



Full wwPDB EM Validation Report ⓘ

Feb 24, 2024 – 10:52 AM EST

PDB ID : 7KZP
EMDB ID : EMD-23085
Title : Structure of the human Fanconi anaemia Core complex
Authors : Wang, S.L.; Pavletich, N.P.
Deposited on : 2020-12-10
Resolution : 3.10 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

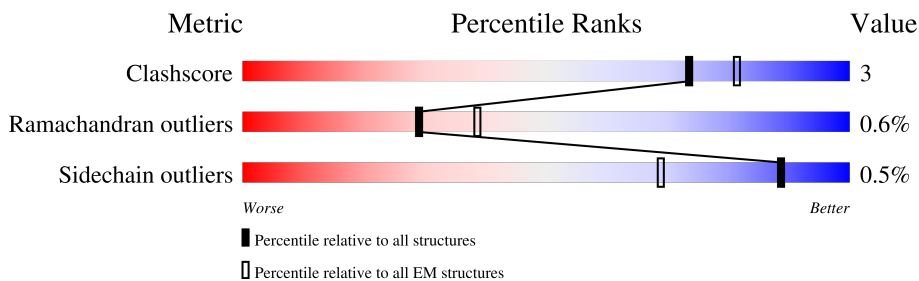
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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 $\leq 5\%$. 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	
1	S	1477	
2	B	884	
2	O	884	
3	C	583	
4	E	555	
5	F	399	
6	G	641	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	641	<p>5% 77% 7% 15%</p>
7	L	394	<p>1% 88% 6% 6%</p>
7	M	394	<p>53% 69% 6% 25%</p>
8	P	906	<p>1% 71% 11% 17%</p>
8	Q	906	<p>17% 75% 8% 17%</p>
9	W	39	<p>13% 85% 15%</p>

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 129871 atoms, of which 65409 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	
			Total	C	H	N	O			S
1	A	1186	18889	6001	9487	1650	1692	59	0	0
1	S	1250	19961	6345	10028	1747	1780	61	0	0

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

Continued on next page...

Continued from previous page...

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
			Total	C	H	N	O	S		
2	B	701	11395	3619	5790	934	1013	39	0	0
2	O	693	11244	3587	5705	916	1000	36	0	0

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

Continued on next page...

Continued from previous page...

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	
			Total	C	H	N	O			S
3	C	550	8838	2826	4442	749	791	30	0	0

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	
			Total	C	H	N	O			S
4	E	170	2654	815	1353	248	231	7	0	0

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

Continued on next page...

Continued from previous page...

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
			Total	C	H	N	O	S		
5	F	340	5466	1730	2740	506	483	7	0	0

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

Continued on next page...

Continued from previous page...

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
			Total	C	H	N	O	S		
6	G	577	9020	2843	4537	778	844	18	0	0
6	H	544	8504	2676	4288	734	790	16	0	0

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

Continued on next page...

Continued from previous page...

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
			Total	C	H	N	O	S		
7	L	370	5951	1914	2977	496	542	22	0	0
7	M	296	4799	1538	2415	402	431	13	0	0

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
			Total	C	H	N	O		
9	W	39	513	179	242	42	50	0	0

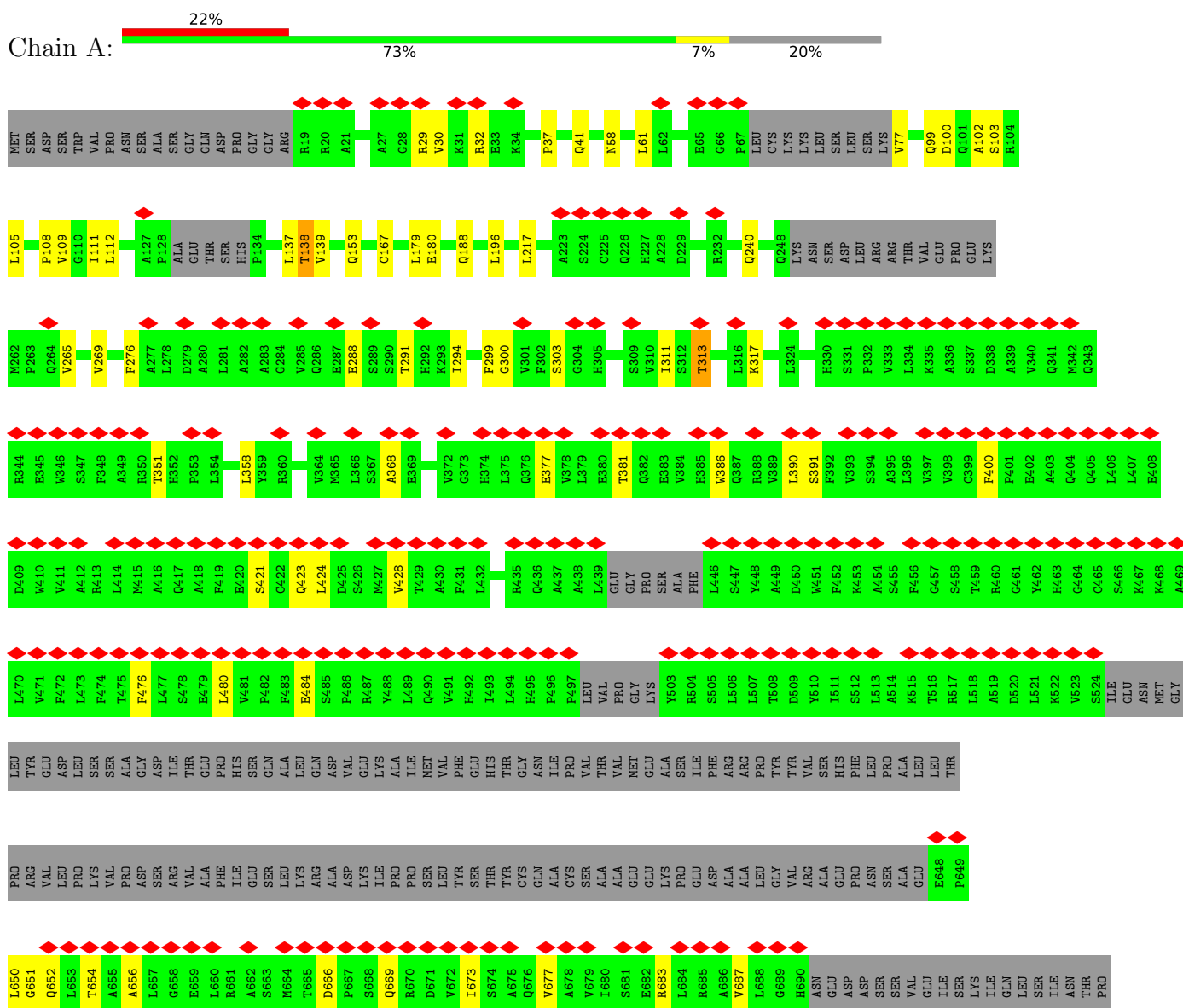
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

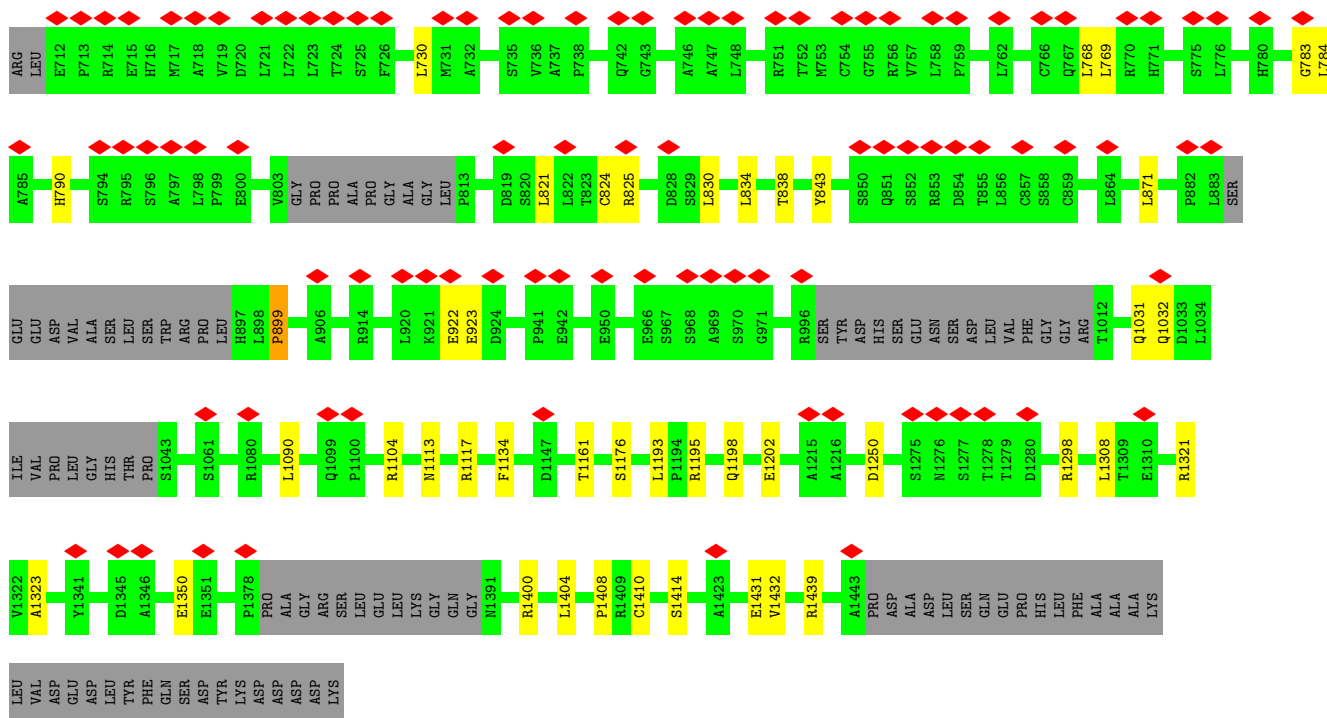
Mol	Chain	Residues	Atoms		AltConf
10	G	1	Total	Zn	0
			1	1	
10	L	2	Total	Zn	0
			2	2	

3 Residue-property plots [i](#)

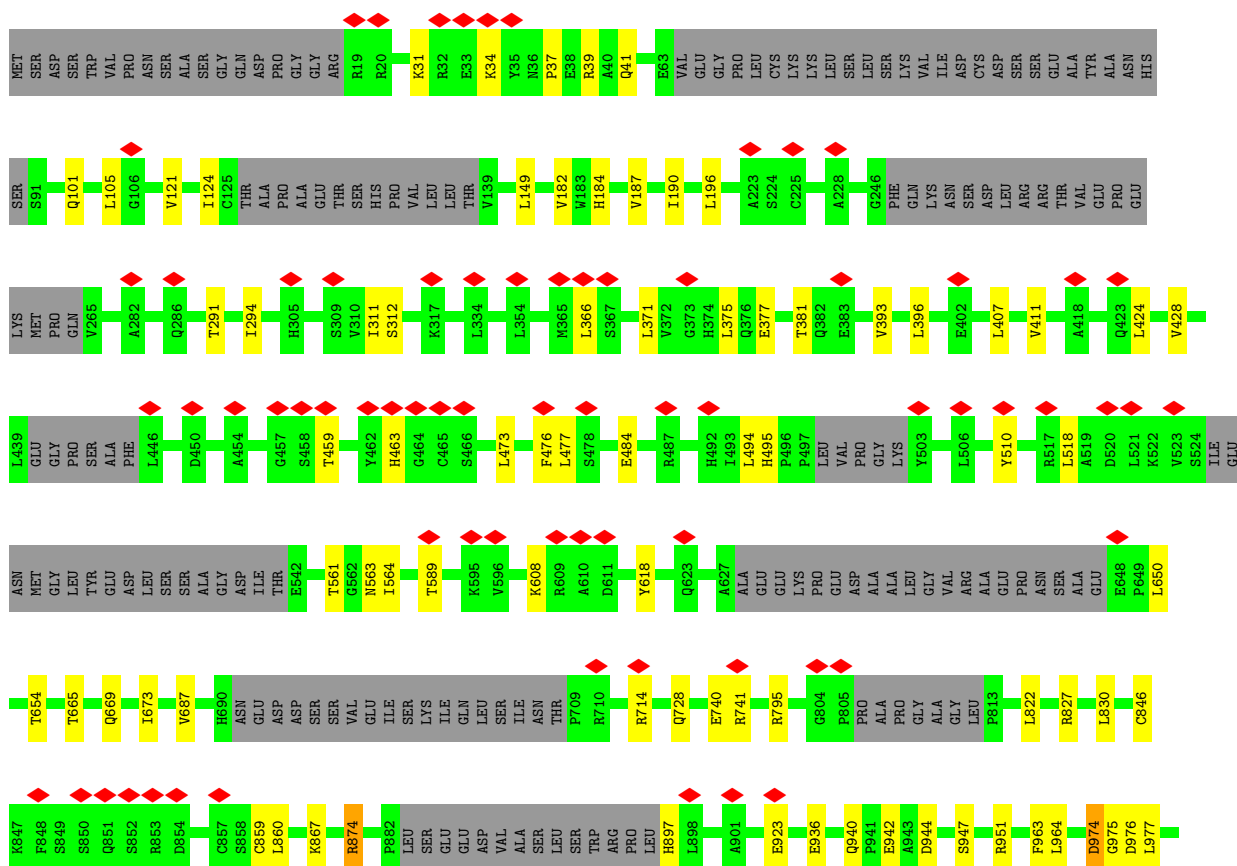
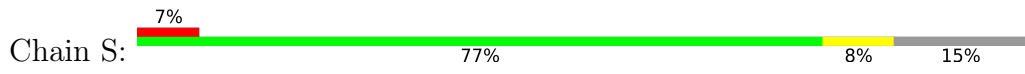
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

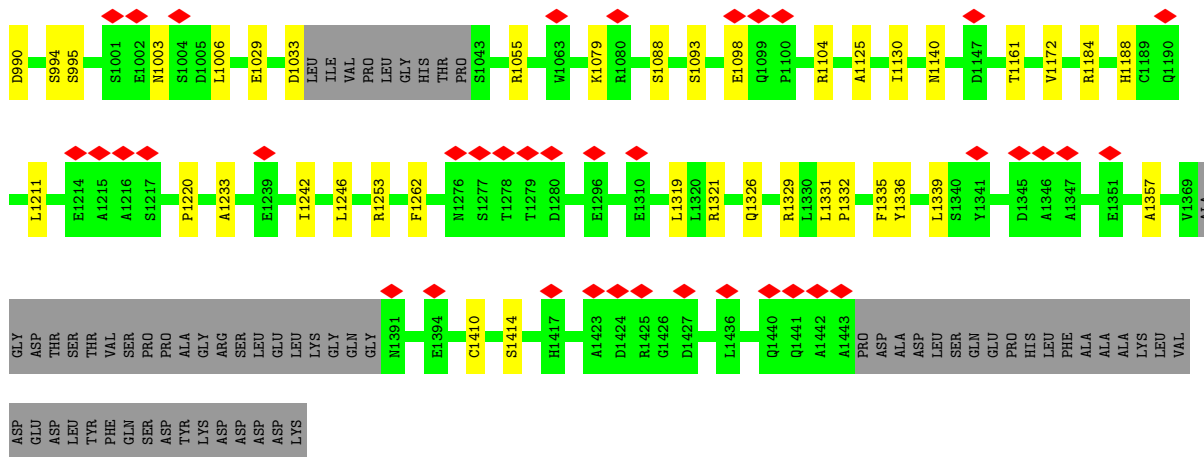
- Molecule 1: Fanconi anemia group A protein



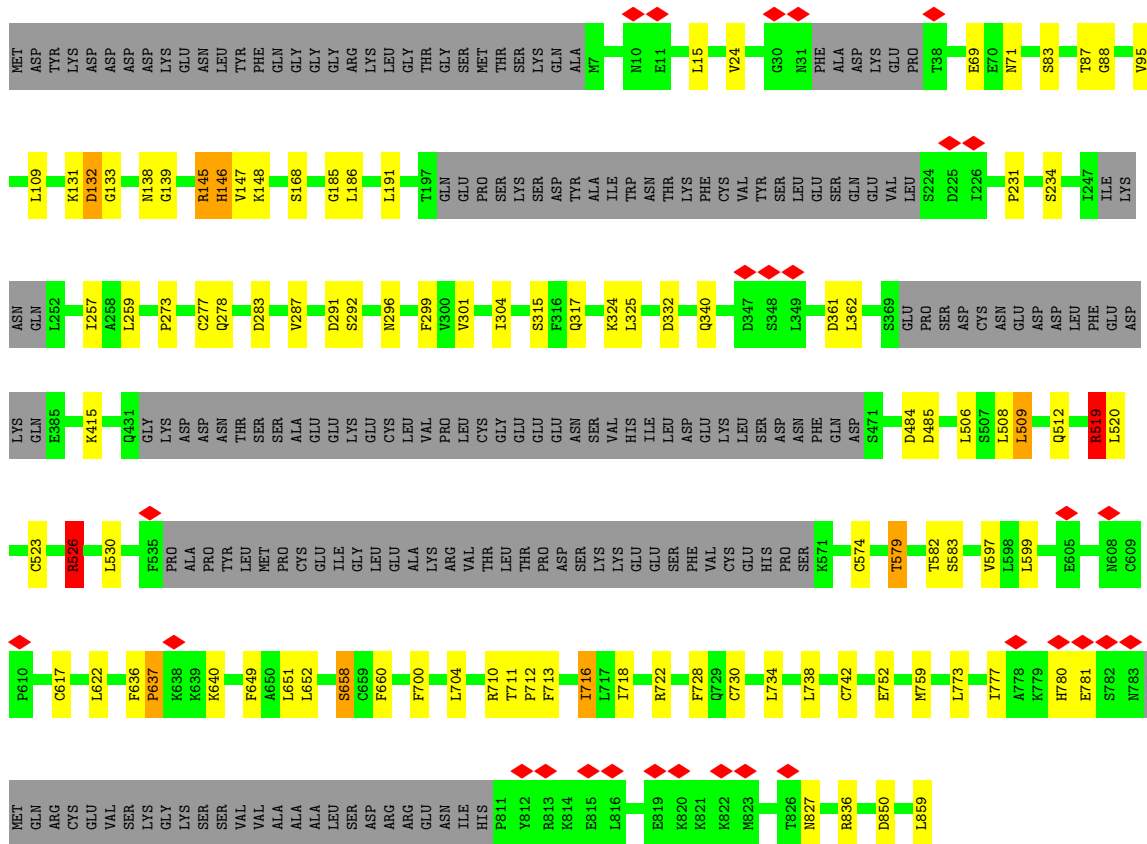


● Molecule 1: Fanconi anemia group A protein



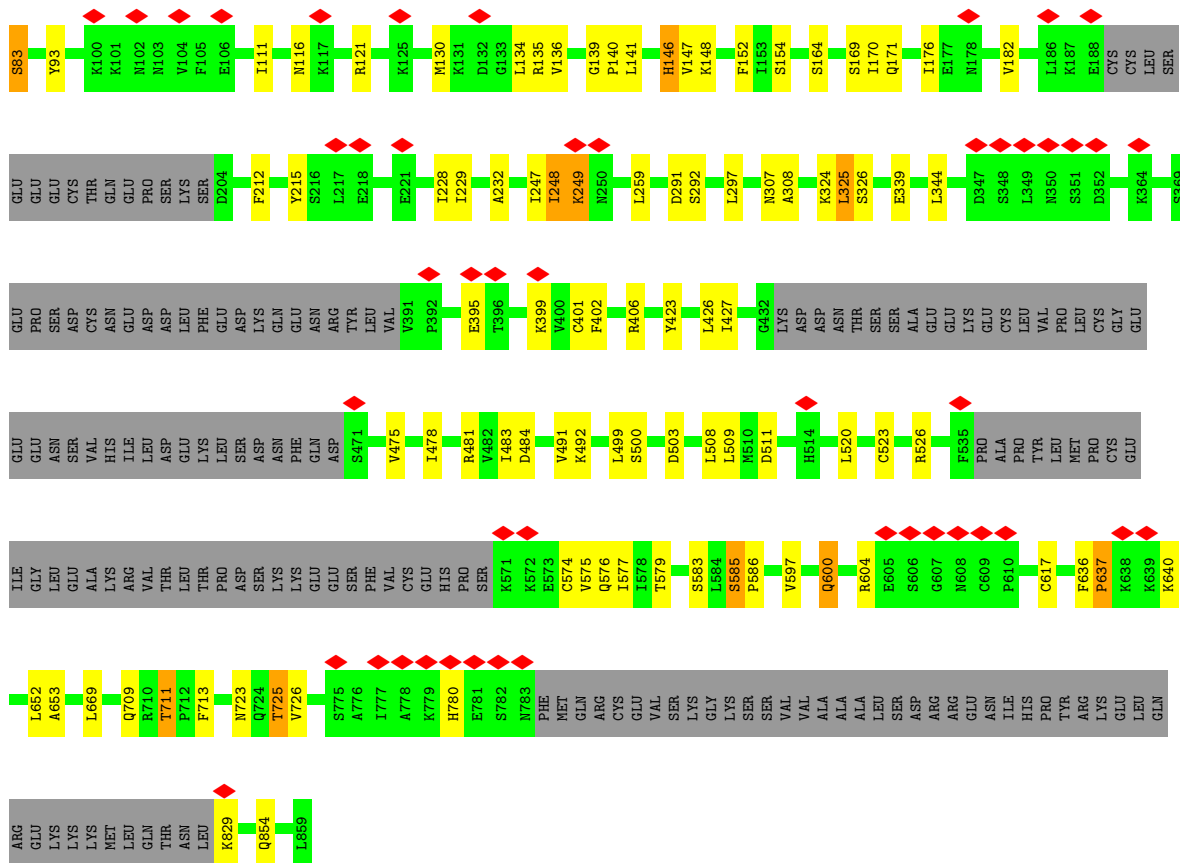


• Molecule 2: Fanconi anemia group B protein

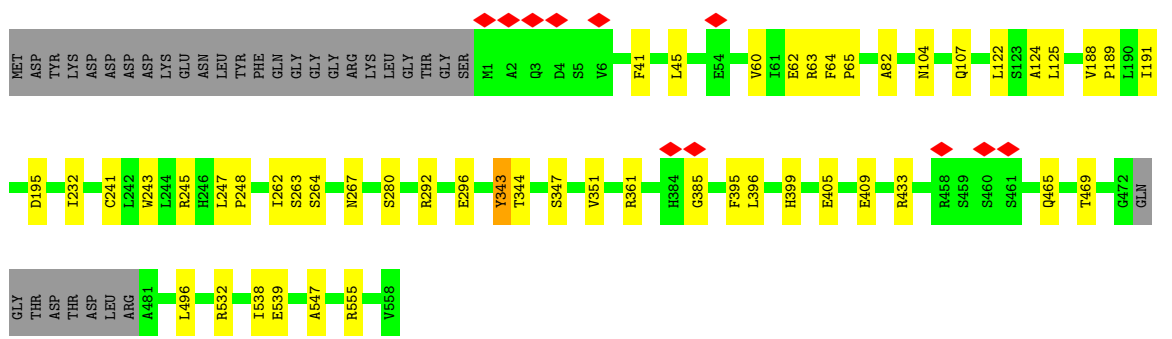
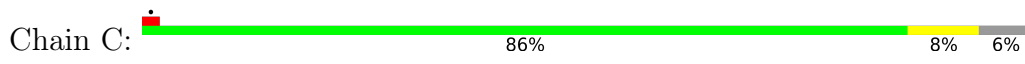


• Molecule 2: Fanconi anemia group B protein

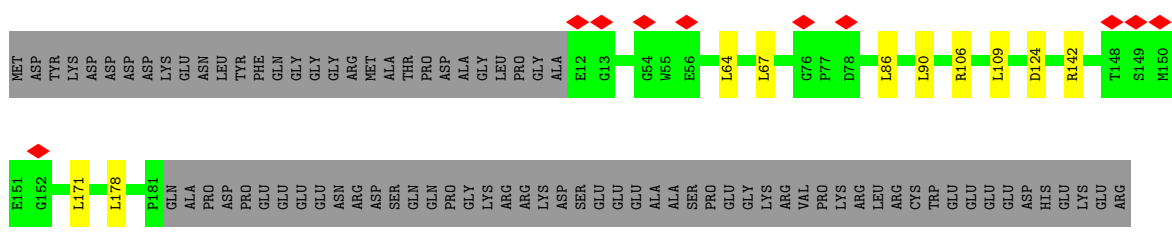


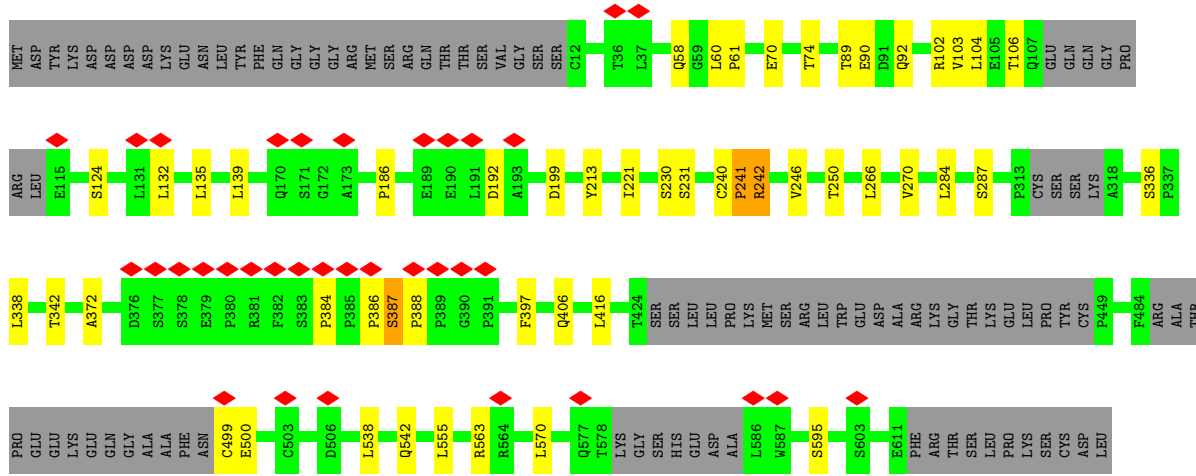


• Molecule 3: Fanconi anemia group C protein

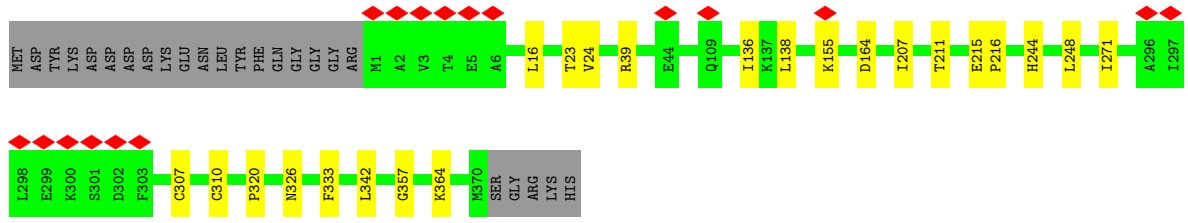
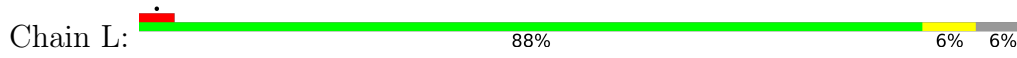


• Molecule 4: Fanconi anemia group E protein

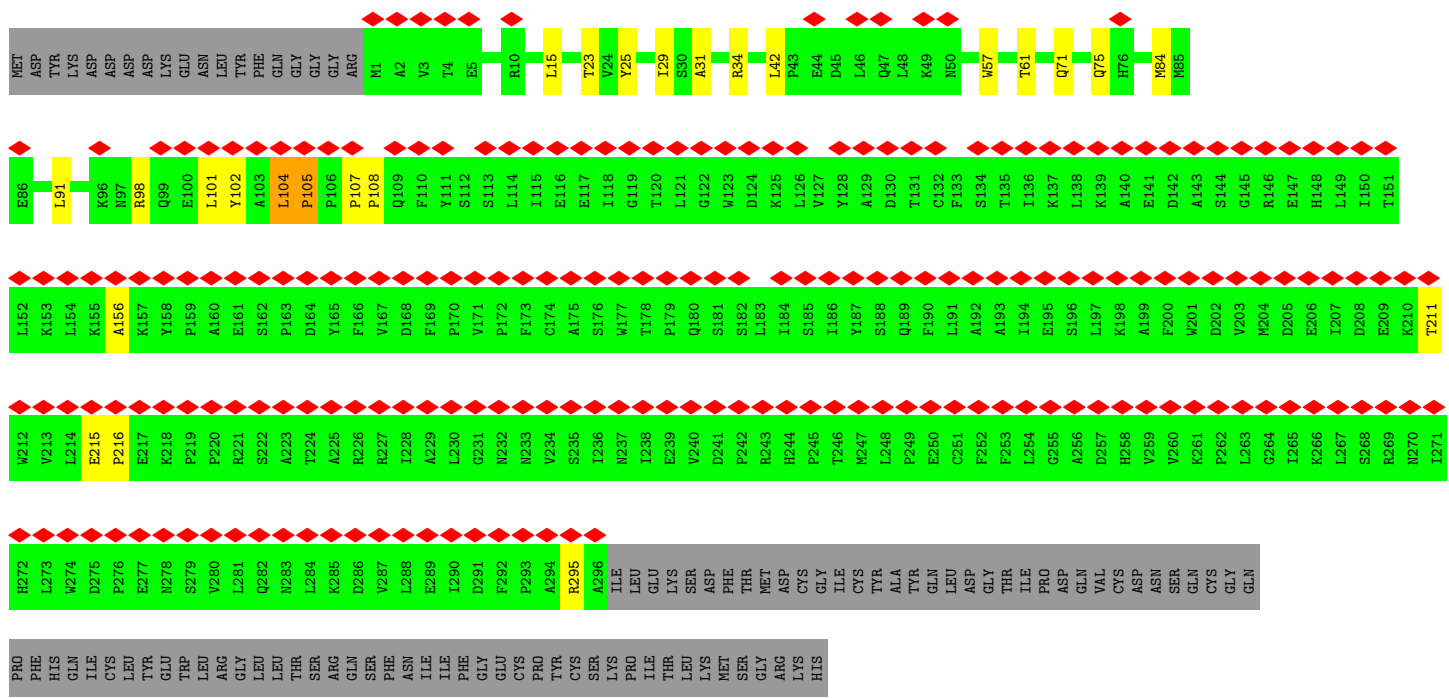


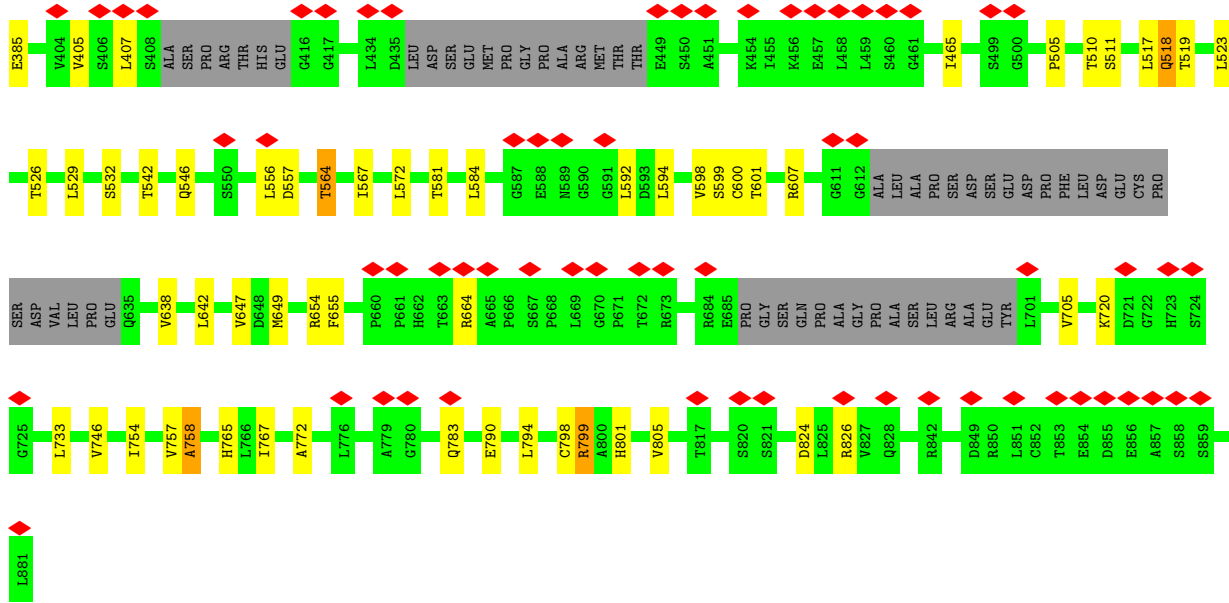


• Molecule 7: E3 ubiquitin-protein ligase FANCL

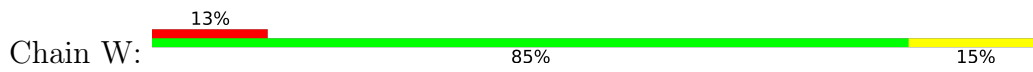


• Molecule 7: E3 ubiquitin-protein ligase FANCL





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	671972	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 ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.208	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	426.68024, 426.68024, 426.68024	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08847, 1.08847, 1.08847	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.50	0/9605	0.66	0/13008
1	S	0.48	0/10153	0.65	1/13749 (0.0%)
2	B	0.90	11/5707 (0.2%)	0.94	7/7686 (0.1%)
2	O	0.66	1/5645 (0.0%)	0.82	2/7610 (0.0%)
3	C	0.72	0/4497	0.81	5/6103 (0.1%)
4	E	0.79	0/1324	0.91	0/1792
5	F	0.52	0/2791	0.70	0/3790
6	G	0.56	1/4568 (0.0%)	0.68	0/6215
6	H	0.59	0/4293	0.74	1/5840 (0.0%)
7	L	0.51	0/3050	0.68	1/4143 (0.0%)
7	M	0.47	0/2445	0.67	0/3323
8	P	0.85	2/5697 (0.0%)	0.97	3/7752 (0.0%)
8	Q	0.56	1/5737 (0.0%)	0.74	1/7810 (0.0%)
9	W	0.43	0/202	0.60	0/281
All	All	0.63	16/65714 (0.0%)	0.76	21/89102 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	S	0	7
2	B	0	10
2	O	0	9
6	G	0	2
6	H	0	4
7	L	0	1
7	M	0	1
8	P	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	Q	0	5
All	All	0	49

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	361	SER	CA-CB	-8.53	1.40	1.52
2	B	718	ILE	C-O	-8.03	1.08	1.23
2	B	658	SER	C-O	-7.69	1.08	1.23
2	B	523	CYS	C-O	-7.07	1.09	1.23
2	B	582	THR	C-O	-6.91	1.10	1.23
2	O	583	SER	CA-CB	-6.90	1.42	1.52
2	B	660	PHE	C-O	-6.87	1.10	1.23
2	B	526	ARG	C-O	-6.80	1.10	1.23
2	B	651	LEU	C-O	-6.76	1.10	1.23
2	B	506	LEU	C-O	-6.61	1.10	1.23
2	B	716	ILE	C-O	-6.40	1.11	1.23
2	B	599	LEU	C-O	-5.66	1.12	1.23
6	G	499	CYS	CB-SG	-5.62	1.72	1.81
8	Q	564	THR	C-O	-5.38	1.13	1.23
2	B	526	ARG	CD-NE	-5.29	1.37	1.46
8	P	566	THR	C-O	-5.06	1.13	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	526	ARG	NE-CZ-NH2	-8.75	115.92	120.30
2	B	526	ARG	NE-CZ-NH1	8.20	124.40	120.30
3	C	243	TRP	CH2-CZ2-CE2	-7.31	110.09	117.40
2	B	728	PHE	CB-CG-CD1	6.63	125.44	120.80
6	H	102	ARG	NE-CZ-NH2	-6.53	117.03	120.30
2	B	722	ARG	NE-CZ-NH1	6.43	123.52	120.30
3	C	292	ARG	CG-CD-NE	-6.34	98.50	111.80
3	C	292	ARG	NE-CZ-NH2	-6.09	117.26	120.30
2	O	725	THR	CA-CB-OG1	-5.92	96.57	109.00
2	B	579	THR	CA-CB-OG1	5.65	120.87	109.00
8	P	578	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	O	481	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	B	759	MET	CG-SD-CE	-5.33	91.67	100.20
8	P	707	SER	N-CA-CB	5.32	118.48	110.50
8	Q	799	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	C	243	TRP	CD2-CE3-CZ3	-5.24	111.99	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	399	LEU	CB-CG-CD1	-5.21	102.15	111.00
3	C	243	TRP	NE1-CE2-CZ2	-5.19	124.69	130.40
2	B	622	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	S	874	ARG	NE-CZ-NH1	5.12	122.86	120.30
7	L	39	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1350	GLU	Peptide
1	A	138	THR	Peptide
1	A	313	THR	Peptide
1	A	484	GLU	Peptide
1	A	899	PRO	Peptide
1	A	922	GLU	Peptide
1	A	923	GLU	Peptide
2	B	132	ASP	Peptide
2	B	139	GLY	Peptide
2	B	145	ARG	Peptide
2	B	146	HIS	Peptide
2	B	191	LEU	Peptide
2	B	259	LEU	Peptide
2	B	324	LYS	Peptide
2	B	519	ARG	Peptide
2	B	636	PHE	Peptide
2	B	637	PRO	Peptide
6	G	388	PRO	Peptide
6	G	563	ARG	Peptide
6	H	132	LEU	Peptide
6	H	186	PRO	Peptide
6	H	386	PRO	Peptide
6	H	563	ARG	Peptide
7	L	215	GLU	Peptide
7	M	215	GLU	Peptide
2	O	146	HIS	Peptide
2	O	154	SER	Peptide
2	O	247	ILE	Peptide
2	O	248	ILE	Peptide
2	O	259	LEU	Peptide
2	O	324	LYS	Peptide
2	O	636	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	O	637	PRO	Peptide
2	O	711	THR	Peptide
8	P	329	ASP	Peptide
8	P	725	GLY	Peptide
8	P	781	PRO	Peptide
8	Q	49	GLN	Peptide
8	Q	584	LEU	Peptide
8	Q	594	LEU	Peptide
8	Q	647	VAL	Peptide
8	Q	720	LYS	Peptide
1	S	31	LYS	Peptide
1	S	484	GLU	Peptide
1	S	495	HIS	Peptide
1	S	561	THR	Peptide
1	S	563	ASN	Peptide
1	S	923	GLU	Peptide
1	S	974	ASP	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	64	0
1	S	9933	10028	9969	64	0
2	B	5605	5790	5768	47	0
2	O	5539	5705	5686	57	0
3	C	4396	4442	4427	29	0
4	E	1301	1353	1352	7	0
5	F	2726	2740	2729	10	0
6	G	4483	4537	4523	22	0
6	H	4216	4288	4273	38	0
7	L	2974	2977	2972	13	0
7	M	2384	2415	2410	22	0
8	P	5598	5681	5652	56	0
8	Q	5631	5724	5694	42	0
9	W	271	242	196	4	0
10	G	1	0	0	0	0
10	L	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	64462	65409	65082	429	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 3.

All (429) 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:A:30:VAL:HG21	6:H:372:ALA:HB1	1.40	1.02
7:M:104:LEU:HG	7:M:105:PRO:HD2	1.42	1.01
2:B:362:LEU:O	8:P:468:ARG:NH2	1.94	1.01
6:H:342:THR:HG21	6:H:384:PRO:HG3	1.42	0.97
7:M:104:LEU:HG	7:M:105:PRO:CD	1.94	0.97
6:H:342:THR:HG21	6:H:384:PRO:CG	1.97	0.93
7:M:107:PRO:HG2	7:M:108:PRO:HD3	1.56	0.88
1:A:30:VAL:HG21	6:H:372:ALA:CB	2.05	0.86
6:G:214:ARG:NH1	6:G:328:LEU:O	2.17	0.78
8:P:796:ASP:OD1	8:P:799:ARG:NH2	2.20	0.74
2:B:292:SER:OG	2:B:361:ASP:OD1	2.06	0.73
2:O:509:LEU:HD22	8:Q:542:THR:HG21	1.69	0.73
6:H:387:SER:HB2	6:H:388:PRO:CD	2.19	0.72
6:H:342:THR:CG2	6:H:384:PRO:HG3	2.20	0.72
1:A:769:LEU:HD13	1:A:821:LEU:HD12	1.72	0.71
8:P:776:LEU:HD13	8:P:879:ILE:HD12	1.73	0.69
1:S:1410:CYS:SG	1:S:1414:SER:OG	2.50	0.69
1:A:652:GLN:O	1:A:683:ARG:NH1	2.26	0.68
1:A:300:GLY:O	1:A:303:SER:OG	2.12	0.68
1:A:30:VAL:CG2	6:H:372:ALA:CB	2.72	0.67
1:A:102:ALA:HB2	1:A:112:LEU:HD12	1.75	0.67
7:L:155:LYS:NZ	7:L:164:ASP:OD1	2.26	0.67
3:C:385:GLY:O	7:L:244:HIS:NE2	2.26	0.67
2:O:723:ASN:OD1	2:O:726:VAL:HG23	1.94	0.67
1:S:494:LEU:HD11	1:S:518:LEU:HD11	1.76	0.67
1:A:1410:CYS:SG	1:A:1414:SER:OG	2.53	0.66
1:A:790:HIS:HE2	1:A:843:TYR:HH	1.41	0.66
7:M:107:PRO:CG	7:M:108:PRO:HD3	2.25	0.66
1:A:32:ARG:HG2	1:A:32:ARG:HH11	1.60	0.66
5:F:289:LEU:HD12	6:G:539:LEU:HD23	1.77	0.66
1:S:822:LEU:O	1:S:867:LYS:NZ	2.27	0.66
6:H:342:THR:CG2	6:H:384:PRO:CG	2.74	0.65
8:P:860:CYS:SG	8:P:861:ALA:N	2.67	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:846:CYS:HG	1:S:897:HIS:N	1.95	0.65
2:O:520:LEU:HD12	8:Q:567:ILE:HG12	1.76	0.65
6:H:406:GLN:OE1	6:H:595:SER:OG	2.15	0.64
5:F:289:LEU:HD12	6:G:539:LEU:CD2	2.28	0.64
2:O:7:MET:N	2:O:13:GLU:O	2.30	0.64
2:B:526:ARG:HD2	8:P:559:ALA:HA	1.78	0.64
2:O:511:ASP:OD2	8:Q:607:ARG:NH1	2.31	0.63
3:C:104:ASN:ND2	3:C:107:GLN:OE1	2.31	0.63
1:S:1033:ASP:OD1	1:S:1093:SER:OG	2.15	0.62
5:F:18:SER:O	5:F:100:ASN:ND2	2.32	0.62
6:H:499:CYS:SG	6:H:500:GLU:N	2.72	0.62
1:A:30:VAL:CG2	6:H:372:ALA:HB1	2.24	0.61
1:S:589:THR:HG23	1:S:1006:LEU:HD13	1.82	0.61
8:P:324:ILE:HG12	8:P:338:LEU:HD23	1.82	0.61
1:A:428:VAL:HG22	1:A:476:PHE:CE1	2.36	0.61
3:C:82:ALA:O	5:F:138:ARG:NH1	2.34	0.61
2:O:146:HIS:O	2:O:148:LYS:N	2.33	0.61
6:G:21:ASP:OD1	6:G:25:ARG:NH1	2.34	0.60
7:M:104:LEU:HG	7:M:105:PRO:HD3	1.81	0.60
2:B:146:HIS:O	2:B:148:LYS:N	2.34	0.60
1:S:1336:TYR:OH	1:S:1357:ALA:O	2.19	0.60
6:H:387:SER:HB2	6:H:388:PRO:HD2	1.83	0.60
1:S:1326:GLN:OE1	1:S:1329:ARG:NH2	2.35	0.60
1:A:651:GLY:O	1:A:654:THR:OG1	2.19	0.59
2:O:483:ILE:HG22	2:O:484:ASP:H	1.67	0.59
1:S:428:VAL:HG22	1:S:476:PHE:CE1	2.37	0.59
2:B:711:THR:O	2:B:713:PHE:N	2.35	0.59
7:M:23:THR:OG1	7:M:42:LEU:O	2.21	0.59
1:A:265:VAL:O	1:A:269:VAL:HG23	2.02	0.59
1:A:830:LEU:HD22	1:A:871:LEU:HD21	1.85	0.59
1:S:366:LEU:HD13	1:S:371:LEU:HD21	1.85	0.59
1:A:1404:LEU:HD21	1:A:1432:VAL:HG22	1.83	0.58
1:S:1335:PHE:HE1	1:S:1339:LEU:HG	1.66	0.58
8:Q:654:ARG:NH2	8:Q:758:ALA:O	2.37	0.58
8:P:502:GLY:O	8:P:504:ARG:NH1	2.37	0.58
2:B:485:ASP:OD1	2:O:725:THR:HG23	2.04	0.58
2:B:509:LEU:HD23	8:P:542:THR:HG21	1.85	0.58
7:M:104:LEU:O	7:M:156:ALA:HB1	2.03	0.58
8:P:24:GLY:O	8:P:27:ARG:NH1	2.37	0.58
8:P:735:TRP:O	8:P:807:ARG:NH1	2.36	0.58
8:Q:733:LEU:HD22	8:Q:746:VAL:HG11	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:829:LYS:N	8:Q:824:ASP:O	2.37	0.58
7:M:34:ARG:NH1	7:M:102:TYR:HD2	2.02	0.58
1:S:974:ASP:O	1:S:976:ASP:N	2.37	0.58
2:O:61:SER:OG	2:O:116:ASN:ND2	2.37	0.58
8:P:74:ARG:HD3	8:P:90:LEU:HD12	1.86	0.58
6:G:39:ARG:NH2	6:G:319:PRO:O	2.37	0.57
2:B:519:ARG:NH1	2:B:520:LEU:O	2.36	0.57
1:A:666:ASP:O	1:A:669:GLN:NE2	2.38	0.57
7:L:207:ILE:O	7:L:211:THR:OG1	2.21	0.57
7:L:342:LEU:HD22	7:L:357:GLY:HA3	1.86	0.57
8:Q:733:LEU:CD2	8:Q:746:VAL:HG11	2.35	0.57
1:S:393:VAL:HA	1:S:396:LEU:HD12	1.87	0.57
1:S:424:LEU:O	1:S:428:VAL:HG23	2.05	0.57
2:B:734:LEU:HD23	2:B:738:LEU:HG	1.86	0.56
2:B:315:SER:O	2:B:315:SER:OG	2.16	0.56
7:M:104:LEU:CG	7:M:105:PRO:CD	2.79	0.56
1:S:1220:PRO:O	1:S:1253:ARG:NH2	2.38	0.56
2:O:500:SER:O	2:O:604:ARG:NH1	2.39	0.56
8:P:765:HIS:CD2	8:P:767:ILE:HD11	2.41	0.56
6:H:342:THR:HG21	6:H:384:PRO:CD	2.35	0.56
2:O:780:HIS:O	8:Q:826:ARG:NH1	2.39	0.56
7:M:98:ARG:HB3	7:M:101:LEU:HD12	1.88	0.56
2:B:69:GLU:OE1	2:B:71:ASN:ND2	2.39	0.55
1:S:947:SER:O	1:S:951:ARG:NH2	2.39	0.55
1:S:1161:THR:O	1:S:1321:ARG:NH2	2.40	0.55
6:H:266:LEU:O	6:H:270:VAL:HG23	2.06	0.55
7:M:29:ILE:HD12	7:M:84:MET:HE3	1.89	0.55
2:O:111:ILE:HD12	2:O:121:ARG:HG3	1.88	0.55
8:Q:311:CYS:SG	8:Q:312:LEU:N	2.80	0.55
2:B:520:LEU:HD12	8:P:567:ILE:HB	1.88	0.55
6:H:538:LEU:O	6:H:542:GLN:NE2	2.40	0.55
8:P:751:LEU:HD13	8:P:754:ILE:HG22	1.89	0.55
1:A:58:ASN:OD1	1:A:77:VAL:N	2.41	0.54
1:A:138:THR:O	1:A:139:VAL:HG23	2.06	0.54
2:B:87:THR:OG1	2:B:88:GLY:N	2.41	0.54
3:C:409:GLU:OE2	3:C:532:ARG:NH1	2.41	0.54
1:A:1250:ASP:O	1:A:1298:ARG:NH1	2.40	0.54
6:G:355:LEU:HD23	6:G:591:LEU:CD2	2.38	0.54
1:S:1140:ASN:OD1	1:S:1184:ARG:NH1	2.41	0.54
1:A:153:GLN:NE2	1:A:188:GLN:O	2.40	0.54
1:A:99:GLN:OE1	1:A:109:VAL:HG21	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:ILE:HG13	3:C:232:ILE:HD12	1.90	0.54
1:S:477:LEU:HD13	1:S:510:TYR:OH	2.08	0.54
8:P:230:GLY:O	8:P:234:THR:OG1	2.23	0.53
1:A:299:PHE:CD1	1:A:358:LEU:HD13	2.43	0.53
2:O:423:TYR:CZ	2:O:427:ILE:HD11	2.44	0.53
1:S:665:THR:HA	9:W:80:VAL:HG22	1.91	0.53
1:S:827:ARG:HA	1:S:830:LEU:HD12	1.89	0.53
8:Q:505:PRO:O	8:Q:532:SER:OG	2.26	0.53
2:O:307:ASN:HA	2:O:325:LEU:HD12	1.90	0.53
2:O:93:TYR:CE2	2:O:136:VAL:HG21	2.44	0.53
7:M:71:GLN:NE2	7:M:75:GLN:OE1	2.42	0.53
1:S:687:VAL:O	1:S:714:ARG:NH1	2.41	0.53
6:G:257:ARG:NH2	6:G:285:GLU:OE2	2.38	0.52
7:L:23:THR:HG23	7:L:24:VAL:HG23	1.91	0.52
2:O:82:VAL:HG13	2:O:83:SER:H	1.75	0.52
2:B:315:SER:O	2:B:317:GLN:N	2.43	0.52
1:A:1032:GLN:OE1	1:A:1104:ARG:NH2	2.43	0.52
8:P:60:PHE:HZ	8:P:88:LEU:HD11	1.74	0.52
1:S:650:LEU:O	1:S:654:THR:HG23	2.09	0.52
1:A:1193:LEU:O	1:A:1198:GLN:NE2	2.43	0.52
2:O:508:LEU:HD12	2:O:523:CYS:SG	2.50	0.52
7:M:211:THR:O	7:M:295:ARG:NH1	2.43	0.52
6:G:392:CYS:SG	6:G:394:PRO:HD2	2.50	0.52
6:H:241:PRO:O	6:H:242:ARG:HB3	2.09	0.52
2:B:332:ASP:HA	2:B:340:GLN:OE1	2.10	0.52
2:O:164:SER:OG	2:O:215:TYR:OH	2.23	0.52
8:P:60:PHE:CZ	8:P:88:LEU:HD11	2.45	0.52
6:H:397:PHE:HD2	6:H:416:LEU:HD11	1.75	0.51
2:O:520:LEU:CD1	8:Q:567:ILE:HG12	2.41	0.51
2:O:579:THR:HG21	2:O:653:ALA:HB2	1.91	0.51
2:O:499:LEU:HD12	2:O:576:GLN:HG2	1.93	0.51
8:Q:337:GLU:OE2	8:Q:339:ARG:NH1	2.43	0.51
1:S:291:THR:HA	1:S:294:ILE:HD12	1.92	0.51
2:B:850:ASP:OD2	8:P:801:HIS:HD2	1.94	0.51
3:C:296:GLU:OE1	4:E:142:ARG:NH1	2.38	0.51
2:O:426:LEU:HD22	8:Q:638:VAL:HG21	1.91	0.51
1:A:1090:LEU:HD12	1:A:1134:PHE:HA	1.93	0.51
3:C:241:CYS:O	3:C:245:ARG:HG2	2.11	0.51
2:O:585:SER:N	2:O:586:PRO:CD	2.74	0.51
5:F:287:TYR:HE2	5:F:289:LEU:HD23	1.77	0.50
8:P:755:GLN:OE1	8:P:765:HIS:ND1	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:GLN:OE1	1:S:1188:HIS:NE2	2.44	0.50
6:H:89:THR:N	6:H:92:GLN:OE1	2.44	0.50
2:O:139:GLY:O	2:O:141:LEU:N	2.43	0.50
2:O:170:ILE:HG22	2:O:170:ILE:O	2.11	0.50
1:S:463:HIS:HD2	1:S:473:LEU:HD11	1.77	0.50
2:O:228:ILE:HG22	2:O:229:ILE:H	1.77	0.50
8:P:398:SER:O	8:P:398:SER:OG	2.24	0.50
1:A:824:CYS:SG	1:A:825:ARG:N	2.85	0.50
1:A:1195:ARG:NH1	1:A:1202:GLU:OE2	2.45	0.50
1:S:963:PHE:CZ	1:S:977:LEU:HD23	2.47	0.49
6:H:342:THR:HB	6:H:384:PRO:HG2	1.94	0.49
1:A:368:ALA:HB2	1:A:400:PHE:CD1	2.47	0.49
6:H:213:TYR:OH	6:H:338:LEU:HD13	2.12	0.49
6:H:241:PRO:O	6:H:242:ARG:CB	2.57	0.49
1:S:990:ASP:OD1	1:S:1055:ARG:NH2	2.43	0.49
1:A:1161:THR:O	1:A:1321:ARG:NH2	2.41	0.49
2:B:231:PRO:O	2:B:234:SER:OG	2.29	0.49
3:C:539:GLU:N	3:C:539:GLU:OE1	2.45	0.49
6:H:60:LEU:HD23	2:O:232:ALA:HB1	1.92	0.49
6:H:555:LEU:HD21	6:H:570:LEU:HB2	1.93	0.49
8:P:399:LEU:O	8:P:423:LEU:O	2.30	0.49
2:B:752:GLU:HB3	2:B:859:LEU:HD21	1.94	0.49
6:G:79:ILE:HG13	6:G:145:LEU:HD21	1.94	0.49
2:O:526:ARG:NH2	2:O:652:LEU:O	2.45	0.49
9:W:77:VAL:HG12	9:W:79:THR:HG23	1.94	0.49
2:B:15:LEU:CD2	2:B:24:VAL:HG22	2.43	0.49
3:C:361:ARG:HD2	3:C:538:ILE:HD12	1.95	0.49
6:G:67:LEU:HD23	6:G:135:LEU:HD22	1.95	0.49
1:A:656:ALA:HB3	1:A:683:ARG:NH2	2.28	0.49
5:F:333:LYS:HD2	5:F:348:THR:HG22	1.94	0.48
8:Q:511:SER:HG	8:Q:526:THR:HG1	1.59	0.48
6:G:448:CYS:SG	6:G:482:LEU:HD22	2.53	0.48
5:F:188:PHE:CZ	5:F:192:LEU:HD11	2.48	0.48
6:H:230:SER:OG	6:H:231:SER:N	2.47	0.48
2:B:530:LEU:HD12	2:B:649:PHE:HE1	1.79	0.48
8:P:339:ARG:NH1	8:P:385:GLU:O	2.47	0.48
8:P:826:ARG:O	8:P:830:LEU:HD12	2.14	0.48
2:B:773:LEU:HD23	2:B:777:ILE:HD12	1.96	0.48
3:C:124:ALA:O	5:F:140:ARG:NH1	2.47	0.48
1:A:768:LEU:HD13	1:A:784:LEU:HD21	1.94	0.48
2:O:577:ILE:O	2:O:577:ILE:HG13	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1079:LYS:HD2	1:S:1130:ILE:HD11	1.96	0.48
1:A:476:PHE:CZ	1:A:480:LEU:HD11	2.48	0.48
1:S:1003:ASN:HA	9:W:1:UNK:H2	1.77	0.48
2:B:185:GLY:O	2:B:186:LEU:HD23	2.14	0.48
7:M:31:ALA:HB3	7:M:91:LEU:HD22	1.96	0.48
8:Q:24:GLY:O	8:Q:27:ARG:NH1	2.46	0.48
1:S:377:GLU:O	1:S:381:THR:OG1	2.18	0.48
1:A:1113:ASN:O	1:A:1117:ARG:NE	2.43	0.47
3:C:62:GLU:OE1	3:C:63:ARG:NH2	2.47	0.47
2:O:395:GLU:OE2	2:O:399:LYS:NZ	2.47	0.47
1:S:963:PHE:HZ	1:S:977:LEU:HD23	1.79	0.47
2:B:512:GLN:NE2	8:P:570:ASP:OD1	2.47	0.47
2:O:169:SER:OG	2:O:171:GLN:NE2	2.47	0.47
2:O:711:THR:O	2:O:713:PHE:N	2.47	0.47
2:O:503:ASP:OD1	2:O:604:ARG:NE	2.44	0.47
2:B:287:VAL:HG12	2:B:301:VAL:HG22	1.95	0.47
6:G:67:LEU:HD23	6:G:135:LEU:CD2	2.43	0.47
8:P:655:PHE:CE1	8:P:754:ILE:HD12	2.48	0.47
1:S:1242:ILE:HG23	1:S:1246:LEU:HD12	1.96	0.47
8:Q:772:ALA:HB2	8:Q:783:GLN:HG3	1.95	0.47
1:S:494:LEU:CD1	1:S:518:LEU:HD11	2.42	0.47
1:S:859:CYS:SG	1:S:860:LEU:N	2.88	0.47
3:C:188:VAL:HB	3:C:189:PRO:HD3	1.95	0.47
2:O:600:GLN:HE22	8:Q:601:THR:HG21	1.80	0.47
8:P:500:GLY:O	8:P:501:THR:OG1	2.25	0.47
8:Q:92:HIS:NE2	8:Q:116:ILE:HD13	2.30	0.47
1:A:137:LEU:O	1:A:137:LEU:HD12	2.14	0.47
6:G:143:VAL:HG11	6:G:166:LEU:HD11	1.97	0.47
6:G:469:GLN:NE2	6:G:523:GLU:OE1	2.47	0.47
8:P:85:LEU:HD12	8:P:130:LEU:HD11	1.96	0.47
8:Q:600:CYS:O	8:Q:642:LEU:O	2.33	0.47
1:A:790:HIS:NE2	1:A:843:TYR:OH	2.35	0.47
7:L:16:LEU:HD11	8:P:483:LEU:CD2	2.45	0.47
8:P:74:ARG:CD	8:P:90:LEU:HD12	2.44	0.47
1:S:1262:PHE:CD1	1:S:1319:LEU:HD22	2.50	0.47
1:A:179:LEU:HD22	1:A:217:LEU:HD11	1.97	0.47
8:Q:546:GLN:HB3	8:Q:564:THR:HG22	1.95	0.47
4:E:124:ASP:N	4:E:124:ASP:OD1	2.48	0.47
8:Q:526:THR:HG22	8:Q:581:THR:HG22	1.97	0.47
1:S:121:VAL:HA	1:S:124:ILE:HD12	1.97	0.47
7:L:326:ASN:HD22	7:L:364:LYS:HG3	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:292:SER:OG	2:O:339:GLU:O	2.24	0.46
8:Q:405:VAL:HG12	8:Q:407:LEU:HG	1.96	0.46
1:S:589:THR:HG23	1:S:1006:LEU:CD1	2.45	0.46
2:B:415:LYS:HZ2	8:P:476:VAL:HG13	1.80	0.46
3:C:122:LEU:O	5:F:140:ARG:NE	2.48	0.46
2:O:130:MET:CE	2:O:134:LEU:HD13	2.45	0.46
6:G:21:ASP:OD1	6:G:195:LEU:HD12	2.15	0.46
2:O:176:ILE:HD12	2:O:182:VAL:HG21	1.97	0.46
2:B:710:ARG:HD2	2:B:711:THR:HG23	1.97	0.46
3:C:433:ARG:NH1	4:E:178:LEU:O	2.43	0.46
2:O:248:ILE:HG22	2:O:249:LYS:H	1.80	0.46
2:O:406:ARG:NH1	8:Q:318:HIS:O	2.47	0.46
8:Q:655:PHE:CE1	8:Q:754:ILE:HD12	2.50	0.46
8:Q:794:LEU:HD23	8:Q:798:CYS:SG	2.56	0.46
1:A:377:GLU:O	1:A:381:THR:OG1	2.27	0.46
3:C:64:PHE:N	3:C:65:PRO:HD2	2.31	0.46
3:C:262:ILE:HG12	4:E:171:LEU:HD12	1.98	0.46
3:C:343:TYR:HD1	3:C:344:THR:HG23	1.80	0.46
2:B:700:PHE:HD1	2:B:730:CYS:HG	1.63	0.46
6:G:242:ARG:NH1	6:G:275:GLU:O	2.49	0.46
6:H:103:VAL:O	6:H:106:THR:OG1	2.31	0.46
6:H:246:VAL:O	6:H:250:THR:HG23	2.15	0.46
7:L:248:LEU:HD21	7:L:271:ILE:HD11	1.98	0.46
8:P:227:LEU:HD21	8:P:336:PRO:HB3	1.98	0.46
4:E:64:LEU:HD23	4:E:67:LEU:HD12	1.97	0.46
2:O:402:PHE:HA	8:Q:465:ILE:HD11	1.99	0.45
8:P:28:VAL:HG23	8:P:400:ASN:ND2	2.30	0.45
8:P:50:GLU:N	8:P:50:GLU:OE1	2.49	0.45
6:H:388:PRO:O	6:H:500:GLU:OE2	2.34	0.45
1:A:834:LEU:O	1:A:838:THR:OG1	2.25	0.45
2:B:145:ARG:NH2	2:B:168:SER:O	2.50	0.45
2:B:277:CYS:SG	2:B:278:GLN:N	2.89	0.45
2:O:426:LEU:CD2	8:Q:638:VAL:HG21	2.47	0.45
8:P:825:LEU:HD21	8:P:881:LEU:HD13	1.98	0.45
8:Q:801:HIS:O	8:Q:805:VAL:HG23	2.17	0.45
1:A:240:GLN:HA	1:A:311:ILE:HD11	1.98	0.45
1:A:291:THR:HA	1:A:294:ILE:HD12	1.98	0.45
3:C:347:SER:O	3:C:351:VAL:HG23	2.16	0.45
8:Q:143:LEU:HD12	8:Q:197:LEU:HD21	1.99	0.45
3:C:247:LEU:N	3:C:248:PRO:CD	2.80	0.45
3:C:267:ASN:O	3:C:555:ARG:NH2	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:224:LEU:HD12	8:Q:227:LEU:HD23	1.99	0.45
3:C:465:GLN:O	3:C:469:THR:HG23	2.16	0.45
6:H:89:THR:HG22	6:H:90:GLU:H	1.81	0.45
2:B:15:LEU:HD22	2:B:24:VAL:HG22	1.97	0.45
8:P:390:LEU:N	8:P:390:LEU:HD23	2.32	0.45
8:P:875:HIS:HB3	8:P:876:PRO:HD3	1.99	0.45
8:P:704:SER:O	8:P:797:ILE:HD11	2.17	0.45
1:S:940:GLN:NE2	1:S:942:GLU:OE2	2.50	0.45
3:C:395:PHE:O	3:C:399:HIS:ND1	2.50	0.44
2:O:574:CYS:SG	2:O:575:VAL:N	2.90	0.44
8:P:47:TYR:CZ	8:P:54:LEU:HB3	2.51	0.44
1:S:1029:GLU:OE2	1:S:1088:SER:OG	2.35	0.44
4:E:106:ARG:HA	4:E:109:LEU:HD12	2.00	0.44
1:A:1176:SER:HA	1:S:964:LEU:HD13	1.99	0.44
5:F:246:GLU:OE2	5:F:246:GLU:N	2.49	0.44
2:O:475:VAL:HG13	2:O:491:VAL:HG13	2.00	0.44
2:O:669:LEU:O	2:O:709:GLN:NE2	2.51	0.44
8:P:25:LYS:N	8:P:26:PRO:CD	2.81	0.44
1:A:100:ASP:O	1:A:103:SER:OG	2.26	0.44
2:B:781:GLU:O	2:B:827:ASN:ND2	2.50	0.44
6:H:284:LEU:O	6:H:287:SER:OG	2.23	0.44
7:M:104:LEU:CG	7:M:105:PRO:HD3	2.44	0.44
2:O:291:ASP:HA	2:O:297:LEU:HD23	1.99	0.44
2:O:478:ILE:HD11	2:O:597:VAL:HG21	1.99	0.44
3:C:60:VAL:HG23	3:C:64:PHE:CE1	2.53	0.44
1:S:37:PRO:O	1:S:41:GLN:NE2	2.50	0.44
1:A:421:SER:OG	1:A:423:GLN:NE2	2.50	0.44
6:G:402:VAL:HG11	6:G:595:SER:HB3	1.99	0.44
1:A:313:THR:HG22	1:A:317:LYS:HG3	2.00	0.44
6:H:58:GLN:NE2	6:H:70:GLU:OE2	2.50	0.44
2:O:134:LEU:HD12	2:O:135:ARG:N	2.33	0.44
8:Q:341:TYR:OH	8:Q:385:GLU:O	2.31	0.44
1:S:184:HIS:HA	1:S:187:VAL:HG12	1.99	0.44
1:A:108:PRO:HG2	1:A:111:ILE:HD12	1.99	0.43
1:A:424:LEU:O	1:A:428:VAL:HG23	2.18	0.43
8:Q:765:HIS:HD2	8:Q:767:ILE:HD11	1.83	0.43
1:S:1088:SER:O	1:S:1104:ARG:NH2	2.50	0.43
1:A:351:THR:HG21	1:A:391:SER:HB2	1.99	0.43
1:A:1408:PRO:O	1:A:1439:ARG:NH1	2.52	0.43
8:P:28:VAL:HG23	8:P:400:ASN:HD21	1.83	0.43
2:B:257:ILE:HD11	2:B:299:PHE:CE1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:149:LEU:HD22	1:S:190:ILE:HG13	1.98	0.43
1:S:1125:ALA:CB	1:S:1172:VAL:HG21	2.47	0.43
6:H:104:LEU:HD21	6:H:124:SER:OG	2.18	0.43
7:M:15:LEU:HD21	7:M:25:TYR:HB3	2.01	0.43
8:P:504:ARG:O	8:P:532:SER:OG	2.30	0.43
8:P:704:SER:OG	8:P:797:ILE:HD12	2.19	0.43
1:S:101:GLN:O	1:S:105:LEU:HG	2.18	0.43
9:W:81:GLY:O	9:W:83:LYS:N	2.52	0.43
7:M:57:TRP:O	7:M:61:THR:HG23	2.18	0.43
2:O:141:LEU:HD11	2:O:152:PHE:HB2	2.00	0.43
2:O:212:PHE:CE2	2:O:229:ILE:HD11	2.53	0.43
1:S:463:HIS:CD2	1:S:473:LEU:HD11	2.54	0.43
6:H:342:THR:CB	6:H:384:PRO:HG3	2.48	0.43
7:L:307:CYS:CB	7:L:310:CYS:SG	3.06	0.43
8:P:751:LEU:HD13	8:P:754:ILE:CG2	2.48	0.43
8:Q:125:LEU:O	8:Q:125:LEU:HD12	2.19	0.43
2:B:484:ASP:OD1	2:B:484:ASP:N	2.50	0.43
6:G:575:GLU:HA	6:G:578:THR:HG22	2.01	0.43
1:S:874:ARG:NH2	1:S:944:ASP:OD1	2.51	0.43
6:H:199:ASP:OD1	6:H:199:ASP:N	2.51	0.42
6:H:221:ILE:HD11	6:H:336:SER:HA	2.00	0.42
6:H:342:THR:CB	6:H:384:PRO:CG	2.97	0.42
7:L:320:PRO:HA	7:L:333:PHE:O	2.19	0.42
7:M:107:PRO:HB2	2:O:401:CYS:SG	2.58	0.42
2:B:95:VAL:HG22	2:B:109:LEU:HD12	2.01	0.42
3:C:405:GLU:N	3:C:405:GLU:OE1	2.52	0.42
2:O:326:SER:OG	2:O:344:LEU:O	2.33	0.42
8:Q:523:LEU:HD12	8:Q:592:LEU:HD21	2.00	0.42
1:S:994:SER:OG	1:S:995:SER:N	2.51	0.42
3:C:41:PHE:CE2	3:C:45:LEU:HD11	2.54	0.42
2:O:308:ALA:N	2:O:325:LEU:HD12	2.34	0.42
3:C:125:LEU:HD23	3:C:125:LEU:H	1.84	0.42
7:M:34:ARG:NH2	7:M:102:TYR:CE2	2.88	0.42
1:A:61:LEU:HD21	1:A:105:LEU:HD11	2.02	0.42
8:P:124:ILE:O	8:P:125:LEU:C	2.58	0.42
2:B:711:THR:O	2:B:711:THR:OG1	2.33	0.42
2:B:777:ILE:HG21	8:P:830:LEU:HD13	2.02	0.42
8:P:778:PRO:HD3	8:P:824:ASP:O	2.20	0.42
1:A:167:CYS:SG	1:A:196:LEU:HD23	2.60	0.42
2:B:83:SER:O	2:B:83:SER:OG	2.29	0.42
3:C:344:THR:HG21	3:C:396:LEU:HD22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:450:LEU:HD12	6:G:512:LEU:HD23	2.02	0.42
1:S:1033:ASP:CG	1:S:1093:SER:HG	2.23	0.42
1:A:137:LEU:N	1:A:180:GLU:OE1	2.46	0.42
7:L:307:CYS:HB3	7:L:310:CYS:SG	2.59	0.42
2:B:850:ASP:OD1	8:P:870:TYR:OH	2.22	0.41
8:Q:529:LEU:CD2	8:Q:572:LEU:HD21	2.50	0.41
1:S:1331:LEU:N	1:S:1332:PRO:HD2	2.34	0.41
1:A:673:ILE:O	1:A:677:VAL:HG23	2.20	0.41
1:A:769:LEU:HD13	1:A:821:LEU:CD1	2.46	0.41
6:G:444:GLU:O	6:G:487:THR:OG1	2.36	0.41
8:P:144:VAL:HG13	8:P:151:LYS:HG2	2.02	0.41
8:Q:517:LEU:O	8:Q:519:THR:N	2.53	0.41
1:A:37:PRO:O	1:A:41:GLN:NE2	2.53	0.41
7:M:107:PRO:CB	2:O:401:CYS:SG	3.09	0.41
8:P:173:VAL:HG12	8:P:174:GLU:H	1.85	0.41
1:S:608:LYS:NZ	1:S:618:TYR:OH	2.45	0.41
1:S:740:GLU:OE1	1:S:741:ARG:NH1	2.53	0.41
1:S:1211:LEU:HD12	1:S:1233:ALA:HB1	2.02	0.41
8:P:139:VAL:CG1	8:P:154:LEU:HD11	2.51	0.41
8:P:769:ARG:NH1	8:P:786:GLU:OE2	2.53	0.41
1:S:34:LYS:O	1:S:39:ARG:NH2	2.54	0.41
1:A:650:LEU:HD21	1:A:687:VAL:HG21	2.02	0.41
1:A:1400:ARG:NH2	1:A:1431:GLU:OE1	2.53	0.41
4:E:67:LEU:HD23	4:E:86:LEU:HD23	2.01	0.41
6:G:163:LEU:HD23	6:G:166:LEU:HD12	2.02	0.41
1:S:182:VAL:HG23	1:S:196:LEU:CD1	2.51	0.41
1:S:366:LEU:CD1	1:S:371:LEU:HD21	2.49	0.41
1:A:730:LEU:HD22	1:A:783:GLY:HA2	2.02	0.41
2:O:854:GLN:OE1	8:Q:799:ARG:NE	2.51	0.41
1:A:351:THR:HG21	1:A:391:SER:CB	2.50	0.41
8:Q:517:LEU:O	8:Q:518:GLN:C	2.59	0.41
1:S:669:GLN:O	1:S:673:ILE:HD12	2.21	0.41
2:B:716:ILE:O	2:B:716:ILE:CG2	2.63	0.41
2:B:777:ILE:O	2:B:780:HIS:N	2.54	0.41
6:G:555:LEU:HD21	6:G:570:LEU:HB2	2.03	0.41
2:O:829:LYS:O	8:Q:826:ARG:NH2	2.54	0.41
1:A:288:GLU:OE1	1:A:288:GLU:N	2.53	0.41
1:A:386:TRP:O	1:A:390:LEU:HD23	2.21	0.41
2:B:283:ASP:HB3	2:B:304:ILE:HD12	2.03	0.41
2:B:508:LEU:CD2	2:B:597:VAL:HG22	2.51	0.41
2:B:530:LEU:HD12	2:B:649:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:136:ILE:HD12	7:L:138:LEU:HD11	2.03	0.41
7:M:34:ARG:CZ	7:M:102:TYR:CD2	3.03	0.41
8:P:712:ALA:HB2	8:P:783:GLN:O	2.20	0.41
1:S:874:ARG:NH1	1:S:936:GLU:OE1	2.54	0.41
1:S:1098:GLU:N	1:S:1098:GLU:OE1	2.53	0.41
1:A:276:PHE:CZ	1:A:291:THR:HG23	2.55	0.41
1:A:1117:ARG:NH1	1:A:1323:ALA:O	2.54	0.41
2:B:652:LEU:HD23	2:B:704:LEU:HD13	2.02	0.41
3:C:263:SER:OG	3:C:264:SER:N	2.54	0.41
6:H:135:LEU:HD12	6:H:139:LEU:HG	2.03	0.41
6:H:221:ILE:HD11	6:H:336:SER:CB	2.51	0.41
6:H:240:CYS:O	6:H:242:ARG:N	2.54	0.41
1:S:375:LEU:HD11	1:S:396:LEU:HD11	2.02	0.41
1:S:407:LEU:O	1:S:411:VAL:HG23	2.21	0.41
2:B:291:ASP:O	2:B:296:ASN:O	2.39	0.40
7:M:34:ARG:CZ	7:M:102:TYR:HD2	2.34	0.40
2:O:492:LYS:HA	2:O:577:ILE:HG22	2.02	0.40
8:Q:705:VAL:HG22	8:Q:790:GLU:HG2	2.04	0.40
8:Q:765:HIS:CD2	8:Q:767:ILE:HD11	2.56	0.40
1:S:311:ILE:HG22	1:S:312:SER:O	2.21	0.40
2:B:836:ARG:NH2	8:P:714:LEU:HD21	2.37	0.40
3:C:496:LEU:HD11	3:C:547:ALA:HB2	2.03	0.40
8:P:472:LEU:O	8:P:476:VAL:HG23	2.21	0.40
8:Q:224:LEU:CD1	8:Q:227:LEU:HD23	2.51	0.40
8:P:707:SER:OG	8:P:788:GLN:OE1	2.19	0.40
7:L:16:LEU:HD11	8:P:483:LEU:HD23	2.02	0.40
2:B:526:ARG:O	2:B:579:THR:HG22	2.22	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	1160/1477 (78%)	1071 (92%)	88 (8%)	1 (0%)	51	83
1	S	1224/1477 (83%)	1135 (93%)	87 (7%)	2 (0%)	47	79
2	B	685/884 (78%)	602 (88%)	74 (11%)	9 (1%)	12	42
2	O	679/884 (77%)	594 (88%)	78 (12%)	7 (1%)	15	49
3	C	546/583 (94%)	503 (92%)	43 (8%)	0	100	100
4	E	168/555 (30%)	161 (96%)	7 (4%)	0	100	100
5	F	336/399 (84%)	318 (95%)	18 (5%)	0	100	100
6	G	567/641 (88%)	519 (92%)	48 (8%)	0	100	100
6	H	532/641 (83%)	482 (91%)	45 (8%)	5 (1%)	17	52
7	L	368/394 (93%)	338 (92%)	29 (8%)	1 (0%)	41	73
7	M	294/394 (75%)	271 (92%)	20 (7%)	3 (1%)	15	49
8	P	726/906 (80%)	640 (88%)	73 (10%)	13 (2%)	8	34
8	Q	732/906 (81%)	650 (89%)	76 (10%)	6 (1%)	19	54
9	W	21/39 (54%)	14 (67%)	7 (33%)	0	100	100
All	All	8038/10180 (79%)	7298 (91%)	693 (9%)	47 (1%)	29	59

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	VAL
6	H	242	ARG
6	H	387	SER
2	O	147	VAL
2	O	249	LYS
8	P	642	LEU
8	Q	518	GLN
1	S	975	GLY
2	B	132	ASP
2	B	133	GLY
8	P	781	PRO
8	P	782	ILE
2	B	325	LEU
6	H	61	PRO
8	P	426	LYS
8	Q	557	ASP
8	Q	649	MET
2	B	138	ASN
2	B	637	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	70	GLU
2	O	83	SER
2	O	637	PRO
8	P	63	GLN
8	P	384	GLU
2	B	131	LYS
6	H	192	ASP
7	M	105	PRO
2	O	325	LEU
8	P	641	PRO
8	Q	556	LEU
8	Q	758	ALA
6	H	241	PRO
8	P	148	ALA
1	S	564	ILE
8	P	383	PRO
8	P	822	ALA
7	M	216	PRO
2	O	140	PRO
8	P	876	PRO
1	A	899	PRO
2	B	273	PRO
7	L	216	PRO
8	P	166	PRO
8	Q	757	VAL
2	B	712	PRO
7	M	104	LEU
8	P	427	GLY

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%)	1032 (100%)	2 (0%)	93	97
1	S	1092/1282 (85%)	1089 (100%)	3 (0%)	92	96
2	B	644/810 (80%)	635 (99%)	9 (1%)	67	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	635/810 (78%)	631 (99%)	4 (1%)	86	94
3	C	480/507 (95%)	477 (99%)	3 (1%)	86	94
4	E	136/467 (29%)	135 (99%)	1 (1%)	84	93
5	F	288/336 (86%)	287 (100%)	1 (0%)	92	96
6	G	483/538 (90%)	482 (100%)	1 (0%)	93	97
6	H	454/538 (84%)	453 (100%)	1 (0%)	93	97
7	L	334/354 (94%)	334 (100%)	0	100	100
7	M	266/354 (75%)	266 (100%)	0	100	100
8	P	627/749 (84%)	622 (99%)	5 (1%)	81	92
8	Q	630/749 (84%)	626 (99%)	4 (1%)	86	94
9	W	22/22 (100%)	22 (100%)	0	100	100
All	All	7125/8798 (81%)	7091 (100%)	34 (0%)	89	94

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	1308	LEU
2	B	509	LEU
2	B	519	ARG
2	B	526	ARG
2	B	574	CYS
2	B	583	SER
2	B	617	CYS
2	B	640	LYS
2	B	658	SER
2	B	742	CYS
3	C	195	ASP
3	C	280	SER
3	C	343	TYR
4	E	90	LEU
5	F	101	ARG
6	G	530	ASP
6	H	74	THR
2	O	585	SER
2	O	600	GLN
2	O	617	CYS
2	O	640	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	P	402	CYS
8	P	526	THR
8	P	599	SER
8	P	643	SER
8	P	839	THR
8	Q	510	THR
8	Q	598	VAL
8	Q	599	SER
8	Q	664	ARG
1	S	459	THR
1	S	728	GLN
1	S	795	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	GLN
1	A	463	HIS
2	B	533	ASN
3	C	58	ASN
3	C	104	ASN
3	C	107	GLN
3	C	354	GLN
3	C	489	HIS
6	G	31	GLN
6	H	58	GLN
6	H	366	HIS
6	H	542	GLN
7	M	18	GLN
7	M	71	GLN
2	O	116	ASN
2	O	171	GLN
2	O	600	GLN
2	O	780	HIS
8	P	237	GLN
8	P	382	GLN
8	P	589	ASN
8	P	801	HIS
8	Q	645	HIS
8	Q	801	HIS
8	Q	832	GLN
1	S	913	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	940	GLN
1	S	1366	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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

All 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	35.90
1	W	95:TRP	C	101:UNK	N	5.65

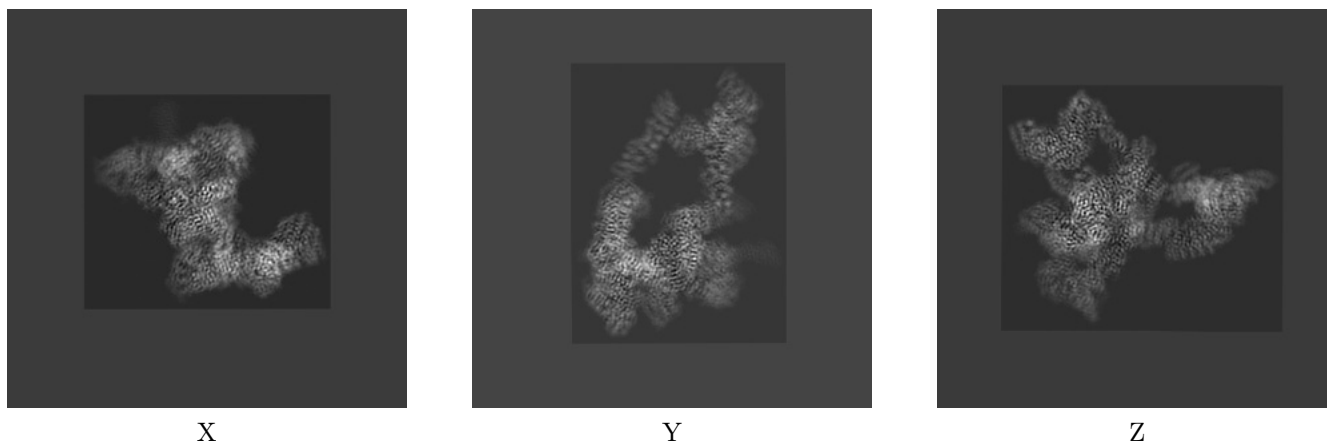
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23085. 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 [i](#)

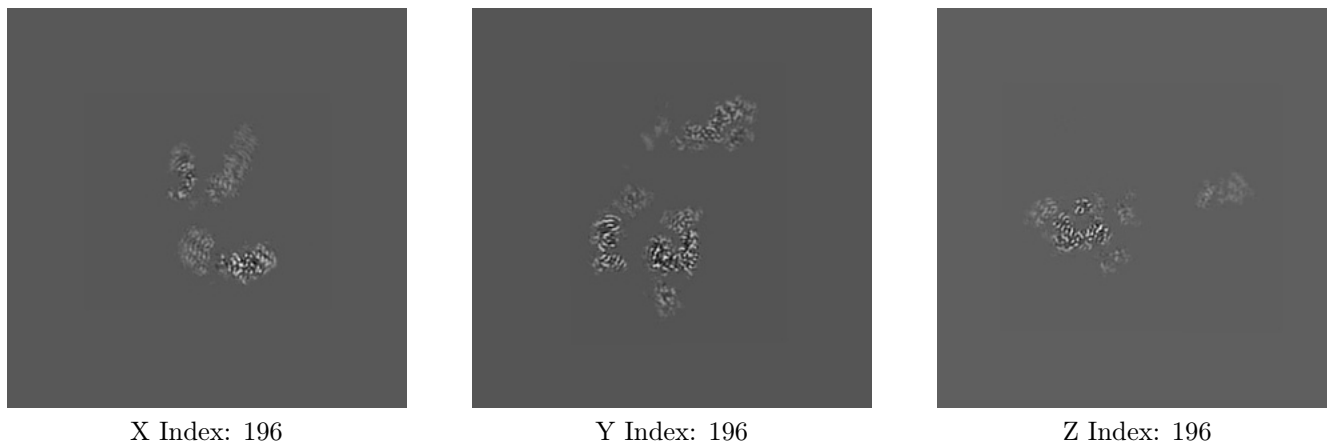
6.1.1 Primary map



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

6.2 Central slices [i](#)

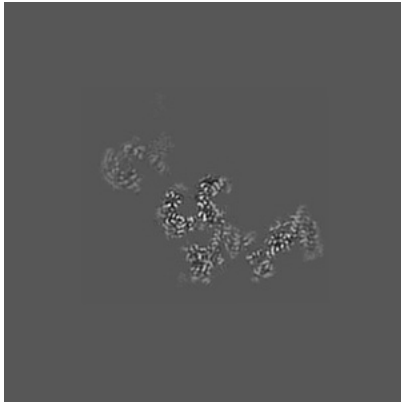
6.2.1 Primary map



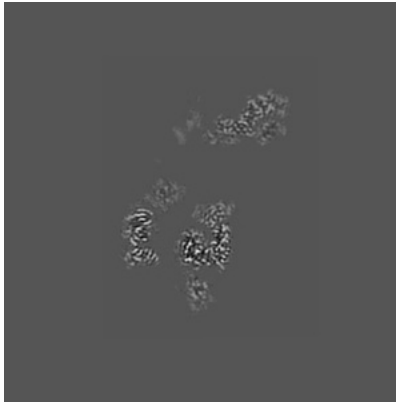
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

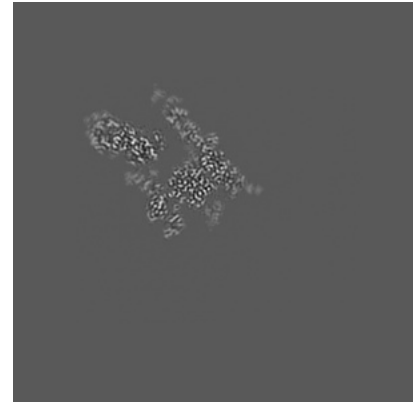
6.3.1 Primary map



X Index: 139



Y Index: 196

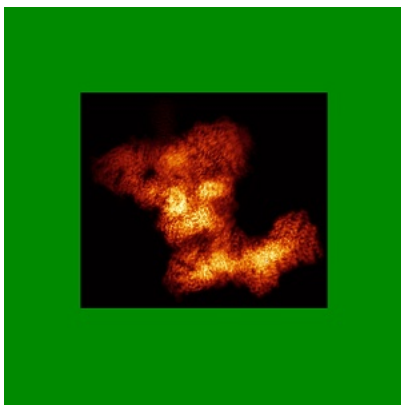


Z Index: 142

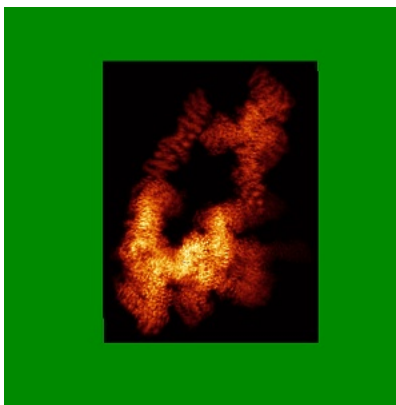
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

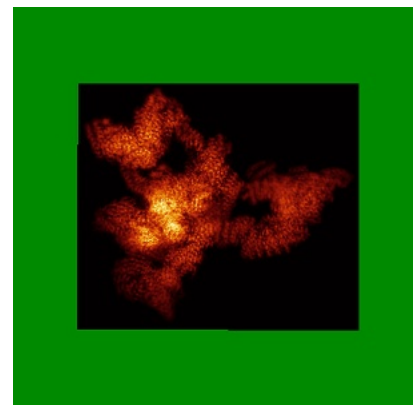
6.4.1 Primary map



X



Y

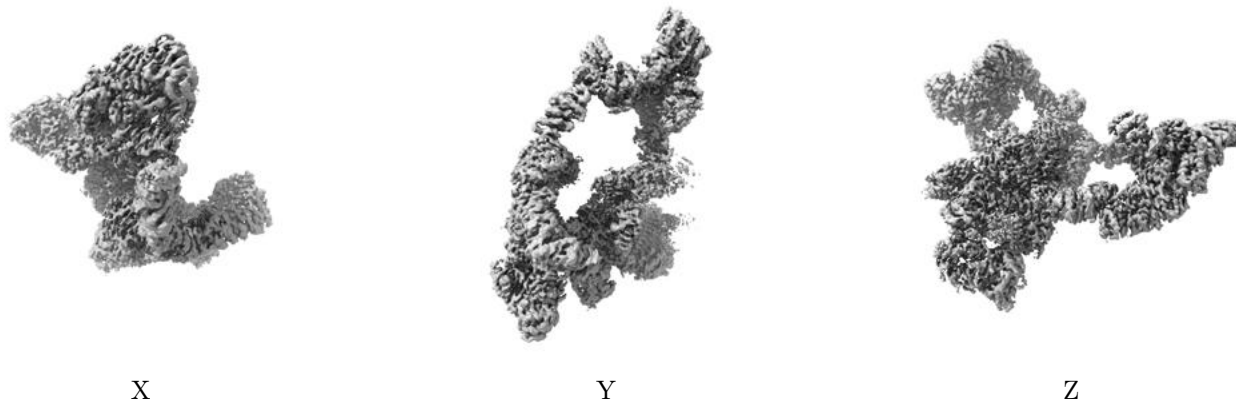


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

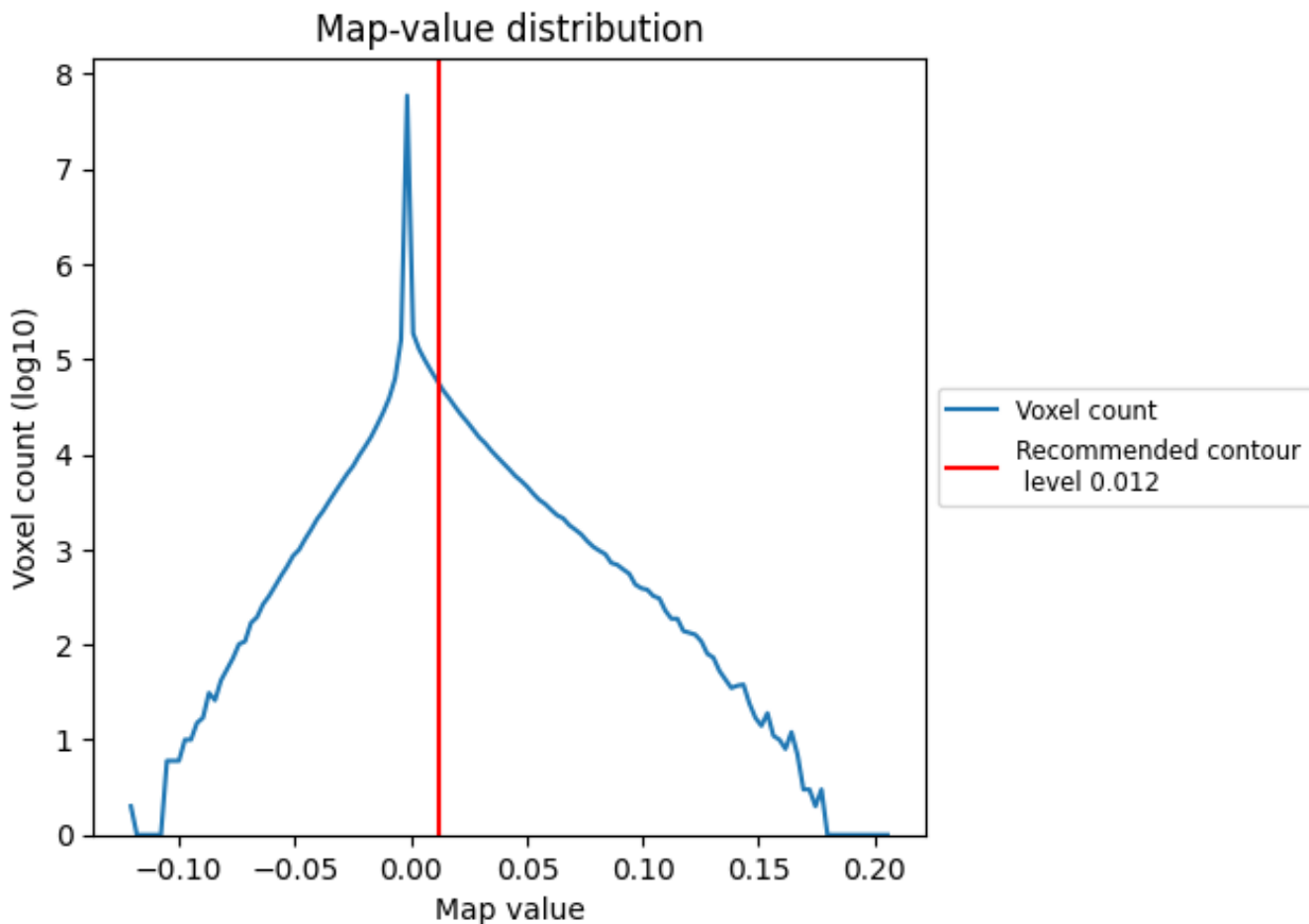
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

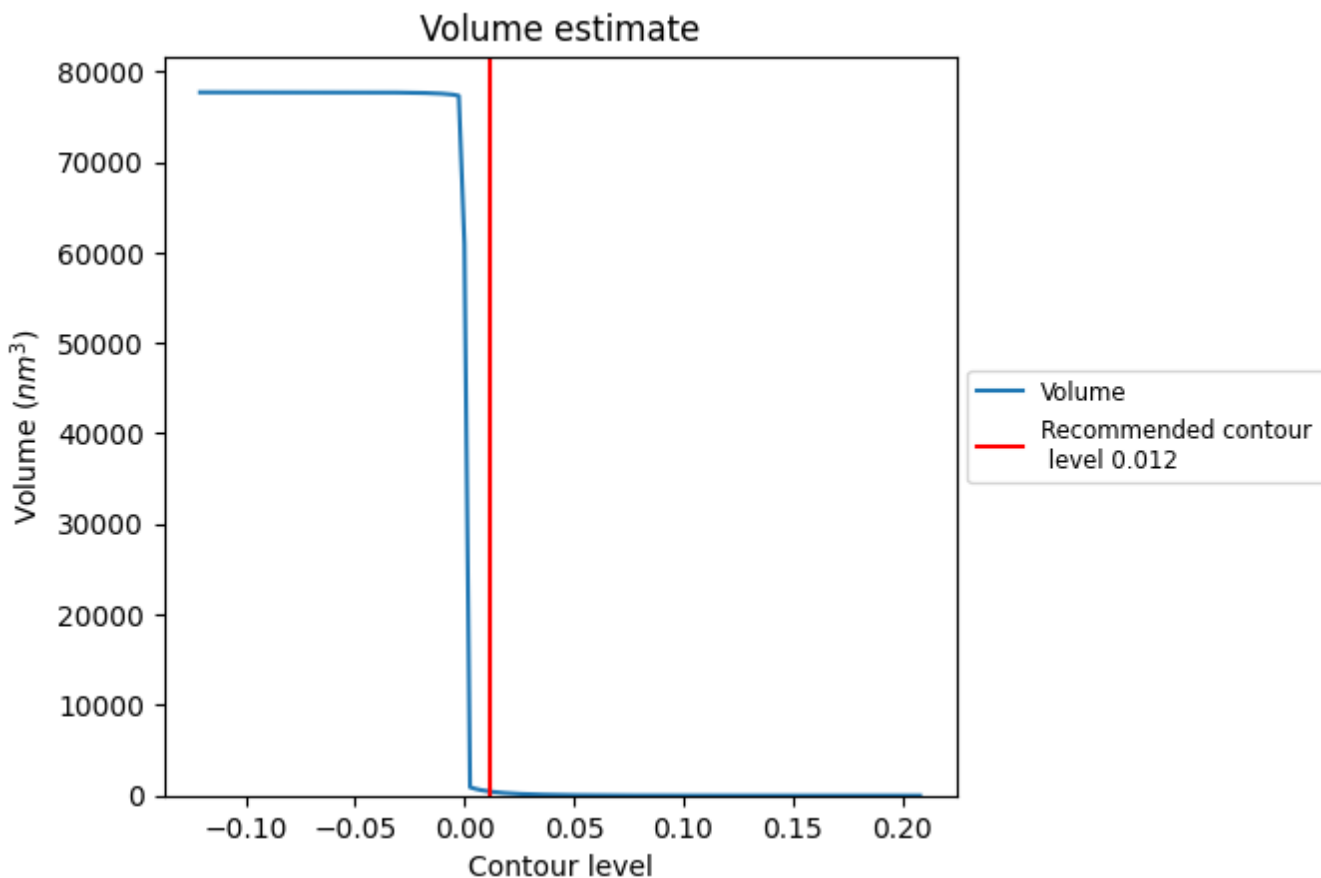
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

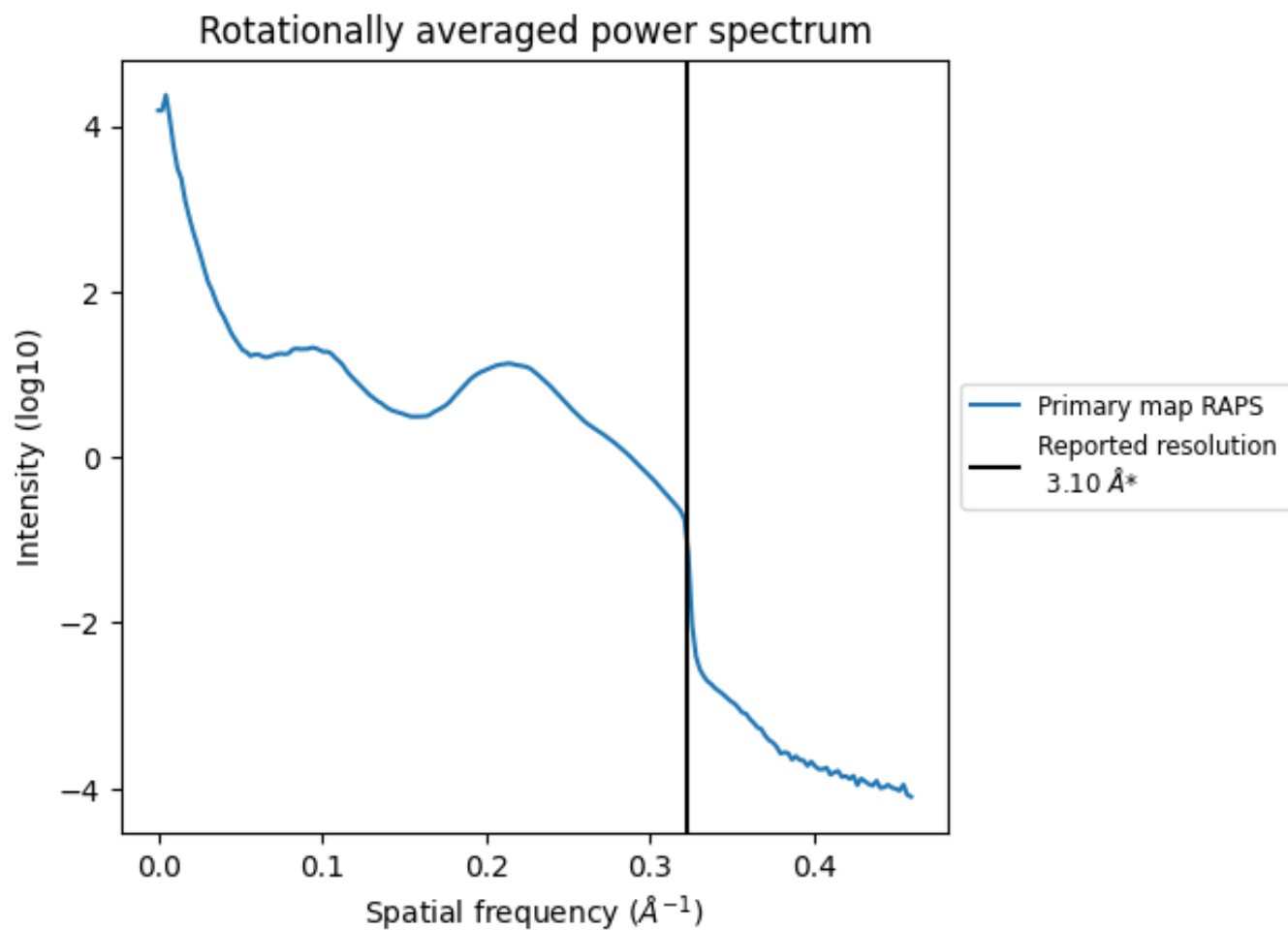
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 436 nm³; this corresponds to an approximate mass of 394 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 0.323 Å⁻¹

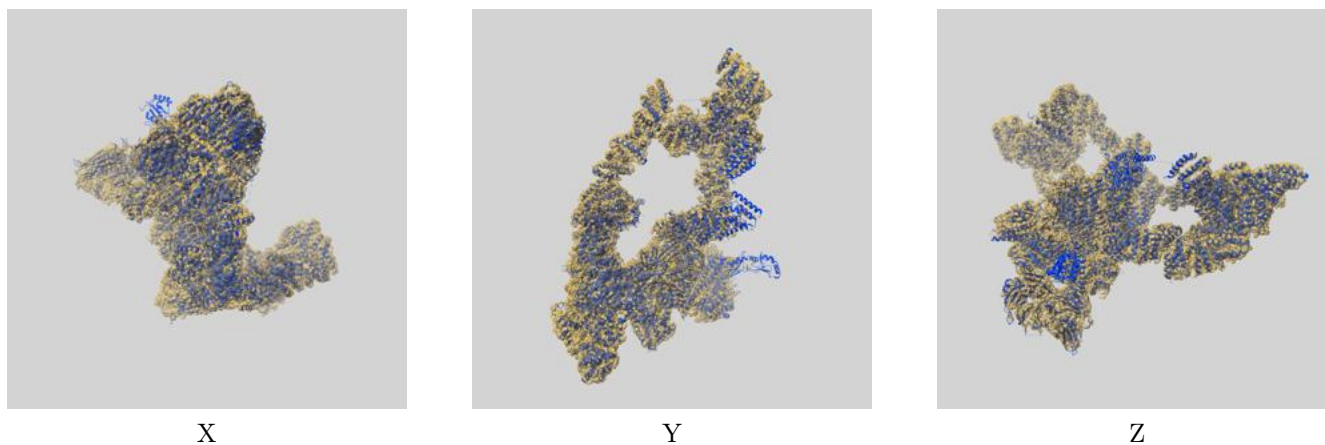
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

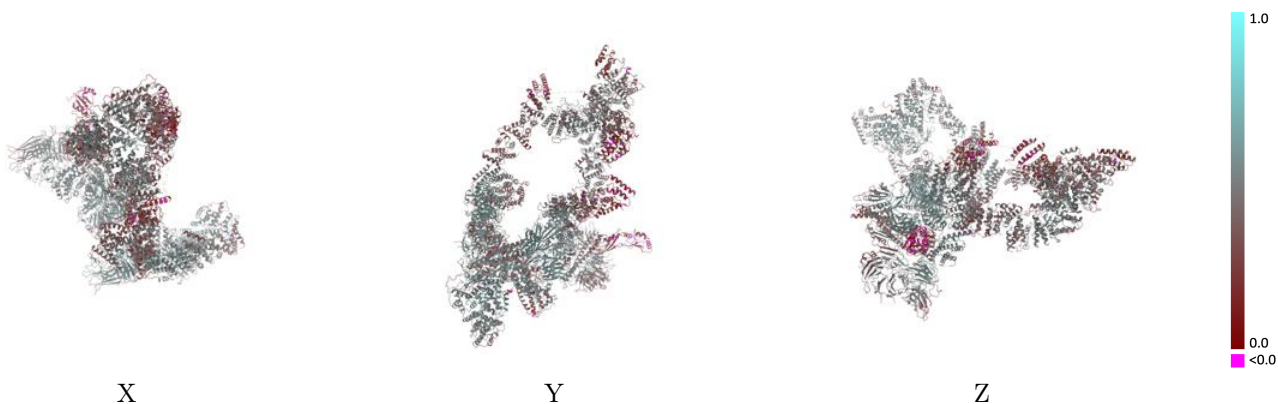
This section contains information regarding the fit between EMDB map EMD-23085 and PDB model 7KZP. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



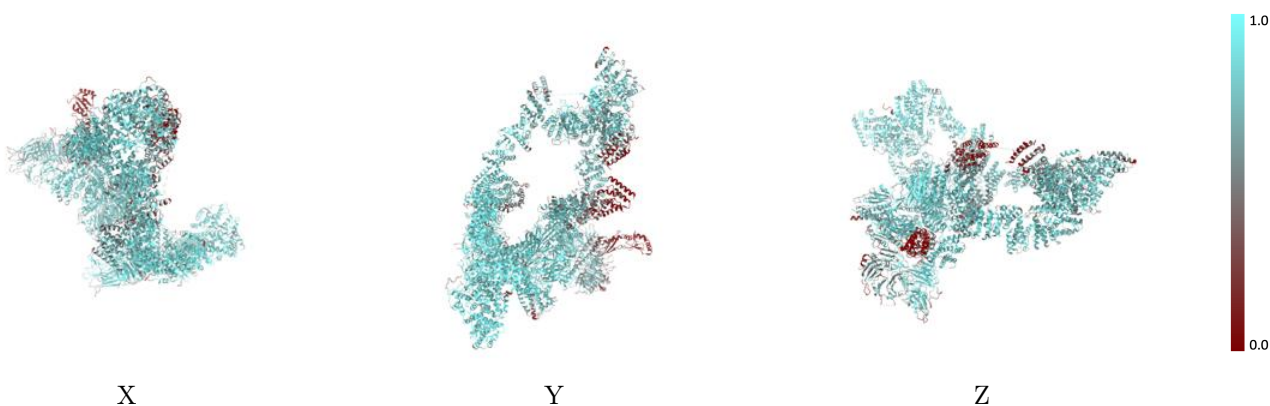
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



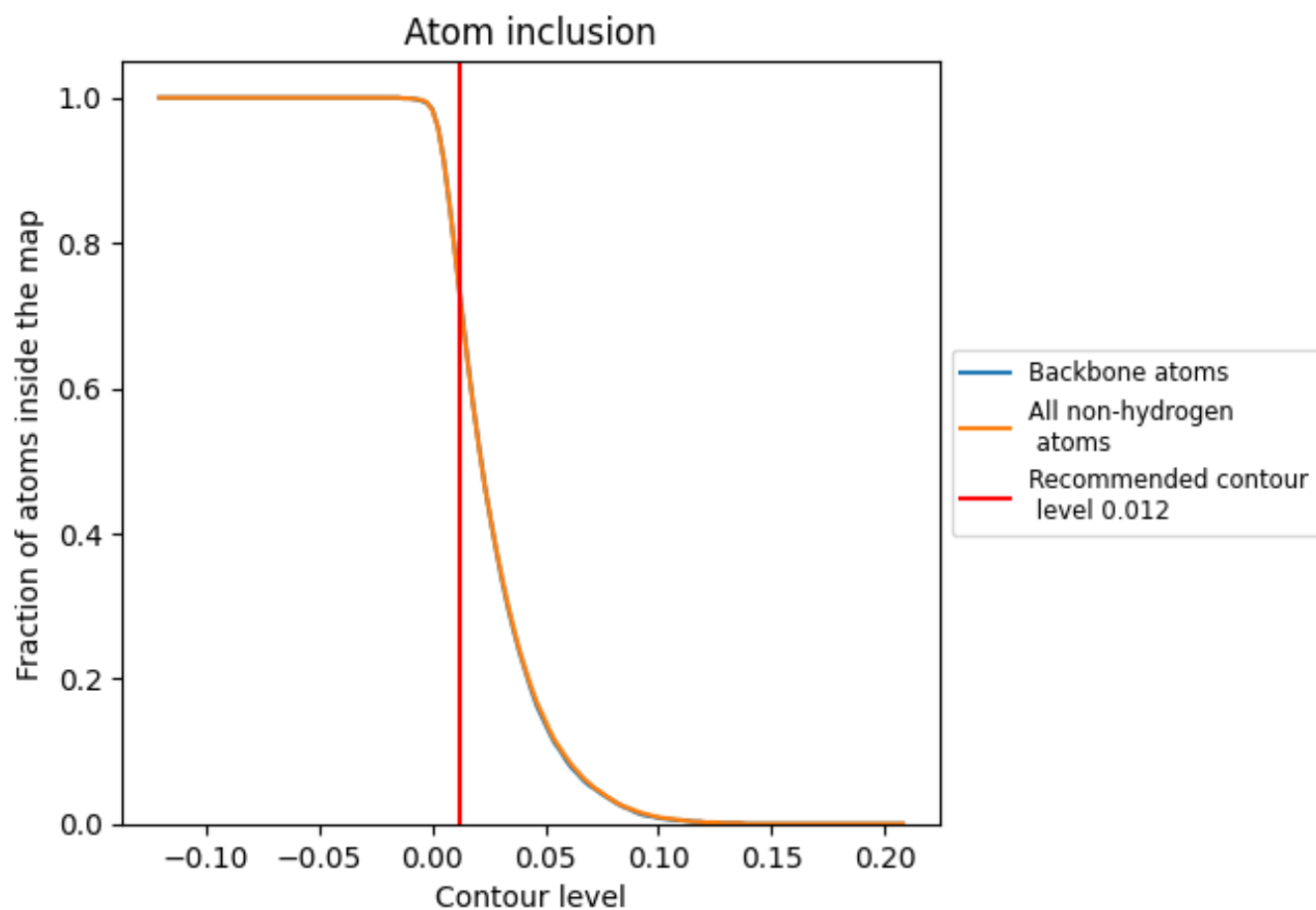
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.012).































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.4370
A	 0.5990	 0.3580
B	 0.8440	 0.5100
C	 0.8730	 0.5080
E	 0.8350	 0.5230
F	 0.8380	 0.4560
G	 0.7470	 0.4510
H	 0.7920	 0.4590
L	 0.8130	 0.4650
M	 0.2570	 0.2370
O	 0.7530	 0.4680
P	 0.8720	 0.5200
Q	 0.6630	 0.4290
S	 0.7350	 0.3900
W	 0.6990	 0.3930

