



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 11:18 pm GMT

PDB ID : 8QY4  
EMDB ID : EMD-18741  
Title : Structure of interleukin 11 (gp130 P496L mutant).  
Authors : Gardner, S.; Bubeck, D.; Jin, Y.  
Deposited on : 2023-10-25  
Resolution : 3.06 Å(reported)

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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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
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

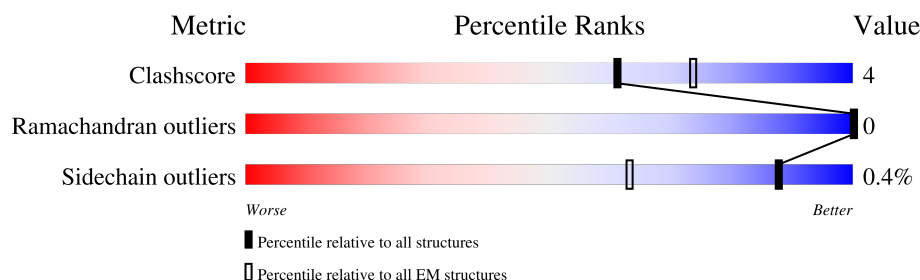
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.06 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  $\geq 3$ , 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	199	<div> <div>16%</div> <div>67%</div> <div>16%</div> <div>•</div> <div>17%</div> </div>
1	D	199	<div> <div>16%</div> <div>68%</div> <div>15%</div> <div>•</div> <div>17%</div> </div>
2	C	917	<div> <div>33%</div> <div>58%</div> <div>6%</div> <div>36%</div> </div>
2	F	917	<div> <div>33%</div> <div>58%</div> <div>6%</div> <div>36%</div> </div>
3	B	422	<div> <div>8%</div> <div>42%</div> <div>•</div> <div>53%</div> </div>
3	E	422	<div> <div>8%</div> <div>43%</div> <div>•</div> <div>53%</div> </div>
4	G	2	<div> <div>100%</div> </div>
4	H	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	I	2	<div><div></div><div>50%</div><div>100%</div></div>
4	J	2	<div><div></div><div>50%</div><div>50%</div></div>
4	K	2	<div><div></div><div>100%</div><div>100%</div></div>
4	L	2	<div><div></div><div>50%</div><div>50%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30094 atoms, of which 14962 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 Interleukin-11.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	165	Total	C	H	N	O	S	0	0
			2599	802	1337	238	220	2		
1	D	165	Total	C	H	N	O	S	0	0
			2599	802	1337	238	220	2		

- Molecule 2 is a protein called Interleukin-6 receptor subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	583	Total	C	H	N	O	S	0	0
			9101	2929	4498	761	894	19		
2	F	583	Total	C	H	N	O	S	0	0
			9101	2929	4498	761	894	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	496	LEU	PRO	engineered mutation	UNP Q00560
F	496	LEU	PRO	engineered mutation	UNP Q00560

- Molecule 3 is a protein called Interleukin-11 receptor subunit alpha.

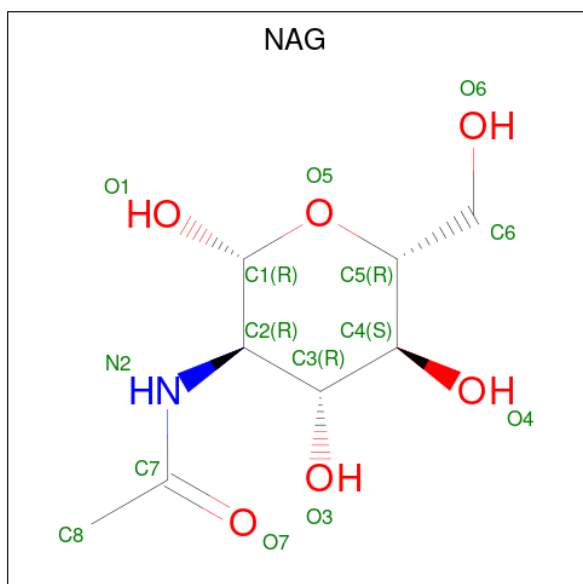
Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	197	Total	C	H	N	O	S	0	0
			3042	989	1495	274	279	5		
3	E	197	Total	C	H	N	O	S	0	0
			3042	989	1495	274	279	5		

- 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	G	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	H	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	I	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	J	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	K	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
4	L	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

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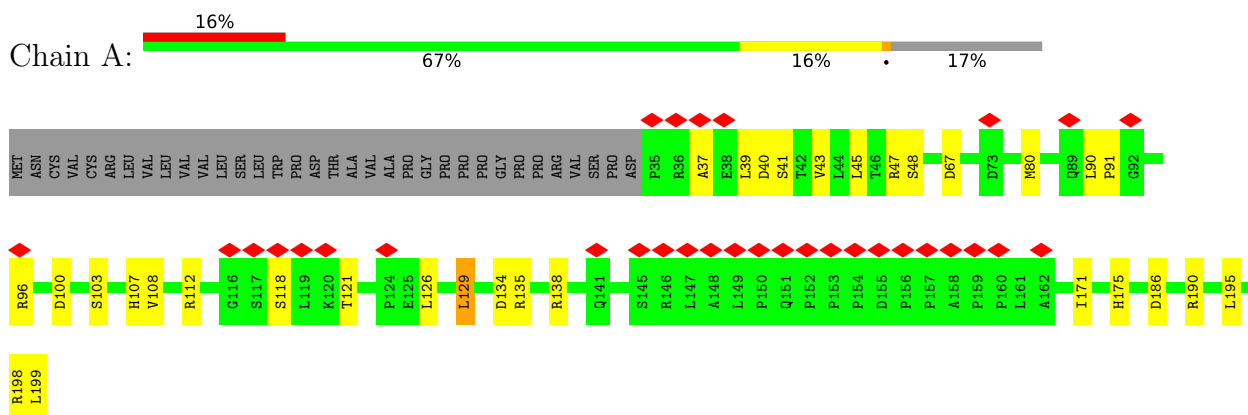
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Mol	Chain	Residues	Atoms					AltConf
5	F	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	F	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	F	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	F	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	F	1	Total	C	H	N	O	0
			28	8	14	1	5	

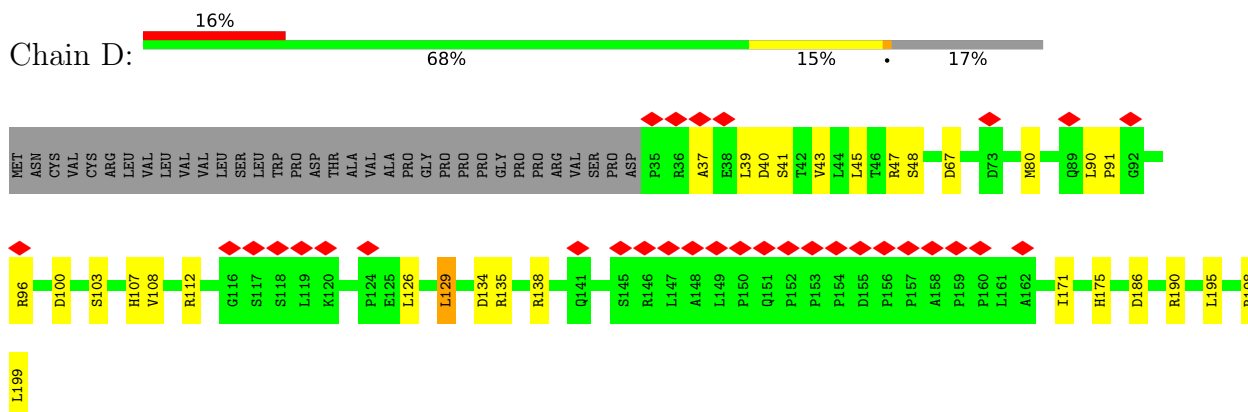
### 3 Residue-property plots [i](#)

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.

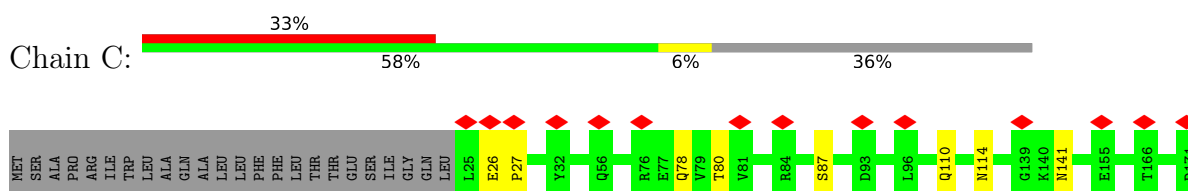
- Molecule 1: Interleukin-11



- Molecule 1: Interleukin-11



- Molecule 2: Interleukin-6 receptor subunit beta







R401	N461	P521	S581	LYS	VAL	GLU	ASP
N402	A462	T522	S582	ARG	HIS	ALA	GLY
K403	P463	V523	D583	ASP	SER	CYS	GLN
V404	C464	R524	T584	ILE	GLY	PRO	MET
K406	V465	T525	L585	LYS	LEU	ILE	ARG
S407	D467	K526	Y586	HIS	GLN	HIS	PHE
A408	V468	K527	M587	TRP	VAL	PHE	GLU
A409	Q469	V528	V588	ASP	PRO	GLU	SER
A410	Q470	G529	R589	ASN	VAL	SER	GLY
V411	E471	K530	M590	VAL	GLN	ASN	MET
L412	D472	N531	A591	PRO	VAL	GLN	THR
T413	A473	E532	A592	ASP	PHE	VAL	ILE
I414	T474	A533	Y593	PRO	ARG	ALA	ASP
P415	V475	V534	T594	SER	SER	GLY	GLU
S416	N476	L535	D595	HIS	GLU	GLU	ILE
P417	R477	A536	E596	TRP	THR	GLU	PRO
H418	T478	W537	G597	ALA	GLN	ASP	GLN
V419	H479	D538	G598	GLN	SER	PHE	SER
T420	L480	Q539	K599	TRP	GLY	VAL	TYR
A421	R481	I540	D600	PRO	ILE	ARG	PRO
A422	G482	P541	G601	HIS	GLY	LEU	CYS
Y423	R483	V542	P602	THR	GLY	GLN	PRO
S424	L484	D543	E603	PRO	SER	GLN	TRP
V425	L485	D544	F604	ARG	PRO	VAL	GLY
V426	L486	Q545	T605	HIS	GLU	SER	PRO
N427	E486	N546	F606	ASN	ASP	GLY	GLY
L428	S487	G547	T607	ASN	ILE	GLN	TYR
K429	K488	F548	THR	SER	SER	GLN	PRO
A430	C489	I549	PRO	LYS	PRO	GLN	TYR
F431	Y490	R550	LYS	ASP	ASP	PRO	GLY
P432	Q491	N551	PHE	GLN	ILE	TYR	GLY
K433	I492	Y552	ALA	MET	VAL	PRO	GLY
D434	T493	S553	GLY	SER	ASP	GLY	ARG
M435	V494	I554	GLY	ASP	GLY	GLN	SER
L436	T495	S555	ILE	GLY	ASP	ARG	VAL
L437	V497	Y556	GLU	ASN	GLU	LEU	LYS
W438	F498	R557	ALA	PHE	ILE	LEU	LEU
V439	A499	T558	VAL	THR	THR	PHE	CYS
E440	T500	S559	VAL	VAL	ALA	GLN	PRO
W441	G501	V560	PRO	SER	ARG	GLY	GLY
T442	P502	G561	VAL	VAL	THR	THR	VAL
P443	G503	K562	CYS	GLU	PHE	ALA	ASP
P444	G504	E563	LEU	GLU	VAL	GLN	ALA
P445	S505	M564	LEU	ASN	ALA	ASN	LEU
K446	S506	V565	THR	ASN	ASN	CYS	THR
P447	S507	V566	LYS	THR	GLN	SER	GLY
V448	L508	H567	LEU	LEU	VAL	TRP	TRP
S449	K509	V568	GLY	VAL	GLY	ALA	PHE
K450	A510	D569	LEU	LEU	LEU	GLY	THR
Y451	Y511	S570	PHE	THR	THR	GLY	ALA
I452	L512	S571	CYS	CYS	GLN	THR	TRP
L453	K513	H572	PHE	ASN	PRO	VAL	PHE
E454	Q514	T573	ASN	ASN	VAL	VAL	
W455	A515	E574	THR	THR	GLY	GLY	
C456	A516	Y575	SER	SER	GLY	GLY	
V457	P517	T576	THR	THR	GLY	GLY	
L458	S459	S577	GLN	GLN	GLY	GLY	
S459	R519	S578	PRO	PRO	GLY	GLY	
E460	G520	S579	ALA	ALA	GLY	GLY	

• Molecule 3: Interleukin-11 receptor subunit alpha



MET	ARG	S138	L287	GLN
SER	ASP	G139	F288	VAL
SER	GLY	L140	H289	ALA
CYS	PRO	P141	R292	VAL
SER	LYS	R142	F298	LEU
GLY	LEU	R143	L299	SER
LEU	LEU	T146	E310	LEU
SER	GLN	T152	S316	ILE
VAL	PRO	V153	T317	THR
VAL	GLY	L154	GLY	LEU
ALA	LEU	GLY	ILE	LEU
ALA	HIS	ASP	ALA	VAL
ALA	GLU	GLY	ALA	VAL
VAL	LEU	GLN	LYS	GLY
VAL	VAL	ARG	ILE	ALA
ALA	ALA	SER	ALA	LEU
ALA	GLN	PRO	ALA	LEU
ALA	ALA	GLY	TRP	LEU
ASP	ASP	S164	GLY	LEU
SER	SER	Q172	GLN	TRP
THR	THR	D173	LEU	LEU
GLY	GLY	P174	HIS	ARG
THR	THR	L175	THR	LEU
ILE	CYS	G176	GLY	ARG
GLN	VAL	A177	GLY	GLY
THR	GLN	A178	ASP	LYS
LEU	THR	E186	VAL	GLY
GLY	ASP	N199	GLY	GLY
ASP	GLY	P200	SER	PRO
ALA	ALA	L201	PRO	LYS
GLY	GLY	L202	ALA	GLY
THR	THR	G202	PHE	GLY
VAL	VAL	A203	LEU	ALA
LYS	LYS	L207	ALA	SER
LEU	THR	L208	ILE	VAL
CYS	GLN	D209	GLN	ILE
PRO	LEU	L212	PRO	PRO
GLY	GLY	R225	HIS	VAL
VAL	TYR	Y226	ARG	ASP
P112	P113	E227	ARG	ARG
A114	W132	Q259	LEU	THR
S135	Q136	A263	LEU	LEU
Q136	I137	Q264	ASP	GLY
I137		A274	ASN	ALA
		E278	ARG	ALA
		V279	SER	GLY
		G286	VAL	GLY
			GLU	GLY

• Molecule 3: Interleukin-11 receptor subunit alpha





- 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	487147	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.202	Depositor
Minimum map value	-5.260	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	1.01	Depositor
Map size (Å)	474.87997, 474.87997, 474.87997	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/1288	0.79	2/1754 (0.1%)
1	D	0.28	0/1288	0.79	2/1754 (0.1%)
2	C	0.27	0/4722	0.55	0/6448
2	F	0.27	0/4722	0.55	0/6448
3	B	0.26	0/1603	0.53	0/2205
3	E	0.26	0/1603	0.53	0/2205
All	All	0.27	0/15226	0.59	4/20814 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	D	199	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	A	129	LEU	CA-CB-CG	5.04	126.88	115.30
1	D	129	LEU	CA-CB-CG	5.02	126.85	115.30

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	1262	1337	1337	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1262	1337	1337	22	0
2	C	4603	4498	4497	34	0
2	F	4603	4498	4497	35	0
3	B	1547	1495	1494	11	0
3	E	1547	1495	1494	11	0
4	G	28	27	25	0	0
4	H	28	27	25	0	0
4	I	28	27	25	0	0
4	J	28	27	25	1	0
4	K	28	27	25	0	0
4	L	28	27	25	1	0
5	C	70	70	65	0	0
5	F	70	70	65	0	0
All	All	15132	14962	14936	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 126 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:F:263:ASP:OD1	2:F:264:ALA:N	2.14	0.80
2:C:263:ASP:OD1	2:C:264:ALA:N	2.14	0.80
2:C:333:LYS:NZ	2:C:454:GLU:OE2	2.16	0.79
2:F:333:LYS:NZ	2:F:454:GLU:OE2	2.16	0.78
2:C:114:ASN:N	1:D:67:ASP:OD1	2.23	0.72

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	163/199 (82%)	159 (98%)	4 (2%)	0	100	100
1	D	163/199 (82%)	159 (98%)	4 (2%)	0	100	100
2	C	581/917 (63%)	551 (95%)	30 (5%)	0	100	100
2	F	581/917 (63%)	550 (95%)	31 (5%)	0	100	100
3	B	193/422 (46%)	185 (96%)	8 (4%)	0	100	100
3	E	193/422 (46%)	185 (96%)	8 (4%)	0	100	100
All	All	1874/3076 (61%)	1789 (96%)	85 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	133/163 (82%)	133 (100%)	0	100	100
1	D	133/163 (82%)	133 (100%)	0	100	100
2	C	521/821 (64%)	520 (100%)	1 (0%)	92	95
2	F	521/821 (64%)	520 (100%)	1 (0%)	92	95
3	B	168/346 (49%)	166 (99%)	2 (1%)	67	82
3	E	168/346 (49%)	166 (99%)	2 (1%)	67	82
All	All	1644/2660 (62%)	1638 (100%)	6 (0%)	88	93

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	298	PHE
3	E	209	ASP
3	E	298	PHE
2	F	326	ARG
2	C	326	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	D	175	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 ⓘ

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	$\# Z  > 2$
4	NAG	G	1	2,4	14,14,15	0.73	0	17,19,21	0.87	0
4	NAG	G	2	4	14,14,15	0.72	0	17,19,21	0.86	0
4	NAG	H	1	2,4	14,14,15	0.73	0	17,19,21	0.87	0
4	NAG	H	2	4	14,14,15	0.72	0	17,19,21	0.87	0
4	NAG	I	1	3,4	14,14,15	0.72	0	17,19,21	0.88	0
4	NAG	I	2	4	14,14,15	0.70	0	17,19,21	0.89	0
4	NAG	J	1	3,4	14,14,15	0.74	0	17,19,21	0.82	0
4	NAG	J	2	4	14,14,15	0.72	0	17,19,21	0.81	0
4	NAG	K	1	3,4	14,14,15	0.72	0	17,19,21	0.88	0
4	NAG	K	2	4	14,14,15	0.70	0	17,19,21	0.89	0
4	NAG	L	1	3,4	14,14,15	0.75	0	17,19,21	0.82	0
4	NAG	L	2	4	14,14,15	0.72	0	17,19,21	0.81	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	G	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	NAG	J	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	NAG	L	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

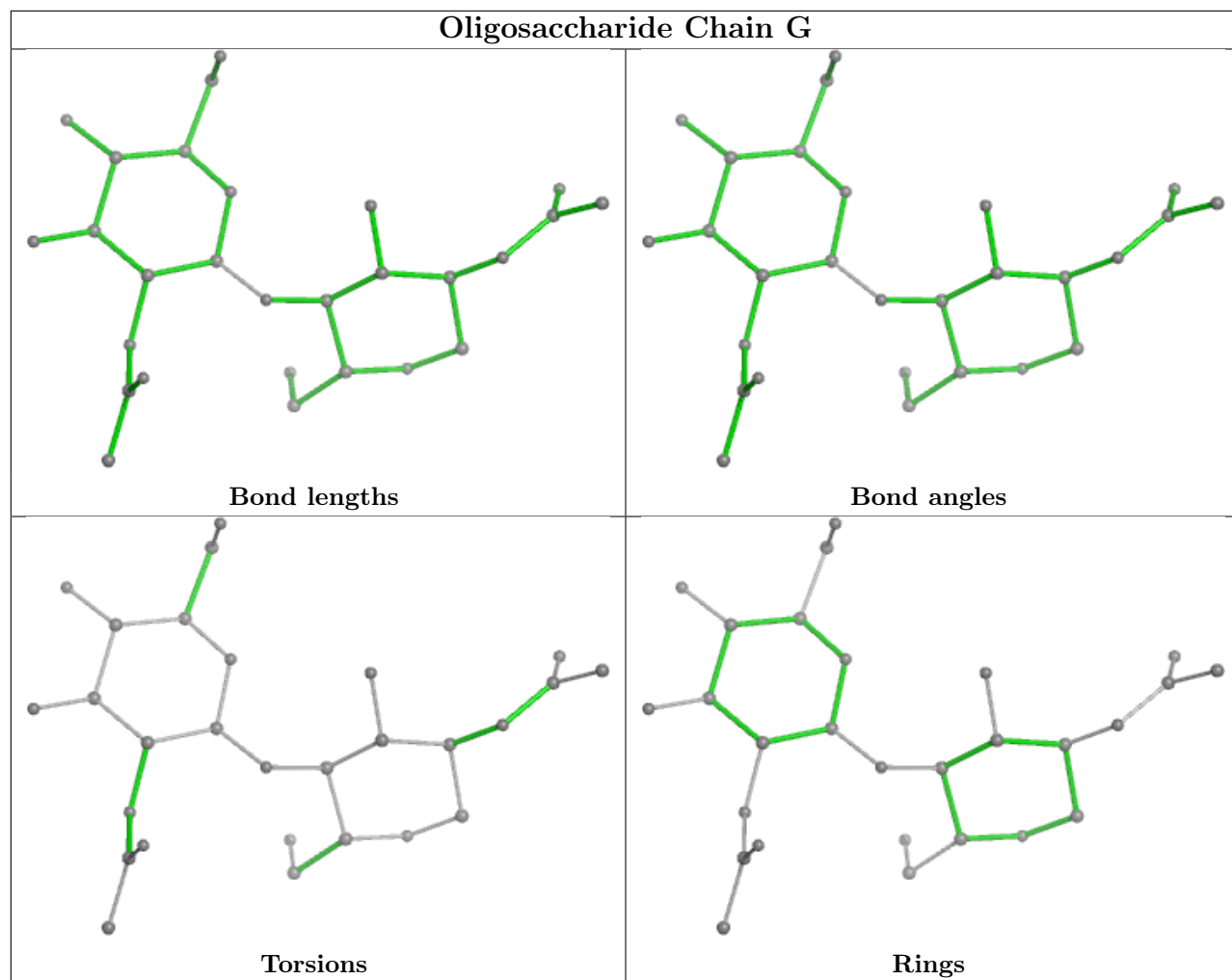
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C3-C2-N2-C7

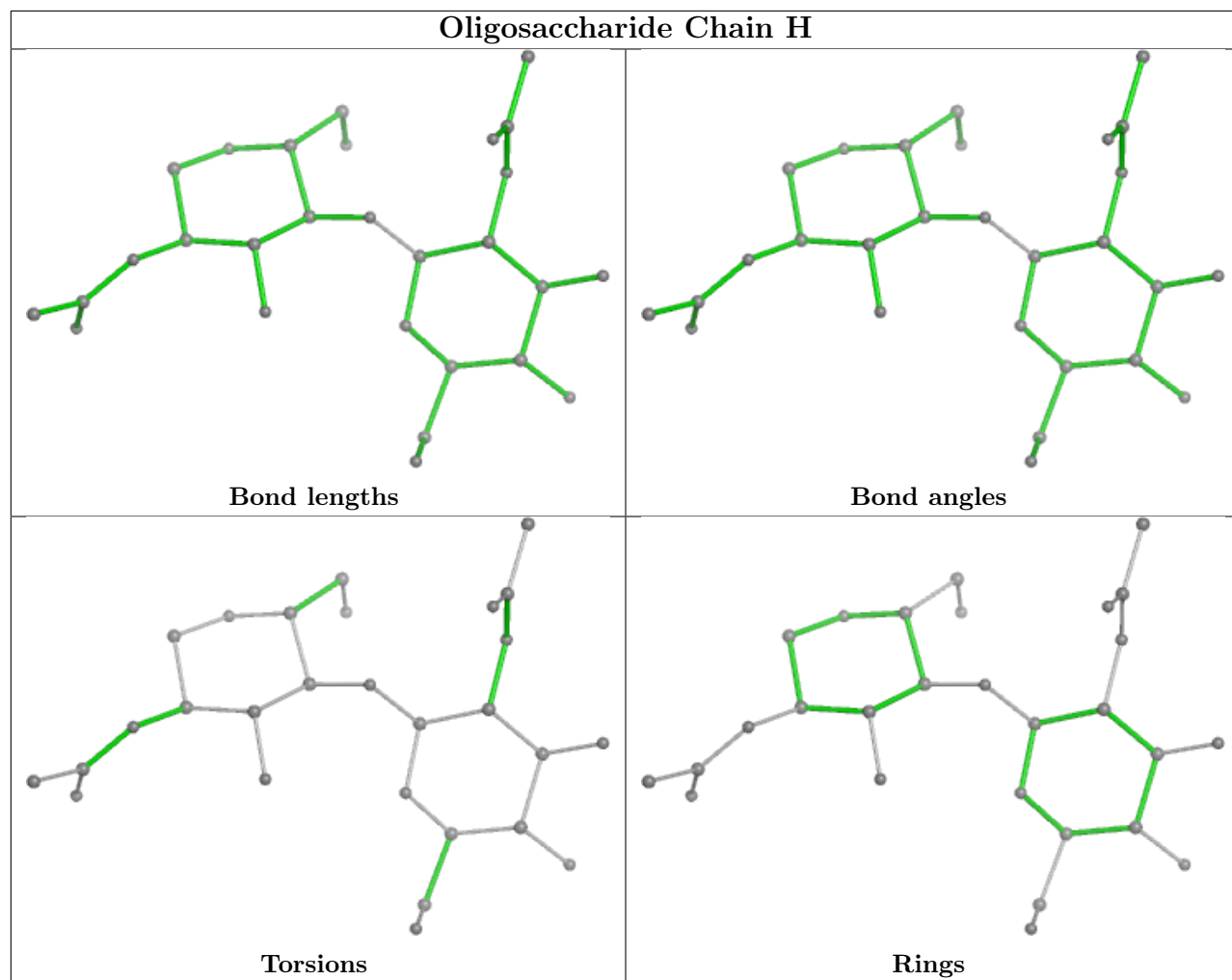
There are no ring outliers.

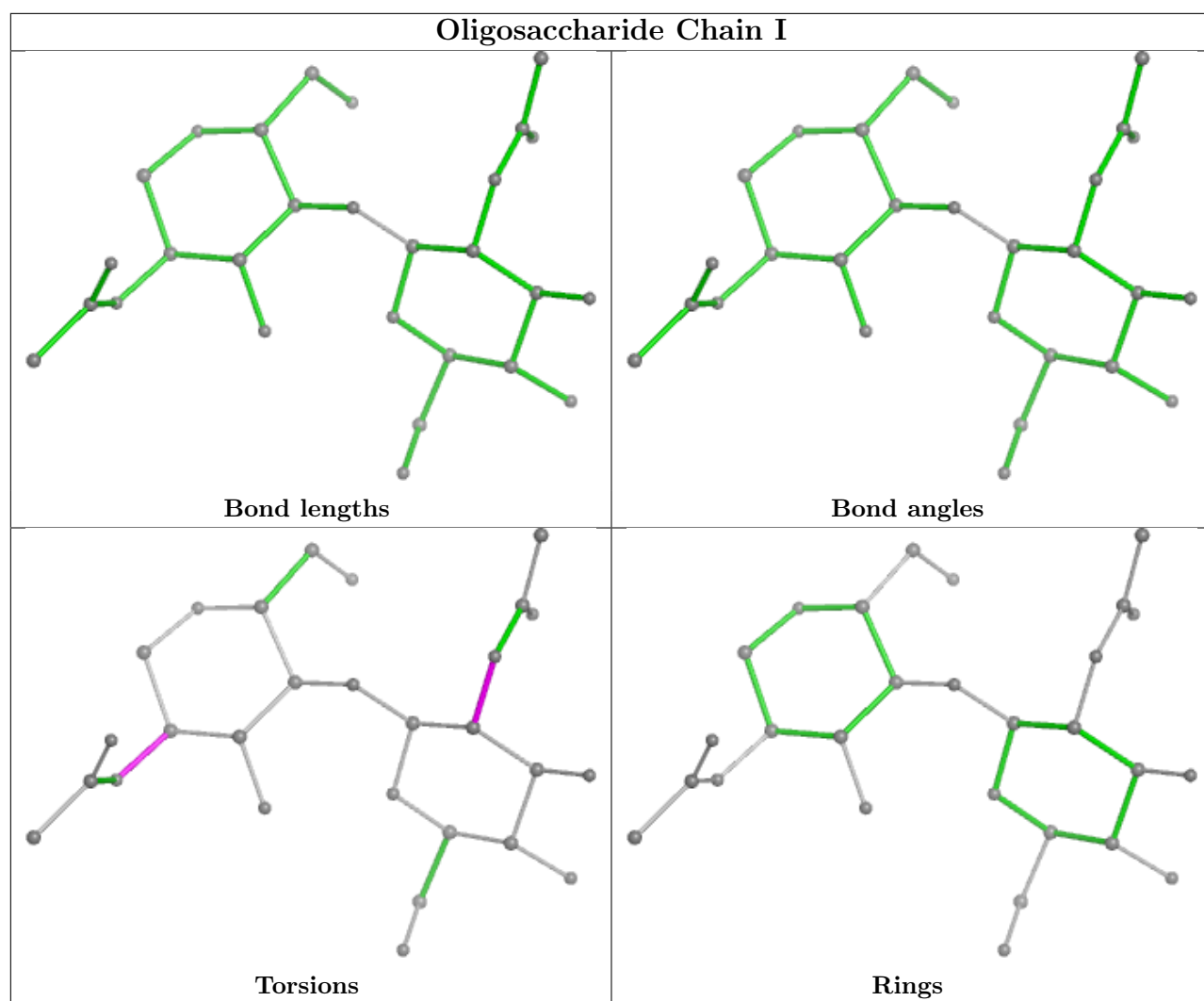
2 monomers are involved in 2 short contacts:

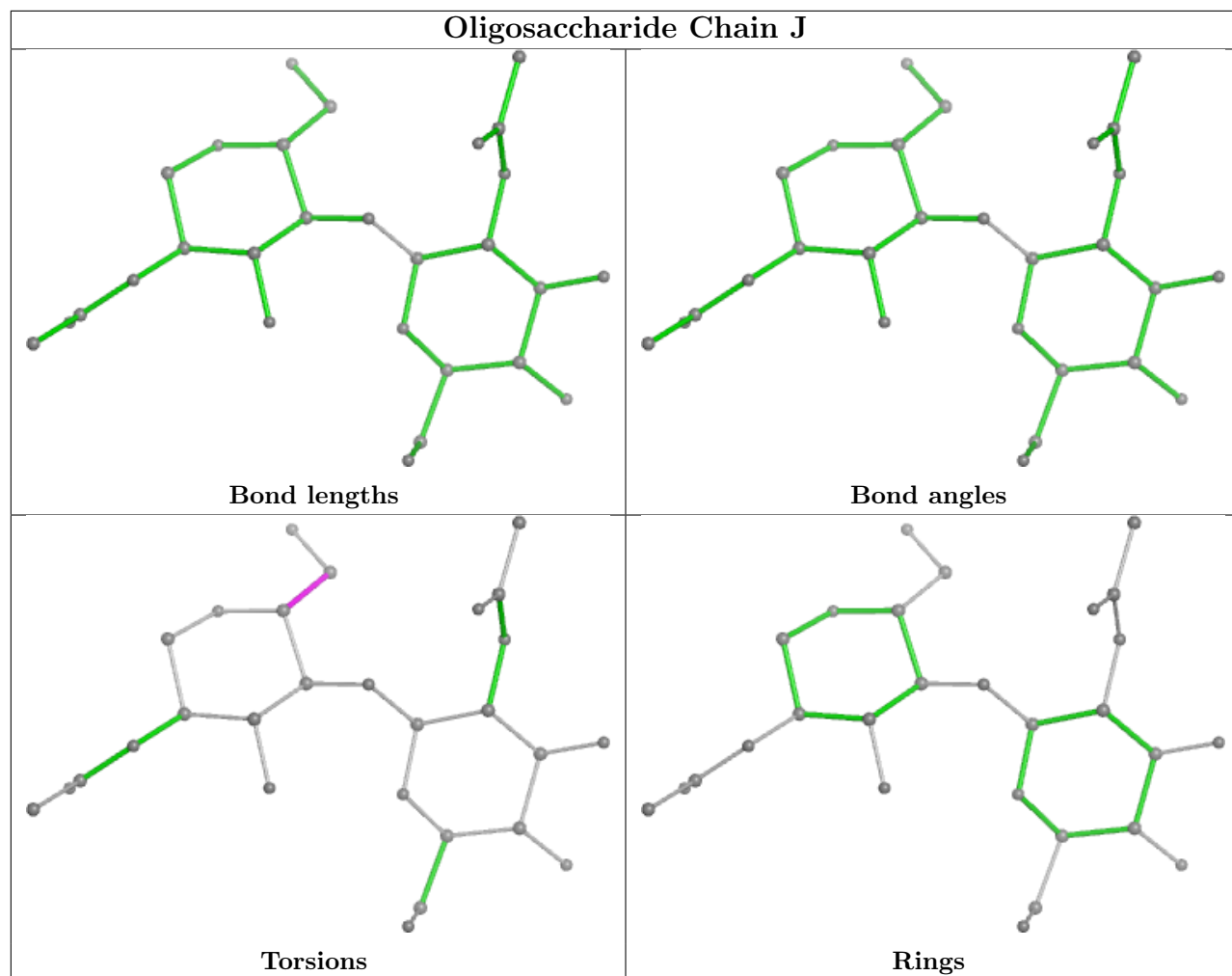
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	2	NAG	1	0
4	J	2	NAG	1	0

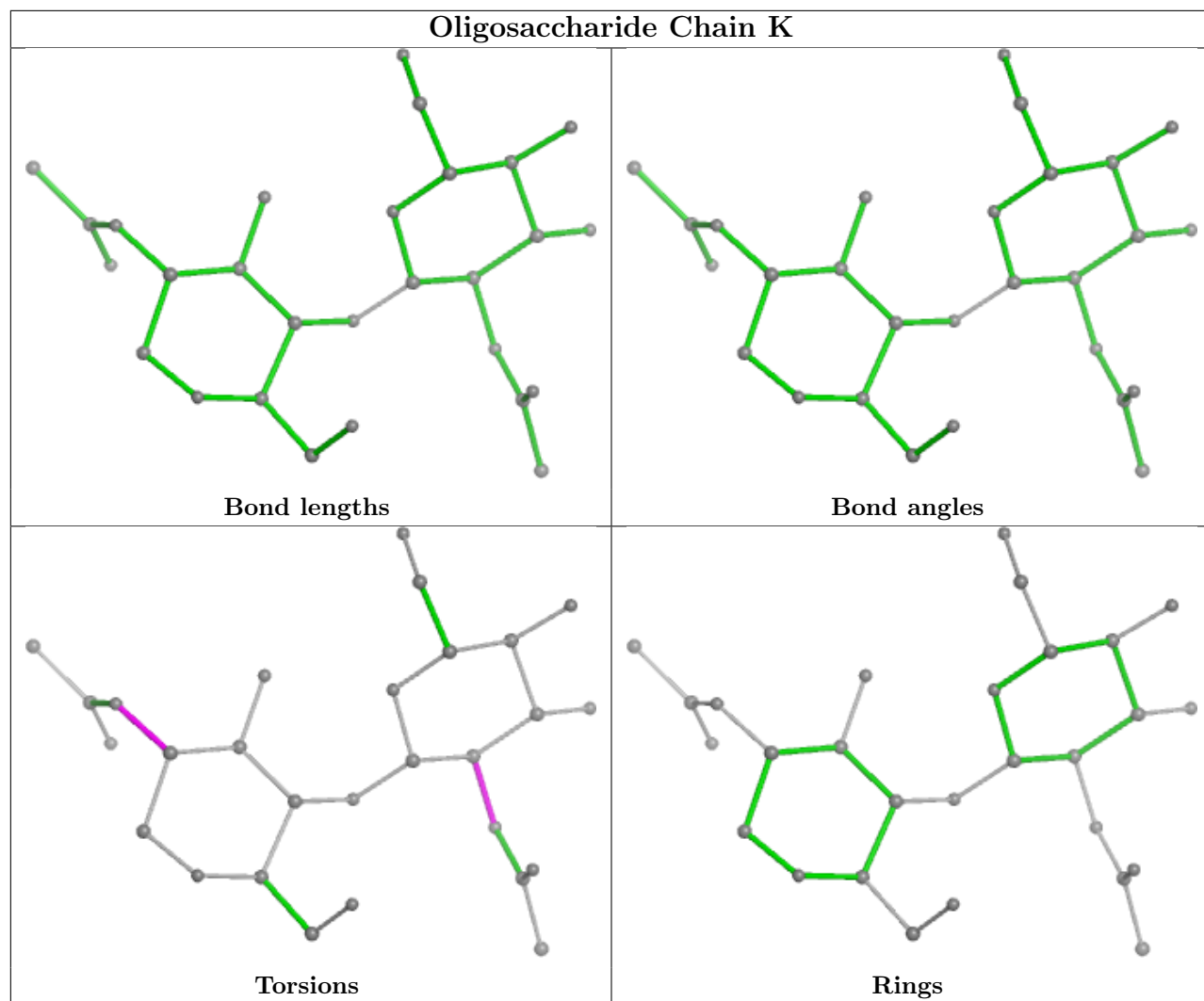
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

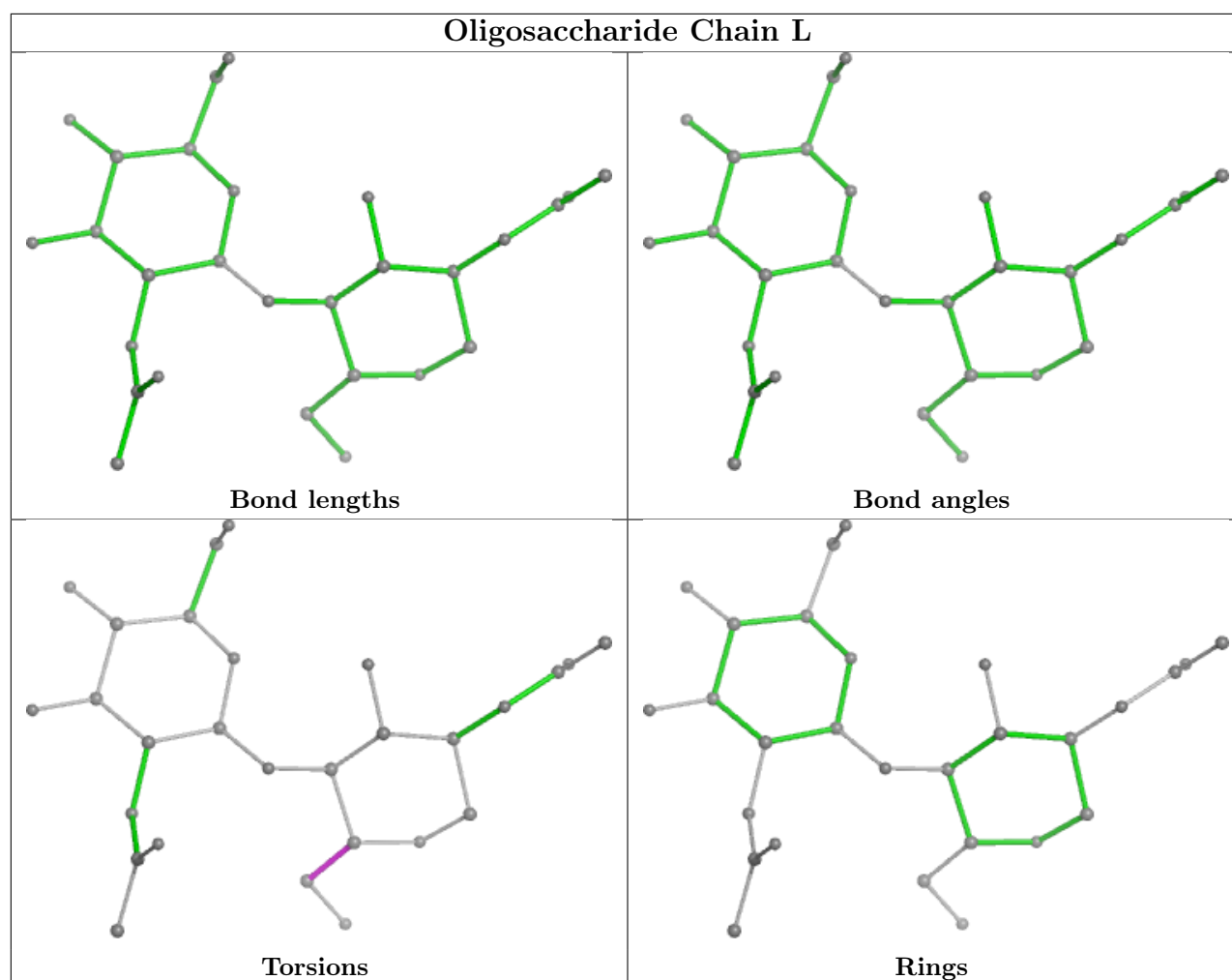












## 5.6 Ligand geometry [i](#)

10 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	C	1004	2	14,14,15	0.75	0	17,19,21	0.96	0
5	NAG	F	1003	2	14,14,15	0.72	0	17,19,21	0.86	0
5	NAG	C	1005	2	14,14,15	0.72	0	17,19,21	0.86	0
5	NAG	C	1002	2	14,14,15	0.73	0	17,19,21	0.88	1 (5%)
5	NAG	C	1001	2	14,14,15	0.72	0	17,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	1003	2	14,14,15	0.72	0	17,19,21	0.86	0
5	NAG	F	1004	2	14,14,15	0.75	0	17,19,21	0.96	0
5	NAG	F	1002	2	14,14,15	0.73	0	17,19,21	0.88	1 (5%)
5	NAG	F	1005	2	14,14,15	0.72	0	17,19,21	0.86	0
5	NAG	F	1001	2	14,14,15	0.72	0	17,19,21	0.87	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
5	NAG	C	1004	2	-	0/6/23/26	0/1/1/1
5	NAG	F	1003	2	-	1/6/23/26	0/1/1/1
5	NAG	C	1005	2	-	0/6/23/26	0/1/1/1
5	NAG	C	1002	2	-	0/6/23/26	0/1/1/1
5	NAG	C	1001	2	-	2/6/23/26	0/1/1/1
5	NAG	C	1003	2	-	1/6/23/26	0/1/1/1
5	NAG	F	1004	2	-	0/6/23/26	0/1/1/1
5	NAG	F	1002	2	-	0/6/23/26	0/1/1/1
5	NAG	F	1005	2	-	0/6/23/26	0/1/1/1
5	NAG	F	1001	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1002	NAG	O5-C1-C2	-2.04	108.06	111.29
5	C	1002	NAG	O5-C1-C2	-2.04	108.06	111.29

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1001	NAG	O5-C5-C6-O6
5	F	1001	NAG	O5-C5-C6-O6
5	C	1001	NAG	C4-C5-C6-O6
5	F	1001	NAG	C4-C5-C6-O6
5	C	1003	NAG	C4-C5-C6-O6

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.

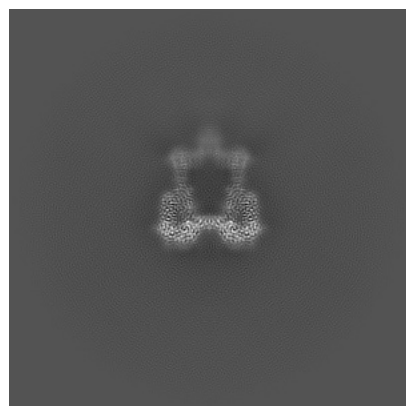
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18741. These allow visual inspection of the internal detail of the map and identification of artifacts.

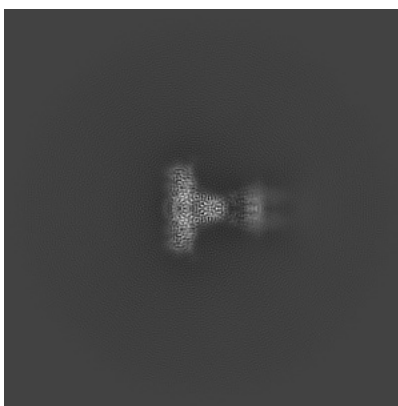
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

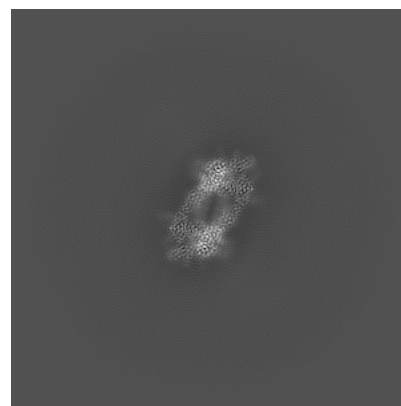
#### 6.1.1 Primary map



X

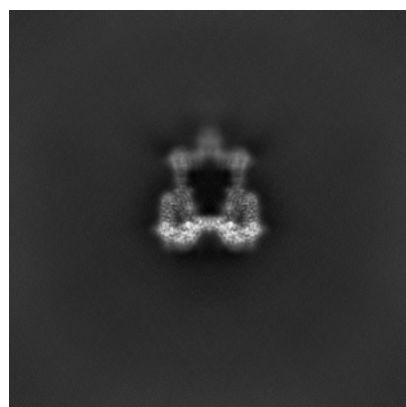


Y

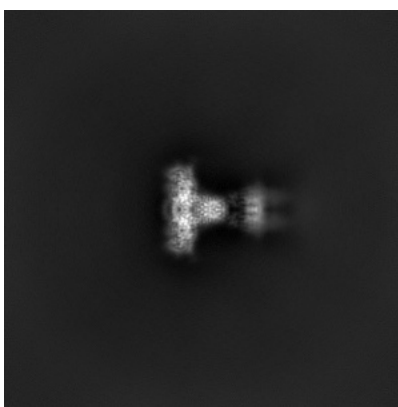


Z

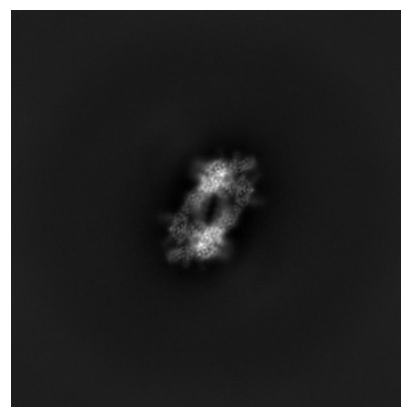
#### 6.1.2 Raw map



X



Y

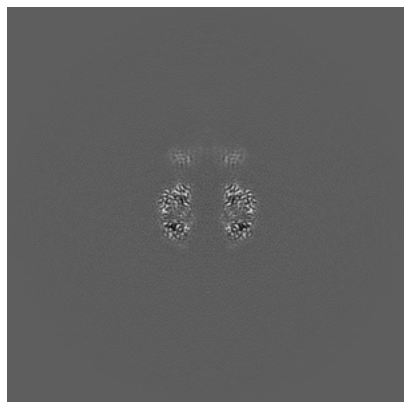


Z

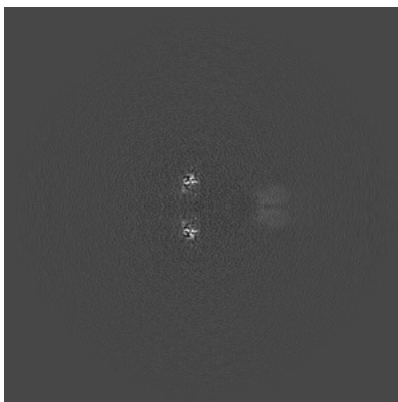
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

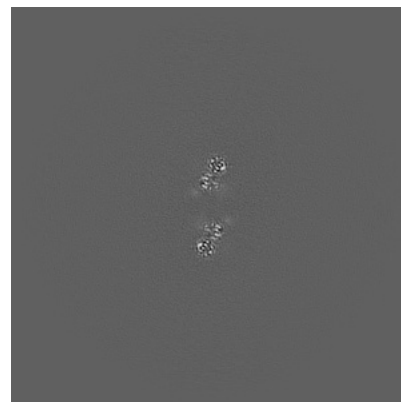
### 6.2.1 Primary map



X Index: 224



Y Index: 224

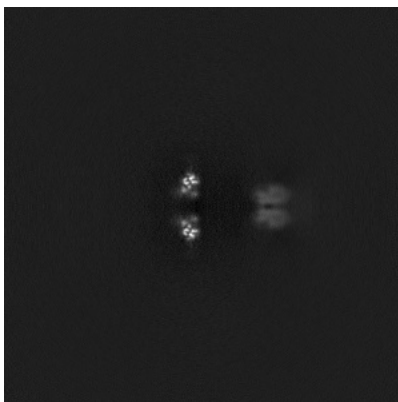


Z Index: 224

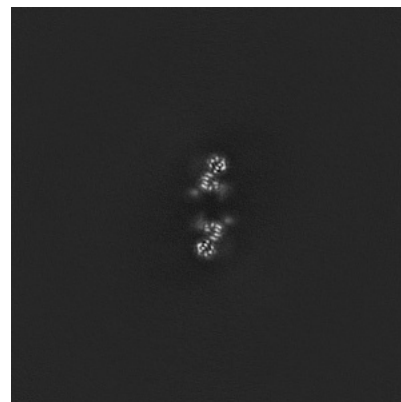
### 6.2.2 Raw map



X Index: 224



Y Index: 224



Z Index: 224

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

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

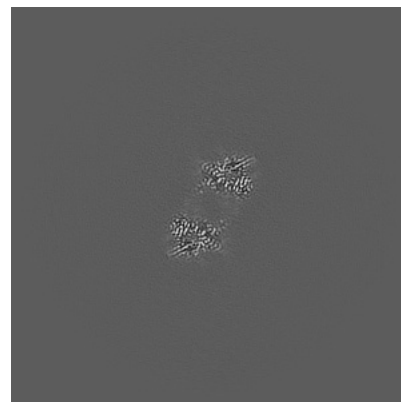
### 6.3.1 Primary map



X Index: 230



Y Index: 267

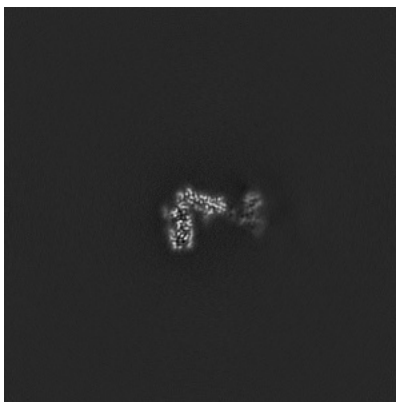


Z Index: 198

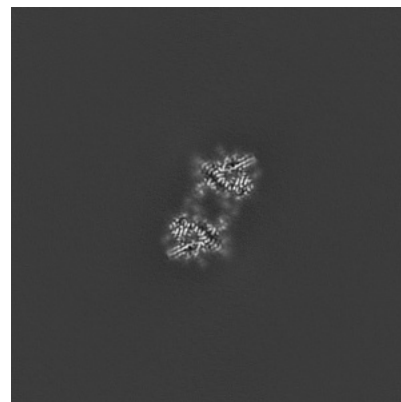
### 6.3.2 Raw map



X Index: 218



Y Index: 200

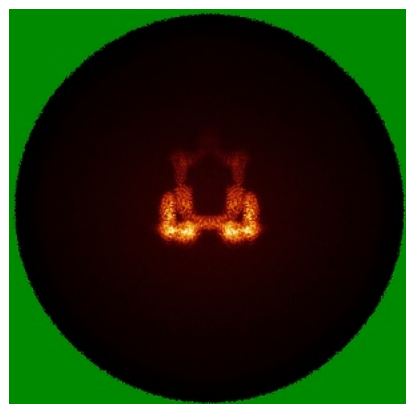


Z Index: 198

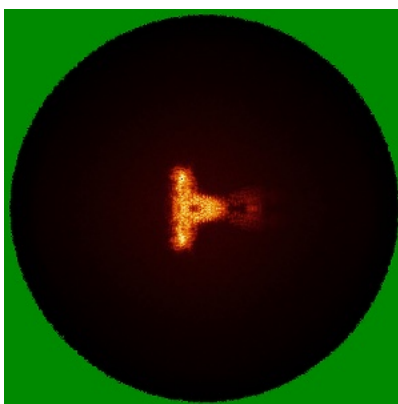
The images above show the largest variance slices of the map in three orthogonal directions.

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

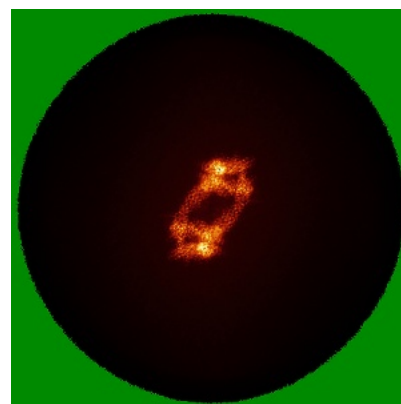
### 6.4.1 Primary map



X

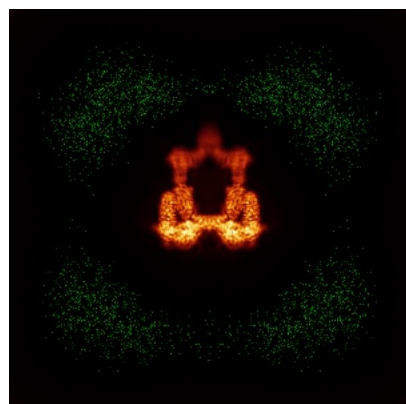


Y

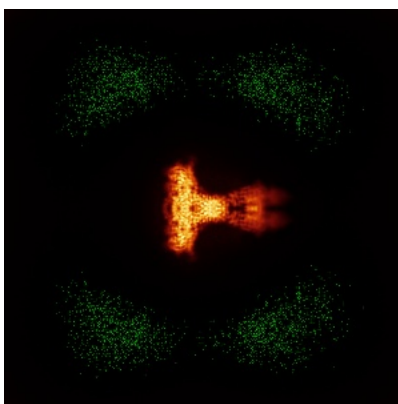


Z

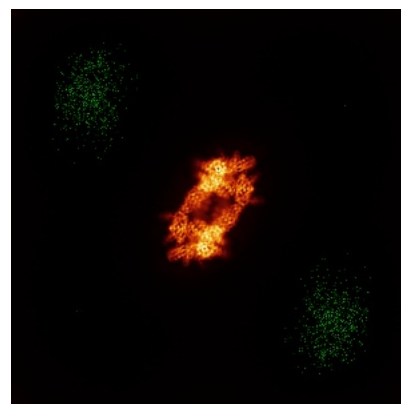
### 6.4.2 Raw map



X



Y



Z

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

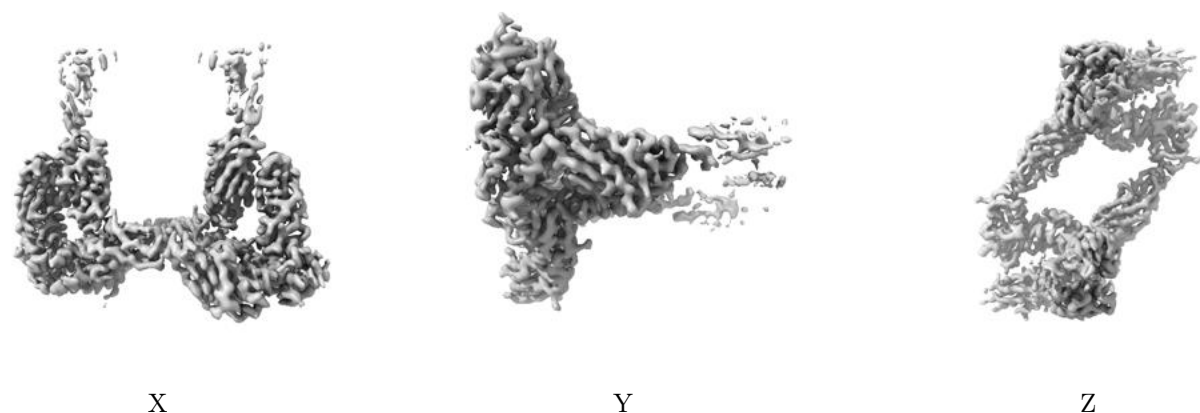
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

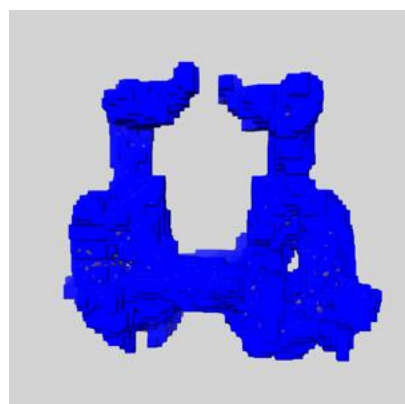
## 6.6 Mask visualisation [i](#)

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

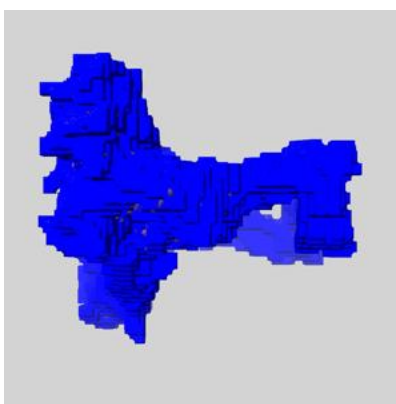
A mask typically either:

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

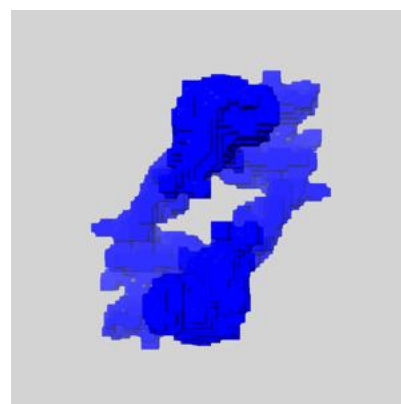
### 6.6.1 emd\_18741\_msk\_1.map [i](#)



X



Y

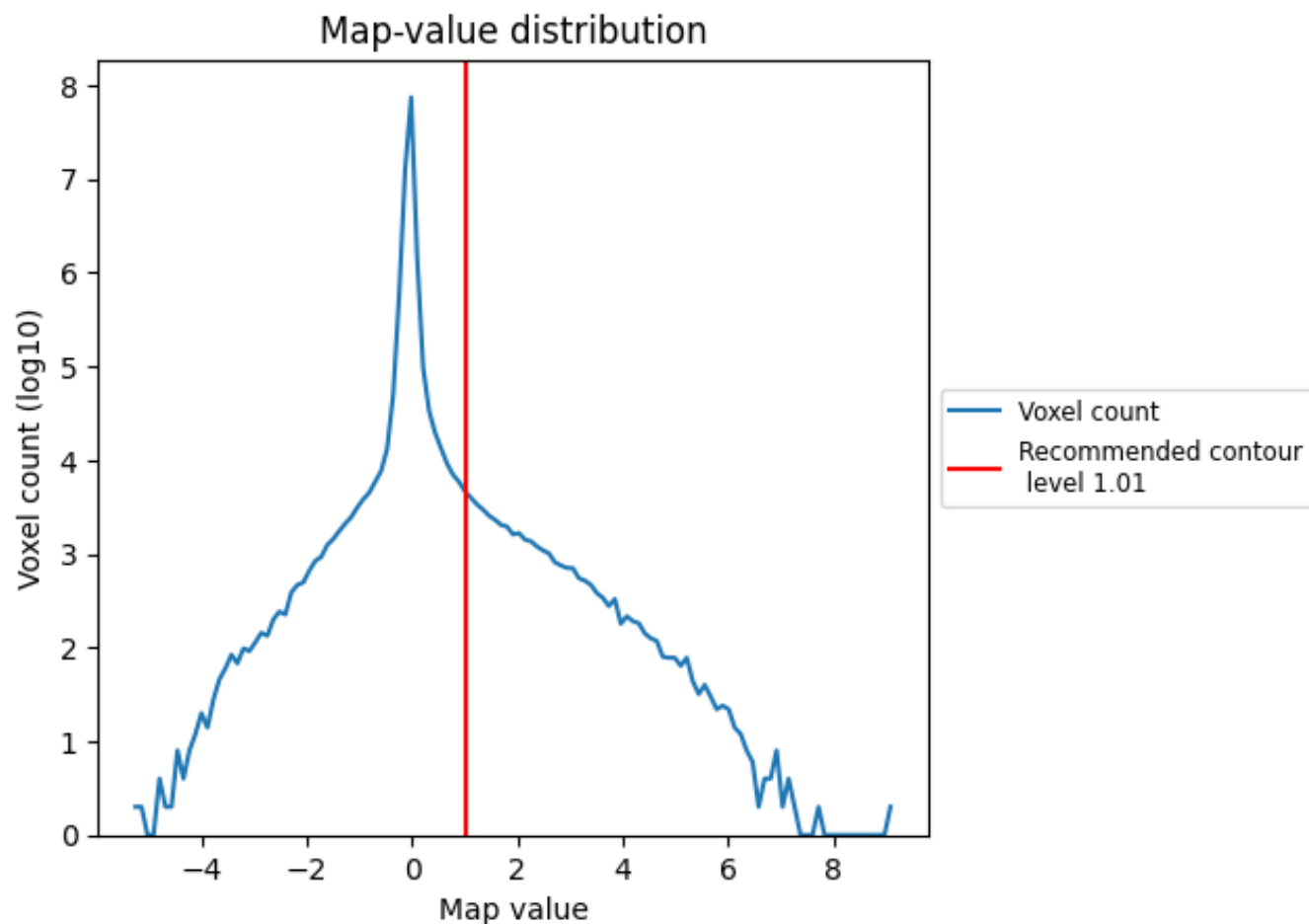


Z

## 7 Map analysis [i](#)

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

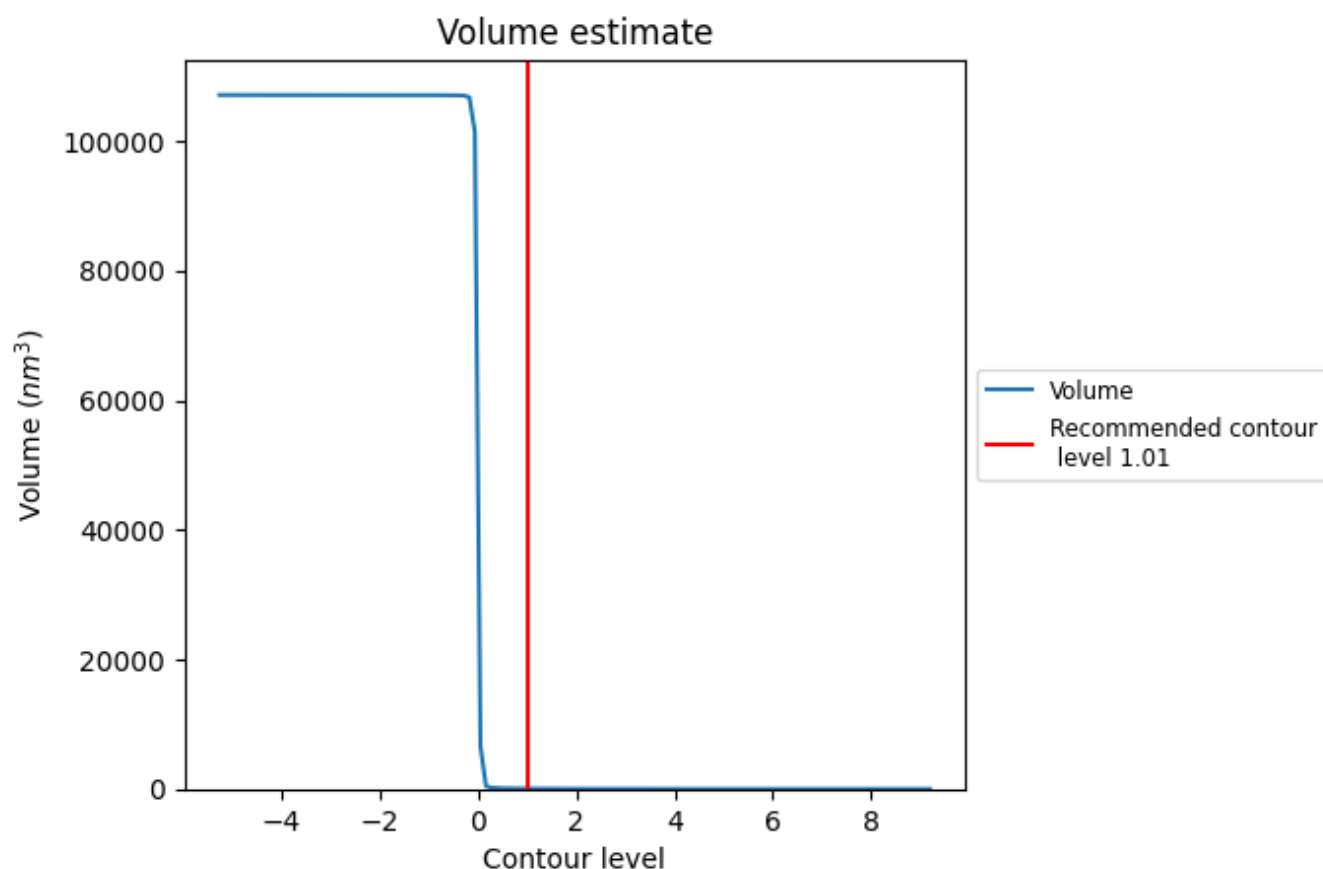
### 7.1 Map-value distribution [i](#)



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



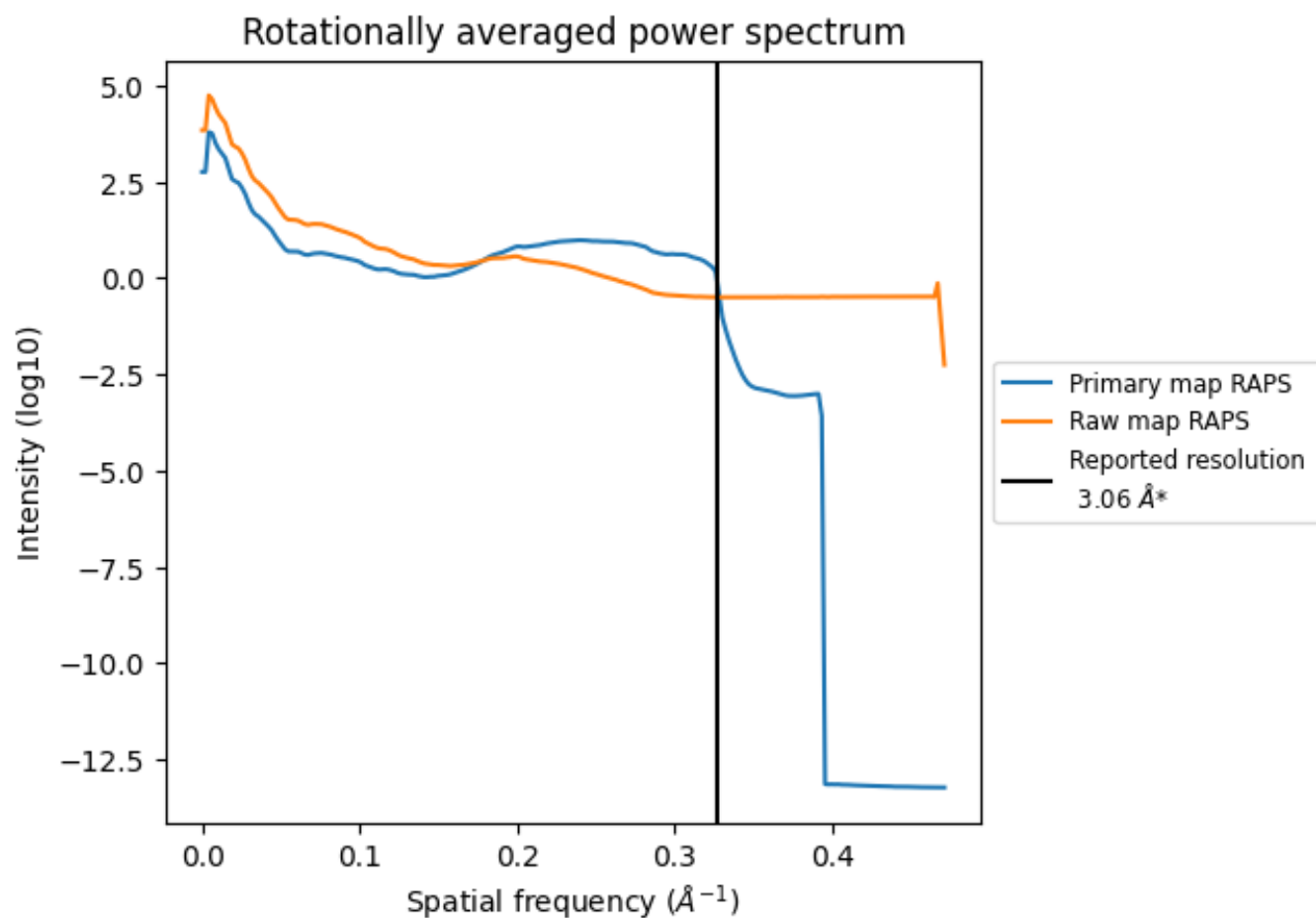
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49  $\text{nm}^3$ ; this corresponds to an approximate mass of 44 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 ⓘ

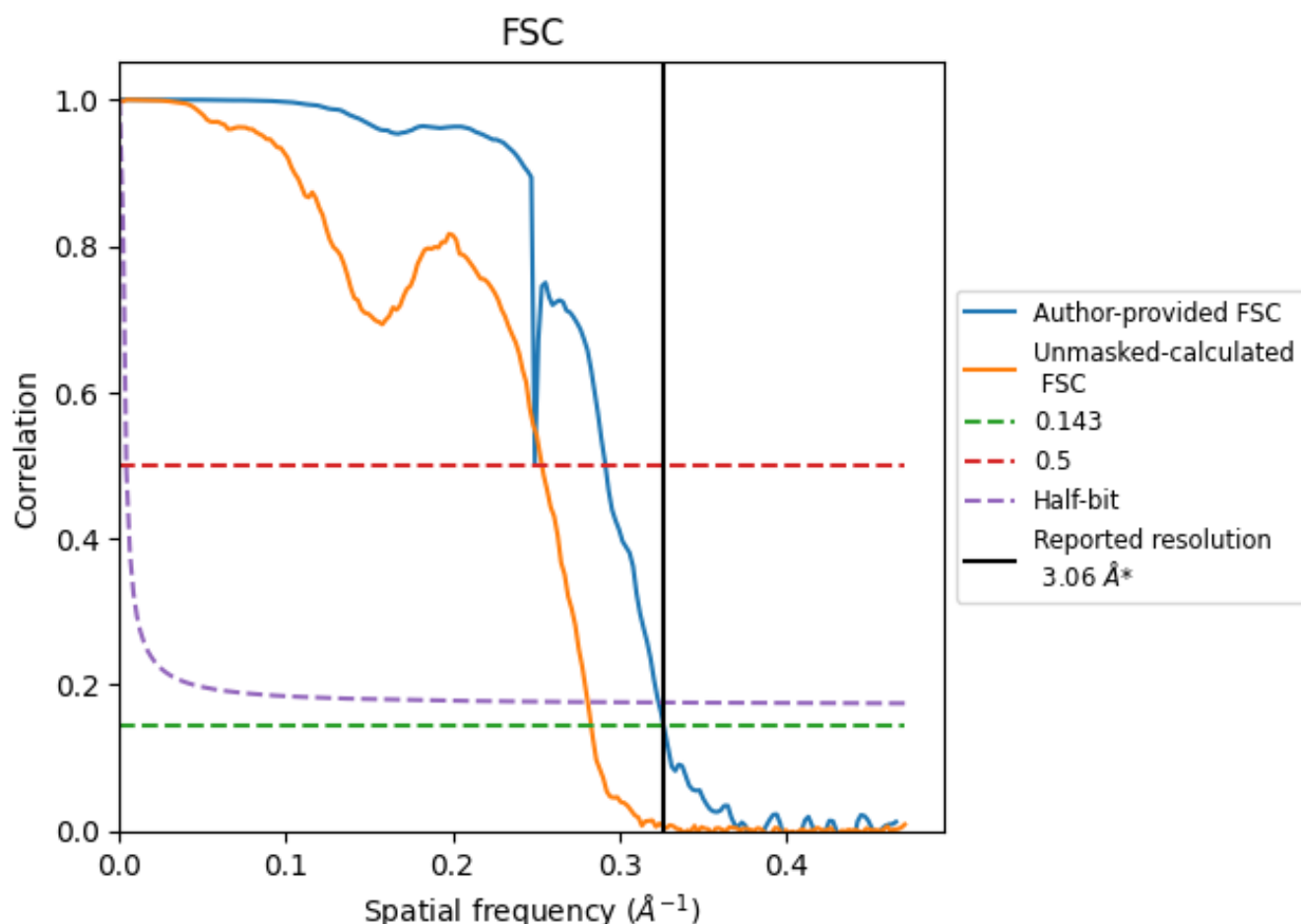


\*Reported resolution corresponds to spatial frequency of 0.327 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.327  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

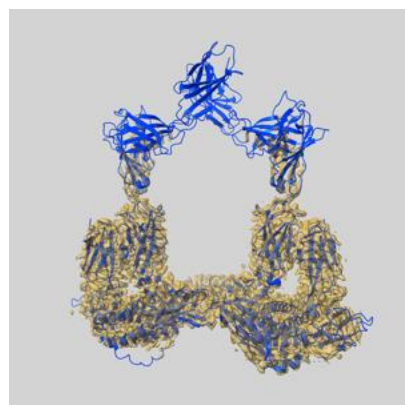
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.43	3.09
Unmasked-calculated*	3.53	3.94	3.55

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 3.06 by more than 10 %

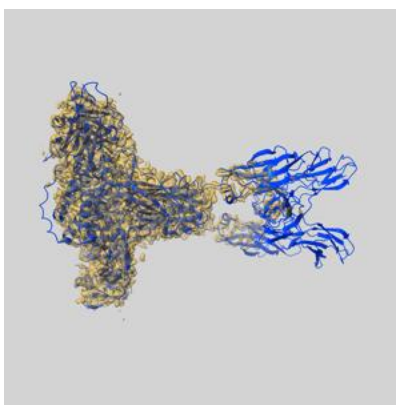
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18741 and PDB model 8QY4. Per-residue inclusion information can be found in section [3](#) on page [7](#).

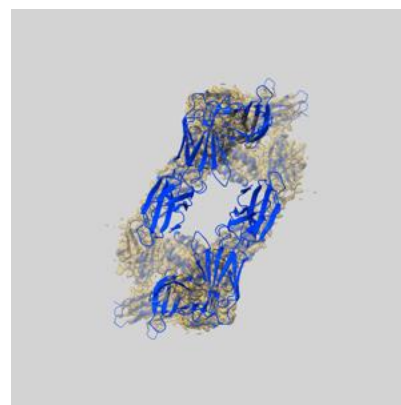
### 9.1 Map-model overlay [i](#)



X



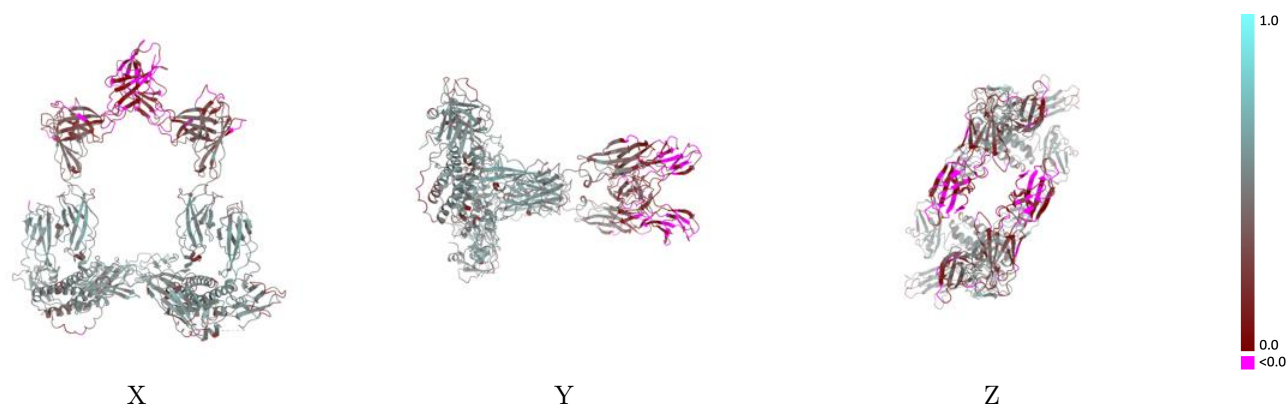
Y



Z

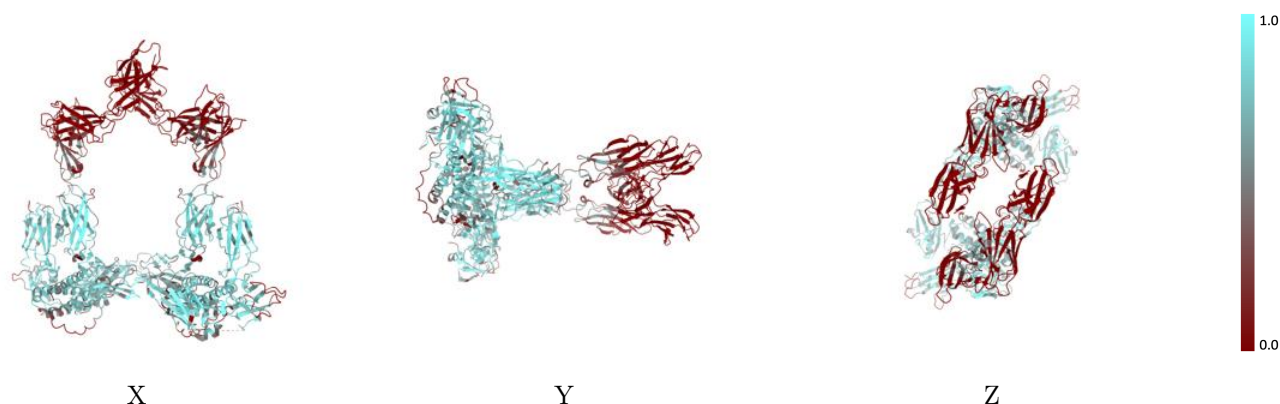
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



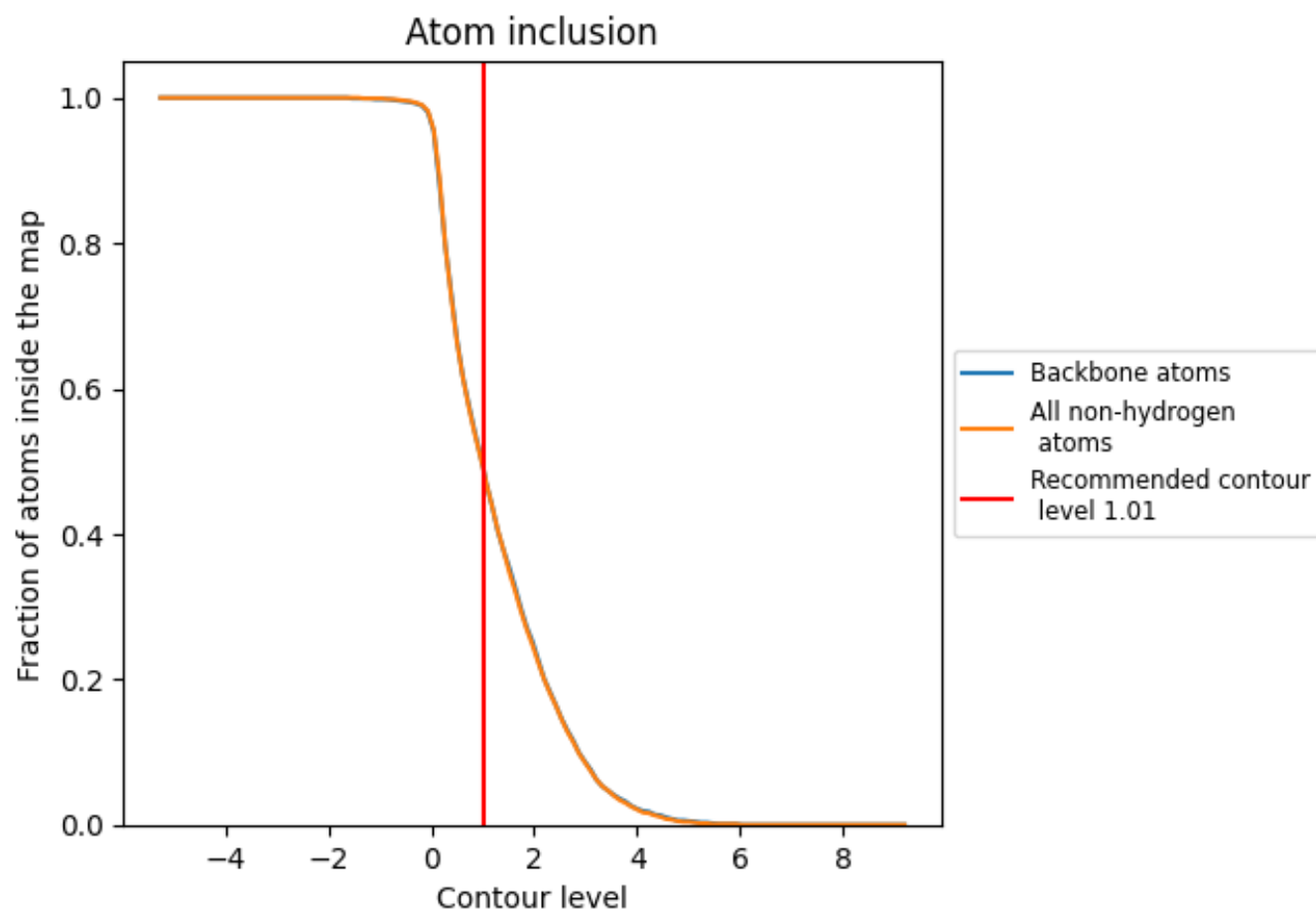
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 49% 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 (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4910	<div></div> 0.4040
A	<div></div> 0.6390	<div></div> 0.4680
B	<div></div> 0.6940	<div></div> 0.5110
C	<div></div> 0.3870	<div></div> 0.3530
D	<div></div> 0.6380	<div></div> 0.4670
E	<div></div> 0.7000	<div></div> 0.5090
F	<div></div> 0.3850	<div></div> 0.3510
G	<div></div> 0.0000	<div></div> 0.3110
H	<div></div> 0.0000	<div></div> 0.3130
I	<div></div> 0.2500	<div></div> 0.3270
J	<div></div> 0.3930	<div></div> 0.4960
K	<div></div> 0.1790	<div></div> 0.3400
L	<div></div> 0.3930	<div></div> 0.5070

