



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 10:30 am BST

PDB ID : 9TLG / pdb_00009tlg
EMDB ID : EMD-56054
Title : Structure of human prothrombinase with meizothrombin
Authors : Faille, A.; Ustok, F.I.; Warren, A.; Huntingon, J.A.
Deposited on : 2025-12-10
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary 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:

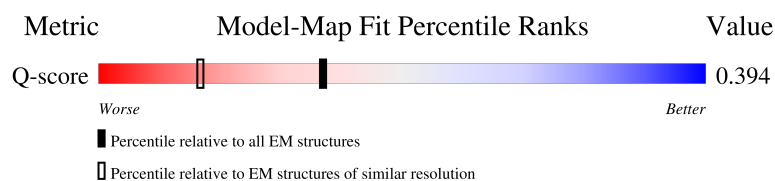
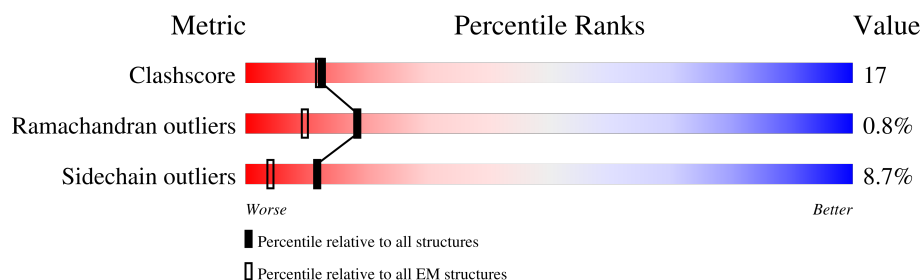
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	709	15% 57% 34% 5%
2	B	651	19% 59% 37% .
3	H	254	15% 55% 34% 8%
4	L	110	11% 29% 16% 5% 50%

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Mol	Chain	Length	Quality of chain
5	P	320	
6	Q	259	
7	X	3	
8	C	5	
8	E	5	
9	D	7	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16551 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 Coagulation factor V heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	673	Total	C	N	O	S	0	0
			5428	3444	913	1042	29		

- Molecule 2 is a protein called Coagulation factor V light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	651	Total	C	N	O	S	0	0
			5305	3376	916	988	25		

- Molecule 3 is a protein called Activated factor Xa heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	233	Total	C	N	O	S	0	0
			1860	1170	330	345	15		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	129	ASN	GLU	engineered mutation	UNP P00742
H	130	GLU	SER	engineered mutation	UNP P00742
H	132	LYS	THR	engineered mutation	UNP P00742
H	134	ASP	LYS	engineered mutation	UNP P00742
H	166	HIS	ASN	engineered mutation	UNP P00742
H	169	MET	LYS	engineered mutation	UNP P00742
H	173	ASP	SER	engineered mutation	UNP P00742
H	175	ARG	ILE	engineered mutation	UNP P00742
H	195	ALA	SER	engineered mutation	UNP P00742
H	233	ARG	ALA	engineered mutation	UNP P00742
H	239	LYS	ASP	engineered mutation	UNP P00742

- Molecule 4 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	55	Total	C	N	O	S	0	0
			416	253	79	76	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	85	MET	THR	engineered mutation	UNP P00742
L	90	ARG	SER	engineered mutation	UNP P00742
L	91	ALA	LEU	engineered mutation	UNP P00742
L	92	PHE	ASP	engineered mutation	UNP P00742
L	101	LYS	HIS	engineered mutation	UNP P00742
L	102	ARG	GLU	engineered mutation	UNP P00742
L	103	VAL	GLU	engineered mutation	UNP P00742
L	105	SER	ASN	engineered mutation	UNP P00742

- Molecule 5 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	152	Total	C	N	O	S	0	0
			1189	730	204	248	7		

- Molecule 6 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	259	Total	C	N	O	S	0	0
			2092	1334	370	374	14		

There is a discrepancy between the modelled and reference sequences:

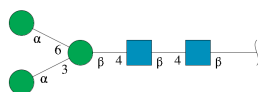
Chain	Residue	Modelled	Actual	Comment	Reference
Q	195	ALA	SER	engineered mutation	UNP P00734

- Molecule 7 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.



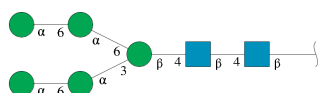
Mol	Chain	Residues	Atoms				AltConf	Trace
7	X	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 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.



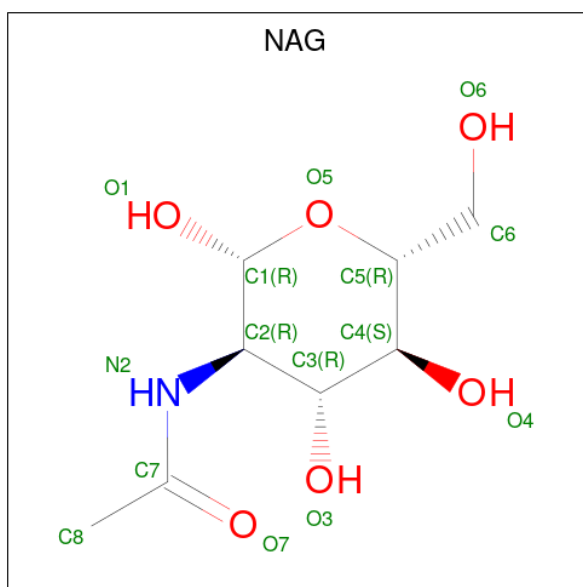
Mol	Chain	Residues	Atoms				AltConf	Trace
8	C	5	Total	C	N	O	0	0
			61	34	2	25		
8	E	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
9	D	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
11	H	1	Total	Ca	0
			1	1	

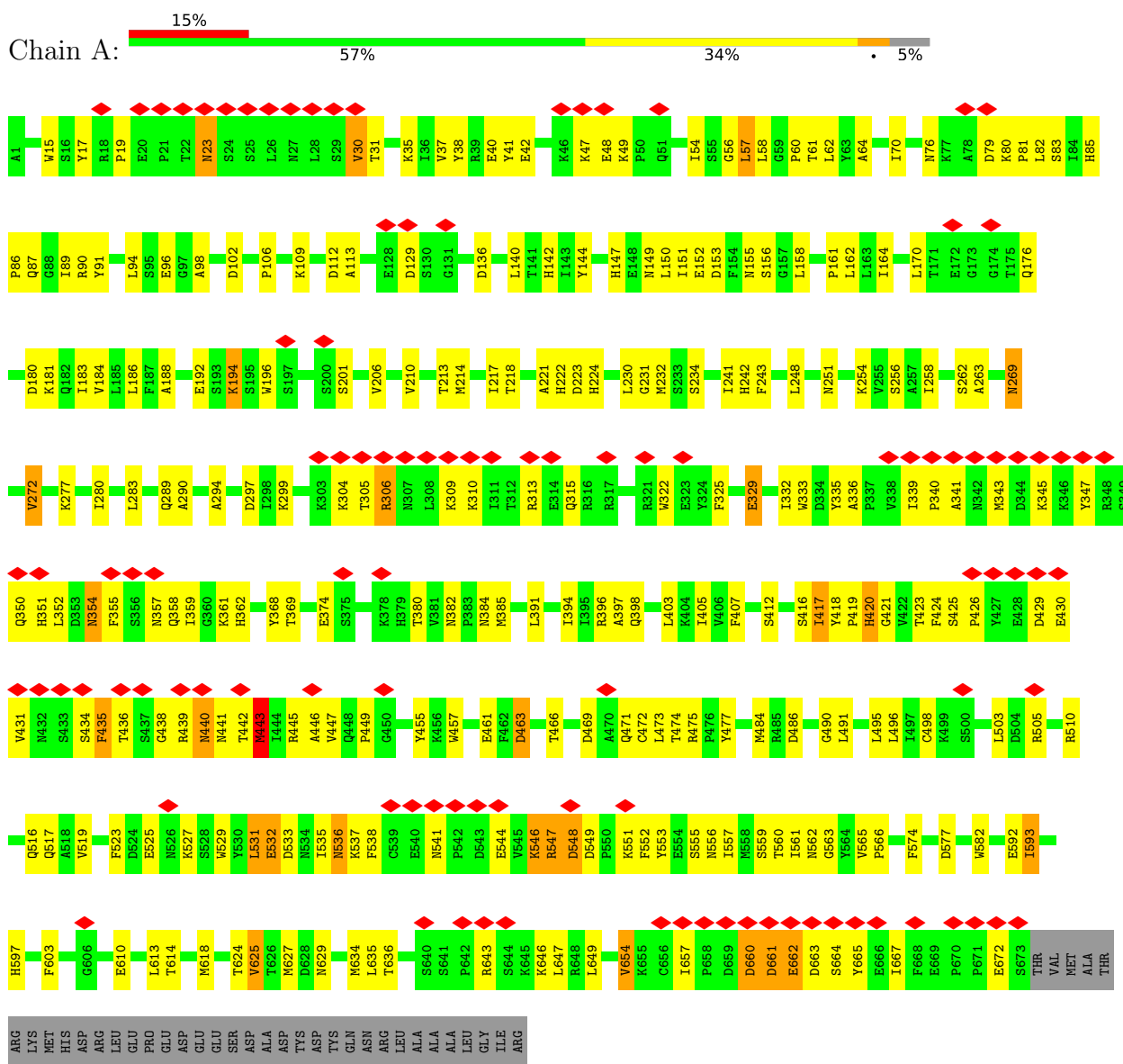
- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
12	H	1	Total	Na	0
			1	1	
12	Q	1	Total	Na	0
			1	1	

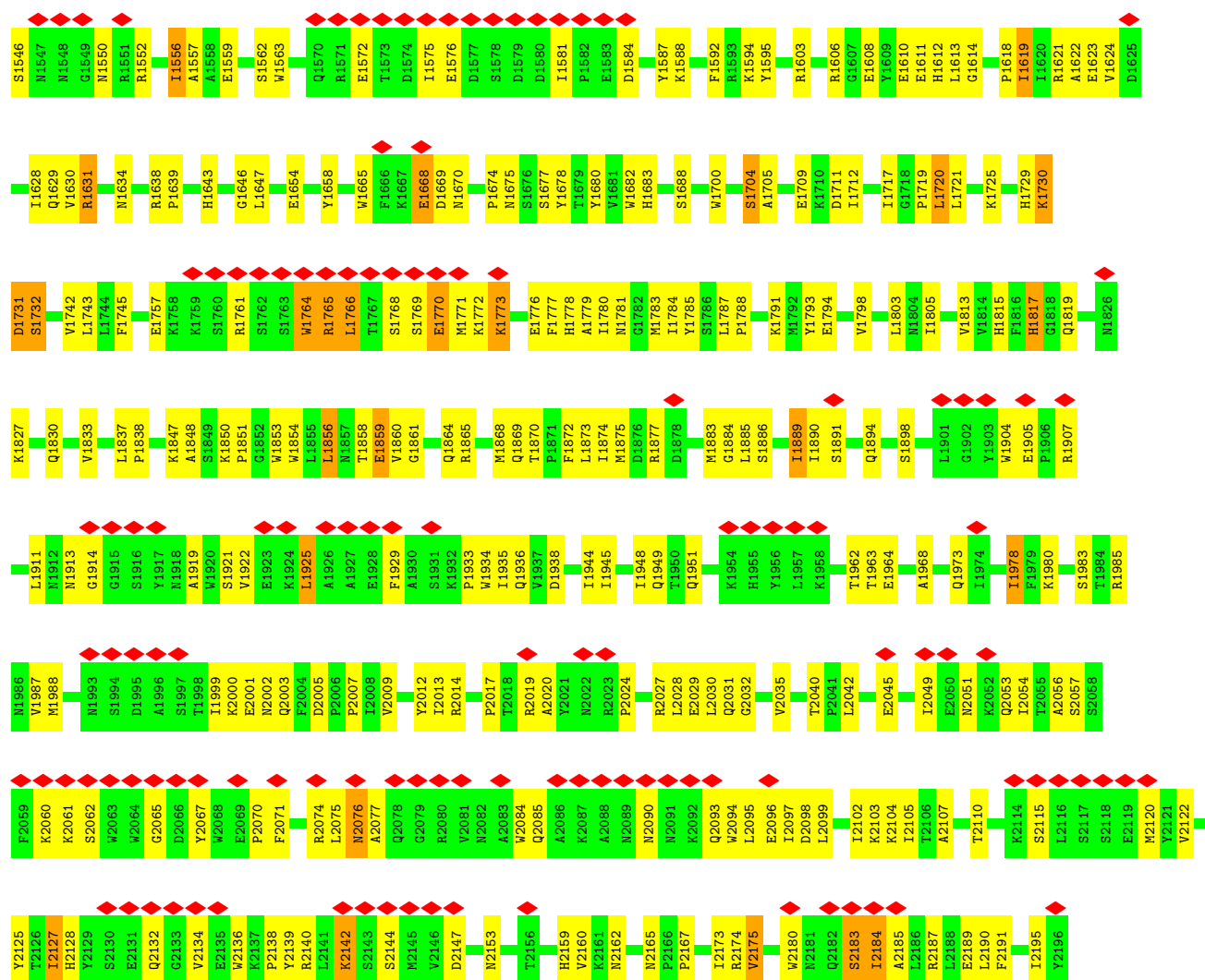
3 Residue-property plots

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.

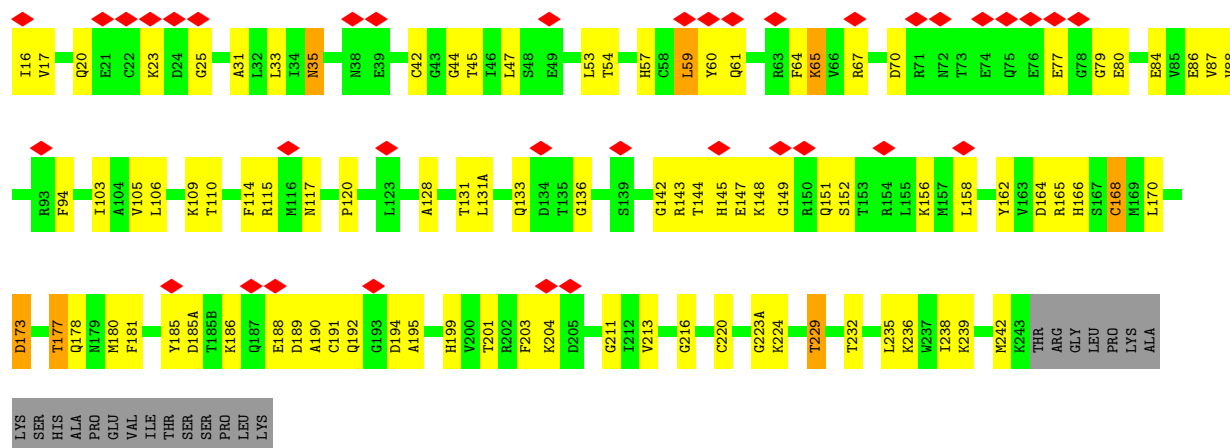
- Molecule 1: Coagulation factor V heavy chain



- Molecule 2: Coagulation factor V light chain



• Molecule 3: Activated factor Xa heavy chain



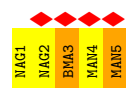
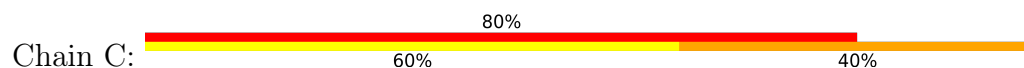
LYS
SER
HIS
ALA
PRO
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VAL
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THR
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LYS



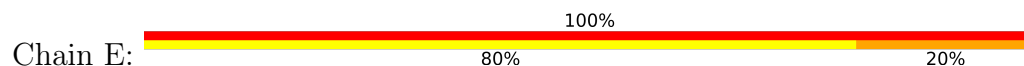
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25376	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.7	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	44.684	Depositor
Minimum map value	-29.948	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6	Depositor
Map size (Å)	314.92798, 314.92798, 314.92798	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/5552	0.38	0/7526
2	B	0.15	0/5448	0.34	0/7370
3	H	0.16	0/1899	0.43	1/2555 (0.0%)
4	L	0.21	0/422	0.74	1/565 (0.2%)
5	P	0.26	0/1213	0.75	0/1638
6	Q	0.13	0/2147	0.33	0/2902
All	All	0.16	0/16681	0.42	2/22556 (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
6	Q	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	134	LYS	N-CA-C	5.53	115.54	108.24
3	H	60	TYR	N-CA-C	-5.50	107.58	114.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	Q	36(A)	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	5428	0	5253	184	0
2	B	5305	0	5152	179	0
3	H	1860	0	1814	68	0
4	L	416	0	406	14	0
5	P	1189	0	1081	74	0
6	Q	2092	0	2063	60	0
7	X	39	0	34	1	0
8	C	61	0	52	1	0
8	E	61	0	52	1	0
9	D	83	0	70	2	0
10	B	14	0	13	2	0
11	H	1	0	0	0	0
12	H	1	0	0	0	0
12	Q	1	0	0	0	0
All	All	16551	0	15990	546	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 17.

The worst 5 of 546 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:P:175:GLY:O	5:P:220:ARG:NH2	2.12	0.82
1:A:603:PHE:HB3	1:A:625:VAL:HG12	1.66	0.78
2:B:1594:LYS:HB2	2:B:1618:PRO:HB3	1.67	0.77
5:P:221:ASN:HB3	5:P:229:VAL:HA	1.67	0.77
1:A:251:ASN:O	2:B:1827:LYS:NZ	2.17	0.76

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	670/709 (94%)	602 (90%)	63 (9%)	5 (1%)	18	49
2	B	649/651 (100%)	593 (91%)	53 (8%)	3 (0%)	24	57
3	H	231/254 (91%)	209 (90%)	22 (10%)	0	100	100
4	L	53/110 (48%)	43 (81%)	8 (15%)	2 (4%)	2	15
5	P	150/320 (47%)	102 (68%)	42 (28%)	6 (4%)	2	13
6	Q	257/259 (99%)	247 (96%)	9 (4%)	1 (0%)	30	61
All	All	2010/2303 (87%)	1796 (89%)	197 (10%)	17 (1%)	18	47

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	ASN
2	B	1584	ASP
2	B	1766	LEU
4	L	90	ARG
5	P	264	SER

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	606/634 (96%)	555 (92%)	51 (8%)	10	35
2	B	576/576 (100%)	532 (92%)	44 (8%)	12	39
3	H	198/216 (92%)	185 (93%)	13 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	46/94 (49%)	38 (83%)	8 (17%)	2	9
5	P	125/271 (46%)	97 (78%)	28 (22%)	1	4
6	Q	224/224 (100%)	213 (95%)	11 (5%)	22	53
All	All	1775/2015 (88%)	1620 (91%)	155 (9%)	12	34

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	138	GLU
5	P	312	LEU
5	P	182	LEU
5	P	245	LEU
6	Q	154	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2085	GLN
3	H	199	HIS
2	B	2128	HIS
3	H	151	GLN
5	P	187	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	TYS	A	665	1	15,16,17	1.94	2 (13%)	18,22,24	1.21	2 (11%)

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
1	TYS	A	665	1	-	2/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	665	TYS	OH-S	6.65	1.68	1.58
1	A	665	TYS	OH-CZ	-3.12	1.37	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	TYS	CG-CB-CA	2.50	119.16	114.10
1	A	665	TYS	O3-S-OH	-2.48	99.87	105.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	665	TYS	CA-CB-CG-CD2
1	A	665	TYS	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

20 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
8	NAG	C	1	8,2	14,14,15	0.76	0	17,19,21	1.32	2 (11%)
8	NAG	C	2	8	14,14,15	0.72	0	17,19,21	1.75	3 (17%)
8	BMA	C	3	8	11,11,12	1.16	1 (9%)	15,15,17	3.70	7 (46%)
8	MAN	C	4	8	11,11,12	0.81	0	15,15,17	1.74	1 (6%)
8	MAN	C	5	8	11,11,12	0.78	0	15,15,17	1.30	1 (6%)
9	NAG	D	1	9	14,14,15	0.79	1 (7%)	17,19,21	2.51	7 (41%)
9	NAG	D	2	9	14,14,15	0.76	0	17,19,21	1.12	1 (5%)
9	BMA	D	3	9	11,11,12	0.92	1 (9%)	15,15,17	2.25	3 (20%)
9	MAN	D	4	9	11,11,12	0.62	0	15,15,17	1.79	1 (6%)
9	MAN	D	5	9	11,11,12	0.72	0	15,15,17	1.12	1 (6%)
9	MAN	D	6	9	11,11,12	0.80	0	15,15,17	1.25	2 (13%)
9	MAN	D	7	9	11,11,12	0.80	0	15,15,17	1.06	0
8	NAG	E	1	8,6	14,14,15	0.63	0	17,19,21	1.15	2 (11%)
8	NAG	E	2	8	14,14,15	0.82	0	17,19,21	2.06	6 (35%)
8	BMA	E	3	8	11,11,12	0.88	0	15,15,17	3.39	8 (53%)
8	MAN	E	4	8	11,11,12	0.60	0	15,15,17	1.80	1 (6%)
8	MAN	E	5	8	11,11,12	0.55	0	15,15,17	2.35	2 (13%)
7	NAG	X	1	7,1	14,14,15	0.77	0	17,19,21	2.38	4 (23%)
7	NAG	X	2	7	14,14,15	0.71	0	17,19,21	0.96	1 (5%)
7	BMA	X	3	7	11,11,12	0.79	0	15,15,17	2.86	5 (33%)

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
8	NAG	C	1	8,2	-	4/6/23/26	0/1/1/1
8	NAG	C	2	8	-	3/6/23/26	0/1/1/1
8	BMA	C	3	8	-	1/2/19/22	0/1/1/1
8	MAN	C	4	8	-	1/2/19/22	0/1/1/1
8	MAN	C	5	8	-	2/2/19/22	1/1/1/1
9	NAG	D	1	9	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	D	2	9	-	0/6/23/26	0/1/1/1
9	BMA	D	3	9	-	1/2/19/22	0/1/1/1
9	MAN	D	4	9	-	2/2/19/22	0/1/1/1
9	MAN	D	5	9	-	2/2/19/22	0/1/1/1
9	MAN	D	6	9	-	1/2/19/22	0/1/1/1
9	MAN	D	7	9	-	1/2/19/22	0/1/1/1
8	NAG	E	1	8,6	-	1/6/23/26	0/1/1/1
8	NAG	E	2	8	-	2/6/23/26	0/1/1/1
8	BMA	E	3	8	-	2/2/19/22	0/1/1/1
8	MAN	E	4	8	-	1/2/19/22	0/1/1/1
8	MAN	E	5	8	-	0/2/19/22	0/1/1/1
7	NAG	X	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	3	BMA	C2-C3	2.86	1.56	1.52
9	D	1	NAG	O5-C1	-2.09	1.40	1.43
9	D	3	BMA	C2-C3	2.04	1.55	1.52

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	3	BMA	C1-O5-C5	10.27	126.11	112.19
8	E	3	BMA	C1-O5-C5	10.27	126.10	112.19
7	X	3	BMA	C1-O5-C5	9.14	124.58	112.19
8	E	5	MAN	C1-O5-C5	8.00	123.03	112.19
9	D	1	NAG	C2-N2-C7	7.71	133.88	122.90

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	X	1	NAG	O5-C5-C6-O6
8	C	5	MAN	C4-C5-C6-O6
9	D	4	MAN	O5-C5-C6-O6
8	C	2	NAG	C1-C2-N2-C7
7	X	1	NAG	C4-C5-C6-O6

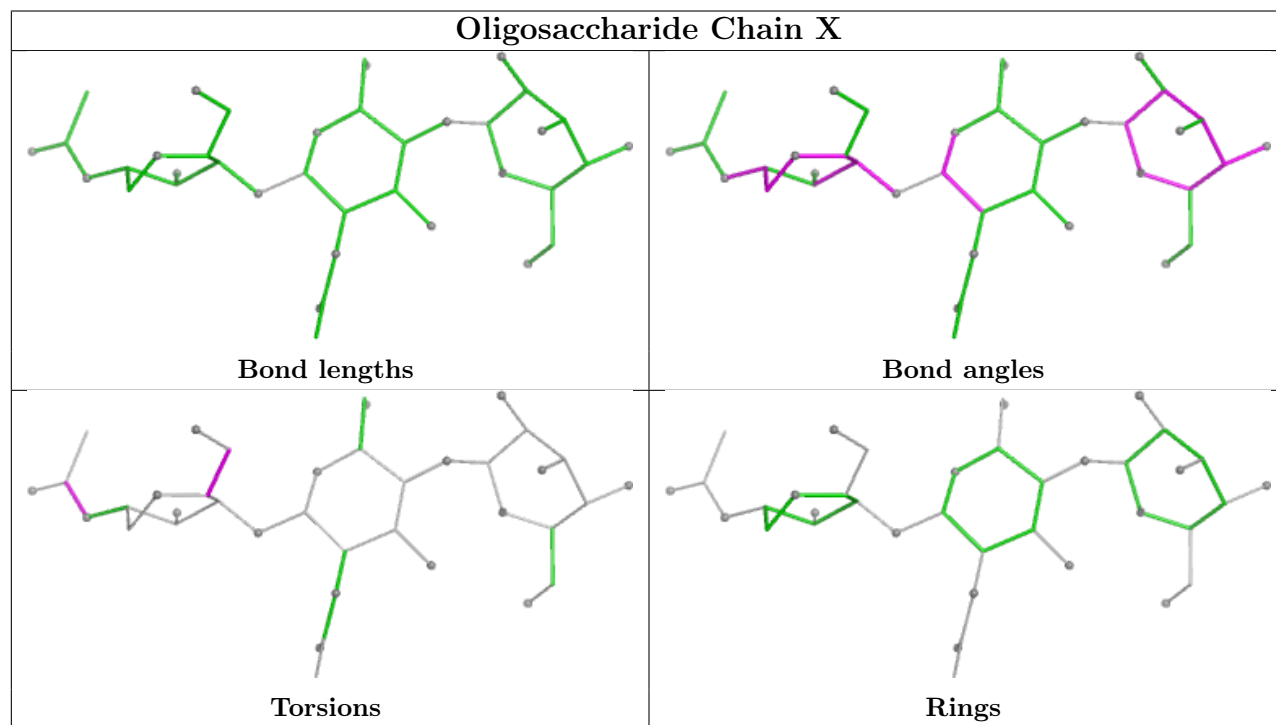
All (1) ring outliers are listed below:

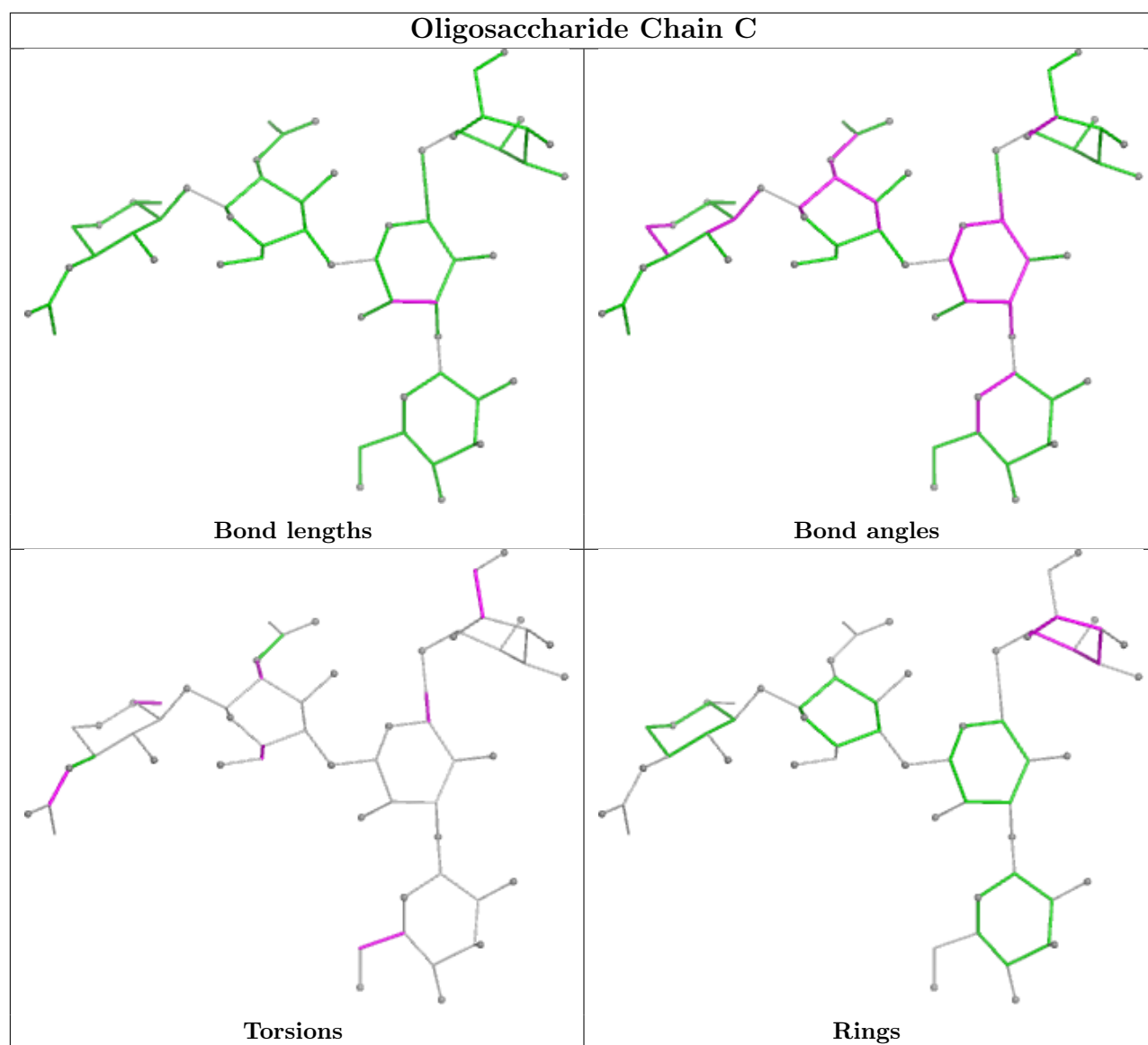
Mol	Chain	Res	Type	Atoms
8	C	5	MAN	C1-C2-C3-C4-C5-O5

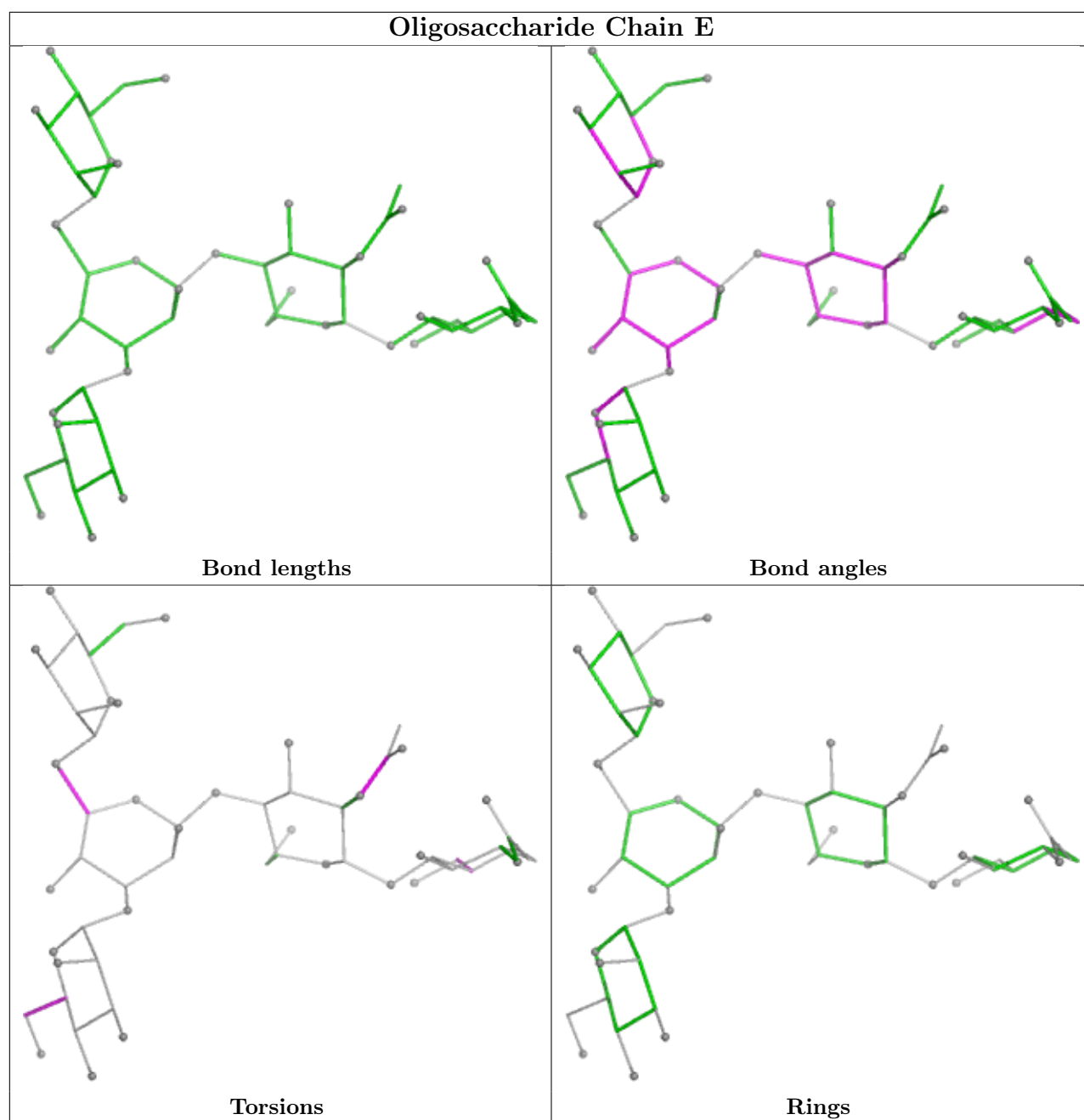
7 monomers are involved in 5 short contacts:

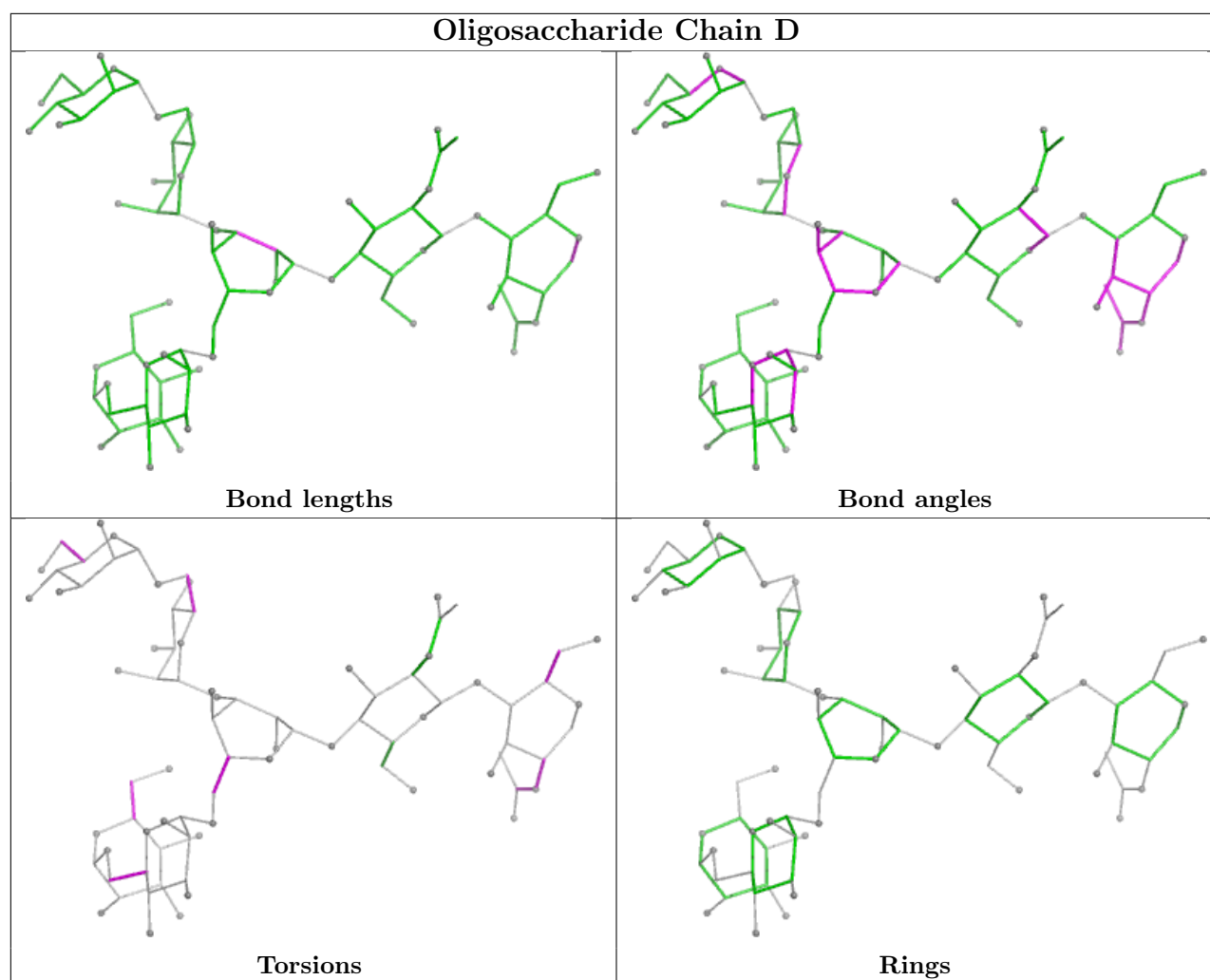
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	7	MAN	1	0
8	E	1	NAG	1	0
8	C	5	MAN	1	0
8	C	3	BMA	1	0
9	D	1	NAG	1	0
9	D	6	MAN	1	0
7	X	1	NAG	1	0

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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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
10	NAG	B	2201	2	14,14,15	0.74	0	17,19,21	1.88	3 (17%)

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
10	NAG	B	2201	2	-	0/6/23/26	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(°)
10	B	2201	NAG	C1-O5-C5	6.52	121.03	112.19
10	B	2201	NAG	C1-C2-N2	2.33	114.47	110.49
10	B	2201	NAG	O5-C1-C2	-2.28	107.68	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	2201	NAG	2	0

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.

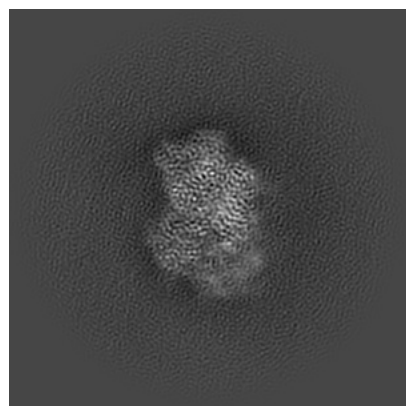
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56054. 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](#)

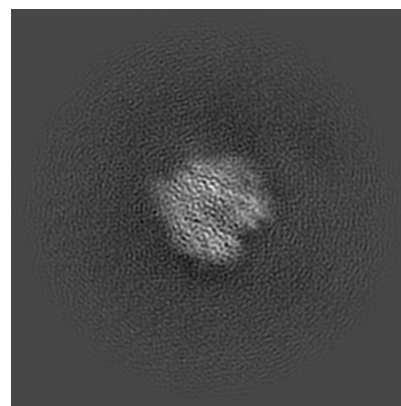
6.1.1 Primary map



X

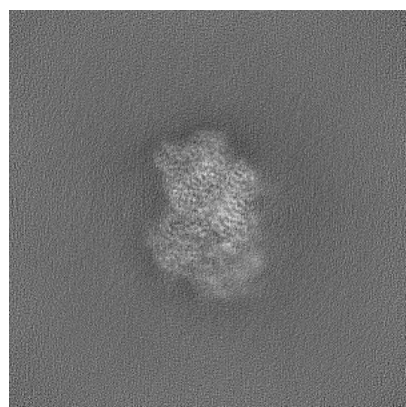


Y

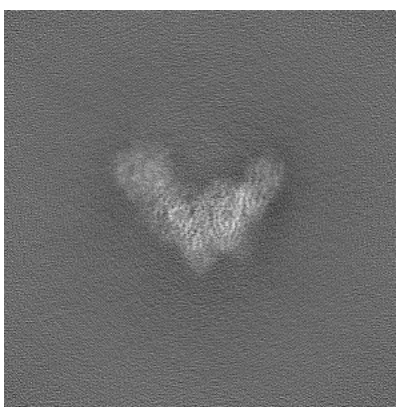


Z

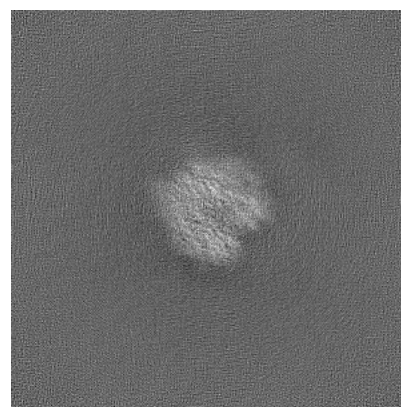
6.1.2 Raw map



X



Y

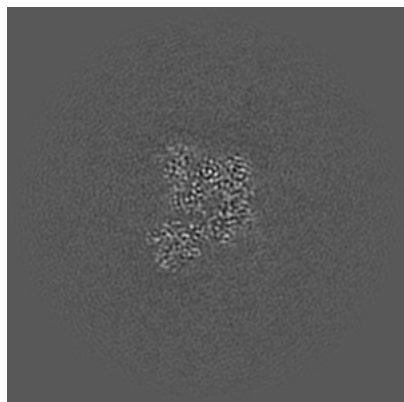


Z

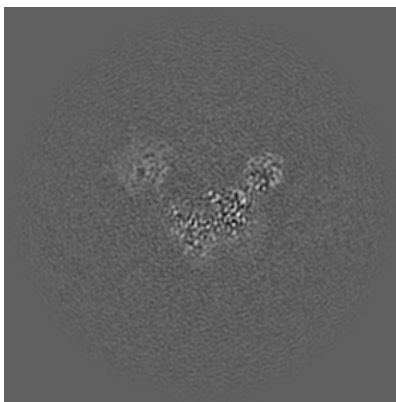
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

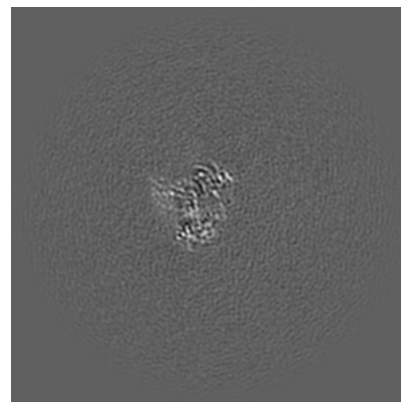
6.2.1 Primary map



X Index: 216

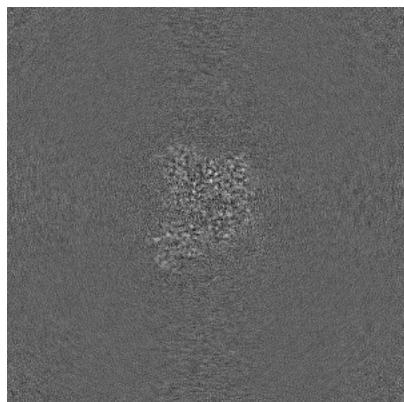


Y Index: 216

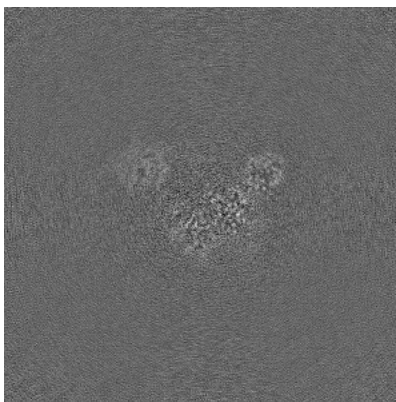


Z Index: 216

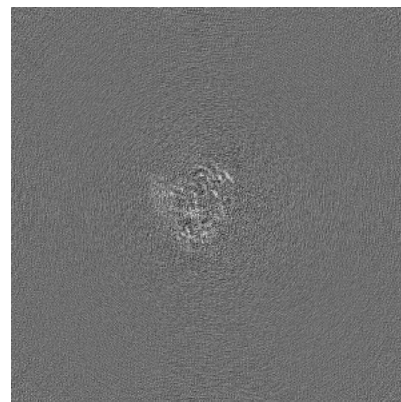
6.2.2 Raw map



X Index: 216



Y Index: 216

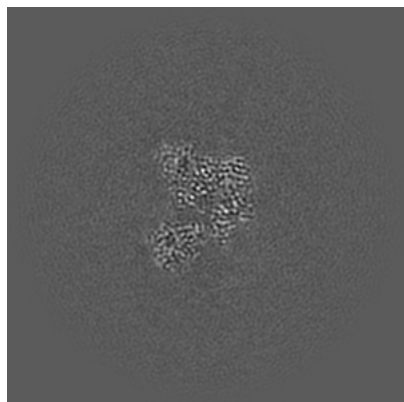


Z Index: 216

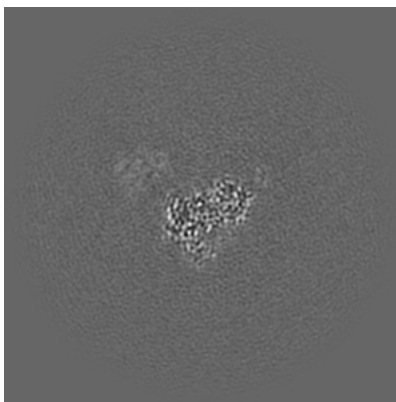
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

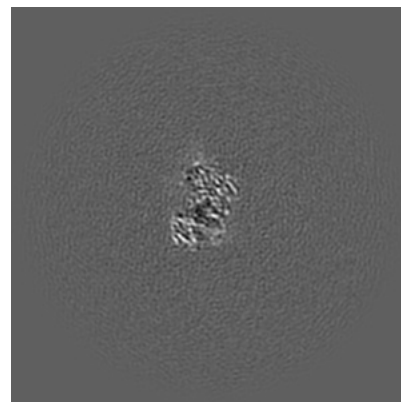
6.3.1 Primary map



X Index: 219

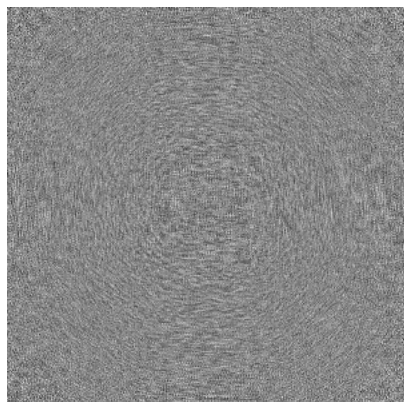


Y Index: 237

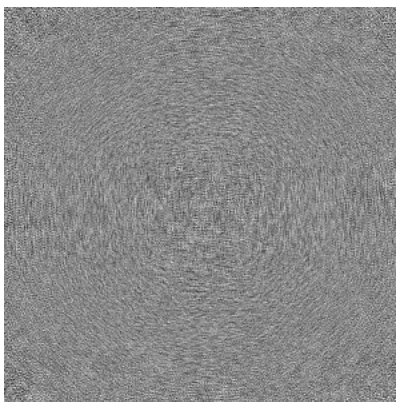


Z Index: 236

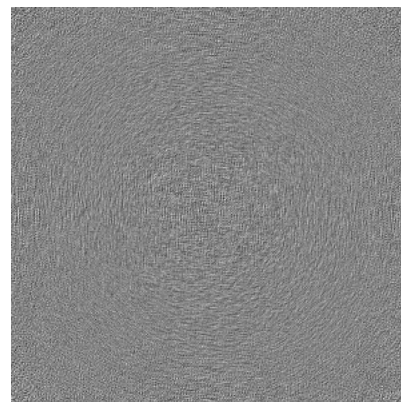
6.3.2 Raw map



X Index: 0



Y Index: 0

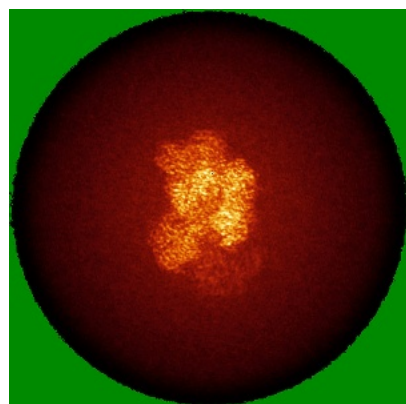


Z Index: 0

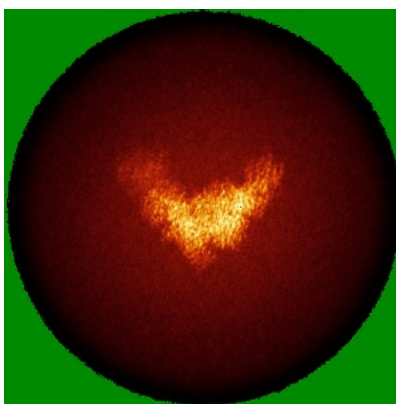
The images above show the largest variance slices of the map in three orthogonal directions.

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

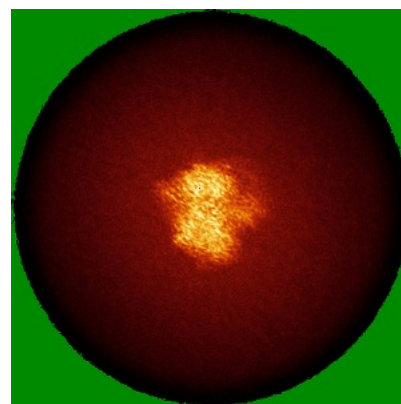
6.4.1 Primary map



X

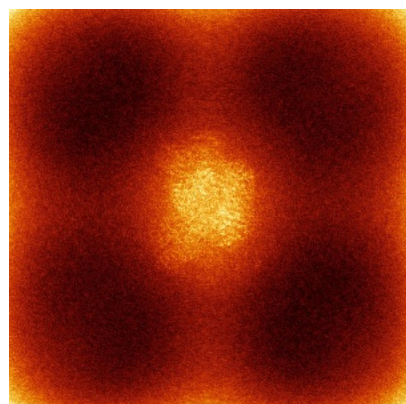


Y

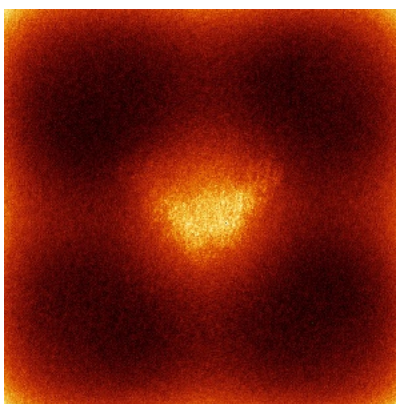


Z

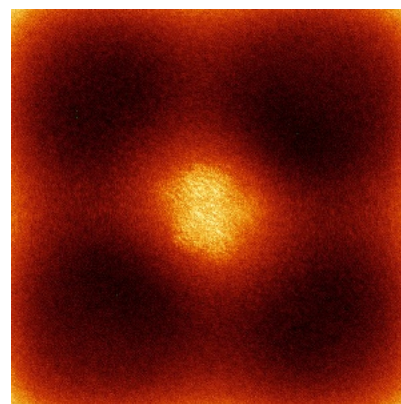
6.4.2 Raw map



X



Y

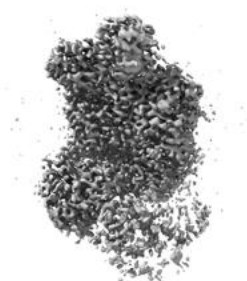


Z

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](#)

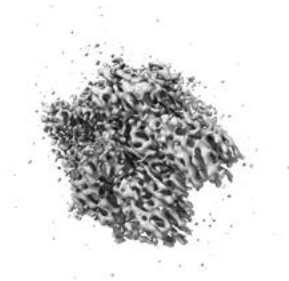
6.5.1 Primary map



X



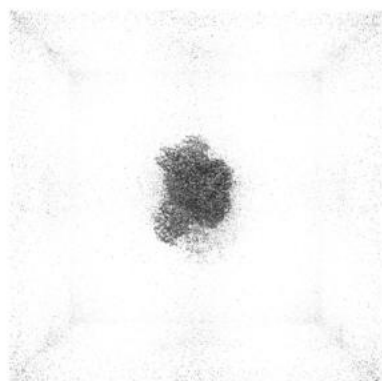
Y



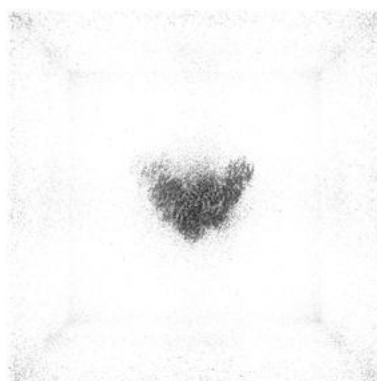
Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

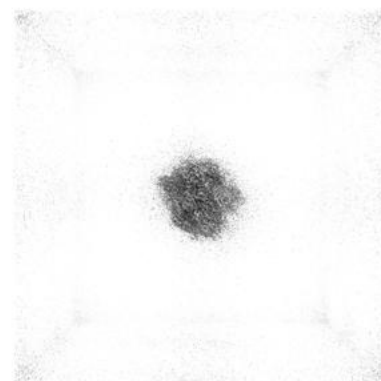
6.5.2 Raw map



X



Y



Z

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.

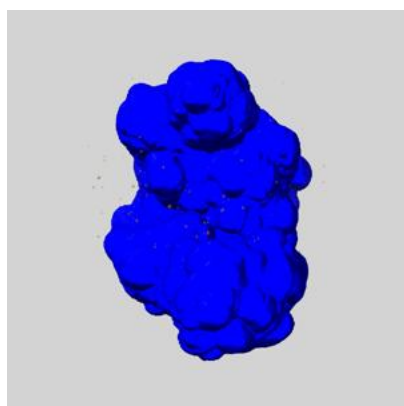
6.6 Mask visualisation [i](#)

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

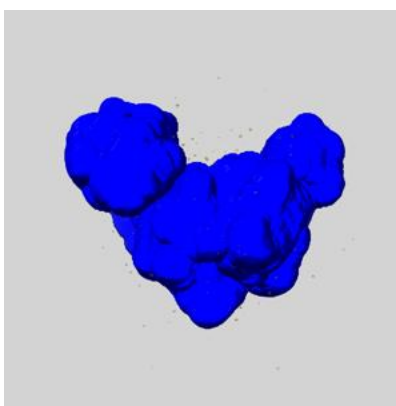
A mask typically either:

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

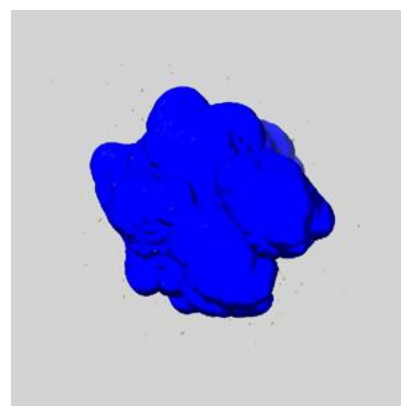
6.6.1 emd_56054_msk_1.map [i](#)



X



Y

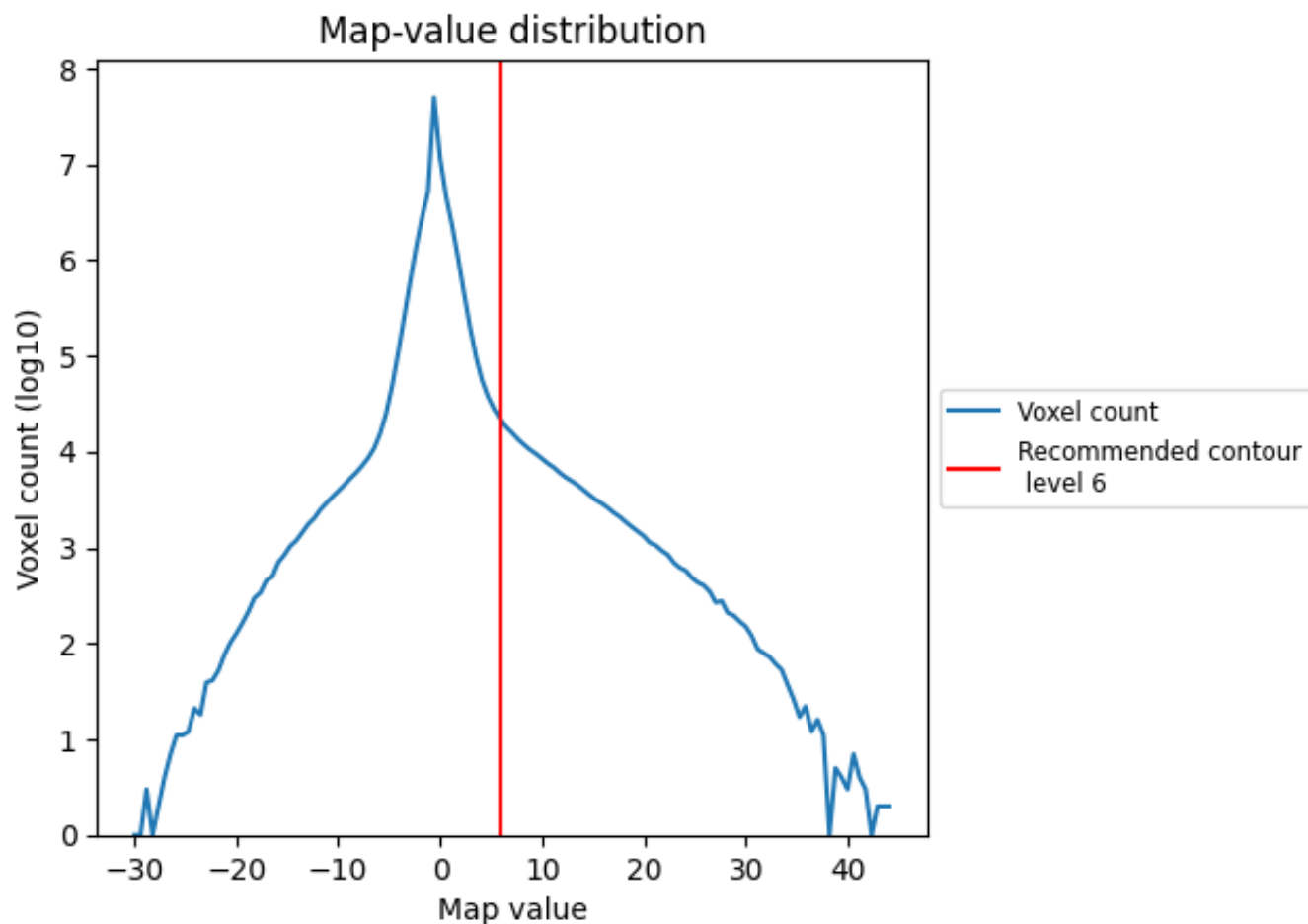


Z

7 Map analysis [i](#)

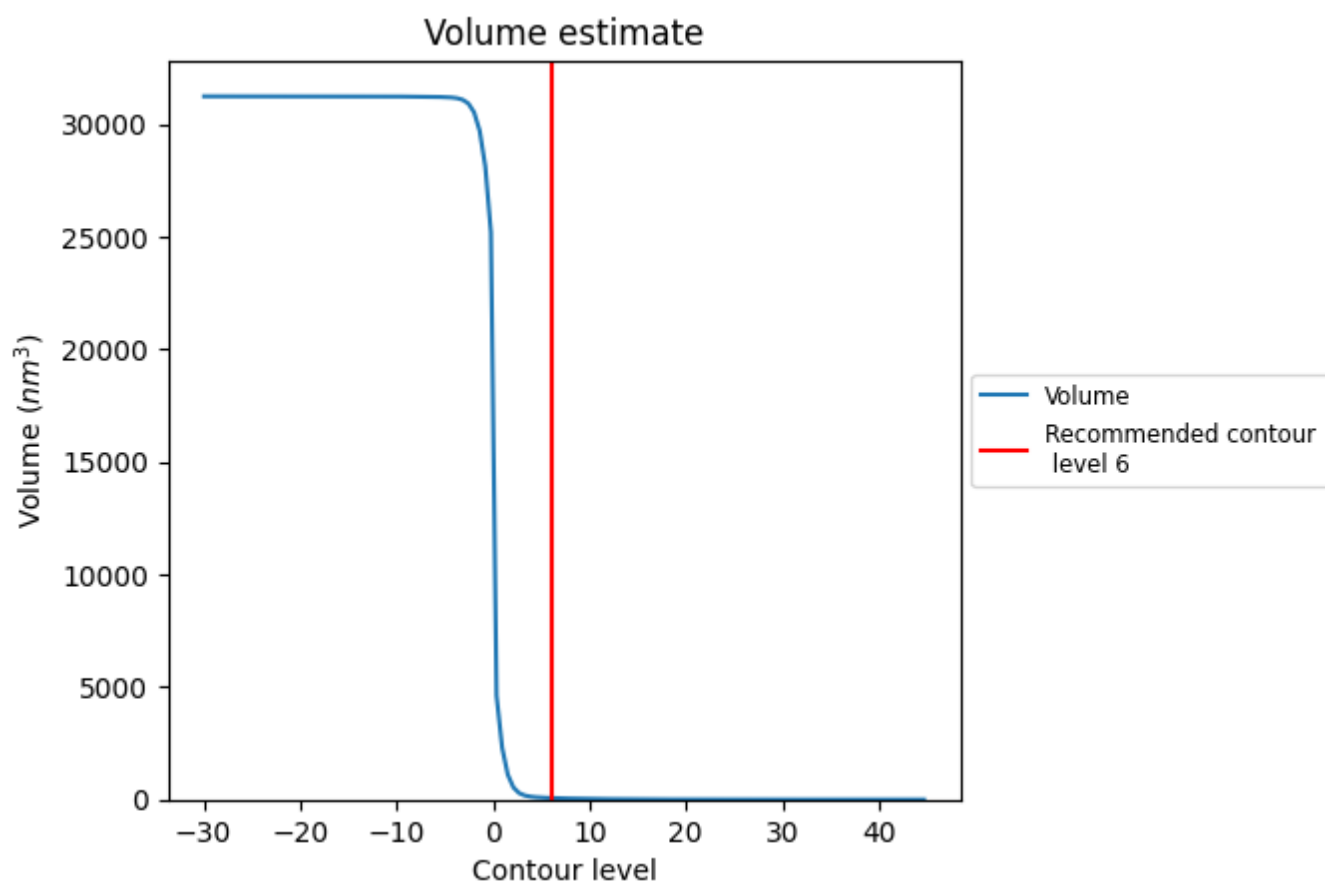
This section contains the results of statistical analysis of the map.

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.

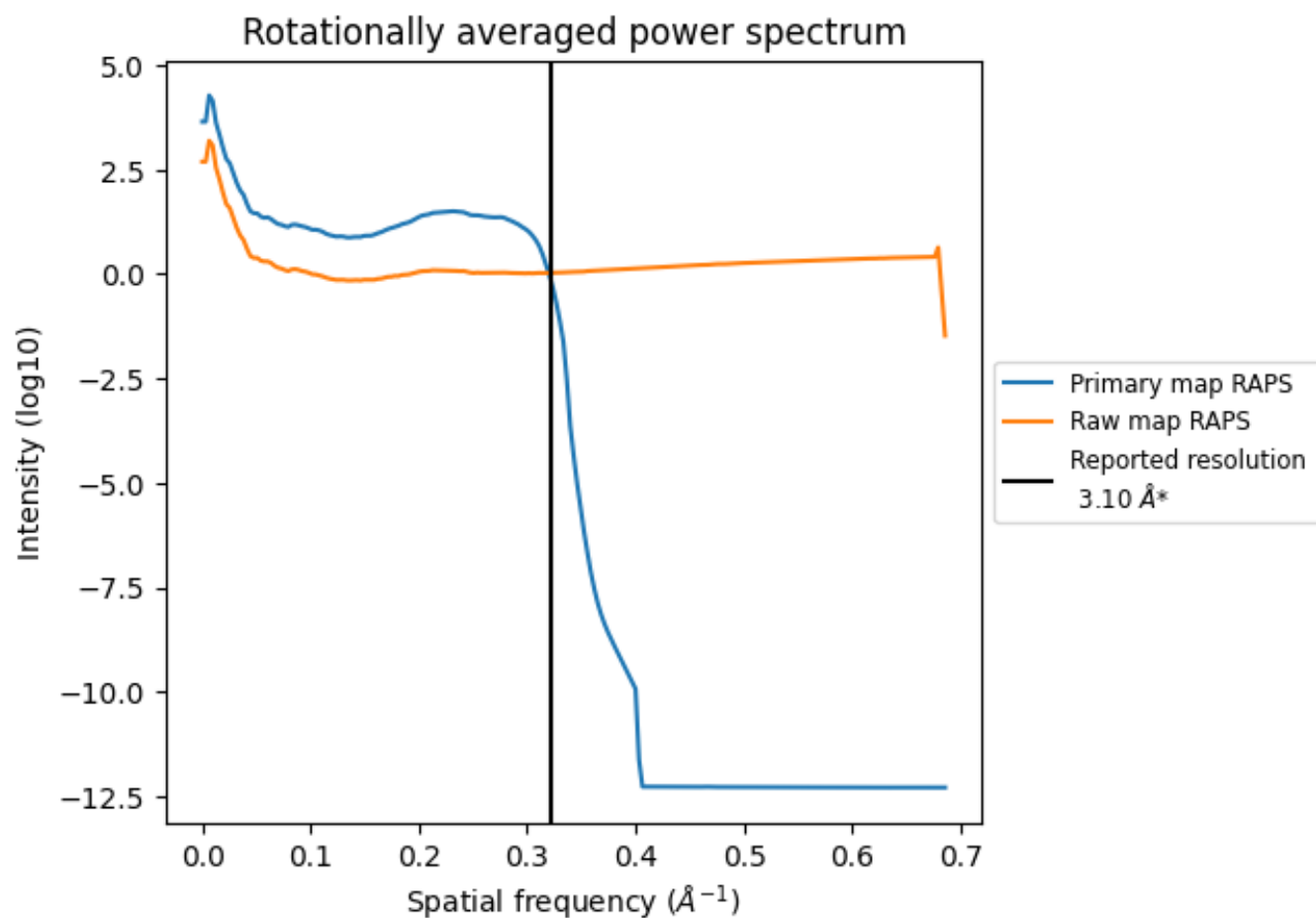
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm^3 ; this corresponds to an approximate mass of 62 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 ⓘ

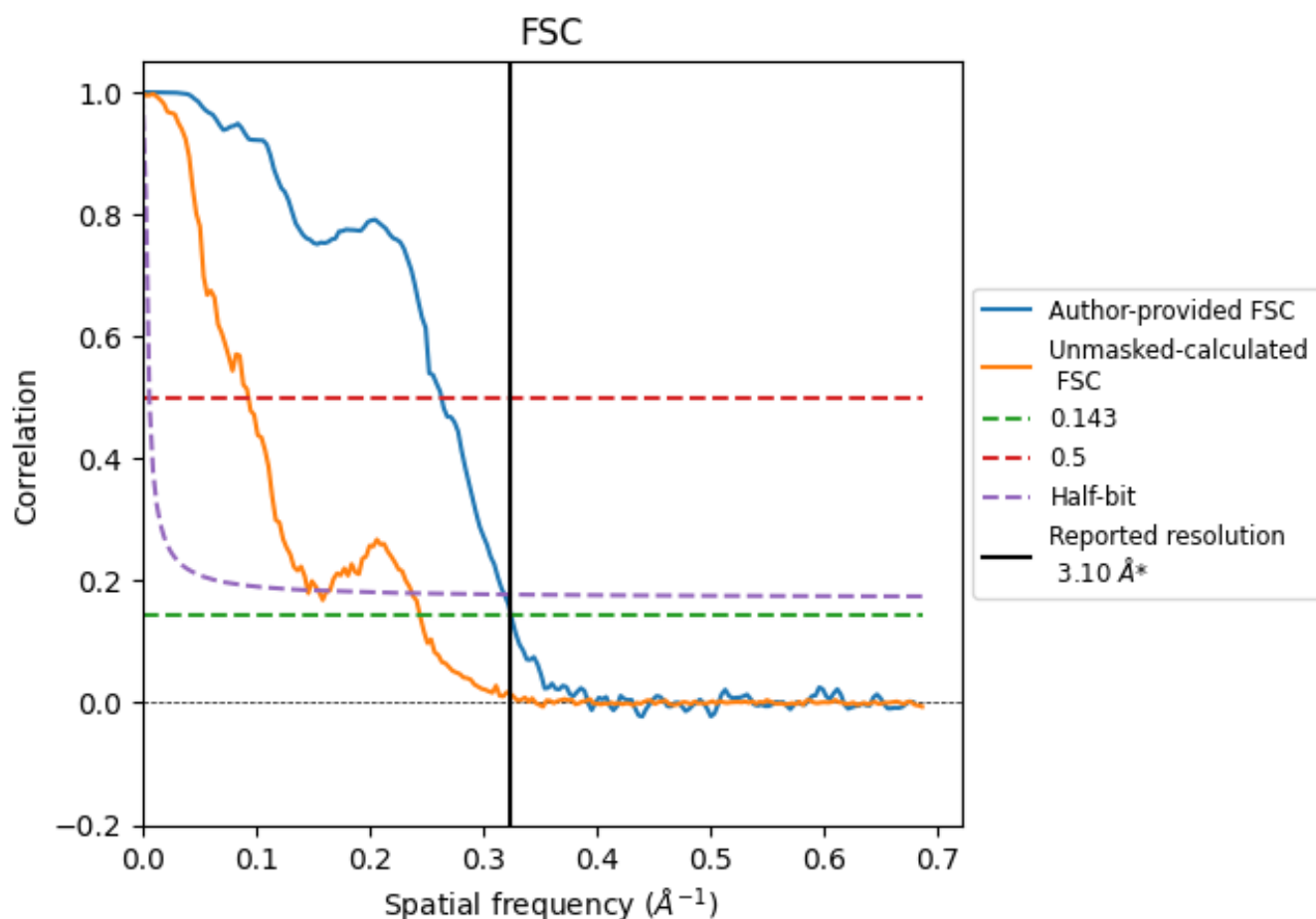


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

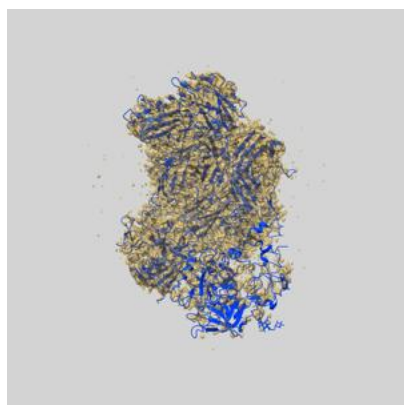
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.80	3.14
Unmasked-calculated*	4.09	10.72	6.87

*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 4.09 differs from the reported value 3.1 by more than 10 %

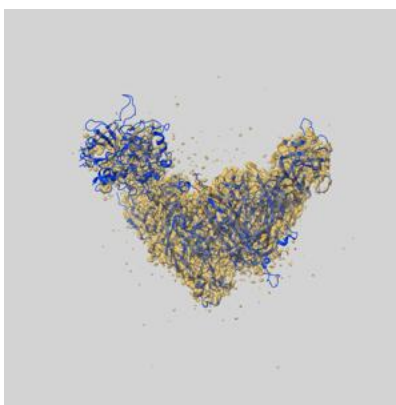
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56054 and PDB model 9TLG. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

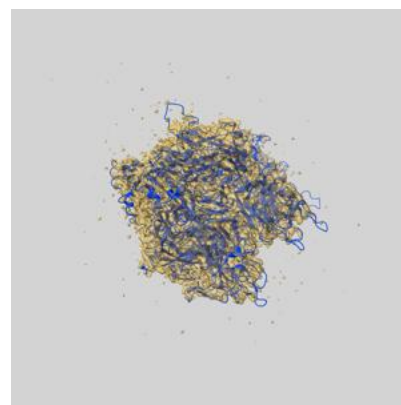
9.1 Map-model overlay [i](#)



X



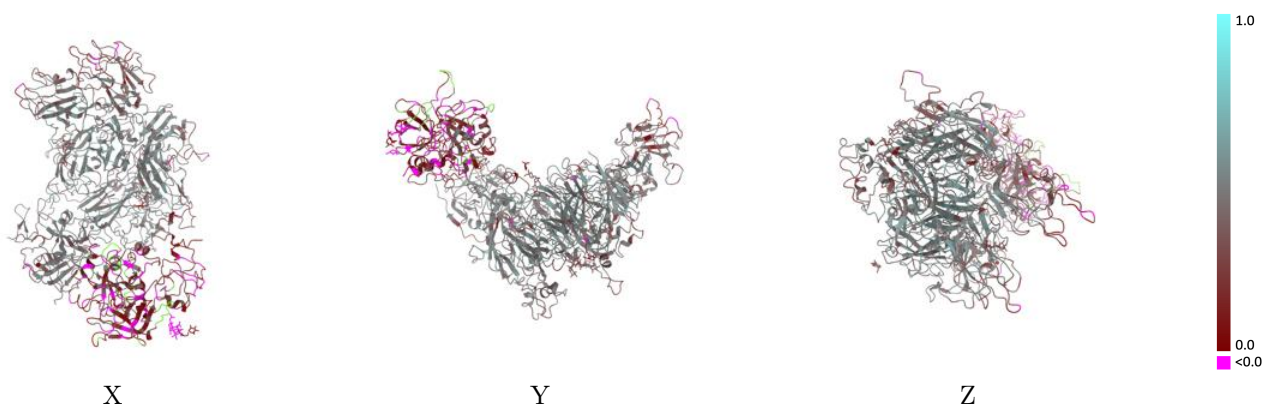
Y



Z

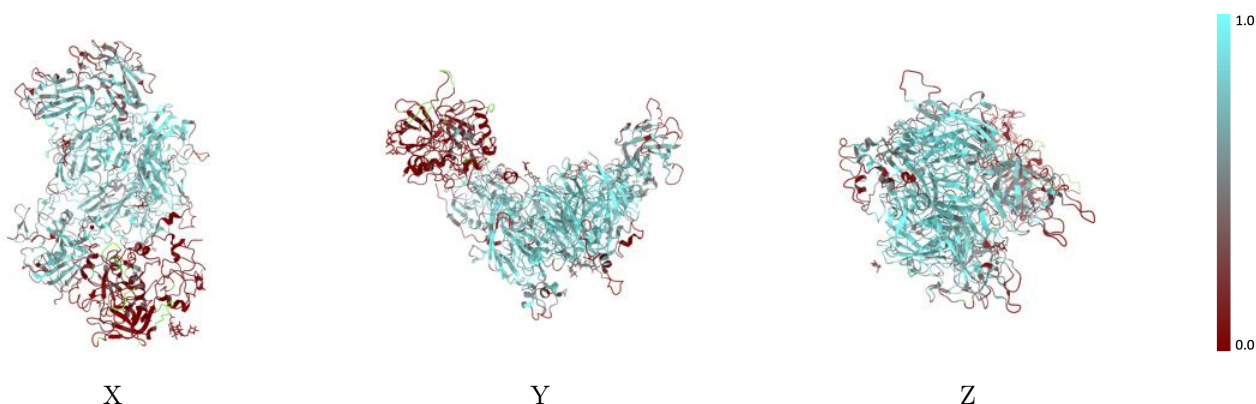
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



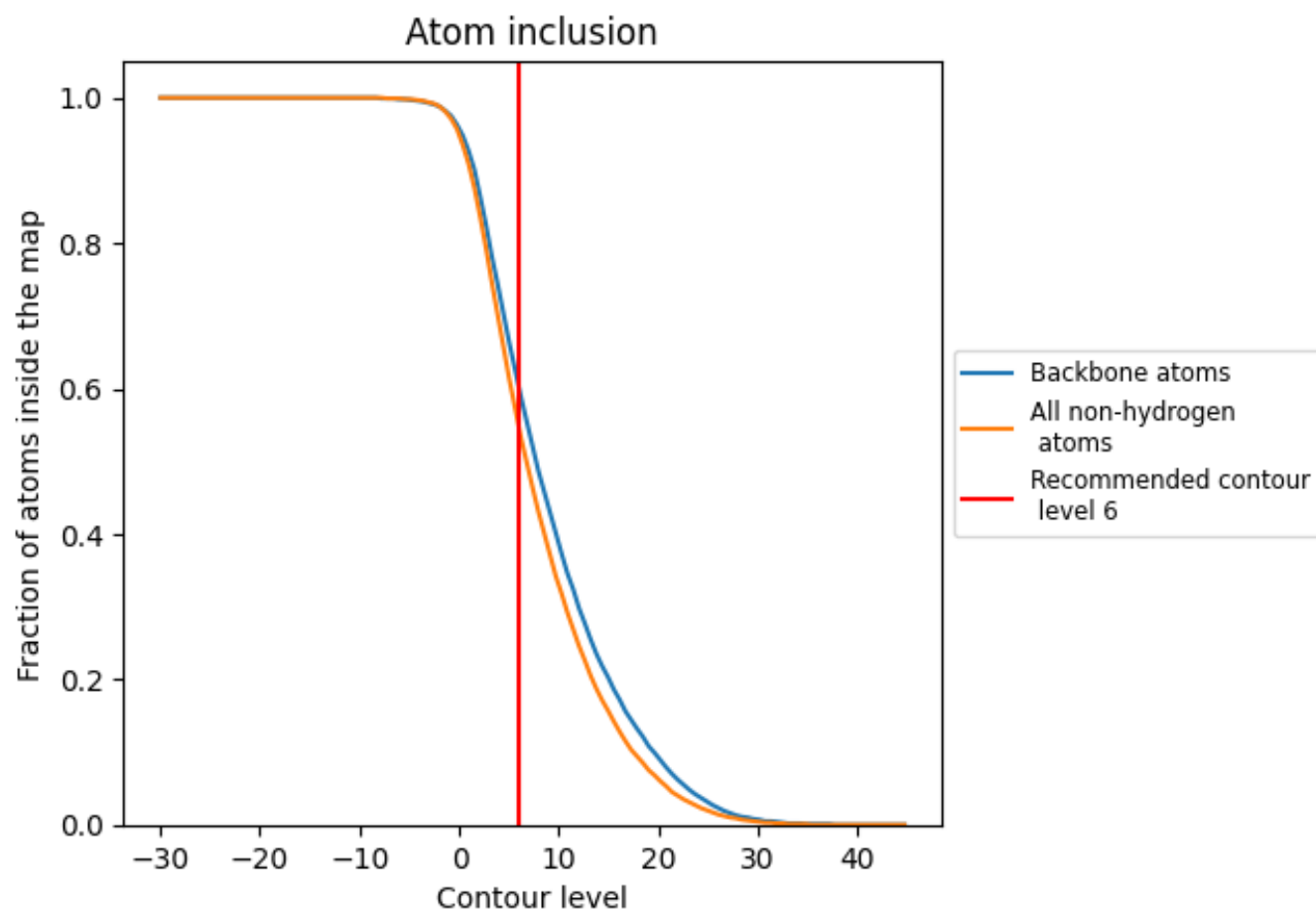
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 55% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5460	0.3940
A	0.6910	0.4600
B	0.6410	0.4430
C	0.1970	0.3220
D	0.4220	0.2930
E	0.0330	-0.0160
H	0.6310	0.4490
L	0.5690	0.4590
P	0.0970	0.1950
Q	0.1350	0.1670
X	0.3080	0.2380

1.0
0.0
<0.0