wwPDB EM Validation Summary Report

Mar 8, 2026 – 05:06 AM UTC

PDB ID	:	9IY6 / pdb_00009iy6
EMDB ID	:	EMD-60986
Title	:	BTN2A1-BTN3A1-BTN3A2 oligomer complex
Authors	:	Xin, W.; Huang, B.; Su, Q.; Zhou, Q.
Deposited on	:	2024-07-30
Resolution	:	10.00 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:

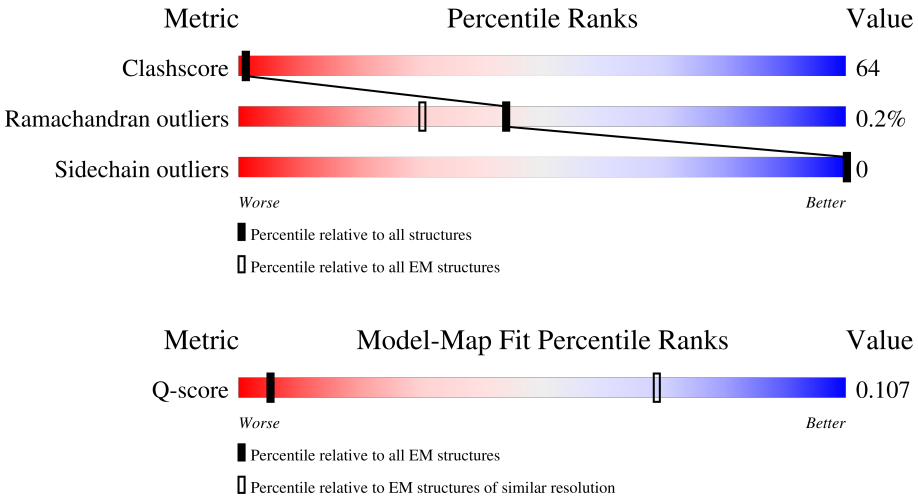
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 10.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	147 (9.50 - 10.50)

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	E	534	6% 34% · 60%
1	F	534	13% 27% · 60%
1	I	534	16% 24% 60%
1	J	534	11% 29% 60%

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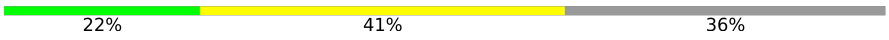
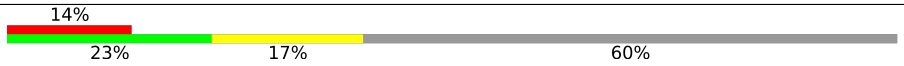
Mol	Chain	Length	Quality of chain
2	G	340	
2	K	340	
3	H	539	
3	L	539	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13310 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 Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	216	Total	C	N	O	S	0	0
			1698	1072	297	318	11		
1	F	216	Total	C	N	O	S	0	0
			1698	1072	297	318	11		
1	I	216	Total	C	N	O	S	0	0
			1698	1072	297	318	11		
1	J	216	Total	C	N	O	S	0	0
			1698	1072	297	318	11		

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	7	MET	-	initiating methionine	UNP Q7KYR7
E	8	ASP	-	expression tag	UNP Q7KYR7
E	9	MET	-	expression tag	UNP Q7KYR7
E	10	ARG	-	expression tag	UNP Q7KYR7
E	11	VAL	-	expression tag	UNP Q7KYR7
E	12	PRO	-	expression tag	UNP Q7KYR7
E	13	ALA	-	expression tag	UNP Q7KYR7
E	14	GLN	-	expression tag	UNP Q7KYR7
E	15	LEU	-	expression tag	UNP Q7KYR7
E	16	LEU	-	expression tag	UNP Q7KYR7
E	17	GLY	-	expression tag	UNP Q7KYR7
E	18	LEU	-	expression tag	UNP Q7KYR7
E	19	LEU	-	expression tag	UNP Q7KYR7
E	20	LEU	-	expression tag	UNP Q7KYR7
E	21	LEU	-	expression tag	UNP Q7KYR7
E	22	TRP	-	expression tag	UNP Q7KYR7
E	23	LEU	-	expression tag	UNP Q7KYR7
E	24	SER	-	expression tag	UNP Q7KYR7
E	25	GLY	-	expression tag	UNP Q7KYR7
E	26	ALA	-	expression tag	UNP Q7KYR7
E	27	ARG	-	expression tag	UNP Q7KYR7
E	28	CYS	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	528	GLY	-	expression tag	UNP Q7KYR7
E	529	SER	-	expression tag	UNP Q7KYR7
E	530	SER	-	expression tag	UNP Q7KYR7
E	531	GLY	-	expression tag	UNP Q7KYR7
E	532	MET	-	expression tag	UNP Q7KYR7
E	533	ASP	-	expression tag	UNP Q7KYR7
E	534	TYR	-	expression tag	UNP Q7KYR7
E	535	LYS	-	expression tag	UNP Q7KYR7
E	536	ASP	-	expression tag	UNP Q7KYR7
E	537	ASP	-	expression tag	UNP Q7KYR7
E	538	ASP	-	expression tag	UNP Q7KYR7
E	539	ASP	-	expression tag	UNP Q7KYR7
E	540	LYS	-	expression tag	UNP Q7KYR7
F	7	MET	-	initiating methionine	UNP Q7KYR7
F	8	ASP	-	expression tag	UNP Q7KYR7
F	9	MET	-	expression tag	UNP Q7KYR7
F	10	ARG	-	expression tag	UNP Q7KYR7
F	11	VAL	-	expression tag	UNP Q7KYR7
F	12	PRO	-	expression tag	UNP Q7KYR7
F	13	ALA	-	expression tag	UNP Q7KYR7
F	14	GLN	-	expression tag	UNP Q7KYR7
F	15	LEU	-	expression tag	UNP Q7KYR7
F	16	LEU	-	expression tag	UNP Q7KYR7
F	17	GLY	-	expression tag	UNP Q7KYR7
F	18	LEU	-	expression tag	UNP Q7KYR7
F	19	LEU	-	expression tag	UNP Q7KYR7
F	20	LEU	-	expression tag	UNP Q7KYR7
F	21	LEU	-	expression tag	UNP Q7KYR7
F	22	TRP	-	expression tag	UNP Q7KYR7
F	23	LEU	-	expression tag	UNP Q7KYR7
F	24	SER	-	expression tag	UNP Q7KYR7
F	25	GLY	-	expression tag	UNP Q7KYR7
F	26	ALA	-	expression tag	UNP Q7KYR7
F	27	ARG	-	expression tag	UNP Q7KYR7
F	28	CYS	-	expression tag	UNP Q7KYR7
F	528	GLY	-	expression tag	UNP Q7KYR7
F	529	SER	-	expression tag	UNP Q7KYR7
F	530	SER	-	expression tag	UNP Q7KYR7
F	531	GLY	-	expression tag	UNP Q7KYR7
F	532	MET	-	expression tag	UNP Q7KYR7
F	533	ASP	-	expression tag	UNP Q7KYR7
F	534	TYR	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	535	LYS	-	expression tag	UNP Q7KYR7
F	536	ASP	-	expression tag	UNP Q7KYR7
F	537	ASP	-	expression tag	UNP Q7KYR7
F	538	ASP	-	expression tag	UNP Q7KYR7
F	539	ASP	-	expression tag	UNP Q7KYR7
F	540	LYS	-	expression tag	UNP Q7KYR7
I	7	MET	-	initiating methionine	UNP Q7KYR7
I	8	ASP	-	expression tag	UNP Q7KYR7
I	9	MET	-	expression tag	UNP Q7KYR7
I	10	ARG	-	expression tag	UNP Q7KYR7
I	11	VAL	-	expression tag	UNP Q7KYR7
I	12	PRO	-	expression tag	UNP Q7KYR7
I	13	ALA	-	expression tag	UNP Q7KYR7
I	14	GLN	-	expression tag	UNP Q7KYR7
I	15	LEU	-	expression tag	UNP Q7KYR7
I	16	LEU	-	expression tag	UNP Q7KYR7
I	17	GLY	-	expression tag	UNP Q7KYR7
I	18	LEU	-	expression tag	UNP Q7KYR7
I	19	LEU	-	expression tag	UNP Q7KYR7
I	20	LEU	-	expression tag	UNP Q7KYR7
I	21	LEU	-	expression tag	UNP Q7KYR7
I	22	TRP	-	expression tag	UNP Q7KYR7
I	23	LEU	-	expression tag	UNP Q7KYR7
I	24	SER	-	expression tag	UNP Q7KYR7
I	25	GLY	-	expression tag	UNP Q7KYR7
I	26	ALA	-	expression tag	UNP Q7KYR7
I	27	ARG	-	expression tag	UNP Q7KYR7
I	28	CYS	-	expression tag	UNP Q7KYR7
I	528	GLY	-	expression tag	UNP Q7KYR7
I	529	SER	-	expression tag	UNP Q7KYR7
I	530	SER	-	expression tag	UNP Q7KYR7
I	531	GLY	-	expression tag	UNP Q7KYR7
I	532	MET	-	expression tag	UNP Q7KYR7
I	533	ASP	-	expression tag	UNP Q7KYR7
I	534	TYR	-	expression tag	UNP Q7KYR7
I	535	LYS	-	expression tag	UNP Q7KYR7
I	536	ASP	-	expression tag	UNP Q7KYR7
I	537	ASP	-	expression tag	UNP Q7KYR7
I	538	ASP	-	expression tag	UNP Q7KYR7
I	539	ASP	-	expression tag	UNP Q7KYR7
I	540	LYS	-	expression tag	UNP Q7KYR7
J	7	MET	-	initiating methionine	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	8	ASP	-	expression tag	UNP Q7KYR7
J	9	MET	-	expression tag	UNP Q7KYR7
J	10	ARG	-	expression tag	UNP Q7KYR7
J	11	VAL	-	expression tag	UNP Q7KYR7
J	12	PRO	-	expression tag	UNP Q7KYR7
J	13	ALA	-	expression tag	UNP Q7KYR7
J	14	GLN	-	expression tag	UNP Q7KYR7
J	15	LEU	-	expression tag	UNP Q7KYR7
J	16	LEU	-	expression tag	UNP Q7KYR7
J	17	GLY	-	expression tag	UNP Q7KYR7
J	18	LEU	-	expression tag	UNP Q7KYR7
J	19	LEU	-	expression tag	UNP Q7KYR7
J	20	LEU	-	expression tag	UNP Q7KYR7
J	21	LEU	-	expression tag	UNP Q7KYR7
J	22	TRP	-	expression tag	UNP Q7KYR7
J	23	LEU	-	expression tag	UNP Q7KYR7
J	24	SER	-	expression tag	UNP Q7KYR7
J	25	GLY	-	expression tag	UNP Q7KYR7
J	26	ALA	-	expression tag	UNP Q7KYR7
J	27	ARG	-	expression tag	UNP Q7KYR7
J	28	CYS	-	expression tag	UNP Q7KYR7
J	528	GLY	-	expression tag	UNP Q7KYR7
J	529	SER	-	expression tag	UNP Q7KYR7
J	530	SER	-	expression tag	UNP Q7KYR7
J	531	GLY	-	expression tag	UNP Q7KYR7
J	532	MET	-	expression tag	UNP Q7KYR7
J	533	ASP	-	expression tag	UNP Q7KYR7
J	534	TYR	-	expression tag	UNP Q7KYR7
J	535	LYS	-	expression tag	UNP Q7KYR7
J	536	ASP	-	expression tag	UNP Q7KYR7
J	537	ASP	-	expression tag	UNP Q7KYR7
J	538	ASP	-	expression tag	UNP Q7KYR7
J	539	ASP	-	expression tag	UNP Q7KYR7
J	540	LYS	-	expression tag	UNP Q7KYR7

- Molecule 2 is a protein called Butyrophilin subfamily 3 member A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	216	Total	C	N	O	S	0	0
			1630	1027	279	316	8		
2	K	216	Total	C	N	O	S	0	0
			1630	1027	279	316	8		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	8	MET	-	initiating methionine	UNP P78410
G	9	ASP	-	expression tag	UNP P78410
G	10	MET	-	expression tag	UNP P78410
G	11	ARG	-	expression tag	UNP P78410
G	12	VAL	-	expression tag	UNP P78410
G	13	PRO	-	expression tag	UNP P78410
G	14	ALA	-	expression tag	UNP P78410
G	15	GLN	-	expression tag	UNP P78410
G	16	LEU	-	expression tag	UNP P78410
G	17	LEU	-	expression tag	UNP P78410
G	18	GLY	-	expression tag	UNP P78410
G	19	LEU	-	expression tag	UNP P78410
G	20	LEU	-	expression tag	UNP P78410
G	21	LEU	-	expression tag	UNP P78410
G	22	LEU	-	expression tag	UNP P78410
G	23	TRP	-	expression tag	UNP P78410
G	24	LEU	-	expression tag	UNP P78410
G	25	SER	-	expression tag	UNP P78410
G	26	GLY	-	expression tag	UNP P78410
G	27	ALA	-	expression tag	UNP P78410
G	28	ARG	-	expression tag	UNP P78410
G	29	CYS	-	expression tag	UNP P78410
G	335	GLY	-	expression tag	UNP P78410
G	336	SER	-	expression tag	UNP P78410
G	337	SER	-	expression tag	UNP P78410
G	338	GLY	-	expression tag	UNP P78410
G	339	MET	-	expression tag	UNP P78410
G	340	ASP	-	expression tag	UNP P78410
G	341	TYR	-	expression tag	UNP P78410
G	342	LYS	-	expression tag	UNP P78410
G	343	ASP	-	expression tag	UNP P78410
G	344	ASP	-	expression tag	UNP P78410
G	345	ASP	-	expression tag	UNP P78410
G	346	ASP	-	expression tag	UNP P78410
G	347	LYS	-	expression tag	UNP P78410
K	8	MET	-	initiating methionine	UNP P78410
K	9	ASP	-	expression tag	UNP P78410
K	10	MET	-	expression tag	UNP P78410
K	11	ARG	-	expression tag	UNP P78410
K	12	VAL	-	expression tag	UNP P78410
K	13	PRO	-	expression tag	UNP P78410
K	14	ALA	-	expression tag	UNP P78410

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Chain	Residue	Modelled	Actual	Comment	Reference
K	15	GLN	-	expression tag	UNP P78410
K	16	LEU	-	expression tag	UNP P78410
K	17	LEU	-	expression tag	UNP P78410
K	18	GLY	-	expression tag	UNP P78410
K	19	LEU	-	expression tag	UNP P78410
K	20	LEU	-	expression tag	UNP P78410
K	21	LEU	-	expression tag	UNP P78410
K	22	LEU	-	expression tag	UNP P78410
K	23	TRP	-	expression tag	UNP P78410
K	24	LEU	-	expression tag	UNP P78410
K	25	SER	-	expression tag	UNP P78410
K	26	GLY	-	expression tag	UNP P78410
K	27	ALA	-	expression tag	UNP P78410
K	28	ARG	-	expression tag	UNP P78410
K	29	CYS	-	expression tag	UNP P78410
K	335	GLY	-	expression tag	UNP P78410
K	336	SER	-	expression tag	UNP P78410
K	337	SER	-	expression tag	UNP P78410
K	338	GLY	-	expression tag	UNP P78410
K	339	MET	-	expression tag	UNP P78410
K	340	ASP	-	expression tag	UNP P78410
K	341	TYR	-	expression tag	UNP P78410
K	342	LYS	-	expression tag	UNP P78410
K	343	ASP	-	expression tag	UNP P78410
K	344	ASP	-	expression tag	UNP P78410
K	345	ASP	-	expression tag	UNP P78410
K	346	ASP	-	expression tag	UNP P78410
K	347	LYS	-	expression tag	UNP P78410

- Molecule 3 is a protein called Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	216	Total	C	N	O	S	0	0
			1629	1025	279	317	8		
3	L	216	Total	C	N	O	S	0	0
			1629	1025	279	317	8		

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	MET	-	initiating methionine	UNP O00481
H	9	ASP	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
H	10	MET	-	expression tag	UNP O00481
H	11	ARG	-	expression tag	UNP O00481
H	12	VAL	-	expression tag	UNP O00481
H	13	PRO	-	expression tag	UNP O00481
H	14	ALA	-	expression tag	UNP O00481
H	15	GLN	-	expression tag	UNP O00481
H	16	LEU	-	expression tag	UNP O00481
H	17	LEU	-	expression tag	UNP O00481
H	18	GLY	-	expression tag	UNP O00481
H	19	LEU	-	expression tag	UNP O00481
H	20	LEU	-	expression tag	UNP O00481
H	21	LEU	-	expression tag	UNP O00481
H	22	LEU	-	expression tag	UNP O00481
H	23	TRP	-	expression tag	UNP O00481
H	24	LEU	-	expression tag	UNP O00481
H	25	SER	-	expression tag	UNP O00481
H	26	GLY	-	expression tag	UNP O00481
H	27	ALA	-	expression tag	UNP O00481
H	28	ARG	-	expression tag	UNP O00481
H	29	CYS	-	expression tag	UNP O00481
H	514	GLY	-	expression tag	UNP O00481
H	515	SER	-	expression tag	UNP O00481
H	516	SER	-	expression tag	UNP O00481
H	517	GLY	-	expression tag	UNP O00481
H	518	ALA	-	expression tag	UNP O00481
H	519	TRP	-	expression tag	UNP O00481
H	520	SER	-	expression tag	UNP O00481
H	521	HIS	-	expression tag	UNP O00481
H	522	PRO	-	expression tag	UNP O00481
H	523	GLN	-	expression tag	UNP O00481
H	524	PHE	-	expression tag	UNP O00481
H	525	GLU	-	expression tag	UNP O00481
H	526	LYS	-	expression tag	UNP O00481
H	527	GLY	-	expression tag	UNP O00481
H	528	GLY	-	expression tag	UNP O00481
H	529	GLY	-	expression tag	UNP O00481
H	530	SER	-	expression tag	UNP O00481
H	531	GLY	-	expression tag	UNP O00481
H	532	GLY	-	expression tag	UNP O00481
H	533	GLY	-	expression tag	UNP O00481
H	534	SER	-	expression tag	UNP O00481
H	535	GLY	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
H	536	GLY	-	expression tag	UNP O00481
H	537	SER	-	expression tag	UNP O00481
H	538	ALA	-	expression tag	UNP O00481
H	539	TRP	-	expression tag	UNP O00481
H	540	SER	-	expression tag	UNP O00481
H	541	HIS	-	expression tag	UNP O00481
H	542	PRO	-	expression tag	UNP O00481
H	543	GLN	-	expression tag	UNP O00481
H	544	PHE	-	expression tag	UNP O00481
H	545	GLU	-	expression tag	UNP O00481
H	546	LYS	-	expression tag	UNP O00481
L	8	MET	-	initiating methionine	UNP O00481
L	9	ASP	-	expression tag	UNP O00481
L	10	MET	-	expression tag	UNP O00481
L	11	ARG	-	expression tag	UNP O00481
L	12	VAL	-	expression tag	UNP O00481
L	13	PRO	-	expression tag	UNP O00481
L	14	ALA	-	expression tag	UNP O00481
L	15	GLN	-	expression tag	UNP O00481
L	16	LEU	-	expression tag	UNP O00481
L	17	LEU	-	expression tag	UNP O00481
L	18	GLY	-	expression tag	UNP O00481
L	19	LEU	-	expression tag	UNP O00481
L	20	LEU	-	expression tag	UNP O00481
L	21	LEU	-	expression tag	UNP O00481
L	22	LEU	-	expression tag	UNP O00481
L	23	TRP	-	expression tag	UNP O00481
L	24	LEU	-	expression tag	UNP O00481
L	25	SER	-	expression tag	UNP O00481
L	26	GLY	-	expression tag	UNP O00481
L	27	ALA	-	expression tag	UNP O00481
L	28	ARG	-	expression tag	UNP O00481
L	29	CYS	-	expression tag	UNP O00481
L	514	GLY	-	expression tag	UNP O00481
L	515	SER	-	expression tag	UNP O00481
L	516	SER	-	expression tag	UNP O00481
L	517	GLY	-	expression tag	UNP O00481
L	518	ALA	-	expression tag	UNP O00481
L	519	TRP	-	expression tag	UNP O00481
L	520	SER	-	expression tag	UNP O00481
L	521	HIS	-	expression tag	UNP O00481
L	522	PRO	-	expression tag	UNP O00481

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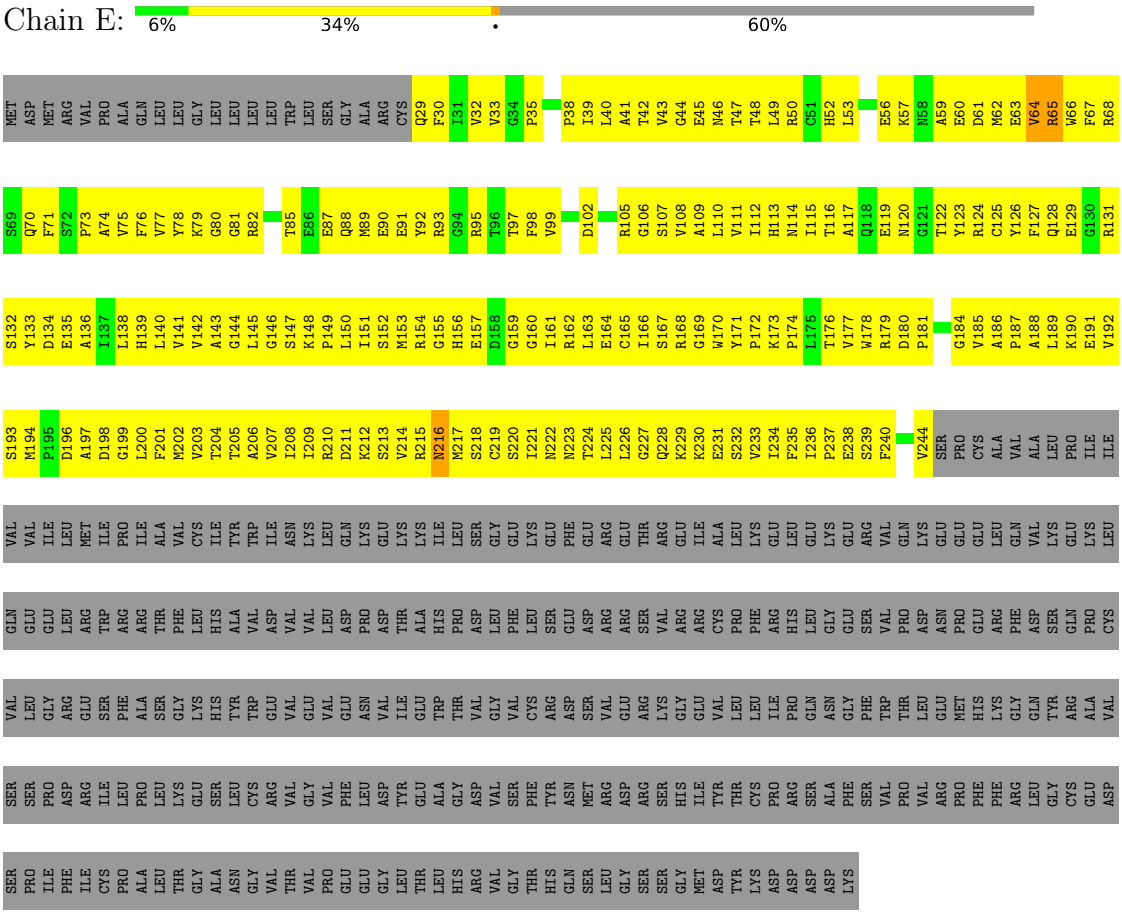
Chain	Residue	Modelled	Actual	Comment	Reference
L	523	GLN	-	expression tag	UNP O00481
L	524	PHE	-	expression tag	UNP O00481
L	525	GLU	-	expression tag	UNP O00481
L	526	LYS	-	expression tag	UNP O00481
L	527	GLY	-	expression tag	UNP O00481
L	528	GLY	-	expression tag	UNP O00481
L	529	GLY	-	expression tag	UNP O00481
L	530	SER	-	expression tag	UNP O00481
L	531	GLY	-	expression tag	UNP O00481
L	532	GLY	-	expression tag	UNP O00481
L	533	GLY	-	expression tag	UNP O00481
L	534	SER	-	expression tag	UNP O00481
L	535	GLY	-	expression tag	UNP O00481
L	536	GLY	-	expression tag	UNP O00481
L	537	SER	-	expression tag	UNP O00481
L	538	ALA	-	expression tag	UNP O00481
L	539	TRP	-	expression tag	UNP O00481
L	540	SER	-	expression tag	UNP O00481
L	541	HIS	-	expression tag	UNP O00481
L	542	PRO	-	expression tag	UNP O00481
L	543	GLN	-	expression tag	UNP O00481
L	544	PHE	-	expression tag	UNP O00481
L	545	GLU	-	expression tag	UNP O00481
L	546	LYS	-	expression tag	UNP O00481

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.

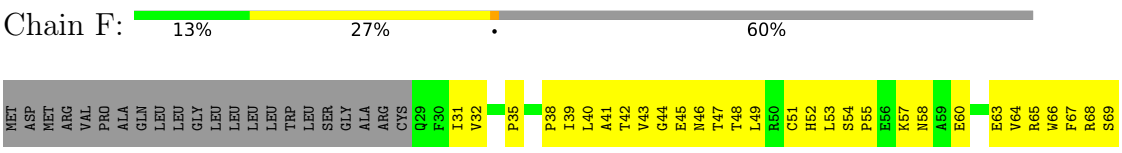
• Molecule 1: Butyrophilin subfamily 2 member A1

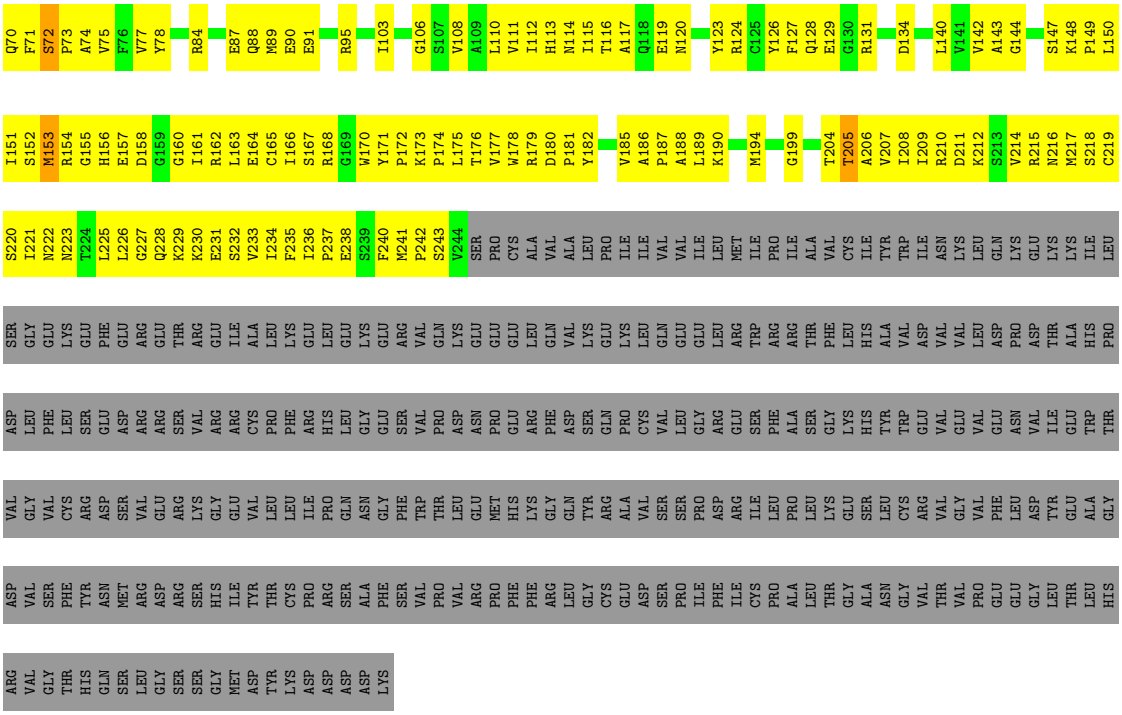
Chain E:



• Molecule 1: Butyrophilin subfamily 2 member A1

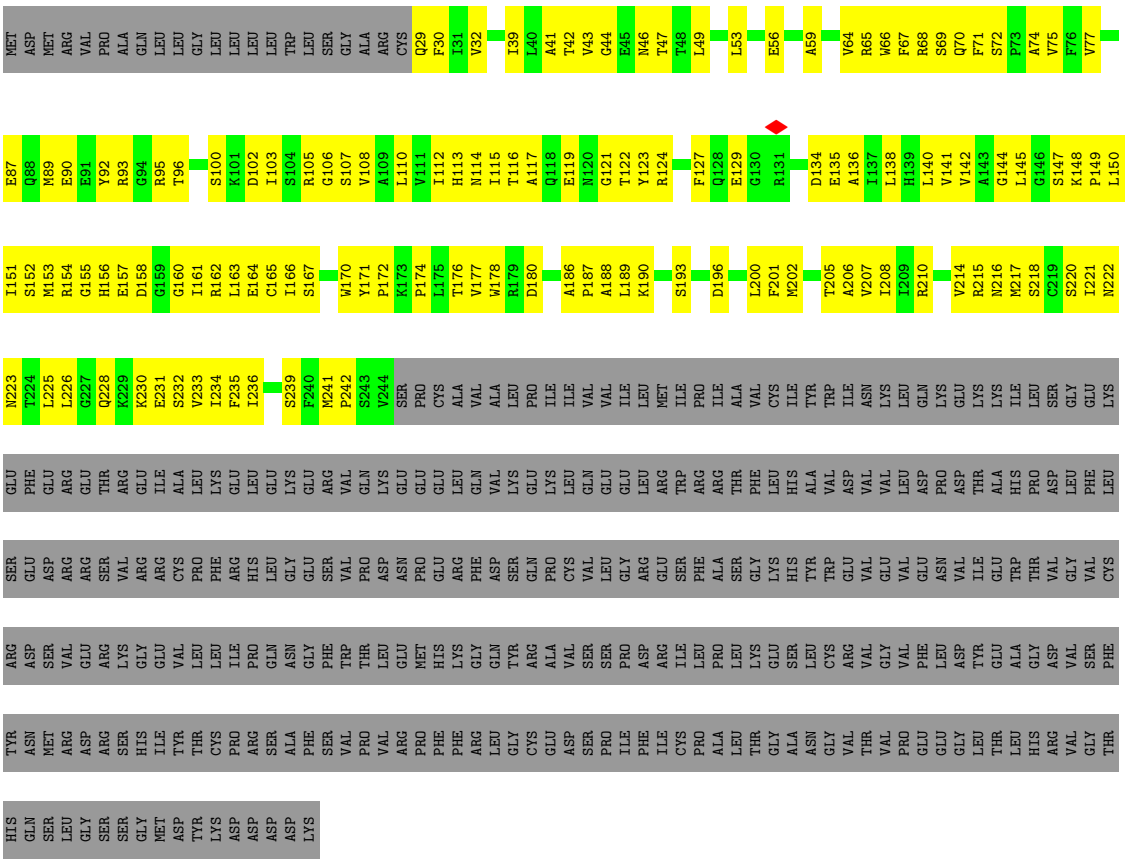
Chain F:





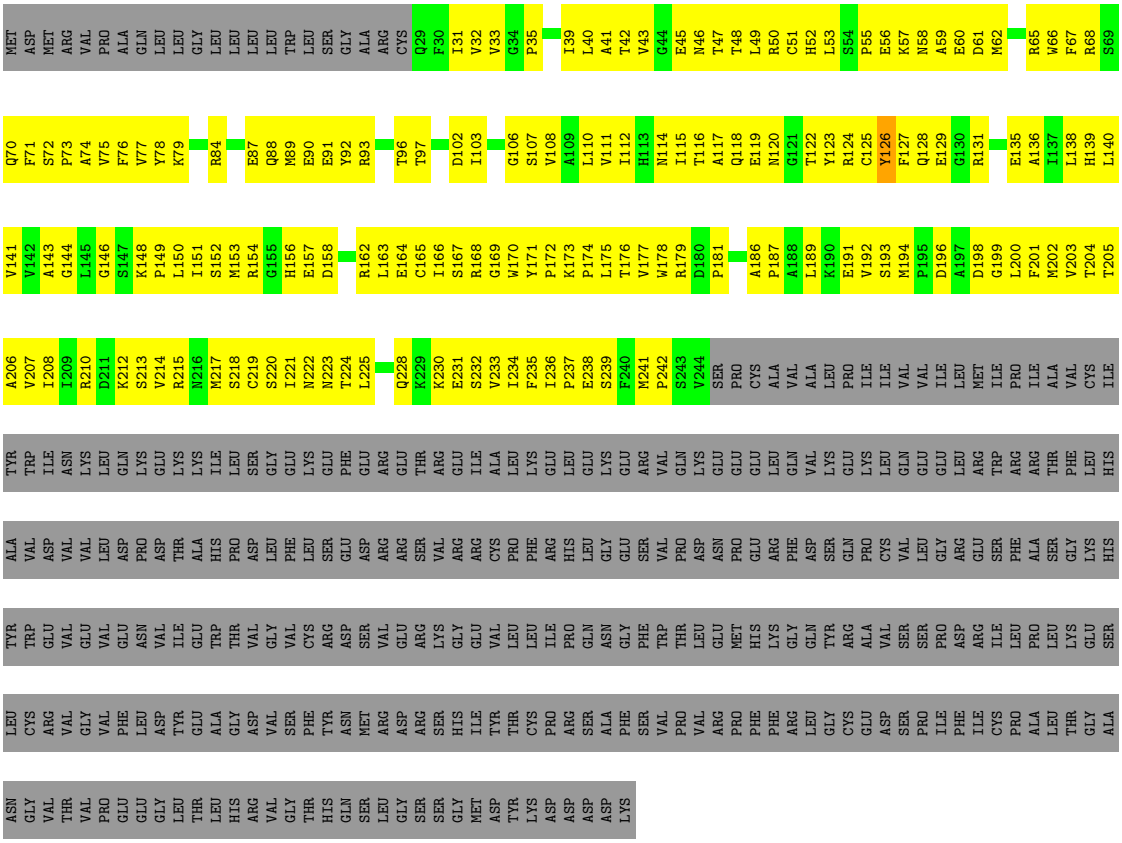
• Molecule 1: Butyrophilin subfamily 2 member A1

Chain I:



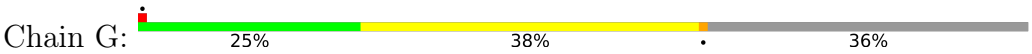
• Molecule 1: Butyrophilin subfamily 2 member A1

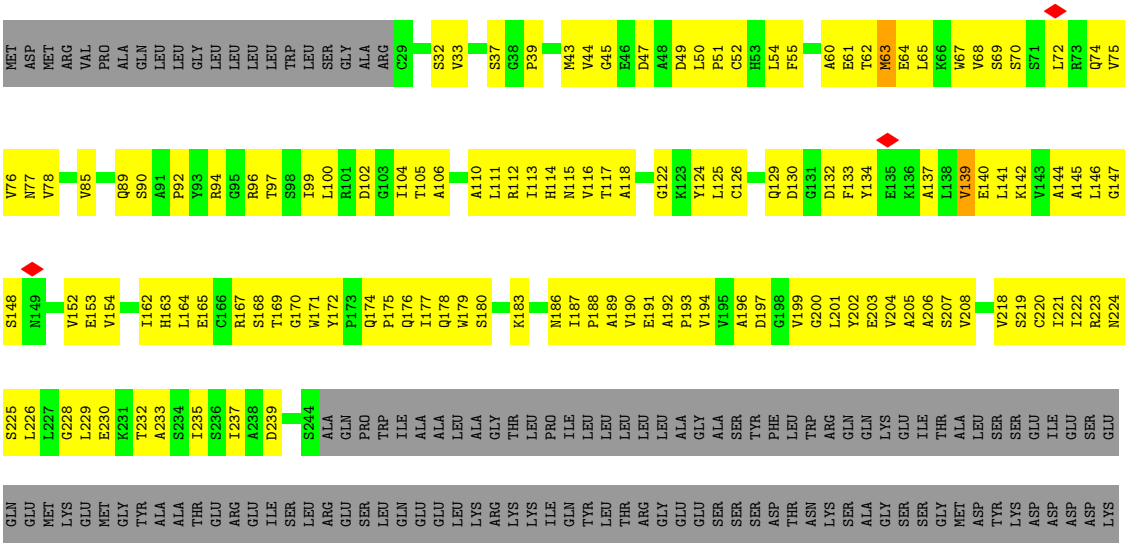
Chain J:



• Molecule 2: Butyrophilin subfamily 3 member A2

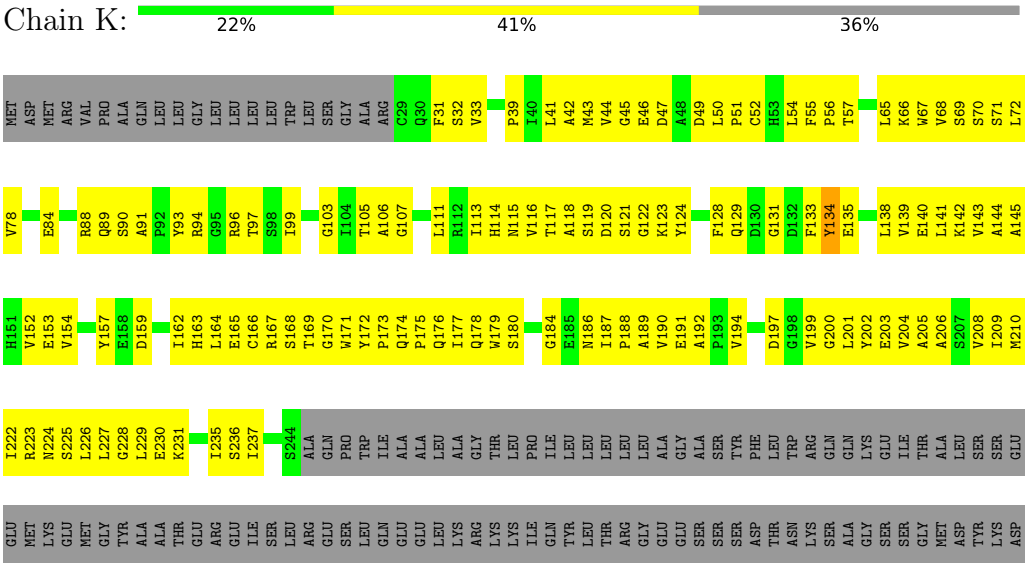
Chain G:





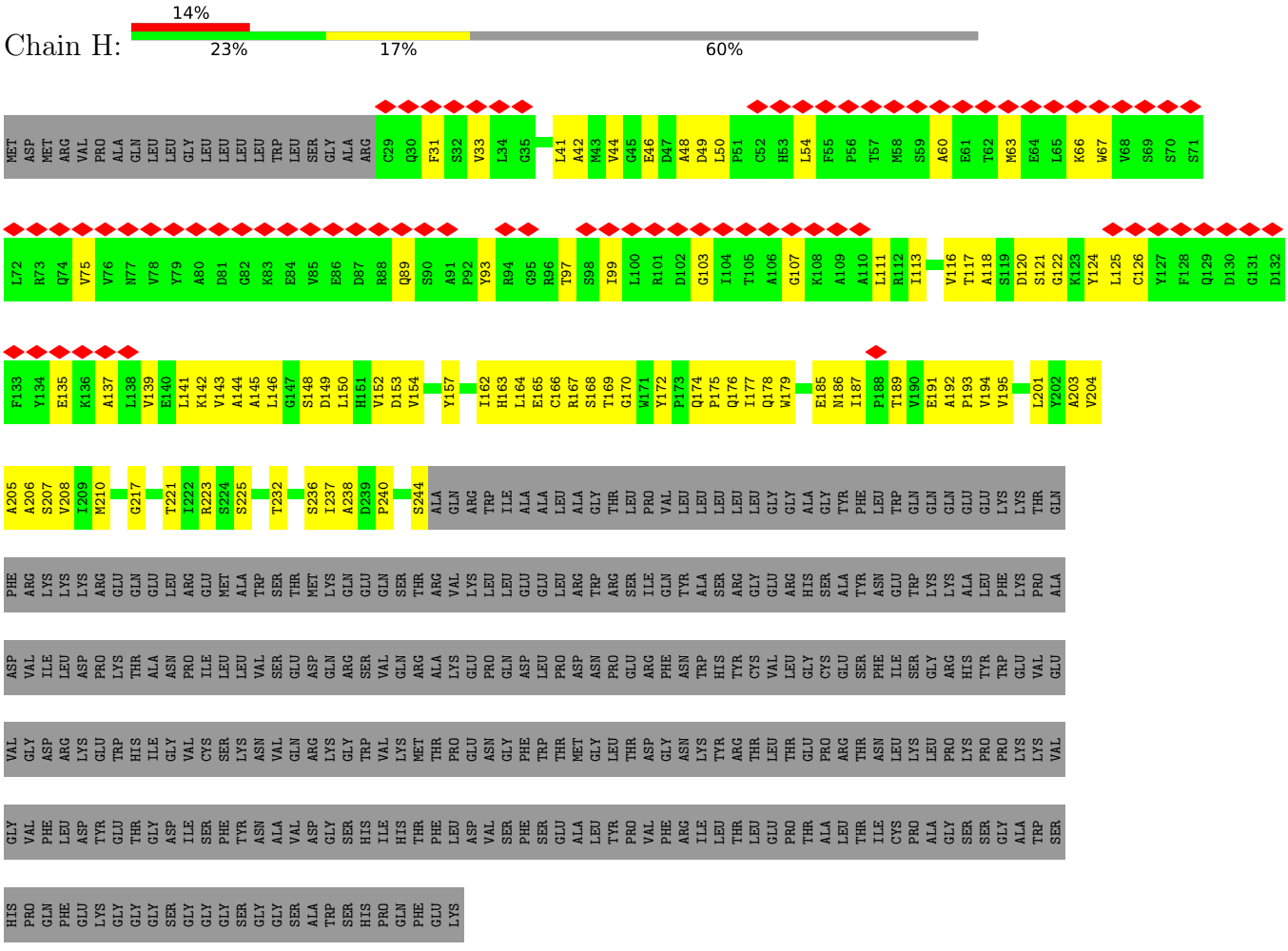
• Molecule 2: Butyrophilin subfamily 3 member A2

Chain K:



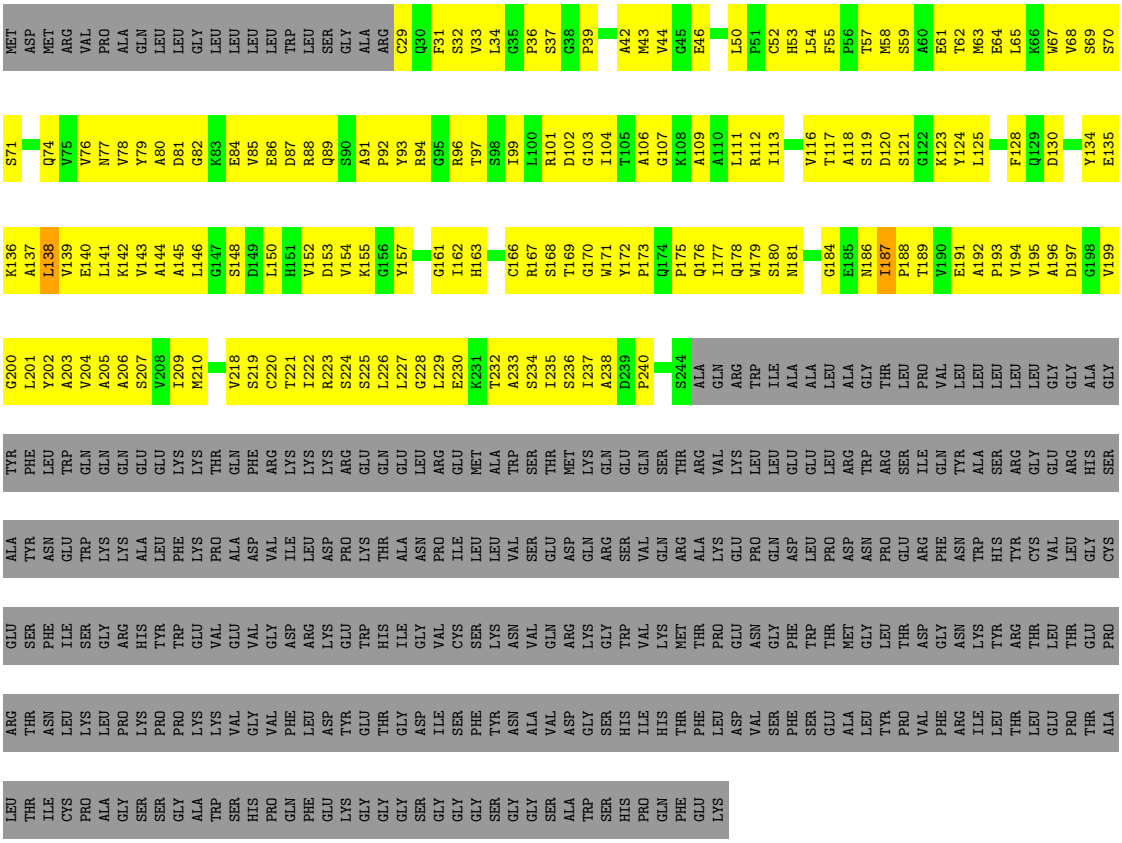
• Molecule 3: Butyrophilin subfamily 3 member A1

Chain H:



• Molecule 3: Butyrophilin subfamily 3 member A1

Chain L:


MET ASP MET ARG VAL PRO ALA GLN LEU LEU GLY LEU LEU LEU LEU TRP LEU SER GLY ALA ARG C29 Q30 F31 S32 V33 L34 G35 P36 S37 G38 P39 A42 M43 V44 G45 E46 L50 P51 C52 H53 L54 F55 P56 T57 M58 S59 A60 E61 T62 M63 E64 L65 K66 W67 V68 S69 S70
S71 Q74 V75 V76 N77 V78 Y79 A80 D81 G82 K83 E84 V85 E86 D87 R88 Q89 S90 A91 P92 Y93 R94 G95 R96 T97 S98 I99 L100 R101 D102 G103 I104 T105 A106 G107 K108 A109 A110 L111 R112 I113 V116 T117 A118 S119 D120 S121 G122 K123 Y124 L125 F128 Q129 D130 Y134 E135
K136 A137 L138 V139 E140 L141 K142 V143 A144 A145 L146 G147 S148 D149 L150 H151 V152 D153 V154 K155 G156 Y157 G161 I162 H163 C166 R167 S168 T169 G170 W171 Y172 P173 Q174 P175 Q176 I177 Q178 W179 S180 N181 G184 E185 N186 I187 P188 T189 V190 E191 A192 P193 V194 V195 A196 D197 G198 V199
G200 L201 Y202 A203 V204 A205 A206 S207 V208 I209 M210 V218 S219 C220 T221 I222 R223 S224 S225 L226 L227 G228 L229 E230 K231 T232 A233 S234 I235 S236 I237 A238 D239 P240 S244 ALA GLN ARG TRP ILE ALA ALA LEU ALA ALA GLY THR LEU PRO VAL LEU LEU LEU LEU LEU GLY GLY ALA GLY
TYR PHE LEU TRP GLN GLN GLN GLU GLU LYS LYS THR GLN PHE ARG LYS LYS LYS ARG GLU GLN LEU GLU LEU ARG GLU MET ALA TRP SER THR MET LYS GLN GLU GLN SER THR ARG VAL LYS LEU LEU GLU GLU LEU ARG TRP ARG SER ILE GLN TYR ALA SER ARG GLY GLU ARG HIS SER
ALA TYR ASN GLU TRP LYS LYS ALA LEU PHE LYS PRO ALA ASP VAL ILE LEU ASP PRO LYS THR ALA ASN PRO ILE LEU LEU VAL SER GLU ASP GLN ARG SER VAL GLN ARG ARG ALA LYS GLU PRO GLN ASP LEU PRO ASP ASN PRO GLU ARG PHE ASN TRP HIS TYR CYS VAL LEU GLY CYS
GLU SER PHE ILE SER GLY ARG HIS TYR TRP GLU VAL GLU VAL GLY ASP ARG LYS GLU TRP HIS ILE GLY VAL CYS SER LYS ASN VAL GLN ARG LYS GLY TRP VAL LYS MET THR PRO GLU ASN GLY PHE TRP THR MET GLY LEU THR ASP GLY ASN LYS TYR ARG THR LEU THR GLU PRO
ARG THR ASN LEU LYS LEU PRO LYS PRO PRO LYS LYS VAL GLY VAL PHE LEU ASP TYR GLU THR GLY ASP ILE SER PHE TYR ASN ALA VAL ASP GLY SER HIS ILE HIS THR PHE LEU ASP VAL SER PHE SER GLU ALA LEU TYR PRO VAL PHE ARG ILE LEU THR LEU GLU PRO THR ALA
LEU THR ILE CYS PRO ALA GLY SER SER GLY ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER GLY ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229039	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.140	Depositor
Minimum map value	-2.825	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.261	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	517.104, 517.104, 517.104	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.3092, 4.3092, 4.3092	Depositor

5 Model quality

5.1 Standard geometry

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	E	0.35	0/1735	0.63	0/2348
1	F	0.26	0/1735	0.54	0/2348
1	I	0.19	0/1735	0.44	0/2348
1	J	0.25	0/1735	0.53	0/2348
2	G	0.23	0/1663	0.51	2/2255 (0.1%)
2	K	0.26	0/1663	0.59	2/2255 (0.1%)
3	H	0.16	0/1662	0.36	0/2254
3	L	0.25	0/1662	0.49	1/2254 (0.0%)
All	All	0.25	0/13590	0.52	5/18410 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3
1	F	0	4
1	J	0	2
3	L	0	1
All	All	0	10

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	134	TYR	CA-C-N	10.83	141.19	121.70
2	K	134	TYR	C-N-CA	10.83	141.19	121.70
2	G	63	MET	CA-C-N	7.50	135.19	121.70
2	G	63	MET	C-N-CA	7.50	135.19	121.70
3	L	187	ILE	N-CA-C	-5.42	103.00	108.96

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	216	ASN	Peptide
1	E	64	VAL	Peptide
1	E	65	ARG	Peptide
1	F	60	GLU	Peptide
1	F	72	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1698	0	1681	464	0
1	F	1698	0	1681	295	0
1	I	1698	0	1681	189	0
1	J	1698	0	1681	260	0
2	G	1630	0	1596	145	0
2	K	1630	0	1596	179	0
3	H	1629	0	1598	91	0
3	L	1629	0	1598	185	0
All	All	13310	0	13112	1686	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 64.

The worst 5 of 1686 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:I:154:ARG:NH1	1:I:164:GLU:OE1	1.95	0.99
3:L:37:SER:OG	3:L:137:ALA:O	1.83	0.97
1:E:40:LEU:HD21	1:E:226:LEU:HD23	1.48	0.96
3:L:180:SER:O	3:L:219:SER:OG	1.86	0.93
2:K:164:LEU:HD13	2:K:235:ILE:HG23	1.50	0.91

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	E	214/534 (40%)	159 (74%)	55 (26%)	0	100	100
1	F	214/534 (40%)	155 (72%)	59 (28%)	0	100	100
1	I	214/534 (40%)	178 (83%)	36 (17%)	0	100	100
1	J	214/534 (40%)	159 (74%)	55 (26%)	0	100	100
2	G	214/340 (63%)	160 (75%)	53 (25%)	1 (0%)	24	63
2	K	214/340 (63%)	154 (72%)	58 (27%)	2 (1%)	14	51
3	H	214/539 (40%)	182 (85%)	32 (15%)	0	100	100
3	L	214/539 (40%)	163 (76%)	50 (23%)	1 (0%)	24	63
All	All	1712/3894 (44%)	1310 (76%)	398 (23%)	4 (0%)	44	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	129	GLN
3	L	138	LEU
2	G	139	VAL
2	K	138	LEU

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	E	187/472 (40%)	187 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	187/472 (40%)	187 (100%)	0	100	100
1	I	187/472 (40%)	187 (100%)	0	100	100
1	J	187/472 (40%)	187 (100%)	0	100	100
2	G	173/278 (62%)	173 (100%)	0	100	100
2	K	173/278 (62%)	173 (100%)	0	100	100
3	H	175/451 (39%)	175 (100%)	0	100	100
3	L	175/451 (39%)	175 (100%)	0	100	100
All	All	1444/3346 (43%)	1444 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	52	HIS
1	F	46	ASN
2	G	74	GLN
2	G	174	GLN

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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

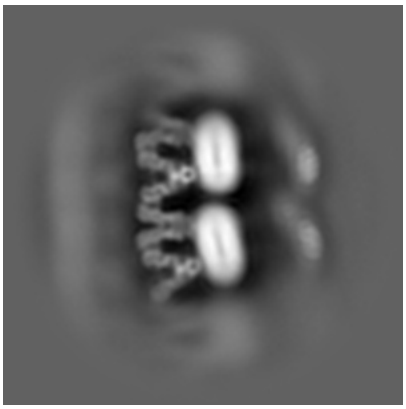
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60986. 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

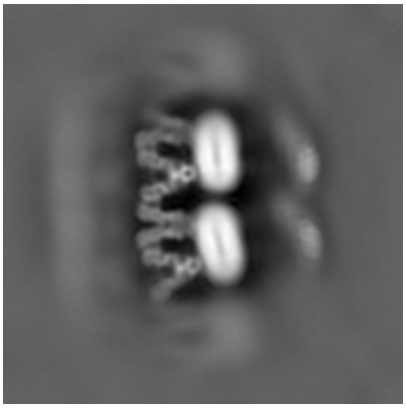


X

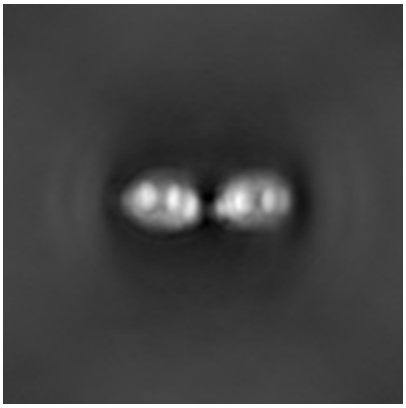
Y

Z

6.1.2 Raw map



X



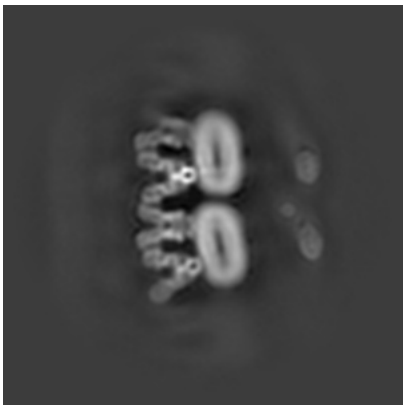
Y

Z

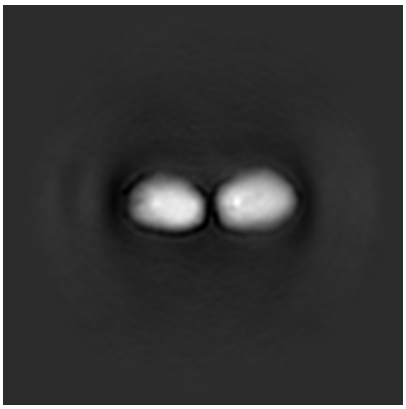
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

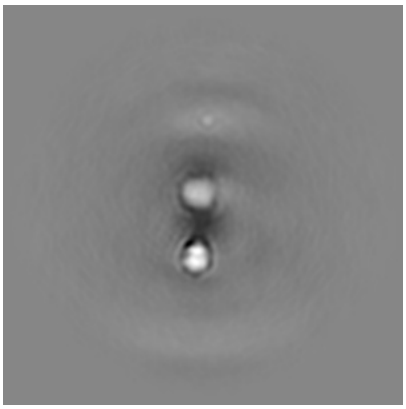
6.2.1 Primary map



X Index: 60

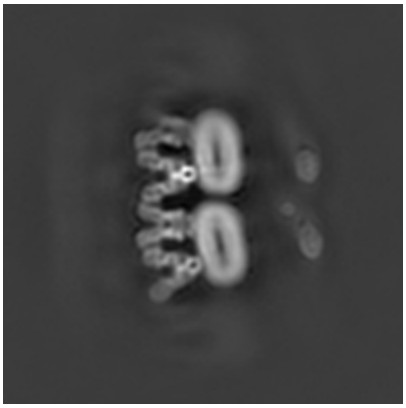


Y Index: 60

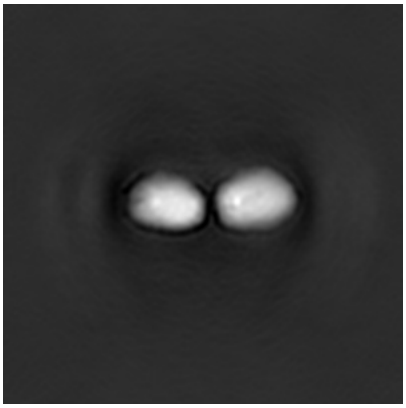


Z Index: 60

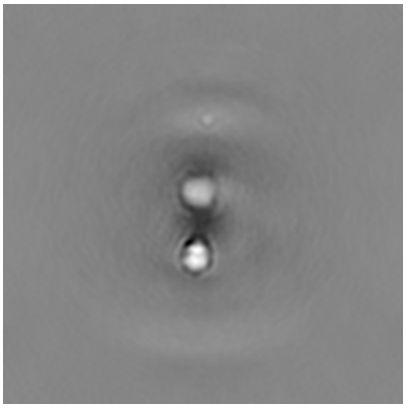
6.2.2 Raw map



X Index: 60



Y Index: 60

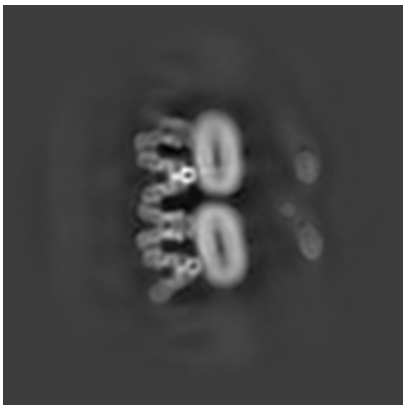


Z Index: 60

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

6.3 Largest variance slices (i)

6.3.1 Primary map

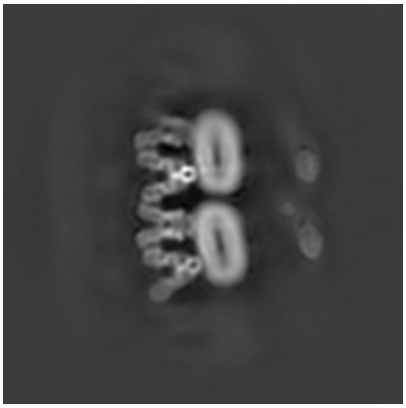


X Index: 60

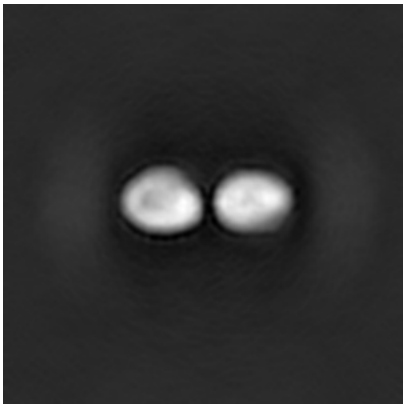
Y Index: 67

Z Index: 70

6.3.2 Raw map



X Index: 60



Y Index: 67

Z Index: 70

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

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

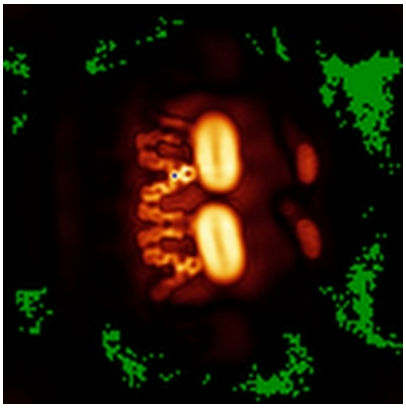
6.4.1 Primary map

X

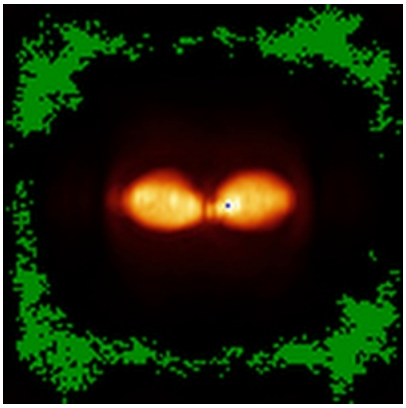
Y

Z

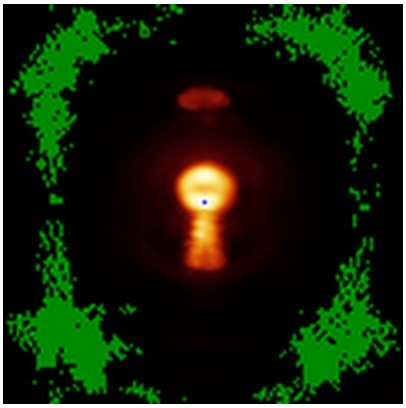
6.4.2 Raw map



X



Y

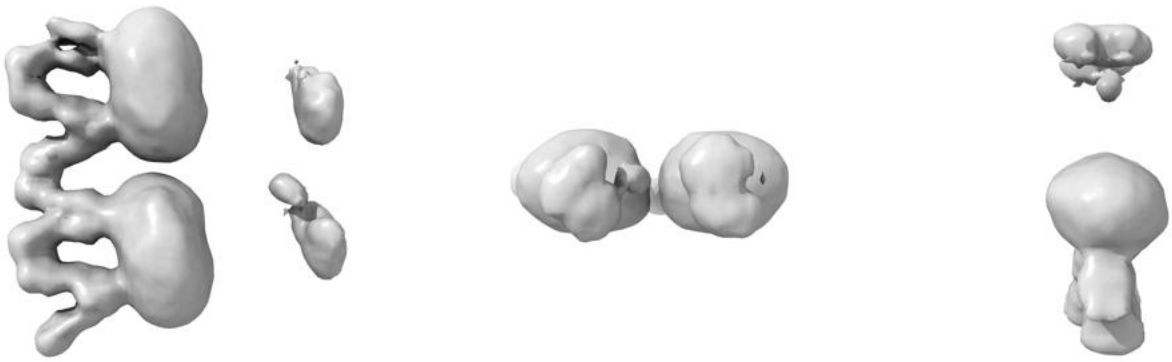


Z

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)

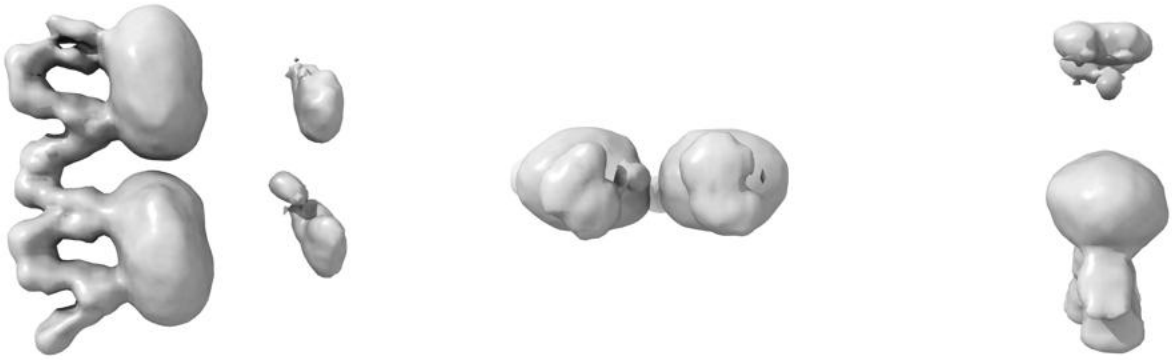
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

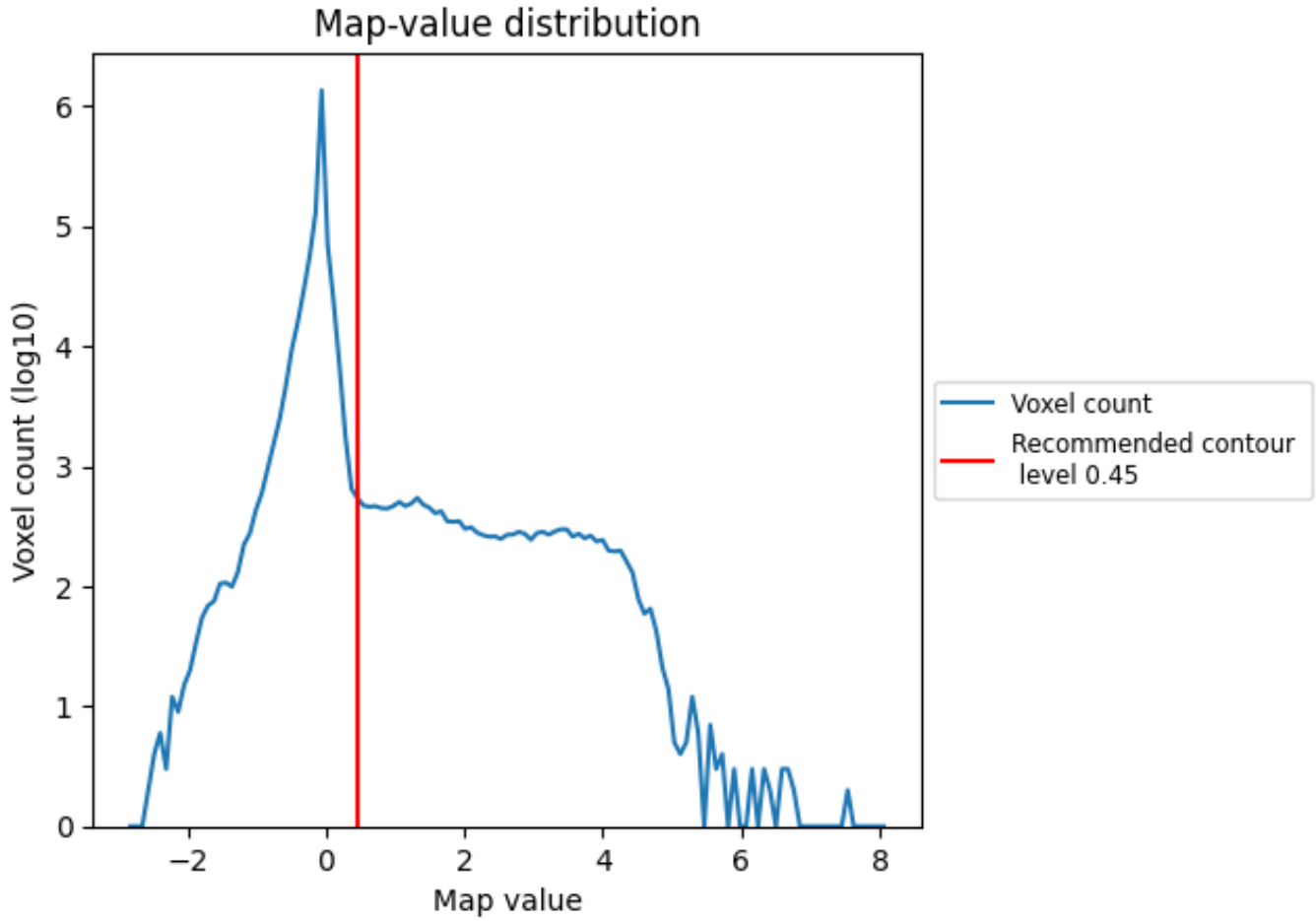
6.6 Mask visualisation (i)

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

7 Map analysis

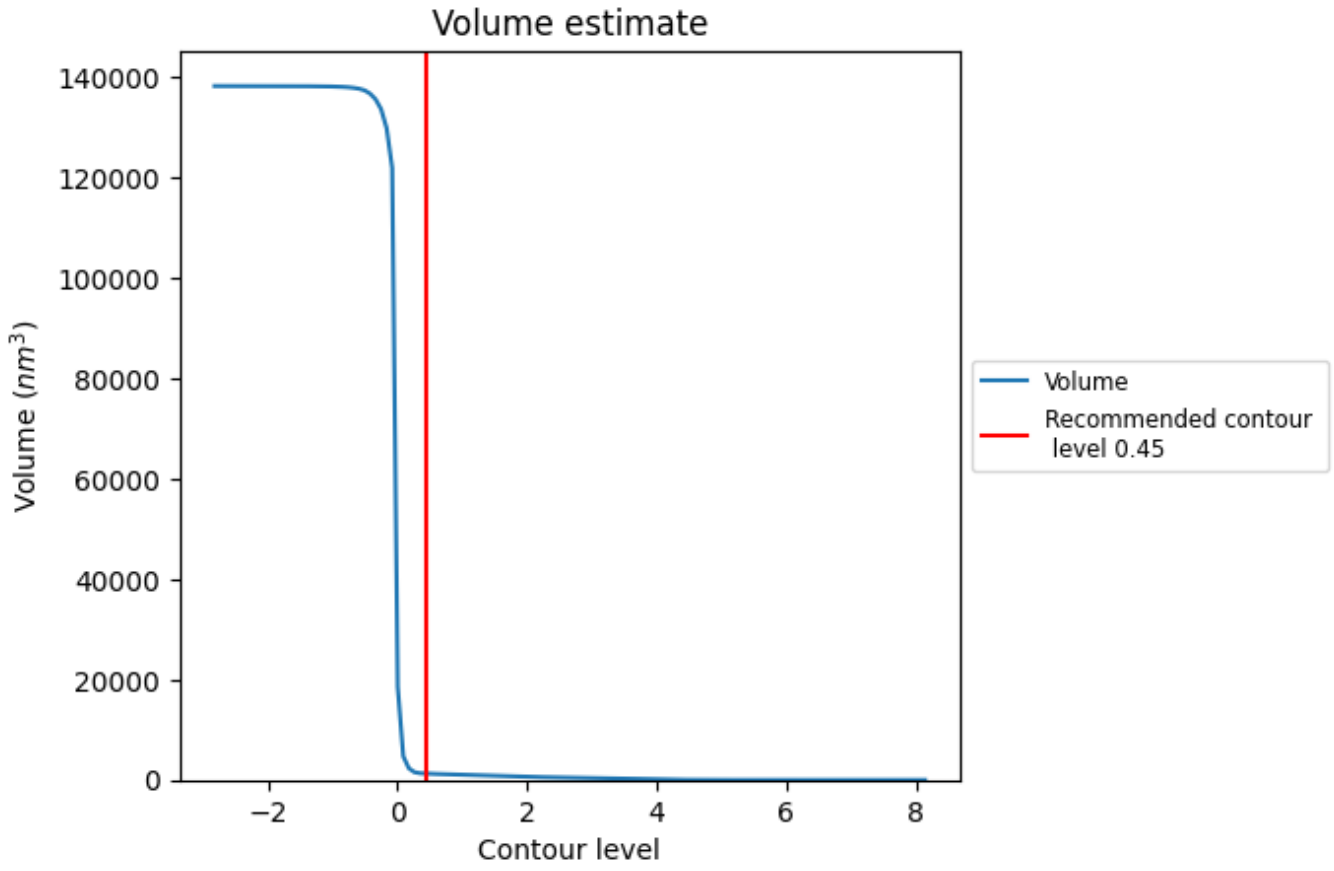
This section contains the results of statistical analysis of the map.

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.

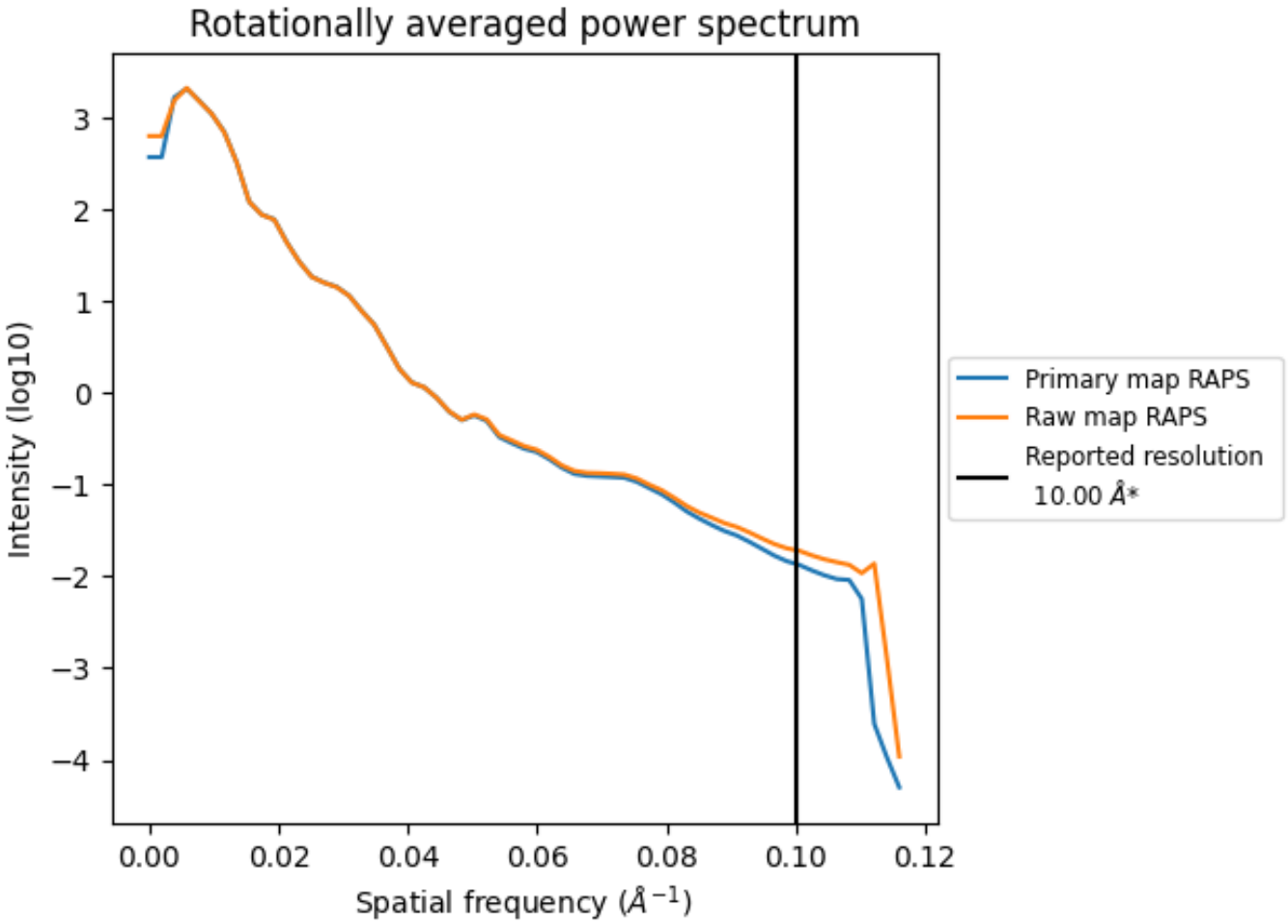
7.2 Volume estimate (i)



The volume at the recommended contour level is 1270 nm^3; this corresponds to an approximate mass of 1147 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)

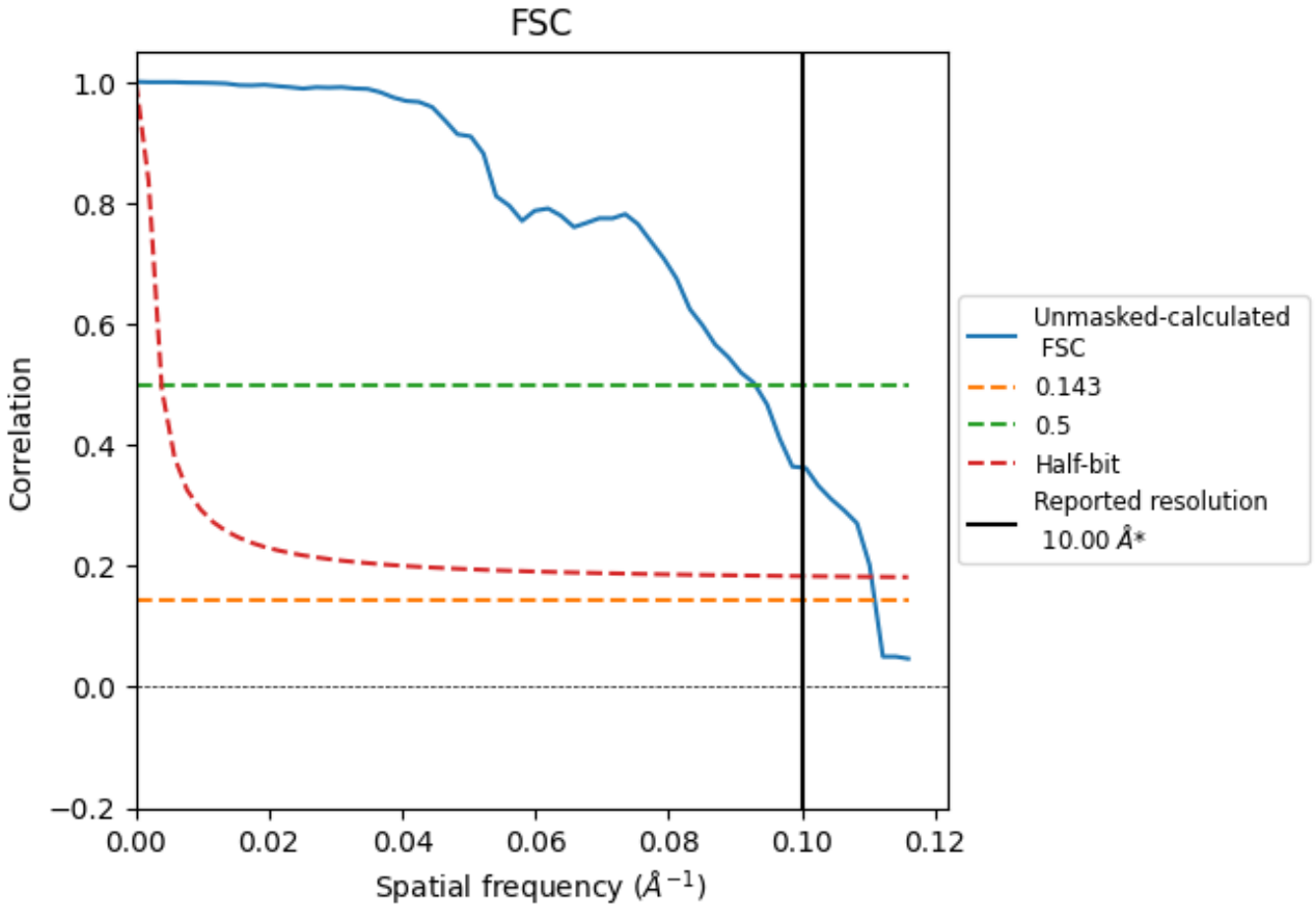


*Reported resolution corresponds to spatial frequency of 0.100 Å^{-1}

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 0.100 Å^{-1}

8.2 Resolution estimates (i)

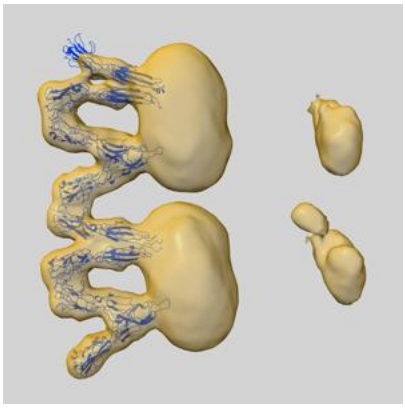
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.01	10.75	9.05

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

9 Map-model fit

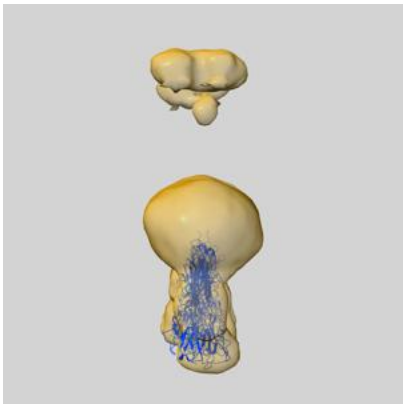
This section contains information regarding the fit between EMDB map EMD-60986 and PDB model 9IY6. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay



X

Y



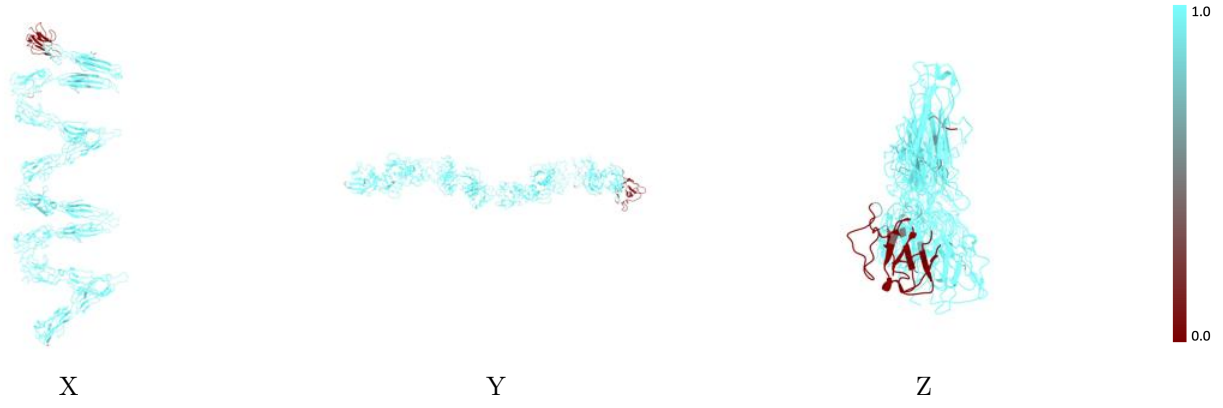
Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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

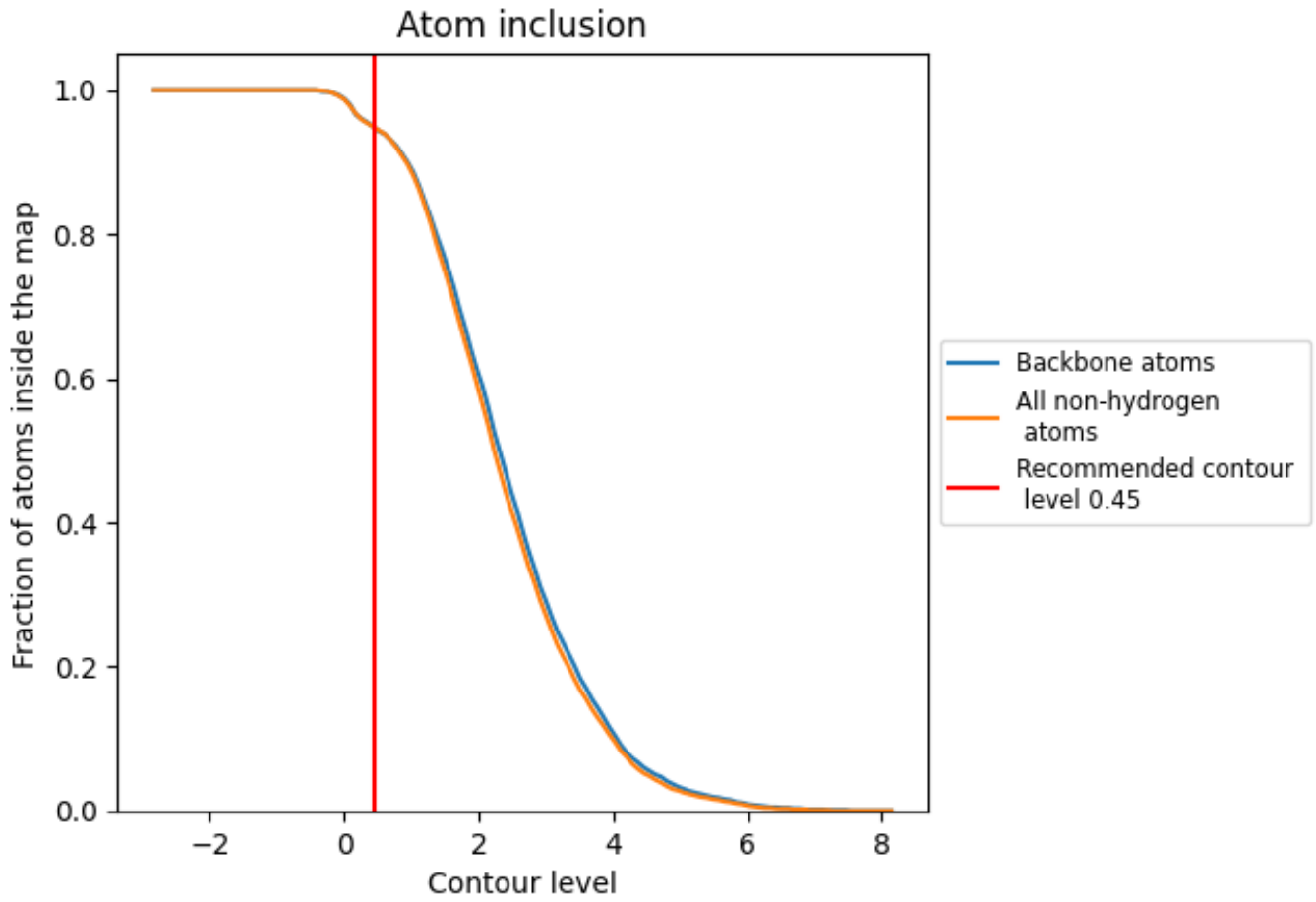
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.1070
E	1.0000	0.1240
F	1.0000	0.1170
G	0.9710	0.1040
H	0.6150	0.0850
I	0.9910	0.1060
J	1.0000	0.1120
K	1.0000	0.1040
L	1.0000	0.1020