



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 09:52 AM EST

PDB ID : 6UE7  
EMDB ID : EMD-20749  
Title : Structure of dimeric sIgA complex  
Authors : Kumar, N.; Arthur, C.P.; Ciferri, C.; Matsumoto, M.L.  
Deposited on : 2019-09-20  
Resolution : 2.90 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](mailto: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>.

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

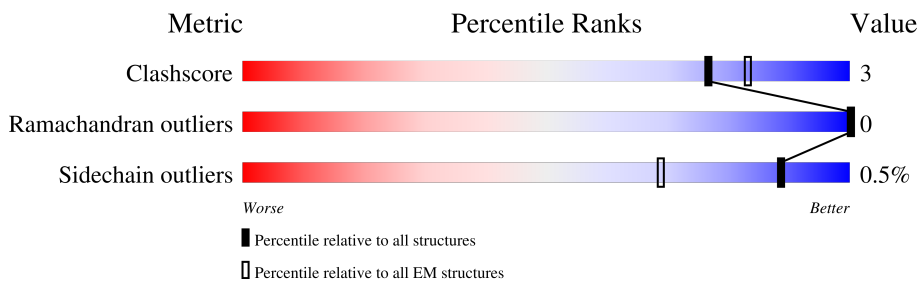
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 2.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	245	79% 11% 9%
1	B	245	88% 6% 6%
1	F	245	86% 8% 6%
1	G	245	87% 9%
2	C	591	84% 7% 10%
3	D	137	93% . .
4	E	3	100%
5	H	2	100%

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Mol	Chain	Length	Quality of chain	
5	I	2	 50%	 50%
5	J	2	 50%	 50%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11701 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 Immunoglobulin heavy constant alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	222	1559	991	267	293	8	0	0
1	B	230	1621	1025	277	310	9	0	0
1	F	231	1632	1036	280	306	10	0	0
1	G	223	1556	990	264	294	8	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ASP	-	expression tag	UNP P01876
A	229	TYR	-	expression tag	UNP P01876
A	230	LYS	-	expression tag	UNP P01876
A	231	ASP	-	expression tag	UNP P01876
A	232	ASP	-	expression tag	UNP P01876
A	233	ASP	-	expression tag	UNP P01876
A	234	ASP	-	expression tag	UNP P01876
A	235	LYS	-	expression tag	UNP P01876
A	236	LEU	-	expression tag	UNP P01876
A	237	VAL	-	expression tag	UNP P01876
A	238	PRO	-	expression tag	UNP P01876
A	239	ARG	-	expression tag	UNP P01876
A	240	GLY	-	expression tag	UNP P01876
A	241	SER	-	expression tag	UNP P01876
B	228	ASP	-	expression tag	UNP P01876
B	229	TYR	-	expression tag	UNP P01876
B	230	LYS	-	expression tag	UNP P01876
B	231	ASP	-	expression tag	UNP P01876
B	232	ASP	-	expression tag	UNP P01876
B	233	ASP	-	expression tag	UNP P01876
B	234	ASP	-	expression tag	UNP P01876
B	235	LYS	-	expression tag	UNP P01876

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Chain	Residue	Modelled	Actual	Comment	Reference
B	236	LEU	-	expression tag	UNP P01876
B	237	VAL	-	expression tag	UNP P01876
B	238	PRO	-	expression tag	UNP P01876
B	239	ARG	-	expression tag	UNP P01876
B	240	GLY	-	expression tag	UNP P01876
B	241	SER	-	expression tag	UNP P01876
F	228	ASP	-	expression tag	UNP P01876
F	229	TYR	-	expression tag	UNP P01876
F	230	LYS	-	expression tag	UNP P01876
F	231	ASP	-	expression tag	UNP P01876
F	232	ASP	-	expression tag	UNP P01876
F	233	ASP	-	expression tag	UNP P01876
F	234	ASP	-	expression tag	UNP P01876
F	235	LYS	-	expression tag	UNP P01876
F	236	LEU	-	expression tag	UNP P01876
F	237	VAL	-	expression tag	UNP P01876
F	238	PRO	-	expression tag	UNP P01876
F	239	ARG	-	expression tag	UNP P01876
F	240	GLY	-	expression tag	UNP P01876
F	241	SER	-	expression tag	UNP P01876
G	228	ASP	-	expression tag	UNP P01876
G	229	TYR	-	expression tag	UNP P01876
G	230	LYS	-	expression tag	UNP P01876
G	231	ASP	-	expression tag	UNP P01876
G	232	ASP	-	expression tag	UNP P01876
G	233	ASP	-	expression tag	UNP P01876
G	234	ASP	-	expression tag	UNP P01876
G	235	LYS	-	expression tag	UNP P01876
G	236	LEU	-	expression tag	UNP P01876
G	237	VAL	-	expression tag	UNP P01876
G	238	PRO	-	expression tag	UNP P01876
G	239	ARG	-	expression tag	UNP P01876
G	240	GLY	-	expression tag	UNP P01876
G	241	SER	-	expression tag	UNP P01876

- Molecule 2 is a protein called Polymeric immunoglobulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	534	4109	2588	709	792	20	0	0

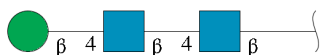
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	586	HIS	-	expression tag	UNP P01833
C	587	HIS	-	expression tag	UNP P01833
C	588	HIS	-	expression tag	UNP P01833
C	589	HIS	-	expression tag	UNP P01833
C	590	HIS	-	expression tag	UNP P01833
C	591	HIS	-	expression tag	UNP P01833

- Molecule 3 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	131	1003	622	179	193	9	0	0

- Molecule 4 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	N	O		
4	E	3	39	22	2	15	0	0

- Molecule 5 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
			Total	C	N	O		
5	H	2	28	16	2	10	0	0
5	I	2	28	16	2	10	0	0
5	J	2	28	16	2	10	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

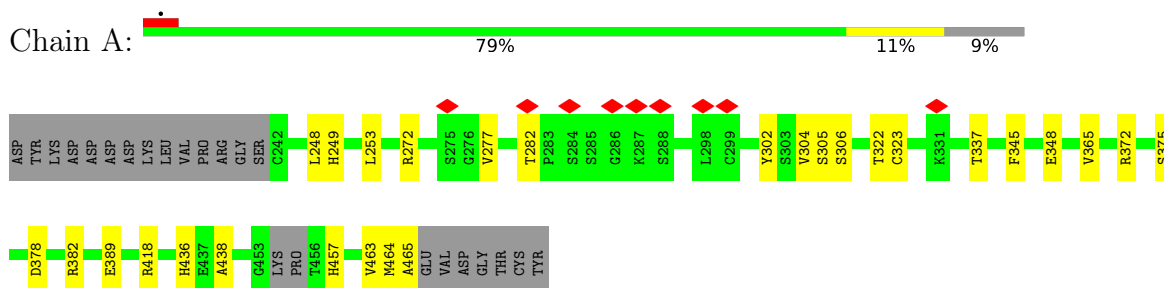


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	Total 14	8	1	5	0
6	B	1	Total 28	16	2	10	0
6	B	1	Total 28	16	2	10	0
6	C	1	Total 56	32	4	20	0
6	C	1	Total 56	32	4	20	0
6	C	1	Total 56	32	4	20	0
6	C	1	Total 56	32	4	20	0

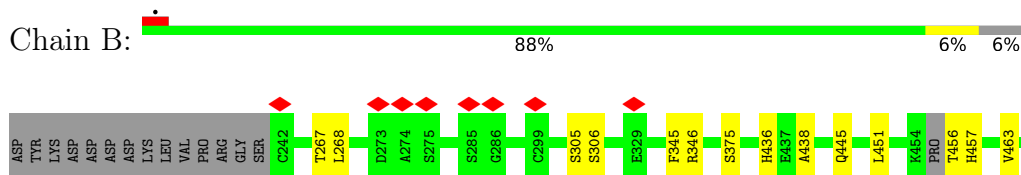
### 3 Residue-property plots [i](#)

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.

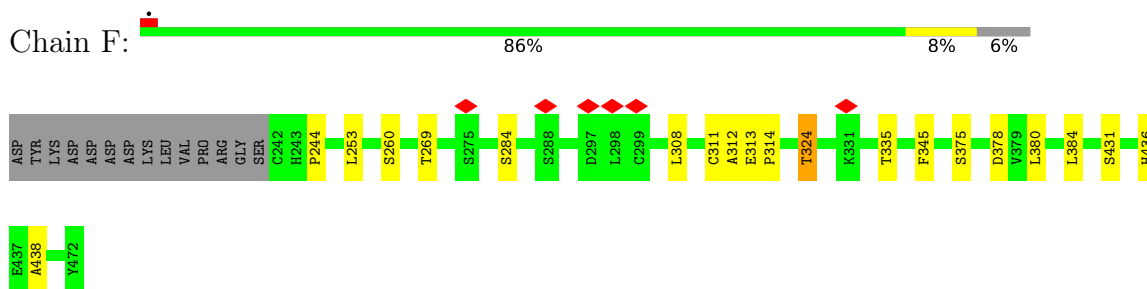
- Molecule 1: Immunoglobulin heavy constant alpha 1



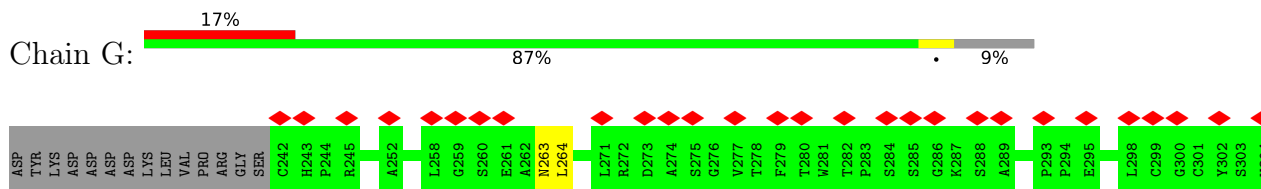
- Molecule 1: Immunoglobulin heavy constant alpha 1



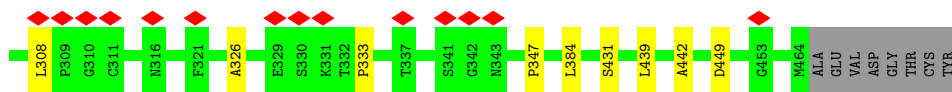
- Molecule 1: Immunoglobulin heavy constant alpha 1



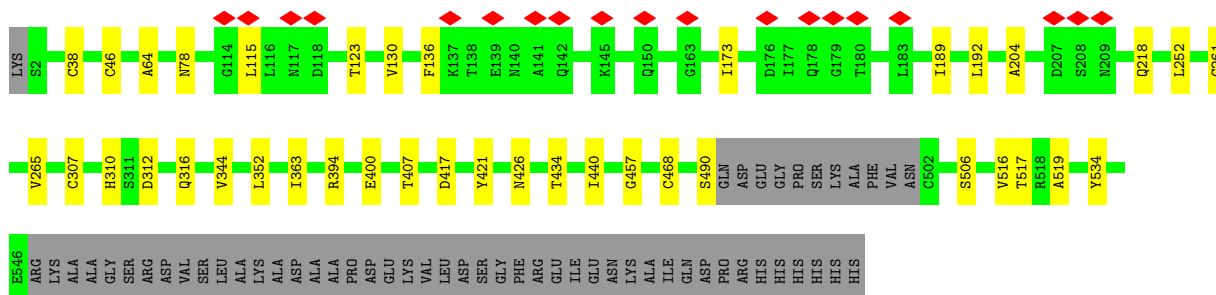
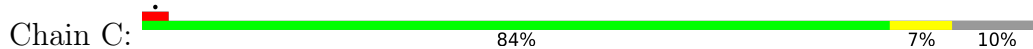
- Molecule 1: Immunoglobulin heavy constant alpha 1



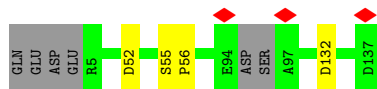




- Molecule 2: Polymeric immunoglobulin receptor



- Molecule 3: Immunoglobulin J chain



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

  
MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	233402	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 ( $e^-/\text{\AA}^2$ )	51.91	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	19.459	Depositor
Minimum map value	-7.666	Depositor
Average map value	-0.014	Depositor
Map value standard deviation	0.361	Depositor
Recommended contour level	3.2	Depositor
Map size (Å)	391.2192, 391.2192, 391.2192	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0188, 1.0188, 1.0188	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, 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	0.35	0/1598	0.59	1/2204 (0.0%)
1	B	0.32	0/1661	0.59	0/2291
1	F	0.36	0/1674	0.58	0/2308
1	G	0.31	0/1597	0.60	0/2208
2	C	0.36	0/4198	0.58	1/5708 (0.0%)
3	D	0.36	0/1017	0.58	0/1387
All	All	0.35	0/11745	0.58	2/16106 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	115	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	464	MET	CA-CB-CG	5.53	122.70	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	55	SER	Peptide

## 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	1559	0	1438	16	0
1	B	1621	0	1482	11	0
1	F	1632	0	1512	16	0
1	G	1556	0	1422	6	0
2	C	4109	0	3986	19	0
3	D	1003	0	982	3	0
4	E	39	0	34	0	0
5	H	28	0	25	0	0
5	I	28	0	25	1	0
5	J	28	0	25	0	0
6	A	14	0	13	0	0
6	B	28	0	26	0	0
6	C	56	0	52	0	0
All	All	11701	0	11022	67	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 3.

All (67) 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)
5:I:1:NAG:O7	5:I:1:NAG:O3	2.05	0.72
1:F:244:PRO:HA	1:F:269:THR:O	1.92	0.70
1:F:260:SER:HA	1:F:312:ALA:HB2	1.77	0.65
1:F:308:LEU:O	1:F:308:LEU:HG	1.98	0.63
1:A:277:VAL:HG21	1:A:304:VAL:HG11	1.81	0.62
1:F:260:SER:CB	1:F:312:ALA:CB	2.82	0.57
1:B:445:GLN:NE2	3:D:52:ASP:OD2	2.37	0.57
1:F:260:SER:CA	1:F:312:ALA:HB2	2.36	0.56
1:B:456:THR:OG1	1:B:457:HIS:N	2.38	0.56
1:F:378:ASP:N	1:F:378:ASP:OD1	2.36	0.55
1:F:260:SER:CB	1:F:312:ALA:HB2	2.37	0.55
1:F:324:THR:HG23	1:F:335:THR:HG22	1.89	0.54
1:G:263:ASN:ND2	1:G:308:LEU:O	2.40	0.54
1:A:322:THR:HG22	1:A:337:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:HIS:ND1	2:C:312:ASP:OD1	2.42	0.52
2:C:400:GLU:HG2	2:C:534:TYR:HE1	1.75	0.51
2:C:457:GLY:H	2:C:516:VAL:HG23	1.75	0.51
1:A:282:THR:OG1	1:A:322:THR:OG1	2.28	0.50
2:C:123:THR:HG22	2:C:218:GLN:HB2	1.94	0.50
1:F:384:LEU:HB2	1:F:431:SER:HB3	1.93	0.50
1:A:463:VAL:HG12	1:A:465:ALA:H	1.76	0.49
1:B:346:ARG:NH2	3:D:132:ASP:OD1	2.44	0.49
1:A:348:GLU:OE1	1:A:372:ARG:NH2	2.43	0.49
2:C:517:THR:HG23	2:C:519:ALA:H	1.77	0.49
1:A:463:VAL:HB	1:B:463:VAL:HA	1.95	0.48
1:F:313:GLU:CB	1:F:314:PRO:CD	2.91	0.48
1:B:345:PHE:HD2	1:B:375:SER:HB2	1.78	0.48
1:A:382:ARG:NH1	1:A:389:GLU:OE2	2.41	0.48
1:A:272:ARG:H	1:A:302:TYR:H	1.62	0.47
1:G:347:PRO:HD2	1:G:439:LEU:HD21	1.95	0.47
1:A:248:LEU:O	1:A:249:HIS:ND1	2.47	0.47
1:F:284:SER:O	1:F:284:SER:OG	2.31	0.47
2:C:252:LEU:HB3	2:C:265:VAL:HG12	1.96	0.47
1:F:436:HIS:CD2	1:F:438:ALA:H	2.32	0.47
2:C:421:TYR:O	2:C:434:THR:HA	2.14	0.47
1:B:451:LEU:HD12	3:D:56:PRO:HB2	1.97	0.47
1:B:305:SER:OG	1:B:306:SER:N	2.46	0.46
2:C:173:ILE:HG13	2:C:189:ILE:HG12	1.97	0.46
1:F:253:LEU:HD23	1:F:380:LEU:HG	1.97	0.46
2:C:130:VAL:HG12	2:C:192:LEU:HD21	1.96	0.46
2:C:352:LEU:HD23	2:C:407:THR:HG22	1.98	0.46
2:C:363:ILE:HB	2:C:426:ASN:HD22	1.81	0.46
1:A:248:LEU:HD11	1:A:323:CYS:HB3	1.98	0.46
2:C:64:ALA:HA	2:C:78:ASN:O	2.16	0.46
1:A:305:SER:OG	1:A:306:SER:N	2.49	0.45
1:A:345:PHE:HD2	1:A:375:SER:HB2	1.81	0.45
2:C:506:SER:O	2:C:506:SER:OG	2.32	0.44
2:C:136:PHE:HB2	2:C:204:ALA:HB2	1.99	0.43
2:C:344:VAL:HG12	2:C:440:ILE:HG13	1.98	0.43
1:A:253:LEU:HD22	1:A:378:ASP:HB3	1.99	0.43
2:C:312:ASP:OD2	2:C:316:GLN:NE2	2.46	0.43
1:B:436:HIS:CD2	1:B:438:ALA:H	2.36	0.43
2:C:394:ARG:NH2	2:C:417:ASP:OD2	2.52	0.43
1:G:439:LEU:HB2	1:G:442:ALA:HA	2.01	0.43
1:G:449:ASP:N	1:G:449:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:O	1:A:418:ARG:HA	2.19	0.42
2:C:490:SER:O	2:C:490:SER:OG	2.37	0.41
1:G:326:ALA:HA	1:G:333:PRO:HB3	2.02	0.41
1:G:384:LEU:HB2	1:G:431:SER:HB3	2.02	0.41
1:A:436:HIS:HD2	1:A:438:ALA:H	1.68	0.41
1:A:457:HIS:HB2	1:B:457:HIS:CD2	2.55	0.41
2:C:38:CYS:HB2	2:C:46:CYS:HB3	1.74	0.41
1:F:260:SER:CB	1:F:312:ALA:HB3	2.50	0.41
1:F:260:SER:CB	1:F:312:ALA:H	2.33	0.41
1:B:468:ASP:OD1	1:B:468:ASP:N	2.39	0.40
1:B:267:THR:OG1	1:B:268:LEU:N	2.55	0.40
1:F:345:PHE:HD2	1:F:375:SER:HB2	1.86	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	218/245 (89%)	198 (91%)	20 (9%)	0	100	100
1	B	226/245 (92%)	203 (90%)	23 (10%)	0	100	100
1	F	229/245 (94%)	203 (89%)	26 (11%)	0	100	100
1	G	221/245 (90%)	192 (87%)	29 (13%)	0	100	100
2	C	530/591 (90%)	488 (92%)	42 (8%)	0	100	100
3	D	127/137 (93%)	109 (86%)	18 (14%)	0	100	100
All	All	1551/1708 (91%)	1393 (90%)	158 (10%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	153/210 (73%)	153 (100%)	0	100	100
1	B	161/210 (77%)	161 (100%)	0	100	100
1	F	162/210 (77%)	160 (99%)	2 (1%)	71	91
1	G	152/210 (72%)	151 (99%)	1 (1%)	84	95
2	C	450/501 (90%)	447 (99%)	3 (1%)	84	95
3	D	114/129 (88%)	114 (100%)	0	100	100
All	All	1192/1470 (81%)	1186 (100%)	6 (0%)	89	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	261	CYS
2	C	307	CYS
2	C	468	CYS
1	F	311	CYS
1	F	324	THR
1	G	264	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	291	GLN
2	C	218	GLN
2	C	412	GLN
2	C	426	ASN
1	F	436	HIS
1	G	263	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

9 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	E	1	4,2	14,14,15	0.80	1 (7%)	17,19,21	0.85	0
4	NAG	E	2	4	14,14,15	0.26	0	17,19,21	1.11	1 (5%)
4	BMA	E	3	4	11,11,12	1.05	2 (18%)	15,15,17	1.57	3 (20%)
5	NAG	H	1	2,5	14,14,15	0.28	0	17,19,21	1.10	2 (11%)
5	NAG	H	2	5	14,14,15	0.41	0	17,19,21	1.00	1 (5%)
5	NAG	I	1	1,5	14,14,15	0.79	0	17,19,21	1.62	3 (17%)
5	NAG	I	2	5	14,14,15	0.32	0	17,19,21	0.44	0
5	NAG	J	1	3,5	14,14,15	0.41	0	17,19,21	0.70	1 (5%)
5	NAG	J	2	5	14,14,15	0.41	0	17,19,21	0.38	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
4	NAG	E	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	3,5	-	2/6/23/26	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	O5-C1	-2.64	1.39	1.43
4	E	3	BMA	C1-C2	2.37	1.57	1.52
4	E	3	BMA	C2-C3	2.35	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C1-C2-N2	-3.95	103.73	110.49
4	E	3	BMA	C1-O5-C5	3.94	117.53	112.19
5	H	1	NAG	C2-N2-C7	3.11	127.33	122.90
5	H	2	NAG	C2-N2-C7	3.07	127.28	122.90
4	E	2	NAG	C2-N2-C7	3.04	127.23	122.90
4	E	3	BMA	C1-C2-C3	2.83	113.15	109.67
5	I	1	NAG	C6-C5-C4	-2.56	107.02	113.00
4	E	3	BMA	O5-C1-C2	2.25	114.24	110.77
5	J	1	NAG	C1-O5-C5	2.14	115.09	112.19
5	H	1	NAG	C1-O5-C5	2.10	115.03	112.19
5	I	1	NAG	O5-C1-C2	-2.01	108.11	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

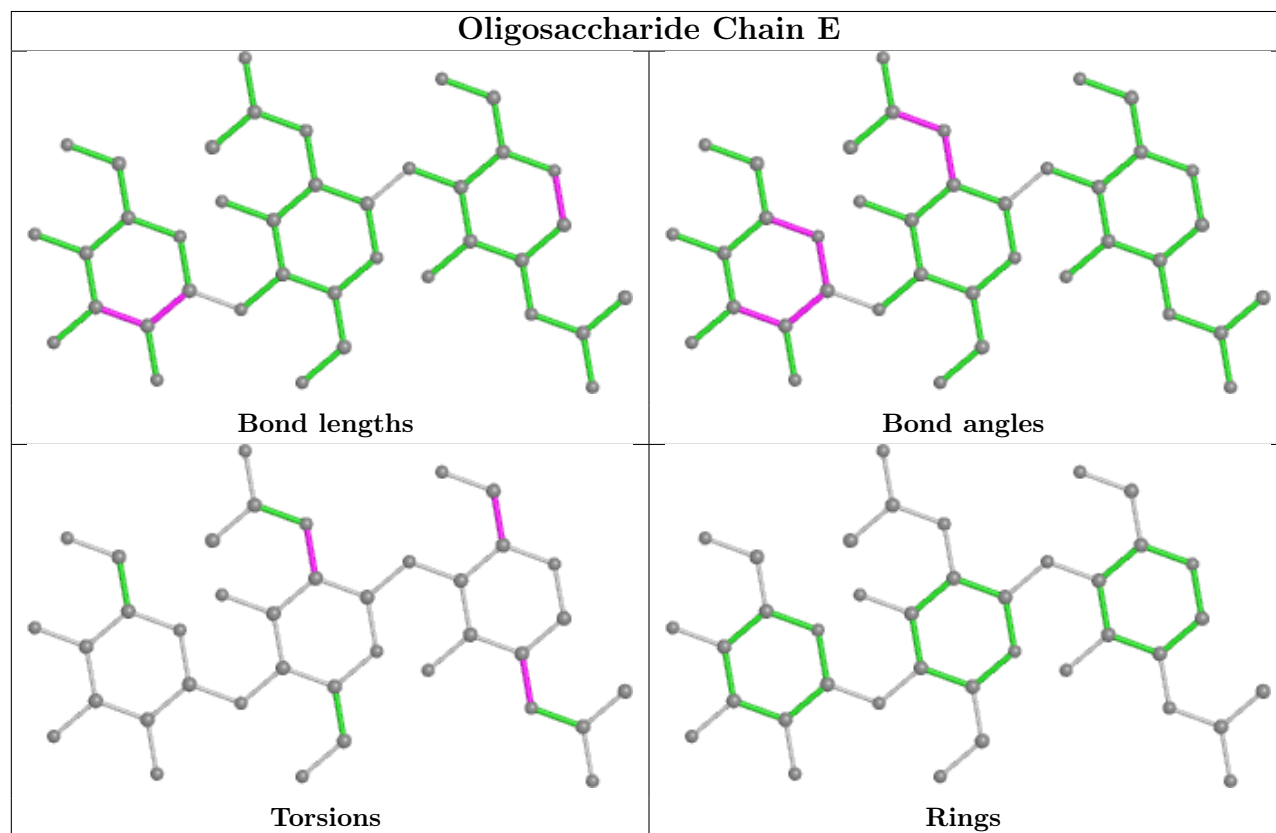
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C3-C2-N2-C7
5	H	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
5	J	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
5	H	1	NAG	C3-C2-N2-C7
5	H	2	NAG	C3-C2-N2-C7

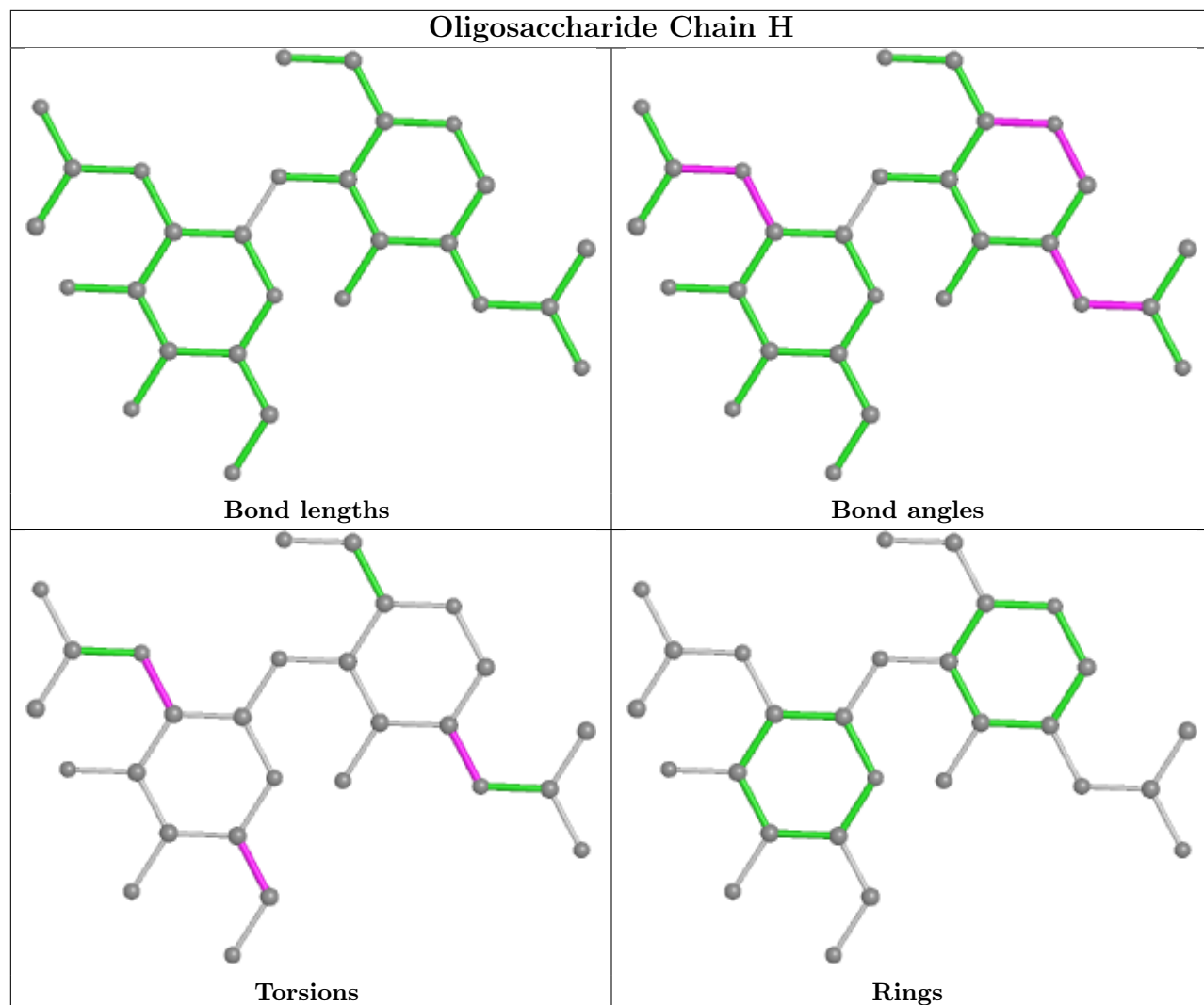
There are no ring outliers.

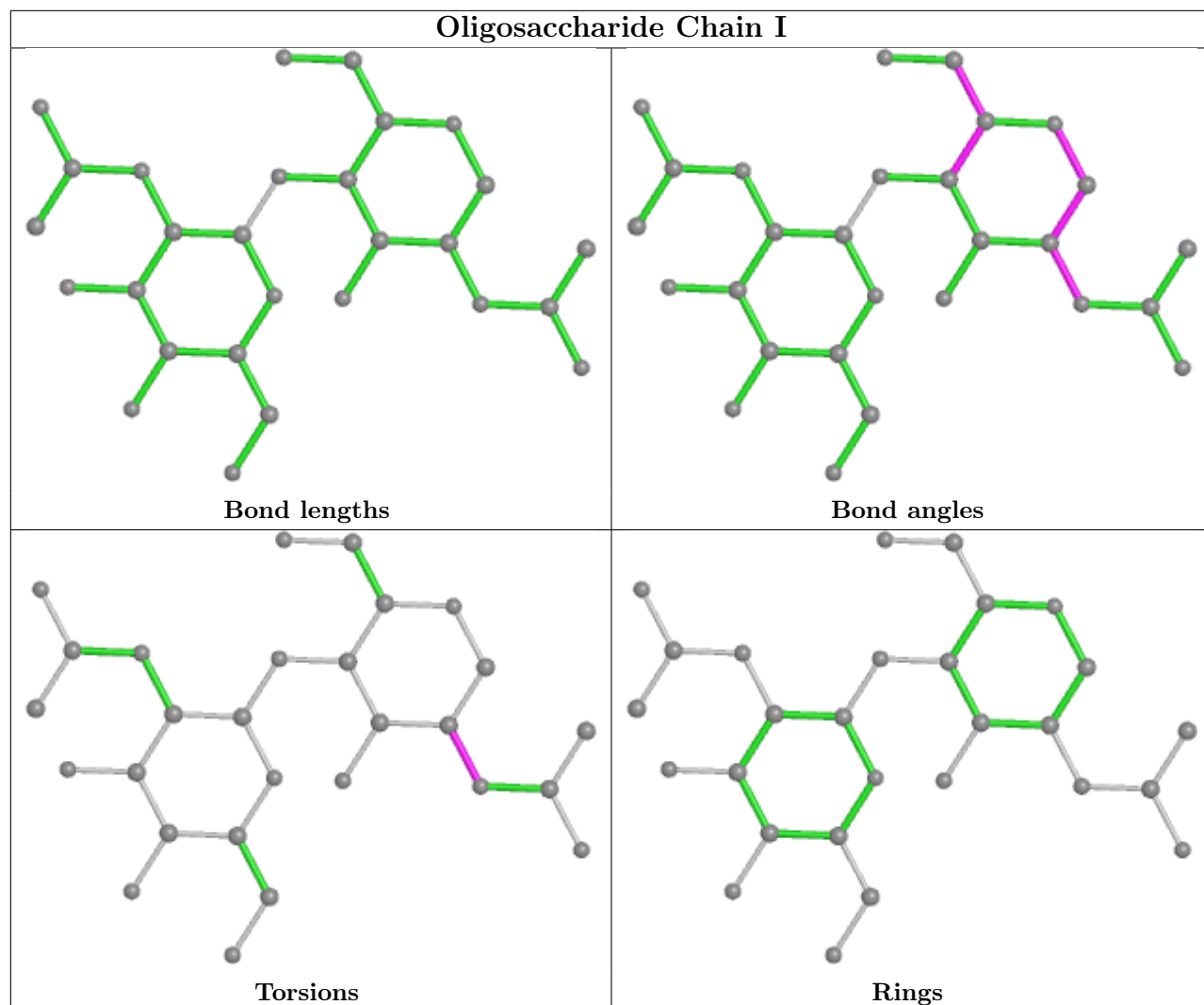
1 monomer is involved in 1 short contact:

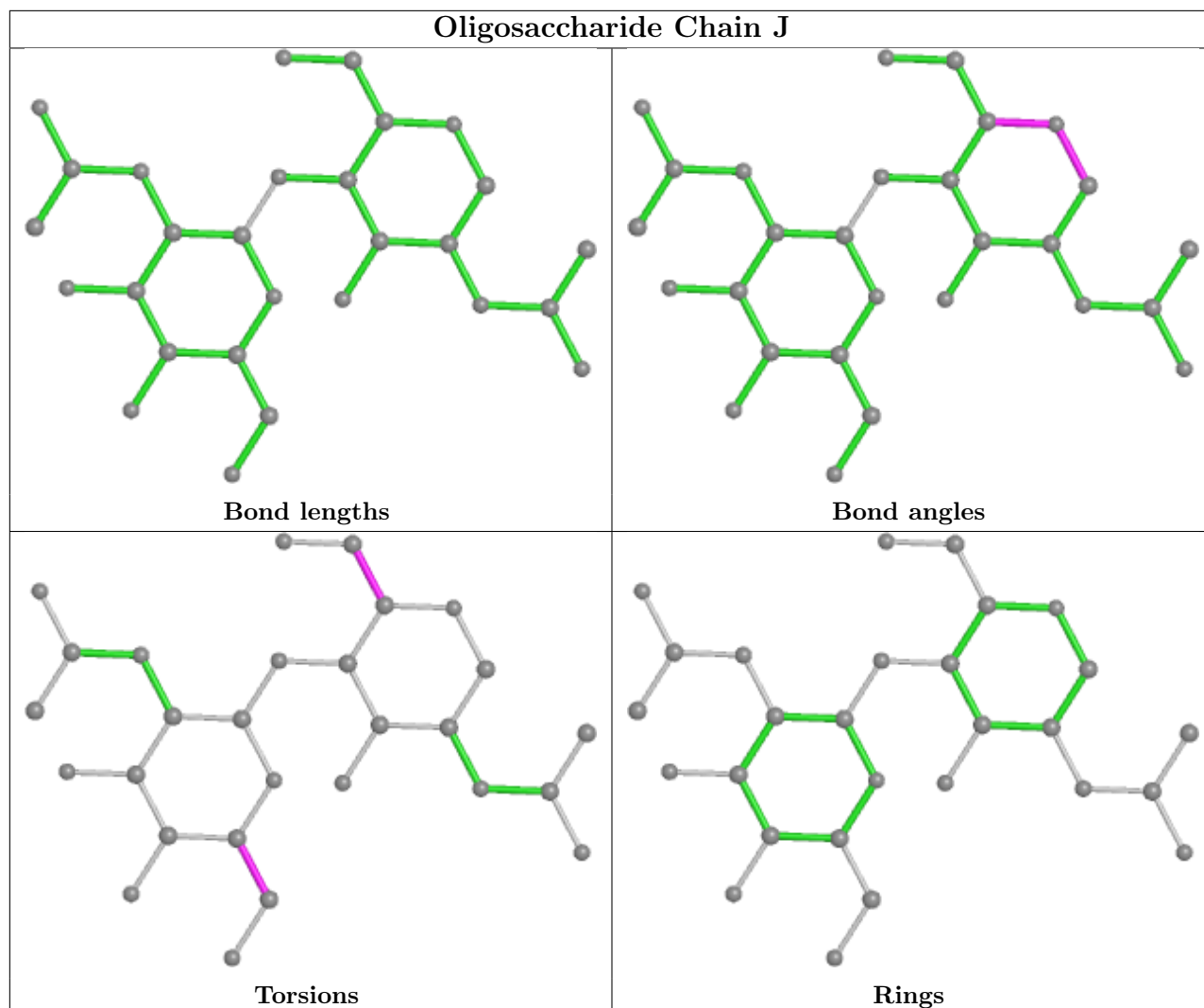
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	1	0

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](#)

7 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	501	1	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
6	NAG	C	605	2	14,14,15	0.52	0	17,19,21	0.61	1 (5%)
6	NAG	C	609	2	14,14,15	0.49	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	B	501	1	14,14,15	0.35	0	17,19,21	0.58	0
6	NAG	B	502	1	14,14,15	0.42	0	17,19,21	0.94	1 (5%)
6	NAG	C	608	2	14,14,15	0.65	0	17,19,21	0.51	0
6	NAG	C	601	2	14,14,15	0.22	0	17,19,21	0.50	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
6	NAG	A	501	1	-	3/6/23/26	0/1/1/1
6	NAG	C	605	2	-	2/6/23/26	0/1/1/1
6	NAG	C	609	2	-	0/6/23/26	0/1/1/1
6	NAG	B	501	1	-	2/6/23/26	0/1/1/1
6	NAG	B	502	1	-	3/6/23/26	0/1/1/1
6	NAG	C	608	2	-	2/6/23/26	0/1/1/1
6	NAG	C	601	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	501	NAG	C2-N2-C7	3.11	127.33	122.90
6	B	502	NAG	C2-N2-C7	3.11	127.33	122.90
6	C	605	NAG	C1-O5-C5	2.13	115.07	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	NAG	O5-C5-C6-O6
6	C	605	NAG	C4-C5-C6-O6
6	B	502	NAG	O5-C5-C6-O6
6	A	501	NAG	C4-C5-C6-O6
6	C	605	NAG	O5-C5-C6-O6
6	B	502	NAG	C4-C5-C6-O6
6	B	501	NAG	C8-C7-N2-C2
6	B	501	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	C	608	NAG	O5-C5-C6-O6
6	C	601	NAG	C4-C5-C6-O6
6	C	608	NAG	C4-C5-C6-O6
6	C	601	NAG	O5-C5-C6-O6
6	A	501	NAG	C3-C2-N2-C7
6	B	502	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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.



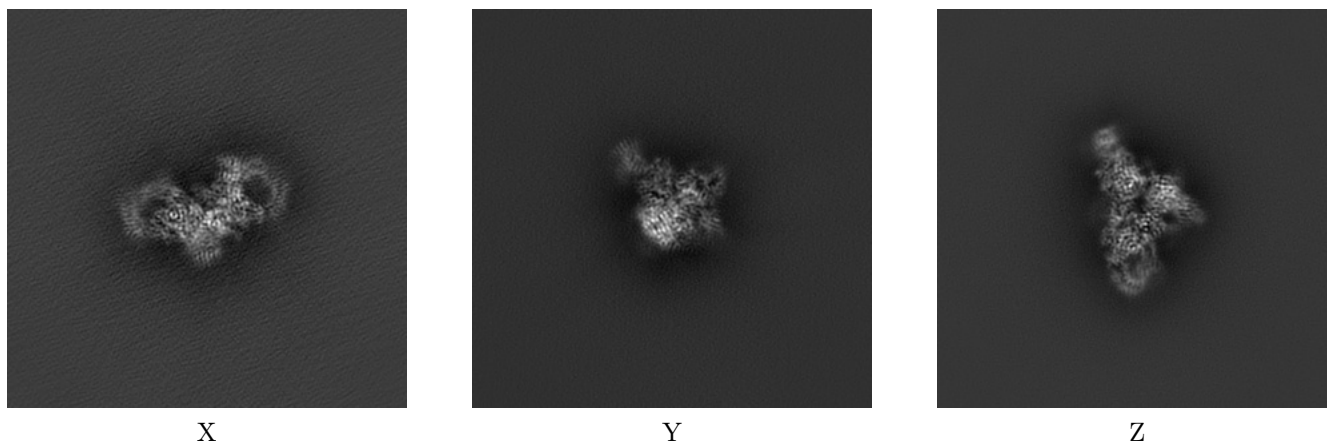
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20749. 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](#)

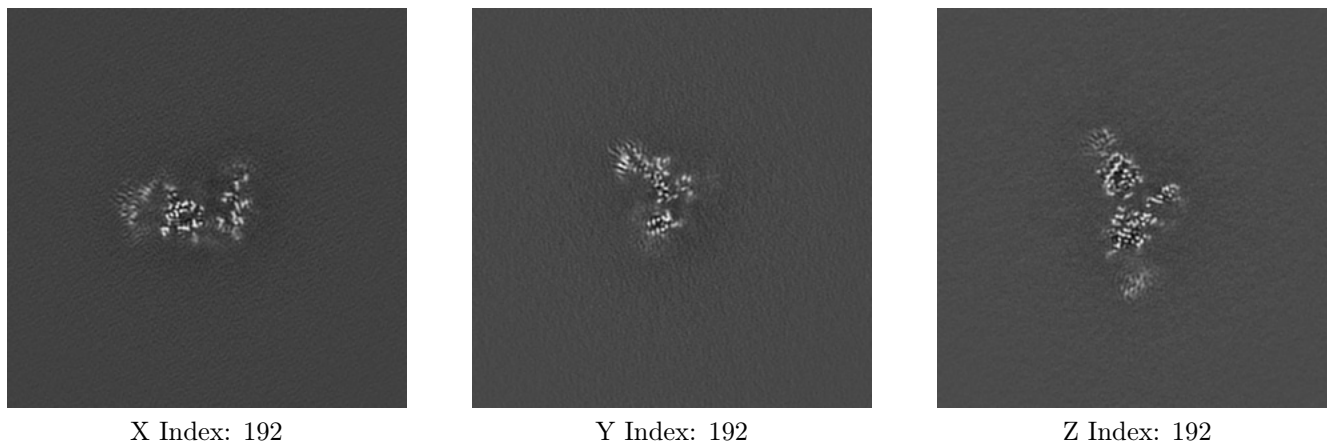
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

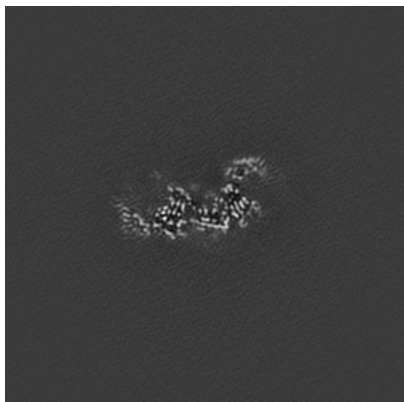
#### 6.2.1 Primary map



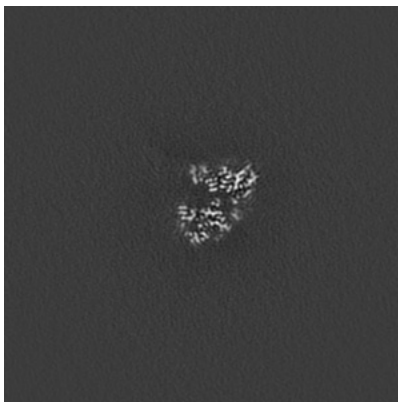
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

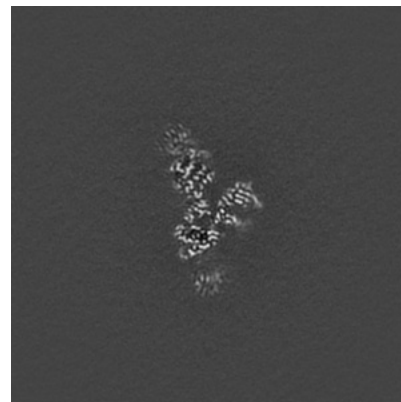
### 6.3.1 Primary map



X Index: 180



Y Index: 213



Z Index: 188

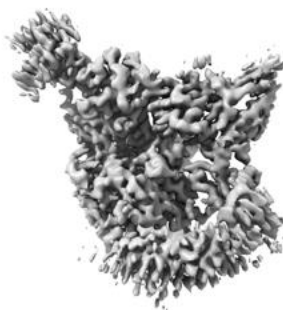
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

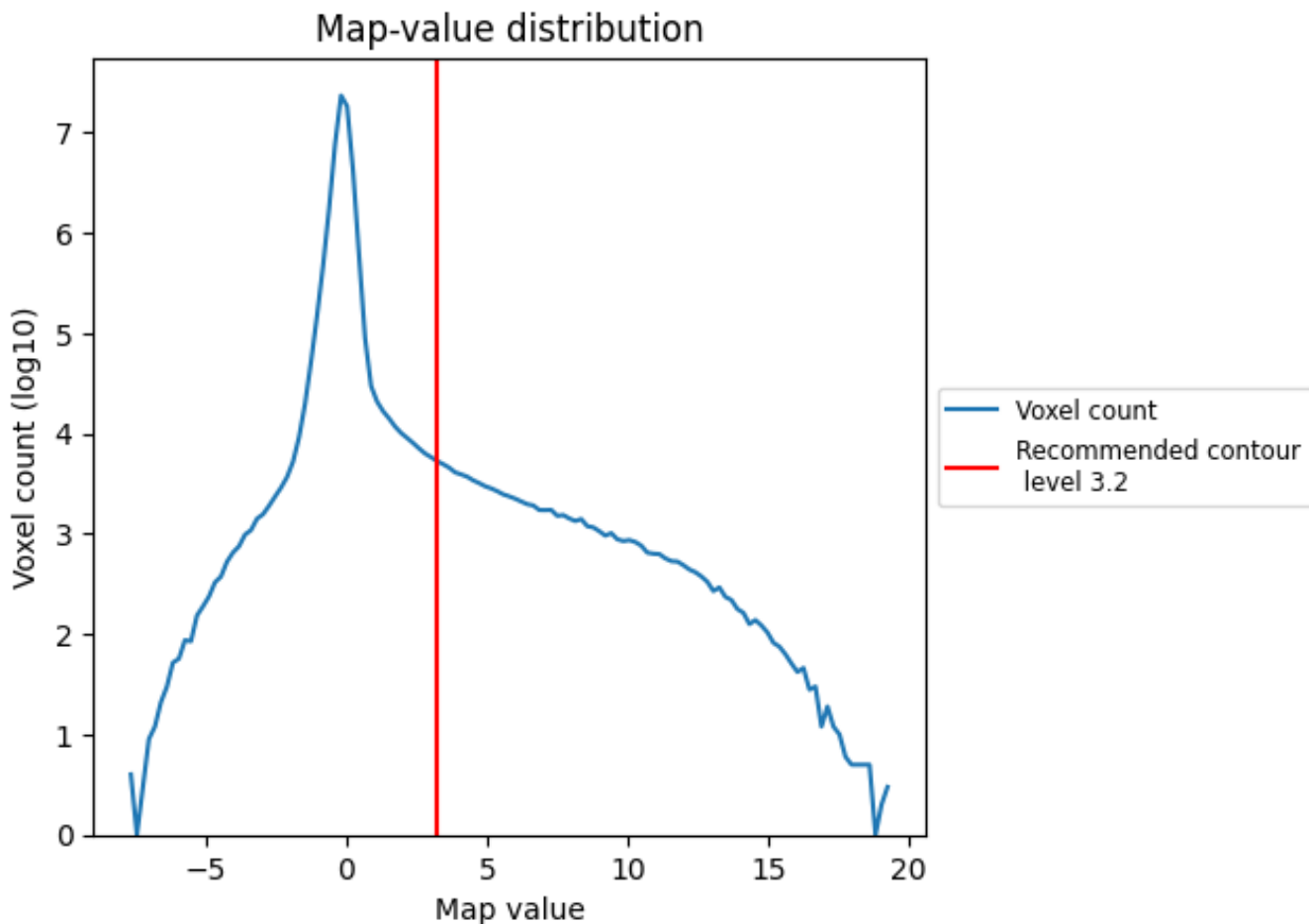
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

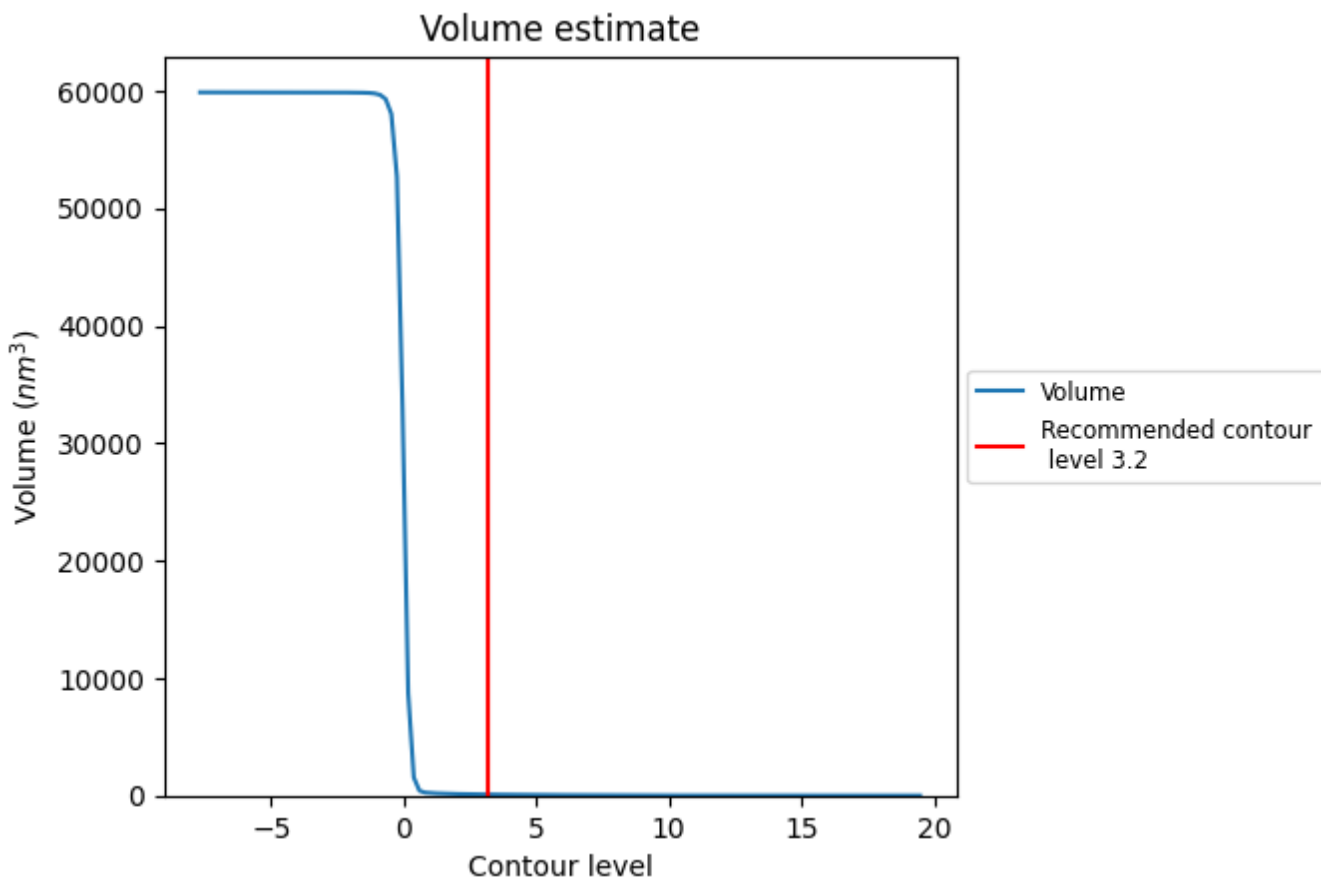
This section contains the results of statistical analysis of the map.

### 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.

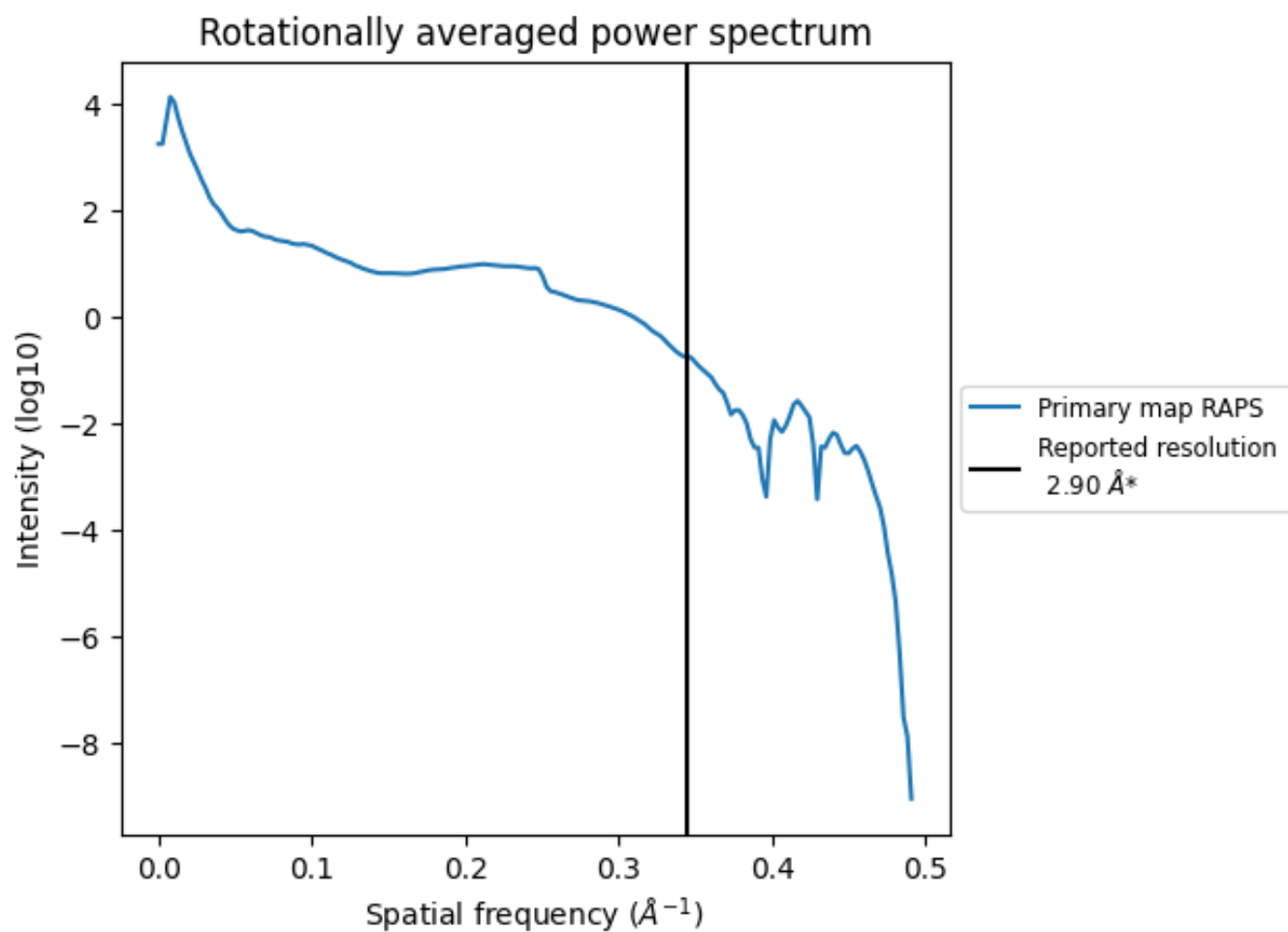
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm<sup>3</sup>; this corresponds to an approximate mass of 81 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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.345 \text{\AA}^{-1}$

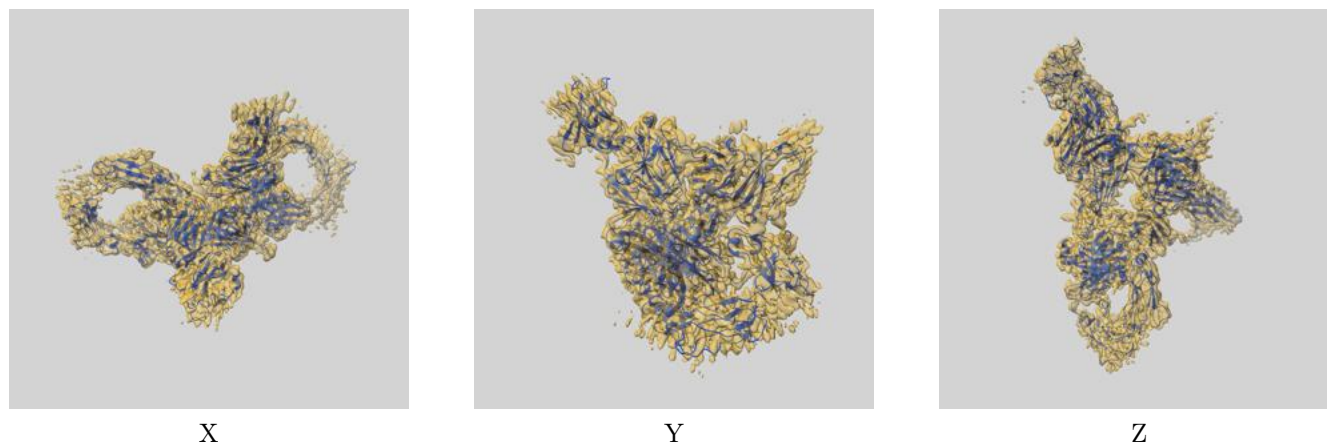
## 8 Fourier-Shell correlation

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-20749 and PDB model 6UE7. Per-residue inclusion information can be found in section 3 on page 8.

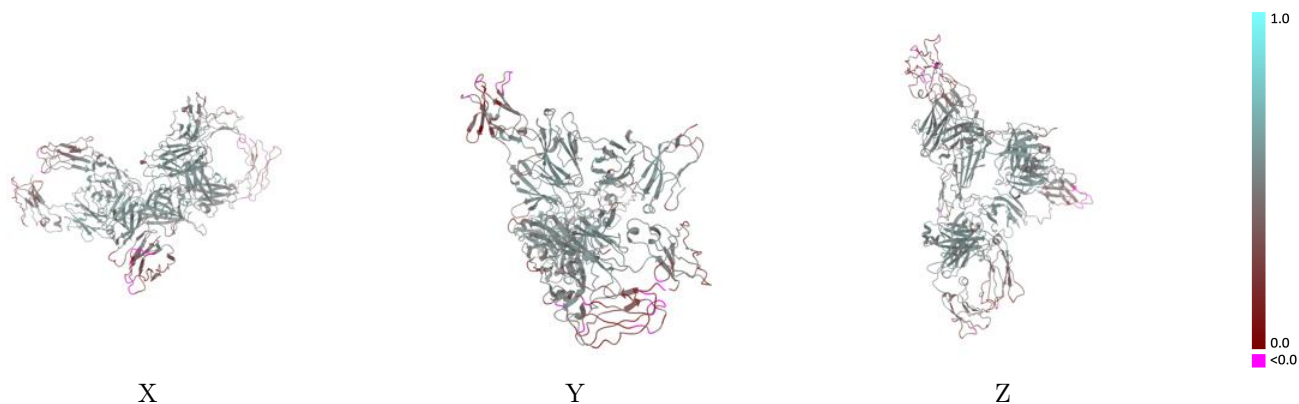
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.2 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](#)



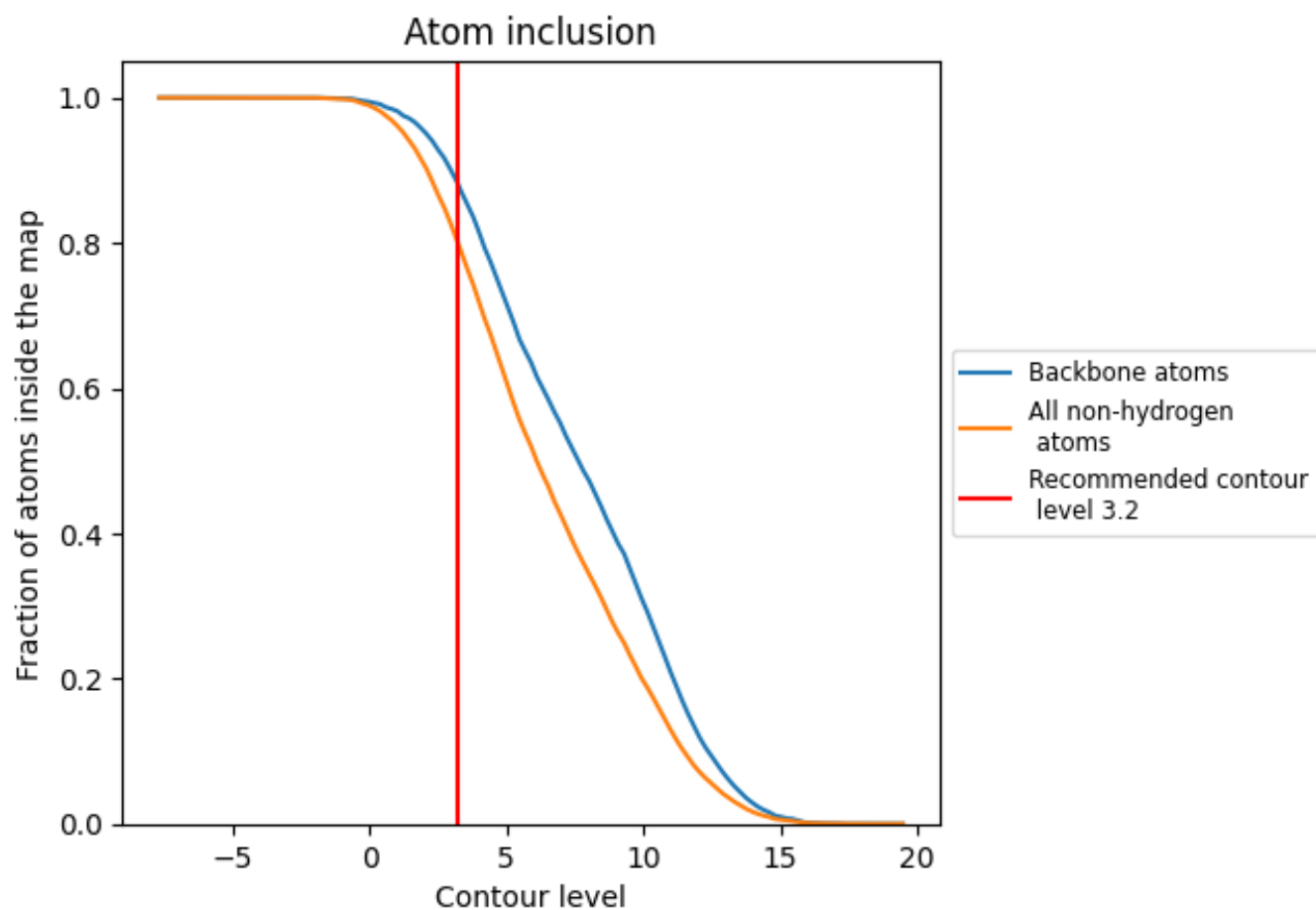
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.2).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8024	 0.4630
A	 0.7934	 0.4530
B	 0.8297	 0.4790
C	 0.8126	 0.4680
D	 0.8628	 0.5080
E	 0.5385	 0.3050
F	 0.8416	 0.4910
G	 0.6855	 0.3910
H	 0.6071	 0.4040
I	 0.7500	 0.4510
J	 0.8929	 0.5100

