Full wwPDB EM Validation Report

Sep 30, 2024 – 12:21 PM JST

PDB ID	:	8WYR
EMDB ID	:	EMD-37936
Title	:	Cryo-EM structure of human CD5L bound to IgM-Fc/J
Authors	:	Wang, Y.X.; Su, C.; Xiao, J.Y.
Deposited on	:	2023-10-31
Resolution	:	3.39 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

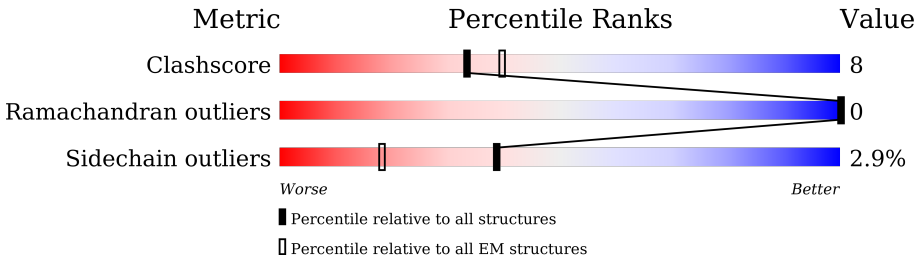
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.39 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	403	14% 44% 13% 42%
1	B	403	15% 43% 14% 43%
1	C	403	15% 42% 13% • 44%
1	D	403	15% 44% 12% 44%
1	E	403	12% 44% 12% 44%
1	F	403	15% 45% 10% • 44%
1	G	403	12% 39% 16% • 44%
1	H	403	13% 45% 12% 42%

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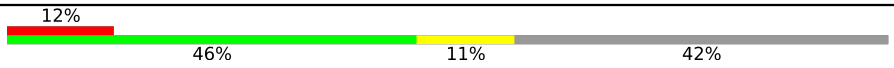
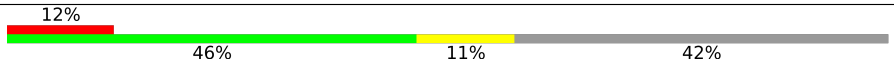
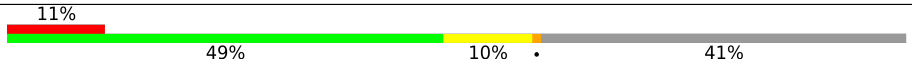
Mol	Chain	Length	Quality of chain
1	K	403	
1	L	403	
2	J	168	
3	M	359	
4	I	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20612 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-2,Isoform 1 of Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		
1	B	230	Total	C	N	O	S	0	0
			1780	1120	302	350	8		
1	C	226	Total	C	N	O	S	0	0
			1757	1107	298	344	8		
1	D	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
1	E	226	Total	C	N	O	S	0	0
			1757	1107	298	344	8		
1	F	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
1	G	225	Total	C	N	O	S	0	0
			1749	1103	297	341	8		
1	H	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		
1	K	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		
1	L	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		

There are 340 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	SER	-	linker	UNP P60568
A	196	ALA	-	linker	UNP P60568
A	197	TRP	-	linker	UNP P60568
A	198	SER	-	linker	UNP P60568
A	199	HIS	-	linker	UNP P60568
A	200	PRO	-	linker	UNP P60568
A	201	GLN	-	linker	UNP P60568
A	202	PHE	-	linker	UNP P60568
A	203	GLU	-	linker	UNP P60568
A	204	LYS	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
A	205	GLY	-	linker	UNP P60568
A	206	GLY	-	linker	UNP P60568
A	207	GLY	-	linker	UNP P60568
A	208	SER	-	linker	UNP P60568
A	209	GLY	-	linker	UNP P60568
A	210	GLY	-	linker	UNP P60568
A	211	GLY	-	linker	UNP P60568
A	212	SER	-	linker	UNP P60568
A	213	GLY	-	linker	UNP P60568
A	214	GLY	-	linker	UNP P60568
A	215	SER	-	linker	UNP P60568
A	216	ALA	-	linker	UNP P60568
A	217	TRP	-	linker	UNP P60568
A	218	SER	-	linker	UNP P60568
A	219	HIS	-	linker	UNP P60568
A	220	PRO	-	linker	UNP P60568
A	221	GLN	-	linker	UNP P60568
A	222	PHE	-	linker	UNP P60568
A	223	GLU	-	linker	UNP P60568
A	224	LYS	-	linker	UNP P60568
A	225	ILE	-	linker	UNP P60568
A	226	ASP	-	linker	UNP P60568
A	227	THR	-	linker	UNP P60568
A	228	THR	-	linker	UNP P60568
B	195	SER	-	linker	UNP P60568
B	196	ALA	-	linker	UNP P60568
B	197	TRP	-	linker	UNP P60568
B	198	SER	-	linker	UNP P60568
B	199	HIS	-	linker	UNP P60568
B	200	PRO	-	linker	UNP P60568
B	201	GLN	-	linker	UNP P60568
B	202	PHE	-	linker	UNP P60568
B	203	GLU	-	linker	UNP P60568
B	204	LYS	-	linker	UNP P60568
B	205	GLY	-	linker	UNP P60568
B	206	GLY	-	linker	UNP P60568
B	207	GLY	-	linker	UNP P60568
B	208	SER	-	linker	UNP P60568
B	209	GLY	-	linker	UNP P60568
B	210	GLY	-	linker	UNP P60568
B	211	GLY	-	linker	UNP P60568
B	212	SER	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
B	213	GLY	-	linker	UNP P60568
B	214	GLY	-	linker	UNP P60568
B	215	SER	-	linker	UNP P60568
B	216	ALA	-	linker	UNP P60568
B	217	TRP	-	linker	UNP P60568
B	218	SER	-	linker	UNP P60568
B	219	HIS	-	linker	UNP P60568
B	220	PRO	-	linker	UNP P60568
B	221	GLN	-	linker	UNP P60568
B	222	PHE	-	linker	UNP P60568
B	223	GLU	-	linker	UNP P60568
B	224	LYS	-	linker	UNP P60568
B	225	ILE	-	linker	UNP P60568
B	226	ASP	-	linker	UNP P60568
B	227	THR	-	linker	UNP P60568
B	228	THR	-	linker	UNP P60568
C	195	SER	-	linker	UNP P60568
C	196	ALA	-	linker	UNP P60568
C	197	TRP	-	linker	UNP P60568
C	198	SER	-	linker	UNP P60568
C	199	HIS	-	linker	UNP P60568
C	200	PRO	-	linker	UNP P60568
C	201	GLN	-	linker	UNP P60568
C	202	PHE	-	linker	UNP P60568
C	203	GLU	-	linker	UNP P60568
C	204	LYS	-	linker	UNP P60568
C	205	GLY	-	linker	UNP P60568
C	206	GLY	-	linker	UNP P60568
C	207	GLY	-	linker	UNP P60568
C	208	SER	-	linker	UNP P60568
C	209	GLY	-	linker	UNP P60568
C	210	GLY	-	linker	UNP P60568
C	211	GLY	-	linker	UNP P60568
C	212	SER	-	linker	UNP P60568
C	213	GLY	-	linker	UNP P60568
C	214	GLY	-	linker	UNP P60568
C	215	SER	-	linker	UNP P60568
C	216	ALA	-	linker	UNP P60568
C	217	TRP	-	linker	UNP P60568
C	218	SER	-	linker	UNP P60568
C	219	HIS	-	linker	UNP P60568
C	220	PRO	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
C	221	GLN	-	linker	UNP P60568
C	222	PHE	-	linker	UNP P60568
C	223	GLU	-	linker	UNP P60568
C	224	LYS	-	linker	UNP P60568
C	225	ILE	-	linker	UNP P60568
C	226	ASP	-	linker	UNP P60568
C	227	THR	-	linker	UNP P60568
C	228	THR	-	linker	UNP P60568
D	195	SER	-	linker	UNP P60568
D	196	ALA	-	linker	UNP P60568
D	197	TRP	-	linker	UNP P60568
D	198	SER	-	linker	UNP P60568
D	199	HIS	-	linker	UNP P60568
D	200	PRO	-	linker	UNP P60568
D	201	GLN	-	linker	UNP P60568
D	202	PHE	-	linker	UNP P60568
D	203	GLU	-	linker	UNP P60568
D	204	LYS	-	linker	UNP P60568
D	205	GLY	-	linker	UNP P60568
D	206	GLY	-	linker	UNP P60568
D	207	GLY	-	linker	UNP P60568
D	208	SER	-	linker	UNP P60568
D	209	GLY	-	linker	UNP P60568
D	210	GLY	-	linker	UNP P60568
D	211	GLY	-	linker	UNP P60568
D	212	SER	-	linker	UNP P60568
D	213	GLY	-	linker	UNP P60568
D	214	GLY	-	linker	UNP P60568
D	215	SER	-	linker	UNP P60568
D	216	ALA	-	linker	UNP P60568
D	217	TRP	-	linker	UNP P60568
D	218	SER	-	linker	UNP P60568
D	219	HIS	-	linker	UNP P60568
D	220	PRO	-	linker	UNP P60568
D	221	GLN	-	linker	UNP P60568
D	222	PHE	-	linker	UNP P60568
D	223	GLU	-	linker	UNP P60568
D	224	LYS	-	linker	UNP P60568
D	225	ILE	-	linker	UNP P60568
D	226	ASP	-	linker	UNP P60568
D	227	THR	-	linker	UNP P60568
D	228	THR	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
E	195	SER	-	linker	UNP P60568
E	196	ALA	-	linker	UNP P60568
E	197	TRP	-	linker	UNP P60568
E	198	SER	-	linker	UNP P60568
E	199	HIS	-	linker	UNP P60568
E	200	PRO	-	linker	UNP P60568
E	201	GLN	-	linker	UNP P60568
E	202	PHE	-	linker	UNP P60568
E	203	GLU	-	linker	UNP P60568
E	204	LYS	-	linker	UNP P60568
E	205	GLY	-	linker	UNP P60568
E	206	GLY	-	linker	UNP P60568
E	207	GLY	-	linker	UNP P60568
E	208	SER	-	linker	UNP P60568
E	209	GLY	-	linker	UNP P60568
E	210	GLY	-	linker	UNP P60568
E	211	GLY	-	linker	UNP P60568
E	212	SER	-	linker	UNP P60568
E	213	GLY	-	linker	UNP P60568
E	214	GLY	-	linker	UNP P60568
E	215	SER	-	linker	UNP P60568
E	216	ALA	-	linker	UNP P60568
E	217	TRP	-	linker	UNP P60568
E	218	SER	-	linker	UNP P60568
E	219	HIS	-	linker	UNP P60568
E	220	PRO	-	linker	UNP P60568
E	221	GLN	-	linker	UNP P60568
E	222	PHE	-	linker	UNP P60568
E	223	GLU	-	linker	UNP P60568
E	224	LYS	-	linker	UNP P60568
E	225	ILE	-	linker	UNP P60568
E	226	ASP	-	linker	UNP P60568
E	227	THR	-	linker	UNP P60568
E	228	THR	-	linker	UNP P60568
F	195	SER	-	linker	UNP P60568
F	196	ALA	-	linker	UNP P60568
F	197	TRP	-	linker	UNP P60568
F	198	SER	-	linker	UNP P60568
F	199	HIS	-	linker	UNP P60568
F	200	PRO	-	linker	UNP P60568
F	201	GLN	-	linker	UNP P60568
F	202	PHE	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
F	203	GLU	-	linker	UNP P60568
F	204	LYS	-	linker	UNP P60568
F	205	GLY	-	linker	UNP P60568
F	206	GLY	-	linker	UNP P60568
F	207	GLY	-	linker	UNP P60568
F	208	SER	-	linker	UNP P60568
F	209	GLY	-	linker	UNP P60568
F	210	GLY	-	linker	UNP P60568
F	211	GLY	-	linker	UNP P60568
F	212	SER	-	linker	UNP P60568
F	213	GLY	-	linker	UNP P60568
F	214	GLY	-	linker	UNP P60568
F	215	SER	-	linker	UNP P60568
F	216	ALA	-	linker	UNP P60568
F	217	TRP	-	linker	UNP P60568
F	218	SER	-	linker	UNP P60568
F	219	HIS	-	linker	UNP P60568
F	220	PRO	-	linker	UNP P60568
F	221	GLN	-	linker	UNP P60568
F	222	PHE	-	linker	UNP P60568
F	223	GLU	-	linker	UNP P60568
F	224	LYS	-	linker	UNP P60568
F	225	ILE	-	linker	UNP P60568
F	226	ASP	-	linker	UNP P60568
F	227	THR	-	linker	UNP P60568
F	228	THR	-	linker	UNP P60568
G	195	SER	-	linker	UNP P60568
G	196	ALA	-	linker	UNP P60568
G	197	TRP	-	linker	UNP P60568
G	198	SER	-	linker	UNP P60568
G	199	HIS	-	linker	UNP P60568
G	200	PRO	-	linker	UNP P60568
G	201	GLN	-	linker	UNP P60568
G	202	PHE	-	linker	UNP P60568
G	203	GLU	-	linker	UNP P60568
G	204	LYS	-	linker	UNP P60568
G	205	GLY	-	linker	UNP P60568
G	206	GLY	-	linker	UNP P60568
G	207	GLY	-	linker	UNP P60568
G	208	SER	-	linker	UNP P60568
G	209	GLY	-	linker	UNP P60568
G	210	GLY	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
G	211	GLY	-	linker	UNP P60568
G	212	SER	-	linker	UNP P60568
G	213	GLY	-	linker	UNP P60568
G	214	GLY	-	linker	UNP P60568
G	215	SER	-	linker	UNP P60568
G	216	ALA	-	linker	UNP P60568
G	217	TRP	-	linker	UNP P60568
G	218	SER	-	linker	UNP P60568
G	219	HIS	-	linker	UNP P60568
G	220	PRO	-	linker	UNP P60568
G	221	GLN	-	linker	UNP P60568
G	222	PHE	-	linker	UNP P60568
G	223	GLU	-	linker	UNP P60568
G	224	LYS	-	linker	UNP P60568
G	225	ILE	-	linker	UNP P60568
G	226	ASP	-	linker	UNP P60568
G	227	THR	-	linker	UNP P60568
G	228	THR	-	linker	UNP P60568
H	195	SER	-	linker	UNP P60568
H	196	ALA	-	linker	UNP P60568
H	197	TRP	-	linker	UNP P60568
H	198	SER	-	linker	UNP P60568
H	199	HIS	-	linker	UNP P60568
H	200	PRO	-	linker	UNP P60568
H	201	GLN	-	linker	UNP P60568
H	202	PHE	-	linker	UNP P60568
H	203	GLU	-	linker	UNP P60568
H	204	LYS	-	linker	UNP P60568
H	205	GLY	-	linker	UNP P60568
H	206	GLY	-	linker	UNP P60568
H	207	GLY	-	linker	UNP P60568
H	208	SER	-	linker	UNP P60568
H	209	GLY	-	linker	UNP P60568
H	210	GLY	-	linker	UNP P60568
H	211	GLY	-	linker	UNP P60568
H	212	SER	-	linker	UNP P60568
H	213	GLY	-	linker	UNP P60568
H	214	GLY	-	linker	UNP P60568
H	215	SER	-	linker	UNP P60568
H	216	ALA	-	linker	UNP P60568
H	217	TRP	-	linker	UNP P60568
H	218	SER	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
H	219	HIS	-	linker	UNP P60568
H	220	PRO	-	linker	UNP P60568
H	221	GLN	-	linker	UNP P60568
H	222	PHE	-	linker	UNP P60568
H	223	GLU	-	linker	UNP P60568
H	224	LYS	-	linker	UNP P60568
H	225	ILE	-	linker	UNP P60568
H	226	ASP	-	linker	UNP P60568
H	227	THR	-	linker	UNP P60568
H	228	THR	-	linker	UNP P60568
K	195	SER	-	linker	UNP P60568
K	196	ALA	-	linker	UNP P60568
K	197	TRP	-	linker	UNP P60568
K	198	SER	-	linker	UNP P60568
K	199	HIS	-	linker	UNP P60568
K	200	PRO	-	linker	UNP P60568
K	201	GLN	-	linker	UNP P60568
K	202	PHE	-	linker	UNP P60568
K	203	GLU	-	linker	UNP P60568
K	204	LYS	-	linker	UNP P60568
K	205	GLY	-	linker	UNP P60568
K	206	GLY	-	linker	UNP P60568
K	207	GLY	-	linker	UNP P60568
K	208	SER	-	linker	UNP P60568
K	209	GLY	-	linker	UNP P60568
K	210	GLY	-	linker	UNP P60568
K	211	GLY	-	linker	UNP P60568
K	212	SER	-	linker	UNP P60568
K	213	GLY	-	linker	UNP P60568
K	214	GLY	-	linker	UNP P60568
K	215	SER	-	linker	UNP P60568
K	216	ALA	-	linker	UNP P60568
K	217	TRP	-	linker	UNP P60568
K	218	SER	-	linker	UNP P60568
K	219	HIS	-	linker	UNP P60568
K	220	PRO	-	linker	UNP P60568
K	221	GLN	-	linker	UNP P60568
K	222	PHE	-	linker	UNP P60568
K	223	GLU	-	linker	UNP P60568
K	224	LYS	-	linker	UNP P60568
K	225	ILE	-	linker	UNP P60568
K	226	ASP	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
K	227	THR	-	linker	UNP P60568
K	228	THR	-	linker	UNP P60568
L	195	SER	-	linker	UNP P60568
L	196	ALA	-	linker	UNP P60568
L	197	TRP	-	linker	UNP P60568
L	198	SER	-	linker	UNP P60568
L	199	HIS	-	linker	UNP P60568
L	200	PRO	-	linker	UNP P60568
L	201	GLN	-	linker	UNP P60568
L	202	PHE	-	linker	UNP P60568
L	203	GLU	-	linker	UNP P60568
L	204	LYS	-	linker	UNP P60568
L	205	GLY	-	linker	UNP P60568
L	206	GLY	-	linker	UNP P60568
L	207	GLY	-	linker	UNP P60568
L	208	SER	-	linker	UNP P60568
L	209	GLY	-	linker	UNP P60568
L	210	GLY	-	linker	UNP P60568
L	211	GLY	-	linker	UNP P60568
L	212	SER	-	linker	UNP P60568
L	213	GLY	-	linker	UNP P60568
L	214	GLY	-	linker	UNP P60568
L	215	SER	-	linker	UNP P60568
L	216	ALA	-	linker	UNP P60568
L	217	TRP	-	linker	UNP P60568
L	218	SER	-	linker	UNP P60568
L	219	HIS	-	linker	UNP P60568
L	220	PRO	-	linker	UNP P60568
L	221	GLN	-	linker	UNP P60568
L	222	PHE	-	linker	UNP P60568
L	223	GLU	-	linker	UNP P60568
L	224	LYS	-	linker	UNP P60568
L	225	ILE	-	linker	UNP P60568
L	226	ASP	-	linker	UNP P60568
L	227	THR	-	linker	UNP P60568
L	228	THR	-	linker	UNP P60568

- Molecule 2 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	127	Total	C	N	O	S	0	0
			1010	622	176	203	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	137	TYR	-	expression tag	UNP P01591
J	138	PRO	-	expression tag	UNP P01591
J	139	TYR	-	expression tag	UNP P01591
J	140	ASP	-	expression tag	UNP P01591
J	141	VAL	-	expression tag	UNP P01591
J	142	PRO	-	expression tag	UNP P01591
J	143	ASP	-	expression tag	UNP P01591
J	144	TYR	-	expression tag	UNP P01591
J	145	ALA	-	expression tag	UNP P01591

- Molecule 3 is a protein called Interleukin-2,CD5 antigen-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	213	Total	C	N	O	S	0	0
			1669	1026	315	309	19		

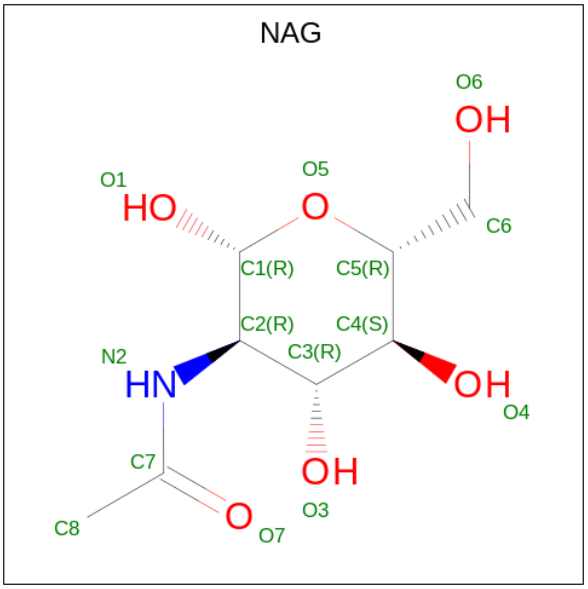
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	10	ARG	-	linker	UNP P60568
M	11	ILE	-	linker	UNP P60568
M	12	HIS	-	linker	UNP P60568
M	13	HIS	-	linker	UNP P60568
M	14	HIS	-	linker	UNP P60568
M	15	HIS	-	linker	UNP P60568
M	16	HIS	-	linker	UNP P60568
M	17	HIS	-	linker	UNP P60568
M	18	HIS	-	linker	UNP P60568
M	19	HIS	-	linker	UNP P60568

- 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	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

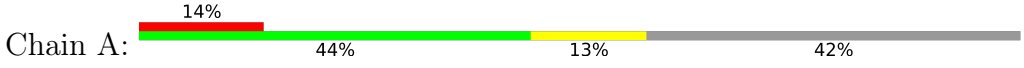
Mol	Chain	Residues	Atoms		AltConf
6	M	2	Total	Ca	0
			2	2	

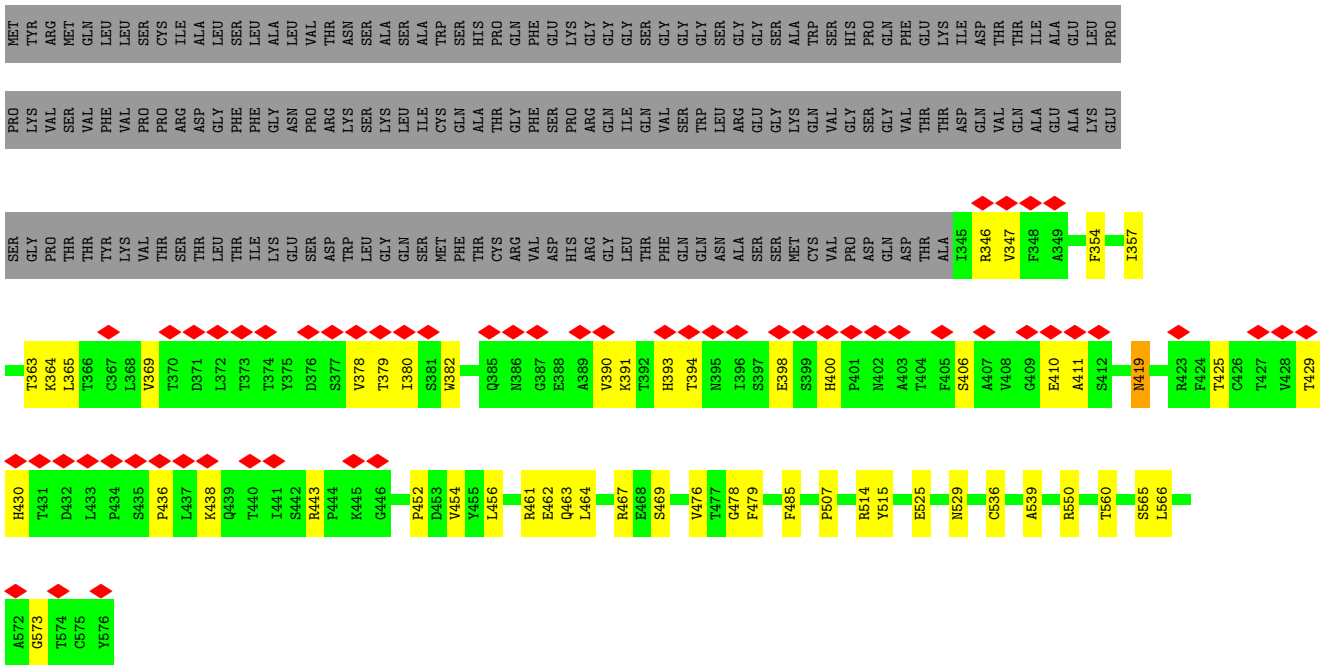
3 Residue-property plots (i)

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-2,Isoform 1 of Immunoglobulin heavy constant mu

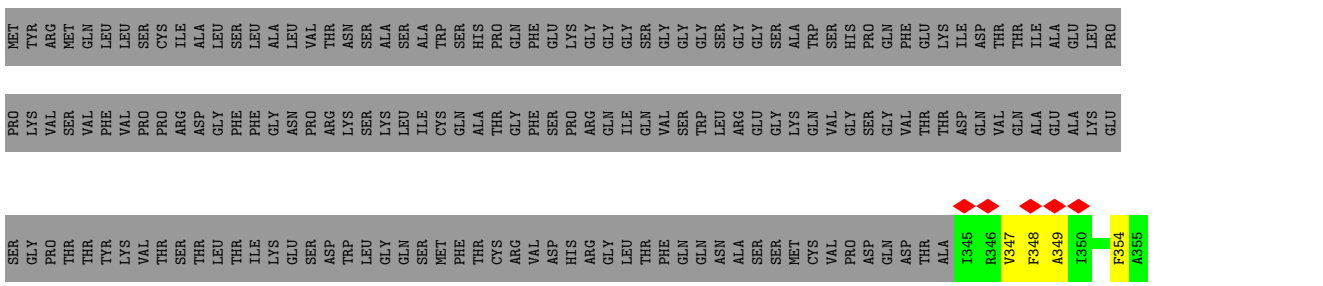
Chain A:

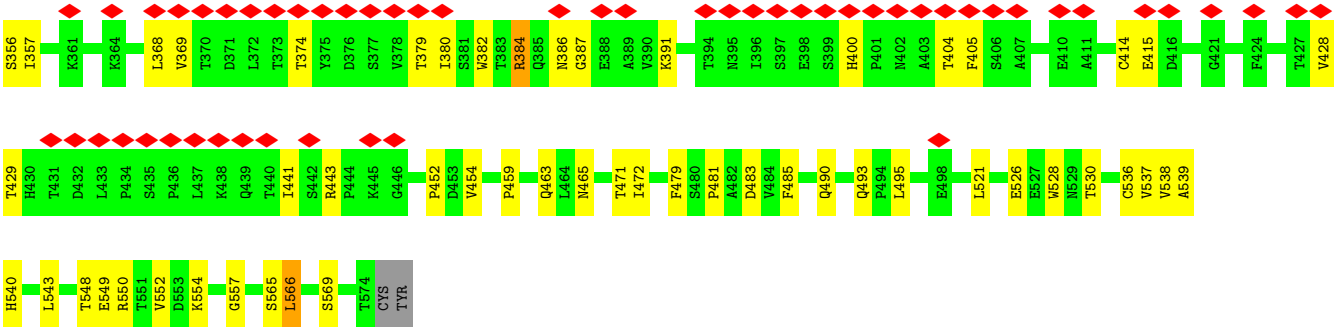




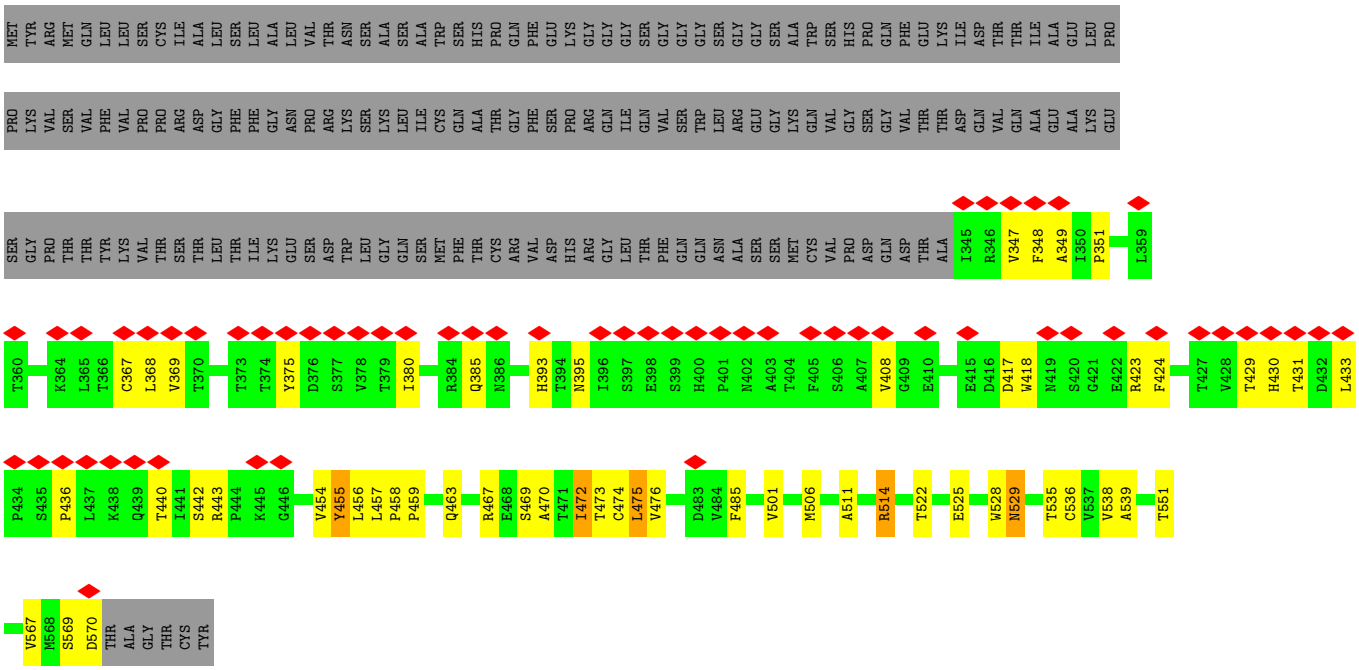
• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu

Chain B:

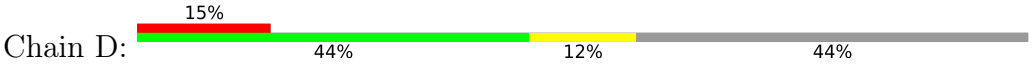


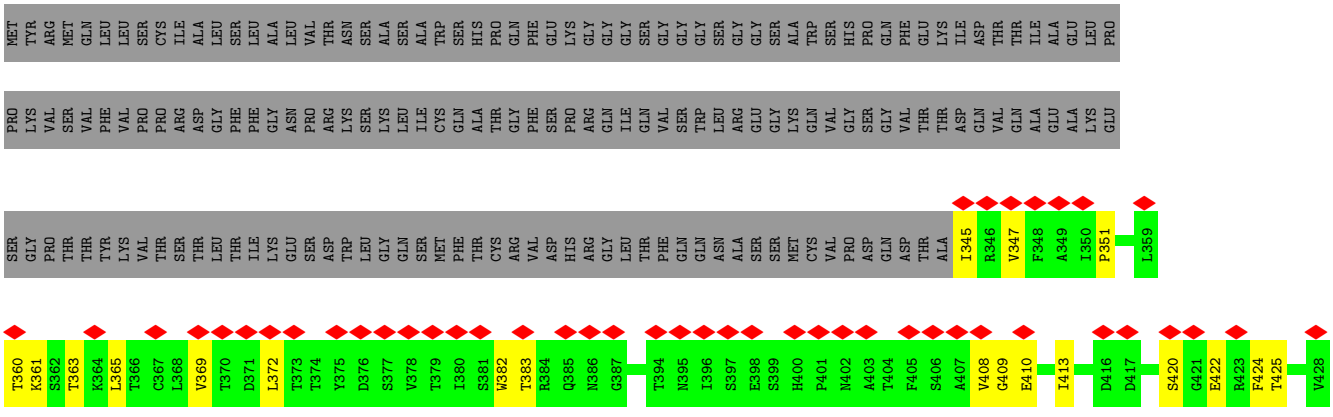


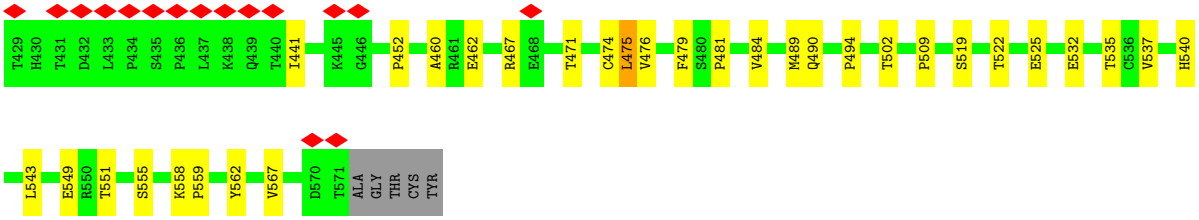
• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu



• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu

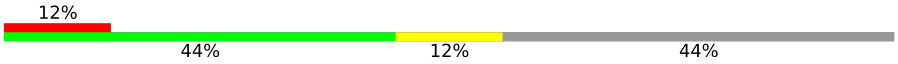


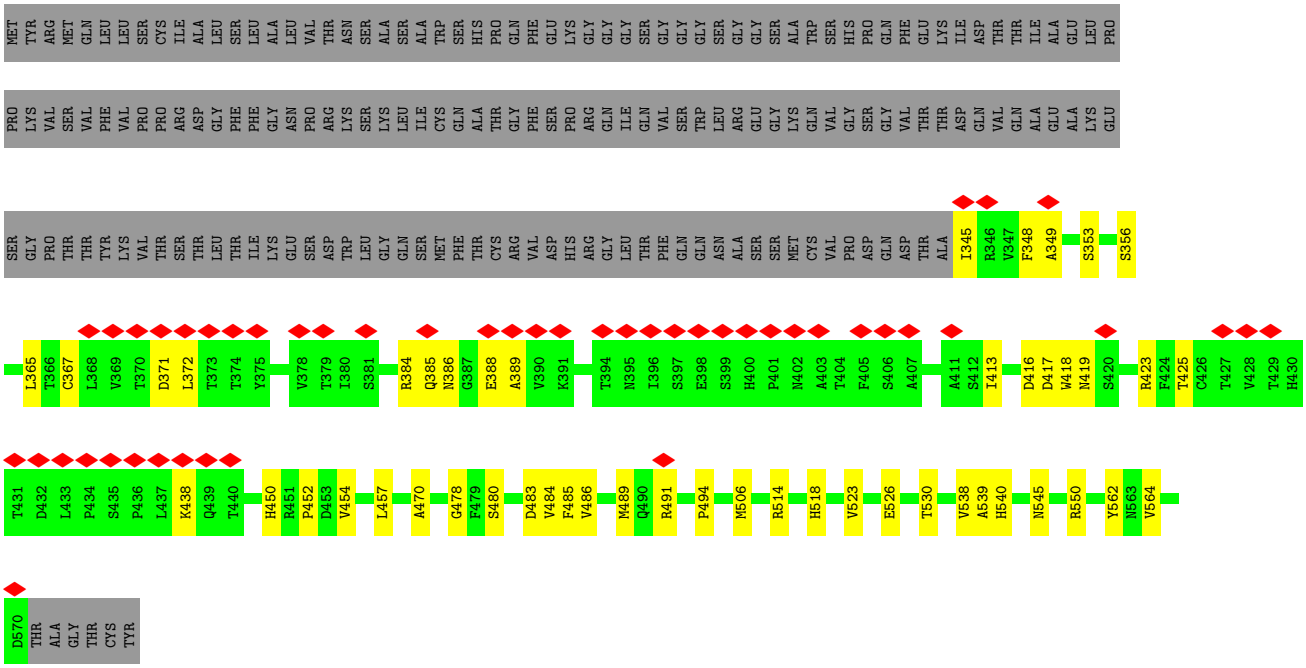




• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu

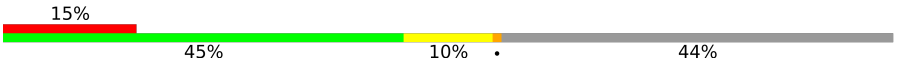
Chain E:

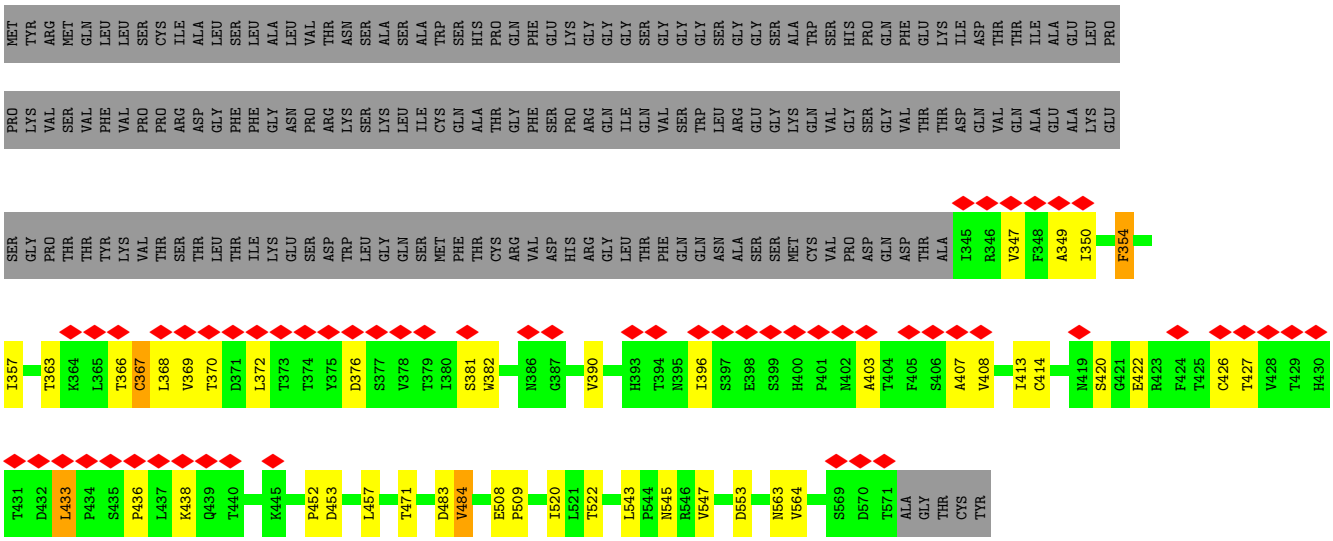




• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu

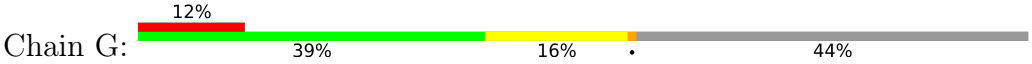
Chain F:

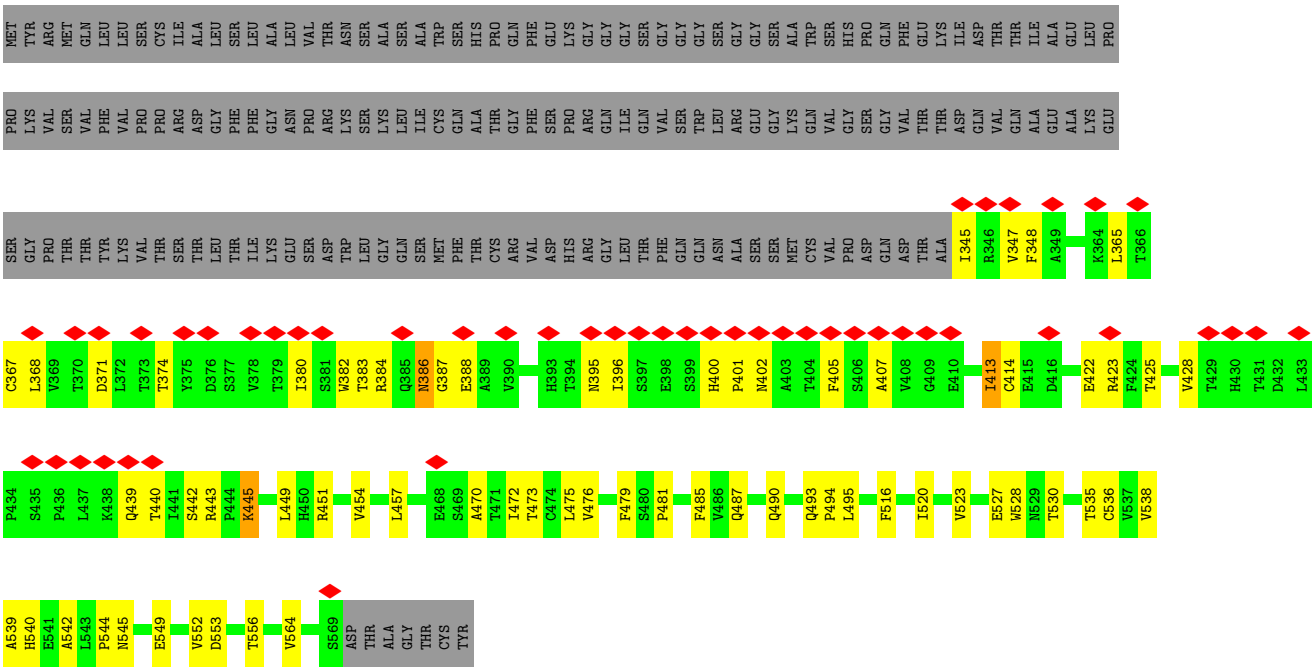




• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu

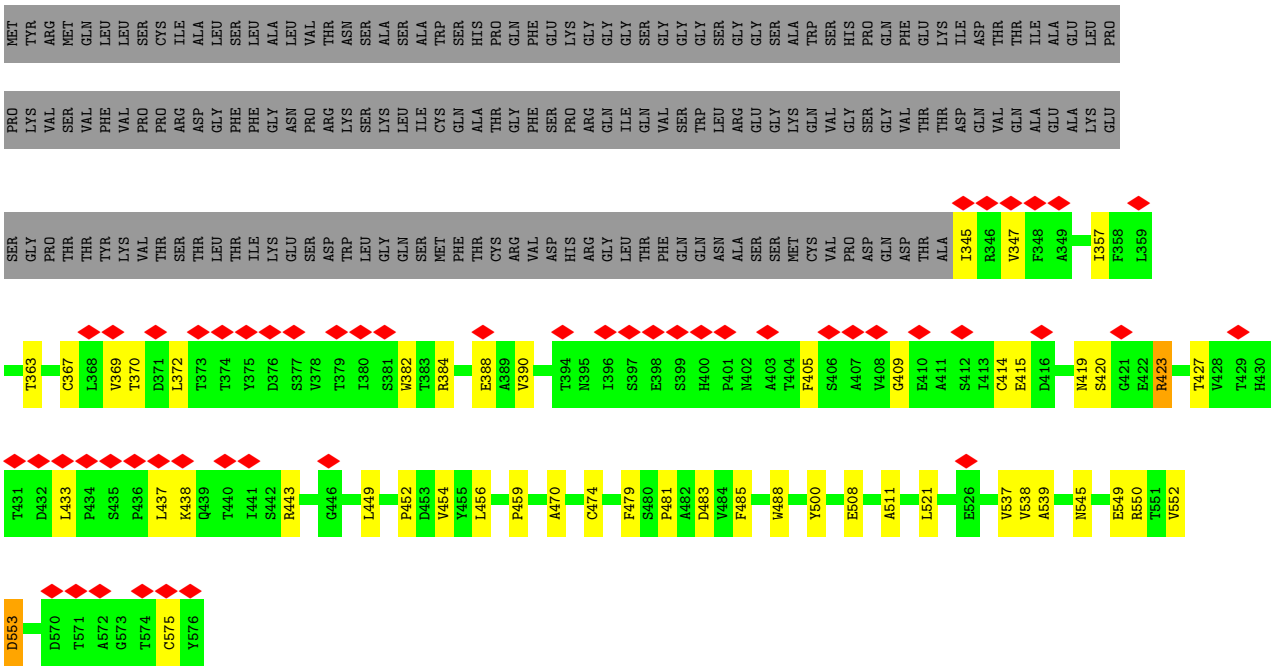
Chain G:





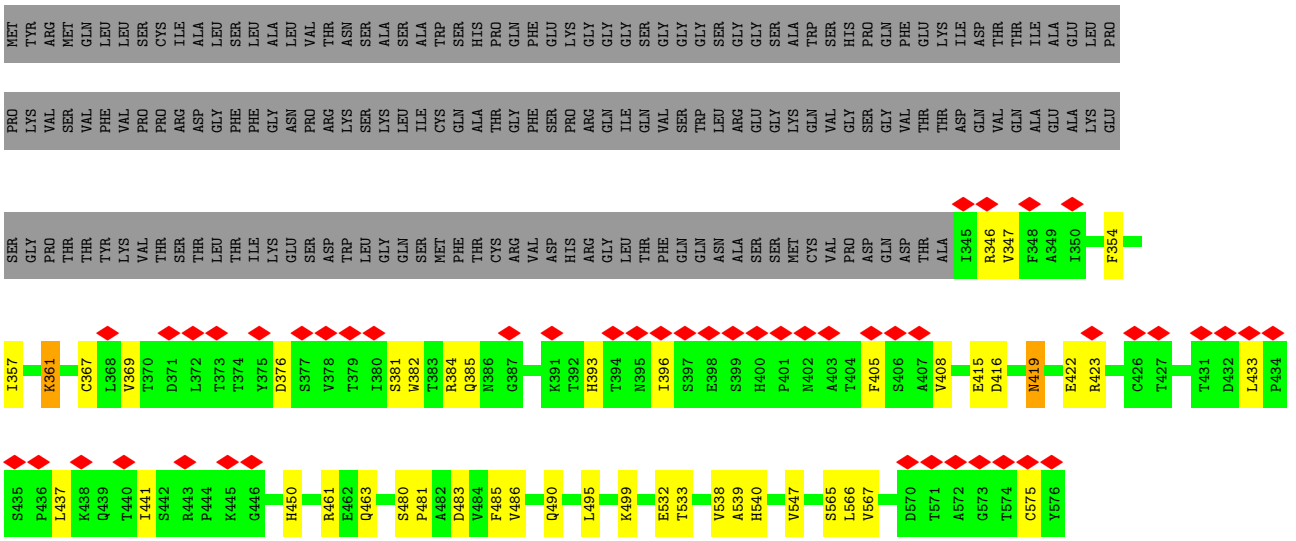
• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu

Chain H:



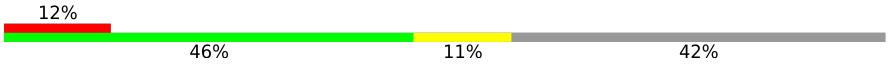
• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu

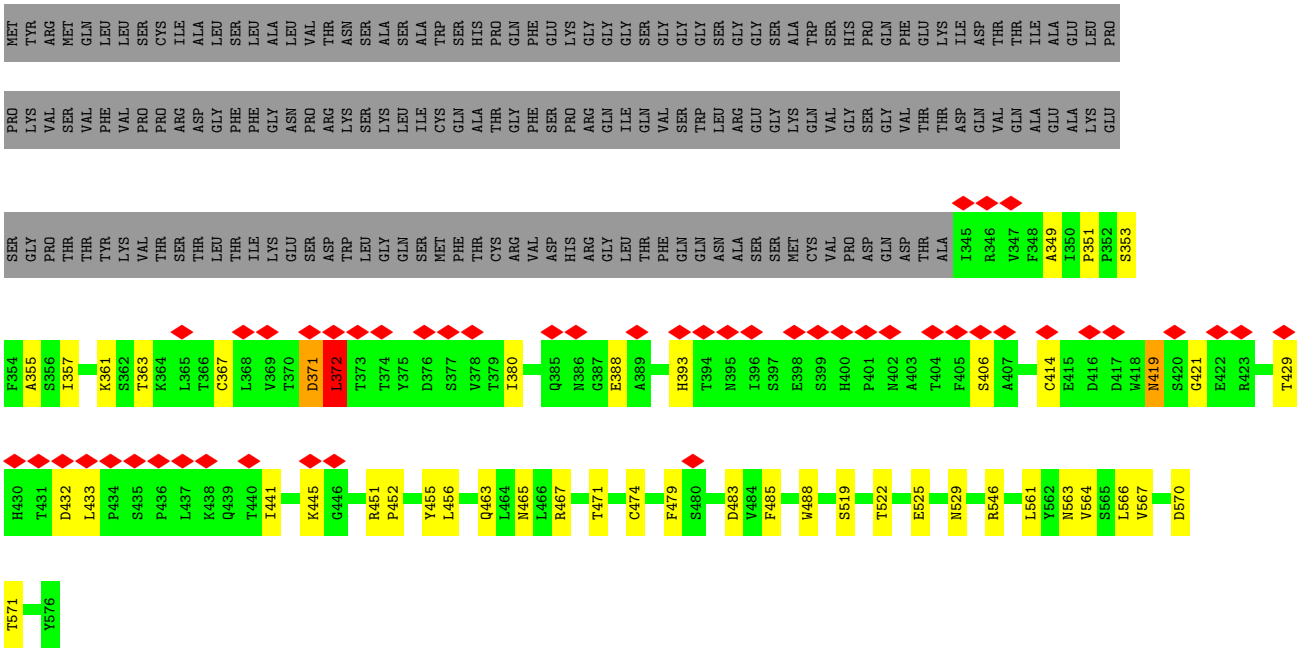
Chain K:



• Molecule 1: Interleukin-2,Isoform 1 of Immunoglobulin heavy constant mu

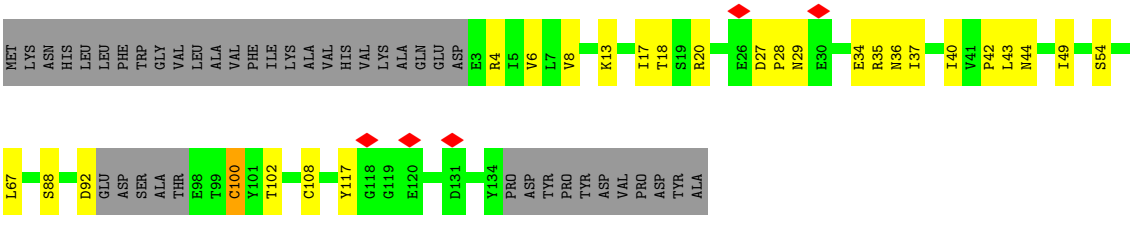
Chain L:





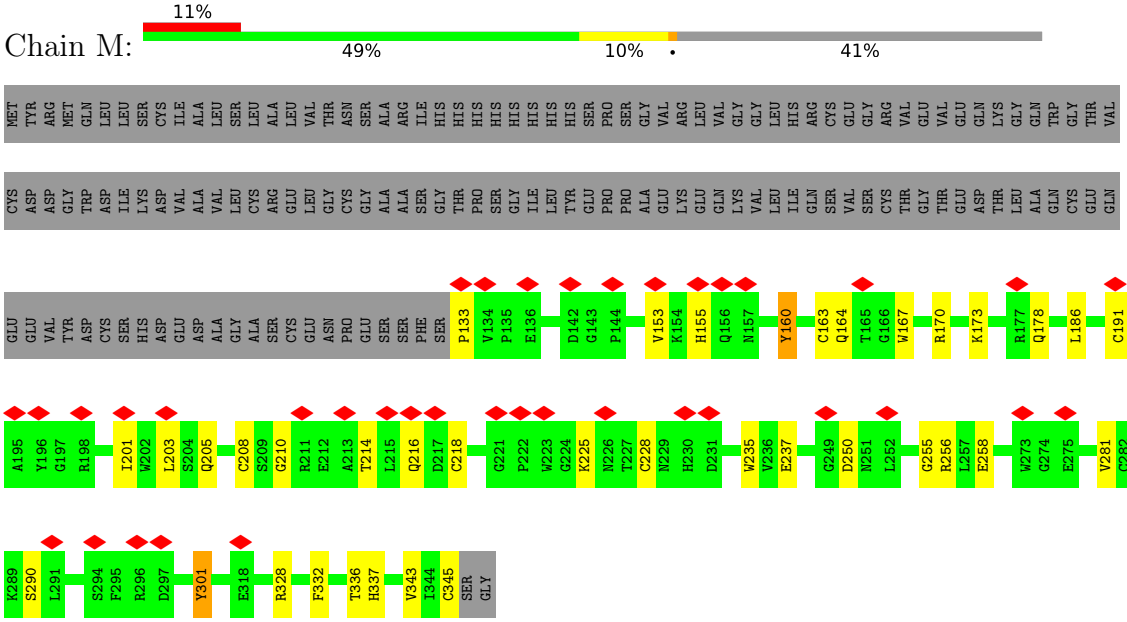
• Molecule 2: Immunoglobulin J chain

Chain J:



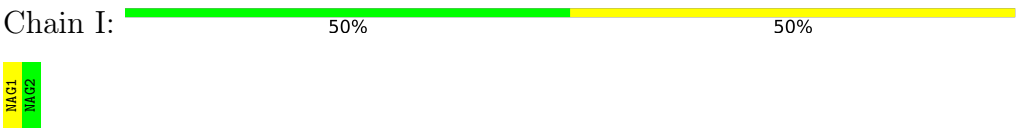
• Molecule 3: Interleukin-2,CD5 antigen-like

Chain M:



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

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	381470	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.542	Depositor
Minimum map value	-0.989	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.35	0/1844	0.61	0/2526
1	B	0.37	0/1825	0.64	0/2500
1	C	0.42	0/1802	0.61	0/2468
1	D	0.39	0/1809	0.67	1/2478 (0.0%)
1	E	0.38	0/1802	0.65	0/2468
1	F	0.43	0/1809	0.75	0/2478
1	G	0.35	0/1794	0.63	0/2457
1	H	0.35	0/1844	0.65	0/2526
1	K	0.34	0/1844	0.61	0/2526
1	L	0.37	0/1844	0.64	1/2526 (0.0%)
2	J	0.38	0/1023	0.70	0/1390
3	M	0.32	0/1710	0.66	0/2311
All	All	0.37	0/20950	0.65	2/28654 (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})
1	D	474	CYS	CA-CB-SG	5.85	124.52	114.00
1	L	372	LEU	CA-CB-CG	5.13	127.11	115.30

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	A	1798	0	1752	32	0
1	B	1780	0	1738	33	0
1	C	1757	0	1716	35	0
1	D	1764	0	1723	32	0
1	E	1757	0	1716	35	0
1	F	1764	0	1724	32	0
1	G	1749	0	1713	37	0
1	H	1798	0	1751	27	0
1	K	1798	0	1750	29	0
1	L	1798	0	1751	33	0
2	J	1010	0	993	20	0
3	M	1669	0	1570	22	0
4	I	28	0	25	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	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	0	0
5	H	14	0	13	0	0
5	K	14	0	13	1	0
5	L	14	0	13	0	0
6	M	2	0	0	0	0
All	All	20612	0	20052	329	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 8.

All (329) 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:L:488:TRP:HE1	1:L:519:SER:HG	1.27	0.81
1:F:547:VAL:HG11	1:G:545:ASN:HD21	1.53	0.72
1:B:472:ILE:HG21	1:B:552:VAL:HG11	1.72	0.72
1:A:454:VAL:HG12	1:A:476:VAL:HG22	1.71	0.71
1:B:537:VAL:HG12	1:B:549:GLU:HG2	1.72	0.71
1:B:454:VAL:HG21	1:B:538:VAL:HG11	1.73	0.71
2:J:43:LEU:HB2	1:L:570:ASP:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:348:PHE:HB2	1:G:368:LEU:HB3	1.74	0.67
1:C:457:LEU:HD22	1:C:475:LEU:HD21	1.75	0.67
1:C:454:VAL:HG21	1:C:538:VAL:HG11	1.79	0.64
3:M:214:THR:HG23	3:M:216:GLN:H	1.61	0.64
1:H:384:ARG:HD2	1:H:388:GLU:HB3	1.80	0.64
1:H:456:LEU:HD23	1:H:552:VAL:HG12	1.80	0.64
1:G:490:GLN:HE21	1:G:495:LEU:HD11	1.63	0.63
1:G:383:THR:HB	1:G:387:GLY:HA2	1.80	0.63
1:H:414:CYS:SG	1:H:415:GLU:N	2.71	0.62
1:G:374:THR:HA	1:G:405:PHE:HB2	1.82	0.62
1:B:400:HIS:HB2	1:B:404:THR:HB	1.82	0.61
1:L:372:LEU:HD12	1:L:433:LEU:HD23	1.81	0.61
1:L:414:CYS:SG	3:M:191:CYS:N	2.72	0.61
1:F:367:CYS:SG	1:F:368:LEU:N	2.74	0.61
1:F:350:ILE:HB	1:F:366:THR:HB	1.83	0.61
1:C:395:ASN:HB2	1:C:408:VAL:HB	1.83	0.60
1:G:485:PHE:HB3	1:G:539:ALA:HB3	1.84	0.60
1:H:357:ILE:HG13	1:H:363:THR:HG22	1.84	0.59
1:C:459:PRO:HD3	1:C:472:ILE:HG23	1.84	0.59
1:G:365:LEU:HD21	1:G:413:ILE:HD11	1.84	0.59
1:K:415:GLU:O	1:K:419:ASN:ND2	2.36	0.59
1:L:452:PRO:HG3	1:L:479:PHE:HB3	1.85	0.59
1:H:545:ASN:OD1	1:H:545:ASN:N	2.36	0.59
1:E:345:ILE:N	1:E:371:ASP:O	2.36	0.58
1:A:365:LEU:HB2	1:A:411:ALA:HB3	1.85	0.58
1:K:385:GLN:HG3	1:K:423:ARG:HB2	1.85	0.58
3:M:235:TRP:HE1	3:M:237:GLU:HG3	1.69	0.58
1:E:485:PHE:HB3	1:E:539:ALA:HB3	1.85	0.58
1:C:347:VAL:HG13	1:C:369:VAL:HG22	1.87	0.57
1:E:416:ASP:HA	1:E:419:ASN:HB2	1.87	0.57
1:A:382:TRP:HB3	1:A:390:VAL:HG23	1.86	0.57
1:H:347:VAL:HG12	1:H:369:VAL:HG12	1.85	0.57
1:A:347:VAL:HA	1:A:369:VAL:HA	1.87	0.56
1:A:461:ARG:HH12	1:B:557:GLY:HA2	1.71	0.56
1:B:414:CYS:SG	1:B:415:GLU:N	2.78	0.56
1:E:457:LEU:HB3	1:F:457:LEU:HD23	1.88	0.56
1:F:545:ASN:OD1	1:G:487:GLN:NE2	2.39	0.56
1:C:501:VAL:HG12	1:D:509:PRO:HG3	1.86	0.56
1:L:471:THR:HG22	1:L:522:THR:HG22	1.87	0.56
1:B:459:PRO:HD3	1:B:472:ILE:HG12	1.88	0.55
1:A:566:LEU:HD13	1:L:566:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:328:ARG:HH21	3:M:332:PHE:HB3	1.71	0.55
1:C:456:LEU:HD21	1:C:472:ILE:HG22	1.89	0.55
1:F:414:CYS:HB3	1:G:414:CYS:HB3	1.88	0.55
1:D:490:GLN:NE2	1:D:532:GLU:OE1	2.40	0.55
1:H:553:ASP:OD2	1:H:553:ASP:N	2.38	0.55
1:K:485:PHE:HB3	1:K:539:ALA:HB3	1.88	0.54
1:B:485:PHE:HB3	1:B:539:ALA:HB3	1.88	0.54
1:C:525:GLU:OE2	1:C:529:ASN:ND2	2.40	0.54
1:D:484:VAL:HG23	1:D:540:HIS:HB2	1.90	0.54
1:E:365:LEU:HD13	1:E:413:ILE:HD13	1.88	0.54
1:L:525:GLU:OE1	1:L:529:ASN:ND2	2.40	0.54
1:E:484:VAL:HG12	1:E:540:HIS:HB2	1.87	0.54
1:F:369:VAL:HG23	1:F:403:ALA:HB1	1.89	0.54
2:J:36:ASN:ND2	1:L:563:ASN:OD1	2.35	0.54
2:J:44:ASN:ND2	1:L:570:ASP:OD2	2.39	0.54
1:A:485:PHE:HB3	1:A:539:ALA:HB3	1.89	0.53
1:C:348:PHE:HB2	1:C:368:LEU:HB2	1.89	0.53
1:C:570:ASP:OD1	1:C:570:ASP:N	2.41	0.53
3:M:164:GLN:NE2	3:M:205:GLN:OE1	2.41	0.53
1:F:363:THR:OG1	1:F:413:ILE:O	2.27	0.53
1:A:461:ARG:HH21	1:A:560:THR:HG22	1.74	0.53
1:F:381:SER:HB2	1:F:427:THR:HB	1.90	0.53
1:D:535:THR:HG22	1:D:551:THR:HG22	1.91	0.53
2:J:6:VAL:HA	2:J:18:THR:HG22	1.90	0.53
2:J:42:PRO:HG3	2:J:102:THR:HG22	1.90	0.53
1:K:381:SER:HA	1:K:393:HIS:HE1	1.74	0.53
1:B:374:THR:HA	1:B:405:PHE:HB2	1.89	0.53
1:C:375:TYR:HB2	1:C:431:THR:HB	1.91	0.52
1:G:454:VAL:HG11	1:G:538:VAL:HG11	1.90	0.52
1:F:347:VAL:HG11	1:F:426:CYS:HB3	1.92	0.52
1:G:400:HIS:ND1	1:G:402:ASN:OD1	2.43	0.52
1:G:425:THR:HG22	1:G:440:THR:H	1.75	0.52
3:M:164:GLN:HB3	3:M:167:TRP:HB2	1.90	0.52
1:B:463:GLN:HE22	1:B:471:THR:HG22	1.75	0.52
1:C:380:ILE:O	1:C:393:HIS:ND1	2.33	0.52
1:E:423:ARG:NH1	1:E:425:THR:OG1	2.43	0.52
1:K:486:VAL:HG22	1:K:538:VAL:HG22	1.92	0.52
1:F:354:PHE:HA	1:F:357:ILE:HG12	1.92	0.52
1:E:486:VAL:HG22	1:E:538:VAL:HG22	1.92	0.51
1:K:369:VAL:HB	1:K:405:PHE:HB3	1.93	0.51
3:M:153:VAL:N	3:M:160:TYR:O	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:485:PHE:HB3	1:H:539:ALA:HB3	1.93	0.51
1:A:379:THR:HB	1:A:429:THR:HB	1.92	0.51
1:B:349:ALA:HB1	1:B:441:ILE:HD11	1.92	0.51
1:A:464:LEU:O	1:A:467:ARG:NH1	2.44	0.51
1:F:471:THR:HG22	1:F:522:THR:HG22	1.93	0.51
1:L:371:ASP:HB3	1:L:406:SER:HB3	1.92	0.51
1:D:555:SER:HA	1:D:558:LYS:HE2	1.93	0.51
1:B:566:LEU:HD13	1:K:566:LEU:HD11	1.94	0.50
1:C:417:ASP:HB3	1:C:424:PHE:HE1	1.74	0.50
1:D:481:PRO:HD2	1:D:540:HIS:CE1	2.47	0.50
1:G:454:VAL:HG12	1:G:476:VAL:HG13	1.93	0.50
1:B:348:PHE:N	1:B:368:LEU:O	2.44	0.50
1:H:345:ILE:HA	1:H:372:LEU:HD13	1.92	0.50
2:J:29:ASN:ND2	1:L:465:ASN:OD1	2.42	0.50
1:L:421:GLY:HA3	1:L:445:LYS:HE2	1.94	0.50
1:B:347:VAL:HG22	1:B:369:VAL:HG13	1.94	0.50
1:C:535:THR:HG22	1:C:551:THR:HG22	1.93	0.50
1:H:452:PRO:HG3	1:H:479:PHE:HB3	1.94	0.50
3:M:256:ARG:NH2	3:M:258:GLU:OE2	2.44	0.50
1:E:454:VAL:HG11	1:E:538:VAL:HG21	1.93	0.50
1:F:414:CYS:HB3	1:G:414:CYS:CB	2.42	0.50
1:H:419:ASN:HA	1:H:443:ARG:HE	1.76	0.50
1:F:433:LEU:HB2	1:F:436:PRO:HD2	1.93	0.50
1:E:564:VAL:HG21	1:F:564:VAL:HG21	1.94	0.49
1:A:354:PHE:HA	1:A:357:ILE:HG12	1.93	0.49
1:G:384:ARG:HH11	1:G:388:GLU:HG3	1.77	0.49
1:G:481:PRO:HB2	1:G:540:HIS:HE2	1.77	0.49
1:L:432:ASP:OD2	1:L:432:ASP:N	2.46	0.49
1:C:442:SER:OG	1:C:443:ARG:N	2.45	0.49
1:G:473:THR:HG22	1:G:520:ILE:HG22	1.95	0.49
1:A:391:LYS:NZ	1:A:394:THR:OG1	2.44	0.49
1:E:478:GLY:HA2	1:E:514:ARG:HB3	1.94	0.49
1:H:420:SER:O	1:H:423:ARG:NH2	2.44	0.49
1:E:386:ASN:ND2	1:E:388:GLU:OE1	2.45	0.49
1:H:537:VAL:HG12	1:H:549:GLU:HB2	1.94	0.49
3:M:201:ILE:HD13	3:M:228:CYS:HB3	1.94	0.49
2:J:13:LYS:HD2	2:J:67:LEU:HD21	1.95	0.49
1:A:463:GLN:NE2	1:A:469:SER:O	2.41	0.49
1:D:537:VAL:HG21	1:E:545:ASN:HD22	1.78	0.48
1:K:565:SER:OG	5:K:601:NAG:O7	2.25	0.48
1:A:573:GLY:O	1:K:461:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:490:GLN:O	1:K:533:THR:OG1	2.30	0.48
1:H:345:ILE:N	1:H:370:THR:O	2.46	0.48
1:L:353:SER:HB2	1:L:483:ASP:HB3	1.94	0.48
1:B:354:PHE:HA	1:B:357:ILE:HD12	1.94	0.48
1:D:365:LEU:HD13	1:D:413:ILE:HB	1.95	0.48
3:M:255:GLY:HA2	3:M:301:TYR:HD2	1.78	0.48
3:M:178:GLN:HB3	3:M:214:THR:HA	1.96	0.48
1:A:478:GLY:HA2	1:A:514:ARG:HB3	1.96	0.48
1:C:385:GLN:HE21	1:C:423:ARG:HH21	1.60	0.48
1:D:345:ILE:HB	1:D:372:LEU:HD22	1.95	0.48
1:C:511:ALA:HB1	1:C:514:ARG:HE	1.79	0.48
1:C:348:PHE:N	1:C:368:LEU:O	2.43	0.48
1:C:567:VAL:HA	1:D:567:VAL:HB	1.95	0.47
1:A:436:PRO:HB2	1:A:438:LYS:HG3	1.94	0.47
1:E:457:LEU:HD23	1:F:457:LEU:HB3	1.96	0.47
1:F:382:TRP:HD1	1:F:390:VAL:HG23	1.79	0.47
3:M:170:ARG:HB3	3:M:210:GLY:HA3	1.96	0.47
1:B:379:THR:O	1:B:429:THR:OG1	2.31	0.47
1:B:528:TRP:CZ2	1:B:554:LYS:HA	2.49	0.47
2:J:44:ASN:ND2	1:L:570:ASP:O	2.48	0.47
1:A:425:THR:HB	1:A:438:LYS:HB3	1.97	0.47
1:H:454:VAL:HG21	1:H:538:VAL:HG11	1.95	0.47
3:M:186:LEU:HB3	3:M:237:GLU:HB2	1.96	0.47
1:E:518:HIS:CD2	1:F:520:ILE:HD11	2.50	0.47
1:F:396:ILE:HG23	1:F:407:ALA:HA	1.97	0.47
2:J:37:ILE:HD12	1:L:564:VAL:HG22	1.96	0.47
1:K:354:PHE:HA	1:K:357:ILE:HG12	1.97	0.47
1:K:376:ASP:OD1	1:K:376:ASP:N	2.47	0.47
1:A:380:ILE:O	1:A:393:HIS:ND1	2.48	0.47
1:F:438:LYS:HA	1:F:438:LYS:HD3	1.76	0.47
1:A:467:ARG:HA	1:A:525:GLU:HG3	1.96	0.47
1:E:483:ASP:O	1:E:540:HIS:HD2	1.97	0.47
1:D:502:THR:HA	1:D:519:SER:HA	1.97	0.47
1:F:508:GLU:HG3	1:F:509:PRO:HD2	1.97	0.47
2:J:20:ARG:NH1	2:J:34:GLU:OE1	2.47	0.47
1:K:495:LEU:HD23	1:K:499:LYS:HD2	1.97	0.47
1:D:467:ARG:HH11	1:D:525:GLU:HB3	1.80	0.46
1:C:349:ALA:HA	1:C:367:CYS:HA	1.98	0.46
1:G:380:ILE:HD11	1:G:428:VAL:HG12	1.97	0.46
1:D:479:PHE:HB2	1:D:540:HIS:CE1	2.51	0.46
1:G:479:PHE:HB2	1:G:540:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:49:ILE:HD13	2:J:100:CYS:O	2.14	0.46
1:C:430:HIS:HB3	1:C:433:LEU:H	1.80	0.46
1:B:382:TRP:HB3	1:B:384:ARG:HH22	1.79	0.46
1:B:526:GLU:O	1:B:530:THR:OG1	2.32	0.46
1:L:349:ALA:HA	1:L:367:CYS:HA	1.98	0.46
1:E:454:VAL:HG23	1:E:550:ARG:HG3	1.97	0.46
1:D:383:THR:OG1	1:D:425:THR:O	2.32	0.46
1:D:420:SER:OG	1:D:422:GLU:OE1	2.33	0.46
1:K:396:ILE:HG22	1:K:408:VAL:H	1.81	0.46
1:K:567:VAL:HB	1:L:567:VAL:HA	1.98	0.46
1:C:463:GLN:HG2	1:C:469:SER:O	2.16	0.46
1:D:413:ILE:HD13	1:D:424:PHE:HE2	1.81	0.46
1:F:349:ALA:HA	1:F:367:CYS:HA	1.98	0.46
2:J:4:ARG:HD2	2:J:20:ARG:HD2	1.97	0.46
2:J:92:ASP:N	2:J:92:ASP:OD1	2.48	0.45
1:A:419:ASN:HB3	1:A:443:ARG:HH21	1.81	0.45
1:B:354:PHE:N	1:B:483:ASP:OD1	2.44	0.45
1:F:452:PRO:HD2	1:F:543:LEU:HG	1.97	0.45
1:K:361:LYS:HD3	1:K:361:LYS:HA	1.86	0.45
1:C:351:PRO:HB3	1:C:418:TRP:CZ2	2.51	0.45
1:D:360:THR:O	1:D:361:LYS:HB3	2.16	0.45
1:G:396:ILE:HG23	1:G:407:ALA:HA	1.96	0.45
1:H:433:LEU:HD13	1:H:437:LEU:HD21	1.98	0.45
1:L:351:PRO:HB3	1:L:441:ILE:HG12	1.98	0.45
1:G:400:HIS:CD2	1:G:401:PRO:HD2	2.51	0.45
1:E:385:GLN:HE22	1:E:423:ARG:H	1.63	0.45
1:E:417:ASP:OD1	1:E:418:TRP:N	2.50	0.45
3:M:163:CYS:HB3	3:M:228:CYS:HB2	1.51	0.45
3:M:208:CYS:HB3	3:M:218:CYS:HB2	1.87	0.45
1:F:420:SER:OG	1:F:422:GLU:OE2	2.34	0.45
1:G:535:THR:HB	1:G:549:GLU:HG3	1.99	0.45
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.74	0.45
1:L:474:CYS:HB3	1:L:519:SER:HB3	1.98	0.45
1:C:455:TYR:HD2	1:C:475:LEU:HD12	1.81	0.45
1:C:467:ARG:HA	1:C:525:GLU:HG3	1.98	0.45
1:D:347:VAL:HA	1:D:369:VAL:HA	1.99	0.45
1:K:367:CYS:SG	1:K:382:TRP:NE1	2.90	0.45
1:E:384:ARG:NH2	1:E:389:ALA:O	2.42	0.45
1:F:382:TRP:H	1:F:390:VAL:HB	1.82	0.45
2:J:37:ILE:HB	1:L:564:VAL:HG13	1.98	0.45
1:G:347:VAL:HG21	1:G:439:GLN:HE21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:GLU:O	1:G:442:SER:OG	2.35	0.44
1:G:449:LEU:HD23	1:G:542:ALA:HA	2.00	0.44
2:J:49:ILE:CD1	2:J:100:CYS:HB3	2.47	0.44
1:L:357:ILE:HD13	1:L:357:ILE:HA	1.85	0.44
1:E:491:ARG:HE	1:E:491:ARG:HB3	1.64	0.44
1:H:508:GLU:HG2	1:H:511:ALA:HB3	1.98	0.44
1:B:493:GLN:OE1	1:B:493:GLN:N	2.47	0.44
1:B:569:SER:HA	1:C:569:SER:HB2	1.98	0.44
1:D:471:THR:HG22	1:D:522:THR:HG22	1.98	0.44
1:A:398:GLU:O	1:A:406:SER:OG	2.35	0.44
1:D:363:THR:HB	1:D:413:ILE:O	2.16	0.44
1:G:472:ILE:HG21	1:G:552:VAL:HG11	2.00	0.44
1:E:450:HIS:N	1:E:480:SER:OG	2.49	0.44
1:K:481:PRO:HD2	1:K:540:HIS:CE1	2.53	0.44
1:H:454:VAL:O	1:H:550:ARG:NH1	2.50	0.44
1:G:345:ILE:N	1:G:371:ASP:O	2.51	0.44
1:A:525:GLU:OE2	1:A:529:ASN:ND2	2.50	0.43
1:C:457:LEU:HD12	1:D:460:ALA:HB2	1.99	0.43
2:J:40:ILE:HD13	1:L:567:VAL:HB	2.00	0.43
3:M:203:LEU:O	3:M:225:LYS:N	2.50	0.43
1:A:565:SER:HA	1:B:565:SER:HB3	2.00	0.43
1:B:380:ILE:HG23	1:B:428:VAL:HG12	1.99	0.43
1:B:386:ASN:OD1	1:B:386:ASN:N	2.47	0.43
1:B:495:LEU:HD13	1:B:521:LEU:HD11	2.00	0.43
1:D:452:PRO:HB3	1:D:476:VAL:HG12	2.00	0.43
1:A:363:THR:O	1:A:363:THR:OG1	2.34	0.43
1:K:490:GLN:NE2	1:K:532:GLU:OE1	2.50	0.43
1:G:457:LEU:HD11	1:G:475:LEU:HD22	2.00	0.43
1:H:449:LEU:HD13	1:H:481:PRO:HG2	1.99	0.43
1:K:450:HIS:N	1:K:480:SER:OG	2.47	0.43
1:B:391:LYS:HD2	1:B:391:LYS:HA	1.80	0.43
1:D:481:PRO:HD2	1:D:540:HIS:HE1	1.81	0.43
1:G:493:GLN:HA	1:G:494:PRO:HD3	1.91	0.43
1:H:545:ASN:HD22	1:K:547:VAL:HG11	1.84	0.43
1:G:451:ARG:HE	1:G:544:PRO:HD3	1.84	0.43
1:L:363:THR:HB	1:L:414:CYS:HA	2.01	0.43
1:A:378:VAL:HG13	1:A:430:HIS:HE1	1.84	0.42
1:D:489:MET:HA	1:D:494:PRO:HA	2.00	0.42
1:D:558:LYS:HA	1:D:559:PRO:HD3	1.83	0.42
1:E:416:ASP:OD1	1:E:416:ASP:N	2.45	0.42
1:G:527:GLU:O	1:G:530:THR:OG1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:553:ASP:H	1:G:556:THR:HG22	1.84	0.42
1:L:355:ALA:HA	1:L:485:PHE:HB2	2.00	0.42
1:L:456:LEU:HA	1:L:456:LEU:HD12	1.72	0.42
1:B:452:PRO:HG3	1:B:479:PHE:HB3	2.01	0.42
1:G:481:PRO:HD2	1:G:540:HIS:CE1	2.53	0.42
1:B:465:ASN:HD22	1:L:571:THR:HB	1.85	0.42
3:M:173:LYS:HB2	3:M:173:LYS:HE2	1.81	0.42
1:F:483:ASP:O	1:F:484:VAL:C	2.57	0.42
1:F:564:VAL:HG22	1:G:564:VAL:HB	2.02	0.42
2:J:35:ARG:HH22	1:K:461:ARG:HH22	1.68	0.42
1:A:393:HIS:HA	1:A:410:GLU:HG3	2.00	0.42
1:A:452:PRO:HB3	1:A:479:PHE:HB3	2.02	0.42
1:D:351:PRO:HB3	1:D:441:ILE:HG12	2.01	0.42
1:E:489:MET:HA	1:E:494:PRO:HA	2.01	0.42
1:F:372:LEU:HD23	1:F:372:LEU:HA	1.90	0.42
3:M:283:LYS:HE3	3:M:283:LYS:HB2	1.83	0.42
1:C:470:ALA:O	1:C:522:THR:HA	2.19	0.42
1:H:382:TRP:HB3	1:H:390:VAL:HG22	2.01	0.42
1:H:500:TYR:HB3	1:H:521:LEU:HD13	2.00	0.42
1:K:382:TRP:HH2	1:K:441:ILE:HD13	1.84	0.42
1:A:364:LYS:HE2	1:A:364:LYS:HB2	1.91	0.42
1:C:456:LEU:HD12	1:C:536:CYS:HB2	2.01	0.42
1:D:452:PRO:HD2	1:D:543:LEU:HG	2.01	0.42
1:G:445:LYS:HB2	1:G:445:LYS:HE2	1.69	0.42
1:B:543:LEU:HD13	1:B:548:THR:HG23	2.01	0.42
1:E:526:GLU:O	1:E:530:THR:OG1	2.34	0.42
1:F:370:THR:HA	1:F:403:ALA:HB2	2.02	0.42
2:J:8:VAL:HG22	2:J:17:ILE:HB	2.01	0.42
1:D:382:TRP:NE1	1:D:409:GLY:O	2.43	0.42
1:D:475:LEU:O	1:D:476:VAL:C	2.57	0.42
1:B:481:PRO:HD2	1:B:540:HIS:CE1	2.55	0.42
1:C:457:LEU:HA	1:C:458:PRO:HD3	1.83	0.42
1:E:349:ALA:HA	1:E:367:CYS:HA	2.01	0.42
1:F:396:ILE:HD13	1:F:408:VAL:HG22	2.02	0.42
1:H:575:CYS:SG	1:K:575:CYS:N	2.93	0.42
1:K:384:ARG:NH2	1:K:422:GLU:OE1	2.53	0.42
1:E:438:LYS:HE2	1:E:438:LYS:HB3	1.85	0.41
1:C:485:PHE:HB3	1:C:539:ALA:HB3	2.02	0.41
3:M:250:ASP:OD1	3:M:301:TYR:OH	2.29	0.41
3:M:290:SER:HA	3:M:345:CYS:HB3	2.02	0.41
1:H:474:CYS:HB2	1:H:488:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:SER:O	1:E:356:SER:OG	2.31	0.41
1:K:347:VAL:HG23	1:K:437:LEU:HD12	2.03	0.41
1:K:433:LEU:HD23	1:K:433:LEU:HA	1.95	0.41
1:D:549:GLU:OE2	1:E:545:ASN:ND2	2.43	0.41
1:E:562:TYR:HB2	1:E:564:VAL:HG23	2.03	0.41
1:B:384:ARG:HG3	1:B:387:GLY:H	1.85	0.41
1:C:423:ARG:HB3	1:C:440:THR:HB	2.02	0.41
1:H:459:PRO:HG3	1:H:470:ALA:HB1	2.02	0.41
2:J:27:ASP:HA	2:J:28:PRO:HD3	1.89	0.41
1:E:545:ASN:OD1	1:E:545:ASN:N	2.39	0.41
1:H:367:CYS:H	1:H:409:GLY:HA3	1.86	0.41
1:A:454:VAL:O	1:A:550:ARG:HG3	2.21	0.41
1:D:408:VAL:HG13	1:D:410:GLU:H	1.86	0.41
1:C:429:THR:HG22	1:C:436:PRO:HB3	2.03	0.41
1:D:462:GLU:H	1:D:462:GLU:HG3	1.70	0.41
1:E:372:LEU:HA	1:E:372:LEU:HD23	1.85	0.41
1:L:463:GLN:NE2	1:L:471:THR:OG1	2.46	0.41
1:A:507:PRO:HA	1:A:515:TYR:HD2	1.84	0.41
1:C:475:LEU:O	1:C:476:VAL:C	2.57	0.41
1:E:452:PRO:HG3	1:E:540:HIS:HB3	2.03	0.41
1:K:346:ARG:HA	1:K:437:LEU:HD13	2.03	0.41
1:A:462:GLU:OE1	1:B:550:ARG:NH1	2.52	0.40
1:E:470:ALA:N	1:E:523:VAL:O	2.53	0.40
1:H:427:THR:HG22	1:H:438:LYS:HG2	2.04	0.40
1:K:463:GLN:HG2	1:L:455:TYR:CZ	2.57	0.40
1:L:361:LYS:HA	1:L:361:LYS:HD2	1.87	0.40
1:G:386:ASN:OD1	1:G:386:ASN:N	2.54	0.40
1:L:419:ASN:OD1	1:L:419:ASN:N	2.54	0.40
3:M:336:THR:OG1	3:M:337:HIS:N	2.54	0.40
1:E:518:HIS:NE2	1:F:520:ILE:HD11	2.36	0.40
1:G:470:ALA:N	1:G:523:VAL:O	2.47	0.40
3:M:281:VAL:HG11	3:M:343:VAL:HG21	2.04	0.40
1:C:459:PRO:HD2	1:C:528:TRP:CZ2	2.56	0.40
1:F:543:LEU:HD23	1:F:543:LEU:HA	1.98	0.40
2:J:27:ASP:OD2	1:L:467:ARG:NH2	2.54	0.40

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	230/403 (57%)	217 (94%)	13 (6%)	0	100	100
1	B	228/403 (57%)	216 (95%)	12 (5%)	0	100	100
1	C	224/403 (56%)	209 (93%)	15 (7%)	0	100	100
1	D	225/403 (56%)	210 (93%)	15 (7%)	0	100	100
1	E	224/403 (56%)	211 (94%)	13 (6%)	0	100	100
1	F	225/403 (56%)	203 (90%)	22 (10%)	0	100	100
1	G	223/403 (55%)	214 (96%)	9 (4%)	0	100	100
1	H	230/403 (57%)	208 (90%)	22 (10%)	0	100	100
1	K	230/403 (57%)	216 (94%)	14 (6%)	0	100	100
1	L	230/403 (57%)	212 (92%)	18 (8%)	0	100	100
2	J	123/168 (73%)	119 (97%)	4 (3%)	0	100	100
3	M	211/359 (59%)	191 (90%)	20 (10%)	0	100	100
All	All	2603/4557 (57%)	2426 (93%)	177 (7%)	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	206/349 (59%)	202 (98%)	4 (2%)	52	71
1	B	204/349 (58%)	198 (97%)	6 (3%)	37	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	202/349 (58%)	194 (96%)	8 (4%)	27 52
1	D	203/349 (58%)	201 (99%)	2 (1%)	73 83
1	E	202/349 (58%)	200 (99%)	2 (1%)	73 83
1	F	203/349 (58%)	195 (96%)	8 (4%)	27 53
1	G	201/349 (58%)	190 (94%)	11 (6%)	18 44
1	H	206/349 (59%)	202 (98%)	4 (2%)	52 71
1	K	206/349 (59%)	202 (98%)	4 (2%)	52 71
1	L	206/349 (59%)	196 (95%)	10 (5%)	21 48
2	J	120/155 (77%)	115 (96%)	5 (4%)	25 51
3	M	182/304 (60%)	178 (98%)	4 (2%)	47 68
All	All	2341/3949 (59%)	2273 (97%)	68 (3%)	39 61

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	ARG
1	A	400	HIS
1	A	419	ASN
1	A	536	CYS
1	B	356	SER
1	B	384	ARG
1	B	443	ARG
1	B	490	GLN
1	B	536	CYS
1	B	566	LEU
1	C	455	TYR
1	C	472	ILE
1	C	473	THR
1	C	474	CYS
1	C	475	LEU
1	C	506	MET
1	C	514	ARG
1	C	529	ASN
1	D	475	LEU
1	D	562	TYR
1	E	348	PHE
1	E	506	MET
1	F	354	PHE

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Mol	Chain	Res	Type
1	F	367	CYS
1	F	376	ASP
1	F	433	LEU
1	F	453	ASP
1	F	484	VAL
1	F	553	ASP
1	F	563	ASN
1	G	367	CYS
1	G	382	TRP
1	G	386	ASN
1	G	395	ASN
1	G	413	ILE
1	G	423	ARG
1	G	443	ARG
1	G	445	LYS
1	G	516	PHE
1	G	528	TRP
1	G	536	CYS
1	H	405	PHE
1	H	423	ARG
1	H	483	ASP
1	H	553	ASP
2	J	54	SER
2	J	88	SER
2	J	100	CYS
2	J	108	CYS
2	J	117	TYR
1	K	361	LYS
1	K	416	ASP
1	K	419	ASN
1	K	483	ASP
1	L	371	ASP
1	L	372	LEU
1	L	380	ILE
1	L	388	GLU
1	L	393	HIS
1	L	419	ASN
1	L	429	THR
1	L	451	ARG
1	L	546	ARG
1	L	561	LEU
3	M	133	PRO

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Mol	Chain	Res	Type
3	M	155	HIS
3	M	160	TYR
3	M	301	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	487	GLN
1	G	490	GLN
1	G	545	ASN
2	J	29	ASN
1	K	393	HIS
1	K	419	ASN
1	L	465	ASN
1	L	529	ASN

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	I	1	2,4	14,14,15	0.20	0	17,19,21	0.63	1 (5%)
4	NAG	I	2	4	14,14,15	0.34	0	17,19,21	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	2,4	-	0/6/23/26	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	2.18	115.15	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

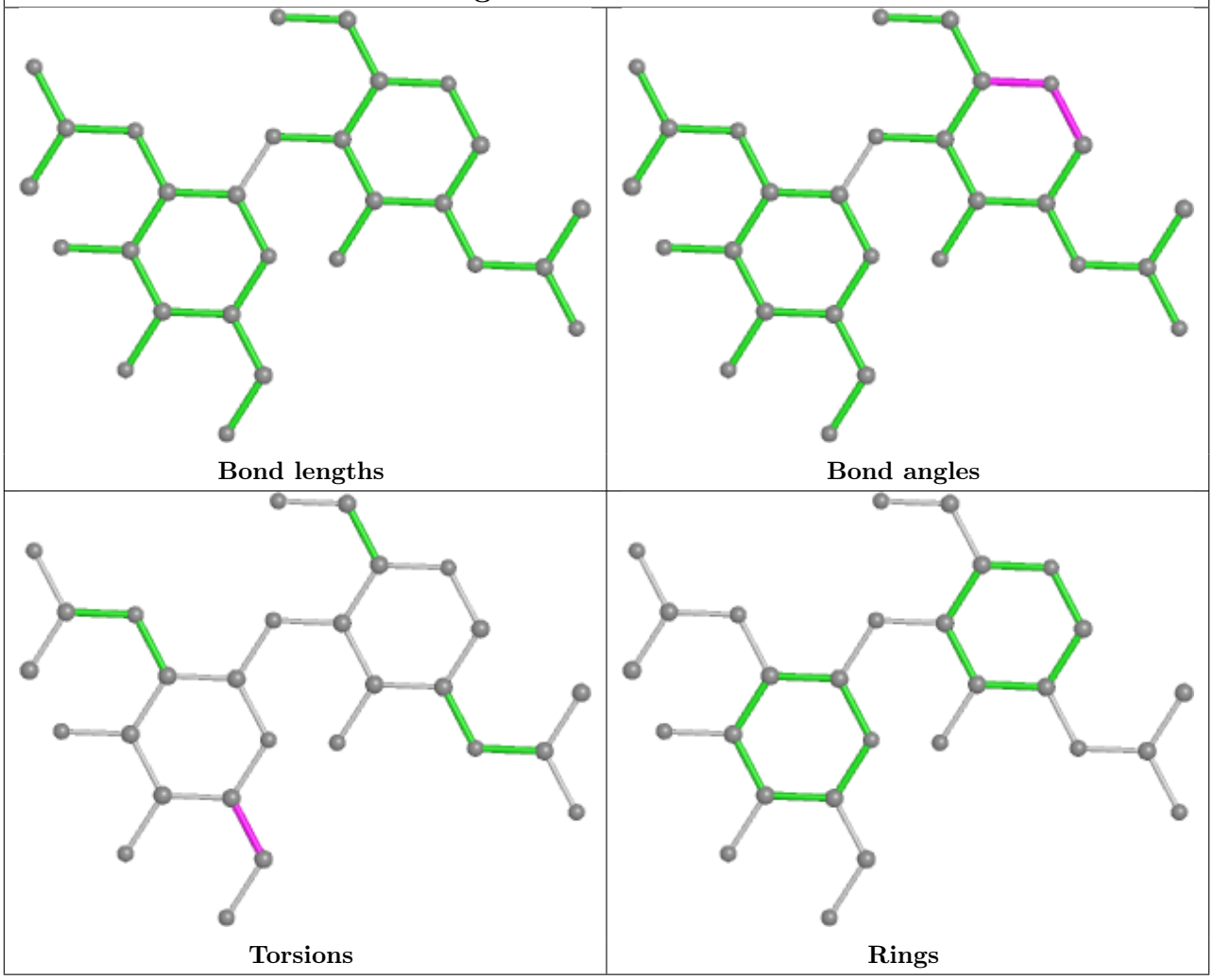
Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6

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)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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	B	601	1	14,14,15	0.41	0	17,19,21	0.55	0
5	NAG	D	601	1	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	C	601	1	14,14,15	0.47	0	17,19,21	0.45	0
5	NAG	F	601	1	14,14,15	0.37	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	G	601	1	14,14,15	0.41	0	17,19,21	0.48	0
5	NAG	L	601	1	14,14,15	0.45	0	17,19,21	0.61	0
5	NAG	A	601	1	14,14,15	0.41	0	17,19,21	0.58	1 (5%)
5	NAG	K	601	1	14,14,15	0.45	0	17,19,21	0.48	0
5	NAG	H	601	1	14,14,15	0.43	0	17,19,21	0.76	1 (5%)
5	NAG	E	601	1	14,14,15	0.29	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
5	NAG	B	601	1	-	0/6/23/26	0/1/1/1
5	NAG	D	601	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	4/6/23/26	0/1/1/1
5	NAG	F	601	1	-	2/6/23/26	0/1/1/1
5	NAG	G	601	1	-	2/6/23/26	0/1/1/1
5	NAG	L	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	K	601	1	-	2/6/23/26	0/1/1/1
5	NAG	H	601	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	601	NAG	C1-O5-C5	2.69	115.84	112.19
5	A	601	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	NAG	C4-C5-C6-O6
5	H	601	NAG	O5-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	F	601	NAG	O5-C5-C6-O6
5	H	601	NAG	C4-C5-C6-O6
5	D	601	NAG	O5-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	F	601	NAG	C4-C5-C6-O6
5	C	601	NAG	C8-C7-N2-C2
5	C	601	NAG	O7-C7-N2-C2
5	K	601	NAG	C8-C7-N2-C2
5	K	601	NAG	O7-C7-N2-C2
5	A	601	NAG	O5-C5-C6-O6
5	G	601	NAG	O5-C5-C6-O6
5	L	601	NAG	C4-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	L	601	NAG	O5-C5-C6-O6
5	D	601	NAG	C4-C5-C6-O6
5	G	601	NAG	C4-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	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.

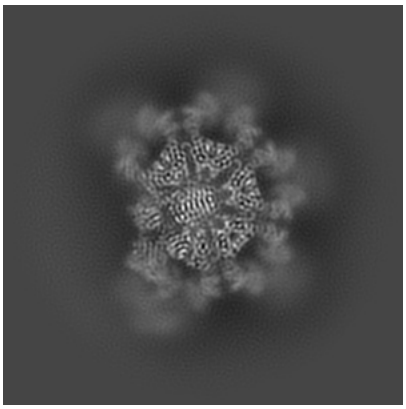
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37936. These allow visual inspection of the internal detail of the map and identification of artifacts.

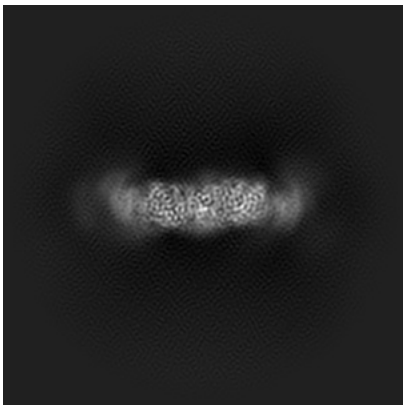
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

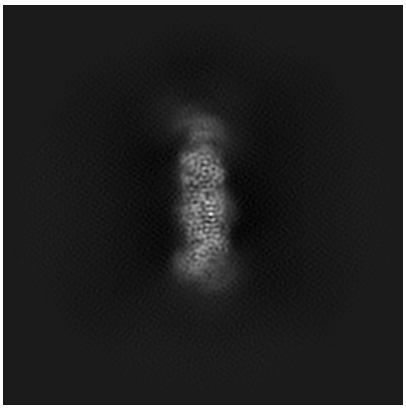
6.1.1 Primary map



X

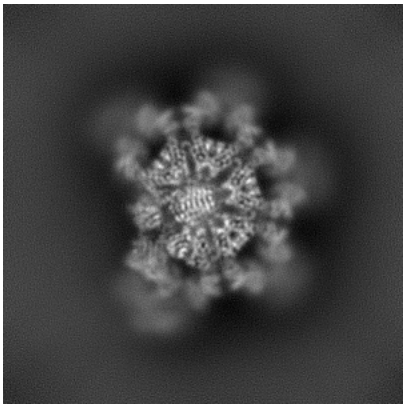


Y

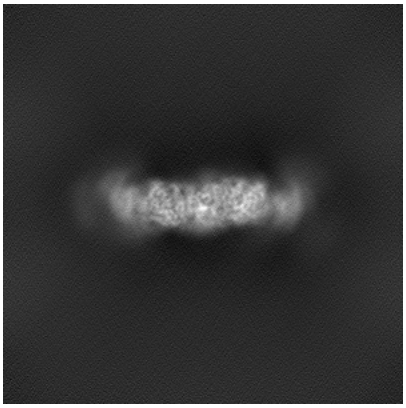


Z

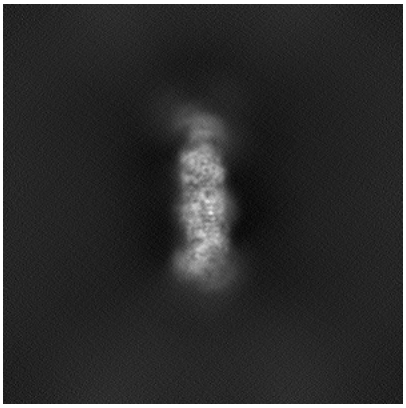
6.1.2 Raw map



X



Y

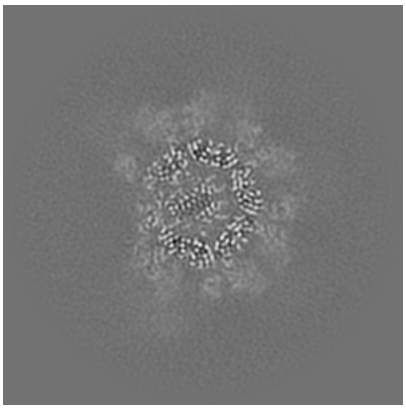


Z

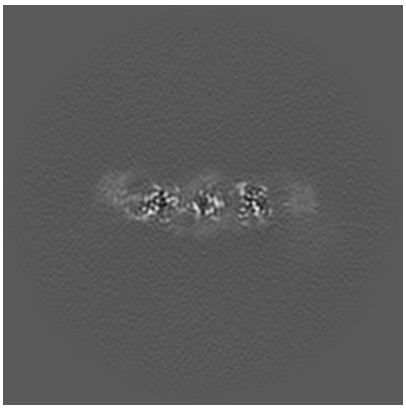
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

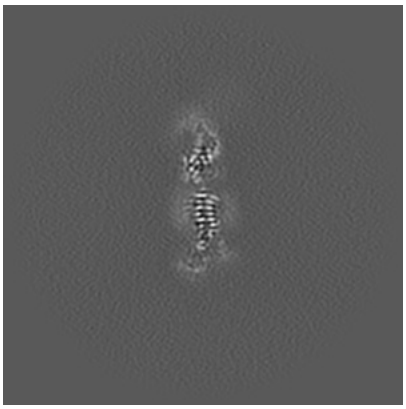
6.2.1 Primary map



X Index: 200

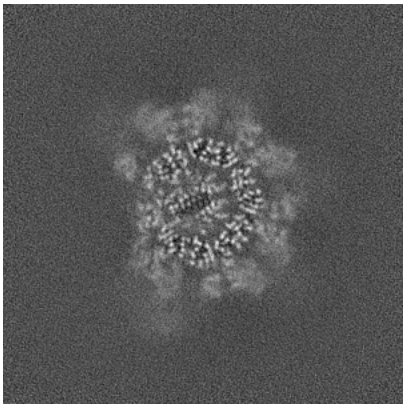


Y Index: 200

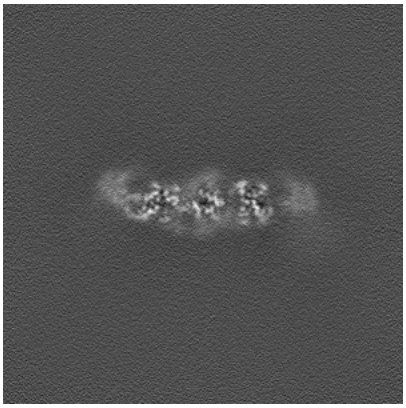


Z Index: 200

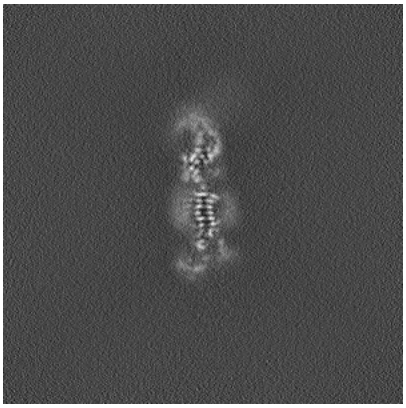
6.2.2 Raw map



X Index: 200



Y Index: 200

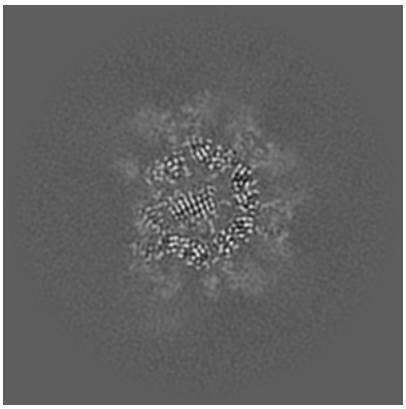


Z Index: 200

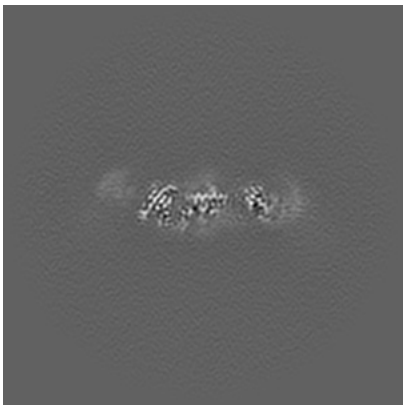
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

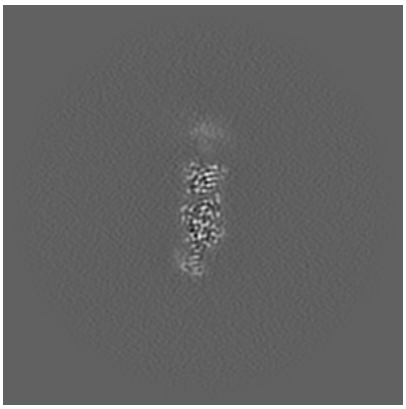
6.3.1 Primary map



X Index: 197

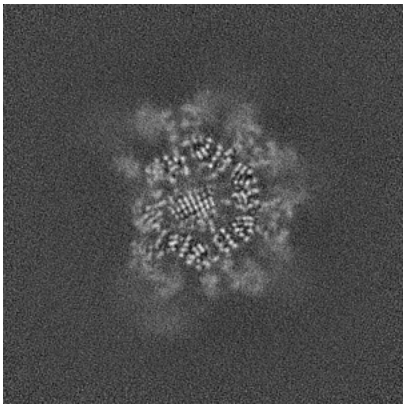


Y Index: 191

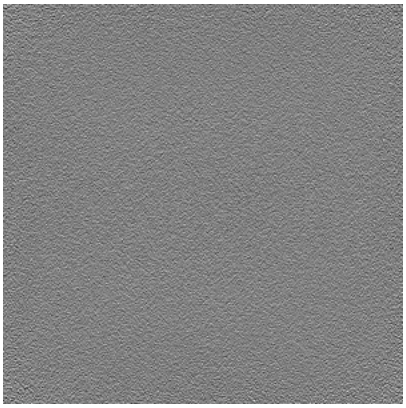


Z Index: 160

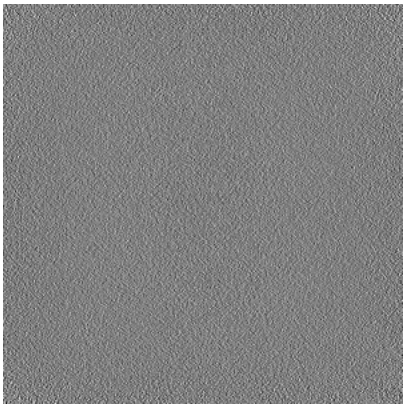
6.3.2 Raw map



X Index: 196



Y Index: 0

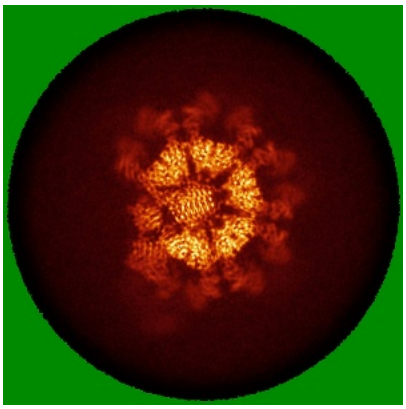


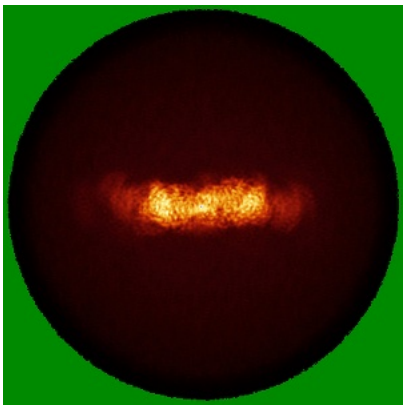
Z Index: 0

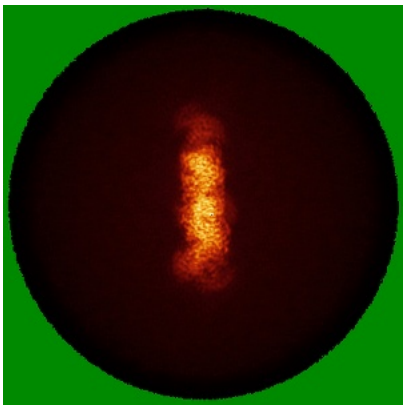
The images above show the largest variance slices of the map in three orthogonal directions.

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

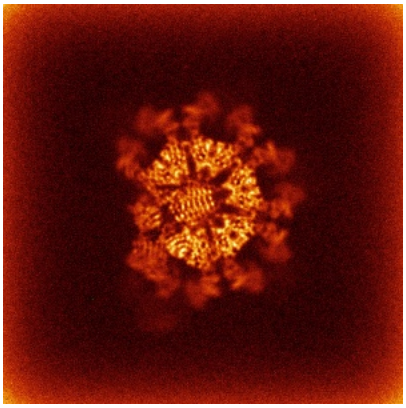
6.4.1 Primary map

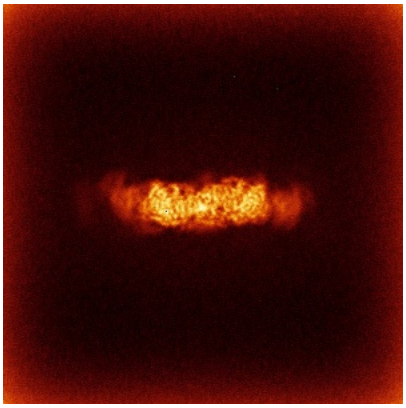

X

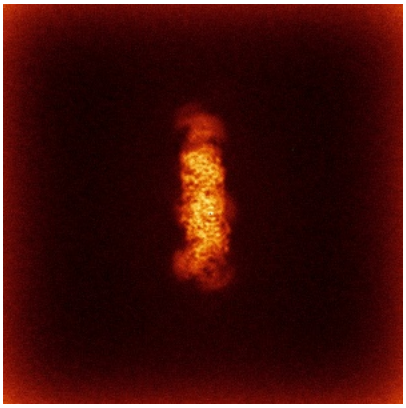

Y


Z

6.4.2 Raw map


X

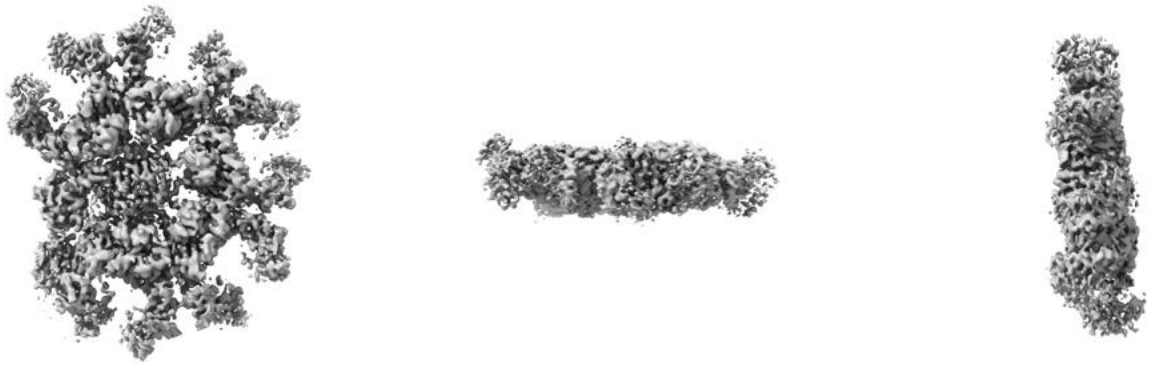

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. 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.

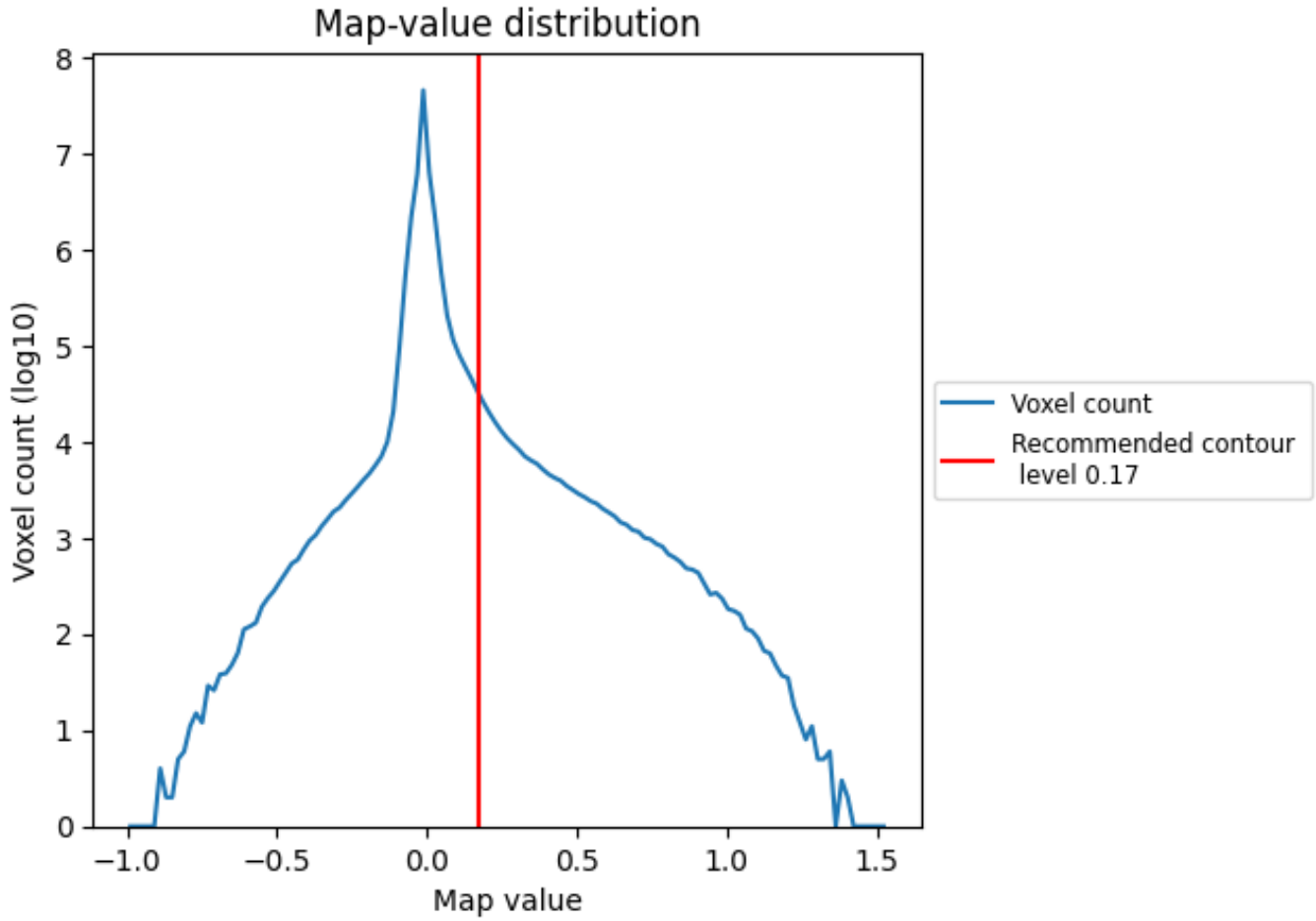
6.6 Mask visualisation (i)

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

7 Map analysis

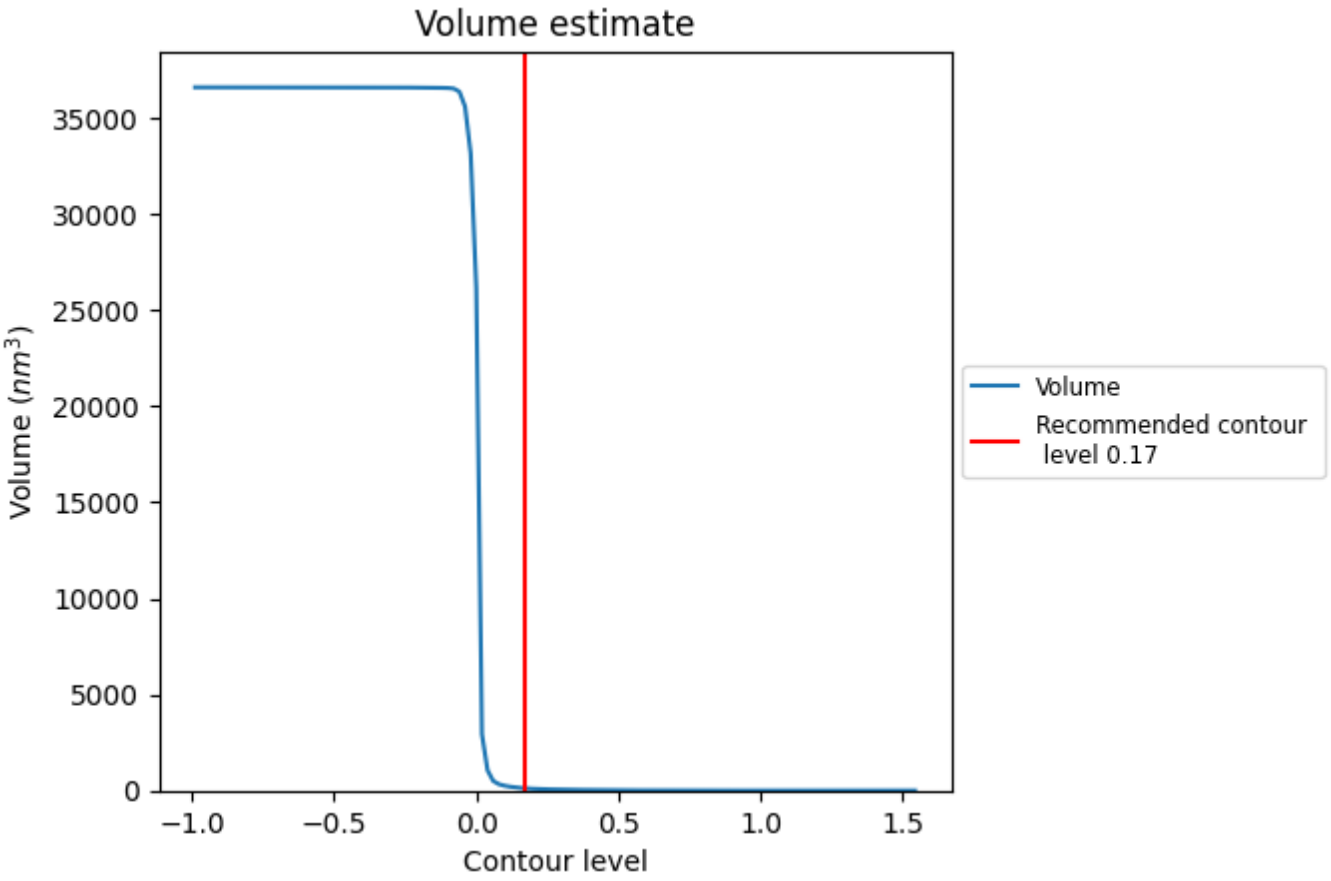
This section contains the results of statistical analysis of the map.

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.

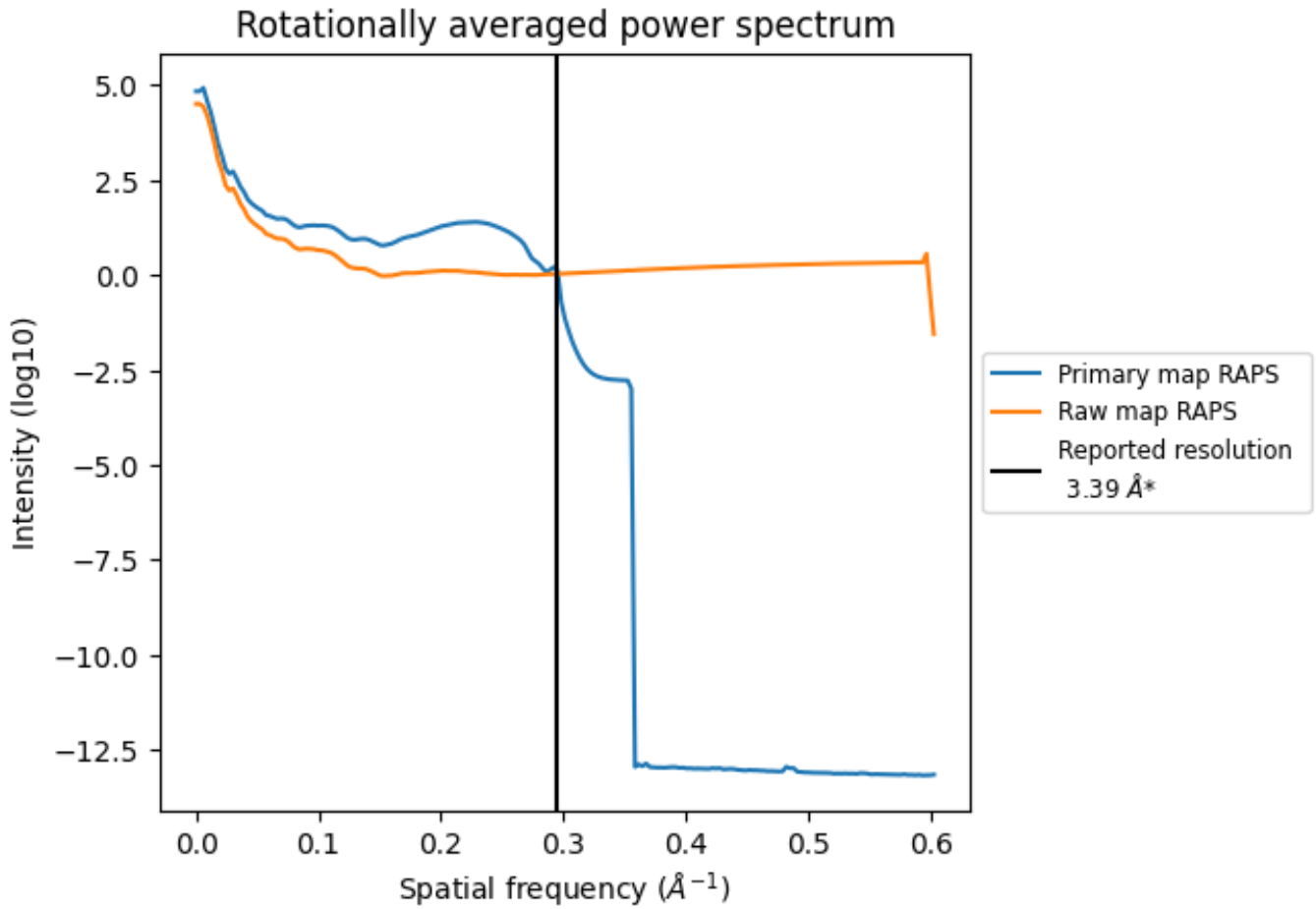
7.2 Volume estimate



The volume at the recommended contour level is 119 nm^3; this corresponds to an approximate mass of 107 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)

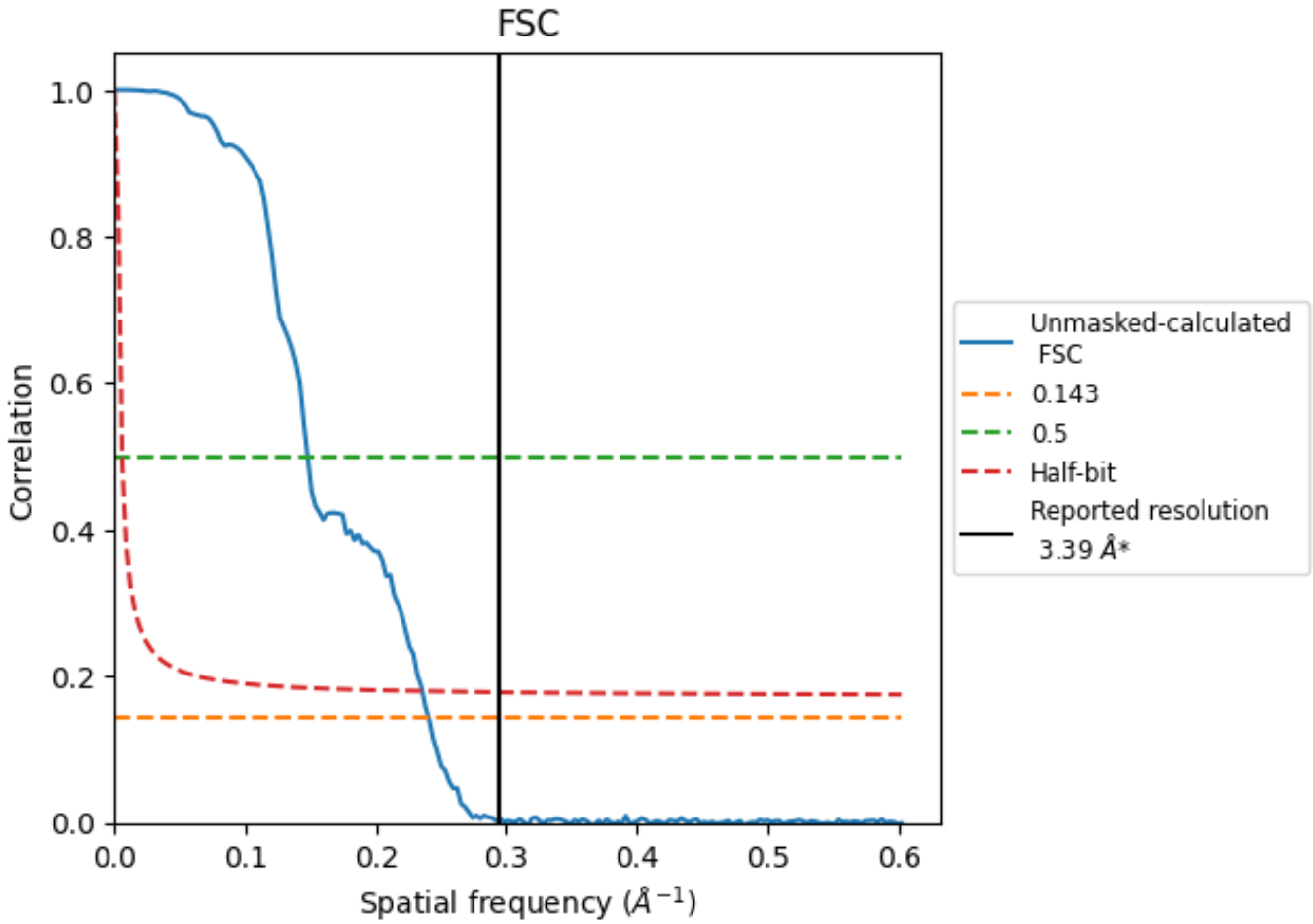


*Reported resolution corresponds to spatial frequency of 0.295 $Å^{-1}$

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 0.295 Å^{-1}

8.2 Resolution estimates (i)

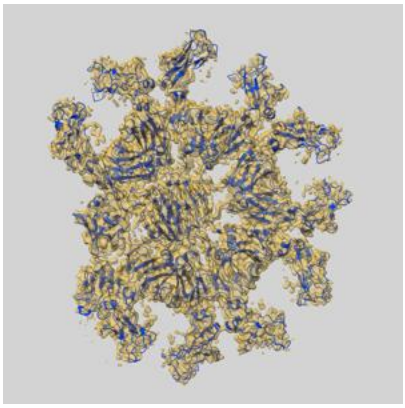
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	6.78	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.39 by more than 10 %

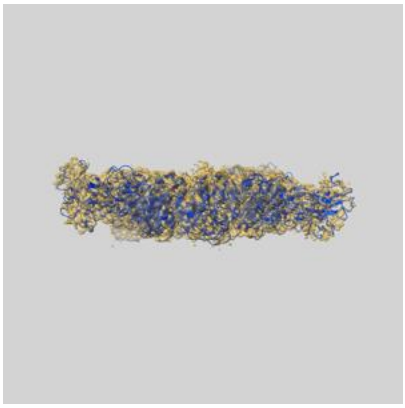
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37936 and PDB model 8WYR. Per-residue inclusion information can be found in section 3 on page 16.

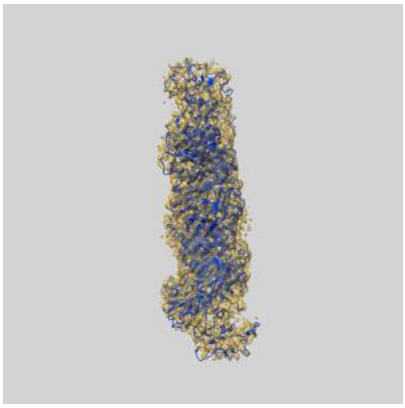
9.1 Map-model overlay



X



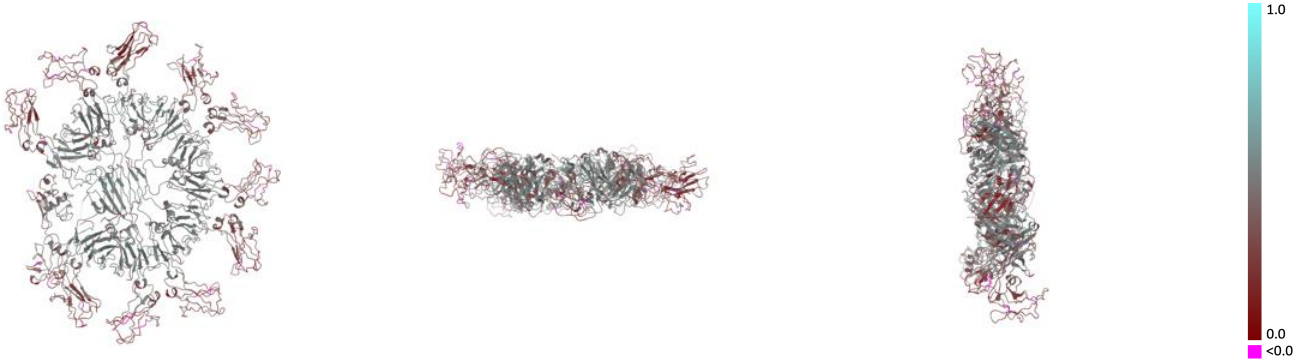
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 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.

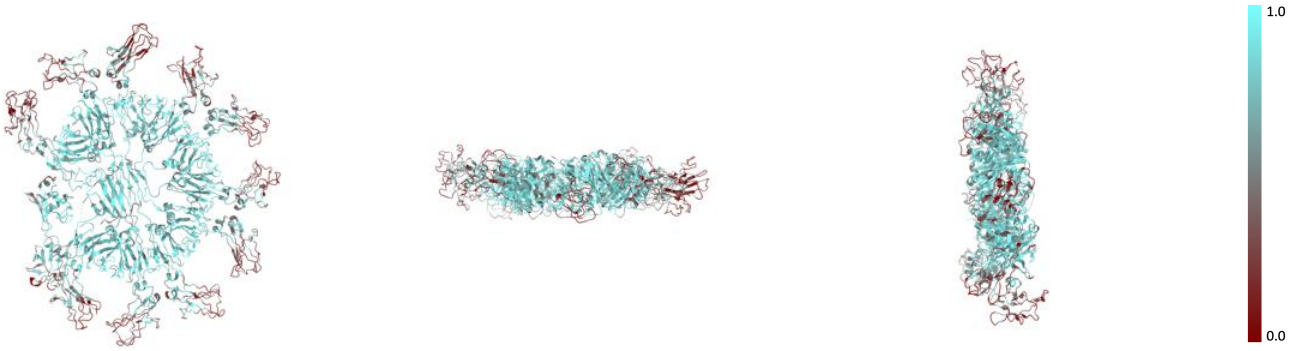
9.2 Q-score mapped to coordinate model (i)



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.

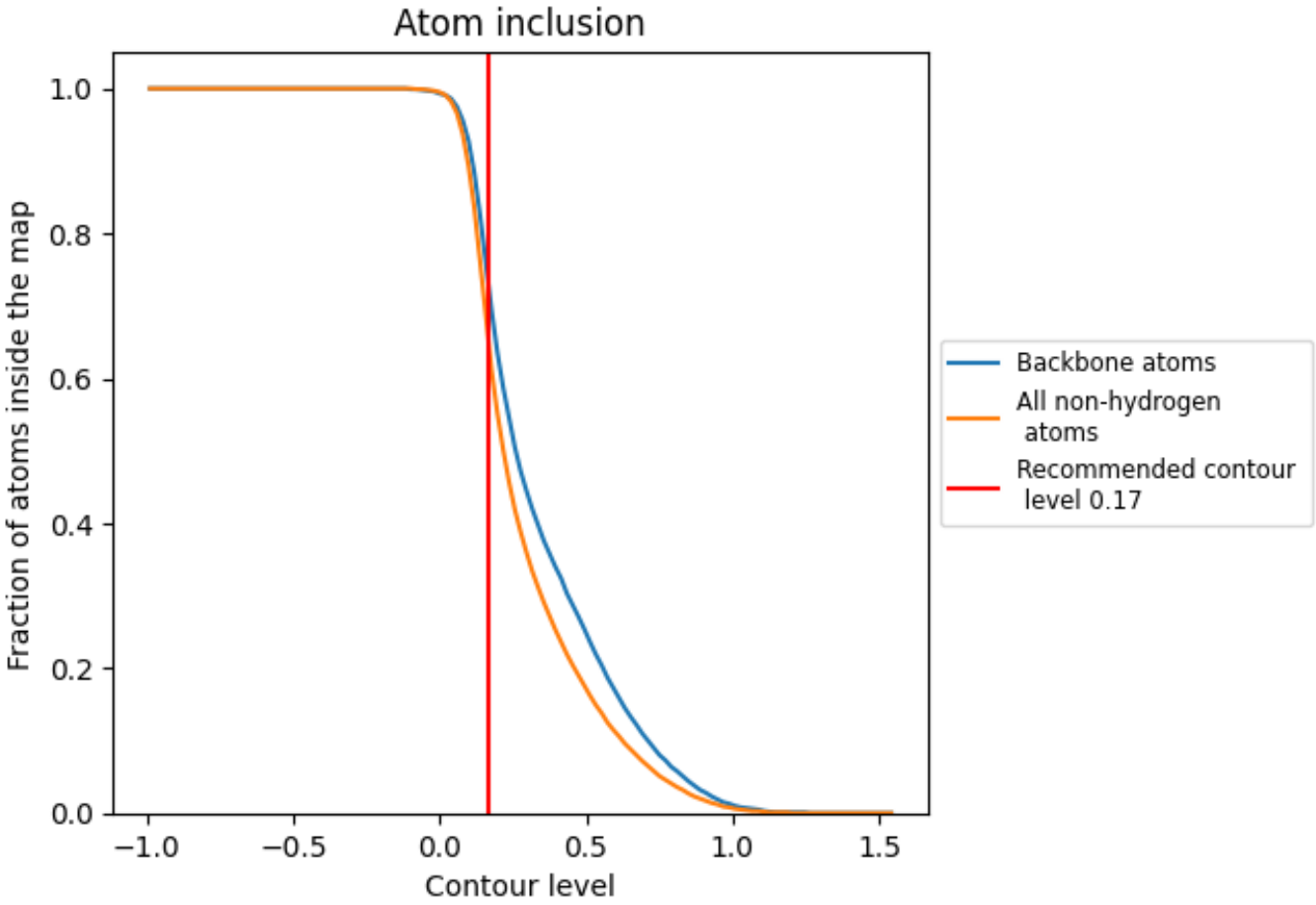
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6380	0.4000
A	0.6080	0.3890
B	0.6110	0.3870
C	0.6080	0.3900
D	0.6030	0.3910
E	0.6430	0.4050
F	0.6180	0.3870
G	0.6480	0.4070
H	0.6490	0.3960
I	0.7860	0.4750
J	0.7800	0.4840
K	0.6400	0.3940
L	0.6700	0.4180
M	0.6450	0.3850