wwPDB EM Validation Summary Report

Oct 27, 2024 – 07:26 PM EDT

PDB ID	:	7UWN
EMDB ID	:	EMD-26837
Title	:	Structure of the IL-17A-IL-17RA-IL-17RC ternary complex
Authors	:	Wilson, S.C.; Caveney, N.A.; Jude, K.M.; Garcia, K.C.
Deposited on	:	2022-05-03
Resolution	:	3.01 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:

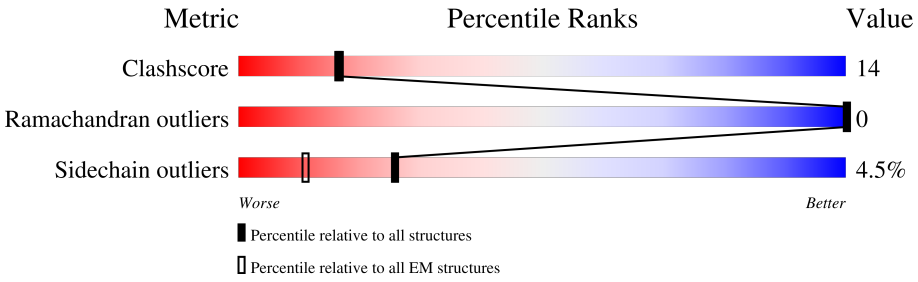
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 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 <=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	170	9% 40% 23% • 35%
1	B	170	9% 40% 24% • 35%
1	D	170	18% 38% 25% 38%
1	E	170	9% 33% 20% • 45%
2	C	319	13% 56% 25% • 17%
2	F	319	10% 49% 23% • 26%
3	G	479	47% 60% 22% • 16%
4	H	2	100% 100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10602 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 Interleukin-17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	111	Total	C	N	O	S	0	0
			887	554	164	163	6		
1	B	111	Total	C	N	O	S	0	0
			885	547	167	164	7		
1	D	106	Total	C	N	O	S	0	0
			853	533	159	155	6		
1	E	93	Total	C	N	O	S	0	0
			752	466	144	136	6		

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q16552
A	157	ALA	-	expression tag	UNP Q16552
A	158	PRO	-	expression tag	UNP Q16552
A	159	GLY	-	expression tag	UNP Q16552
A	160	SER	-	expression tag	UNP Q16552
A	161	ALA	-	expression tag	UNP Q16552
A	162	LEU	-	expression tag	UNP Q16552
A	163	GLU	-	expression tag	UNP Q16552
A	164	VAL	-	expression tag	UNP Q16552
A	165	LEU	-	expression tag	UNP Q16552
A	166	PHE	-	expression tag	UNP Q16552
A	167	GLN	-	expression tag	UNP Q16552
A	168	GLY	-	expression tag	UNP Q16552
A	169	PRO	-	expression tag	UNP Q16552
A	170	GLY	-	expression tag	UNP Q16552
A	171	ALA	-	expression tag	UNP Q16552
A	172	ALA	-	expression tag	UNP Q16552
A	173	GLY	-	expression tag	UNP Q16552
A	174	LEU	-	expression tag	UNP Q16552
A	175	ASN	-	expression tag	UNP Q16552
A	176	ASP	-	expression tag	UNP Q16552
A	177	ILE	-	expression tag	UNP Q16552

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Chain	Residue	Modelled	Actual	Comment	Reference
A	178	PHE	-	expression tag	UNP Q16552
A	179	GLU	-	expression tag	UNP Q16552
A	180	ALA	-	expression tag	UNP Q16552
A	181	GLN	-	expression tag	UNP Q16552
A	182	LYS	-	expression tag	UNP Q16552
A	183	ILE	-	expression tag	UNP Q16552
A	184	GLU	-	expression tag	UNP Q16552
A	185	TRP	-	expression tag	UNP Q16552
A	186	HIS	-	expression tag	UNP Q16552
A	187	GLU	-	expression tag	UNP Q16552
A	188	HIS	-	expression tag	UNP Q16552
A	189	HIS	-	expression tag	UNP Q16552
A	190	HIS	-	expression tag	UNP Q16552
A	191	HIS	-	expression tag	UNP Q16552
A	192	HIS	-	expression tag	UNP Q16552
A	193	HIS	-	expression tag	UNP Q16552
B	156	GLY	-	expression tag	UNP Q16552
B	157	ALA	-	expression tag	UNP Q16552
B	158	PRO	-	expression tag	UNP Q16552
B	159	GLY	-	expression tag	UNP Q16552
B	160	SER	-	expression tag	UNP Q16552
B	161	ALA	-	expression tag	UNP Q16552
B	162	LEU	-	expression tag	UNP Q16552
B	163	GLU	-	expression tag	UNP Q16552
B	164	VAL	-	expression tag	UNP Q16552
B	165	LEU	-	expression tag	UNP Q16552
B	166	PHE	-	expression tag	UNP Q16552
B	167	GLN	-	expression tag	UNP Q16552
B	168	GLY	-	expression tag	UNP Q16552
B	169	PRO	-	expression tag	UNP Q16552
B	170	GLY	-	expression tag	UNP Q16552
B	171	ALA	-	expression tag	UNP Q16552
B	172	ALA	-	expression tag	UNP Q16552
B	173	GLY	-	expression tag	UNP Q16552
B	174	LEU	-	expression tag	UNP Q16552
B	175	ASN	-	expression tag	UNP Q16552
B	176	ASP	-	expression tag	UNP Q16552
B	177	ILE	-	expression tag	UNP Q16552
B	178	PHE	-	expression tag	UNP Q16552
B	179	GLU	-	expression tag	UNP Q16552
B	180	ALA	-	expression tag	UNP Q16552
B	181	GLN	-	expression tag	UNP Q16552

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Chain	Residue	Modelled	Actual	Comment	Reference
B	182	LYS	-	expression tag	UNP Q16552
B	183	ILE	-	expression tag	UNP Q16552
B	184	GLU	-	expression tag	UNP Q16552
B	185	TRP	-	expression tag	UNP Q16552
B	186	HIS	-	expression tag	UNP Q16552
B	187	GLU	-	expression tag	UNP Q16552
B	188	HIS	-	expression tag	UNP Q16552
B	189	HIS	-	expression tag	UNP Q16552
B	190	HIS	-	expression tag	UNP Q16552
B	191	HIS	-	expression tag	UNP Q16552
B	192	HIS	-	expression tag	UNP Q16552
B	193	HIS	-	expression tag	UNP Q16552
D	156	GLY	-	expression tag	UNP Q16552
D	157	ALA	-	expression tag	UNP Q16552
D	158	PRO	-	expression tag	UNP Q16552
D	159	GLY	-	expression tag	UNP Q16552
D	160	SER	-	expression tag	UNP Q16552
D	161	ALA	-	expression tag	UNP Q16552
D	162	LEU	-	expression tag	UNP Q16552
D	163	GLU	-	expression tag	UNP Q16552
D	164	VAL	-	expression tag	UNP Q16552
D	165	LEU	-	expression tag	UNP Q16552
D	166	PHE	-	expression tag	UNP Q16552
D	167	GLN	-	expression tag	UNP Q16552
D	168	GLY	-	expression tag	UNP Q16552
D	169	PRO	-	expression tag	UNP Q16552
D	170	GLY	-	expression tag	UNP Q16552
D	171	ALA	-	expression tag	UNP Q16552
D	172	ALA	-	expression tag	UNP Q16552
D	173	GLY	-	expression tag	UNP Q16552
D	174	LEU	-	expression tag	UNP Q16552
D	175	ASN	-	expression tag	UNP Q16552
D	176	ASP	-	expression tag	UNP Q16552
D	177	ILE	-	expression tag	UNP Q16552
D	178	PHE	-	expression tag	UNP Q16552
D	179	GLU	-	expression tag	UNP Q16552
D	180	ALA	-	expression tag	UNP Q16552
D	181	GLN	-	expression tag	UNP Q16552
D	182	LYS	-	expression tag	UNP Q16552
D	183	ILE	-	expression tag	UNP Q16552
D	184	GLU	-	expression tag	UNP Q16552
D	185	TRP	-	expression tag	UNP Q16552

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Chain	Residue	Modelled	Actual	Comment	Reference
D	186	HIS	-	expression tag	UNP Q16552
D	187	GLU	-	expression tag	UNP Q16552
D	188	HIS	-	expression tag	UNP Q16552
D	189	HIS	-	expression tag	UNP Q16552
D	190	HIS	-	expression tag	UNP Q16552
D	191	HIS	-	expression tag	UNP Q16552
D	192	HIS	-	expression tag	UNP Q16552
D	193	HIS	-	expression tag	UNP Q16552
E	156	GLY	-	expression tag	UNP Q16552
E	157	ALA	-	expression tag	UNP Q16552
E	158	PRO	-	expression tag	UNP Q16552
E	159	GLY	-	expression tag	UNP Q16552
E	160	SER	-	expression tag	UNP Q16552
E	161	ALA	-	expression tag	UNP Q16552
E	162	LEU	-	expression tag	UNP Q16552
E	163	GLU	-	expression tag	UNP Q16552
E	164	VAL	-	expression tag	UNP Q16552
E	165	LEU	-	expression tag	UNP Q16552
E	166	PHE	-	expression tag	UNP Q16552
E	167	GLN	-	expression tag	UNP Q16552
E	168	GLY	-	expression tag	UNP Q16552
E	169	PRO	-	expression tag	UNP Q16552
E	170	GLY	-	expression tag	UNP Q16552
E	171	ALA	-	expression tag	UNP Q16552
E	172	ALA	-	expression tag	UNP Q16552
E	173	GLY	-	expression tag	UNP Q16552
E	174	LEU	-	expression tag	UNP Q16552
E	175	ASN	-	expression tag	UNP Q16552
E	176	ASP	-	expression tag	UNP Q16552
E	177	ILE	-	expression tag	UNP Q16552
E	178	PHE	-	expression tag	UNP Q16552
E	179	GLU	-	expression tag	UNP Q16552
E	180	ALA	-	expression tag	UNP Q16552
E	181	GLN	-	expression tag	UNP Q16552
E	182	LYS	-	expression tag	UNP Q16552
E	183	ILE	-	expression tag	UNP Q16552
E	184	GLU	-	expression tag	UNP Q16552
E	185	TRP	-	expression tag	UNP Q16552
E	186	HIS	-	expression tag	UNP Q16552
E	187	GLU	-	expression tag	UNP Q16552
E	188	HIS	-	expression tag	UNP Q16552
E	189	HIS	-	expression tag	UNP Q16552

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Chain	Residue	Modelled	Actual	Comment	Reference
E	190	HIS	-	expression tag	UNP Q16552
E	191	HIS	-	expression tag	UNP Q16552
E	192	HIS	-	expression tag	UNP Q16552
E	193	HIS	-	expression tag	UNP Q16552

- Molecule 2 is a protein called Interleukin-17 receptor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	264	Total	C	N	O	S	0	0
			2147	1355	391	386	15		
2	F	237	Total	C	N	O	S	0	0
			1888	1195	337	345	11		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	318	SER	-	expression tag	UNP Q96F46
C	319	ALA	-	expression tag	UNP Q96F46
C	320	ALA	-	expression tag	UNP Q96F46
C	321	LEU	-	expression tag	UNP Q96F46
C	322	GLU	-	expression tag	UNP Q96F46
C	323	VAL	-	expression tag	UNP Q96F46
C	324	LEU	-	expression tag	UNP Q96F46
C	325	PHE	-	expression tag	UNP Q96F46
C	326	GLN	-	expression tag	UNP Q96F46
C	327	GLY	-	expression tag	UNP Q96F46
C	328	PRO	-	expression tag	UNP Q96F46
C	329	GLY	-	expression tag	UNP Q96F46
C	330	ALA	-	expression tag	UNP Q96F46
C	331	ALA	-	expression tag	UNP Q96F46
C	332	GLU	-	expression tag	UNP Q96F46
C	333	ASP	-	expression tag	UNP Q96F46
C	334	GLN	-	expression tag	UNP Q96F46
C	335	VAL	-	expression tag	UNP Q96F46
C	336	ASP	-	expression tag	UNP Q96F46
C	337	PRO	-	expression tag	UNP Q96F46
C	338	ARG	-	expression tag	UNP Q96F46
C	339	LEU	-	expression tag	UNP Q96F46
C	340	ILE	-	expression tag	UNP Q96F46
C	341	ASP	-	expression tag	UNP Q96F46
C	342	GLY	-	expression tag	UNP Q96F46
C	343	LYS	-	expression tag	UNP Q96F46

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Chain	Residue	Modelled	Actual	Comment	Reference
C	344	HIS	-	expression tag	UNP Q96F46
C	345	HIS	-	expression tag	UNP Q96F46
C	346	HIS	-	expression tag	UNP Q96F46
C	347	HIS	-	expression tag	UNP Q96F46
C	348	HIS	-	expression tag	UNP Q96F46
C	349	HIS	-	expression tag	UNP Q96F46
C	350	HIS	-	expression tag	UNP Q96F46
C	351	HIS	-	expression tag	UNP Q96F46
F	318	SER	-	expression tag	UNP Q96F46
F	319	ALA	-	expression tag	UNP Q96F46
F	320	ALA	-	expression tag	UNP Q96F46
F	321	LEU	-	expression tag	UNP Q96F46
F	322	GLU	-	expression tag	UNP Q96F46
F	323	VAL	-	expression tag	UNP Q96F46
F	324	LEU	-	expression tag	UNP Q96F46
F	325	PHE	-	expression tag	UNP Q96F46
F	326	GLN	-	expression tag	UNP Q96F46
F	327	GLY	-	expression tag	UNP Q96F46
F	328	PRO	-	expression tag	UNP Q96F46
F	329	GLY	-	expression tag	UNP Q96F46
F	330	ALA	-	expression tag	UNP Q96F46
F	331	ALA	-	expression tag	UNP Q96F46
F	332	GLU	-	expression tag	UNP Q96F46
F	333	ASP	-	expression tag	UNP Q96F46
F	334	GLN	-	expression tag	UNP Q96F46
F	335	VAL	-	expression tag	UNP Q96F46
F	336	ASP	-	expression tag	UNP Q96F46
F	337	PRO	-	expression tag	UNP Q96F46
F	338	ARG	-	expression tag	UNP Q96F46
F	339	LEU	-	expression tag	UNP Q96F46
F	340	ILE	-	expression tag	UNP Q96F46
F	341	ASP	-	expression tag	UNP Q96F46
F	342	GLY	-	expression tag	UNP Q96F46
F	343	LYS	-	expression tag	UNP Q96F46
F	344	HIS	-	expression tag	UNP Q96F46
F	345	HIS	-	expression tag	UNP Q96F46
F	346	HIS	-	expression tag	UNP Q96F46
F	347	HIS	-	expression tag	UNP Q96F46
F	348	HIS	-	expression tag	UNP Q96F46
F	349	HIS	-	expression tag	UNP Q96F46
F	350	HIS	-	expression tag	UNP Q96F46
F	351	HIS	-	expression tag	UNP Q96F46

- Molecule 3 is a protein called Isoform 5 of Interleukin-17 receptor C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	403	Total	C	N	O	S	0	0
			3036	1929	525	561	21		

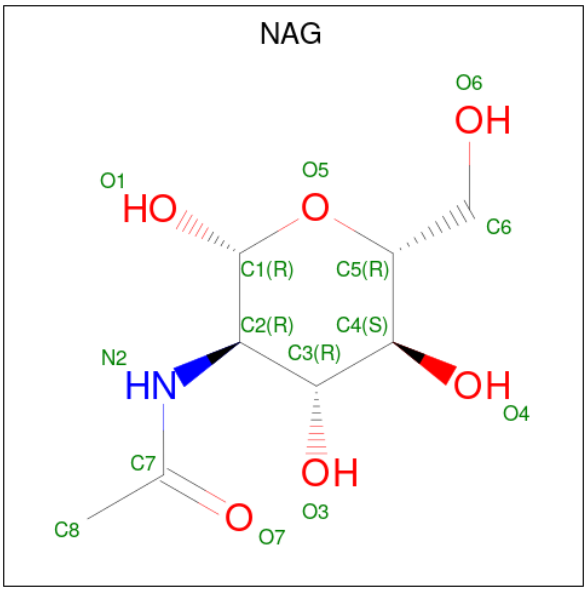
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	111	LEU	SER	conflict	UNP Q8NAC3
G	307	ARG	GLN	conflict	UNP Q8NAC3
G	466	ALA	-	expression tag	UNP Q8NAC3
G	467	ALA	-	expression tag	UNP Q8NAC3
G	468	ALA	-	expression tag	UNP Q8NAC3
G	469	LEU	-	expression tag	UNP Q8NAC3
G	470	GLU	-	expression tag	UNP Q8NAC3
G	471	VAL	-	expression tag	UNP Q8NAC3
G	472	LEU	-	expression tag	UNP Q8NAC3
G	473	PHE	-	expression tag	UNP Q8NAC3
G	474	GLN	-	expression tag	UNP Q8NAC3
G	475	GLY	-	expression tag	UNP Q8NAC3
G	476	PRO	-	expression tag	UNP Q8NAC3
G	477	GLY	-	expression tag	UNP Q8NAC3
G	478	ALA	-	expression tag	UNP Q8NAC3
G	479	ALA	-	expression tag	UNP Q8NAC3
G	480	GLU	-	expression tag	UNP Q8NAC3
G	481	ASP	-	expression tag	UNP Q8NAC3
G	482	GLN	-	expression tag	UNP Q8NAC3
G	483	VAL	-	expression tag	UNP Q8NAC3
G	484	ASP	-	expression tag	UNP Q8NAC3
G	485	PRO	-	expression tag	UNP Q8NAC3
G	486	ARG	-	expression tag	UNP Q8NAC3
G	487	LEU	-	expression tag	UNP Q8NAC3
G	488	ILE	-	expression tag	UNP Q8NAC3
G	489	ASP	-	expression tag	UNP Q8NAC3
G	490	GLY	-	expression tag	UNP Q8NAC3
G	491	LYS	-	expression tag	UNP Q8NAC3
G	492	HIS	-	expression tag	UNP Q8NAC3
G	493	HIS	-	expression tag	UNP Q8NAC3
G	494	HIS	-	expression tag	UNP Q8NAC3
G	495	HIS	-	expression tag	UNP Q8NAC3
G	496	HIS	-	expression tag	UNP Q8NAC3
G	497	HIS	-	expression tag	UNP Q8NAC3
G	498	HIS	-	expression tag	UNP Q8NAC3
G	499	HIS	-	expression tag	UNP Q8NAC3

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

- 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 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0
5	C	1	Total C N O 14 8 1 5	0
5	F	1	Total C N O 14 8 1 5	0
5	F	1	Total C N O 14 8 1 5	0

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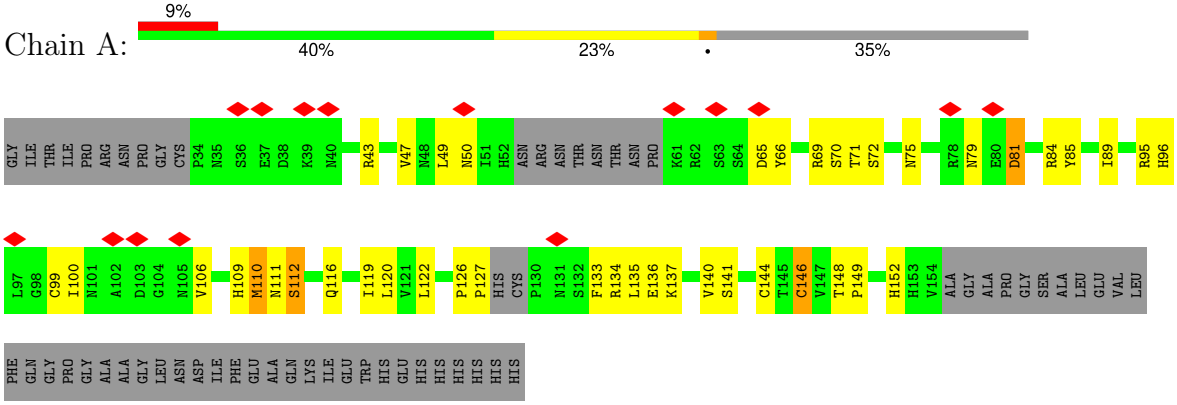
Mol	Chain	Residues	Atoms				AltConf
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	

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.

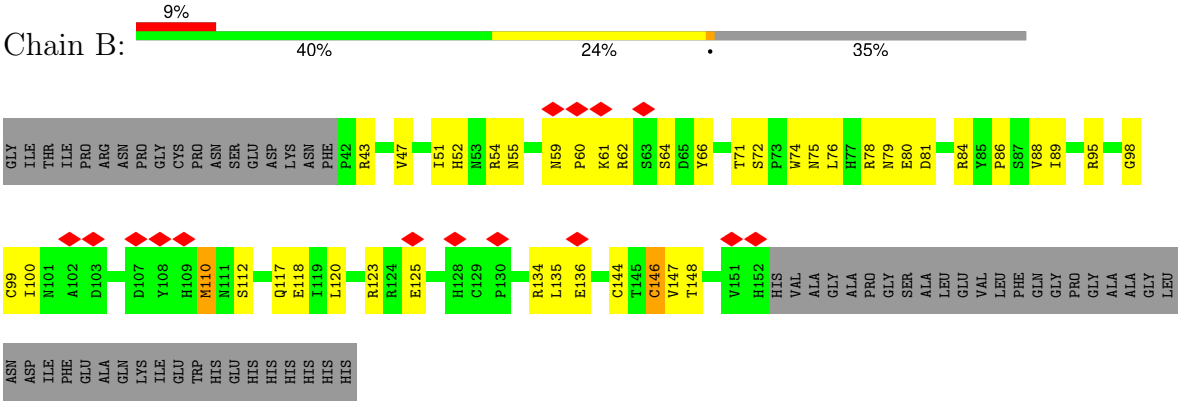
• Molecule 1: Interleukin-17A

Chain A:



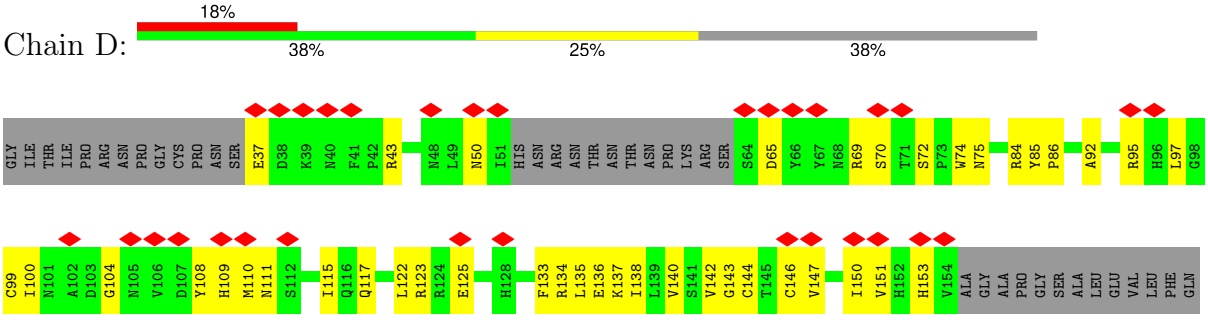
• Molecule 1: Interleukin-17A

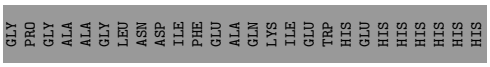
Chain B:



• Molecule 1: Interleukin-17A

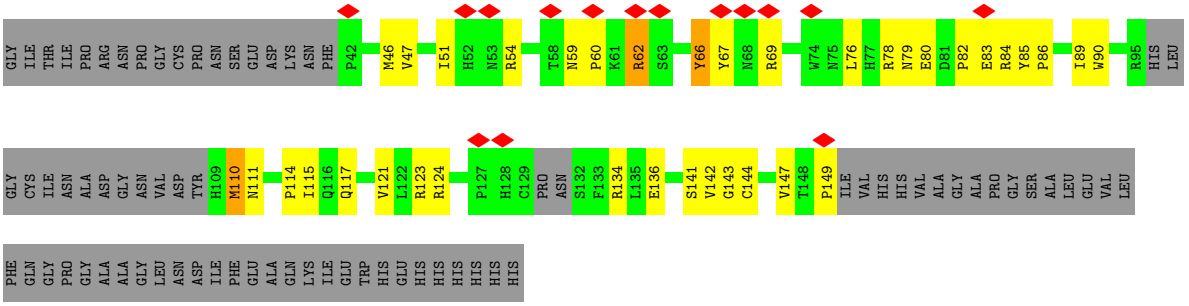
Chain D:





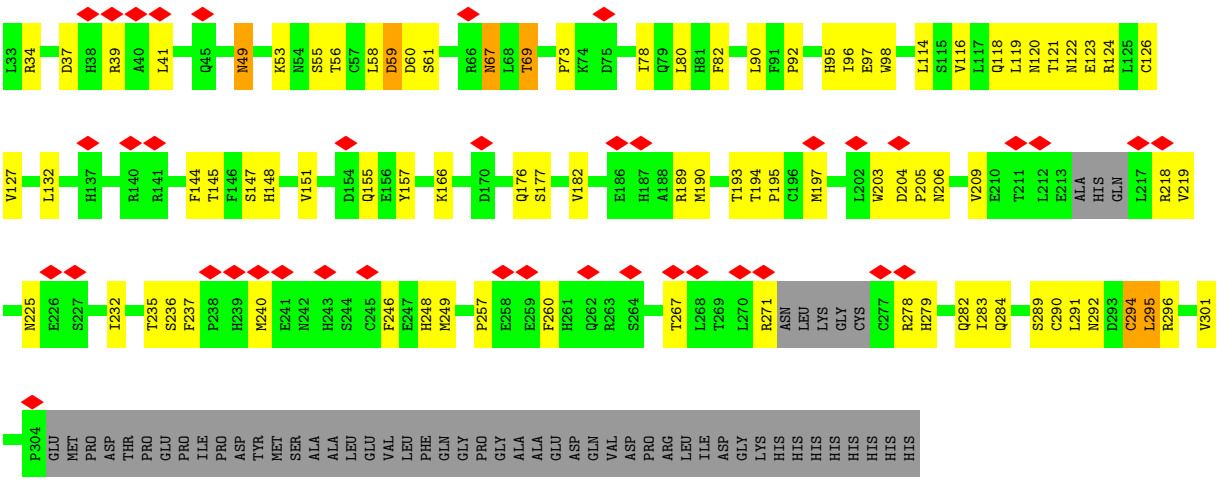
• Molecule 1: Interleukin-17A

Chain E:



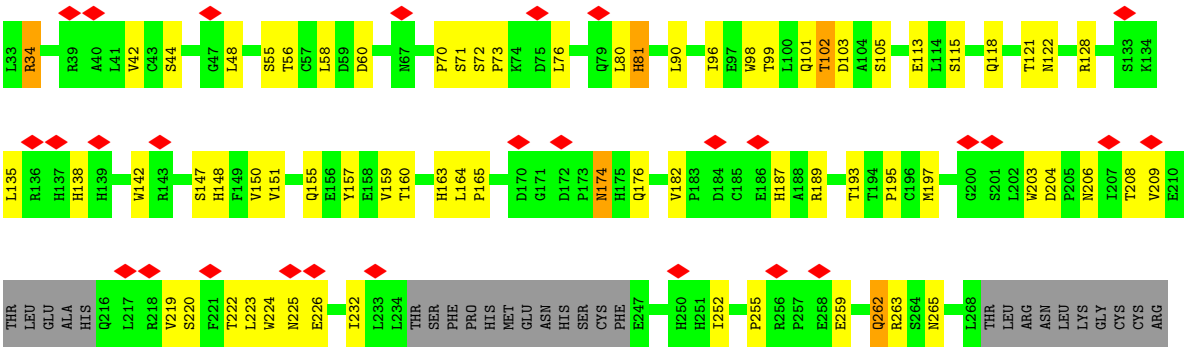
• Molecule 2: Interleukin-17 receptor A

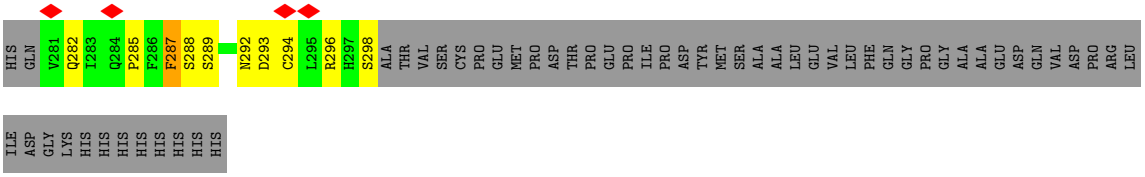
Chain C:



• Molecule 2: Interleukin-17 receptor A

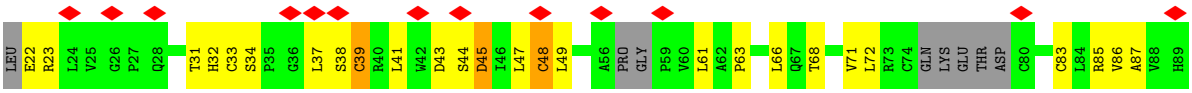
Chain F:

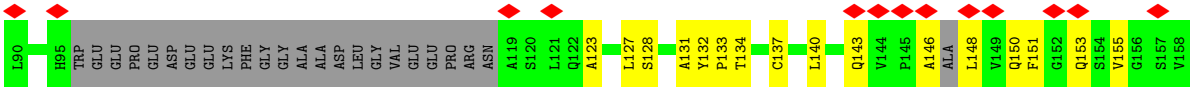


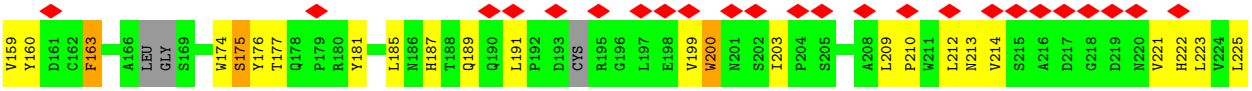


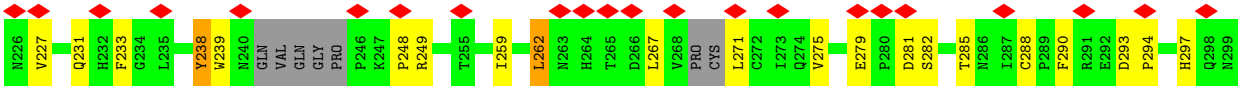
• Molecule 3: Isoform 5 of Interleukin-17 receptor C

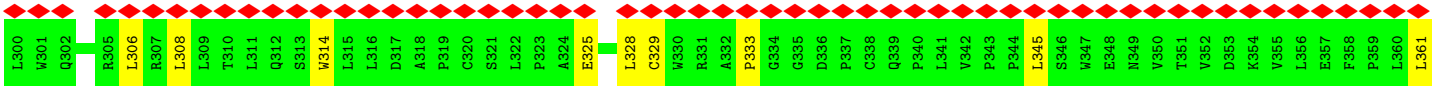
Chain G:

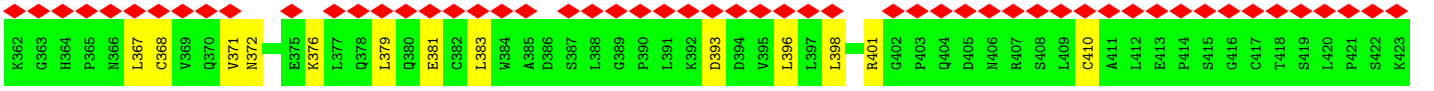


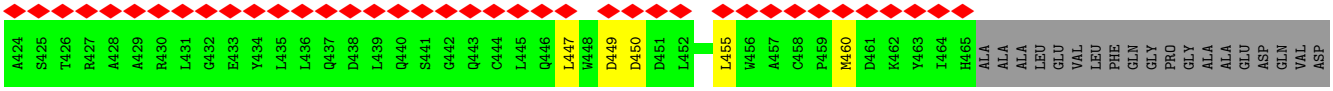


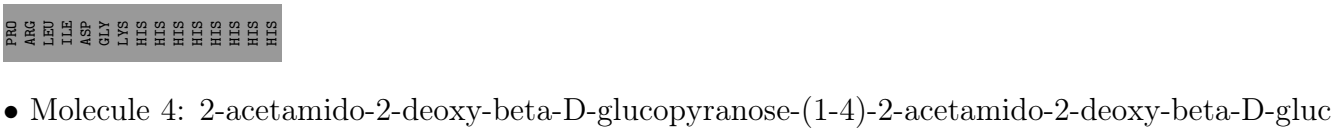












• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	542344	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.997	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	272.896, 272.896, 272.896	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	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	A	0.29	0/910	0.53	0/1240
1	B	0.26	0/908	0.52	0/1241
1	D	0.27	0/875	0.56	0/1194
1	E	0.29	0/770	0.59	0/1048
2	C	0.26	0/2211	0.51	0/3013
2	F	0.29	0/1942	0.51	0/2654
3	G	0.26	0/3108	0.49	0/4258
All	All	0.27	0/10724	0.52	0/14648

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	887	0	839	42	0
1	B	885	0	842	41	0
1	D	853	0	815	31	0
1	E	752	0	727	27	0
2	C	2147	0	2046	63	0
2	F	1888	0	1768	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	3036	0	2896	72	0
4	H	28	0	25	0	0
5	A	14	0	13	0	0
5	C	56	0	52	0	0
5	F	28	0	26	1	0
5	G	28	0	26	1	0
All	All	10602	0	10075	288	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 14.

The worst 5 of 288 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:72:SER:O	2:F:101:GLN:NE2	2.13	0.80
1:B:88:VAL:O	2:C:124:ARG:NH2	2.17	0.76
2:C:225:ASN:HA	2:C:260:PHE:HD2	1.49	0.75
1:B:125:GLU:OE2	1:B:134:ARG:NH1	2.21	0.73
1:B:74:TRP:HB3	1:B:144:CYS:HB3	1.72	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	105/170 (62%)	99 (94%)	6 (6%)	0	100	100
1	B	109/170 (64%)	104 (95%)	5 (5%)	0	100	100
1	D	102/170 (60%)	93 (91%)	9 (9%)	0	100	100
1	E	87/170 (51%)	81 (93%)	6 (7%)	0	100	100
2	C	258/319 (81%)	241 (93%)	17 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	229/319 (72%)	209 (91%)	20 (9%)	0	100	100
3	G	385/479 (80%)	370 (96%)	15 (4%)	0	100	100
All	All	1275/1797 (71%)	1197 (94%)	78 (6%)	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	102/152 (67%)	97 (95%)	5 (5%)	21	53
1	B	102/152 (67%)	97 (95%)	5 (5%)	21	53
1	D	98/152 (64%)	97 (99%)	1 (1%)	73	88
1	E	88/152 (58%)	82 (93%)	6 (7%)	13	40
2	C	248/297 (84%)	237 (96%)	11 (4%)	24	56
2	F	213/297 (72%)	203 (95%)	10 (5%)	22	54
3	G	325/414 (78%)	310 (95%)	15 (5%)	23	55
All	All	1176/1616 (73%)	1123 (96%)	53 (4%)	26	56

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	34	ARG
2	F	287	PHE
3	G	262	LEU
2	F	81	HIS
2	F	174	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	118	GLN
2	F	138	HIS
3	G	150	GLN
2	F	148	HIS
2	C	250	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)

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	H	1	4,2	14,14,15	0.33	0	17,19,21	0.39	0
4	NAG	H	2	4	14,14,15	0.28	0	17,19,21	0.54	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	H	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	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.

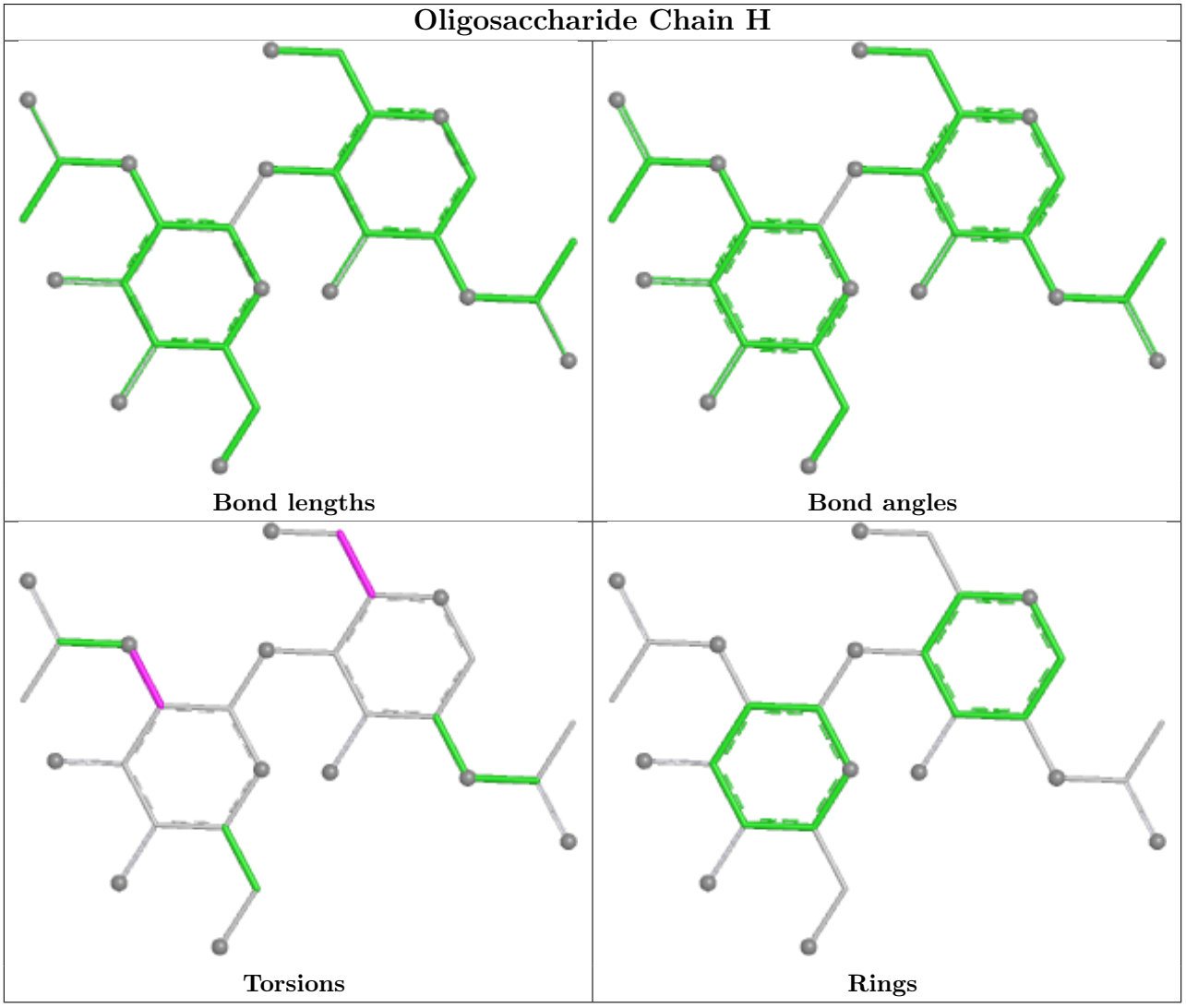
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7
4	H	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C3-C2-N2-C7

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)

9 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	A	201	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	G	501	3	14,14,15	0.46	0	17,19,21	0.65	1 (5%)
5	NAG	F	401	2	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
5	NAG	C	402	2	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	C	403	2	14,14,15	0.32	0	17,19,21	0.50	0
5	NAG	C	404	2	14,14,15	0.22	0	17,19,21	0.46	0
5	NAG	F	402	2	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	C	401	2	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	G	502	3	14,14,15	0.24	0	17,19,21	0.40	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	A	201	1	-	0/6/23/26	0/1/1/1
5	NAG	G	501	3	-	0/6/23/26	0/1/1/1
5	NAG	F	401	2	-	5/6/23/26	0/1/1/1
5	NAG	C	402	2	-	2/6/23/26	0/1/1/1
5	NAG	C	403	2	-	2/6/23/26	0/1/1/1
5	NAG	C	404	2	-	4/6/23/26	0/1/1/1
5	NAG	F	402	2	-	0/6/23/26	0/1/1/1
5	NAG	C	401	2	-	1/6/23/26	0/1/1/1
5	NAG	G	502	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	401	NAG	C2-N2-C7	4.53	128.97	122.90
5	F	401	NAG	C1-C2-N2	2.11	113.75	110.43
5	G	501	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	403	NAG	C4-C5-C6-O6
5	C	404	NAG	C4-C5-C6-O6
5	C	403	NAG	O5-C5-C6-O6
5	C	404	NAG	O5-C5-C6-O6
5	C	404	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	501	NAG	1	0
5	F	401	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.

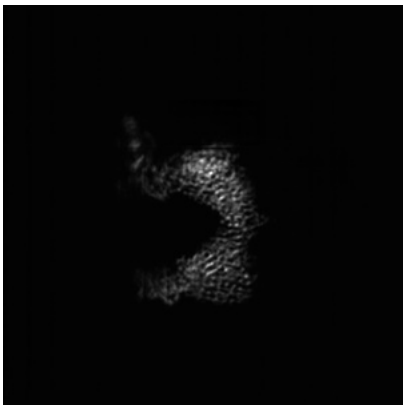
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26837. These allow visual inspection of the internal detail of the map and identification of artifacts.

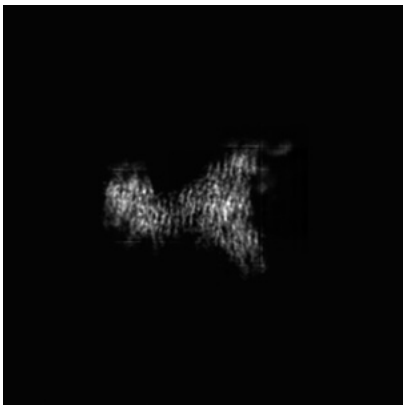
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

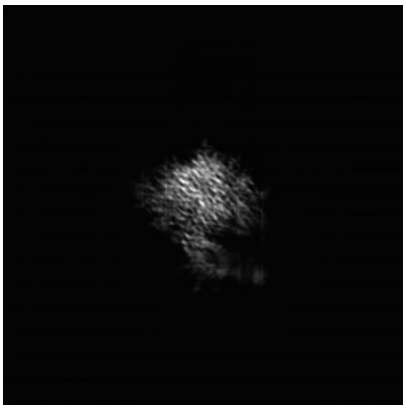
6.1.1 Primary map



X

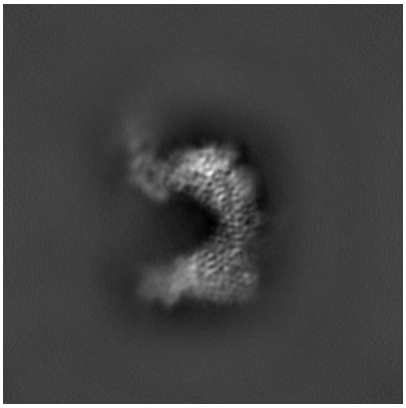


Y

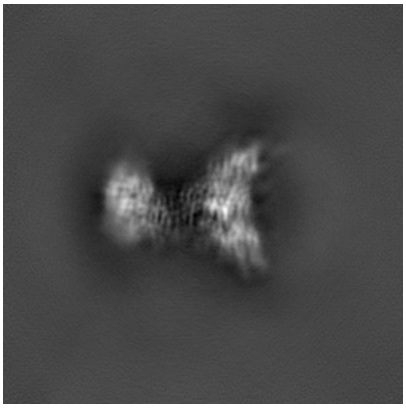


Z

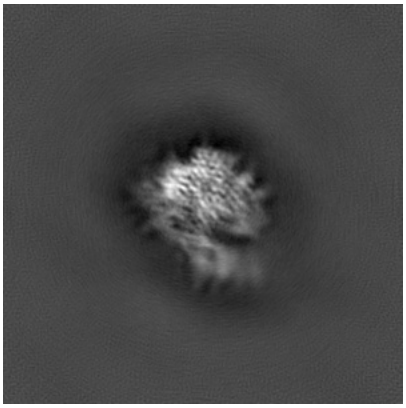
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

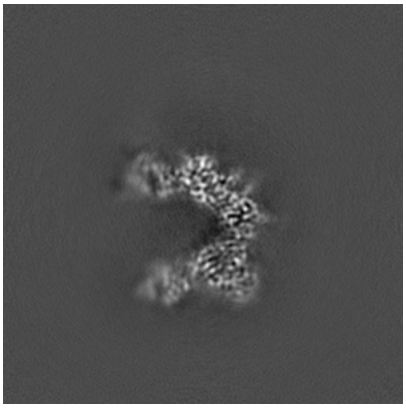
6.2.1 Primary map

X Index: 128

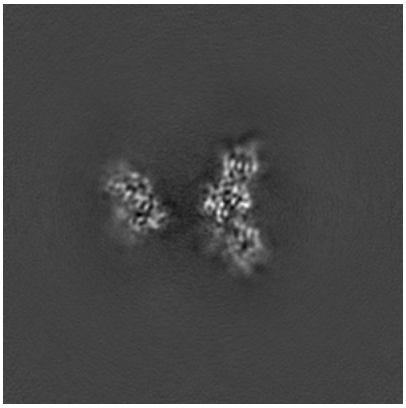
Y Index: 128

Z Index: 128

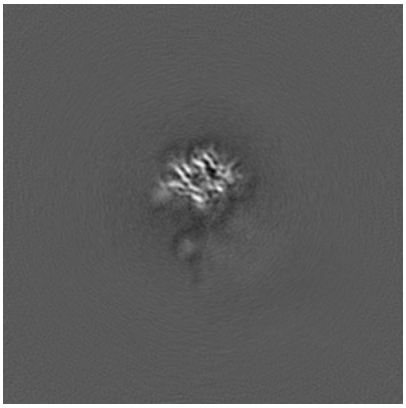
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

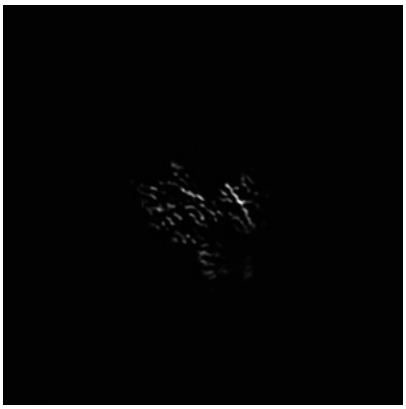
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

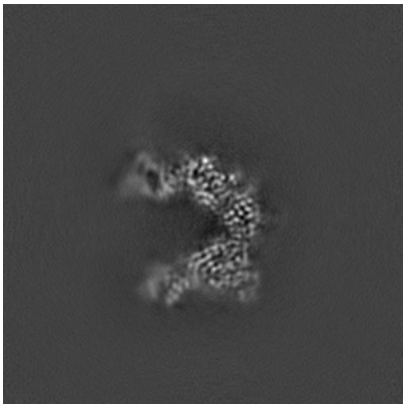
X Index: 126

Y Index: 133

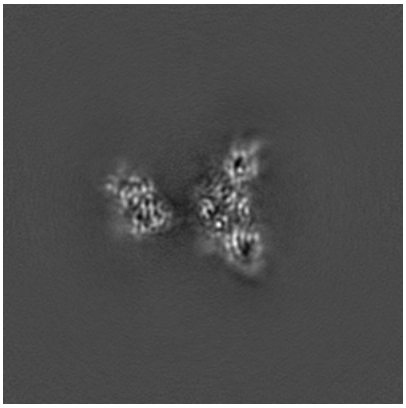


Z Index: 151

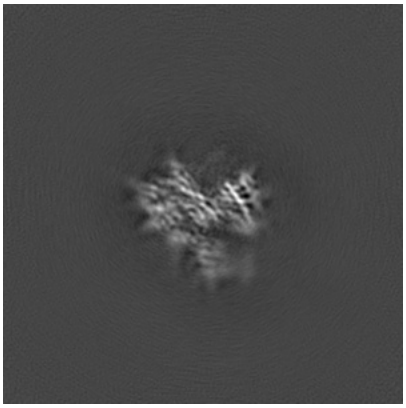
6.3.2 Raw map



X Index: 126



Y Index: 132

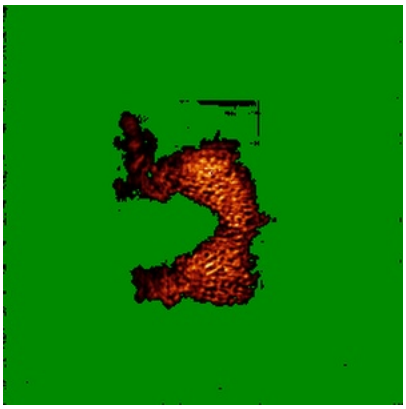


Z Index: 151

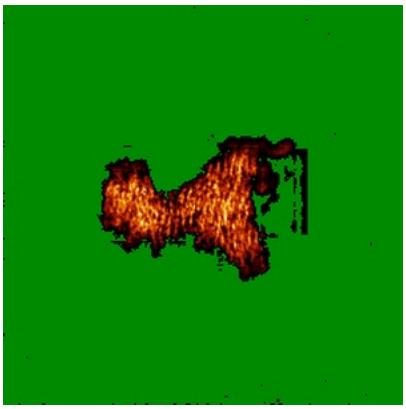
The images above show the largest variance slices of the map in three orthogonal directions.

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

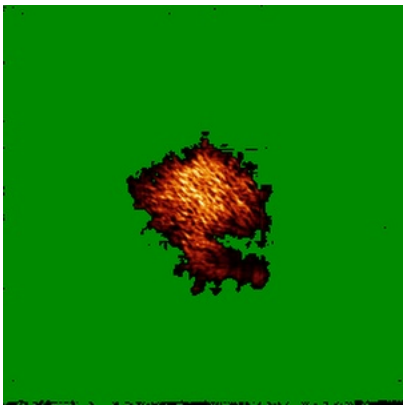
6.4.1 Primary map



X

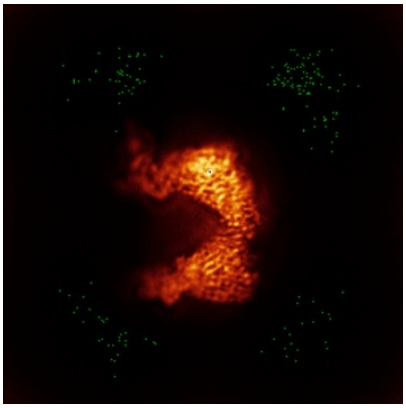


Y

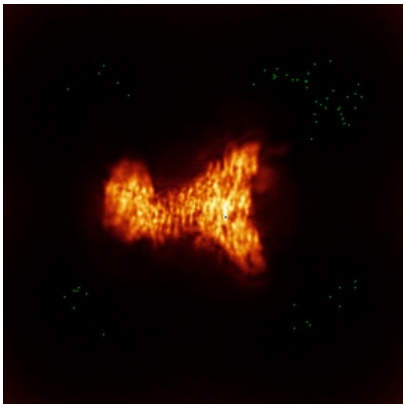


Z

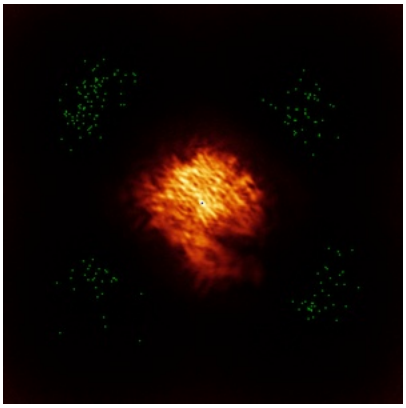
6.4.2 Raw map



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.

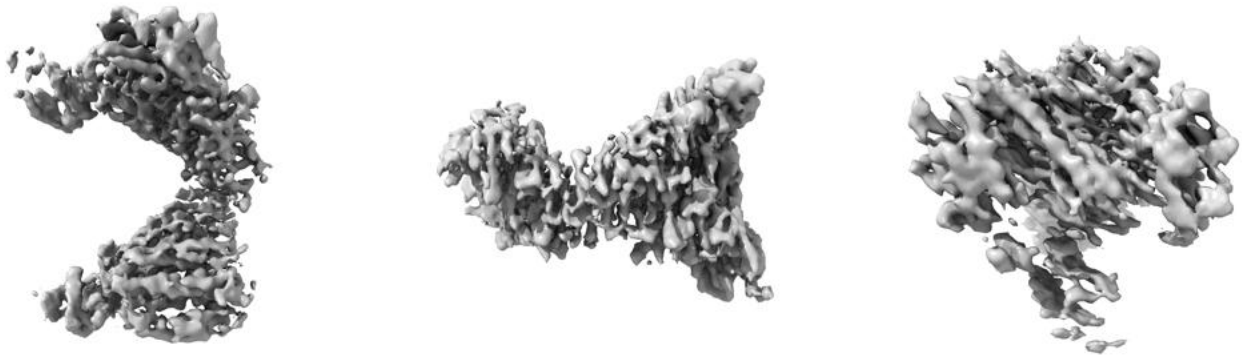
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

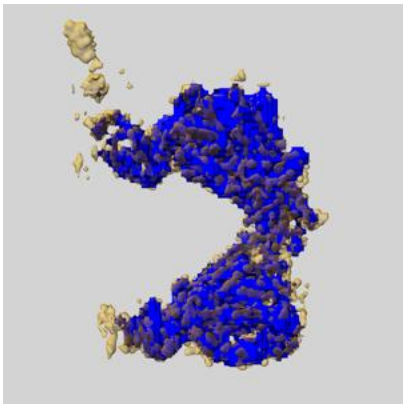
6.6 Mask visualisation (i)

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

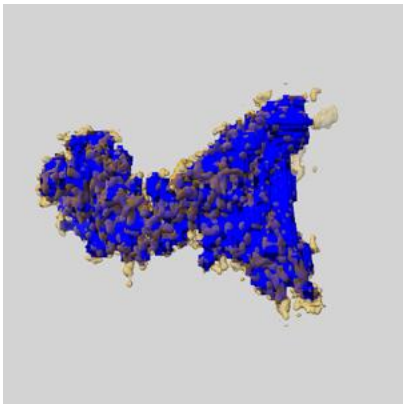
A mask typically either:

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

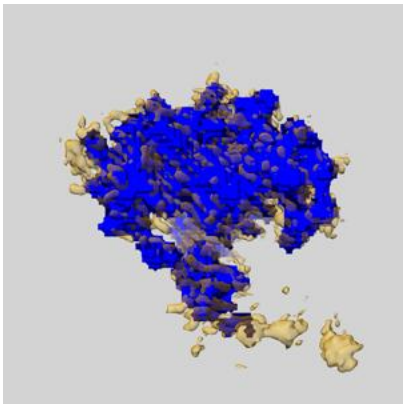
6.6.1 emd_26837_msk_1.map (i)



X



Y

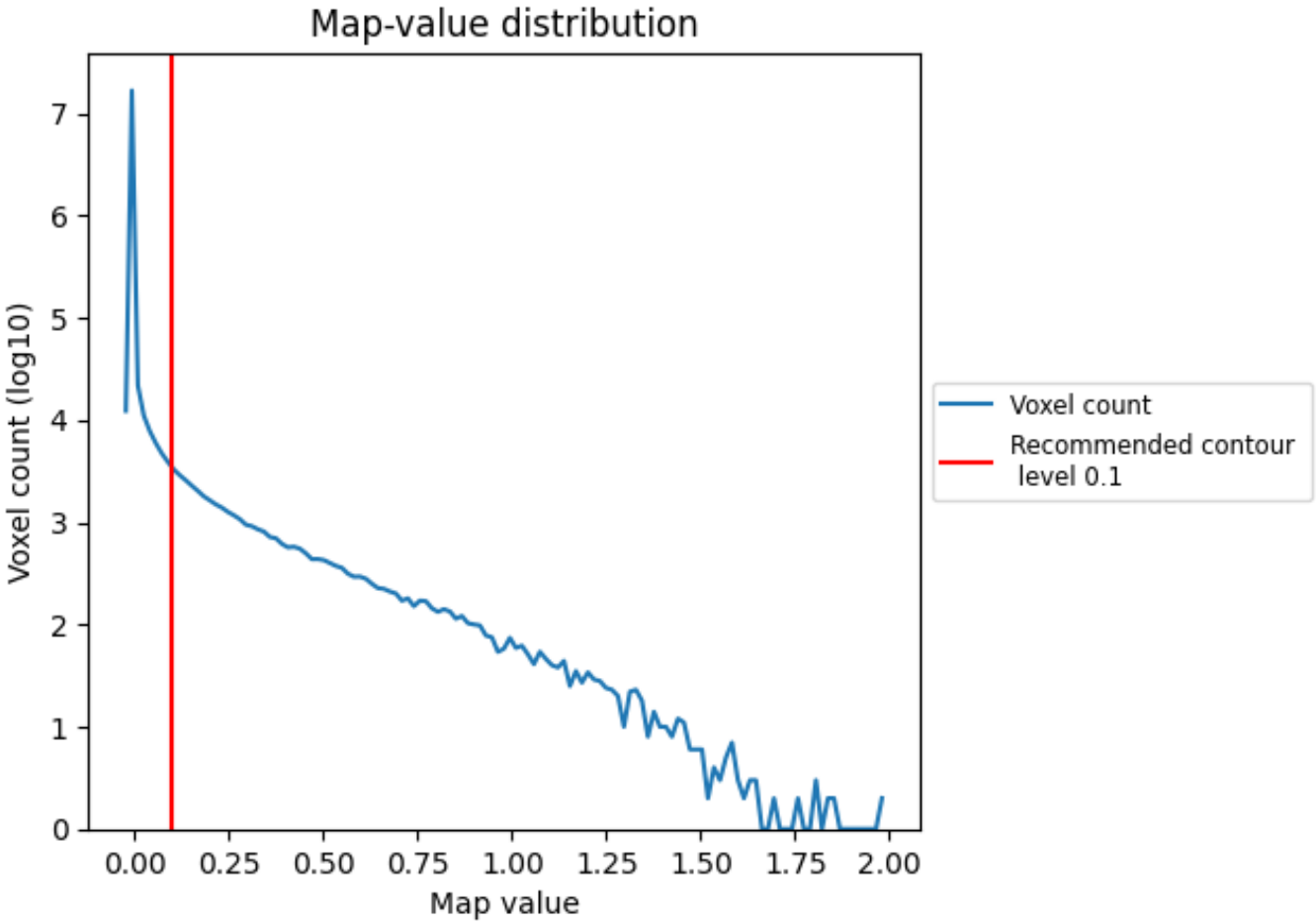


Z

7 Map analysis

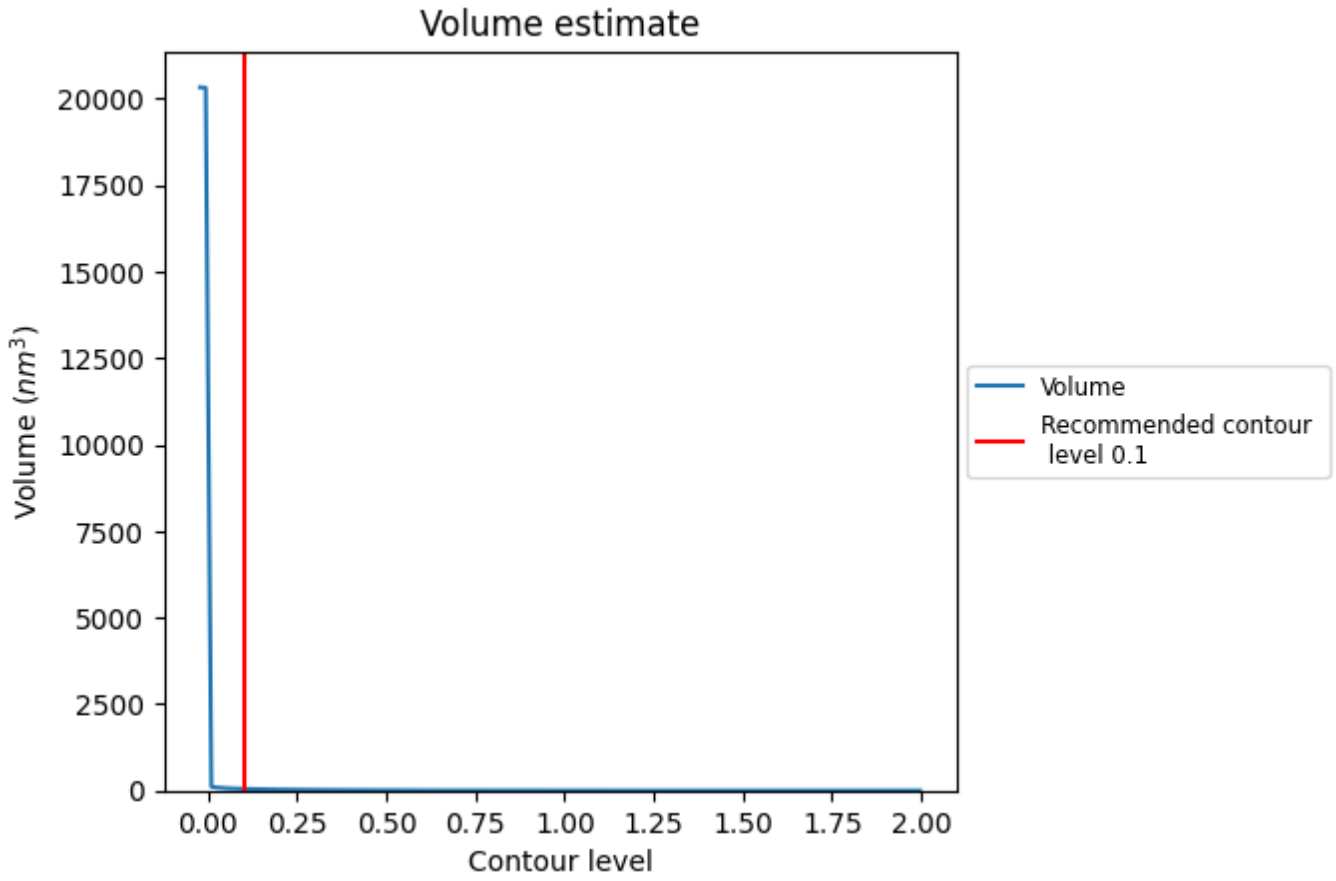
This section contains the results of statistical analysis of the map.

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.

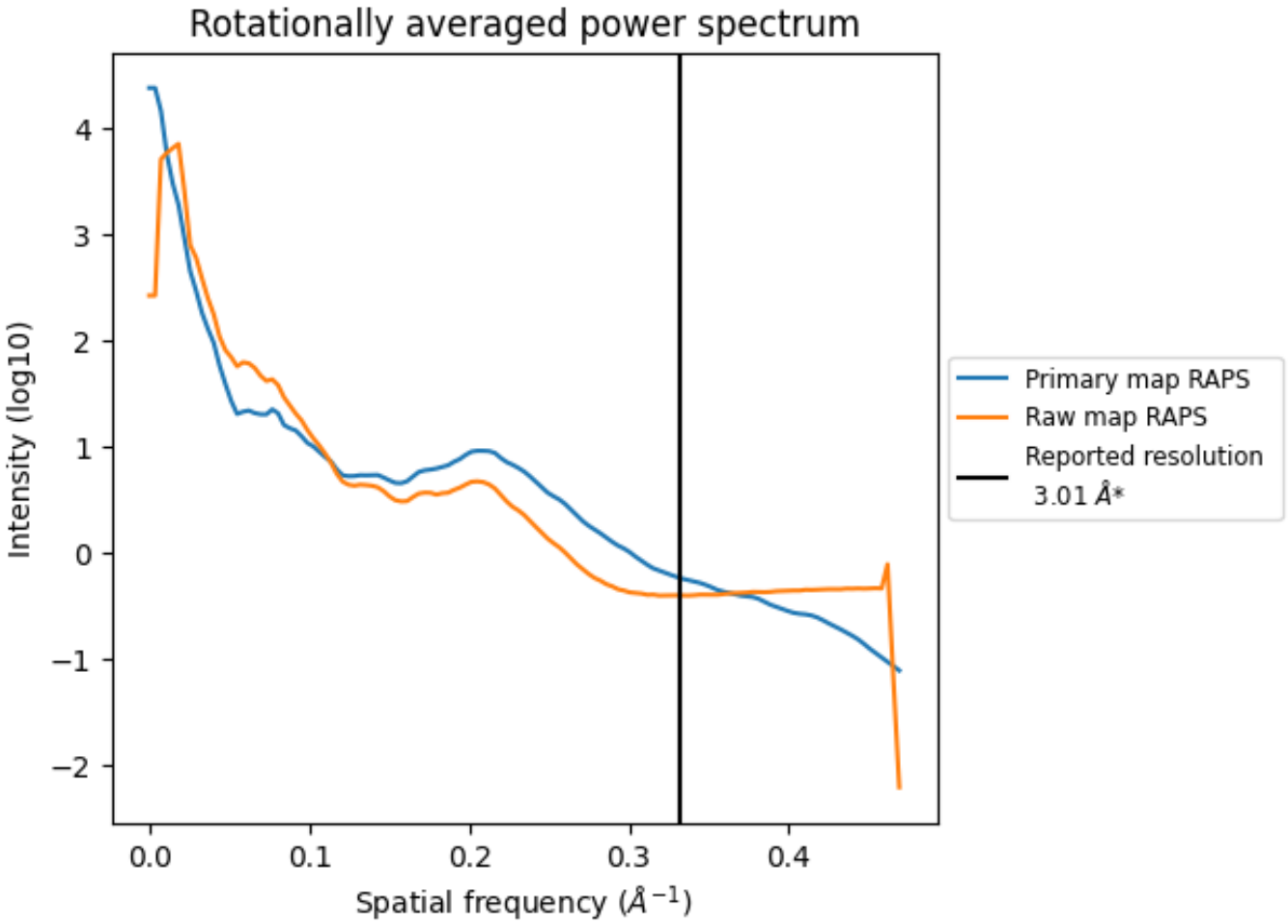
7.2 Volume estimate (i)



The volume at the recommended contour level is 48 nm^3; this corresponds to an approximate mass of 43 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)

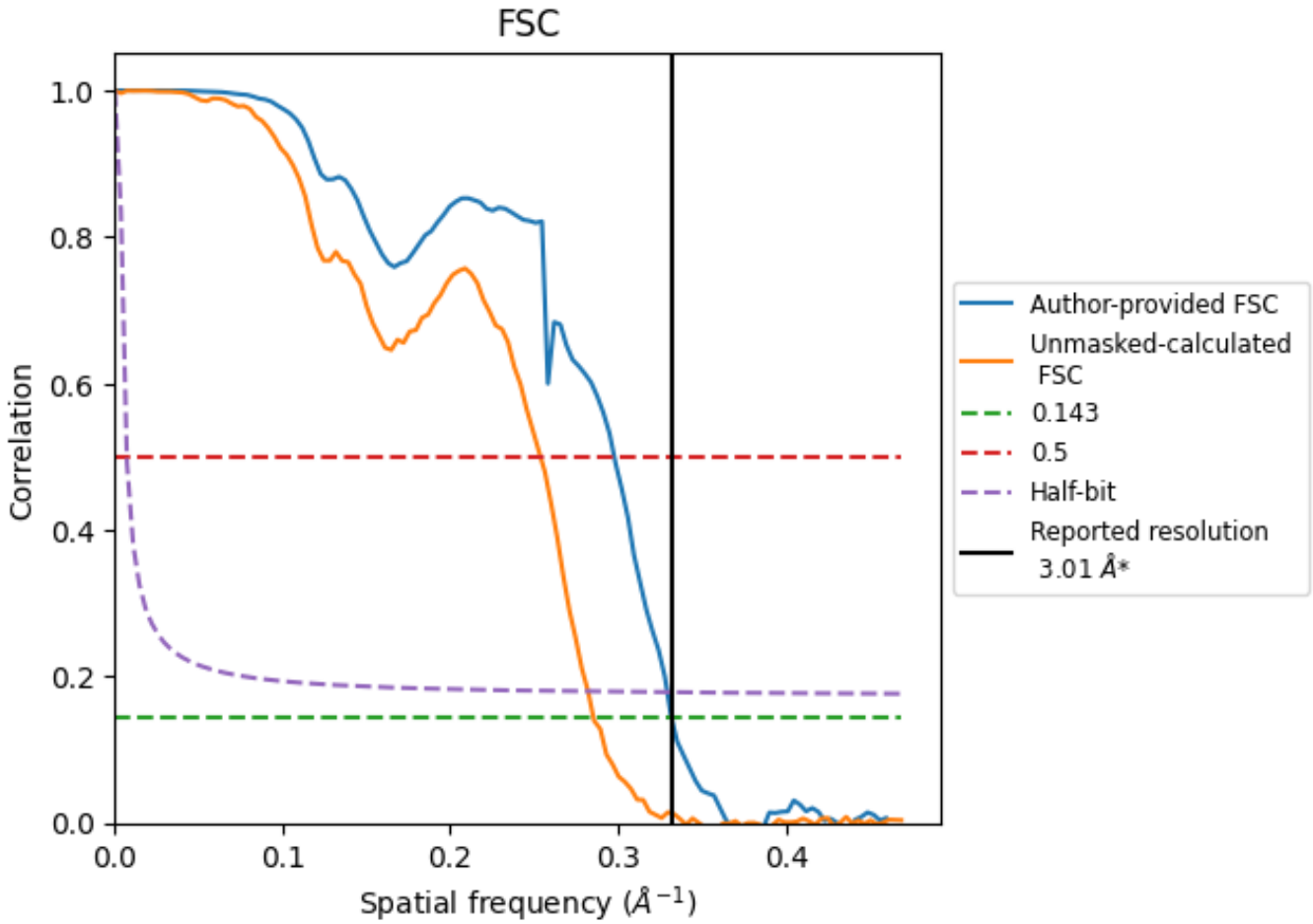


*Reported resolution corresponds to spatial frequency of 0.332 Å^{-1}

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 0.332 Å^{-1}

8.2 Resolution estimates (i)

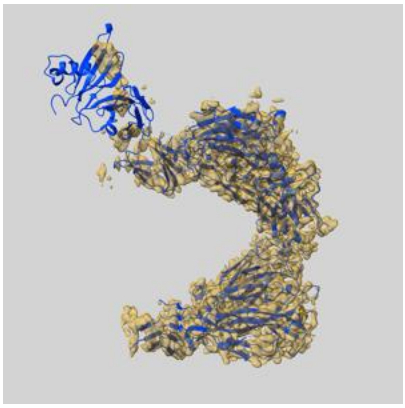
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.36	3.04
Unmasked-calculated*	3.50	3.94	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.50 differs from the reported value 3.01 by more than 10 %

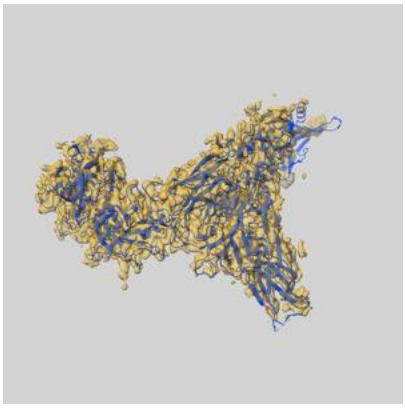
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26837 and PDB model 7UWN. Per-residue inclusion information can be found in section 3 on page 12.

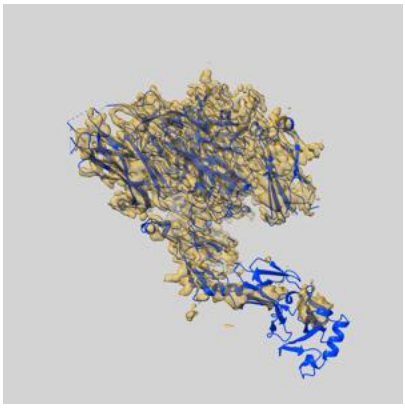
9.1 Map-model overlay



X



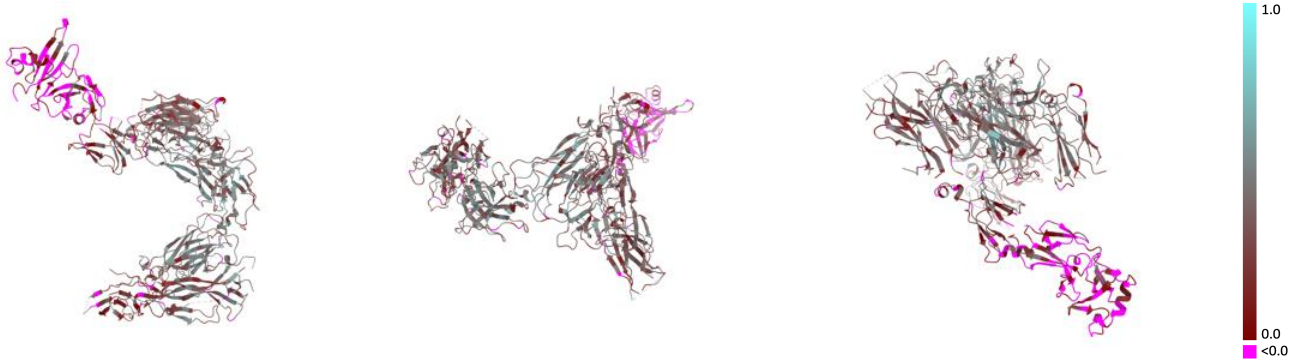
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

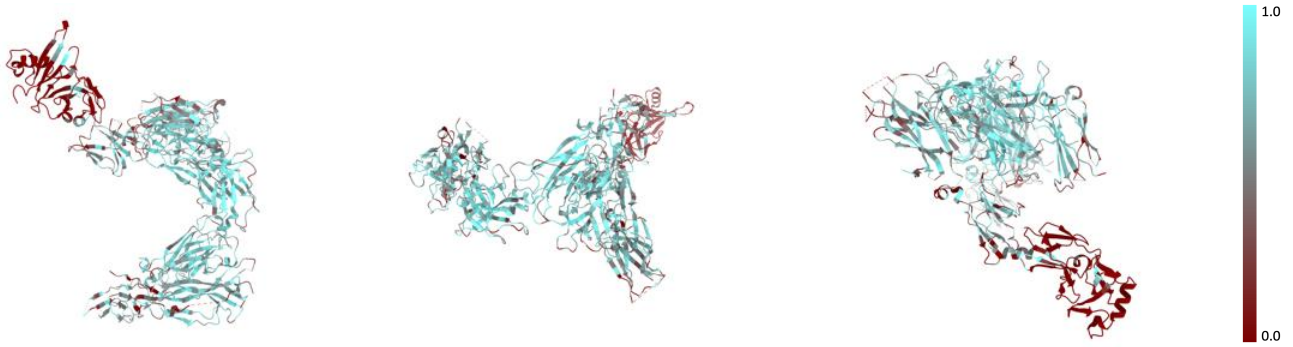
9.2 Q-score mapped to coordinate model (i)



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.

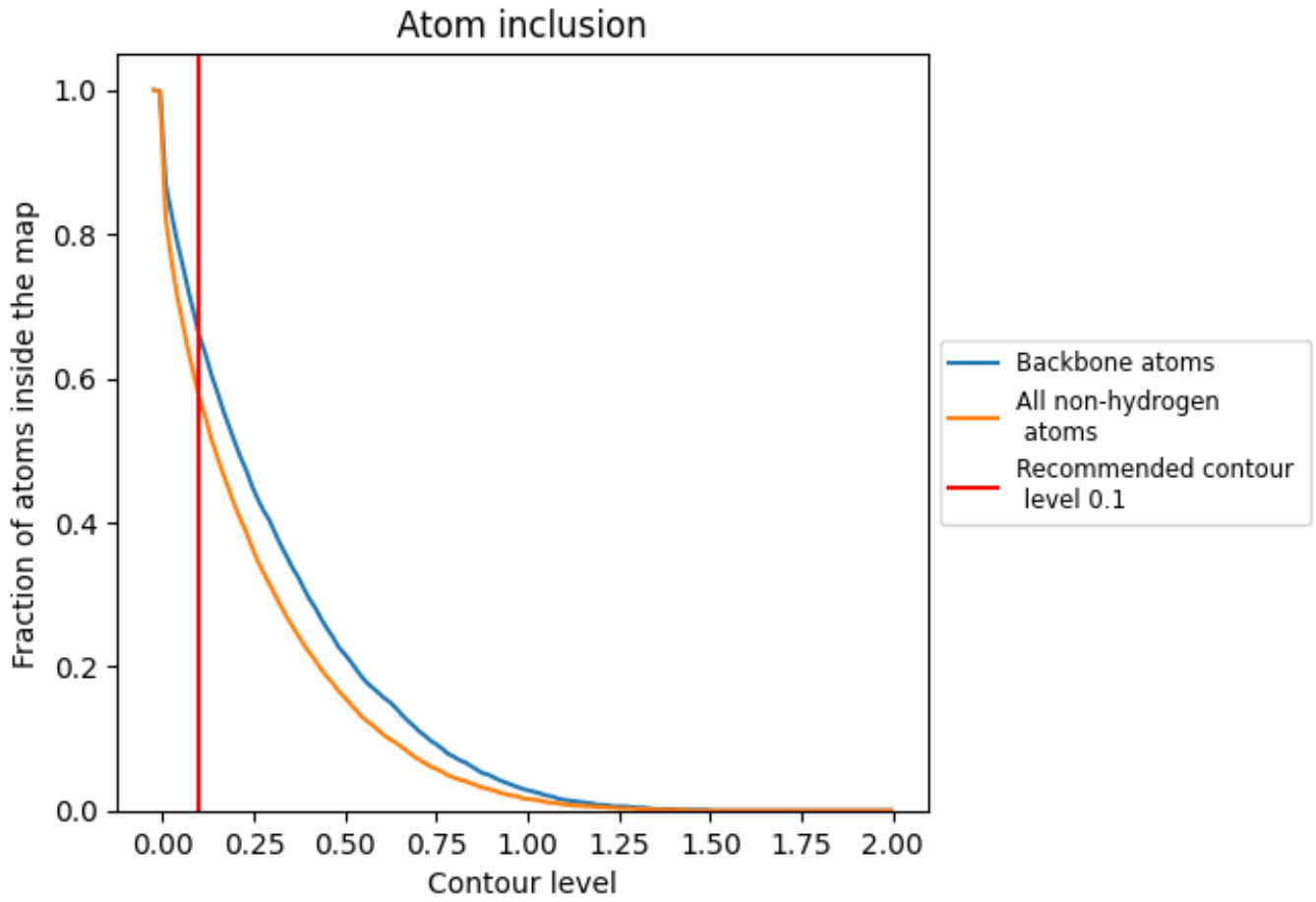
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 57% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5750	0.3160
A	0.6850	0.3860
B	0.6750	0.4040
C	0.6800	0.3890
D	0.5730	0.3290
E	0.6190	0.3400
F	0.6940	0.3670
G	0.3580	0.1780
H	0.3210	0.3130