



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 10:40 PM EDT

PDB ID : 8G4N
EMDB ID : EMD-29727
Title : Native GABA-A receptor from the mouse brain, alpha1-beta2-gamma2 subtype, in complex with GABA, Zolpidem, and endogenous neurosteroids
Authors : Sun, C.; Gouaux, E.
Deposited on : 2023-02-10
Resolution : 2.67 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

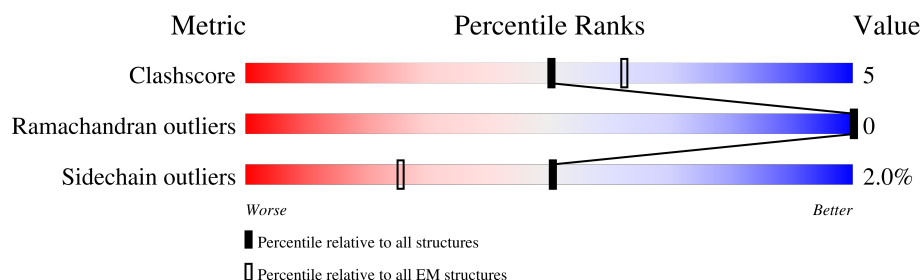
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.67 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	455	
1	C	455	
2	B	512	
2	E	512	
3	D	474	
4	H	223	
4	J	223	
5	K	213	

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Mol	Chain	Length	Quality of chain
5	L	213	<div><div></div><div>45%</div><div></div><div>51%</div></div>
6	O	3	<div><div></div><div>33%</div><div></div><div>100%</div></div>
7	F	5	<div><div></div><div>60%</div><div></div><div>40%</div></div>
7	G	5	<div><div></div><div>40%</div><div></div><div>60%</div></div>
7	M	5	<div><div></div><div>60%</div><div></div><div>80%</div><div></div><div>20%</div></div>
7	R	5	<div><div></div><div>40%</div><div></div><div>80%</div><div></div><div>20%</div></div>
7	U	5	<div><div></div><div>40%</div><div></div><div>60%</div><div></div><div>40%</div></div>
8	I	7	<div><div></div><div>29%</div><div></div><div>57%</div><div></div><div>14%</div></div>

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 18308 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 Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	346	Total	C	N	O	S	0	0
			2803	1811	471	505	16		
1	C	346	Total	C	N	O	S	0	0
			2803	1811	471	505	16		

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	333	Total	C	N	O	S	0	0
			2725	1787	436	486	16		
2	E	333	Total	C	N	O	S	0	0
			2726	1787	437	486	16		

- Molecule 3 is a protein called Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	318	Total	C	N	O	S	0	0
			2605	1698	428	465	14		

- Molecule 4 is a protein called Heavy Chain of 8E3 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	117	Total	C	N	O	S	0	0
			920	587	152	177	4		
4	J	117	Total	C	N	O	S	0	0
			920	587	152	177	4		

- Molecule 5 is a protein called Light Chain of 8E3 Fab.

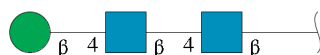
Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	105	Total	C	N	O	S	0	0
			796	505	132	155	4		

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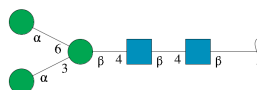
Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	105	Total	C	N	O	S	0	0
			792	503	131	154	4		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



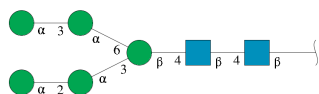
Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	3	Total	C	N	O		0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



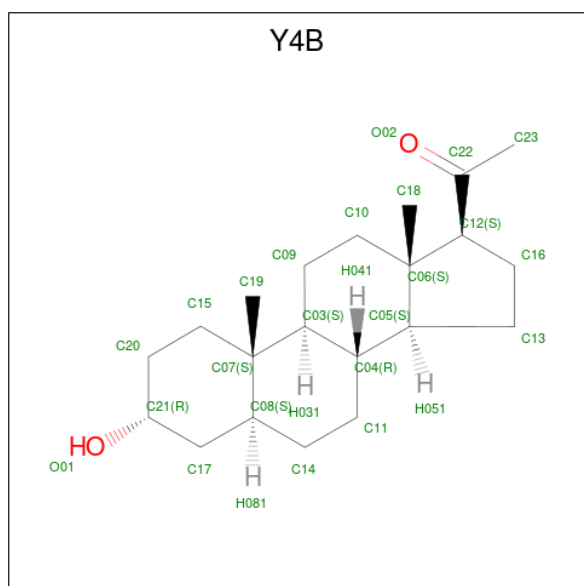
Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	5	Total	C	N	O		0	0
			61	34	2	25			
7	R	5	Total	C	N	O		0	0
			61	34	2	25			
7	U	5	Total	C	N	O		0	0
			61	34	2	25			
7	F	5	Total	C	N	O		0	0
			61	34	2	25			
7	G	5	Total	C	N	O		0	0
			61	34	2	25			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



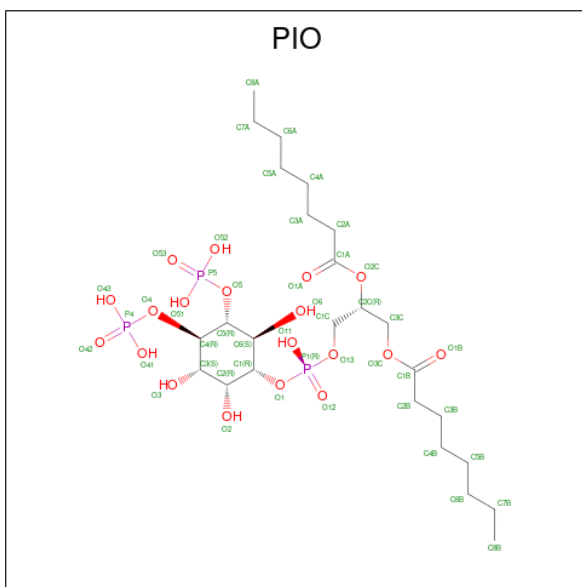
Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 9 is allopregnanolone (three-letter code: Y4B) (formula: $C_{21}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).



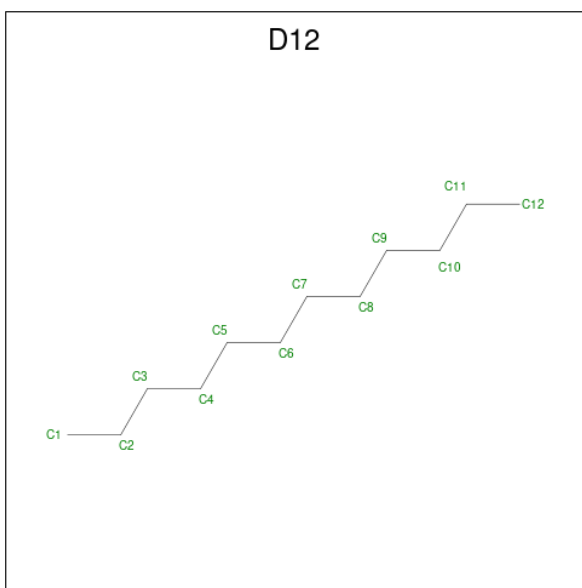
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			23	21	2	
9	C	1	Total	C	O	0
			23	21	2	

- Molecule 10 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: $C_{25}H_{49}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total 47	C 25	O 19	P 3	0
10	C	1	Total 47	C 25	O 19	P 3	0

- Molecule 11 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



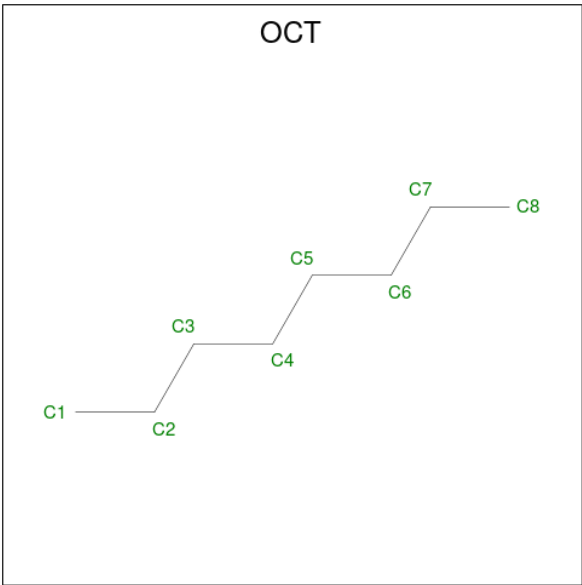
Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C 12 12	0
11	A	1	Total C 12 12	0

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Mol	Chain	Residues	Atoms	AltConf
11	B	1	Total C 12 12	0
11	B	1	Total C 12 12	0
11	B	1	Total C 12 12	0
11	B	1	Total C 12 12	0
11	B	1	Total C 12 12	0
11	B	1	Total C 12 12	0
11	B	1	Total C 12 12	0
11	C	1	Total C 12 12	0
11	C	1	Total C 12 12	0
11	D	1	Total C 12 12	0
11	D	1	Total C 12 12	0
11	E	1	Total C 12 12	0
11	E	1	Total C 12 12	0
11	E	1	Total C 12 12	0
11	E	1	Total C 12 12	0

- Molecule 12 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



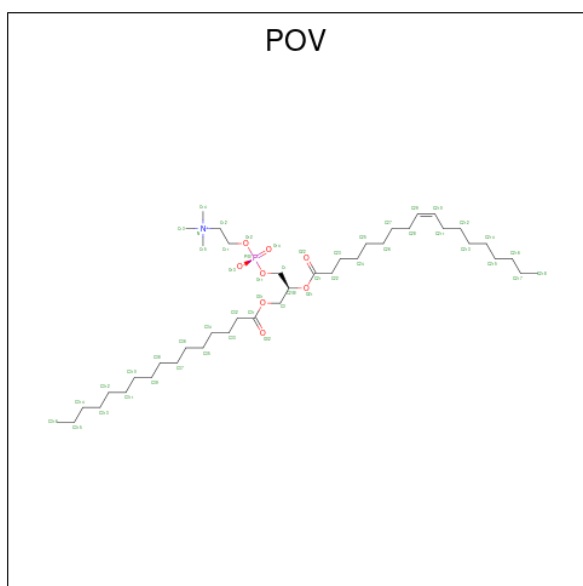
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C 8 8	0
12	A	1	Total C 8 8	0
12	A	1	Total C 8 8	0
12	A	1	Total C 8 8	0
12	C	1	Total C 8 8	0
12	C	1	Total C 8 8	0
12	C	1	Total C 8 8	0
12	C	1	Total C 8 8	0
12	D	1	Total C 8 8	0
12	D	1	Total C 8 8	0
12	D	1	Total C 8 8	0
12	D	1	Total C 8 8	0
12	E	1	Total C 8 8	0
12	E	1	Total C 8 8	0

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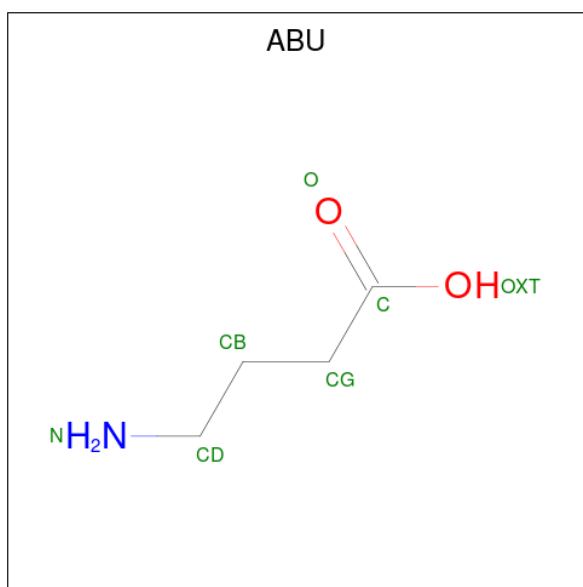
Mol	Chain	Residues	Atoms		AltConf
12	E	1	Total	C	0
			8	8	
12	E	1	Total	C	0
			8	8	
12	E	1	Total	C	0
			8	8	

- Molecule 13 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



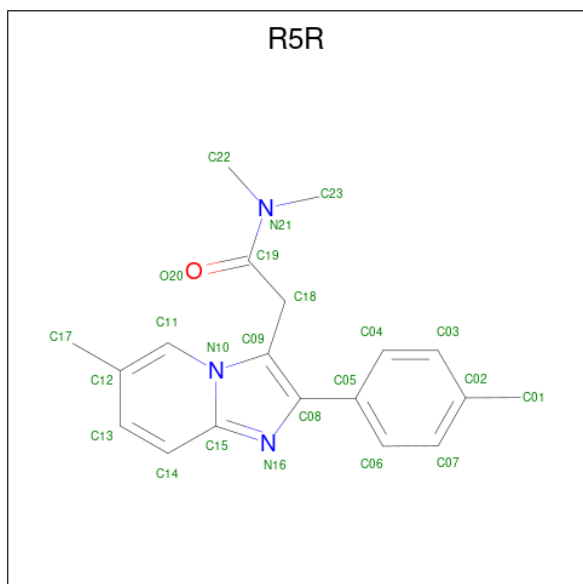
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	E	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 14 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: C₄H₉NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	N	O	0
			7	4	1	2	
14	E	1	Total	C	N	O	0
			7	4	1	2	

- Molecule 15 is Zolpidem (three-letter code: R5R) (formula: $C_{19}H_{21}N_3O$) (labeled as "Ligand of Interest" by depositor).

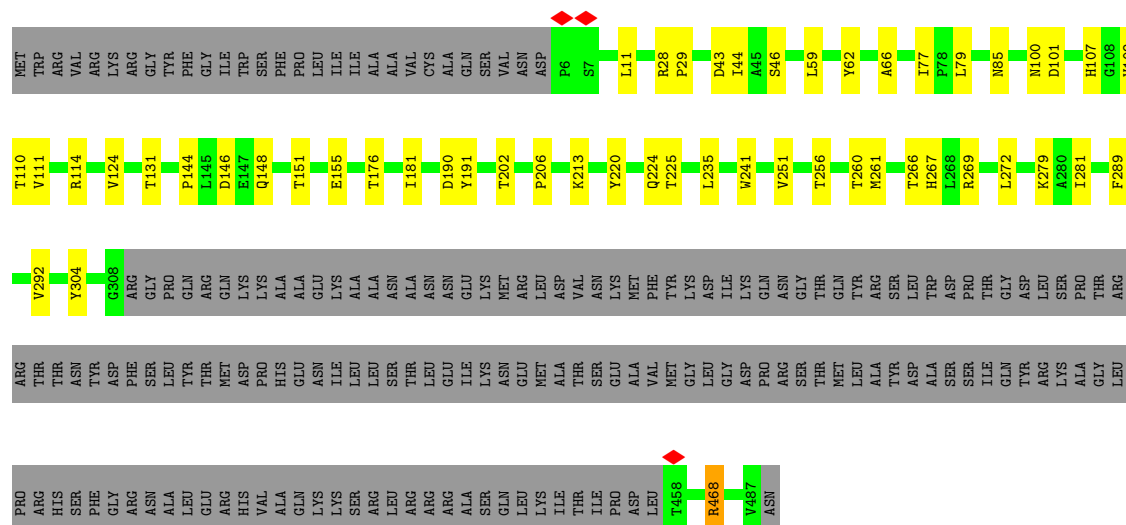


Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	N	O	0
			23	19	3	1	

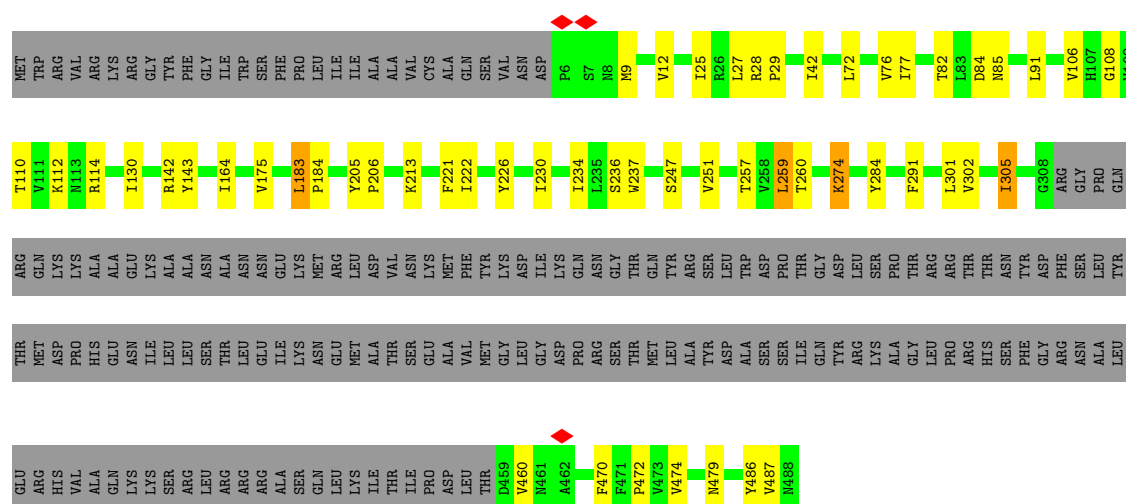
- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



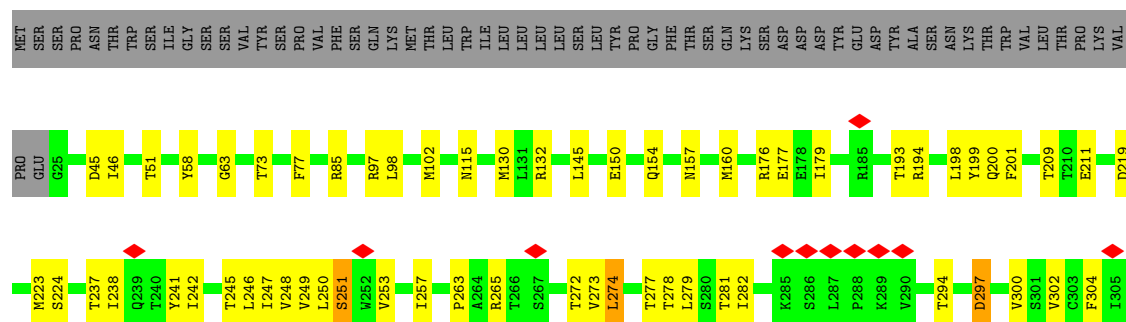
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
16	D	1	14	8	1	5	0



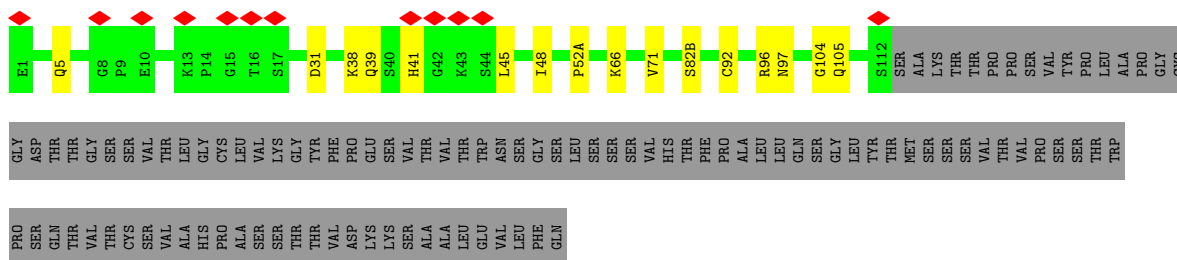
• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-2



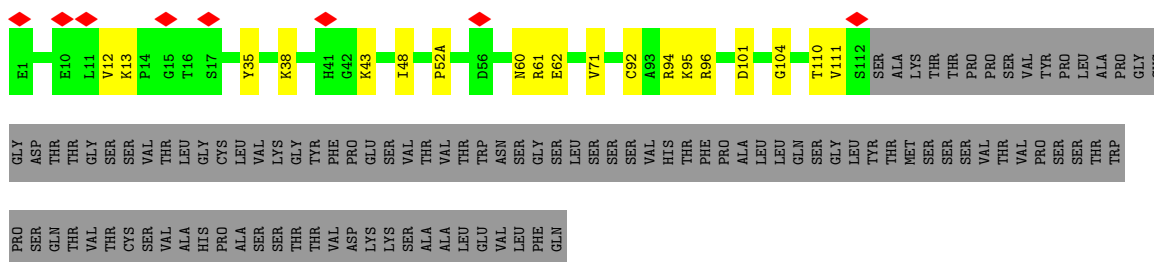
• Molecule 3: Gamma-aminobutyric acid receptor subunit gamma-2



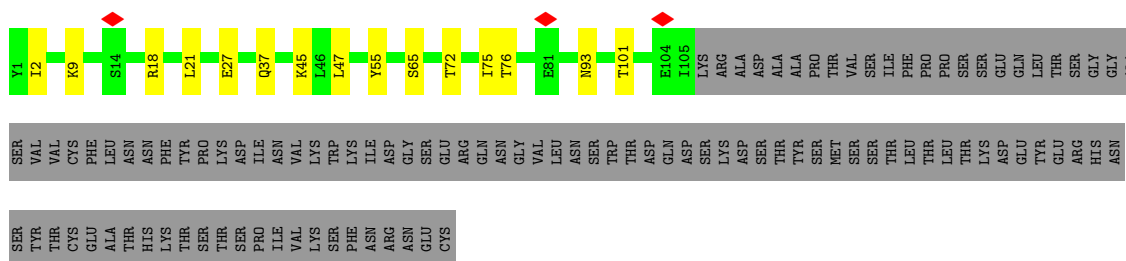
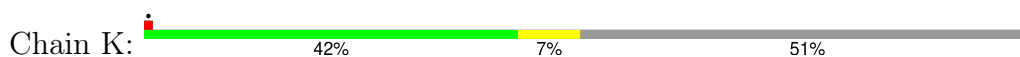
- Molecule 4: Heavy Chain of 8E3 Fab



- Molecule 4: Heavy Chain of 8E3 Fab



- Molecule 5: Light Chain of 8E3 Fab



- Molecule 5: Light Chain of 8E3 Fab

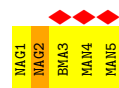
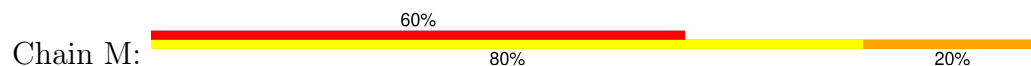




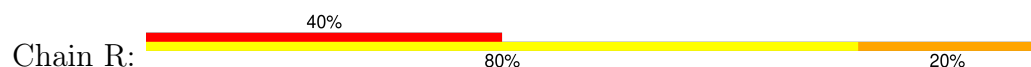
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



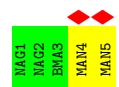
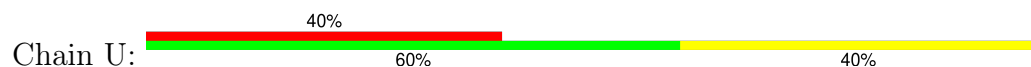
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



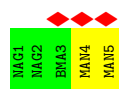
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



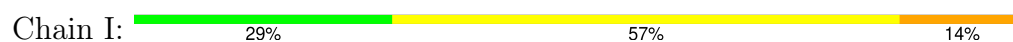
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.623	Depositor
Minimum map value	-0.295	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	297.36, 297.36, 297.36	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG, Y4B, OCT, D12, POV, ABU, R5R, PIO

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	0.27	0/2874	0.50	0/3904
1	C	0.27	0/2874	0.49	0/3904
2	B	0.27	0/2796	0.49	0/3806
2	E	0.27	0/2797	0.49	0/3807
3	D	0.26	0/2676	0.50	0/3646
4	H	0.26	0/946	0.46	0/1284
4	J	0.26	0/946	0.45	0/1284
5	K	0.27	0/815	0.47	0/1108
5	L	0.27	0/811	0.50	0/1103
All	All	0.27	0/17535	0.49	0/23846

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2803	0	2782	32	0
1	C	2803	0	2782	35	0
2	B	2725	0	2729	31	0
2	E	2726	0	2728	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2605	0	2581	41	0
4	H	920	0	863	7	0
4	J	920	0	863	8	0
5	K	796	0	756	10	0
5	L	792	0	750	5	0
6	O	39	0	34	0	0
7	F	61	0	52	0	0
7	G	61	0	52	4	0
7	M	61	0	52	2	0
7	R	61	0	52	2	0
7	U	61	0	52	0	0
8	I	83	0	70	1	0
9	A	23	0	0	1	0
9	C	23	0	0	0	0
10	A	47	0	44	2	0
10	C	47	0	44	0	0
11	A	24	0	52	0	0
11	B	84	0	182	2	0
11	C	24	0	52	0	0
11	D	24	0	52	0	0
11	E	48	0	104	0	0
12	A	32	0	72	1	0
12	C	32	0	72	1	0
12	D	32	0	72	0	0
12	E	40	0	90	0	0
13	A	52	0	82	1	0
13	B	52	0	82	0	0
13	C	104	0	164	4	0
13	E	52	0	82	6	0
14	C	7	0	0	1	0
14	E	7	0	0	0	0
15	C	23	0	0	0	0
16	D	14	0	13	0	0
All	All	18308	0	18457	198	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 5.

All (198) 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:C:85:LEU:HD13	1:C:89:MET:HG3	1.69	0.75
2:E:213:LYS:HB2	7:G:1:NAG:H82	1.74	0.68
2:B:43:ASP:HB2	2:B:62:TYR:HB2	1.76	0.68
2:B:146:ASP:OD2	2:B:148:GLN:NE2	2.27	0.67
1:C:404:GLY:HA3	13:C:511:POV:H313	1.76	0.67
1:C:109:HIS:NE2	1:C:133:THR:OG1	2.23	0.67
5:L:18:ARG:NH1	5:L:20:THR:OG1	2.28	0.66
2:E:284:TYR:OH	2:E:479:ASN:OD1	2.13	0.66
3:D:51:THR:HB	3:D:179:ILE:HD13	1.78	0.65
1:C:176:ARG:NH1	5:K:93:ASN:OD1	2.29	0.65
2:B:220:TYR:OH	2:B:224:GLN:NE2	2.29	0.65
3:D:209:THR:OG1	3:D:224:SER:OG	2.14	0.65
3:D:45:ASP:OD1	3:D:85:ARG:NH1	2.30	0.64
1:A:85:LEU:HD13	1:A:89:MET:HG3	1.78	0.64
1:A:167:VAL:HG23	1:A:210:VAL:HG21	1.80	0.63
1:A:248:ARG:NH1	1:A:387:SER:O	2.32	0.62
1:A:119:ARG:NH2	2:E:205:TYR:OH	2.33	0.62
1:A:263:LEU:HD22	2:B:260:THR:HG21	1.81	0.62
1:C:190:TYR:O	1:C:221:LYS:NZ	2.32	0.62
1:C:61:ILE:HG23	1:C:134:VAL:HG13	1.81	0.62
13:E:510:POV:H35	13:E:510:POV:H29	1.82	0.62
7:M:2:NAG:H83	7:M:2:NAG:H3	1.83	0.60
1:A:400:PRO:HB2	13:E:510:POV:H38	1.81	0.60
2:E:291:PHE:HE2	2:E:474:VAL:HG13	1.66	0.60
1:C:167:VAL:HA	1:C:210:VAL:HG11	1.83	0.60
2:B:11:LEU:HG	2:B:77:ILE:HD11	1.84	0.59
12:C:505:OCT:H22	13:C:512:POV:H28A	1.84	0.59
2:E:42:ILE:HB	2:E:175:VAL:HG22	1.84	0.59
3:D:198:LEU:HD11	3:D:201:PHE:HB2	1.85	0.59
7:G:2:NAG:H83	7:G:2:NAG:H3	1.85	0.58
1:C:204:SER:OG	1:C:207:GLY:O	2.19	0.57
7:M:1:NAG:H61	7:M:2:NAG:H82	1.86	0.57
8:I:2:NAG:H3	8:I:2:NAG:H83	1.86	0.57
3:D:238:ILE:HA	3:D:242:ILE:HD12	1.87	0.57
2:B:269:ARG:NH1	1:C:228:GLN:OE1	2.36	0.57
2:E:28:ARG:NH1	2:E:29:PRO:O	2.38	0.57
7:R:2:NAG:H83	7:R:2:NAG:H3	1.87	0.57
5:K:21:LEU:HD22	5:K:101:THR:HG21	1.86	0.57
3:D:294:THR:OG1	3:D:297:ASP:OD1	2.21	0.56
1:C:245:TRP:CD2	1:C:396:ARG:HD3	2.41	0.56
4:H:66:LYS:NZ	4:H:82(B):SER:O	2.39	0.56
1:C:165:GLU:OE2	3:D:97:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:274:LEU:O	3:D:277:THR:OG1	2.22	0.56
1:C:117:LEU:HG	1:C:129:THR:HB	1.88	0.55
1:C:238:ILE:O	1:C:242:VAL:HG23	2.06	0.55
1:A:263:LEU:HD11	2:B:256:THR:HB	1.89	0.55
1:C:75:LYS:NZ	1:C:123:ASP:O	2.40	0.54
2:B:28:ARG:NH1	2:B:29:PRO:O	2.41	0.54
2:B:85:ASN:HB2	2:B:114:ARG:HB2	1.89	0.54
1:C:262:VAL:HG21	1:C:300:LEU:HD12	1.90	0.54
4:J:101:ASP:OD1	5:K:55:TYR:OH	2.19	0.54
1:A:74:LEU:HD12	1:A:126:LEU:HD11	1.91	0.53
1:A:256:VAL:HA	1:A:259:VAL:HG22	1.91	0.53
3:D:160:MET:SD	3:D:160:MET:N	2.83	0.52
1:C:190:TYR:OH	1:C:220:ARG:NH2	2.42	0.52
2:E:142:ARG:NH2	2:E:486:TYR:O	2.41	0.52
2:B:241:TRP:CD2	2:B:468:ARG:HD2	2.45	0.52
3:D:154:GLN:N	3:D:154:GLN:OE1	2.43	0.52
1:A:109:HIS:NE2	1:A:133:THR:OG1	2.24	0.52
2:E:183:LEU:HD23	2:E:184:PRO:HD2	1.92	0.52
1:C:66:ARG:HG2	1:C:129:THR:HG23	1.92	0.51
2:E:106:VAL:HG21	2:E:112:LYS:HE3	1.91	0.51
2:B:202:THR:OG1	14:C:501:ABU:O	2.22	0.51
4:H:38:LYS:HB2	4:H:48:ILE:HD11	1.93	0.51
1:A:317:ASP:OD1	1:A:318:GLY:N	2.44	0.50
3:D:237:THR:HA	3:D:241:TYR:HB2	1.92	0.50
1:C:86:ASN:OD1	1:C:86:ASN:N	2.44	0.50
2:E:76:VAL:HG23	2:E:77:ILE:HG23	1.93	0.50
5:K:37:GLN:HB2	5:K:47:LEU:HD11	1.93	0.50
1:A:390:LYS:NZ	10:A:502:PIO:O1A	2.44	0.50
3:D:245:THR:O	3:D:249:VAL:HG23	2.12	0.50
1:A:276:LEU:H	1:A:276:LEU:HD23	1.77	0.49
4:H:96:ARG:NH1	4:H:97:ASN:OD1	2.45	0.49
3:D:273:VAL:HG13	3:D:274:LEU:HD22	1.94	0.49
2:E:85:ASN:HB2	2:E:114:ARG:HB3	1.93	0.49
1:C:256:VAL:HA	1:C:259:VAL:HG12	1.94	0.49
1:C:415:LEU:HD11	13:C:512:POV:H33A	1.94	0.49
5:K:18:ARG:HD2	5:K:76:THR:HA	1.95	0.49
2:B:46:SER:HA	2:B:181:ILE:HD12	1.94	0.49
1:A:226:VAL:HA	1:A:230:TYR:HB2	1.95	0.48
1:C:278:LYS:HE3	3:D:200:GLN:HA	1.94	0.48
3:D:274:LEU:HD12	2:E:260:THR:HG21	1.94	0.48
2:E:236:SER:HB3	2:E:257:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:GLY:HA2	2:E:112:LYS:HA	1.94	0.48
2:E:291:PHE:CE2	2:E:474:VAL:HG13	2.48	0.48
3:D:250:LEU:O	3:D:253:VAL:HG12	2.13	0.48
1:A:259:VAL:O	1:A:263:LEU:HG	2.14	0.48
5:L:104:GLU:OE1	5:L:105:ILE:N	2.46	0.48
3:D:176:ARG:N	3:D:219:ASP:O	2.44	0.48
3:D:277:THR:HG22	3:D:304:PHE:HE1	1.78	0.48
1:A:238:ILE:O	1:A:242:VAL:HG23	2.14	0.47
5:K:2:ILE:HD12	5:K:27:GLU:HB2	1.95	0.47
5:K:65:SER:OG	5:K:72:THR:OG1	2.32	0.47
1:A:38:THR:HB	1:A:166:VAL:HG12	1.97	0.47
1:C:226:VAL:HA	1:C:230:TYR:HB2	1.96	0.47
1:A:116:LYS:HG2	1:A:130:MET:HB3	1.96	0.47
1:A:258:GLY:HA3	1:A:300:LEU:HD13	1.97	0.47
2:B:100:ASN:ND2	2:B:151:THR:O	2.46	0.47
1:C:245:TRP:CE2	1:C:396:ARG:HD3	2.50	0.47
3:D:247:ILE:HG13	3:D:272:THR:HG23	1.97	0.47
4:J:62:GLU:OE1	4:J:62:GLU:N	2.48	0.47
2:B:44:ILE:HD12	2:B:59:LEU:HD11	1.97	0.46
2:B:272:LEU:HD22	2:B:279:LYS:HE3	1.97	0.46
2:E:470:PHE:O	2:E:474:VAL:HG12	2.15	0.46
3:D:251:SER:OG	3:D:307:VAL:HG12	2.15	0.46
3:D:46:ILE:HG22	2:E:9:MET:SD	2.55	0.46
1:C:293:TYR:CE1	3:D:246:LEU:HD13	2.51	0.46
1:C:392:ASP:O	1:C:396:ARG:HG3	2.15	0.46
3:D:63:GLY:N	3:D:73:THR:O	2.49	0.46
1:A:111:MET:HG2	1:A:112:THR:HA	1.97	0.46
4:J:60:ASN:OD1	4:J:61:ARG:N	2.49	0.45
7:G:3:BMA:O2	7:G:4:MAN:O5	2.32	0.45
1:A:312:ARG:NH1	10:A:502:PIO:O52	2.45	0.45
1:C:198:ASP:OD1	1:C:199:SER:N	2.46	0.45
5:L:6:GLN:NE2	5:L:99:GLY:O	2.49	0.45
13:E:510:POV:H34	13:E:510:POV:H37	1.49	0.45
3:D:302:VAL:HG21	3:D:425:PHE:CE1	2.52	0.45
2:B:144:PRO:HD3	2:B:281:ILE:HB	1.99	0.45
5:L:81:GLU:N	5:L:81:GLU:OE1	2.50	0.45
2:B:289:PHE:HA	2:B:292:VAL:HG12	1.98	0.45
2:B:304:TYR:HE2	11:B:502:D12:H71	1.82	0.45
4:J:92:CYS:O	4:J:104:GLY:N	2.50	0.45
1:A:389:SER:HB3	1:A:392:ASP:HB2	1.98	0.45
4:H:39:GLN:HB2	4:H:45:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:297:ASP:HA	3:D:300:VAL:HG22	1.99	0.44
3:D:274:LEU:HD13	3:D:274:LEU:HA	1.69	0.44
3:D:278:THR:O	3:D:281:THR:OG1	2.29	0.44
4:H:5:GLN:NE2	4:H:105:GLN:OE1	2.50	0.44
2:B:251:VAL:HG21	1:C:253:ALA:HB1	1.99	0.44
4:H:92:CYS:O	4:H:104:GLY:N	2.50	0.44
1:C:154:LEU:HB3	1:C:214:THR:HG23	2.00	0.44
13:E:510:POV:H28A	13:E:510:POV:H21A	1.45	0.44
1:C:312:ARG:O	1:C:386:ASN:ND2	2.50	0.44
3:D:130:MET:SD	3:D:132:ARG:HG3	2.58	0.44
2:E:106:VAL:HG12	2:E:130:ILE:HG12	2.00	0.44
3:D:98:LEU:HD13	3:D:102:MET:HG3	1.99	0.43
3:D:279:LEU:O	3:D:282:ILE:HG13	2.18	0.43
4:J:52(A):PRO:HB3	4:J:71:VAL:HG21	1.99	0.43
1:A:50:GLY:HA2	1:A:186:ARG:HB2	2.01	0.43
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.84	0.43
2:B:261:MET:HG3	2:B:292:VAL:HG11	1.99	0.43
3:D:145:LEU:HD11	2:E:110:THR:HG22	1.99	0.43
9:A:501:Y4B:O02	2:E:301:LEU:HD23	2.17	0.43
2:E:237:TRP:CH2	2:E:472:PRO:HA	2.54	0.43
3:D:248:VAL:HA	3:D:251:SER:HG	1.84	0.43
2:E:302:VAL:HG13	2:E:460:VAL:HB	2.00	0.43
2:B:213:LYS:HB2	7:R:1:NAG:H81	2.01	0.43
4:J:35:TYR:CE1	4:J:95:LYS:HD2	2.54	0.43
1:C:68:SER:HA	1:C:126:LEU:O	2.18	0.43
7:G:3:BMA:O2	7:G:4:MAN:O6	2.30	0.43
3:D:115:ASN:O	3:D:150:GLU:N	2.45	0.43
12:A:506:OCT:H62	13:A:509:POV:H38	2.01	0.42
2:B:190:ASP:OD1	2:B:191:TYR:N	2.52	0.42
2:E:143:TYR:HH	2:E:221:PHE:HE2	1.67	0.42
4:J:38:LYS:HB2	4:J:48:ILE:HD11	2.02	0.42
2:E:247:SER:O	2:E:251:VAL:HB	2.18	0.42
13:C:511:POV:H35	13:C:511:POV:H32A	1.83	0.42
2:B:155:GLU:HG3	2:B:206:PRO:O	2.19	0.42
3:D:411:ASP:O	3:D:415:ARG:HG3	2.18	0.42
2:E:72:LEU:HD11	2:E:91:LEU:HD22	2.01	0.42
13:E:510:POV:H24	13:E:510:POV:O32	2.20	0.42
3:D:157:ASN:OD1	3:D:157:ASN:N	2.51	0.42
1:A:98:THR:O	2:B:110:THR:HB	2.20	0.42
1:C:43:ASP:HB2	1:C:171:THR:HG22	2.01	0.42
1:A:110:ASN:HA	1:A:114:PRO:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:MET:HG2	1:A:293:TYR:HA	2.01	0.42
3:D:193:THR:OG1	3:D:194:ARG:NH2	2.53	0.42
2:B:266:THR:HG23	1:C:228:GLN:NE2	2.35	0.41
3:D:257:ILE:O	3:D:265:ARG:NH2	2.46	0.41
4:H:52(A):PRO:HB3	4:H:71:VAL:HG21	2.01	0.41
1:A:224:TYR:CD2	2:E:274:LYS:HG3	2.56	0.41
1:A:262:VAL:HG11	2:B:235:LEU:HD22	2.02	0.41
5:L:24:ARG:NH1	5:L:70:ASP:OD1	2.44	0.41
2:B:66:ALA:HA	2:B:124:VAL:O	2.20	0.41
2:E:230:ILE:O	2:E:234:ILE:HG12	2.21	0.41
5:K:37:GLN:O	5:K:45:LYS:N	2.49	0.41
1:A:43:ASP:HB3	1:A:171:THR:HG22	2.02	0.41
2:B:110:THR:HG22	2:B:111:VAL:HG13	2.02	0.41
5:K:9:LYS:HA	5:K:9:LYS:HD2	1.94	0.41
2:B:43:ASP:OD1	2:B:176:THR:OG1	2.38	0.41
1:C:252:PRO:HG3	3:D:263:PRO:HG2	2.03	0.41
3:D:177:GLU:OE1	3:D:177:GLU:N	2.50	0.41
2:E:12:VAL:HG22	2:E:77:ILE:HD13	2.03	0.41
2:B:107:HIS:NE2	2:B:131:THR:OG1	2.34	0.41
2:E:222:ILE:HA	2:E:226:TYR:HB2	2.02	0.41
2:B:269:ARG:HH12	1:C:228:GLN:HB2	1.86	0.41
2:E:25:ILE:H	2:E:25:ILE:HD12	1.85	0.41
2:E:301:LEU:HD22	2:E:305:ILE:HD13	2.01	0.41
2:E:164:ILE:HG23	2:E:206:PRO:HG3	2.02	0.41
3:D:58:TYR:HB3	3:D:77:PHE:HB2	2.03	0.40
3:D:247:ILE:HD12	3:D:247:ILE:HA	1.93	0.40
2:E:259:LEU:HA	2:E:259:LEU:HD13	1.76	0.40
4:J:12:VAL:O	4:J:111:VAL:HA	2.22	0.40
1:A:248:ARG:HD3	1:A:310:THR:HG23	2.02	0.40
11:B:503:D12:H72	11:B:503:D12:H41	1.82	0.40
1:A:245:TRP:CH2	13:E:510:POV:H3	2.56	0.40
1:C:258:GLY:O	1:C:262:VAL:HG23	2.21	0.40
5:K:18:ARG:HA	5:K:75:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	342/455 (75%)	336 (98%)	6 (2%)	0	100	100
1	C	342/455 (75%)	337 (98%)	5 (2%)	0	100	100
2	B	329/512 (64%)	321 (98%)	8 (2%)	0	100	100
2	E	329/512 (64%)	321 (98%)	8 (2%)	0	100	100
3	D	314/474 (66%)	306 (98%)	8 (2%)	0	100	100
4	H	115/223 (52%)	111 (96%)	4 (4%)	0	100	100
4	J	115/223 (52%)	113 (98%)	2 (2%)	0	100	100
5	K	103/213 (48%)	99 (96%)	4 (4%)	0	100	100
5	L	103/213 (48%)	99 (96%)	4 (4%)	0	100	100
All	All	2092/3280 (64%)	2043 (98%)	49 (2%)	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	308/404 (76%)	305 (99%)	3 (1%)	73	88
1	C	308/404 (76%)	301 (98%)	7 (2%)	45	72
2	B	303/457 (66%)	297 (98%)	6 (2%)	50	76
2	E	303/457 (66%)	295 (97%)	8 (3%)	41	68
3	D	292/436 (67%)	286 (98%)	6 (2%)	48	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	98/195 (50%)	96 (98%)	2 (2%)	50	76
4	J	98/195 (50%)	93 (95%)	5 (5%)	20	42
5	K	83/188 (44%)	83 (100%)	0	100	100
5	L	82/188 (44%)	81 (99%)	1 (1%)	67	85
All	All	1875/2924 (64%)	1837 (98%)	38 (2%)	50	76

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	257	PHE
1	A	293	TYR
2	B	79	LEU
2	B	101	ASP
2	B	109	VAL
2	B	225	THR
2	B	267	HIS
2	B	468	ARG
1	C	43	ASP
1	C	48	SER
1	C	87	ASN
1	C	214	THR
1	C	231	LEU
1	C	257	PHE
1	C	273	ARG
3	D	199	TYR
3	D	211	GLU
3	D	223	MET
3	D	251	SER
3	D	274	LEU
3	D	297	ASP
2	E	27	LEU
2	E	82	THR
2	E	84	ASP
2	E	183	LEU
2	E	259	LEU
2	E	274	LYS
2	E	305	ILE
2	E	487	VAL
4	H	31	ASP
4	H	41	HIS

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Mol	Chain	Res	Type
4	J	13	LYS
4	J	43	LYS
4	J	94	ARG
4	J	96	ARG
4	J	110	THR
5	L	104	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
2	B	224	GLN
1	C	115	ASN
3	D	80	GLN
2	E	64	GLN
2	E	224	GLN
4	H	5	GLN
4	H	105	GLN
5	L	6	GLN

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](#)

35 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
7	NAG	F	1	2,7	14,14,15	0.26	0	17,19,21	0.45	0
7	NAG	F	2	7	14,14,15	0.20	0	17,19,21	0.45	0
7	BMA	F	3	7	11,11,12	0.61	0	15,15,17	0.72	0
7	MAN	F	4	7	11,11,12	0.93	2 (18%)	15,15,17	1.48	2 (13%)
7	MAN	F	5	7	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
7	NAG	G	1	2,7	14,14,15	0.40	0	17,19,21	0.43	0
7	NAG	G	2	7	14,14,15	0.45	0	17,19,21	1.35	2 (11%)
7	BMA	G	3	7	11,11,12	0.99	0	15,15,17	1.01	1 (6%)
7	MAN	G	4	7	11,11,12	0.82	1 (9%)	15,15,17	1.11	2 (13%)
7	MAN	G	5	7	11,11,12	0.79	0	15,15,17	1.16	2 (13%)
8	NAG	I	1	8,1	14,14,15	0.28	0	17,19,21	0.55	0
8	NAG	I	2	8	14,14,15	0.41	0	17,19,21	1.33	2 (11%)
8	BMA	I	3	8	11,11,12	0.52	0	15,15,17	0.81	0
8	MAN	I	4	8	11,11,12	0.50	0	15,15,17	1.02	2 (13%)
8	MAN	I	5	8	11,11,12	0.48	0	15,15,17	0.97	2 (13%)
8	MAN	I	6	8	11,11,12	0.60	0	15,15,17	0.95	2 (13%)
8	MAN	I	7	8	11,11,12	0.54	0	15,15,17	1.16	2 (13%)
7	NAG	M	1	2,7	14,14,15	0.43	0	17,19,21	0.55	0
7	NAG	M	2	7	14,14,15	0.45	0	17,19,21	1.36	1 (5%)
7	BMA	M	3	7	11,11,12	0.70	0	15,15,17	0.92	1 (6%)
7	MAN	M	4	7	11,11,12	0.89	1 (9%)	15,15,17	1.22	2 (13%)
7	MAN	M	5	7	11,11,12	0.66	0	15,15,17	0.91	1 (6%)
6	NAG	O	1	3,6	14,14,15	0.43	0	17,19,21	0.53	0
6	NAG	O	2	6	14,14,15	0.25	0	17,19,21	0.48	0
6	BMA	O	3	6	11,11,12	0.59	0	15,15,17	0.63	0
7	NAG	R	1	2,7	14,14,15	0.36	0	17,19,21	0.56	0
7	NAG	R	2	7	14,14,15	0.47	0	17,19,21	1.40	2 (11%)
7	BMA	R	3	7	11,11,12	0.86	1 (9%)	15,15,17	0.91	1 (6%)
7	MAN	R	4	7	11,11,12	0.65	0	15,15,17	1.08	2 (13%)
7	MAN	R	5	7	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
7	NAG	U	1	1,7	14,14,15	0.38	0	17,19,21	0.55	0
7	NAG	U	2	7	14,14,15	0.21	0	17,19,21	0.68	0
7	BMA	U	3	7	11,11,12	0.55	0	15,15,17	0.73	0
7	MAN	U	4	7	11,11,12	0.69	0	15,15,17	0.92	1 (6%)
7	MAN	U	5	7	11,11,12	0.59	0	15,15,17	1.00	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
7	NAG	F	1	2,7	-	4/6/23/26	0/1/1/1
7	NAG	F	2	7	-	2/6/23/26	0/1/1/1
7	BMA	F	3	7	-	2/2/19/22	0/1/1/1
7	MAN	F	4	7	-	1/2/19/22	1/1/1/1
7	MAN	F	5	7	-	1/2/19/22	0/1/1/1
7	NAG	G	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	6/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	2/2/19/22	1/1/1/1
7	MAN	G	5	7	-	0/2/19/22	1/1/1/1
8	NAG	I	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	4/6/23/26	0/1/1/1
8	BMA	I	3	8	-	2/2/19/22	0/1/1/1
8	MAN	I	4	8	-	1/2/19/22	0/1/1/1
8	MAN	I	5	8	-	1/2/19/22	0/1/1/1
8	MAN	I	6	8	-	0/2/19/22	0/1/1/1
8	MAN	I	7	8	-	0/2/19/22	0/1/1/1
7	NAG	M	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	6/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
7	MAN	M	4	7	-	0/2/19/22	1/1/1/1
7	MAN	M	5	7	-	1/2/19/22	0/1/1/1
6	NAG	O	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
7	NAG	R	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	R	2	7	-	5/6/23/26	0/1/1/1
7	BMA	R	3	7	-	1/2/19/22	0/1/1/1
7	MAN	R	4	7	-	0/2/19/22	0/1/1/1
7	MAN	R	5	7	-	0/2/19/22	0/1/1/1
7	NAG	U	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	U	2	7	-	2/6/23/26	0/1/1/1
7	BMA	U	3	7	-	0/2/19/22	0/1/1/1
7	MAN	U	4	7	-	1/2/19/22	0/1/1/1
7	MAN	U	5	7	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	3	BMA	C1-C2	2.34	1.57	1.52
7	F	4	MAN	C1-C2	2.18	1.57	1.52
7	M	4	MAN	C1-C2	2.17	1.57	1.52
7	F	4	MAN	O5-C5	2.04	1.47	1.43
7	G	4	MAN	C1-C2	2.00	1.57	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	4	MAN	C1-O5-C5	4.75	118.56	112.19
7	R	2	NAG	C2-N2-C7	4.63	129.11	122.90
8	I	2	NAG	C2-N2-C7	4.58	129.04	122.90
7	M	2	NAG	C2-N2-C7	4.57	129.03	122.90
7	G	2	NAG	C2-N2-C7	4.54	128.99	122.90
7	M	4	MAN	C1-O5-C5	3.79	117.26	112.19
7	G	5	MAN	C1-O5-C5	3.47	116.84	112.19
8	I	7	MAN	C1-O5-C5	3.38	116.72	112.19
7	G	4	MAN	C1-O5-C5	3.29	116.60	112.19
7	R	4	MAN	C1-O5-C5	2.89	116.06	112.19
7	R	5	MAN	C1-O5-C5	2.70	115.80	112.19
7	F	5	MAN	C1-O5-C5	2.70	115.80	112.19
7	U	5	MAN	C1-O5-C5	2.66	115.76	112.19
8	I	4	MAN	C1-O5-C5	2.64	115.72	112.19
7	G	3	BMA	O3-C3-C2	2.62	115.40	110.05
8	I	5	MAN	C1-O5-C5	2.48	115.51	112.19
8	I	4	MAN	O2-C2-C3	-2.36	105.27	110.15
8	I	6	MAN	O2-C2-C3	-2.36	105.27	110.15
7	U	5	MAN	O2-C2-C3	-2.28	105.42	110.15
7	R	2	NAG	C1-C2-N2	2.26	113.99	110.43
8	I	7	MAN	O2-C2-C3	-2.24	105.52	110.15
8	I	5	MAN	O2-C2-C3	-2.21	105.58	110.15
7	M	5	MAN	O2-C2-C3	-2.19	105.62	110.15
7	U	4	MAN	O2-C2-C3	-2.18	105.63	110.15
7	G	2	NAG	C1-C2-N2	2.18	113.87	110.43
7	F	5	MAN	O2-C2-C3	-2.18	105.64	110.15
7	F	4	MAN	O2-C2-C3	-2.15	105.69	110.15
7	R	4	MAN	O2-C2-C3	-2.15	105.71	110.15
7	M	4	MAN	O2-C2-C3	-2.14	105.72	110.15
7	R	5	MAN	O2-C2-C3	-2.13	105.73	110.15
7	G	5	MAN	O2-C2-C3	-2.13	105.74	110.15
7	G	4	MAN	O2-C2-C3	-2.12	105.75	110.15
8	I	2	NAG	C1-C2-N2	2.12	113.77	110.43
7	R	3	BMA	O2-C2-C3	-2.11	105.79	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	6	MAN	C1-O5-C5	2.07	114.95	112.19
7	M	3	BMA	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	3	BMA	C4-C5-C6-O6
7	F	2	NAG	C4-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
7	F	3	BMA	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
7	F	2	NAG	O5-C5-C6-O6
7	G	1	NAG	C4-C5-C6-O6
7	M	2	NAG	C4-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
8	I	3	BMA	O5-C5-C6-O6
7	F	1	NAG	O5-C5-C6-O6
7	G	4	MAN	O5-C5-C6-O6
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
7	M	1	NAG	C8-C7-N2-C2
7	M	1	NAG	O7-C7-N2-C2
7	M	2	NAG	C8-C7-N2-C2
7	M	2	NAG	O7-C7-N2-C2
7	R	2	NAG	C8-C7-N2-C2
7	R	2	NAG	O7-C7-N2-C2
7	F	1	NAG	C8-C7-N2-C2
7	F	1	NAG	O7-C7-N2-C2
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2
8	I	2	NAG	C8-C7-N2-C2
8	I	2	NAG	O7-C7-N2-C2
7	U	1	NAG	C4-C5-C6-O6
7	F	1	NAG	C4-C5-C6-O6
8	I	3	BMA	C4-C5-C6-O6
8	I	5	MAN	O5-C5-C6-O6
7	F	4	MAN	O5-C5-C6-O6
7	R	3	BMA	O5-C5-C6-O6
7	F	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	G	4	MAN	C4-C5-C6-O6
7	U	4	MAN	O5-C5-C6-O6
8	I	4	MAN	O5-C5-C6-O6
7	M	5	MAN	O5-C5-C6-O6
7	U	2	NAG	C1-C2-N2-C7
8	I	1	NAG	C1-C2-N2-C7
7	G	2	NAG	C4-C5-C6-O6
7	U	1	NAG	C3-C2-N2-C7
7	U	2	NAG	C3-C2-N2-C7
7	G	2	NAG	O5-C5-C6-O6
7	M	2	NAG	C1-C2-N2-C7
7	R	2	NAG	C1-C2-N2-C7
7	U	1	NAG	C1-C2-N2-C7
7	G	2	NAG	C1-C2-N2-C7
8	I	2	NAG	C1-C2-N2-C7
7	M	2	NAG	C3-C2-N2-C7
7	R	2	NAG	C3-C2-N2-C7
7	G	2	NAG	C3-C2-N2-C7
8	I	1	NAG	C3-C2-N2-C7
8	I	2	NAG	C3-C2-N2-C7
7	R	2	NAG	C4-C5-C6-O6

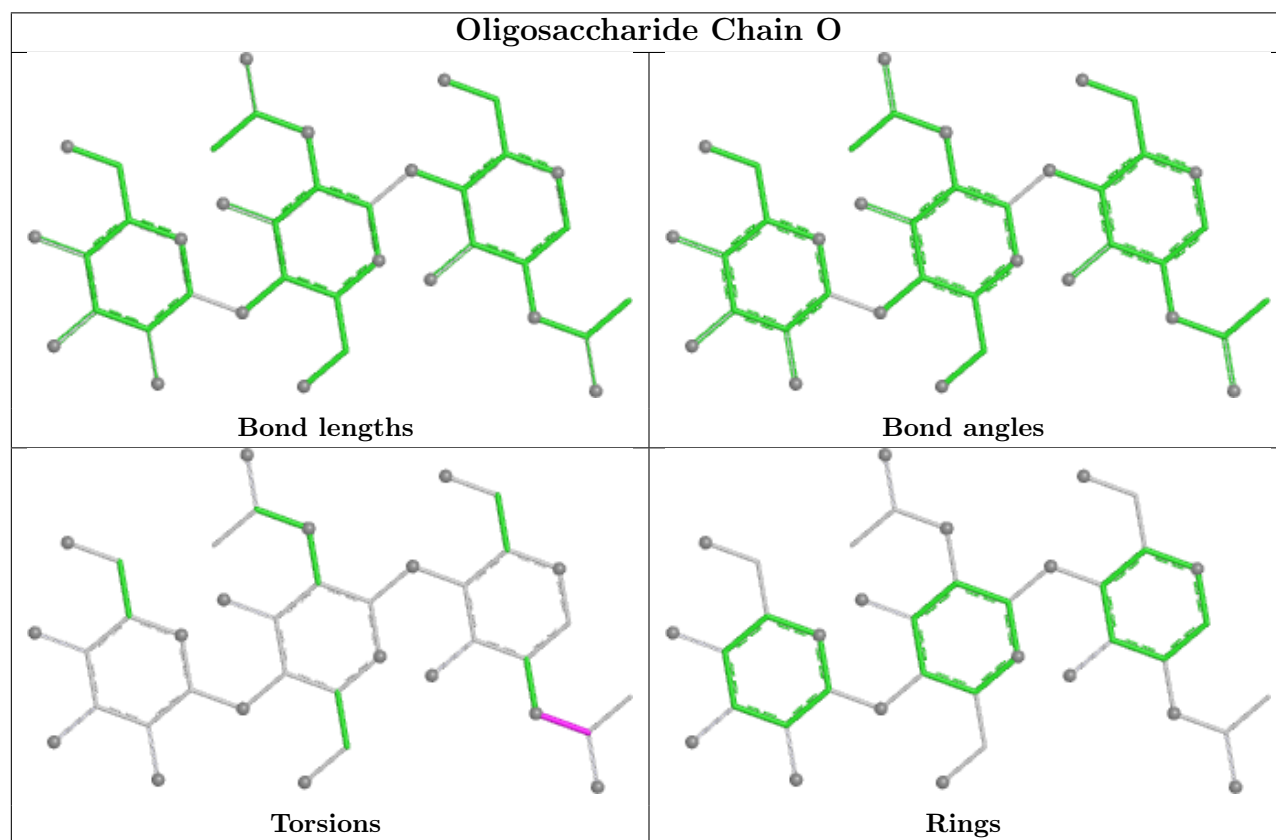
All (4) ring outliers are listed below:

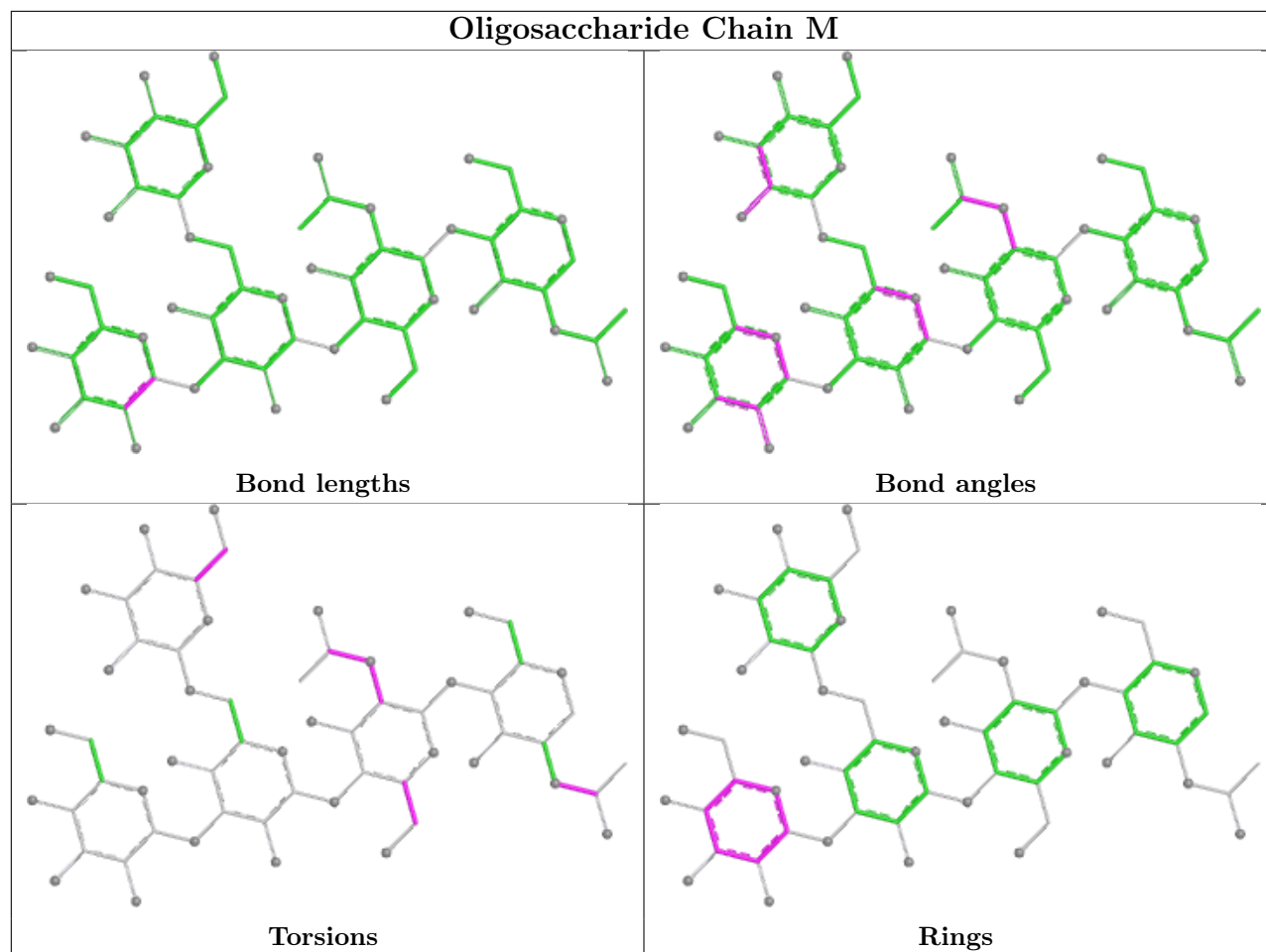
Mol	Chain	Res	Type	Atoms
7	F	4	MAN	C1-C2-C3-C4-C5-O5
7	G	4	MAN	C1-C2-C3-C4-C5-O5
7	G	5	MAN	C1-C2-C3-C4-C5-O5
7	M	4	MAN	C1-C2-C3-C4-C5-O5

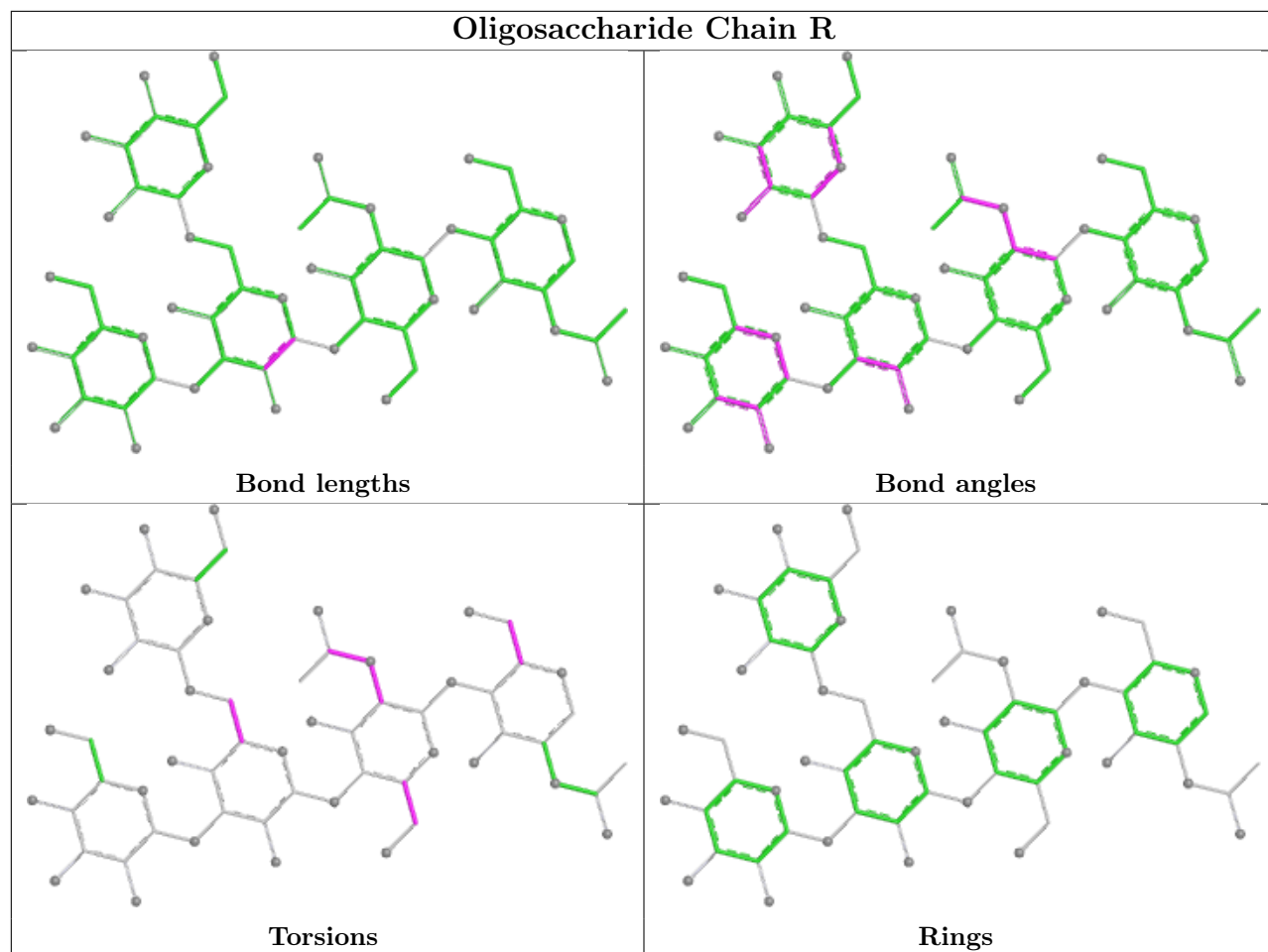
9 monomers are involved in 9 short contacts:

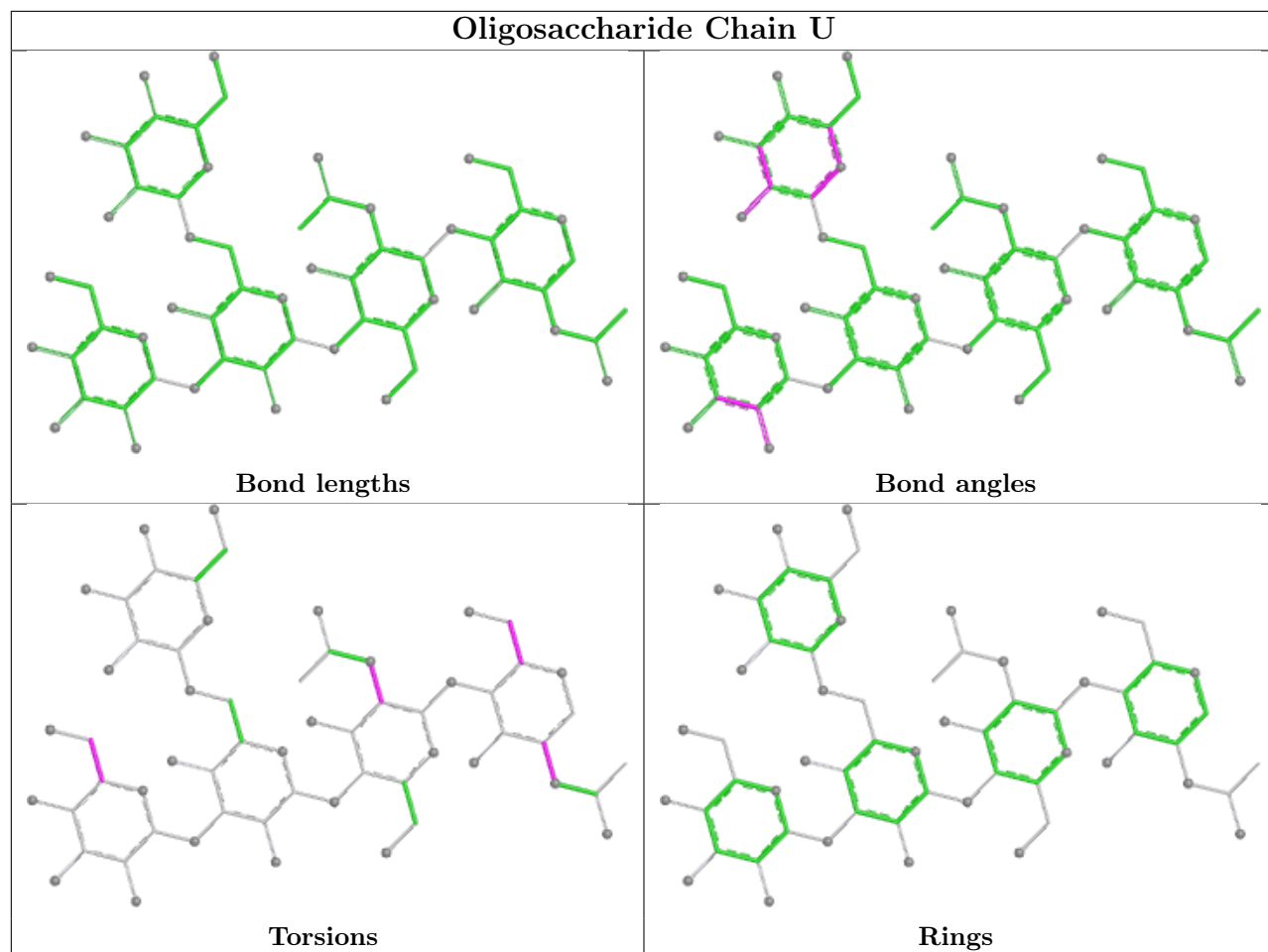
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	1	NAG	1	0
7	G	1	NAG	1	0
7	G	2	NAG	1	0
7	R	2	NAG	1	0
7	G	4	MAN	2	0
7	G	3	BMA	2	0
7	M	1	NAG	1	0
8	I	2	NAG	1	0
7	M	2	NAG	2	0

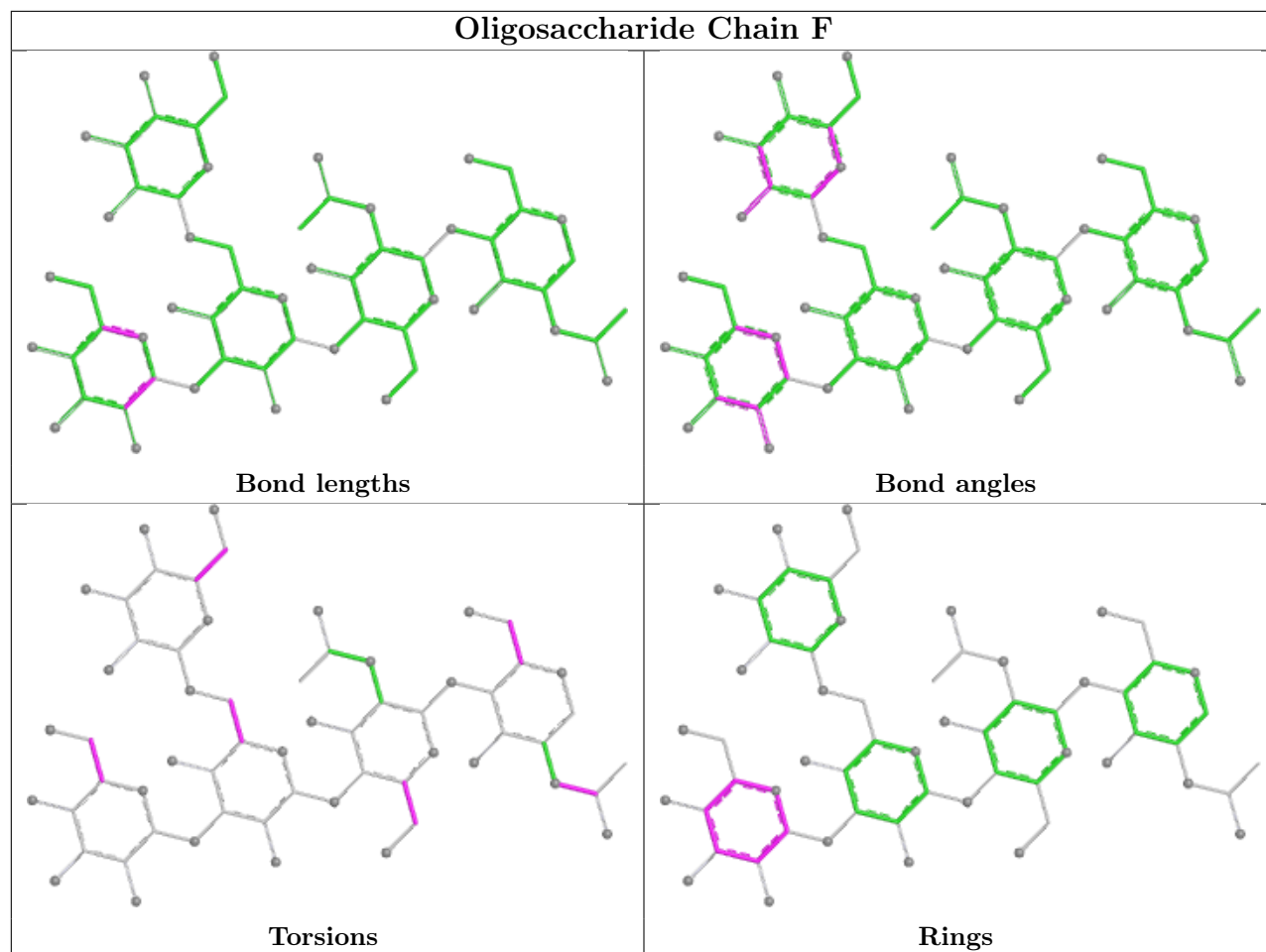
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

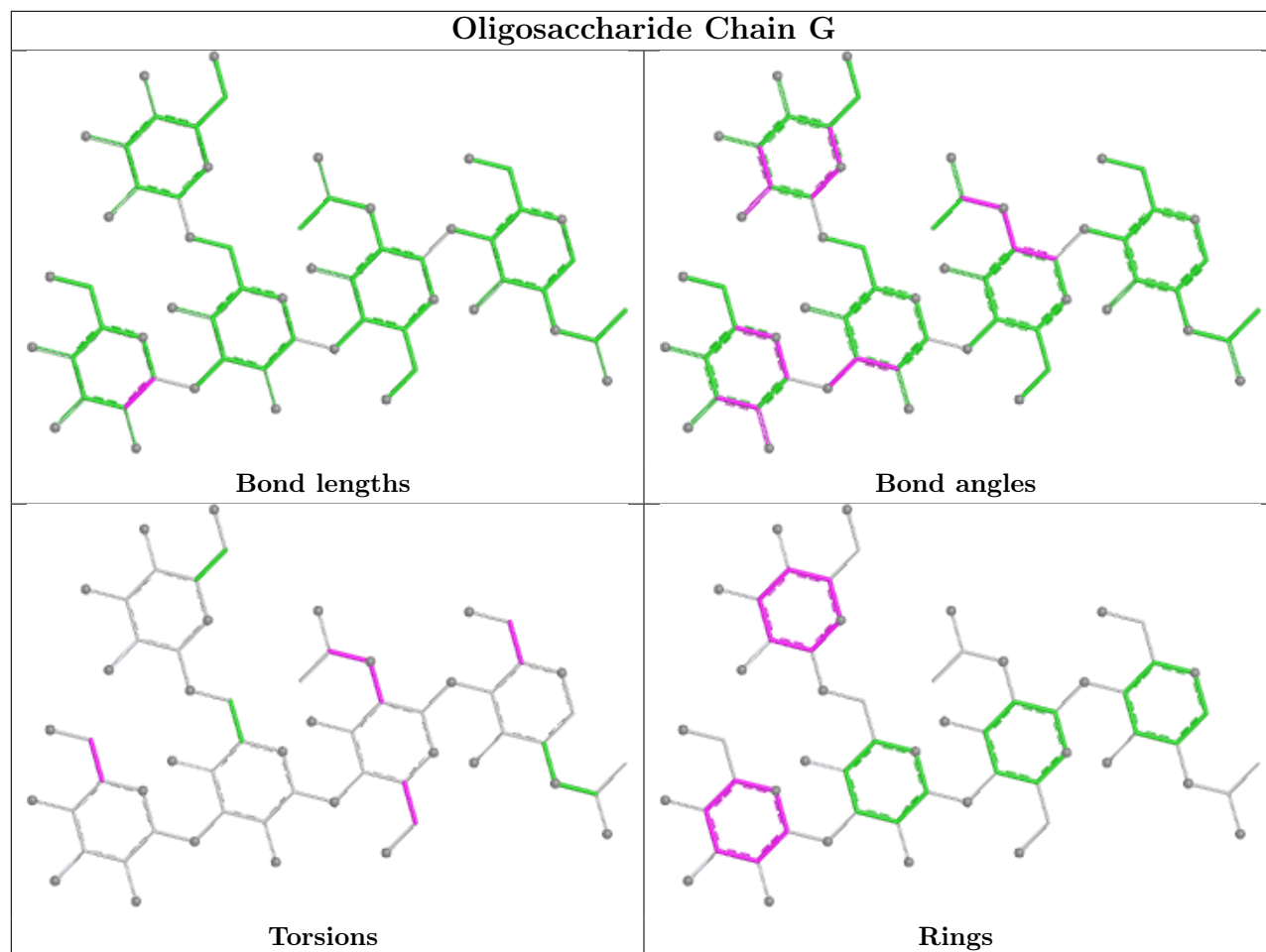


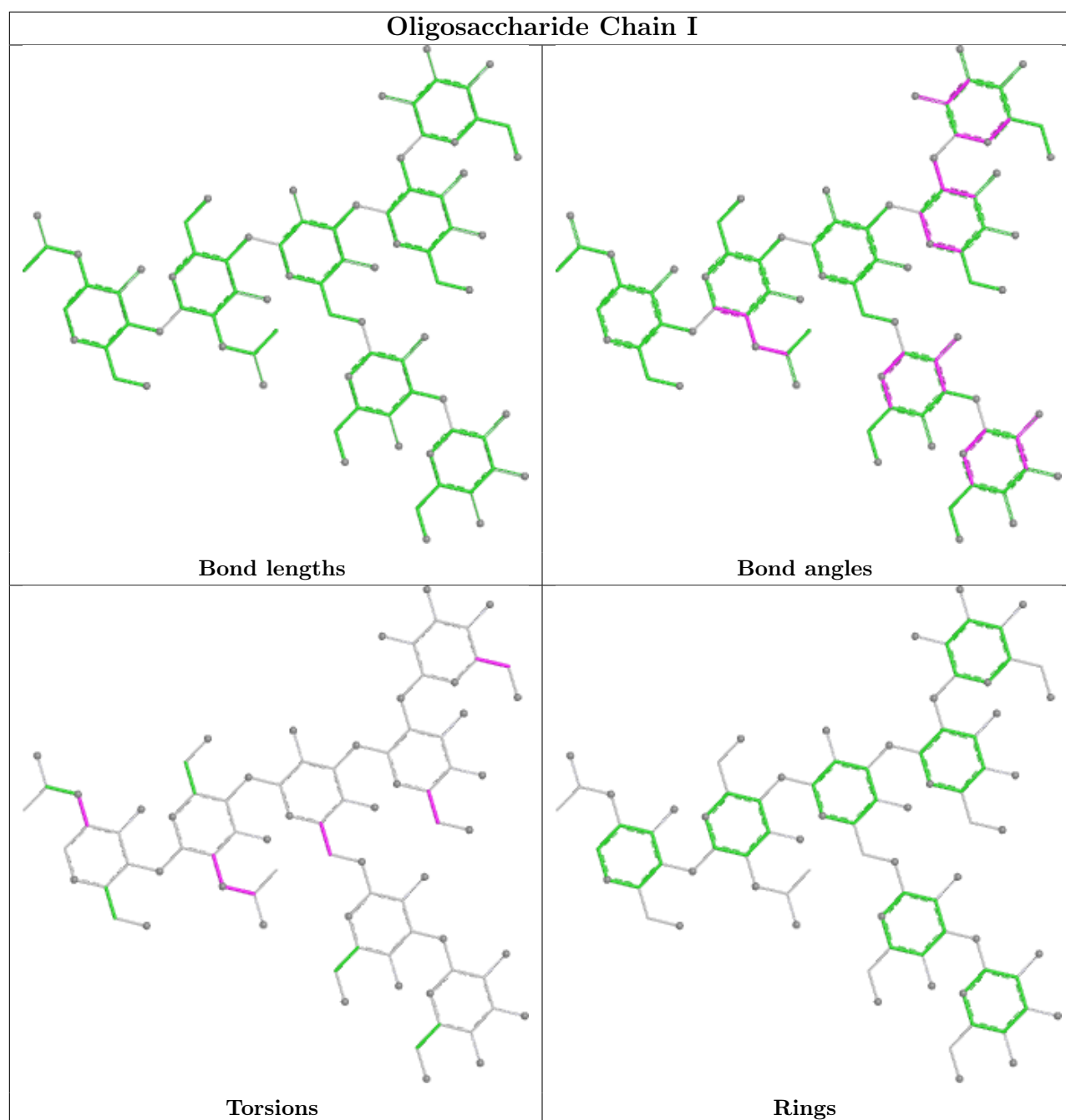












5.6 Ligand geometry [i](#)

47 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	POV	C	512	-	51,51,51	1.16	5 (9%)	57,59,59	1.08	2 (3%)
12	OCT	E	505	-	7,7,7	0.24	0	6,6,6	0.19	0
12	OCT	A	508	-	7,7,7	0.25	0	6,6,6	0.18	0
12	OCT	C	506	-	7,7,7	0.25	0	6,6,6	0.18	0
11	D12	E	504	-	11,11,11	0.23	0	10,10,10	0.21	0
11	D12	E	502	-	11,11,11	0.22	0	10,10,10	0.21	0
12	OCT	D	503	-	7,7,7	0.25	0	6,6,6	0.17	0
14	ABU	C	501	-	6,6,6	0.95	0	6,6,6	1.26	1 (16%)
14	ABU	E	501	-	6,6,6	0.88	0	6,6,6	1.40	0
11	D12	B	506	-	11,11,11	0.24	0	10,10,10	0.18	0
12	OCT	E	506	-	7,7,7	0.24	0	6,6,6	0.20	0
12	OCT	A	505	-	7,7,7	0.25	0	6,6,6	0.19	0
9	Y4B	C	504	-	26,26,26	1.45	3 (11%)	42,42,42	2.35	18 (42%)
13	POV	A	509	-	51,51,51	1.14	6 (11%)	57,59,59	1.07	3 (5%)
12	OCT	D	507	-	7,7,7	0.25	0	6,6,6	0.17	0
11	D12	B	507	-	11,11,11	0.23	0	10,10,10	0.19	0
12	OCT	C	510	-	7,7,7	0.24	0	6,6,6	0.17	0
12	OCT	D	502	-	7,7,7	0.24	0	6,6,6	0.17	0
12	OCT	E	503	-	7,7,7	0.25	0	6,6,6	0.18	0
11	D12	B	504	-	11,11,11	0.23	0	10,10,10	0.26	0
10	PIO	C	503	-	47,47,47	1.40	10 (21%)	62,65,65	1.24	7 (11%)
13	POV	B	508	-	51,51,51	1.15	5 (9%)	57,59,59	1.11	3 (5%)
11	D12	C	508	-	11,11,11	0.24	0	10,10,10	0.19	0
12	OCT	E	507	-	7,7,7	0.25	0	6,6,6	0.18	0
11	D12	A	504	-	11,11,11	0.24	0	10,10,10	0.18	0
11	D12	B	502	-	11,11,11	0.22	0	10,10,10	0.23	0
11	D12	E	508	-	11,11,11	0.22	0	10,10,10	0.21	0
11	D12	D	506	-	11,11,11	0.23	0	10,10,10	0.20	0
12	OCT	E	509	-	7,7,7	0.26	0	6,6,6	0.16	0
16	NAG	D	501	3	14,14,15	0.24	0	17,19,21	0.42	0
9	Y4B	A	501	-	26,26,26	1.40	4 (15%)	42,42,42	2.33	18 (42%)
11	D12	D	505	-	11,11,11	0.24	0	10,10,10	0.18	0
12	OCT	C	507	-	7,7,7	0.23	0	6,6,6	0.20	0
12	OCT	A	506	-	7,7,7	0.25	0	6,6,6	0.16	0
12	OCT	C	505	-	7,7,7	0.24	0	6,6,6	0.18	0
15	R5R	C	502	-	22,25,25	2.37	5 (22%)	21,36,36	1.10	1 (4%)
10	PIO	A	502	-	47,47,47	1.43	11 (23%)	62,65,65	1.37	9 (14%)
11	D12	B	503	-	11,11,11	0.21	0	10,10,10	0.26	0
12	OCT	A	507	-	7,7,7	0.25	0	6,6,6	0.16	0
11	D12	B	505	-	11,11,11	0.24	0	10,10,10	0.19	0
11	D12	B	501	-	11,11,11	0.24	0	10,10,10	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	D12	C	509	-	11,11,11	0.23	0	10,10,10	0.18	0
11	D12	A	503	-	11,11,11	0.22	0	10,10,10	0.21	0
11	D12	E	511	-	11,11,11	0.22	0	10,10,10	0.21	0
12	OCT	D	504	-	7,7,7	0.25	0	6,6,6	0.18	0
13	POV	C	511	-	51,51,51	1.18	5 (9%)	57,59,59	1.14	3 (5%)
13	POV	E	510	-	51,51,51	1.18	5 (9%)	57,59,59	1.15	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	POV	C	512	-	-	21/55/55/55	-
12	OCT	E	505	-	-	2/5/5/5	-
12	OCT	A	508	-	-	1/5/5/5	-
12	OCT	C	506	-	-	1/5/5/5	-
11	D12	E	504	-	-	2/9/9/9	-
11	D12	E	502	-	-	4/9/9/9	-
12	OCT	D	503	-	-	4/5/5/5	-
14	ABU	C	501	-	-	3/4/4/4	-
14	ABU	E	501	-	-	2/4/4/4	-
11	D12	B	506	-	-	0/9/9/9	-
12	OCT	E	506	-	-	1/5/5/5	-
12	OCT	A	505	-	-	1/5/5/5	-
9	Y4B	C	504	-	-	0/4/62/62	0/4/4/4
13	POV	A	509	-	-	28/55/55/55	-
12	OCT	D	507	-	-	1/5/5/5	-
11	D12	B	507	-	-	3/9/9/9	-
12	OCT	C	510	-	-	1/5/5/5	-
12	OCT	D	502	-	-	1/5/5/5	-
12	OCT	E	503	-	-	1/5/5/5	-
11	D12	B	504	-	-	0/9/9/9	-
10	PIO	C	503	-	-	13/44/68/68	0/1/1/1
13	POV	B	508	-	-	24/55/55/55	-
11	D12	C	508	-	-	4/9/9/9	-
12	OCT	E	507	-	-	0/5/5/5	-
11	D12	A	504	-	-	3/9/9/9	-
11	D12	B	502	-	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	D12	E	508	-	-	1/9/9/9	-
11	D12	D	506	-	-	1/9/9/9	-
12	OCT	E	509	-	-	0/5/5/5	-
16	NAG	D	501	3	-	4/6/23/26	0/1/1/1
9	Y4B	A	501	-	-	0/4/62/62	0/4/4/4
11	D12	D	505	-	-	1/9/9/9	-
12	OCT	C	507	-	-	1/5/5/5	-
12	OCT	A	506	-	-	1/5/5/5	-
12	OCT	C	505	-	-	1/5/5/5	-
15	R5R	C	502	-	-	3/12/12/12	0/3/3/3
10	PIO	A	502	-	-	15/44/68/68	0/1/1/1
11	D12	B	503	-	-	1/9/9/9	-
12	OCT	A	507	-	-	3/5/5/5	-
11	D12	B	505	-	-	2/9/9/9	-
11	D12	B	501	-	-	2/9/9/9	-
11	D12	C	509	-	-	3/9/9/9	-
11	D12	A	503	-	-	3/9/9/9	-
11	D12	E	511	-	-	2/9/9/9	-
12	OCT	D	504	-	-	2/5/5/5	-
13	POV	C	511	-	-	24/55/55/55	-
13	POV	E	510	-	-	24/55/55/55	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	502	R5R	C19-N21	9.15	1.45	1.34
13	E	510	POV	C29-C210	4.09	1.54	1.31
9	C	504	Y4B	C07-C03	4.03	1.63	1.56
13	C	511	POV	C29-C210	3.99	1.54	1.31
13	C	512	POV	C29-C210	3.79	1.53	1.31
13	B	508	POV	C29-C210	3.75	1.53	1.31
13	A	509	POV	C29-C210	3.74	1.53	1.31
9	C	504	Y4B	C04-C05	3.63	1.60	1.53
9	A	501	Y4B	C07-C03	3.61	1.62	1.56
9	A	501	Y4B	C04-C05	3.52	1.60	1.53
15	C	502	R5R	C05-C08	3.36	1.52	1.49
10	A	502	PIO	P4-O4	3.29	1.65	1.59
10	C	503	PIO	P4-O4	3.29	1.65	1.59
10	A	502	PIO	P5-O5	3.24	1.65	1.59
10	C	503	PIO	P5-O5	3.07	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	502	R5R	C15-N16	2.84	1.36	1.33
13	C	512	POV	O21-C2	-2.70	1.40	1.46
10	A	502	PIO	O2C-C2C	-2.67	1.40	1.46
9	A	501	Y4B	C04-C03	2.66	1.58	1.53
13	C	511	POV	O21-C2	-2.60	1.40	1.46
15	C	502	R5R	C18-C09	2.59	1.53	1.50
13	C	512	POV	O31-C31	2.52	1.40	1.33
13	B	508	POV	O21-C21	2.50	1.41	1.34
13	C	511	POV	O31-C31	2.46	1.40	1.33
9	C	504	Y4B	C04-C03	2.45	1.58	1.53
10	C	503	PIO	O3C-C1B	2.45	1.40	1.33
13	B	508	POV	O31-C31	2.43	1.40	1.33
10	A	502	PIO	O3C-C1B	2.41	1.40	1.33
13	A	509	POV	O21-C21	2.40	1.41	1.34
13	E	510	POV	O31-C31	2.39	1.40	1.33
10	C	503	PIO	O2C-C1A	2.36	1.40	1.34
10	A	502	PIO	P5-O51	-2.35	1.46	1.54
13	A	509	POV	O21-C2	-2.35	1.41	1.46
13	A	509	POV	O31-C31	2.31	1.40	1.33
10	A	502	PIO	P4-O43	-2.31	1.46	1.54
13	C	511	POV	O21-C21	2.30	1.40	1.34
13	E	510	POV	O21-C21	2.29	1.40	1.34
10	A	502	PIO	P4-O41	-2.28	1.46	1.54
10	C	503	PIO	P5-O51	-2.28	1.46	1.54
10	C	503	PIO	P4-O41	-2.27	1.46	1.54
10	C	503	PIO	P4-O43	-2.27	1.46	1.54
10	A	502	PIO	P5-O52	-2.26	1.46	1.54
10	C	503	PIO	P5-O52	-2.25	1.46	1.54
13	E	510	POV	O21-C2	-2.23	1.41	1.46
10	C	503	PIO	O2C-C2C	-2.20	1.41	1.46
10	A	502	PIO	O2C-C1A	2.17	1.40	1.34
13	C	511	POV	O31-C3	-2.16	1.40	1.45
10	A	502	PIO	O3C-C3C	-2.16	1.40	1.45
13	A	509	POV	O31-C3	-2.14	1.40	1.45
13	C	512	POV	O31-C3	-2.12	1.40	1.45
9	A	501	Y4B	C15-C07	2.11	1.57	1.54
13	C	512	POV	O21-C21	2.11	1.40	1.34
13	B	508	POV	O31-C3	-2.11	1.40	1.45
10	C	503	PIO	O3C-C3C	-2.06	1.40	1.45
13	B	508	POV	O21-C2	-2.06	1.41	1.46
10	A	502	PIO	P1-O11	-2.05	1.45	1.55
13	E	510	POV	O31-C3	-2.04	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	502	R5R	O20-C19	-2.03	1.18	1.23
13	A	509	POV	P-O13	-2.01	1.46	1.55

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	504	Y4B	C10-C06-C12	5.09	122.22	116.11
9	A	501	Y4B	C10-C06-C12	4.60	121.63	116.11
9	A	501	Y4B	C07-C03-C04	4.47	116.97	112.43
9	C	504	Y4B	C09-C03-C04	-4.37	105.69	111.78
9	A	501	Y4B	C09-C03-C04	-4.20	105.92	111.78
9	C	504	Y4B	C07-C03-C04	4.13	116.62	112.43
13	E	510	POV	O21-C21-C22	4.09	120.34	111.48
9	C	504	Y4B	O02-C22-C23	-4.05	114.02	121.17
10	C	503	PIO	O2C-C1A-C2A	4.05	120.24	111.48
9	A	501	Y4B	O02-C22-C23	-4.04	114.03	121.17
13	C	511	POV	O21-C21-C22	4.00	120.13	111.48
9	C	504	Y4B	C23-C22-C12	3.95	124.48	117.65
9	A	501	Y4B	C13-C05-C04	3.91	125.34	119.10
13	A	509	POV	O21-C21-C22	3.86	119.83	111.48
9	C	504	Y4B	C13-C05-C04	3.84	125.22	119.10
9	A	501	Y4B	C23-C22-C12	3.78	124.20	117.65
10	A	502	PIO	O2C-C1A-C2A	3.75	119.60	111.48
10	A	502	PIO	C6-C1-C2	-3.70	105.73	110.86
13	C	512	POV	O21-C21-C22	3.64	119.36	111.48
9	C	504	Y4B	C13-C05-C06	-3.64	99.56	103.84
9	A	501	Y4B	C13-C05-C06	-3.55	99.66	103.84
9	A	501	Y4B	C16-C12-C06	-3.44	101.14	104.21
13	B	508	POV	O21-C21-C22	3.40	118.85	111.48
9	C	504	Y4B	C14-C08-C07	-3.38	106.63	112.31
9	C	504	Y4B	C16-C12-C06	-3.28	101.27	104.21
9	C	504	Y4B	C18-C06-C10	-3.28	105.78	110.61
9	A	501	Y4B	C18-C06-C10	-3.19	105.91	110.61
9	A	501	Y4B	C14-C08-C07	-3.09	107.14	112.31
9	A	501	Y4B	C12-C06-C05	3.08	102.94	99.72
13	C	511	POV	O31-C31-C32	2.99	120.94	111.83
10	C	503	PIO	O3C-C1B-C2B	2.88	120.63	111.83
13	B	508	POV	O31-C31-C32	2.75	120.22	111.83
13	C	512	POV	O31-C31-C32	2.72	120.12	111.83
13	E	510	POV	O31-C31-C32	2.63	119.84	111.83
9	A	501	Y4B	C20-C15-C07	2.62	117.15	112.74
9	C	504	Y4B	C12-C06-C05	2.60	102.44	99.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	502	PIO	O3C-C1B-C2B	2.59	119.72	111.83
13	E	510	POV	O31-C3-C2	2.55	115.76	108.40
9	C	504	Y4B	C14-C11-C04	2.55	116.23	112.16
10	A	502	PIO	O1-C1-C2	2.54	114.11	108.73
9	C	504	Y4B	C15-C07-C03	2.53	115.27	111.34
10	A	502	PIO	O11-P1-O12	-2.52	100.73	112.44
9	A	501	Y4B	C06-C05-C04	-2.49	110.87	114.41
10	C	503	PIO	O11-P1-O12	-2.47	100.96	112.44
9	C	504	Y4B	C09-C03-C07	2.45	116.67	113.91
13	A	509	POV	O31-C31-C32	2.44	119.28	111.83
13	B	508	POV	O13-P-O14	-2.42	101.17	112.44
9	A	501	Y4B	C17-C21-C20	-2.39	107.70	110.62
13	A	509	POV	O13-P-O14	-2.35	101.52	112.44
9	A	501	Y4B	C14-C11-C04	2.30	115.83	112.16
15	C	502	R5R	C18-C19-N21	2.27	120.45	117.39
9	C	504	Y4B	C05-C04-C03	2.25	112.03	109.09
9	A	501	Y4B	C15-C07-C03	2.23	114.80	111.34
10	A	502	PIO	O51-P5-O5	2.20	114.41	105.85
9	C	504	Y4B	C20-C15-C07	2.17	116.40	112.74
10	A	502	PIO	O43-P4-O4	2.15	114.24	105.85
9	C	504	Y4B	C18-C06-C12	-2.15	106.78	110.35
10	A	502	PIO	O41-P4-O4	2.14	114.20	105.85
10	C	503	PIO	O41-P4-O4	2.13	114.16	105.85
10	A	502	PIO	O52-P5-O5	2.12	114.11	105.85
10	C	503	PIO	O43-P4-O4	2.11	114.09	105.85
9	A	501	Y4B	C09-C03-C07	2.11	116.28	113.91
10	C	503	PIO	O52-P5-O5	2.11	114.05	105.85
14	C	501	ABU	OXT-C-CG	2.10	120.63	114.00
10	C	503	PIO	O51-P5-O5	2.09	114.01	105.85
9	A	501	Y4B	C05-C04-C03	2.09	111.81	109.09
13	C	511	POV	O13-P-O14	-2.05	102.91	112.44
13	E	510	POV	O13-P-O14	-2.04	102.94	112.44
9	C	504	Y4B	C19-C07-C15	-2.04	105.06	108.31

There are no chirality outliers.

All (219) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	502	PIO	C2-C1-O1-P1
10	A	502	PIO	C1C-O13-P1-O1
10	A	502	PIO	C1C-O13-P1-O12
10	A	502	PIO	O2C-C2C-C3C-O3C

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Mol	Chain	Res	Type	Atoms
10	C	503	PIO	C1C-O13-P1-O1
10	C	503	PIO	C1C-O13-P1-O12
10	C	503	PIO	C2A-C1A-O2C-C2C
13	A	509	POV	C1-O11-P-O12
13	A	509	POV	C1-O11-P-O13
13	A	509	POV	C1-O11-P-O14
13	B	508	POV	C1-O11-P-O12
13	B	508	POV	C1-O11-P-O13
15	C	502	R5R	C04-C05-C08-N16
15	C	502	R5R	C06-C05-C08-N16
13	A	509	POV	O32-C31-O31-C3
13	E	510	POV	O32-C31-O31-C3
13	E	510	POV	C32-C31-O31-C3
10	C	503	PIO	O1A-C1A-O2C-C2C
13	A	509	POV	C32-C31-O31-C3
13	A	509	POV	C22-C21-O21-C2
16	D	501	NAG	O5-C5-C6-O6
10	C	503	PIO	C1B-C2B-C3B-C4B
16	D	501	NAG	C8-C7-N2-C2
16	D	501	NAG	O7-C7-N2-C2
13	A	509	POV	O22-C21-O21-C2
14	C	501	ABU	CD-CB-CG-C
13	B	508	POV	C31-C32-C33-C34
13	C	512	POV	C31-C32-C33-C34
16	D	501	NAG	C4-C5-C6-O6
10	C	503	PIO	C2B-C1B-O3C-C3C
13	B	508	POV	C32-C31-O31-C3
13	E	510	POV	C22-C21-O21-C2
13	E	510	POV	O22-C21-O21-C2
10	C	503	PIO	O1B-C1B-O3C-C3C
10	C	503	PIO	C3B-C4B-C5B-C6B
11	D	505	D12	C5-C6-C7-C8
13	C	511	POV	C39-C310-C311-C312
13	E	510	POV	C212-C213-C214-C215
10	A	502	PIO	C3B-C4B-C5B-C6B
12	D	503	OCT	C3-C4-C5-C6
13	A	509	POV	C311-C312-C313-C314
13	C	511	POV	C212-C213-C214-C215
13	E	510	POV	C24-C25-C26-C27
10	A	502	PIO	C4A-C5A-C6A-C7A
11	B	507	D12	C4-C5-C6-C7
10	A	502	PIO	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
13	B	508	POV	C210-C211-C212-C213
13	B	508	POV	O32-C31-O31-C3
13	E	510	POV	C312-C313-C314-C315
13	C	511	POV	C311-C310-C39-C38
13	C	512	POV	C211-C212-C213-C214
13	A	509	POV	C39-C310-C311-C312
12	C	507	OCT	C2-C3-C4-C5
13	C	511	POV	C1-C2-C3-O31
11	A	503	D12	C3-C4-C5-C6
11	B	505	D12	C4-C5-C6-C7
13	A	509	POV	C212-C213-C214-C215
13	C	511	POV	C35-C36-C37-C38
13	E	510	POV	C34-C35-C36-C37
11	C	508	D12	C6-C7-C8-C9
12	A	506	OCT	C2-C3-C4-C5
11	C	509	D12	C7-C8-C9-C10
12	A	508	OCT	C4-C5-C6-C7
13	C	511	POV	C211-C212-C213-C214
13	A	509	POV	C31-C32-C33-C34
13	A	509	POV	C310-C311-C312-C313
12	D	507	OCT	C3-C4-C5-C6
13	A	509	POV	C23-C24-C25-C26
13	C	511	POV	C310-C311-C312-C313
13	C	512	POV	C22-C23-C24-C25
13	B	508	POV	C214-C215-C216-C217
13	C	511	POV	C33-C34-C35-C36
13	C	512	POV	C212-C213-C214-C215
13	C	511	POV	C36-C37-C38-C39
10	A	502	PIO	C2B-C3B-C4B-C5B
13	A	509	POV	C26-C27-C28-C29
13	C	511	POV	C26-C27-C28-C29
13	E	510	POV	C313-C314-C315-C316
11	E	504	D12	C4-C5-C6-C7
13	A	509	POV	C32-C33-C34-C35
13	E	510	POV	C311-C310-C39-C38
13	B	508	POV	C26-C27-C28-C29
13	C	512	POV	C23-C24-C25-C26
13	C	511	POV	C29-C210-C211-C212
13	B	508	POV	C212-C213-C214-C215
13	E	510	POV	C33-C34-C35-C36
11	A	504	D12	C5-C6-C7-C8
13	A	509	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
11	E	511	D12	C5-C6-C7-C8
13	B	508	POV	C311-C312-C313-C314
13	B	508	POV	C36-C37-C38-C39
11	D	506	D12	C4-C5-C6-C7
13	C	512	POV	C312-C313-C314-C315
13	B	508	POV	O11-C1-C2-C3
13	E	510	POV	C23-C24-C25-C26
10	C	503	PIO	C4A-C5A-C6A-C7A
13	B	508	POV	C39-C310-C311-C312
10	A	502	PIO	C1C-C2C-C3C-O3C
13	B	508	POV	C25-C26-C27-C28
11	B	502	D12	C9-C10-C11-C12
11	E	502	D12	C4-C5-C6-C7
13	C	512	POV	C39-C310-C311-C312
10	A	502	PIO	C3A-C4A-C5A-C6A
11	A	503	D12	C7-C8-C9-C10
12	C	505	OCT	C2-C3-C4-C5
13	E	510	POV	C21-C22-C23-C24
13	E	510	POV	C36-C37-C38-C39
13	E	510	POV	C3-C2-O21-C21
13	C	512	POV	C26-C27-C28-C29
13	B	508	POV	C33-C34-C35-C36
13	B	508	POV	O11-C1-C2-O21
13	C	512	POV	C37-C38-C39-C310
12	A	507	OCT	C2-C3-C4-C5
12	D	502	OCT	C2-C3-C4-C5
11	C	508	D12	C9-C10-C11-C12
12	E	505	OCT	C5-C6-C7-C8
13	A	509	POV	C34-C35-C36-C37
12	C	510	OCT	C5-C6-C7-C8
12	D	503	OCT	C5-C6-C7-C8
11	E	502	D12	C9-C10-C11-C12
13	B	508	POV	C313-C314-C315-C316
11	C	509	D12	C3-C4-C5-C6
11	B	502	D12	C11-C10-C9-C8
11	B	507	D12	C11-C10-C9-C8
12	D	503	OCT	C1-C2-C3-C4
13	A	509	POV	O11-C1-C2-C3
11	E	508	D12	C6-C7-C8-C9
13	C	511	POV	C24-C25-C26-C27
12	E	505	OCT	C3-C4-C5-C6
12	C	506	OCT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
11	B	507	D12	C9-C10-C11-C12
12	A	507	OCT	C1-C2-C3-C4
12	A	507	OCT	C3-C4-C5-C6
11	B	505	D12	C9-C10-C11-C12
13	E	510	POV	C213-C214-C215-C216
13	C	511	POV	C214-C215-C216-C217
13	A	509	POV	O11-C1-C2-O21
13	C	512	POV	C311-C312-C313-C314
11	B	502	D12	C7-C8-C9-C10
13	C	511	POV	C21-C22-C23-C24
11	C	509	D12	C4-C5-C6-C7
13	A	509	POV	C25-C26-C27-C28
10	A	502	PIO	C5A-C6A-C7A-C8A
13	C	511	POV	C23-C24-C25-C26
13	C	511	POV	O11-C1-C2-C3
12	D	504	OCT	C2-C3-C4-C5
13	A	509	POV	C1-C2-O21-C21
13	B	508	POV	C3-C2-O21-C21
12	D	503	OCT	C2-C3-C4-C5
11	E	502	D12	C3-C4-C5-C6
13	A	509	POV	C12-C11-O12-P
13	C	511	POV	C12-C11-O12-P
13	C	512	POV	C12-C11-O12-P
13	E	510	POV	C12-C11-O12-P
13	C	511	POV	C34-C35-C36-C37
11	C	508	D12	C7-C8-C9-C10
10	A	502	PIO	C4B-C5B-C6B-C7B
11	A	503	D12	C4-C5-C6-C7
13	C	511	POV	O11-C1-C2-O21
13	E	510	POV	O11-C1-C2-O21
13	C	511	POV	O21-C2-C3-O31
10	C	503	PIO	C1C-O13-P1-O11
13	B	508	POV	C1-O11-P-O14
13	C	512	POV	C1-O11-P-O12
13	C	512	POV	C1-O11-P-O14
13	E	510	POV	C1-O11-P-O14
13	C	511	POV	C215-C216-C217-C218
10	C	503	PIO	C1C-C2C-O2C-C1A
13	C	512	POV	O11-C1-C2-C3
11	B	503	D12	C4-C5-C6-C7
13	A	509	POV	C35-C36-C37-C38
13	B	508	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
13	E	510	POV	C31-C32-C33-C34
13	C	511	POV	C32-C31-O31-C3
11	C	508	D12	C1-C2-C3-C4
13	C	511	POV	O32-C31-O31-C3
13	C	512	POV	C311-C310-C39-C38
11	B	501	D12	C1-C2-C3-C4
10	C	503	PIO	C5B-C6B-C7B-C8B
13	E	510	POV	C311-C312-C313-C314
13	A	509	POV	C2-C1-O11-P
10	A	502	PIO	C3-C4-O4-P4
12	E	503	OCT	C4-C5-C6-C7
12	E	506	OCT	C3-C4-C5-C6
11	E	511	D12	C6-C7-C8-C9
13	B	508	POV	C21-C22-C23-C24
11	E	504	D12	C3-C4-C5-C6
10	A	502	PIO	O1B-C1B-O3C-C3C
13	A	509	POV	C11-C12-N-C14
13	C	512	POV	C11-C12-N-C14
10	A	502	PIO	C2B-C1B-O3C-C3C
13	C	512	POV	C215-C216-C217-C218
14	E	501	ABU	O-C-CG-CB
12	A	505	OCT	C1-C2-C3-C4
13	B	508	POV	O21-C2-C3-O31
13	C	511	POV	C32-C33-C34-C35
13	E	510	POV	O11-C1-C2-C3
11	A	504	D12	C6-C7-C8-C9
13	A	509	POV	C11-C12-N-C15
14	E	501	ABU	OXT-C-CG-CB
13	E	510	POV	C37-C38-C39-C310
13	B	508	POV	O12-C11-C12-N
11	E	502	D12	C2-C3-C4-C5
11	B	501	D12	C4-C5-C6-C7
11	A	504	D12	C7-C8-C9-C10
12	D	504	OCT	C3-C4-C5-C6
10	C	503	PIO	C4-O4-P4-O41
13	C	512	POV	C32-C33-C34-C35
13	A	509	POV	C11-C12-N-C13
13	C	512	POV	C11-C12-N-C13
15	C	502	R5R	C09-C18-C19-O20
14	C	501	ABU	OXT-C-CG-CB
13	C	512	POV	C11-C12-N-C15
13	C	512	POV	C213-C214-C215-C216

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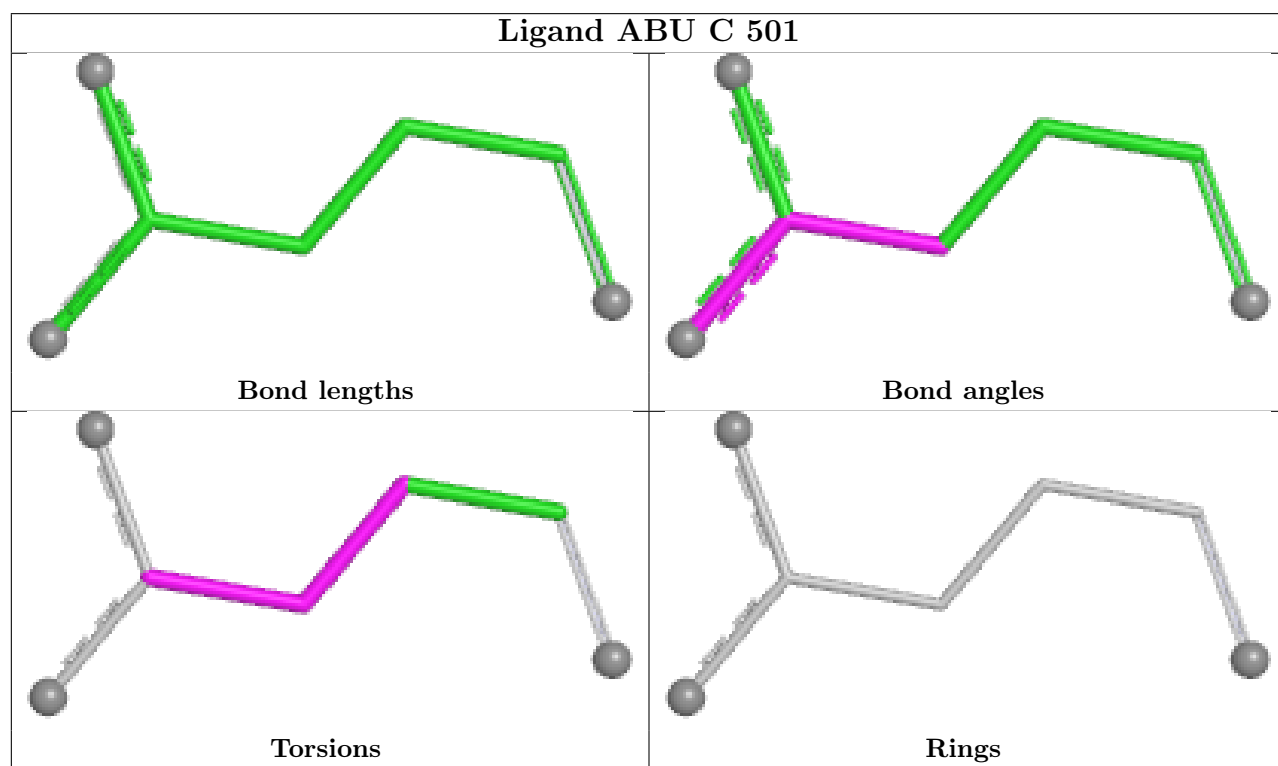
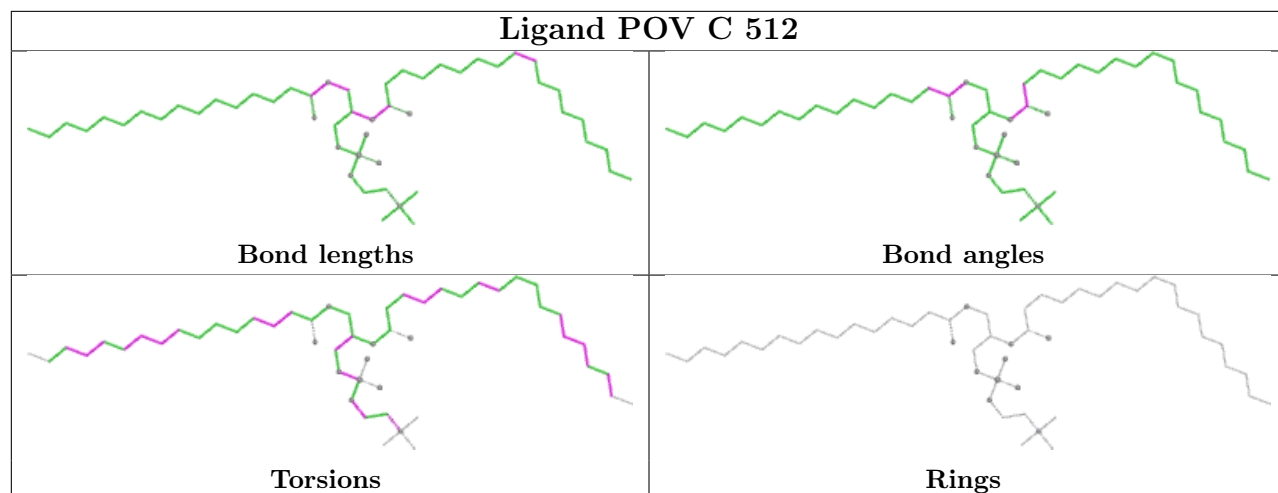
Mol	Chain	Res	Type	Atoms
13	B	508	POV	O21-C21-C22-C23
14	C	501	ABU	O-C-CG-CB
11	B	502	D12	C4-C5-C6-C7
13	A	509	POV	O31-C31-C32-C33
13	E	510	POV	O31-C31-C32-C33

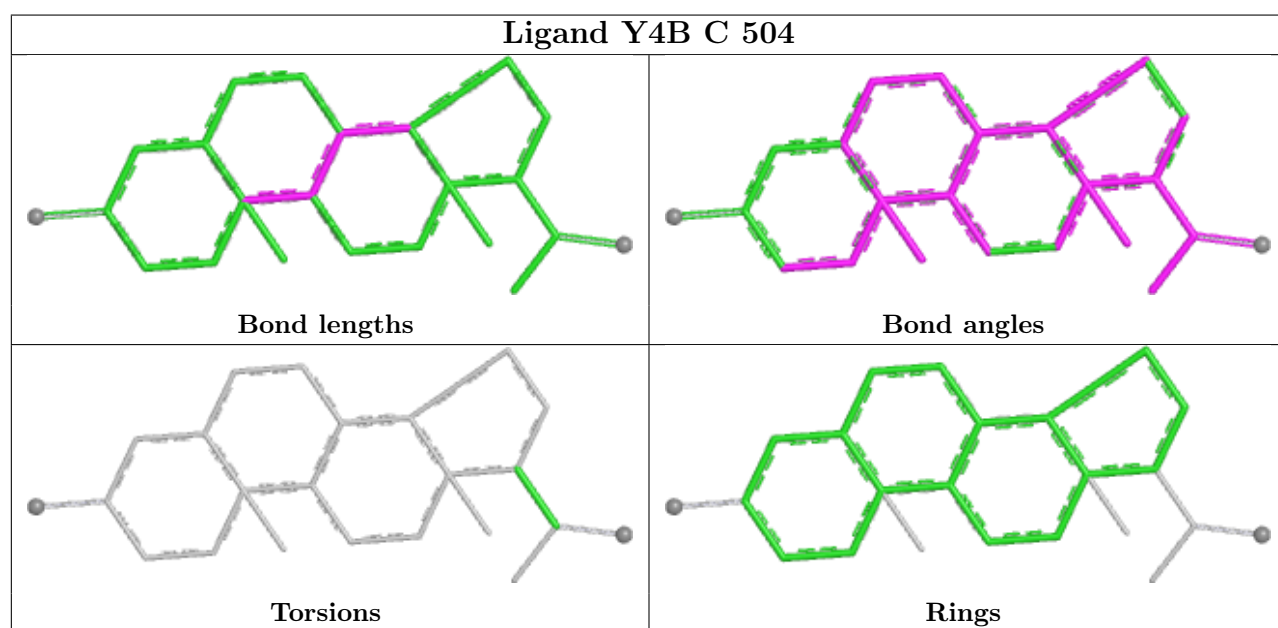
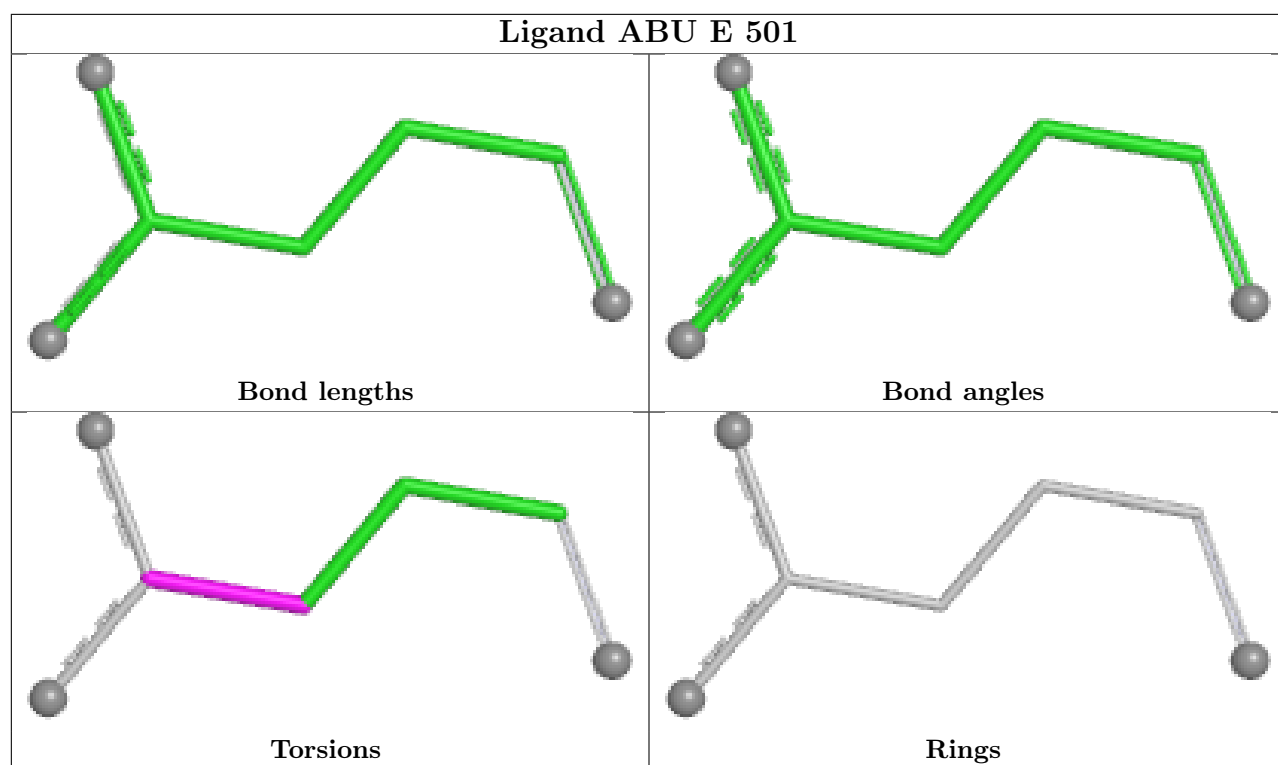
There are no ring outliers.

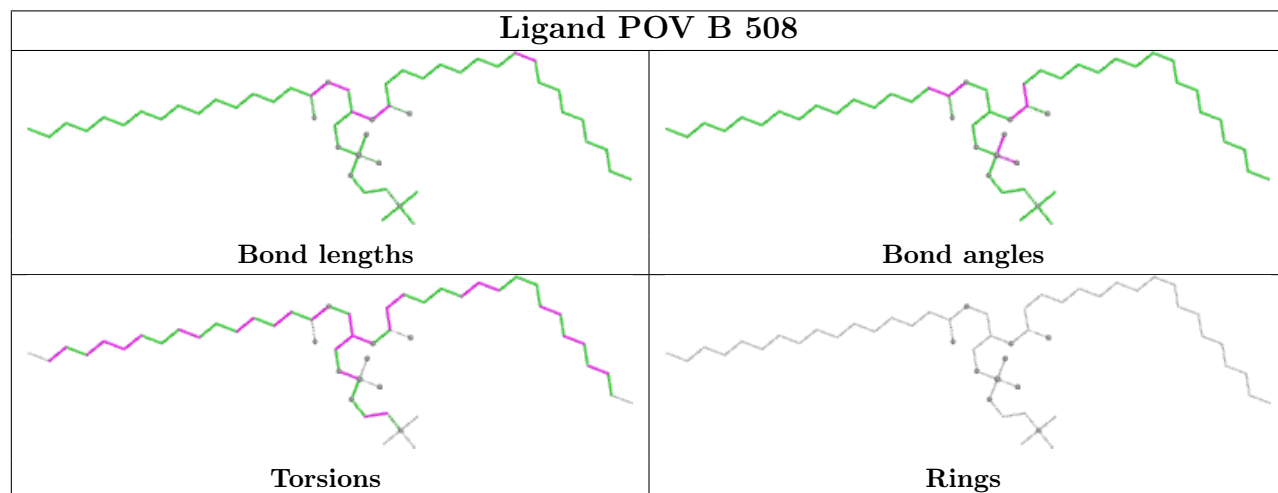
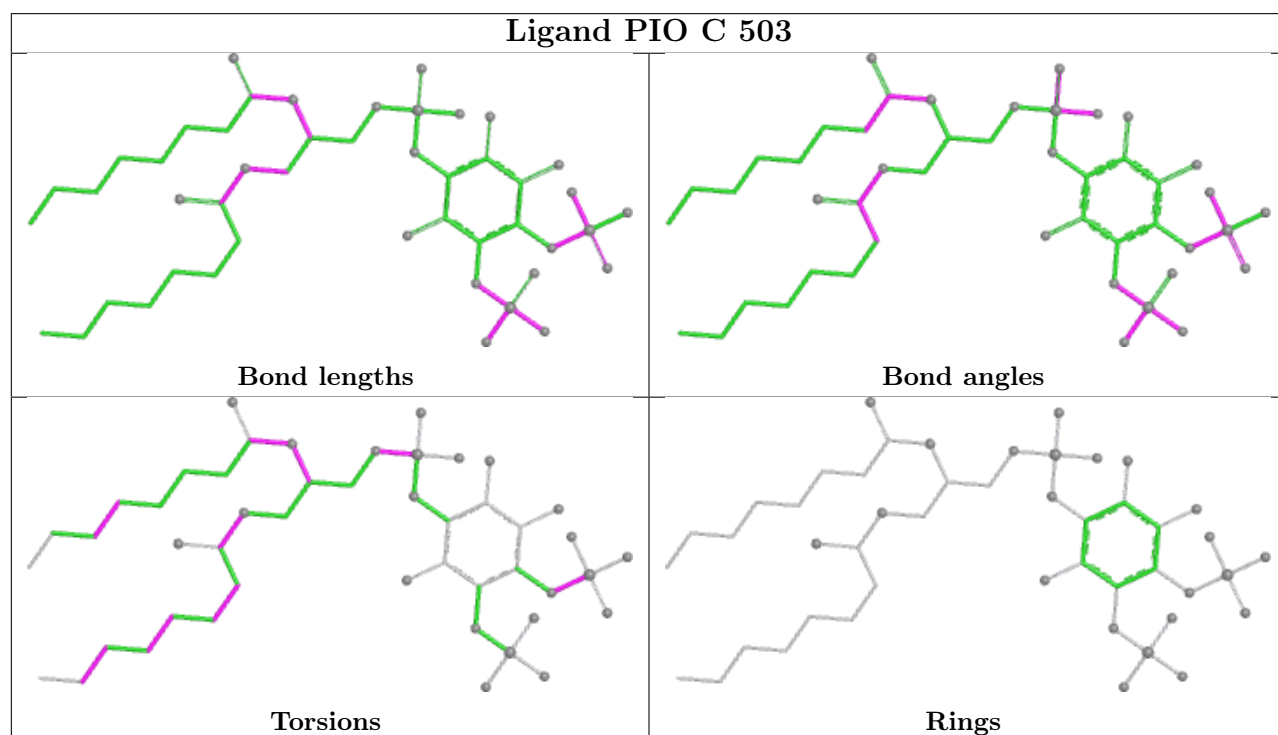
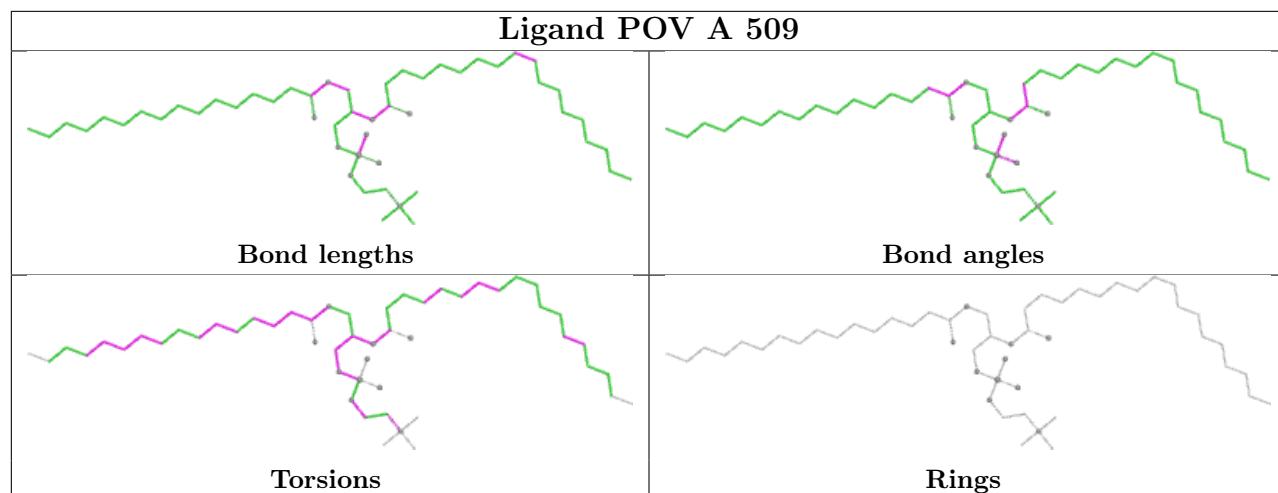
11 monomers are involved in 17 short contacts:

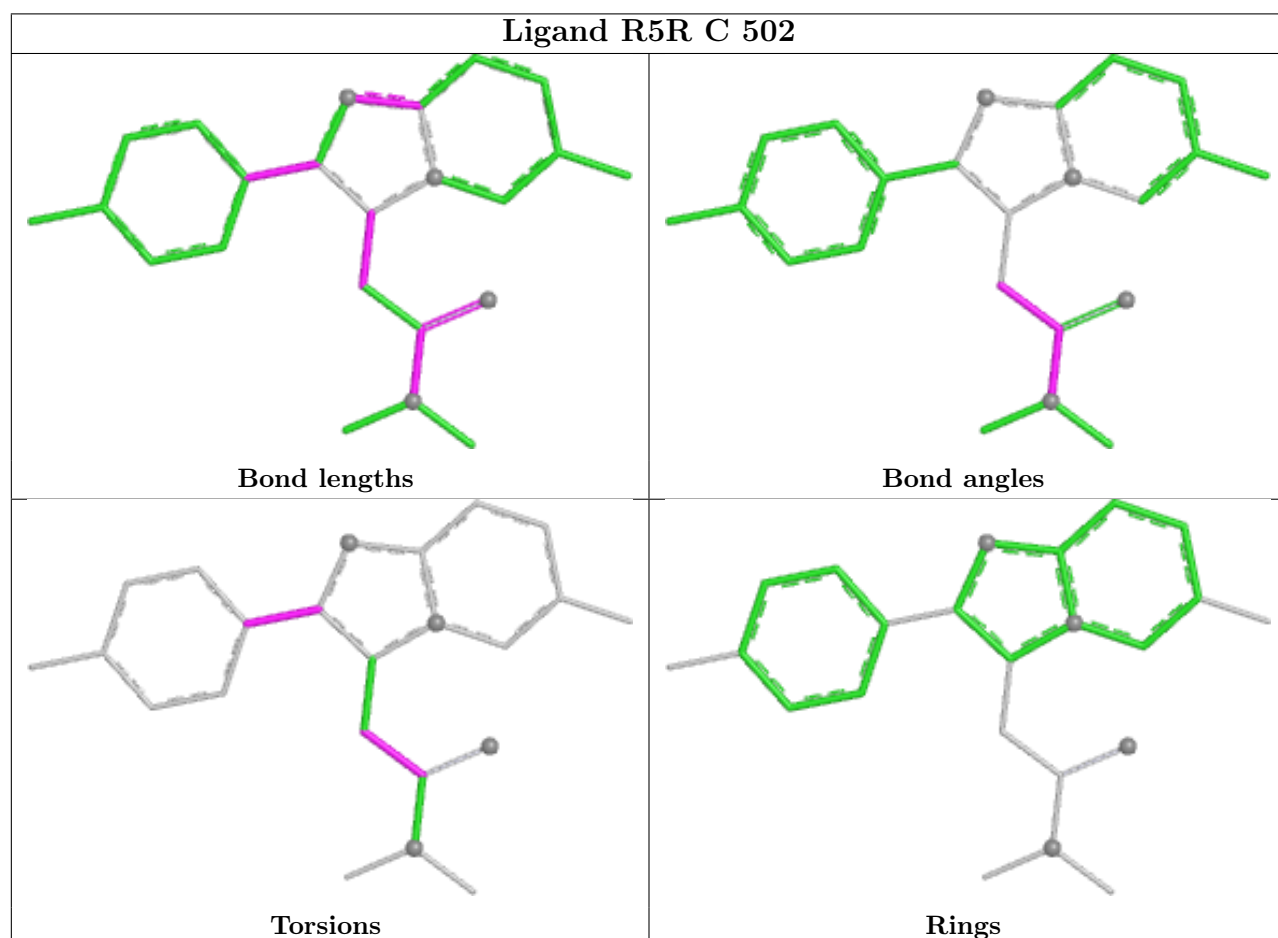
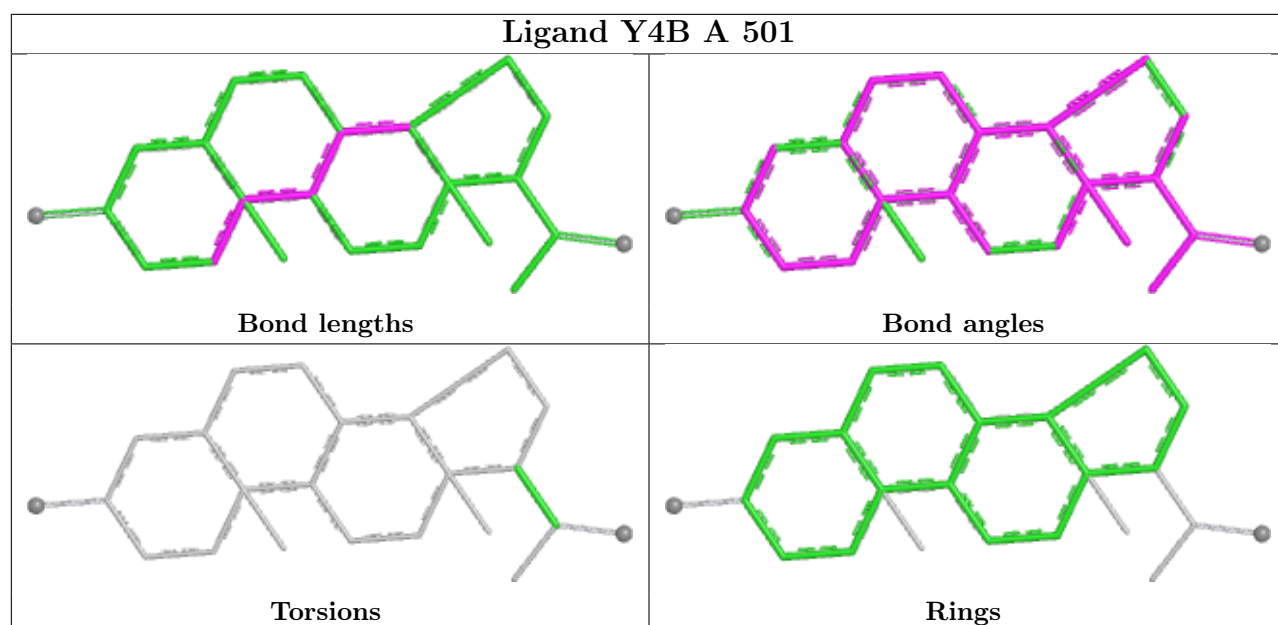
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	512	POV	2	0
14	C	501	ABU	1	0
13	A	509	POV	1	0
11	B	502	D12	1	0
9	A	501	Y4B	1	0
12	A	506	OCT	1	0
12	C	505	OCT	1	0
10	A	502	PIO	2	0
11	B	503	D12	1	0
13	C	511	POV	2	0
13	E	510	POV	6	0

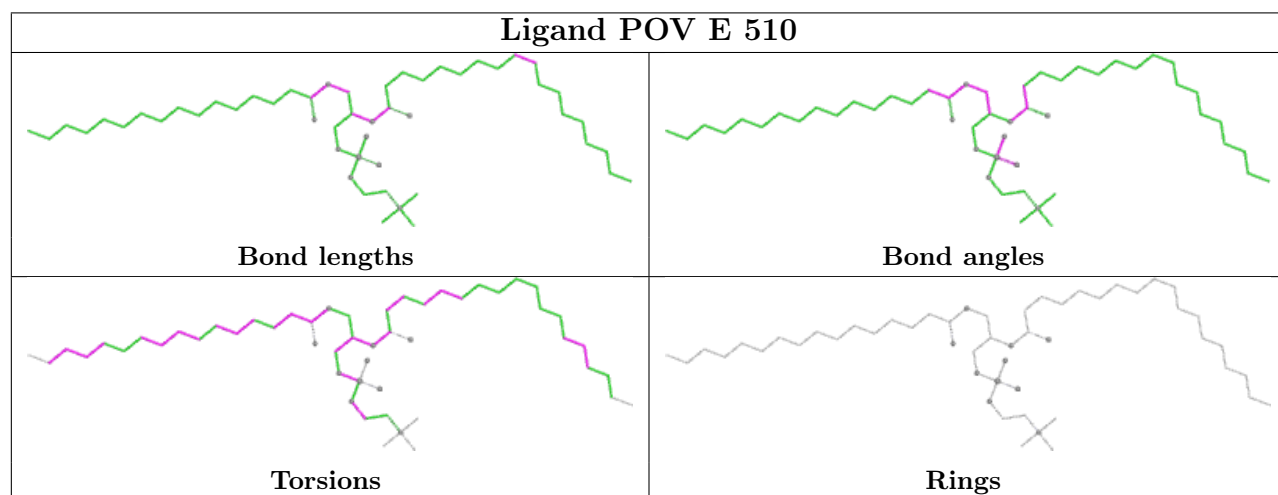
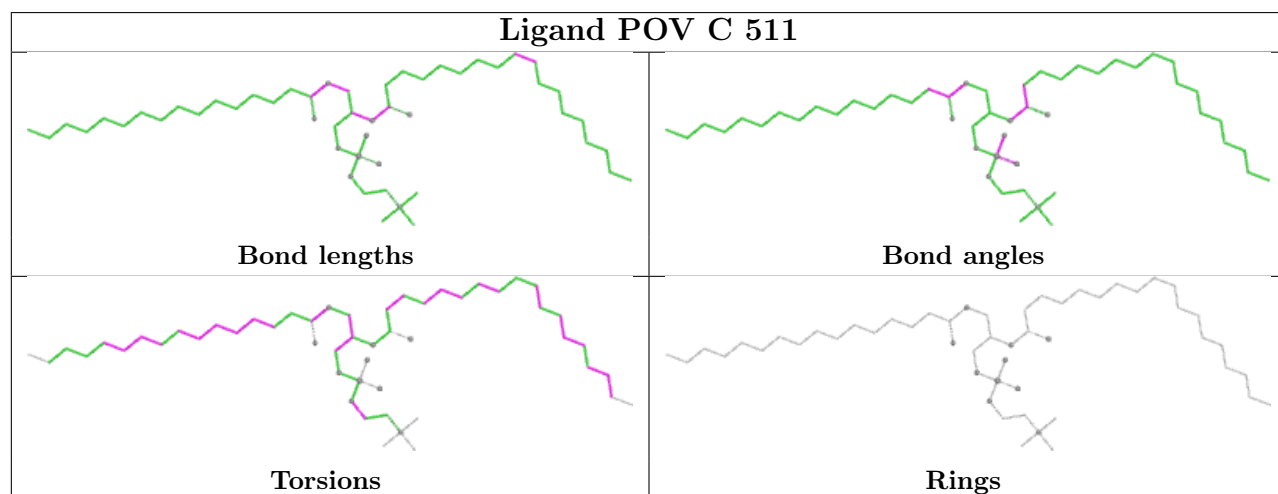
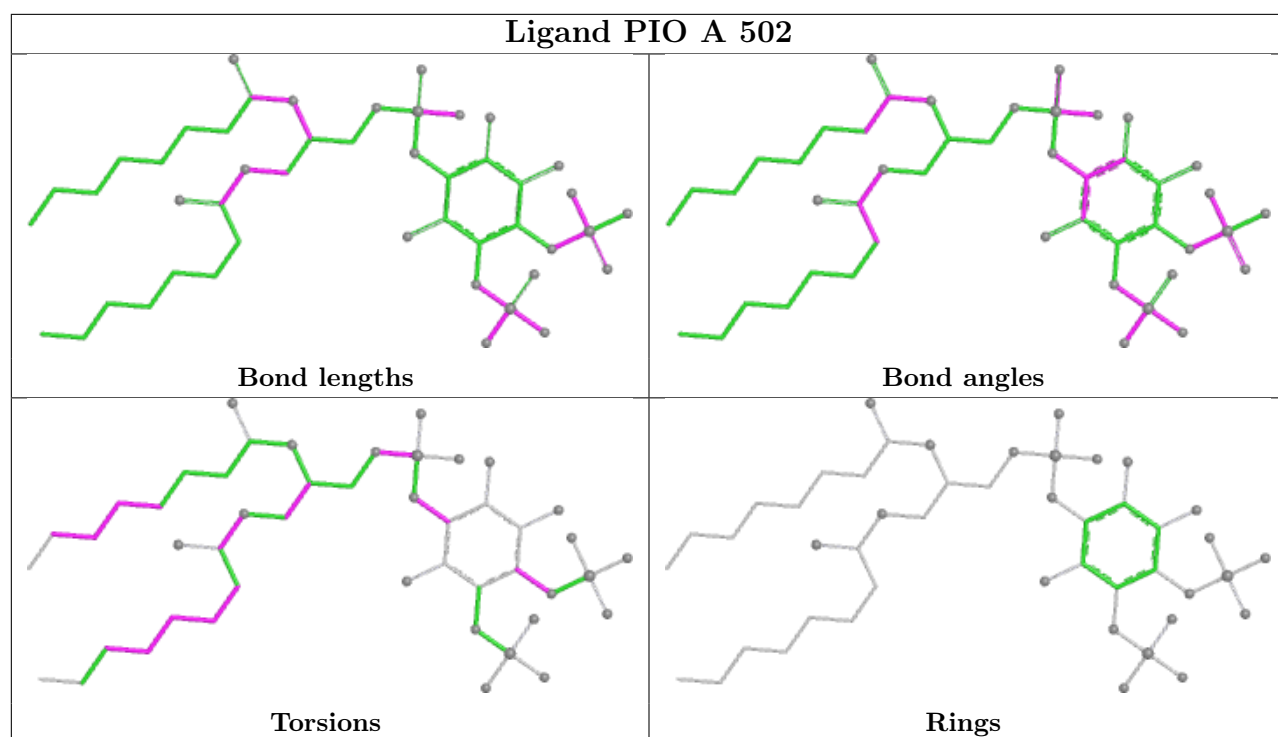
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

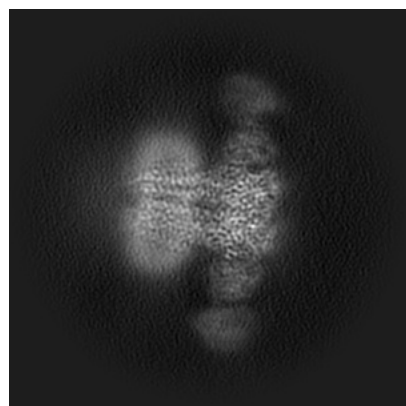
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29727. These allow visual inspection of the internal detail of the map and identification of artifacts.

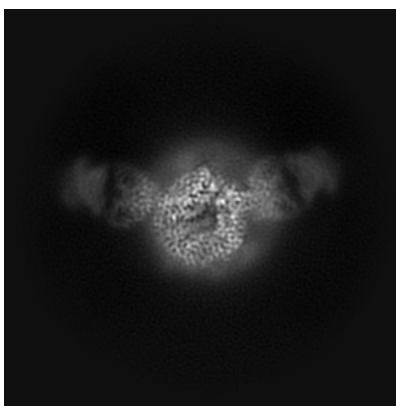
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

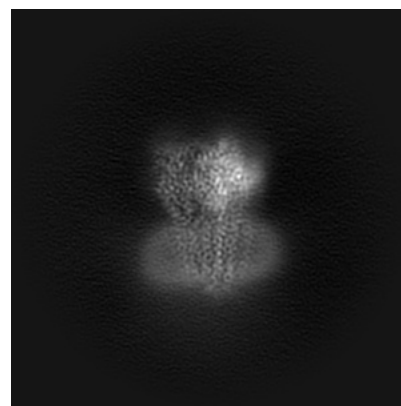
6.1.1 Primary map



X

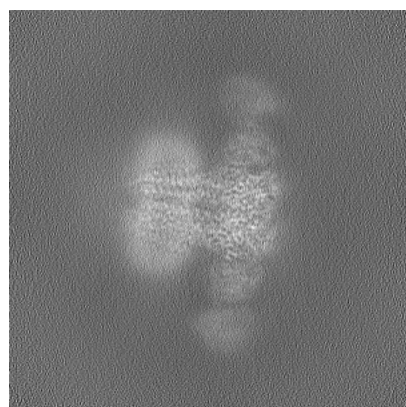


Y

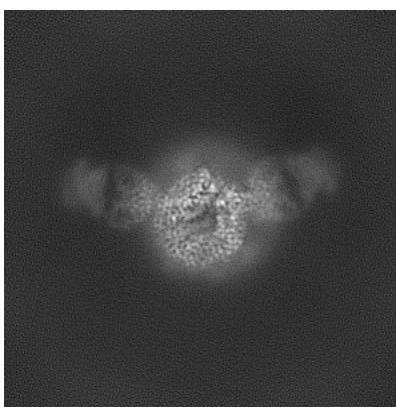


Z

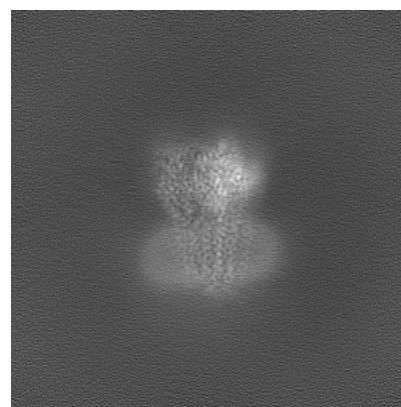
6.1.2 Raw map



X



Y

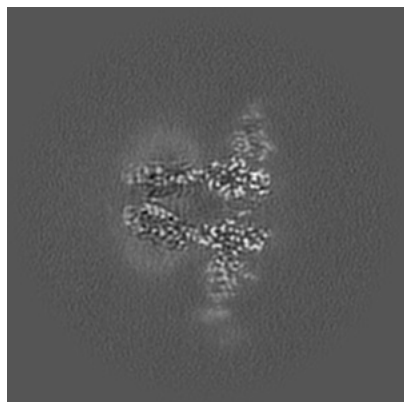


Z

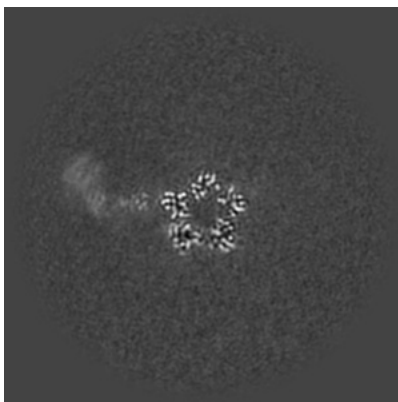
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

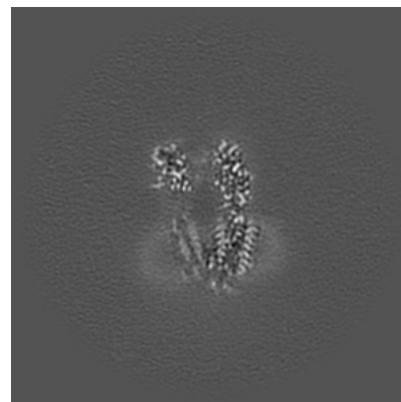
6.2.1 Primary map



X Index: 180

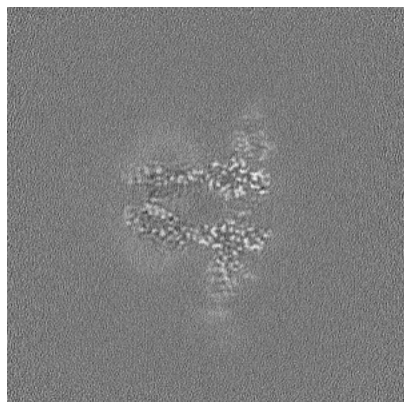


Y Index: 180

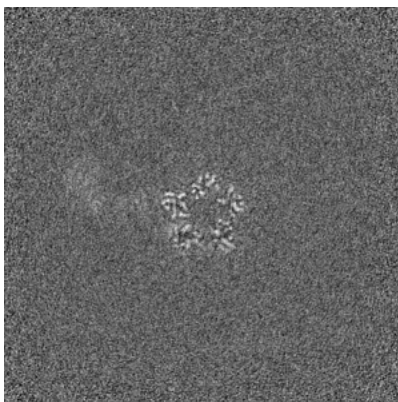


Z Index: 180

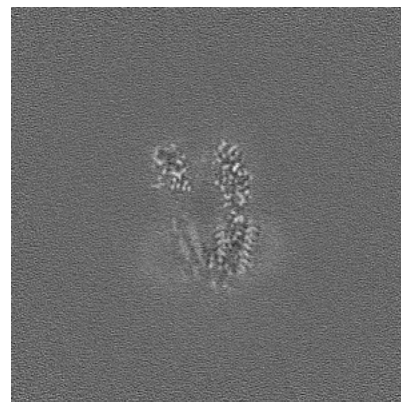
6.2.2 Raw map



X Index: 180



Y Index: 180

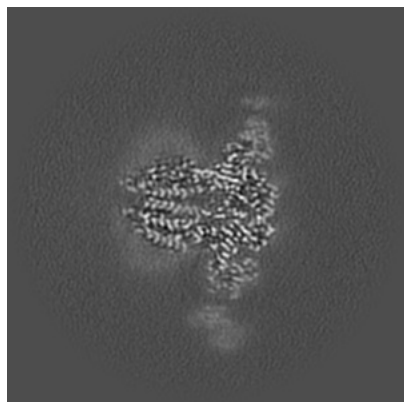


Z Index: 180

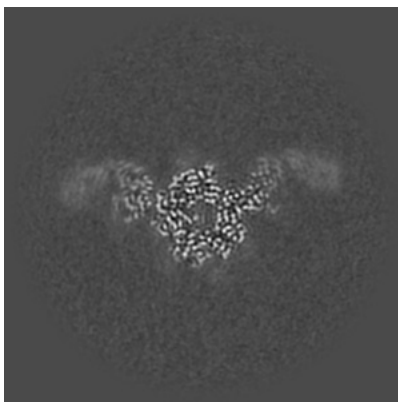
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

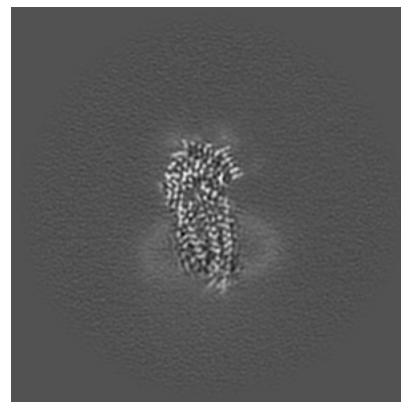
6.3.1 Primary map



X Index: 188

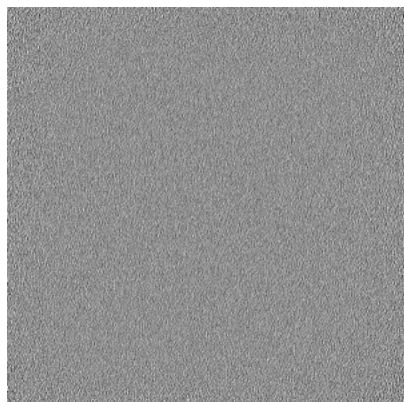


Y Index: 204

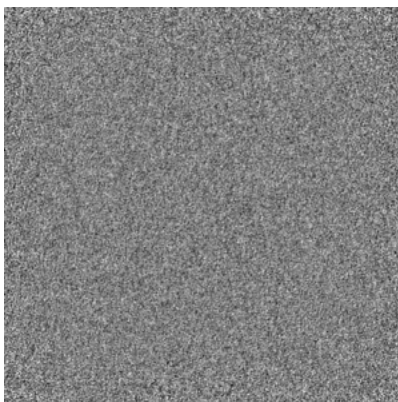


Z Index: 203

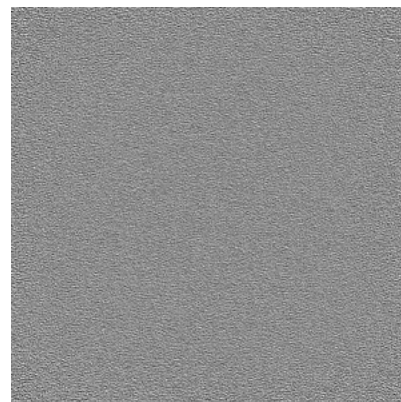
6.3.2 Raw map



X Index: 0



Y Index: 0

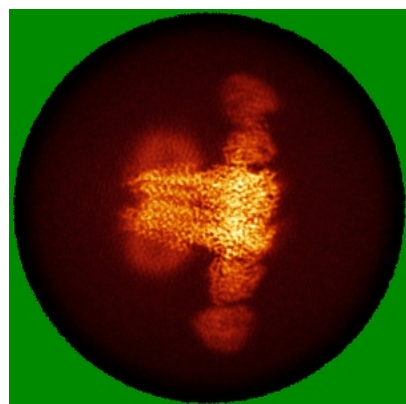


Z Index: 0

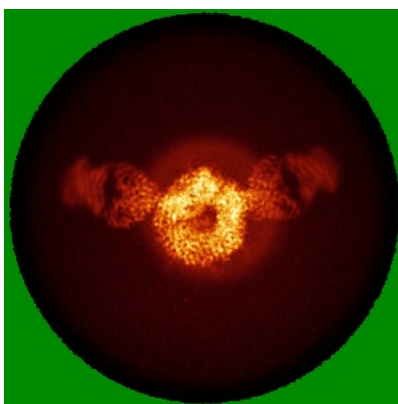
The images above show the largest variance slices of the map in three orthogonal directions.

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

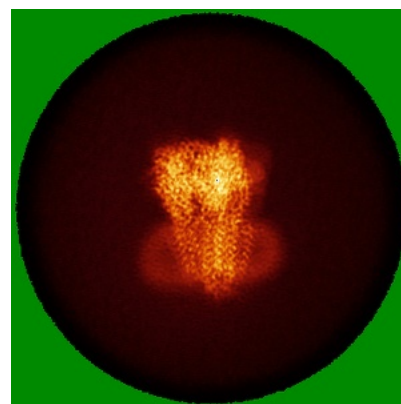
6.4.1 Primary map



X

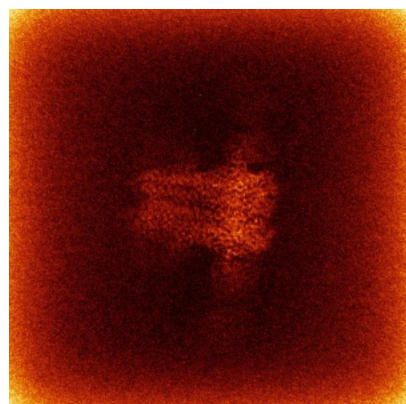


Y

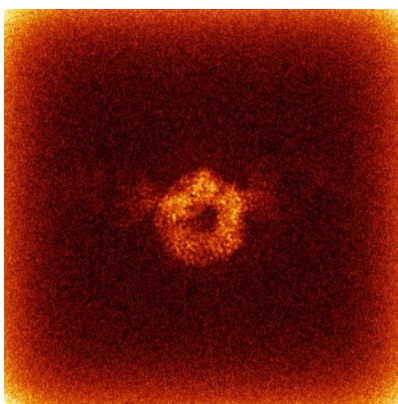


Z

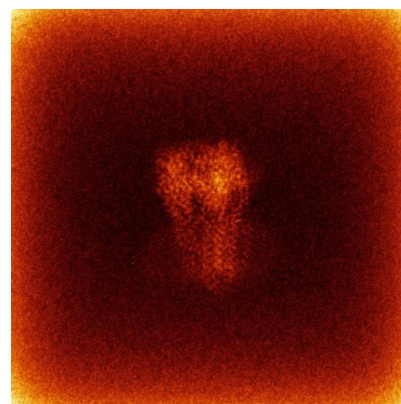
6.4.2 Raw map



X



Y

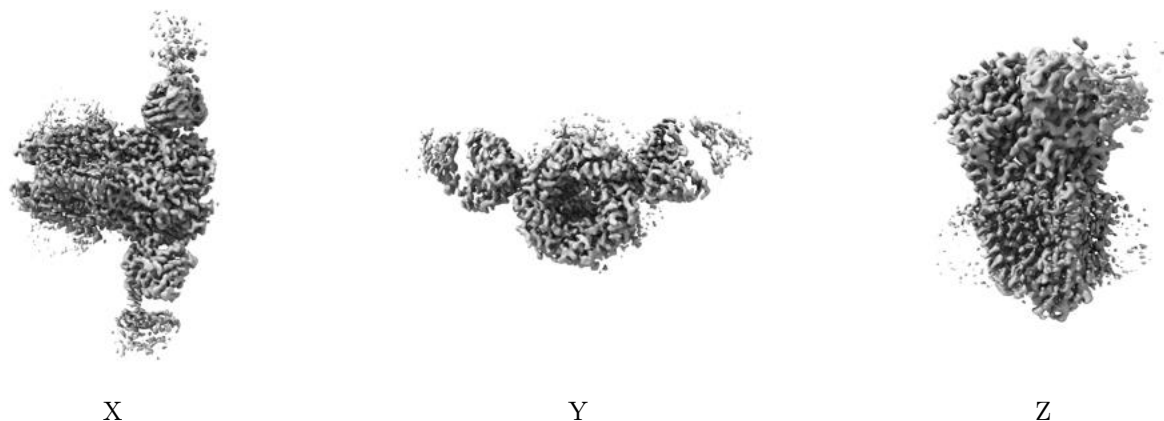


Z

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.

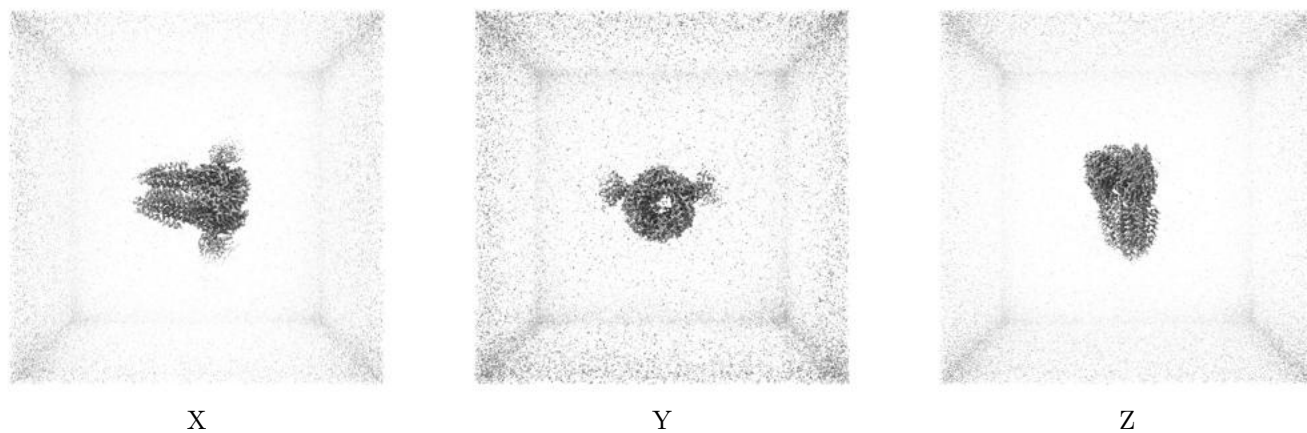
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

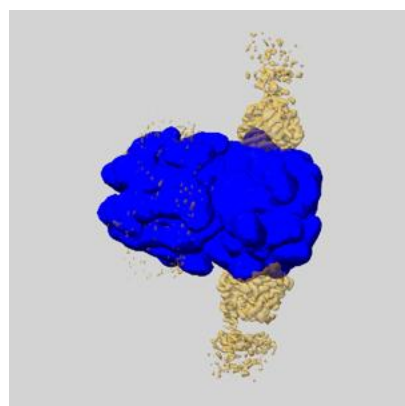
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

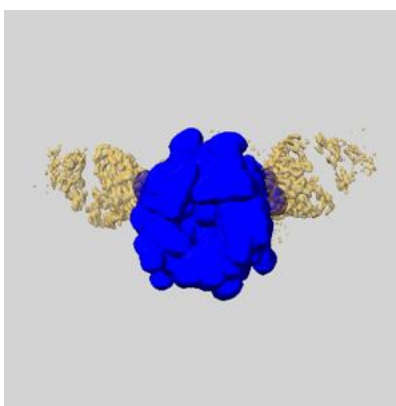
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

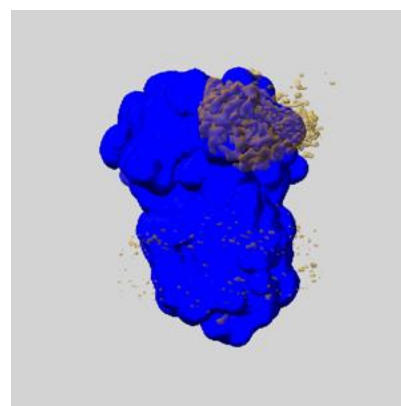
6.6.1 emd_29727_msk_1.map [i](#)



X



Y

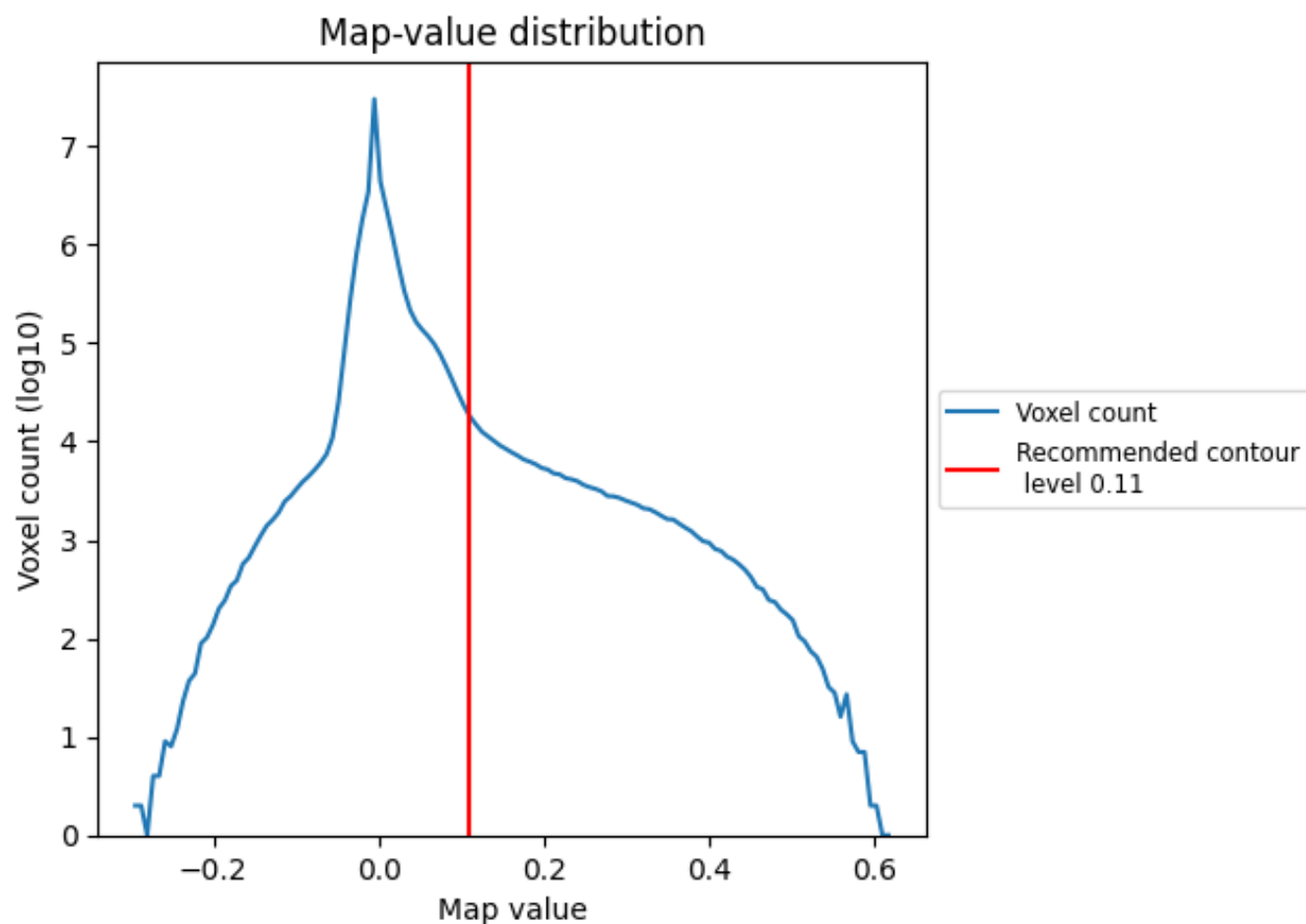


Z

7 Map analysis [i](#)

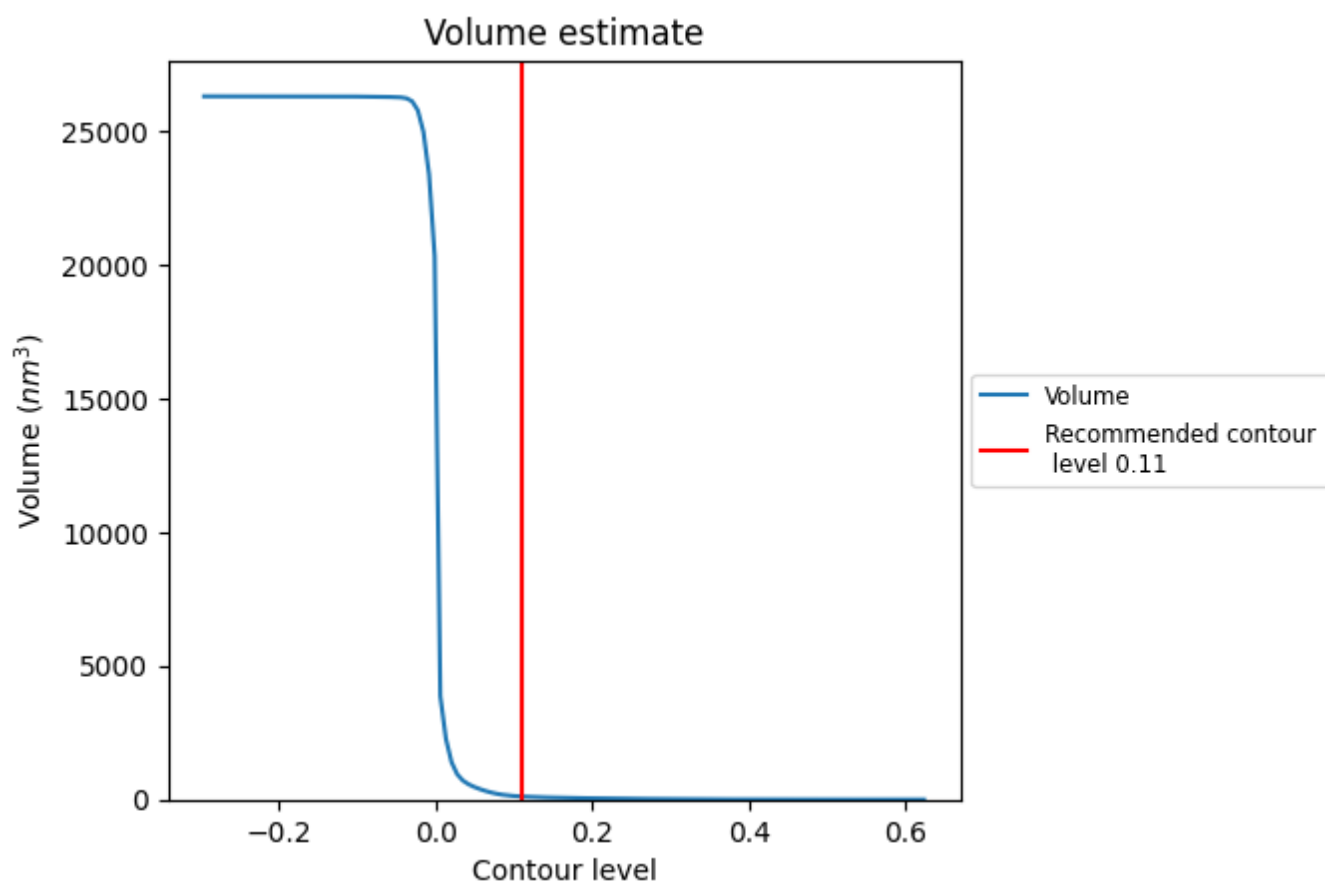
This section contains the results of statistical analysis of the map.

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.

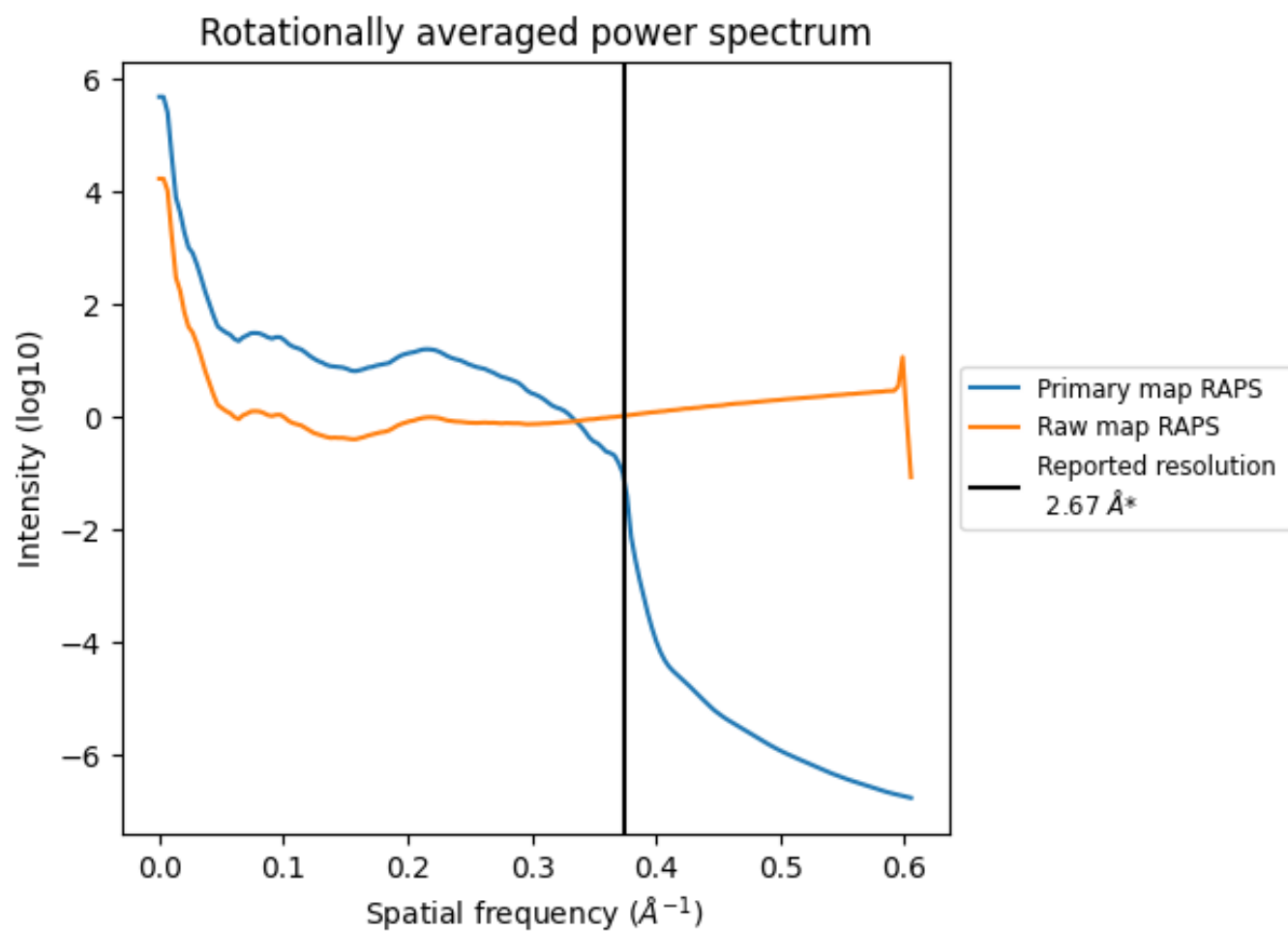
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

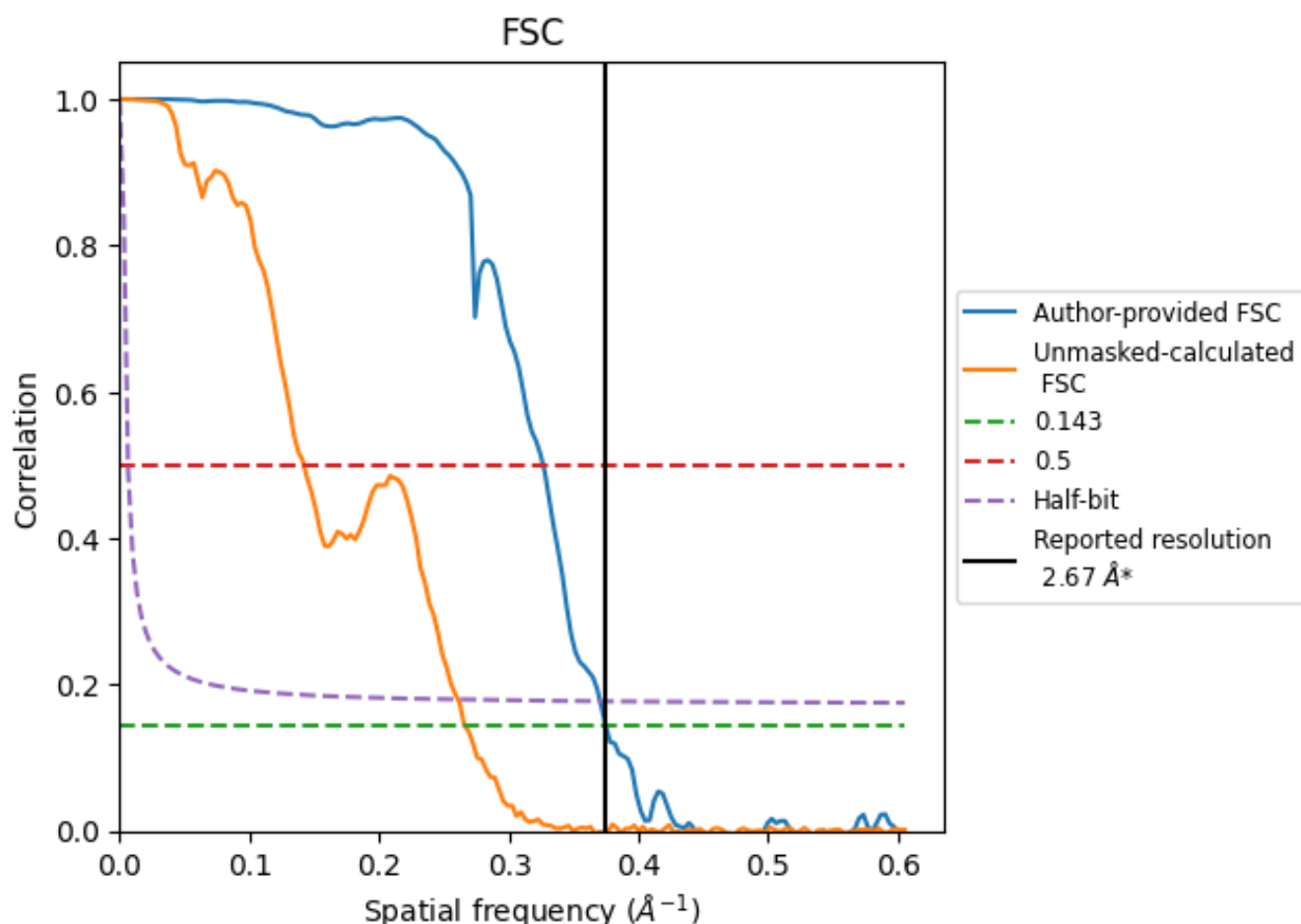


*Reported resolution corresponds to spatial frequency of 0.375 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.375 \AA^{-1}

8.2 Resolution estimates [i](#)

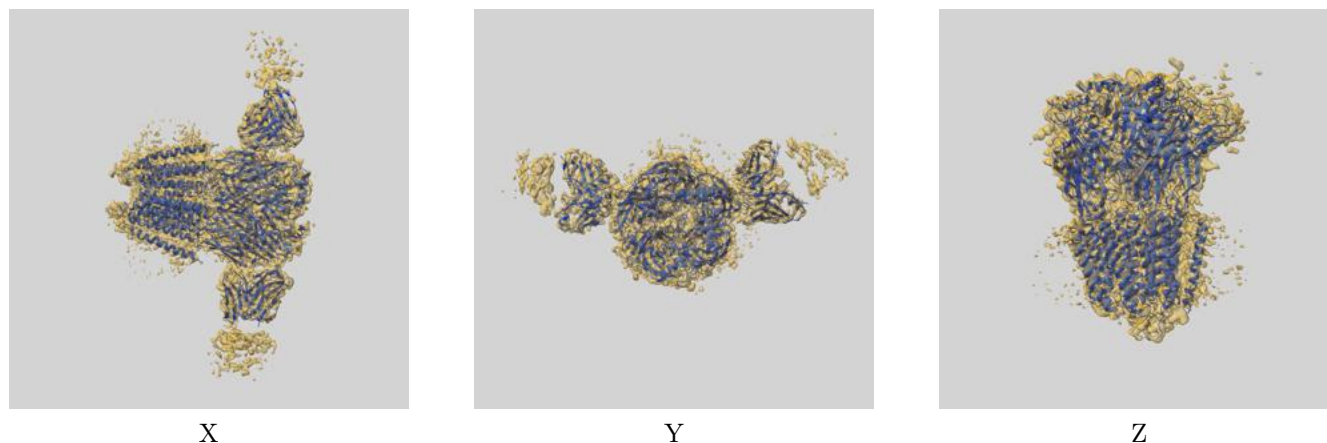
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	3.06	2.70
Unmasked-calculated*	3.76	7.04	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 2.67 by more than 10 %

9 Map-model fit [i](#)

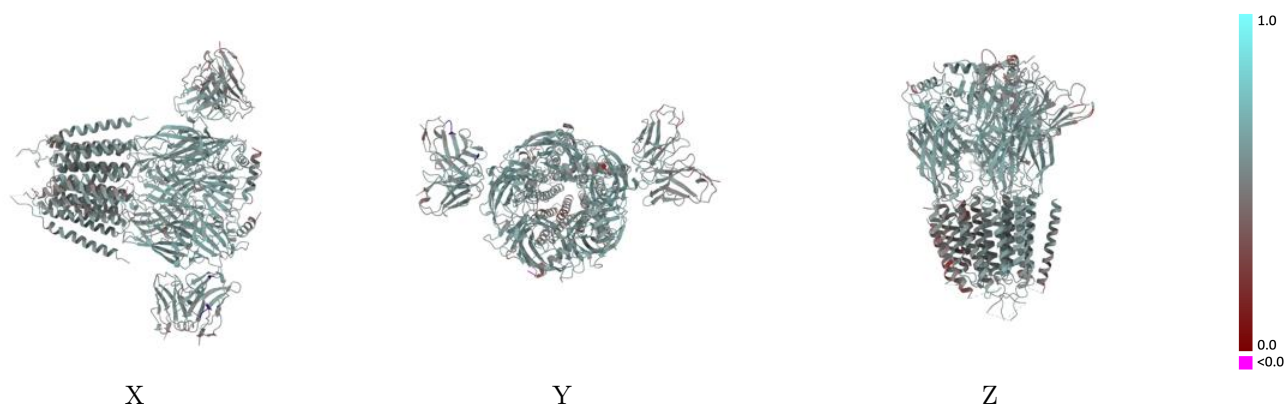
This section contains information regarding the fit between EMDB map EMD-29727 and PDB model 8G4N. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



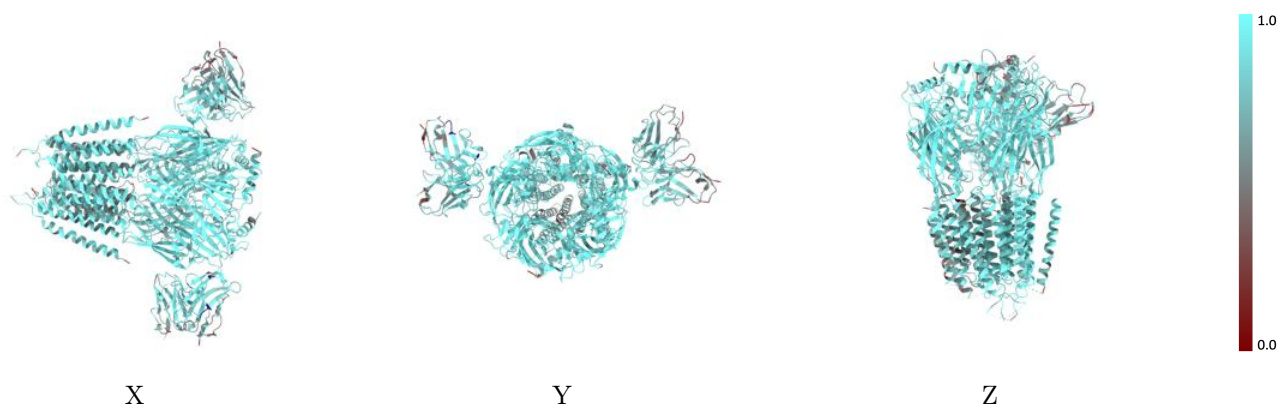
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



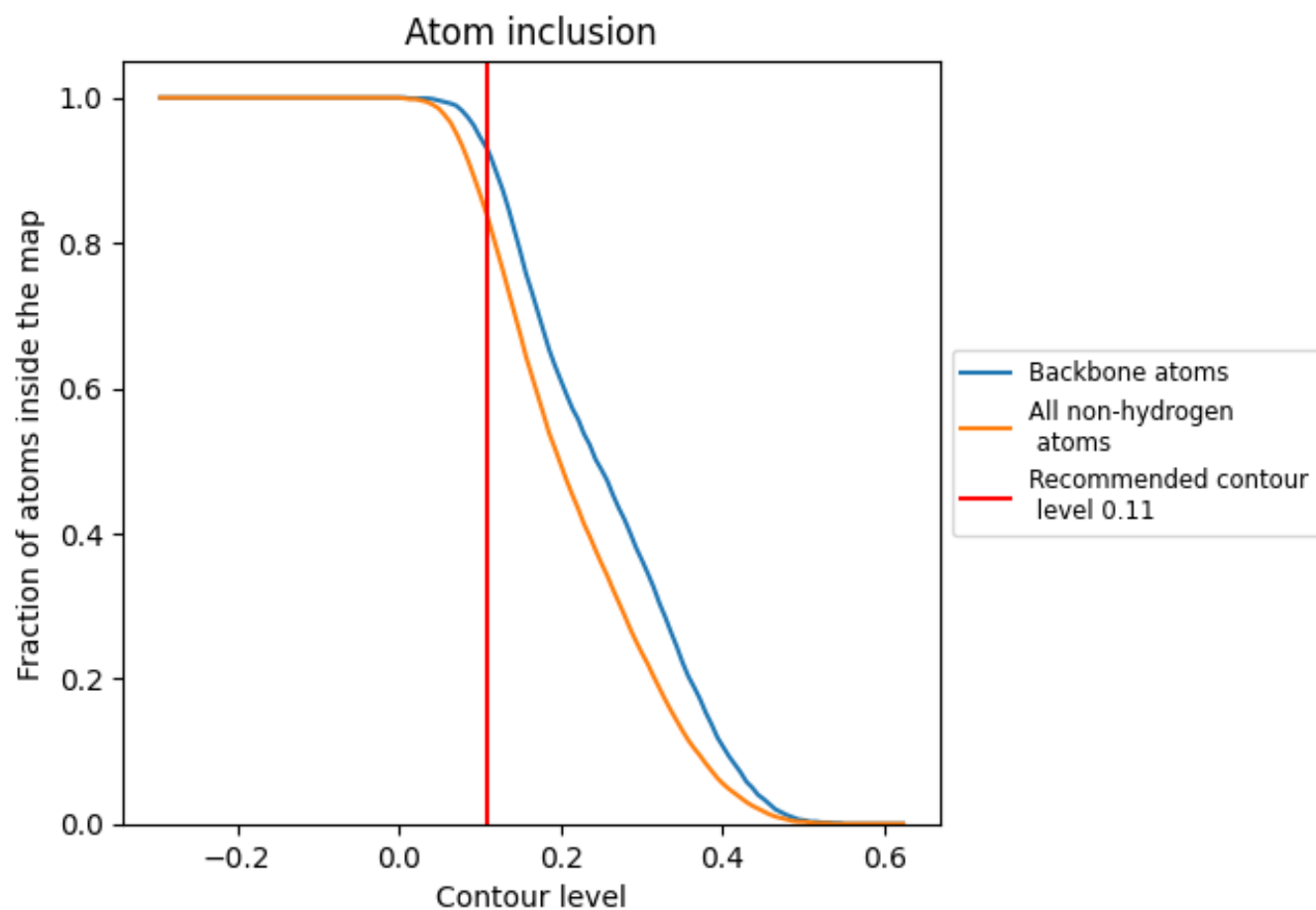
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 84% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.5430
A	 0.8880	 0.5700
B	 0.8860	 0.5620
C	 0.8820	 0.5640
D	 0.7980	 0.5170
E	 0.8580	 0.5430
F	 0.3440	 0.3570
G	 0.5570	 0.4380
H	 0.7100	 0.5070
I	 0.8070	 0.5320
J	 0.7620	 0.5200
K	 0.8070	 0.5350
L	 0.7340	 0.5160
M	 0.3440	 0.3830
O	 0.4360	 0.4130
R	 0.5410	 0.4230
U	 0.5250	 0.4950

