



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 08:39 AM EDT

PDB ID : 8FOI
EMDB ID : EMD-29350
Title : Native GABA-A receptor from the mouse brain, alpha1-beta2-gamma2 subtype, in complex with GABA and allopregnanolone
Authors : Sun, C.; Gouaux, E.
Deposited on : 2022-12-30
Resolution : 2.50 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

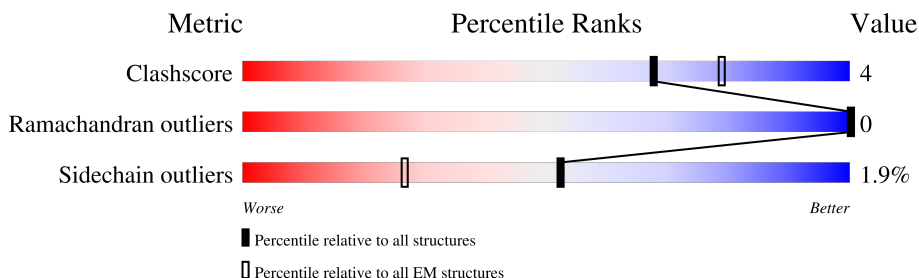
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	70% 6% 24%
1	C	455	69% 7% 24%
2	B	512	58% 7% 35%
2	E	512	56% 8% 35%
3	D	474	58% 9% 33%
4	H	223	47% 5% 48%
4	J	223	50% 48%
5	K	213	44% 6% 51%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	L	213	
6	F	7	
7	G	5	
7	I	5	
7	M	5	
7	O	5	
7	P	5	
8	N	3	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 36827 atoms, of which 18541 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	H	N	O	S	0	0
			5585	1811	2782	471	505	16		
1	C	346	Total	C	H	N	O	S	0	0
			5585	1811	2782	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	H	N	O	S	0	0
			5454	1787	2729	436	486	16		
2	E	333	Total	C	H	N	O	S	0	0
			5455	1787	2728	437	487	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	H	N	O	S	0	0
			5186	1698	2581	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	H	N	O	S	0	0
			1783	587	863	152	177	4		
4	J	117	Total	C	H	N	O	S	0	0
			1783	587	863	152	177	4		

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

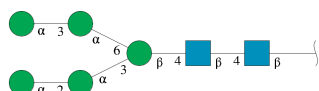
Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	105	Total	C	H	N	O	S	0	0
			1552	505	756	132	155	4		

Continued on next page...

Continued from previous page...

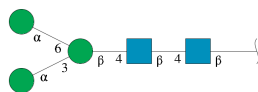
Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	105	Total	C	H	N	O	S	0	0
			1542	503	750	131	154	4		

- Molecule 6 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.



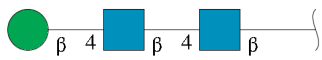
Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	7	Total	C	H	N	O		0	0
			153	46	70	2	35			

- 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.



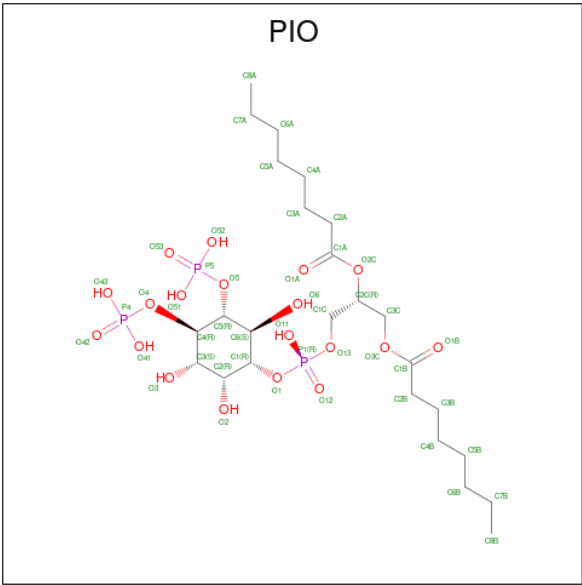
Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	5	Total	C	H	N	O		0	0
			113	34	52	2	25			
7	I	5	Total	C	H	N	O		0	0
			113	34	52	2	25			
7	M	5	Total	C	H	N	O		0	0
			113	34	52	2	25			
7	O	5	Total	C	H	N	O		0	0
			113	34	52	2	25			
7	P	5	Total	C	H	N	O		0	0
			113	34	52	2	25			

- Molecule 8 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.



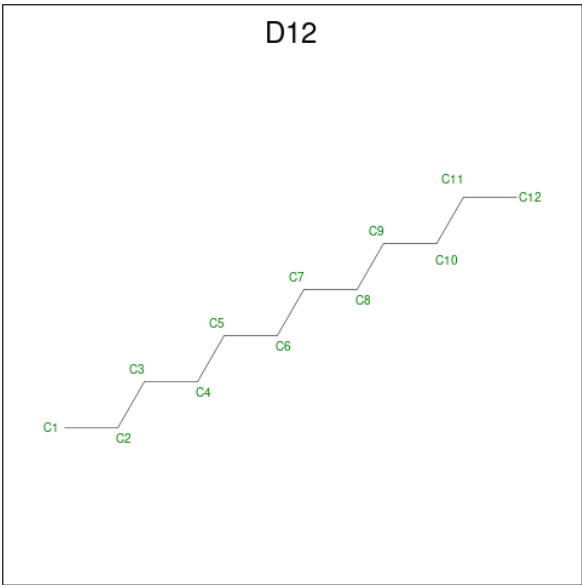
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
8	N	3	73	22	34	2	15	0	0

- Molecule 9 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: C₂₅H₄₉O₁₉P₃).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
9	A	1	91	25	44	19	3	0
9	C	1	91	25	44	19	3	0

- Molecule 10 is DODECANE (three-letter code: D12) (formula: C₁₂H₂₆).



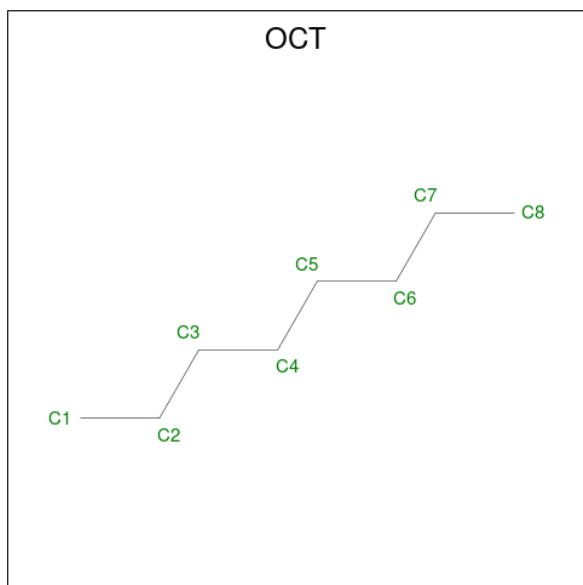
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	H	0
			38	12	26	
10	A	1	Total	C	H	0
			38	12	26	
10	B	1	Total	C	H	0
			38	12	26	
10	B	1	Total	C	H	0
			38	12	26	
10	B	1	Total	C	H	0
			38	12	26	
10	B	1	Total	C	H	0
			38	12	26	
10	B	1	Total	C	H	0
			38	12	26	
10	B	1	Total	C	H	0
			38	12	26	
10	C	1	Total	C	H	0
			38	12	26	
10	C	1	Total	C	H	0
			38	12	26	
10	D	1	Total	C	H	0
			38	12	26	
10	D	1	Total	C	H	0
			38	12	26	
10	E	1	Total	C	H	0
			38	12	26	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
10	E	1	Total	C	H	0
			38	12	26	
10	E	1	Total	C	H	0
			38	12	26	
10	E	1	Total	C	H	0
			38	12	26	

- Molecule 11 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



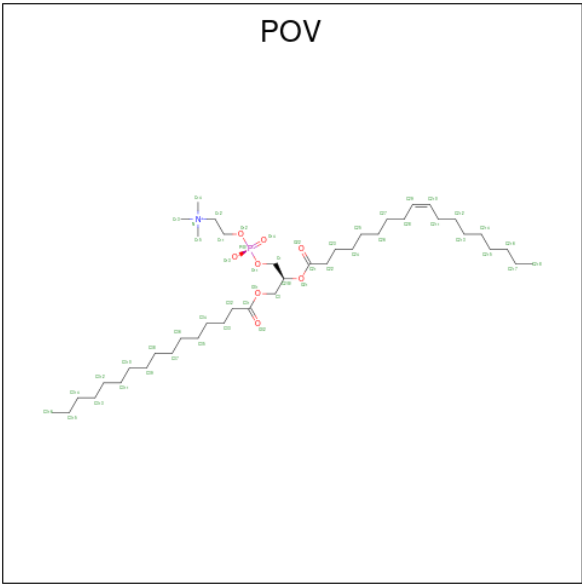
Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	H	0
			26	8	18	
11	A	1	Total	C	H	0
			26	8	18	
11	A	1	Total	C	H	0
			26	8	18	
11	A	1	Total	C	H	0
			26	8	18	
11	C	1	Total	C	H	0
			26	8	18	
11	C	1	Total	C	H	0
			26	8	18	
11	C	1	Total	C	H	0
			26	8	18	
11	D	1	Total	C	H	0
			26	8	18	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
11	D	1	26	8	18	0
11	D	1	26	8	18	0
11	D	1	26	8	18	0
11	D	1	26	8	18	0
11	E	1	26	8	18	0
11	E	1	26	8	18	0
11	E	1	26	8	18	0
11	E	1	26	8	18	0
11	E	1	26	8	18	0

- Molecule 12 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



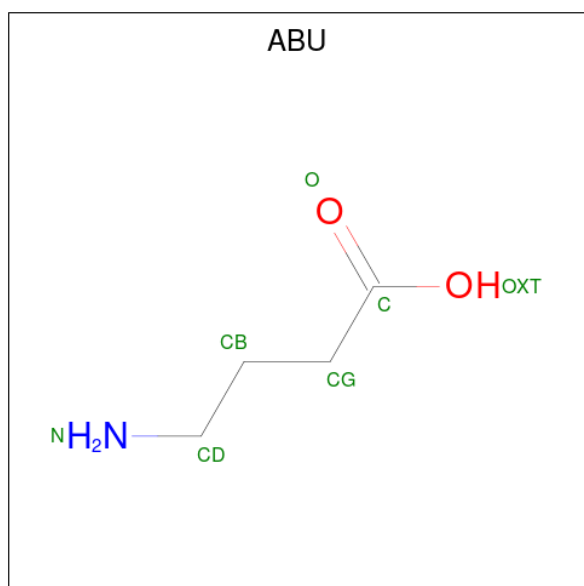
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
12	A	1	134	42	82	1	8	1	0
12	A	1	134	42	82	1	8	1	0

Continued on next page...

Continued from previous page...

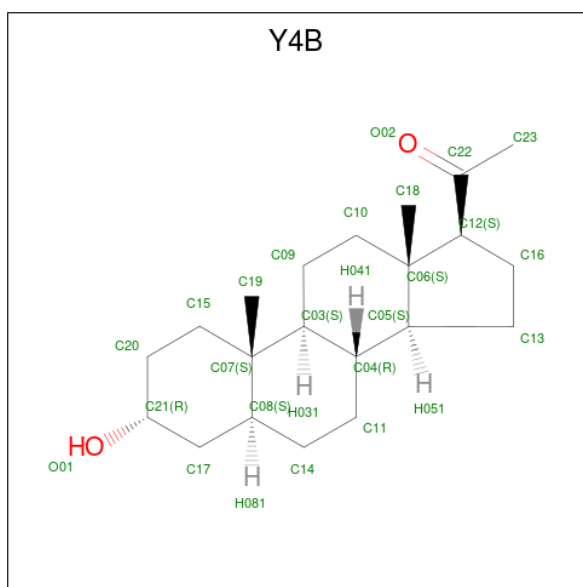
Mol	Chain	Residues	Atoms					AltConf	
12	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
12	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
12	E	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

- Molecule 13 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



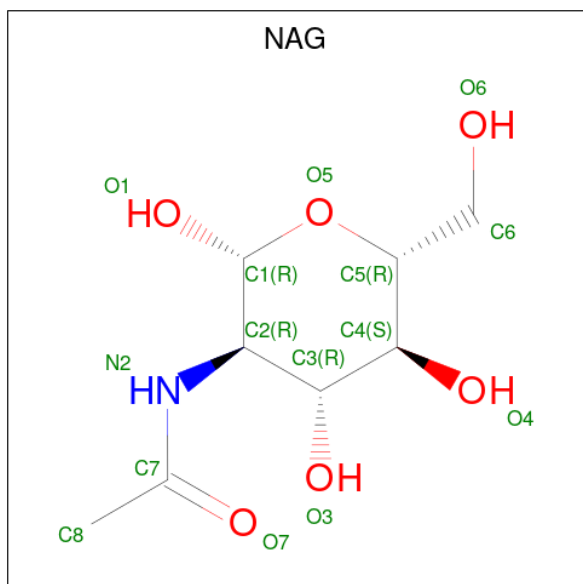
Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	H	N	O	0
			15	4	8	1	2	
13	E	1	Total	C	H	N	O	0
			15	4	8	1	2	

- Molecule 14 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
14	B	1	Total	C	H	O	0
			57	21	34	2	
14	E	1	Total	C	H	O	0
			57	21	34	2	

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

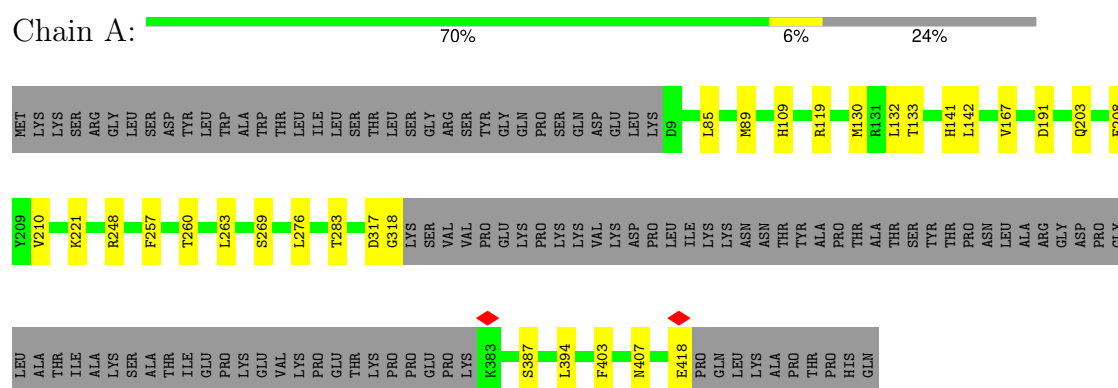


Mol	Chain	Residues	Atoms					AltConf
15	D	1	Total	C	H	N	O	0
			27	8	13	1	5	

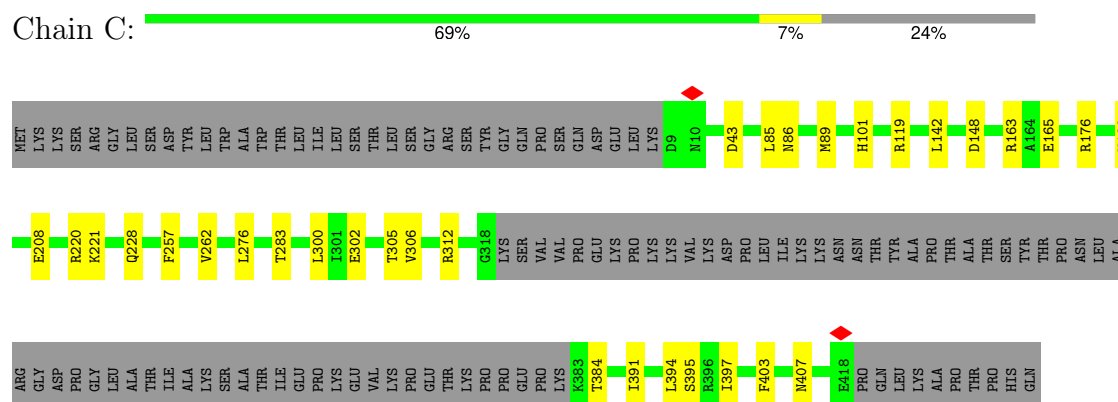
3 Residue-property plots

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.

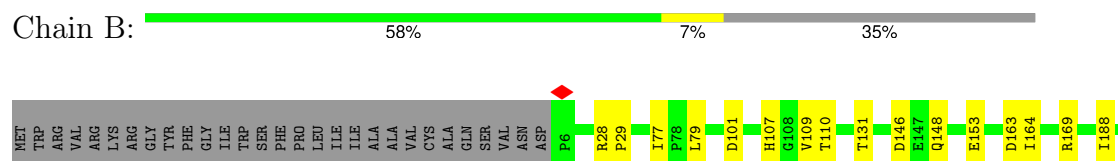
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

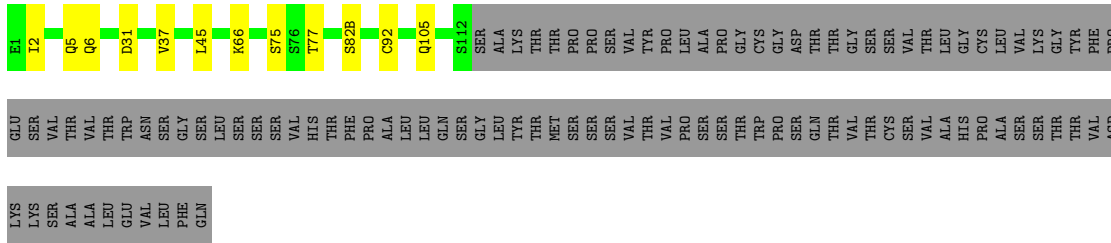


- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-1

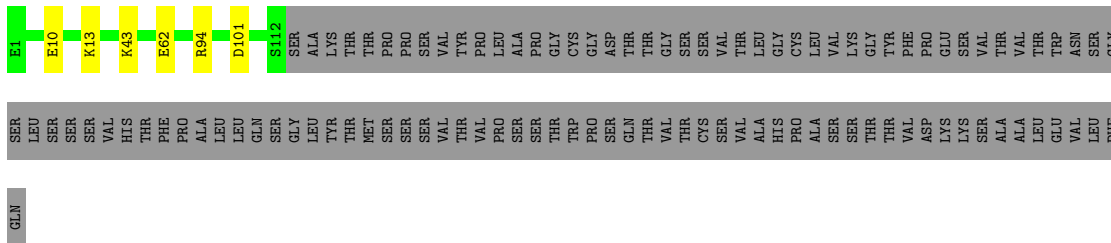


- Molecule 2: Gamma-aminobutyric acid receptor subunit beta-2

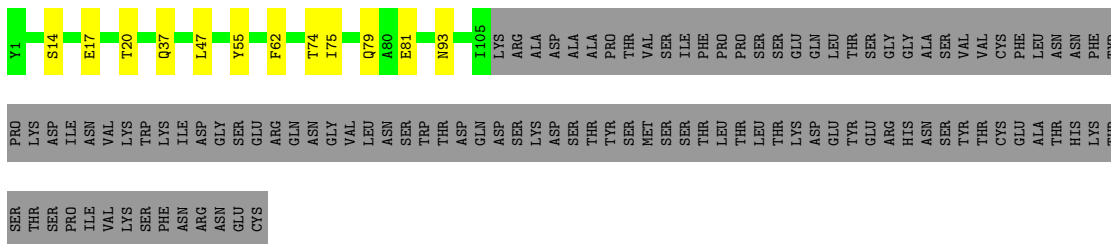




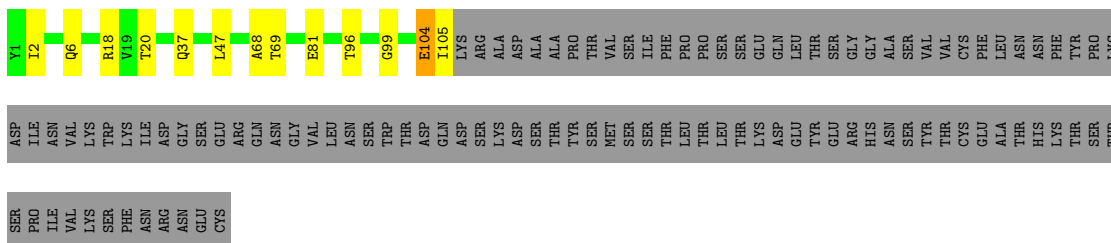
- Molecule 4: Heavy Chain of 8E3 Fab



- Molecule 5: Light Chain of 8E3-Fab



- Molecule 5: Light Chain of 8E3-Fab

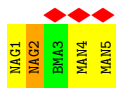


- Molecule 6: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

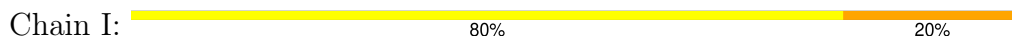




- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



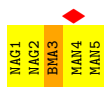
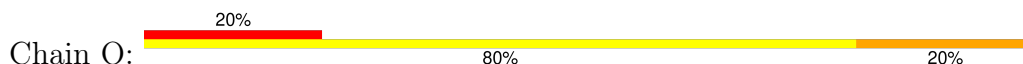
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



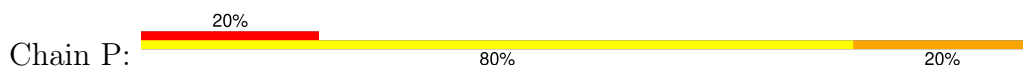
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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: 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, C1	Depositor
Number of particles used	299655	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	0.799	Depositor
Minimum map value	-0.346	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	299.16, 299.16, 299.16	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83100003, 0.83100003, 0.83100003	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.26	0/2874	0.53	0/3904
1	C	0.27	0/2874	0.53	0/3904
2	B	0.27	0/2796	0.51	0/3806
2	E	0.27	0/2798	0.52	0/3807
3	D	0.26	0/2676	0.52	0/3646
4	H	0.27	0/946	0.46	0/1284
4	J	0.28	0/946	0.48	0/1284
5	K	0.28	0/815	0.51	0/1108
5	L	0.29	0/811	0.53	0/1103
All	All	0.27	0/17536	0.52	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 [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	2803	2782	2782	18	0
1	C	2803	2782	2782	20	0
2	B	2725	2729	2729	23	0
2	E	2727	2728	2728	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2605	2581	2581	25	0
4	H	920	863	863	6	0
4	J	920	863	863	3	0
5	K	796	756	756	8	0
5	L	792	750	750	7	0
6	F	83	70	70	1	0
7	G	61	52	52	1	0
7	I	61	52	52	3	0
7	M	61	52	52	0	0
7	O	61	52	52	1	0
7	P	61	52	52	1	0
8	N	39	34	34	0	0
9	A	47	44	44	1	0
9	C	47	44	44	2	0
10	A	24	52	52	0	0
10	B	84	182	182	1	0
10	C	24	52	52	0	0
10	D	24	52	52	0	0
10	E	48	104	104	0	0
11	A	32	72	72	0	0
11	C	24	54	54	0	0
11	D	40	90	90	0	0
11	E	40	90	90	0	0
12	A	104	164	164	1	0
12	C	104	164	164	3	0
12	E	52	82	82	0	0
13	B	7	8	0	1	0
13	E	7	8	0	0	0
14	B	23	34	0	0	0
14	E	23	34	0	0	0
15	D	14	13	13	0	0
All	All	18286	18541	18457	131	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 (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:NH1	1:A:387:SER:O	2.18	0.76
3:D:274:LEU:O	3:D:277:THR:OG1	2.04	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:247:ILE:HD12	3:D:250:LEU:HD12	1.70	0.74
2:E:76:VAL:HG23	2:E:77:ILE:HG23	1.69	0.74
1:A:263:LEU:HD22	2:B:260:THR:HG21	1.70	0.73
1:A:191:ASP:OD1	1:A:221:LYS:NZ	2.19	0.73
1:C:176:ARG:NH1	5:K:93:ASN:OD1	2.23	0.72
4:J:62:GLU:OE1	4:J:62:GLU:N	2.26	0.68
3:D:45:ASP:OD1	3:D:85:ARG:NH1	2.27	0.67
2:B:107:HIS:HE2	2:B:131:THR:HG1	1.42	0.67
2:E:284:TYR:OH	2:E:479:ASN:OD1	2.12	0.67
3:D:294:THR:OG1	3:D:297:ASP:OD1	2.15	0.64
2:B:269:ARG:NH1	1:C:228:GLN:OE1	2.31	0.63
1:A:109:HIS:NE2	1:A:133:THR:OG1	2.20	0.63
3:D:263:PRO:O	3:D:267:SER:OG	2.09	0.63
2:E:235:LEU:O	2:E:238:VAL:HG12	1.98	0.63
2:B:461:ASN:O	2:B:465:ARG:N	2.32	0.62
2:E:291:PHE:HE2	2:E:474:VAL:HG13	1.64	0.62
7:I:2:NAG:H3	7:I:2:NAG:H83	1.82	0.61
2:E:470:PHE:O	2:E:474:VAL:HG12	2.01	0.60
6:F:2:NAG:H83	6:F:2:NAG:H3	1.83	0.60
2:B:202:THR:OG1	13:B:501:ABU:O	2.11	0.60
2:B:220:TYR:OH	2:B:224:GLN:NE2	2.35	0.60
1:A:403:PHE:O	1:A:407:ASN:ND2	2.36	0.59
2:E:252:ALA:O	2:E:256:THR:OG1	2.11	0.59
1:A:167:VAL:HG23	1:A:210:VAL:HG21	1.85	0.58
5:L:2:ILE:O	5:L:96:THR:OG1	2.19	0.58
3:D:122:HIS:HE2	3:D:146:THR:HG1	1.49	0.57
2:E:470:PHE:CZ	2:E:474:VAL:HG11	2.40	0.57
5:K:14:SER:N	5:K:17:GLU:OE2	2.39	0.56
1:C:85:LEU:HD13	1:C:89:MET:HG3	1.88	0.56
3:D:154:GLN:N	3:D:154:GLN:OE1	2.38	0.56
2:E:183:LEU:HD23	2:E:184:PRO:HD2	1.87	0.56
10:B:508:D12:H81	12:C:608:POV:H210	1.87	0.56
7:G:2:NAG:H83	7:G:2:NAG:H3	1.88	0.56
1:A:317:ASP:OD1	1:A:318:GLY:N	2.40	0.55
2:E:298:GLU:O	2:E:302:VAL:HG23	2.07	0.54
4:H:5:GLN:NE2	4:H:105:GLN:OE1	2.40	0.54
5:L:18:ARG:NH1	5:L:20:THR:OG1	2.40	0.54
2:E:143:TYR:HH	2:E:221:PHE:HE2	1.56	0.54
2:B:213:LYS:HB2	7:I:1:NAG:H82	1.88	0.54
2:B:272:LEU:HD22	2:B:279:LYS:HE3	1.90	0.53
2:B:107:HIS:NE2	2:B:131:THR:OG1	2.31	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD13	1:A:89:MET:HG3	1.89	0.53
3:D:247:ILE:CD1	3:D:250:LEU:HD12	2.39	0.53
1:C:312:ARG:NE	1:C:384:THR:OG1	2.39	0.53
1:A:119:ARG:NH2	2:E:205:TYR:OH	2.42	0.52
3:D:46:ILE:HG22	2:E:9:MET:SD	2.49	0.52
3:D:270:ILE:O	3:D:274:LEU:HD23	2.10	0.52
2:B:188:ILE:O	2:B:188:ILE:HG23	2.10	0.52
5:L:104:GLU:OE1	5:L:105:ILE:N	2.43	0.52
7:O:2:NAG:O3	7:O:3:BMA:O5	2.22	0.52
3:D:63:GLY:N	3:D:73:THR:O	2.42	0.51
3:D:269:GLY:O	3:D:273:VAL:HG12	2.10	0.51
1:A:263:LEU:CD2	2:B:260:THR:HG21	2.41	0.51
2:B:275:ILE:HD13	2:B:277:TYR:CD1	2.45	0.51
2:E:239:SER:HB2	2:E:253:LEU:HD23	1.91	0.51
2:B:202:THR:HG22	1:C:119:ARG:NH1	2.26	0.51
7:I:1:NAG:H62	7:I:2:NAG:H82	1.93	0.51
5:K:81:GLU:N	5:K:81:GLU:OE1	2.42	0.50
5:K:17:GLU:OE1	5:K:17:GLU:N	2.44	0.50
5:K:20:THR:HG22	5:K:74:THR:HG22	1.92	0.50
3:D:257:ILE:O	3:D:265:ARG:NH2	2.42	0.50
4:H:66:LYS:NZ	4:H:82(B):SER:O	2.45	0.50
1:A:130:MET:SD	2:B:110:THR:HG23	2.51	0.49
1:C:165:GLU:OE2	3:D:97:ARG:NH1	2.43	0.49
1:C:391:ILE:O	1:C:395:SER:OG	2.27	0.49
1:C:403:PHE:O	1:C:407:ASN:ND2	2.42	0.49
1:A:260:THR:HG21	2:E:255:ILE:CG2	2.42	0.49
2:B:28:ARG:NH1	2:B:29:PRO:O	2.46	0.49
1:A:276:LEU:H	1:A:276:LEU:HD23	1.77	0.49
2:E:475:PHE:O	2:E:479:ASN:ND2	2.41	0.48
2:B:298:GLU:O	2:B:302:VAL:HG23	2.14	0.48
1:C:305:THR:HG21	9:C:601:PIO:H3B	1.96	0.48
4:H:37:VAL:HG11	4:H:45:LEU:HD22	1.96	0.47
1:C:142:LEU:HD13	1:C:276:LEU:HD22	1.96	0.47
1:C:86:ASN:OD1	1:C:86:ASN:N	2.47	0.47
1:C:302:GLU:O	1:C:306:VAL:HG23	2.14	0.47
1:A:130:MET:HE2	1:A:132:LEU:HD21	1.97	0.47
12:C:607:POV:H15B	12:C:607:POV:O12	2.15	0.47
4:H:6:GLN:NE2	4:H:92:CYS:SG	2.88	0.47
1:A:142:LEU:O	1:A:283:THR:HG22	2.15	0.47
2:B:275:ILE:HD12	2:B:275:ILE:O	2.15	0.47
2:B:146:ASP:OD2	2:B:148:GLN:NE2	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:68:ALA:O	5:L:69:THR:OG1	2.25	0.46
3:D:253:VAL:HG13	3:D:268:LEU:HD21	1.98	0.46
5:L:81:GLU:N	5:L:81:GLU:OE1	2.49	0.46
5:L:6:GLN:NE2	5:L:99:GLY:O	2.49	0.46
2:B:275:ILE:HD13	2:B:277:TYR:CE1	2.52	0.45
3:D:273:VAL:HG13	3:D:274:LEU:HD22	1.98	0.45
1:C:190:TYR:OH	1:C:220:ARG:NH2	2.49	0.45
4:J:101:ASP:OD1	5:K:55:TYR:OH	2.22	0.45
5:K:62:PHE:CD2	5:K:75:ILE:HD12	2.52	0.45
1:C:148:ASP:OD1	1:C:148:ASP:N	2.50	0.44
2:E:173:ASN:N	2:E:173:ASN:OD1	2.49	0.44
1:C:142:LEU:O	1:C:283:THR:HG22	2.17	0.44
12:A:609:POV:H15B	12:A:609:POV:O12	2.17	0.44
1:C:397:ILE:HD11	12:C:607:POV:O31	2.17	0.44
2:E:262:THR:O	2:E:266:THR:HG23	2.17	0.44
1:C:262:VAL:HG11	3:D:250:LEU:HD11	2.00	0.43
1:C:394:LEU:HD22	9:C:601:PIO:H6AA	2.00	0.43
1:A:394:LEU:HD12	9:A:601:PIO:H4A	2.00	0.43
2:E:28:ARG:NH1	2:E:29:PRO:O	2.52	0.43
4:H:75:SER:O	4:H:77:THR:N	2.50	0.42
3:D:160:MET:SD	3:D:160:MET:N	2.91	0.42
2:E:47:ILE:HD12	2:E:188:ILE:HD11	2.00	0.42
2:E:48:ASP:N	2:E:48:ASP:OD1	2.51	0.42
2:E:238:VAL:HG13	2:E:253:LEU:HD21	2.01	0.42
3:D:244:CYS:O	3:D:248:VAL:HG23	2.20	0.42
3:D:281:THR:O	3:D:285:LYS:N	2.51	0.42
5:K:37:GLN:HB2	5:K:47:LEU:HD11	2.02	0.41
5:L:37:GLN:HB2	5:L:47:LEU:HD11	2.01	0.41
4:J:10:GLU:N	4:J:10:GLU:OE1	2.53	0.41
7:P:2:NAG:H83	7:P:2:NAG:H3	2.01	0.41
2:B:77:ILE:N	2:B:77:ILE:HD12	2.35	0.41
2:B:469:ILE:O	2:B:473:VAL:HG23	2.20	0.41
3:D:274:LEU:CD1	2:E:260:THR:HG21	2.50	0.41
2:E:42:ILE:HB	2:E:175:VAL:HG22	2.03	0.41
2:B:164:ILE:HG23	2:B:206:PRO:HG3	2.03	0.41
2:E:104:SER:HB3	2:E:132:THR:HG22	2.02	0.41
1:A:418:GLU:OE1	1:A:418:GLU:N	2.50	0.41
3:D:62:ILE:HD12	3:D:196:TRP:CZ3	2.56	0.41
3:D:233:MET:O	3:D:237:THR:HG23	2.20	0.41
3:D:161:ASP:OD1	3:D:163:HIS:NE2	2.52	0.41
3:D:215:THR:OG1	3:D:216:THR:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:VAL:HG21	2:E:112:LYS:HE3	2.02	0.40
1:A:203:GLN:NE2	1:A:208:GLU:OE2	2.54	0.40
2:B:153:GLU:OE1	2:B:207:ARG:NH1	2.52	0.40
1:C:163:ARG:N	1:C:208:GLU:O	2.47	0.40
1:C:190:TYR:O	1:C:221:LYS:NZ	2.47	0.40
4:H:2:ILE:N	4:H:2:ILE:HD12	2.36	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%)	338 (99%)	4 (1%)	0	100	100
1	C	342/455 (75%)	334 (98%)	8 (2%)	0	100	100
2	B	329/512 (64%)	322 (98%)	7 (2%)	0	100	100
2	E	329/512 (64%)	319 (97%)	10 (3%)	0	100	100
3	D	314/474 (66%)	307 (98%)	7 (2%)	0	100	100
4	H	115/223 (52%)	111 (96%)	4 (4%)	0	100	100
4	J	115/223 (52%)	112 (97%)	3 (3%)	0	100	100
5	K	103/213 (48%)	97 (94%)	6 (6%)	0	100	100
5	L	103/213 (48%)	99 (96%)	4 (4%)	0	100	100
All	All	2092/3280 (64%)	2039 (98%)	53 (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%)	304 (99%)	4 (1%)	65	85
2	B	303/457 (66%)	297 (98%)	6 (2%)	50	75
2	E	303/457 (66%)	293 (97%)	10 (3%)	33	59
3	D	292/436 (67%)	286 (98%)	6 (2%)	48	74
4	H	98/195 (50%)	97 (99%)	1 (1%)	73	88
4	J	98/195 (50%)	95 (97%)	3 (3%)	35	62
5	K	83/188 (44%)	82 (99%)	1 (1%)	67	86
5	L	82/188 (44%)	81 (99%)	1 (1%)	67	86
All	All	1875/2924 (64%)	1840 (98%)	35 (2%)	52	77

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	257	PHE
1	A	269	SER
2	B	79	LEU
2	B	101	ASP
2	B	109	VAL
2	B	163	ASP
2	B	169	ARG
2	B	225	THR
1	C	43	ASP
1	C	101	HIS
1	C	257	PHE
1	C	300	LEU
3	D	199	TYR
3	D	211	GLU
3	D	251	SER
3	D	297	ASP
3	D	423	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	427	LEU
2	E	59	LEU
2	E	132	THR
2	E	169	ARG
2	E	172	ASP
2	E	173	ASN
2	E	183	LEU
2	E	190	ASP
2	E	274	LYS
2	E	461	ASN
2	E	487	VAL
4	H	31	ASP
4	J	13	LYS
4	J	43	LYS
4	J	94	ARG
5	K	79	GLN
5	L	104	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	173	ASN
2	B	224	GLN
2	E	224	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
6	NAG	F	1	1,6	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	F	2	6	14,14,15	0.30	0	17,19,21	1.30	1 (5%)
6	BMA	F	3	6	11,11,12	0.49	0	15,15,17	0.81	0
6	MAN	F	4	6	11,11,12	0.57	0	15,15,17	0.95	2 (13%)
6	MAN	F	5	6	11,11,12	0.49	0	15,15,17	0.89	1 (6%)
6	MAN	F	6	6	11,11,12	0.61	0	15,15,17	0.94	2 (13%)
6	MAN	F	7	6	11,11,12	0.59	0	15,15,17	0.92	2 (13%)
7	NAG	G	1	2,7	14,14,15	0.33	0	17,19,21	0.66	1 (5%)
7	NAG	G	2	7	14,14,15	1.38	1 (7%)	17,19,21	1.45	2 (11%)
7	BMA	G	3	7	11,11,12	0.39	0	15,15,17	0.72	0
7	MAN	G	4	7	11,11,12	0.66	0	15,15,17	1.17	2 (13%)
7	MAN	G	5	7	11,11,12	0.67	0	15,15,17	0.93	1 (6%)
7	NAG	I	1	2,7	14,14,15	0.42	0	17,19,21	0.63	0
7	NAG	I	2	7	14,14,15	0.33	0	17,19,21	1.41	2 (11%)
7	BMA	I	3	7	11,11,12	0.77	1 (9%)	15,15,17	0.95	0
7	MAN	I	4	7	11,11,12	0.73	1 (9%)	15,15,17	1.09	2 (13%)
7	MAN	I	5	7	11,11,12	0.66	0	15,15,17	0.91	1 (6%)
7	NAG	M	1	1,7	14,14,15	0.47	0	17,19,21	0.61	0
7	NAG	M	2	7	14,14,15	0.23	0	17,19,21	0.64	0
7	BMA	M	3	7	11,11,12	0.55	0	15,15,17	0.70	0
7	MAN	M	4	7	11,11,12	0.61	0	15,15,17	0.91	1 (6%)
7	MAN	M	5	7	11,11,12	0.66	0	15,15,17	0.91	1 (6%)
8	NAG	N	1	3,8	14,14,15	0.45	0	17,19,21	0.75	1 (5%)
8	NAG	N	2	8	14,14,15	0.31	0	17,19,21	0.48	0
8	BMA	N	3	8	11,11,12	0.61	0	15,15,17	0.64	0
7	NAG	O	1	2,7	14,14,15	0.22	0	17,19,21	0.80	1 (5%)
7	NAG	O	2	7	14,14,15	0.16	0	17,19,21	0.69	0
7	BMA	O	3	7	11,11,12	0.43	0	15,15,17	0.95	1 (6%)
7	MAN	O	4	7	11,11,12	0.59	0	15,15,17	1.13	2 (13%)
7	MAN	O	5	7	11,11,12	0.97	0	15,15,17	1.66	3 (20%)
7	NAG	P	1	2,7	14,14,15	0.44	0	17,19,21	0.68	1 (5%)
7	NAG	P	2	7	14,14,15	0.20	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	P	3	7	11,11,12	0.78	0	15,15,17	1.14	2 (13%)
7	MAN	P	4	7	11,11,12	0.61	0	15,15,17	1.24	2 (13%)
7	MAN	P	5	7	11,11,12	0.63	0	15,15,17	1.02	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
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	4/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
6	MAN	F	4	6	-	2/2/19/22	0/1/1/1
6	MAN	F	5	6	-	2/2/19/22	0/1/1/1
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1
6	MAN	F	7	6	-	0/2/19/22	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	-	0/2/19/22	1/1/1/1
7	MAN	G	5	7	-	1/2/19/22	0/1/1/1
7	NAG	I	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	6/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	2/2/19/22	0/1/1/1
7	NAG	M	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
7	MAN	M	4	7	-	1/2/19/22	0/1/1/1
7	MAN	M	5	7	-	0/2/19/22	0/1/1/1
8	NAG	N	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	1/6/23/26	0/1/1/1
8	BMA	N	3	8	-	0/2/19/22	0/1/1/1
7	NAG	O	1	2,7	-	4/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	O	4	7	-	1/2/19/22	1/1/1/1
7	MAN	O	5	7	-	2/2/19/22	0/1/1/1
7	NAG	P	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	4/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	1/1/1/1
7	MAN	P	5	7	-	0/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	2	NAG	O5-C1	-4.68	1.35	1.43
7	I	3	BMA	C1-C2	2.17	1.57	1.52
7	I	4	MAN	C1-C2	2.08	1.57	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	5	MAN	C1-O5-C5	5.01	118.90	112.19
7	I	2	NAG	C2-N2-C7	4.51	128.94	122.90
6	F	2	NAG	C2-N2-C7	4.23	128.57	122.90
7	P	2	NAG	C2-N2-C7	4.22	128.56	122.90
7	P	4	MAN	C1-O5-C5	3.82	117.31	112.19
7	G	2	NAG	C2-N2-C7	3.73	127.89	122.90
7	G	4	MAN	C1-O5-C5	3.56	116.95	112.19
7	O	4	MAN	C1-O5-C5	3.54	116.93	112.19
7	P	5	MAN	C1-O5-C5	2.92	116.10	112.19
7	G	2	NAG	C4-C3-C2	2.90	115.27	111.02
7	P	3	BMA	O3-C3-C2	2.77	115.70	110.05
7	I	4	MAN	C1-O5-C5	2.60	115.66	112.19
7	P	3	BMA	C1-O5-C5	2.46	115.48	112.19
6	F	4	MAN	O2-C2-C3	-2.45	105.08	110.15
7	P	2	NAG	C1-C2-N2	2.38	114.18	110.43
6	F	6	MAN	O2-C2-C3	-2.35	105.28	110.15
7	O	1	NAG	C2-N2-C7	2.27	125.94	122.90
7	G	5	MAN	O2-C2-C3	-2.23	105.53	110.15
7	M	5	MAN	O2-C2-C3	-2.22	105.56	110.15
7	O	3	BMA	C1-O5-C5	2.20	115.14	112.19
6	F	4	MAN	C1-O5-C5	2.20	115.13	112.19
7	I	4	MAN	O2-C2-C3	-2.19	105.61	110.15
8	N	1	NAG	C2-N2-C7	2.18	125.82	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	5	MAN	C1-O5-C5	2.16	115.08	112.19
6	F	7	MAN	C1-O5-C5	2.15	115.06	112.19
6	F	7	MAN	O2-C2-C3	-2.14	105.72	110.15
7	P	4	MAN	O2-C2-C3	-2.14	105.72	110.15
7	G	4	MAN	O2-C2-C3	-2.13	105.75	110.15
7	I	5	MAN	O2-C2-C3	-2.12	105.75	110.15
7	M	4	MAN	O2-C2-C3	-2.12	105.76	110.15
7	P	1	NAG	C1-O5-C5	2.11	115.02	112.19
7	O	5	MAN	C3-C4-C5	2.10	114.03	110.23
7	O	5	MAN	O2-C2-C3	-2.08	105.84	110.15
7	I	2	NAG	C1-C2-N2	2.07	113.70	110.43
7	P	5	MAN	O2-C2-C3	-2.07	105.86	110.15
7	G	1	NAG	C2-N2-C7	2.07	125.67	122.90
7	O	4	MAN	O2-C2-C3	-2.06	105.88	110.15
6	F	6	MAN	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
7	O	1	NAG	C8-C7-N2-C2
7	O	1	NAG	O7-C7-N2-C2
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
8	N	1	NAG	C8-C7-N2-C2
8	N	1	NAG	O7-C7-N2-C2
7	O	2	NAG	O5-C5-C6-O6
7	I	5	MAN	O5-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
7	I	5	MAN	C4-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
6	F	4	MAN	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
7	M	1	NAG	C4-C5-C6-O6
7	M	4	MAN	O5-C5-C6-O6
7	G	5	MAN	O5-C5-C6-O6
7	O	4	MAN	O5-C5-C6-O6
6	F	1	NAG	C1-C2-N2-C7
7	M	1	NAG	C1-C2-N2-C7
7	M	2	NAG	C1-C2-N2-C7
7	P	2	NAG	C1-C2-N2-C7
6	F	1	NAG	C3-C2-N2-C7
6	F	2	NAG	C3-C2-N2-C7
7	G	2	NAG	C3-C2-N2-C7
7	I	2	NAG	C3-C2-N2-C7
7	M	2	NAG	C3-C2-N2-C7
8	N	2	NAG	C3-C2-N2-C7
7	I	2	NAG	C4-C5-C6-O6
6	F	2	NAG	C1-C2-N2-C7
7	G	2	NAG	C1-C2-N2-C7
7	I	2	NAG	C1-C2-N2-C7
7	M	1	NAG	C3-C2-N2-C7
7	P	2	NAG	C3-C2-N2-C7
7	I	2	NAG	O5-C5-C6-O6

All (4) ring outliers are listed below:

Continued on next page...

Continued from previous page...

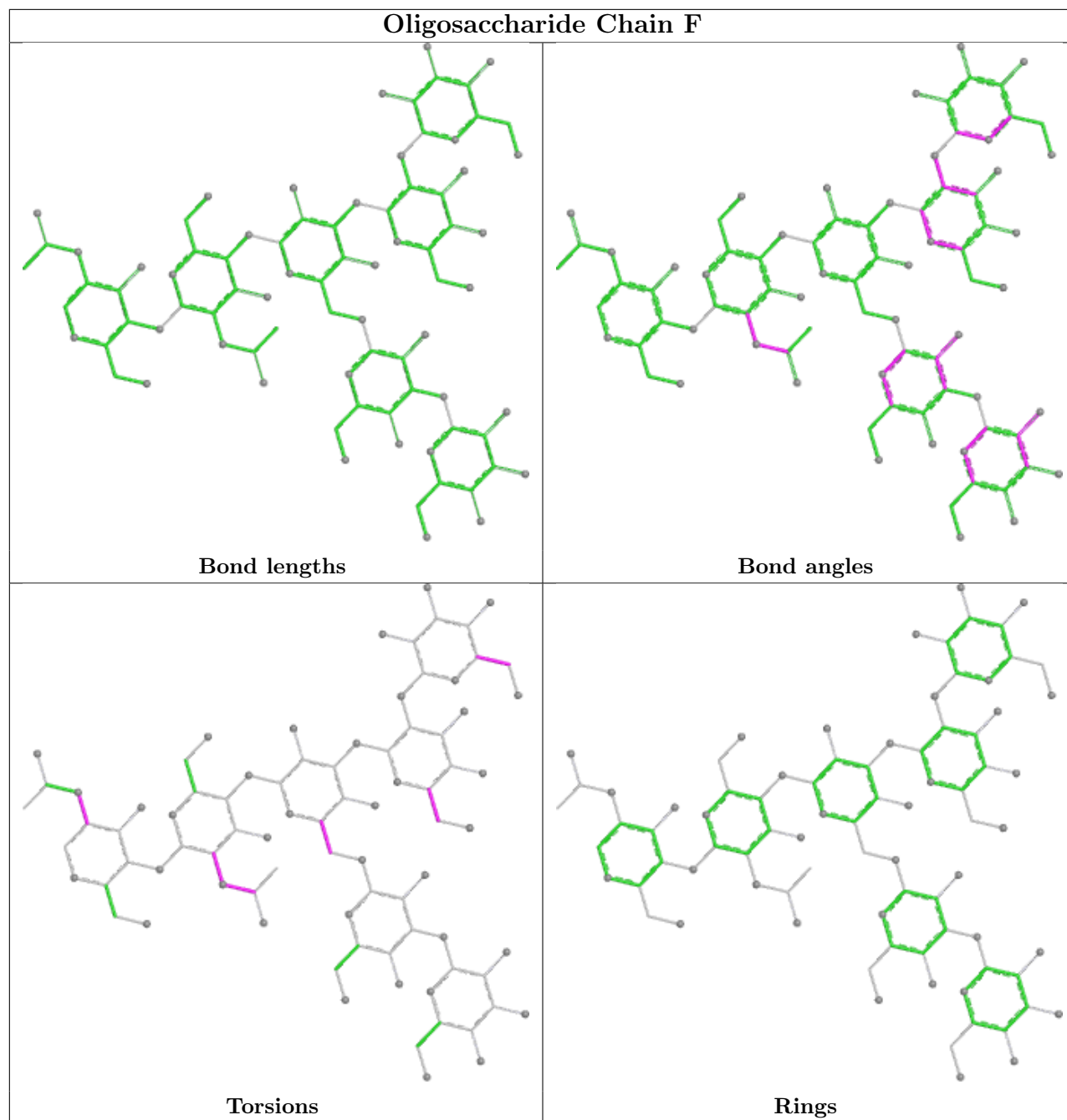
Mol	Chain	Res	Type	Atoms
-----	-------	-----	------	-------

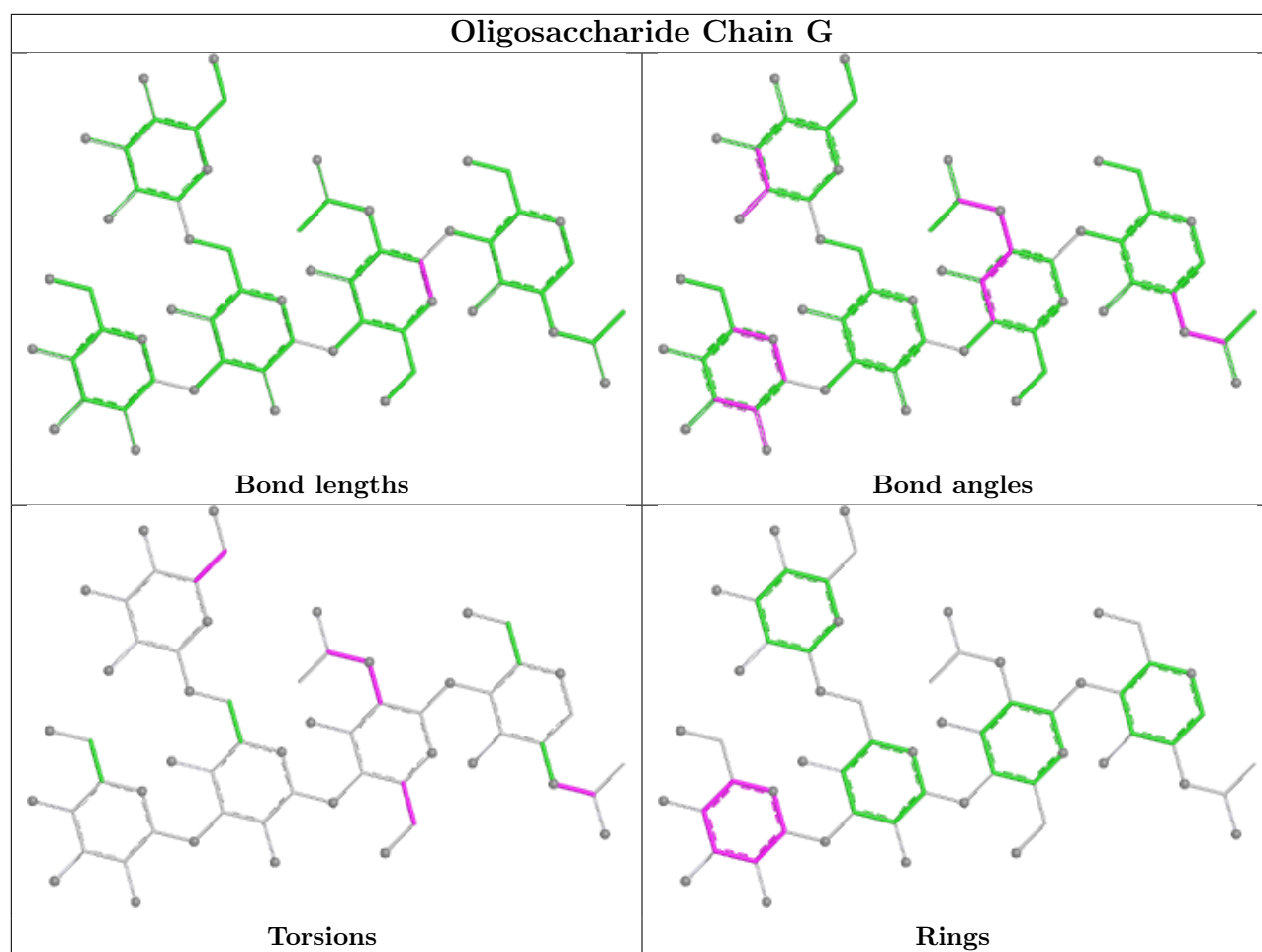
Mol	Chain	Res	Type	Atoms
7	P	5	MAN	C1-C2-C3-C4-C5-O5
7	O	4	MAN	C1-C2-C3-C4-C5-O5
7	G	4	MAN	C1-C2-C3-C4-C5-O5
7	P	4	MAN	C1-C2-C3-C4-C5-O5

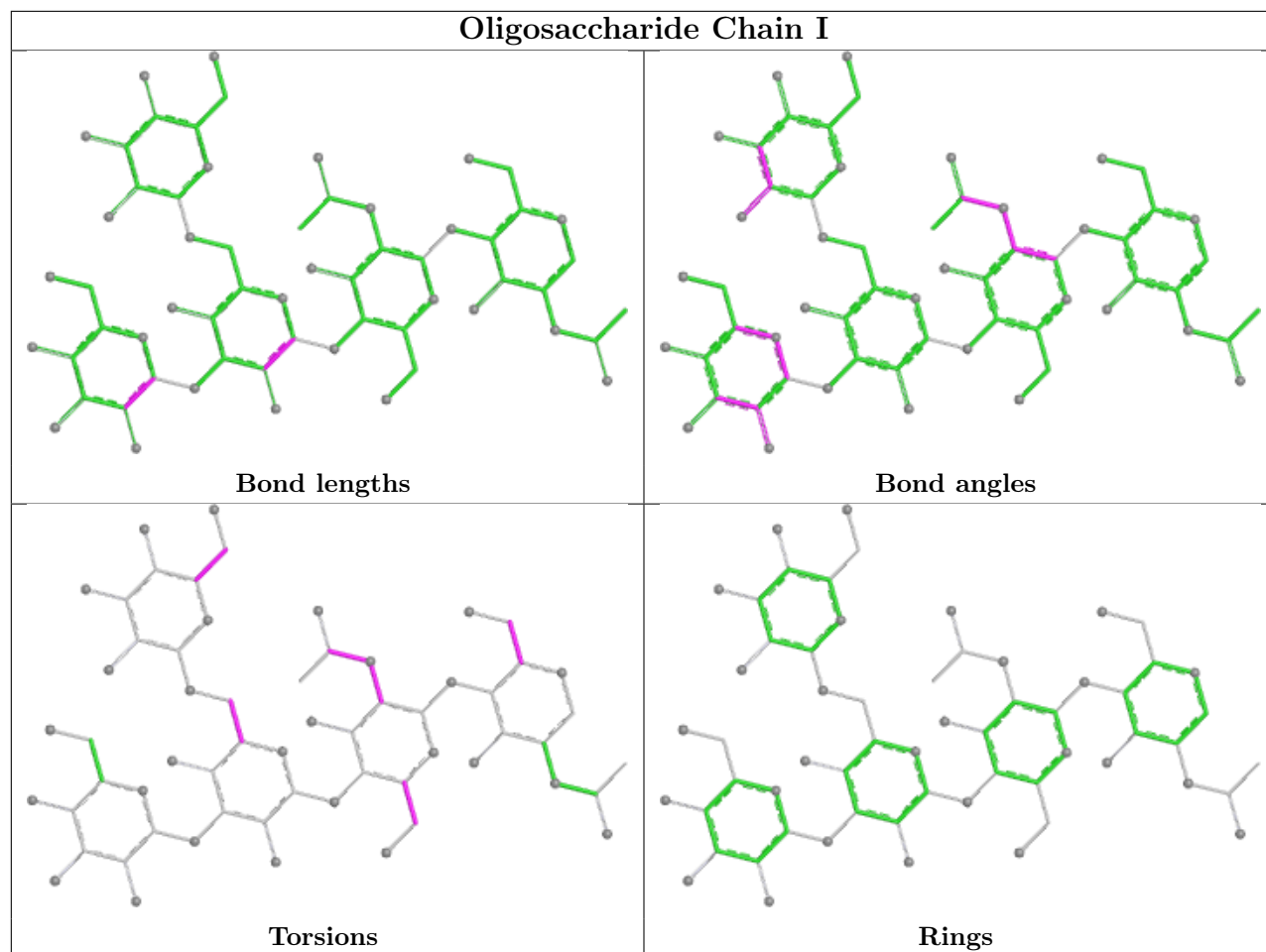
7 monomers are involved in 7 short contacts:

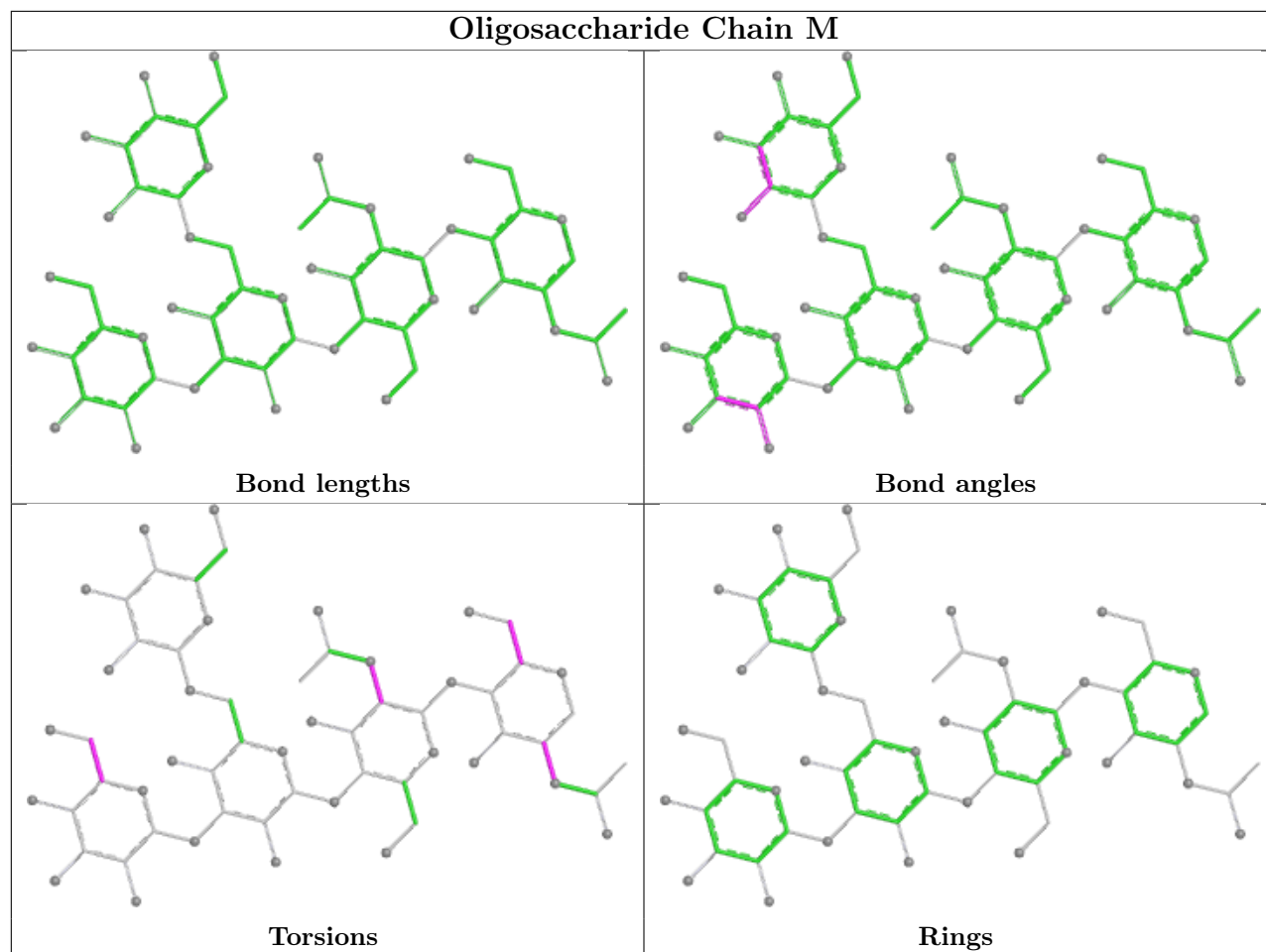
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	O	3	BMA	1	0
7	P	2	NAG	1	0
6	F	2	NAG	1	0
7	G	2	NAG	1	0
7	I	2	NAG	2	0
7	O	2	NAG	1	0
7	I	1	NAG	2	0

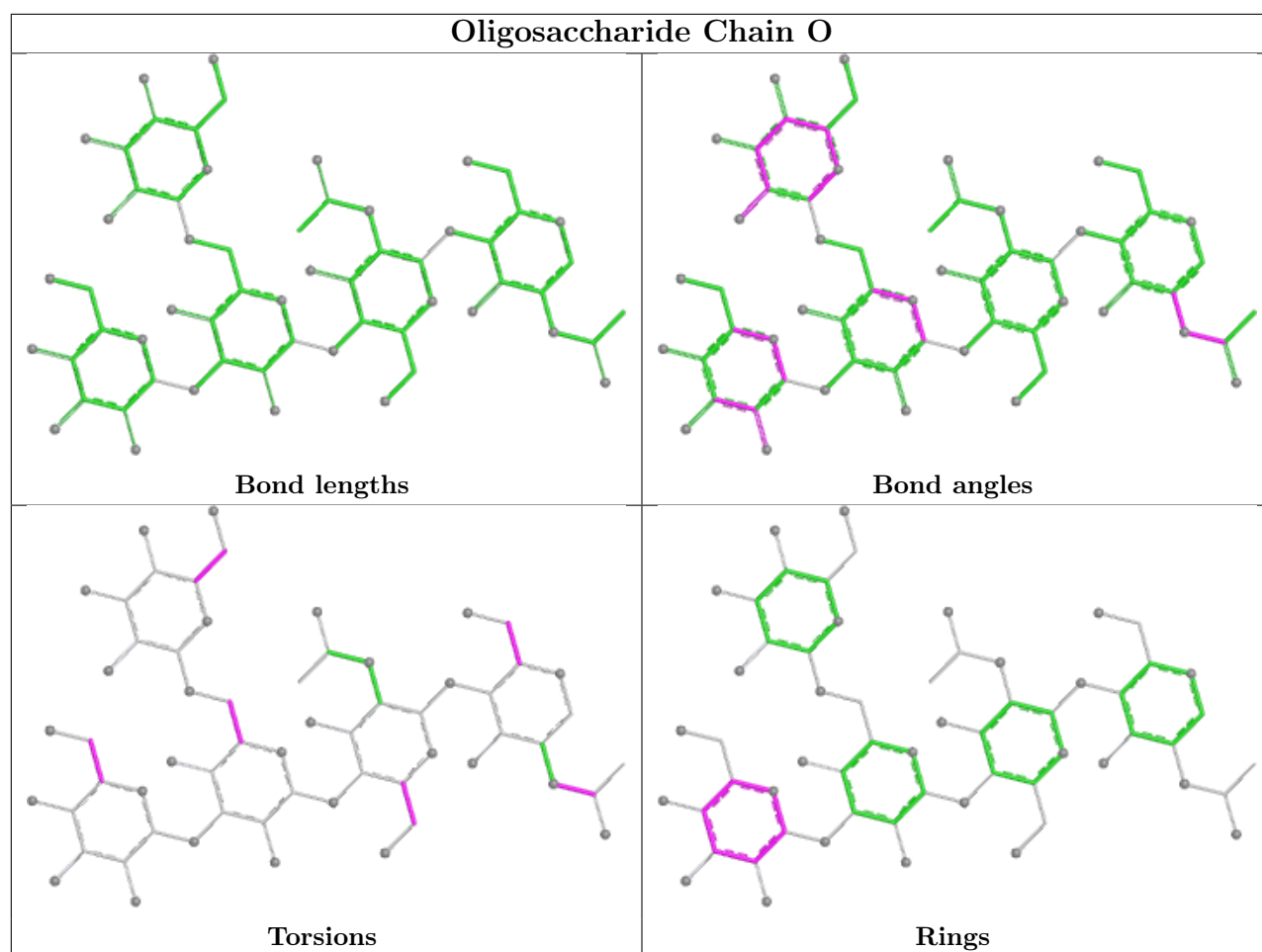
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

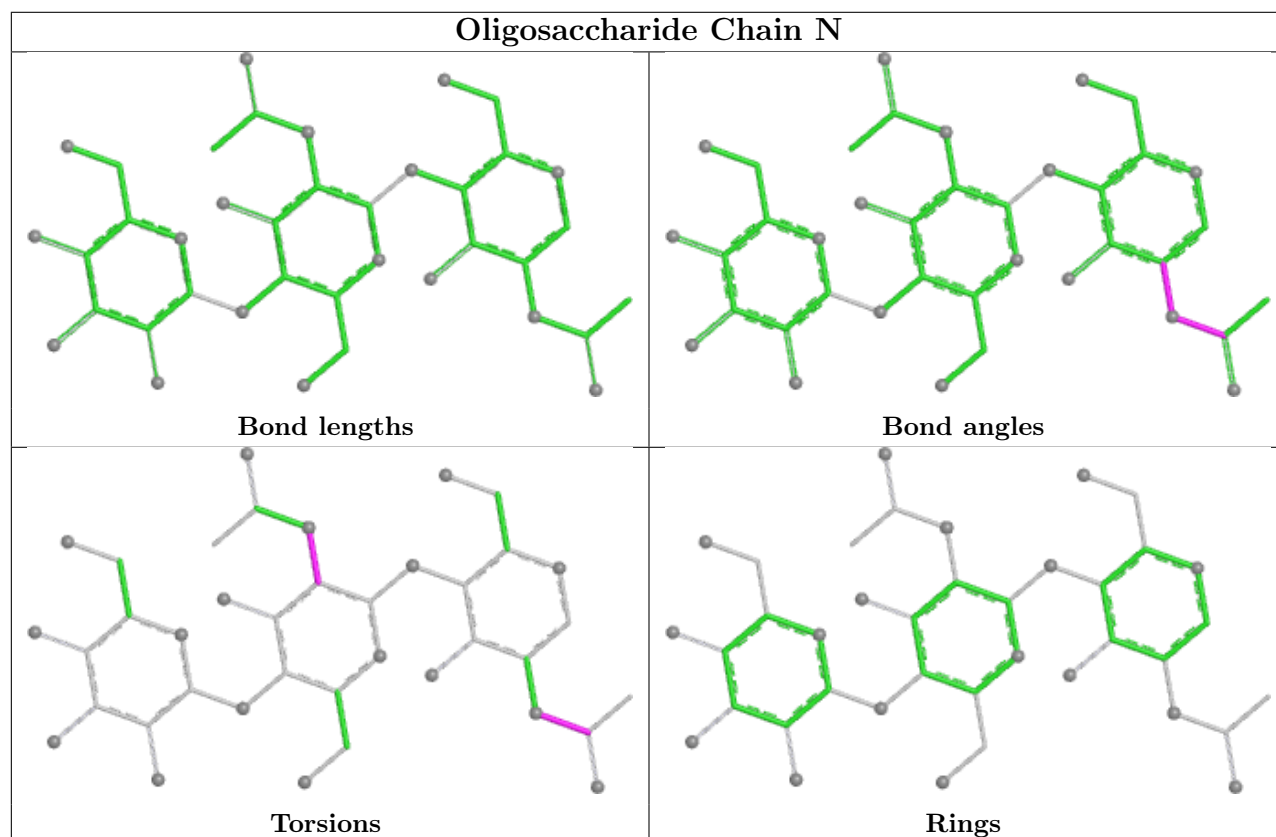
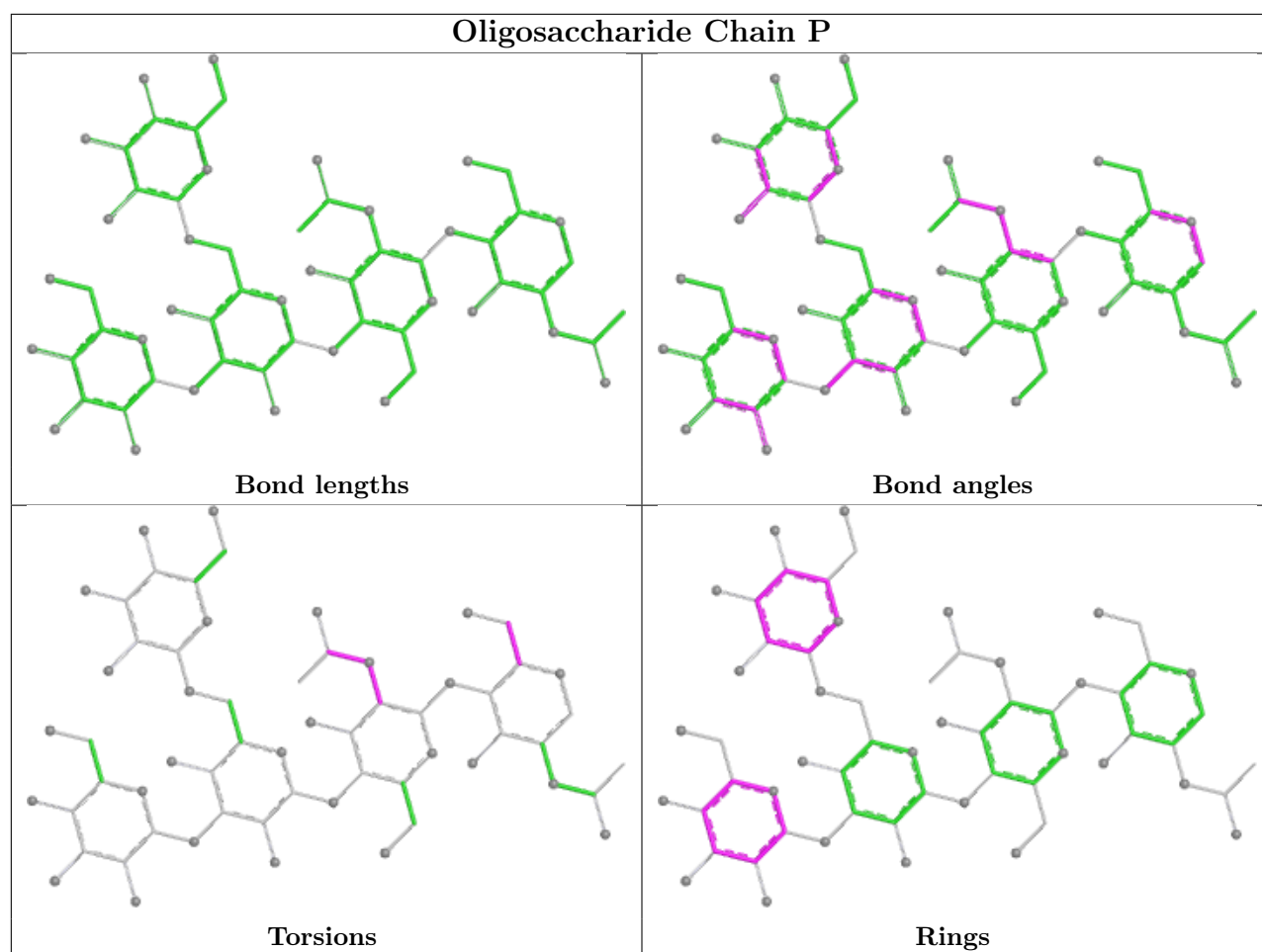












5.6 Ligand geometry ⓘ

46 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
12	POV	C	607	-	51,51,51	1.13	5 (9%)	57,59,59	1.02	3 (5%)
10	D12	A	602	-	11,11,11	0.26	0	10,10,10	0.13	0
11	OCT	E	506	-	7,7,7	0.25	0	6,6,6	0.18	0
11	OCT	E	508	-	7,7,7	0.24	0	6,6,6	0.18	0
10	D12	C	605	-	11,11,11	0.24	0	10,10,10	0.15	0
12	POV	E	511	-	51,51,51	1.12	5 (9%)	57,59,59	1.12	3 (5%)
14	Y4B	E	501	-	26,26,26	1.85	8 (30%)	42,42,42	2.19	12 (28%)
10	D12	A	603	-	11,11,11	0.26	0	10,10,10	0.12	0
11	OCT	D	508	-	7,7,7	0.26	0	6,6,6	0.14	0
10	D12	E	512	-	11,11,11	0.24	0	10,10,10	0.16	0
10	D12	B	504	-	11,11,11	0.24	0	10,10,10	0.20	0
10	D12	E	509	-	11,11,11	0.25	0	10,10,10	0.18	0
11	OCT	E	510	-	7,7,7	0.23	0	6,6,6	0.21	0
11	OCT	C	603	-	7,7,7	0.24	0	6,6,6	0.16	0
10	D12	E	503	-	11,11,11	0.24	0	10,10,10	0.19	0
11	OCT	A	607	-	7,7,7	0.25	0	6,6,6	0.17	0
11	OCT	C	602	-	7,7,7	0.24	0	6,6,6	0.18	0
12	POV	C	608	-	51,51,51	1.14	4 (7%)	57,59,59	0.96	3 (5%)
11	OCT	A	605	-	7,7,7	0.25	0	6,6,6	0.13	0
11	OCT	E	504	-	7,7,7	0.25	0	6,6,6	0.18	0
11	OCT	D	503	-	7,7,7	0.26	0	6,6,6	0.14	0
10	D12	B	505	-	11,11,11	0.24	0	10,10,10	0.17	0
11	OCT	E	507	-	7,7,7	0.24	0	6,6,6	0.20	0
14	Y4B	B	502	-	26,26,26	1.17	2 (7%)	42,42,42	2.03	14 (33%)
11	OCT	A	604	-	7,7,7	0.25	0	6,6,6	0.17	0
10	D12	B	503	-	11,11,11	0.24	0	10,10,10	0.19	0
10	D12	D	507	-	11,11,11	0.24	0	10,10,10	0.19	0
10	D12	D	506	-	11,11,11	0.25	0	10,10,10	0.15	0
12	POV	A	609	-	51,51,51	1.12	6 (11%)	57,59,59	1.02	3 (5%)
10	D12	C	606	-	11,11,11	0.28	0	10,10,10	0.15	0
10	D12	B	508	-	11,11,11	0.23	0	10,10,10	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	D12	B	506	-	11,11,11	0.23	0	10,10,10	0.29	0
11	OCT	D	505	-	7,7,7	0.24	0	6,6,6	0.14	0
13	ABU	E	502	-	6,6,6	0.85	0	6,6,6	1.44	1 (16%)
12	POV	A	608	-	51,51,51	1.13	4 (7%)	57,59,59	1.04	3 (5%)
10	D12	E	505	-	11,11,11	0.24	0	10,10,10	0.18	0
11	OCT	D	504	-	7,7,7	0.26	0	6,6,6	0.15	0
11	OCT	D	502	-	7,7,7	0.25	0	6,6,6	0.14	0
9	PIO	C	601	-	47,47,47	1.41	9 (19%)	62,65,65	1.22	7 (11%)
13	ABU	B	501	-	6,6,6	0.96	0	6,6,6	1.45	1 (16%)
15	NAG	D	501	3	14,14,15	0.26	0	17,19,21	0.71	1 (5%)
11	OCT	A	606	-	7,7,7	0.25	0	6,6,6	0.16	0
11	OCT	C	604	-	7,7,7	0.24	0	6,6,6	0.17	0
9	PIO	A	601	-	47,47,47	1.43	11 (23%)	62,65,65	1.26	9 (14%)
10	D12	B	507	-	11,11,11	0.24	0	10,10,10	0.18	0
10	D12	B	509	-	11,11,11	0.23	0	10,10,10	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	POV	C	607	-	-	27/55/55/55	-
10	D12	A	602	-	-	2/9/9/9	-
11	OCT	E	506	-	-	0/5/5/5	-
11	OCT	E	508	-	-	0/5/5/5	-
10	D12	C	605	-	-	1/9/9/9	-
12	POV	E	511	-	-	28/55/55/55	-
14	Y4B	E	501	-	-	0/4/62/62	0/4/4/4
10	D12	A	603	-	-	3/9/9/9	-
11	OCT	D	508	-	-	1/5/5/5	-
10	D12	E	512	-	-	2/9/9/9	-
10	D12	B	504	-	-	1/9/9/9	-
10	D12	E	509	-	-	2/9/9/9	-
11	OCT	E	510	-	-	1/5/5/5	-
11	OCT	C	603	-	-	0/5/5/5	-
10	D12	E	503	-	-	1/9/9/9	-
11	OCT	A	607	-	-	1/5/5/5	-
11	OCT	C	602	-	-	2/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	POV	C	608	-	-	26/55/55/55	-
11	OCT	A	605	-	-	3/5/5/5	-
11	OCT	E	504	-	-	1/5/5/5	-
11	OCT	D	503	-	-	2/5/5/5	-
10	D12	B	505	-	-	1/9/9/9	-
11	OCT	E	507	-	-	1/5/5/5	-
14	Y4B	B	502	-	-	0/4/62/62	0/4/4/4
11	OCT	A	604	-	-	1/5/5/5	-
10	D12	B	503	-	-	0/9/9/9	-
10	D12	D	507	-	-	1/9/9/9	-
10	D12	D	506	-	-	2/9/9/9	-
12	POV	A	609	-	-	29/55/55/55	-
10	D12	C	606	-	-	5/9/9/9	-
10	D12	B	508	-	-	1/9/9/9	-
10	D12	B	506	-	-	0/9/9/9	-
11	OCT	D	505	-	-	1/5/5/5	-
13	ABU	E	502	-	-	2/4/4/4	-
12	POV	A	608	-	-	26/55/55/55	-
10	D12	E	505	-	-	4/9/9/9	-
11	OCT	D	504	-	-	2/5/5/5	-
11	OCT	D	502	-	-	1/5/5/5	-
9	PIO	C	601	-	-	14/44/68/68	0/1/1/1
13	ABU	B	501	-	-	4/4/4/4	-
15	NAG	D	501	3	-	4/6/23/26	0/1/1/1
11	OCT	A	606	-	-	2/5/5/5	-
11	OCT	C	604	-	-	1/5/5/5	-
9	PIO	A	601	-	-	18/44/68/68	0/1/1/1
10	D12	B	507	-	-	1/9/9/9	-
10	D12	B	509	-	-	1/9/9/9	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	501	Y4B	C19-C07	-4.02	1.47	1.54
12	C	608	POV	C29-C210	3.78	1.53	1.31
12	E	511	POV	C29-C210	3.73	1.52	1.31
12	C	607	POV	C29-C210	3.73	1.52	1.31
12	A	608	POV	C29-C210	3.72	1.52	1.31
12	A	609	POV	C29-C210	3.69	1.52	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	E	501	Y4B	C09-C03	-3.52	1.48	1.53
9	A	601	PIO	P5-O5	3.30	1.65	1.59
9	A	601	PIO	P4-O4	3.24	1.65	1.59
9	C	601	PIO	P4-O4	3.22	1.65	1.59
14	E	501	Y4B	O01-C21	-3.17	1.34	1.43
14	E	501	Y4B	C17-C21	-3.12	1.46	1.52
9	C	601	PIO	P5-O5	3.10	1.65	1.59
14	E	501	Y4B	C14-C08	-2.92	1.46	1.53
9	C	601	PIO	O3C-C1B	2.65	1.41	1.33
12	C	608	POV	O21-C2	-2.63	1.40	1.46
12	A	608	POV	O31-C31	2.56	1.40	1.33
12	C	608	POV	O31-C31	2.54	1.40	1.33
9	A	601	PIO	O2C-C2C	-2.50	1.40	1.46
9	A	601	PIO	O3C-C1B	2.50	1.40	1.33
12	A	609	POV	O21-C21	2.50	1.41	1.34
12	C	607	POV	O21-C2	-2.49	1.40	1.46
9	C	601	PIO	O2C-C1A	2.45	1.41	1.34
12	A	608	POV	O21-C21	2.43	1.41	1.34
12	C	607	POV	O31-C31	2.41	1.40	1.33
12	E	511	POV	O21-C21	2.41	1.41	1.34
14	E	501	Y4B	C12-C22	-2.40	1.48	1.51
14	B	502	Y4B	C09-C03	-2.40	1.49	1.53
12	A	609	POV	O31-C31	2.37	1.40	1.33
12	E	511	POV	O31-C31	2.31	1.40	1.33
9	C	601	PIO	P5-O51	-2.31	1.46	1.54
9	A	601	PIO	O2C-C1A	2.30	1.40	1.34
12	C	607	POV	O21-C21	2.28	1.40	1.34
9	A	601	PIO	P5-O51	-2.28	1.46	1.54
9	A	601	PIO	P4-O41	-2.27	1.46	1.54
12	C	608	POV	O21-C21	2.27	1.40	1.34
9	C	601	PIO	P4-O43	-2.27	1.46	1.54
9	C	601	PIO	P4-O41	-2.27	1.46	1.54
9	A	601	PIO	P5-O52	-2.27	1.46	1.54
9	C	601	PIO	P5-O52	-2.26	1.46	1.54
9	A	601	PIO	P4-O43	-2.26	1.46	1.54
12	E	511	POV	O21-C2	-2.19	1.41	1.46
12	E	511	POV	O31-C3	-2.13	1.40	1.45
14	E	501	Y4B	C11-C04	-2.12	1.49	1.53
12	C	607	POV	O31-C3	-2.12	1.40	1.45
12	A	609	POV	O31-C3	-2.12	1.40	1.45
12	A	609	POV	O21-C2	-2.11	1.41	1.46
12	A	608	POV	O21-C2	-2.09	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	PIO	P1-O11	-2.08	1.45	1.55
9	A	601	PIO	O3C-C3C	-2.07	1.40	1.45
9	C	601	PIO	O2C-C2C	-2.04	1.41	1.46
14	E	501	Y4B	C17-C08	-2.04	1.50	1.53
14	B	502	Y4B	C10-C06	-2.02	1.50	1.54
12	A	609	POV	P-O13	-2.00	1.46	1.55

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	501	Y4B	C09-C03-C04	-6.02	103.38	111.78
14	B	502	Y4B	C09-C03-C04	-4.87	104.98	111.78
14	E	501	Y4B	C07-C03-C04	4.86	117.37	112.43
14	E	501	Y4B	O02-C22-C23	-4.84	112.63	121.17
14	E	501	Y4B	C23-C22-C12	4.54	125.50	117.65
12	E	511	POV	O21-C21-C22	4.34	120.87	111.48
12	C	607	POV	O21-C21-C22	4.24	120.65	111.48
14	B	502	Y4B	O02-C22-C23	-4.19	113.77	121.17
14	B	502	Y4B	C07-C03-C04	4.17	116.67	112.43
9	C	601	PIO	O2C-C1A-C2A	4.10	120.34	111.48
12	A	609	POV	O21-C21-C22	3.64	119.36	111.48
14	B	502	Y4B	C13-C05-C04	3.60	124.84	119.10
14	B	502	Y4B	C18-C06-C10	-3.51	105.43	110.61
14	E	501	Y4B	C13-C05-C04	3.50	124.69	119.10
12	A	608	POV	O21-C21-C22	3.39	118.83	111.48
9	A	601	PIO	O2C-C1A-C2A	3.38	118.79	111.48
14	B	502	Y4B	C23-C22-C12	3.29	123.33	117.65
14	E	501	Y4B	C13-C05-C06	-3.20	100.08	103.84
14	E	501	Y4B	C10-C06-C12	3.15	119.89	116.11
12	C	608	POV	O21-C21-C22	3.11	118.20	111.48
14	E	501	Y4B	O01-C21-C17	-3.08	103.72	109.84
14	E	501	Y4B	C18-C06-C10	-2.99	106.20	110.61
14	B	502	Y4B	C16-C12-C06	-2.91	101.61	104.21
12	A	608	POV	O31-C31-C32	2.87	120.60	111.83
14	E	501	Y4B	C19-C07-C15	-2.83	103.80	108.31
14	E	501	Y4B	C16-C12-C06	-2.83	101.68	104.21
9	A	601	PIO	O3C-C1B-C2B	2.72	120.11	111.83
12	C	608	POV	O31-C31-C32	2.70	120.08	111.83
12	C	607	POV	O31-C31-C32	2.66	119.94	111.83
13	B	501	ABU	OXT-C-CG	2.64	122.34	114.00
12	E	511	POV	O31-C31-C32	2.60	119.77	111.83
14	B	502	Y4B	C10-C06-C12	2.59	119.22	116.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	E	501	Y4B	C15-C07-C03	2.56	115.31	111.34
9	C	601	PIO	O11-P1-O12	-2.55	100.58	112.44
12	A	609	POV	O31-C31-C32	2.48	119.40	111.83
12	A	608	POV	O13-P-O14	-2.45	101.04	112.44
12	E	511	POV	O13-P-O14	-2.43	101.15	112.44
12	C	608	POV	O13-P-O14	-2.42	101.17	112.44
15	D	501	NAG	C2-N2-C7	2.40	126.12	122.90
14	B	502	Y4B	C14-C08-C07	-2.37	108.34	112.31
12	A	609	POV	O13-P-O14	-2.35	101.51	112.44
9	A	601	PIO	O11-P1-O12	-2.34	101.56	112.44
12	C	607	POV	O13-P-O14	-2.33	101.62	112.44
14	B	502	Y4B	C13-C05-C06	-2.31	101.13	103.84
14	B	502	Y4B	C09-C03-C07	2.29	116.49	113.91
9	A	601	PIO	C6-C1-C2	-2.24	107.75	110.86
9	C	601	PIO	O3C-C1B-C2B	2.24	118.67	111.83
9	A	601	PIO	O1-C1-C2	2.23	113.45	108.73
9	A	601	PIO	O41-P4-O4	2.22	114.49	105.85
9	A	601	PIO	O51-P5-O5	2.22	114.48	105.85
9	A	601	PIO	O52-P5-O5	2.17	114.32	105.85
9	C	601	PIO	O52-P5-O5	2.16	114.26	105.85
14	B	502	Y4B	C19-C07-C08	2.15	114.03	110.44
9	C	601	PIO	O41-P4-O4	2.13	114.14	105.85
9	A	601	PIO	O43-P4-O4	2.11	114.08	105.85
9	C	601	PIO	O51-P5-O5	2.11	114.06	105.85
14	B	502	Y4B	C20-C15-C07	2.08	116.25	112.74
14	B	502	Y4B	C15-C07-C03	2.06	114.54	111.34
9	C	601	PIO	O43-P4-O4	2.04	113.81	105.85
13	E	502	ABU	CB-CG-C	-2.03	109.22	114.51

There are no chirality outliers.

All (226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	PIO	C2-C1-O1-P1
9	A	601	PIO	C1C-O13-P1-O1
9	A	601	PIO	C1C-O13-P1-O12
9	A	601	PIO	O2C-C2C-C3C-O3C
9	C	601	PIO	C1C-O13-P1-O11
12	A	608	POV	C1-O11-P-O12
12	A	608	POV	C1-O11-P-O13
12	A	608	POV	C11-O12-P-O13
12	A	608	POV	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	A	609	POV	C1-O11-P-O12
12	A	609	POV	C1-O11-P-O13
12	A	609	POV	C1-O11-P-O14
12	A	609	POV	C11-O12-P-O13
12	A	609	POV	O12-C11-C12-N
12	C	607	POV	O12-C11-C12-N
12	C	608	POV	C11-O12-P-O13
12	C	608	POV	C11-O12-P-O14
12	C	608	POV	O12-C11-C12-N
12	E	511	POV	O12-C11-C12-N
12	E	511	POV	C22-C21-O21-C2
13	B	501	ABU	CD-CB-CG-C
12	E	511	POV	O32-C31-O31-C3
12	E	511	POV	O22-C21-O21-C2
12	E	511	POV	C32-C31-O31-C3
12	A	609	POV	O32-C31-O31-C3
15	D	501	NAG	O5-C5-C6-O6
12	A	609	POV	C32-C31-O31-C3
12	E	511	POV	C211-C210-C29-C28
9	C	601	PIO	C2A-C1A-O2C-C2C
15	D	501	NAG	C4-C5-C6-O6
9	C	601	PIO	O1A-C1A-O2C-C2C
15	D	501	NAG	C8-C7-N2-C2
15	D	501	NAG	O7-C7-N2-C2
9	C	601	PIO	C1B-C2B-C3B-C4B
12	A	609	POV	C31-C32-C33-C34
9	A	601	PIO	C1B-C2B-C3B-C4B
12	C	608	POV	C31-C32-C33-C34
12	A	608	POV	C32-C31-O31-C3
12	C	607	POV	C22-C21-O21-C2
12	C	607	POV	O22-C21-O21-C2
12	E	511	POV	C3-C2-O21-C21
10	C	606	D12	C11-C10-C9-C8
11	C	602	OCT	C2-C3-C4-C5
12	A	608	POV	C312-C313-C314-C315
12	A	609	POV	C212-C213-C214-C215
12	E	511	POV	C24-C25-C26-C27
12	A	608	POV	C33-C34-C35-C36
12	C	607	POV	C311-C310-C39-C38
12	A	608	POV	O32-C31-O31-C3
12	C	607	POV	C33-C34-C35-C36
12	C	608	POV	C311-C312-C313-C314

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	A	608	POV	C214-C215-C216-C217
12	A	609	POV	C22-C21-O21-C2
12	C	607	POV	C37-C38-C39-C310
12	C	607	POV	C311-C312-C313-C314
9	A	601	PIO	C2B-C1B-O3C-C3C
10	E	505	D12	C4-C5-C6-C7
12	C	608	POV	C39-C310-C311-C312
10	B	509	D12	C4-C5-C6-C7
11	C	602	OCT	C4-C5-C6-C7
9	C	601	PIO	C4B-C5B-C6B-C7B
9	A	601	PIO	C3B-C4B-C5B-C6B
12	A	609	POV	C39-C310-C311-C312
10	D	506	D12	C5-C6-C7-C8
12	A	609	POV	O22-C21-O21-C2
10	C	605	D12	C7-C8-C9-C10
12	A	609	POV	C214-C215-C216-C217
10	A	602	D12	C5-C6-C7-C8
10	E	512	D12	C7-C8-C9-C10
12	C	607	POV	C35-C36-C37-C38
12	C	607	POV	C212-C213-C214-C215
12	E	511	POV	C211-C212-C213-C214
12	C	608	POV	C22-C23-C24-C25
12	E	511	POV	C311-C312-C313-C314
12	C	608	POV	C312-C313-C314-C315
12	C	608	POV	C214-C215-C216-C217
10	B	507	D12	C3-C4-C5-C6
11	E	504	OCT	C4-C5-C6-C7
9	A	601	PIO	O1B-C1B-O3C-C3C
11	C	604	OCT	C2-C3-C4-C5
12	A	609	POV	C311-C310-C39-C38
10	B	504	D12	C11-C10-C9-C8
12	C	608	POV	C213-C214-C215-C216
12	A	608	POV	C26-C27-C28-C29
12	C	608	POV	C26-C27-C28-C29
12	E	511	POV	C23-C24-C25-C26
10	E	503	D12	C4-C5-C6-C7
12	A	608	POV	C39-C310-C311-C312
12	A	609	POV	C311-C312-C313-C314
12	E	511	POV	C35-C36-C37-C38
12	A	609	POV	C310-C311-C312-C313
12	C	607	POV	C39-C310-C311-C312
10	E	509	D12	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	E	511	POV	C312-C313-C314-C315
12	C	608	POV	C25-C26-C27-C28
12	C	607	POV	C210-C211-C212-C213
12	C	607	POV	O11-C1-C2-C3
12	C	607	POV	C22-C23-C24-C25
12	E	511	POV	C214-C215-C216-C217
11	D	504	OCT	C2-C3-C4-C5
9	A	601	PIO	C1C-C2C-C3C-O3C
12	C	607	POV	C1-C2-C3-O31
12	C	607	POV	C32-C31-O31-C3
12	E	511	POV	C37-C38-C39-C310
11	A	605	OCT	C2-C3-C4-C5
9	C	601	PIO	C4A-C5A-C6A-C7A
12	C	607	POV	C26-C27-C28-C29
12	C	608	POV	C210-C211-C212-C213
12	E	511	POV	C26-C27-C28-C29
10	A	602	D12	C6-C7-C8-C9
12	A	609	POV	C312-C313-C314-C315
12	A	609	POV	C25-C26-C27-C28
11	D	502	OCT	C3-C4-C5-C6
12	C	608	POV	C212-C213-C214-C215
11	A	607	OCT	C4-C5-C6-C7
11	A	604	OCT	C1-C2-C3-C4
10	C	606	D12	C4-C5-C6-C7
10	D	506	D12	C7-C8-C9-C10
12	E	511	POV	C39-C310-C311-C312
10	C	606	D12	C7-C8-C9-C10
12	A	608	POV	O11-C1-C2-C3
11	D	505	OCT	C5-C6-C7-C8
10	E	505	D12	C1-C2-C3-C4
12	C	607	POV	O32-C31-O31-C3
12	E	511	POV	C213-C214-C215-C216
9	A	601	PIO	C1A-C2A-C3A-C4A
12	A	609	POV	C22-C23-C24-C25
12	E	511	POV	C212-C213-C214-C215
12	C	607	POV	C313-C314-C315-C316
10	B	505	D12	C2-C3-C4-C5
11	D	504	OCT	C3-C4-C5-C6
10	C	606	D12	C5-C6-C7-C8
11	A	605	OCT	C4-C5-C6-C7
12	C	607	POV	C211-C212-C213-C214
12	C	607	POV	C215-C216-C217-C218

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	601	PIO	C3-C4-O4-P4
12	C	608	POV	C35-C36-C37-C38
12	E	511	POV	C313-C314-C315-C316
12	C	608	POV	C313-C314-C315-C316
12	A	609	POV	O11-C1-C2-O21
12	C	607	POV	O11-C1-C2-O21
12	C	608	POV	C12-C11-O12-P
12	C	607	POV	O21-C2-C3-O31
12	C	608	POV	C36-C37-C38-C39
9	C	601	PIO	C2B-C3B-C4B-C5B
9	C	601	PIO	C5A-C6A-C7A-C8A
12	A	608	POV	C36-C37-C38-C39
12	C	607	POV	C213-C214-C215-C216
12	C	607	POV	C25-C26-C27-C28
12	A	609	POV	C213-C214-C215-C216
11	D	503	OCT	C3-C4-C5-C6
10	A	603	D12	C3-C4-C5-C6
12	C	607	POV	C24-C25-C26-C27
9	C	601	PIO	C1C-O13-P1-O1
12	A	608	POV	C1-O11-P-O14
12	A	608	POV	C11-O12-P-O11
12	A	608	POV	C11-O12-P-O14
12	A	609	POV	C11-O12-P-O11
12	C	608	POV	C1-O11-P-O12
12	C	608	POV	C1-O11-P-O14
12	C	608	POV	C11-O12-P-O11
10	E	505	D12	C5-C6-C7-C8
12	C	608	POV	C34-C35-C36-C37
9	C	601	PIO	C1C-C2C-O2C-C1A
12	A	609	POV	O11-C1-C2-C3
9	A	601	PIO	O13-C1C-C2C-O2C
12	C	607	POV	C214-C215-C216-C217
11	E	510	OCT	C4-C5-C6-C7
13	B	501	ABU	CG-CB-CD-N
12	A	608	POV	C212-C213-C214-C215
10	E	512	D12	C5-C6-C7-C8
9	A	601	PIO	C5B-C6B-C7B-C8B
12	A	608	POV	C25-C26-C27-C28
11	A	606	OCT	C1-C2-C3-C4
12	E	511	POV	C22-C23-C24-C25
12	E	511	POV	C2-C1-O11-P
11	D	508	OCT	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	603	D12	C5-C6-C7-C8
12	A	609	POV	C1-C2-O21-C21
9	A	601	PIO	C5A-C6A-C7A-C8A
10	E	509	D12	C6-C7-C8-C9
9	A	601	PIO	C4B-C5B-C6B-C7B
9	A	601	PIO	C5-C4-O4-P4
11	A	605	OCT	C3-C4-C5-C6
9	A	601	PIO	C4-O4-P4-O42
10	A	603	D12	C4-C5-C6-C7
12	A	608	POV	C211-C212-C213-C214
13	B	501	ABU	OXT-C-CG-CB
9	A	601	PIO	O13-C1C-C2C-C3C
10	C	606	D12	C9-C10-C11-C12
11	D	503	OCT	C1-C2-C3-C4
12	C	608	POV	C37-C38-C39-C310
12	A	609	POV	C24-C25-C26-C27
12	E	511	POV	C215-C216-C217-C218
12	A	608	POV	C1-C2-O21-C21
13	B	501	ABU	O-C-CG-CB
12	C	608	POV	C29-C210-C211-C212
12	E	511	POV	C310-C311-C312-C313
12	A	608	POV	O31-C31-C32-C33
13	E	502	ABU	O-C-CG-CB
13	E	502	ABU	OXT-C-CG-CB
12	C	608	POV	C211-C212-C213-C214
9	C	601	PIO	C1-O1-P1-O11
12	E	511	POV	O31-C31-C32-C33
10	D	507	D12	C11-C10-C9-C8
12	A	609	POV	O31-C31-C32-C33
12	C	607	POV	C310-C311-C312-C313
9	C	601	PIO	C3B-C4B-C5B-C6B
12	A	608	POV	C3-C2-O21-C21
12	E	511	POV	C33-C34-C35-C36
12	A	608	POV	C311-C312-C313-C314
12	E	511	POV	C25-C26-C27-C28
12	A	609	POV	O32-C31-C32-C33
12	E	511	POV	O32-C31-C32-C33
12	A	609	POV	C210-C211-C212-C213
12	A	609	POV	C215-C216-C217-C218
12	A	608	POV	O32-C31-C32-C33
12	A	608	POV	C27-C28-C29-C210
12	A	608	POV	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

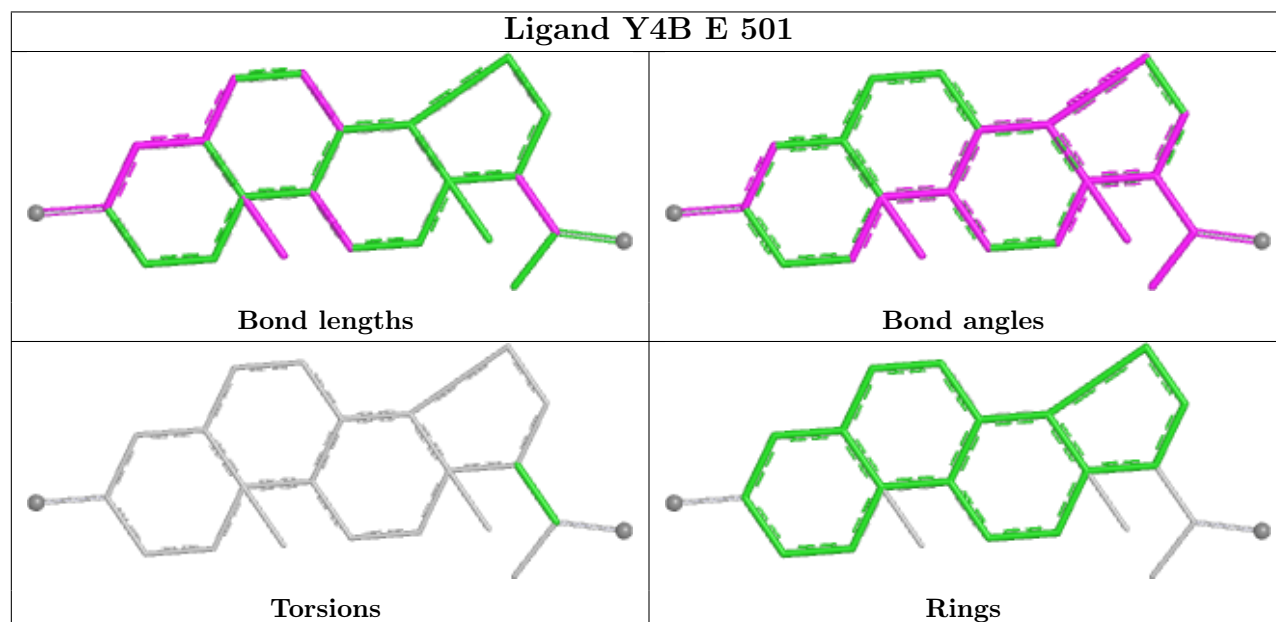
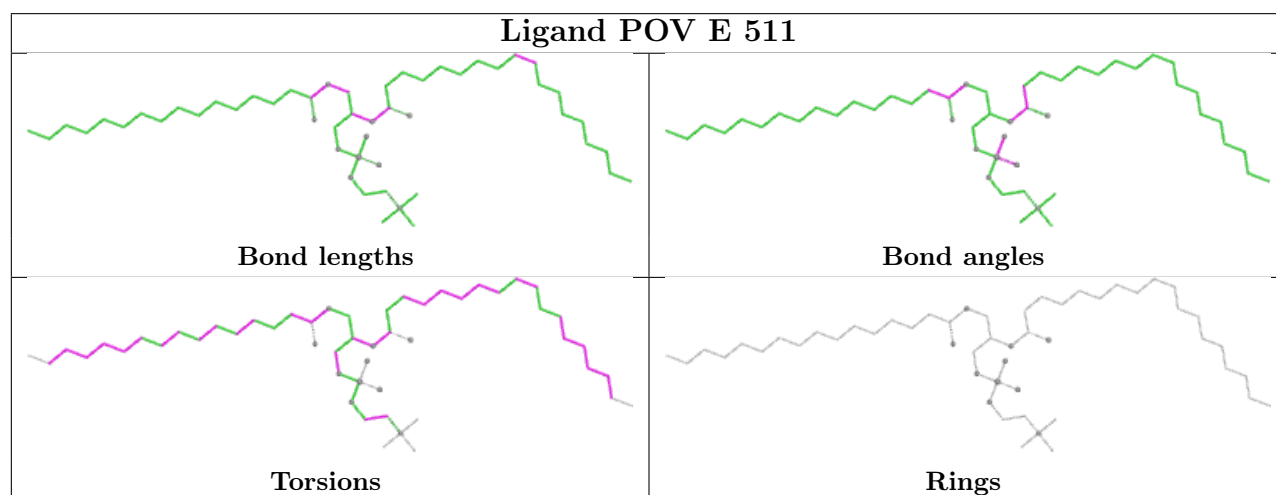
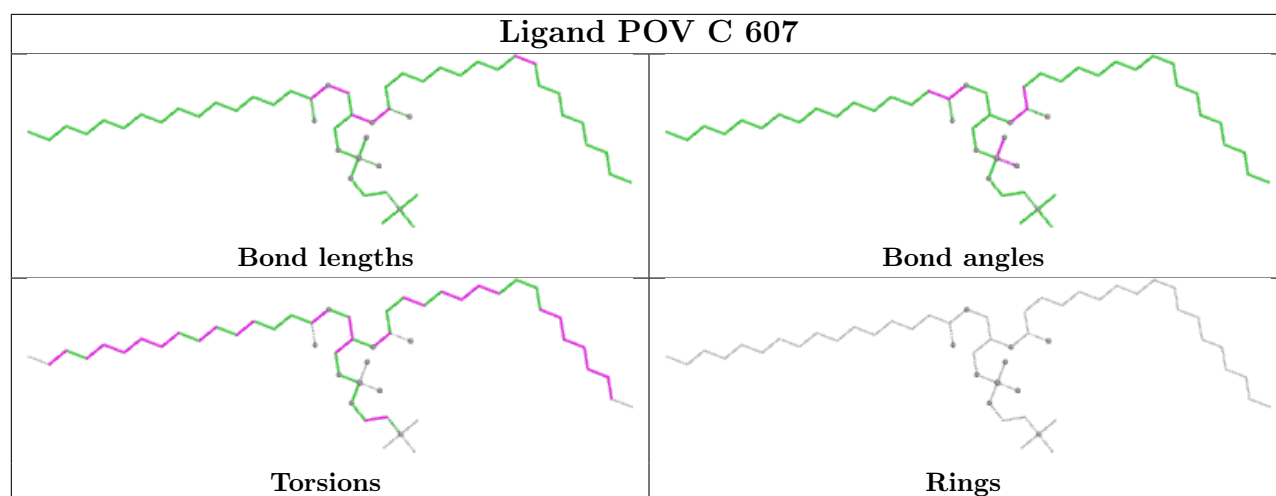
Mol	Chain	Res	Type	Atoms
12	C	608	POV	C32-C33-C34-C35
9	C	601	PIO	C2A-C3A-C4A-C5A
11	E	507	OCT	C3-C4-C5-C6
11	A	606	OCT	C4-C5-C6-C7
9	C	601	PIO	O2C-C1A-C2A-C3A
10	B	508	D12	C6-C7-C8-C9
10	E	505	D12	C7-C8-C9-C10

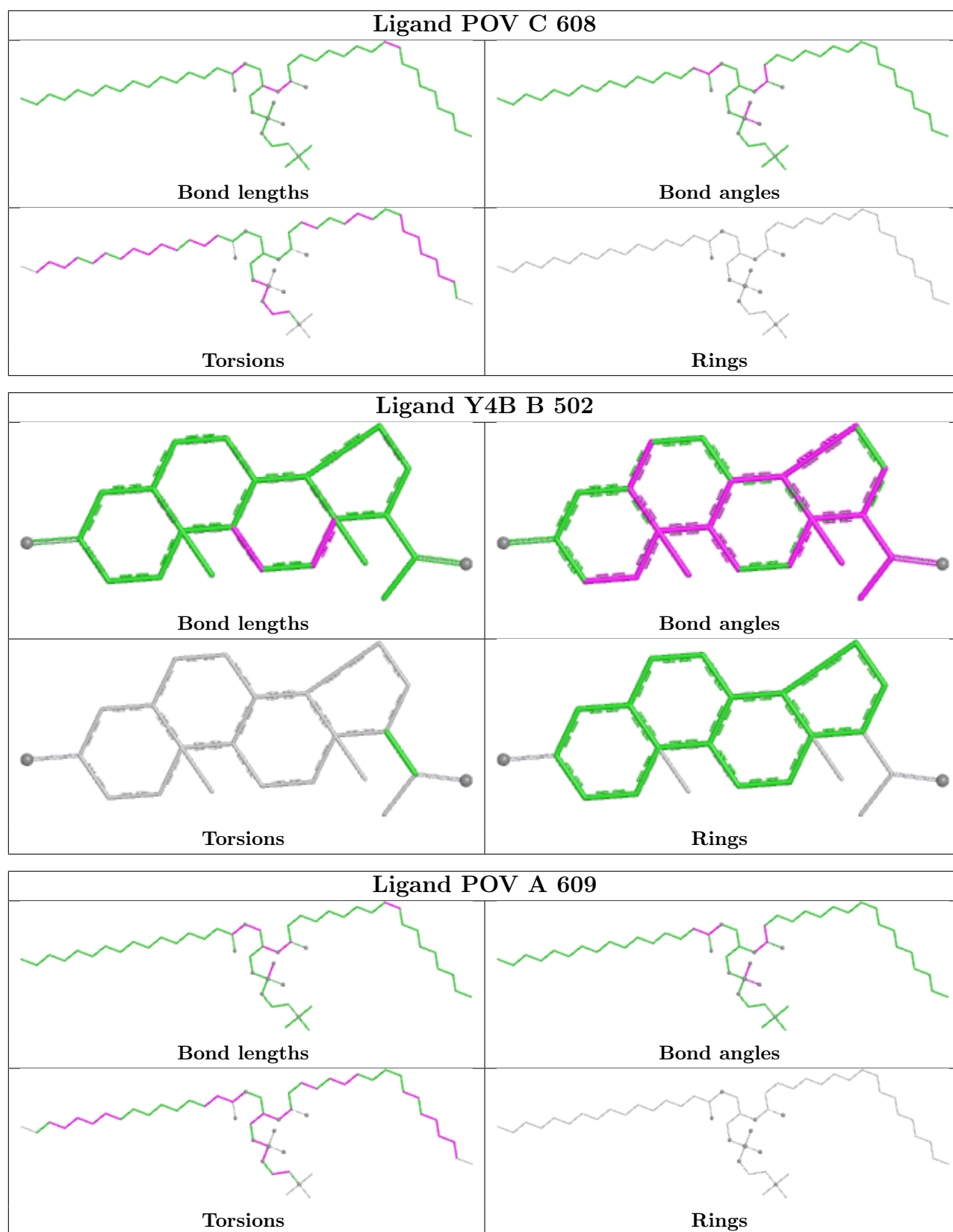
There are no ring outliers.

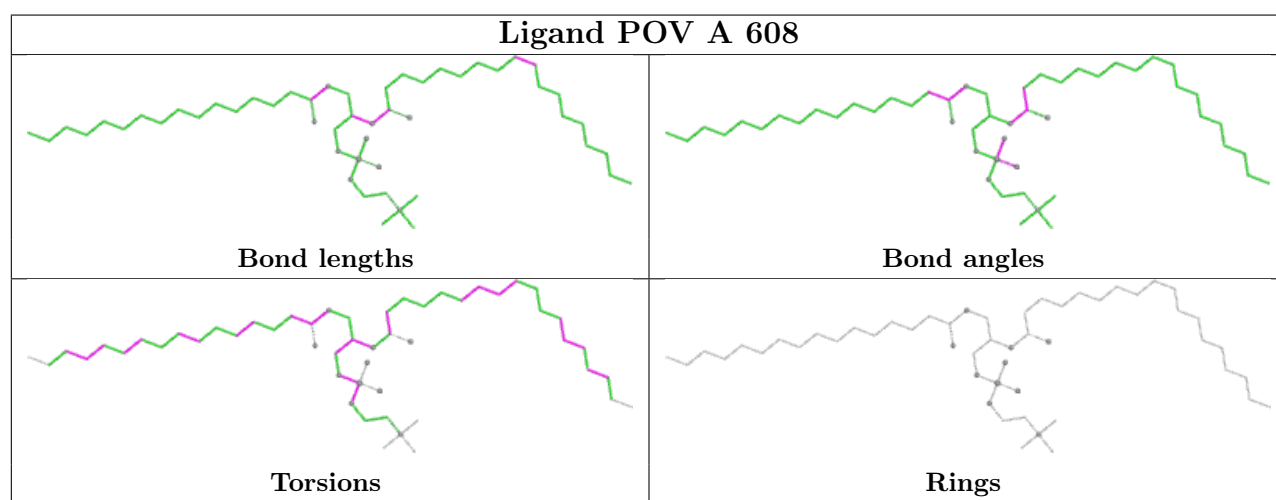
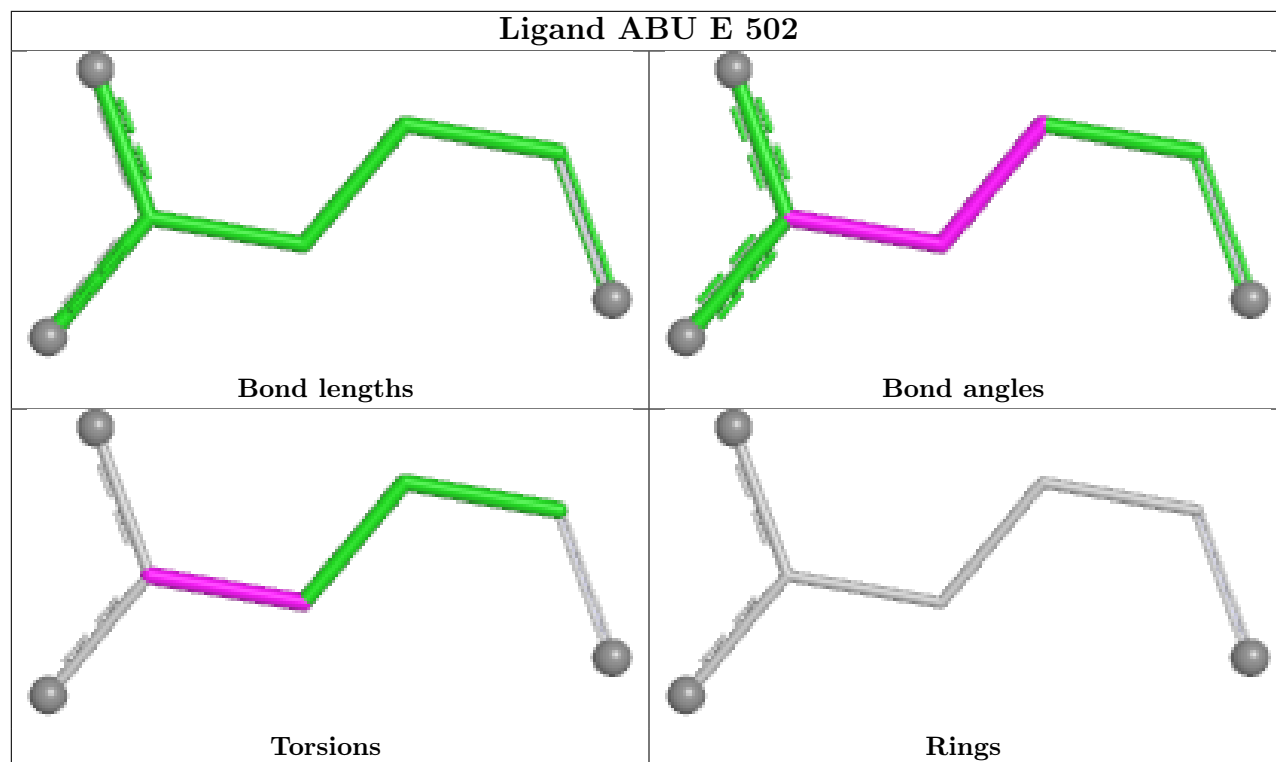
7 monomers are involved in 8 short contacts:

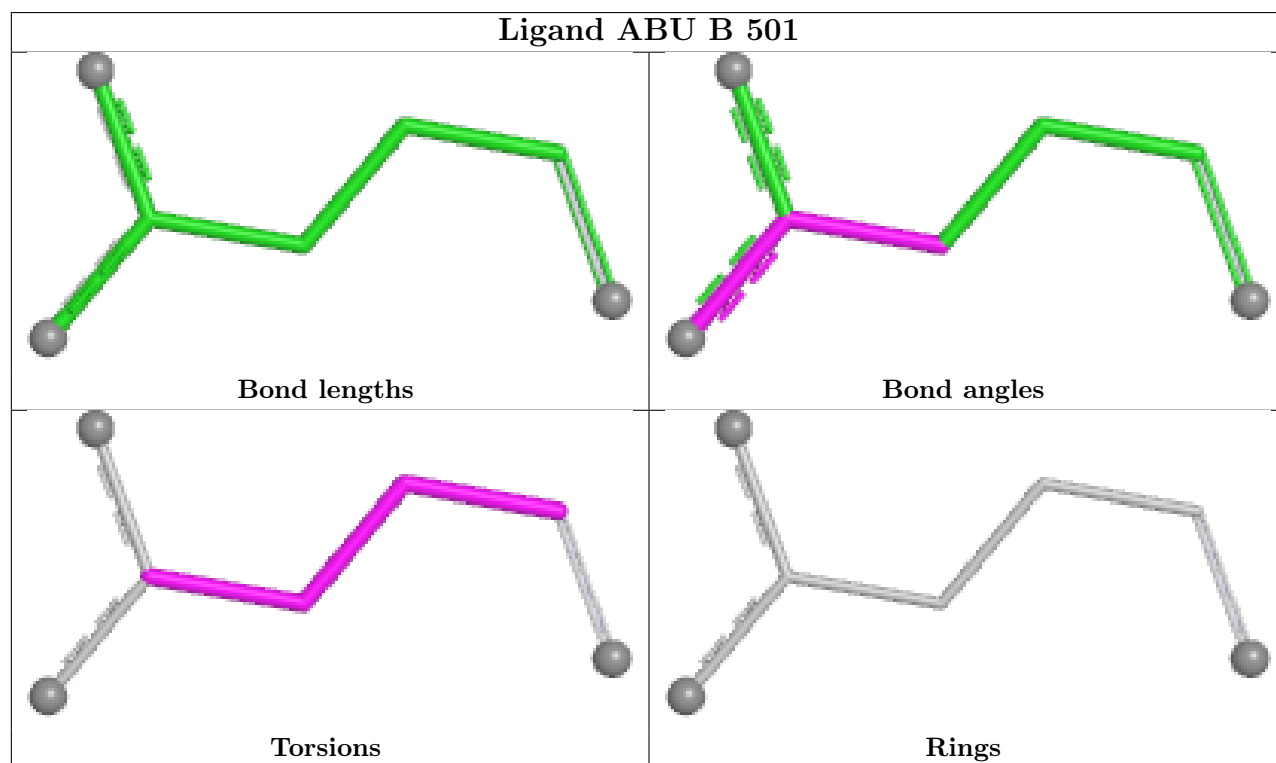
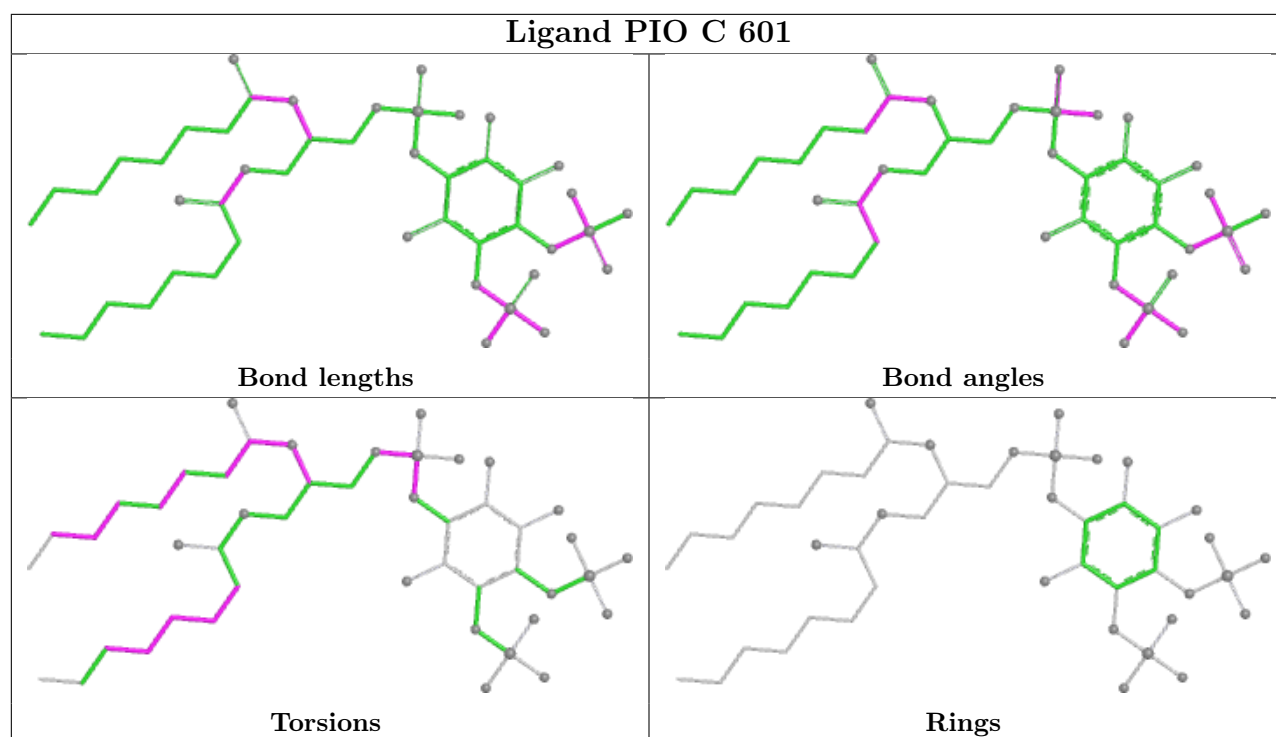
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	607	POV	2	0
12	C	608	POV	1	0
12	A	609	POV	1	0
10	B	508	D12	1	0
9	C	601	PIO	2	0
13	B	501	ABU	1	0
9	A	601	PIO	1	0

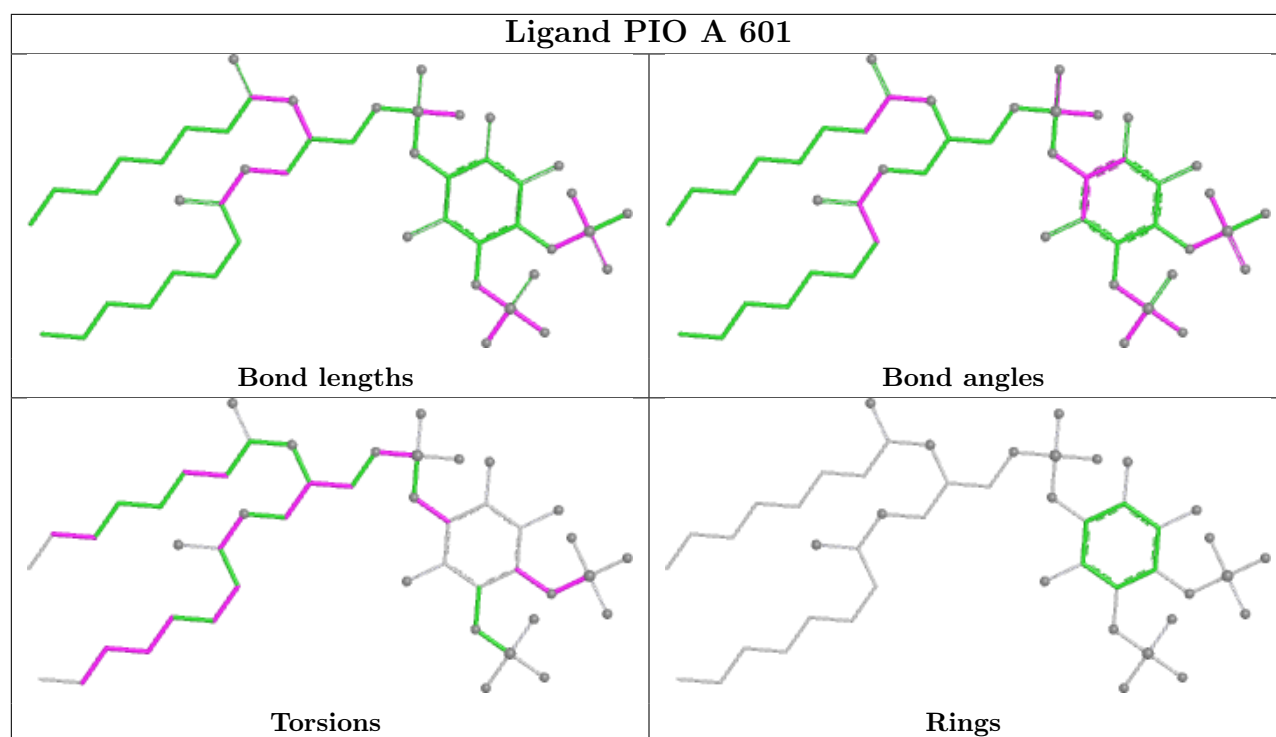
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

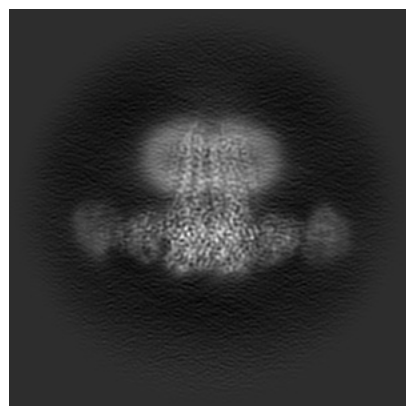
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29350. These allow visual inspection of the internal detail of the map and identification of artifacts.

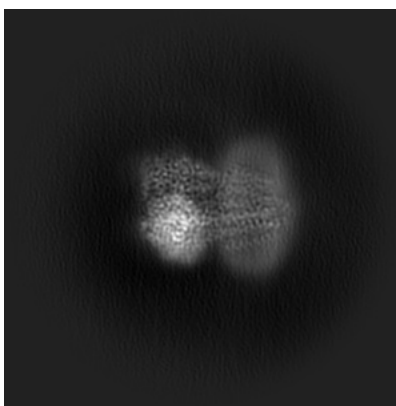
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

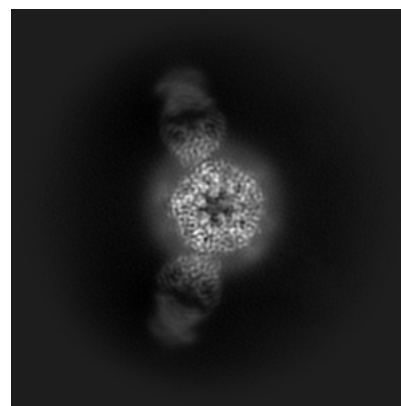
6.1.1 Primary map



X

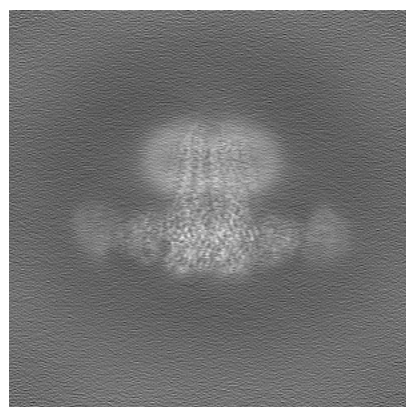


Y

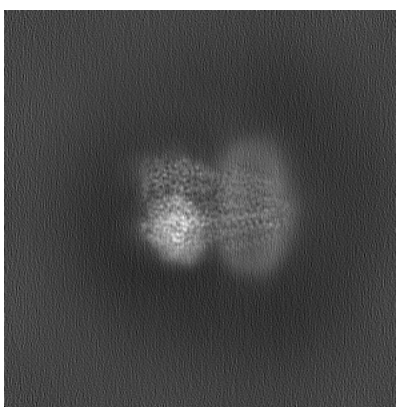


Z

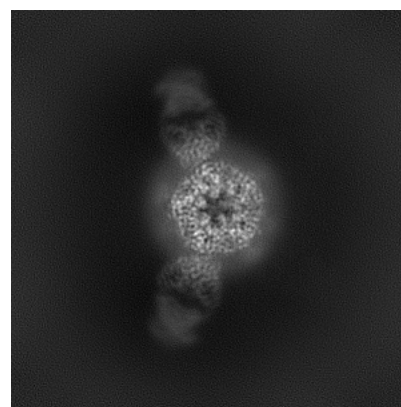
6.1.2 Raw map



X



Y

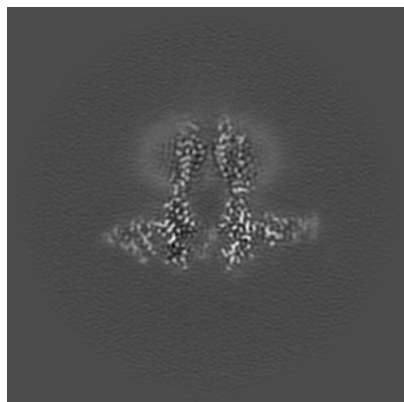


Z

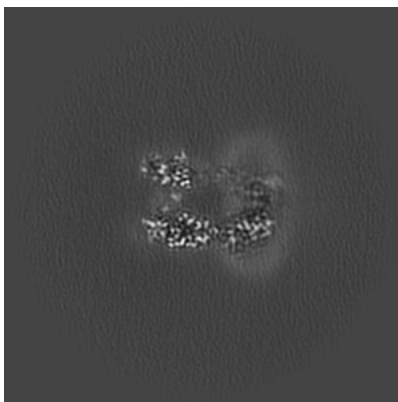
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

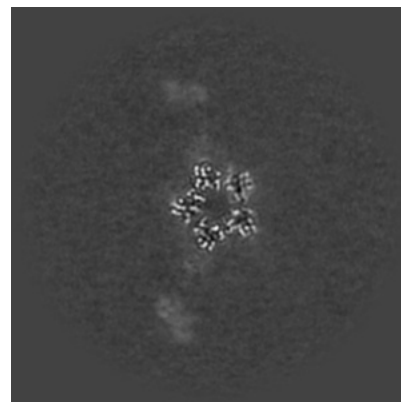
6.2.1 Primary map



X Index: 180

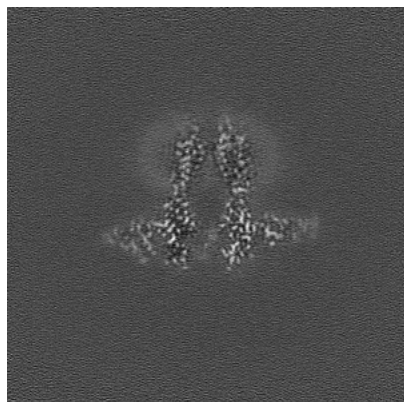


Y Index: 180

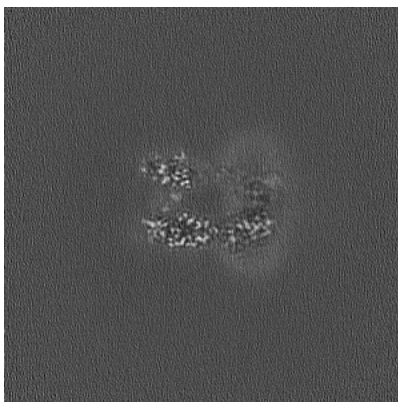


Z Index: 180

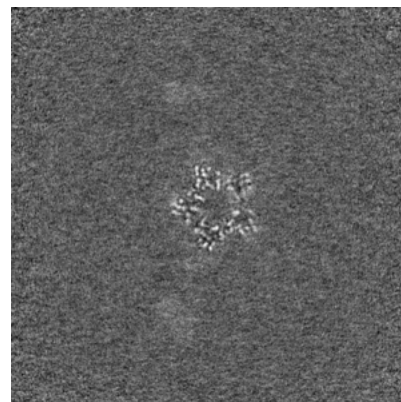
6.2.2 Raw map



X Index: 180



Y Index: 180

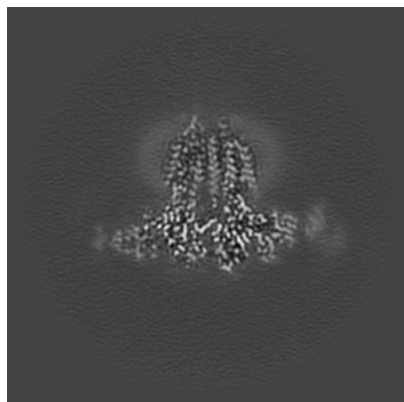


Z Index: 180

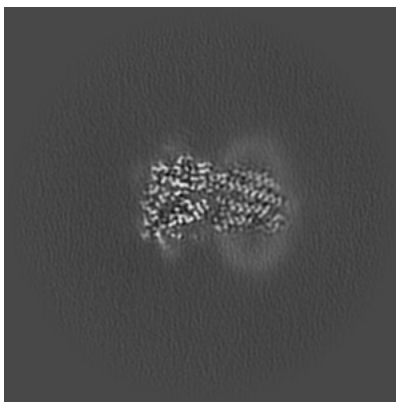
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

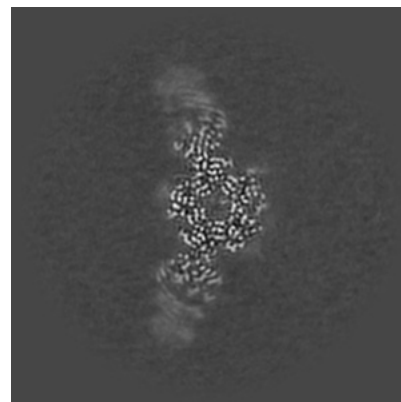
6.3.1 Primary map



X Index: 172

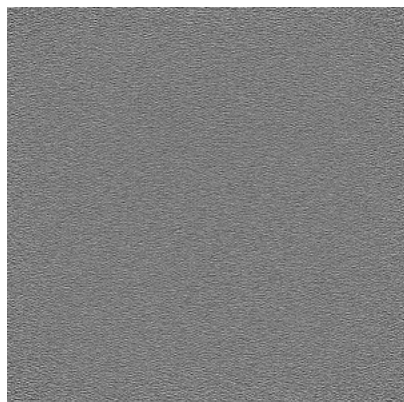


Y Index: 161

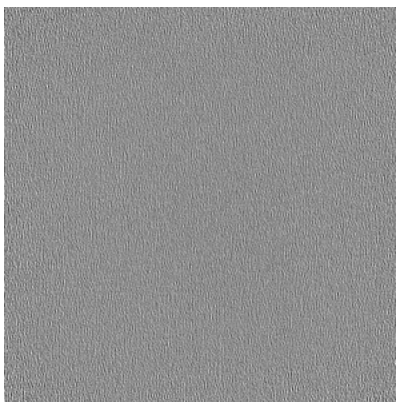


Z Index: 160

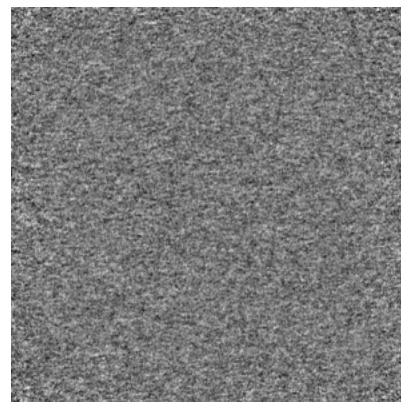
6.3.2 Raw map



X Index: 0



Y Index: 0

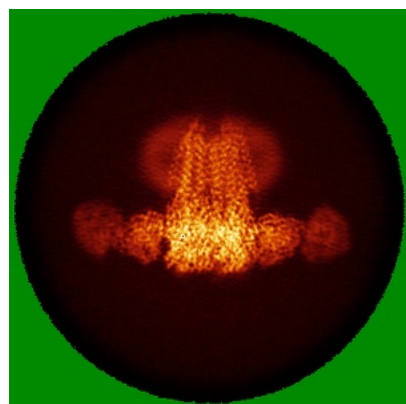


Z Index: 0

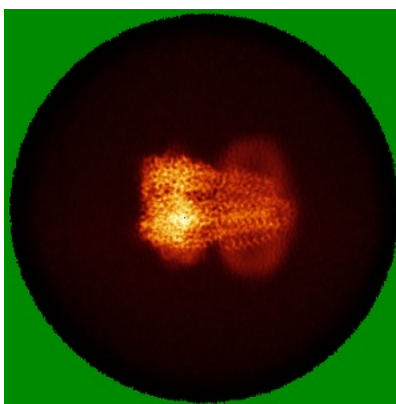
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

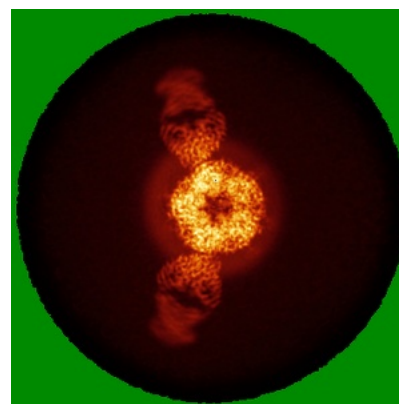
6.4.1 Primary map



X

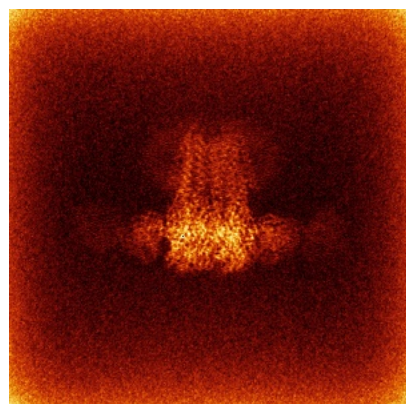


Y

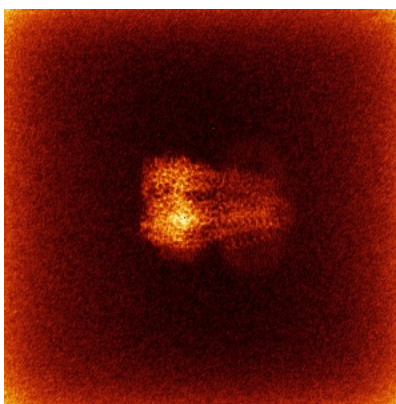


Z

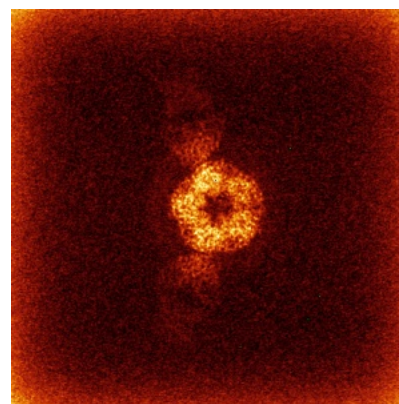
6.4.2 Raw map



X



Y

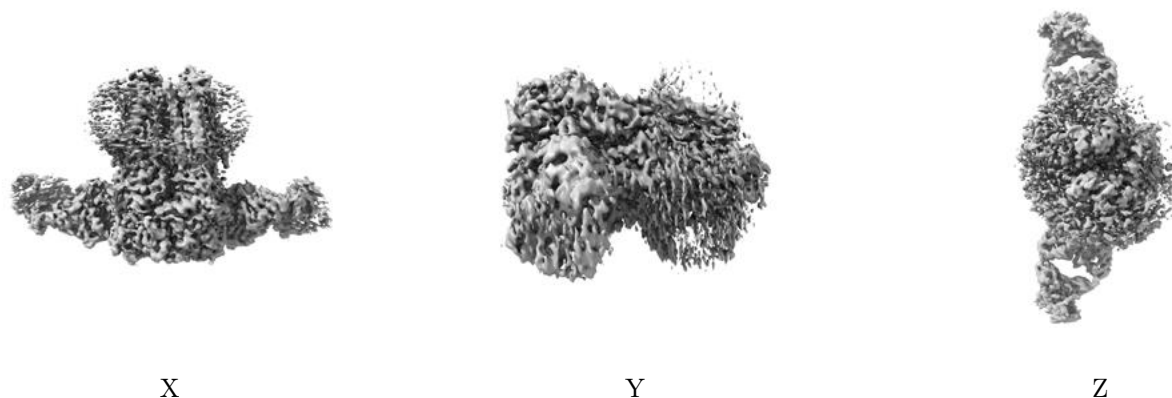


Z

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.

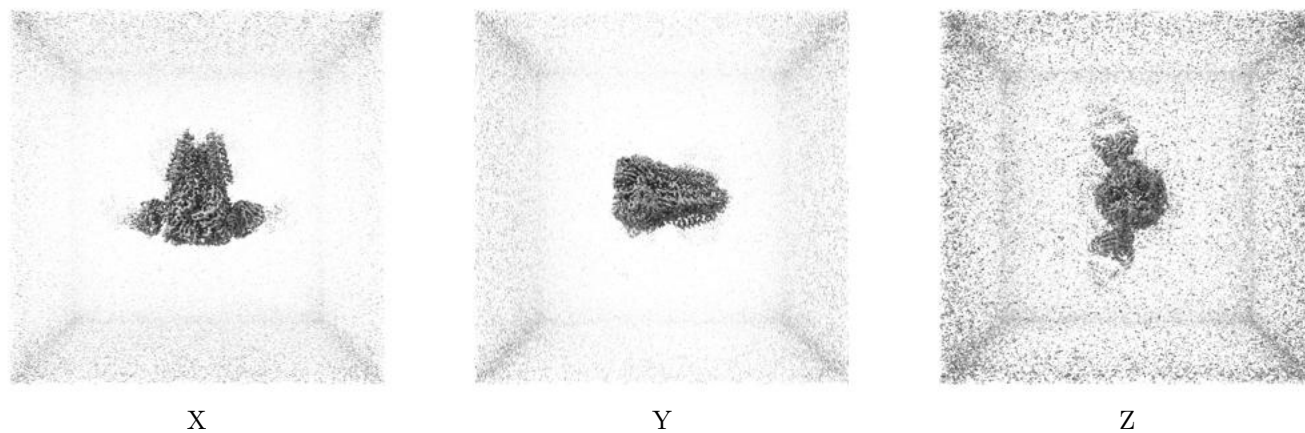
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

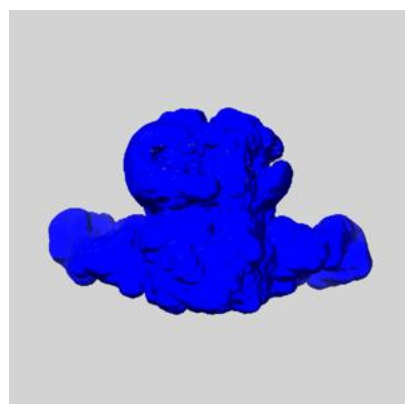
6.6 Mask visualisation [i](#)

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

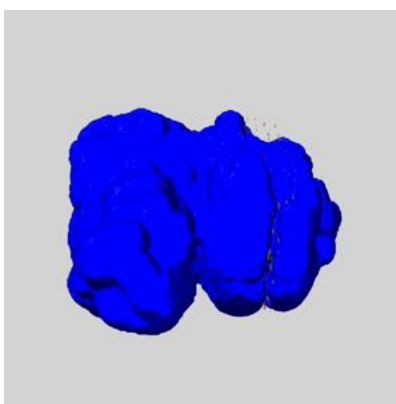
A mask typically either:

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

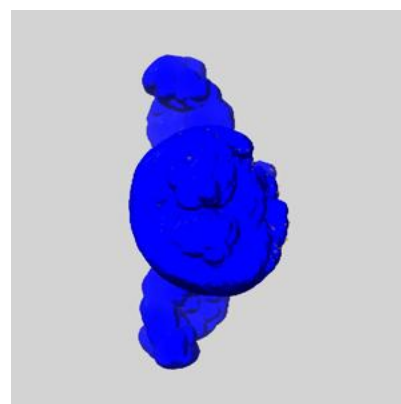
6.6.1 emd_29350_msk_1.map [i](#)



X



Y

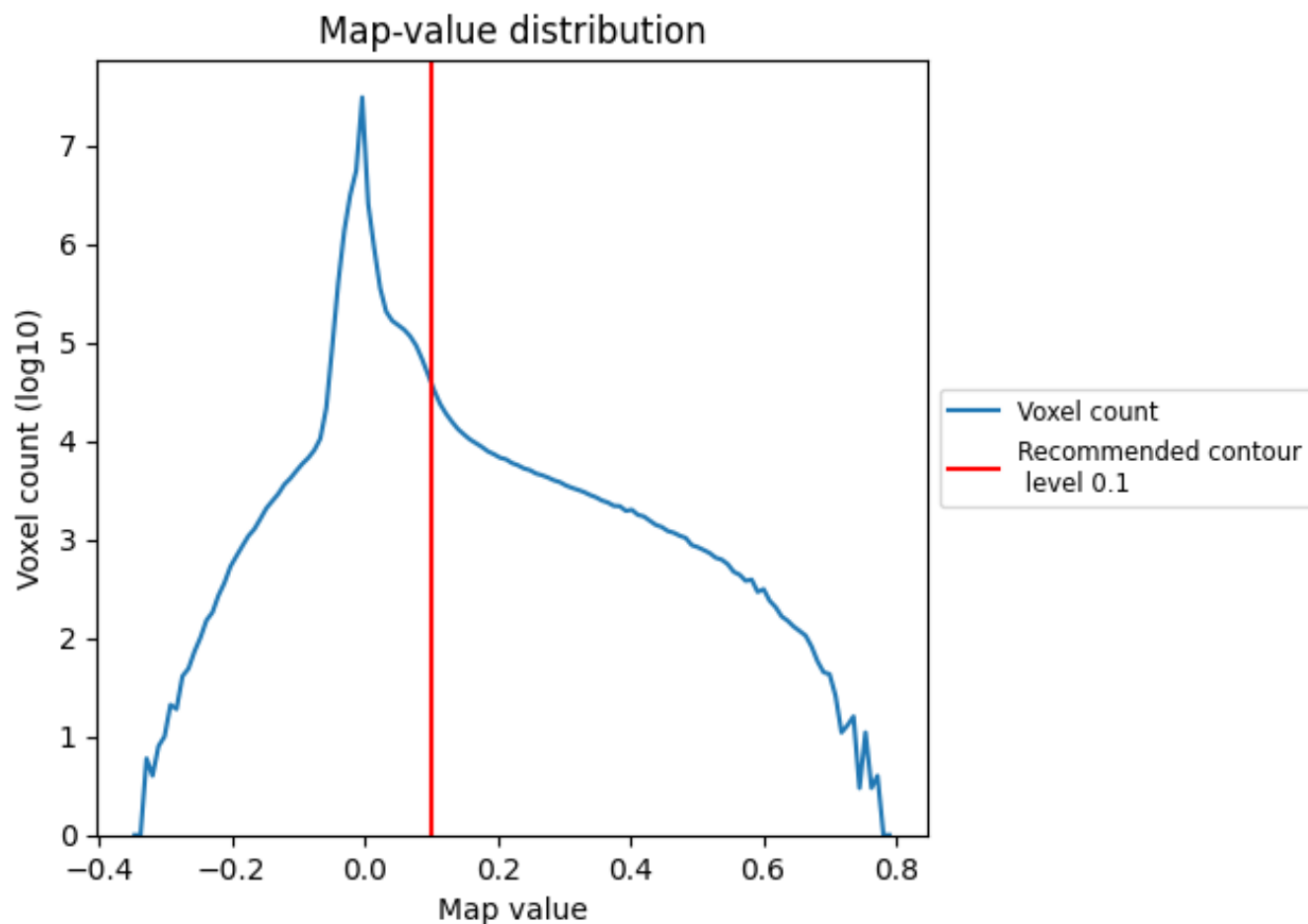


Z

7 Map analysis [i](#)

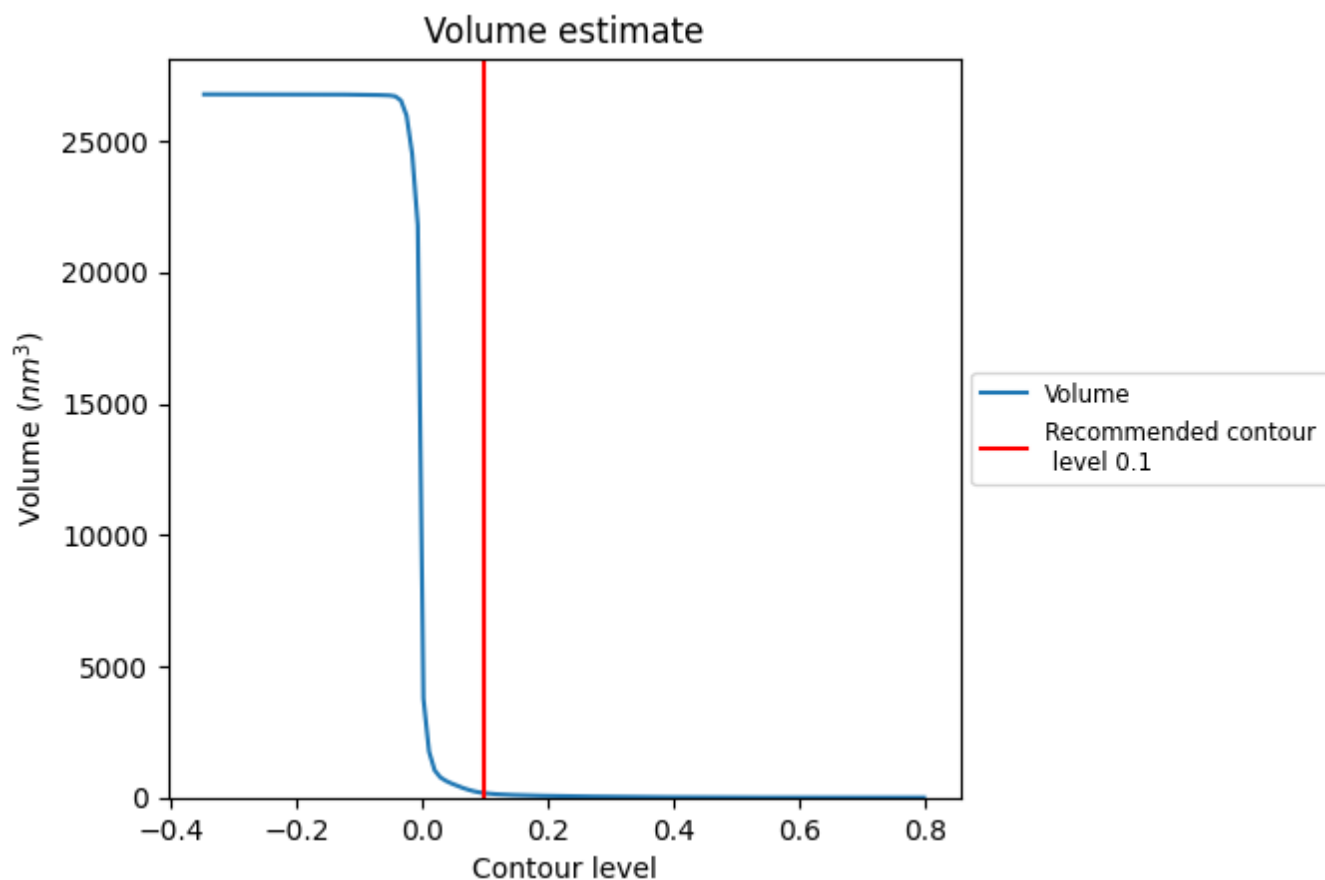
This section contains the results of statistical analysis of the map.

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.

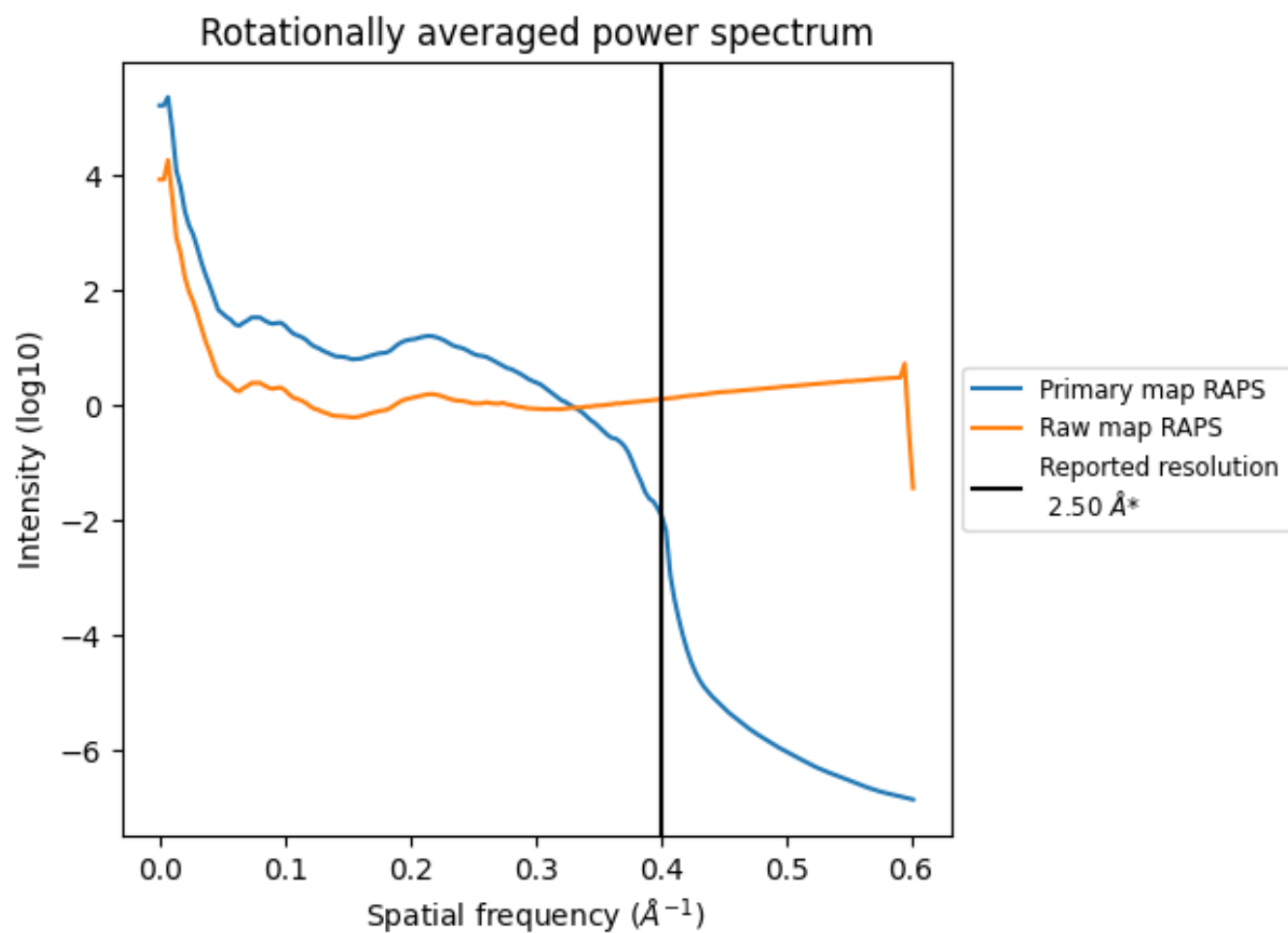
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm^3 ; this corresponds to an approximate mass of 152 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 ⓘ

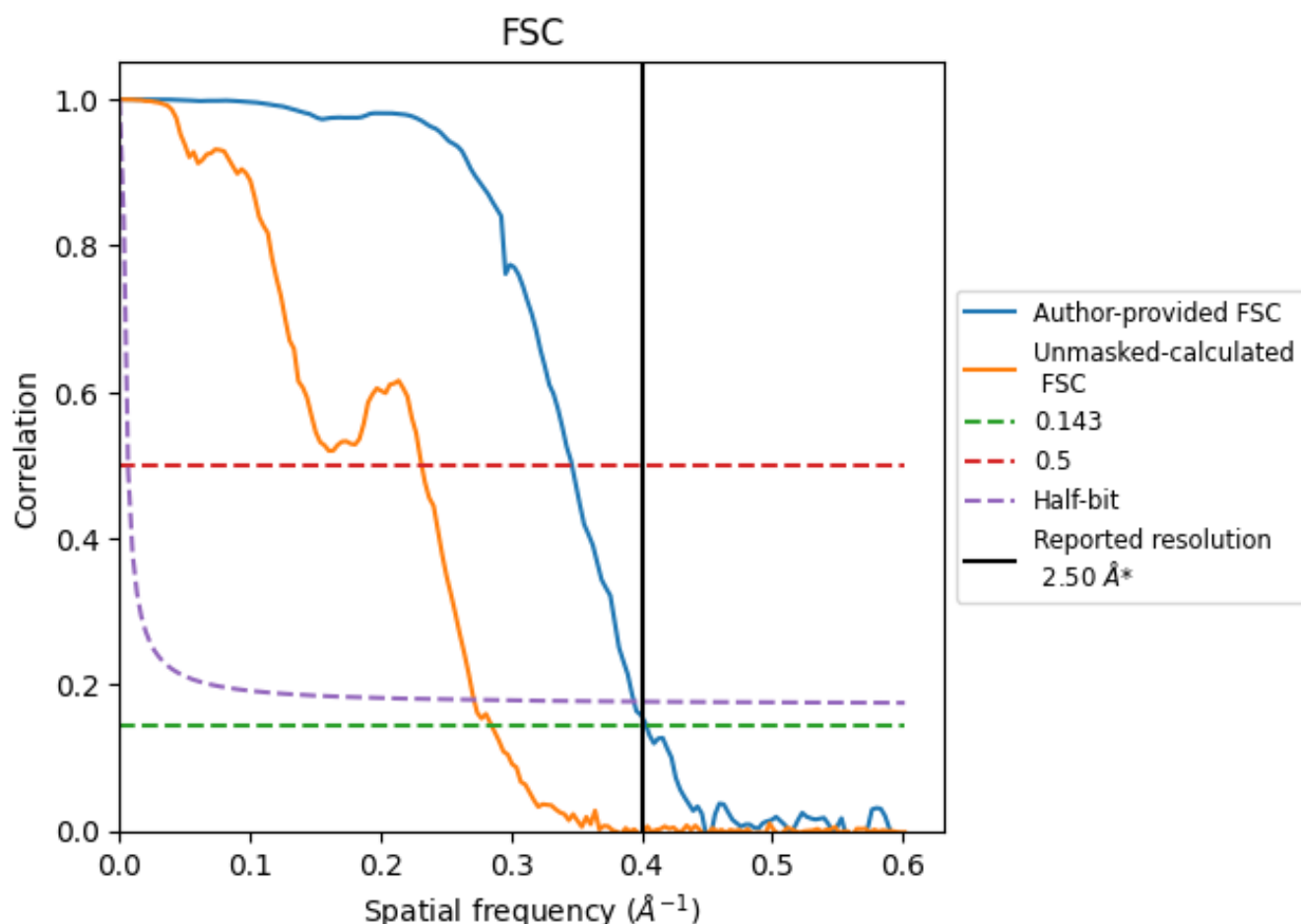


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 \AA^{-1}

8.2 Resolution estimates [i](#)

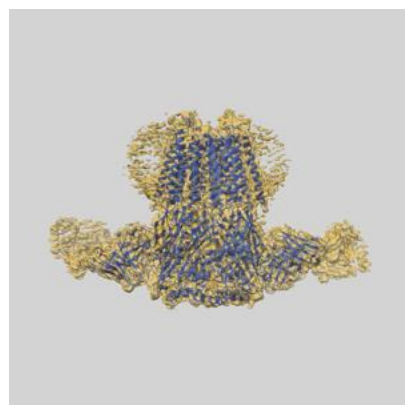
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.48	2.89	2.54
Unmasked-calculated*	3.51	4.32	3.68

*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 3.51 differs from the reported value 2.5 by more than 10 %

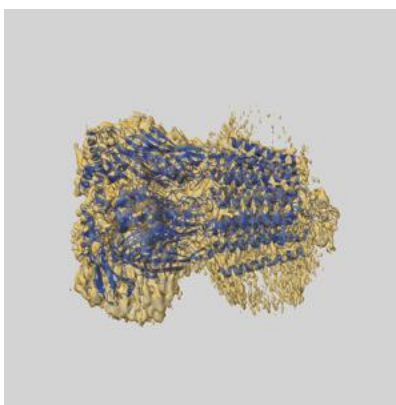
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29350 and PDB model 8FOI. Per-residue inclusion information can be found in section [3](#) on page [12](#).

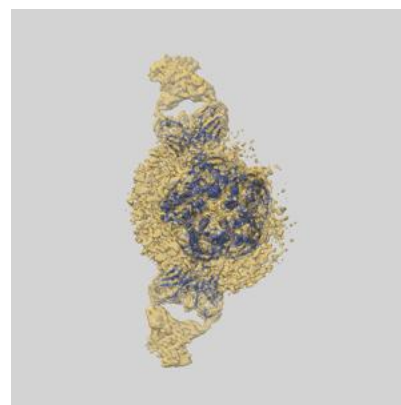
9.1 Map-model overlay [i](#)



X



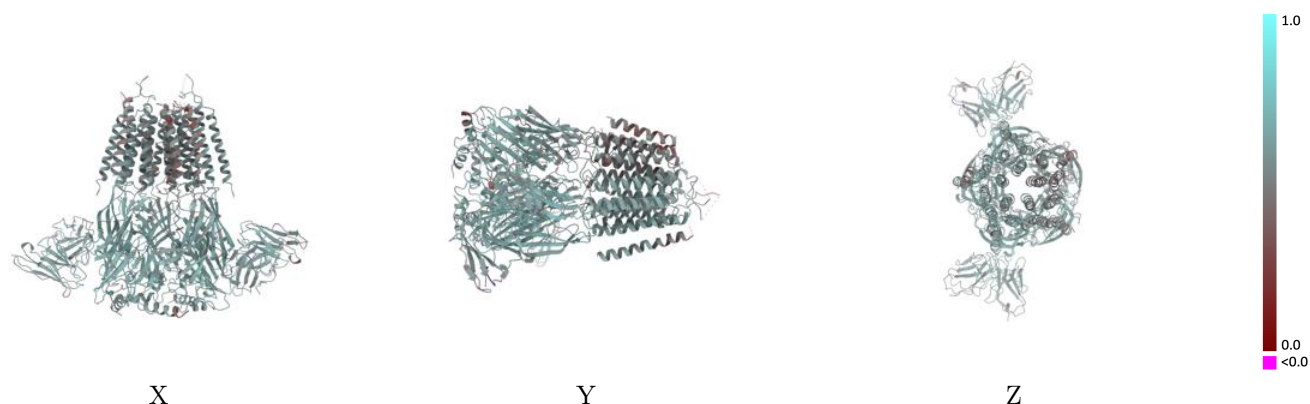
Y



Z

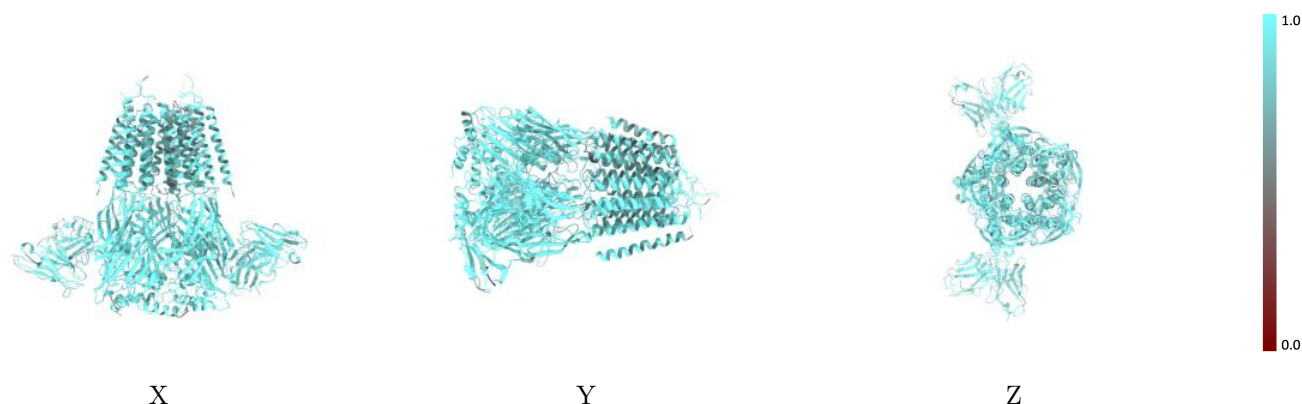
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



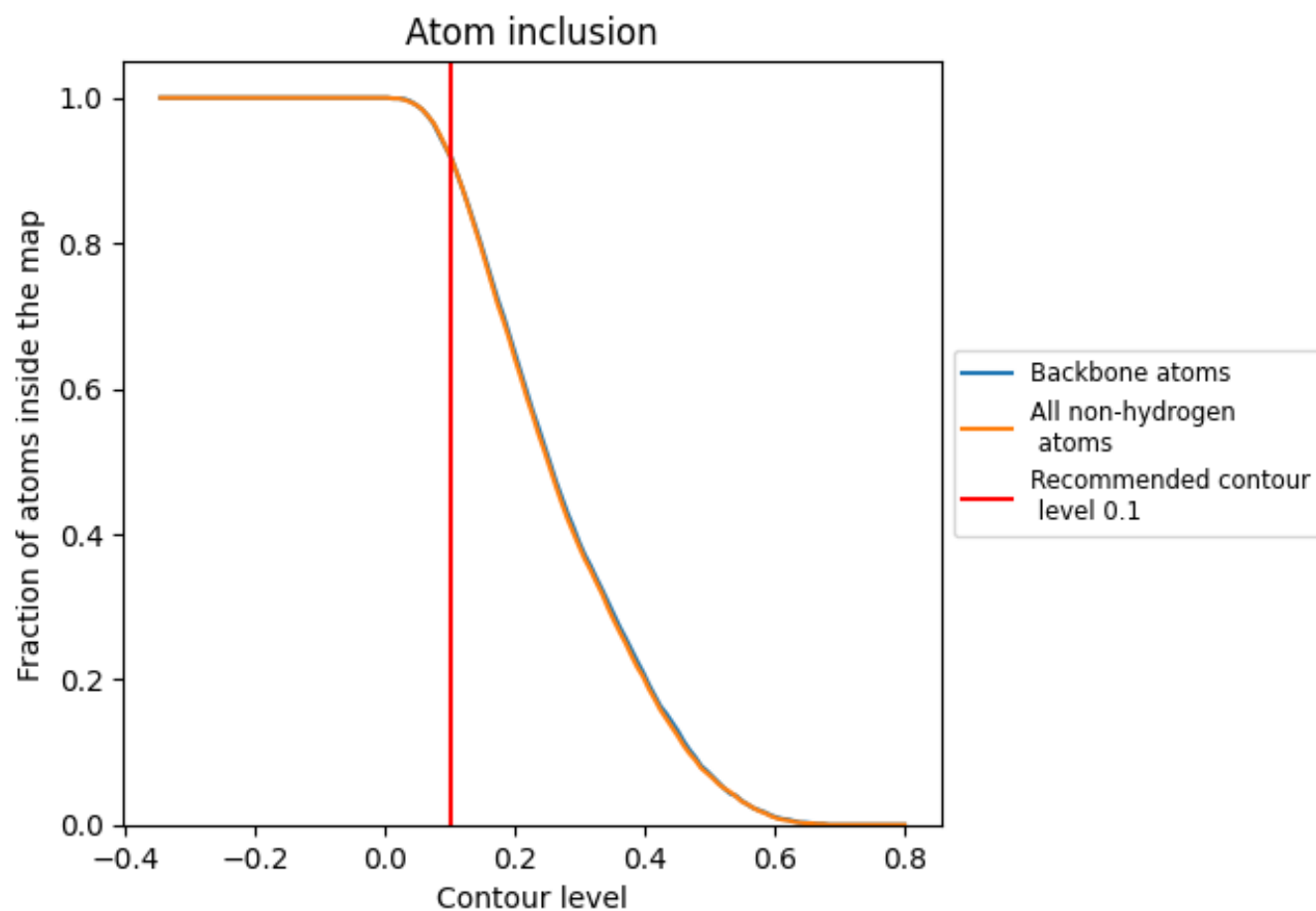
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9190	<div></div> 0.5640
A	<div></div> 0.9390	<div></div> 0.5900
B	<div></div> 0.9430	<div></div> 0.5820
C	<div></div> 0.9380	<div></div> 0.5820
D	<div></div> 0.8830	<div></div> 0.5290
E	<div></div> 0.9180	<div></div> 0.5620
F	<div></div> 0.9160	<div></div> 0.5460
G	<div></div> 0.4260	<div></div> 0.2810
H	<div></div> 0.9120	<div></div> 0.5530
I	<div></div> 0.8530	<div></div> 0.4460
J	<div></div> 0.9310	<div></div> 0.5570
K	<div></div> 0.9290	<div></div> 0.5580
L	<div></div> 0.9020	<div></div> 0.5480
M	<div></div> 0.8360	<div></div> 0.4850
N	<div></div> 0.5900	<div></div> 0.4110
O	<div></div> 0.5570	<div></div> 0.3760
P	<div></div> 0.7380	<div></div> 0.4440

1.0

0.0

<0.0