Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 07:18 am GMT

PDB ID	:	7OKQ
EMDB ID	:	EMD-12964
Title	:	Cryo-EM Structure of the DDB1-DCAF1-CUL4A-RBX1 Complex
Authors	:	Mohamed, W.I.; Schenk, A.D.; Kempf, G.; Cavadini, S.; Thoma, N.H.
Deposited on	:	2021-05-18
Resolution	:	8.40 Å(reported)
Based on initial models	:	2HYE, 5JK7

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:

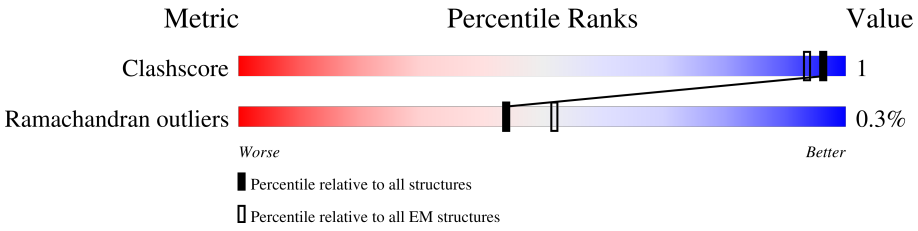
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 8.40 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

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	1159	97%
1	E	1159	97%
1	I	1159	97%
1	M	1159	97%
2	B	1525	21% 78%
2	F	1525	21% 78%
2	J	1525	22% 78%
2	N	1525	22% 78%
3	C	742	96%

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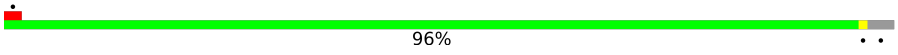
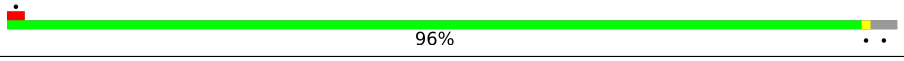
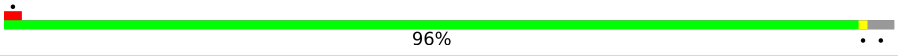
Mol	Chain	Length	Quality of chain
3	G	742	
3	K	742	
3	O	742	
4	D	116	
4	H	116	
4	L	116	
4	P	116	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 44608 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	1135	Total 5594	C 3324	N 1135	O 1135	0	0
1	E	1135	Total 5594	C 3324	N 1135	O 1135	0	0
1	I	1135	Total 5594	C 3324	N 1135	O 1135	0	0
1	M	1135	Total 5594	C 3324	N 1135	O 1135	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q16531
A	-17	HIS	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	HIS	-	expression tag	UNP Q16531
A	-11	VAL	-	expression tag	UNP Q16531
A	-10	ASP	-	expression tag	UNP Q16531
A	-9	GLU	-	expression tag	UNP Q16531
A	-8	ASN	-	expression tag	UNP Q16531
A	-7	LEU	-	expression tag	UNP Q16531
A	-6	TYR	-	expression tag	UNP Q16531
A	-5	PHE	-	expression tag	UNP Q16531
A	-4	GLN	-	expression tag	UNP Q16531
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
E	-18	MET	-	initiating methionine	UNP Q16531
E	-17	HIS	-	expression tag	UNP Q16531
E	-16	HIS	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP Q16531
E	-14	HIS	-	expression tag	UNP Q16531
E	-13	HIS	-	expression tag	UNP Q16531
E	-12	HIS	-	expression tag	UNP Q16531
E	-11	VAL	-	expression tag	UNP Q16531
E	-10	ASP	-	expression tag	UNP Q16531
E	-9	GLU	-	expression tag	UNP Q16531
E	-8	ASN	-	expression tag	UNP Q16531
E	-7	LEU	-	expression tag	UNP Q16531
E	-6	TYR	-	expression tag	UNP Q16531
E	-5	PHE	-	expression tag	UNP Q16531
E	-4	GLN	-	expression tag	UNP Q16531
E	-3	GLY	-	expression tag	UNP Q16531
E	-2	GLY	-	expression tag	UNP Q16531
E	-1	GLY	-	expression tag	UNP Q16531
E	0	ARG	-	expression tag	UNP Q16531
I	-18	MET	-	initiating methionine	UNP Q16531
I	-17	HIS	-	expression tag	UNP Q16531
I	-16	HIS	-	expression tag	UNP Q16531
I	-15	HIS	-	expression tag	UNP Q16531
I	-14	HIS	-	expression tag	UNP Q16531
I	-13	HIS	-	expression tag	UNP Q16531
I	-12	HIS	-	expression tag	UNP Q16531
I	-11	VAL	-	expression tag	UNP Q16531
I	-10	ASP	-	expression tag	UNP Q16531
I	-9	GLU	-	expression tag	UNP Q16531
I	-8	ASN	-	expression tag	UNP Q16531
I	-7	LEU	-	expression tag	UNP Q16531
I	-6	TYR	-	expression tag	UNP Q16531
I	-5	PHE	-	expression tag	UNP Q16531
I	-4	GLN	-	expression tag	UNP Q16531
I	-3	GLY	-	expression tag	UNP Q16531
I	-2	GLY	-	expression tag	UNP Q16531
I	-1	GLY	-	expression tag	UNP Q16531
I	0	ARG	-	expression tag	UNP Q16531
M	-18	MET	-	initiating methionine	UNP Q16531
M	-17	HIS	-	expression tag	UNP Q16531
M	-16	HIS	-	expression tag	UNP Q16531
M	-15	HIS	-	expression tag	UNP Q16531
M	-14	HIS	-	expression tag	UNP Q16531
M	-13	HIS	-	expression tag	UNP Q16531
M	-12	HIS	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-11	VAL	-	expression tag	UNP Q16531
M	-10	ASP	-	expression tag	UNP Q16531
M	-9	GLU	-	expression tag	UNP Q16531
M	-8	ASN	-	expression tag	UNP Q16531
M	-7	LEU	-	expression tag	UNP Q16531
M	-6	TYR	-	expression tag	UNP Q16531
M	-5	PHE	-	expression tag	UNP Q16531
M	-4	GLN	-	expression tag	UNP Q16531
M	-3	GLY	-	expression tag	UNP Q16531
M	-2	GLY	-	expression tag	UNP Q16531
M	-1	GLY	-	expression tag	UNP Q16531
M	0	ARG	-	expression tag	UNP Q16531

- Molecule 2 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	331	Total	C	N	O	0	0
			1635	973	331	331		
2	F	331	Total	C	N	O	0	0
			1635	973	331	331		
2	J	331	Total	C	N	O	0	0
			1635	973	331	331		
2	N	331	Total	C	N	O	0	0
			1635	973	331	331		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP Q9Y4B6
B	-16	ALA	-	expression tag	UNP Q9Y4B6
B	-15	SER	-	expression tag	UNP Q9Y4B6
B	-14	TRP	-	expression tag	UNP Q9Y4B6
B	-13	SER	-	expression tag	UNP Q9Y4B6
B	-12	HIS	-	expression tag	UNP Q9Y4B6
B	-11	PRO	-	expression tag	UNP Q9Y4B6
B	-10	GLN	-	expression tag	UNP Q9Y4B6
B	-9	PHE	-	expression tag	UNP Q9Y4B6
B	-8	GLU	-	expression tag	UNP Q9Y4B6
B	-7	LYS	-	expression tag	UNP Q9Y4B6
B	-6	LEU	-	expression tag	UNP Q9Y4B6
B	-5	GLU	-	expression tag	UNP Q9Y4B6
B	-4	VAL	-	expression tag	UNP Q9Y4B6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	LEU	-	expression tag	UNP Q9Y4B6
B	-2	PHE	-	expression tag	UNP Q9Y4B6
B	-1	GLN	-	expression tag	UNP Q9Y4B6
B	0	GLY	-	expression tag	UNP Q9Y4B6
B	1	PRO	-	expression tag	UNP Q9Y4B6
F	-17	MET	-	initiating methionine	UNP Q9Y4B6
F	-16	ALA	-	expression tag	UNP Q9Y4B6
F	-15	SER	-	expression tag	UNP Q9Y4B6
F	-14	TRP	-	expression tag	UNP Q9Y4B6
F	-13	SER	-	expression tag	UNP Q9Y4B6
F	-12	HIS	-	expression tag	UNP Q9Y4B6
F	-11	PRO	-	expression tag	UNP Q9Y4B6
F	-10	GLN	-	expression tag	UNP Q9Y4B6
F	-9	PHE	-	expression tag	UNP Q9Y4B6
F	-8	GLU	-	expression tag	UNP Q9Y4B6
F	-7	LYS	-	expression tag	UNP Q9Y4B6
F	-6	LEU	-	expression tag	UNP Q9Y4B6
F	-5	GLU	-	expression tag	UNP Q9Y4B6
F	-4	VAL	-	expression tag	UNP Q9Y4B6
F	-3	LEU	-	expression tag	UNP Q9Y4B6
F	-2	PHE	-	expression tag	UNP Q9Y4B6
F	-1	GLN	-	expression tag	UNP Q9Y4B6
F	0	GLY	-	expression tag	UNP Q9Y4B6
F	1	PRO	-	expression tag	UNP Q9Y4B6
J	-17	MET	-	initiating methionine	UNP Q9Y4B6
J	-16	ALA	-	expression tag	UNP Q9Y4B6
J	-15	SER	-	expression tag	UNP Q9Y4B6
J	-14	TRP	-	expression tag	UNP Q9Y4B6
J	-13	SER	-	expression tag	UNP Q9Y4B6
J	-12	HIS	-	expression tag	UNP Q9Y4B6
J	-11	PRO	-	expression tag	UNP Q9Y4B6
J	-10	GLN	-	expression tag	UNP Q9Y4B6
J	-9	PHE	-	expression tag	UNP Q9Y4B6
J	-8	GLU	-	expression tag	UNP Q9Y4B6
J	-7	LYS	-	expression tag	UNP Q9Y4B6
J	-6	LEU	-	expression tag	UNP Q9Y4B6
J	-5	GLU	-	expression tag	UNP Q9Y4B6
J	-4	VAL	-	expression tag	UNP Q9Y4B6
J	-3	LEU	-	expression tag	UNP Q9Y4B6
J	-2	PHE	-	expression tag	UNP Q9Y4B6
J	-1	GLN	-	expression tag	UNP Q9Y4B6
J	0	GLY	-	expression tag	UNP Q9Y4B6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1	PRO	-	expression tag	UNP Q9Y4B6
N	-17	MET	-	initiating methionine	UNP Q9Y4B6
N	-16	ALA	-	expression tag	UNP Q9Y4B6
N	-15	SER	-	expression tag	UNP Q9Y4B6
N	-14	TRP	-	expression tag	UNP Q9Y4B6
N	-13	SER	-	expression tag	UNP Q9Y4B6
N	-12	HIS	-	expression tag	UNP Q9Y4B6
N	-11	PRO	-	expression tag	UNP Q9Y4B6
N	-10	GLN	-	expression tag	UNP Q9Y4B6
N	-9	PHE	-	expression tag	UNP Q9Y4B6
N	-8	GLU	-	expression tag	UNP Q9Y4B6
N	-7	LYS	-	expression tag	UNP Q9Y4B6
N	-6	LEU	-	expression tag	UNP Q9Y4B6
N	-5	GLU	-	expression tag	UNP Q9Y4B6
N	-4	VAL	-	expression tag	UNP Q9Y4B6
N	-3	LEU	-	expression tag	UNP Q9Y4B6
N	-2	PHE	-	expression tag	UNP Q9Y4B6
N	-1	GLN	-	expression tag	UNP Q9Y4B6
N	0	GLY	-	expression tag	UNP Q9Y4B6
N	1	PRO	-	expression tag	UNP Q9Y4B6

- Molecule 3 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	719	Total	C	N	O	0	0
			3564	2126	719	719		
3	G	719	Total	C	N	O	0	0
			3564	2126	719	719		
3	K	719	Total	C	N	O	0	0
			3564	2126	719	719		
3	O	719	Total	C	N	O	0	0
			3564	2126	719	719		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	MET	-	initiating methionine	UNP Q13619
C	19	HIS	-	expression tag	UNP Q13619
C	20	HIS	-	expression tag	UNP Q13619
C	21	HIS	-	expression tag	UNP Q13619
C	22	HIS	-	expression tag	UNP Q13619
C	23	HIS	-	expression tag	UNP Q13619

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	HIS	-	expression tag	UNP Q13619
C	25	VAL	-	expression tag	UNP Q13619
C	26	ASP	-	expression tag	UNP Q13619
C	27	GLU	-	expression tag	UNP Q13619
C	28	GLU	-	expression tag	UNP Q13619
C	29	ASN	-	expression tag	UNP Q13619
C	30	LEU	-	expression tag	UNP Q13619
C	31	TYR	-	expression tag	UNP Q13619
C	32	PHE	-	expression tag	UNP Q13619
C	33	GLN	-	expression tag	UNP Q13619
C	34	GLY	-	expression tag	UNP Q13619
C	37	ARG	ALA	conflict	UNP Q13619
G	18	MET	-	initiating methionine	UNP Q13619
G	19	HIS	-	expression tag	UNP Q13619
G	20	HIS	-	expression tag	UNP Q13619
G	21	HIS	-	expression tag	UNP Q13619
G	22	HIS	-	expression tag	UNP Q13619
G	23	HIS	-	expression tag	UNP Q13619
G	24	HIS	-	expression tag	UNP Q13619
G	25	VAL	-	expression tag	UNP Q13619
G	26	ASP	-	expression tag	UNP Q13619
G	27	GLU	-	expression tag	UNP Q13619
G	28	GLU	-	expression tag	UNP Q13619
G	29	ASN	-	expression tag	UNP Q13619
G	30	LEU	-	expression tag	UNP Q13619
G	31	TYR	-	expression tag	UNP Q13619
G	32	PHE	-	expression tag	UNP Q13619
G	33	GLN	-	expression tag	UNP Q13619
G	34	GLY	-	expression tag	UNP Q13619
G	37	ARG	ALA	conflict	UNP Q13619
K	18	MET	-	initiating methionine	UNP Q13619
K	19	HIS	-	expression tag	UNP Q13619
K	20	HIS	-	expression tag	UNP Q13619
K	21	HIS	-	expression tag	UNP Q13619
K	22	HIS	-	expression tag	UNP Q13619
K	23	HIS	-	expression tag	UNP Q13619
K	24	HIS	-	expression tag	UNP Q13619
K	25	VAL	-	expression tag	UNP Q13619
K	26	ASP	-	expression tag	UNP Q13619
K	27	GLU	-	expression tag	UNP Q13619
K	28	GLU	-	expression tag	UNP Q13619
K	29	ASN	-	expression tag	UNP Q13619

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Chain	Residue	Modelled	Actual	Comment	Reference
K	30	LEU	-	expression tag	UNP Q13619
K	31	TYR	-	expression tag	UNP Q13619
K	32	PHE	-	expression tag	UNP Q13619
K	33	GLN	-	expression tag	UNP Q13619
K	34	GLY	-	expression tag	UNP Q13619
K	37	ARG	ALA	conflict	UNP Q13619
O	18	MET	-	initiating methionine	UNP Q13619
O	19	HIS	-	expression tag	UNP Q13619
O	20	HIS	-	expression tag	UNP Q13619
O	21	HIS	-	expression tag	UNP Q13619
O	22	HIS	-	expression tag	UNP Q13619
O	23	HIS	-	expression tag	UNP Q13619
O	24	HIS	-	expression tag	UNP Q13619
O	25	VAL	-	expression tag	UNP Q13619
O	26	ASP	-	expression tag	UNP Q13619
O	27	GLU	-	expression tag	UNP Q13619
O	28	GLU	-	expression tag	UNP Q13619
O	29	ASN	-	expression tag	UNP Q13619
O	30	LEU	-	expression tag	UNP Q13619
O	31	TYR	-	expression tag	UNP Q13619
O	32	PHE	-	expression tag	UNP Q13619
O	33	GLN	-	expression tag	UNP Q13619
O	34	GLY	-	expression tag	UNP Q13619
O	37	ARG	ALA	conflict	UNP Q13619

- Molecule 4 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	72	Total	C	N	O	0	0
			359	215	72	72		
4	H	72	Total	C	N	O	0	0
			359	215	72	72		
4	L	72	Total	C	N	O	0	0
			359	215	72	72		
4	P	72	Total	C	N	O	0	0
			359	215	72	72		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	insertion	UNP P62877
D	-5	HIS	ALA	conflict	UNP P62877

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	ALA	conflict	UNP P62877
D	-3	HIS	ALA	conflict	UNP P62877
D	-2	HIS	MET	conflict	UNP P62877
D	-1	HIS	ASP	conflict	UNP P62877
D	2	GLU	-	insertion	UNP P62877
D	3	ASN	-	insertion	UNP P62877
D	4	LEU	-	insertion	UNP P62877
D	5	TYR	-	insertion	UNP P62877
D	6	PHE	-	insertion	UNP P62877
D	7	GLN	-	insertion	UNP P62877
D	8	GLY	-	insertion	UNP P62877
D	9	GLY	THR	conflict	UNP P62877
D	10	GLY	PRO	conflict	UNP P62877
D	11	ARG	SER	conflict	UNP P62877
H	-6	HIS	-	insertion	UNP P62877
H	-5	HIS	ALA	conflict	UNP P62877
H	-4	HIS	ALA	conflict	UNP P62877
H	-3	HIS	ALA	conflict	UNP P62877
H	-2	HIS	MET	conflict	UNP P62877
H	-1	HIS	ASP	conflict	UNP P62877
H	2	GLU	-	insertion	UNP P62877
H	3	ASN	-	insertion	UNP P62877
H	4	LEU	-	insertion	UNP P62877
H	5	TYR	-	insertion	UNP P62877
H	6	PHE	-	insertion	UNP P62877
H	7	GLN	-	insertion	UNP P62877
H	8	GLY	-	insertion	UNP P62877
H	9	GLY	THR	conflict	UNP P62877
H	10	GLY	PRO	conflict	UNP P62877
H	11	ARG	SER	conflict	UNP P62877
L	-6	HIS	-	insertion	UNP P62877
L	-5	HIS	ALA	conflict	UNP P62877
L	-4	HIS	ALA	conflict	UNP P62877
L	-3	HIS	ALA	conflict	UNP P62877
L	-2	HIS	MET	conflict	UNP P62877
L	-1	HIS	ASP	conflict	UNP P62877
L	2	GLU	-	insertion	UNP P62877
L	3	ASN	-	insertion	UNP P62877
L	4	LEU	-	insertion	UNP P62877
L	5	TYR	-	insertion	UNP P62877
L	6	PHE	-	insertion	UNP P62877
L	7	GLN	-	insertion	UNP P62877

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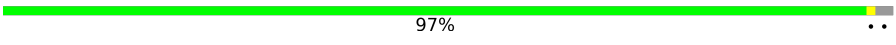
Chain	Residue	Modelled	Actual	Comment	Reference
L	8	GLY	-	insertion	UNP P62877
L	9	GLY	THR	conflict	UNP P62877
L	10	GLY	PRO	conflict	UNP P62877
L	11	ARG	SER	conflict	UNP P62877
P	-6	HIS	-	insertion	UNP P62877
P	-5	HIS	ALA	conflict	UNP P62877
P	-4	HIS	ALA	conflict	UNP P62877
P	-3	HIS	ALA	conflict	UNP P62877
P	-2	HIS	MET	conflict	UNP P62877
P	-1	HIS	ASP	conflict	UNP P62877
P	2	GLU	-	insertion	UNP P62877
P	3	ASN	-	insertion	UNP P62877
P	4	LEU	-	insertion	UNP P62877
P	5	TYR	-	insertion	UNP P62877
P	6	PHE	-	insertion	UNP P62877
P	7	GLN	-	insertion	UNP P62877
P	8	GLY	-	insertion	UNP P62877
P	9	GLY	THR	conflict	UNP P62877
P	10	GLY	PRO	conflict	UNP P62877
P	11	ARG	SER	conflict	UNP P62877

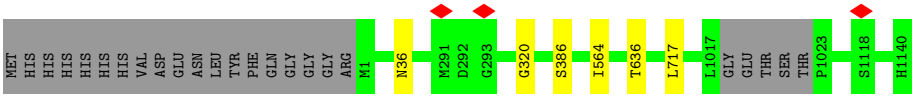
3 Residue-property plots (i)

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: DNA damage-binding protein 1

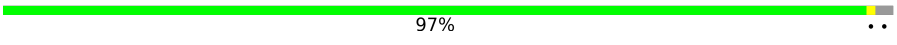
Chain A:

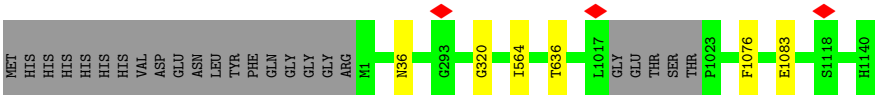




• Molecule 1: DNA damage-binding protein 1

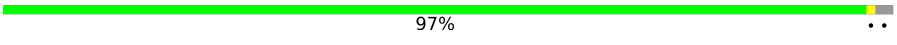
Chain E:

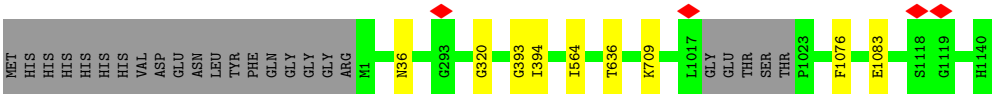




• Molecule 1: DNA damage-binding protein 1

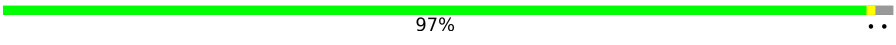
Chain I:

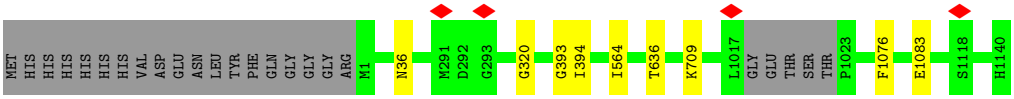




• Molecule 1: DNA damage-binding protein 1

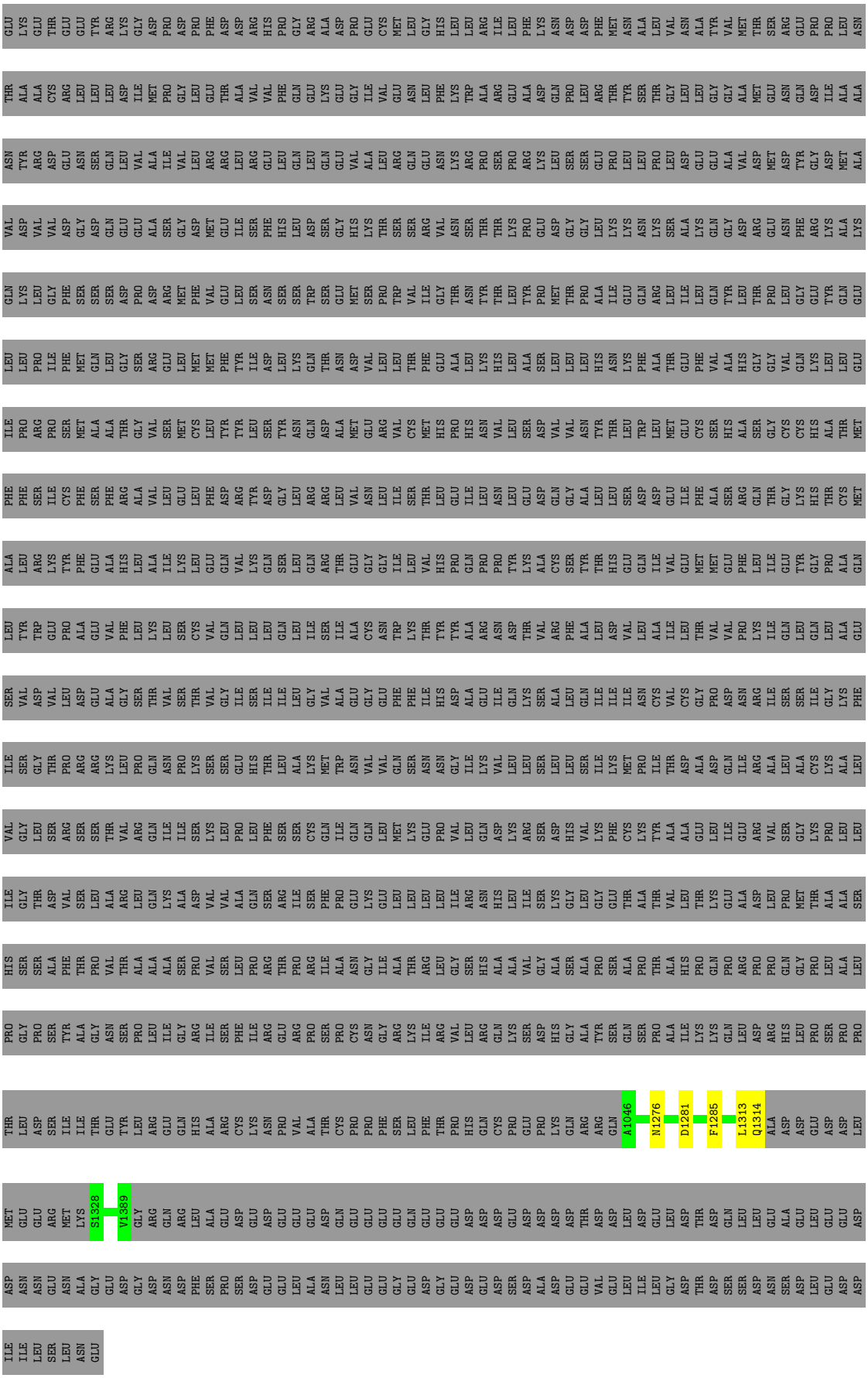
Chain M:





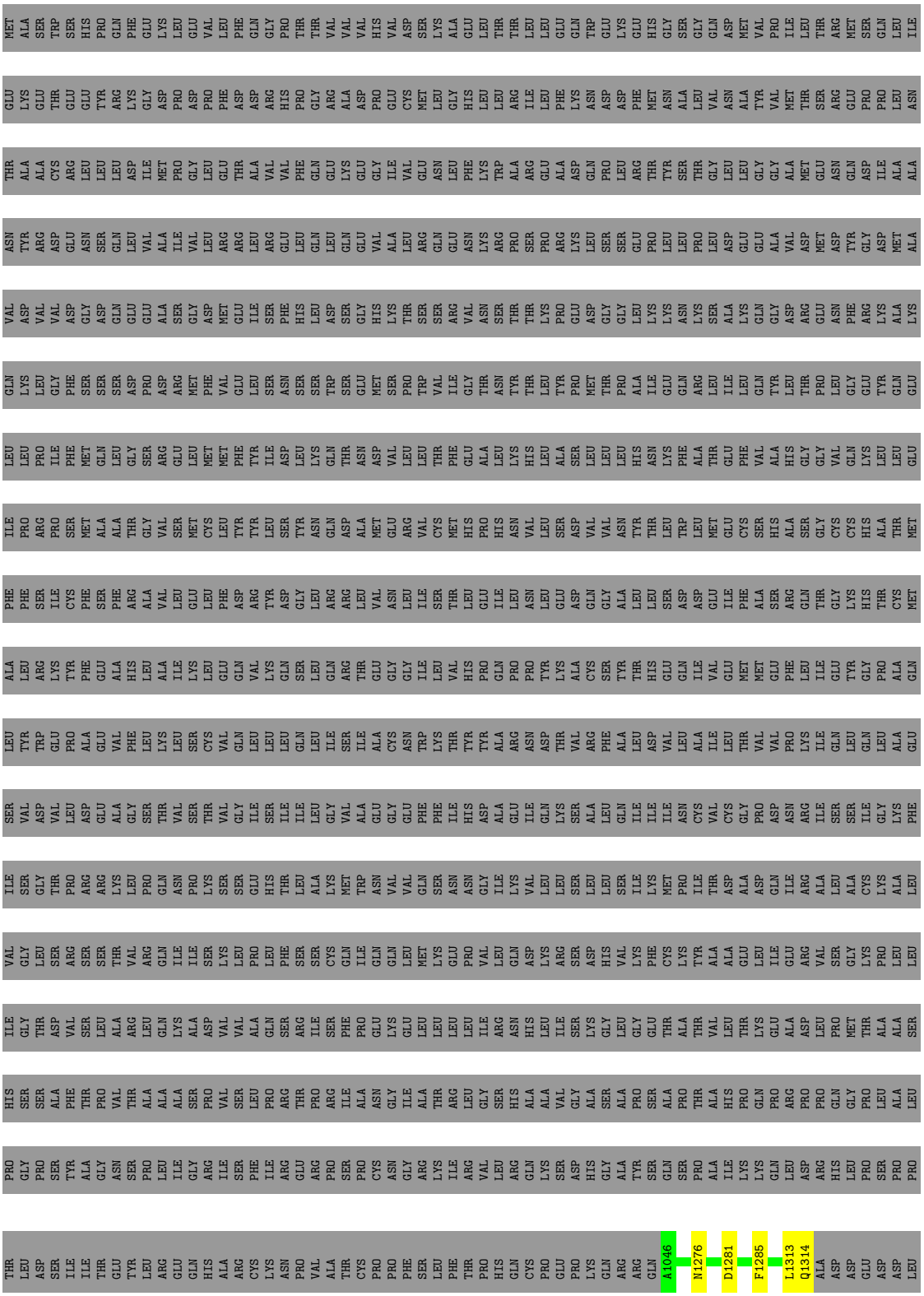
• Molecule 2: DDB1- and CUL4-associated factor 1

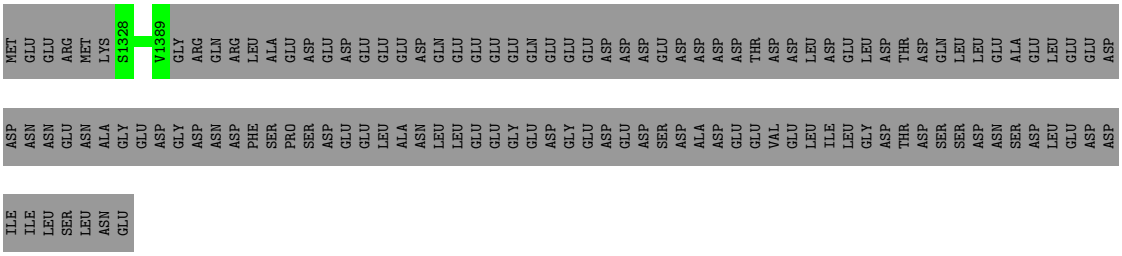
Chain B:


A1046
N1276
D1281
F1285
L1313
Q1314
S1328
V1389

• Molecule 2: DDB1- and CUL4-associated factor 1

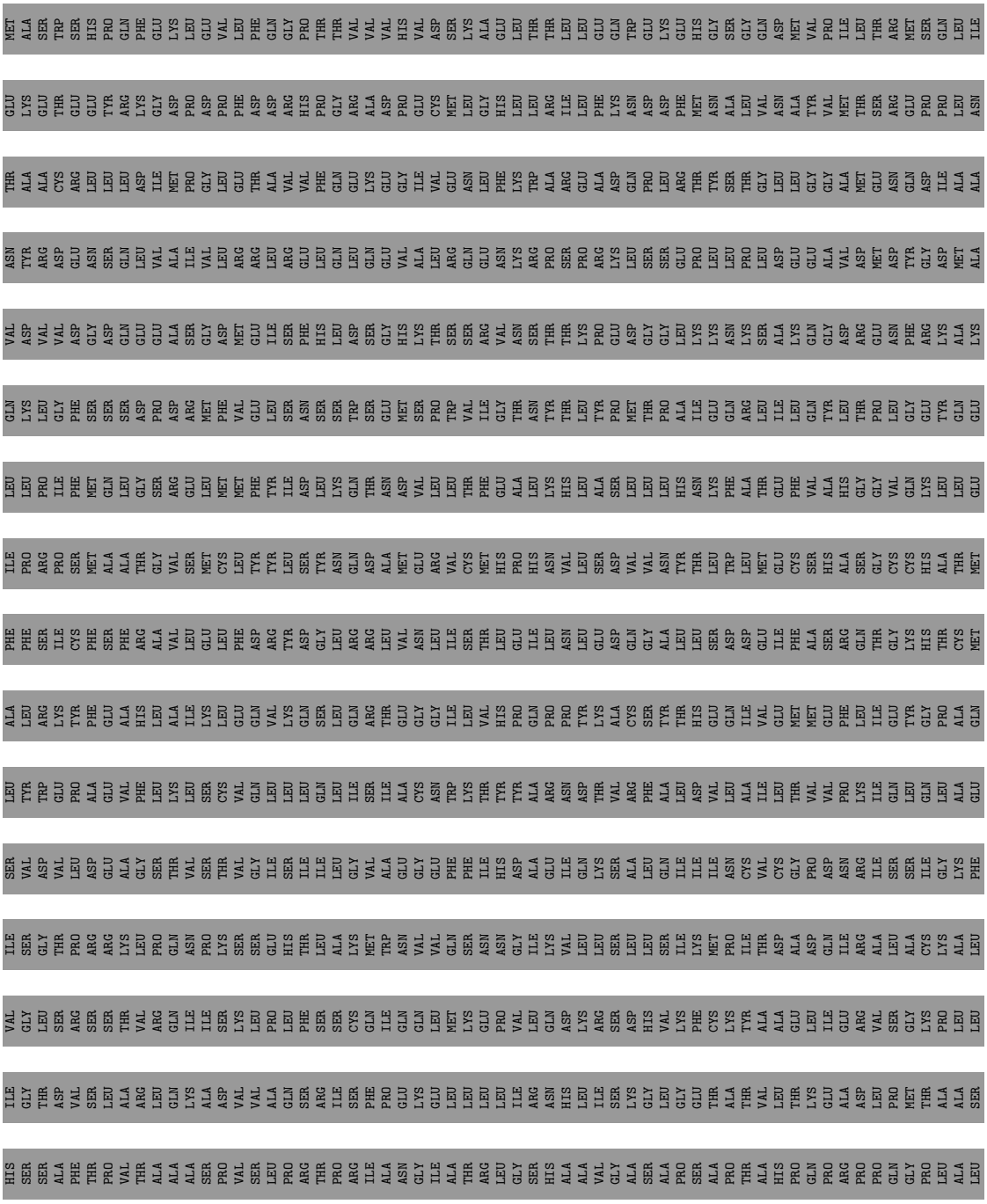
Chain F: 21% 78%





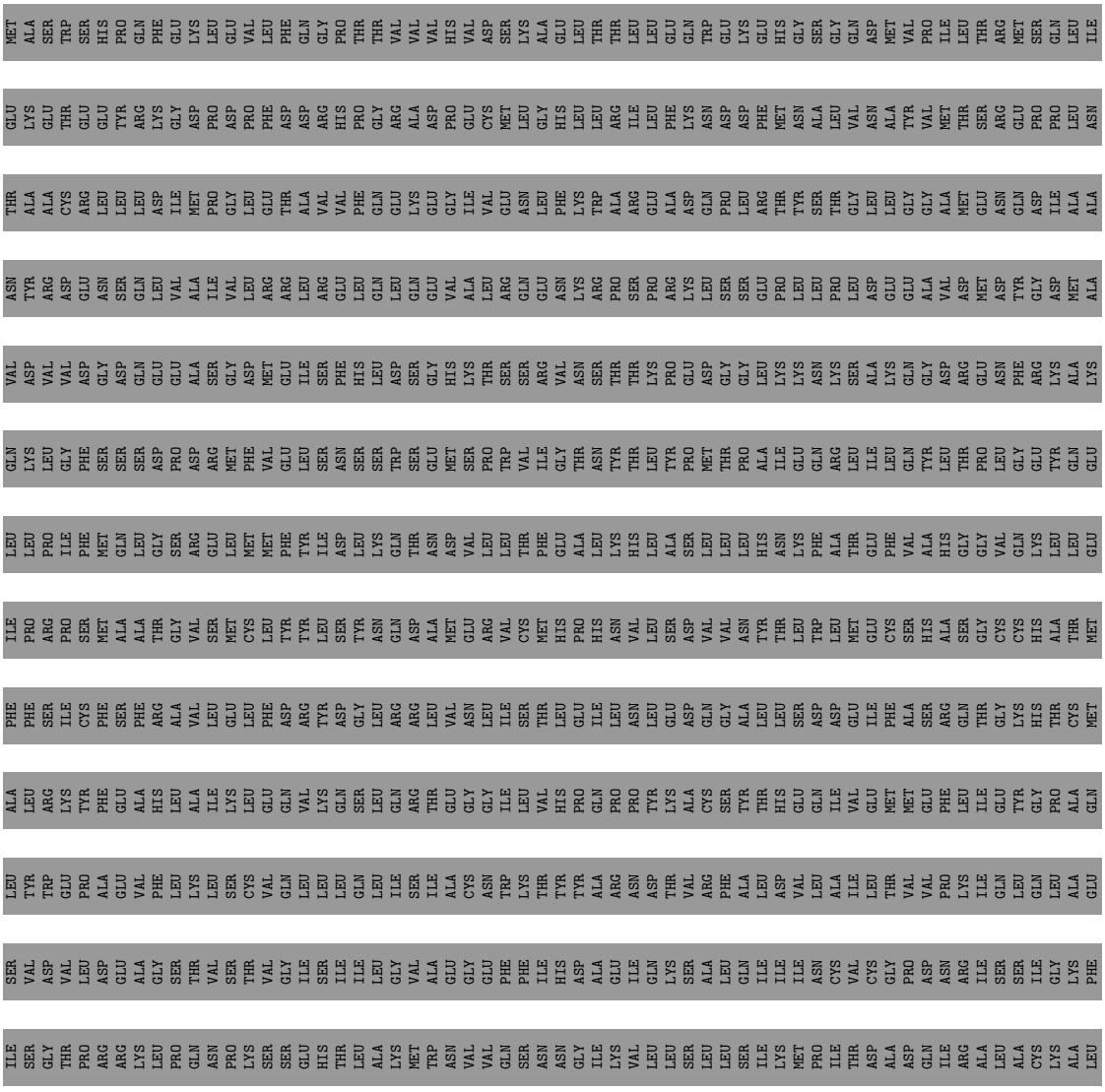
• Molecule 2: DDB1- and CUL4-associated factor 1

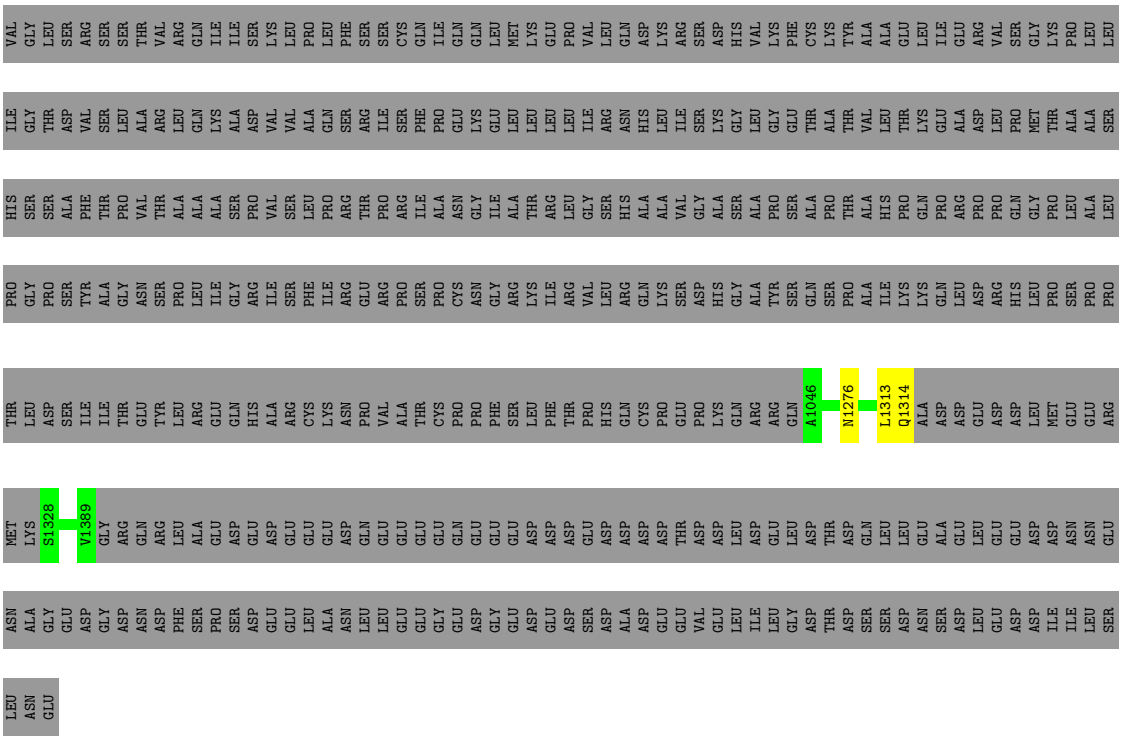
Chain J: 22% 78%



• Molecule 2: DDB1- and CUL4-associated factor 1

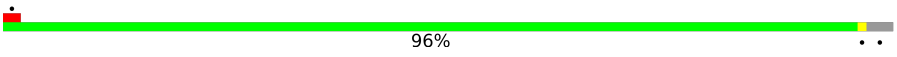
Chain N:

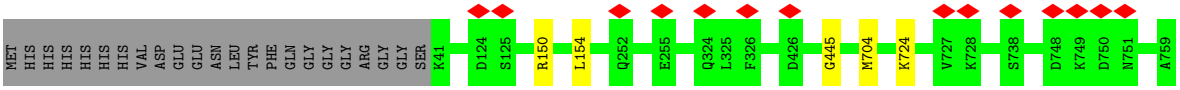




• Molecule 3: Cullin-4A

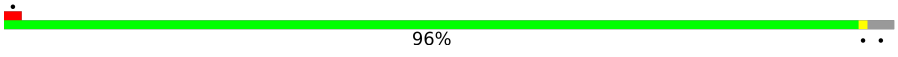
Chain C:

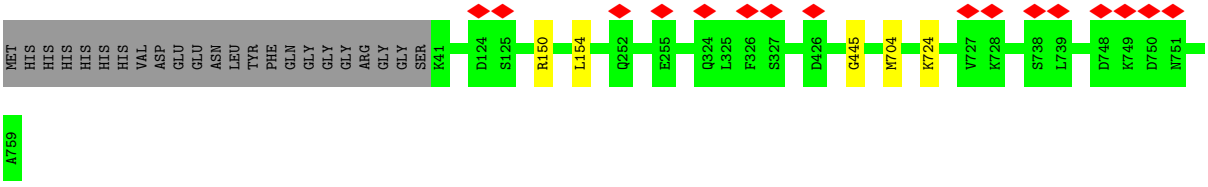




• Molecule 3: Cullin-4A

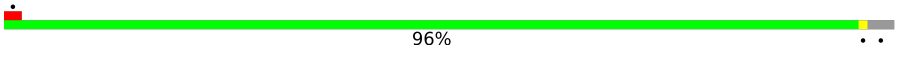
Chain G:

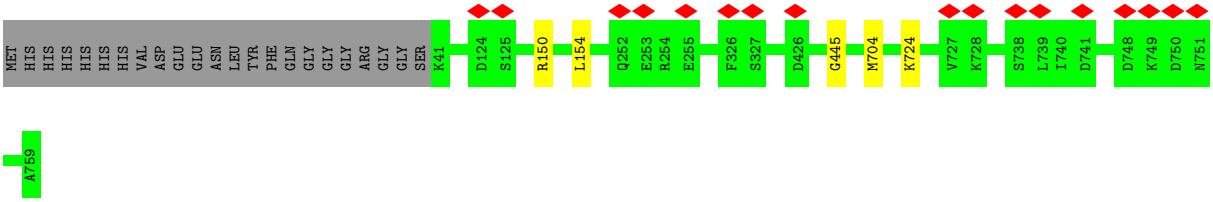




• Molecule 3: Cullin-4A

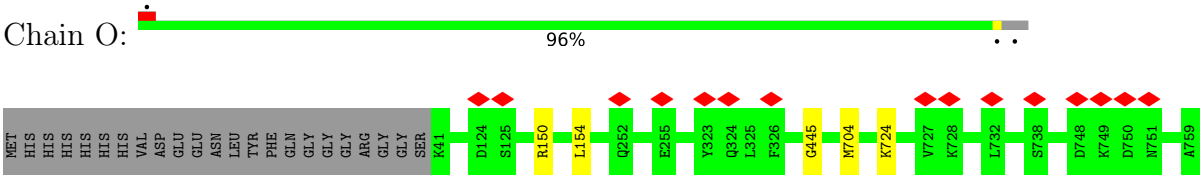
Chain K:





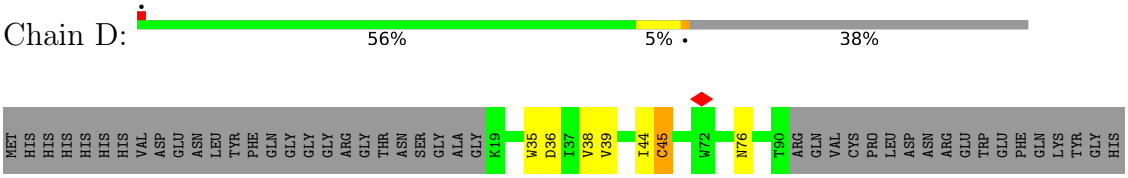
• Molecule 3: Cullin-4A

Chain O:



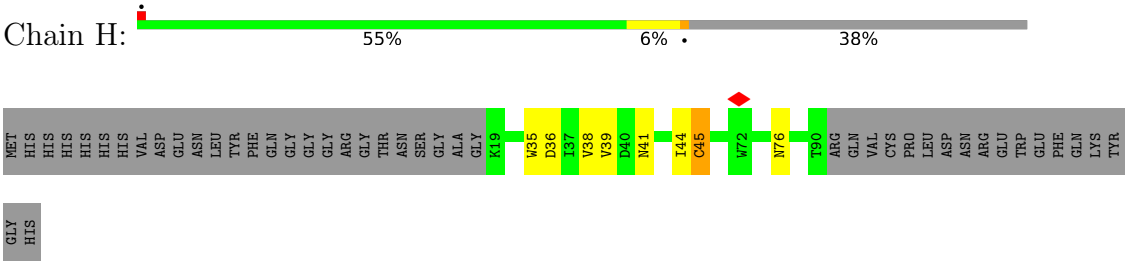
• Molecule 4: E3 ubiquitin-protein ligase RBX1

Chain D:



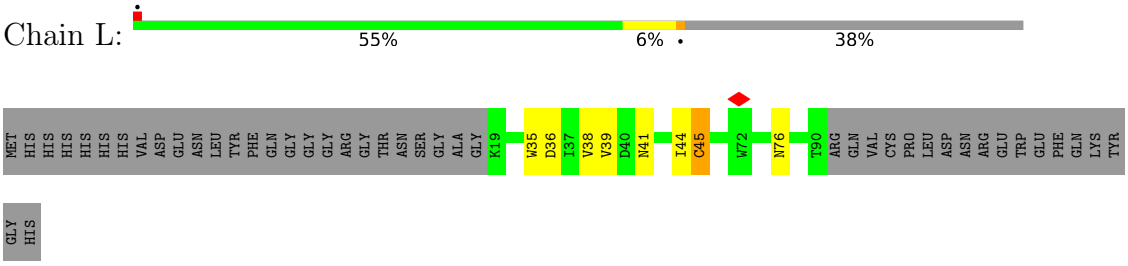
• Molecule 4: E3 ubiquitin-protein ligase RBX1

Chain H:



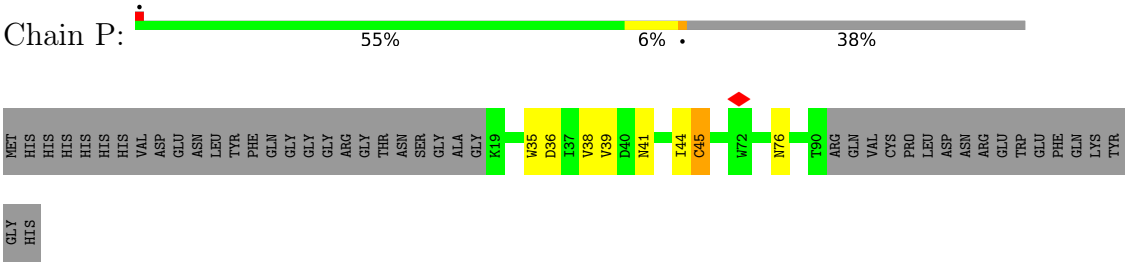
• Molecule 4: E3 ubiquitin-protein ligase RBX1

Chain L:



• Molecule 4: E3 ubiquitin-protein ligase RBX1

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14000	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 ($e^-/Å^2$)	45	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	0.032	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00856	Depositor
Map size (Å)	457.6, 457.6, 457.6	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.76, 1.76, 1.76	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.55	0/5592	0.62	0/7777
1	E	0.34	0/5592	0.53	0/7777
1	I	0.35	0/5592	0.53	0/7777
1	M	0.34	0/5592	0.53	0/7777
2	B	0.32	0/1633	0.51	0/2271
2	F	0.32	0/1633	0.51	0/2271
2	J	0.32	0/1633	0.51	0/2271
2	N	0.32	0/1633	0.51	0/2271
3	C	0.31	0/3563	0.47	0/4968
3	G	0.31	0/3563	0.47	0/4968
3	K	0.31	0/3563	0.47	0/4968
3	O	0.31	0/3563	0.47	0/4968
4	D	0.39	0/358	0.83	1/499 (0.2%)
4	H	0.40	0/358	0.83	1/499 (0.2%)
4	L	0.40	0/358	0.83	1/499 (0.2%)
4	P	0.40	0/358	0.83	1/499 (0.2%)
All	All	0.36	0/44584	0.53	4/62060 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	38	VAL	CB-CA-C	5.10	121.09	111.40
4	D	38	VAL	CB-CA-C	5.09	121.08	111.40
4	L	38	VAL	CB-CA-C	5.09	121.08	111.40
4	H	38	VAL	CB-CA-C	5.09	121.07	111.40

There are no chirality outliers.

There are no planarity outliers.

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	5594	0	2489	1	0
1	E	5594	0	2489	1	0
1	I	5594	0	2489	3	0
1	M	5594	0	2489	3	0
2	B	1635	0	729	2	0
2	F	1635	0	729	2	0
2	J	1635	0	729	1	0
2	N	1635	0	729	1	0
3	C	3564	0	1545	2	0
3	G	3564	0	1545	2	0
3	K	3564	0	1545	2	0
3	O	3564	0	1545	2	0
4	D	359	0	171	5	0
4	H	359	0	171	7	0
4	L	359	0	171	7	0
4	P	359	0	171	7	0
All	All	44608	0	19736	48	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 1.

All (48) 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)
4:L:39:VAL:C	4:L:41:ASN:H	2.01	0.63
4:P:39:VAL:C	4:P:41:ASN:H	2.01	0.62
4:H:39:VAL:C	4:H:41:ASN:H	2.01	0.62
2:J:1313:LEU:O	2:J:1314:GLN:C	2.41	0.59
2:N:1313:LEU:O	2:N:1314:GLN:C	2.41	0.59
4:H:35:TRP:N	4:H:76:ASN:O	2.36	0.58
4:L:35:TRP:N	4:L:76:ASN:O	2.36	0.58
4:P:35:TRP:N	4:P:76:ASN:O	2.36	0.58
2:F:1313:LEU:O	2:F:1314:GLN:C	2.41	0.58
2:B:1313:LEU:O	2:B:1314:GLN:C	2.41	0.58
4:D:35:TRP:N	4:D:76:ASN:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:35:TRP:CB	4:H:76:ASN:O	2.52	0.57
4:L:35:TRP:CB	4:L:76:ASN:O	2.52	0.57
4:P:35:TRP:CB	4:P:76:ASN:O	2.52	0.57
4:H:39:VAL:C	4:H:41:ASN:N	2.58	0.56
4:L:39:VAL:C	4:L:41:ASN:N	2.58	0.55
4:L:44:ILE:O	4:L:45:CYS:CB	2.55	0.55
4:P:44:ILE:O	4:P:45:CYS:CB	2.55	0.55
4:P:39:VAL:C	4:P:41:ASN:N	2.58	0.55
4:D:44:ILE:O	4:D:45:CYS:CB	2.55	0.53
4:H:44:ILE:O	4:H:45:CYS:CB	2.55	0.53
4:D:35:TRP:CB	4:D:76:ASN:O	2.59	0.51
3:C:445:GLY:N	3:C:724:LYS:O	2.46	0.48
3:G:445:GLY:N	3:G:724:LYS:O	2.46	0.48
3:K:445:GLY:N	3:K:724:LYS:O	2.46	0.47
3:O:445:GLY:N	3:O:724:LYS:O	2.46	0.47
1:E:1076:PHE:N	1:E:1083:GLU:O	2.47	0.47
4:D:36:ASP:O	4:D:39:VAL:CB	2.64	0.46
4:H:36:ASP:O	4:H:39:VAL:CB	2.64	0.46
4:P:36:ASP:O	4:P:39:VAL:CB	2.64	0.45
4:L:36:ASP:O	4:L:39:VAL:CB	2.64	0.45
1:M:1076:PHE:N	1:M:1083:GLU:O	2.47	0.45
1:I:1076:PHE:N	1:I:1083:GLU:O	2.47	0.45
4:L:36:ASP:O	4:L:39:VAL:N	2.49	0.45
4:P:36:ASP:O	4:P:39:VAL:N	2.49	0.45
4:D:36:ASP:O	4:D:39:VAL:N	2.49	0.45
4:H:36:ASP:O	4:H:39:VAL:N	2.49	0.44
1:M:393:GLY:N	1:M:709:LYS:O	2.50	0.44
1:I:393:GLY:N	1:I:709:LYS:O	2.50	0.44
1:A:386:SER:HA	1:A:717:LEU:H	1.84	0.42
3:C:150:ARG:O	3:C:154:LEU:N	2.53	0.42
3:G:150:ARG:O	3:G:154:LEU:N	2.53	0.42
3:K:150:ARG:O	3:K:154:LEU:N	2.53	0.41
3:O:150:ARG:O	3:O:154:LEU:N	2.53	0.41
2:F:1281:ASP:O	2:F:1285:PHE:N	2.50	0.41
2:B:1281:ASP:O	2:B:1285:PHE:N	2.51	0.41
1:I:394:ILE:HA	1:I:709:LYS:HA	2.03	0.40
1:M:394:ILE:HA	1:M:709:LYS:HA	2.03	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	1131/1159 (98%)	1088 (96%)	39 (3%)	4 (0%)	34	72
1	E	1131/1159 (98%)	1083 (96%)	44 (4%)	4 (0%)	34	72
1	I	1131/1159 (98%)	1085 (96%)	42 (4%)	4 (0%)	34	72
1	M	1131/1159 (98%)	1085 (96%)	42 (4%)	4 (0%)	34	72
2	B	327/1525 (21%)	311 (95%)	15 (5%)	1 (0%)	41	77
2	F	327/1525 (21%)	311 (95%)	15 (5%)	1 (0%)	41	77
2	J	327/1525 (21%)	311 (95%)	15 (5%)	1 (0%)	41	77
2	N	327/1525 (21%)	311 (95%)	15 (5%)	1 (0%)	41	77
3	C	717/742 (97%)	702 (98%)	14 (2%)	1 (0%)	51	86
3	G	717/742 (97%)	702 (98%)	14 (2%)	1 (0%)	51	86
3	K	717/742 (97%)	701 (98%)	15 (2%)	1 (0%)	51	86
3	O	717/742 (97%)	702 (98%)	14 (2%)	1 (0%)	51	86
4	D	70/116 (60%)	61 (87%)	8 (11%)	1 (1%)	11	46
4	H	70/116 (60%)	61 (87%)	8 (11%)	1 (1%)	11	46
4	L	70/116 (60%)	61 (87%)	8 (11%)	1 (1%)	11	46
4	P	70/116 (60%)	61 (87%)	8 (11%)	1 (1%)	11	46
All	All	8980/14168 (63%)	8636 (96%)	316 (4%)	28 (0%)	44	77

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	45	CYS
4	H	45	CYS
4	L	45	CYS
4	P	45	CYS
1	A	36	ASN
1	A	636	THR

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Mol	Chain	Res	Type
2	B	1276	ASN
1	E	36	ASN
1	E	636	THR
2	F	1276	ASN
1	I	36	ASN
1	I	636	THR
2	J	1276	ASN
1	M	36	ASN
1	M	636	THR
2	N	1276	ASN
3	C	704	MET
3	G	704	MET
3	K	704	MET
3	O	704	MET
1	A	564	ILE
1	E	564	ILE
1	I	564	ILE
1	M	564	ILE
1	A	320	GLY
1	E	320	GLY
1	I	320	GLY
1	M	320	GLY

5.3.2 Protein sidechains (i)

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

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

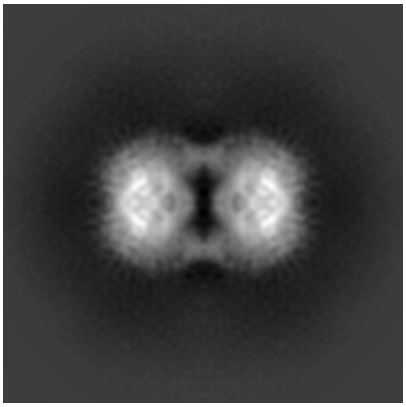
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12964. 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.

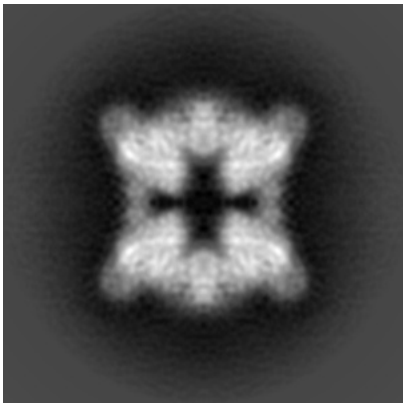
6.1 Orthogonal projections

6.1.1 Primary map



X

Y

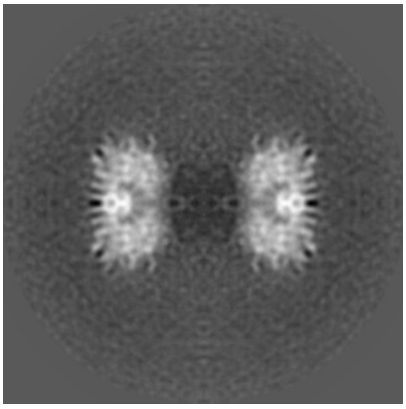


Z

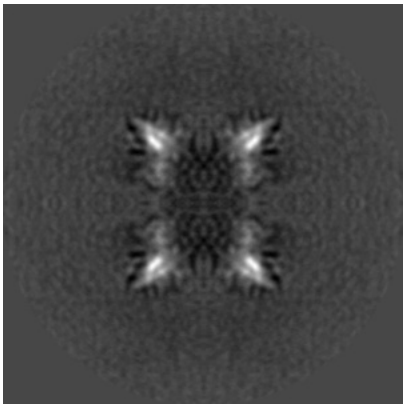
The images above show the map projected in three orthogonal directions.

6.2 Central slices

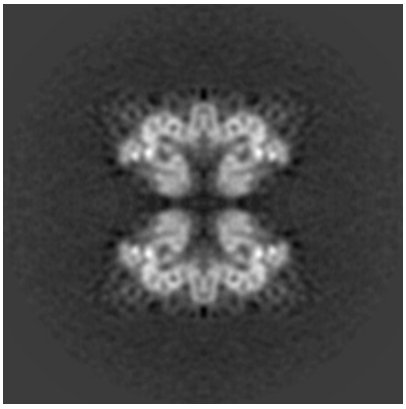
6.2.1 Primary map



X Index: 130



Y Index: 130

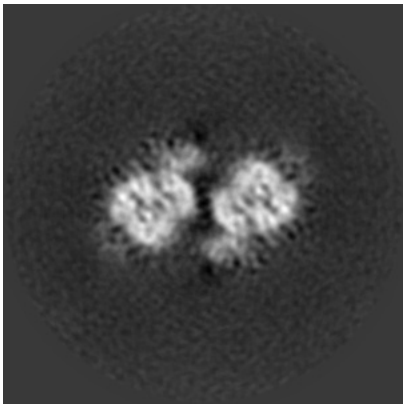


Z Index: 130

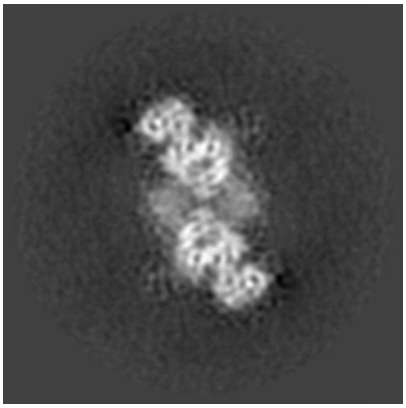
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

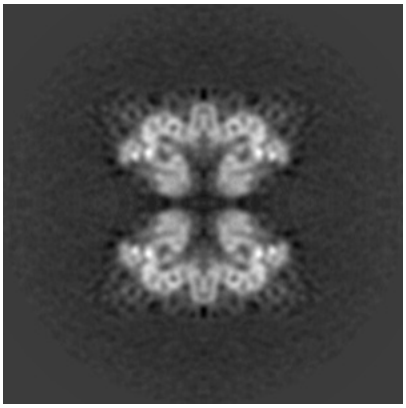
6.3.1 Primary map



X Index: 106



Y Index: 173

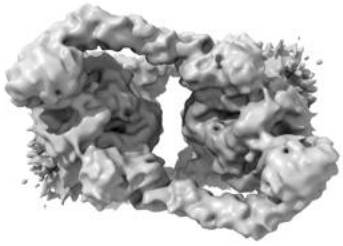


Z Index: 130

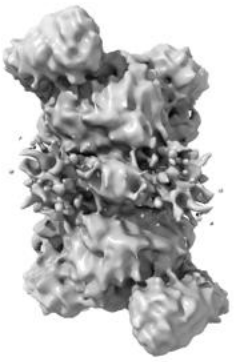
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

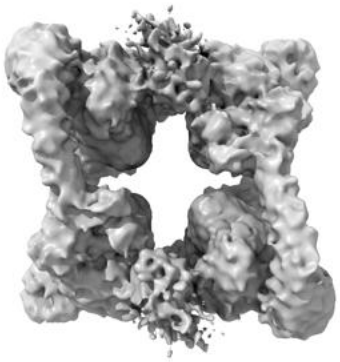
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00856. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

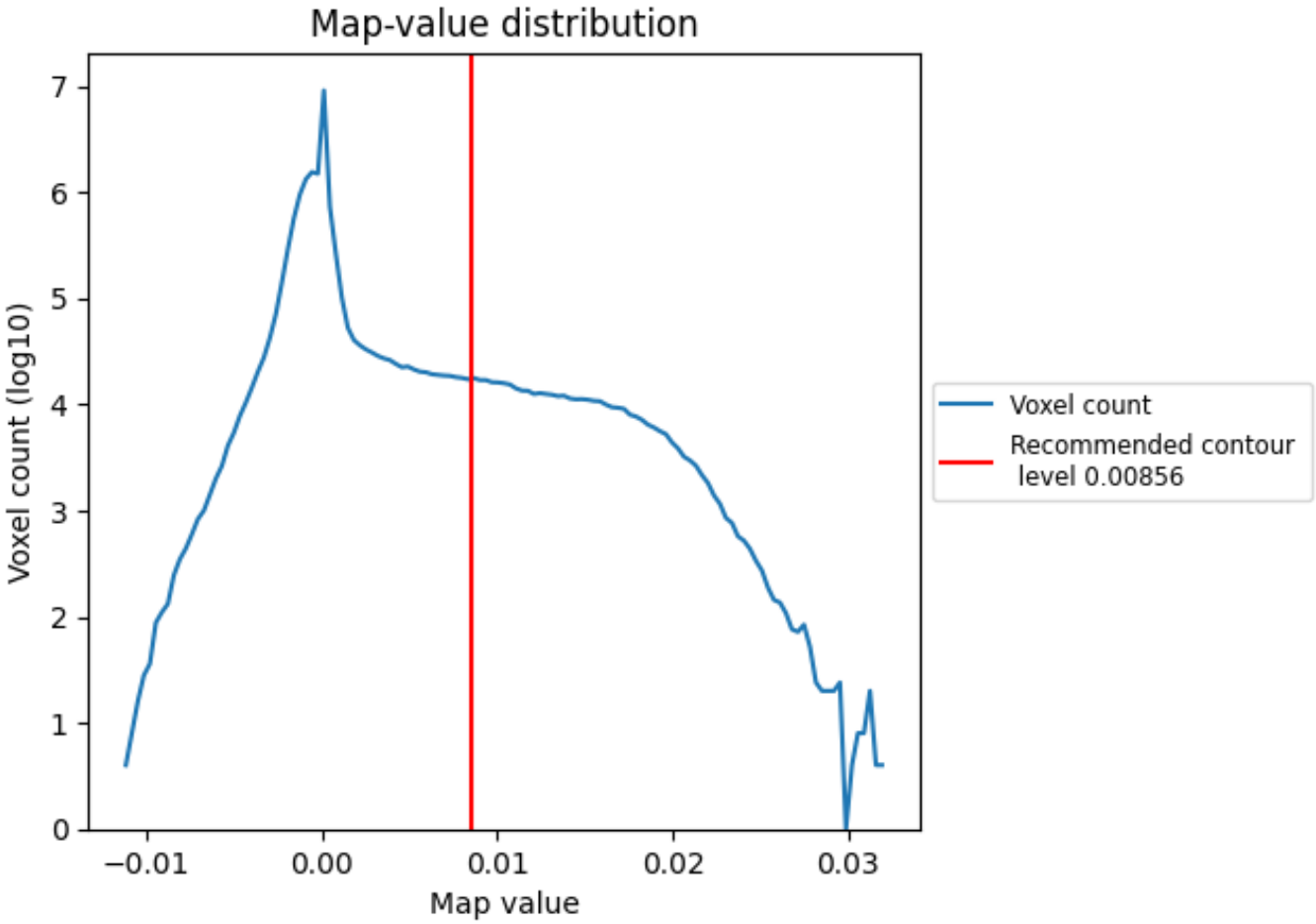
6.5 Mask visualisation (i)

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

7 Map analysis

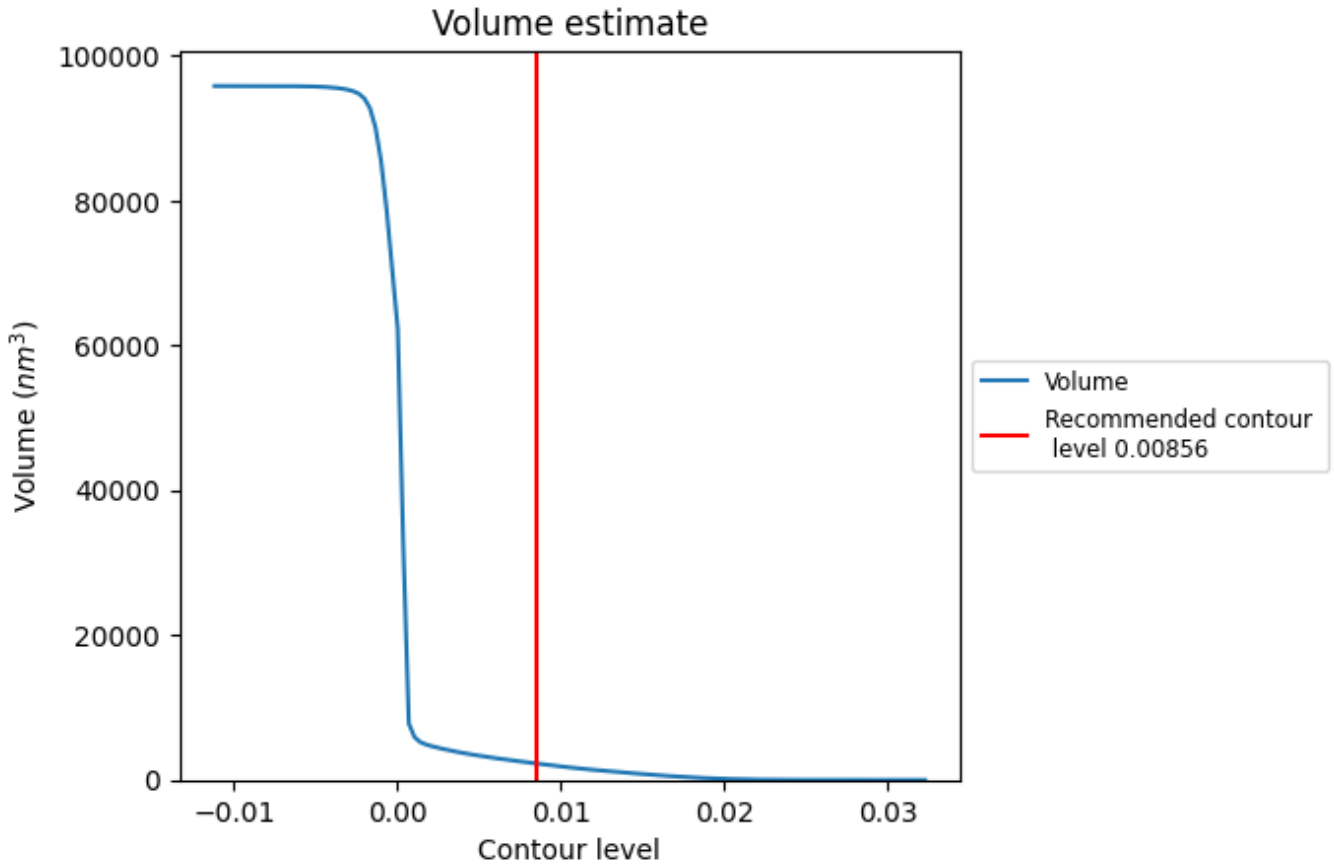
This section contains the results of statistical analysis of the map.

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.

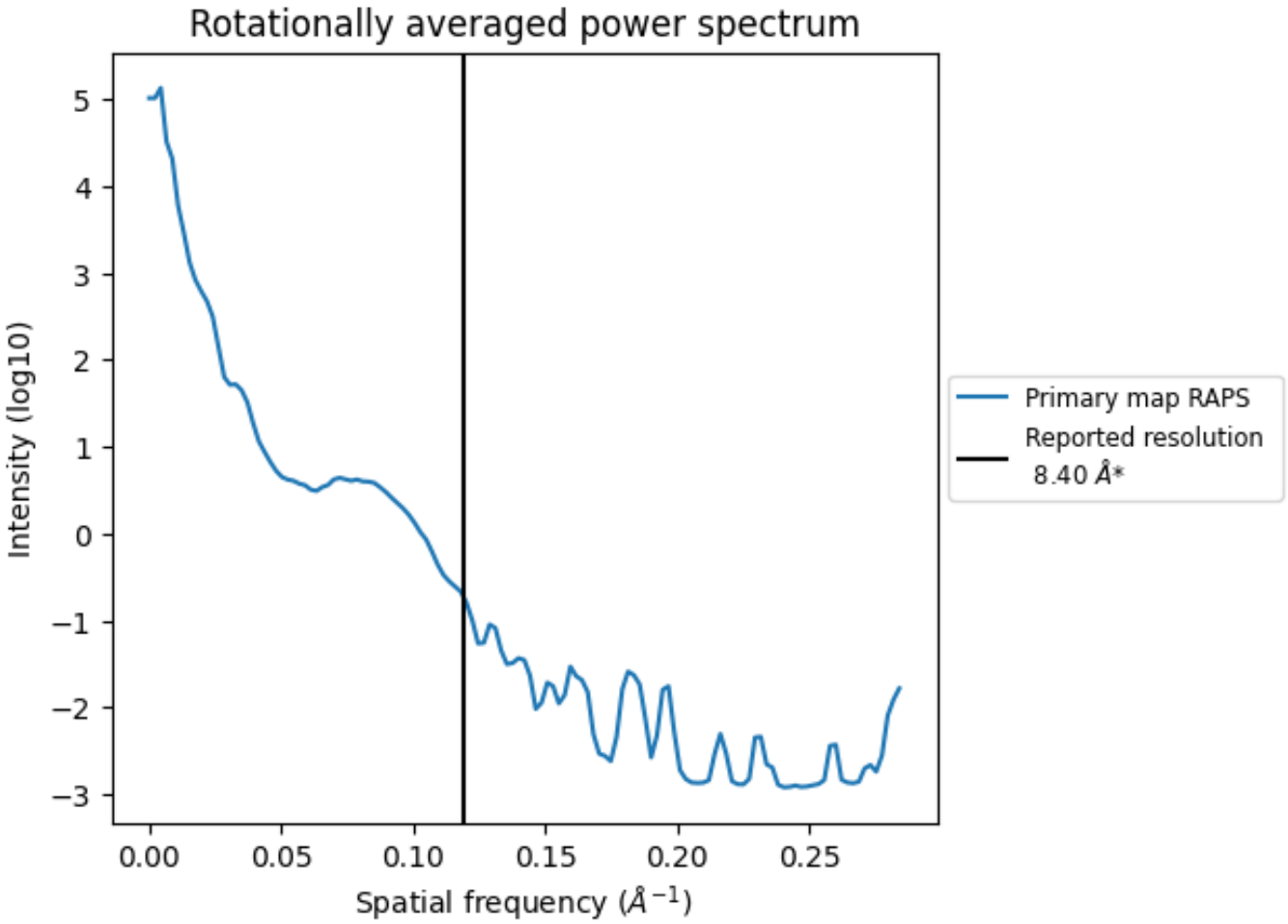
7.2 Volume estimate



The volume at the recommended contour level is 2255 nm^3; this corresponds to an approximate mass of 2037 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 0.119 Å^{-1}

8 Fourier-Shell correlation

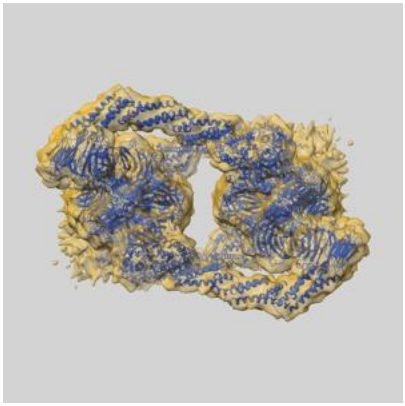
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

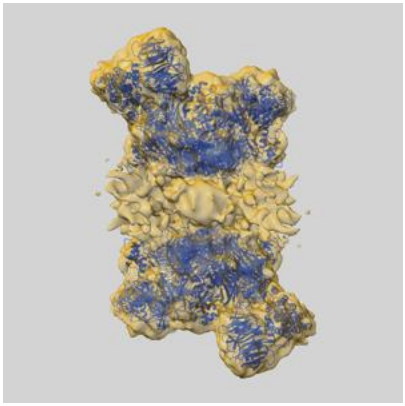
This section contains information regarding the fit between EMDB map EMD-12964 and PDB model 7OKQ. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlays

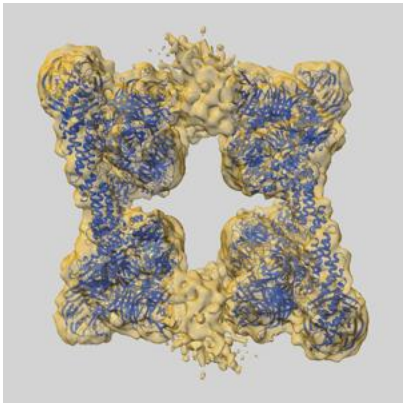
9.1.1 Map-model overlay



X

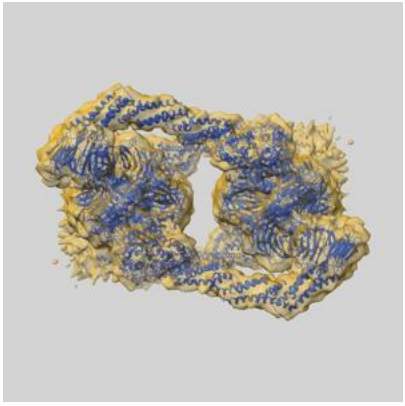


Y

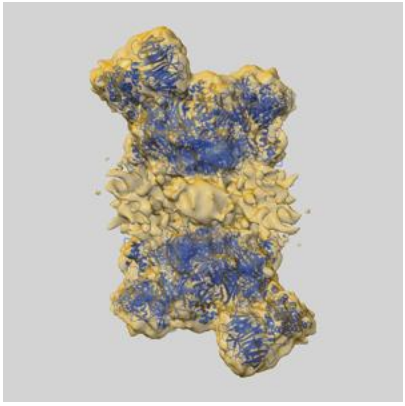


Z

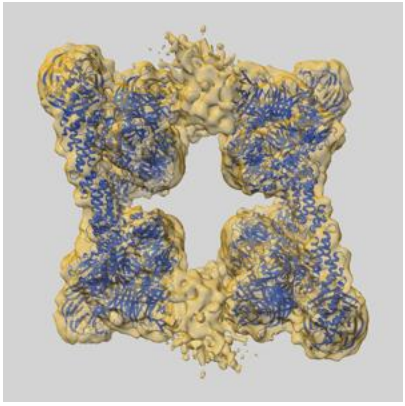
9.1.2 Map-model assembly overlay



X



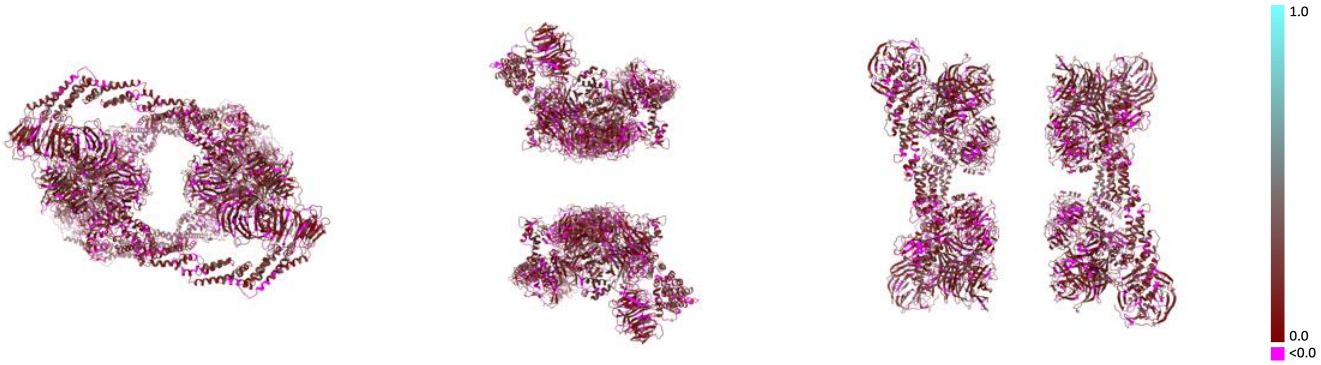
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00856 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

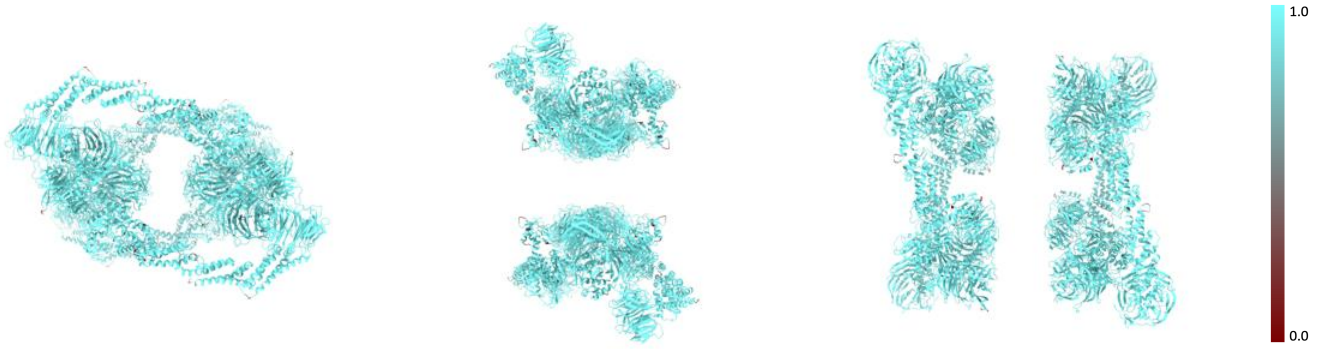
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

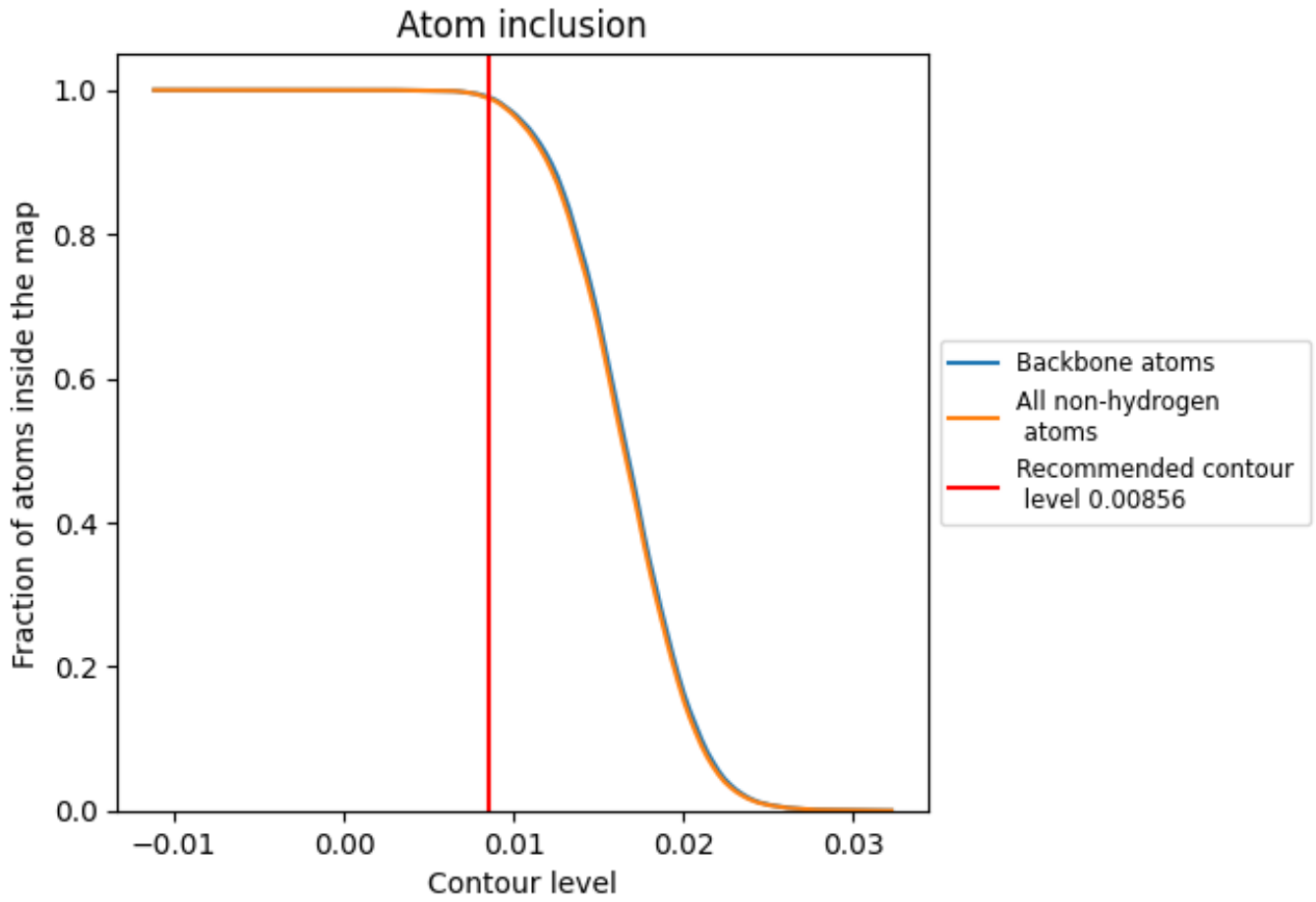
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00856).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.00856) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9883	0.1240
A	0.9941	0.1290
B	0.9994	0.1030
C	0.9750	0.1340
D	0.9833	0.0850
E	0.9952	0.1300
F	1.0000	0.1100
G	0.9736	0.1260
H	0.9833	0.0790
I	0.9932	0.1310
J	1.0000	0.1120
K	0.9728	0.1160
L	0.9861	0.0780
M	0.9941	0.1250
N	1.0000	0.0980
O	0.9750	0.1360
P	0.9833	0.0880