



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:32 AM UTC

PDB ID : 7WPZ / pdb_00007wpz
EMDB ID : EMD-32693
Title : Structure of PDF-2180-COV RBD binding to Bat37 ACE2
Authors : Cao, L.; Wang, X.; Tortorici, M.A.; Veisler, D.
Deposited on : 2022-01-24
Resolution : 3.80 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

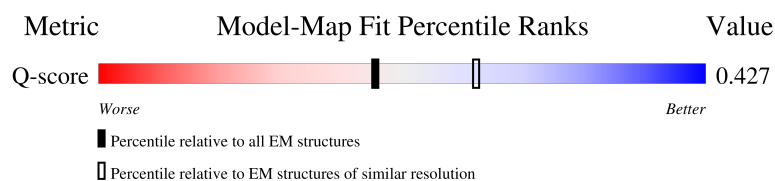
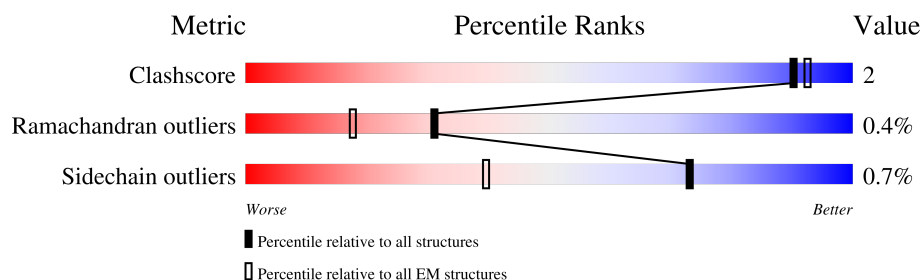
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	595	
2	B	204	
3	D	2	
3	E	2	

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Mol	Chain	Length	Quality of chain
3	J	2	 100%
4	C	5	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5756 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	595	Total	C	N	O	S	0	0
			4361	2810	781	745	25		

There are 24 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

- Molecule 2 is a protein called Spike glycoprotein.

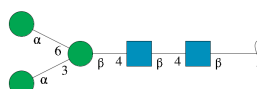
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	192	Total	C	N	O	S	0	0
			1194	748	223	217	6		

- Molecule 3 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
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	C	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

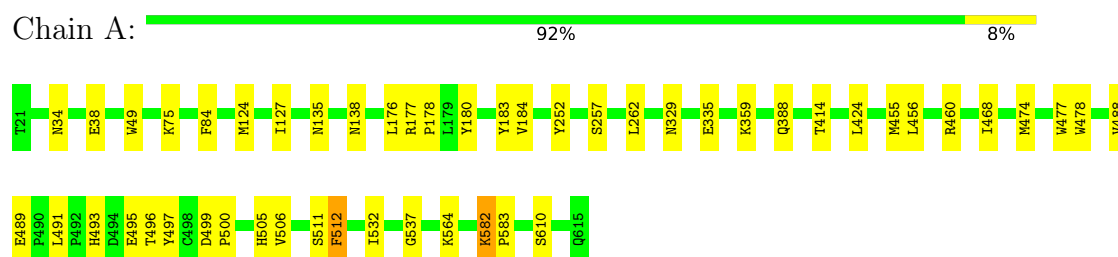


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

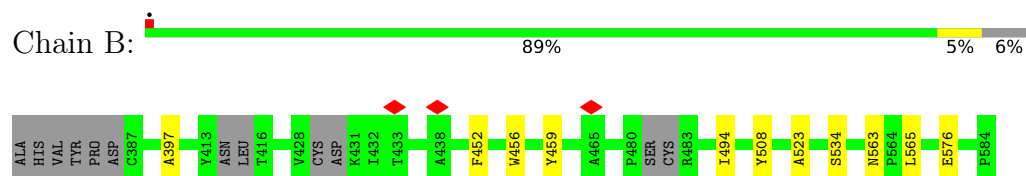
3 Residue-property plots

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



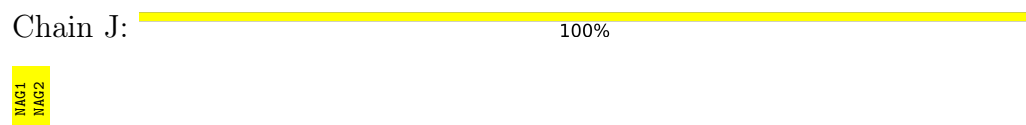
- Molecule 2: Spike glycoprotein



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



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



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



MAG1
MAG2

● Molecule 4: 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

Chain C:

100%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.250	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	209.92, 209.92, 209.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: BMA, MAN, NAG

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	0.70	1/4488 (0.0%)	1.01	36/6123 (0.6%)
2	B	0.70	0/1224	1.21	13/1689 (0.8%)
All	All	0.70	1/5712 (0.0%)	1.05	49/7812 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	LEU	CA-C	5.20	1.57	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	494	ILE	N-CA-C	-8.06	92.58	109.34
1	A	537	GLY	CA-C-N	7.80	127.80	119.76
1	A	537	GLY	C-N-CA	7.80	127.80	119.76
1	A	489	GLU	CA-C-N	7.22	126.92	119.56
1	A	489	GLU	C-N-CA	7.22	126.92	119.56
1	A	335	GLU	CA-C-N	7.03	126.95	119.85
1	A	335	GLU	C-N-CA	7.03	126.95	119.85
2	B	576	GLU	CA-C-N	6.86	126.84	119.78
2	B	576	GLU	C-N-CA	6.86	126.84	119.78
2	B	523	ALA	N-CA-C	-6.67	101.09	110.50
1	A	468	ILE	CA-C-N	6.40	126.37	119.78
1	A	468	ILE	C-N-CA	6.40	126.37	119.78
1	A	135	ASN	CA-C-N	6.25	125.88	119.56
1	A	135	ASN	C-N-CA	6.25	125.88	119.56
1	A	138	ASN	CA-C-N	6.22	127.62	119.84
1	A	138	ASN	C-N-CA	6.22	127.62	119.84
1	A	414	THR	CA-C-N	6.20	126.66	119.47
1	A	414	THR	C-N-CA	6.20	126.66	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ILE	N-CA-C	-6.15	104.51	110.72
1	A	506	VAL	N-CA-C	-6.13	106.94	111.90
1	A	388	GLN	CA-C-N	6.12	126.09	119.78
1	A	388	GLN	C-N-CA	6.12	126.09	119.78
2	B	534	SER	CA-C-N	5.98	126.09	119.87
2	B	534	SER	C-N-CA	5.98	126.09	119.87
2	B	452	PHE	CA-C-N	5.88	125.81	119.76
2	B	452	PHE	C-N-CA	5.88	125.81	119.76
1	A	488	VAL	N-CA-C	5.87	117.20	108.46
1	A	257	SER	CA-C-N	5.85	125.99	119.32
1	A	257	SER	C-N-CA	5.85	125.99	119.32
1	A	424	LEU	CA-C-N	5.77	125.72	119.78
1	A	424	LEU	C-N-CA	5.77	125.72	119.78
1	A	564	LYS	CA-C-N	5.72	125.65	119.76
1	A	564	LYS	C-N-CA	5.72	125.65	119.76
1	A	252	TYR	CA-C-N	5.52	125.45	119.76
1	A	252	TYR	C-N-CA	5.52	125.45	119.76
1	A	582	LYS	CA-C-N	5.50	125.85	119.47
1	A	582	LYS	C-N-CA	5.50	125.85	119.47
2	B	508	TYR	N-CA-C	5.42	116.52	108.60
2	B	563	ASN	CA-C-N	5.37	124.99	119.56
2	B	563	ASN	C-N-CA	5.37	124.99	119.56
1	A	532	ILE	N-CA-CB	5.35	118.60	110.58
1	A	84	PHE	CA-C-N	5.30	125.22	119.76
1	A	84	PHE	C-N-CA	5.30	125.22	119.76
2	B	397	ALA	CA-C-N	5.28	125.48	120.31
2	B	397	ALA	C-N-CA	5.28	125.48	120.31
1	A	262	LEU	CA-C-N	5.19	125.44	119.83
1	A	262	LEU	C-N-CA	5.19	125.44	119.83
1	A	610	SER	CA-C-N	5.03	125.05	119.32
1	A	610	SER	C-N-CA	5.03	125.05	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4361	0	3690	17	0
2	B	1194	0	771	1	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	J	28	0	25	0	0
4	C	61	0	52	0	0
5	A	42	0	39	1	0
5	B	14	0	13	0	0
All	All	5756	0	4640	18	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 2.

All (18) 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:456:LEU:HD13	1:A:477:TRP:CZ3	2.31	0.65
2:B:456:TRP:CG	2:B:459:TYR:HH	2.17	0.62
1:A:124:MET:HE1	1:A:180:TYR:HD1	1.64	0.61
1:A:127:ILE:HB	1:A:176:LEU:HD21	1.88	0.56
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.88	0.55
1:A:460:ARG:HH12	1:A:511:SER:HA	1.71	0.55
1:A:456:LEU:HD13	1:A:477:TRP:HZ3	1.73	0.53
1:A:329:ASN:OD1	5:A:701:NAG:C7	2.61	0.49
1:A:493:HIS:HB3	1:A:497:TYR:CD1	2.48	0.48
1:A:474:MET:HE1	1:A:499:ASP:H	1.79	0.47
1:A:180:TYR:O	1:A:184:VAL:HG23	2.16	0.46
1:A:49:TRP:CZ3	1:A:359:LYS:HB2	2.52	0.45
1:A:505:HIS:HB2	1:A:512:PHE:HE2	1.81	0.45
1:A:34:ASN:O	1:A:38:GLU:HG3	2.15	0.45
1:A:477:TRP:HD1	1:A:478:TRP:CD1	2.35	0.43
1:A:582:LYS:HB2	1:A:583:PRO:HD3	1.99	0.43
1:A:499:ASP:N	1:A:500:PRO:CD	2.81	0.43
1:A:455:MET:HE1	1:A:477:TRP:CH2	2.56	0.41

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	593/595 (100%)	581 (98%)	10 (2%)	2 (0%)	36	67
2	B	184/204 (90%)	176 (96%)	7 (4%)	1 (0%)	24	57
All	All	777/799 (97%)	757 (97%)	17 (2%)	3 (0%)	31	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	GLU
1	A	496	THR
2	B	565	LEU

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	345/531 (65%)	342 (99%)	3 (1%)	70	74
2	B	58/180 (32%)	58 (100%)	0	100	100
All	All	403/711 (57%)	400 (99%)	3 (1%)	73	77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	183	TYR
1	A	512	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	59	ASN
1	A	77	GLN
1	A	97	GLN
1	A	374	HIS
1	A	378	HIS
1	A	445	ASN
1	A	535	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	C	1	1,4	14,14,15	1.70	2 (14%)	17,19,21	1.10	1 (5%)
4	NAG	C	2	4	14,14,15	1.59	2 (14%)	17,19,21	1.02	1 (5%)
4	BMA	C	3	4	11,11,12	1.22	1 (9%)	15,15,17	0.58	0
4	MAN	C	4	4	11,11,12	1.46	2 (18%)	15,15,17	0.65	0
4	MAN	C	5	4	11,11,12	1.33	3 (27%)	15,15,17	0.59	0
3	NAG	D	1	1,3	14,14,15	1.84	2 (14%)	17,19,21	1.03	1 (5%)
3	NAG	D	2	3	14,14,15	1.63	2 (14%)	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	1.78	2 (14%)	17,19,21	0.97	1 (5%)
3	NAG	E	2	3	14,14,15	1.59	2 (14%)	17,19,21	0.87	1 (5%)
3	NAG	J	1	1,3	14,14,15	1.67	3 (21%)	17,19,21	1.02	1 (5%)
3	NAG	J	2	3	14,14,15	1.62	2 (14%)	17,19,21	0.98	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
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	2/2/19/22	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	5.20	1.59	1.52
3	E	1	NAG	C1-C2	4.84	1.58	1.52
4	C	1	NAG	C1-C2	4.53	1.58	1.52
3	E	2	NAG	C1-C2	4.27	1.58	1.52
3	J	1	NAG	C1-C2	4.24	1.58	1.52
3	D	2	NAG	C1-C2	4.02	1.57	1.52
3	J	2	NAG	C1-C2	4.00	1.57	1.52
4	C	2	NAG	C1-C2	3.93	1.57	1.52
3	D	1	NAG	O5-C5	3.01	1.49	1.43
3	J	2	NAG	O5-C5	3.01	1.49	1.43
4	C	2	NAG	O5-C5	2.83	1.48	1.43
3	J	1	NAG	O5-C5	2.80	1.48	1.43
4	C	1	NAG	O5-C5	2.79	1.48	1.43
3	E	1	NAG	O5-C5	2.75	1.48	1.43
4	C	3	BMA	C2-C3	2.58	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C5	2.49	1.48	1.43
3	E	2	NAG	O5-C5	2.39	1.48	1.43
4	C	4	MAN	O5-C5	2.37	1.48	1.43
4	C	5	MAN	O5-C5	2.34	1.48	1.43
4	C	4	MAN	C1-C2	2.34	1.57	1.52
4	C	5	MAN	C2-C3	2.11	1.55	1.52
3	J	1	NAG	C3-C2	2.07	1.56	1.52
4	C	5	MAN	C1-C2	2.04	1.57	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C8-C7-N2	2.54	120.33	116.12
4	C	2	NAG	C8-C7-N2	2.47	120.22	116.12
4	C	1	NAG	C8-C7-N2	2.38	120.07	116.12
3	D	2	NAG	C8-C7-N2	2.33	119.97	116.12
3	J	2	NAG	C8-C7-N2	2.29	119.92	116.12
3	J	1	NAG	C8-C7-N2	2.25	119.85	116.12
3	E	2	NAG	C8-C7-N2	2.23	119.82	116.12
3	E	1	NAG	C8-C7-N2	2.09	119.58	116.12

There are no chirality outliers.

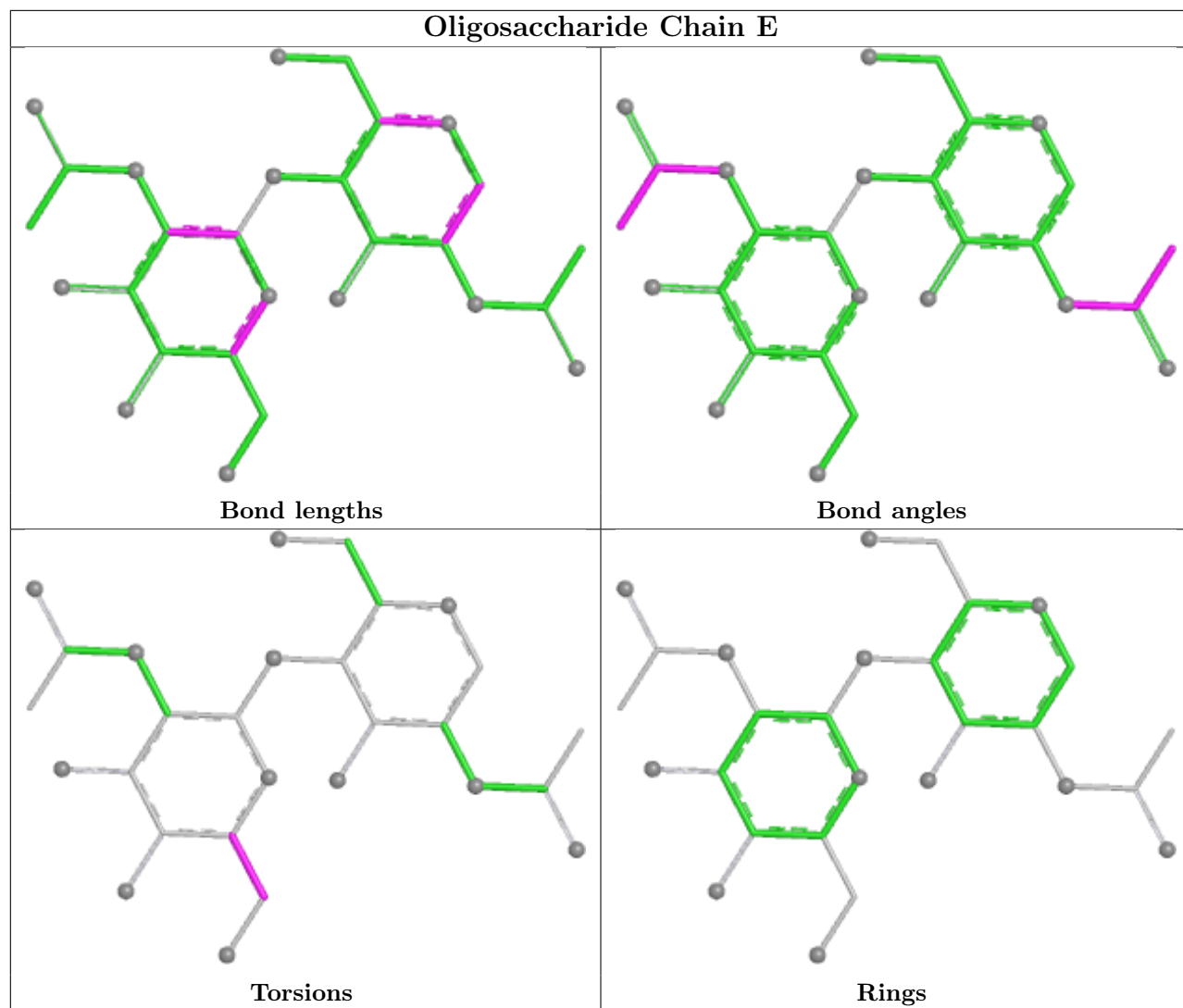
All (3) torsion outliers are listed below:

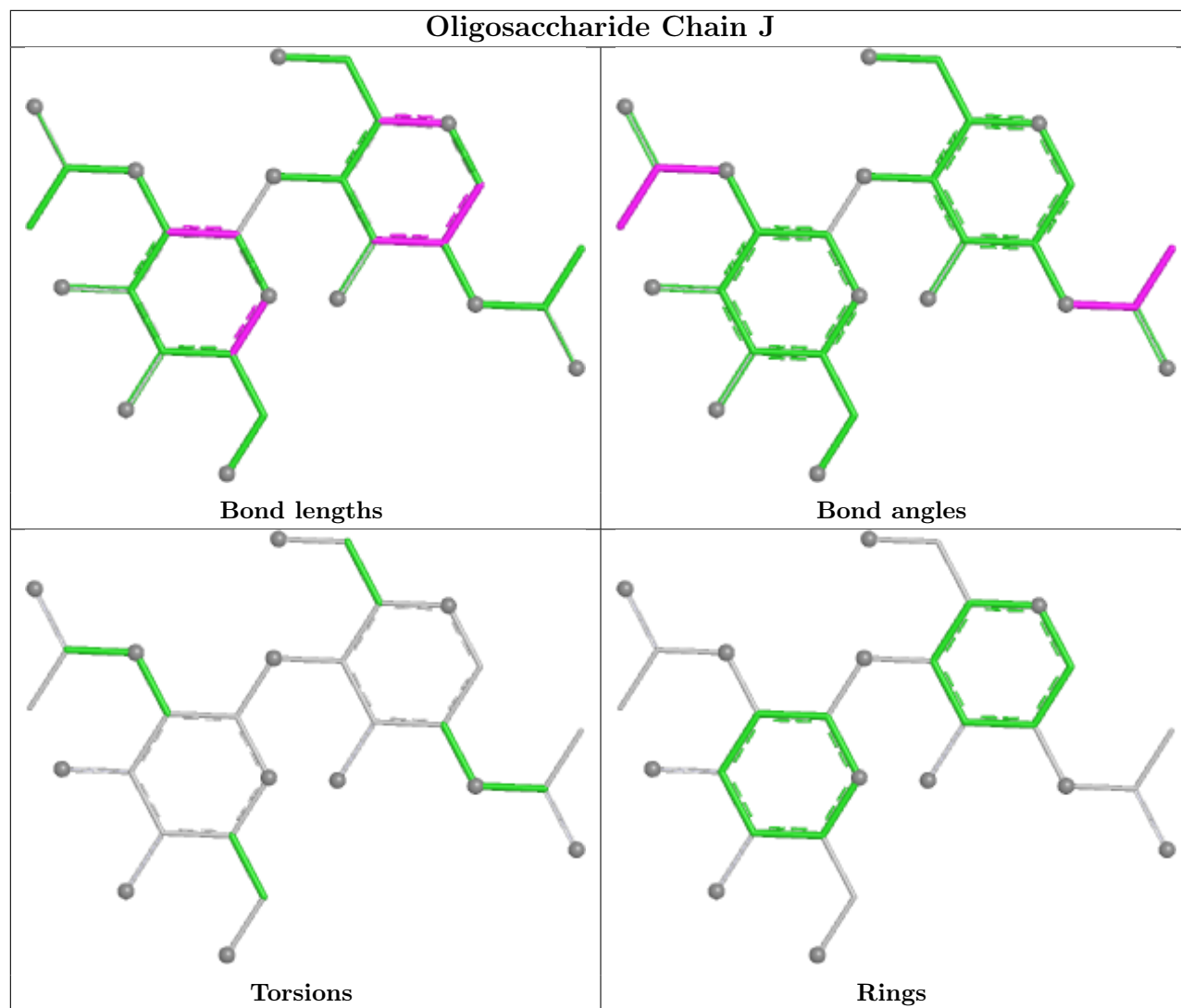
Mol	Chain	Res	Type	Atoms
4	C	4	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	C	4	MAN	C4-C5-C6-O6

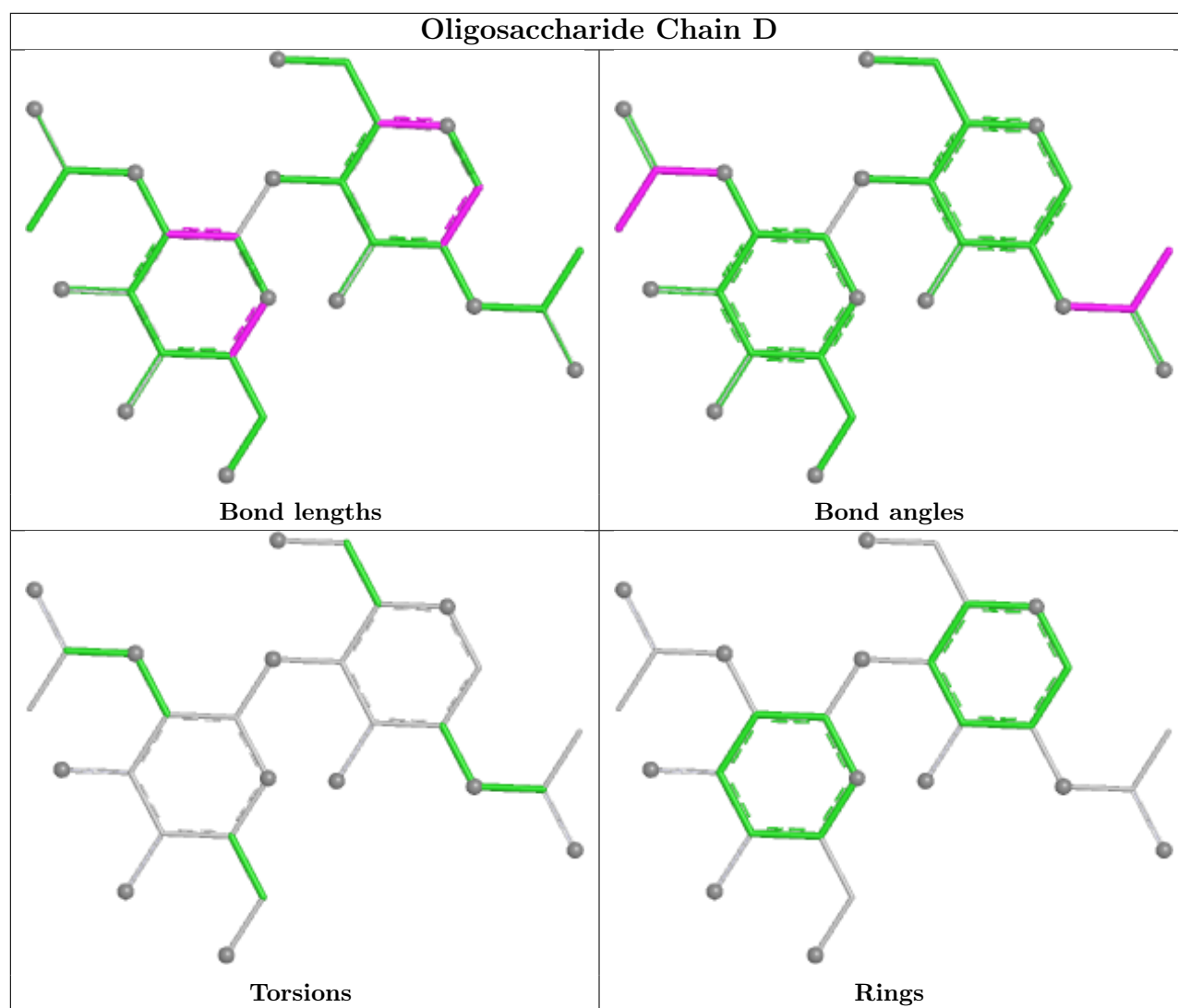
There are no ring outliers.

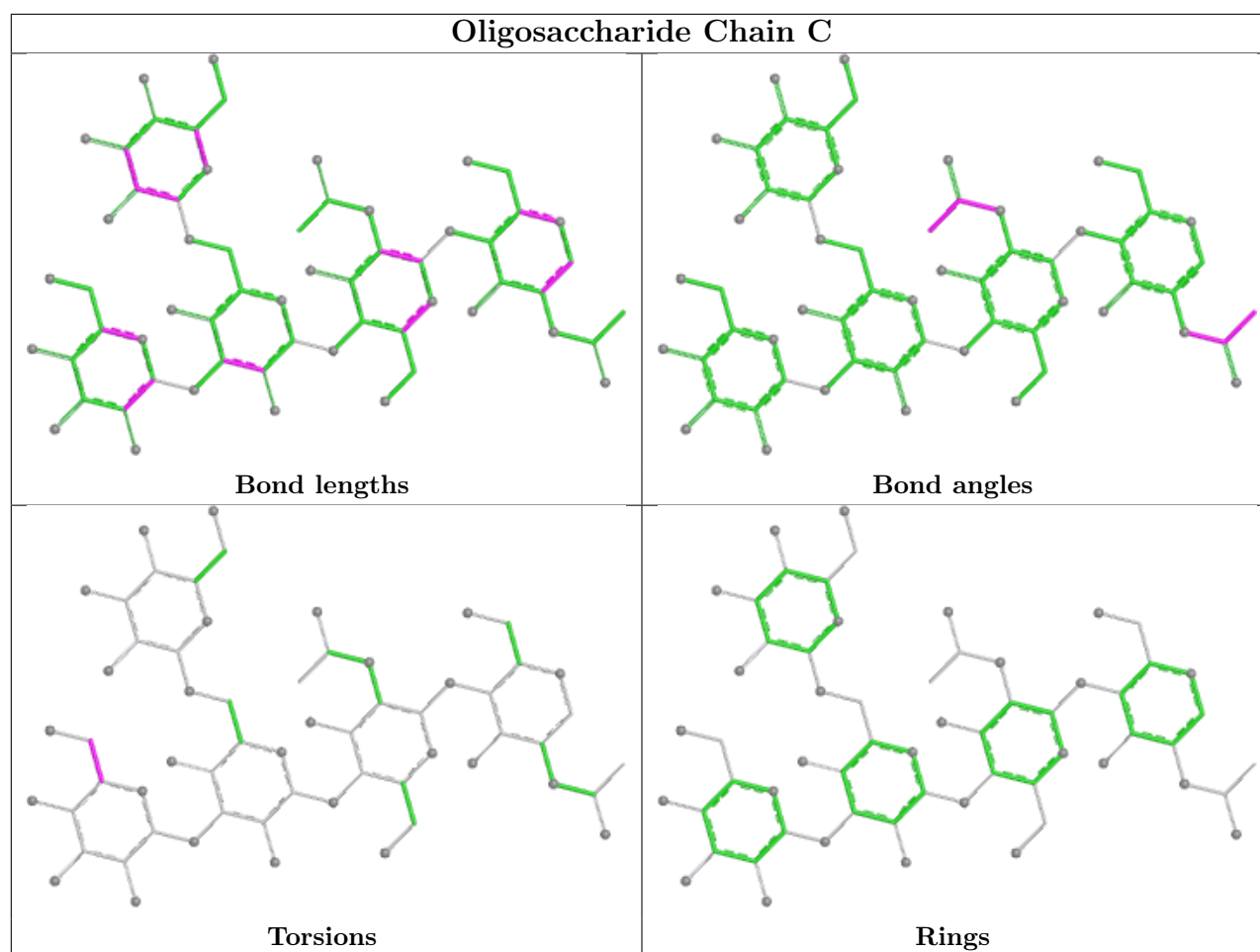
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
5	NAG	A	701	1	14,14,15	1.68	2 (14%)	17,19,21	1.02	1 (5%)
5	NAG	A	702	1	14,14,15	1.79	2 (14%)	17,19,21	1.07	2 (11%)
5	NAG	A	703	1	14,14,15	1.53	2 (14%)	17,19,21	1.01	1 (5%)
5	NAG	B	601	2	14,14,15	1.62	2 (14%)	17,19,21	0.85	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
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	NAG	A	702	1	-	0/6/23/26	0/1/1/1
5	NAG	A	703	1	-	0/6/23/26	0/1/1/1
5	NAG	B	601	2	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	NAG	C1-C2	5.11	1.59	1.52
5	A	701	NAG	C1-C2	4.61	1.58	1.52
5	B	601	NAG	C1-C2	4.32	1.58	1.52
5	A	703	NAG	C1-C2	4.04	1.57	1.52
5	A	701	NAG	O5-C5	2.55	1.48	1.43
5	B	601	NAG	O5-C5	2.39	1.48	1.43
5	A	703	NAG	O5-C5	2.37	1.48	1.43
5	A	702	NAG	O5-C5	2.34	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	NAG	C8-C7-N2	2.80	120.76	116.12
5	A	703	NAG	C8-C7-N2	2.63	120.48	116.12
5	A	702	NAG	C1-C2-N2	-2.21	106.96	110.43
5	B	601	NAG	C8-C7-N2	2.11	119.61	116.12
5	A	702	NAG	C8-C7-N2	2.04	119.50	116.12

There are no chirality outliers.

There are no torsion outliers.

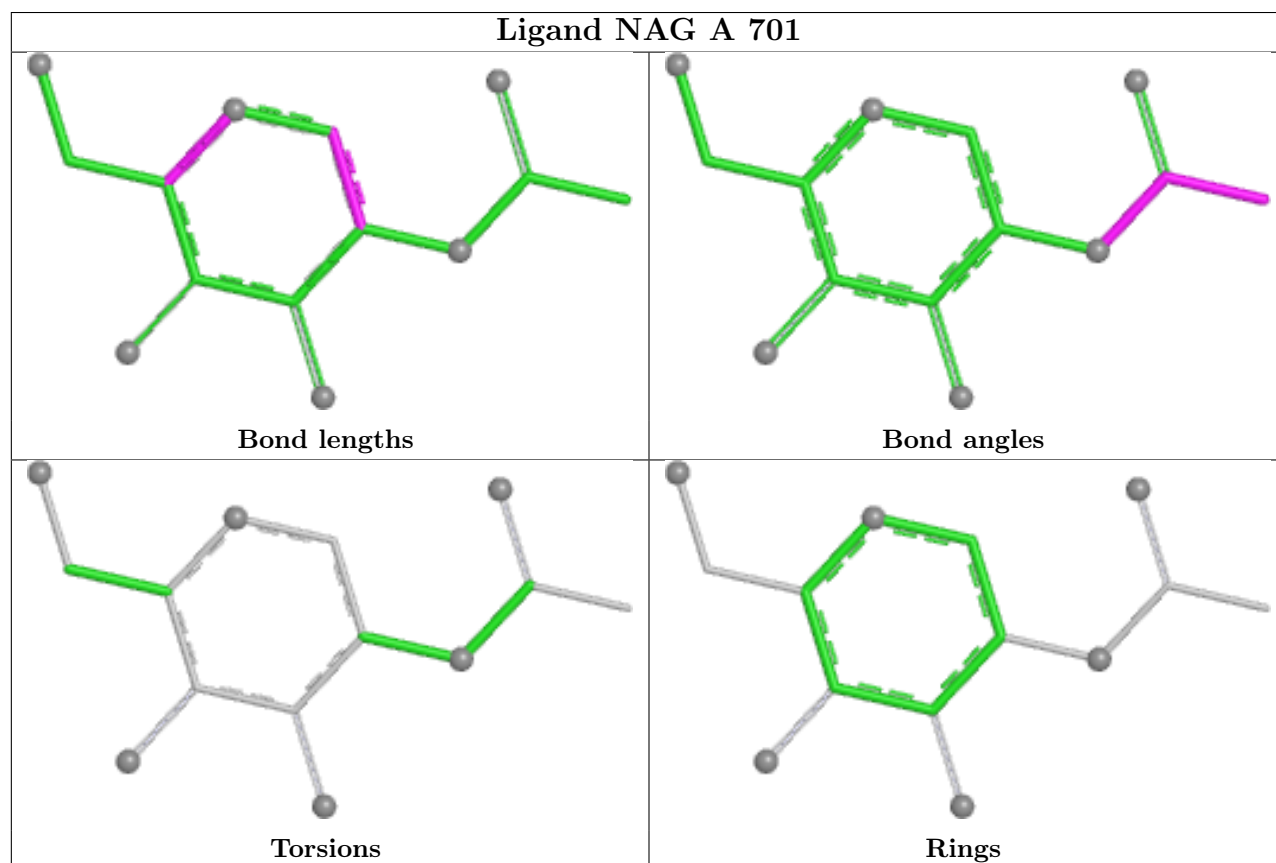
There are no ring outliers.

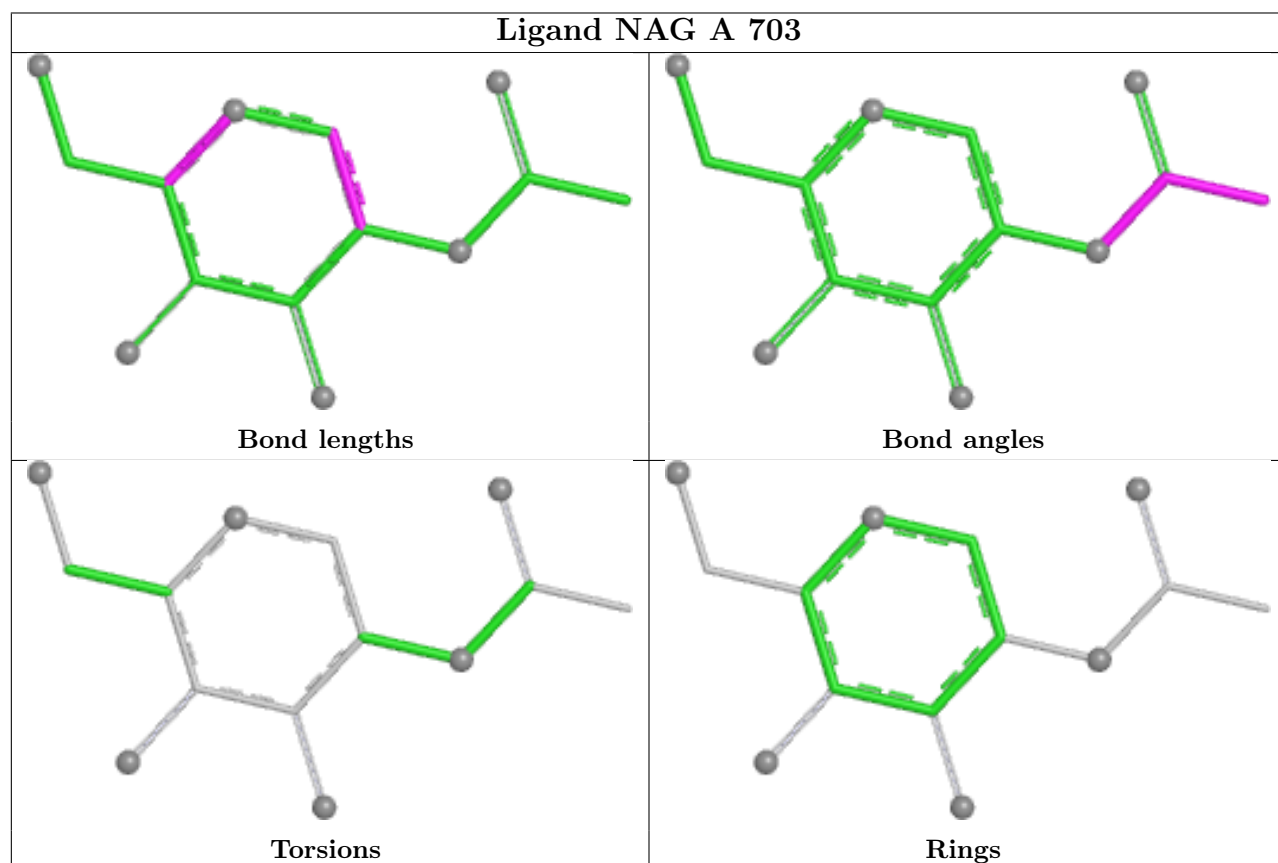
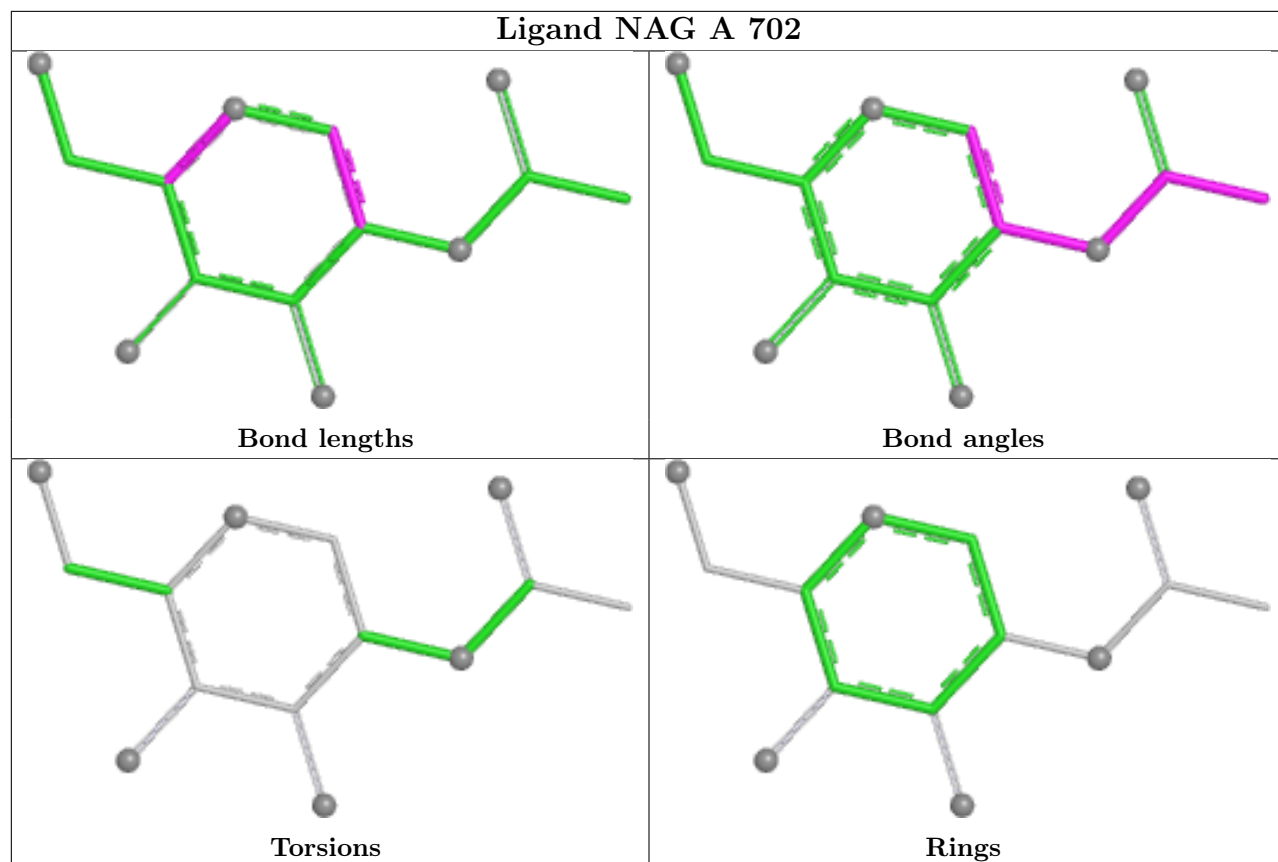
1 monomer is involved in 1 short contact:

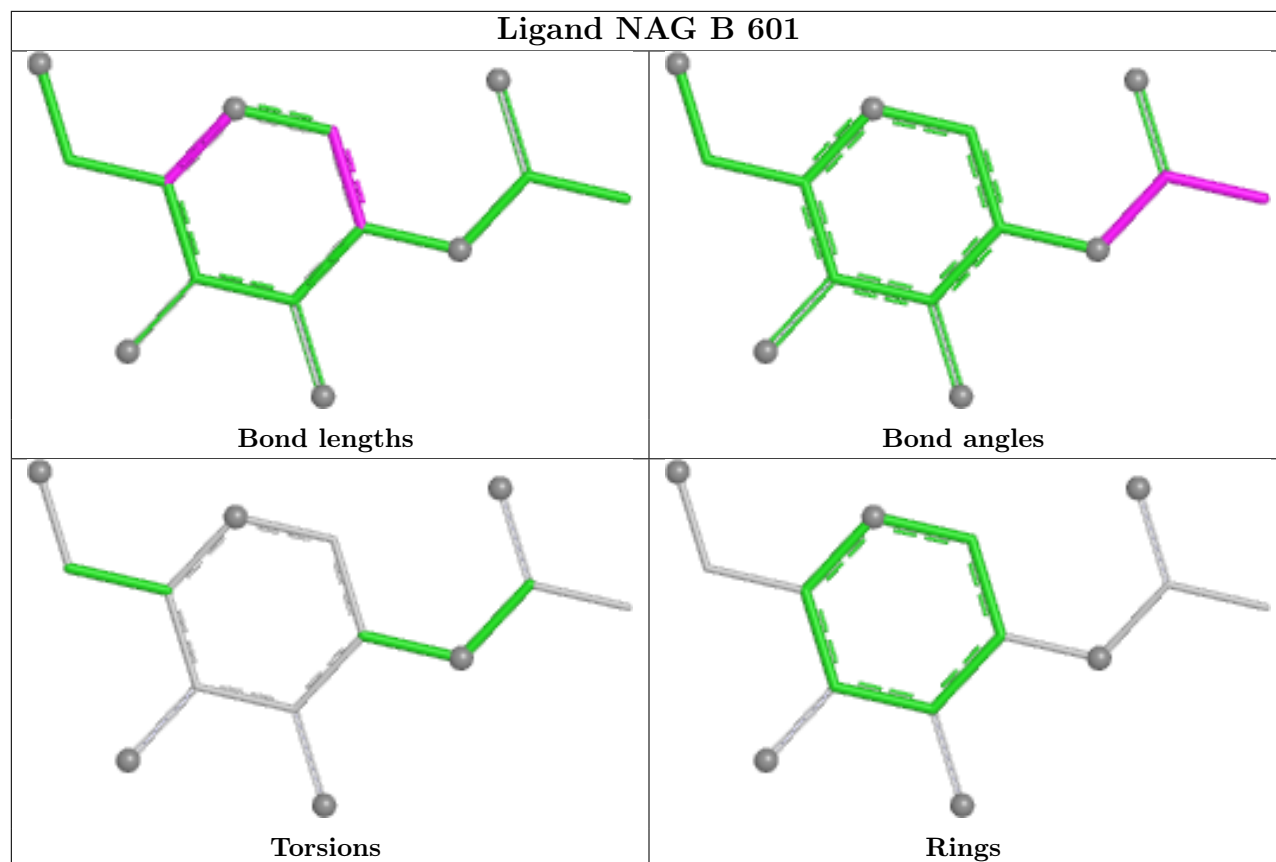
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	NAG	1	0

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

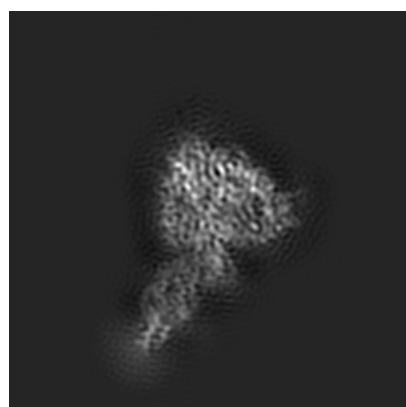
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32693. These allow visual inspection of the internal detail of the map and identification of artifacts.

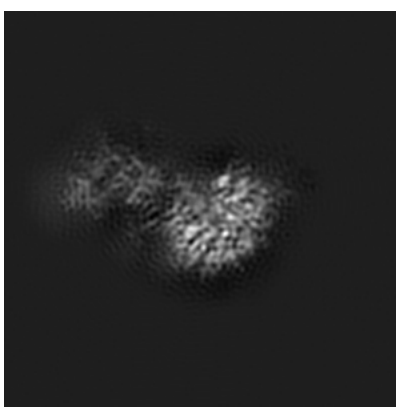
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

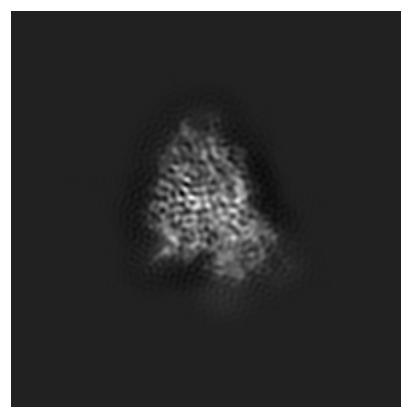
6.1.1 Primary map



X



Y

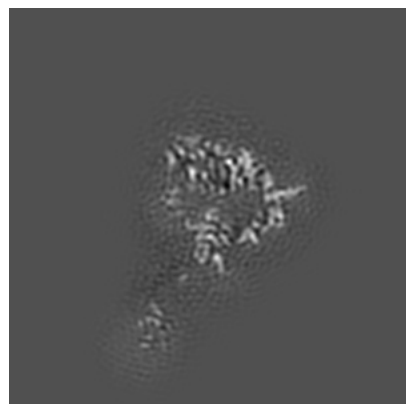


Z

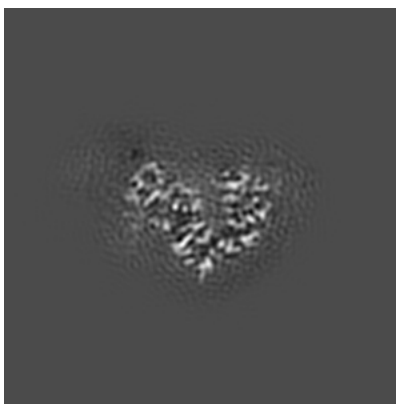
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128

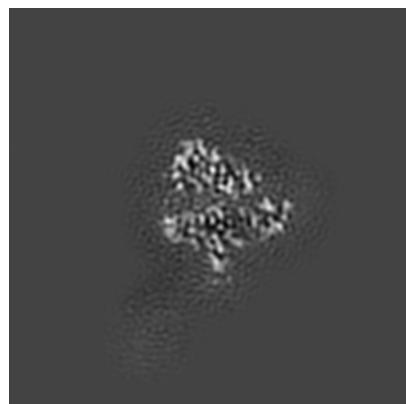


Z Index: 128

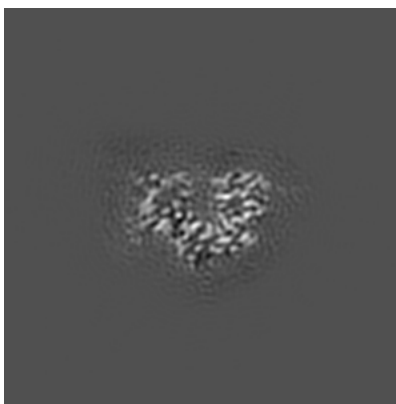
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 118



Y Index: 135

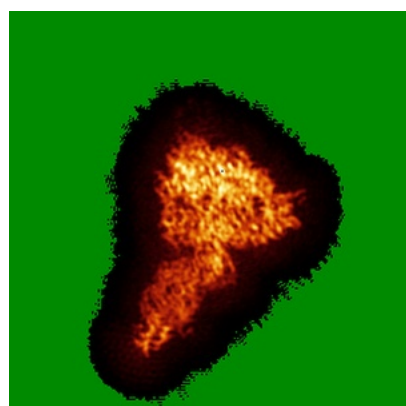


Z Index: 142

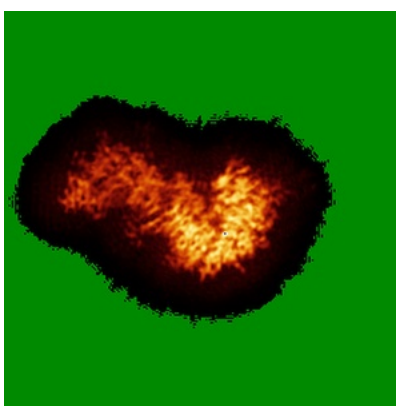
The images above show the largest variance slices of the map in three orthogonal directions.

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

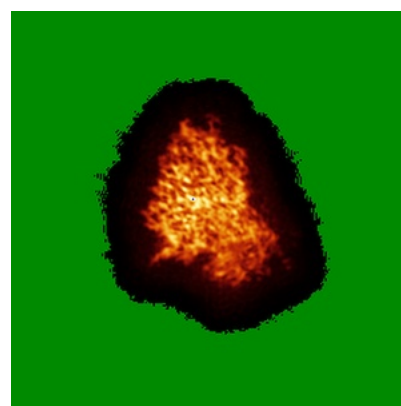
6.4.1 Primary map



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

This section was not generated.

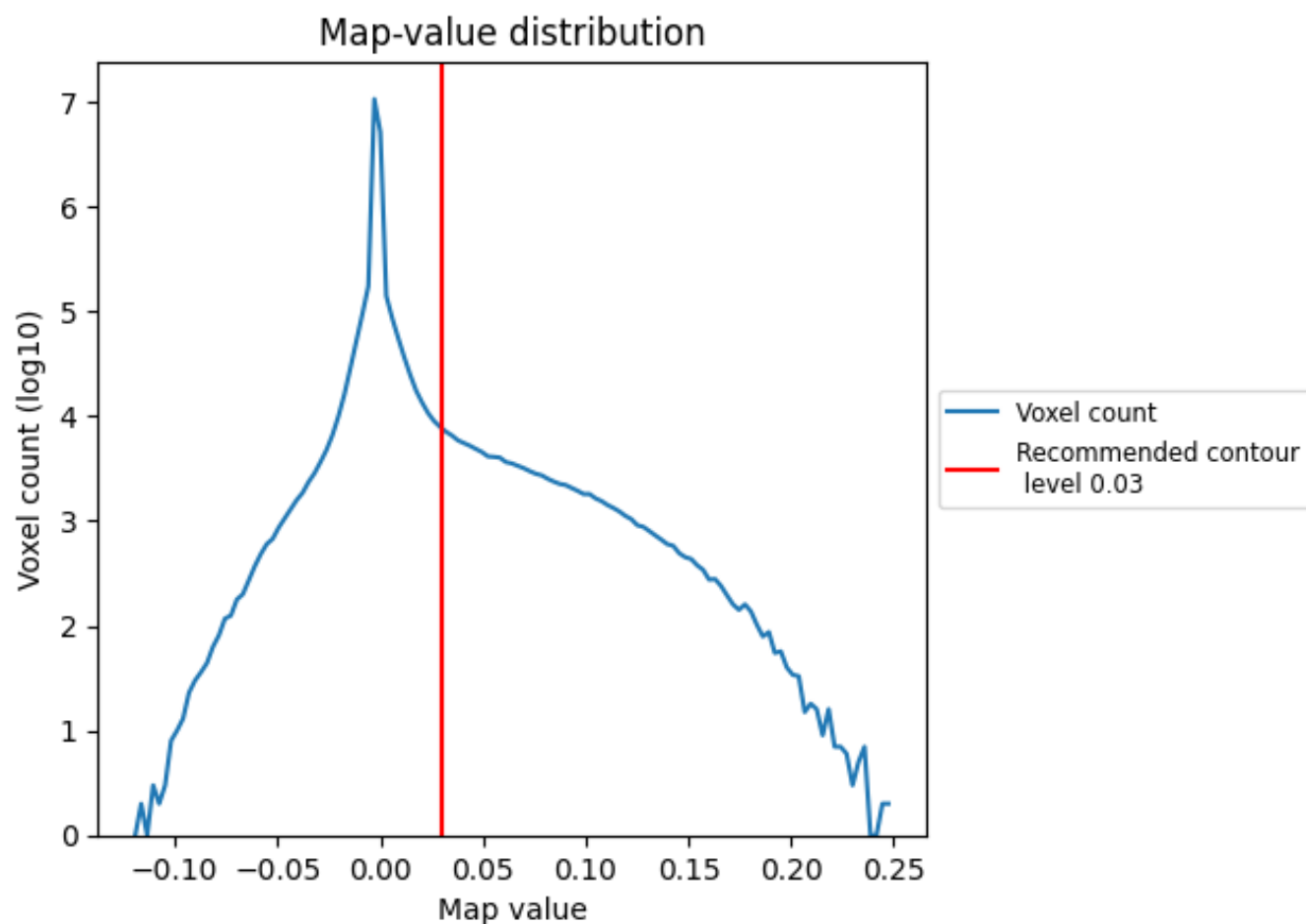
6.6 Mask visualisation

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

7 Map analysis [i](#)

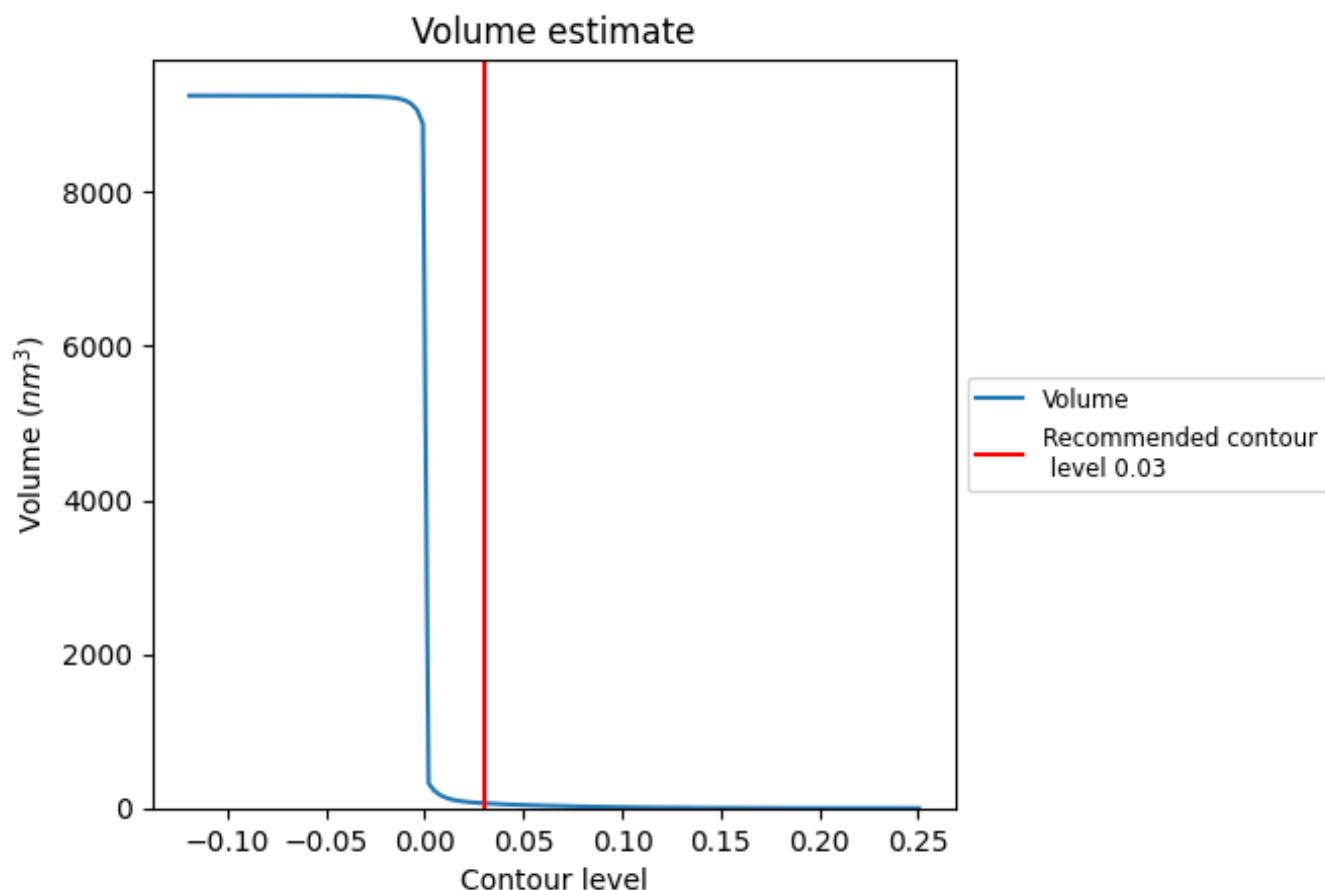
This section contains the results of statistical analysis of the map.

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.

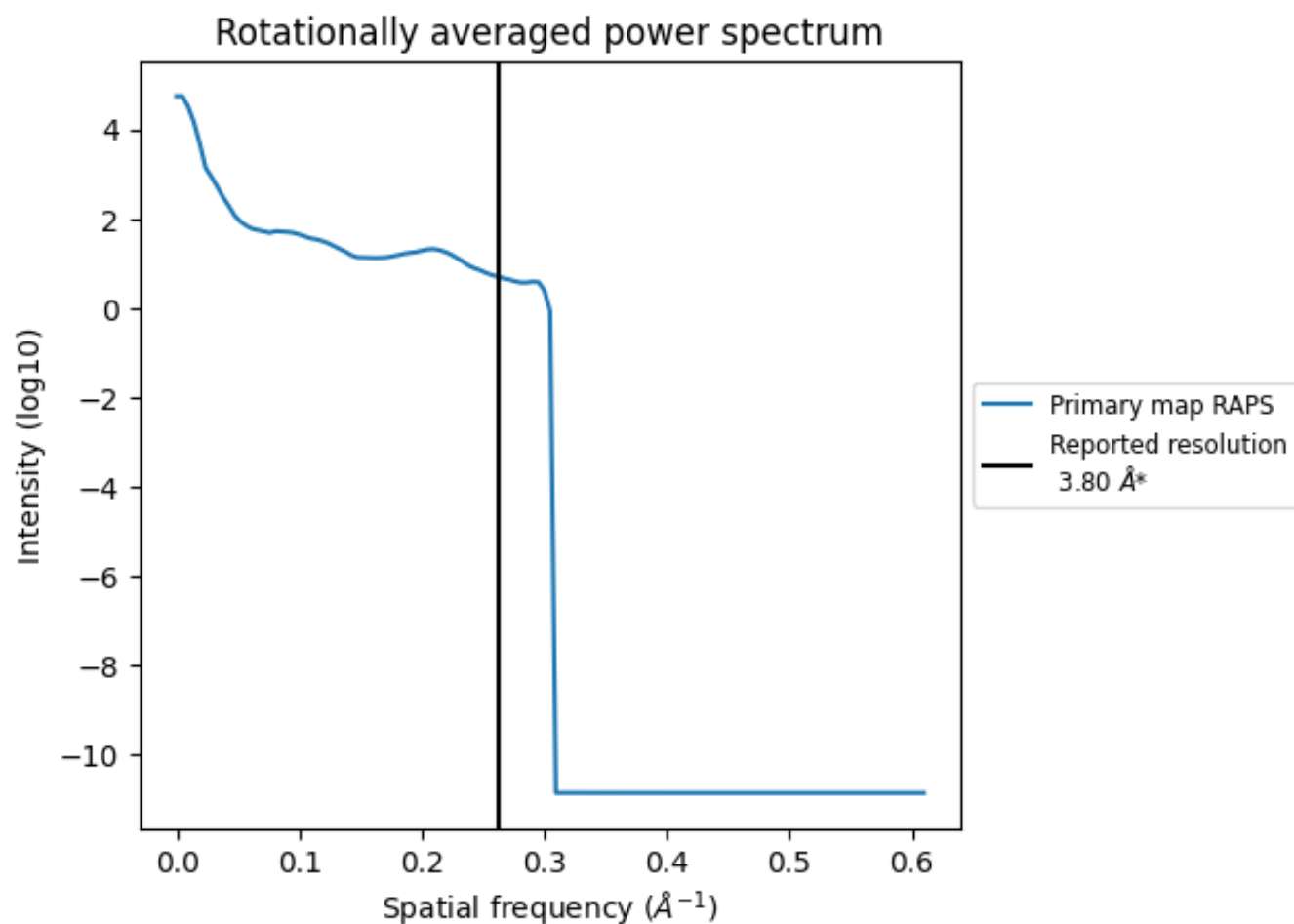
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 58 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 $0.263 \text{ \AA}^{-1}$

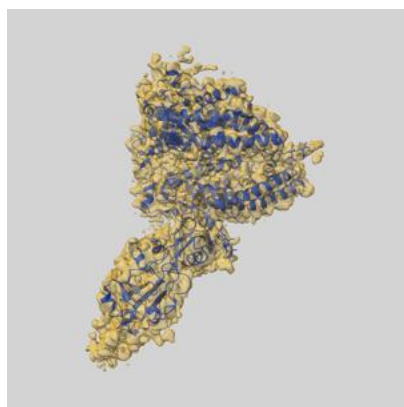
8 Fourier-Shell correlation ⓘ

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

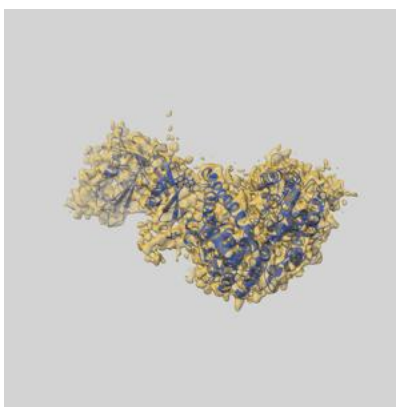
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32693 and PDB model 7WPZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

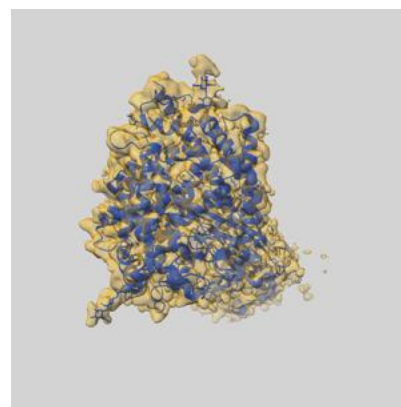
9.1 Map-model overlay [i](#)



X



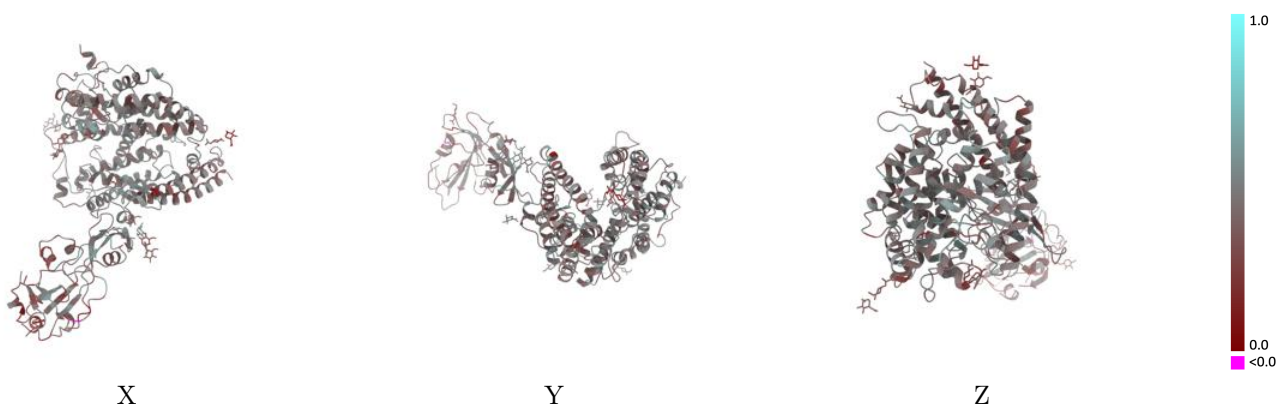
Y



Z

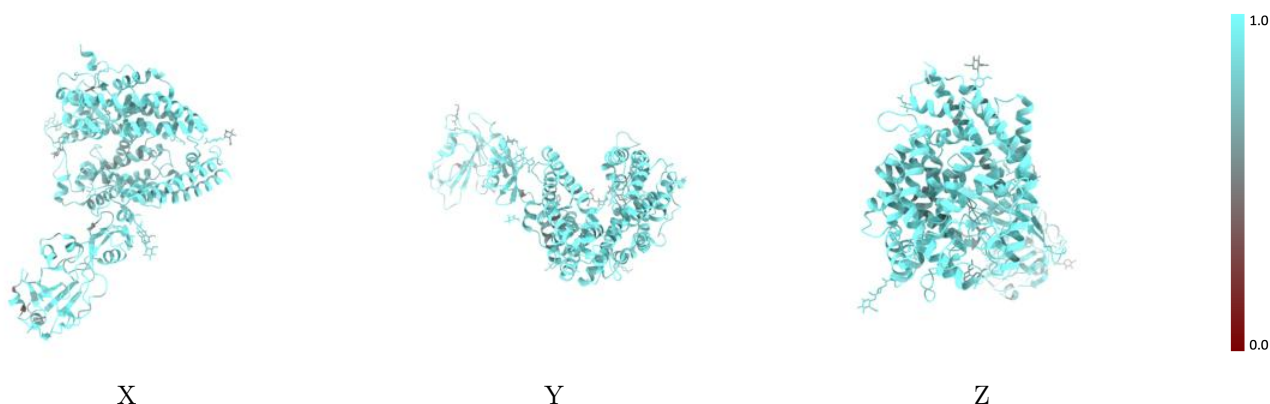
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



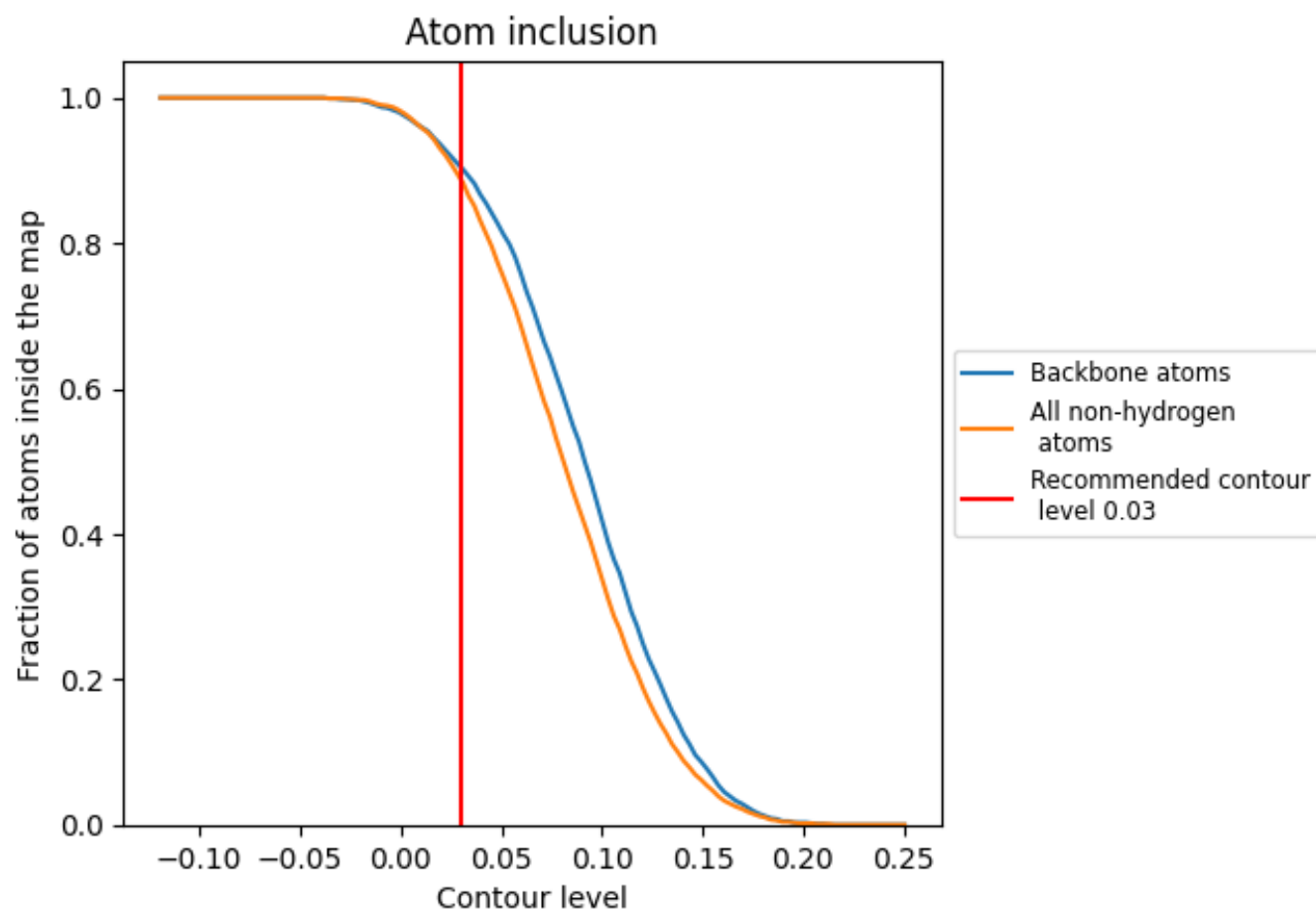
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.4270
A	0.9010	0.4380
B	0.8560	0.3950
C	0.8030	0.3930
D	0.7140	0.2080
E	0.6070	0.2820
J	0.7860	0.3490

1.0

0.0

<0.0