



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 03:22 PM JST

PDB ID : 7D5K
EMDB ID : EMD-30583
Title : CryoEM structure of cotton cellulose synthase isoform 7
Authors : Guan, Z.Y.; Xue, Y.; Yin, P.; Zhang, X.L.
Deposited on : 2020-09-26
Resolution : 3.50 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:

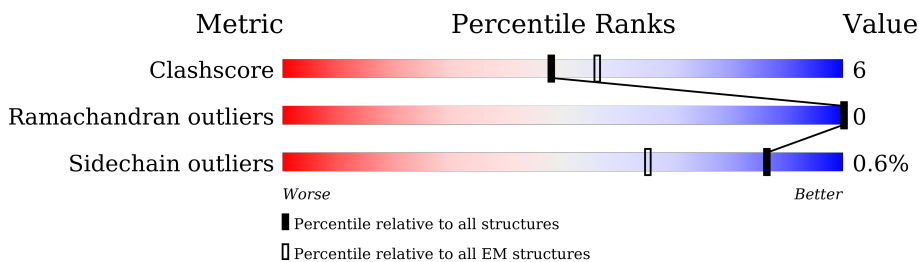
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 ≥ 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	1042	
1	B	1042	
1	C	1042	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

Continued on next page...

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Mol	Chain	Length	Quality of chain
2	I	2	 100% 100%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17667 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.

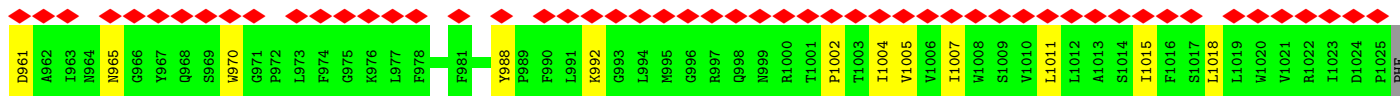
- Molecule 1 is a protein called Cellulose synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	727	5843	3829	976	1004	34	0	0
1	B	727	5843	3829	976	1004	34	0	0
1	C	727	5843	3829	976	1004	34	0	0

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



Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	O		
2	D	2	23	12	11	0	0
2	E	2	23	12	11	0	0
2	F	2	23	12	11	0	0
2	G	2	23	12	11	0	0
2	H	2	23	12	11	0	0
2	I	2	23	12	11	0	0



VAL
LEU
LYS
THR
LYS
GLY
PRO
ASP
THR
THR
GLN
CYS
ILE
ASN
CYS

• Molecule 1: Cellulose synthase



MET
GLU
ALA
SER
ALA
LEU
VAL
ALA
SER
GLN
HIS
ASN
ARG
GLY
ASN
GLU
GLU
LEU
VAL
VAL
ILE
HIS
GLY
HIS
GLU
GLU
PRO

PHE
PRO
CYS
VAL
ARG
CYS
TYR
TYR
GLU
GLU
SER
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ARG
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HIS
GLN
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THR
ARG
TYR
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ALA
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ILE
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LEU
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ARG
VAL
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PRO
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ALA
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ASP
ASP
TYR
ASP
MET
SER
MET
ASP
GLU
A235
R236
R241
K242

I250
R254
M255
R260
F266
F267
L268
R271
I272
L273
M274
A279
L282
V287
E290
M292
F295
S296
M297
P303
K304
W305
F306
P307
E311
T312
R323
E326
A331
D334
I335
T350
V354
I357
Y362
I367
S368
C369
Y370

I403
E404
P405
R432
Y438
K442
D464
D475
I480
H490
D491
T492
E493
G494
L497
P498
V503
S504
R505
R508
L523
V524
R525
F535
M536
L537
D540
C541
D542
H543
N547
A551
R552
E553
A554
M555
C568
Q571
F572
D580
R581

H582
D583
R584
A586
N587
T590
D594
L600
I603
P606
T611
V614
F615
R616
G622
G628
PRO
LYS
ARG
PRO
MET
VAL
SER
CYS
GLY
CYS
CYS
PRO
CYS
PHE
GLY
ARG
ARG
LYS
ASP
LYS
LYS
TYR
PRO
LYS
GLY
GLY
ASN
GLU
ASN
GLY
PRO

S676
Q677
M678
M679
F680
E681
K682
P703
S704
S705
S706
E713
V717
I718
E723
I735
Y736
Y736
E741
R752
G753
W754
L763
P764
A765
G768
D776
R777
L778
M779
Q780
W781
L782
R783
A799
M800

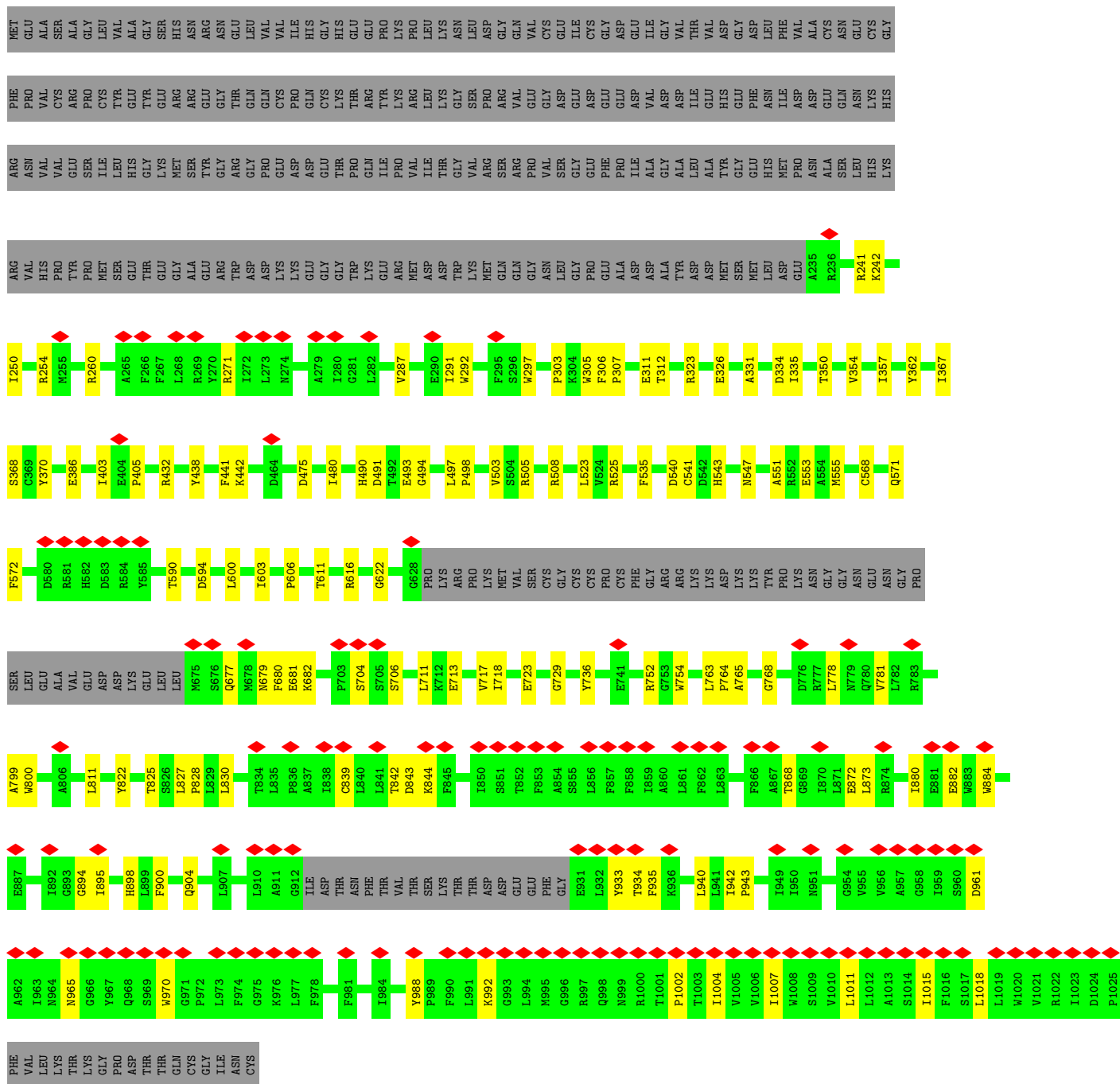
A806
L811
Y822
T825
S826
L827
P828
T834
L835
F836
C839
L840
L841
T842
D843
K844
F845
I860
S851
T862
F863
A864
S855
L856
F857
F858
I859
A860
F862
L863
F866
A867
T868
G869
I870
L871
E872
L873
L880
F881
E882
W883
W884
E887
Q888
I892
G893
G894

H898
L899
F900
Q904
L907
L910
A911
G912
ILE
ASP
THR
ASN
PHE
THR
VAL
THR
SER
LYS
THR
THR
ASP
ASP
GLU
GLU
PHE
GLY
E931
L932
Y933
T934
F935
K936
L940
L941
I942
P943
I949
V1010
N951
G954
V955
V956
G958
L1018
I959
S960
D961
A962
I963
N964
N965
G966
I967
Q968

S969
W970
G971
P972
L973
F974
G975
K976
L977
F978
F981
Y988
F989
F990
L991
K992
G993
L994
M995
G996
R997
Q998
N999
R1000
P1002
T1003
I1004
V1005
V1006
I1007
W1008
S1009
L1011
L1012
A1013
S1014
I1015
F1016
S1017
L1018
L1019
W1020
V1021
R1022
I1023
D1024
P1025
PHE
VAL
LEU
LYS
THR
THR
LYS
GLY
PRO
ASP

THR
THR
GLN
CYS
GLY
ILE
ASN
CYS

• Molecule 1: Cellulose synthase



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



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

Chain E:  100%
100%



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

Chain F:  100%



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

Chain G:  100%



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

Chain H:  100%



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

Chain I:  100%
100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	185759	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.685	Depositor
Minimum map value	-2.101	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	304.36002, 304.36002, 304.36002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC

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	0.26	0/6016	0.49	0/8175
1	B	0.26	0/6016	0.49	0/8175
1	C	0.26	0/6016	0.49	0/8175
All	All	0.26	0/18048	0.49	0/24525

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5843	0	5879	77	0
1	B	5843	0	5879	76	0
1	C	5843	0	5879	76	0
2	D	23	0	21	2	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
2	I	23	0	21	0	0
All	All	17667	0	17763	224	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 6.

The worst 5 of 224 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:ASP:HB2	1:C:611:THR:HG21	1.63	0.80
1:A:540:ASP:HB2	1:A:611:THR:HG21	1.63	0.79
1:B:540:ASP:HB2	1:B:611:THR:HG21	1.63	0.79
1:B:260:ARG:NH1	1:B:868:THR:OG1	2.22	0.73
1:A:260:ARG:NH1	1:A:868:THR:OG1	2.22	0.72

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	721/1042 (69%)	665 (92%)	56 (8%)	0	100	100
1	B	721/1042 (69%)	665 (92%)	56 (8%)	0	100	100
1	C	721/1042 (69%)	665 (92%)	56 (8%)	0	100	100
All	All	2163/3126 (69%)	1995 (92%)	168 (8%)	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	630/902 (70%)	626 (99%)	4 (1%)	86	94
1	B	630/902 (70%)	626 (99%)	4 (1%)	86	94
1	C	630/902 (70%)	626 (99%)	4 (1%)	86	94
All	All	1890/2706 (70%)	1878 (99%)	12 (1%)	86	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	682	LYS
1	C	242	LYS
1	C	682	LYS
1	C	432	ARG
1	A	682	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	898	HIS
1	C	490	HIS
1	C	898	HIS
1	A	898	HIS
1	A	490	HIS

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](#)

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	$\# Z > 2$
2	BGC	D	1	2	12,12,12	0.18	0	17,17,17	0.33	0
2	BGC	D	2	2	11,11,12	0.19	0	15,15,17	0.49	0
2	BGC	E	1	2	12,12,12	0.14	0	17,17,17	0.11	0
2	BGC	E	2	2	11,11,12	0.20	0	15,15,17	0.40	0
2	BGC	F	1	2	12,12,12	0.18	0	17,17,17	0.33	0
2	BGC	F	2	2	11,11,12	0.19	0	15,15,17	0.49	0
2	BGC	G	1	2	12,12,12	0.14	0	17,17,17	0.12	0
2	BGC	G	2	2	11,11,12	0.20	0	15,15,17	0.40	0
2	BGC	H	1	2	12,12,12	0.17	0	17,17,17	0.33	0
2	BGC	H	2	2	11,11,12	0.20	0	15,15,17	0.49	0
2	BGC	I	1	2	12,12,12	0.14	0	17,17,17	0.12	0
2	BGC	I	2	2	11,11,12	0.19	0	15,15,17	0.41	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
2	BGC	D	1	2	-	2/2/22/22	0/1/1/1
2	BGC	D	2	2	-	1/2/19/22	0/1/1/1
2	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	E	2	2	-	2/2/19/22	0/1/1/1
2	BGC	F	1	2	-	2/2/22/22	0/1/1/1
2	BGC	F	2	2	-	1/2/19/22	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	BGC	G	2	2	-	2/2/19/22	0/1/1/1
2	BGC	H	1	2	-	2/2/22/22	0/1/1/1
2	BGC	H	2	2	-	1/2/19/22	0/1/1/1
2	BGC	I	1	2	-	2/2/22/22	0/1/1/1
2	BGC	I	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

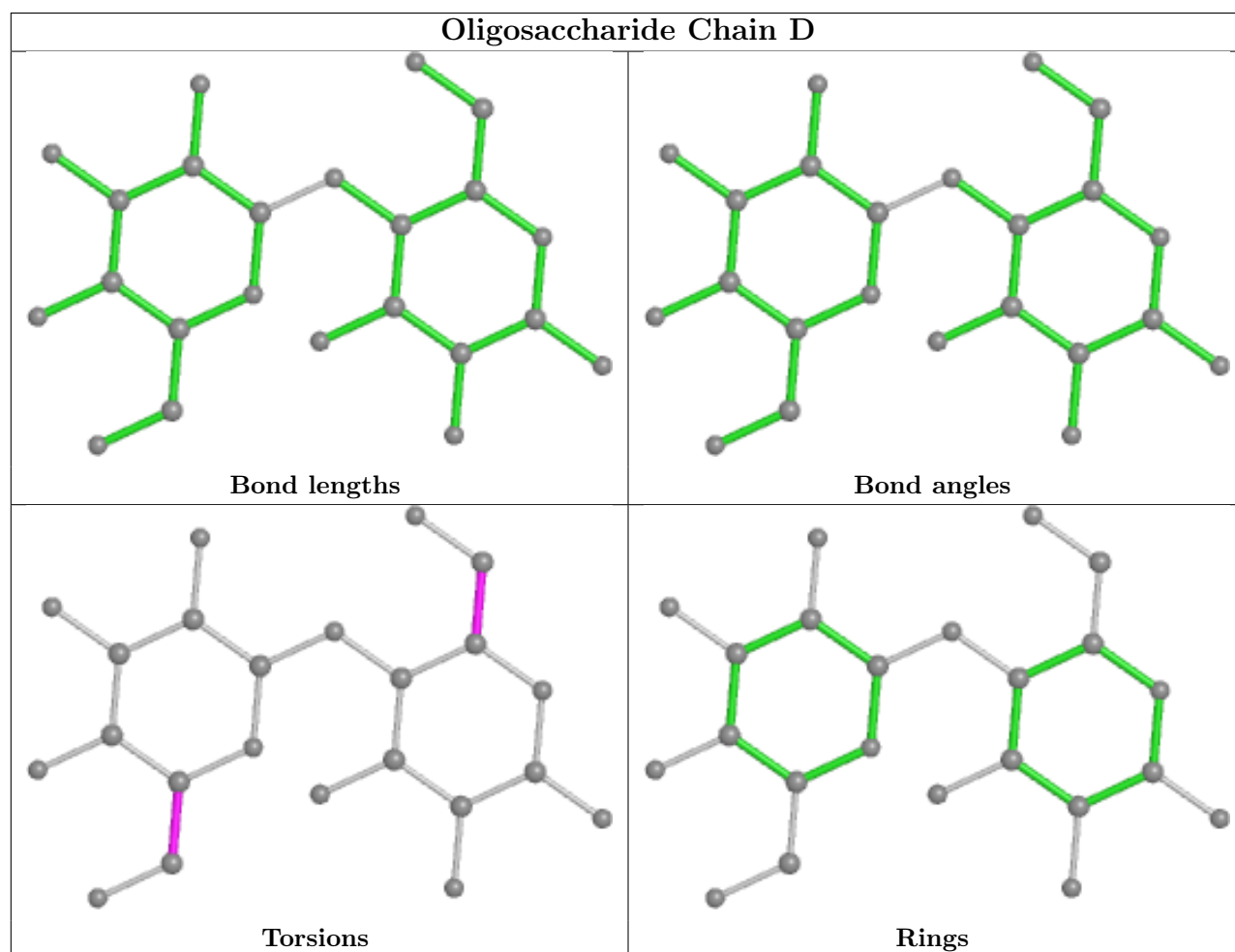
Mol	Chain	Res	Type	Atoms
2	E	2	BGC	O5-C5-C6-O6
2	G	2	BGC	O5-C5-C6-O6
2	I	2	BGC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6

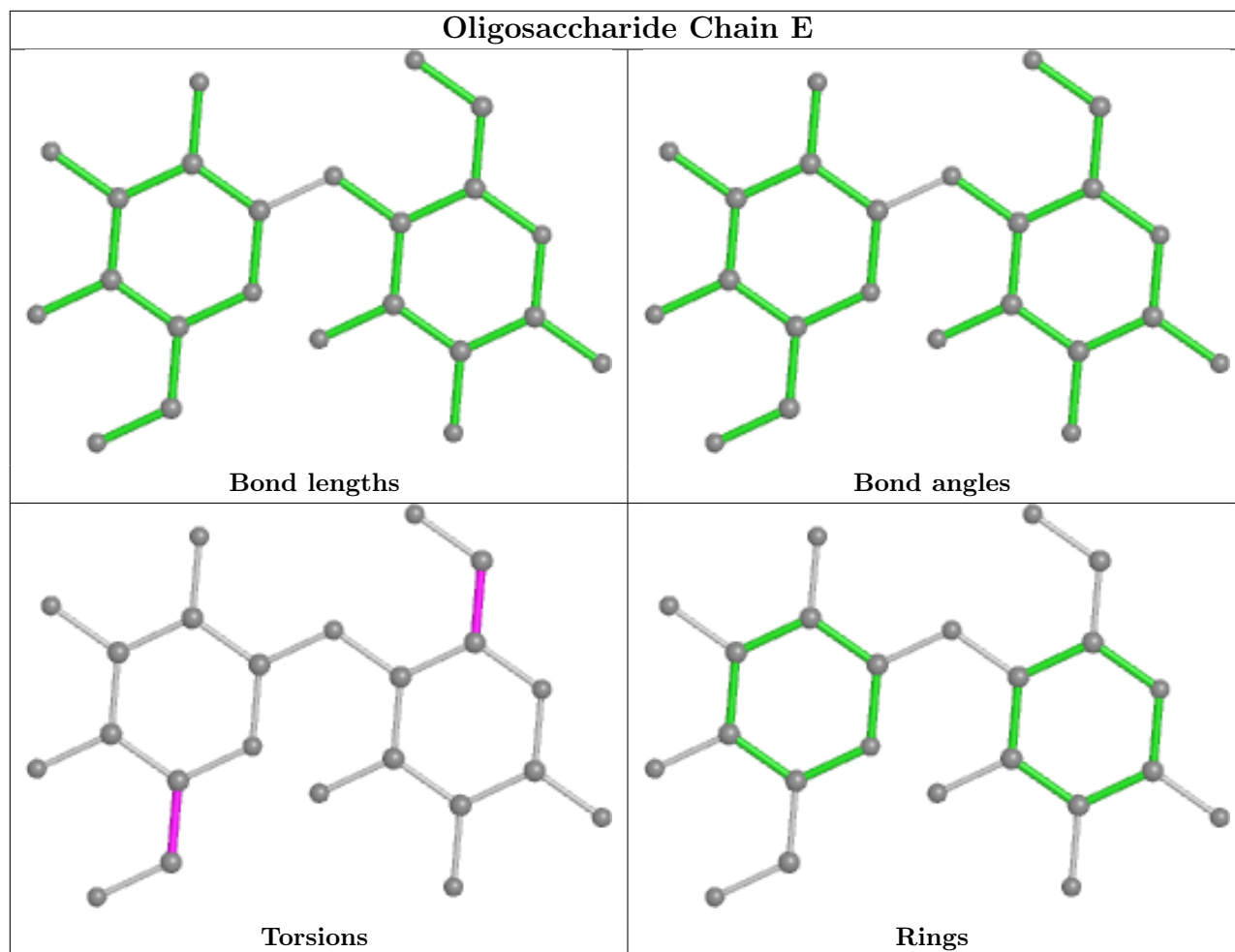
There are no ring outliers.

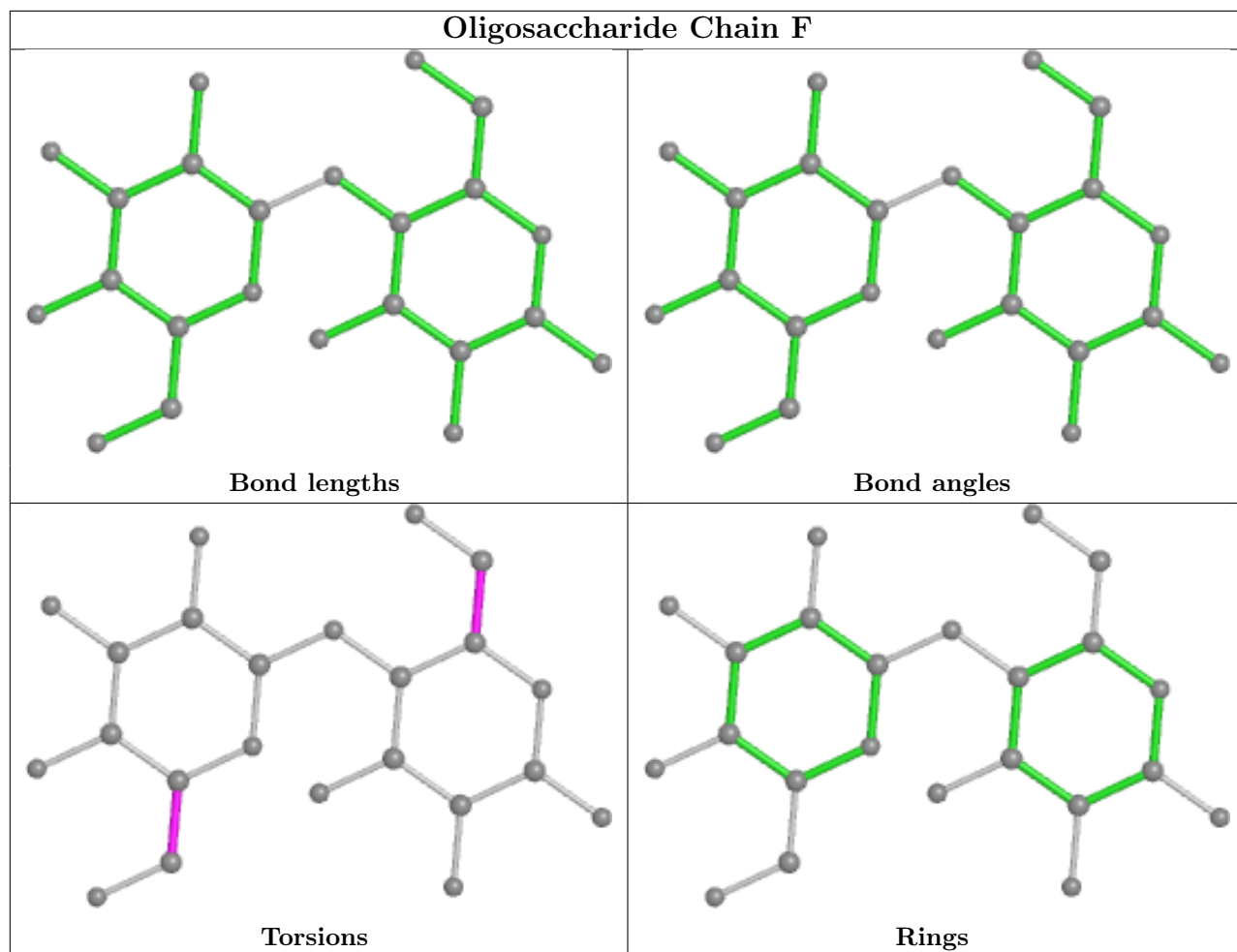
2 monomers are involved in 2 short contacts:

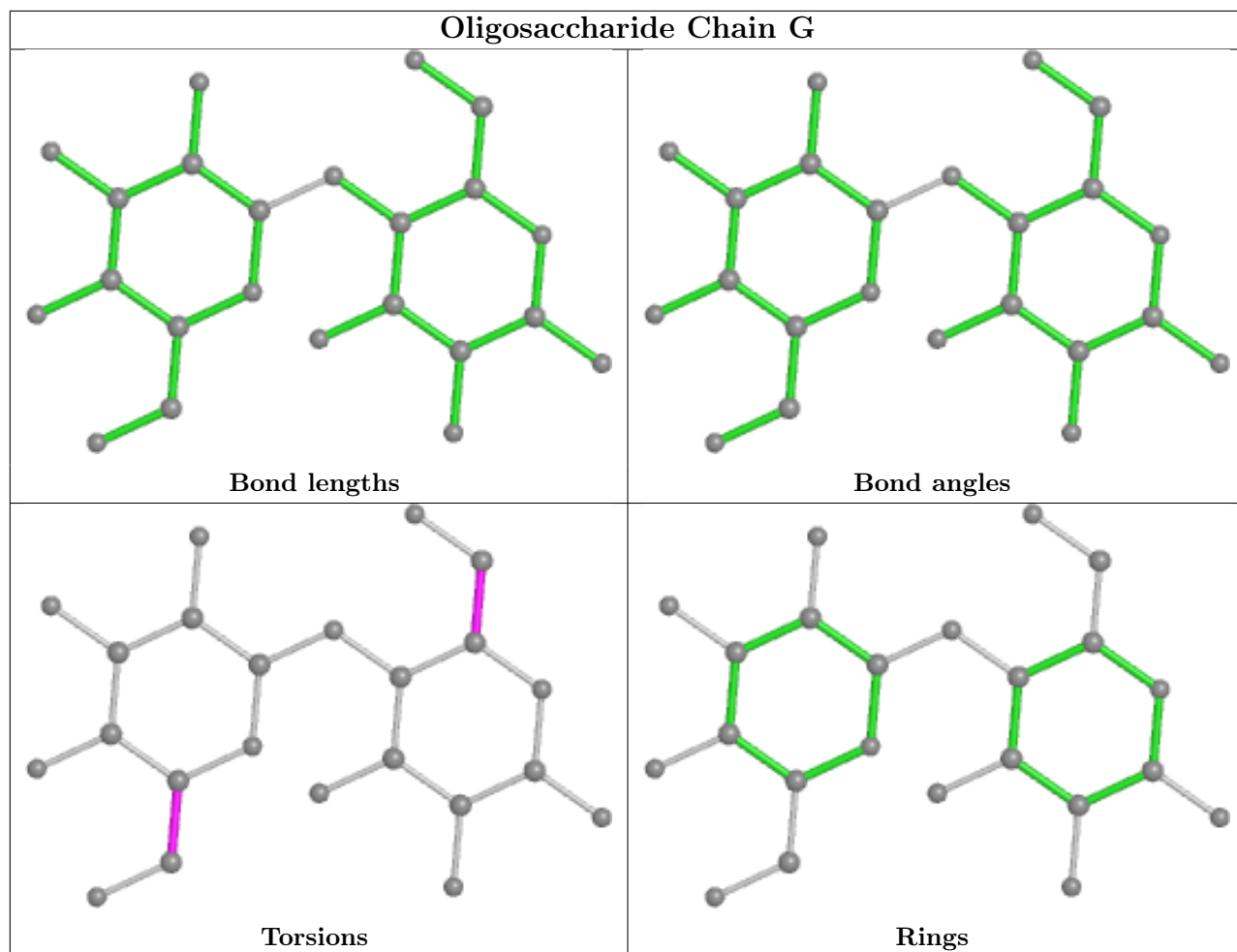
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	BGC	1	0
2	D	1	BGC	1	0

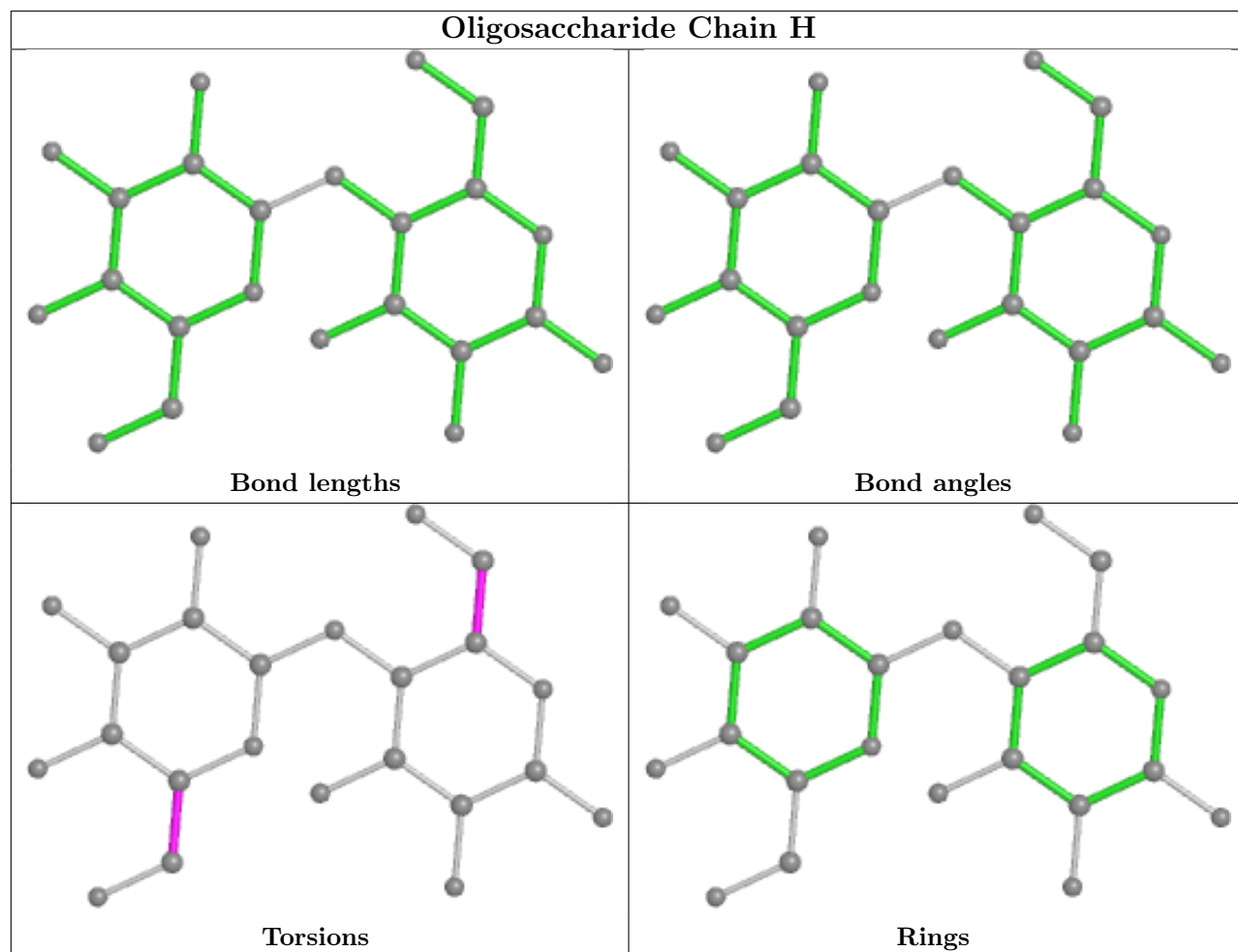
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

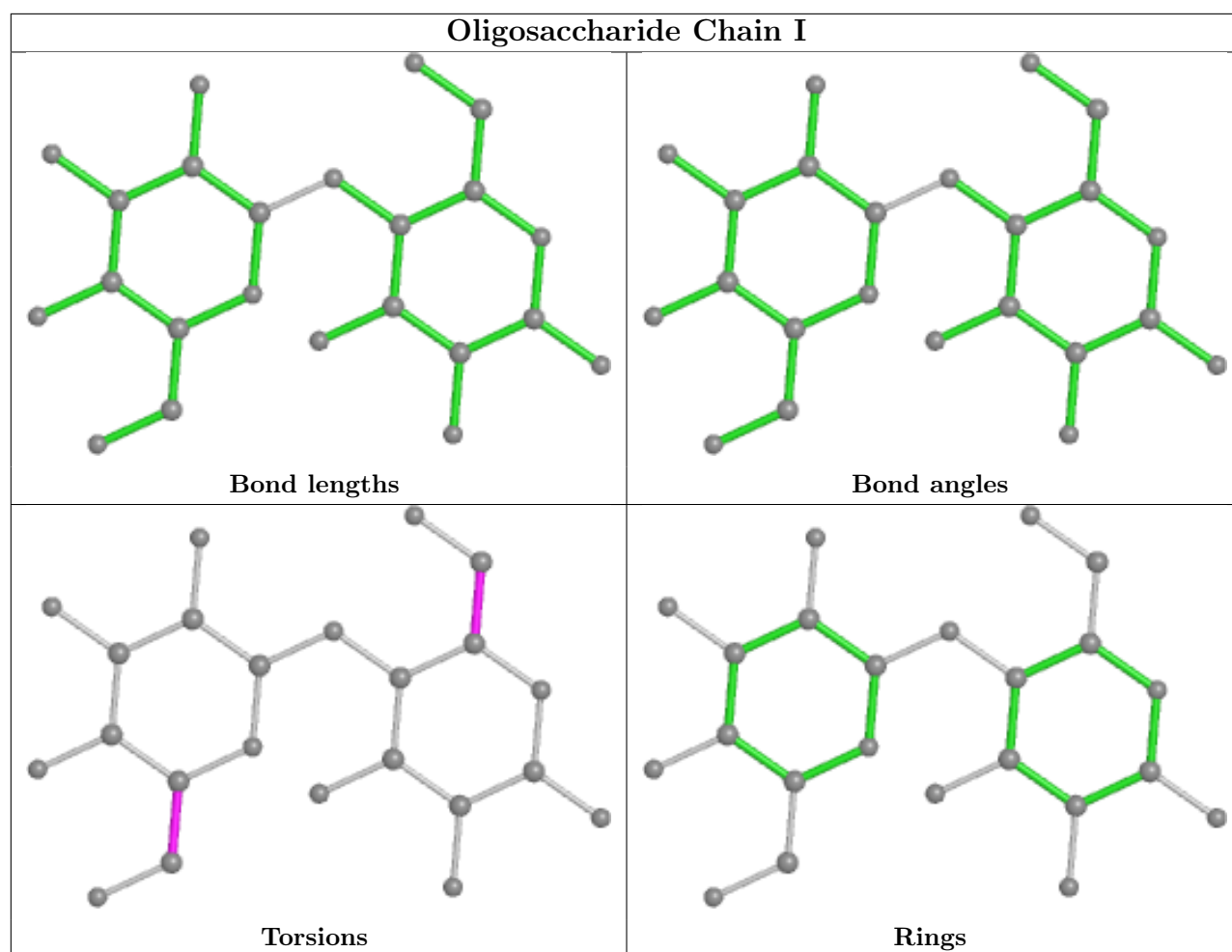












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

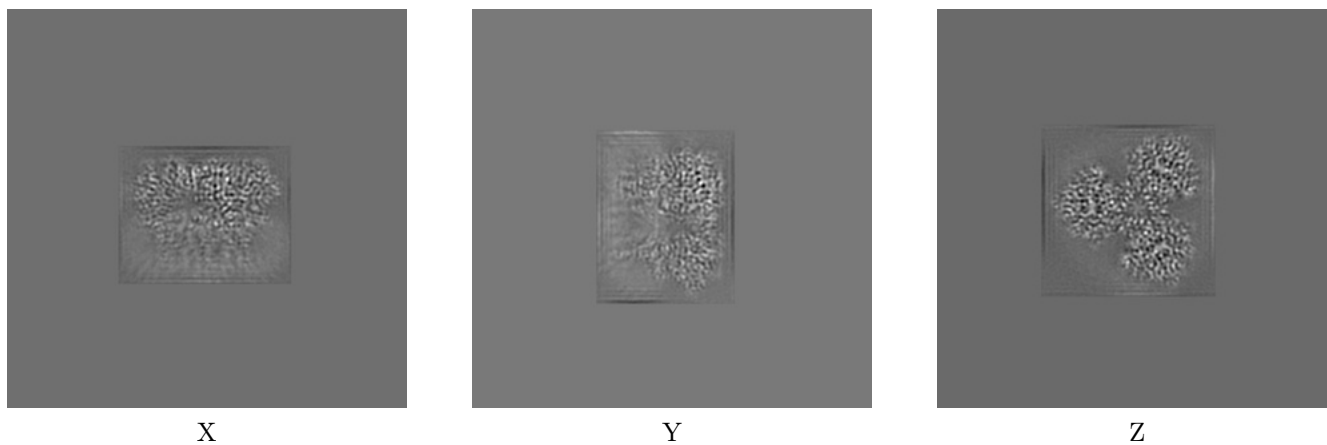
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30583. 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](#)

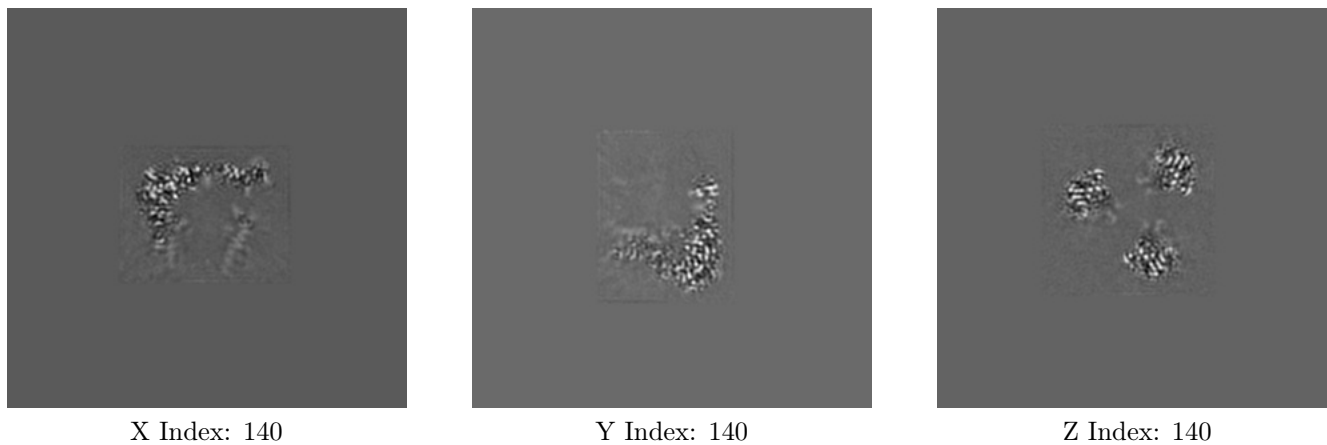
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



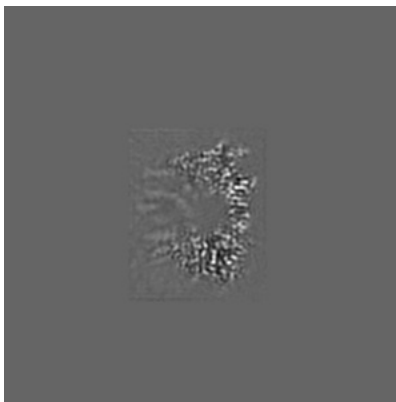
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

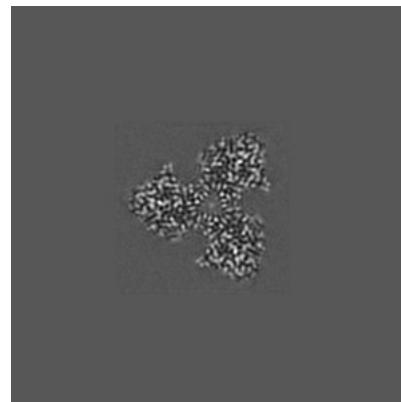
6.3.1 Primary map



X Index: 160



Y Index: 153

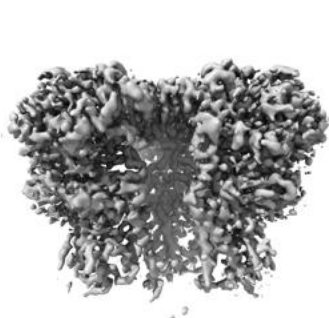


Z Index: 160

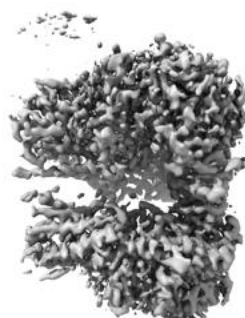
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

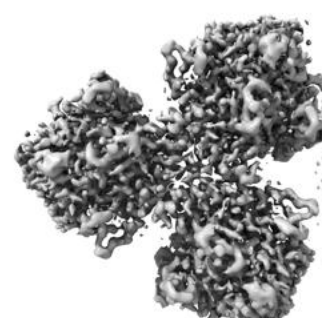
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

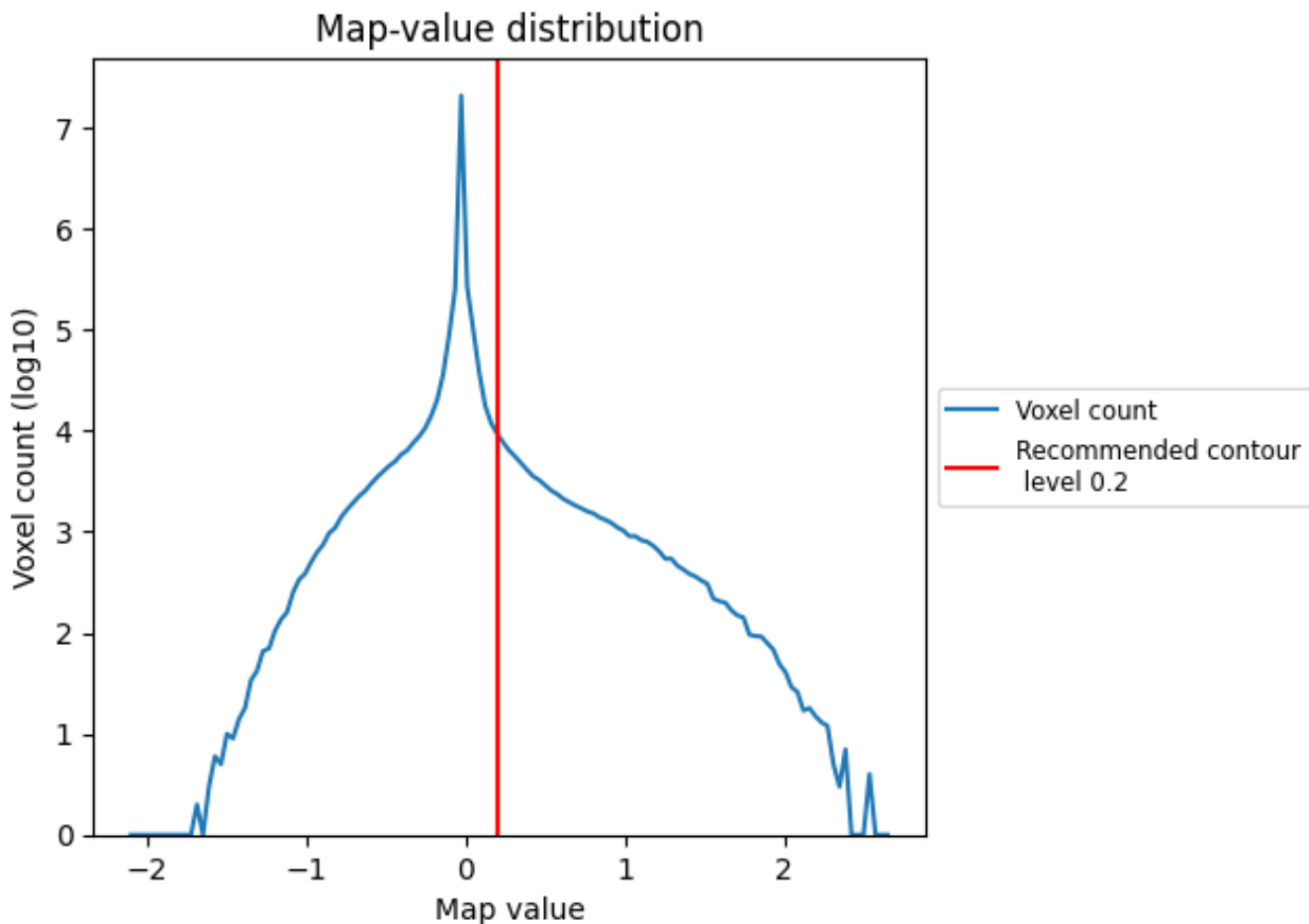
6.5 Mask visualisation

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

7 Map analysis [i](#)

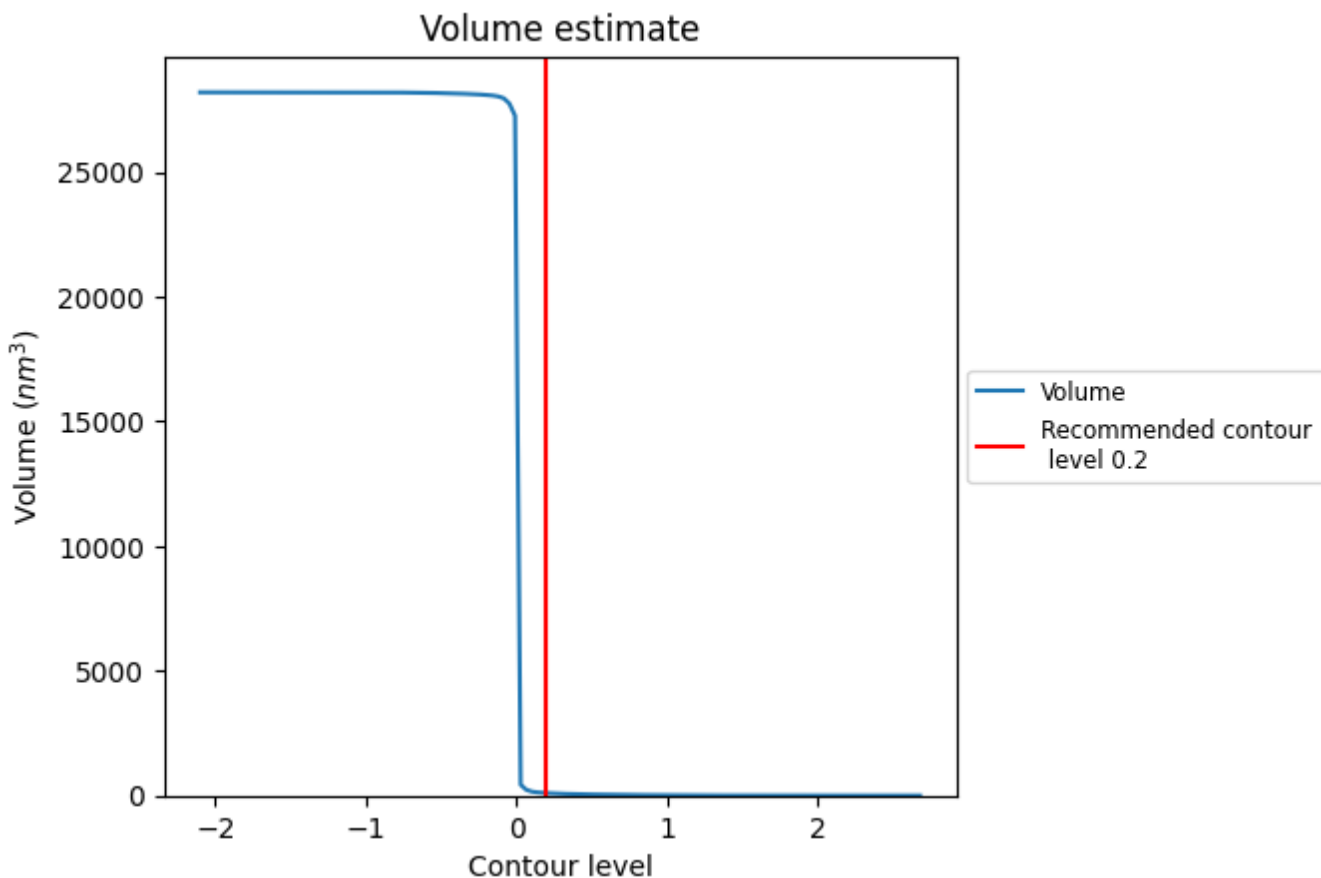
This section contains the results of statistical analysis of the map.

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.

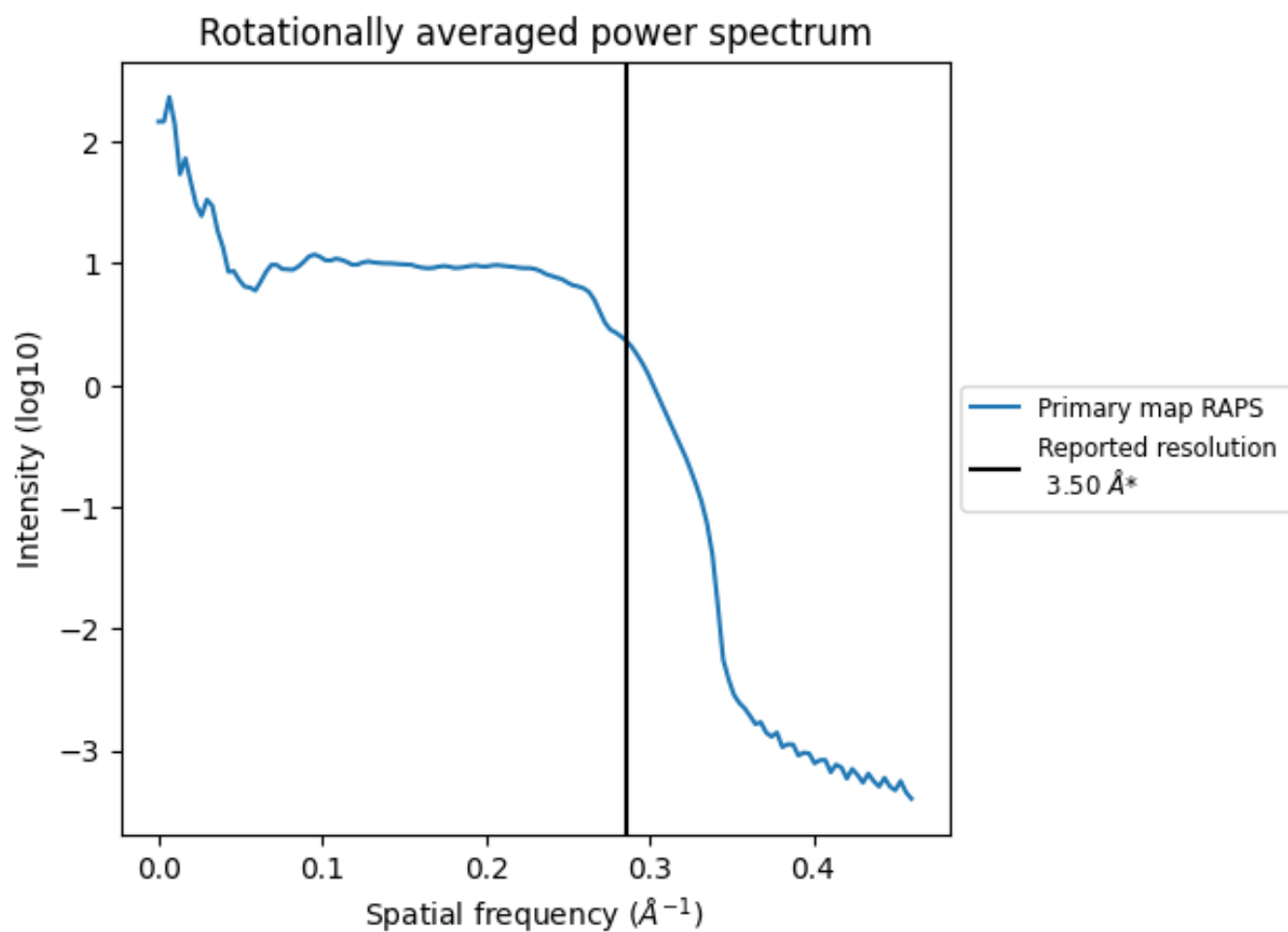
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm³; this corresponds to an approximate mass of 91 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 0.286\AA^{-1}

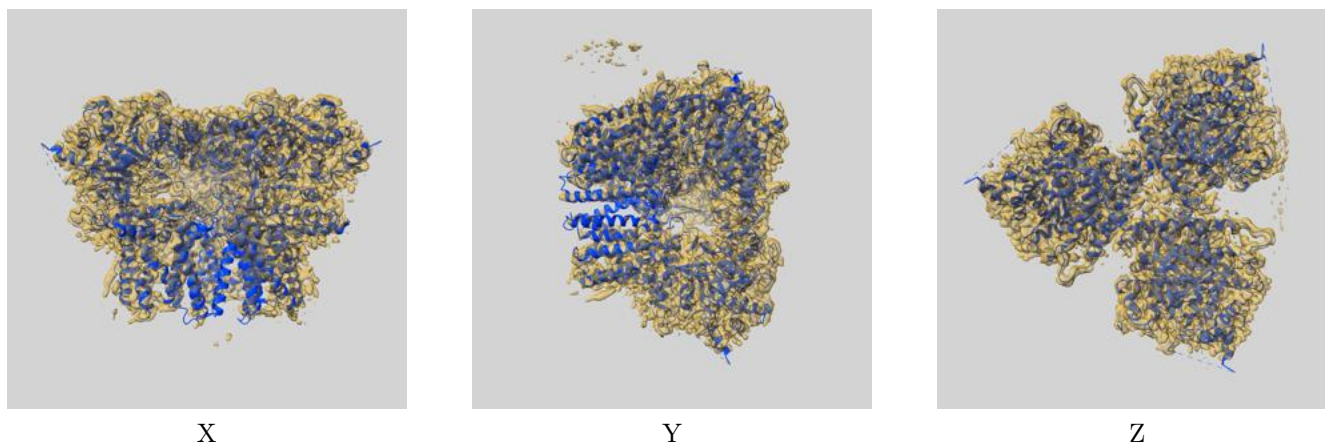
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

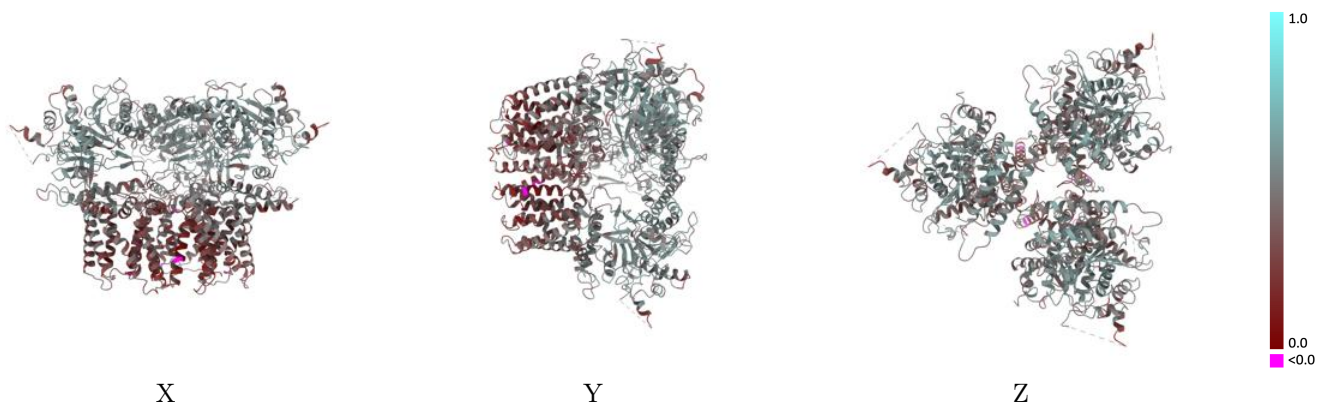
This section contains information regarding the fit between EMDB map EMD-30583 and PDB model 7D5K. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



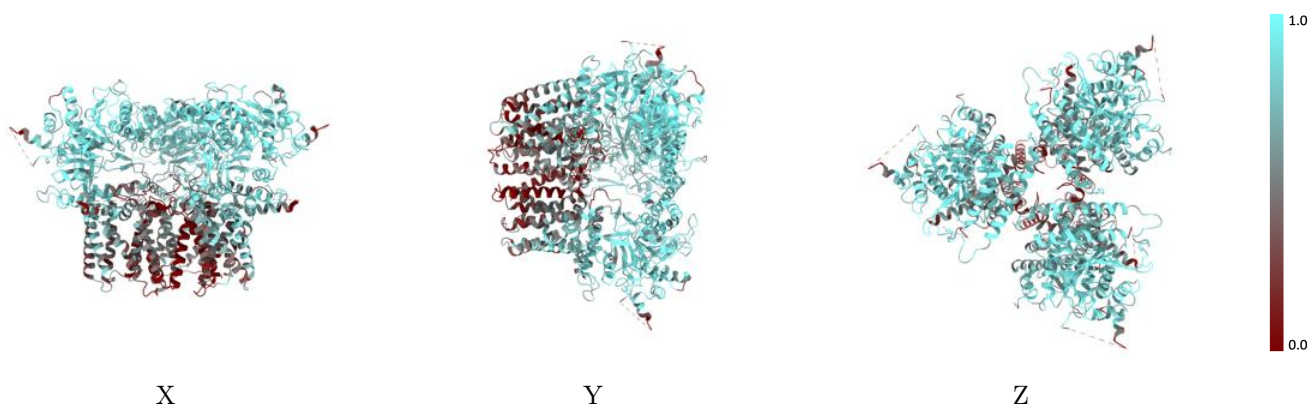
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



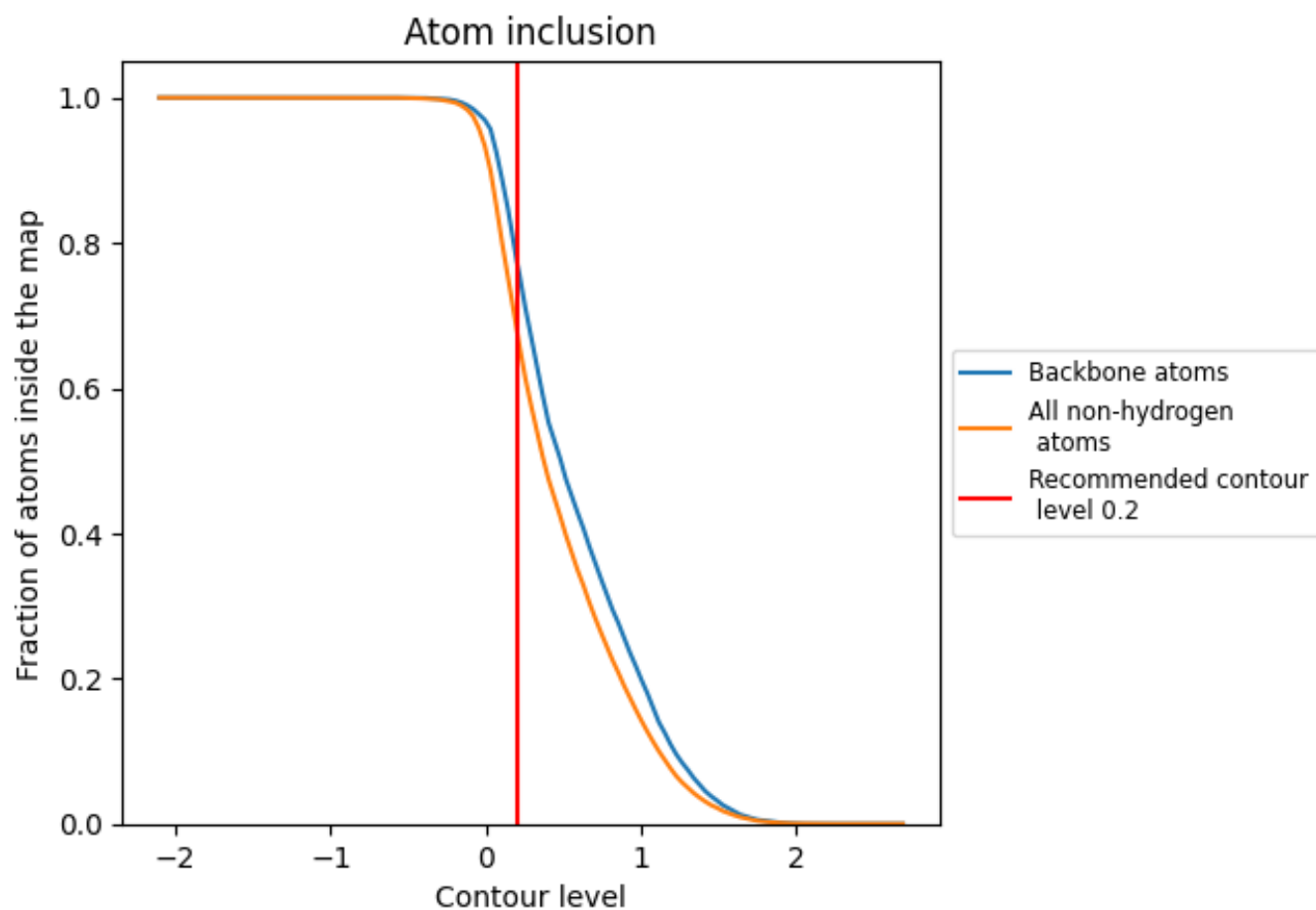
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6782	 0.4400
A	 0.6789	 0.4390
B	 0.6817	 0.4400
C	 0.6780	 0.4410
D	 0.6522	 0.4440
E	 0.2609	 0.2950
F	 0.7826	 0.4490
G	 0.4783	 0.4340
H	 0.6522	 0.4620
I	 0.2609	 0.3460

