wwPDB EM Validation Summary Report

Apr 28, 2024 – 02:32 AM JST

PDB ID	:	7Y0J
EMDB ID	:	EMD-33547
Title	:	Cryo-EM structure of human IgM-Fc in complex with the J chain and the P. falciparum TM284VAR1
Authors	:	Ji, C.; Xiao, J.
Deposited on	:	2022-06-05
Resolution	:	3.62 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:

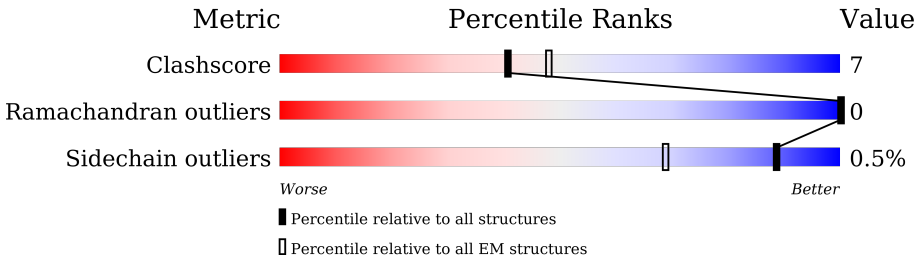
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.62 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 <=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	M	2373	8% · 89%
2	A	383	49% 11% 39%
2	B	383	49% 10% 40%
2	C	383	53% 7% 40%
2	D	383	48% 10% 42%
2	E	383	48% 11% 42%
2	F	383	45% 12% 42%
2	G	383	46% 13% 42%

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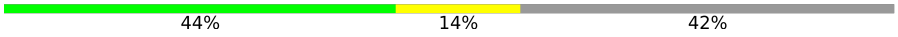
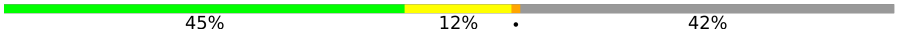
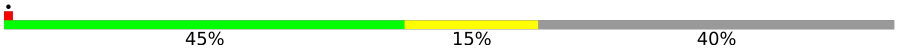
Mol	Chain	Length	Quality of chain
2	H	383	
2	K	383	
2	L	383	
3	J	136	
4	I	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20717 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 Erythrocyte membrane protein 2 variant TM284var1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	254	Total	C	N	O	S	0	0
			2161	1373	368	406	14		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	2368	HIS	-	expression tag	UNP I1X0L2
M	2369	HIS	-	expression tag	UNP I1X0L2
M	2370	HIS	-	expression tag	UNP I1X0L2
M	2371	HIS	-	expression tag	UNP I1X0L2
M	2372	HIS	-	expression tag	UNP I1X0L2
M	2373	HIS	-	expression tag	UNP I1X0L2

- Molecule 2 is a protein called Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		
2	B	228	Total	C	N	O	S	0	0
			1769	1114	300	347	8		
2	C	230	Total	C	N	O	S	0	0
			1779	1120	302	349	8		
2	D	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
2	E	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
2	F	221	Total	C	N	O	S	0	0
			1723	1087	292	336	8		
2	G	224	Total	C	N	O	S	0	0
			1742	1100	296	338	8		
2	H	222	Total	C	N	O	S	0	0
			1730	1092	293	337	8		
2	K	223	Total	C	N	O	S	0	0
			1737	1095	295	339	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	228	Total	C	N	O	S	0	0
			1773	1116	299	349	9		

There are 350 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	ALA	-	expression tag	UNP P01871
A	195	SER	-	expression tag	UNP P01871
A	196	ALA	-	expression tag	UNP P01871
A	197	TRP	-	expression tag	UNP P01871
A	198	SER	-	expression tag	UNP P01871
A	199	HIS	-	expression tag	UNP P01871
A	200	PRO	-	expression tag	UNP P01871
A	201	GLN	-	expression tag	UNP P01871
A	202	PHE	-	expression tag	UNP P01871
A	203	GLU	-	expression tag	UNP P01871
A	204	LYS	-	expression tag	UNP P01871
A	205	GLY	-	expression tag	UNP P01871
A	206	GLY	-	expression tag	UNP P01871
A	207	GLY	-	expression tag	UNP P01871
A	208	SER	-	expression tag	UNP P01871
A	209	GLY	-	expression tag	UNP P01871
A	210	GLY	-	expression tag	UNP P01871
A	211	GLY	-	expression tag	UNP P01871
A	212	SER	-	expression tag	UNP P01871
A	213	GLY	-	expression tag	UNP P01871
A	214	GLY	-	expression tag	UNP P01871
A	215	SER	-	expression tag	UNP P01871
A	216	ALA	-	expression tag	UNP P01871
A	217	TRP	-	expression tag	UNP P01871
A	218	SER	-	expression tag	UNP P01871
A	219	HIS	-	expression tag	UNP P01871
A	220	PRO	-	expression tag	UNP P01871
A	221	GLN	-	expression tag	UNP P01871
A	222	PHE	-	expression tag	UNP P01871
A	223	GLU	-	expression tag	UNP P01871
A	224	LYS	-	expression tag	UNP P01871
A	225	ILE	-	expression tag	UNP P01871
A	226	ASP	-	expression tag	UNP P01871
A	227	THR	-	expression tag	UNP P01871
A	228	THR	-	expression tag	UNP P01871
B	194	ALA	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	SER	-	expression tag	UNP P01871
B	196	ALA	-	expression tag	UNP P01871
B	197	TRP	-	expression tag	UNP P01871
B	198	SER	-	expression tag	UNP P01871
B	199	HIS	-	expression tag	UNP P01871
B	200	PRO	-	expression tag	UNP P01871
B	201	GLN	-	expression tag	UNP P01871
B	202	PHE	-	expression tag	UNP P01871
B	203	GLU	-	expression tag	UNP P01871
B	204	LYS	-	expression tag	UNP P01871
B	205	GLY	-	expression tag	UNP P01871
B	206	GLY	-	expression tag	UNP P01871
B	207	GLY	-	expression tag	UNP P01871
B	208	SER	-	expression tag	UNP P01871
B	209	GLY	-	expression tag	UNP P01871
B	210	GLY	-	expression tag	UNP P01871
B	211	GLY	-	expression tag	UNP P01871
B	212	SER	-	expression tag	UNP P01871
B	213	GLY	-	expression tag	UNP P01871
B	214	GLY	-	expression tag	UNP P01871
B	215	SER	-	expression tag	UNP P01871
B	216	ALA	-	expression tag	UNP P01871
B	217	TRP	-	expression tag	UNP P01871
B	218	SER	-	expression tag	UNP P01871
B	219	HIS	-	expression tag	UNP P01871
B	220	PRO	-	expression tag	UNP P01871
B	221	GLN	-	expression tag	UNP P01871
B	222	PHE	-	expression tag	UNP P01871
B	223	GLU	-	expression tag	UNP P01871
B	224	LYS	-	expression tag	UNP P01871
B	225	ILE	-	expression tag	UNP P01871
B	226	ASP	-	expression tag	UNP P01871
B	227	THR	-	expression tag	UNP P01871
B	228	THR	-	expression tag	UNP P01871
C	194	ALA	-	expression tag	UNP P01871
C	195	SER	-	expression tag	UNP P01871
C	196	ALA	-	expression tag	UNP P01871
C	197	TRP	-	expression tag	UNP P01871
C	198	SER	-	expression tag	UNP P01871
C	199	HIS	-	expression tag	UNP P01871
C	200	PRO	-	expression tag	UNP P01871
C	201	GLN	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
C	202	PHE	-	expression tag	UNP P01871
C	203	GLU	-	expression tag	UNP P01871
C	204	LYS	-	expression tag	UNP P01871
C	205	GLY	-	expression tag	UNP P01871
C	206	GLY	-	expression tag	UNP P01871
C	207	GLY	-	expression tag	UNP P01871
C	208	SER	-	expression tag	UNP P01871
C	209	GLY	-	expression tag	UNP P01871
C	210	GLY	-	expression tag	UNP P01871
C	211	GLY	-	expression tag	UNP P01871
C	212	SER	-	expression tag	UNP P01871
C	213	GLY	-	expression tag	UNP P01871
C	214	GLY	-	expression tag	UNP P01871
C	215	SER	-	expression tag	UNP P01871
C	216	ALA	-	expression tag	UNP P01871
C	217	TRP	-	expression tag	UNP P01871
C	218	SER	-	expression tag	UNP P01871
C	219	HIS	-	expression tag	UNP P01871
C	220	PRO	-	expression tag	UNP P01871
C	221	GLN	-	expression tag	UNP P01871
C	222	PHE	-	expression tag	UNP P01871
C	223	GLU	-	expression tag	UNP P01871
C	224	LYS	-	expression tag	UNP P01871
C	225	ILE	-	expression tag	UNP P01871
C	226	ASP	-	expression tag	UNP P01871
C	227	THR	-	expression tag	UNP P01871
C	228	THR	-	expression tag	UNP P01871
D	194	ALA	-	expression tag	UNP P01871
D	195	SER	-	expression tag	UNP P01871
D	196	ALA	-	expression tag	UNP P01871
D	197	TRP	-	expression tag	UNP P01871
D	198	SER	-	expression tag	UNP P01871
D	199	HIS	-	expression tag	UNP P01871
D	200	PRO	-	expression tag	UNP P01871
D	201	GLN	-	expression tag	UNP P01871
D	202	PHE	-	expression tag	UNP P01871
D	203	GLU	-	expression tag	UNP P01871
D	204	LYS	-	expression tag	UNP P01871
D	205	GLY	-	expression tag	UNP P01871
D	206	GLY	-	expression tag	UNP P01871
D	207	GLY	-	expression tag	UNP P01871
D	208	SER	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
D	209	GLY	-	expression tag	UNP P01871
D	210	GLY	-	expression tag	UNP P01871
D	211	GLY	-	expression tag	UNP P01871
D	212	SER	-	expression tag	UNP P01871
D	213	GLY	-	expression tag	UNP P01871
D	214	GLY	-	expression tag	UNP P01871
D	215	SER	-	expression tag	UNP P01871
D	216	ALA	-	expression tag	UNP P01871
D	217	TRP	-	expression tag	UNP P01871
D	218	SER	-	expression tag	UNP P01871
D	219	HIS	-	expression tag	UNP P01871
D	220	PRO	-	expression tag	UNP P01871
D	221	GLN	-	expression tag	UNP P01871
D	222	PHE	-	expression tag	UNP P01871
D	223	GLU	-	expression tag	UNP P01871
D	224	LYS	-	expression tag	UNP P01871
D	225	ILE	-	expression tag	UNP P01871
D	226	ASP	-	expression tag	UNP P01871
D	227	THR	-	expression tag	UNP P01871
D	228	THR	-	expression tag	UNP P01871
E	194	ALA	-	expression tag	UNP P01871
E	195	SER	-	expression tag	UNP P01871
E	196	ALA	-	expression tag	UNP P01871
E	197	TRP	-	expression tag	UNP P01871
E	198	SER	-	expression tag	UNP P01871
E	199	HIS	-	expression tag	UNP P01871
E	200	PRO	-	expression tag	UNP P01871
E	201	GLN	-	expression tag	UNP P01871
E	202	PHE	-	expression tag	UNP P01871
E	203	GLU	-	expression tag	UNP P01871
E	204	LYS	-	expression tag	UNP P01871
E	205	GLY	-	expression tag	UNP P01871
E	206	GLY	-	expression tag	UNP P01871
E	207	GLY	-	expression tag	UNP P01871
E	208	SER	-	expression tag	UNP P01871
E	209	GLY	-	expression tag	UNP P01871
E	210	GLY	-	expression tag	UNP P01871
E	211	GLY	-	expression tag	UNP P01871
E	212	SER	-	expression tag	UNP P01871
E	213	GLY	-	expression tag	UNP P01871
E	214	GLY	-	expression tag	UNP P01871
E	215	SER	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
E	216	ALA	-	expression tag	UNP P01871
E	217	TRP	-	expression tag	UNP P01871
E	218	SER	-	expression tag	UNP P01871
E	219	HIS	-	expression tag	UNP P01871
E	220	PRO	-	expression tag	UNP P01871
E	221	GLN	-	expression tag	UNP P01871
E	222	PHE	-	expression tag	UNP P01871
E	223	GLU	-	expression tag	UNP P01871
E	224	LYS	-	expression tag	UNP P01871
E	225	ILE	-	expression tag	UNP P01871
E	226	ASP	-	expression tag	UNP P01871
E	227	THR	-	expression tag	UNP P01871
E	228	THR	-	expression tag	UNP P01871
F	194	ALA	-	expression tag	UNP P01871
F	195	SER	-	expression tag	UNP P01871
F	196	ALA	-	expression tag	UNP P01871
F	197	TRP	-	expression tag	UNP P01871
F	198	SER	-	expression tag	UNP P01871
F	199	HIS	-	expression tag	UNP P01871
F	200	PRO	-	expression tag	UNP P01871
F	201	GLN	-	expression tag	UNP P01871
F	202	PHE	-	expression tag	UNP P01871
F	203	GLU	-	expression tag	UNP P01871
F	204	LYS	-	expression tag	UNP P01871
F	205	GLY	-	expression tag	UNP P01871
F	206	GLY	-	expression tag	UNP P01871
F	207	GLY	-	expression tag	UNP P01871
F	208	SER	-	expression tag	UNP P01871
F	209	GLY	-	expression tag	UNP P01871
F	210	GLY	-	expression tag	UNP P01871
F	211	GLY	-	expression tag	UNP P01871
F	212	SER	-	expression tag	UNP P01871
F	213	GLY	-	expression tag	UNP P01871
F	214	GLY	-	expression tag	UNP P01871
F	215	SER	-	expression tag	UNP P01871
F	216	ALA	-	expression tag	UNP P01871
F	217	TRP	-	expression tag	UNP P01871
F	218	SER	-	expression tag	UNP P01871
F	219	HIS	-	expression tag	UNP P01871
F	220	PRO	-	expression tag	UNP P01871
F	221	GLN	-	expression tag	UNP P01871
F	222	PHE	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
F	223	GLU	-	expression tag	UNP P01871
F	224	LYS	-	expression tag	UNP P01871
F	225	ILE	-	expression tag	UNP P01871
F	226	ASP	-	expression tag	UNP P01871
F	227	THR	-	expression tag	UNP P01871
F	228	THR	-	expression tag	UNP P01871
G	194	ALA	-	expression tag	UNP P01871
G	195	SER	-	expression tag	UNP P01871
G	196	ALA	-	expression tag	UNP P01871
G	197	TRP	-	expression tag	UNP P01871
G	198	SER	-	expression tag	UNP P01871
G	199	HIS	-	expression tag	UNP P01871
G	200	PRO	-	expression tag	UNP P01871
G	201	GLN	-	expression tag	UNP P01871
G	202	PHE	-	expression tag	UNP P01871
G	203	GLU	-	expression tag	UNP P01871
G	204	LYS	-	expression tag	UNP P01871
G	205	GLY	-	expression tag	UNP P01871
G	206	GLY	-	expression tag	UNP P01871
G	207	GLY	-	expression tag	UNP P01871
G	208	SER	-	expression tag	UNP P01871
G	209	GLY	-	expression tag	UNP P01871
G	210	GLY	-	expression tag	UNP P01871
G	211	GLY	-	expression tag	UNP P01871
G	212	SER	-	expression tag	UNP P01871
G	213	GLY	-	expression tag	UNP P01871
G	214	GLY	-	expression tag	UNP P01871
G	215	SER	-	expression tag	UNP P01871
G	216	ALA	-	expression tag	UNP P01871
G	217	TRP	-	expression tag	UNP P01871
G	218	SER	-	expression tag	UNP P01871
G	219	HIS	-	expression tag	UNP P01871
G	220	PRO	-	expression tag	UNP P01871
G	221	GLN	-	expression tag	UNP P01871
G	222	PHE	-	expression tag	UNP P01871
G	223	GLU	-	expression tag	UNP P01871
G	224	LYS	-	expression tag	UNP P01871
G	225	ILE	-	expression tag	UNP P01871
G	226	ASP	-	expression tag	UNP P01871
G	227	THR	-	expression tag	UNP P01871
G	228	THR	-	expression tag	UNP P01871
H	194	ALA	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
H	195	SER	-	expression tag	UNP P01871
H	196	ALA	-	expression tag	UNP P01871
H	197	TRP	-	expression tag	UNP P01871
H	198	SER	-	expression tag	UNP P01871
H	199	HIS	-	expression tag	UNP P01871
H	200	PRO	-	expression tag	UNP P01871
H	201	GLN	-	expression tag	UNP P01871
H	202	PHE	-	expression tag	UNP P01871
H	203	GLU	-	expression tag	UNP P01871
H	204	LYS	-	expression tag	UNP P01871
H	205	GLY	-	expression tag	UNP P01871
H	206	GLY	-	expression tag	UNP P01871
H	207	GLY	-	expression tag	UNP P01871
H	208	SER	-	expression tag	UNP P01871
H	209	GLY	-	expression tag	UNP P01871
H	210	GLY	-	expression tag	UNP P01871
H	211	GLY	-	expression tag	UNP P01871
H	212	SER	-	expression tag	UNP P01871
H	213	GLY	-	expression tag	UNP P01871
H	214	GLY	-	expression tag	UNP P01871
H	215	SER	-	expression tag	UNP P01871
H	216	ALA	-	expression tag	UNP P01871
H	217	TRP	-	expression tag	UNP P01871
H	218	SER	-	expression tag	UNP P01871
H	219	HIS	-	expression tag	UNP P01871
H	220	PRO	-	expression tag	UNP P01871
H	221	GLN	-	expression tag	UNP P01871
H	222	PHE	-	expression tag	UNP P01871
H	223	GLU	-	expression tag	UNP P01871
H	224	LYS	-	expression tag	UNP P01871
H	225	ILE	-	expression tag	UNP P01871
H	226	ASP	-	expression tag	UNP P01871
H	227	THR	-	expression tag	UNP P01871
H	228	THR	-	expression tag	UNP P01871
K	194	ALA	-	expression tag	UNP P01871
K	195	SER	-	expression tag	UNP P01871
K	196	ALA	-	expression tag	UNP P01871
K	197	TRP	-	expression tag	UNP P01871
K	198	SER	-	expression tag	UNP P01871
K	199	HIS	-	expression tag	UNP P01871
K	200	PRO	-	expression tag	UNP P01871
K	201	GLN	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
K	202	PHE	-	expression tag	UNP P01871
K	203	GLU	-	expression tag	UNP P01871
K	204	LYS	-	expression tag	UNP P01871
K	205	GLY	-	expression tag	UNP P01871
K	206	GLY	-	expression tag	UNP P01871
K	207	GLY	-	expression tag	UNP P01871
K	208	SER	-	expression tag	UNP P01871
K	209	GLY	-	expression tag	UNP P01871
K	210	GLY	-	expression tag	UNP P01871
K	211	GLY	-	expression tag	UNP P01871
K	212	SER	-	expression tag	UNP P01871
K	213	GLY	-	expression tag	UNP P01871
K	214	GLY	-	expression tag	UNP P01871
K	215	SER	-	expression tag	UNP P01871
K	216	ALA	-	expression tag	UNP P01871
K	217	TRP	-	expression tag	UNP P01871
K	218	SER	-	expression tag	UNP P01871
K	219	HIS	-	expression tag	UNP P01871
K	220	PRO	-	expression tag	UNP P01871
K	221	GLN	-	expression tag	UNP P01871
K	222	PHE	-	expression tag	UNP P01871
K	223	GLU	-	expression tag	UNP P01871
K	224	LYS	-	expression tag	UNP P01871
K	225	ILE	-	expression tag	UNP P01871
K	226	ASP	-	expression tag	UNP P01871
K	227	THR	-	expression tag	UNP P01871
K	228	THR	-	expression tag	UNP P01871
L	194	ALA	-	expression tag	UNP P01871
L	195	SER	-	expression tag	UNP P01871
L	196	ALA	-	expression tag	UNP P01871
L	197	TRP	-	expression tag	UNP P01871
L	198	SER	-	expression tag	UNP P01871
L	199	HIS	-	expression tag	UNP P01871
L	200	PRO	-	expression tag	UNP P01871
L	201	GLN	-	expression tag	UNP P01871
L	202	PHE	-	expression tag	UNP P01871
L	203	GLU	-	expression tag	UNP P01871
L	204	LYS	-	expression tag	UNP P01871
L	205	GLY	-	expression tag	UNP P01871
L	206	GLY	-	expression tag	UNP P01871
L	207	GLY	-	expression tag	UNP P01871
L	208	SER	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
L	209	GLY	-	expression tag	UNP P01871
L	210	GLY	-	expression tag	UNP P01871
L	211	GLY	-	expression tag	UNP P01871
L	212	SER	-	expression tag	UNP P01871
L	213	GLY	-	expression tag	UNP P01871
L	214	GLY	-	expression tag	UNP P01871
L	215	SER	-	expression tag	UNP P01871
L	216	ALA	-	expression tag	UNP P01871
L	217	TRP	-	expression tag	UNP P01871
L	218	SER	-	expression tag	UNP P01871
L	219	HIS	-	expression tag	UNP P01871
L	220	PRO	-	expression tag	UNP P01871
L	221	GLN	-	expression tag	UNP P01871
L	222	PHE	-	expression tag	UNP P01871
L	223	GLU	-	expression tag	UNP P01871
L	224	LYS	-	expression tag	UNP P01871
L	225	ILE	-	expression tag	UNP P01871
L	226	ASP	-	expression tag	UNP P01871
L	227	THR	-	expression tag	UNP P01871
L	228	THR	-	expression tag	UNP P01871

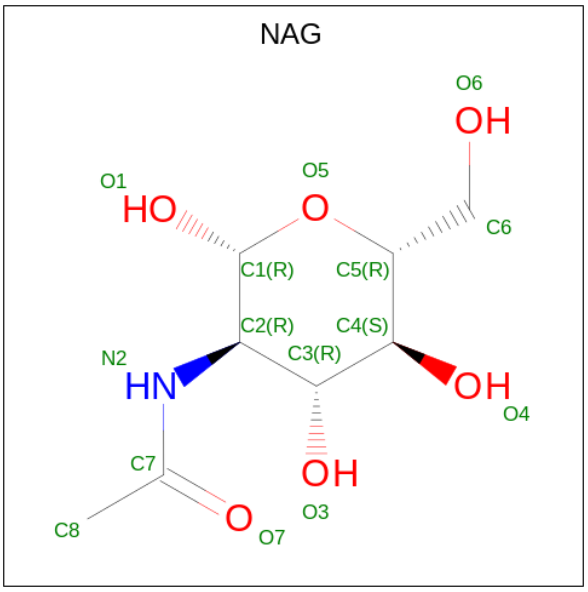
- Molecule 3 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	106	Total	C	N	O	S	0	0
			851	528	150	166	7		

- 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	I	2	Total	C	N	O	0	0
			28	16	2	10		

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



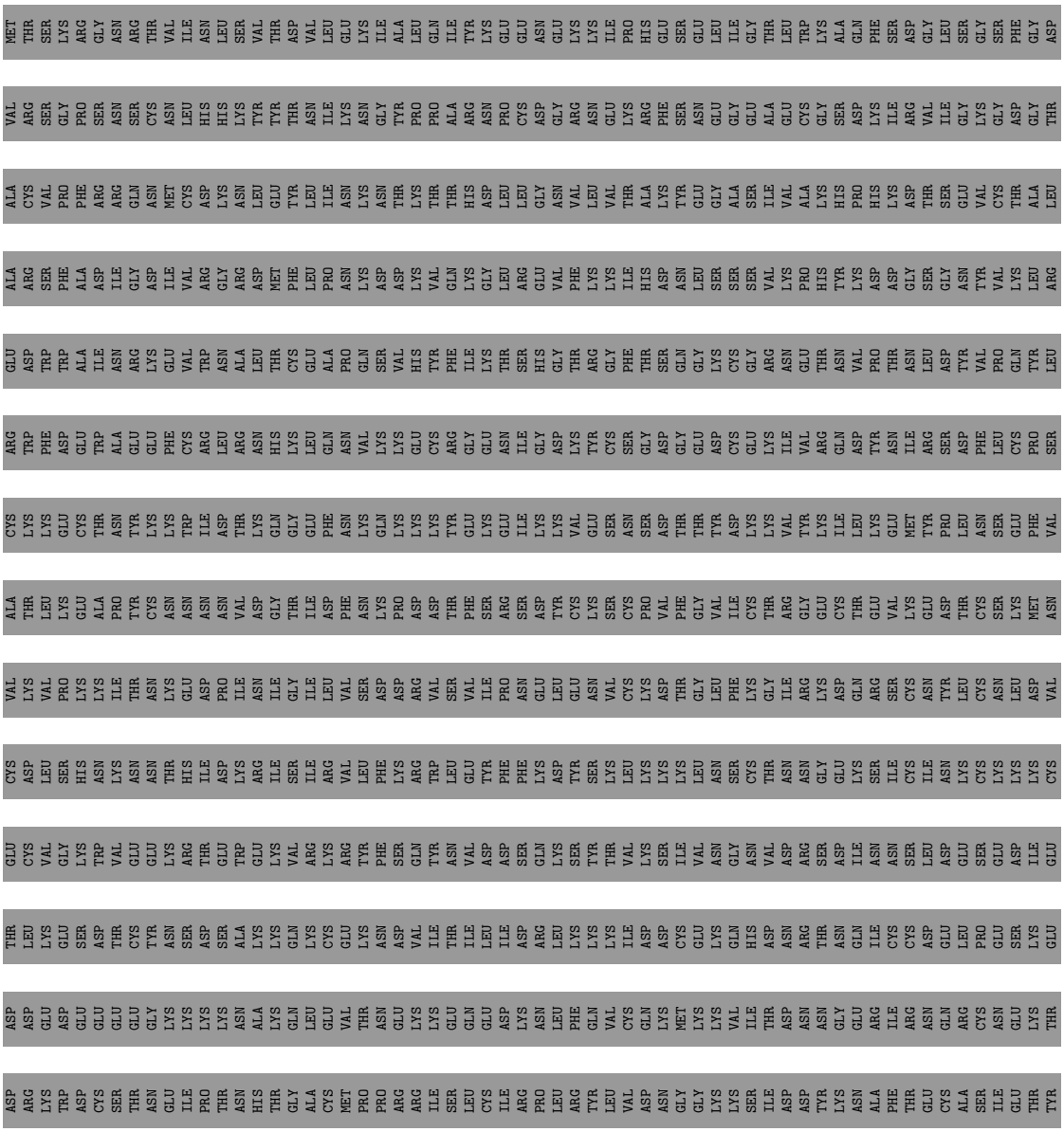
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	K	1	Total	C	N	O	0
			14	8	1	5	
5	L	1	Total	C	N	O	0
			14	8	1	5	

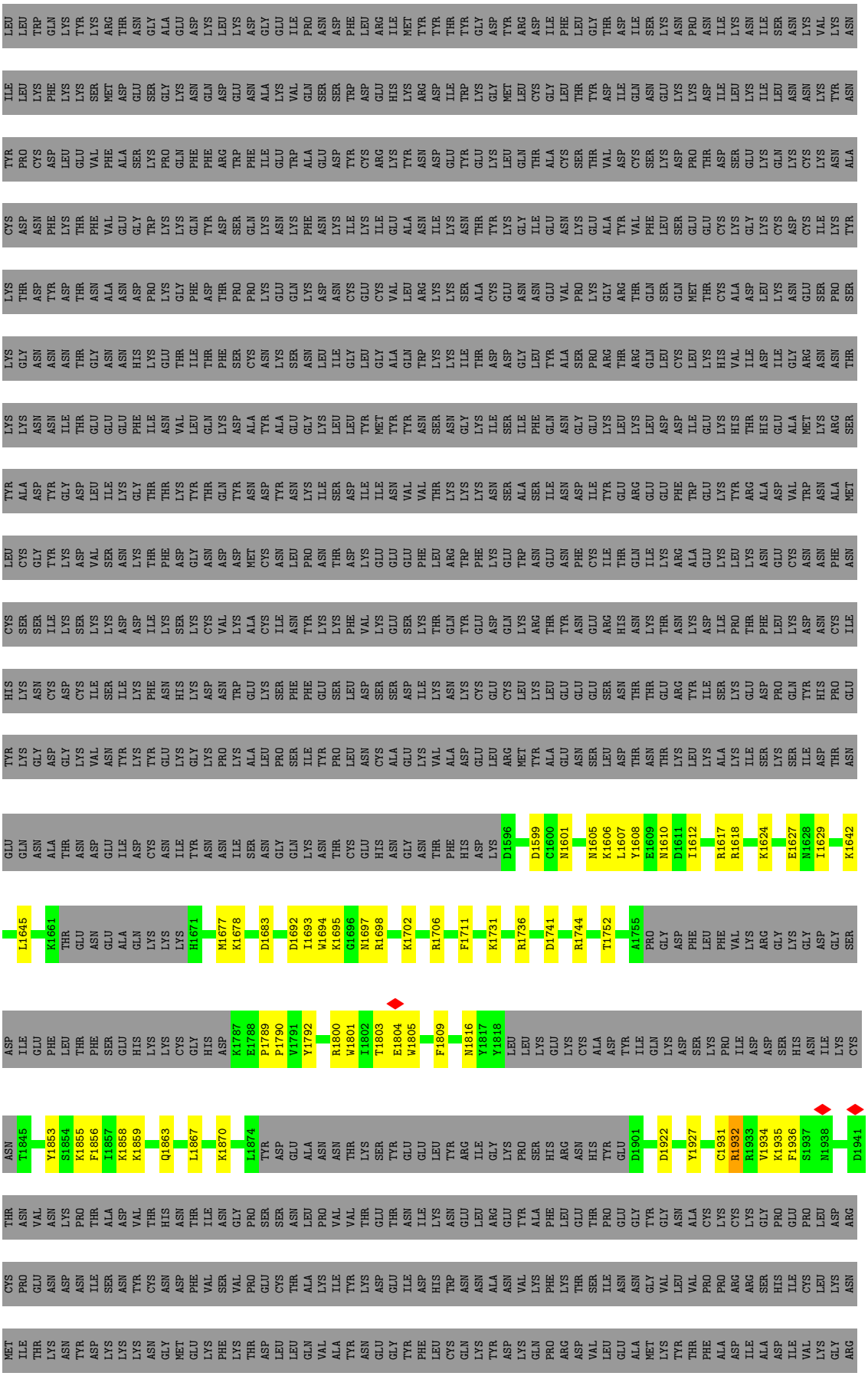
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Erythrocyte membrane protein 2 variant TM284var1

Chain M: 8% 89%




D1596
D1599
C1600
N1601
N1605
K1606
L1607
Y1608
E1609
N1610
D1611
I1612
R1617
R1618
K1624
E1627
N1628
I1629
K1642
L1645
K1661
H1671
M1677
K1678
D1683
D1692
I1693
W1694
K1695
G1696
N1697
R1698
K1702
R1706
F1711
K1731
R1736
D1741
R1744
T1752
A1755
K1787
E1788
P1789
P1790
V1791
Y1792
R1800
W1801
I1802
T1803
E1804
W1805
F1809
N1816
Y1817
Y1818
T1845
Y1853
S1854
K1855
F1856
I1857
K1858
K1859
Q1863
L1867
K1870
L1874
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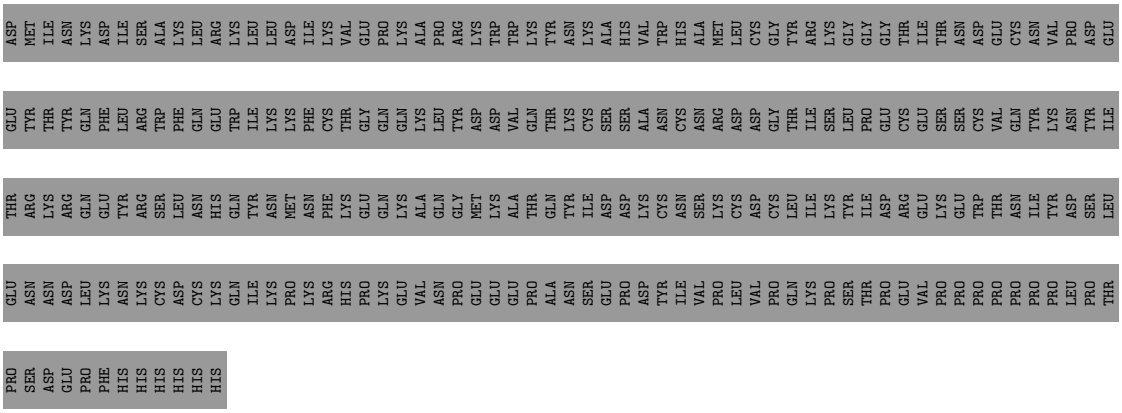
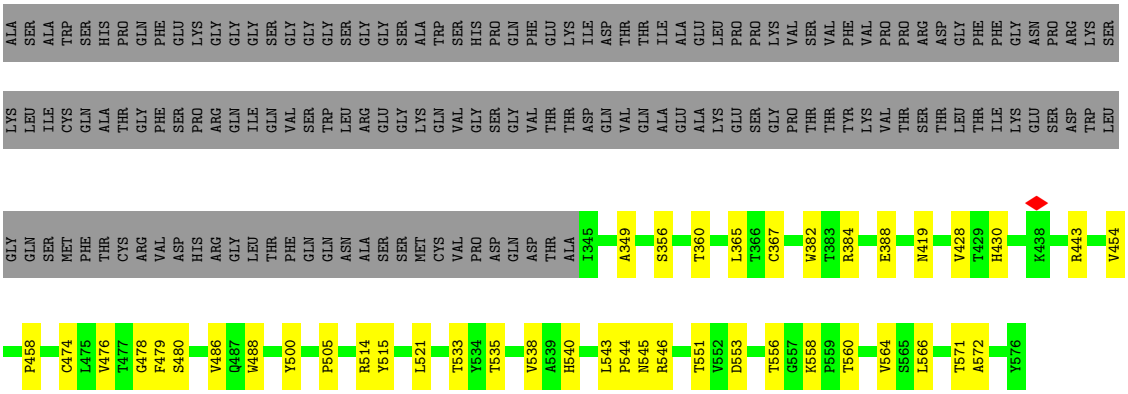
D1922
Y1927
C1931
R1932
R1933
V1934
K1935
F1936
S1937
N1938
D1941



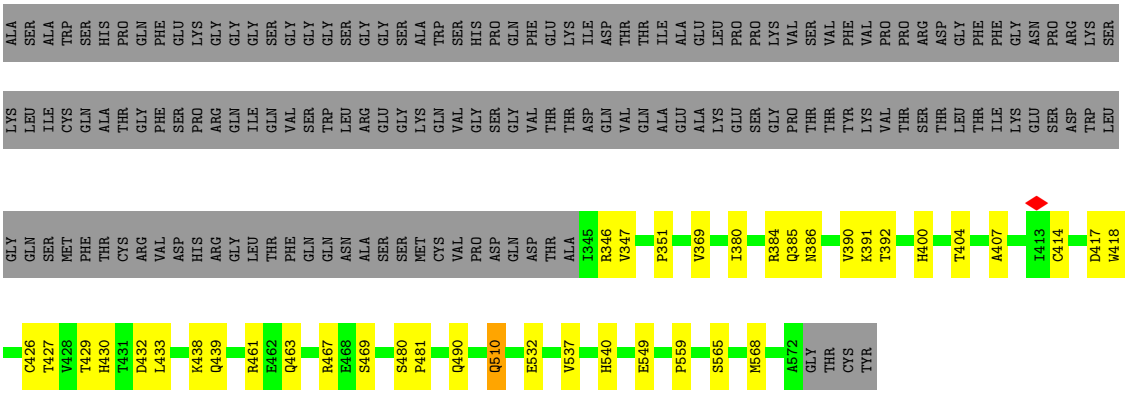
• Molecule 2: Immunoglobulin heavy constant mu

Chain A:



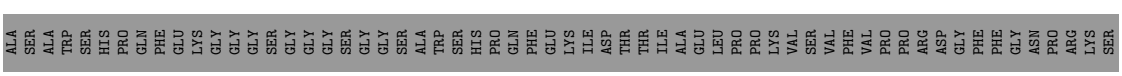
• Molecule 2: Immunoglobulin heavy constant mu

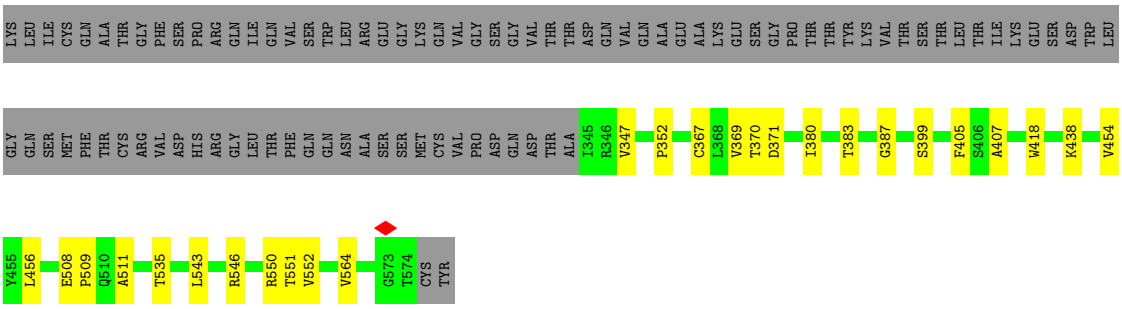
Chain B:



• Molecule 2: Immunoglobulin heavy constant mu

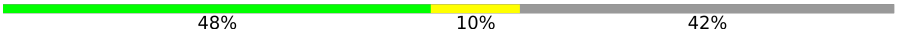
Chain C:

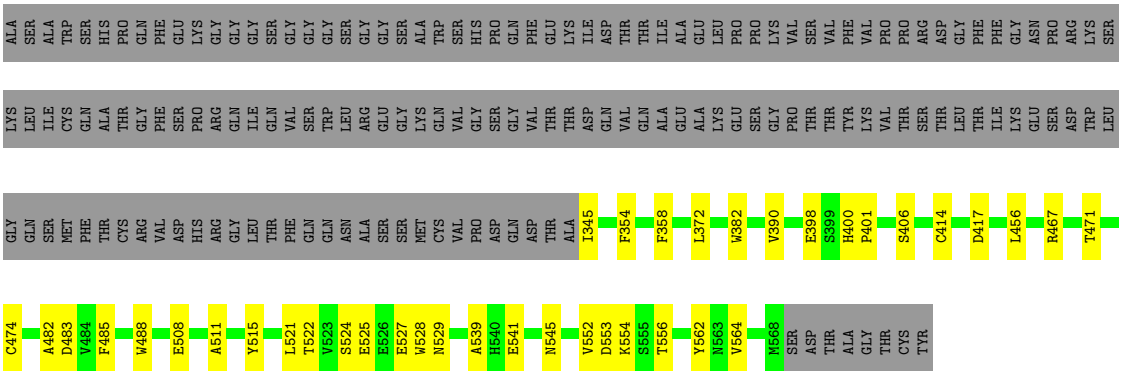




• Molecule 2: Immunoglobulin heavy constant mu

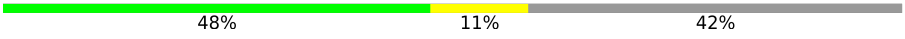
Chain D:

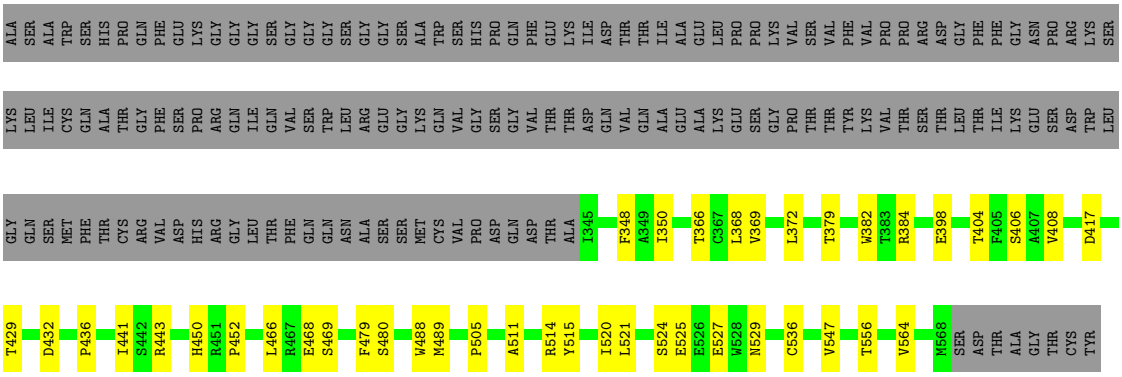




• Molecule 2: Immunoglobulin heavy constant mu

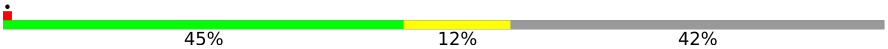
Chain E:

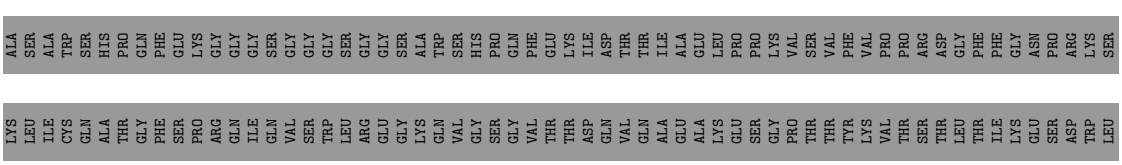


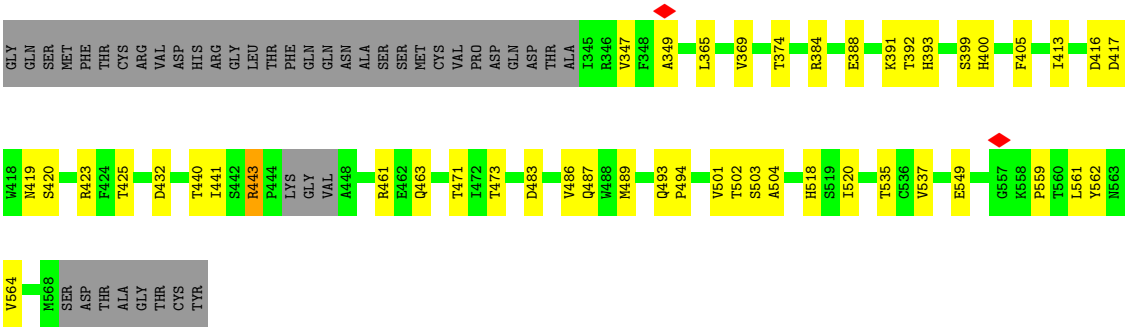


• Molecule 2: Immunoglobulin heavy constant mu

Chain F:

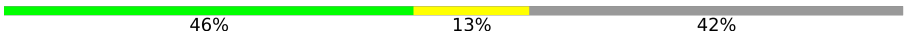


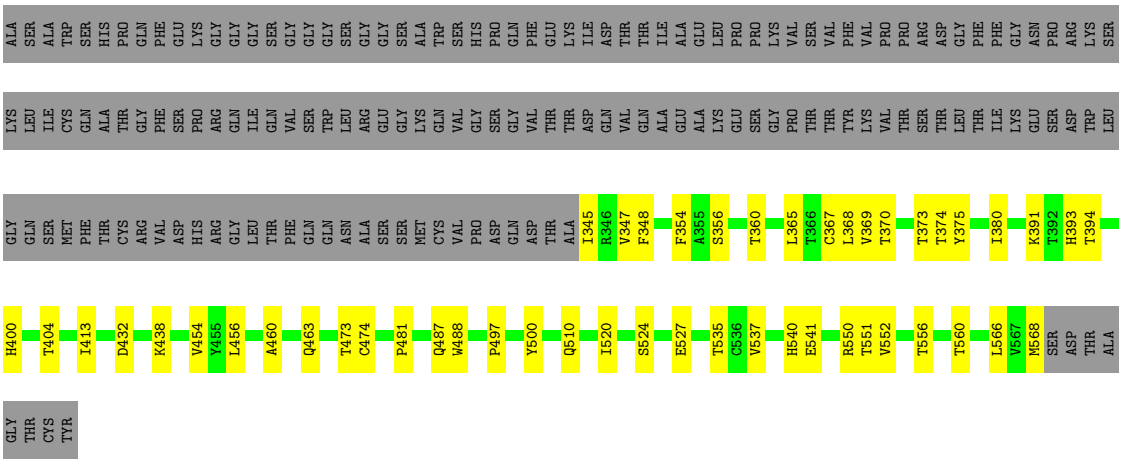




• Molecule 2: Immunoglobulin heavy constant mu

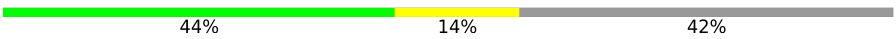
Chain G:

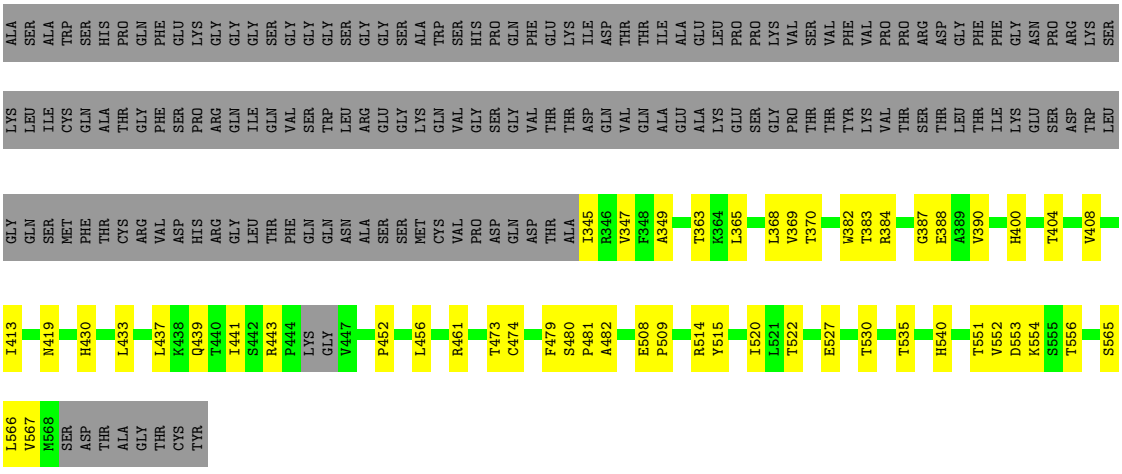




• Molecule 2: Immunoglobulin heavy constant mu

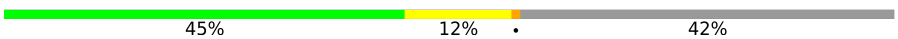
Chain H:

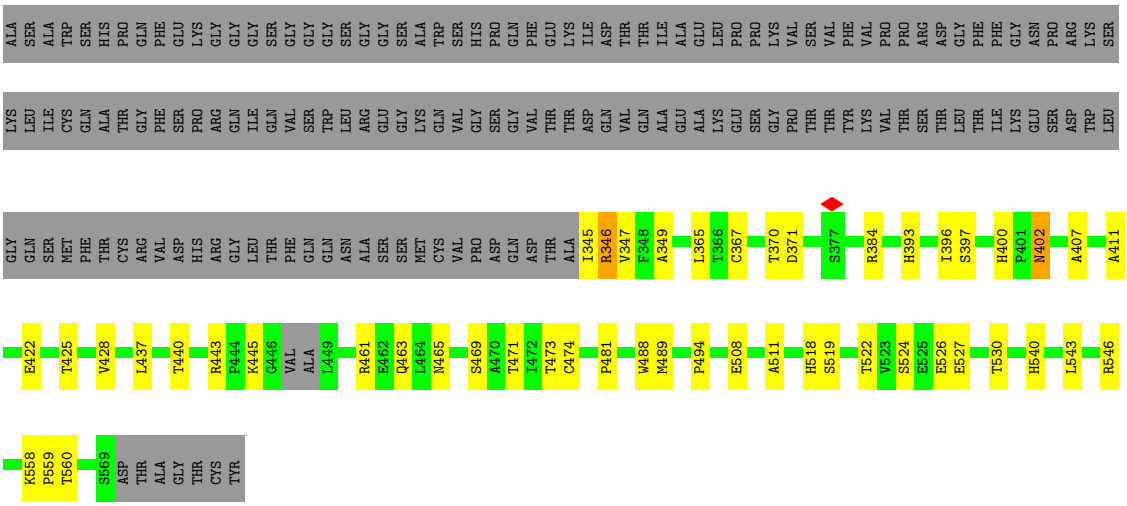




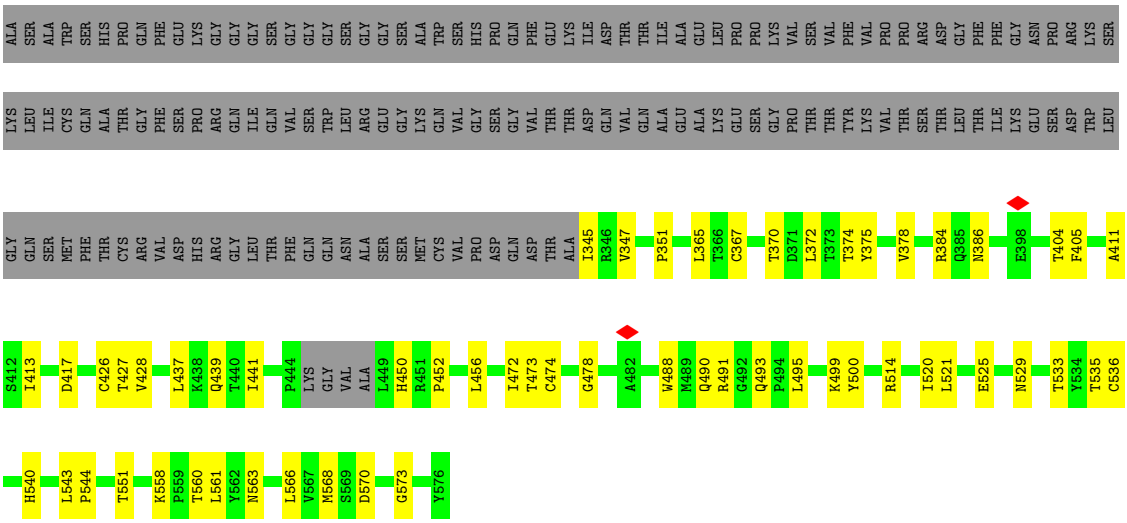
• Molecule 2: Immunoglobulin heavy constant mu

Chain K:

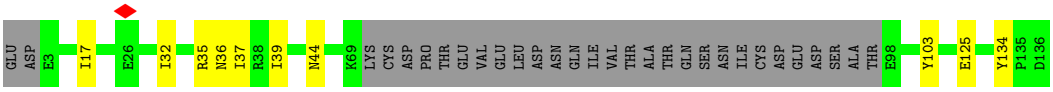




• Molecule 2: Immunoglobulin heavy constant mu



• Molecule 3: Immunoglobulin J chain



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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	849826	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 ($e^-/Å^2$)	59.74	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.736	Depositor
Minimum map value	-1.778	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	340.0, 340.0, 340.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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	M	0.27	0/2207	0.51	0/2968
2	A	0.25	0/1844	0.54	0/2526
2	B	0.25	0/1814	0.54	0/2485
2	C	0.27	0/1824	0.53	0/2498
2	D	0.26	0/1788	0.54	1/2449 (0.0%)
2	E	0.25	0/1788	0.54	0/2449
2	F	0.25	0/1767	0.55	1/2420 (0.0%)
2	G	0.25	0/1787	0.51	0/2447
2	H	0.25	0/1774	0.53	0/2430
2	K	0.25	0/1781	0.53	0/2437
2	L	0.24	0/1818	0.53	0/2490
3	J	0.26	0/864	0.56	0/1173
All	All	0.25	0/21056	0.53	2/28772 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	483	ASP	CB-CG-OD1	6.17	123.85	118.30
2	F	432	ASP	CB-CG-OD2	5.51	123.26	118.30

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	M	2161	0	2110	42	0
2	A	1798	0	1753	30	0
2	B	1769	0	1729	27	0
2	C	1779	0	1739	16	0
2	D	1743	0	1708	27	0
2	E	1743	0	1710	27	0
2	F	1723	0	1682	28	0
2	G	1742	0	1708	30	0
2	H	1730	0	1691	30	0
2	K	1737	0	1698	30	0
2	L	1773	0	1722	38	0
3	J	851	0	844	10	0
4	I	28	0	25	0	0
5	A	14	0	13	1	0
5	B	14	0	13	2	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
5	G	14	0	13	1	0
5	H	14	0	13	1	0
5	K	14	0	13	2	0
5	L	14	0	13	2	0
All	All	20717	0	20249	307	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 7.

The worst 5 of 307 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:M:1629:ILE:HG22	1:M:1706:ARG:HD3	1.67	0.77
2:G:556:THR:O	2:H:461:ARG:NH2	2.24	0.71
2:C:367:CYS:HB3	2:C:380:ILE:HD11	1.73	0.70
2:K:402:ASN:O	2:K:402:ASN:ND2	2.22	0.69
2:G:391:LYS:NZ	2:G:394:THR:OG1	2.26	0.68

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	M	244/2373 (10%)	234 (96%)	10 (4%)	0	100	100
2	A	230/383 (60%)	217 (94%)	13 (6%)	0	100	100
2	B	226/383 (59%)	215 (95%)	11 (5%)	0	100	100
2	C	228/383 (60%)	214 (94%)	14 (6%)	0	100	100
2	D	222/383 (58%)	211 (95%)	11 (5%)	0	100	100
2	E	222/383 (58%)	210 (95%)	12 (5%)	0	100	100
2	F	217/383 (57%)	203 (94%)	14 (6%)	0	100	100
2	G	222/383 (58%)	214 (96%)	8 (4%)	0	100	100
2	H	218/383 (57%)	208 (95%)	10 (5%)	0	100	100
2	K	219/383 (57%)	210 (96%)	9 (4%)	0	100	100
2	L	224/383 (58%)	211 (94%)	13 (6%)	0	100	100
3	J	102/136 (75%)	92 (90%)	10 (10%)	0	100	100
All	All	2574/6339 (41%)	2439 (95%)	135 (5%)	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	M	240/2195 (11%)	238 (99%)	2 (1%)	81	91
2	A	206/331 (62%)	206 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	203/331 (61%)	201 (99%)	2 (1%)	76 88
2	C	204/331 (62%)	204 (100%)	0	100 100
2	D	200/331 (60%)	200 (100%)	0	100 100
2	E	200/331 (60%)	198 (99%)	2 (1%)	76 88
2	F	198/331 (60%)	196 (99%)	2 (1%)	76 88
2	G	200/331 (60%)	200 (100%)	0	100 100
2	H	199/331 (60%)	199 (100%)	0	100 100
2	K	200/331 (60%)	197 (98%)	3 (2%)	65 83
2	L	204/331 (62%)	204 (100%)	0	100 100
3	J	100/128 (78%)	100 (100%)	0	100 100
All	All	2354/5633 (42%)	2343 (100%)	11 (0%)	89 95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	443	ARG
2	K	346	ARG
2	K	465	ASN
2	K	402	ASN
2	E	443	ARG

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

Mol	Chain	Res	Type
2	F	518	HIS
2	G	510	GLN
2	K	510	GLN
2	B	439	GLN
1	M	1610	ASN

5.3.3 RNA

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)

2 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	I	1	3,4	14,14,15	0.45	0	17,19,21	0.69	1 (5%)
4	NAG	I	2	4	14,14,15	0.45	0	17,19,21	0.46	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	I	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1	NAG	C1-O5-C5	2.20	115.17	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

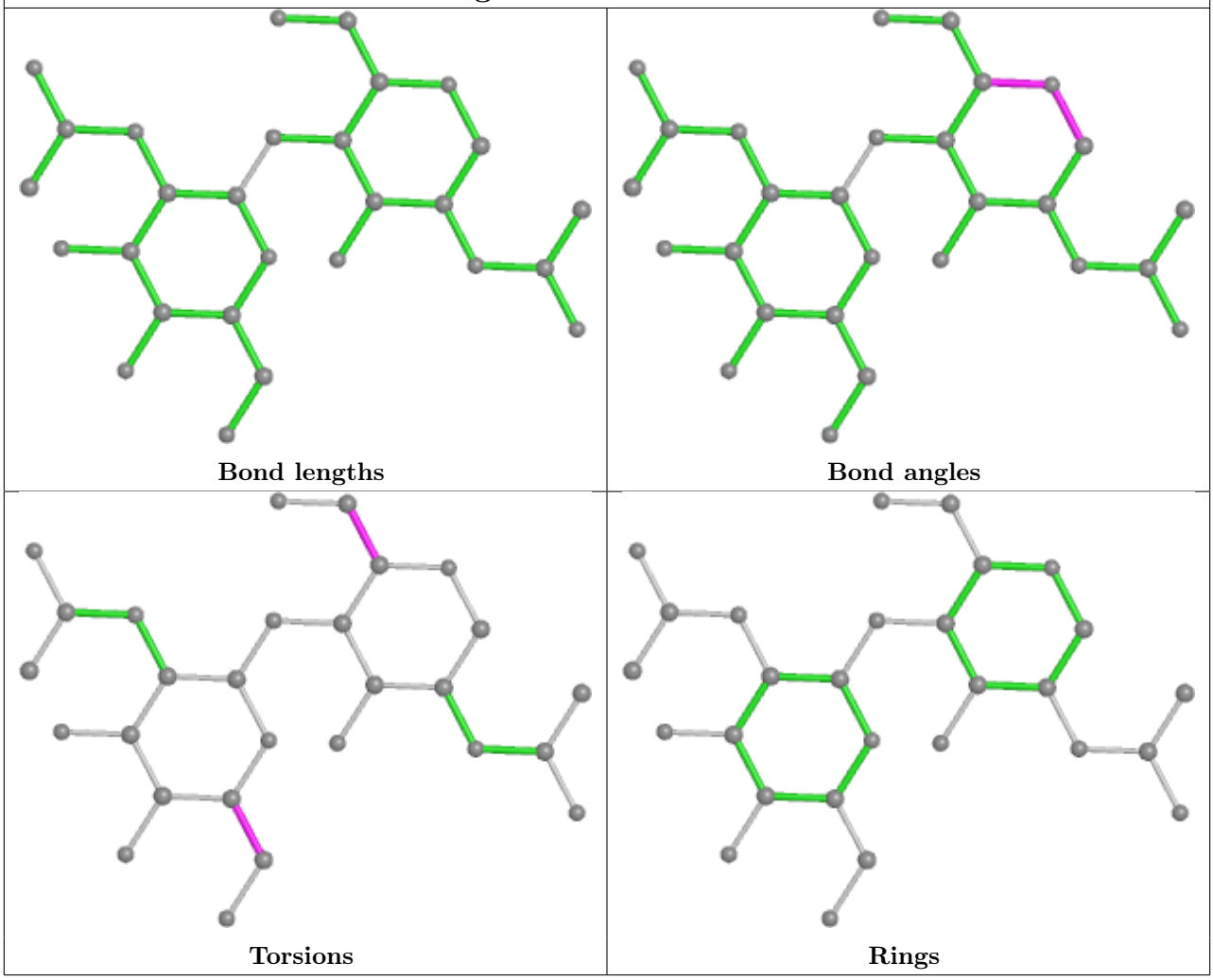
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6

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.

Oligosaccharide Chain I



5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	601	2	14,14,15	0.16	0	17,19,21	0.38	0
5	NAG	H	601	2	14,14,15	0.40	0	17,19,21	0.41	0
5	NAG	K	601	2	14,14,15	0.25	0	17,19,21	0.34	0
5	NAG	B	601	2	14,14,15	0.27	0	17,19,21	0.49	0
5	NAG	F	601	2	14,14,15	0.33	0	17,19,21	0.45	0
5	NAG	L	601	2	14,14,15	0.32	0	17,19,21	0.47	0
5	NAG	D	601	2	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	G	601	2	14,14,15	0.26	0	17,19,21	0.39	0
5	NAG	E	601	2	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	A	601	2	14,14,15	0.35	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
5	NAG	C	601	2	-	4/6/23/26	0/1/1/1
5	NAG	H	601	2	-	3/6/23/26	0/1/1/1
5	NAG	K	601	2	-	4/6/23/26	0/1/1/1
5	NAG	B	601	2	-	0/6/23/26	0/1/1/1
5	NAG	F	601	2	-	2/6/23/26	0/1/1/1
5	NAG	L	601	2	-	1/6/23/26	0/1/1/1
5	NAG	D	601	2	-	1/6/23/26	0/1/1/1
5	NAG	G	601	2	-	1/6/23/26	0/1/1/1
5	NAG	E	601	2	-	2/6/23/26	0/1/1/1
5	NAG	A	601	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	601	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	K	601	NAG	O5-C5-C6-O6
5	F	601	NAG	O5-C5-C6-O6
5	H	601	NAG	O5-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	601	NAG	1	0
5	K	601	NAG	2	0
5	B	601	NAG	2	0
5	L	601	NAG	2	0
5	G	601	NAG	1	0
5	A	601	NAG	1	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.

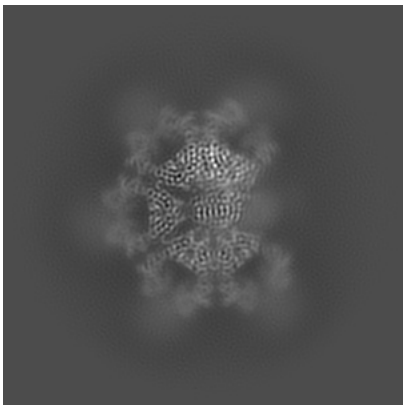
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33547. These allow visual inspection of the internal detail of the map and identification of artifacts.

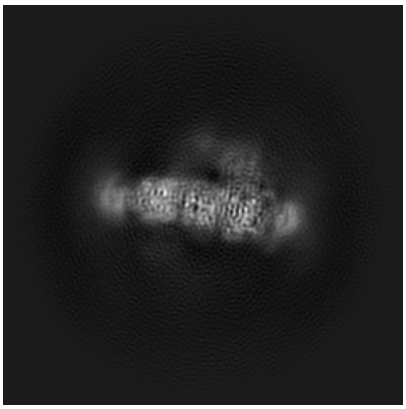
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

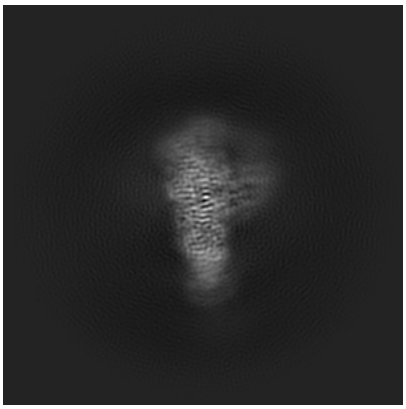
6.1.1 Primary map



X

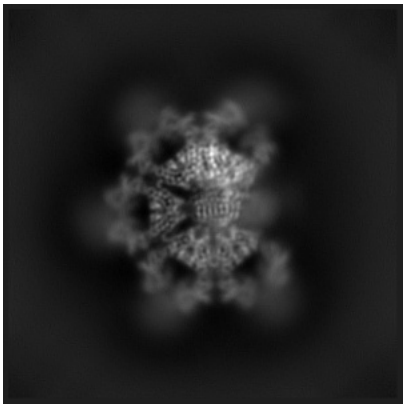


Y

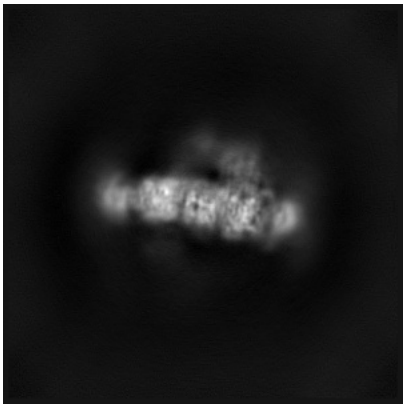


Z

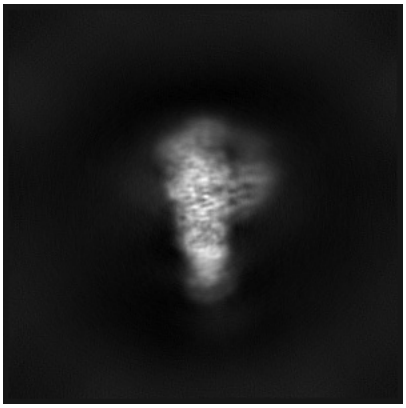
6.1.2 Raw map



X



Y

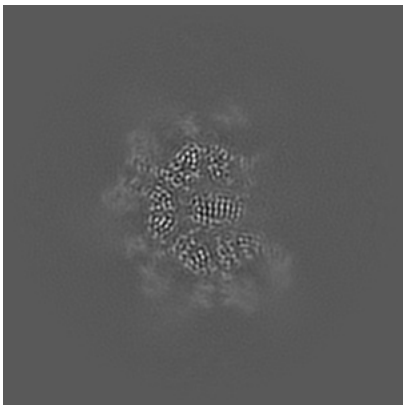


Z

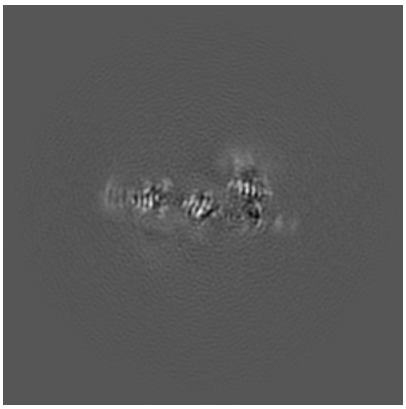
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

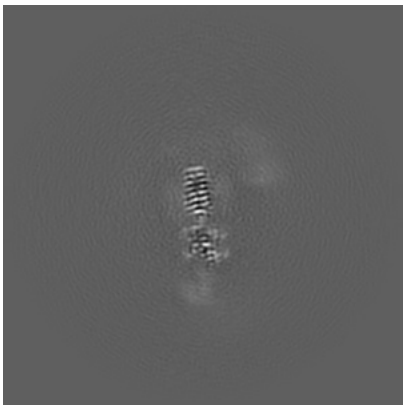
6.2.1 Primary map



X Index: 200

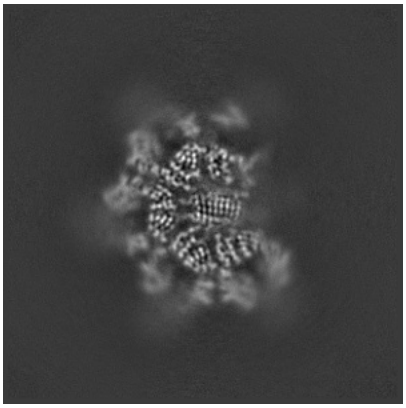


Y Index: 200

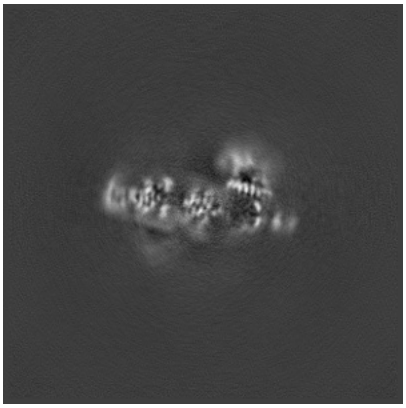


Z Index: 200

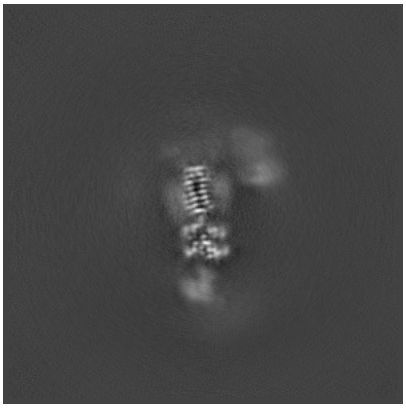
6.2.2 Raw map



X Index: 200



Y Index: 200

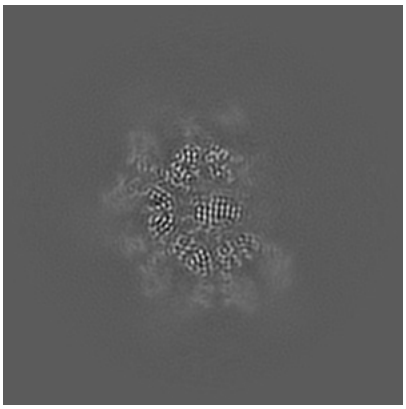


Z Index: 200

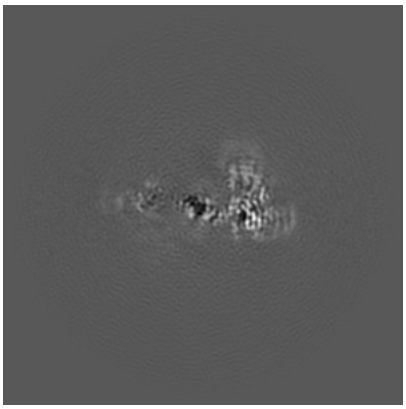
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

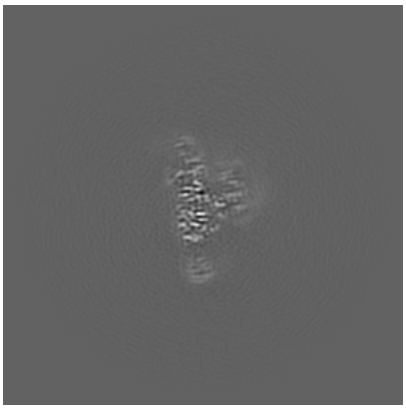
6.3.1 Primary map



X Index: 202

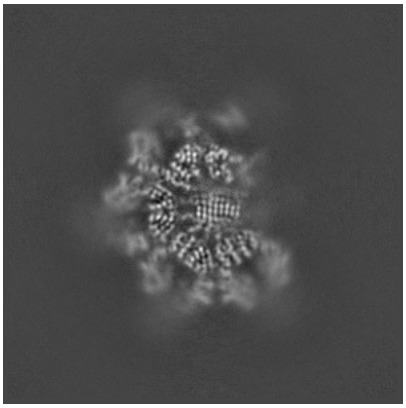


Y Index: 209

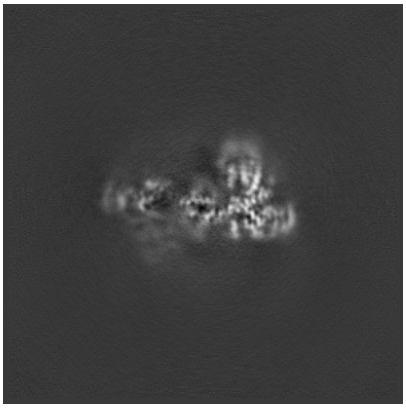


Z Index: 243

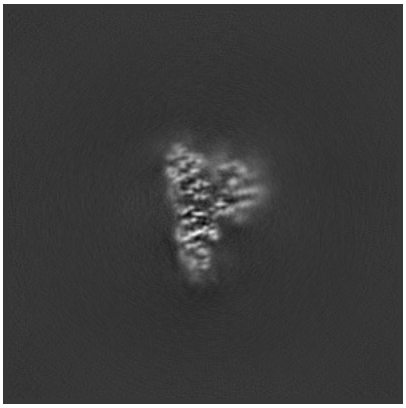
6.3.2 Raw map



X Index: 202



Y Index: 208

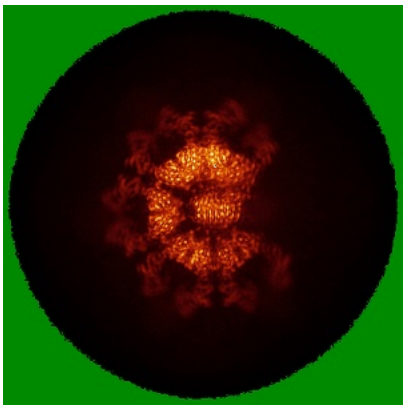


Z Index: 236

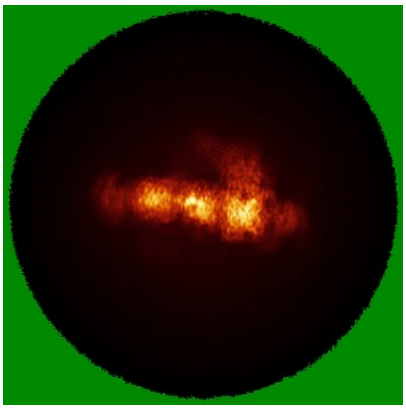
The images above show the largest variance slices of the map in three orthogonal directions.

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

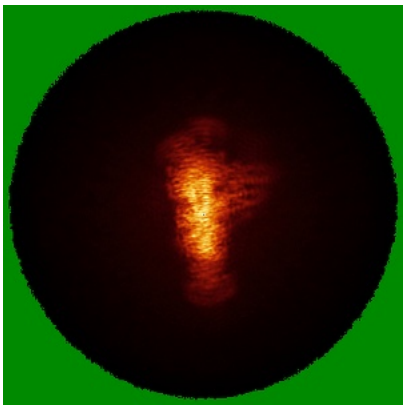
6.4.1 Primary map



X

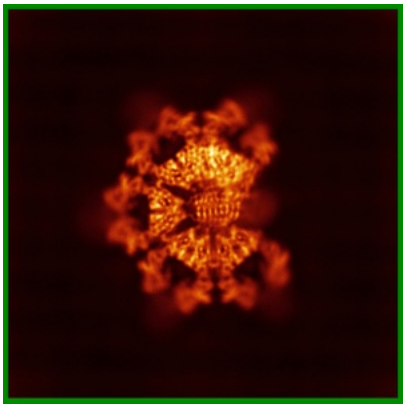


Y

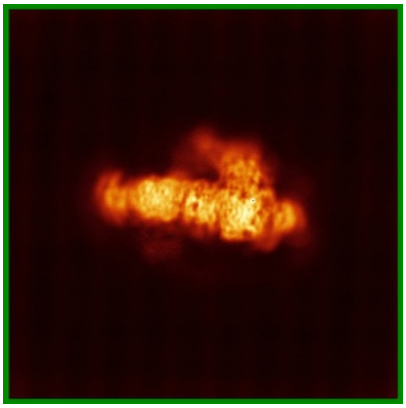


Z

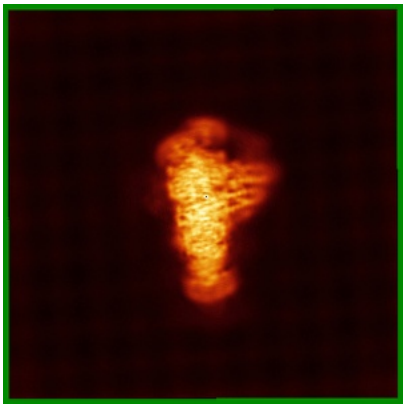
6.4.2 Raw map



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 0.13. 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.

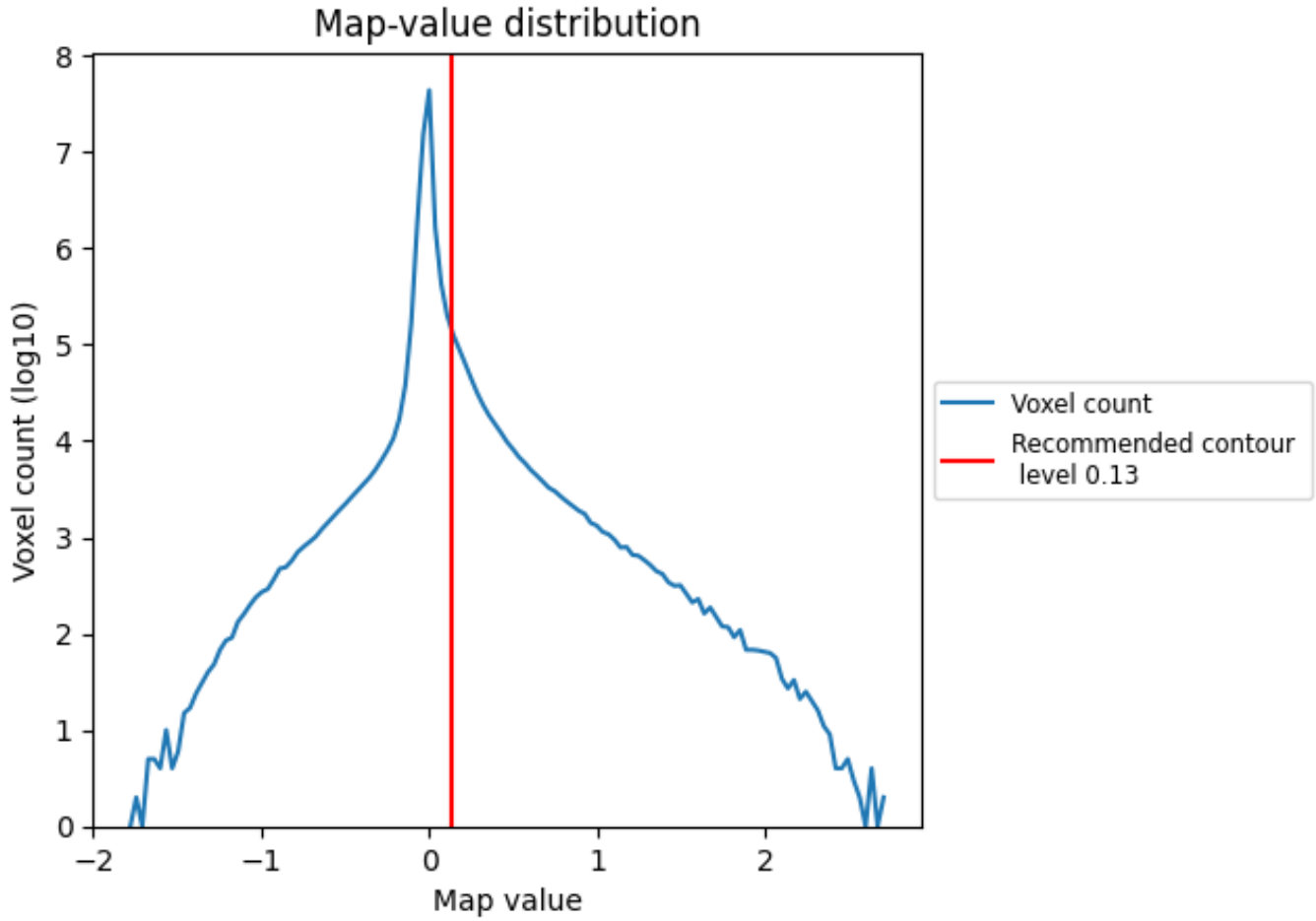
6.6 Mask visualisation (i)

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

7 Map analysis

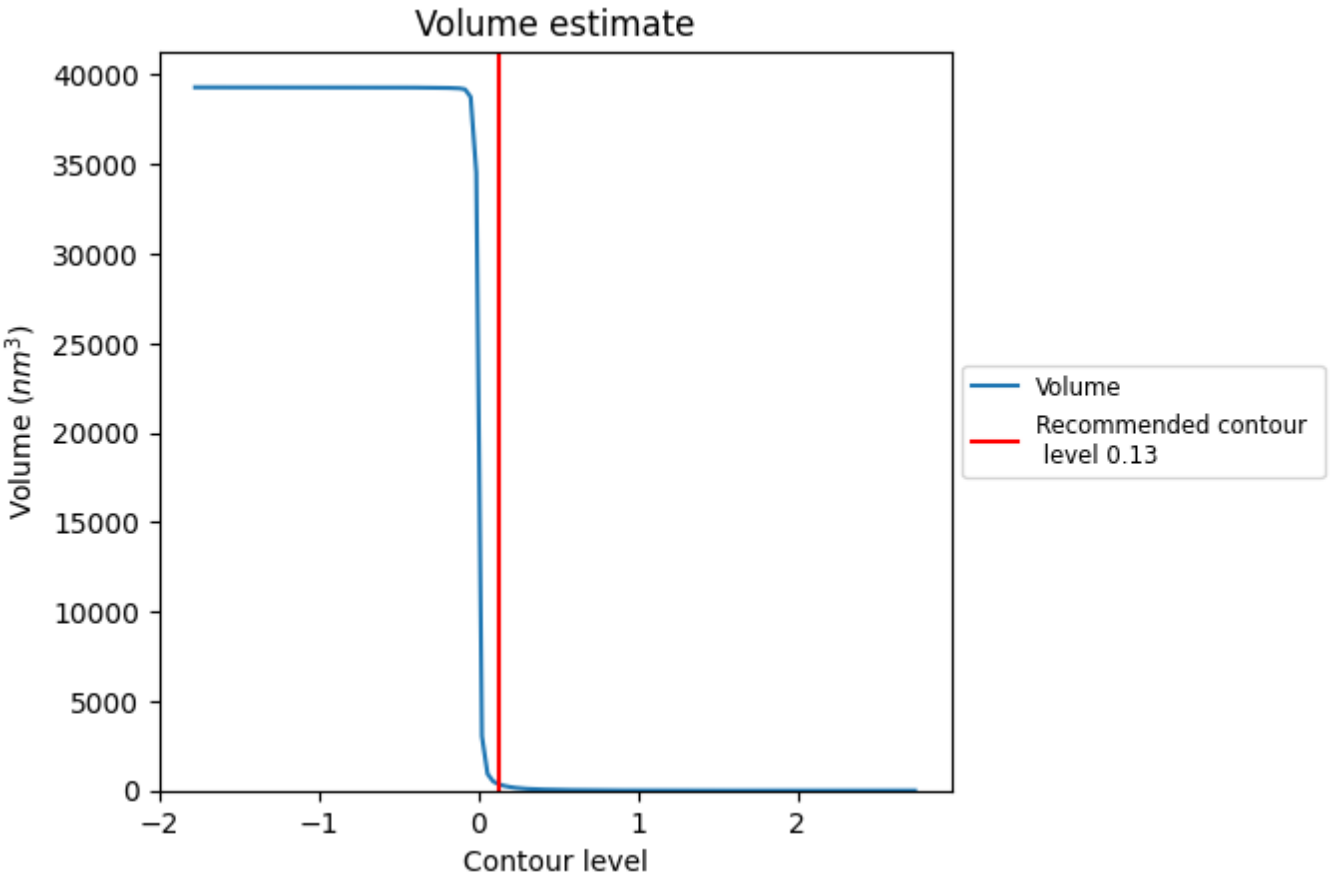
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

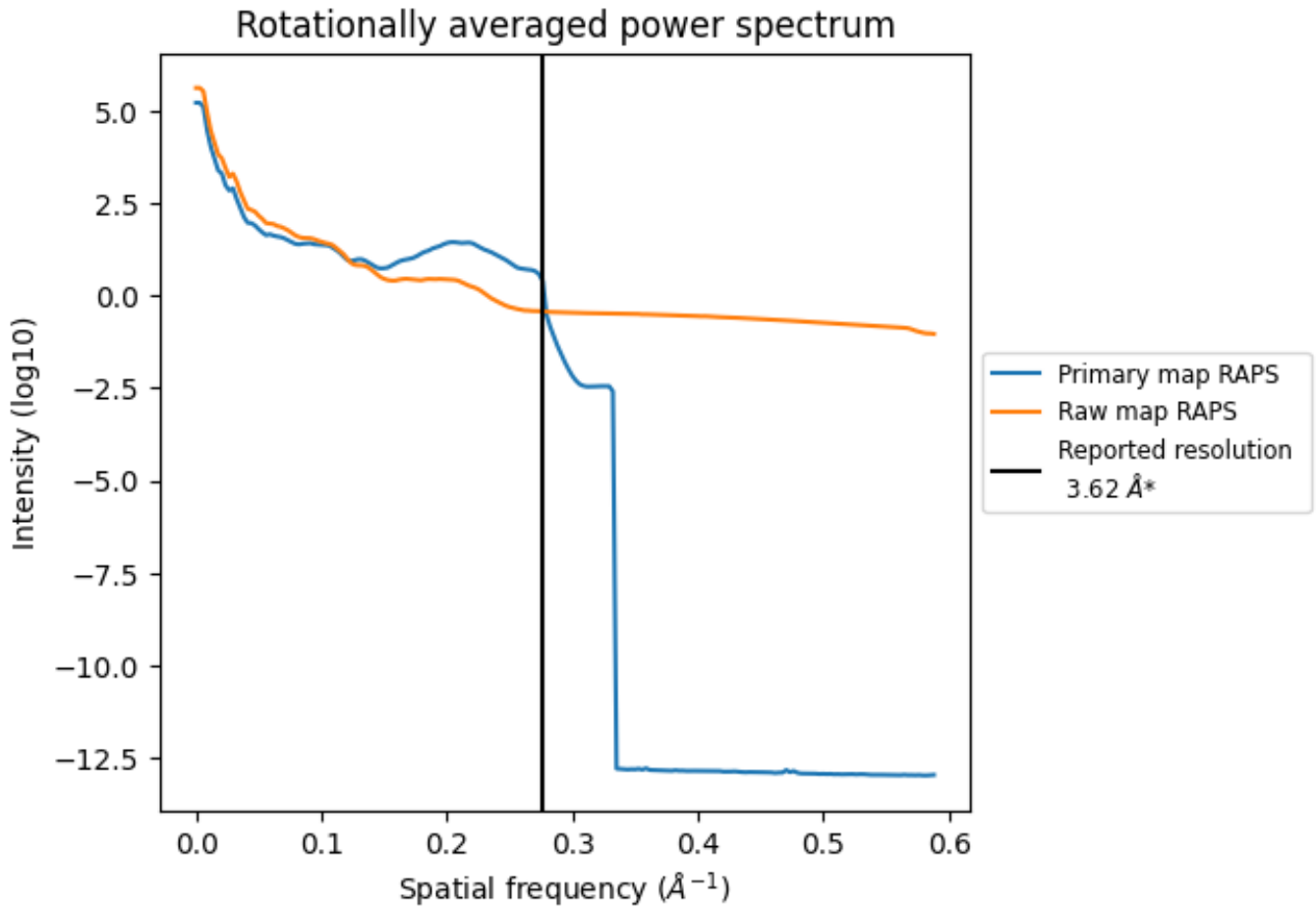
7.2 Volume estimate (i)



The volume at the recommended contour level is 344 nm^3; this corresponds to an approximate mass of 310 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)

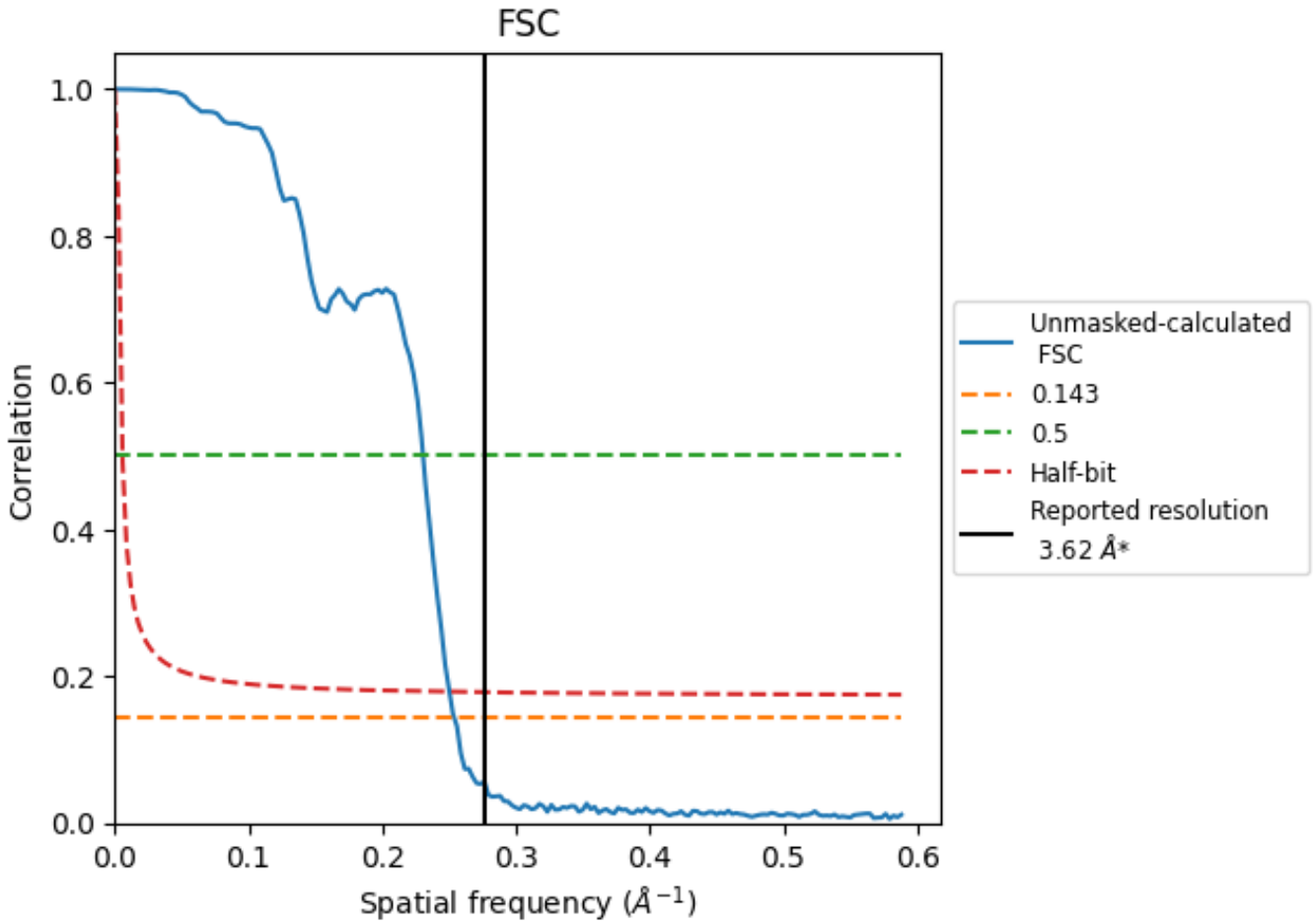


*Reported resolution corresponds to spatial frequency of 0.276 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.276 Å^{-1}

8.2 Resolution estimates (i)

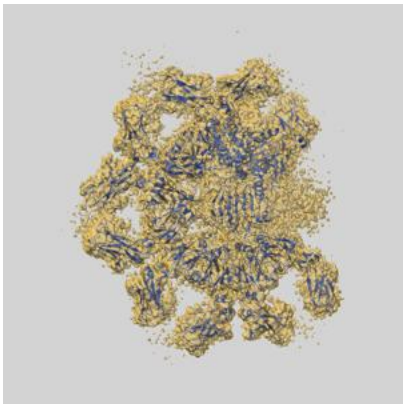
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	4.34	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

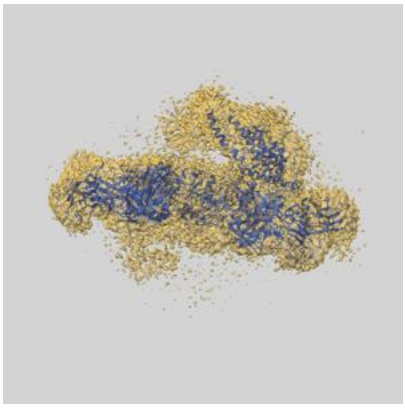
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33547 and PDB model 7Y0J. Per-residue inclusion information can be found in section 3 on page 15.

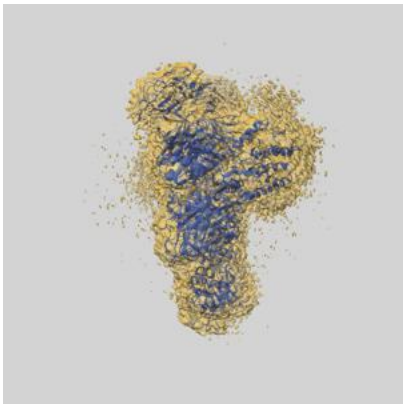
9.1 Map-model overlay



X



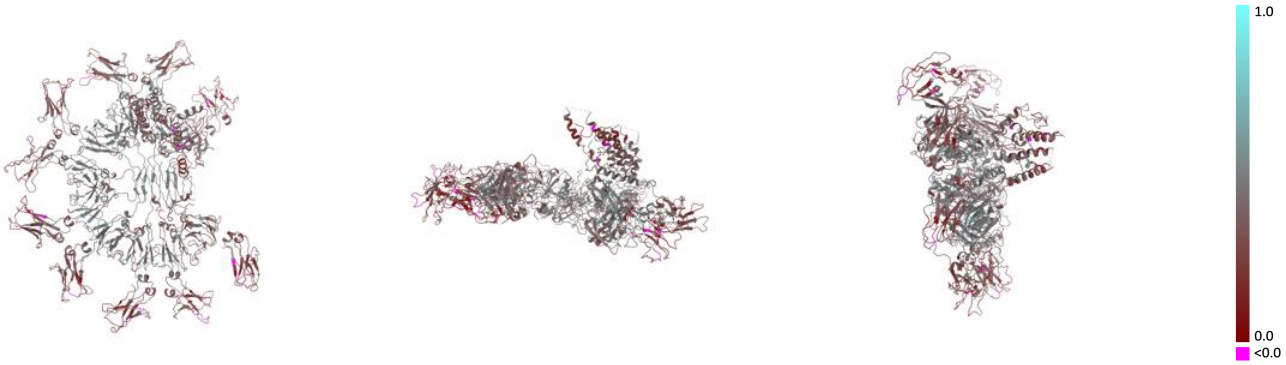
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

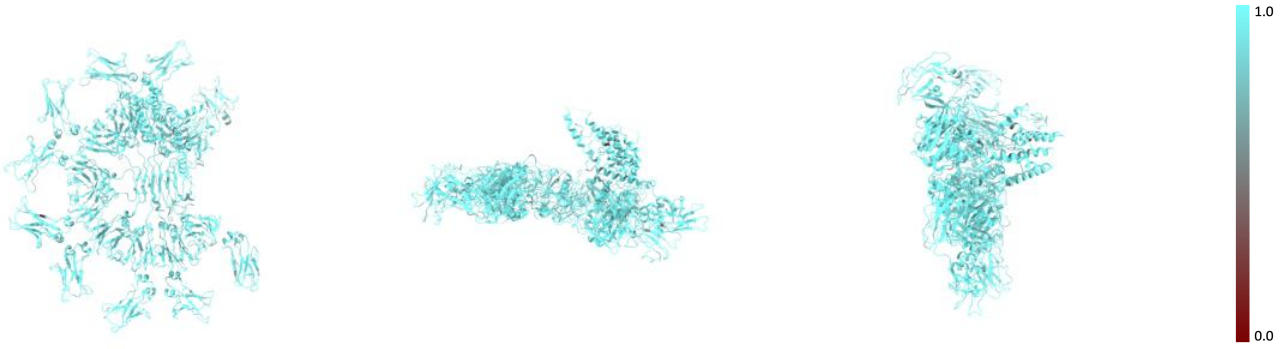
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

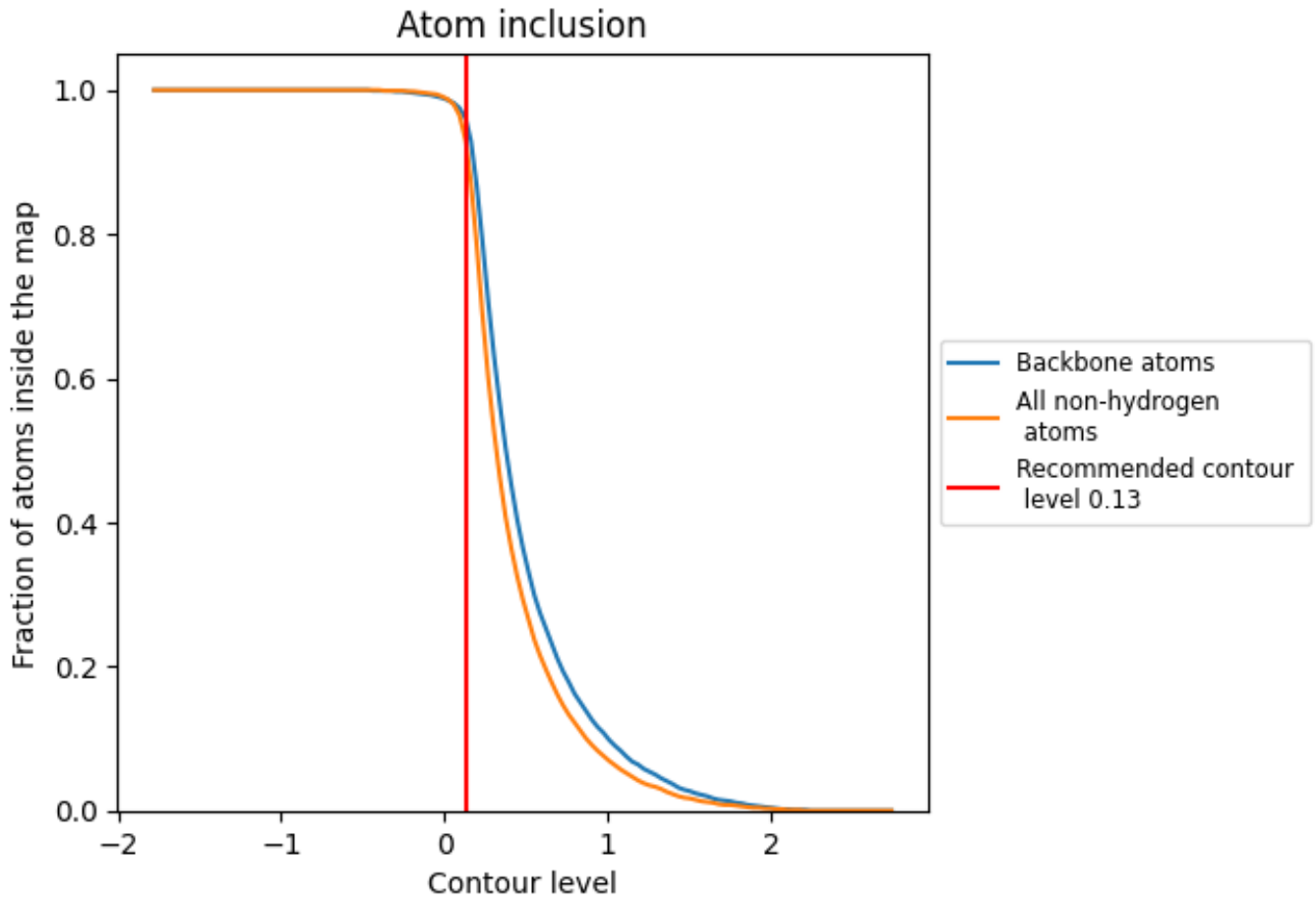
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9290	0.3730
A	0.9210	0.3490
B	0.9450	0.4090
C	0.9380	0.4170
D	0.9440	0.4030
E	0.9320	0.3740
F	0.9310	0.3770
G	0.9330	0.3830
H	0.9390	0.3580
I	0.9640	0.3540
J	0.9010	0.4060
K	0.9180	0.3510
L	0.9010	0.3120
M	0.9270	0.3620