



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 03:31 am GMT

PDB ID : 7A5R
EMDB ID : EMD-11648
Title : Complex of SARS-CoV-2 spike and CR3022 Fab (Non-Uniform Refinement)
Authors : Wrobel, A.G.; Benton, D.J.; Rosenthal, P.B.; Gamblin, S.J.
Deposited on : 2020-08-21
Resolution : 3.70 Å(reported)
Based on initial model : 6W41

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.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

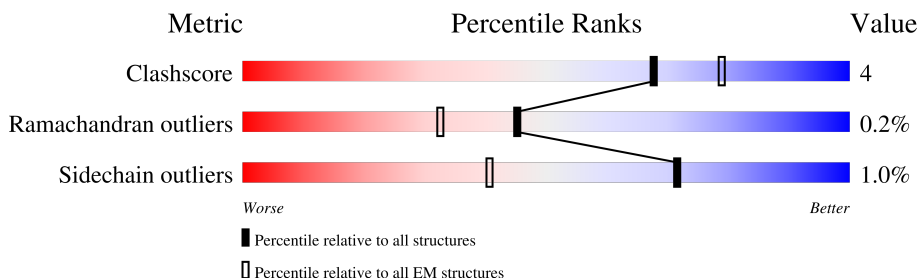
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY









The reported resolution of this entry is 3.70 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 ≥ 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	H	256	
1	I	256	
2	L	240	
2	M	240	
3	A	1286	
3	B	1286	
4	C	2	
4	D	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10608 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 CR3022 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	213	Total	C	N	O	S	0	0
			1595	1017	259	311	8		
1	I	213	Total	C	N	O	S	0	0
			1595	1017	259	311	8		

- Molecule 2 is a protein called CR3022 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	202	Total	C	N	O	S	0	0
			1568	989	255	320	4		
2	M	202	Total	C	N	O	S	0	0
			1568	989	255	320	4		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	264	Total	C	N	O	S	0	0
			2113	1358	358	389	8		
3	B	264	Total	C	N	O	S	0	0
			2113	1358	358	389	8		

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP P0DTC2
A	-29	GLY	-	expression tag	UNP P0DTC2
A	-28	ILE	-	expression tag	UNP P0DTC2
A	-27	LEU	-	expression tag	UNP P0DTC2
A	-26	PRO	-	expression tag	UNP P0DTC2
A	-25	SER	-	expression tag	UNP P0DTC2
A	-24	PRO	-	expression tag	UNP P0DTC2
A	-23	GLY	-	expression tag	UNP P0DTC2
A	-22	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	PRO	-	expression tag	UNP P0DTC2
A	-20	ALA	-	expression tag	UNP P0DTC2
A	-19	LEU	-	expression tag	UNP P0DTC2
A	-18	LEU	-	expression tag	UNP P0DTC2
A	-17	SER	-	expression tag	UNP P0DTC2
A	-16	LEU	-	expression tag	UNP P0DTC2
A	-15	VAL	-	expression tag	UNP P0DTC2
A	-14	SER	-	expression tag	UNP P0DTC2
A	-13	LEU	-	expression tag	UNP P0DTC2
A	-12	LEU	-	expression tag	UNP P0DTC2
A	-11	SER	-	expression tag	UNP P0DTC2
A	-10	VAL	-	expression tag	UNP P0DTC2
A	-9	LEU	-	expression tag	UNP P0DTC2
A	-8	LEU	-	expression tag	UNP P0DTC2
A	-7	MET	-	expression tag	UNP P0DTC2
A	-6	GLY	-	expression tag	UNP P0DTC2
A	-5	CYS	-	expression tag	UNP P0DTC2
A	-4	VAL	-	expression tag	UNP P0DTC2
A	-3	ALA	-	expression tag	UNP P0DTC2
A	-2	GLU	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	GLY	-	expression tag	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
A	1212	GLU	-	expression tag	UNP P0DTC2
A	1213	ASN	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	PHE	-	expression tag	UNP P0DTC2
A	1217	GLN	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	ILE	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	ARG	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLN	-	expression tag	UNP P0DTC2
A	1234	ALA	-	expression tag	UNP P0DTC2
A	1235	TYR	-	expression tag	UNP P0DTC2
A	1236	VAL	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	ASP	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	TRP	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	LEU	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	THR	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
B	-30	MET	-	initiating methionine	UNP P0DTC2
B	-29	GLY	-	expression tag	UNP P0DTC2
B	-28	ILE	-	expression tag	UNP P0DTC2
B	-27	LEU	-	expression tag	UNP P0DTC2
B	-26	PRO	-	expression tag	UNP P0DTC2
B	-25	SER	-	expression tag	UNP P0DTC2
B	-24	PRO	-	expression tag	UNP P0DTC2
B	-23	GLY	-	expression tag	UNP P0DTC2
B	-22	MET	-	expression tag	UNP P0DTC2
B	-21	PRO	-	expression tag	UNP P0DTC2
B	-20	ALA	-	expression tag	UNP P0DTC2
B	-19	LEU	-	expression tag	UNP P0DTC2
B	-18	LEU	-	expression tag	UNP P0DTC2

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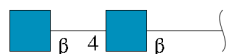
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P0DTC2
B	-16	LEU	-	expression tag	UNP P0DTC2
B	-15	VAL	-	expression tag	UNP P0DTC2
B	-14	SER	-	expression tag	UNP P0DTC2
B	-13	LEU	-	expression tag	UNP P0DTC2
B	-12	LEU	-	expression tag	UNP P0DTC2
B	-11	SER	-	expression tag	UNP P0DTC2
B	-10	VAL	-	expression tag	UNP P0DTC2
B	-9	LEU	-	expression tag	UNP P0DTC2
B	-8	LEU	-	expression tag	UNP P0DTC2
B	-7	MET	-	expression tag	UNP P0DTC2
B	-6	GLY	-	expression tag	UNP P0DTC2
B	-5	CYS	-	expression tag	UNP P0DTC2
B	-4	VAL	-	expression tag	UNP P0DTC2
B	-3	ALA	-	expression tag	UNP P0DTC2
B	-2	GLU	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	GLY	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2
B	1211	ARG	-	expression tag	UNP P0DTC2
B	1212	GLU	-	expression tag	UNP P0DTC2
B	1213	ASN	-	expression tag	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	PHE	-	expression tag	UNP P0DTC2
B	1217	GLN	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	TYR	-	expression tag	UNP P0DTC2
B	1225	ILE	-	expression tag	UNP P0DTC2
B	1226	PRO	-	expression tag	UNP P0DTC2
B	1227	GLU	-	expression tag	UNP P0DTC2
B	1228	ALA	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLN	-	expression tag	UNP P0DTC2
B	1234	ALA	-	expression tag	UNP P0DTC2
B	1235	TYR	-	expression tag	UNP P0DTC2
B	1236	VAL	-	expression tag	UNP P0DTC2
B	1237	ARG	-	expression tag	UNP P0DTC2
B	1238	LYS	-	expression tag	UNP P0DTC2
B	1239	ASP	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	TRP	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	LEU	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	THR	-	expression tag	UNP P0DTC2
B	1248	PHE	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2

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

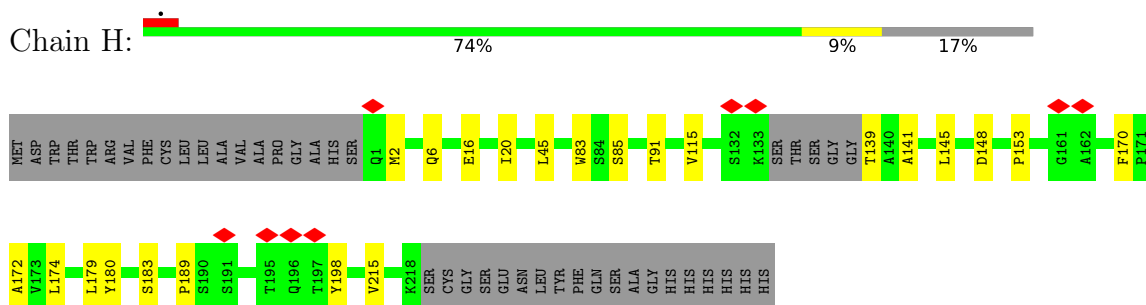


Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

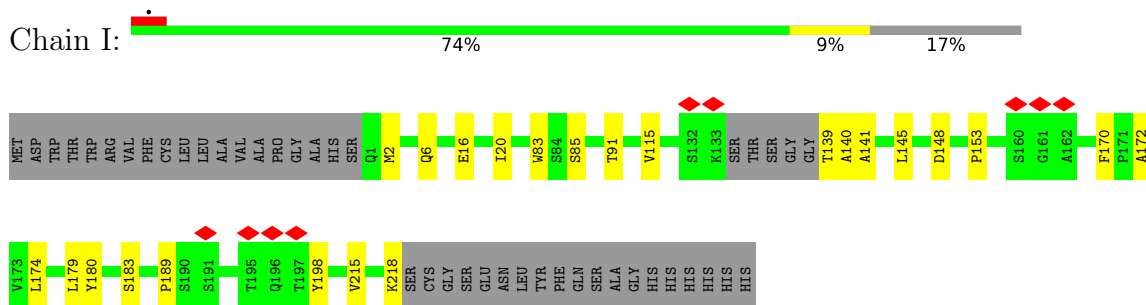
3 Residue-property plots [i](#)

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.

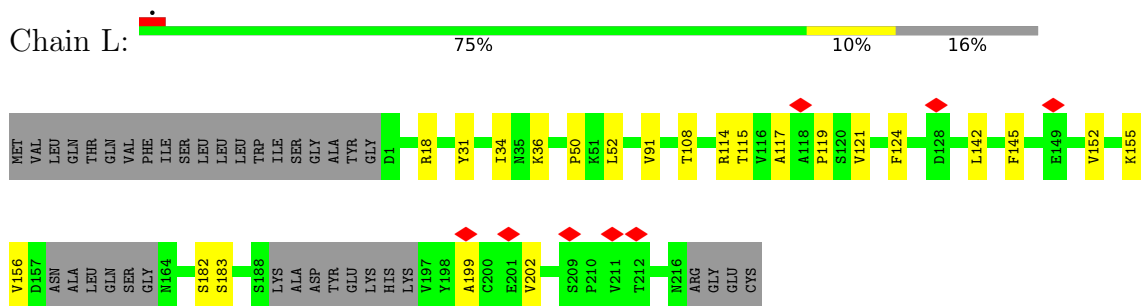
- Molecule 1: CR3022 Fab Heavy Chain



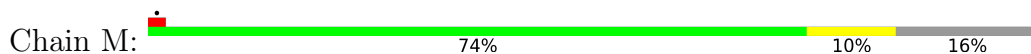
- Molecule 1: CR3022 Fab Heavy Chain

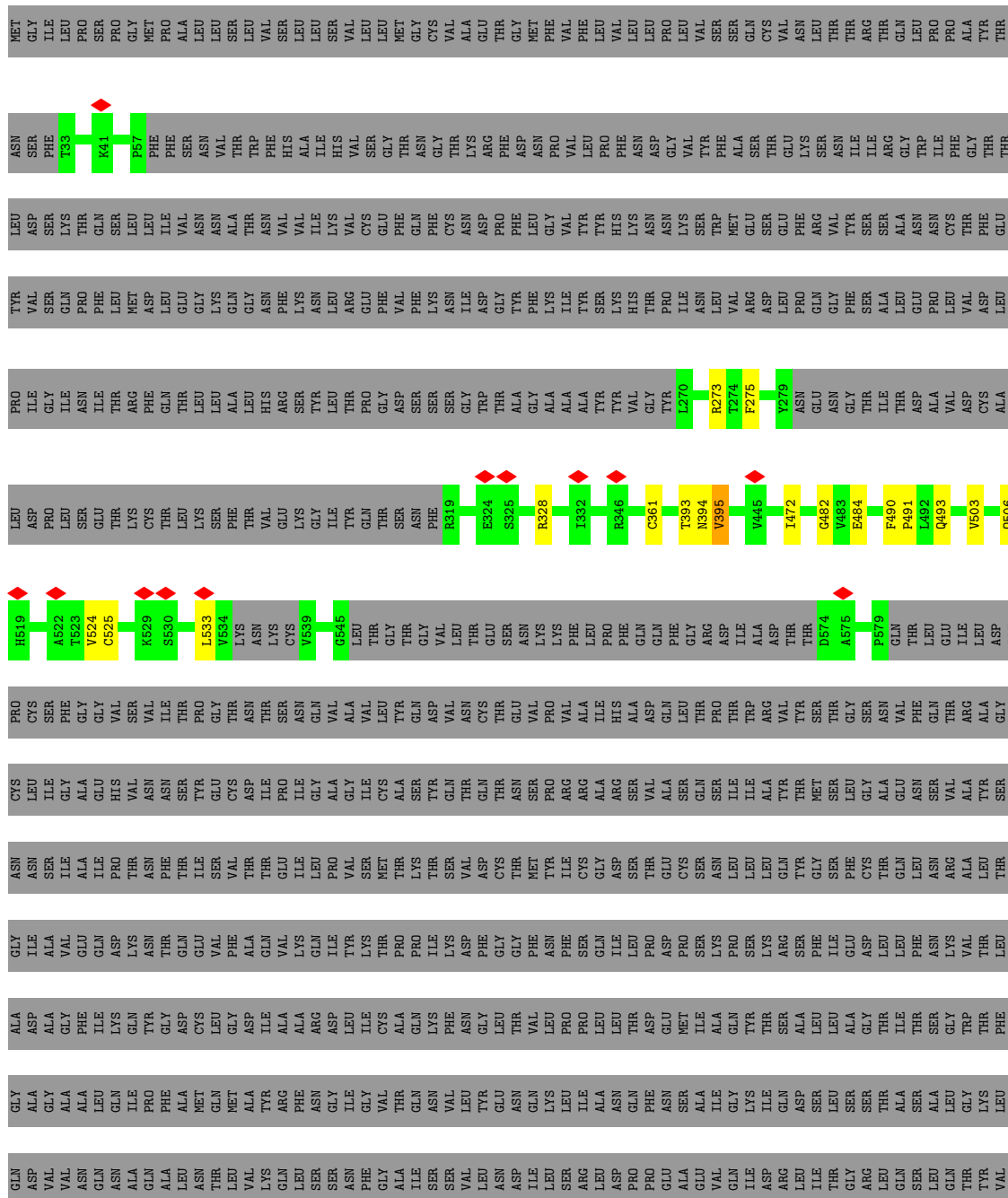


- Molecule 2: CR3022 Fab Light Chain



- Molecule 2: CR3022 Fab Light Chain







LEU	ARG	ASN	VAL	GLN	LEU	GLY
SER	ASN	CYS	THR	THR	GLY	THR
THR	ASN	ASP	THR	TYR	LYS	PHI
PHI	VAL	VAL	VAL	VAL	GLN	GLY
LEU	VAL	VAL	PRO	THR	GLN	GLY
GLY	ALA	ILE	ALA	GLN	ASP	ALA
HIS	LYS	GLY	GLN	GLN	VAL	GLY
HIS	ASN	ILE	GLU	ILE	VAL	HIS
HIS	LEU	VAL	LYS	ILE	ASN	LEU
HIS	ASN	ASN	ASN	ARG	GLN	ALA
HIS	GLU	ASN	PHI	ALA	ASN	GLN
	SER	THR	THR	ALA	ALA	ILE
	LEU	VAL	THR	GLU	GLN	PRO
	ILE	TYR	ALA	ILE	ALA	PHI
	ASP	ASP	PRO	ARG	LEU	ALA
	LEU	PRO	ALA	ALA	ASN	MET
	GLN	LEU	ILE	SER	THR	GLN
	GLU	GLN	CYS	ALA	LEU	MET
	LEU	PRO	HIS	ASN	VAL	ALA
	GLY	GLU	ASP	LEU	LYS	TYR
	LYS	LEU	GLY	ALA	GLN	ARG
	TYR	ASP	LYS	ALA	LEU	PHI
	GLU	SER	ALA	THR	SER	ASN
	GLN	PHI	HIS	LYS	SER	GLY
	SER	LYS	PHI	MET	ASN	ILE
	GLY	GLU	PRO	SER	PHI	GLY
	ARG	GLU	ARG	GLU	GLY	VAL
	GLU	LEU	GLY	CYS	ILE	THR
	ASN	ASP	GLY	VAL	ILE	GLN
	LEU	LYS	VAL	LEU	SER	ASN
	TYR	TYR	PHI	GLY	SER	VAL
	PHI	PHI	VAL	GLN	VAL	LEU
	GLN	LYS	SER	LYS	LEU	TYR
	GLY	ASN	ASN	LYS	ASN	GLU
	GLY	HIS	GLY	ARG	ASP	ASN
	GLY	THR	THR	VAL	ILE	GLN
	GLY	SER	HIS	ASP	LEU	LYS
	SER	PRO	TRP	PHI	SER	LEU
	GLY	ASP	PHI	CYS	ARG	ILE
	TYR	VAL	VAL	GLY	LEU	ALA
	ILE	ASP	THR	LYS	ASP	ASN
	PRO	LEU	GLN	GLY	PRO	GLN
	GLU	GLY	ARG	TYR	PRO	PHI
	ALA	ASP	ASN	HIS	GLU	ASN
	PRO	ILE	PHI	LEU	ALA	SER
	ARG	SER	TYR	MET	GLU	ALA
	ASP	GLY	GLU	SER	VAL	ILE
	GLN	ILE	PRO	PHI	GLN	GLY
	GLY	ASN	GLN	PRO	ILE	LYS
	ALA	ALA	ILE	GLN	ASP	ILE
	TYR	SER	ILE	SER	ARG	GLN
	VAL	VAL	THR	ALA	LEU	ASP
	ARG	VAL	THR	PRO	ILE	SER
	LYS	ASN	ASP	HIS	THR	LEU
	ASP	ILE	ASN	GLY	GLY	SER
	GLY	GLN	THR	VAL	ARG	SER
	GLY	LYS	PHI	VAL	LEU	THR
	TRP	GLU	VAL	PHE	GLN	ALA
	VAL	ILE	GLY	THR	LEU	SER
		ASP		HIS	THR	ALA

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

Chain C:  100%

NAG1
NAG2

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

Chain D:  100%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	88000	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 ($e^-/\text{\AA}^2$)	33.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.547	Depositor
Minimum map value	-2.113	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	H	0.28	0/1636	0.51	0/2228
1	I	0.29	0/1636	0.51	0/2228
2	L	0.30	0/1602	0.54	0/2180
2	M	0.30	0/1602	0.54	0/2180
3	A	0.28	0/2169	0.51	0/2947
3	B	0.28	0/2169	0.51	0/2947
All	All	0.29	0/10814	0.52	0/14710

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 [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	H	1595	0	1579	15	0
1	I	1595	0	1579	18	0
2	L	1568	0	1517	16	0
2	M	1568	0	1517	19	0
3	A	2113	0	2033	9	0
3	B	2113	0	2033	10	0
4	C	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	25	0	0
All	All	10608	0	10308	76	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 76 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:H:174:LEU:O	1:H:174:LEU:HD12	1.55	1.05
1:I:174:LEU:HD12	1:I:174:LEU:O	1.55	1.05
2:M:119:PRO:HB3	2:M:145:PHE:HB3	1.68	0.76
2:L:119:PRO:HB3	2:L:145:PHE:HB3	1.68	0.73
1:H:91:THR:HA	1:H:115:VAL:O	1.90	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	H	209/256 (82%)	197 (94%)	11 (5%)	1 (0%)	25	57
1	I	209/256 (82%)	197 (94%)	11 (5%)	1 (0%)	25	57
2	L	196/240 (82%)	184 (94%)	12 (6%)	0	100	100
2	M	196/240 (82%)	184 (94%)	12 (6%)	0	100	100
3	A	254/1286 (20%)	227 (89%)	27 (11%)	0	100	100
3	B	254/1286 (20%)	227 (89%)	27 (11%)	0	100	100
All	All	1318/3564 (37%)	1216 (92%)	100 (8%)	2 (0%)	45	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	153	PRO
1	I	153	PRO

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	H	180/214 (84%)	178 (99%)	2 (1%)	70	80
1	I	180/214 (84%)	178 (99%)	2 (1%)	70	80
2	L	181/212 (85%)	180 (99%)	1 (1%)	84	90
2	M	181/212 (85%)	180 (99%)	1 (1%)	84	90
3	A	234/1115 (21%)	231 (99%)	3 (1%)	65	77
3	B	234/1115 (21%)	231 (99%)	3 (1%)	65	77
All	All	1190/3082 (39%)	1178 (99%)	12 (1%)	71	82

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

Mol	Chain	Res	Type
3	B	395	VAL
3	B	525	CYS
1	I	6	GLN
2	M	31	TYR
3	A	361	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	106	GLN
1	I	77	ASN
3	A	321	GLN
3	B	49	HIS
3	B	271	GLN

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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1	4,3	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	C	2	4	14,14,15	0.25	0	17,19,21	0.49	0
4	NAG	D	1	4,3	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.48	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	C	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	4/6/23/26	0/1/1/1
4	NAG	D	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

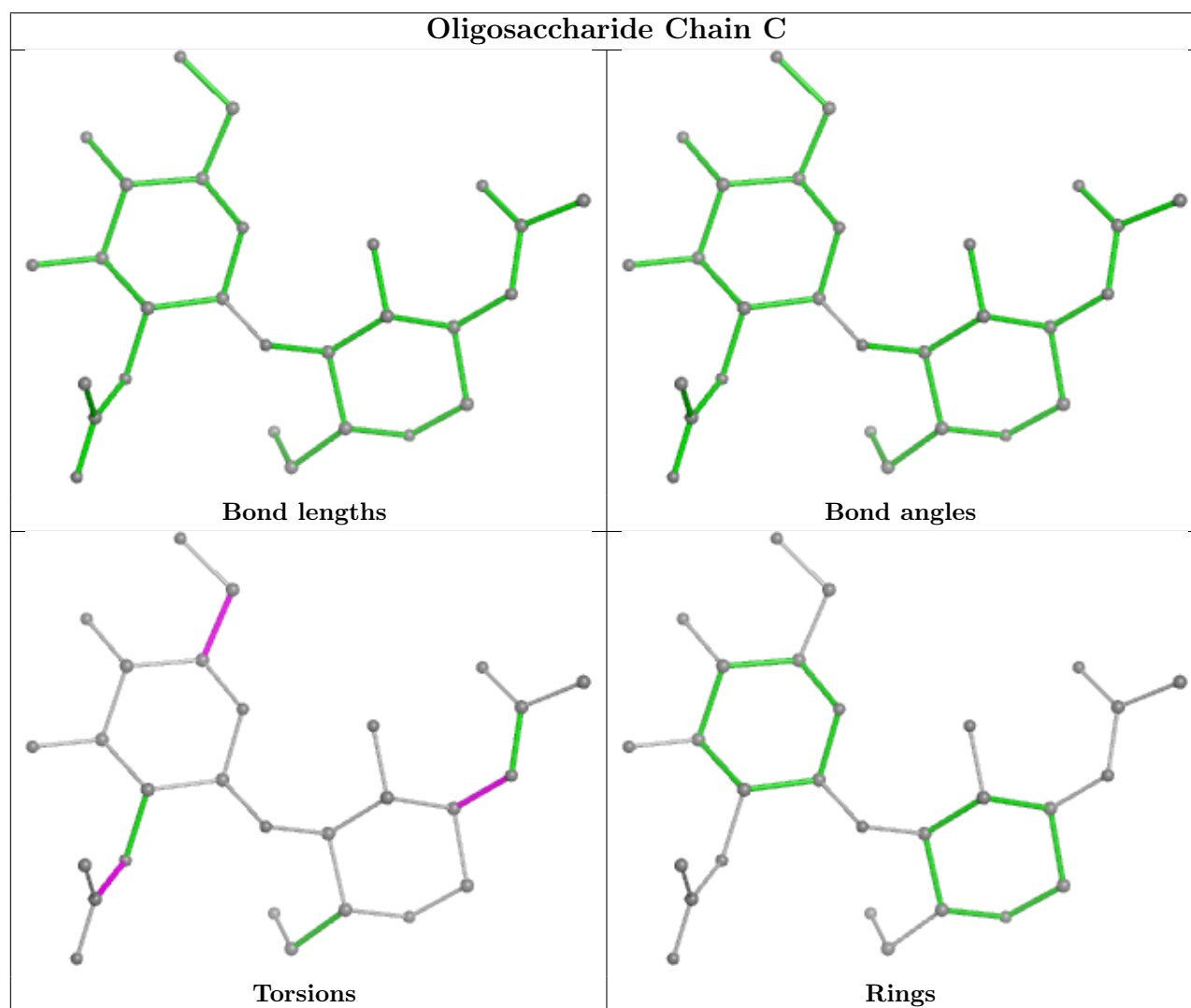
5 of 10 torsion outliers are listed below:

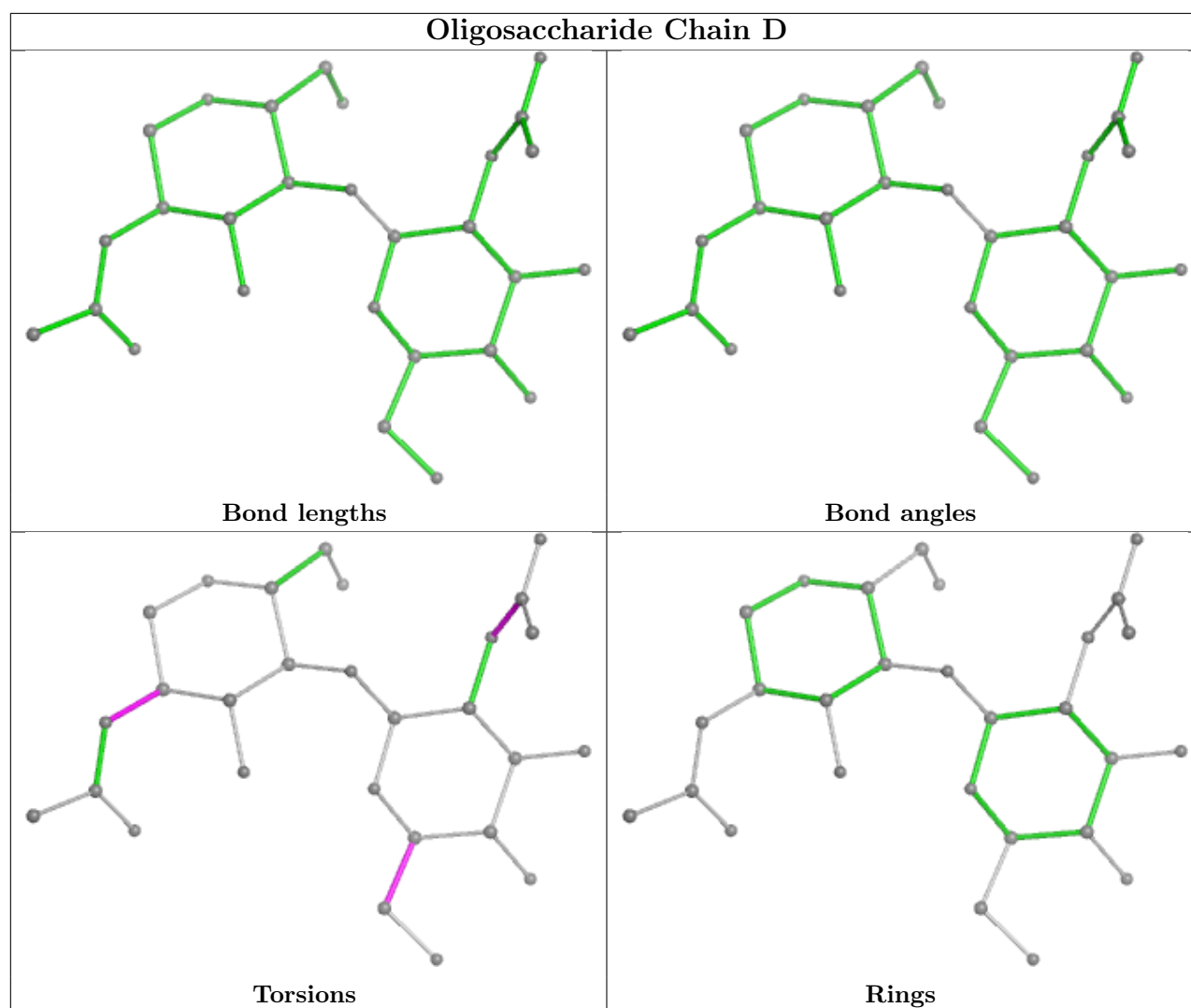
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

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-11648. These allow visual inspection of the internal detail of the map and identification of artifacts.

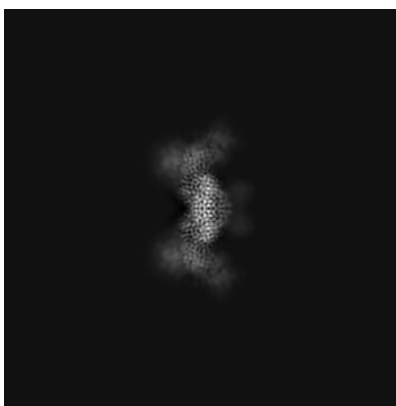
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

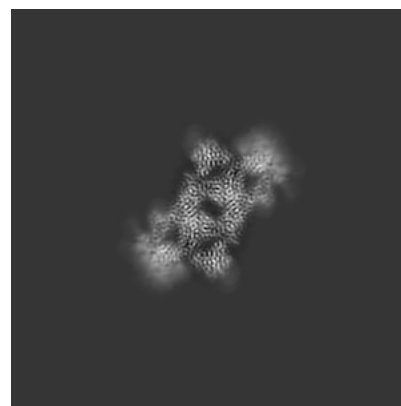
6.1.1 Primary map



X

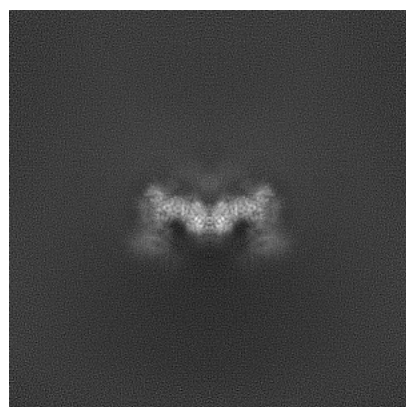


Y

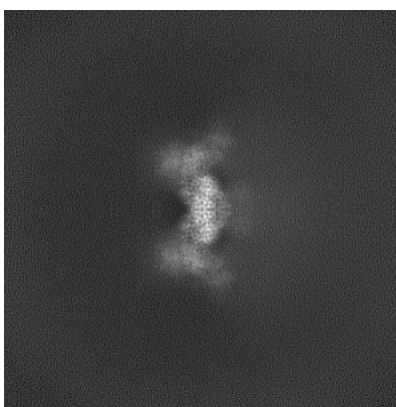


Z

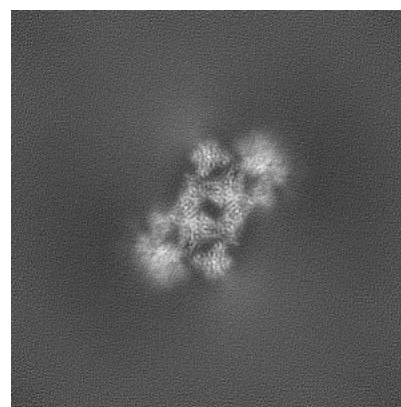
6.1.2 Raw map



X



Y



Z

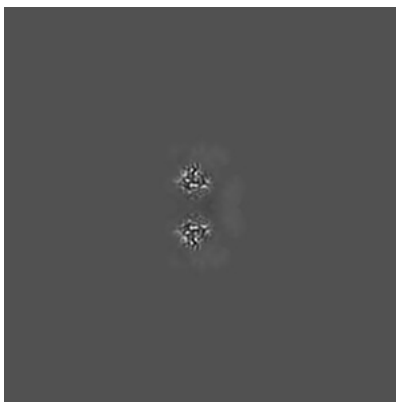
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

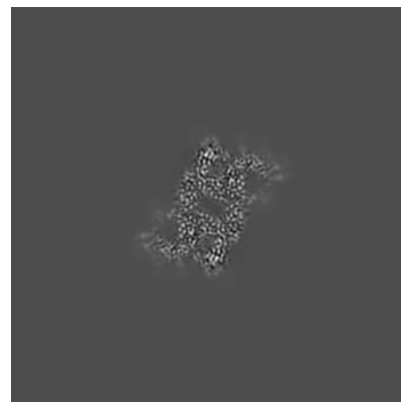
6.2.1 Primary map



X Index: 200

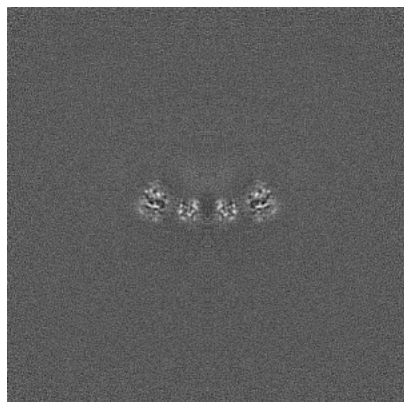


Y Index: 200

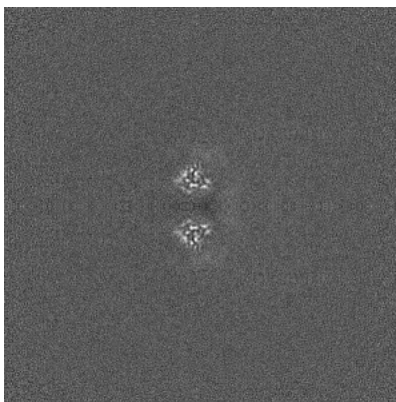


Z Index: 200

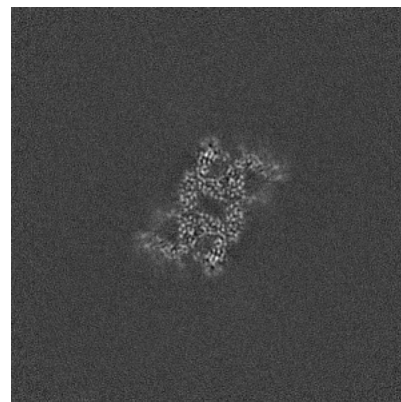
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

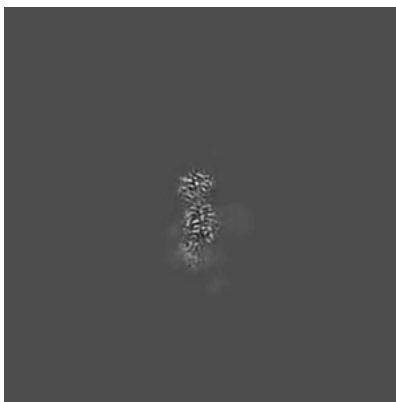
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

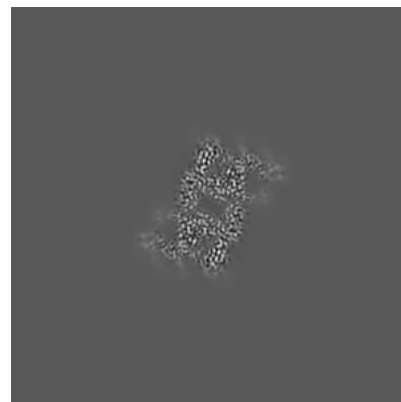
6.3.1 Primary map



X Index: 207

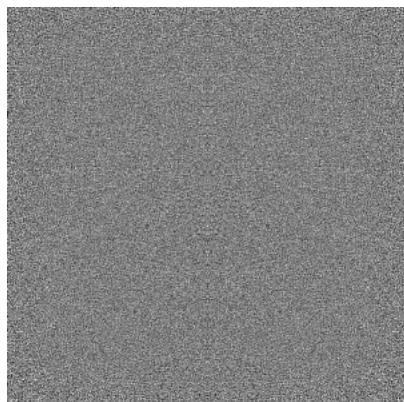


Y Index: 188

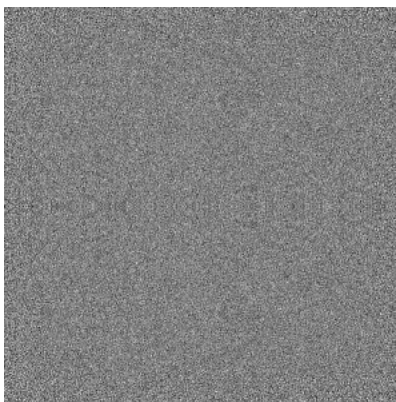


Z Index: 201

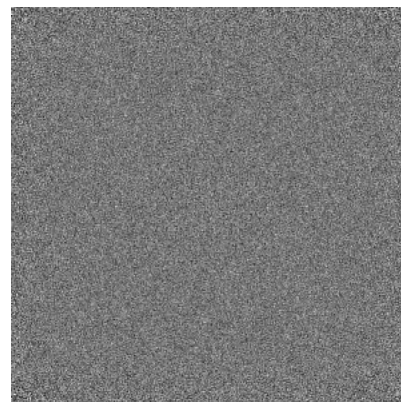
6.3.2 Raw map



X Index: 0



Y Index: 0

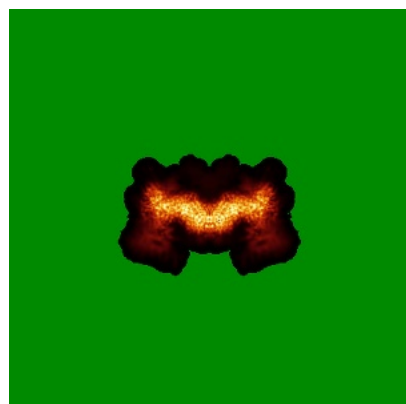


Z Index: 0

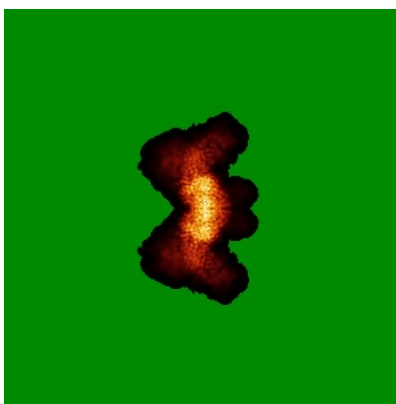
The images above show the largest variance slices of the map in three orthogonal directions.

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

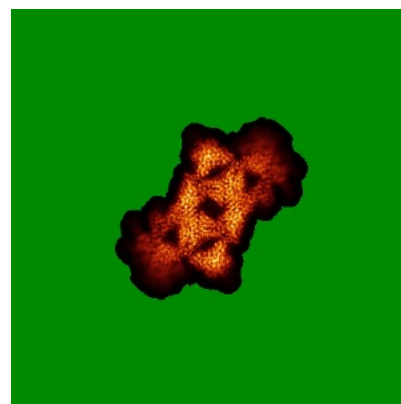
6.4.1 Primary map



X

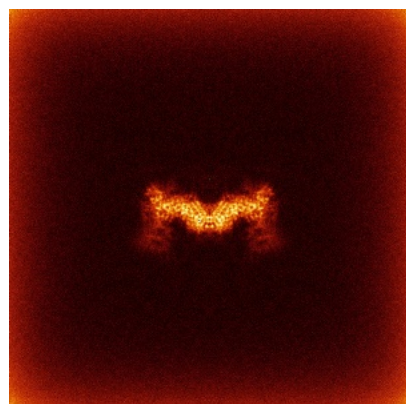


Y

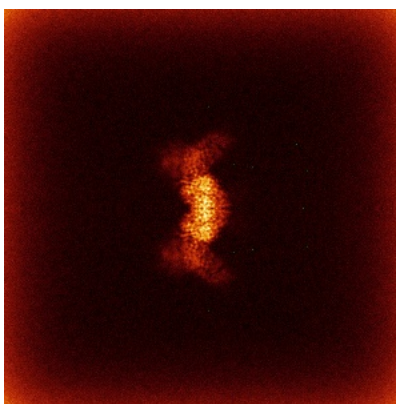


Z

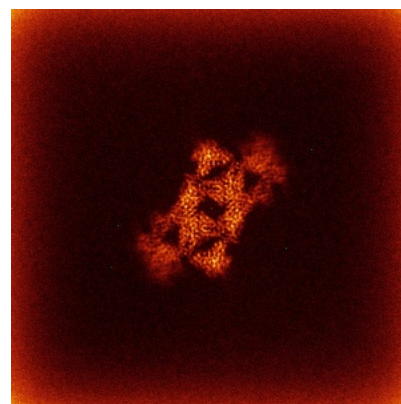
6.4.2 Raw map



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.

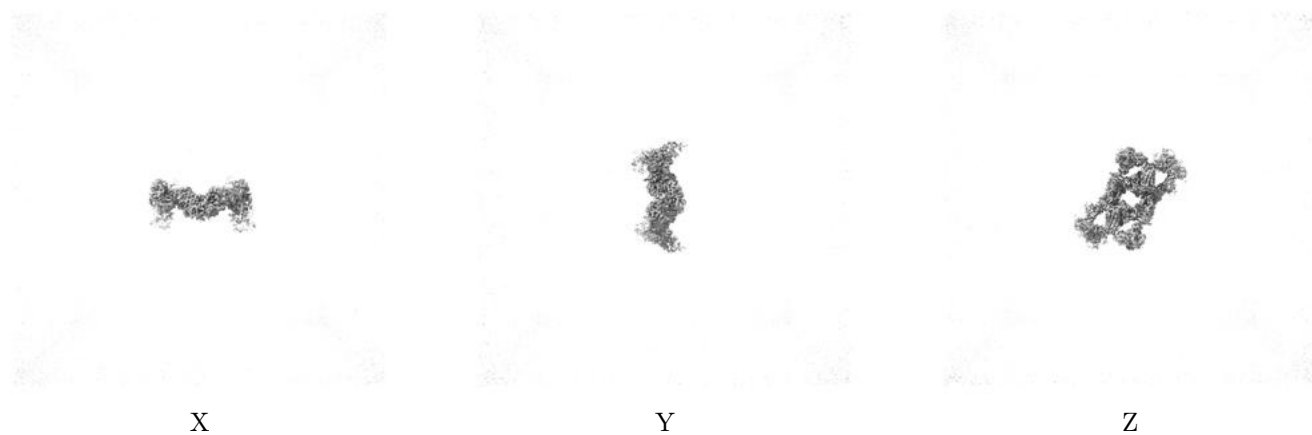
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

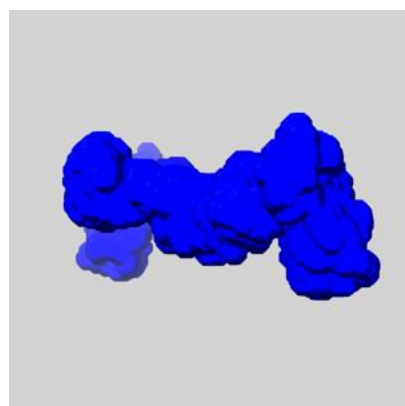
6.6 Mask visualisation [i](#)

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

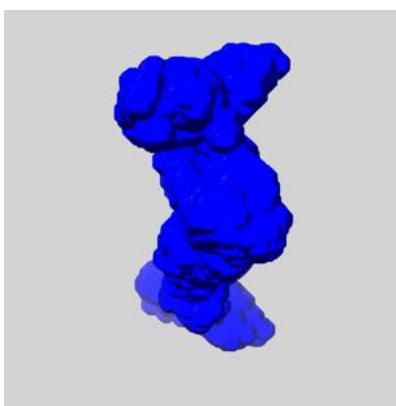
A mask typically either:

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

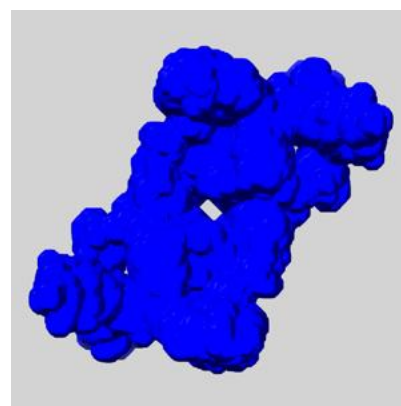
6.6.1 emd_11648_msk_1.map [i](#)



X



Y

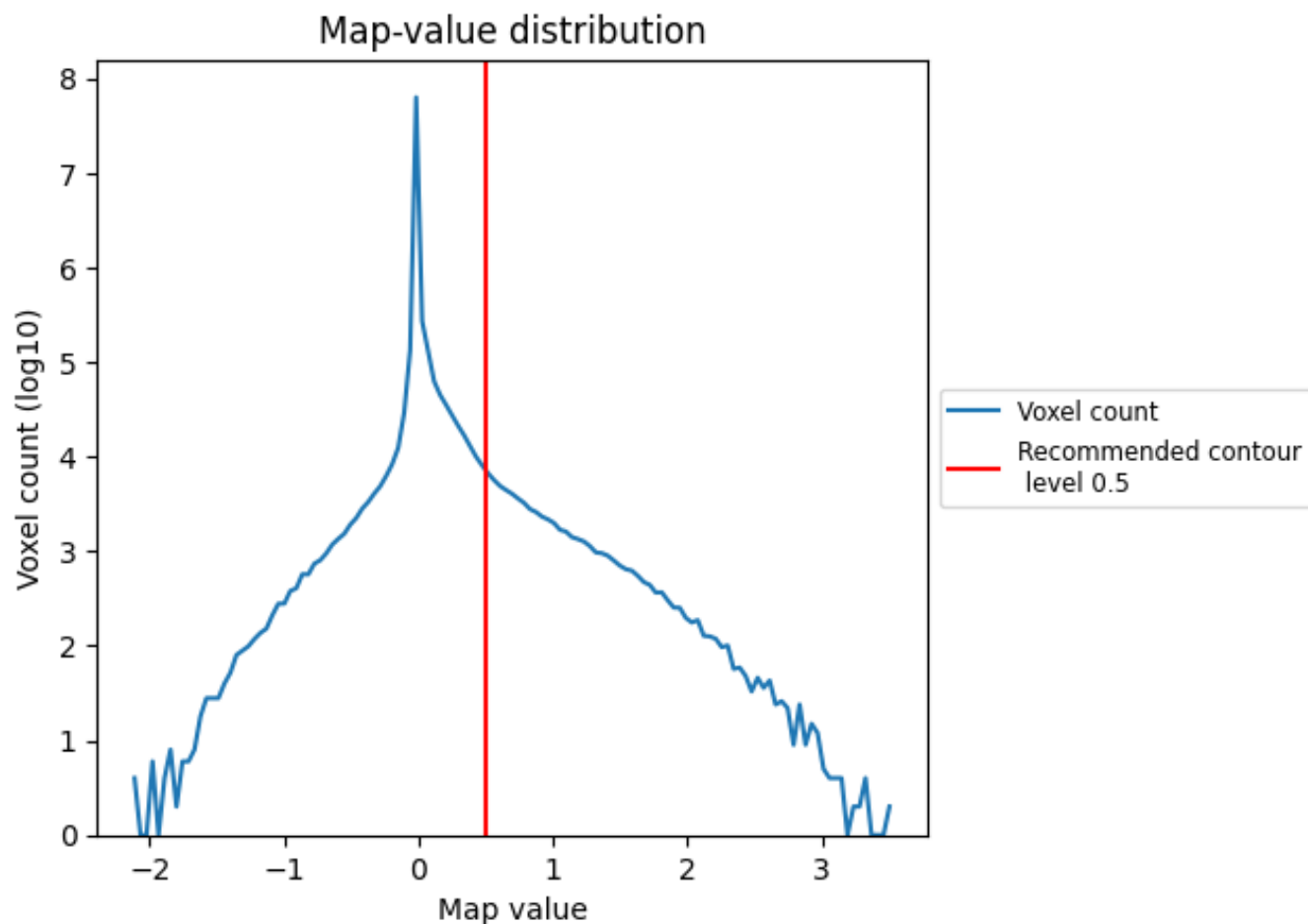


Z

7 Map analysis [i](#)

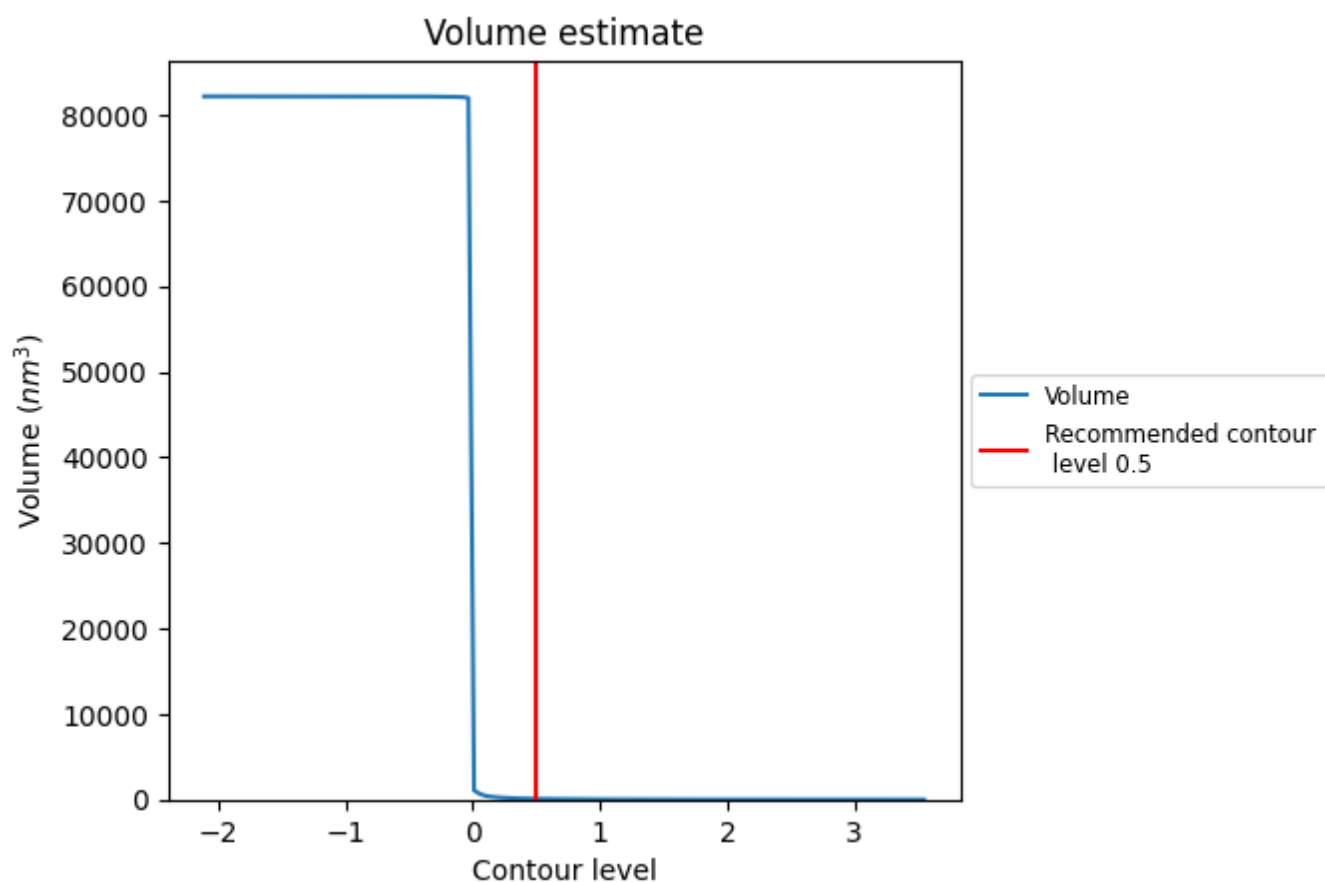
This section contains the results of statistical analysis of the map.

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.

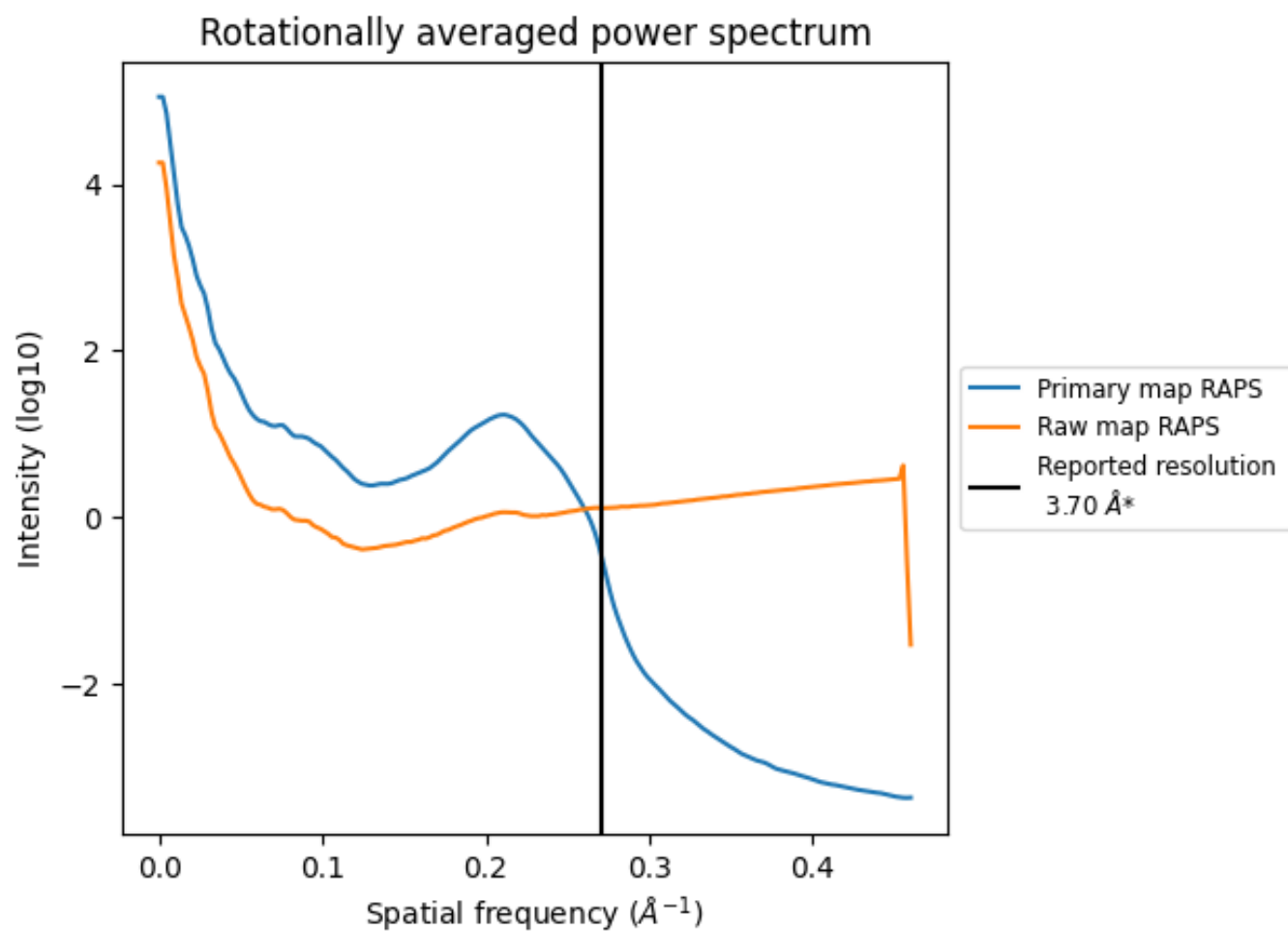
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm³; this corresponds to an approximate mass of 77 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 ⓘ

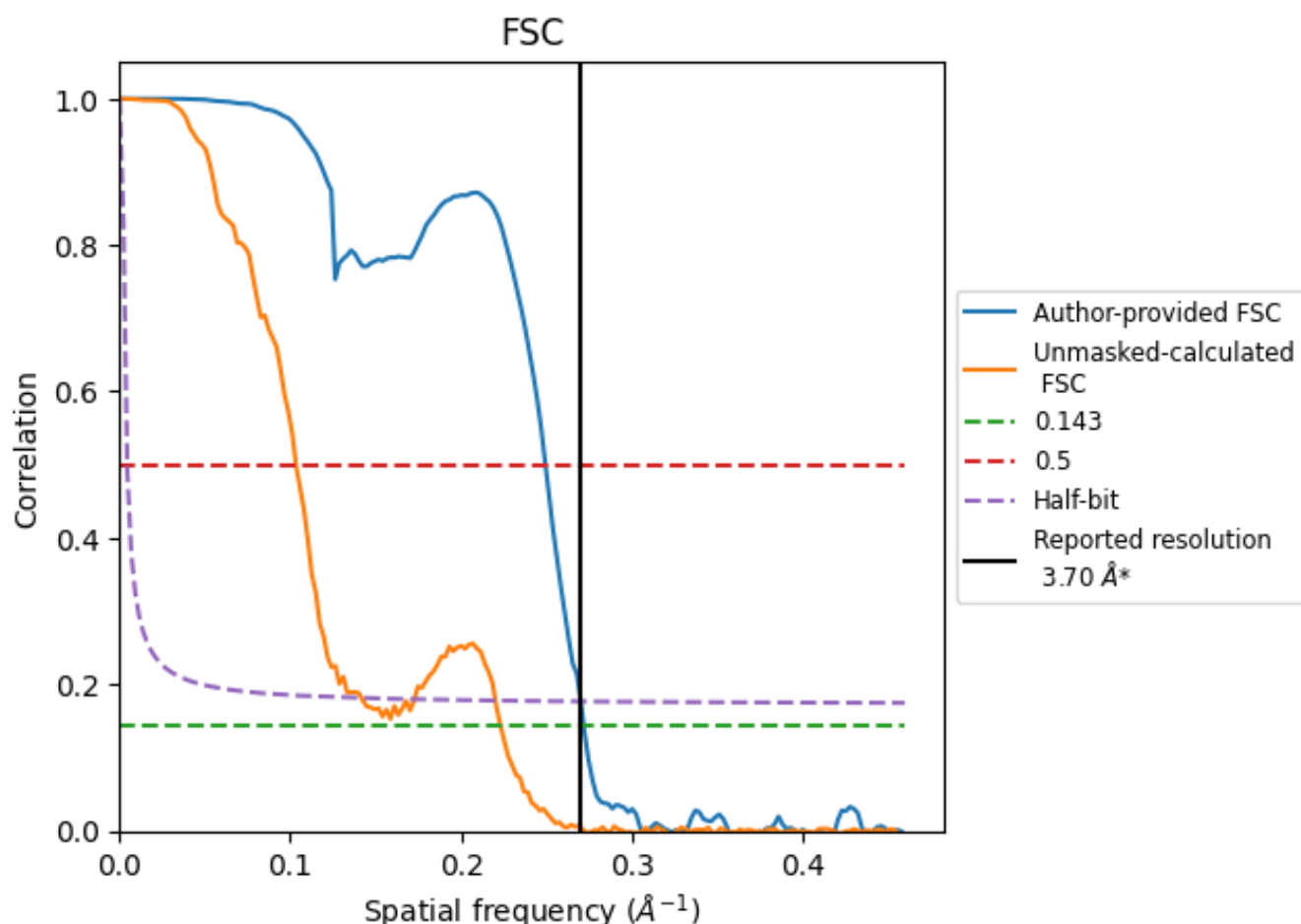


*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

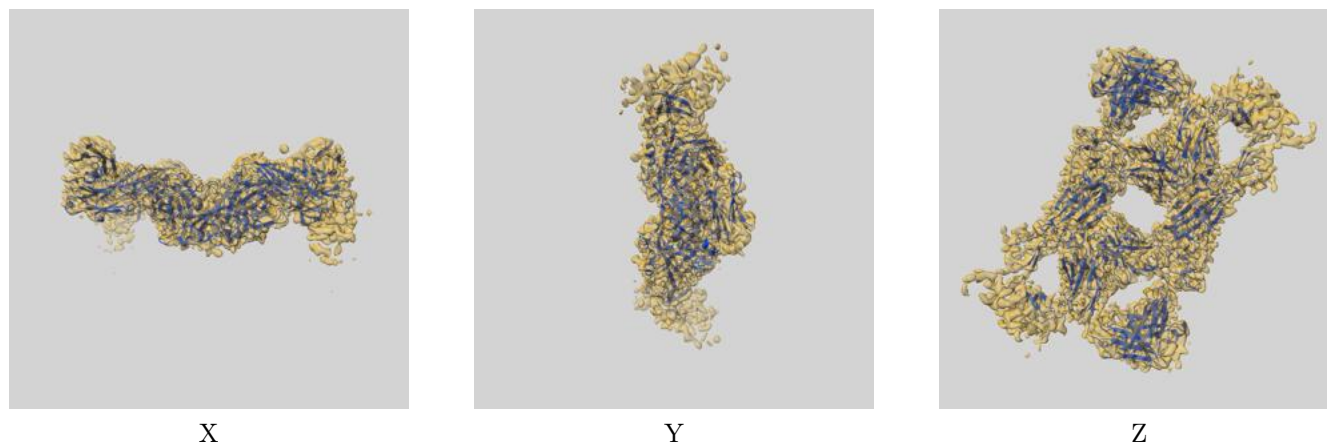
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.01	3.70
Unmasked-calculated*	4.48	9.67	7.05

*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 4.48 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

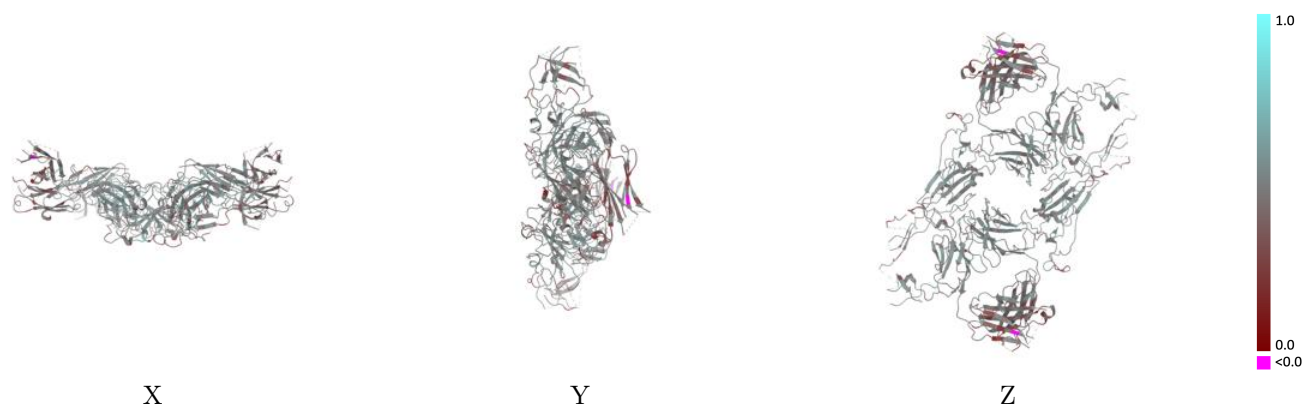
This section contains information regarding the fit between EMDB map EMD-11648 and PDB model 7A5R. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



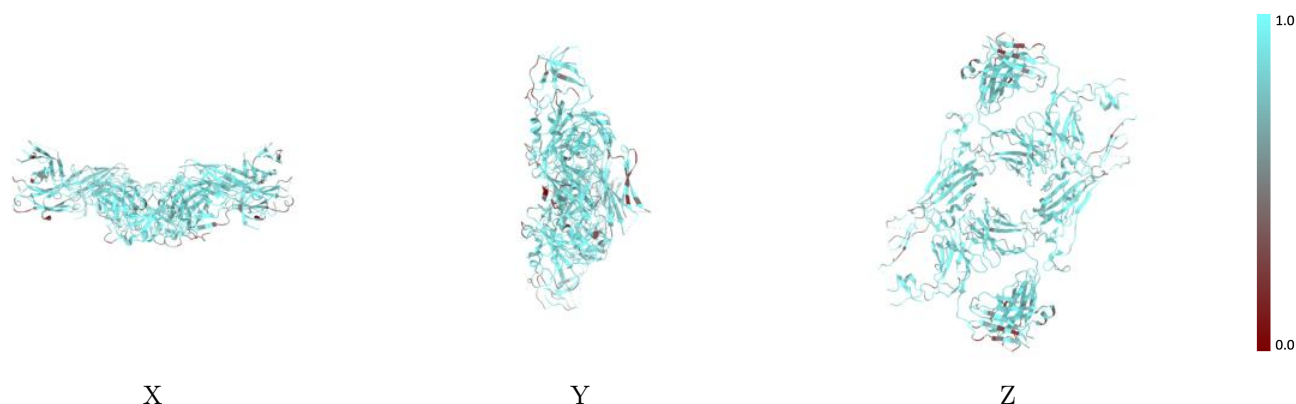
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



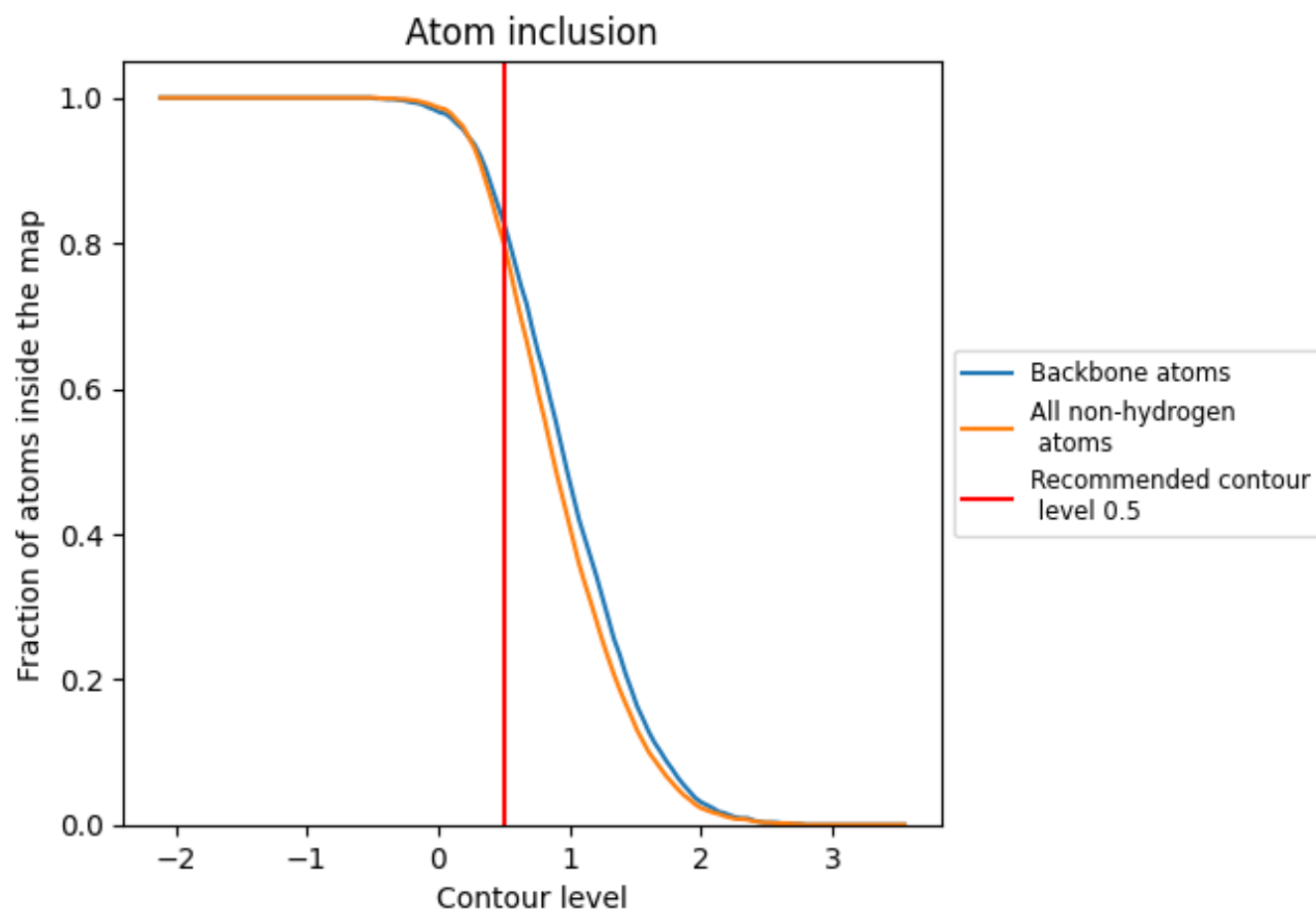
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7990	<div><div></div></div> 0.4720
A	<div><div></div></div> 0.8070	<div><div></div></div> 0.4800
B	<div><div></div></div> 0.8070	<div><div></div></div> 0.4780
C	<div><div></div></div> 0.6070	<div><div></div></div> 0.4310
D	<div><div></div></div> 0.6070	<div><div></div></div> 0.4320
H	<div><div></div></div> 0.7970	<div><div></div></div> 0.4740
I	<div><div></div></div> 0.7950	<div><div></div></div> 0.4700
L	<div><div></div></div> 0.7970	<div><div></div></div> 0.4640
M	<div><div></div></div> 0.7940	<div><div></div></div> 0.4620

1.0

0.0

<0.0