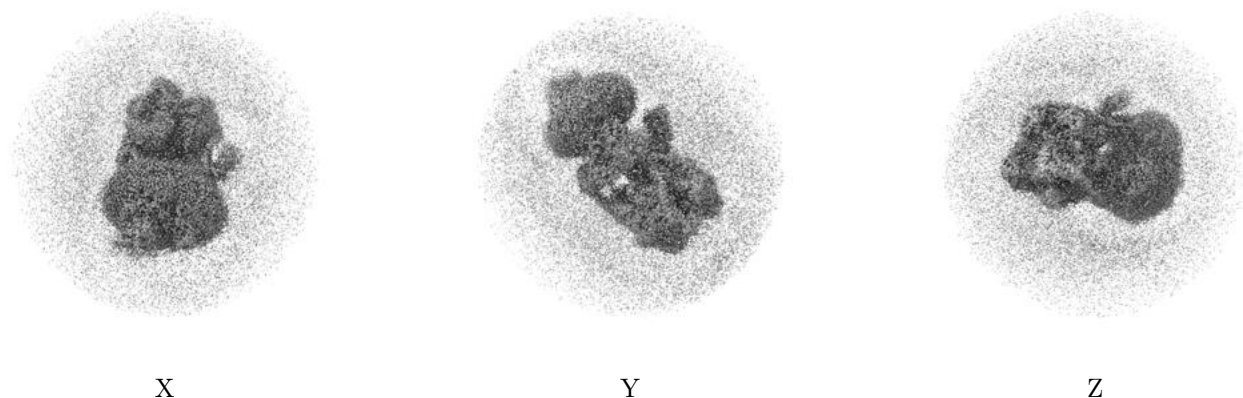


Z

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

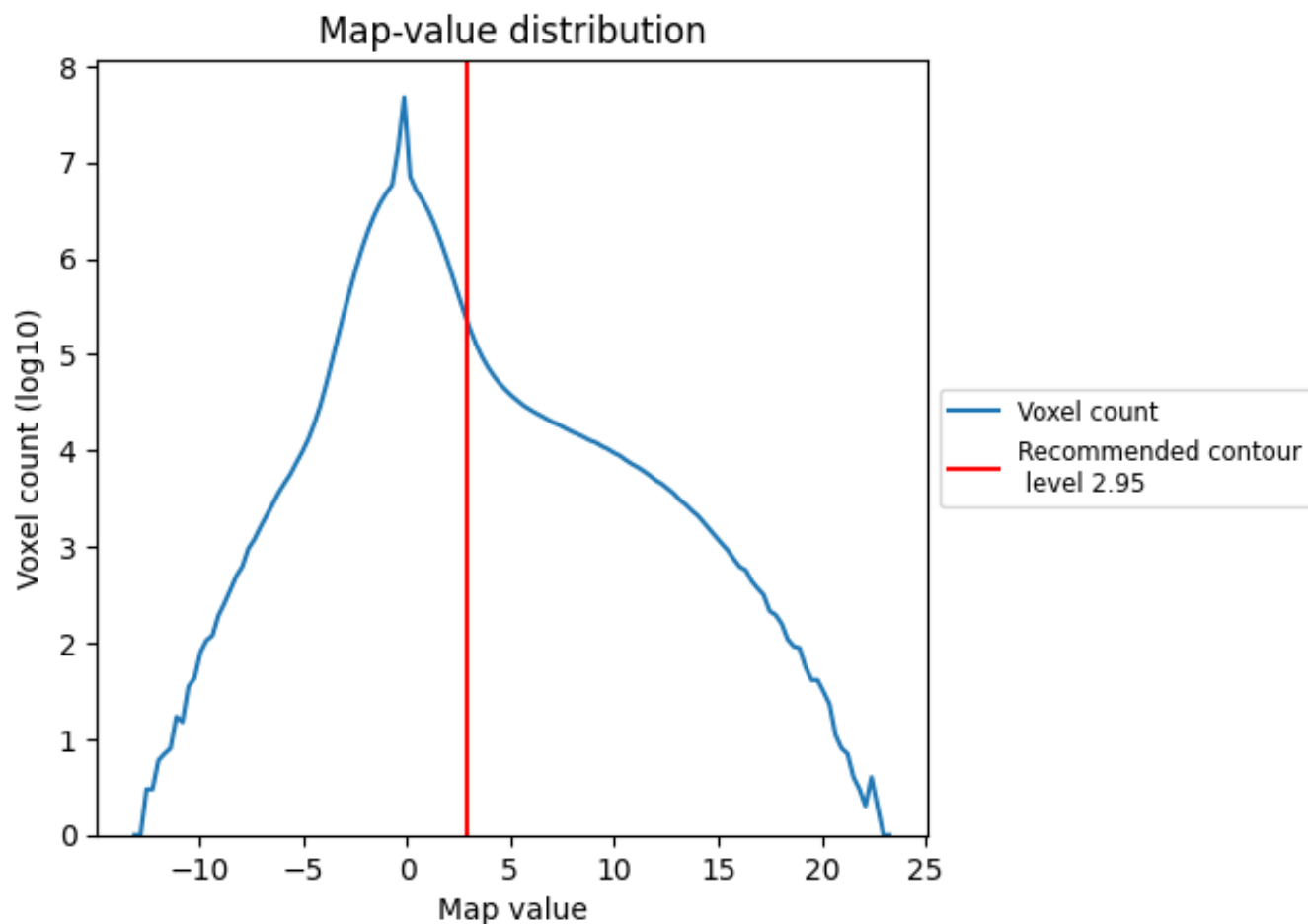
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

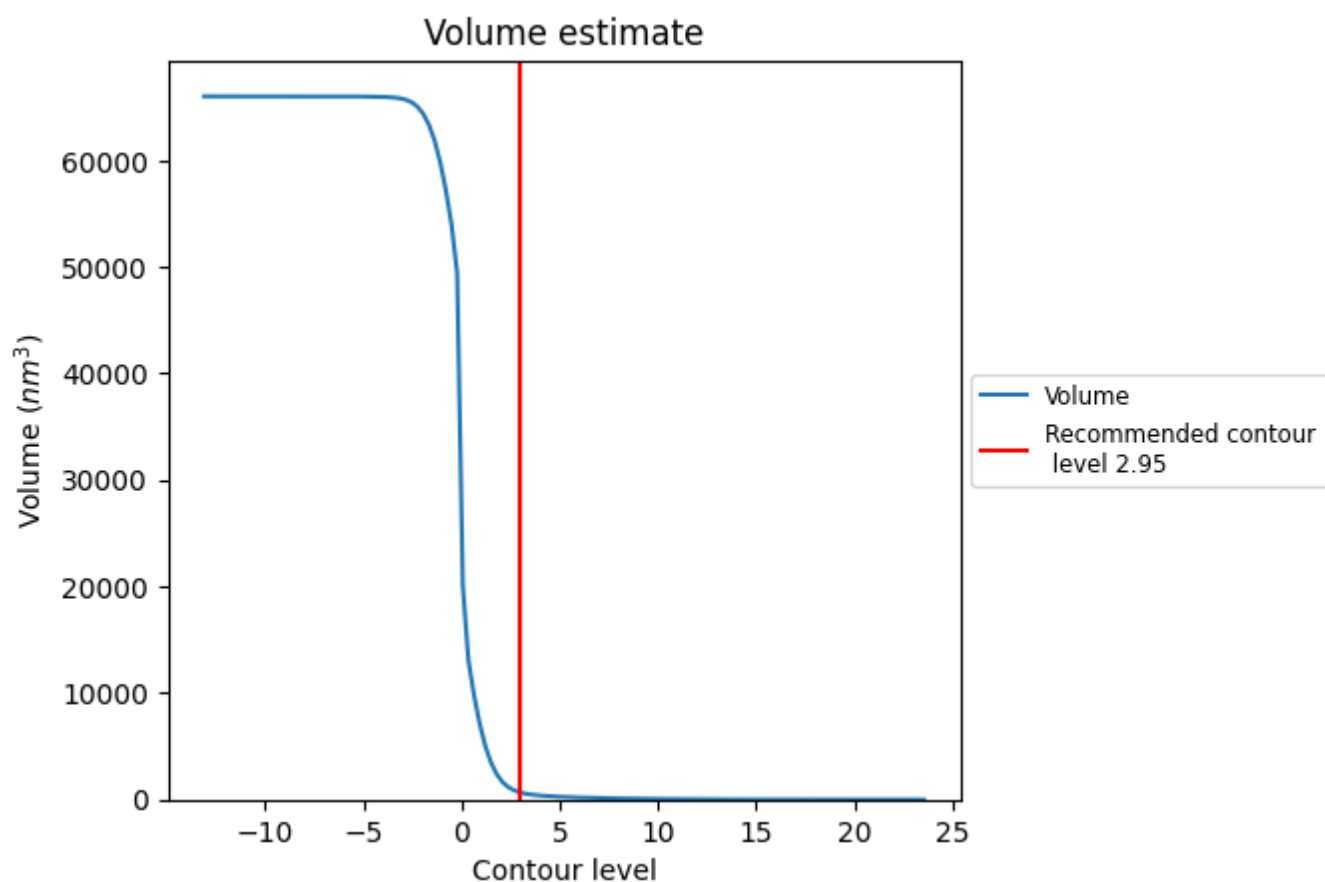
This section contains the results of statistical analysis of the map.

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.

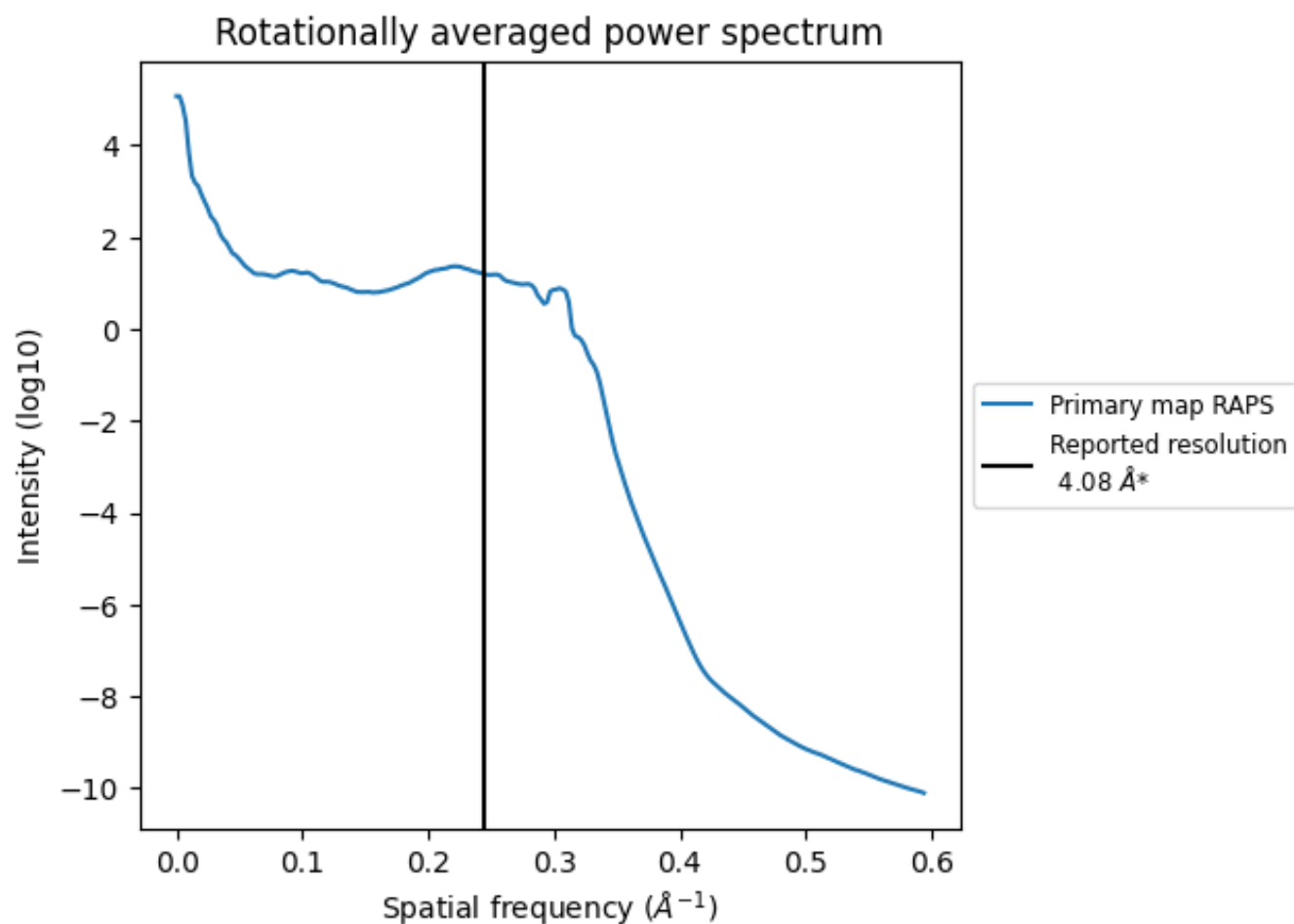
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 688 nm³; this corresponds to an approximate mass of 622 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 0.245 Å⁻¹

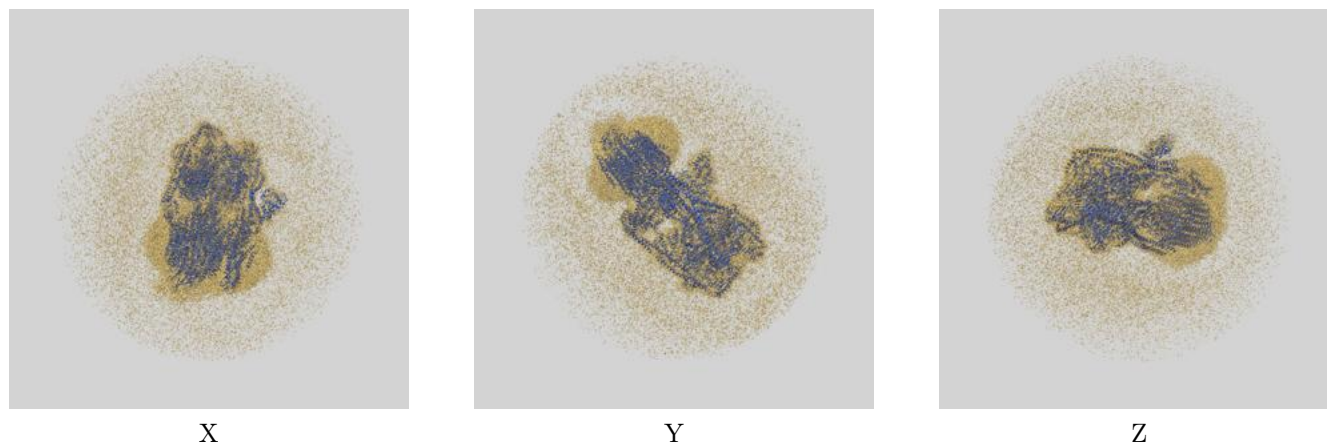
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

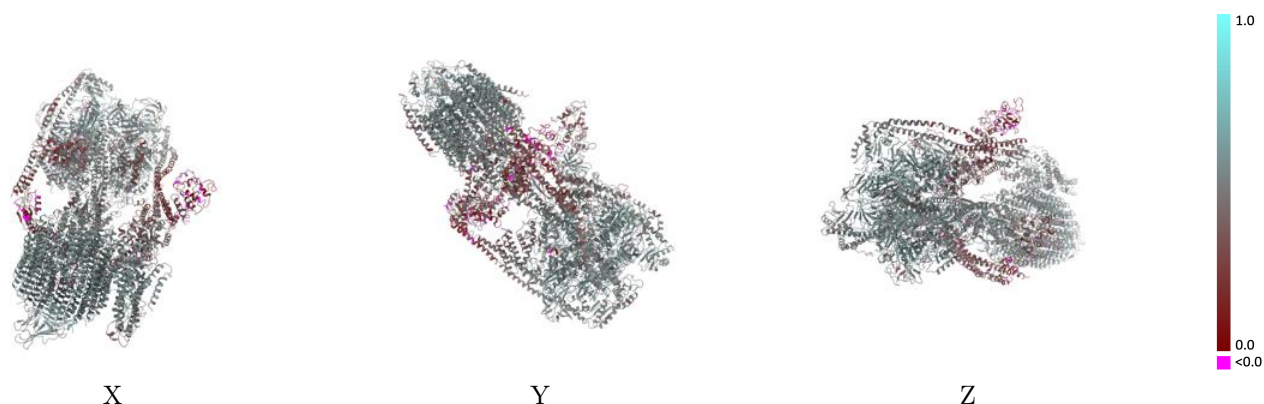
This section contains information regarding the fit between EMDB map EMD-26623 and PDB model 7UNF. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



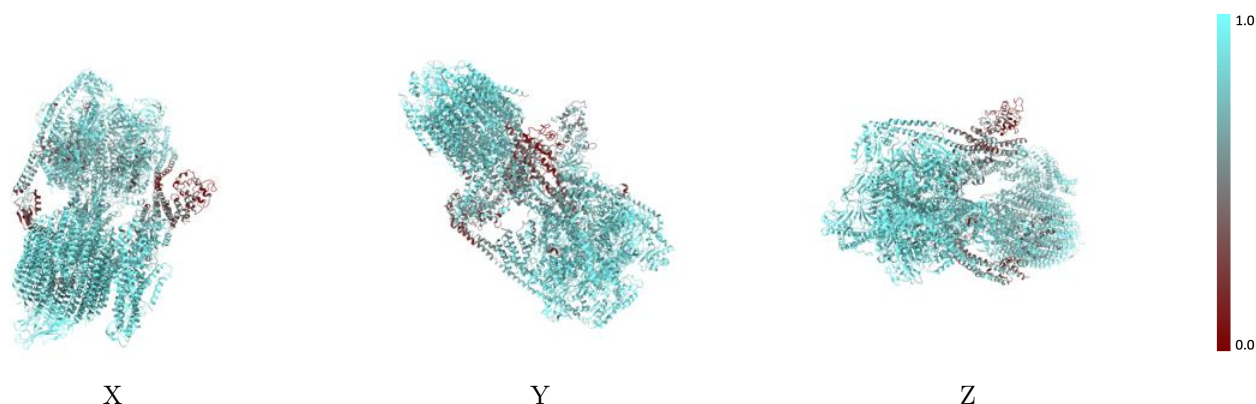
The images above show the 3D surface view of the map at the recommended contour level 2.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



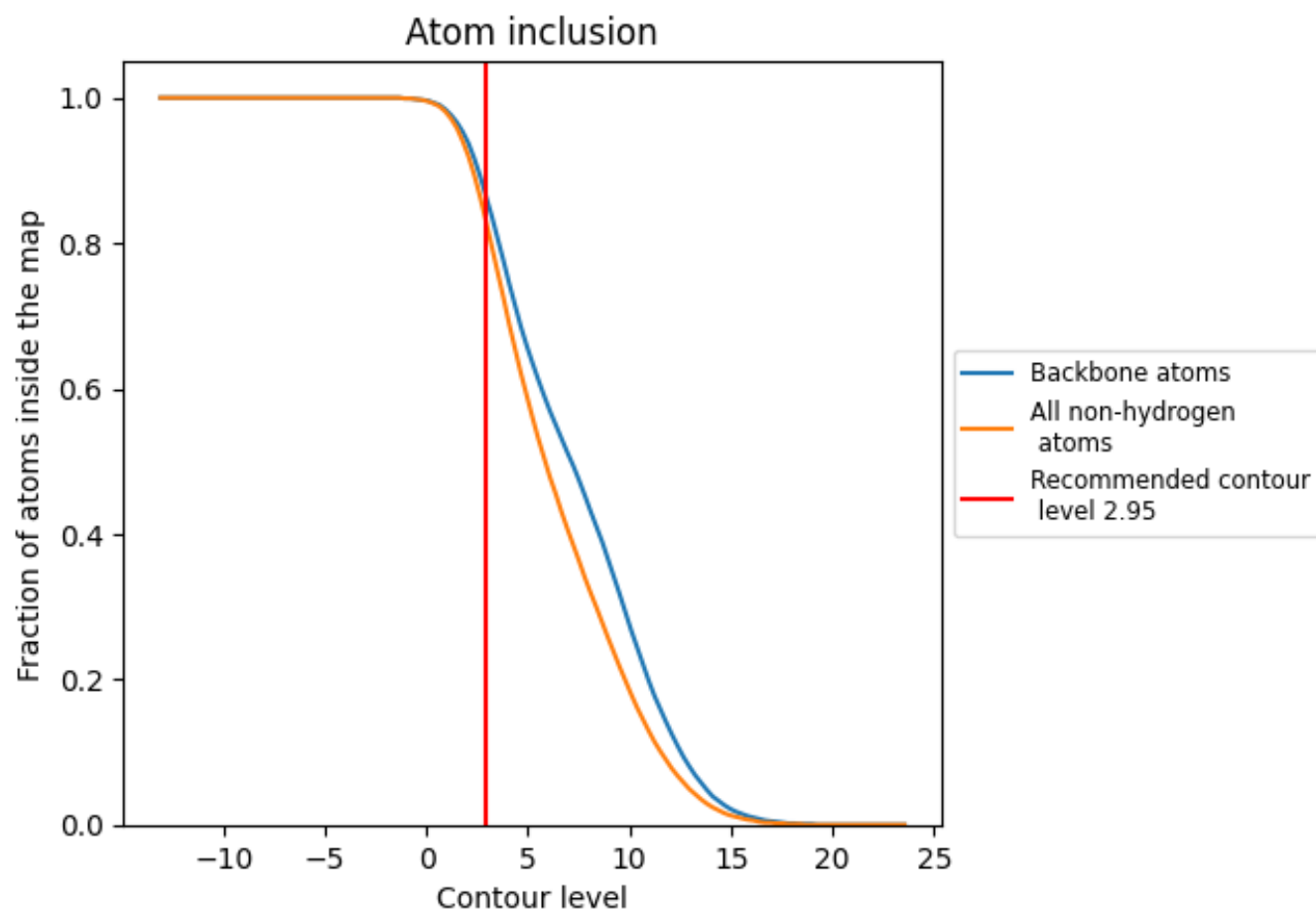
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.95).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (2.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.4790
0	 0.9290	 0.5470
1	 0.9230	 0.5530
2	 0.9260	 0.5430
3	 0.9200	 0.5410
4	 0.9110	 0.5350
5	 0.9020	 0.5330
6	 0.9170	 0.5310
7	 0.9120	 0.5350
8	 0.9060	 0.5360
9	 0.9160	 0.5420
C	 0.4590	 0.2100
D	 0.8250	 0.4910
F	 0.7760	 0.4620
H	 0.4550	 0.2370
L	 0.8590	 0.4970
M	 0.8900	 0.5200
N	 0.8300	 0.4760
O	 0.8880	 0.5350
P	 0.9030	 0.5400
Q	 0.8990	 0.5380
U	 0.7120	 0.4090
a	 0.8150	 0.4390
b	 0.7450	 0.4440
c	 0.8240	 0.4590
d	 0.8080	 0.4660
e	 0.6130	 0.3810
f	 0.7050	 0.3810
g	 0.7690	 0.4000
k	 0.8660	 0.5200
m	 0.8870	 0.5030
n	 0.8310	 0.4410
r	 0.9020	 0.5450
s	 0.9200	 0.5280
t	 0.8830	 0.5000
w	 0.7730	 0.4010

