



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:47 PM UTC

PDB ID : 7OKQ / pdb_00007okq
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 : 5JK7, 2HYE

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:

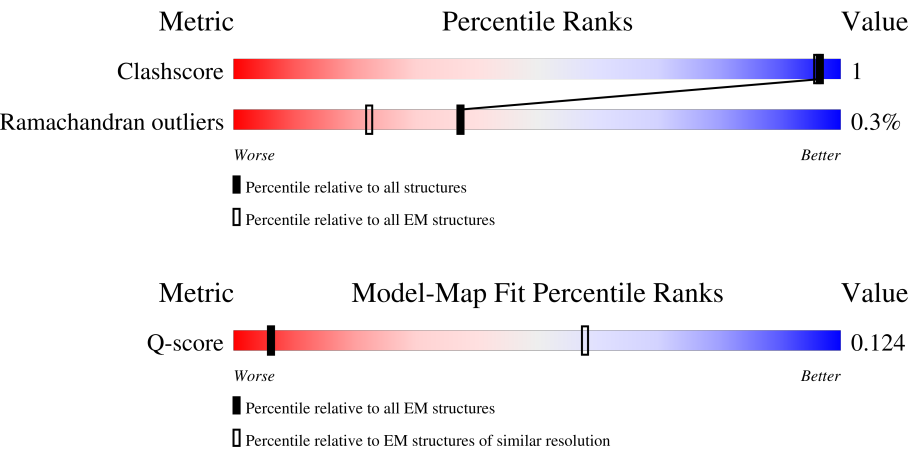
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	298 (7.90 - 8.90)

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	1159	95%
1	E	1159	95%
1	I	1159	94%
1	M	1159	94%
2	B	1525	21% 78%

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Mol	Chain	Length	Quality of chain
2	F	1525	21%78%
2	J	1525	21%78%
2	N	1525	21%78%
3	C	742	94%
3	G	742	94%
3	K	742	95%
3	O	742	95%
4	D	116	54%6%38%
4	H	116	54%6%38%
4	L	116	54%6%38%
4	P	116	54%6%38%

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	C	N	O	0	0
			5594	3324	1135	1135		
1	E	1135	Total	C	N	O	0	0
			5594	3324	1135	1135		
1	I	1135	Total	C	N	O	0	0
			5594	3324	1135	1135		
1	M	1135	Total	C	N	O	0	0
			5594	3324	1135	1135		

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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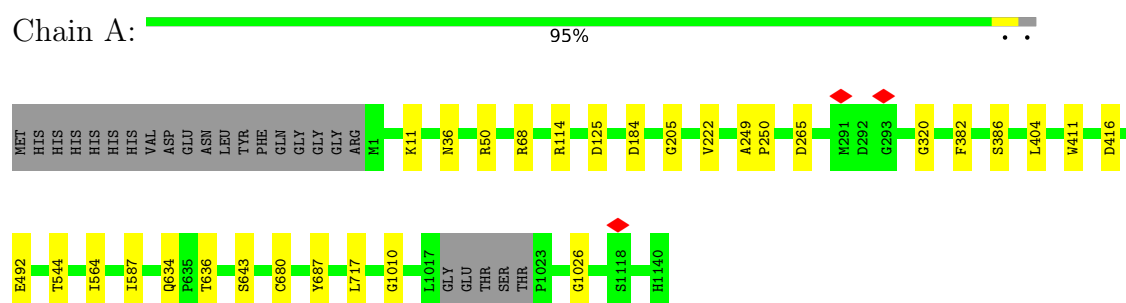
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Chain	Residue	Modelled	Actual	Comment	Reference
L	8	GLY	-	insertion	UNP P62877
L	9	GLY	THR	conflict	UNP P62877
L	10	GLY	PRO	conflict	UNP P62877
L	11	ARG	SER	conflict	UNP P62877
P	-6	HIS	-	insertion	UNP P62877
P	-5	HIS	ALA	conflict	UNP P62877
P	-4	HIS	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

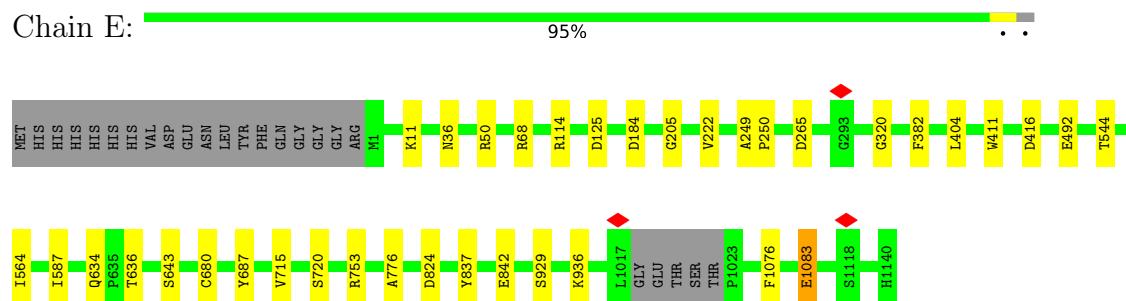
3 Residue-property plots

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.

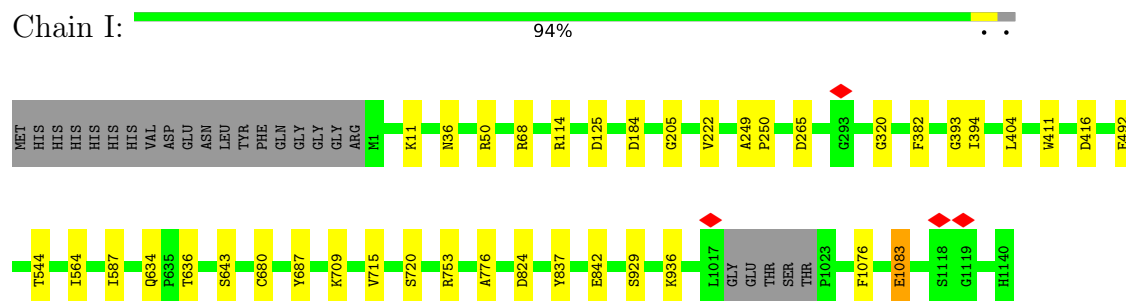
- Molecule 1: DNA damage-binding protein 1



- Molecule 1: DNA damage-binding protein 1

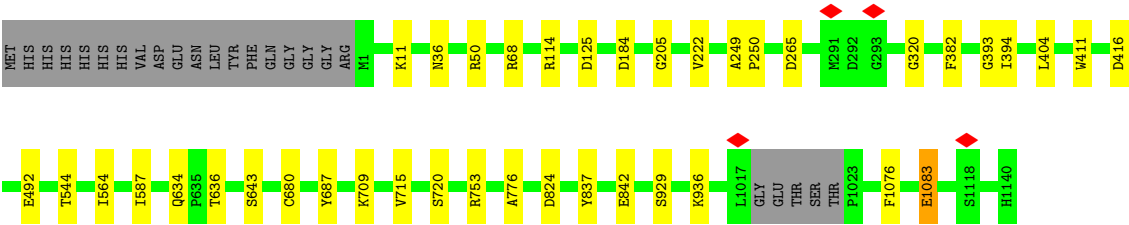


- Molecule 1: DNA damage-binding protein 1



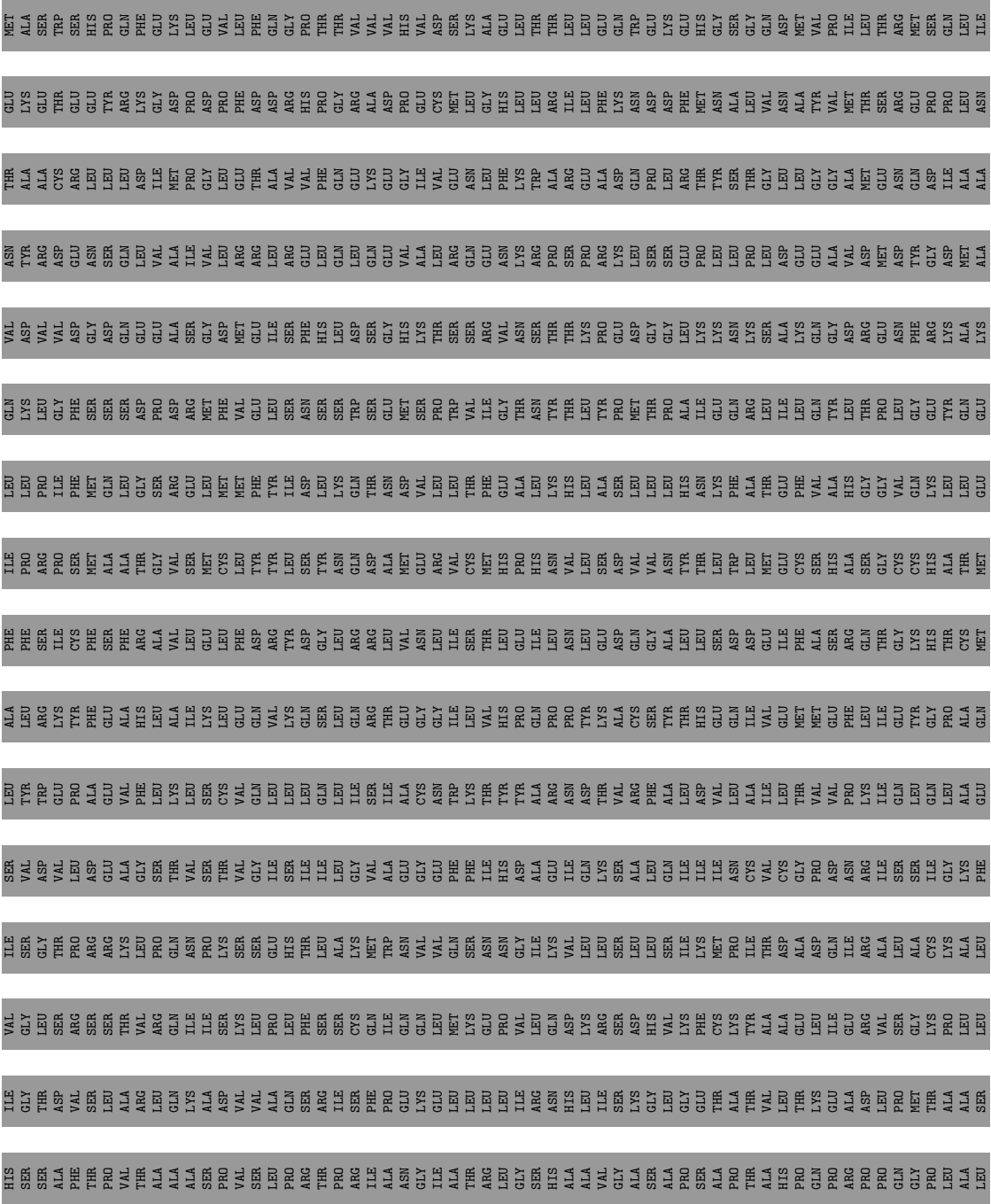
- Molecule 1: DNA damage-binding protein 1





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

Chain B: 21% 78%

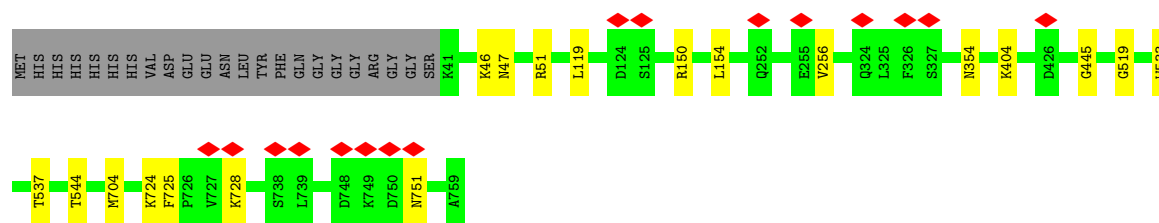




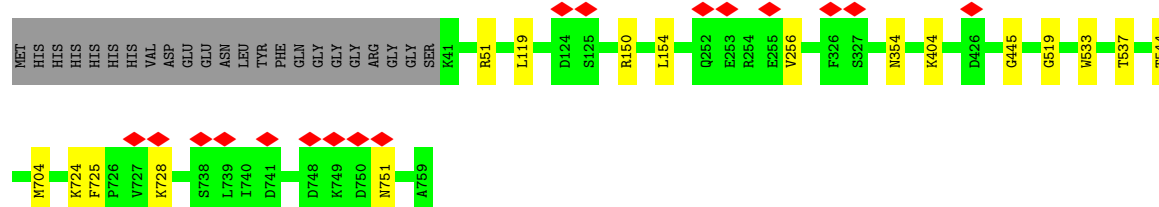




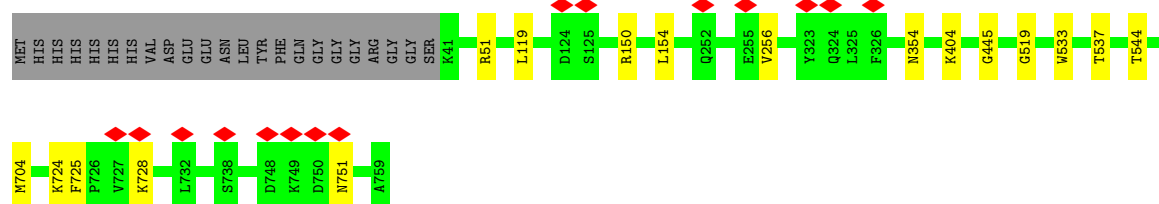
- Molecule 2: DDB1- and CUL4-associated factor 1



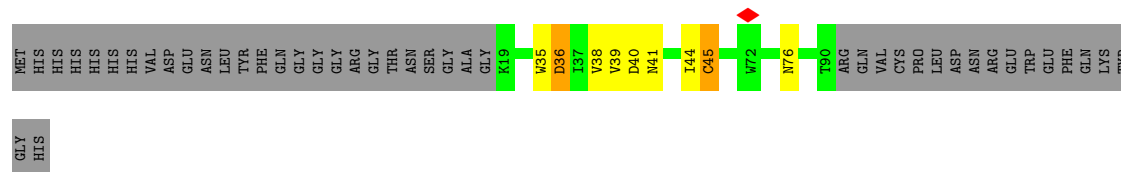
- Molecule 3: Cullin-4A



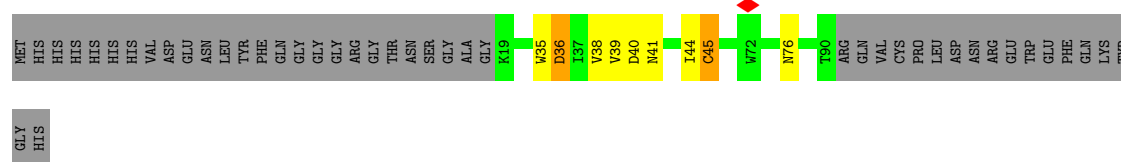
- Molecule 3: Cullin-4A



- Molecule 4: E3 ubiquitin-protein ligase RBX1



- Molecule 4: E3 ubiquitin-protein ligase RBX1

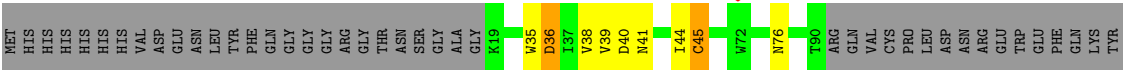


- Molecule 4: E3 ubiquitin-protein ligase RBX1



GLY
HIS

• Molecule 4: E3 ubiquitin-protein ligase RBX1



GLY
HIS

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.87	0/5592	1.26	44/7777 (0.6%)
1	E	0.52	0/5592	1.14	61/7777 (0.8%)
1	I	0.52	0/5592	1.15	61/7777 (0.8%)
1	M	0.51	0/5592	1.14	61/7777 (0.8%)
2	B	0.48	0/1633	1.09	16/2271 (0.7%)
2	F	0.48	0/1633	1.10	16/2271 (0.7%)
2	J	0.48	0/1633	1.10	16/2271 (0.7%)
2	N	0.48	0/1633	1.09	16/2271 (0.7%)
3	C	0.49	0/3563	0.98	24/4968 (0.5%)
3	G	0.49	0/3563	0.98	24/4968 (0.5%)
3	K	0.49	0/3563	0.98	24/4968 (0.5%)
3	O	0.49	0/3563	0.98	24/4968 (0.5%)
4	D	0.62	0/358	1.37	5/499 (1.0%)
4	H	0.64	0/358	1.36	5/499 (1.0%)
4	L	0.64	0/358	1.36	4/499 (0.8%)
4	P	0.64	0/358	1.36	5/499 (1.0%)
All	All	0.56	0/44584	1.11	406/62060 (0.7%)

There are no bond length outliers.

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	36	ASP	N-CA-C	-11.06	98.92	110.97
4	H	36	ASP	N-CA-C	-11.05	98.92	110.97
4	D	36	ASP	N-CA-C	-11.05	98.93	110.97
4	P	36	ASP	N-CA-C	-11.02	98.96	110.97
3	O	354	ASN	CA-C-N	8.30	128.03	119.56
3	O	354	ASN	C-N-CA	8.30	128.03	119.56
3	G	354	ASN	CA-C-N	8.27	128.00	119.56
3	G	354	ASN	C-N-CA	8.27	128.00	119.56
3	K	354	ASN	CA-C-N	8.26	127.98	119.56
3	K	354	ASN	C-N-CA	8.26	127.98	119.56
3	C	354	ASN	CA-C-N	8.25	127.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	354	ASN	C-N-CA	8.25	127.97	119.56
3	O	256	VAL	CA-C-N	7.64	128.09	120.52
3	O	256	VAL	C-N-CA	7.64	128.09	120.52
3	G	256	VAL	CA-C-N	7.64	128.08	120.52
3	G	256	VAL	C-N-CA	7.64	128.08	120.52
3	C	256	VAL	CA-C-N	7.63	128.07	120.52
3	C	256	VAL	C-N-CA	7.63	128.07	120.52
3	K	256	VAL	CA-C-N	7.60	128.05	120.52
3	K	256	VAL	C-N-CA	7.60	128.05	120.52
1	I	114	ARG	CA-C-N	7.59	127.55	120.03
1	I	114	ARG	C-N-CA	7.59	127.55	120.03
1	M	114	ARG	CA-C-N	7.58	127.53	120.03
1	M	114	ARG	C-N-CA	7.58	127.53	120.03
2	J	1291	VAL	CA-C-N	7.56	127.27	119.56
2	J	1291	VAL	C-N-CA	7.56	127.27	119.56
1	A	114	ARG	CA-C-N	7.56	127.51	120.03
1	A	114	ARG	C-N-CA	7.56	127.51	120.03
1	E	114	ARG	CA-C-N	7.55	127.50	120.03
1	E	114	ARG	C-N-CA	7.55	127.50	120.03
2	B	1291	VAL	CA-C-N	7.54	127.25	119.56
2	B	1291	VAL	C-N-CA	7.54	127.25	119.56
2	N	1291	VAL	CA-C-N	7.54	127.25	119.56
2	N	1291	VAL	C-N-CA	7.54	127.25	119.56
1	E	687	TYR	CA-C-N	7.52	127.16	119.56
1	E	687	TYR	C-N-CA	7.52	127.16	119.56
2	F	1291	VAL	CA-C-N	7.52	127.23	119.56
2	F	1291	VAL	C-N-CA	7.52	127.23	119.56
1	A	687	TYR	CA-C-N	7.52	127.15	119.56
1	A	687	TYR	C-N-CA	7.52	127.15	119.56
1	M	687	TYR	CA-C-N	7.49	127.13	119.56
1	M	687	TYR	C-N-CA	7.49	127.13	119.56
1	I	687	TYR	CA-C-N	7.48	127.12	119.56
1	I	687	TYR	C-N-CA	7.48	127.12	119.56
1	A	265	ASP	CA-C-N	7.45	127.12	119.82
1	A	265	ASP	C-N-CA	7.45	127.12	119.82
1	E	265	ASP	CA-C-N	7.44	127.11	119.82
1	E	265	ASP	C-N-CA	7.44	127.11	119.82
1	I	404	LEU	CA-C-N	7.42	127.38	120.03
1	I	404	LEU	C-N-CA	7.42	127.38	120.03
1	M	404	LEU	CA-C-N	7.42	127.37	120.03
1	M	404	LEU	C-N-CA	7.42	127.37	120.03
1	A	404	LEU	CA-C-N	7.42	127.37	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	LEU	C-N-CA	7.42	127.37	120.03
1	M	265	ASP	CA-C-N	7.40	127.07	119.82
1	M	265	ASP	C-N-CA	7.40	127.07	119.82
1	I	265	ASP	CA-C-N	7.40	127.07	119.82
1	I	265	ASP	C-N-CA	7.40	127.07	119.82
1	E	776	ALA	CA-C-N	7.36	127.31	120.03
1	E	776	ALA	C-N-CA	7.36	127.31	120.03
3	K	519	GLY	CA-C-N	7.35	127.51	119.87
3	K	519	GLY	C-N-CA	7.35	127.51	119.87
1	E	404	LEU	CA-C-N	7.34	127.30	120.03
1	E	404	LEU	C-N-CA	7.34	127.30	120.03
3	O	519	GLY	CA-C-N	7.33	127.50	119.87
3	O	519	GLY	C-N-CA	7.33	127.50	119.87
1	M	776	ALA	CA-C-N	7.32	127.28	120.03
1	M	776	ALA	C-N-CA	7.32	127.28	120.03
1	I	776	ALA	CA-C-N	7.31	127.27	120.03
1	I	776	ALA	C-N-CA	7.31	127.27	120.03
3	G	519	GLY	CA-C-N	7.30	127.47	119.87
3	G	519	GLY	C-N-CA	7.30	127.47	119.87
3	C	519	GLY	CA-C-N	7.29	127.45	119.87
3	C	519	GLY	C-N-CA	7.29	127.45	119.87
2	J	1216	ASN	CA-C-N	7.28	126.98	119.56
2	J	1216	ASN	C-N-CA	7.28	126.98	119.56
2	F	1216	ASN	CA-C-N	7.21	126.92	119.56
2	F	1216	ASN	C-N-CA	7.21	126.92	119.56
2	N	1216	ASN	CA-C-N	7.18	126.88	119.56
2	N	1216	ASN	C-N-CA	7.18	126.88	119.56
2	B	1216	ASN	CA-C-N	7.17	126.88	119.56
2	B	1216	ASN	C-N-CA	7.17	126.88	119.56
1	I	936	LYS	CA-C-N	7.08	126.78	119.56
1	I	936	LYS	C-N-CA	7.08	126.78	119.56
1	M	936	LYS	CA-C-N	7.08	126.78	119.56
1	M	936	LYS	C-N-CA	7.08	126.78	119.56
1	E	936	LYS	CA-C-N	7.04	126.74	119.56
1	E	936	LYS	C-N-CA	7.04	126.74	119.56
2	F	1267	HIS	CA-C-N	6.97	126.67	119.56
2	F	1267	HIS	C-N-CA	6.97	126.67	119.56
2	N	1267	HIS	CA-C-N	6.97	126.67	119.56
2	N	1267	HIS	C-N-CA	6.97	126.67	119.56
2	B	1267	HIS	CA-C-N	6.93	126.63	119.56
2	B	1267	HIS	C-N-CA	6.93	126.63	119.56
2	J	1267	HIS	CA-C-N	6.92	126.62	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1267	HIS	C-N-CA	6.92	126.62	119.56
3	O	725	PHE	CA-C-N	6.92	126.94	119.89
3	O	725	PHE	C-N-CA	6.92	126.94	119.89
3	G	725	PHE	CA-C-N	6.89	126.92	119.89
3	G	725	PHE	C-N-CA	6.89	126.92	119.89
3	K	725	PHE	CA-C-N	6.89	126.91	119.89
3	K	725	PHE	C-N-CA	6.89	126.91	119.89
1	A	492	GLU	CA-C-N	6.85	126.81	119.28
1	A	492	GLU	C-N-CA	6.85	126.81	119.28
1	I	492	GLU	CA-C-N	6.84	126.81	119.28
1	I	492	GLU	C-N-CA	6.84	126.81	119.28
3	C	725	PHE	CA-C-N	6.81	126.84	119.89
3	C	725	PHE	C-N-CA	6.81	126.84	119.89
1	M	492	GLU	CA-C-N	6.81	126.77	119.28
1	M	492	GLU	C-N-CA	6.81	126.77	119.28
1	E	492	GLU	CA-C-N	6.80	126.76	119.28
1	E	492	GLU	C-N-CA	6.80	126.76	119.28
1	E	205	GLY	CA-C-N	6.66	126.91	119.32
1	E	205	GLY	C-N-CA	6.66	126.91	119.32
1	M	205	GLY	CA-C-N	6.63	126.88	119.32
1	M	205	GLY	C-N-CA	6.63	126.88	119.32
1	A	205	GLY	CA-C-N	6.62	126.87	119.32
1	A	205	GLY	C-N-CA	6.62	126.87	119.32
1	I	205	GLY	CA-C-N	6.60	126.84	119.32
1	I	205	GLY	C-N-CA	6.60	126.84	119.32
2	J	1231	ASN	CA-C-N	6.59	126.28	119.56
2	J	1231	ASN	C-N-CA	6.59	126.28	119.56
2	N	1231	ASN	CA-C-N	6.57	126.27	119.56
2	N	1231	ASN	C-N-CA	6.57	126.27	119.56
1	E	842	GLU	CA-C-N	6.54	126.45	119.85
1	E	842	GLU	C-N-CA	6.54	126.45	119.85
1	I	837	TYR	CA-C-N	6.53	127.05	119.47
1	I	837	TYR	C-N-CA	6.53	127.05	119.47
1	M	837	TYR	CA-C-N	6.53	127.04	119.47
1	M	837	TYR	C-N-CA	6.53	127.04	119.47
2	B	1231	ASN	CA-C-N	6.53	126.22	119.56
2	B	1231	ASN	C-N-CA	6.53	126.22	119.56
1	E	837	TYR	CA-C-N	6.53	127.04	119.47
1	E	837	TYR	C-N-CA	6.53	127.04	119.47
1	I	842	GLU	CA-C-N	6.53	126.44	119.85
1	I	842	GLU	C-N-CA	6.53	126.44	119.85
2	F	1231	ASN	CA-C-N	6.50	126.19	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1231	ASN	C-N-CA	6.50	126.19	119.56
1	M	842	GLU	CA-C-N	6.50	126.41	119.85
1	M	842	GLU	C-N-CA	6.50	126.41	119.85
2	B	1046	ALA	CA-C-N	6.47	126.39	119.85
2	B	1046	ALA	C-N-CA	6.47	126.39	119.85
2	J	1142	GLU	CA-C-N	6.46	126.64	120.31
2	J	1142	GLU	C-N-CA	6.46	126.64	120.31
2	J	1046	ALA	CA-C-N	6.46	126.37	119.85
2	J	1046	ALA	C-N-CA	6.46	126.37	119.85
2	F	1142	GLU	CA-C-N	6.42	126.61	120.31
2	F	1142	GLU	C-N-CA	6.42	126.61	120.31
2	F	1046	ALA	CA-C-N	6.42	126.33	119.85
2	F	1046	ALA	C-N-CA	6.42	126.33	119.85
2	B	1142	GLU	CA-C-N	6.42	126.60	120.31
2	B	1142	GLU	C-N-CA	6.42	126.60	120.31
2	N	1046	ALA	CA-C-N	6.41	126.33	119.85
2	N	1046	ALA	C-N-CA	6.41	126.33	119.85
2	N	1142	GLU	CA-C-N	6.41	126.59	120.31
2	N	1142	GLU	C-N-CA	6.41	126.59	120.31
1	I	250	PRO	CA-C-N	6.38	126.01	119.56
1	I	250	PRO	C-N-CA	6.38	126.01	119.56
1	I	753	ARG	CA-C-N	6.36	126.33	119.78
1	I	753	ARG	C-N-CA	6.36	126.33	119.78
1	M	250	PRO	CA-C-N	6.36	125.98	119.56
1	M	250	PRO	C-N-CA	6.36	125.98	119.56
1	M	753	ARG	CA-C-N	6.35	126.32	119.78
1	M	753	ARG	C-N-CA	6.35	126.32	119.78
1	A	250	PRO	CA-C-N	6.35	125.97	119.56
1	A	250	PRO	C-N-CA	6.35	125.97	119.56
1	E	250	PRO	CA-C-N	6.34	125.96	119.56
1	E	250	PRO	C-N-CA	6.34	125.96	119.56
1	I	715	VAL	CA-C-N	6.33	126.71	119.93
1	I	715	VAL	C-N-CA	6.33	126.71	119.93
1	E	184	ASP	CA-C-N	6.33	126.02	119.82
1	E	184	ASP	C-N-CA	6.33	126.02	119.82
1	E	753	ARG	CA-C-N	6.33	126.30	119.78
1	E	753	ARG	C-N-CA	6.33	126.30	119.78
1	M	715	VAL	CA-C-N	6.31	126.69	119.93
1	M	715	VAL	C-N-CA	6.31	126.69	119.93
1	M	184	ASP	CA-C-N	6.30	126.00	119.82
1	M	184	ASP	C-N-CA	6.30	126.00	119.82
3	C	533	TRP	CA-C-N	6.29	126.26	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	533	TRP	C-N-CA	6.29	126.26	119.78
1	E	715	VAL	CA-C-N	6.29	126.66	119.93
1	E	715	VAL	C-N-CA	6.29	126.66	119.93
1	I	184	ASP	CA-C-N	6.29	125.98	119.82
1	I	184	ASP	C-N-CA	6.29	125.98	119.82
1	M	222	VAL	CA-C-N	6.28	126.25	119.78
1	M	222	VAL	C-N-CA	6.28	126.25	119.78
1	M	411	TRP	CA-C-N	6.27	126.48	119.90
1	M	411	TRP	C-N-CA	6.27	126.48	119.90
1	I	411	TRP	CA-C-N	6.26	126.48	119.90
1	I	411	TRP	C-N-CA	6.26	126.48	119.90
3	K	533	TRP	CA-C-N	6.26	126.23	119.78
3	K	533	TRP	C-N-CA	6.26	126.23	119.78
1	E	411	TRP	CA-C-N	6.26	126.47	119.90
1	E	411	TRP	C-N-CA	6.26	126.47	119.90
4	D	40	ASP	N-CA-C	-6.26	99.44	109.39
1	E	222	VAL	CA-C-N	6.26	126.22	119.78
1	E	222	VAL	C-N-CA	6.26	126.22	119.78
1	M	634	GLN	CA-C-N	6.25	126.15	119.28
1	M	634	GLN	C-N-CA	6.25	126.15	119.28
1	A	184	ASP	CA-C-N	6.25	125.94	119.82
1	A	184	ASP	C-N-CA	6.25	125.94	119.82
3	G	533	TRP	CA-C-N	6.24	126.21	119.78
3	G	533	TRP	C-N-CA	6.24	126.21	119.78
1	A	222	VAL	CA-C-N	6.24	126.21	119.78
1	A	222	VAL	C-N-CA	6.24	126.21	119.78
1	I	634	GLN	CA-C-N	6.24	126.14	119.28
1	I	634	GLN	C-N-CA	6.24	126.14	119.28
1	A	411	TRP	CA-C-N	6.24	126.45	119.90
1	A	411	TRP	C-N-CA	6.24	126.45	119.90
3	O	533	TRP	CA-C-N	6.23	126.20	119.78
3	O	533	TRP	C-N-CA	6.23	126.20	119.78
1	E	634	GLN	CA-C-N	6.23	126.13	119.28
1	E	634	GLN	C-N-CA	6.23	126.13	119.28
1	I	222	VAL	CA-C-N	6.22	126.19	119.78
1	I	222	VAL	C-N-CA	6.22	126.19	119.78
1	E	249	ALA	CA-C-N	6.21	126.78	120.38
1	E	249	ALA	C-N-CA	6.21	126.78	120.38
1	A	634	GLN	CA-C-N	6.21	126.11	119.28
1	A	634	GLN	C-N-CA	6.21	126.11	119.28
1	M	382	PHE	CB-CA-C	-6.20	109.43	116.63
1	I	824	ASP	CA-C-N	6.20	126.32	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	824	ASP	C-N-CA	6.20	126.32	119.87
1	I	382	PHE	CB-CA-C	-6.20	109.44	116.63
1	A	587	ILE	CA-C-N	6.20	125.96	119.76
1	A	587	ILE	C-N-CA	6.20	125.96	119.76
1	A	382	PHE	CB-CA-C	-6.19	109.45	116.63
3	G	51	ARG	CA-C-N	6.19	125.81	119.56
3	G	51	ARG	C-N-CA	6.19	125.81	119.56
3	C	751	ASN	CA-C-N	6.18	126.64	119.47
3	C	751	ASN	C-N-CA	6.18	126.64	119.47
1	I	587	ILE	CA-C-N	6.18	125.94	119.76
1	I	587	ILE	C-N-CA	6.18	125.94	119.76
1	M	824	ASP	CA-C-N	6.18	126.30	119.87
1	M	824	ASP	C-N-CA	6.18	126.30	119.87
1	E	382	PHE	CB-CA-C	-6.18	109.46	116.63
1	E	587	ILE	CA-C-N	6.18	125.94	119.76
1	E	587	ILE	C-N-CA	6.18	125.94	119.76
3	C	51	ARG	CA-C-N	6.17	125.85	119.56
3	C	51	ARG	C-N-CA	6.17	125.85	119.56
1	E	824	ASP	CA-C-N	6.17	126.29	119.87
1	E	824	ASP	C-N-CA	6.17	126.29	119.87
1	A	249	ALA	CA-C-N	6.17	126.73	120.38
1	A	249	ALA	C-N-CA	6.17	126.73	120.38
1	I	416	ASP	CA-C-N	6.16	125.84	119.56
1	I	416	ASP	C-N-CA	6.16	125.84	119.56
3	K	751	ASN	CA-C-N	6.16	126.61	119.47
3	K	751	ASN	C-N-CA	6.16	126.61	119.47
1	M	416	ASP	CA-C-N	6.16	125.84	119.56
1	M	416	ASP	C-N-CA	6.16	125.84	119.56
1	A	416	ASP	CA-C-N	6.15	125.84	119.56
1	A	416	ASP	C-N-CA	6.15	125.84	119.56
3	G	751	ASN	CA-C-N	6.15	126.60	119.47
3	G	751	ASN	C-N-CA	6.15	126.60	119.47
1	M	587	ILE	CA-C-N	6.15	125.91	119.76
1	M	587	ILE	C-N-CA	6.15	125.91	119.76
3	O	751	ASN	CA-C-N	6.14	126.59	119.47
3	O	751	ASN	C-N-CA	6.14	126.59	119.47
1	E	416	ASP	CA-C-N	6.14	125.82	119.56
1	E	416	ASP	C-N-CA	6.14	125.82	119.56
1	I	249	ALA	CA-C-N	6.14	126.70	120.38
1	I	249	ALA	C-N-CA	6.14	126.70	120.38
1	E	544	THR	CA-C-N	6.13	126.08	119.76
1	E	544	THR	C-N-CA	6.13	126.08	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	249	ALA	CA-C-N	6.12	126.68	120.38
1	M	249	ALA	C-N-CA	6.12	126.68	120.38
3	G	728	LYS	CA-C-N	6.11	126.00	119.28
3	G	728	LYS	C-N-CA	6.11	126.00	119.28
3	O	51	ARG	CA-C-N	6.11	125.79	119.56
3	O	51	ARG	C-N-CA	6.11	125.79	119.56
1	M	544	THR	CA-C-N	6.10	126.04	119.76
1	M	544	THR	C-N-CA	6.10	126.04	119.76
1	A	544	THR	CA-C-N	6.09	126.03	119.76
1	A	544	THR	C-N-CA	6.09	126.03	119.76
3	K	51	ARG	CA-C-N	6.09	125.77	119.56
3	K	51	ARG	C-N-CA	6.09	125.77	119.56
3	C	728	LYS	CA-C-N	6.07	125.96	119.28
3	C	728	LYS	C-N-CA	6.07	125.96	119.28
3	K	728	LYS	CA-C-N	6.07	125.95	119.28
3	K	728	LYS	C-N-CA	6.07	125.95	119.28
2	N	1060	PHE	CA-C-N	6.06	127.41	119.84
2	N	1060	PHE	C-N-CA	6.06	127.41	119.84
2	F	1060	PHE	CA-C-N	6.05	127.41	119.84
2	F	1060	PHE	C-N-CA	6.05	127.41	119.84
1	E	1083	GLU	CA-C-N	6.05	125.96	119.85
1	E	1083	GLU	C-N-CA	6.05	125.96	119.85
1	I	544	THR	CA-C-N	6.05	125.99	119.76
1	I	544	THR	C-N-CA	6.05	125.99	119.76
2	B	1060	PHE	CA-C-N	6.04	127.39	119.84
2	B	1060	PHE	C-N-CA	6.04	127.39	119.84
2	J	1060	PHE	CA-C-N	6.04	127.39	119.84
2	J	1060	PHE	C-N-CA	6.04	127.39	119.84
2	F	1081	ARG	CA-C-N	6.04	125.98	119.76
2	F	1081	ARG	C-N-CA	6.04	125.98	119.76
3	O	537	THR	CA-C-N	6.03	126.22	120.31
3	O	537	THR	C-N-CA	6.03	126.22	120.31
3	G	537	THR	CA-C-N	6.03	126.22	120.31
3	G	537	THR	C-N-CA	6.03	126.22	120.31
2	B	1081	ARG	CA-C-N	6.02	125.96	119.76
2	B	1081	ARG	C-N-CA	6.02	125.96	119.76
3	O	728	LYS	CA-C-N	6.02	125.90	119.28
3	O	728	LYS	C-N-CA	6.02	125.90	119.28
1	I	1083	GLU	CA-C-N	6.01	125.92	119.85
1	I	1083	GLU	C-N-CA	6.01	125.92	119.85
3	C	537	THR	CA-C-N	6.00	126.19	120.31
3	C	537	THR	C-N-CA	6.00	126.19	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1083	GLU	CA-C-N	6.00	125.91	119.85
1	M	1083	GLU	C-N-CA	6.00	125.91	119.85
2	J	1081	ARG	CA-C-N	5.99	125.93	119.76
2	J	1081	ARG	C-N-CA	5.99	125.93	119.76
3	K	537	THR	CA-C-N	5.98	126.17	120.31
3	K	537	THR	C-N-CA	5.98	126.17	120.31
3	C	119	LEU	CA-C-N	5.98	125.68	119.82
3	C	119	LEU	C-N-CA	5.98	125.68	119.82
4	P	38	VAL	CB-CA-C	5.97	121.09	111.29
4	D	38	VAL	CB-CA-C	5.97	121.08	111.29
2	N	1081	ARG	CA-C-N	5.97	125.91	119.76
2	N	1081	ARG	C-N-CA	5.97	125.91	119.76
4	L	38	VAL	CB-CA-C	5.97	121.08	111.29
4	H	38	VAL	CB-CA-C	5.97	121.07	111.29
3	G	119	LEU	CA-C-N	5.95	125.65	119.82
3	G	119	LEU	C-N-CA	5.95	125.65	119.82
3	K	119	LEU	CA-C-N	5.94	125.64	119.82
3	K	119	LEU	C-N-CA	5.94	125.64	119.82
3	O	119	LEU	CA-C-N	5.93	125.63	119.82
3	O	119	LEU	C-N-CA	5.93	125.63	119.82
1	E	50	ARG	CA-C-N	5.87	125.77	119.85
1	E	50	ARG	C-N-CA	5.87	125.77	119.85
1	I	50	ARG	CA-C-N	5.86	125.77	119.85
1	I	50	ARG	C-N-CA	5.86	125.77	119.85
1	E	680	CYS	CA-C-N	5.85	125.61	119.76
1	E	680	CYS	C-N-CA	5.85	125.61	119.76
1	A	1010	GLY	CA-C-O	-5.84	118.20	122.23
1	A	50	ARG	CA-C-N	5.84	125.75	119.85
1	A	50	ARG	C-N-CA	5.84	125.75	119.85
1	M	50	ARG	CA-C-N	5.84	125.75	119.85
1	M	50	ARG	C-N-CA	5.84	125.75	119.85
1	M	11	LYS	CA-C-N	5.79	125.74	119.78
1	M	11	LYS	C-N-CA	5.79	125.74	119.78
1	A	680	CYS	CA-C-N	5.78	125.54	119.76
1	A	680	CYS	C-N-CA	5.78	125.54	119.76
1	M	680	CYS	CA-C-N	5.77	125.53	119.76
1	M	680	CYS	C-N-CA	5.77	125.53	119.76
1	E	11	LYS	CA-C-N	5.76	125.71	119.78
1	E	11	LYS	C-N-CA	5.76	125.71	119.78
1	I	680	CYS	CA-C-N	5.75	125.51	119.76
1	I	680	CYS	C-N-CA	5.75	125.51	119.76
1	I	11	LYS	CA-C-N	5.75	125.70	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	11	LYS	C-N-CA	5.75	125.70	119.78
1	I	929	SER	CB-CA-C	-5.74	109.43	117.23
1	A	11	LYS	CA-C-N	5.73	125.68	119.78
1	A	11	LYS	C-N-CA	5.73	125.68	119.78
1	M	929	SER	CB-CA-C	-5.73	109.44	117.23
1	E	720	SER	CA-C-N	5.70	125.90	120.31
1	E	720	SER	C-N-CA	5.70	125.90	120.31
1	I	720	SER	CA-C-N	5.69	125.89	120.31
1	I	720	SER	C-N-CA	5.69	125.89	120.31
1	E	929	SER	CB-CA-C	-5.67	109.52	117.23
1	M	720	SER	CA-C-N	5.66	125.86	120.31
1	M	720	SER	C-N-CA	5.66	125.86	120.31
4	P	36	ASP	N-CA-CB	5.63	118.14	109.91
4	L	36	ASP	N-CA-CB	5.63	118.13	109.91
4	D	36	ASP	N-CA-CB	5.61	118.10	109.91
1	E	643	SER	CA-C-O	5.61	121.19	117.94
4	H	36	ASP	N-CA-CB	5.60	118.08	109.91
3	K	544	THR	CA-C-N	5.59	125.69	119.32
3	K	544	THR	C-N-CA	5.59	125.69	119.32
3	G	544	THR	CA-C-N	5.58	125.68	119.32
3	G	544	THR	C-N-CA	5.58	125.68	119.32
1	E	68	ARG	CA-C-N	5.57	126.80	119.84
1	E	68	ARG	C-N-CA	5.57	126.80	119.84
1	A	68	ARG	CA-C-N	5.56	126.79	119.84
1	A	68	ARG	C-N-CA	5.56	126.79	119.84
3	C	544	THR	CA-C-N	5.55	125.64	119.32
3	C	544	THR	C-N-CA	5.55	125.64	119.32
1	I	68	ARG	CA-C-N	5.54	126.77	119.84
1	I	68	ARG	C-N-CA	5.54	126.77	119.84
1	M	68	ARG	CA-C-N	5.54	126.77	119.84
1	M	68	ARG	C-N-CA	5.54	126.77	119.84
1	M	643	SER	CA-C-O	5.54	121.15	117.94
3	O	544	THR	CA-C-N	5.54	125.63	119.32
3	O	544	THR	C-N-CA	5.54	125.63	119.32
1	A	643	SER	CA-C-O	5.50	121.13	117.94
1	I	643	SER	CA-C-O	5.50	121.13	117.94
1	A	1026	GLY	CA-C-O	-5.42	117.90	122.29
1	I	125	ASP	CA-C-N	5.16	124.82	119.56
1	I	125	ASP	C-N-CA	5.16	124.82	119.56
1	E	125	ASP	CA-C-N	5.15	124.81	119.56
1	E	125	ASP	C-N-CA	5.15	124.81	119.56
1	M	125	ASP	CA-C-N	5.13	124.79	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	125	ASP	C-N-CA	5.13	124.79	119.56
1	A	125	ASP	CA-C-N	5.12	124.78	119.56
1	A	125	ASP	C-N-CA	5.12	124.78	119.56
4	P	40	ASP	N-CA-C	-5.07	100.00	110.80
4	L	40	ASP	N-CA-C	-5.05	100.04	110.80
4	H	40	ASP	N-CA-C	-5.05	100.05	110.80
4	D	36	ASP	CA-C-O	-5.04	115.71	121.00
3	C	404	LYS	CA-C-N	5.02	125.30	119.47
3	C	404	LYS	C-N-CA	5.02	125.30	119.47
3	K	404	LYS	CA-C-N	5.02	125.30	119.47
3	K	404	LYS	C-N-CA	5.02	125.30	119.47
4	H	36	ASP	CA-C-O	-5.01	115.74	121.00
3	O	404	LYS	CA-C-N	5.01	125.28	119.47
3	O	404	LYS	C-N-CA	5.01	125.28	119.47
4	P	36	ASP	CA-C-O	-5.00	115.74	121.00
3	G	404	LYS	CA-C-N	5.00	125.27	119.47
3	G	404	LYS	C-N-CA	5.00	125.27	119.47

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	3	0
3	G	3564	0	1545	3	0
3	K	3564	0	1545	2	0
3	O	3564	0	1545	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	359	0	171	6	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	51	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 (51) 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:H:39:VAL:C	4:H:41:ASN:H	2.01	0.69
4:L:39:VAL:C	4:L:41:ASN:H	2.01	0.67
4:P:39:VAL:C	4:P:41:ASN:H	2.01	0.67
2:J:1313:LEU:O	2:J:1314:GLN:C	2.41	0.64
2:N:1313:LEU:O	2:N:1314:GLN:C	2.41	0.64
2:F:1313:LEU:O	2:F:1314:GLN:C	2.41	0.63
2:B:1313:LEU:O	2:B:1314:GLN:C	2.41	0.62
4:L:39:VAL:C	4:L:41:ASN:N	2.58	0.60
4:P:39:VAL:C	4:P:41:ASN:N	2.58	0.60
4:H:39:VAL:C	4:H:41:ASN:N	2.58	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
4:D:35:TRP:N	4:D:76:ASN:O	2.35	0.58
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:46:LYS:O	3:C:47:ASN:C	2.62	0.42
3:G:46:LYS:O	3:G:47:ASN:C	2.62	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
4:D:39:VAL:C	4:D:41:ASN:N	2.78	0.40
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	30	67
1	E	1131/1159 (98%)	1083 (96%)	44 (4%)	4 (0%)	30	67
1	I	1131/1159 (98%)	1085 (96%)	42 (4%)	4 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	1131/1159 (98%)	1085 (96%)	42 (4%)	4 (0%)	30	67
2	B	327/1525 (21%)	311 (95%)	15 (5%)	1 (0%)	36	72
2	F	327/1525 (21%)	311 (95%)	15 (5%)	1 (0%)	36	72
2	J	327/1525 (21%)	311 (95%)	15 (5%)	1 (0%)	36	72
2	N	327/1525 (21%)	311 (95%)	15 (5%)	1 (0%)	36	72
3	C	717/742 (97%)	702 (98%)	14 (2%)	1 (0%)	48	83
3	G	717/742 (97%)	702 (98%)	14 (2%)	1 (0%)	48	83
3	K	717/742 (97%)	701 (98%)	15 (2%)	1 (0%)	48	83
3	O	717/742 (97%)	702 (98%)	14 (2%)	1 (0%)	48	83
4	D	70/116 (60%)	61 (87%)	8 (11%)	1 (1%)	9	40
4	H	70/116 (60%)	61 (87%)	8 (11%)	1 (1%)	9	40
4	L	70/116 (60%)	61 (87%)	8 (11%)	1 (1%)	9	40
4	P	70/116 (60%)	61 (87%)	8 (11%)	1 (1%)	9	40
All	All	8980/14168 (63%)	8636 (96%)	316 (4%)	28 (0%)	37	72

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
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

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Mol	Chain	Res	Type
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

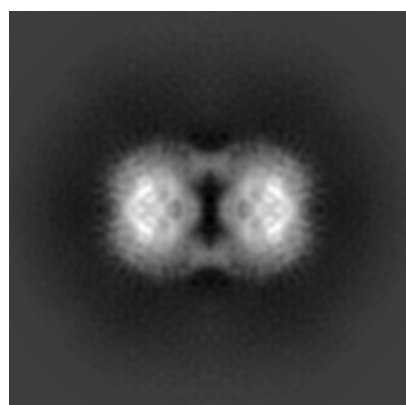
6 Map visualisation [i](#)

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.

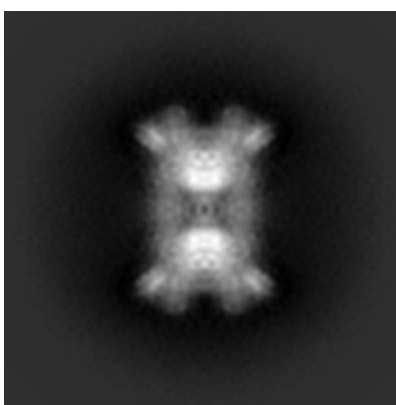
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

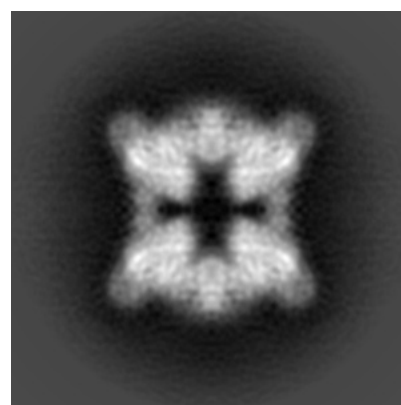
6.1.1 Primary map



X



Y

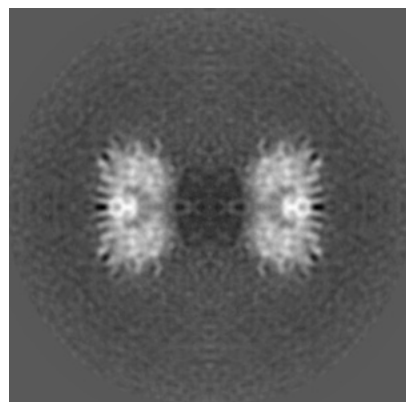


Z

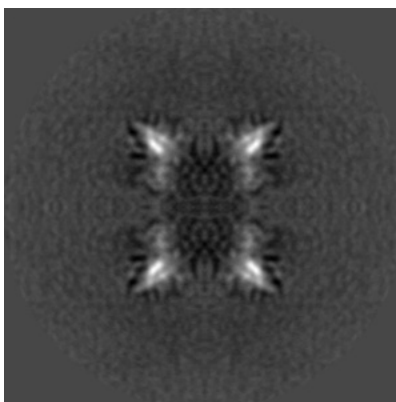
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

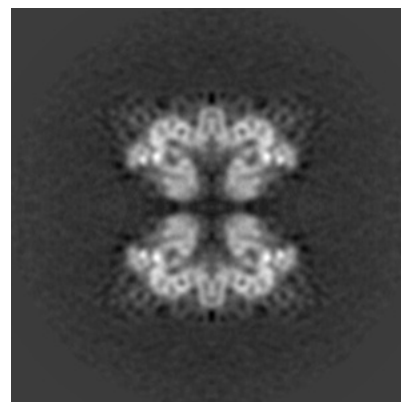
6.2.1 Primary map



X Index: 130



Y Index: 130

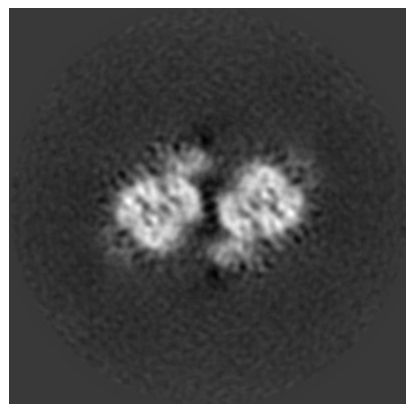


Z Index: 130

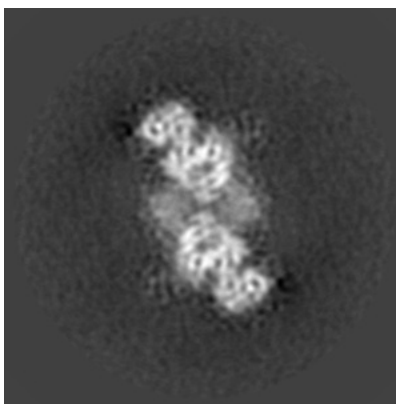
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

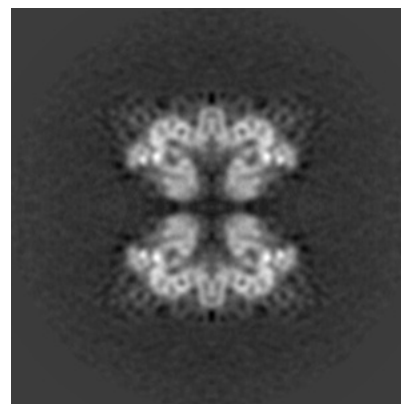
6.3.1 Primary map



X Index: 106



Y Index: 173

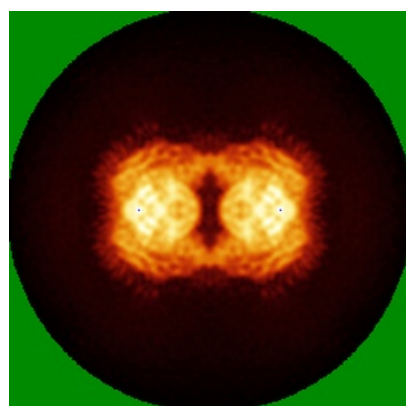


Z Index: 130

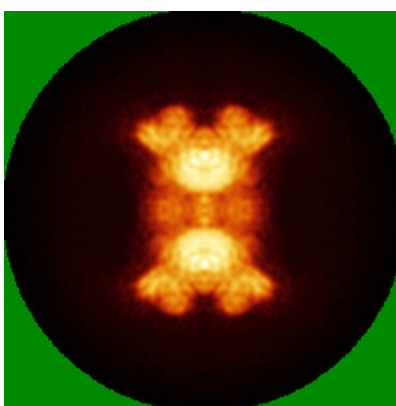
The images above show the largest variance slices of the map in three orthogonal directions.

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

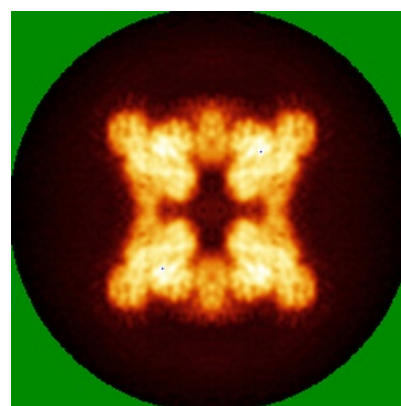
6.4.1 Primary map



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

This section was not generated.

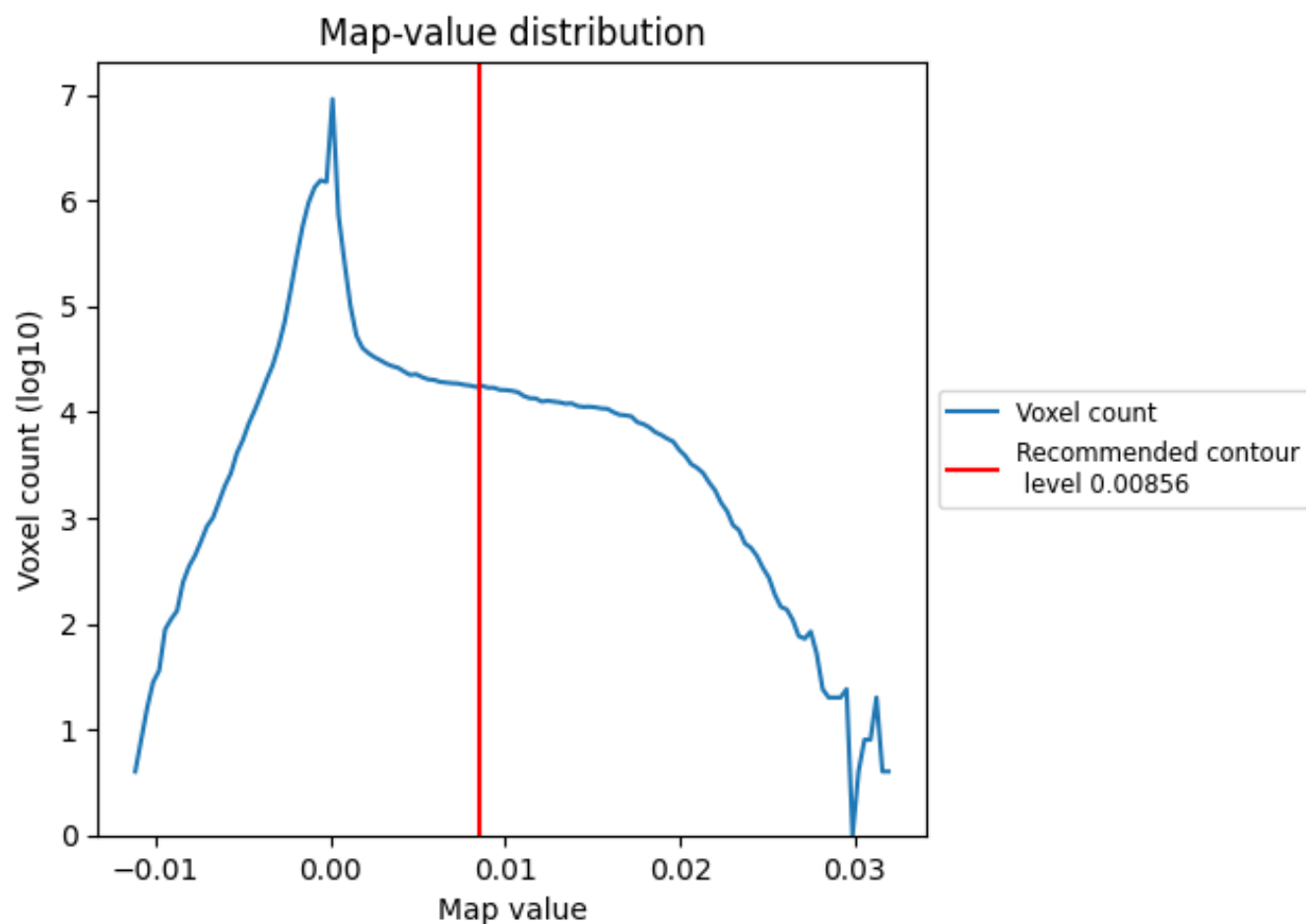
6.6 Mask visualisation

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

7 Map analysis [i](#)

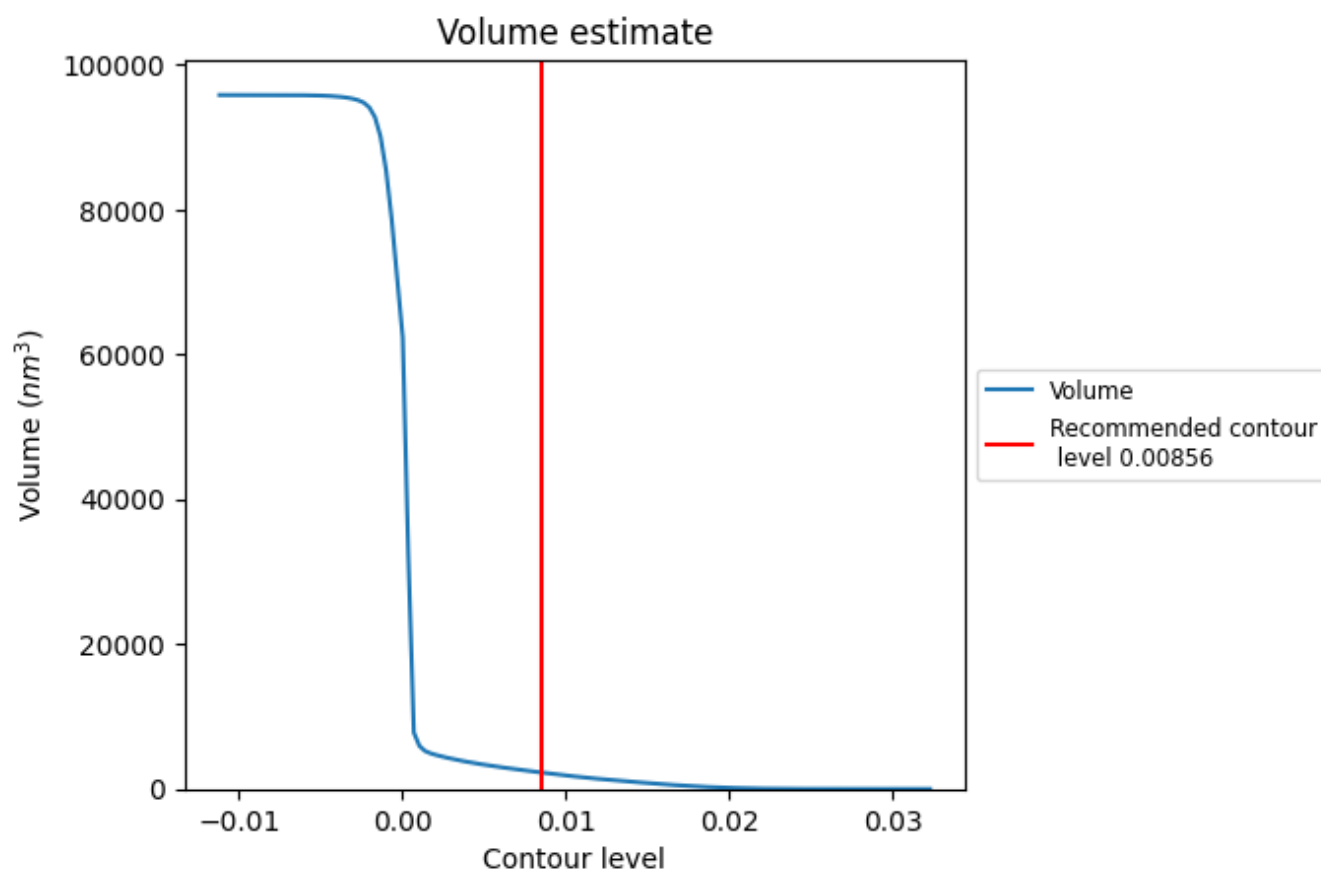
This section contains the results of statistical analysis of the map.

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.

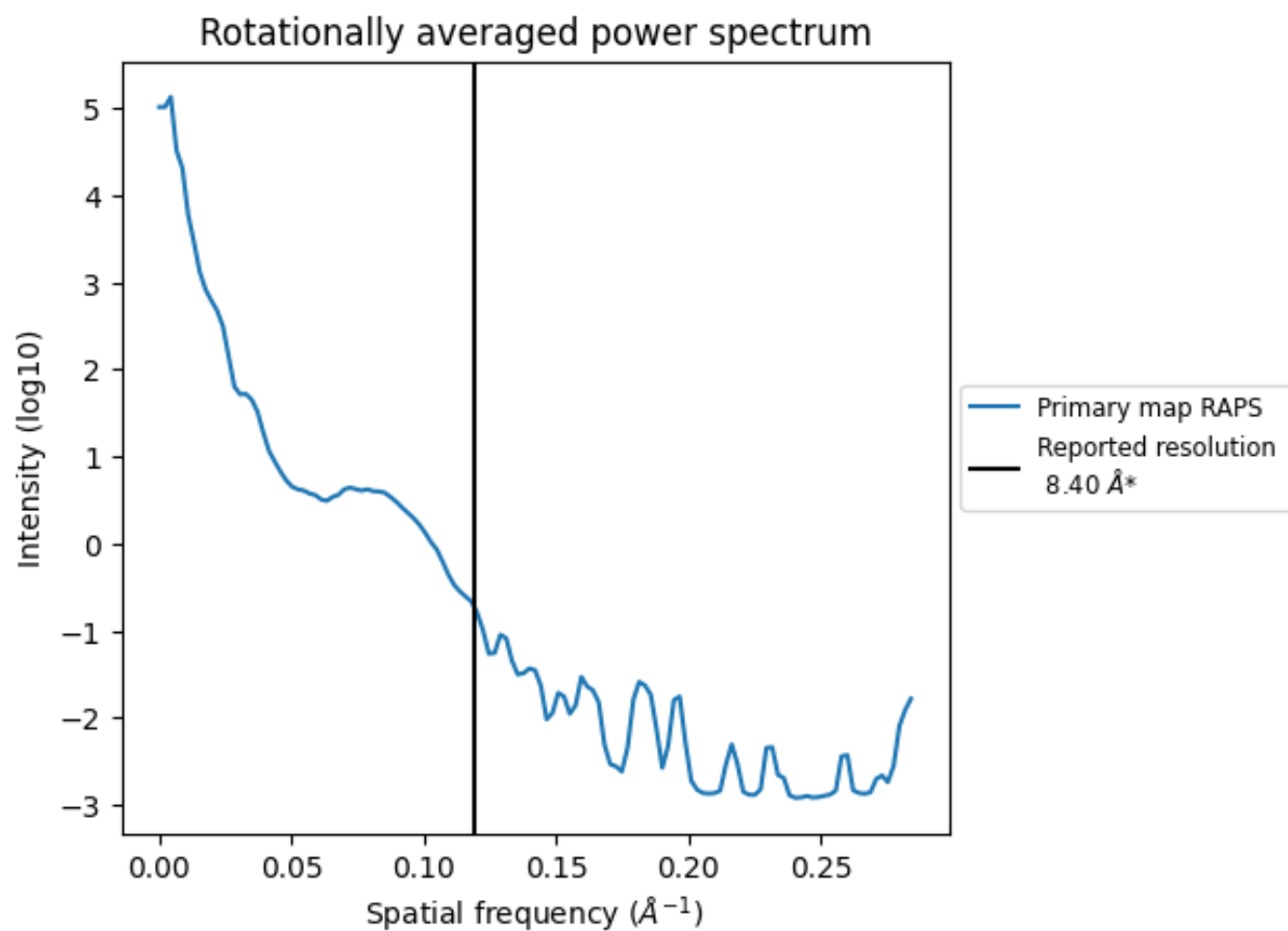
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2255 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.119 Å⁻¹

8 Fourier-Shell correlation ⓘ

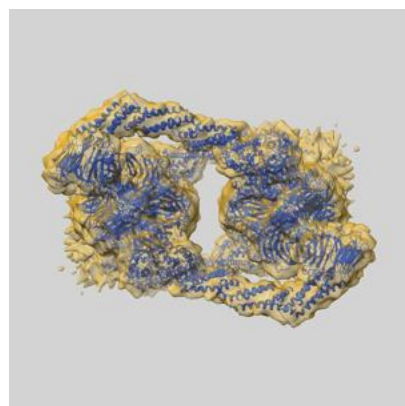
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

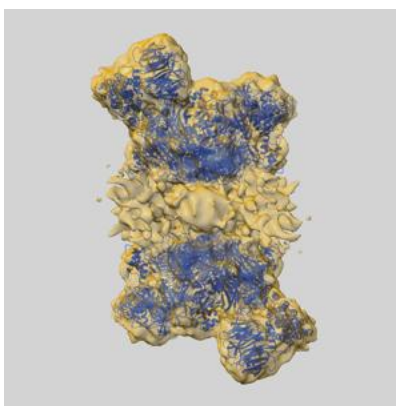
This section contains information regarding the fit between EMDB map EMD-12964 and PDB model 7OKQ. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlays

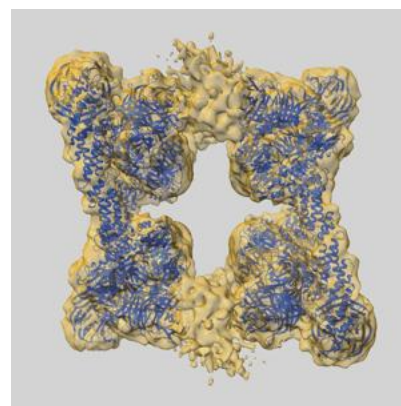
9.1.1 Map-model overlay [i](#)



X

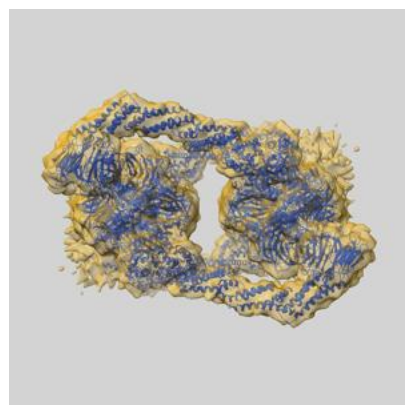


Y

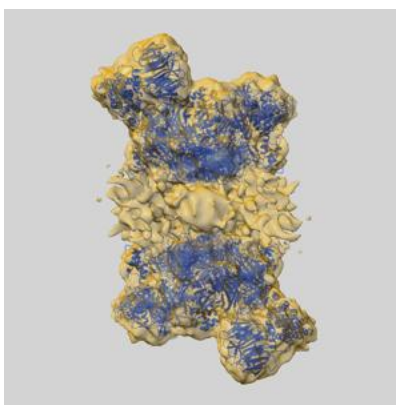


Z

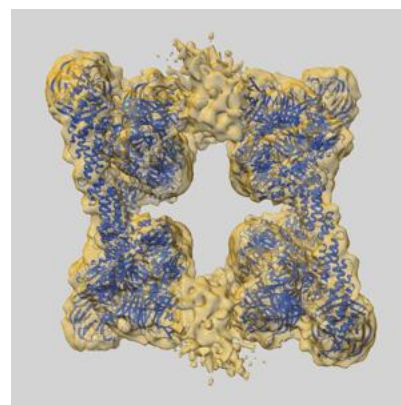
9.1.2 Map-model assembly overlay [i](#)



X



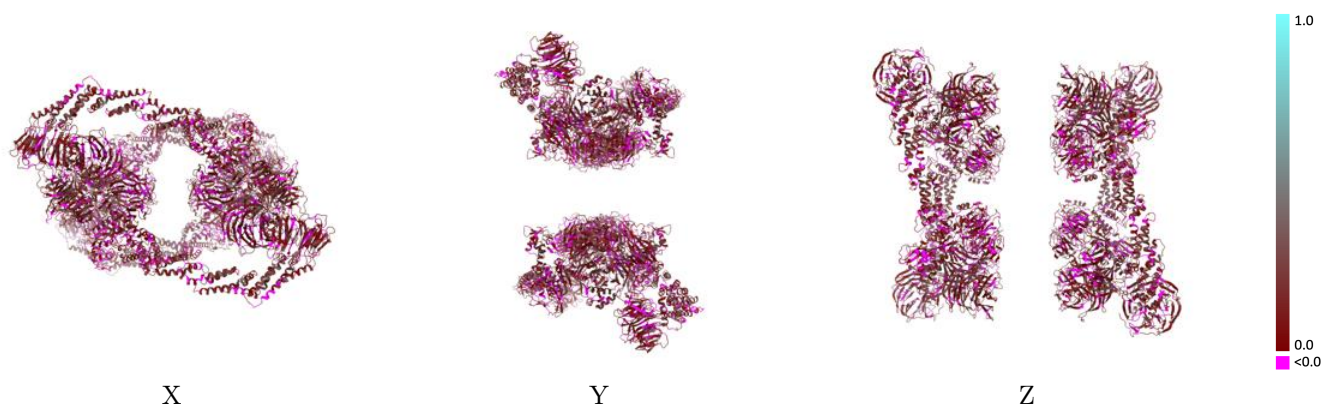
Y



Z

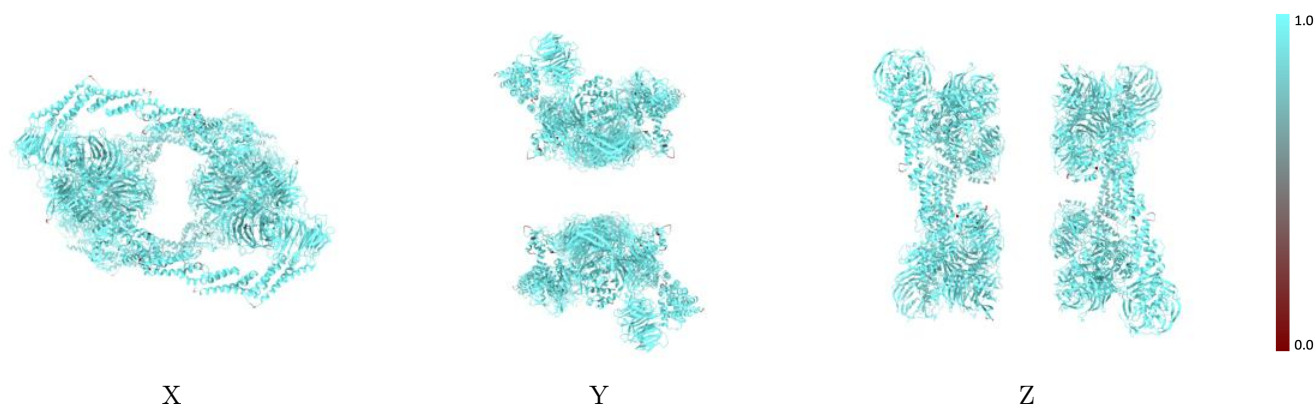
The images above show the 3D surface view of the map at the recommended contour level 0.00856 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



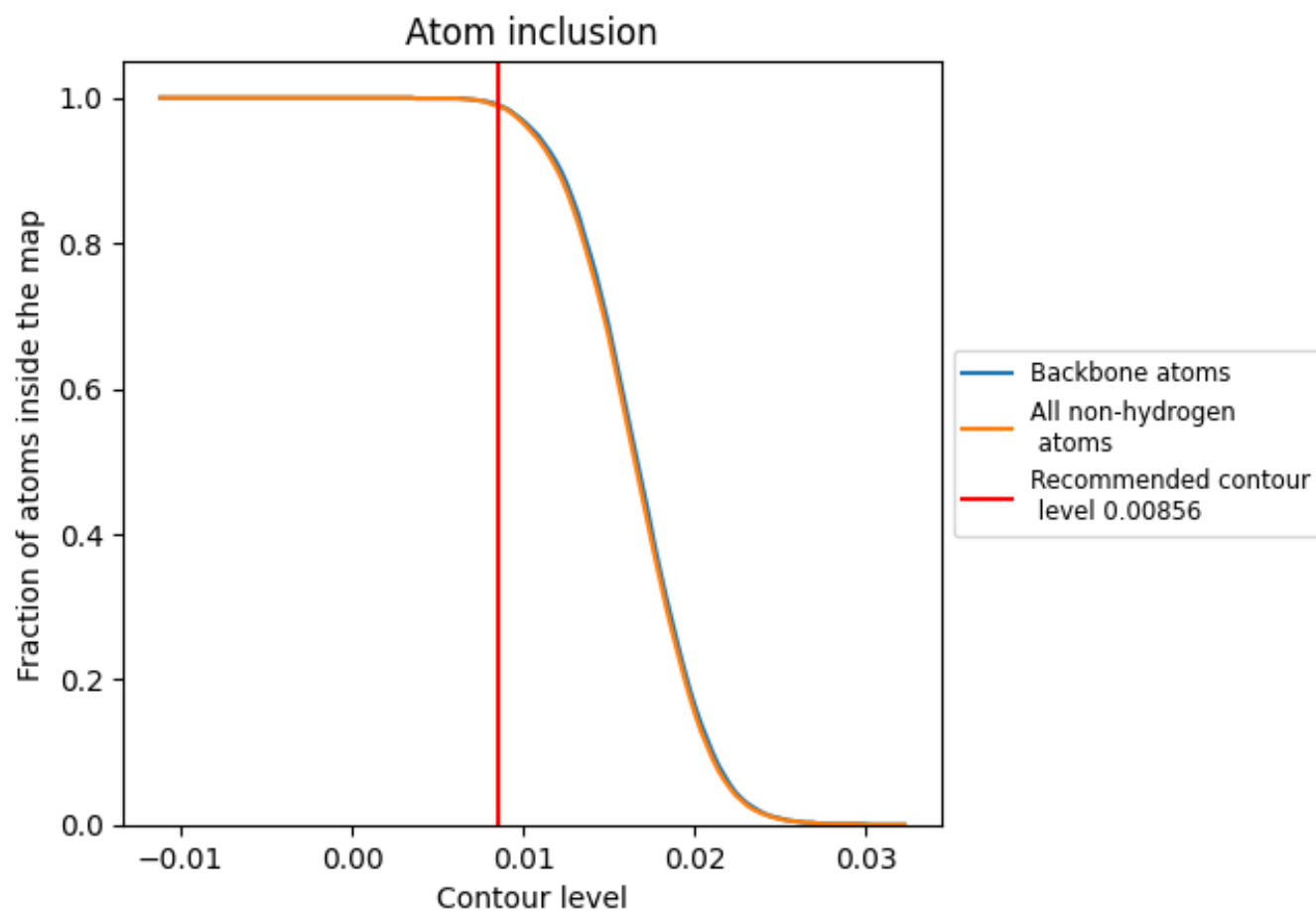
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.9880	 0.1240
A	 0.9940	 0.1290
B	 0.9990	 0.1030
C	 0.9750	 0.1340
D	 0.9830	 0.0850
E	 0.9950	 0.1300
F	 1.0000	 0.1100
G	 0.9740	 0.1260
H	 0.9830	 0.0790
I	 0.9930	 0.1310
J	 1.0000	 0.1120
K	 0.9730	 0.1160
L	 0.9860	 0.0780
M	 0.9940	 0.1250
N	 1.0000	 0.0980
O	 0.9750	 0.1360
P	 0.9830	 0.0880

