



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 08:02 PM JST

PDB ID : 7WPO
EMDB ID : EMD-32686
Title : Structure of NeoCOV RBD binding to Bat37 ACE2
Authors : Cao, L.; Wang, X.; Tortorici, M.A.; Veerler, D.
Deposited on : 2022-01-24
Resolution : 3.50 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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

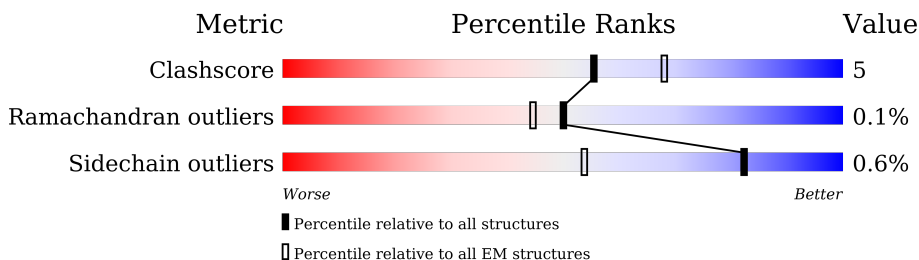
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	692	
2	B	194	
3	C	5	
4	E	2	
4	G	2	
5	P	3	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6829 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	680	Total	C	N	O	S	0	0
			5279	3400	910	937	32		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLU	GLY	conflict	UNP A0A7J7V5I6
A	28	ASP	GLU	conflict	UNP A0A7J7V5I6
A	36	GLU	LYS	conflict	UNP A0A7J7V5I6
A	58	GLU	LYS	conflict	UNP A0A7J7V5I6
A	80	ARG	LEU	conflict	UNP A0A7J7V5I6
A	91	ASN	ASP	conflict	UNP A0A7J7V5I6
A	92	LEU	SER	conflict	UNP A0A7J7V5I6
A	197	GLU	LYS	conflict	UNP A0A7J7V5I6
A	211	GLY	TRP	conflict	UNP A0A7J7V5I6
A	212	GLU	GLY	conflict	UNP A0A7J7V5I6
A	221	GLN	HIS	conflict	UNP A0A7J7V5I6
A	305	GLU	ASP	conflict	UNP A0A7J7V5I6
A	321	TYR	ARG	conflict	UNP A0A7J7V5I6
A	322	SER	ASN	conflict	UNP A0A7J7V5I6
A	325	GLN	PRO	conflict	UNP A0A7J7V5I6
A	330	ASN	LYS	conflict	UNP A0A7J7V5I6
A	353	GLU	LYS	conflict	UNP A0A7J7V5I6
A	432	ASN	LEU	conflict	UNP A0A7J7V5I6
A	436	ILE	LYS	conflict	UNP A0A7J7V5I6
A	536	GLU	GLN	conflict	UNP A0A7J7V5I6
A	568	TYR	LEU	conflict	UNP A0A7J7V5I6
A	571	ASN	GLU	conflict	UNP A0A7J7V5I6
A	575	ARG	GLY	conflict	UNP A0A7J7V5I6
A	597	LYS	GLU	conflict	UNP A0A7J7V5I6
A	617	LEU	ILE	conflict	UNP A0A7J7V5I6
A	664	THR	ARG	conflict	UNP A0A7J7V5I6

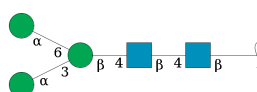
- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1325	843	232	242	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	431	ALA	ILE	conflict	UNP U5NJG5

- Molecule 3 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.



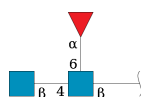
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	5	Total	C	N	O	0	0
			61	34	2	25		

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



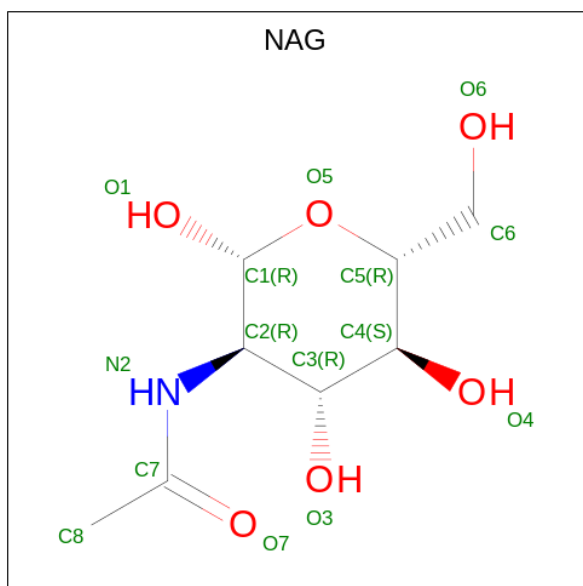
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

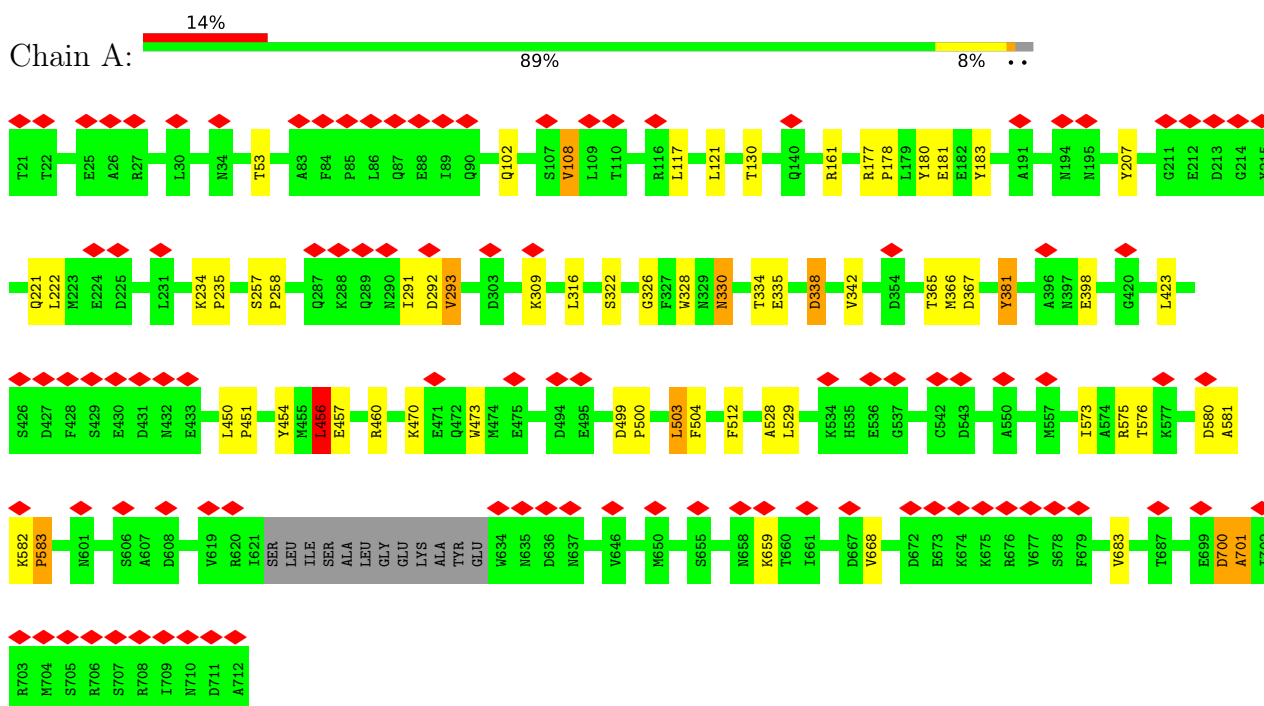


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

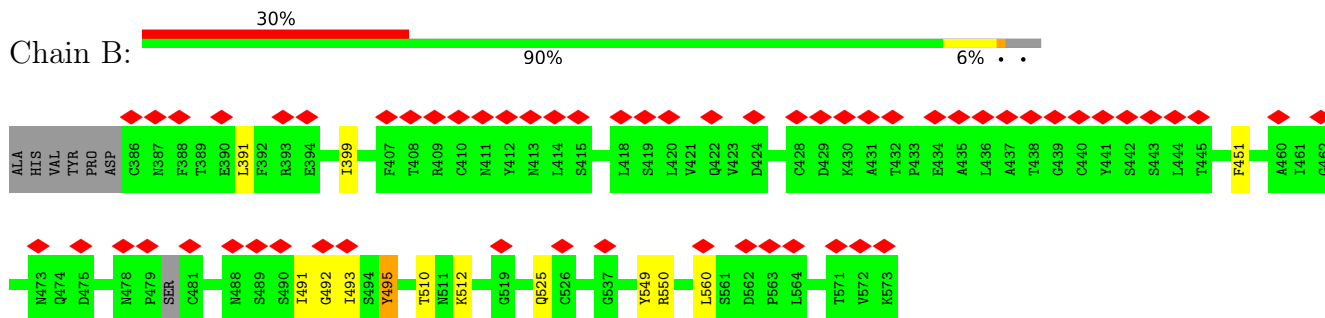
3 Residue-property plots

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: Angiotensin-converting enzyme



• Molecule 2: Spike glycoprotein



• Molecule 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



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]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	62545	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.035	Depositor
Minimum map value	-2.022	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.67	Depositor
Map size (Å)	209.92, 209.92, 209.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	1/5422 (0.0%)	0.82	19/7369 (0.3%)
2	B	0.59	0/1360	0.76	3/1868 (0.2%)
All	All	0.69	1/6782 (0.0%)	0.81	22/9237 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	583	PRO	N-CD	-8.95	1.35	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	LEU	CB-CG-CD2	9.97	127.95	111.00
1	A	161	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	A	583	PRO	CA-N-CD	6.86	121.30	111.70
1	A	701	ALA	N-CA-CB	6.72	119.51	110.10
2	B	391	LEU	CD1-CG-CD2	6.64	130.42	110.50
1	A	456	LEU	CD1-CG-CD2	6.55	130.16	110.50
1	A	583	PRO	N-CA-CB	-6.40	95.56	102.60
1	A	659	LYS	N-CA-CB	6.33	121.98	110.60
1	A	330	ASN	N-CA-C	5.79	126.64	111.00
2	B	495	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	A	381	TYR	CB-CG-CD2	-5.57	117.66	121.00
2	B	391	LEU	CB-CG-CD1	-5.54	101.58	111.00
1	A	454	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	A	161	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	A	108	VAL	CB-CA-C	-5.43	101.08	111.40
1	A	293	VAL	N-CA-CB	-5.39	99.64	111.50
1	A	291	ILE	CB-CA-C	-5.37	100.87	111.60
1	A	221	GLN	CB-CA-C	-5.37	99.67	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	700	ASP	CB-CA-C	-5.33	99.75	110.40
1	A	456	LEU	CB-CG-CD2	-5.33	101.95	111.00
1	A	583	PRO	N-CD-CG	-5.19	95.42	103.20
1	A	222	LEU	N-CA-C	-5.07	97.31	111.00

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	5279	0	4902	50	0
2	B	1325	0	1094	12	0
3	C	61	0	52	0	0
4	E	28	0	25	1	0
4	G	28	0	25	0	0
5	P	38	0	34	0	0
6	A	56	0	52	0	0
6	B	14	0	13	0	0
All	All	6829	0	6197	62	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 (62) 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)
2:B:495:TYR:CD2	2:B:560:LEU:HD22	1.93	1.04
2:B:495:TYR:CE2	2:B:560:LEU:HD23	1.99	0.98
2:B:495:TYR:CZ	2:B:560:LEU:HB3	2.06	0.90
2:B:495:TYR:CD2	2:B:560:LEU:CD2	2.54	0.89
1:A:316:LEU:HD21	1:A:322:SER:HB2	1.58	0.84
2:B:495:TYR:CE2	2:B:560:LEU:CD2	2.63	0.82
1:A:582:LYS:HB2	1:A:583:PRO:HD3	1.60	0.82
1:A:365:THR:HG22	1:A:367:ASP:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:O	1:A:121:LEU:HD13	1.83	0.78
1:A:503:LEU:HD12	1:A:504:PHE:H	1.52	0.74
1:A:575:ARG:O	1:A:576:THR:HG23	1.88	0.72
1:A:580:ASP:HB3	1:A:582:LYS:HG2	1.75	0.68
1:A:499:ASP:N	1:A:500:PRO:CD	2.56	0.68
1:A:108:VAL:HG22	1:A:108:VAL:O	1.94	0.67
1:A:575:ARG:O	1:A:576:THR:CG2	2.45	0.65
1:A:326:GLY:O	1:A:330:ASN:HB2	1.97	0.65
1:A:503:LEU:HD12	1:A:504:PHE:N	2.14	0.62
1:A:456:LEU:HG	1:A:460:ARG:HH21	1.67	0.59
1:A:700:ASP:OD1	1:A:701:ALA:N	2.36	0.58
1:A:334:THR:HG22	1:A:335:GLU:N	2.18	0.57
1:A:181:GLU:HG2	1:A:473:TRP:CZ3	2.40	0.56
1:A:292:ASP:HA	1:A:366:MET:CE	2.36	0.55
1:A:457:GLU:OE2	1:A:512:PHE:HB3	2.07	0.55
1:A:207:TYR:CE1	1:A:398:GLU:OE2	2.60	0.54
1:A:582:LYS:CB	1:A:583:PRO:HD3	2.22	0.54
1:A:450:LEU:N	1:A:451:PRO:HD2	2.23	0.54
1:A:582:LYS:N	1:A:583:PRO:CD	2.71	0.54
1:A:257:SER:OG	1:A:258:PRO:HD2	2.09	0.53
1:A:293:VAL:HG21	1:A:423:LEU:HD21	1.91	0.52
2:B:495:TYR:CE2	2:B:560:LEU:HB3	2.46	0.51
1:A:117:LEU:O	1:A:121:LEU:CD1	2.58	0.51
1:A:234:LYS:N	1:A:235:PRO:CD	2.73	0.51
1:A:668:VAL:HG22	1:A:683:VAL:HG12	1.93	0.51
1:A:499:ASP:N	1:A:500:PRO:HD2	2.25	0.51
2:B:491:ILE:O	2:B:493:ILE:N	2.44	0.50
1:A:365:THR:HG22	1:A:366:MET:N	2.27	0.50
2:B:495:TYR:CE1	2:B:560:LEU:HB3	2.47	0.49
1:A:365:THR:HG22	1:A:367:ASP:N	2.22	0.48
1:A:334:THR:CG2	1:A:335:GLU:N	2.77	0.47
1:A:575:ARG:C	1:A:576:THR:HG23	2.34	0.47
1:A:102:GLN:O	4:E:1:NAG:H82	2.15	0.46
1:A:309:LYS:HG2	1:A:328:TRP:CH2	2.50	0.46
1:A:117:LEU:CD1	1:A:121:LEU:HD11	2.46	0.46
1:A:316:LEU:HD21	1:A:322:SER:CB	2.37	0.45
1:A:338:ASP:OD1	1:A:338:ASP:N	2.49	0.45
1:A:528:ALA:HB1	1:A:573:ILE:O	2.16	0.45
2:B:510:THR:C	2:B:512:LYS:N	2.69	0.45
1:A:180:TYR:O	1:A:183:TYR:HB3	2.16	0.45
1:A:130:THR:O	1:A:130:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:O	1:A:342:VAL:HG12	2.17	0.45
1:A:181:GLU:CD	1:A:470:LYS:HD2	2.37	0.45
2:B:525:GLN:NE2	2:B:549:TYR:OH	2.50	0.44
1:A:292:ASP:HA	1:A:366:MET:HE2	2.00	0.44
1:A:234:LYS:HB3	1:A:235:PRO:HD3	2.00	0.43
1:A:117:LEU:HD11	1:A:121:LEU:HD11	2.01	0.42
1:A:177:ARG:HB3	1:A:178:PRO:HD3	2.02	0.41
1:A:529:LEU:HG	1:A:573:ILE:HD11	2.02	0.41
2:B:399:ILE:HD11	2:B:451:PHE:CD1	2.56	0.41
1:A:117:LEU:CD1	1:A:121:LEU:CD1	2.98	0.41
1:A:117:LEU:HD12	1:A:121:LEU:CD1	2.51	0.41
1:A:581:ALA:O	1:A:582:LYS:C	2.60	0.41
2:B:495:TYR:CG	2:B:560:LEU:HD22	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	676/692 (98%)	663 (98%)	13 (2%)	0	100	100
2	B	183/194 (94%)	173 (94%)	9 (5%)	1 (0%)	25	59
All	All	859/886 (97%)	836 (97%)	22 (3%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	492	GLY

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	513/620 (83%)	510 (99%)	3 (1%)	84	91
2	B	109/168 (65%)	108 (99%)	1 (1%)	75	86
All	All	622/788 (79%)	618 (99%)	4 (1%)	82	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	ASP
1	A	381	TYR
1	A	456	LEU
2	B	550	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	160	GLN
1	A	221	GLN
2	B	478	ASN
2	B	525	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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
3	NAG	C	1	3,1	14,14,15	1.71	1 (7%)	17,19,21	0.97	1 (5%)
3	NAG	C	2	3	14,14,15	1.32	1 (7%)	17,19,21	1.02	1 (5%)
3	BMA	C	3	3	11,11,12	1.17	1 (9%)	15,15,17	0.63	0
3	MAN	C	4	3	11,11,12	1.33	2 (18%)	15,15,17	0.67	0
3	MAN	C	5	3	11,11,12	1.40	3 (27%)	15,15,17	0.59	0
4	NAG	E	1	1,4	14,14,15	1.59	2 (14%)	17,19,21	1.04	2 (11%)
4	NAG	E	2	4	14,14,15	1.36	2 (14%)	17,19,21	0.97	1 (5%)
4	NAG	G	1	1,4	14,14,15	1.62	1 (7%)	17,19,21	1.08	1 (5%)
4	NAG	G	2	4	14,14,15	1.42	2 (14%)	17,19,21	0.89	1 (5%)
5	NAG	P	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	1.40	3 (17%)
5	NAG	P	2	5	14,14,15	1.42	2 (14%)	17,19,21	0.97	1 (5%)
5	FUC	P	3	5	10,10,11	1.53	2 (20%)	14,14,16	0.62	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	FUC	P	3	5	-	-	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	4.87	1.59	1.52
4	G	1	NAG	C1-C2	4.39	1.58	1.52
4	E	1	NAG	C1-C2	4.11	1.58	1.52
4	G	2	NAG	C1-C2	3.43	1.57	1.52
5	P	2	NAG	C1-C2	3.39	1.57	1.52
5	P	1	NAG	C1-C2	3.18	1.57	1.52
4	E	2	NAG	C1-C2	3.11	1.57	1.52
3	C	2	NAG	C1-C2	2.87	1.56	1.52
5	P	3	FUC	C1-C2	2.77	1.58	1.52
3	C	5	MAN	O5-C5	2.53	1.48	1.43
4	E	2	NAG	O5-C5	2.41	1.48	1.43
4	G	2	NAG	O5-C5	2.38	1.48	1.43
4	E	1	NAG	C4-C5	2.22	1.57	1.53
3	C	5	MAN	C1-C2	2.21	1.57	1.52
3	C	4	MAN	C2-C3	2.13	1.55	1.52
5	P	3	FUC	C4-C5	2.12	1.57	1.52
5	P	2	NAG	C3-C2	2.09	1.57	1.52
3	C	5	MAN	C4-C5	2.08	1.57	1.53
3	C	4	MAN	O5-C5	2.04	1.47	1.43
3	C	3	BMA	O5-C1	2.04	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C8-C7-N2	2.84	120.91	116.10
5	P	1	NAG	C8-C7-N2	2.76	120.78	116.10
4	E	1	NAG	C8-C7-N2	2.71	120.69	116.10
4	E	2	NAG	C8-C7-N2	2.57	120.46	116.10
5	P	2	NAG	C8-C7-N2	2.32	120.02	116.10
4	G	2	NAG	C8-C7-N2	2.28	119.96	116.10
5	P	1	NAG	C2-N2-C7	-2.19	119.78	122.90
3	C	2	NAG	C8-C7-N2	2.13	119.71	116.10
5	P	1	NAG	O7-C7-C8	-2.07	118.22	122.06
4	E	1	NAG	O7-C7-C8	-2.01	118.32	122.06
3	C	1	NAG	O5-C1-C2	-2.01	108.12	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

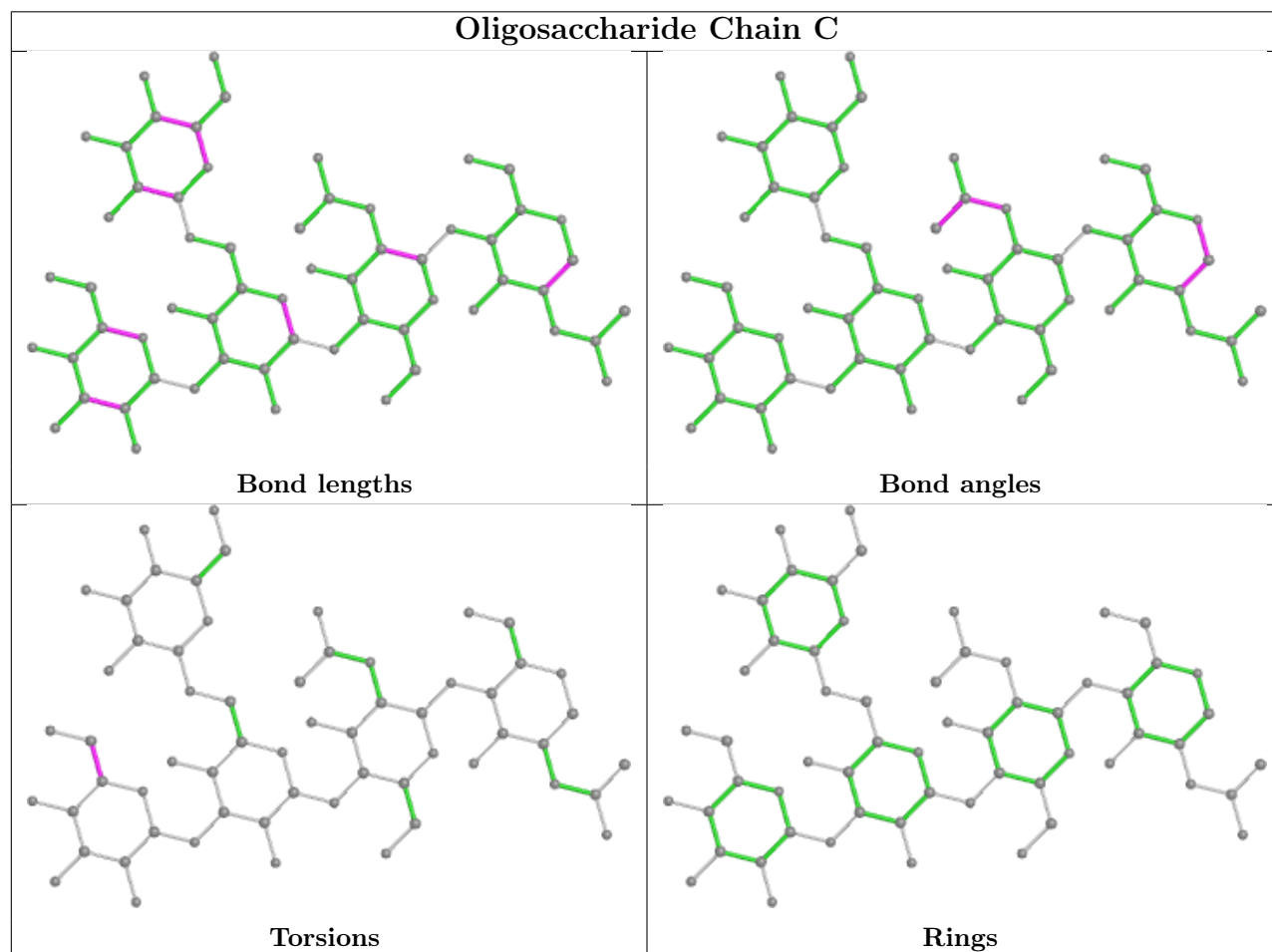
Mol	Chain	Res	Type	Atoms
5	P	1	NAG	O5-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6

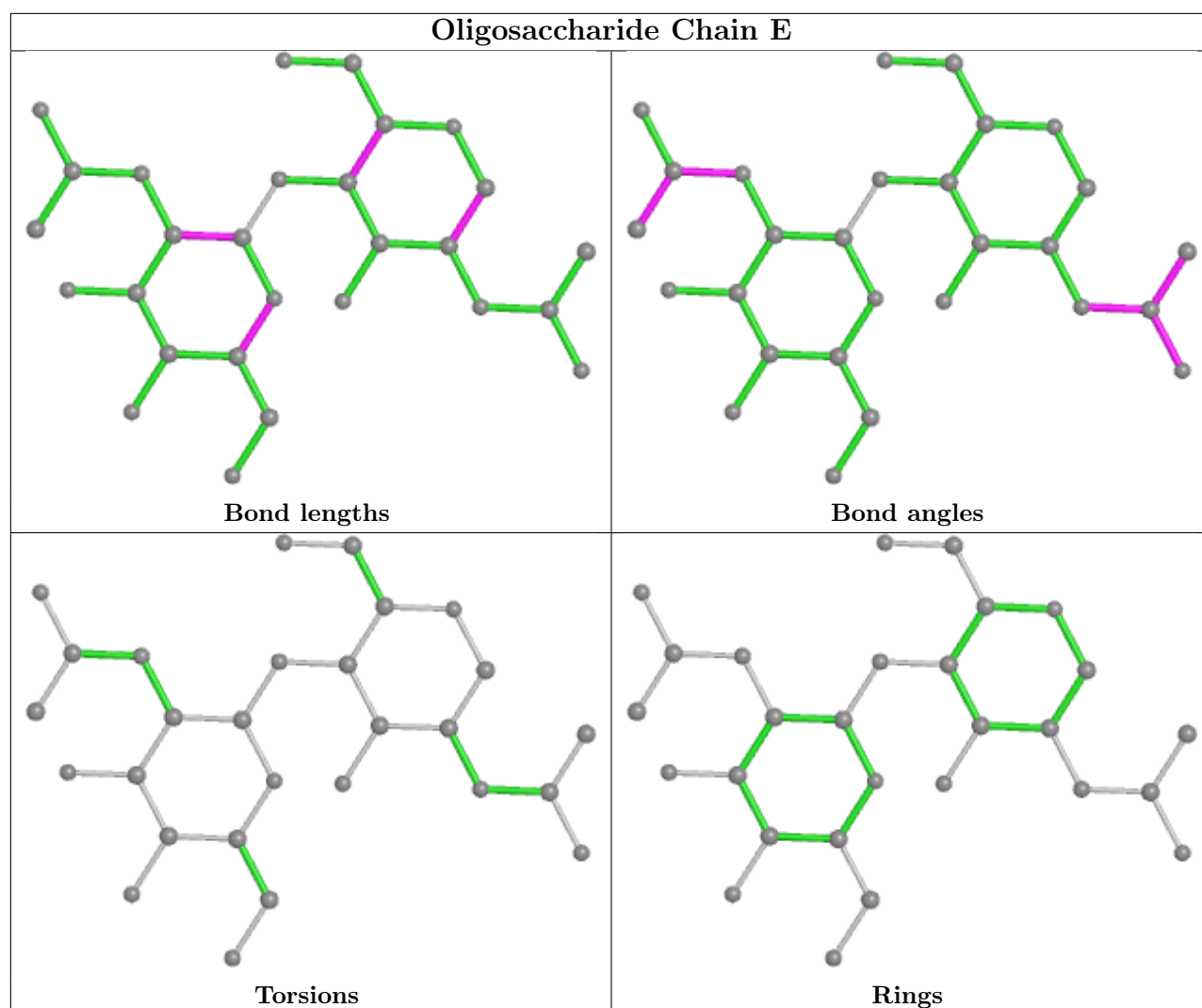
There are no ring outliers.

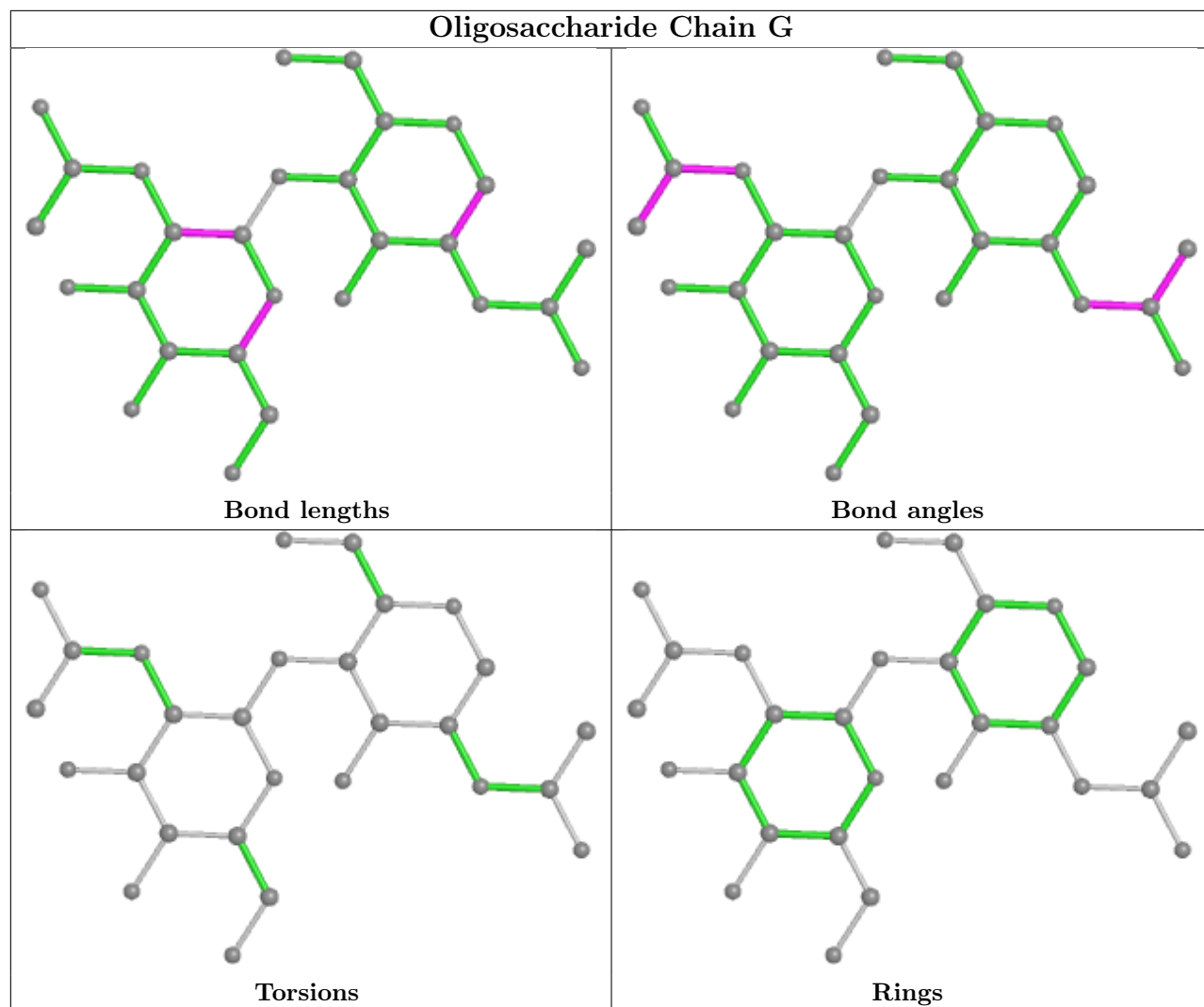
1 monomer is involved in 1 short contact:

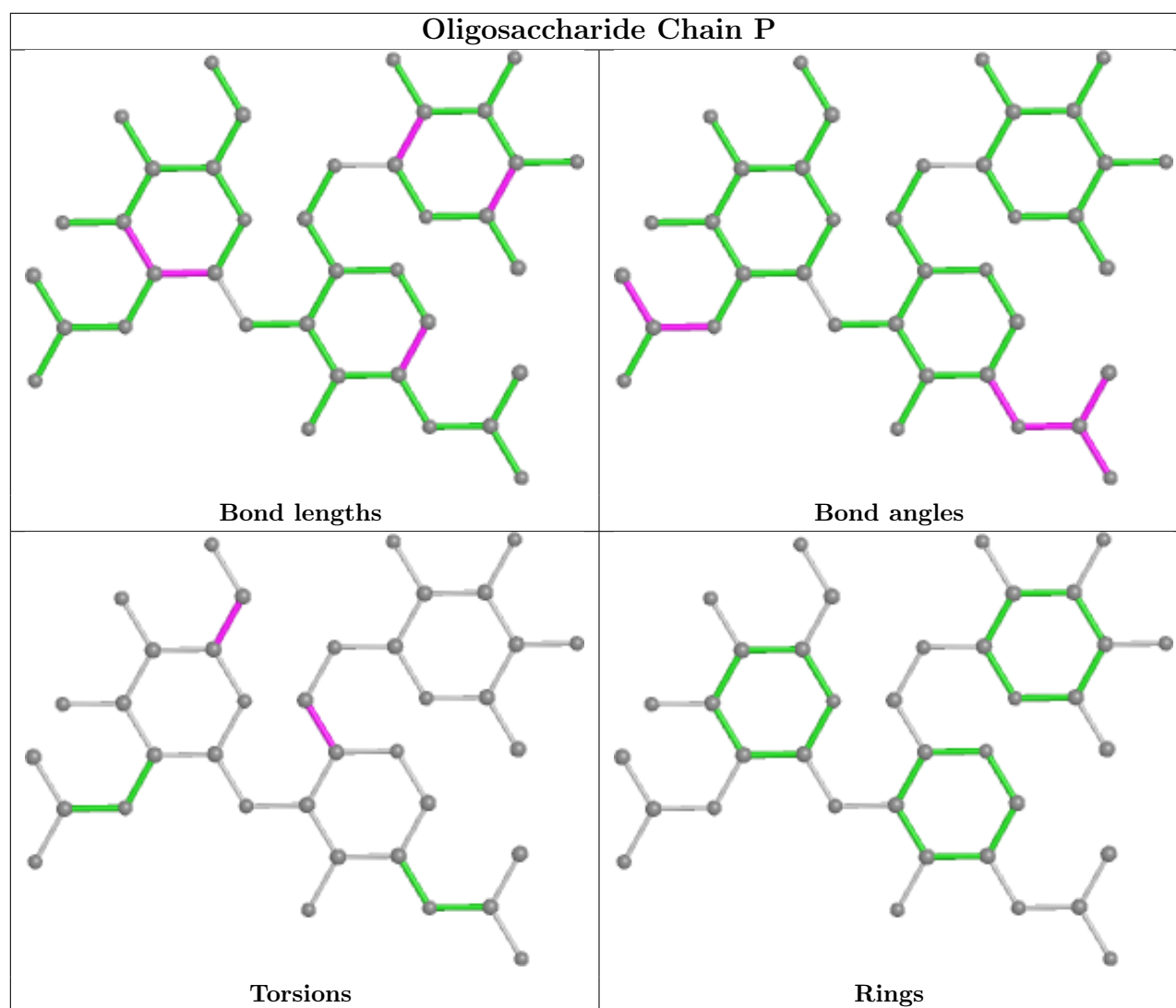
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
6	NAG	A	802	1	14,14,15	1.58	2 (14%)	17,19,21	1.04	1 (5%)
6	NAG	A	804	1	14,14,15	1.65	3 (21%)	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	801	1	14,14,15	1.77	3 (21%)	17,19,21	1.17	2 (11%)
6	NAG	A	803	1	14,14,15	1.64	2 (14%)	17,19,21	0.98	1 (5%)
6	NAG	B	601	2	14,14,15	1.64	2 (14%)	17,19,21	0.94	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	802	1	-	0/6/23/26	0/1/1/1
6	NAG	A	804	1	-	0/6/23/26	0/1/1/1
6	NAG	A	801	1	-	0/6/23/26	0/1/1/1
6	NAG	A	803	1	-	2/6/23/26	0/1/1/1
6	NAG	B	601	2	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	NAG	C1-C2	4.57	1.59	1.52
6	B	601	NAG	C1-C2	4.54	1.59	1.52
6	A	803	NAG	C1-C2	4.44	1.59	1.52
6	A	804	NAG	C1-C2	4.18	1.58	1.52
6	A	802	NAG	C1-C2	4.15	1.58	1.52
6	A	801	NAG	O5-C5	2.73	1.49	1.43
6	A	804	NAG	O5-C5	2.55	1.48	1.43
6	A	803	NAG	O5-C5	2.37	1.48	1.43
6	A	802	NAG	O5-C5	2.29	1.48	1.43
6	B	601	NAG	O5-C5	2.24	1.48	1.43
6	A	801	NAG	C2-N2	2.09	1.49	1.46
6	A	804	NAG	C3-C2	2.08	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	NAG	C8-C7-N2	3.31	121.69	116.10
6	B	601	NAG	C8-C7-N2	2.61	120.51	116.10
6	A	803	NAG	C8-C7-N2	2.56	120.43	116.10
6	A	802	NAG	C8-C7-N2	2.54	120.39	116.10
6	A	801	NAG	O7-C7-C8	-2.53	117.35	122.06
6	A	804	NAG	C8-C7-N2	2.32	120.03	116.10

There are no chirality outliers.

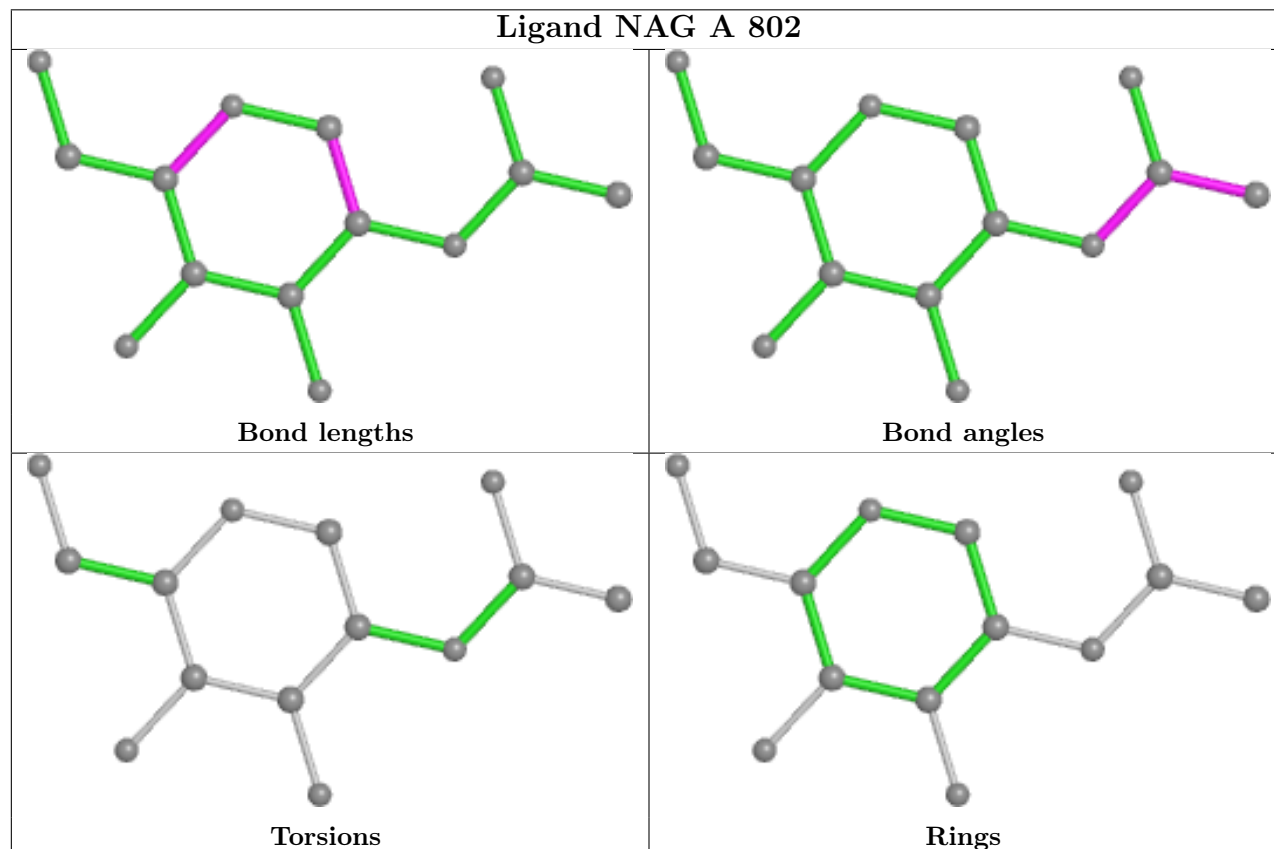
All (2) torsion outliers are listed below:

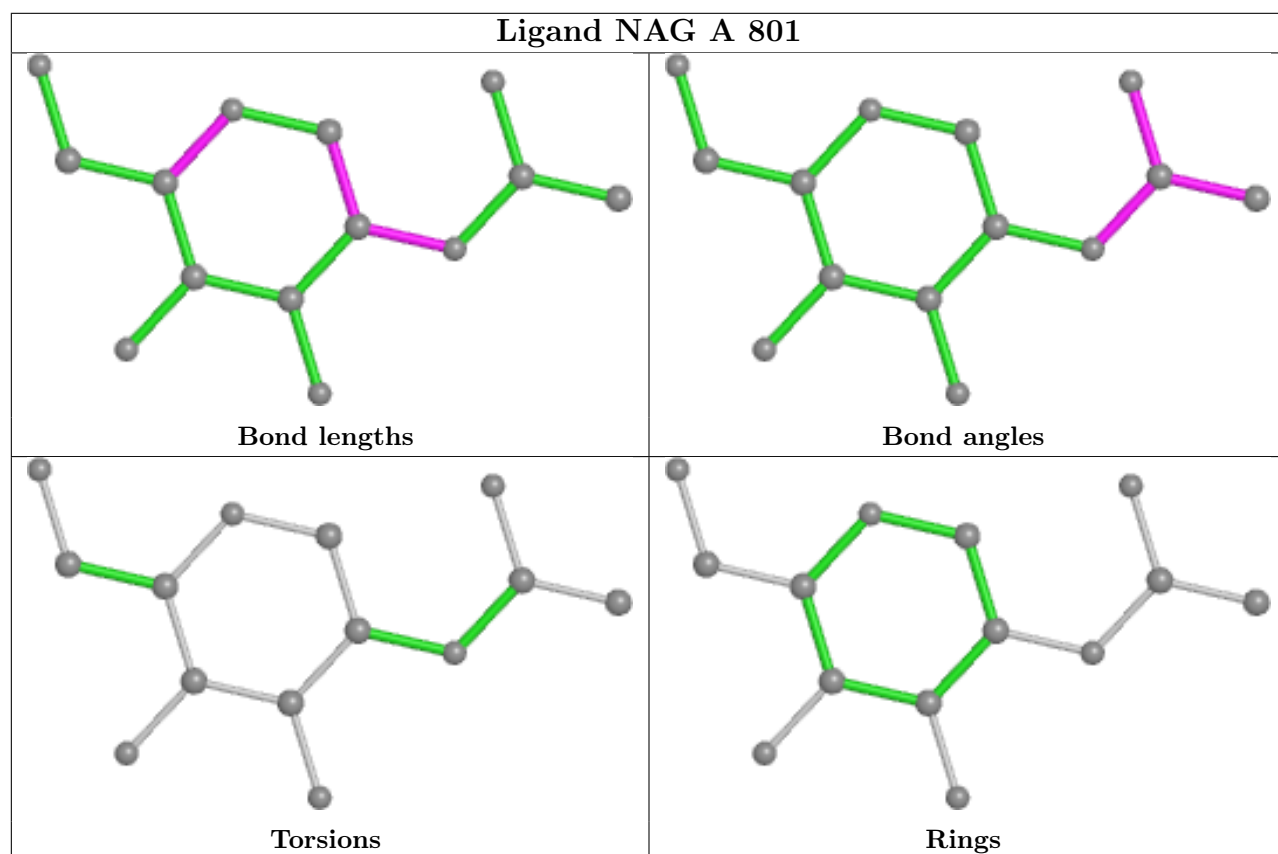
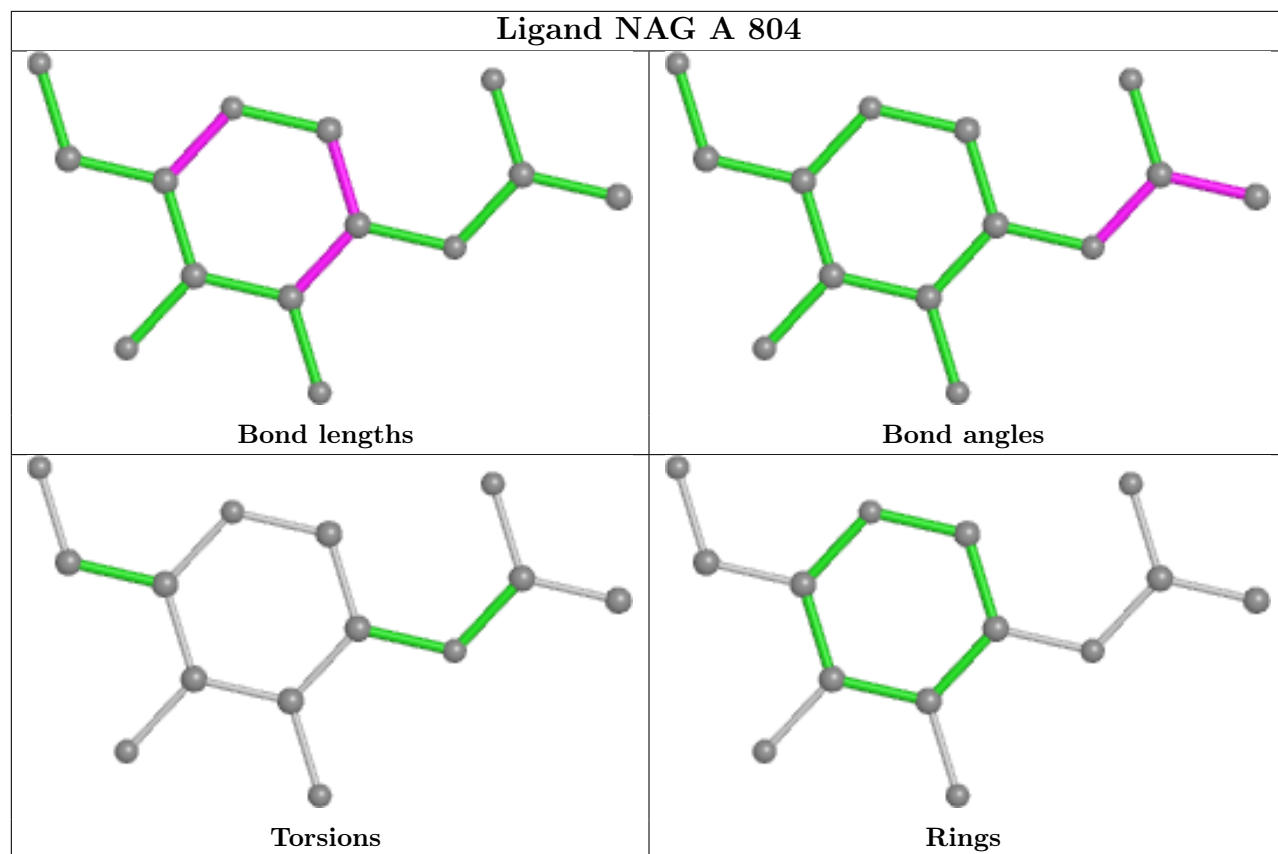
Mol	Chain	Res	Type	Atoms
6	A	803	NAG	C4-C5-C6-O6
6	A	803	NAG	O5-C5-C6-O6

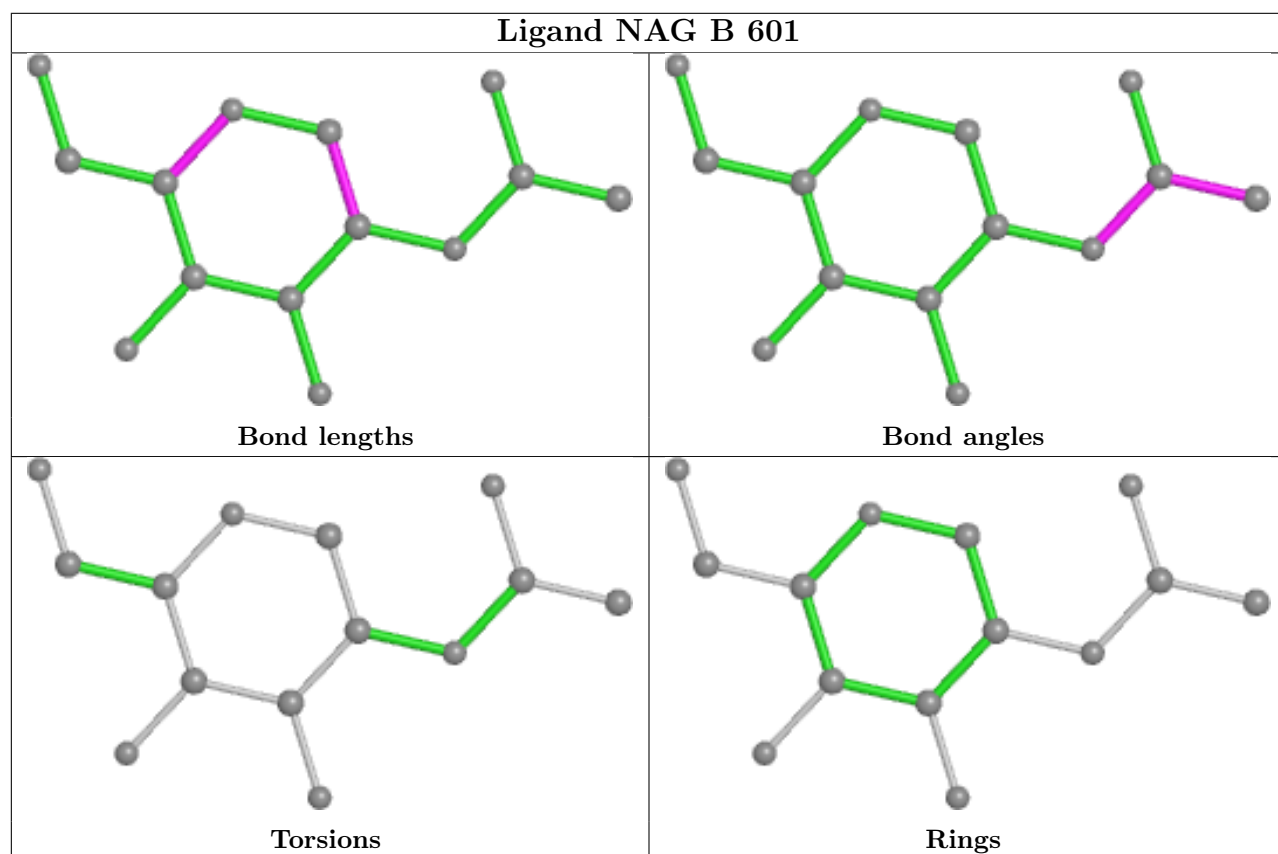
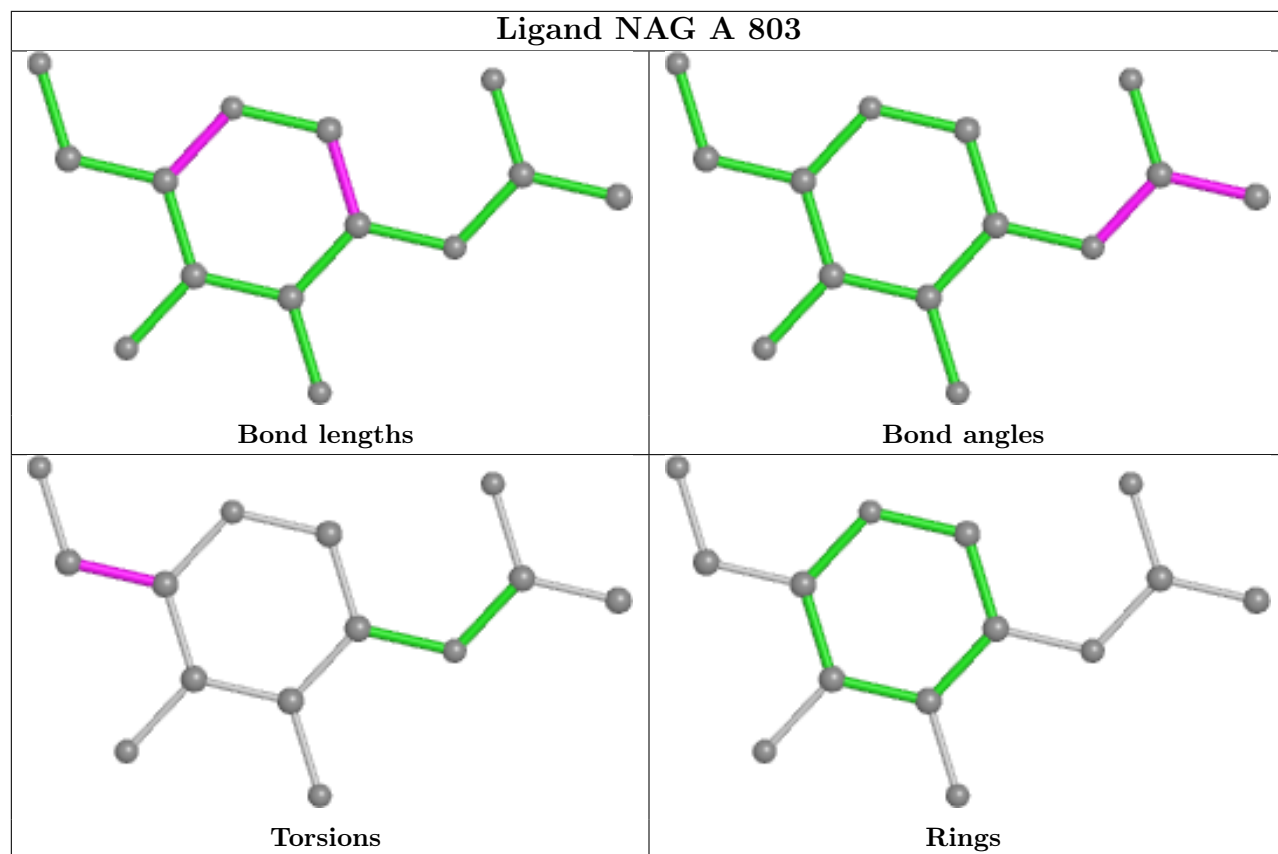
There are no ring outliers.

No monomer is involved in short contacts.

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

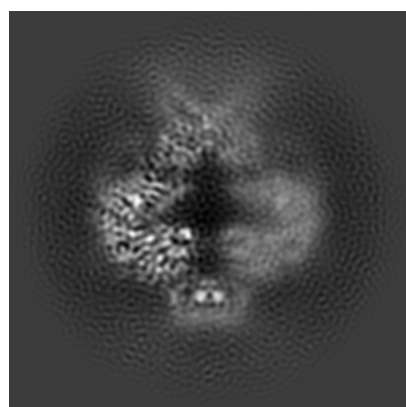
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32686. These allow visual inspection of the internal detail of the map and identification of artifacts.

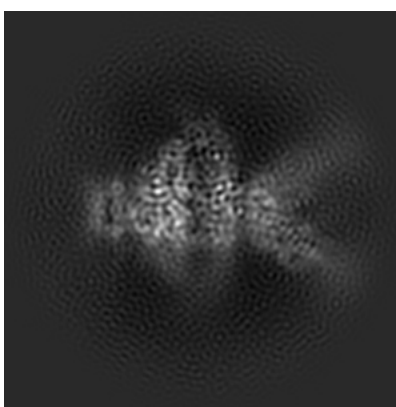
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

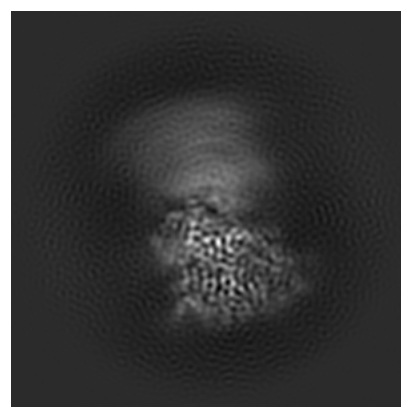
6.1.1 Primary map



X



Y

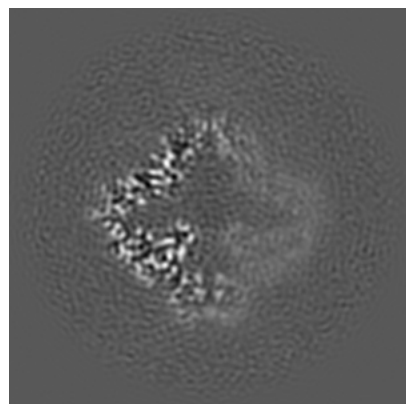


Z

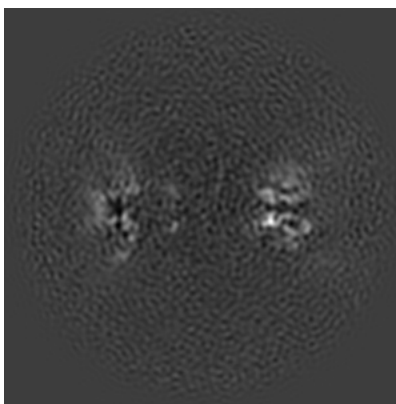
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

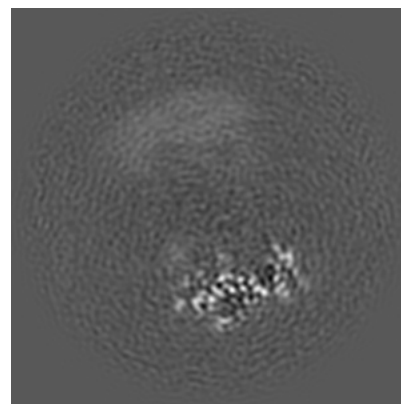
6.2.1 Primary map



X Index: 128



Y Index: 128

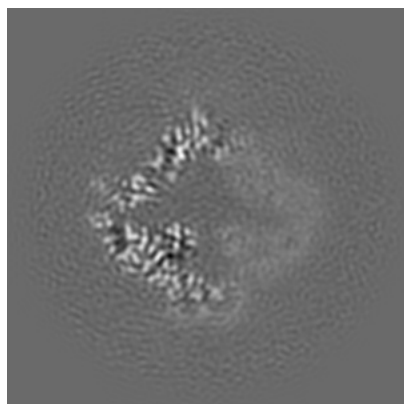


Z Index: 128

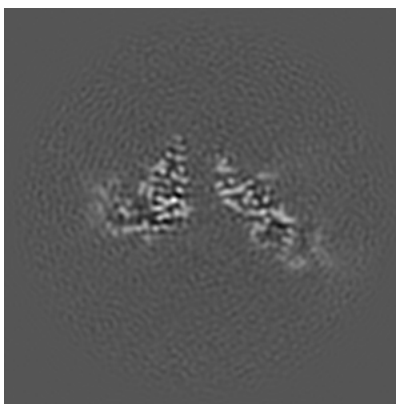
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

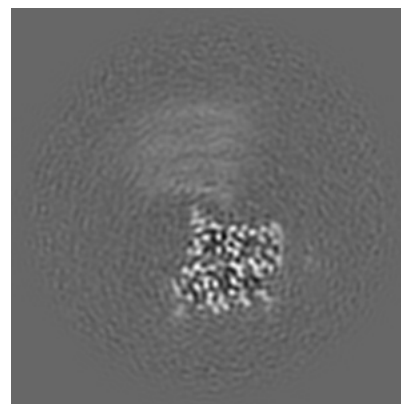
6.3.1 Primary map



X Index: 124



Y Index: 109

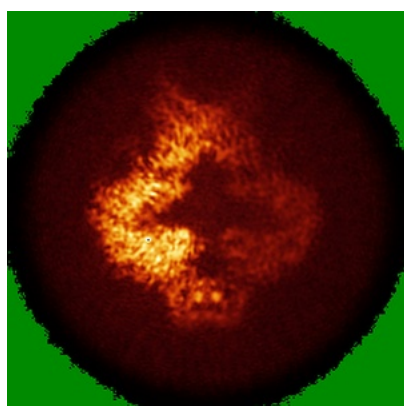


Z Index: 110

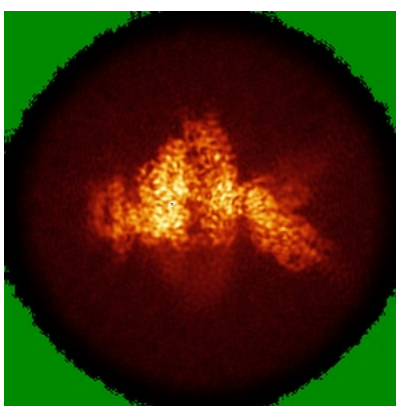
The images above show the largest variance slices of the map in three orthogonal directions.

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

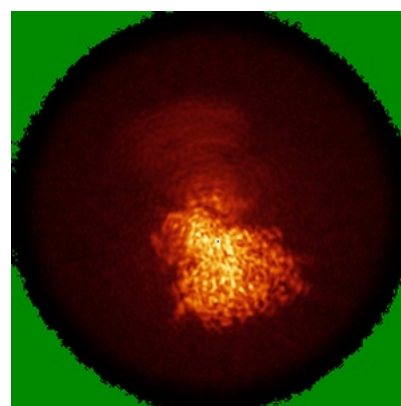
6.4.1 Primary map



X



Y

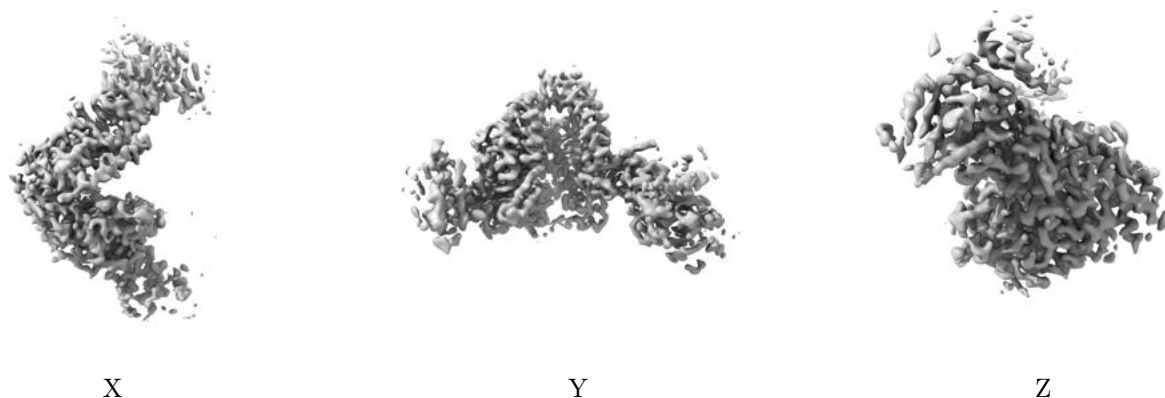


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.67. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

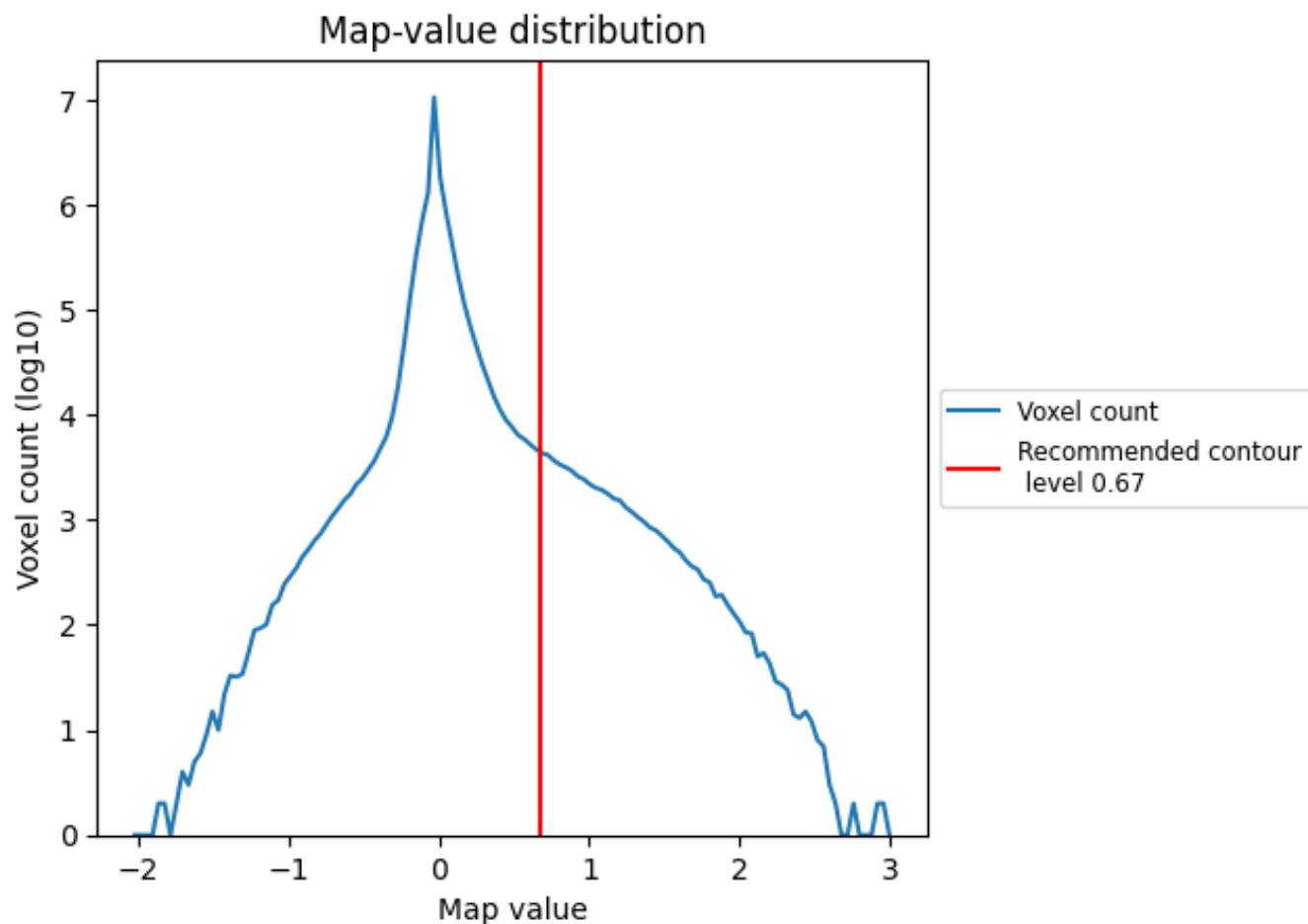
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

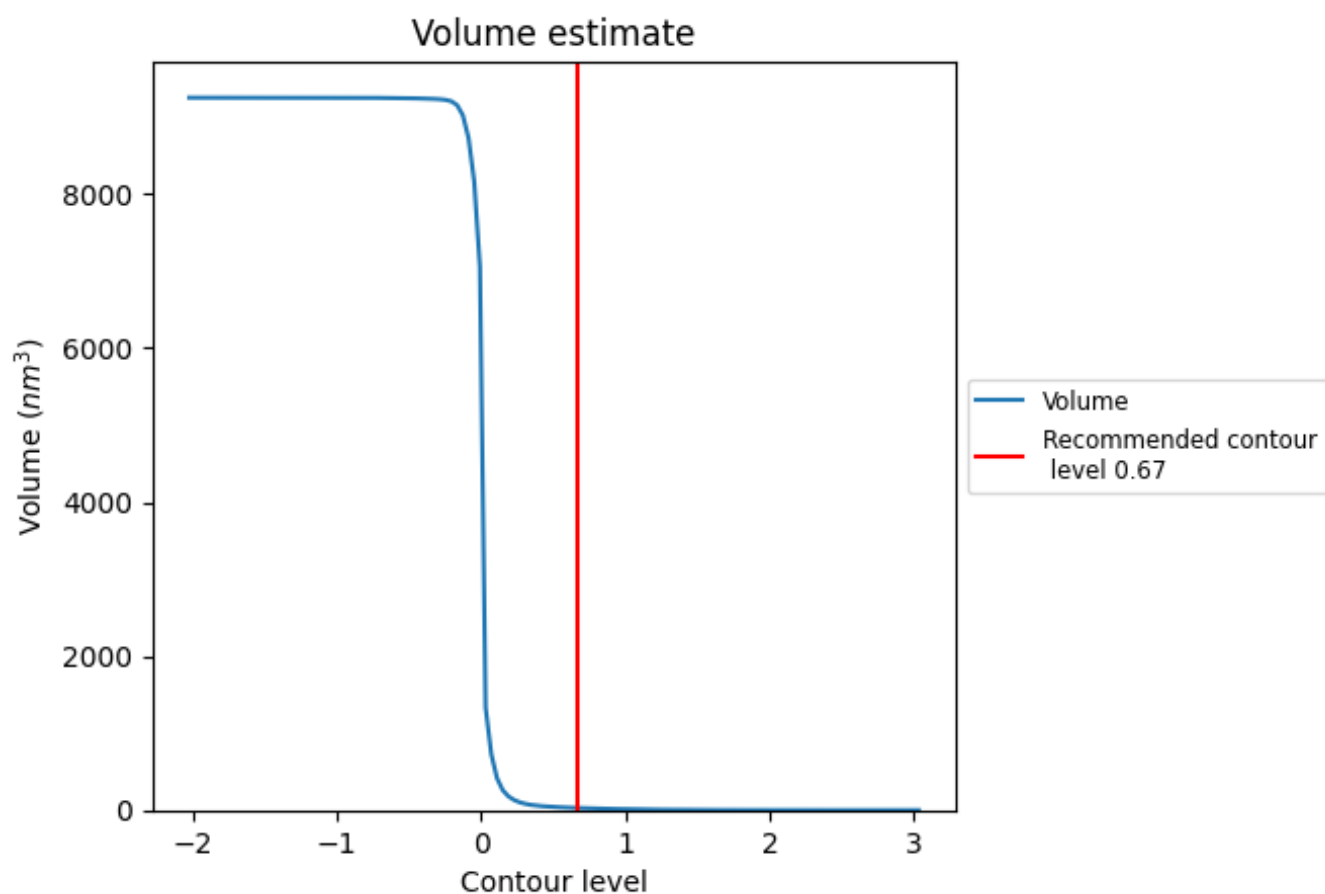
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

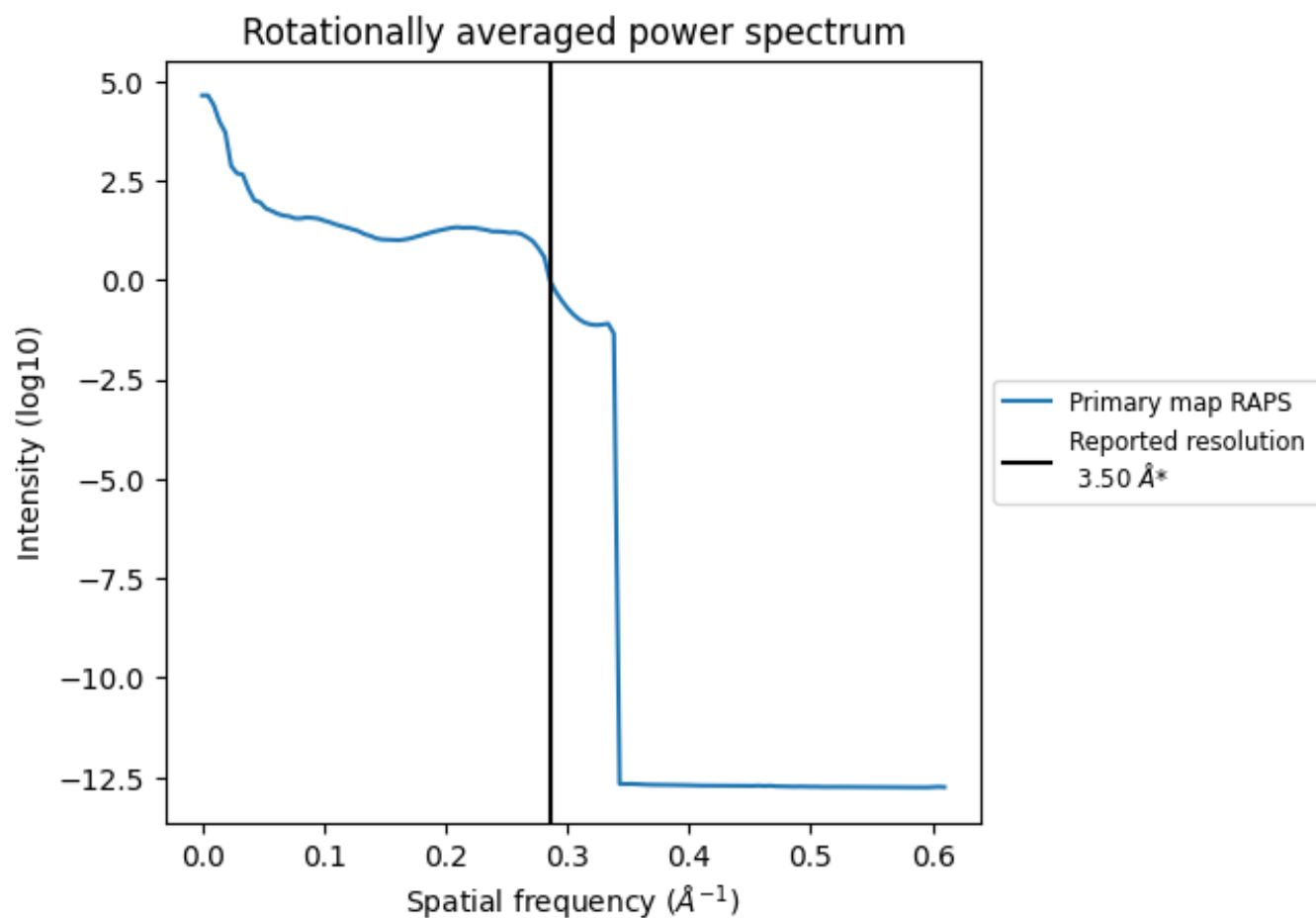
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 28 nm³; this corresponds to an approximate mass of 25 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 0.286 Å⁻¹

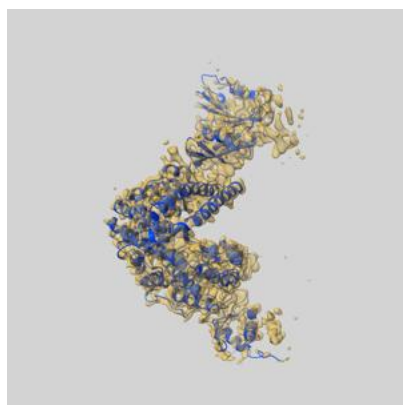
8 Fourier-Shell correlation ⓘ

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

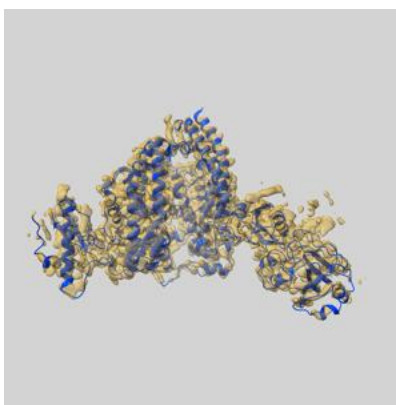
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32686 and PDB model 7WPO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

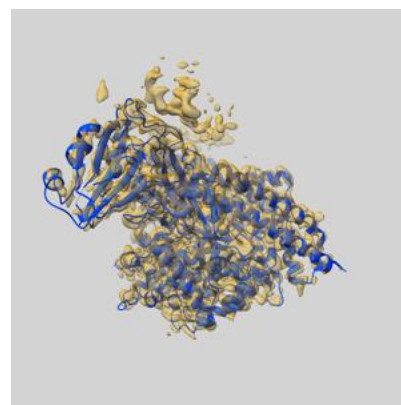
9.1 Map-model overlay [i](#)



X



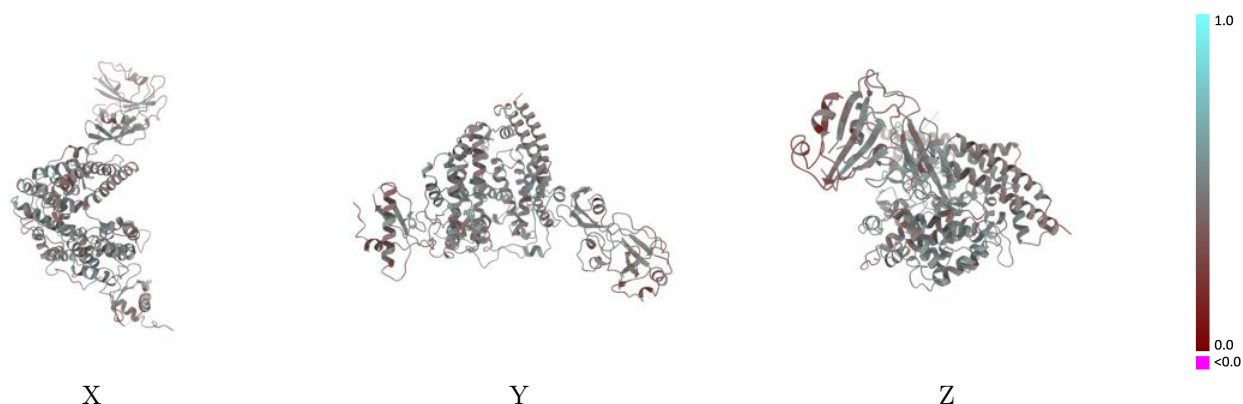
Y



Z

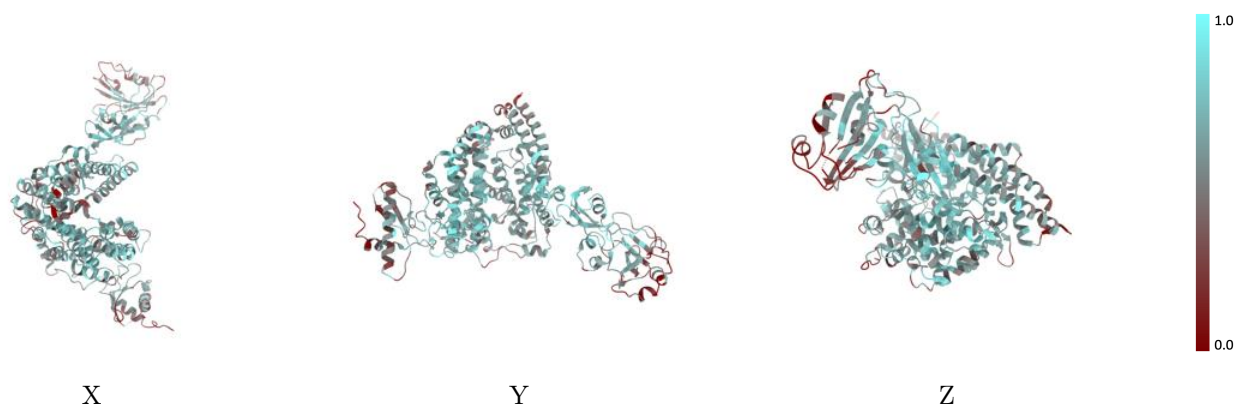
The images above show the 3D surface view of the map at the recommended contour level 0.67 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



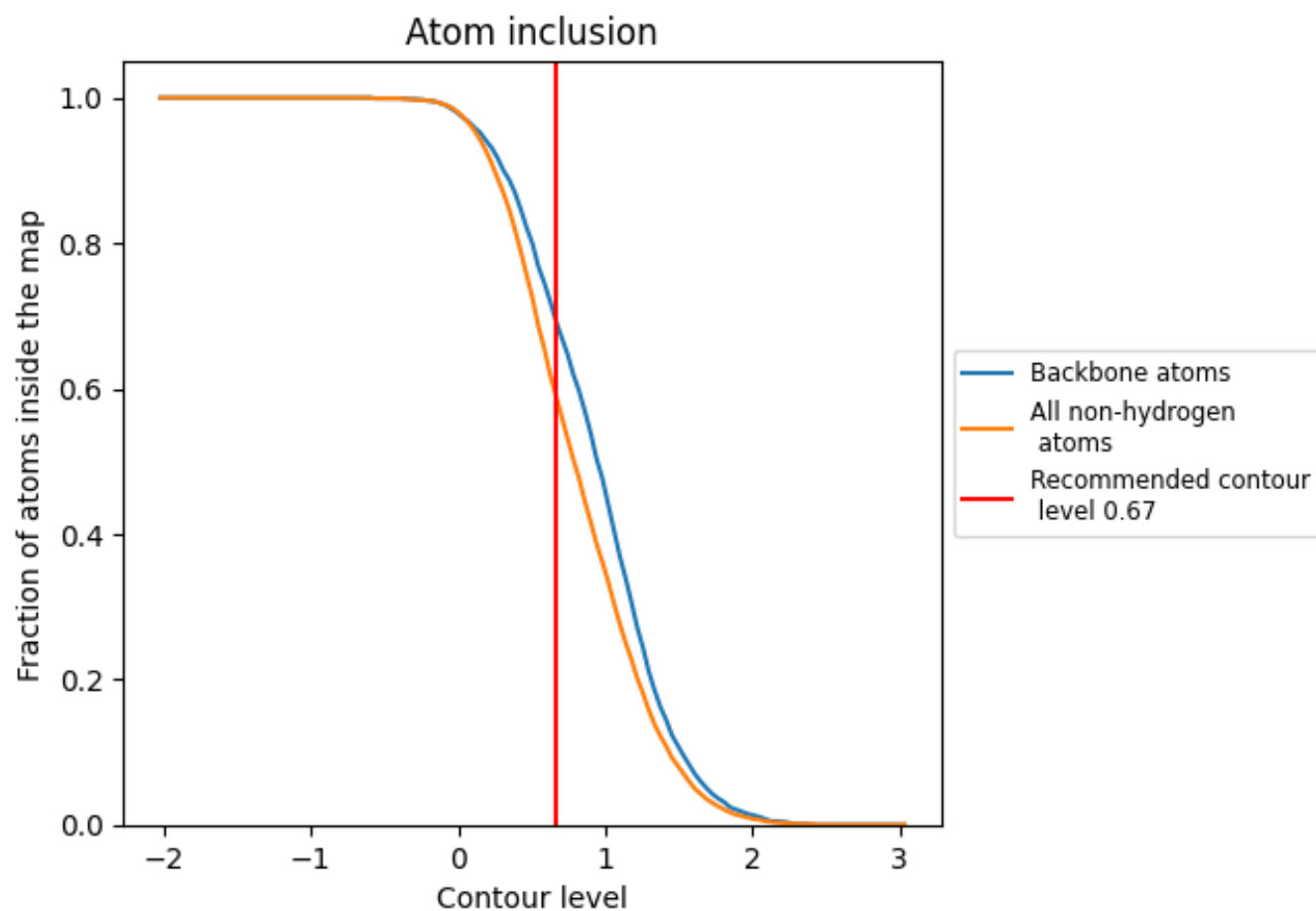
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.67).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 59% 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 (0.67) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5860	<div></div> 0.4580
A	<div></div> 0.6040	<div></div> 0.4680
B	<div></div> 0.5360	<div></div> 0.4310
C	<div></div> 0.5570	<div></div> 0.4360
E	<div></div> 0.4290	<div></div> 0.4200
G	<div></div> 0.1070	<div></div> 0.2030
P	<div></div> 0.3420	<div></div> 0.3370

1.0

0.0

<0.0