wwPDB EM Validation Summary Report

Nov 27, 2022 – 09:20 PM EST

PDB ID	:	7KZS
EMDB ID	:	EMD-23088
Title	:	Structure of the human fanconi anaemia Core-UBE2T-ID-DNA complex in open state
Authors	:	Wang, S.L.; Pavletich, N.P.
Deposited on	:	2020-12-10
Resolution	:	4.20 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:

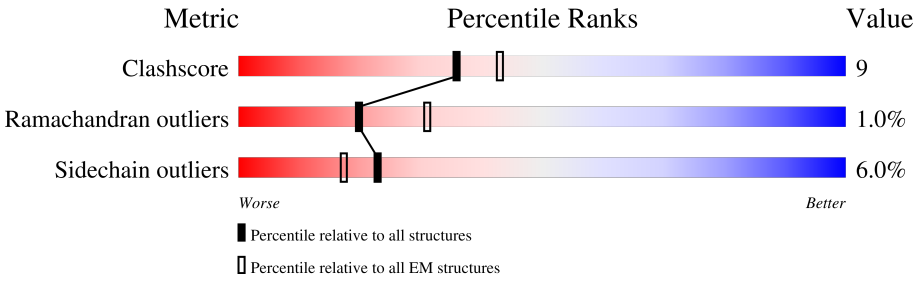
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1477	11% 62% 17% • 20%
1	S	1477	6% 68% 16% • 15%
2	B	884	• 53% 22% • 21%
2	O	884	• 60% 17% • 21%
3	C	583	• 73% 20% • 6%
4	E	555	• 45% 26% • 25%
5	F	399	• 67% 18% 15%
6	G	641	6% 69% 20% • 10%

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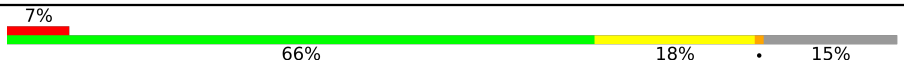
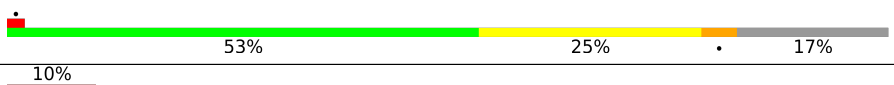
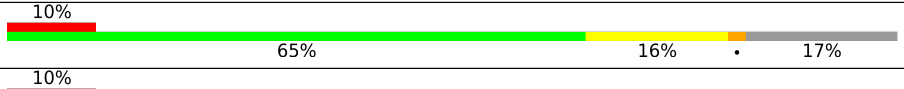
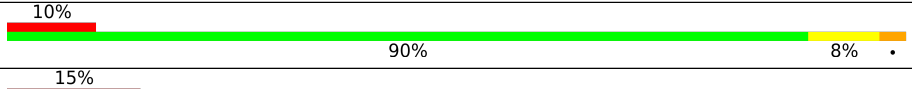
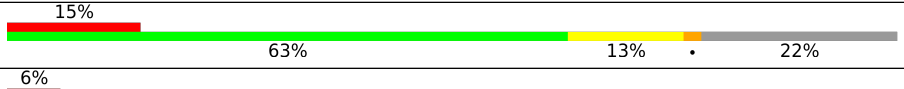
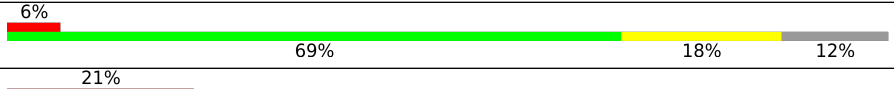
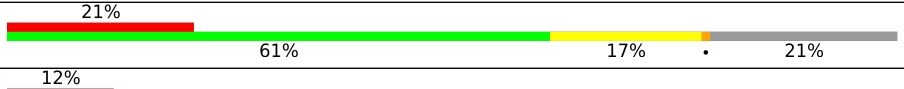
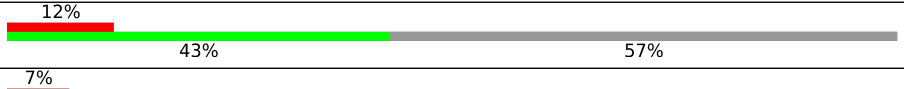
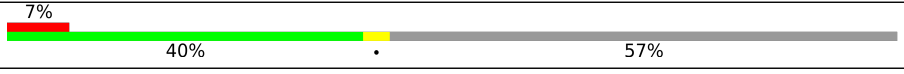
Mol	Chain	Length	Quality of chain
6	H	641	
7	L	394	
7	M	394	
8	P	906	
8	Q	906	
9	W	39	
10	X	197	
11	U	1328	
12	V	1451	
13	Y	58	
14	Z	58	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 176779 atoms, of which 88975 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 Fanconi anemia group A protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1186	Total	C	H	N	O	S	0	0
			18889	6001	9487	1650	1692	59		
1	S	1250	Total	C	H	N	O	S	0	0
			19961	6345	10028	1747	1780	61		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1456	ALA	-	expression tag	UNP O15360
A	1457	ALA	-	expression tag	UNP O15360
A	1458	ALA	-	expression tag	UNP O15360
A	1459	LYS	-	expression tag	UNP O15360
A	1460	LEU	-	expression tag	UNP O15360
A	1461	VAL	-	expression tag	UNP O15360
A	1462	ASP	-	expression tag	UNP O15360
A	1463	GLU	-	expression tag	UNP O15360
A	1464	ASP	-	expression tag	UNP O15360
A	1465	LEU	-	expression tag	UNP O15360
A	1466	TYR	-	expression tag	UNP O15360
A	1467	PHE	-	expression tag	UNP O15360
A	1468	GLN	-	expression tag	UNP O15360
A	1469	SER	-	expression tag	UNP O15360
A	1470	ASP	-	expression tag	UNP O15360
A	1471	TYR	-	expression tag	UNP O15360
A	1472	LYS	-	expression tag	UNP O15360
A	1473	ASP	-	expression tag	UNP O15360
A	1474	ASP	-	expression tag	UNP O15360
A	1475	ASP	-	expression tag	UNP O15360
A	1476	ASP	-	expression tag	UNP O15360
A	1477	LYS	-	expression tag	UNP O15360
S	1456	ALA	-	expression tag	UNP O15360
S	1457	ALA	-	expression tag	UNP O15360
S	1458	ALA	-	expression tag	UNP O15360
S	1459	LYS	-	expression tag	UNP O15360

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Chain	Residue	Modelled	Actual	Comment	Reference
S	1460	LEU	-	expression tag	UNP O15360
S	1461	VAL	-	expression tag	UNP O15360
S	1462	ASP	-	expression tag	UNP O15360
S	1463	GLU	-	expression tag	UNP O15360
S	1464	ASP	-	expression tag	UNP O15360
S	1465	LEU	-	expression tag	UNP O15360
S	1466	TYR	-	expression tag	UNP O15360
S	1467	PHE	-	expression tag	UNP O15360
S	1468	GLN	-	expression tag	UNP O15360
S	1469	SER	-	expression tag	UNP O15360
S	1470	ASP	-	expression tag	UNP O15360
S	1471	TYR	-	expression tag	UNP O15360
S	1472	LYS	-	expression tag	UNP O15360
S	1473	ASP	-	expression tag	UNP O15360
S	1474	ASP	-	expression tag	UNP O15360
S	1475	ASP	-	expression tag	UNP O15360
S	1476	ASP	-	expression tag	UNP O15360
S	1477	LYS	-	expression tag	UNP O15360

- Molecule 2 is a protein called Fanconi anemia group B protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	701	Total	C	H	N	O	S	0	0
			11395	3619	5790	934	1013	39		
2	O	699	Total	C	H	N	O	S	0	0
			11353	3622	5759	926	1010	36		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	initiating methionine	UNP Q8NB91
B	-23	ASP	-	expression tag	UNP Q8NB91
B	-22	TYR	-	expression tag	UNP Q8NB91
B	-21	LYS	-	expression tag	UNP Q8NB91
B	-20	ASP	-	expression tag	UNP Q8NB91
B	-19	ASP	-	expression tag	UNP Q8NB91
B	-18	ASP	-	expression tag	UNP Q8NB91
B	-17	ASP	-	expression tag	UNP Q8NB91
B	-16	LYS	-	expression tag	UNP Q8NB91
B	-15	GLU	-	expression tag	UNP Q8NB91
B	-14	ASN	-	expression tag	UNP Q8NB91
B	-13	LEU	-	expression tag	UNP Q8NB91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	TYR	-	expression tag	UNP Q8NB91
B	-11	PHE	-	expression tag	UNP Q8NB91
B	-10	GLN	-	expression tag	UNP Q8NB91
B	-9	GLY	-	expression tag	UNP Q8NB91
B	-8	GLY	-	expression tag	UNP Q8NB91
B	-7	GLY	-	expression tag	UNP Q8NB91
B	-6	ARG	-	expression tag	UNP Q8NB91
B	-5	LYS	-	expression tag	UNP Q8NB91
B	-4	LEU	-	expression tag	UNP Q8NB91
B	-3	GLY	-	expression tag	UNP Q8NB91
B	-2	THR	-	expression tag	UNP Q8NB91
B	-1	GLY	-	expression tag	UNP Q8NB91
B	0	SER	-	expression tag	UNP Q8NB91
O	-24	MET	-	initiating methionine	UNP Q8NB91
O	-23	ASP	-	expression tag	UNP Q8NB91
O	-22	TYR	-	expression tag	UNP Q8NB91
O	-21	LYS	-	expression tag	UNP Q8NB91
O	-20	ASP	-	expression tag	UNP Q8NB91
O	-19	ASP	-	expression tag	UNP Q8NB91
O	-18	ASP	-	expression tag	UNP Q8NB91
O	-17	ASP	-	expression tag	UNP Q8NB91
O	-16	LYS	-	expression tag	UNP Q8NB91
O	-15	GLU	-	expression tag	UNP Q8NB91
O	-14	ASN	-	expression tag	UNP Q8NB91
O	-13	LEU	-	expression tag	UNP Q8NB91
O	-12	TYR	-	expression tag	UNP Q8NB91
O	-11	PHE	-	expression tag	UNP Q8NB91
O	-10	GLN	-	expression tag	UNP Q8NB91
O	-9	GLY	-	expression tag	UNP Q8NB91
O	-8	GLY	-	expression tag	UNP Q8NB91
O	-7	GLY	-	expression tag	UNP Q8NB91
O	-6	ARG	-	expression tag	UNP Q8NB91
O	-5	LYS	-	expression tag	UNP Q8NB91
O	-4	LEU	-	expression tag	UNP Q8NB91
O	-3	GLY	-	expression tag	UNP Q8NB91
O	-2	THR	-	expression tag	UNP Q8NB91
O	-1	GLY	-	expression tag	UNP Q8NB91
O	0	SER	-	expression tag	UNP Q8NB91

- Molecule 3 is a protein called Fanconi anemia group C protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	550	Total	C	H	N	O	S	0	0
			8838	2826	4442	749	791	30		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	MET	-	initiating methionine	UNP Q00597
C	-23	ASP	-	expression tag	UNP Q00597
C	-22	TYR	-	expression tag	UNP Q00597
C	-21	LYS	-	expression tag	UNP Q00597
C	-20	ASP	-	expression tag	UNP Q00597
C	-19	ASP	-	expression tag	UNP Q00597
C	-18	ASP	-	expression tag	UNP Q00597
C	-17	ASP	-	expression tag	UNP Q00597
C	-16	LYS	-	expression tag	UNP Q00597
C	-15	GLU	-	expression tag	UNP Q00597
C	-14	ASN	-	expression tag	UNP Q00597
C	-13	LEU	-	expression tag	UNP Q00597
C	-12	TYR	-	expression tag	UNP Q00597
C	-11	PHE	-	expression tag	UNP Q00597
C	-10	GLN	-	expression tag	UNP Q00597
C	-9	GLY	-	expression tag	UNP Q00597
C	-8	GLY	-	expression tag	UNP Q00597
C	-7	GLY	-	expression tag	UNP Q00597
C	-6	ARG	-	expression tag	UNP Q00597
C	-5	LYS	-	expression tag	UNP Q00597
C	-4	LEU	-	expression tag	UNP Q00597
C	-3	GLY	-	expression tag	UNP Q00597
C	-2	THR	-	expression tag	UNP Q00597
C	-1	GLY	-	expression tag	UNP Q00597
C	0	SER	-	expression tag	UNP Q00597

- Molecule 4 is a protein called Fanconi anemia group E protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	419	Total	C	H	N	O	S	0	0
			6614	2048	3390	560	592	24		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	MET	-	initiating methionine	UNP Q9HB96
E	-17	ASP	-	expression tag	UNP Q9HB96

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	TYR	-	expression tag	UNP Q9HB96
E	-15	LYS	-	expression tag	UNP Q9HB96
E	-14	ASP	-	expression tag	UNP Q9HB96
E	-13	ASP	-	expression tag	UNP Q9HB96
E	-12	ASP	-	expression tag	UNP Q9HB96
E	-11	ASP	-	expression tag	UNP Q9HB96
E	-10	LYS	-	expression tag	UNP Q9HB96
E	-9	GLU	-	expression tag	UNP Q9HB96
E	-8	ASN	-	expression tag	UNP Q9HB96
E	-7	LEU	-	expression tag	UNP Q9HB96
E	-6	TYR	-	expression tag	UNP Q9HB96
E	-5	PHE	-	expression tag	UNP Q9HB96
E	-4	GLN	-	expression tag	UNP Q9HB96
E	-3	GLY	-	expression tag	UNP Q9HB96
E	-2	GLY	-	expression tag	UNP Q9HB96
E	-1	GLY	-	expression tag	UNP Q9HB96
E	0	ARG	-	expression tag	UNP Q9HB96

- Molecule 5 is a protein called Fanconi anemia group F protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	340	Total	C	H	N	O	S	0	0
			5466	1730	2740	506	483	7		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-24	MET	-	initiating methionine	UNP Q9NPI8
F	-23	ASP	-	expression tag	UNP Q9NPI8
F	-22	TYR	-	expression tag	UNP Q9NPI8
F	-21	LYS	-	expression tag	UNP Q9NPI8
F	-20	ASP	-	expression tag	UNP Q9NPI8
F	-19	ASP	-	expression tag	UNP Q9NPI8
F	-18	ASP	-	expression tag	UNP Q9NPI8
F	-17	ASP	-	expression tag	UNP Q9NPI8
F	-16	LYS	-	expression tag	UNP Q9NPI8
F	-15	GLU	-	expression tag	UNP Q9NPI8
F	-14	ASN	-	expression tag	UNP Q9NPI8
F	-13	LEU	-	expression tag	UNP Q9NPI8
F	-12	TYR	-	expression tag	UNP Q9NPI8
F	-11	PHE	-	expression tag	UNP Q9NPI8
F	-10	GLN	-	expression tag	UNP Q9NPI8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	GLY	-	expression tag	UNP Q9NPI8
F	-8	GLY	-	expression tag	UNP Q9NPI8
F	-7	GLY	-	expression tag	UNP Q9NPI8
F	-6	ARG	-	expression tag	UNP Q9NPI8
F	-5	LYS	-	expression tag	UNP Q9NPI8
F	-4	LEU	-	expression tag	UNP Q9NPI8
F	-3	GLY	-	expression tag	UNP Q9NPI8
F	-2	THR	-	expression tag	UNP Q9NPI8
F	-1	GLY	-	expression tag	UNP Q9NPI8
F	0	SER	-	expression tag	UNP Q9NPI8

- Molecule 6 is a protein called Fanconi anemia group G protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	577	Total	C	H	N	O	S	0	0
			9020	2843	4537	778	844	18		
6	H	544	Total	C	H	N	O	S	0	0
			8504	2676	4288	734	790	16		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	MET	-	initiating methionine	UNP O15287
G	-17	ASP	-	expression tag	UNP O15287
G	-16	TYR	-	expression tag	UNP O15287
G	-15	LYS	-	expression tag	UNP O15287
G	-14	ASP	-	expression tag	UNP O15287
G	-13	ASP	-	expression tag	UNP O15287
G	-12	ASP	-	expression tag	UNP O15287
G	-11	ASP	-	expression tag	UNP O15287
G	-10	LYS	-	expression tag	UNP O15287
G	-9	GLU	-	expression tag	UNP O15287
G	-8	ASN	-	expression tag	UNP O15287
G	-7	LEU	-	expression tag	UNP O15287
G	-6	TYR	-	expression tag	UNP O15287
G	-5	PHE	-	expression tag	UNP O15287
G	-4	GLN	-	expression tag	UNP O15287
G	-3	GLY	-	expression tag	UNP O15287
G	-2	GLY	-	expression tag	UNP O15287
G	-1	GLY	-	expression tag	UNP O15287
G	0	ARG	-	expression tag	UNP O15287
H	-18	MET	-	initiating methionine	UNP O15287

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	ASP	-	expression tag	UNP O15287
H	-16	TYR	-	expression tag	UNP O15287
H	-15	LYS	-	expression tag	UNP O15287
H	-14	ASP	-	expression tag	UNP O15287
H	-13	ASP	-	expression tag	UNP O15287
H	-12	ASP	-	expression tag	UNP O15287
H	-11	ASP	-	expression tag	UNP O15287
H	-10	LYS	-	expression tag	UNP O15287
H	-9	GLU	-	expression tag	UNP O15287
H	-8	ASN	-	expression tag	UNP O15287
H	-7	LEU	-	expression tag	UNP O15287
H	-6	TYR	-	expression tag	UNP O15287
H	-5	PHE	-	expression tag	UNP O15287
H	-4	GLN	-	expression tag	UNP O15287
H	-3	GLY	-	expression tag	UNP O15287
H	-2	GLY	-	expression tag	UNP O15287
H	-1	GLY	-	expression tag	UNP O15287
H	0	ARG	-	expression tag	UNP O15287

- Molecule 7 is a protein called E3 ubiquitin-protein ligase FANCL.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	370	Total	C	H	N	O	S	0	0
			5951	1914	2977	496	542	22		
7	M	370	Total	C	H	N	O	S	0	0
			5951	1914	2977	496	542	22		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-18	MET	-	initiating methionine	UNP Q9NW38
L	-17	ASP	-	expression tag	UNP Q9NW38
L	-16	TYR	-	expression tag	UNP Q9NW38
L	-15	LYS	-	expression tag	UNP Q9NW38
L	-14	ASP	-	expression tag	UNP Q9NW38
L	-13	ASP	-	expression tag	UNP Q9NW38
L	-12	ASP	-	expression tag	UNP Q9NW38
L	-11	ASP	-	expression tag	UNP Q9NW38
L	-10	LYS	-	expression tag	UNP Q9NW38
L	-9	GLU	-	expression tag	UNP Q9NW38
L	-8	ASN	-	expression tag	UNP Q9NW38
L	-7	LEU	-	expression tag	UNP Q9NW38

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	TYR	-	expression tag	UNP Q9NW38
L	-5	PHE	-	expression tag	UNP Q9NW38
L	-4	GLN	-	expression tag	UNP Q9NW38
L	-3	GLY	-	expression tag	UNP Q9NW38
L	-2	GLY	-	expression tag	UNP Q9NW38
L	-1	GLY	-	expression tag	UNP Q9NW38
L	0	ARG	-	expression tag	UNP Q9NW38
M	-18	MET	-	initiating methionine	UNP Q9NW38
M	-17	ASP	-	expression tag	UNP Q9NW38
M	-16	TYR	-	expression tag	UNP Q9NW38
M	-15	LYS	-	expression tag	UNP Q9NW38
M	-14	ASP	-	expression tag	UNP Q9NW38
M	-13	ASP	-	expression tag	UNP Q9NW38
M	-12	ASP	-	expression tag	UNP Q9NW38
M	-11	ASP	-	expression tag	UNP Q9NW38
M	-10	LYS	-	expression tag	UNP Q9NW38
M	-9	GLU	-	expression tag	UNP Q9NW38
M	-8	ASN	-	expression tag	UNP Q9NW38
M	-7	LEU	-	expression tag	UNP Q9NW38
M	-6	TYR	-	expression tag	UNP Q9NW38
M	-5	PHE	-	expression tag	UNP Q9NW38
M	-4	GLN	-	expression tag	UNP Q9NW38
M	-3	GLY	-	expression tag	UNP Q9NW38
M	-2	GLY	-	expression tag	UNP Q9NW38
M	-1	GLY	-	expression tag	UNP Q9NW38
M	0	ARG	-	expression tag	UNP Q9NW38

- Molecule 8 is a protein called Fanconi anemia core complex-associated protein 100.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	748	Total	C	H	N	O	S	0	0
			11279	3520	5681	972	1058	48		
8	Q	754	Total	C	H	N	O	S	0	0
			11355	3548	5724	978	1058	47		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-24	MET	-	initiating methionine	UNP Q0VG06
P	-23	ASP	-	expression tag	UNP Q0VG06
P	-22	TYR	-	expression tag	UNP Q0VG06
P	-21	LYS	-	expression tag	UNP Q0VG06

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-20	ASP	-	expression tag	UNP Q0VG06
P	-19	HIS	-	expression tag	UNP Q0VG06
P	-18	ASP	-	expression tag	UNP Q0VG06
P	-17	GLY	-	expression tag	UNP Q0VG06
P	-16	ASP	-	expression tag	UNP Q0VG06
P	-15	TYR	-	expression tag	UNP Q0VG06
P	-14	LYS	-	expression tag	UNP Q0VG06
P	-13	ASP	-	expression tag	UNP Q0VG06
P	-12	HIS	-	expression tag	UNP Q0VG06
P	-11	ASP	-	expression tag	UNP Q0VG06
P	-10	ILE	-	expression tag	UNP Q0VG06
P	-9	ASP	-	expression tag	UNP Q0VG06
P	-8	TYR	-	expression tag	UNP Q0VG06
P	-7	LYS	-	expression tag	UNP Q0VG06
P	-6	ASP	-	expression tag	UNP Q0VG06
P	-5	ASP	-	expression tag	UNP Q0VG06
P	-4	ASP	-	expression tag	UNP Q0VG06
P	-3	ASP	-	expression tag	UNP Q0VG06
P	-2	LYS	-	expression tag	UNP Q0VG06
P	-1	GLY	-	expression tag	UNP Q0VG06
P	0	SER	-	expression tag	UNP Q0VG06
Q	-24	MET	-	initiating methionine	UNP Q0VG06
Q	-23	ASP	-	expression tag	UNP Q0VG06
Q	-22	TYR	-	expression tag	UNP Q0VG06
Q	-21	LYS	-	expression tag	UNP Q0VG06
Q	-20	ASP	-	expression tag	UNP Q0VG06
Q	-19	HIS	-	expression tag	UNP Q0VG06
Q	-18	ASP	-	expression tag	UNP Q0VG06
Q	-17	GLY	-	expression tag	UNP Q0VG06
Q	-16	ASP	-	expression tag	UNP Q0VG06
Q	-15	TYR	-	expression tag	UNP Q0VG06
Q	-14	LYS	-	expression tag	UNP Q0VG06
Q	-13	ASP	-	expression tag	UNP Q0VG06
Q	-12	HIS	-	expression tag	UNP Q0VG06
Q	-11	ASP	-	expression tag	UNP Q0VG06
Q	-10	ILE	-	expression tag	UNP Q0VG06
Q	-9	ASP	-	expression tag	UNP Q0VG06
Q	-8	TYR	-	expression tag	UNP Q0VG06
Q	-7	LYS	-	expression tag	UNP Q0VG06
Q	-6	ASP	-	expression tag	UNP Q0VG06
Q	-5	ASP	-	expression tag	UNP Q0VG06
Q	-4	ASP	-	expression tag	UNP Q0VG06

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-3	ASP	-	expression tag	UNP Q0VG06
Q	-2	LYS	-	expression tag	UNP Q0VG06
Q	-1	GLY	-	expression tag	UNP Q0VG06
Q	0	SER	-	expression tag	UNP Q0VG06

- Molecule 9 is a protein called Fanconi anemia core complex-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	39	Total	C	H	N	O	0	0
			513	179	242	42	50		

- Molecule 10 is a protein called Ubiquitin-conjugating enzyme E2 T.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	X	153	Total	C	H	N	O	S	0	0
			2484	789	1251	216	221	7		

- Molecule 11 is a protein called Fanconi anemia, complementation group I.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	U	1168	Total	C	H	N	O	S	0	0
			18882	5933	9626	1549	1720	54		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	877	LEU	ILE	conflict	UNP B7ZMF2
U	1235	VAL	ALA	conflict	UNP B7ZMF2
U	1274	SER	ASN	conflict	UNP B7ZMF2

- Molecule 12 is a protein called Fanconi anemia group D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	V	1153	Total	C	H	N	O	S	0	0
			18733	5970	9475	1527	1709	52		

- Molecule 13 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	Y	25	Total	C	H	N	O	P	0	0
			796	243	280	99	149	25		

- Molecule 14 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Z	25	Total	C	H	N	O	P	0	0
			790	241	281	92	151	25		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

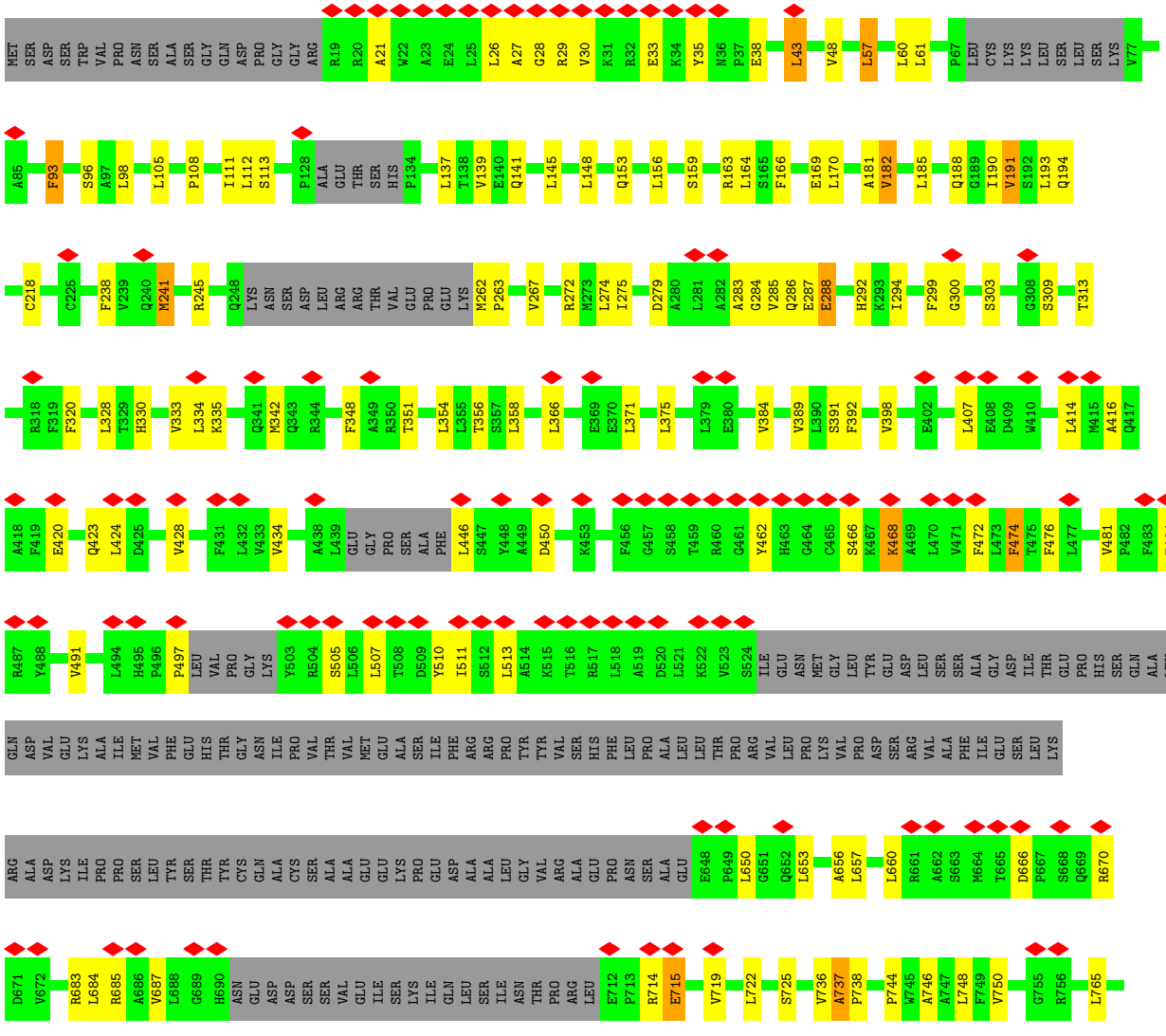
Mol	Chain	Residues	Atoms		AltConf
15	G	1	Total	Zn	0
			1	1	
15	L	2	Total	Zn	0
			2	2	
15	M	2	Total	Zn	0
			2	2	

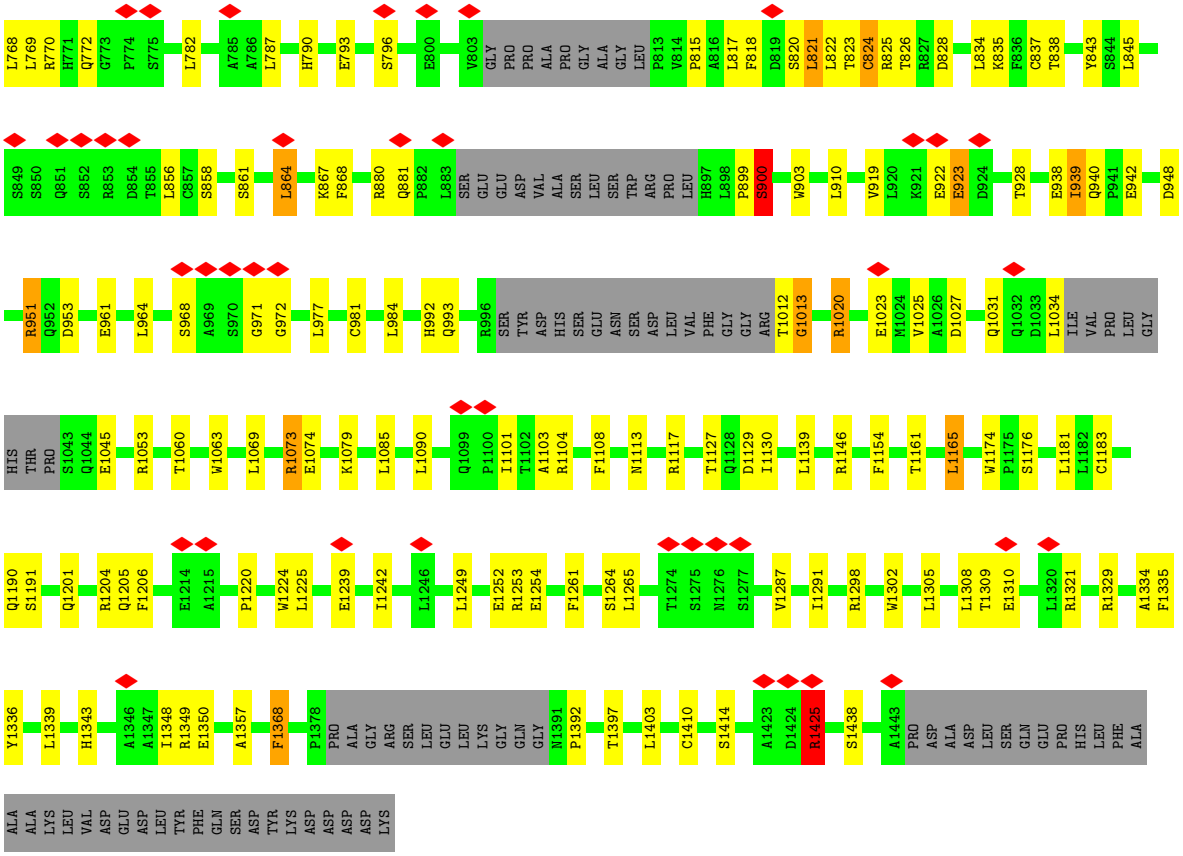
3 Residue-property plots (i)

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: Fanconi anemia group A protein

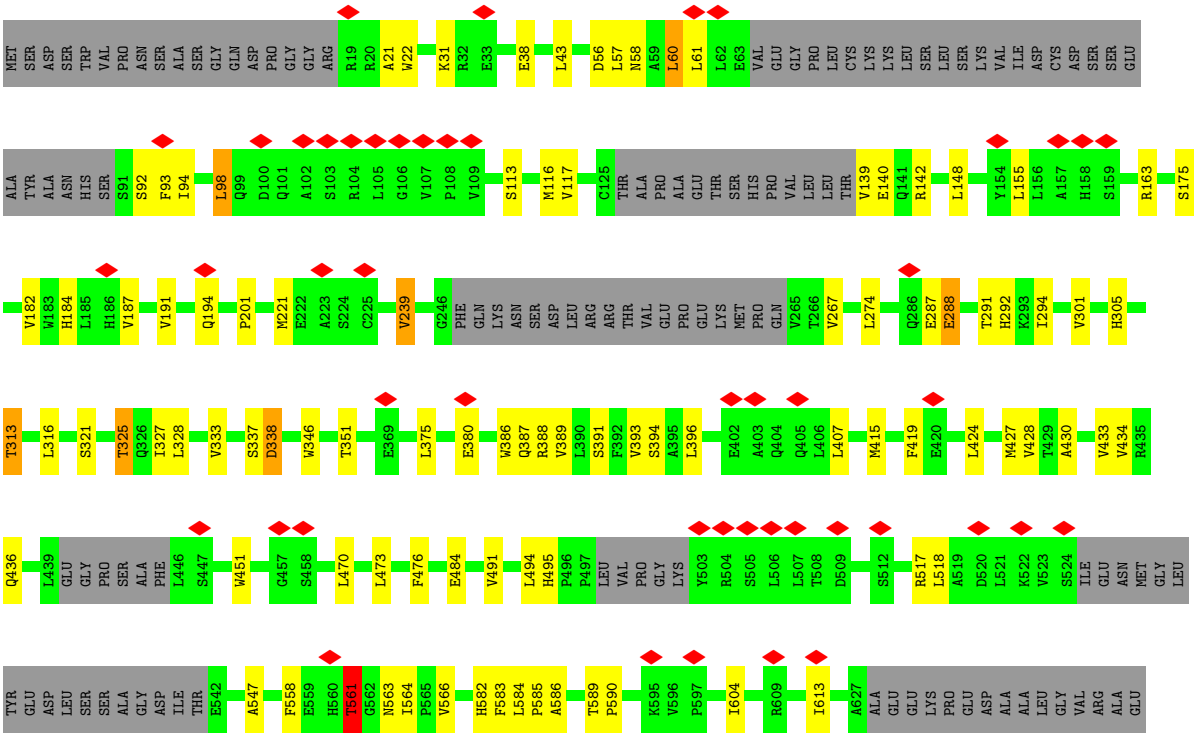
Chain A:

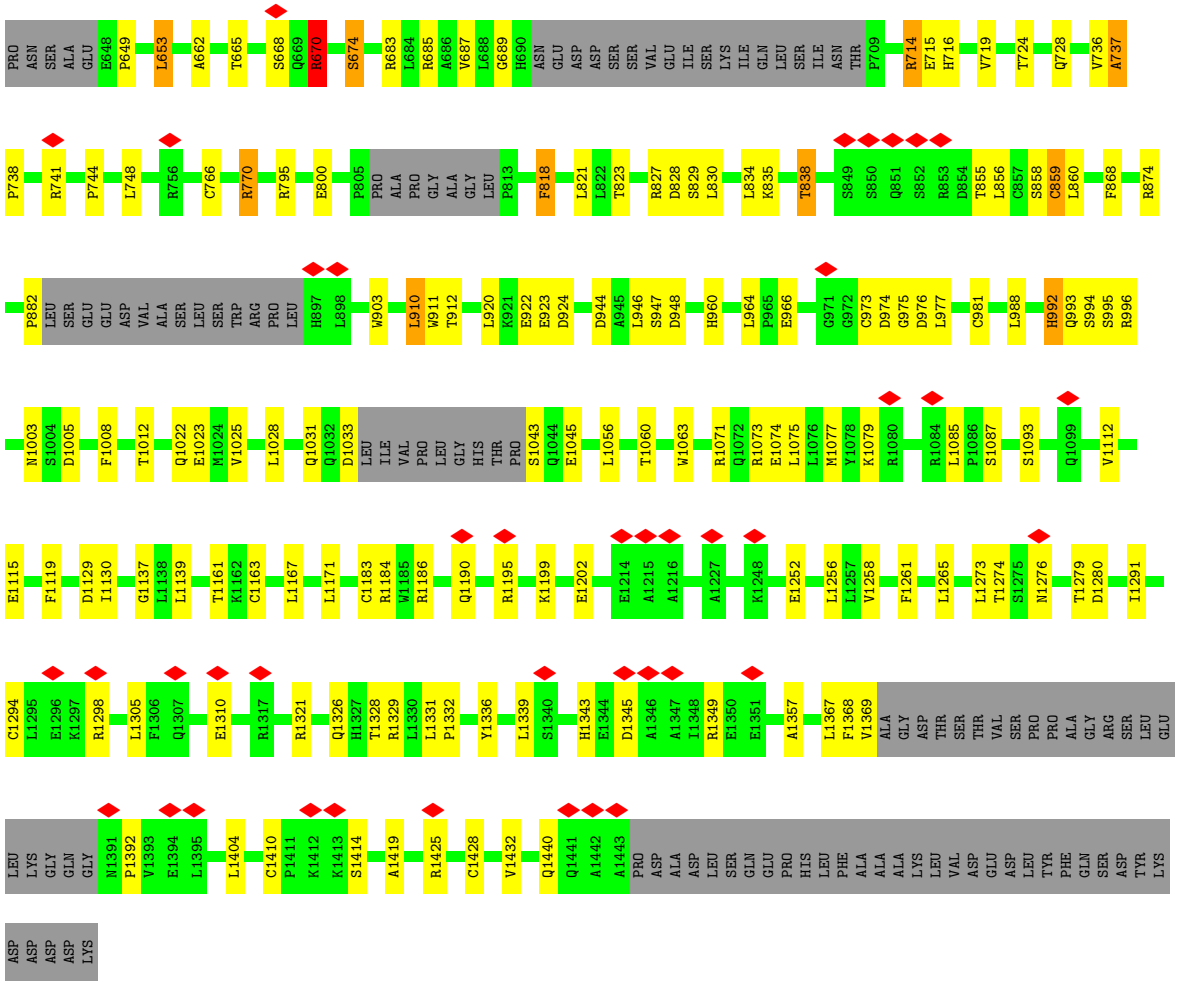




• Molecule 1: Fanconi anemia group A protein

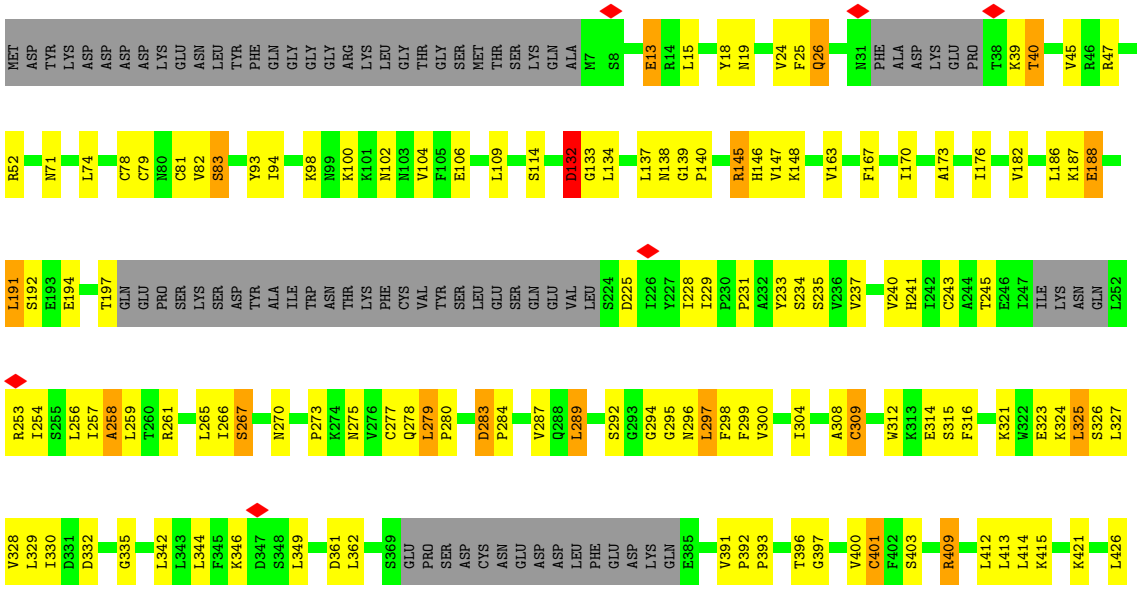
Chain S:

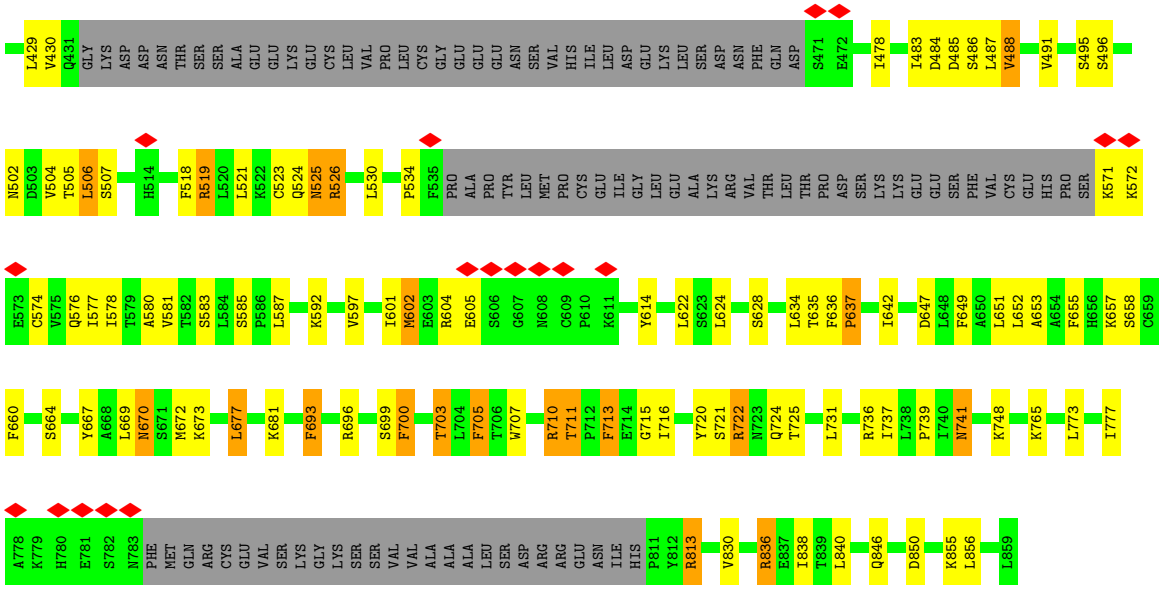




• Molecule 2: Fanconi anemia group B protein

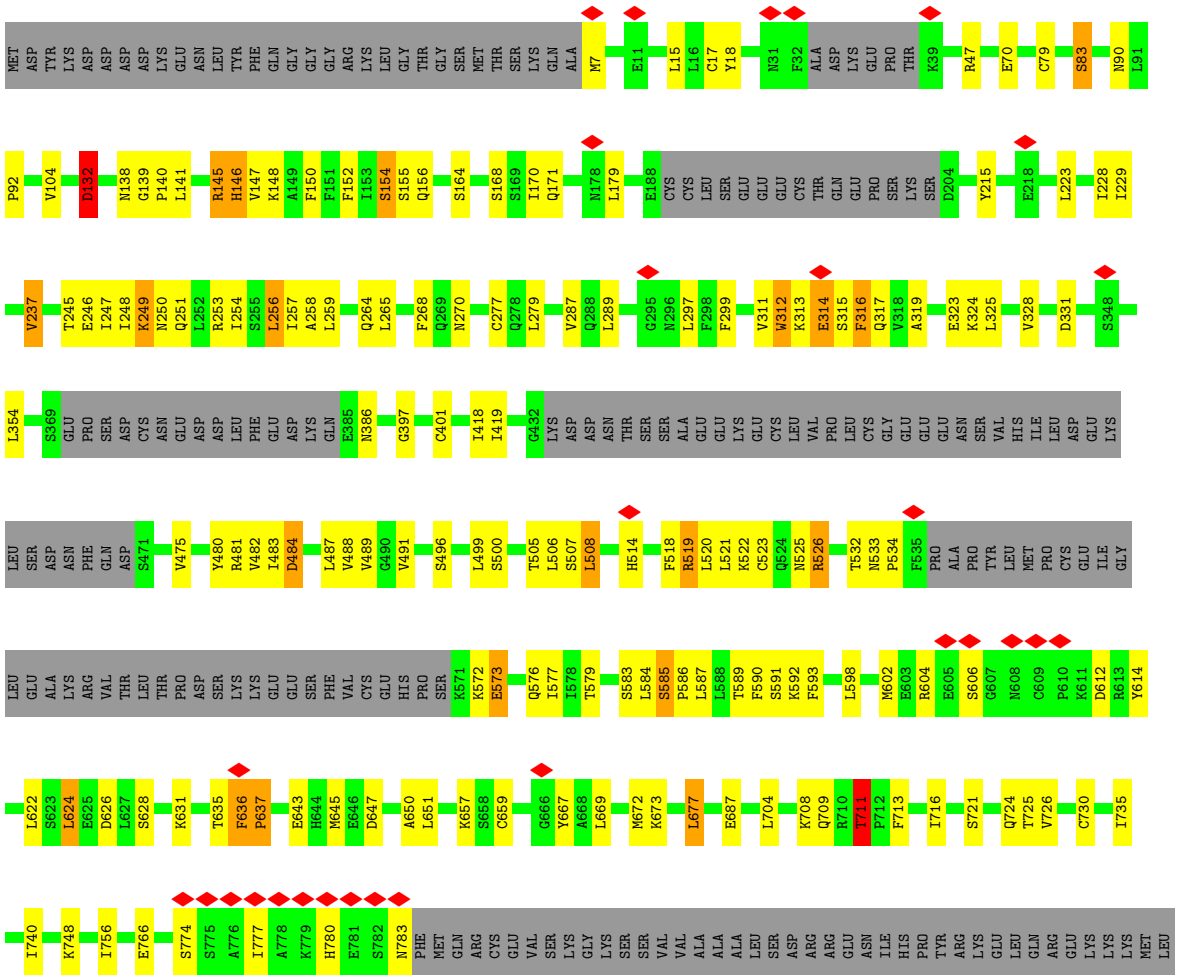
Chain B:





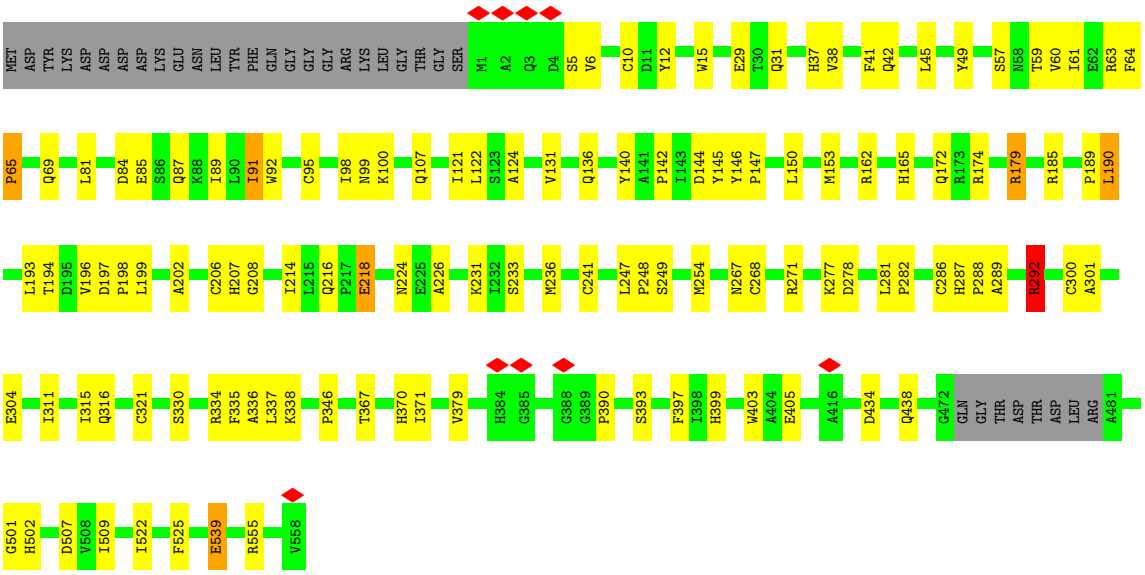
• Molecule 2: Fanconi anemia group B protein

Chain O:



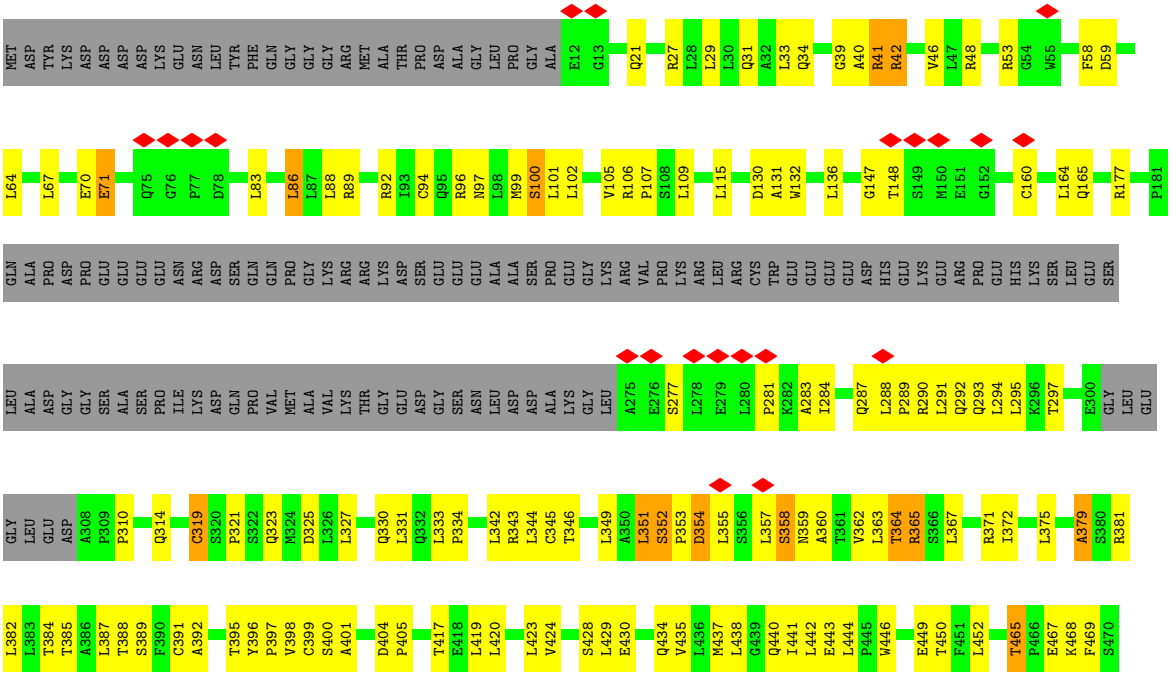
• Molecule 3: Fanconi anemia group C protein

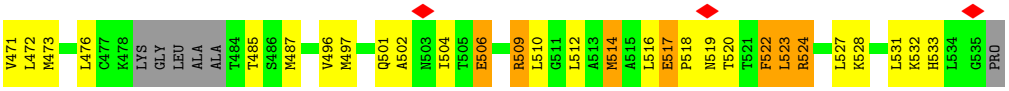
Chain C:



• Molecule 4: Fanconi anemia group E protein

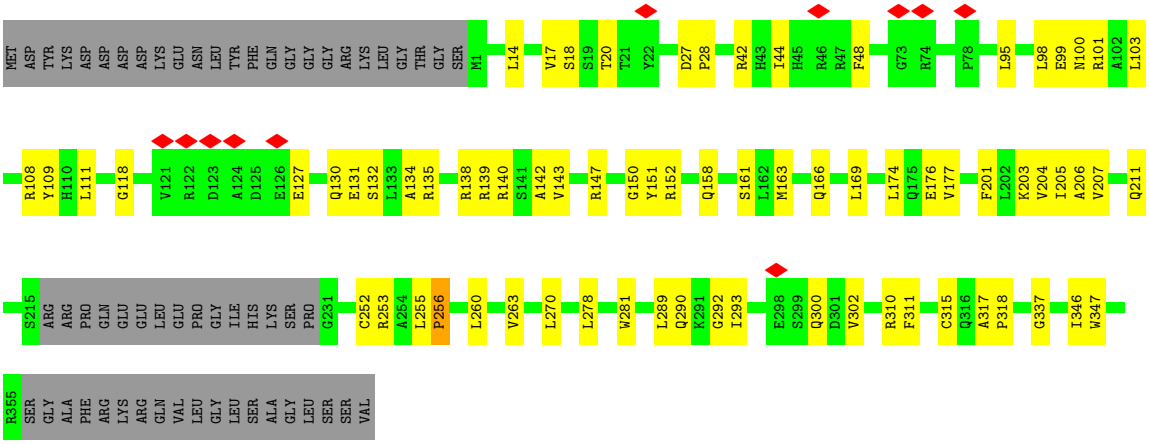
Chain E:





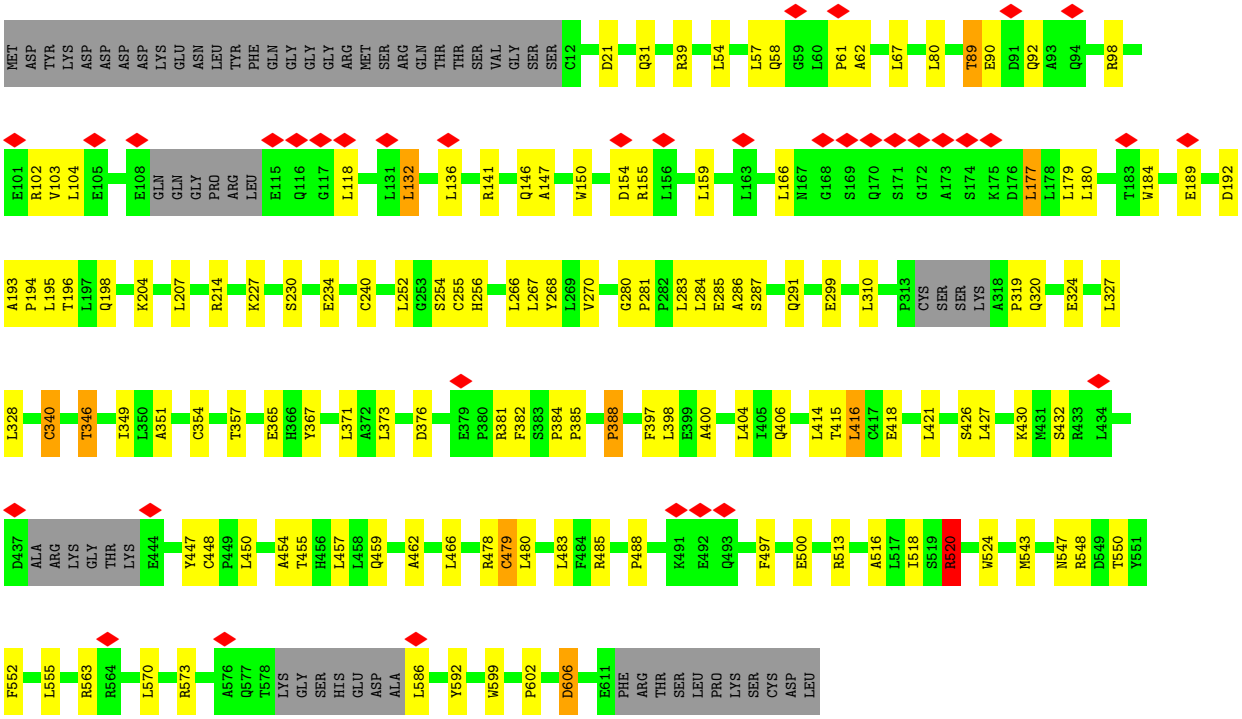
• Molecule 5: Fanconi anemia group F protein

Chain F:



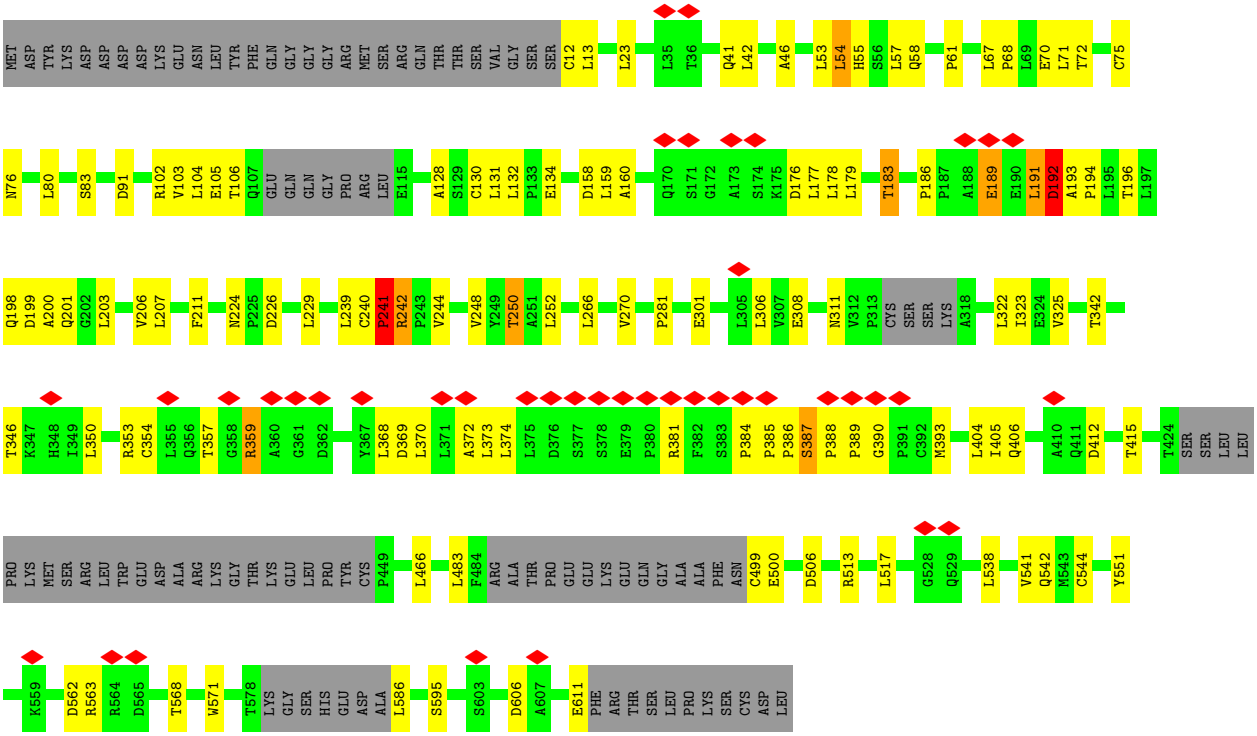
• Molecule 6: Fanconi anemia group G protein

Chain G:



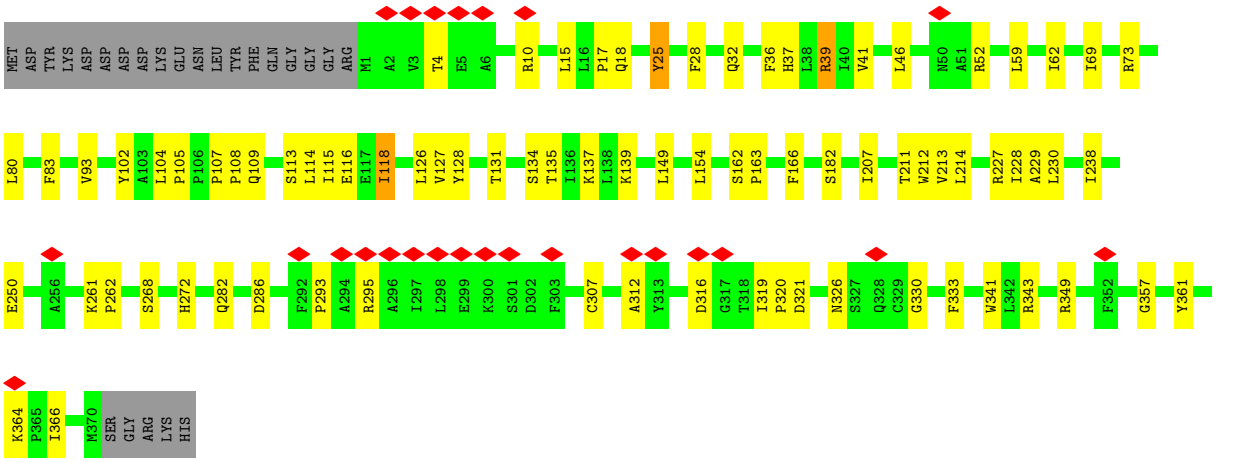
• Molecule 6: Fanconi anemia group G protein

Chain H:



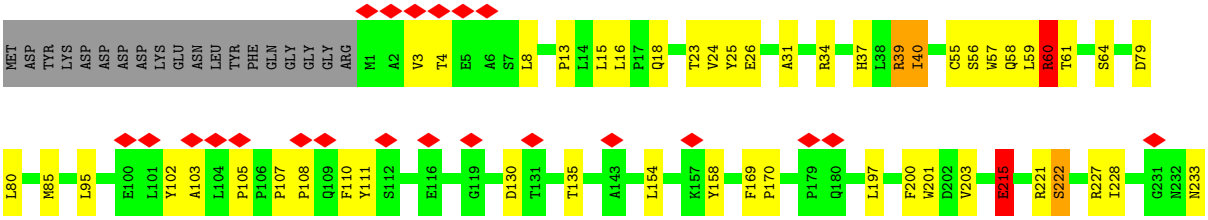
• Molecule 7: E3 ubiquitin-protein ligase FANCL

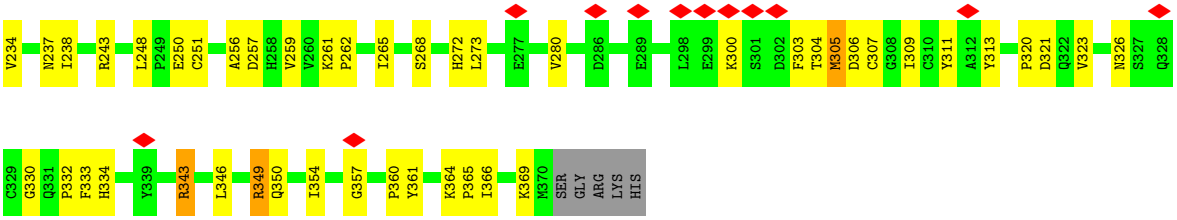
Chain L:



• Molecule 7: E3 ubiquitin-protein ligase FANCL

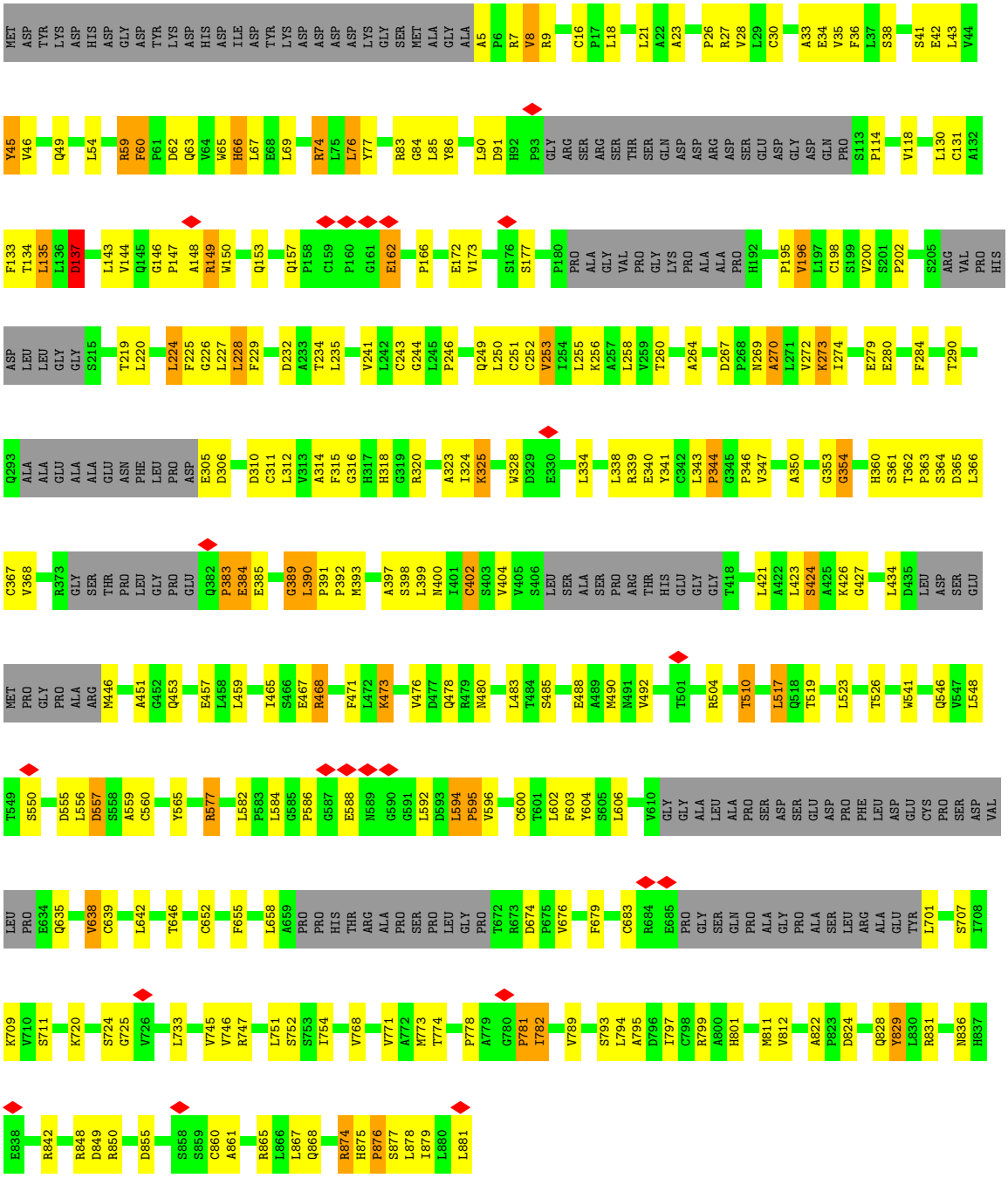
Chain M:





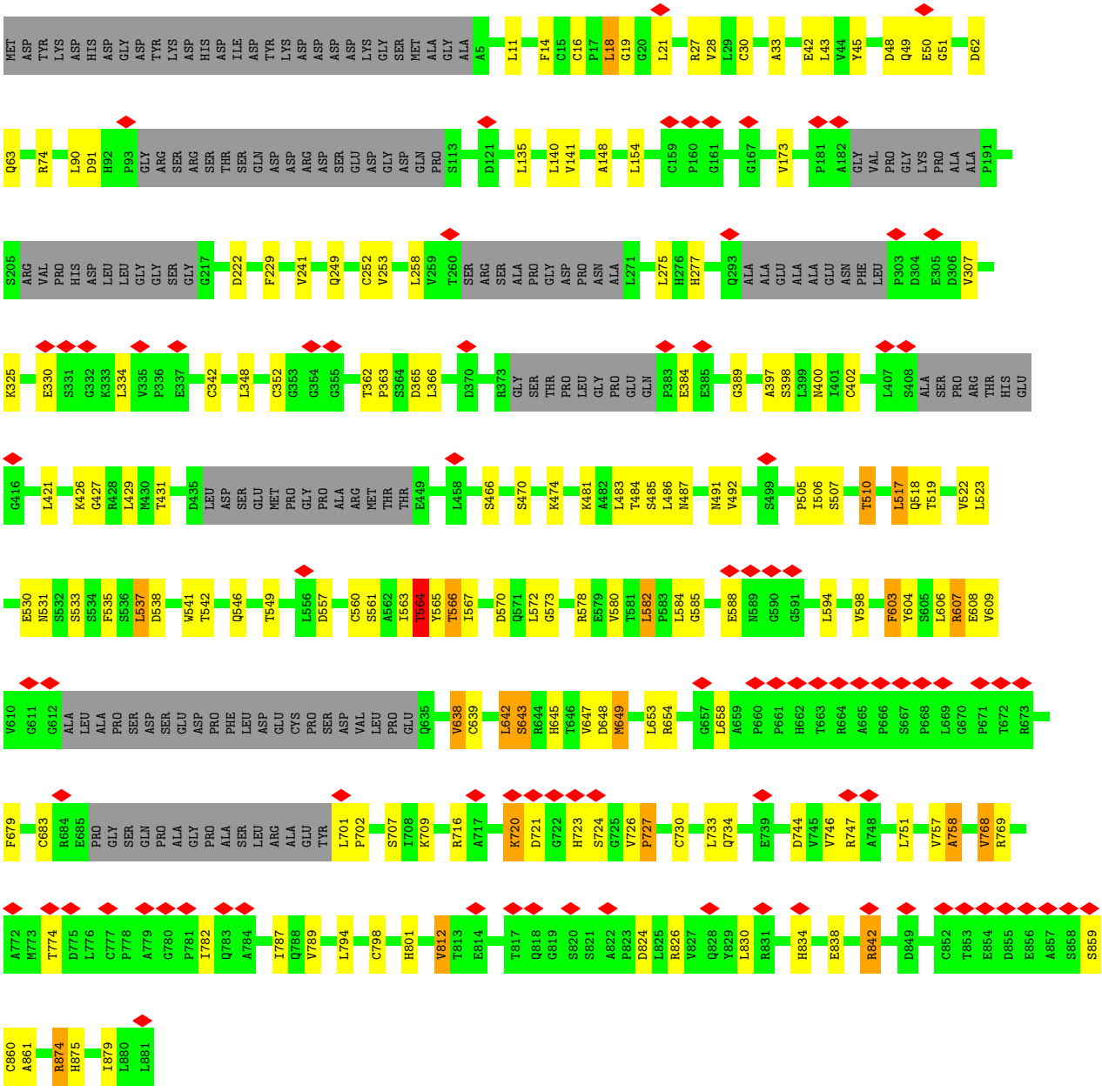
• Molecule 8: Fanconi anemia core complex-associated protein 100

Chain P:



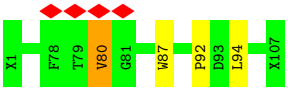
• Molecule 8: Fanconi anemia core complex-associated protein 100

Chain Q:



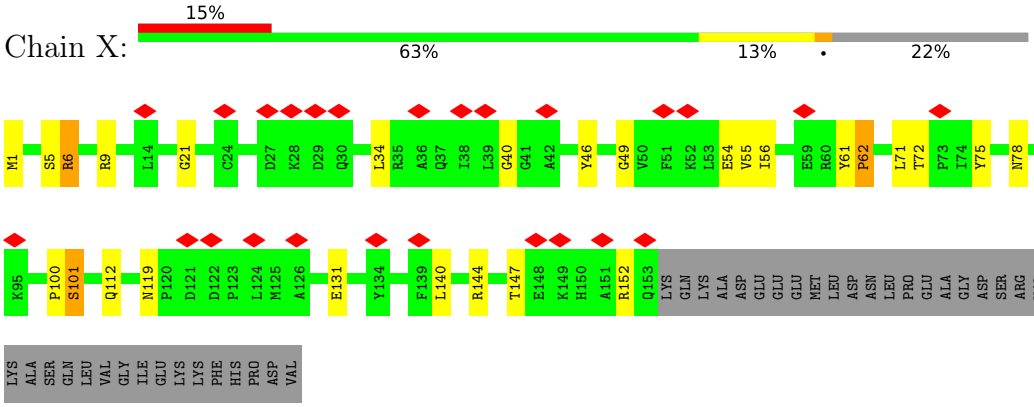
• Molecule 9: Fanconi anemia core complex-associated protein 20

Chain W:



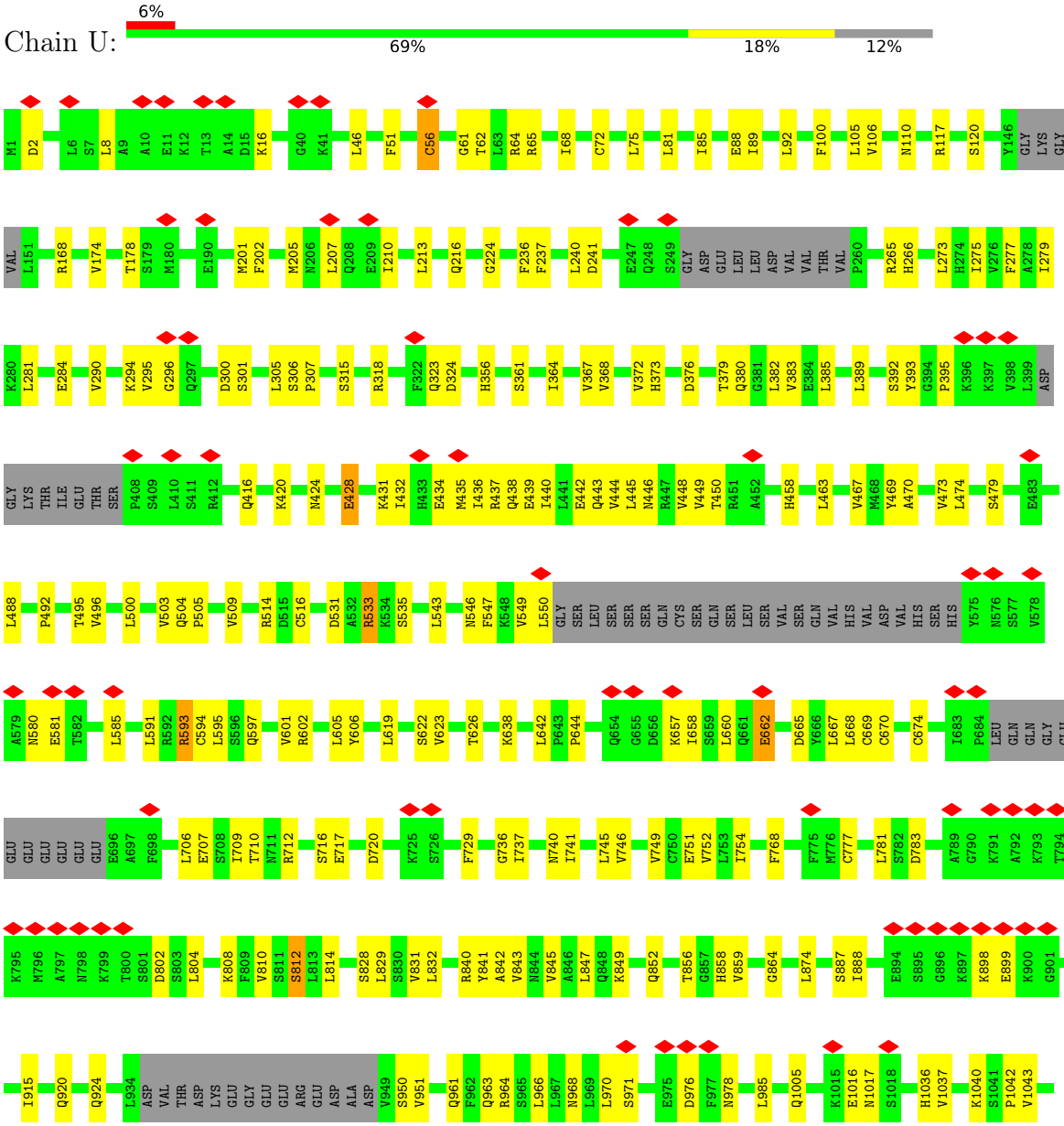
• Molecule 10: Ubiquitin-conjugating enzyme E2 T

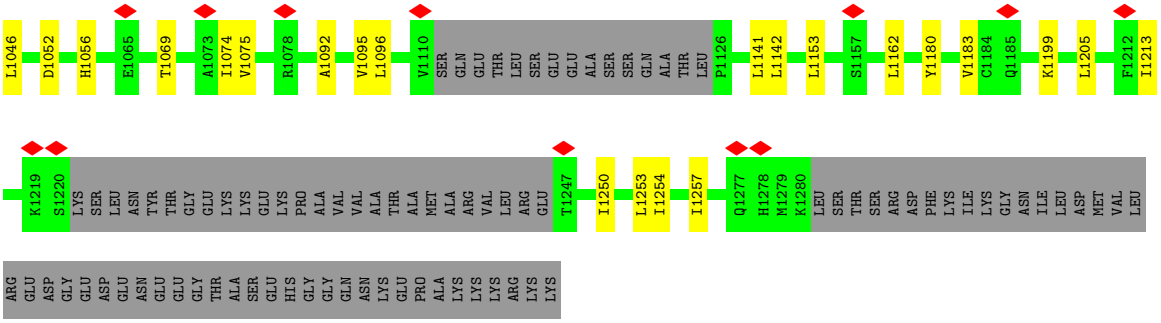
Chain X:



• Molecule 11: Fanconi anemia, complementation group I

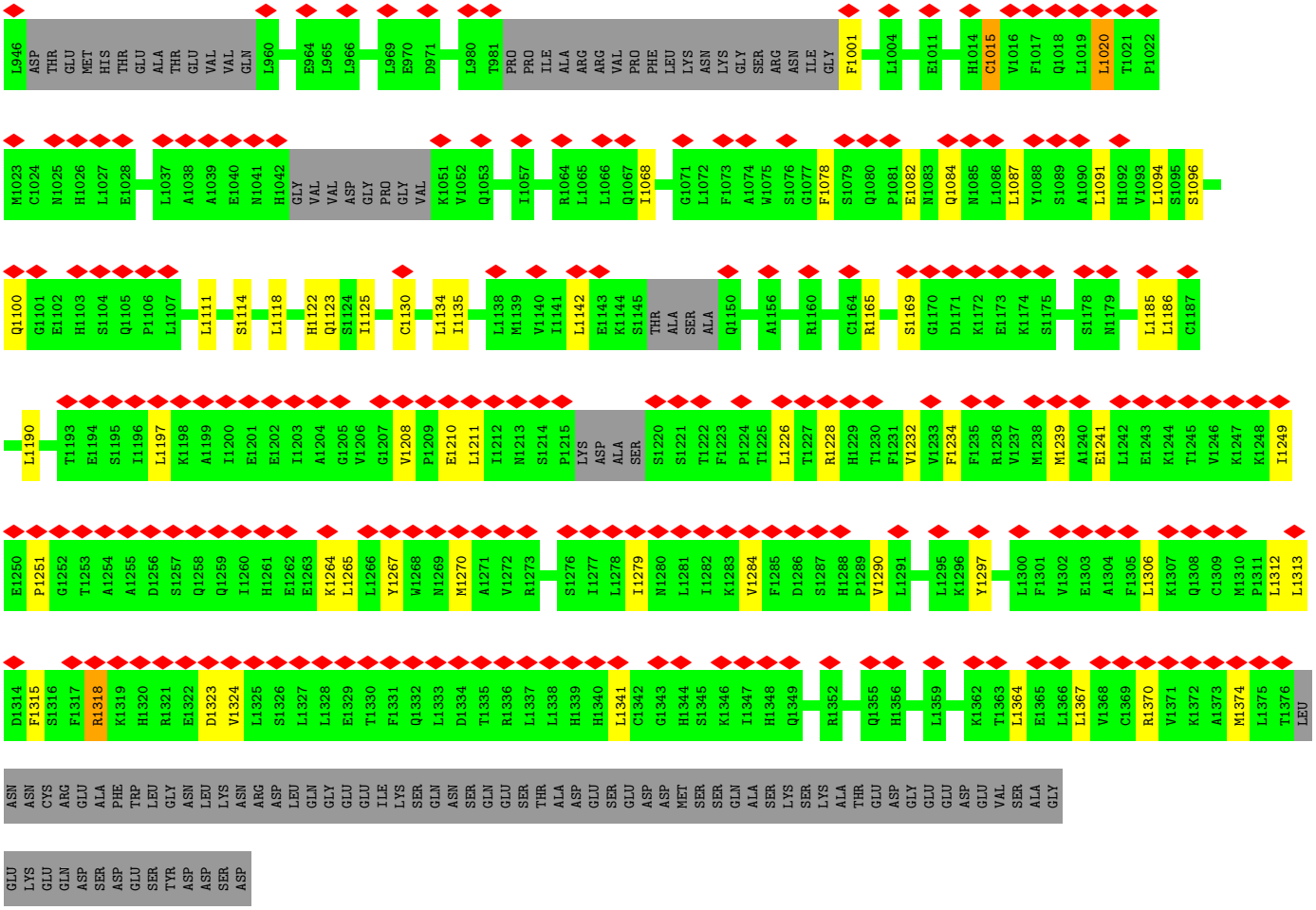
Chain U:





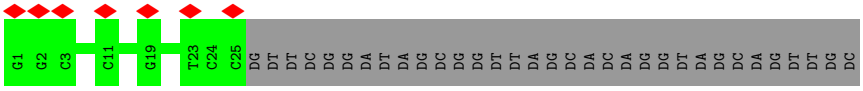
• Molecule 12: Fanconi anemia group D2 protein

Chain V:



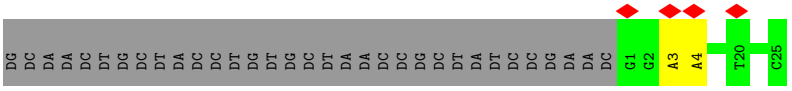
• Molecule 13: DNA (25-MER)

Chain Y:



• Molecule 14: DNA (25-MER)

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40749	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 ($e^-/Å^2$)	36.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0065	Depositor
Map size (Å)	473.088, 473.088, 473.088	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.72	0/9605	0.97	9/13008 (0.1%)
1	S	0.72	0/10153	0.98	6/13749 (0.0%)
2	B	0.80	2/5707 (0.0%)	1.16	13/7686 (0.2%)
2	O	0.75	1/5701 (0.0%)	1.04	3/7686 (0.0%)
3	C	0.76	0/4497	1.07	4/6103 (0.1%)
4	E	0.83	0/3274	1.22	10/4438 (0.2%)
5	F	0.74	0/2791	1.09	1/3790 (0.0%)
6	G	0.76	0/4568	1.05	3/6215 (0.0%)
6	H	0.72	0/4293	0.98	3/5840 (0.1%)
7	L	0.76	2/3050 (0.1%)	1.04	5/4143 (0.1%)
7	M	0.75	2/3050 (0.1%)	1.03	9/4143 (0.2%)
8	P	0.82	1/5697 (0.0%)	1.23	9/7752 (0.1%)
8	Q	0.73	0/5737	1.04	5/7810 (0.1%)
9	W	0.65	0/202	0.88	0/281
10	X	0.77	0/1267	1.00	1/1722 (0.1%)
11	U	0.73	0/9400	0.98	3/12676 (0.0%)
12	V	0.74	0/9433	0.97	0/12760
13	Y	0.45	0/579	0.89	0/892
14	Z	0.48	0/569	0.96	0/875
All	All	0.75	8/89573 (0.0%)	1.04	84/121569 (0.1%)

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	A	0	8
1	S	0	6
2	B	0	12
2	O	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3
4	E	0	7
5	F	0	2
6	G	0	5
6	H	0	2
7	L	0	2
7	M	0	1
8	P	0	20
8	Q	0	10
10	X	0	4
11	U	0	4
12	V	0	9
All	All	0	104

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	330	GLY	C-N	-11.74	1.07	1.34
7	M	321	ASP	C-N	-10.48	1.09	1.34
7	M	330	GLY	C-N	-8.72	1.14	1.34
2	B	721	SER	CA-CB	-8.20	1.40	1.52
7	L	321	ASP	C-N	-6.40	1.19	1.34

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	321	ASP	O-C-N	-9.79	107.04	122.70
7	M	321	ASP	C-N-CA	9.52	145.50	121.70
8	P	315	PHE	CB-CA-C	-8.47	93.45	110.40
7	M	39	ARG	NE-CZ-NH1	8.28	124.44	120.30
8	Q	727	PRO	N-CD-CG	-7.88	91.38	103.20

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	GLY	Peptide
1	A	484	GLU	Peptide
1	A	824	CYS	Peptide
1	A	899	PRO	Peptide
1	A	922	GLU	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	A	9402	9487	9431	163	0
1	S	9933	10028	9969	124	0
2	B	5605	5790	5768	143	0
2	O	5594	5759	5740	104	0
3	C	4396	4442	4427	77	0
4	E	3224	3390	3384	110	0
5	F	2726	2740	2729	48	0
6	G	4483	4537	4523	72	0
6	H	4216	4288	4273	84	0
7	L	2974	2977	2970	52	0
7	M	2974	2977	2970	74	0
8	P	5598	5681	5652	173	0
8	Q	5631	5724	5694	96	0
9	W	271	242	196	8	0
10	X	1233	1251	1248	20	0
11	U	9256	9626	9595	148	0
12	V	9258	9475	9422	163	0
13	Y	516	280	280	0	0
14	Z	509	281	281	1	0
15	G	1	0	0	0	0
15	L	2	0	0	0	0
15	M	2	0	0	0	0
All	All	87804	88975	88552	1500	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 9.

The worst 5 of 1500 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)
8:Q:466:SER:CB	7:M:107:PRO:HB2	1.35	1.55
6:H:342:THR:CG2	6:H:384:PRO:HG3	1.41	1.50
8:Q:466:SER:HB2	7:M:107:PRO:CB	1.59	1.31
6:H:387:SER:OG	6:H:388:PRO:HD3	1.17	1.31
6:H:342:THR:HG21	6:H:384:PRO:CG	1.63	1.27

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	1160/1477 (78%)	1061 (92%)	93 (8%)	6 (0%)	29 68
1	S	1224/1477 (83%)	1115 (91%)	100 (8%)	9 (1%)	22 62
2	B	685/884 (78%)	591 (86%)	78 (11%)	16 (2%)	6 37
2	O	685/884 (78%)	590 (86%)	79 (12%)	16 (2%)	6 37
3	C	546/583 (94%)	475 (87%)	69 (13%)	2 (0%)	34 72
4	E	411/555 (74%)	370 (90%)	39 (10%)	2 (0%)	29 68
5	F	336/399 (84%)	310 (92%)	25 (7%)	1 (0%)	41 76
6	G	567/641 (88%)	510 (90%)	56 (10%)	1 (0%)	47 80
6	H	532/641 (83%)	484 (91%)	42 (8%)	6 (1%)	14 52
7	L	368/394 (93%)	328 (89%)	40 (11%)	0	100 100
7	M	368/394 (93%)	328 (89%)	38 (10%)	2 (0%)	29 68
8	P	726/906 (80%)	616 (85%)	94 (13%)	16 (2%)	6 38
8	Q	732/906 (81%)	636 (87%)	81 (11%)	15 (2%)	7 40
9	W	21/39 (54%)	13 (62%)	7 (33%)	1 (5%)	2 24
10	X	151/197 (77%)	146 (97%)	3 (2%)	2 (1%)	12 48
11	U	1150/1328 (87%)	1053 (92%)	91 (8%)	6 (0%)	29 68
12	V	1131/1451 (78%)	1047 (93%)	78 (7%)	6 (0%)	29 68
All	All	10793/13156 (82%)	9673 (90%)	1013 (9%)	107 (1%)	20 54

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	GLU
1	A	737	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	132	ASP
2	B	133	GLY
2	B	147	VAL

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	1034/1282 (81%)	957 (93%)	77 (7%)	13 40
1	S	1092/1282 (85%)	1018 (93%)	74 (7%)	16 43
2	B	644/810 (80%)	585 (91%)	59 (9%)	9 31
2	O	641/810 (79%)	595 (93%)	46 (7%)	14 41
3	C	480/507 (95%)	459 (96%)	21 (4%)	28 54
4	E	358/467 (77%)	326 (91%)	32 (9%)	9 34
5	F	288/336 (86%)	284 (99%)	4 (1%)	67 80
6	G	483/538 (90%)	444 (92%)	39 (8%)	11 38
6	H	454/538 (84%)	418 (92%)	36 (8%)	12 39
7	L	334/354 (94%)	322 (96%)	12 (4%)	35 60
7	M	334/354 (94%)	316 (95%)	18 (5%)	22 50
8	P	627/749 (84%)	557 (89%)	70 (11%)	6 25
8	Q	630/749 (84%)	584 (93%)	46 (7%)	14 41
9	W	22/22 (100%)	21 (96%)	1 (4%)	27 54
10	X	136/175 (78%)	132 (97%)	4 (3%)	42 64
11	U	1066/1204 (88%)	1041 (98%)	25 (2%)	50 70
12	V	1065/1324 (80%)	1046 (98%)	19 (2%)	59 76
All	All	9688/11501 (84%)	9105 (94%)	583 (6%)	23 47

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	491	VAL
12	V	509	MET
1	S	800	GLU
1	S	380	GLU
7	M	40	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	102	ASN
11	U	625	GLN
8	Q	875	HIS
11	U	618	GLN
12	V	146	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	W	2
7	L	2
7	M	2

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	9:UNK	C	73:GLU	N	37.33
1	W	95:TRP	C	101:UNK	N	7.01
1	L	321:ASP	C	322:GLN	N	1.19
1	M	330:GLY	C	331:GLN	N	1.14
1	M	321:ASP	C	322:GLN	N	1.09

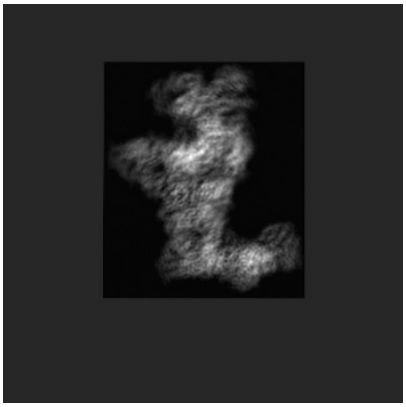
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23088. These allow visual inspection of the internal detail of the map and identification of artifacts.

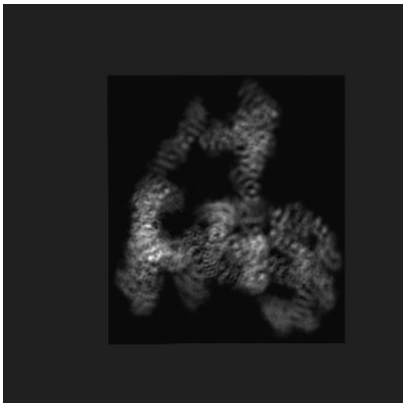
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

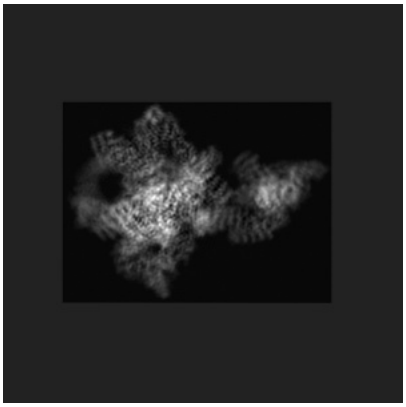
6.1.1 Primary map



X



Y



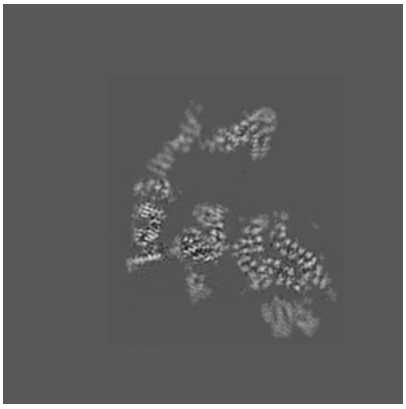
Z

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

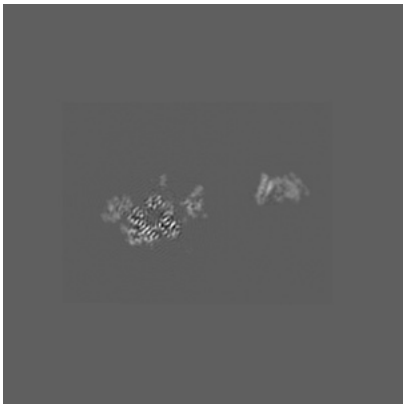
6.2 Central slices

6.2.1 Primary map

X Index: 224



Y Index: 224

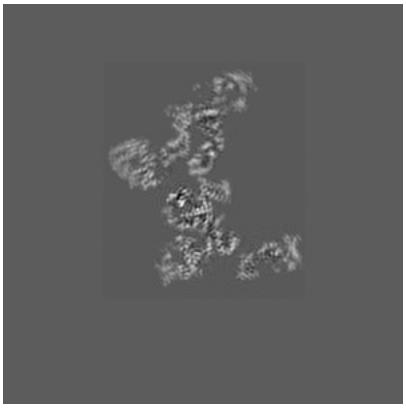


Z Index: 224

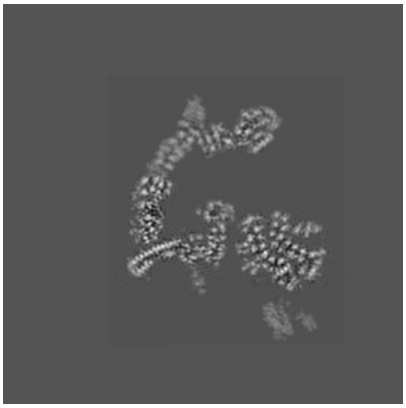
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

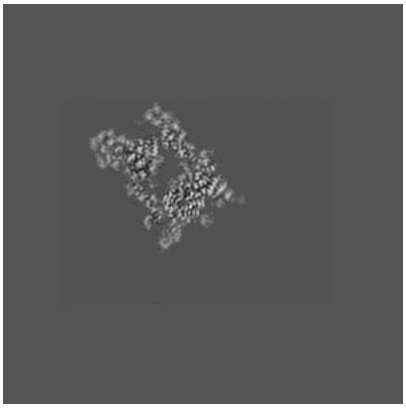
6.3.1 Primary map



X Index: 175



Y Index: 231



Z Index: 161

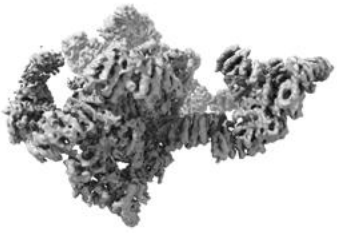
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

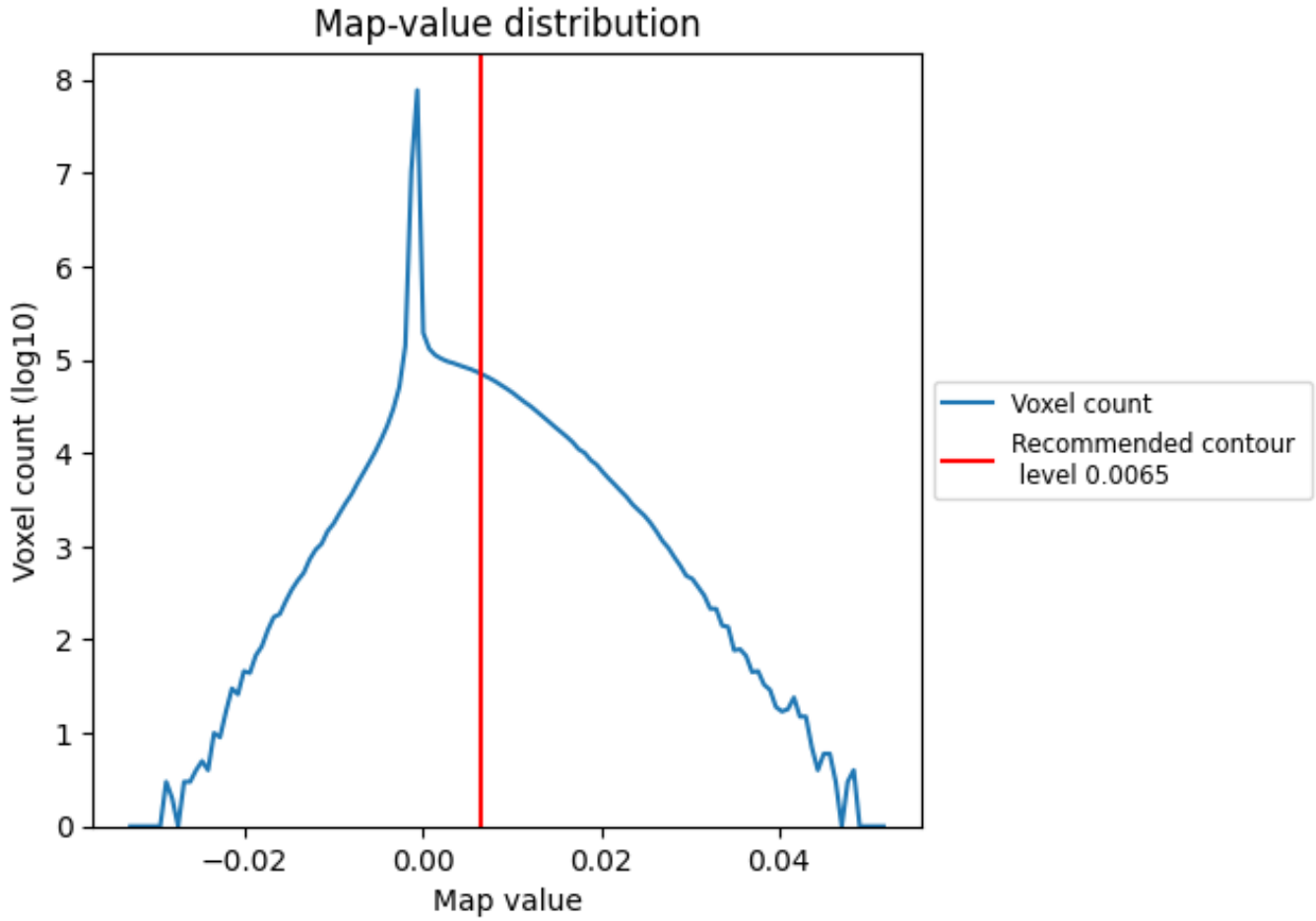
6.5 Mask visualisation (i)

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

7 Map analysis

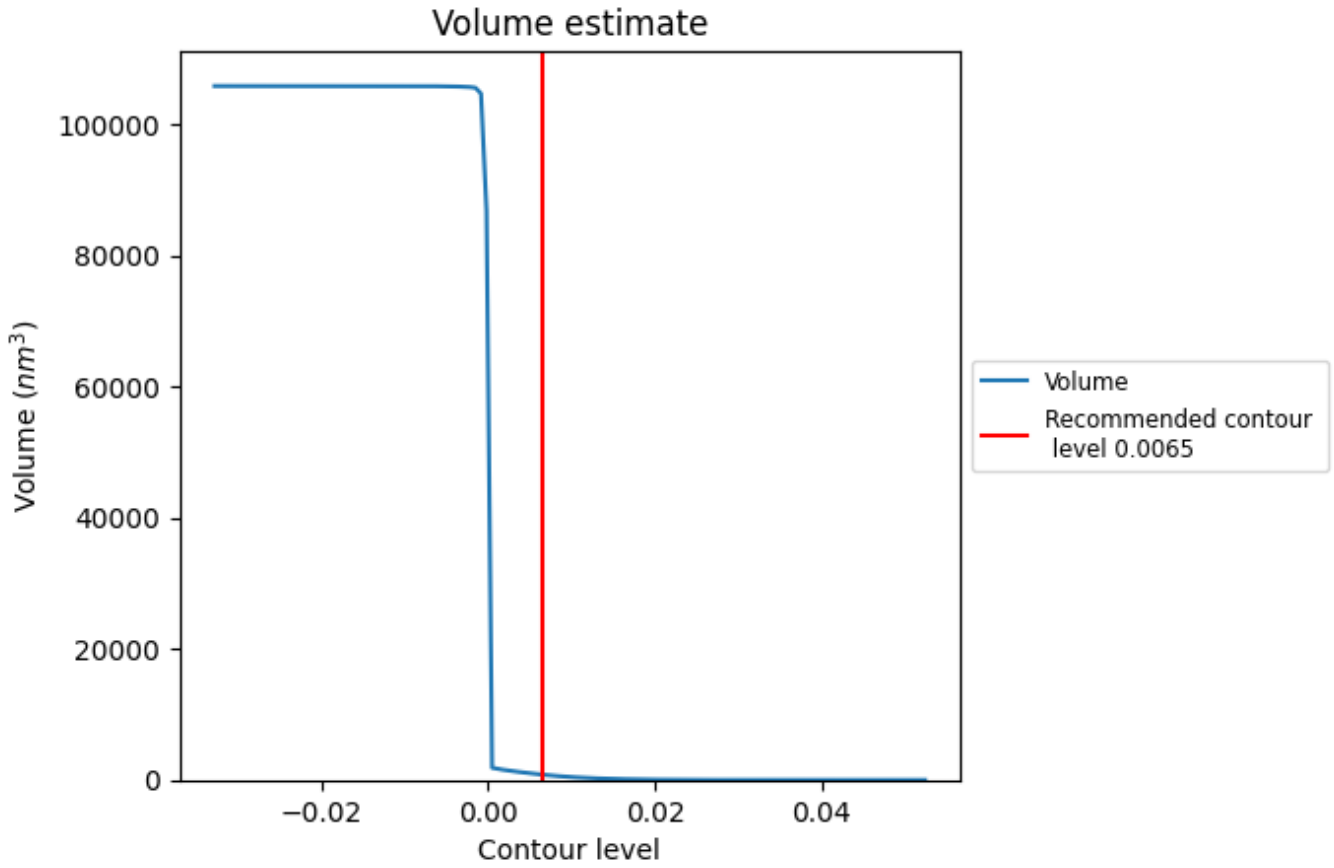
This section contains the results of statistical analysis of the map.

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.

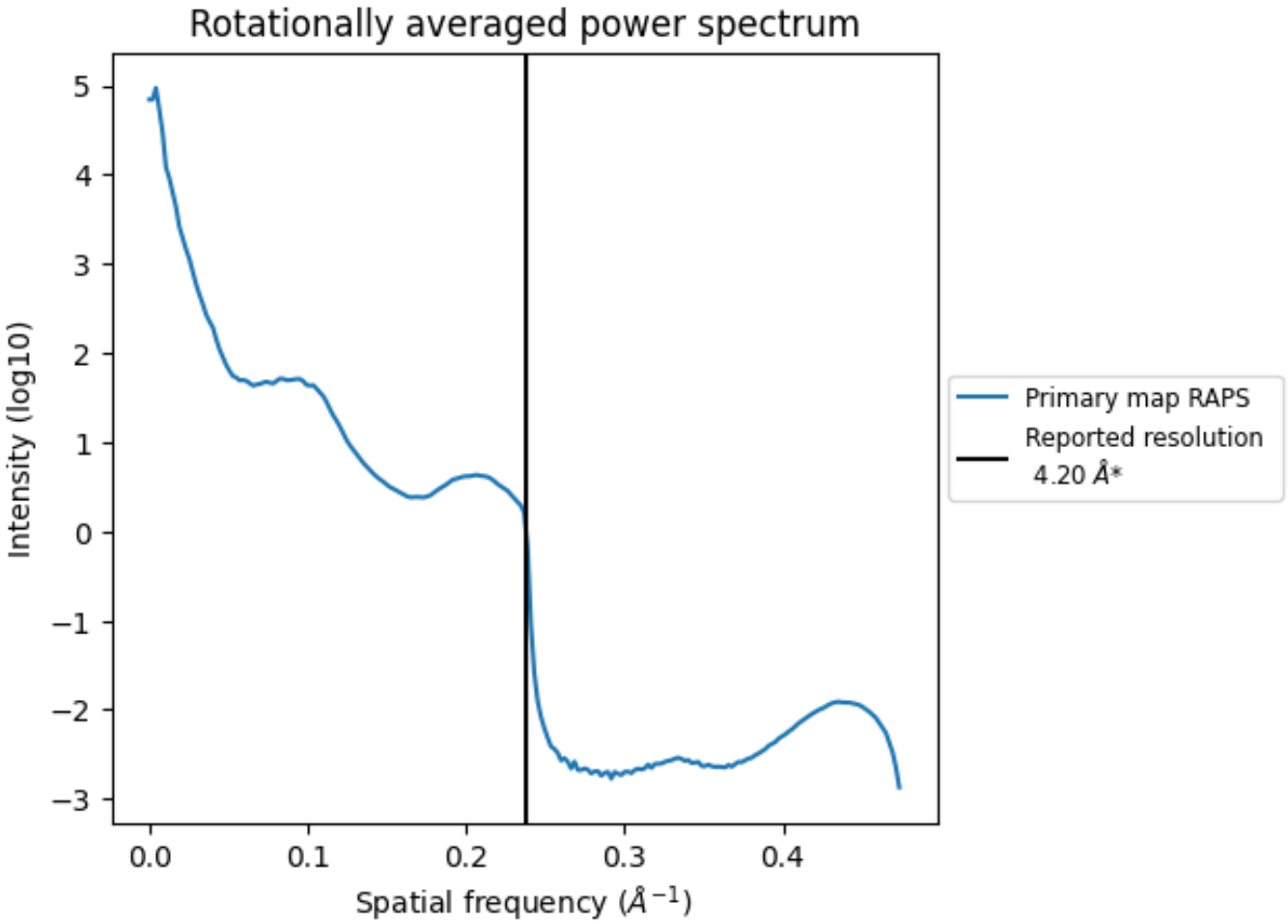
7.2 Volume estimate



The volume at the recommended contour level is 814 nm^3; this corresponds to an approximate mass of 736 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 0.238 Å^{-1}

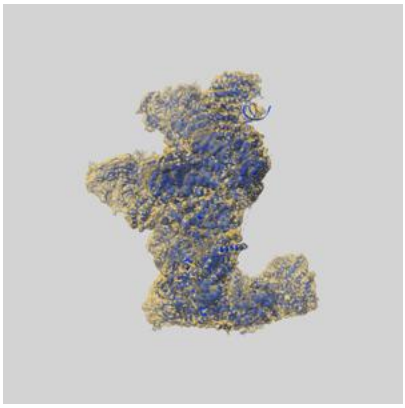
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

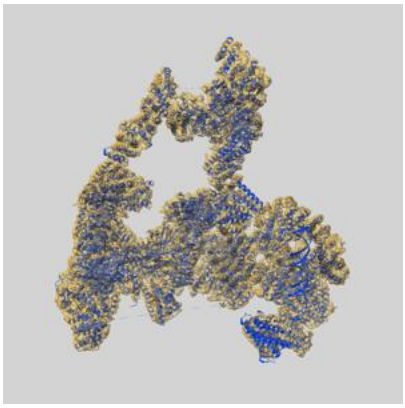
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23088 and PDB model 7KZS. Per-residue inclusion information can be found in section 3 on page 15.

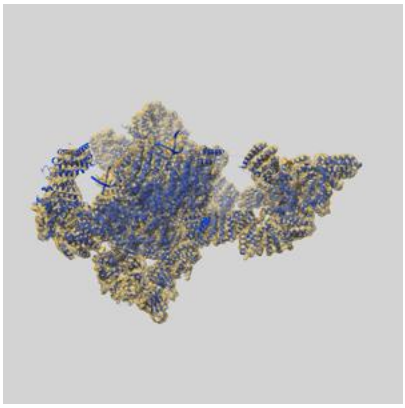
9.1 Map-model overlay



X



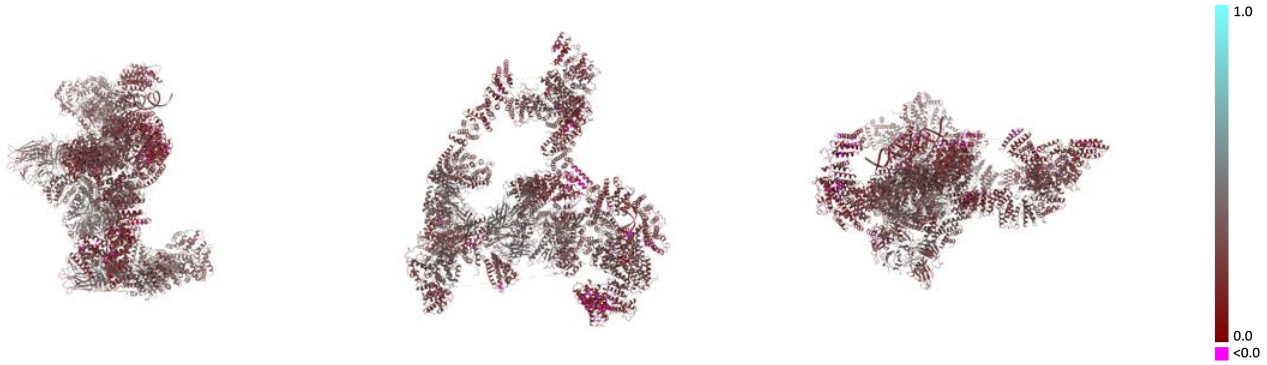
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0065 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.

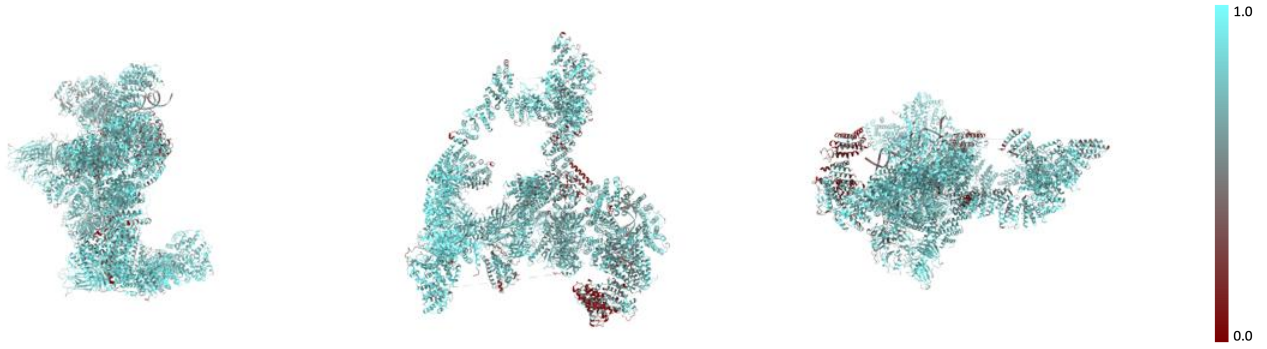
9.2 Q-score mapped to coordinate model



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.

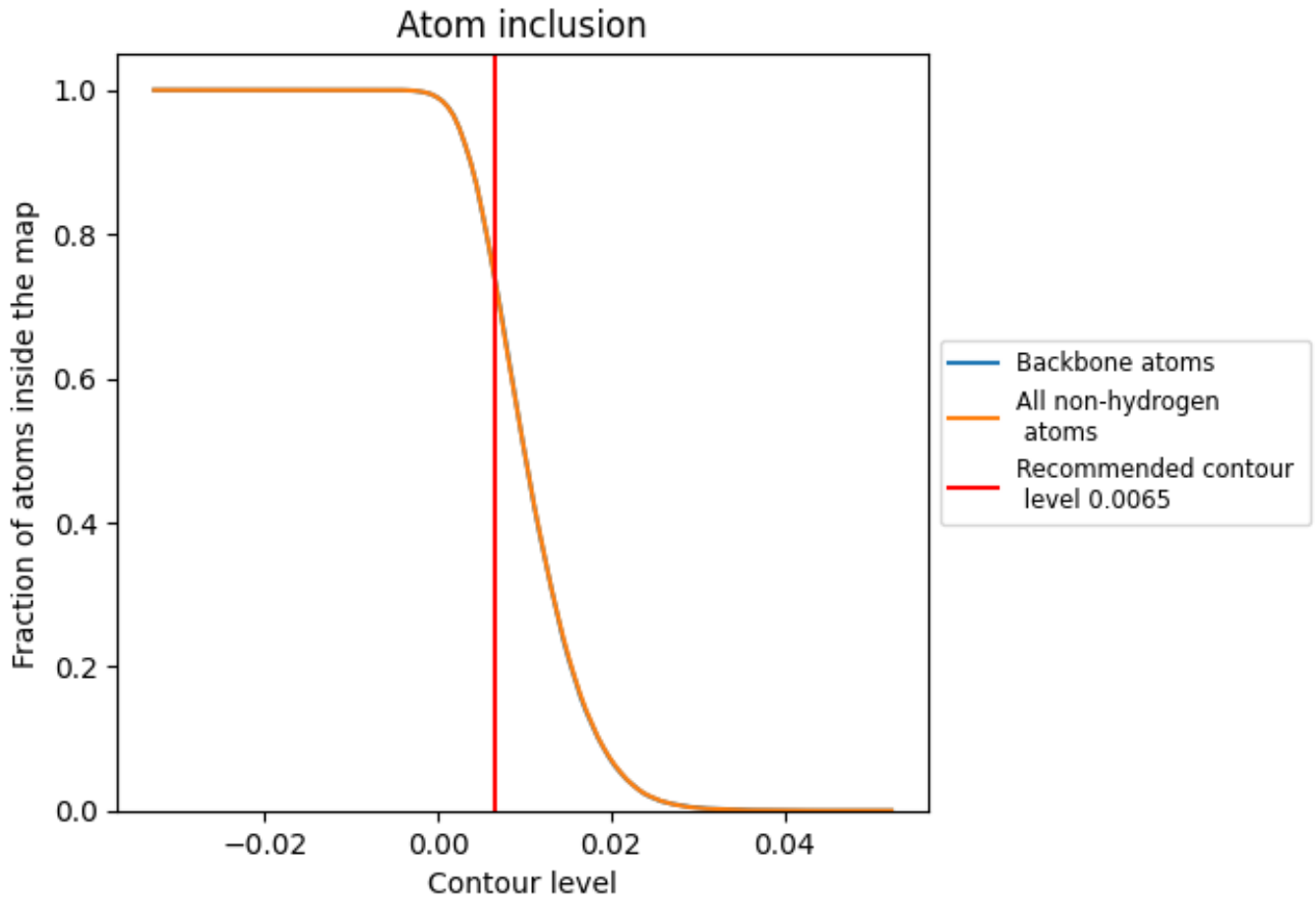
9.3 Atom inclusion mapped to coordinate model



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 (0.0065).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7433	0.3030
A	0.7100	0.2660
B	0.8210	0.3720
C	0.8499	0.3360
E	0.7622	0.3170
F	0.8583	0.3420
G	0.8046	0.3130
H	0.7513	0.2860
L	0.7836	0.3250
M	0.7467	0.3110
O	0.7950	0.3470
P	0.8456	0.4000
Q	0.7230	0.3350
S	0.7549	0.2680
U	0.7377	0.2760
V	0.5945	0.2420
W	0.7546	0.3090
X	0.6211	0.2640
Y	0.5678	0.1830
Z	0.5560	0.1910