



Full wwPDB EM Validation Report ⓘ

Jun 6, 2026 – 12:18 PM EDT

PDB ID : 9O04 / pdb_00009o04
EMDB ID : EMD-49966
Title : CryoEM structure of the FBXO42-CCDC6-PP2Ac degradasome
Authors : Hsu, P.L.; Michaelian, N.; Azumaya, C.; Coassolo, S.; Yauch, R.L.
Deposited on : 2025-04-02
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

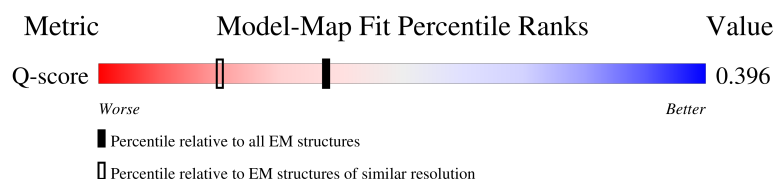
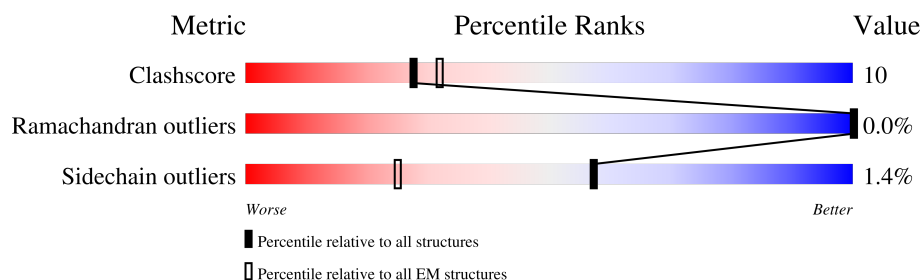
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



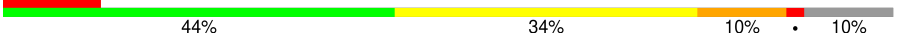
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	490	 22% 5% 73%
1	B	490	 21% 6% 73%
2	C	691	 43% 12% 45%
2	G	691	 46% 10% 45%

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Mol	Chain	Length	Quality of chain
3	D	336	
3	E	336	
3	I	336	
3	J	336	
3	K	336	
3	L	336	
3	M	336	
3	N	336	
4	F	151	
4	H	151	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29353 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 Coiled-coil domain-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	133	Total	C	N	O	S	1	0
			1136	707	203	223	3		
1	B	131	Total	C	N	O	S	0	0
			1110	692	195	220	3		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q16204
A	-14	HIS	-	expression tag	UNP Q16204
A	-13	HIS	-	expression tag	UNP Q16204
A	-12	HIS	-	expression tag	UNP Q16204
A	-11	HIS	-	expression tag	UNP Q16204
A	-10	HIS	-	expression tag	UNP Q16204
A	-9	HIS	-	expression tag	UNP Q16204
A	-8	GLY	-	expression tag	UNP Q16204
A	-7	GLU	-	expression tag	UNP Q16204
A	-6	ASN	-	expression tag	UNP Q16204
A	-5	LEU	-	expression tag	UNP Q16204
A	-4	TYR	-	expression tag	UNP Q16204
A	-3	PHE	-	expression tag	UNP Q16204
A	-2	GLN	-	expression tag	UNP Q16204
A	-1	GLY	-	expression tag	UNP Q16204
A	0	SER	-	expression tag	UNP Q16204
B	-15	MET	-	initiating methionine	UNP Q16204
B	-14	HIS	-	expression tag	UNP Q16204
B	-13	HIS	-	expression tag	UNP Q16204
B	-12	HIS	-	expression tag	UNP Q16204
B	-11	HIS	-	expression tag	UNP Q16204
B	-10	HIS	-	expression tag	UNP Q16204
B	-9	HIS	-	expression tag	UNP Q16204
B	-8	GLY	-	expression tag	UNP Q16204
B	-7	GLU	-	expression tag	UNP Q16204
B	-6	ASN	-	expression tag	UNP Q16204

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	expression tag	UNP Q16204
B	-4	TYR	-	expression tag	UNP Q16204
B	-3	PHE	-	expression tag	UNP Q16204
B	-2	GLN	-	expression tag	UNP Q16204
B	-1	GLY	-	expression tag	UNP Q16204
B	0	SER	-	expression tag	UNP Q16204

- Molecule 2 is a protein called F-box only protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	382	Total	C	N	O	S	0	0
			3029	1944	521	542	22		
2	G	383	Total	C	N	O	S	0	0
			3036	1949	522	543	22		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	27	MET	-	initiating methionine	UNP Q6P3S6
C	28	ASP	-	expression tag	UNP Q6P3S6
C	29	TYR	-	expression tag	UNP Q6P3S6
C	30	LYS	-	expression tag	UNP Q6P3S6
C	31	ASP	-	expression tag	UNP Q6P3S6
C	32	ASP	-	expression tag	UNP Q6P3S6
C	33	ASP	-	expression tag	UNP Q6P3S6
C	34	ASP	-	expression tag	UNP Q6P3S6
C	35	LYS	-	expression tag	UNP Q6P3S6
C	36	GLY	-	expression tag	UNP Q6P3S6
C	37	GLU	-	expression tag	UNP Q6P3S6
C	38	ASN	-	expression tag	UNP Q6P3S6
C	39	LEU	-	expression tag	UNP Q6P3S6
C	40	TYR	-	expression tag	UNP Q6P3S6
C	41	PHE	-	expression tag	UNP Q6P3S6
C	42	GLN	-	expression tag	UNP Q6P3S6
C	43	GLY	-	expression tag	UNP Q6P3S6
C	44	SER	ASN	conflict	UNP Q6P3S6
G	27	MET	-	initiating methionine	UNP Q6P3S6
G	28	ASP	-	expression tag	UNP Q6P3S6
G	29	TYR	-	expression tag	UNP Q6P3S6
G	30	LYS	-	expression tag	UNP Q6P3S6
G	31	ASP	-	expression tag	UNP Q6P3S6
G	32	ASP	-	expression tag	UNP Q6P3S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	33	ASP	-	expression tag	UNP Q6P3S6
G	34	ASP	-	expression tag	UNP Q6P3S6
G	35	LYS	-	expression tag	UNP Q6P3S6
G	36	GLY	-	expression tag	UNP Q6P3S6
G	37	GLU	-	expression tag	UNP Q6P3S6
G	38	ASN	-	expression tag	UNP Q6P3S6
G	39	LEU	-	expression tag	UNP Q6P3S6
G	40	TYR	-	expression tag	UNP Q6P3S6
G	41	PHE	-	expression tag	UNP Q6P3S6
G	42	GLN	-	expression tag	UNP Q6P3S6
G	43	GLY	-	expression tag	UNP Q6P3S6
G	44	SER	ASN	conflict	UNP Q6P3S6

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	295	Total	C	N	O	S	1	0
			2401	1524	411	451	15		
3	E	291	Total	C	N	O	S	0	0
			2344	1485	402	442	15		
3	I	291	Total	C	N	O	S	0	0
			2344	1485	402	442	15		
3	J	294	Total	C	N	O	S	0	0
			2377	1510	405	447	15		
3	K	291	Total	C	N	O	S	0	0
			2344	1485	402	442	15		
3	L	291	Total	C	N	O	S	0	0
			2344	1485	402	442	15		
3	M	291	Total	C	N	O	S	0	0
			2344	1485	402	442	15		
3	N	291	Total	C	N	O	S	0	0
			2344	1485	402	442	15		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-26	MET	-	initiating methionine	UNP P67775
D	-25	ASP	-	expression tag	UNP P67775
D	-24	TYR	-	expression tag	UNP P67775
D	-23	LYS	-	expression tag	UNP P67775
D	-22	ASP	-	expression tag	UNP P67775

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	ASP	-	expression tag	UNP P67775
D	-20	ASP	-	expression tag	UNP P67775
D	-19	ASP	-	expression tag	UNP P67775
D	-18	LYS	-	expression tag	UNP P67775
D	-17	GLY	-	expression tag	UNP P67775
D	-16	GLU	-	expression tag	UNP P67775
D	-15	ASN	-	expression tag	UNP P67775
D	-14	LEU	-	expression tag	UNP P67775
D	-13	TYR	-	expression tag	UNP P67775
D	-12	PHE	-	expression tag	UNP P67775
D	-11	GLN	-	expression tag	UNP P67775
D	-10	GLY	-	expression tag	UNP P67775
D	-9	SER	-	expression tag	UNP P67775
D	-8	TYR	-	expression tag	UNP P67775
D	-7	PRO	-	expression tag	UNP P67775
D	-6	TYR	-	expression tag	UNP P67775
D	-5	ASP	-	expression tag	UNP P67775
D	-4	VAL	-	expression tag	UNP P67775
D	-3	PRO	-	expression tag	UNP P67775
D	-2	ASP	-	expression tag	UNP P67775
D	-1	TYR	-	expression tag	UNP P67775
D	0	ALA	-	expression tag	UNP P67775
E	-26	MET	-	initiating methionine	UNP P67775
E	-25	ASP	-	expression tag	UNP P67775
E	-24	TYR	-	expression tag	UNP P67775
E	-23	LYS	-	expression tag	UNP P67775
E	-22	ASP	-	expression tag	UNP P67775
E	-21	ASP	-	expression tag	UNP P67775
E	-20	ASP	-	expression tag	UNP P67775
E	-19	ASP	-	expression tag	UNP P67775
E	-18	LYS	-	expression tag	UNP P67775
E	-17	GLY	-	expression tag	UNP P67775
E	-16	GLU	-	expression tag	UNP P67775
E	-15	ASN	-	expression tag	UNP P67775
E	-14	LEU	-	expression tag	UNP P67775
E	-13	TYR	-	expression tag	UNP P67775
E	-12	PHE	-	expression tag	UNP P67775
E	-11	GLN	-	expression tag	UNP P67775
E	-10	GLY	-	expression tag	UNP P67775
E	-9	SER	-	expression tag	UNP P67775
E	-8	TYR	-	expression tag	UNP P67775
E	-7	PRO	-	expression tag	UNP P67775

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	TYR	-	expression tag	UNP P67775
E	-5	ASP	-	expression tag	UNP P67775
E	-4	VAL	-	expression tag	UNP P67775
E	-3	PRO	-	expression tag	UNP P67775
E	-2	ASP	-	expression tag	UNP P67775
E	-1	TYR	-	expression tag	UNP P67775
E	0	ALA	-	expression tag	UNP P67775
I	-26	MET	-	initiating methionine	UNP P67775
I	-25	ASP	-	expression tag	UNP P67775
I	-24	TYR	-	expression tag	UNP P67775
I	-23	LYS	-	expression tag	UNP P67775
I	-22	ASP	-	expression tag	UNP P67775
I	-21	ASP	-	expression tag	UNP P67775
I	-20	ASP	-	expression tag	UNP P67775
I	-19	ASP	-	expression tag	UNP P67775
I	-18	LYS	-	expression tag	UNP P67775
I	-17	GLY	-	expression tag	UNP P67775
I	-16	GLU	-	expression tag	UNP P67775
I	-15	ASN	-	expression tag	UNP P67775
I	-14	LEU	-	expression tag	UNP P67775
I	-13	TYR	-	expression tag	UNP P67775
I	-12	PHE	-	expression tag	UNP P67775
I	-11	GLN	-	expression tag	UNP P67775
I	-10	GLY	-	expression tag	UNP P67775
I	-9	SER	-	expression tag	UNP P67775
I	-8	TYR	-	expression tag	UNP P67775
I	-7	PRO	-	expression tag	UNP P67775
I	-6	TYR	-	expression tag	UNP P67775
I	-5	ASP	-	expression tag	UNP P67775
I	-4	VAL	-	expression tag	UNP P67775
I	-3	PRO	-	expression tag	UNP P67775
I	-2	ASP	-	expression tag	UNP P67775
I	-1	TYR	-	expression tag	UNP P67775
I	0	ALA	-	expression tag	UNP P67775
J	-26	MET	-	initiating methionine	UNP P67775
J	-25	ASP	-	expression tag	UNP P67775
J	-24	TYR	-	expression tag	UNP P67775
J	-23	LYS	-	expression tag	UNP P67775
J	-22	ASP	-	expression tag	UNP P67775
J	-21	ASP	-	expression tag	UNP P67775
J	-20	ASP	-	expression tag	UNP P67775
J	-19	ASP	-	expression tag	UNP P67775

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-18	LYS	-	expression tag	UNP P67775
J	-17	GLY	-	expression tag	UNP P67775
J	-16	GLU	-	expression tag	UNP P67775
J	-15	ASN	-	expression tag	UNP P67775
J	-14	LEU	-	expression tag	UNP P67775
J	-13	TYR	-	expression tag	UNP P67775
J	-12	PHE	-	expression tag	UNP P67775
J	-11	GLN	-	expression tag	UNP P67775
J	-10	GLY	-	expression tag	UNP P67775
J	-9	SER	-	expression tag	UNP P67775
J	-8	TYR	-	expression tag	UNP P67775
J	-7	PRO	-	expression tag	UNP P67775
J	-6	TYR	-	expression tag	UNP P67775
J	-5	ASP	-	expression tag	UNP P67775
J	-4	VAL	-	expression tag	UNP P67775
J	-3	PRO	-	expression tag	UNP P67775
J	-2	ASP	-	expression tag	UNP P67775
J	-1	TYR	-	expression tag	UNP P67775
J	0	ALA	-	expression tag	UNP P67775
K	-26	MET	-	initiating methionine	UNP P67775
K	-25	ASP	-	expression tag	UNP P67775
K	-24	TYR	-	expression tag	UNP P67775
K	-23	LYS	-	expression tag	UNP P67775
K	-22	ASP	-	expression tag	UNP P67775
K	-21	ASP	-	expression tag	UNP P67775
K	-20	ASP	-	expression tag	UNP P67775
K	-19	ASP	-	expression tag	UNP P67775
K	-18	LYS	-	expression tag	UNP P67775
K	-17	GLY	-	expression tag	UNP P67775
K	-16	GLU	-	expression tag	UNP P67775
K	-15	ASN	-	expression tag	UNP P67775
K	-14	LEU	-	expression tag	UNP P67775
K	-13	TYR	-	expression tag	UNP P67775
K	-12	PHE	-	expression tag	UNP P67775
K	-11	GLN	-	expression tag	UNP P67775
K	-10	GLY	-	expression tag	UNP P67775
K	-9	SER	-	expression tag	UNP P67775
K	-8	TYR	-	expression tag	UNP P67775
K	-7	PRO	-	expression tag	UNP P67775
K	-6	TYR	-	expression tag	UNP P67775
K	-5	ASP	-	expression tag	UNP P67775
K	-4	VAL	-	expression tag	UNP P67775

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	PRO	-	expression tag	UNP P67775
K	-2	ASP	-	expression tag	UNP P67775
K	-1	TYR	-	expression tag	UNP P67775
K	0	ALA	-	expression tag	UNP P67775
L	-26	MET	-	initiating methionine	UNP P67775
L	-25	ASP	-	expression tag	UNP P67775
L	-24	TYR	-	expression tag	UNP P67775
L	-23	LYS	-	expression tag	UNP P67775
L	-22	ASP	-	expression tag	UNP P67775
L	-21	ASP	-	expression tag	UNP P67775
L	-20	ASP	-	expression tag	UNP P67775
L	-19	ASP	-	expression tag	UNP P67775
L	-18	LYS	-	expression tag	UNP P67775
L	-17	GLY	-	expression tag	UNP P67775
L	-16	GLU	-	expression tag	UNP P67775
L	-15	ASN	-	expression tag	UNP P67775
L	-14	LEU	-	expression tag	UNP P67775
L	-13	TYR	-	expression tag	UNP P67775
L	-12	PHE	-	expression tag	UNP P67775
L	-11	GLN	-	expression tag	UNP P67775
L	-10	GLY	-	expression tag	UNP P67775
L	-9	SER	-	expression tag	UNP P67775
L	-8	TYR	-	expression tag	UNP P67775
L	-7	PRO	-	expression tag	UNP P67775
L	-6	TYR	-	expression tag	UNP P67775
L	-5	ASP	-	expression tag	UNP P67775
L	-4	VAL	-	expression tag	UNP P67775
L	-3	PRO	-	expression tag	UNP P67775
L	-2	ASP	-	expression tag	UNP P67775
L	-1	TYR	-	expression tag	UNP P67775
L	0	ALA	-	expression tag	UNP P67775
M	-26	MET	-	initiating methionine	UNP P67775
M	-25	ASP	-	expression tag	UNP P67775
M	-24	TYR	-	expression tag	UNP P67775
M	-23	LYS	-	expression tag	UNP P67775
M	-22	ASP	-	expression tag	UNP P67775
M	-21	ASP	-	expression tag	UNP P67775
M	-20	ASP	-	expression tag	UNP P67775
M	-19	ASP	-	expression tag	UNP P67775
M	-18	LYS	-	expression tag	UNP P67775
M	-17	GLY	-	expression tag	UNP P67775
M	-16	GLU	-	expression tag	UNP P67775

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-15	ASN	-	expression tag	UNP P67775
M	-14	LEU	-	expression tag	UNP P67775
M	-13	TYR	-	expression tag	UNP P67775
M	-12	PHE	-	expression tag	UNP P67775
M	-11	GLN	-	expression tag	UNP P67775
M	-10	GLY	-	expression tag	UNP P67775
M	-9	SER	-	expression tag	UNP P67775
M	-8	TYR	-	expression tag	UNP P67775
M	-7	PRO	-	expression tag	UNP P67775
M	-6	TYR	-	expression tag	UNP P67775
M	-5	ASP	-	expression tag	UNP P67775
M	-4	VAL	-	expression tag	UNP P67775
M	-3	PRO	-	expression tag	UNP P67775
M	-2	ASP	-	expression tag	UNP P67775
M	-1	TYR	-	expression tag	UNP P67775
M	0	ALA	-	expression tag	UNP P67775
N	-26	MET	-	initiating methionine	UNP P67775
N	-25	ASP	-	expression tag	UNP P67775
N	-24	TYR	-	expression tag	UNP P67775
N	-23	LYS	-	expression tag	UNP P67775
N	-22	ASP	-	expression tag	UNP P67775
N	-21	ASP	-	expression tag	UNP P67775
N	-20	ASP	-	expression tag	UNP P67775
N	-19	ASP	-	expression tag	UNP P67775
N	-18	LYS	-	expression tag	UNP P67775
N	-17	GLY	-	expression tag	UNP P67775
N	-16	GLU	-	expression tag	UNP P67775
N	-15	ASN	-	expression tag	UNP P67775
N	-14	LEU	-	expression tag	UNP P67775
N	-13	TYR	-	expression tag	UNP P67775
N	-12	PHE	-	expression tag	UNP P67775
N	-11	GLN	-	expression tag	UNP P67775
N	-10	GLY	-	expression tag	UNP P67775
N	-9	SER	-	expression tag	UNP P67775
N	-8	TYR	-	expression tag	UNP P67775
N	-7	PRO	-	expression tag	UNP P67775
N	-6	TYR	-	expression tag	UNP P67775
N	-5	ASP	-	expression tag	UNP P67775
N	-4	VAL	-	expression tag	UNP P67775
N	-3	PRO	-	expression tag	UNP P67775
N	-2	ASP	-	expression tag	UNP P67775
N	-1	TYR	-	expression tag	UNP P67775

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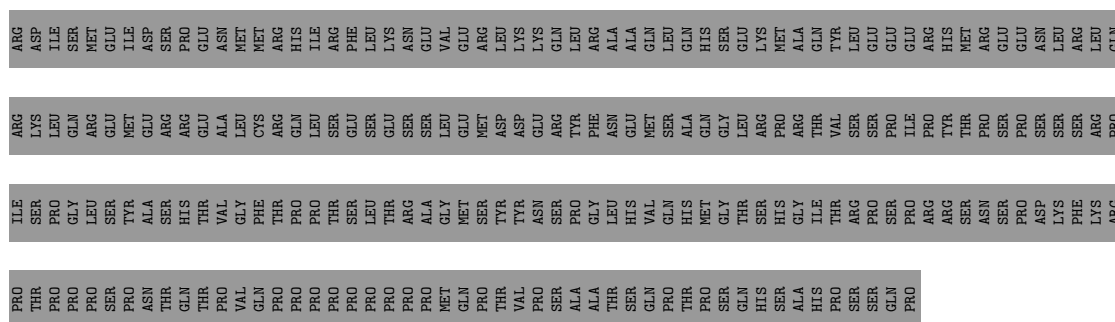
Chain	Residue	Modelled	Actual	Comment	Reference
N	0	ALA	-	expression tag	UNP P67775

- Molecule 4 is a protein called SKP1.

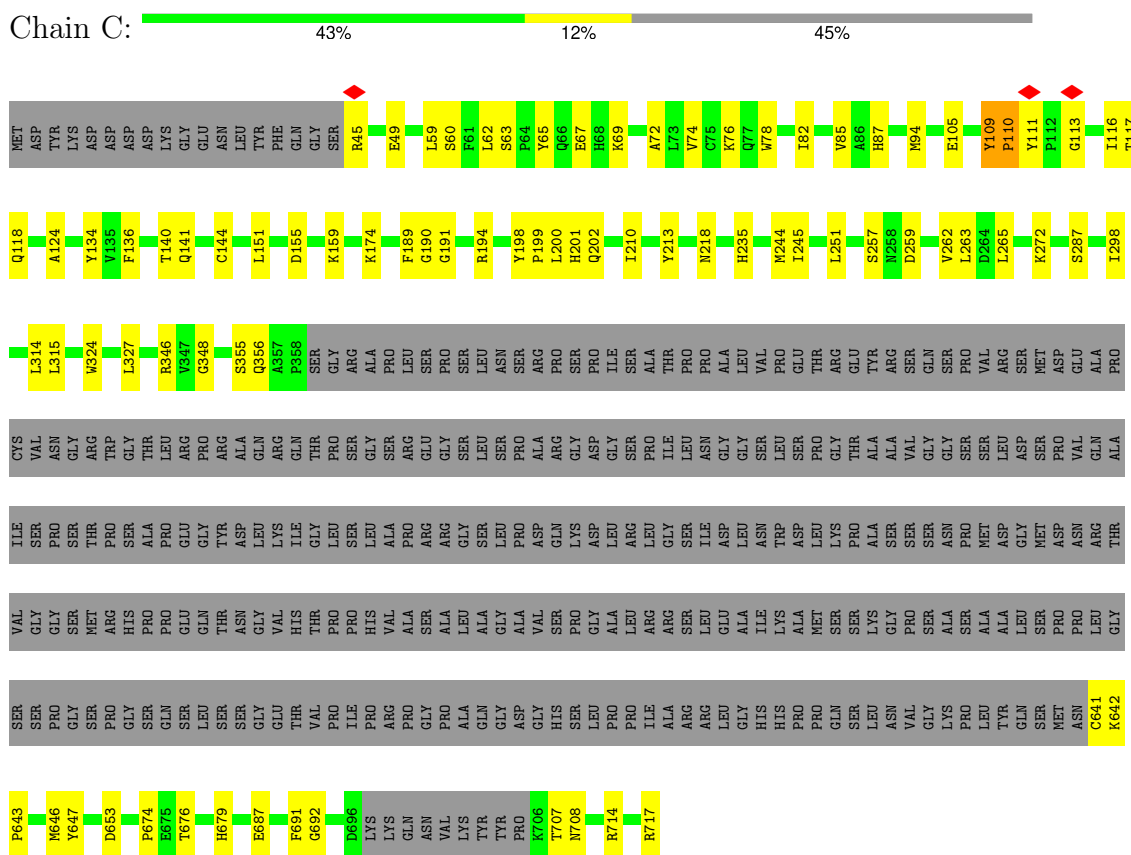
Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	136	Total	C	N	O	S	0	0
			1092	696	177	214	5		
4	H	136	Total	C	N	O	S	0	0
			1092	696	177	214	5		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

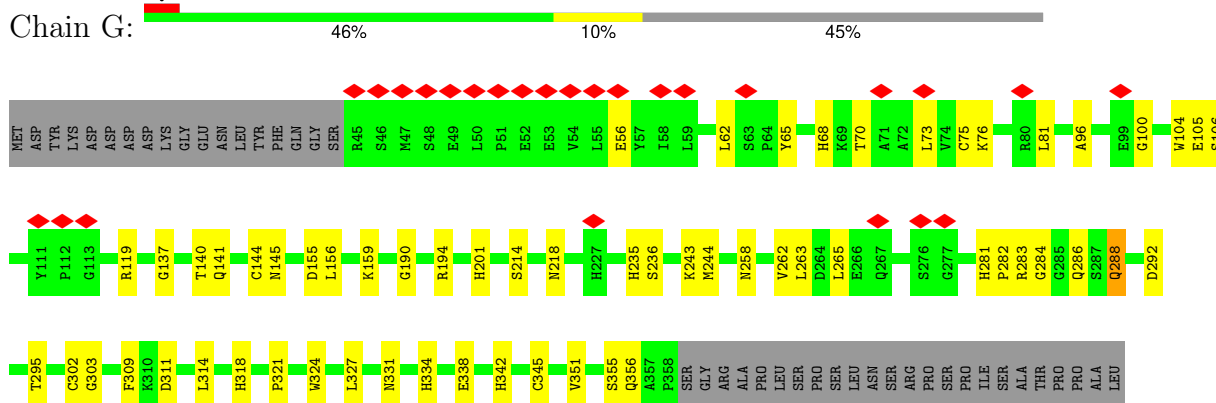
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mn	0
			1	1	
5	D	2	Total	Mn	0
			2	2	
5	E	2	Total	Mn	0
			2	2	
5	I	2	Total	Mn	0
			2	2	
5	J	2	Total	Mn	0
			2	2	
5	K	2	Total	Mn	0
			2	2	
5	L	2	Total	Mn	0
			2	2	
5	M	1	Total	Mn	0
			1	1	
5	N	2	Total	Mn	0
			2	2	

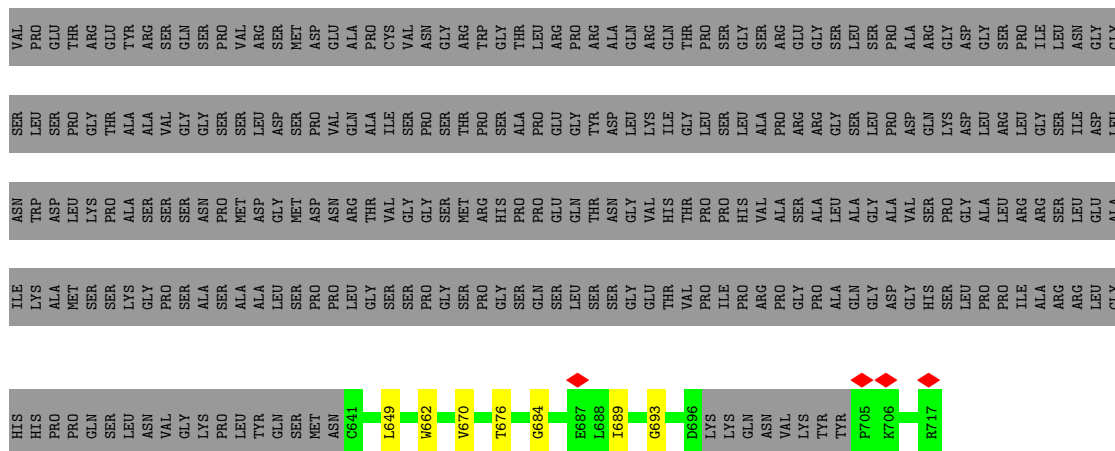


- Molecule 2: F-box only protein 42

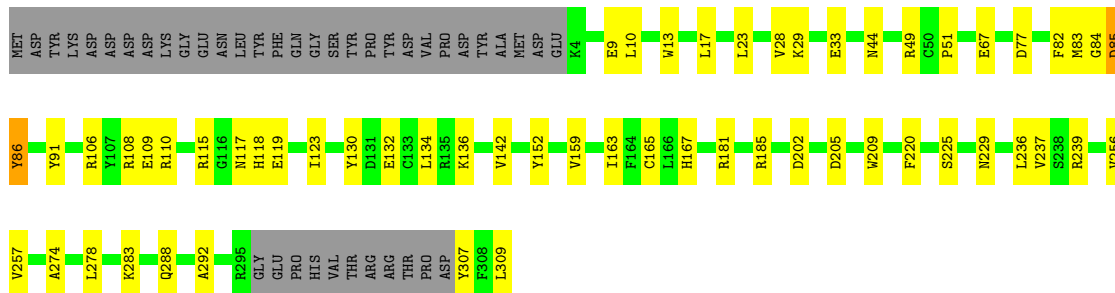


- Molecule 2: F-box only protein 42

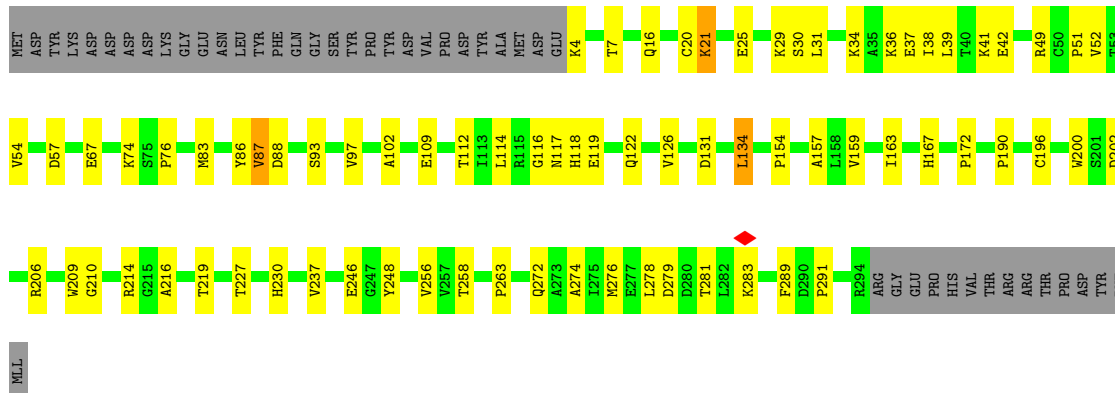




- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

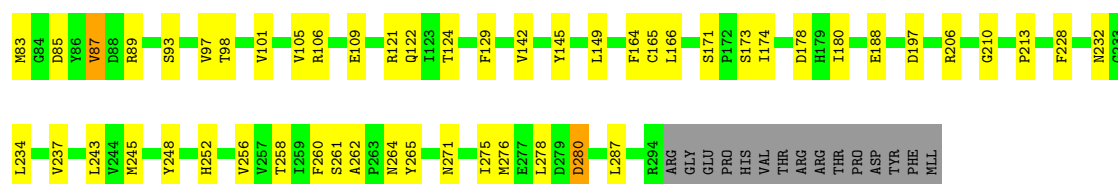


- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



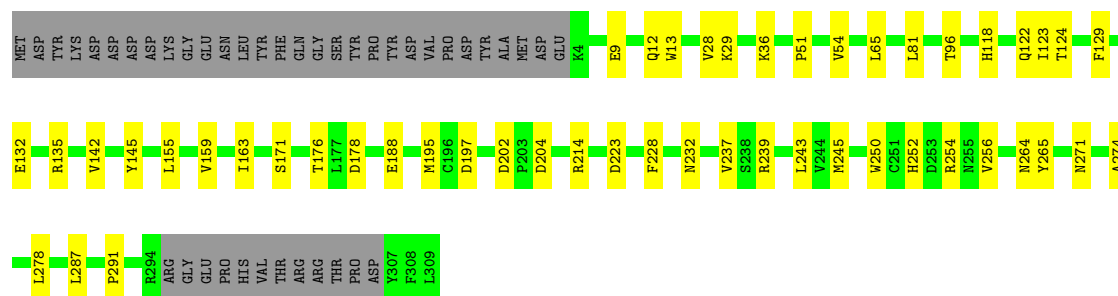
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform





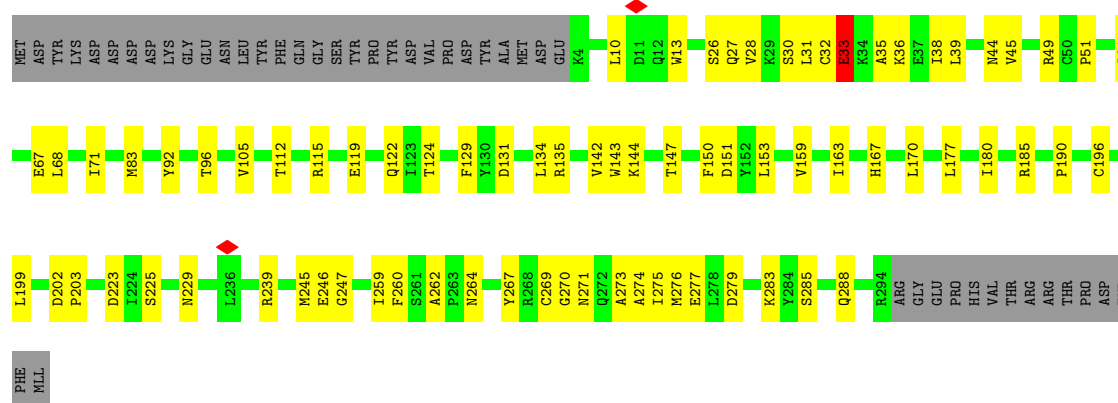
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain J: 73% 15% 12%



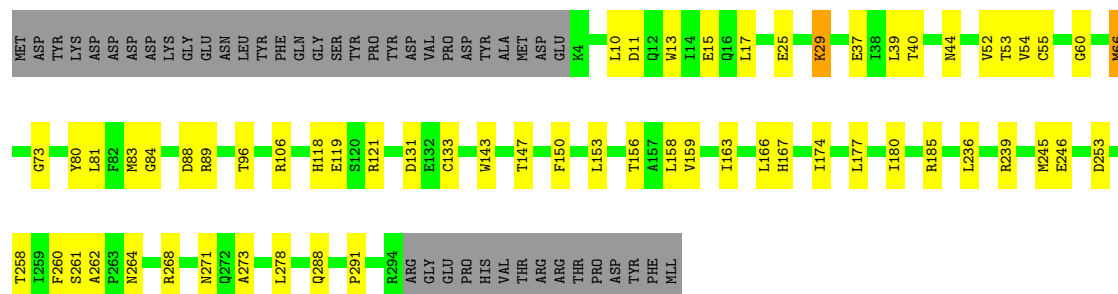
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain K: 64% 23% 13%



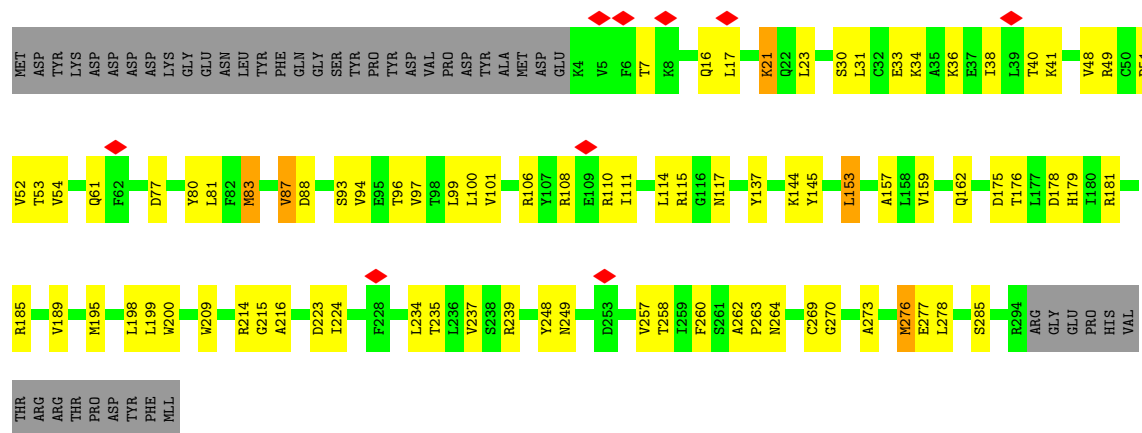
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain L: 68% 18% 13%



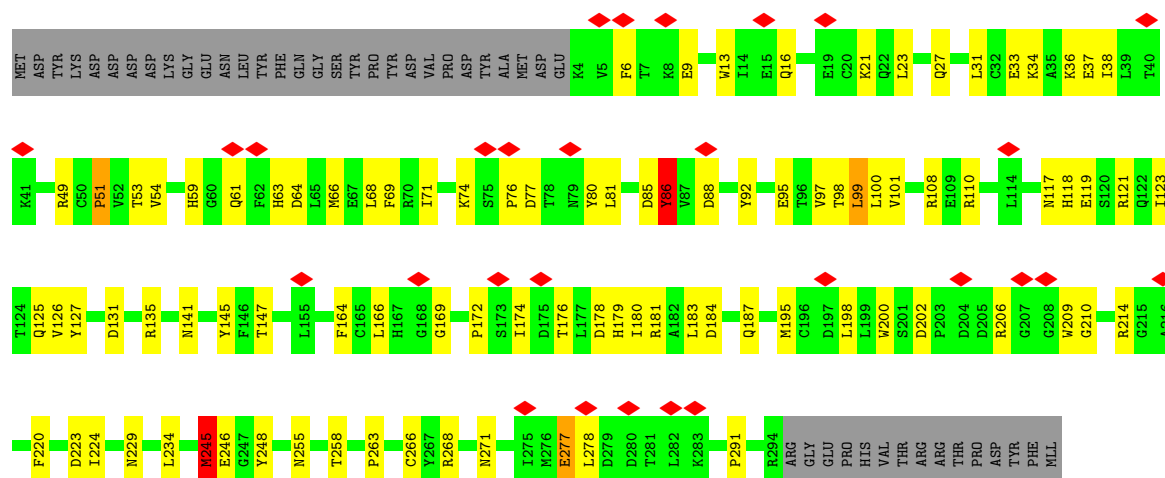
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain M: 



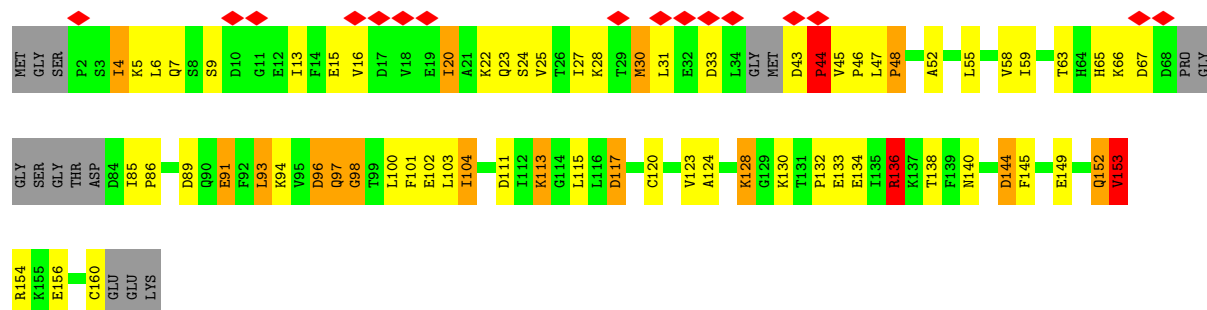
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain N: 

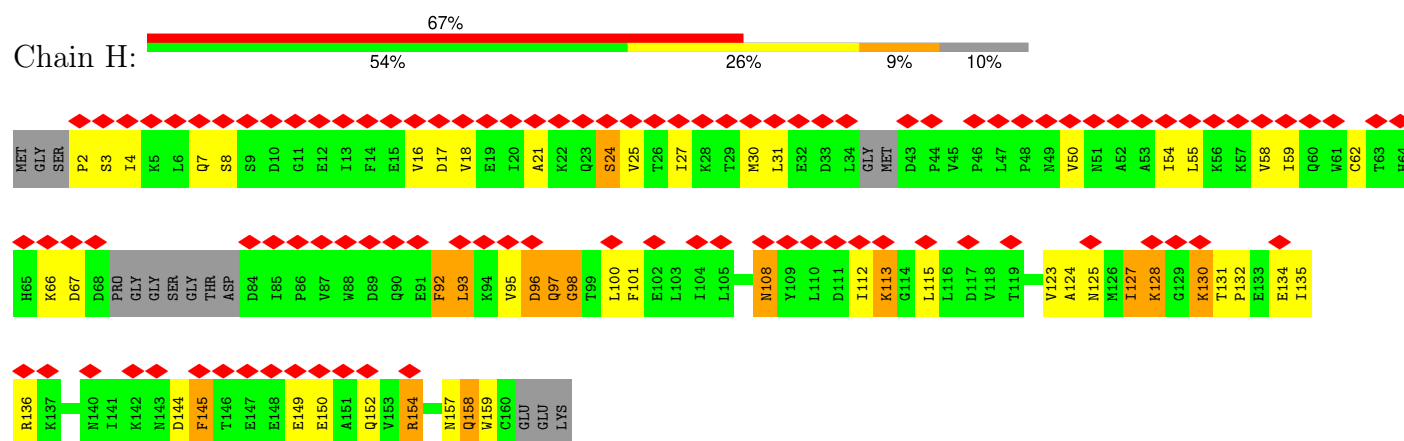


- Molecule 4: SKP1

Chain F: 



- Molecule 4: SKP1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	155244	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	60.354	Depositor
Minimum map value	-41.314	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.067	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	402.24, 402.24, 402.24	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.838, 0.838, 0.838	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.42	0/1145	0.80	1/1526 (0.1%)
1	B	0.33	0/1118	0.76	0/1490
2	C	0.31	0/3128	0.62	2/4256 (0.0%)
2	G	0.25	0/3136	0.60	0/4267
3	D	0.24	0/2449	0.56	0/3318
3	E	0.32	0/2401	0.84	6/3257 (0.2%)
3	I	0.27	0/2401	0.71	2/3257 (0.1%)
3	J	0.24	0/2425	0.59	0/3288
3	K	0.32	0/2401	0.85	2/3257 (0.1%)
3	L	0.29	0/2401	0.75	3/3257 (0.1%)
3	M	0.32	0/2401	0.87	5/3257 (0.2%)
3	N	0.39	0/2401	1.00	11/3257 (0.3%)
4	F	0.56	1/1109 (0.1%)	1.59	26/1499 (1.7%)
4	H	0.56	0/1109	1.55	22/1499 (1.5%)
All	All	0.33	1/30025 (0.0%)	0.84	80/40685 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	1
4	F	0	1
4	H	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	44	PRO	N-CD	6.25	1.56	1.47

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	86	TYR	N-CA-C	21.98	141.69	112.90
4	F	97	GLN	N-CA-C	21.36	140.06	112.72
4	H	97	GLN	N-CA-C	19.87	136.79	112.54
4	F	23	GLN	N-CA-C	17.93	133.02	111.33
4	H	97	GLN	CB-CA-C	-17.16	74.44	110.31
4	H	96	ASP	CB-CA-C	-15.02	78.55	109.65
4	F	140	ASN	CB-CA-C	-11.96	86.62	110.42
4	H	159	TRP	N-CA-CB	-11.92	93.13	110.65
4	H	158	GLN	CB-CA-C	10.91	132.13	110.42
4	F	97	GLN	CB-CA-C	-10.77	92.70	110.37
4	H	93	LEU	N-CA-CB	-10.61	98.15	110.35
4	H	97	GLN	N-CA-CB	-10.10	93.63	110.39
4	H	108	ASN	N-CA-C	10.01	121.95	111.14
4	H	92	PHE	CA-CB-CG	9.88	123.68	113.80
4	F	23	GLN	CB-CA-C	-9.47	94.58	110.68
3	N	86	TYR	CB-CA-C	-9.36	90.87	109.67
4	F	133	GLU	N-CA-C	9.21	120.92	111.07
3	K	33	GLU	CA-CB-CG	9.10	132.31	114.10
4	F	152	GLN	N-CA-C	8.95	124.32	113.23
4	H	113	LYS	N-CA-C	8.82	120.58	110.97
2	C	110	PRO	CB-CA-C	-8.54	97.47	111.56
4	H	96	ASP	N-CA-CB	-8.31	98.38	110.26
4	H	96	ASP	CA-CB-CG	8.10	120.69	112.60
4	F	152	GLN	CB-CA-C	-7.83	93.66	109.55
4	F	96	ASP	N-CA-C	7.66	122.66	111.02
4	H	108	ASN	CB-CA-C	-7.46	99.11	110.90
3	M	185	ARG	CA-CB-CG	7.41	128.91	114.10
3	N	277	GLU	CA-CB-CG	7.40	128.90	114.10
4	F	133	GLU	CB-CA-C	-7.18	99.61	110.88
3	N	99	LEU	CA-CB-CG	6.63	139.50	116.30
4	F	128	LYS	N-CA-C	6.56	120.74	112.87
4	F	113	LYS	N-CA-C	6.54	121.18	111.96
4	H	159	TRP	N-CA-C	6.54	122.22	113.72
3	N	85	ASP	N-CA-C	6.41	120.02	111.30
3	N	33	GLU	CA-CB-CG	6.28	126.67	114.10
3	E	134	LEU	CA-CB-CG	6.22	138.06	116.30
4	F	20	ILE	N-CA-C	-6.21	106.38	111.91
4	H	24	SER	CA-C-N	6.16	128.54	120.60
4	H	24	SER	C-N-CA	6.16	128.54	120.60
3	N	246	GLU	CA-CB-CG	6.12	126.34	114.10
3	E	20	CYS	CA-CB-SG	5.93	128.05	114.40
4	F	98	GLY	CA-C-N	5.87	128.61	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	98	GLY	C-N-CA	5.87	128.61	120.63
3	L	84	GLY	N-CA-C	5.87	123.75	115.30
4	F	4	ILE	N-CA-C	5.79	121.39	109.34
3	N	33	GLU	N-CA-CB	5.75	118.58	110.12
3	K	33	GLU	N-CA-CB	5.72	118.62	110.16
3	M	145	TYR	CA-CB-CG	5.69	124.14	113.90
4	H	113	LYS	CB-CA-C	-5.68	102.21	110.96
3	L	66	MET	CB-CG-SD	5.58	129.45	112.70
1	A	195	LEU	N-CA-C	-5.58	105.20	111.28
4	F	91	GLU	CA-CB-CG	5.56	125.23	114.10
4	H	24	SER	N-CA-C	-5.56	98.28	108.02
4	H	3	SER	N-CA-C	5.51	118.11	108.52
3	L	29	LYS	CA-CB-CG	5.46	125.03	114.10
3	E	29	LYS	CA-CB-CG	5.42	124.94	114.10
4	F	48	PRO	N-CA-C	-5.37	107.64	114.35
3	E	87	VAL	N-CA-C	5.35	114.50	106.42
3	E	36	LYS	CA-CB-CG	5.35	124.80	114.10
3	M	21	LYS	CA-CB-CG	5.33	124.76	114.10
4	F	153	VAL	N-CA-C	-5.32	98.27	109.34
3	I	87	VAL	CG1-CB-CG2	-5.32	99.11	110.80
3	N	51	PRO	CA-N-CD	-5.28	104.61	112.00
4	H	98	GLY	N-CA-C	-5.27	106.02	112.77
4	H	92	PHE	N-CA-C	-5.25	106.00	112.72
3	E	86	TYR	N-CA-C	5.25	117.08	111.36
3	M	144	LYS	CA-CB-CG	5.23	124.56	114.10
4	H	98	GLY	O-C-N	5.21	127.24	122.19
4	F	113	LYS	CA-C-N	5.17	125.68	119.94
4	F	113	LYS	C-N-CA	5.17	125.68	119.94
3	N	245	MET	CB-CG-SD	5.17	128.22	112.70
2	C	109	TYR	CB-CA-C	5.15	120.32	110.17
4	F	140	ASN	CA-C-N	5.15	128.92	122.43
4	F	140	ASN	C-N-CA	5.15	128.92	122.43
3	M	276	MET	CB-CG-SD	5.15	128.15	112.70
3	I	21	LYS	CB-CG-CD	5.13	123.11	111.30
4	F	124	ALA	CA-C-N	5.09	127.42	120.54
4	F	124	ALA	C-N-CA	5.09	127.42	120.54
3	N	245	MET	CA-CB-CG	5.09	124.27	114.10
4	F	136	ARG	N-CA-C	-5.07	106.84	112.57

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	136	ARG	Sidechain
4	H	136	ARG	Sidechain
4	H	154	ARG	Sidechain
3	N	86	TYR	Mainchain

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	1136	0	1157	23	0
1	B	1110	0	1136	26	0
2	C	3029	0	2932	60	0
2	G	3036	0	2940	43	0
3	D	2401	0	2301	33	0
3	E	2344	0	2245	43	0
3	I	2344	0	2245	42	0
3	J	2377	0	2272	30	0
3	K	2344	0	2245	51	0
3	L	2344	0	2245	34	0
3	M	2344	0	2245	53	0
3	N	2344	0	2245	69	0
4	F	1092	0	1096	57	0
4	H	1092	0	1096	38	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	I	2	0	0	0	0
5	J	2	0	0	0	0
5	K	2	0	0	0	0
5	L	2	0	0	0	0
5	M	1	0	0	0	0
5	N	2	0	0	0	0
All	All	29353	0	28400	560	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 10.

All (560) 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:F:97:GLN:O	4:F:101:PHE:CE2	1.99	1.14
4:F:97:GLN:O	4:F:101:PHE:CD2	2.15	0.98
4:F:97:GLN:O	4:F:101:PHE:HE2	1.48	0.90
1:B:211:GLU:HG2	3:M:214:ARG:HH21	1.42	0.85
4:F:98:GLY:O	4:F:102:GLU:HG2	1.77	0.84
4:F:5:LYS:HB2	4:F:44:PRO:HG3	1.58	0.84
4:H:130:LYS:HB3	4:H:135:ILE:HG13	1.59	0.82
3:N:206:ARG:HH22	3:N:210:GLY:HA3	1.47	0.78
4:F:7:GLN:HG3	4:F:44:PRO:HB2	1.66	0.78
3:M:248:TYR:HA	3:M:258:THR:O	1.82	0.78
3:E:248:TYR:HA	3:E:258:THR:O	1.86	0.76
4:F:6:LEU:HD12	4:F:45:VAL:HB	1.68	0.76
4:F:113:LYS:O	4:F:117:ASP:OD1	2.03	0.76
3:L:121:ARG:HG3	3:L:147:THR:HG21	1.68	0.75
4:F:5:LYS:O	4:F:44:PRO:HA	1.87	0.75
2:G:68:HIS:HB3	4:H:158:GLN:OE1	1.89	0.73
4:F:152:GLN:O	4:F:152:GLN:HG3	1.88	0.72
2:G:73:LEU:HD22	4:H:154:ARG:HE	1.54	0.71
4:F:52:ALA:HA	4:F:55:LEU:HB2	1.71	0.71
3:N:51:PRO:HA	3:N:278:LEU:O	1.91	0.71
3:N:59:HIS:HD2	3:N:88:ASP:HB3	1.54	0.70
3:E:16:GLN:O	3:E:21:LYS:NZ	2.24	0.69
3:M:51:PRO:HA	3:M:278:LEU:O	1.93	0.69
3:N:248:TYR:HA	3:N:258:THR:O	1.94	0.68
1:A:200:ILE:HD12	3:N:245:MET:HB2	1.75	0.67
2:C:198:TYR:HA	2:C:200:LEU:H	1.58	0.67
3:I:83:MET:HE1	3:I:165:CYS:HB3	1.78	0.66
4:F:25:VAL:HB	4:F:111:ASP:HB3	1.76	0.66
1:A:211:GLU:OE1	3:N:214:ARG:NH1	2.30	0.65
4:F:89:ASP:O	4:F:93:LEU:HB2	1.97	0.65
3:L:10:LEU:HD21	3:L:106:ARG:HB2	1.77	0.65
3:D:237:VAL:HB	3:D:256:VAL:HG12	1.79	0.65
2:G:73:LEU:HD11	4:H:150:GLU:HG3	1.79	0.65
3:E:206:ARG:HH22	3:E:210:GLY:HA3	1.62	0.64
1:B:191:THR:O	1:B:194:GLN:HB3	1.97	0.64
4:F:152:GLN:O	4:F:156:GLU:HG2	1.98	0.64
2:C:62:LEU:HA	4:F:128:LYS:HZ1	1.63	0.63
4:F:152:GLN:O	4:F:152:GLN:CG	2.45	0.63
4:H:4:ILE:HB	4:H:31:LEU:HD11	1.80	0.63
3:N:266:CYS:HB3	3:N:268:ARG:HE	1.63	0.63
2:G:201:HIS:HB3	3:J:135:ARG:HH21	1.64	0.63
3:N:121:ARG:HG3	3:N:147:THR:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASN:O	1:A:186:ILE:HG12	1.99	0.62
4:H:98:GLY:HA2	4:H:101:PHE:CD2	2.35	0.62
1:A:121:GLN:NE2	3:K:122:GLN:OE1	2.32	0.62
1:B:206:LEU:HD21	3:N:268:ARG:HH12	1.65	0.62
2:C:155:ASP:O	2:C:159:LYS:N	2.33	0.62
3:I:87:VAL:HG11	3:I:97:VAL:HB	1.82	0.62
2:G:214:SER:O	2:G:218:ASN:N	2.33	0.62
3:L:60:GLY:HA2	3:L:96:THR:HG21	1.81	0.62
3:N:209:TRP:HE1	3:N:220:PHE:HB3	1.65	0.62
3:N:9:GLU:OE2	3:N:34:LYS:NZ	2.34	0.61
3:M:48:VAL:HB	3:M:159:VAL:HG22	1.81	0.61
2:C:45:ARG:HG2	2:C:49:GLU:HG2	1.82	0.61
2:C:105:GLU:OE1	2:C:714:ARG:NH2	2.33	0.61
3:N:172:PRO:HB3	3:N:209:TRP:HZ3	1.66	0.61
3:E:237:VAL:HB	3:E:256:VAL:HG12	1.82	0.60
3:E:281:THR:HG23	3:E:283:LYS:HG2	1.83	0.60
3:D:28:VAL:HG11	3:D:142:VAL:HG13	1.82	0.60
3:N:59:HIS:CD2	3:N:88:ASP:HB3	2.33	0.60
4:F:22:LYS:HA	4:F:31:LEU:HD11	1.84	0.60
3:L:245:MET:HA	3:L:271:ASN:HB2	1.82	0.60
2:C:87:HIS:ND1	4:F:160:CYS:SG	2.69	0.60
2:C:69:LYS:HD2	4:F:154:ARG:HD2	1.83	0.60
3:J:28:VAL:HG11	3:J:142:VAL:HG13	1.84	0.60
2:C:63:SER:H	4:F:128:LYS:NZ	1.99	0.60
1:A:138:GLU:OE1	3:L:89:ARG:NH2	2.34	0.60
1:A:138:GLU:HG3	1:B:138:GLU:HG2	1.82	0.60
3:L:239:ARG:NH1	3:L:258:THR:OG1	2.35	0.60
3:M:80:TYR:HB2	3:M:111:ILE:HG22	1.84	0.60
3:L:44:ASN:OD1	3:L:185:ARG:NH1	2.35	0.59
3:M:209:TRP:HE1	3:M:224:ILE:HG21	1.67	0.59
3:N:69:PHE:HE2	3:N:74:LYS:HA	1.66	0.59
2:C:245:ILE:HG13	2:C:262:VAL:HG22	1.84	0.59
1:B:206:LEU:HD21	3:N:268:ARG:HH22	1.67	0.59
1:B:206:LEU:HA	1:B:209:GLU:HB3	1.84	0.59
3:D:225:SER:O	3:D:229:ASN:ND2	2.30	0.59
3:K:38:ILE:HD13	3:K:105:VAL:HG12	1.84	0.59
2:C:641:CYS:SG	2:C:642:LYS:N	2.75	0.59
3:J:202:ASP:OD1	3:J:239:ARG:NH2	2.36	0.59
4:H:124:ALA:O	4:H:128:LYS:N	2.33	0.58
4:H:2:PRO:HG2	4:H:31:LEU:HD22	1.83	0.58
3:I:280:ASP:OD1	3:I:280:ASP:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:16:GLN:HG3	3:N:21:LYS:HB2	1.85	0.58
1:A:194:GLN:O	1:A:198:GLU:N	2.33	0.58
3:K:28:VAL:HG11	3:K:142:VAL:HG13	1.85	0.58
3:M:7:THR:O	3:M:106:ARG:NH1	2.36	0.58
3:J:171:SER:HB3	3:J:197:ASP:HB2	1.86	0.58
3:N:117:ASN:HB2	3:N:200:TRP:HE1	1.69	0.58
2:C:94:MET:HE3	2:C:348:GLY:HA3	1.85	0.58
3:I:174:ILE:HG21	3:I:180:ILE:HG13	1.86	0.58
3:K:159:VAL:HB	3:K:163:ILE:HB	1.85	0.58
3:J:9:GLU:OE2	3:J:13:TRP:NE1	2.37	0.58
3:N:38:ILE:HG23	3:N:108:ARG:HD2	1.86	0.58
3:L:54:VAL:HG22	3:L:81:LEU:HD22	1.85	0.58
3:L:39:LEU:HD12	3:L:153:LEU:HA	1.86	0.57
3:E:131:ASP:HA	3:E:134:LEU:HD23	1.86	0.57
4:H:157:ASN:O	4:H:158:GLN:HG3	2.04	0.57
4:F:97:GLN:O	4:F:101:PHE:HD2	1.81	0.57
3:J:228:PHE:O	3:J:232:ASN:ND2	2.32	0.57
3:D:77:ASP:O	3:D:110:ARG:NH2	2.34	0.57
3:I:237:VAL:HB	3:I:256:VAL:HG12	1.87	0.56
3:E:87:VAL:HG12	3:E:93:SER:HB3	1.87	0.56
2:G:676:THR:HB	2:G:693:GLY:HA3	1.88	0.56
3:L:264:ASN:HB2	3:L:291:PRO:HG3	1.88	0.56
3:L:83:MET:O	3:L:167:HIS:ND1	2.36	0.56
4:H:4:ILE:HD13	4:H:31:LEU:HD21	1.88	0.56
3:J:54:VAL:HG22	3:J:81:LEU:HD22	1.88	0.56
3:K:147:THR:HA	3:K:150:PHE:HB2	1.88	0.56
3:E:206:ARG:NH2	3:E:219:THR:OG1	2.39	0.55
3:J:51:PRO:HA	3:J:278:LEU:O	2.05	0.55
3:D:9[A]:GLU:OE2	3:D:13:TRP:NE1	2.39	0.55
2:G:62:LEU:HD23	4:H:128:LYS:HZ3	1.71	0.55
3:K:247:GLY:HA3	3:K:274:ALA:HB3	1.88	0.55
3:K:269:CYS:SG	3:K:270:GLY:N	2.79	0.55
3:N:174:ILE:HG12	3:N:179:HIS:HB3	1.88	0.55
3:E:248:TYR:H	3:E:274:ALA:HB3	1.72	0.55
3:K:259:ILE:HD11	3:K:276:MET:HE3	1.86	0.55
2:C:201:HIS:HE2	3:D:91:TYR:HA	1.72	0.55
3:E:4:LYS:O	3:E:7:THR:OG1	2.25	0.55
3:E:83:MET:O	3:E:167:HIS:ND1	2.35	0.55
1:B:157:ALA:HA	3:J:245:MET:HE3	1.88	0.55
2:C:144:CYS:HA	2:C:194:ARG:HD2	1.88	0.55
3:J:176:THR:HG22	3:J:178:ASP:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:141:GLN:OE1	2:G:145:ASN:ND2	2.40	0.54
3:J:223:ASP:OD1	3:J:223:ASP:N	2.39	0.54
2:C:69:LYS:HD2	4:F:154:ARG:HA	1.88	0.54
4:H:145:PHE:HB3	4:H:149:GLU:HG2	1.89	0.54
3:E:202:ASP:OD2	3:E:202:ASP:N	2.41	0.54
2:G:314:LEU:O	2:G:324:TRP:HA	2.07	0.54
3:I:206:ARG:HH21	3:I:210:GLY:HA3	1.73	0.54
3:K:13:TRP:NE1	3:K:27:GLN:OE1	2.40	0.54
4:F:91:GLU:HA	4:F:94:LYS:HG2	1.90	0.54
2:G:351:VAL:HG22	2:G:649:LEU:HB3	1.90	0.54
2:C:110:PRO:O	2:C:113:GLY:N	2.30	0.54
3:I:275:ILE:HG12	3:I:287:LEU:HB2	1.89	0.54
3:E:31:LEU:HD21	3:E:102:ALA:HB2	1.89	0.53
3:M:223:ASP:OD2	3:M:224:ILE:N	2.40	0.53
3:N:164:PHE:HB2	3:N:234:LEU:HD22	1.89	0.53
4:F:6:LEU:HD12	4:F:45:VAL:H	1.74	0.53
3:E:117:ASN:OD1	3:E:200:TRP:NE1	2.41	0.53
3:L:163:ILE:HG23	3:L:236:LEU:HB3	1.91	0.53
3:E:227:THR:HA	3:E:230:HIS:CD2	2.43	0.53
2:C:76:LYS:NZ	4:F:144:ASP:O	2.42	0.53
2:C:60:SER:O	2:C:717:ARG:NH1	2.35	0.53
1:A:112:ILE:HD12	3:E:126:VAL:HG13	1.90	0.53
4:H:108:ASN:OD1	4:H:108:ASN:C	2.52	0.53
4:F:55:LEU:O	4:F:59:ILE:HG12	2.09	0.52
2:G:105:GLU:HG2	2:G:106:SER:H	1.74	0.52
3:N:184:ASP:OD1	3:N:187:GLN:NE2	2.42	0.52
3:N:88:ASP:HB2	3:N:118:HIS:CD2	2.44	0.52
1:B:168:GLU:OE1	3:J:214:ARG:NH1	2.41	0.52
4:F:120:CYS:HA	4:F:123:VAL:HG12	1.91	0.52
3:M:115:ARG:HD2	3:M:153:LEU:HB2	1.92	0.52
3:N:245:MET:HA	3:N:271:ASN:HD22	1.73	0.52
3:E:49:ARG:NH2	3:E:109:GLU:OE1	2.42	0.52
3:M:33:GLU:OE1	3:M:36:LYS:NZ	2.41	0.52
2:C:653:ASP:N	2:C:653:ASP:OD1	2.43	0.52
3:I:17:LEU:HD11	3:I:98:THR:HB	1.91	0.52
4:F:65:HIS:HE1	4:F:86:PRO:HG2	1.74	0.52
3:M:87:VAL:HG21	3:M:93:SER:HA	1.92	0.52
3:M:195:MET:HA	3:M:198:LEU:HG	1.92	0.52
2:C:72:ALA:HB2	2:C:82:ILE:HG21	1.92	0.51
4:H:66:LYS:HG3	4:H:67:ASP:H	1.76	0.51
3:M:83:MET:HE1	3:M:239:ARG:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:TYR:HA	2:C:200:LEU:N	2.26	0.51
3:E:88:ASP:OD1	3:E:118:HIS:HB3	2.10	0.51
4:H:108:ASN:OD1	4:H:108:ASN:O	2.29	0.51
3:K:223:ASP:N	3:K:223:ASP:OD1	2.41	0.51
3:E:74:LYS:HG3	3:E:76:PRO:HD2	1.93	0.51
3:E:159:VAL:O	3:E:163:ILE:HB	2.11	0.51
3:L:246:GLU:N	3:L:246:GLU:OE1	2.43	0.51
2:C:82:ILE:HA	2:C:85:VAL:HG12	1.92	0.51
2:G:338:GLU:O	2:G:342:HIS:ND1	2.43	0.51
1:B:201:ASP:O	1:B:205:THR:OG1	2.28	0.51
4:F:6:LEU:HD12	4:F:45:VAL:CB	2.40	0.51
4:F:9:SER:HB2	4:F:48:PRO:HA	1.93	0.51
3:M:263:PRO:HD3	3:M:273:ALA:HB2	1.93	0.51
3:K:115:ARG:HB2	3:K:153:LEU:HB2	1.91	0.51
3:I:121:ARG:NH1	3:I:188:GLU:OE1	2.40	0.51
3:I:228:PHE:O	3:I:232:ASN:ND2	2.43	0.51
3:L:159:VAL:HG13	3:L:163:ILE:HB	1.92	0.51
3:M:94:VAL:HG11	3:M:137:TYR:HE1	1.76	0.51
2:G:119:ARG:NH1	2:G:137:GLY:O	2.44	0.51
4:H:97:GLN:O	4:H:100:LEU:HB2	2.10	0.51
2:C:117:THR:HG22	2:C:118:GLN:H	1.76	0.50
3:I:87:VAL:HB	3:I:93:SER:HB3	1.92	0.50
4:F:7:GLN:HA	4:F:13:ILE:HG23	1.93	0.50
3:J:245:MET:HA	3:J:271:ASN:HB2	1.93	0.50
3:D:82:PHE:HB3	3:D:86:TYR:CE1	2.46	0.50
3:I:171:SER:HB3	3:I:197:ASP:HB3	1.93	0.50
3:N:63:HIS:HA	3:N:66:MET:HG3	1.93	0.50
2:C:287:SER:O	2:C:298:ILE:HA	2.12	0.50
3:K:279:ASP:OD1	3:K:279:ASP:N	2.44	0.50
3:J:65:LEU:HD22	3:J:96:THR:HG23	1.93	0.50
3:E:263:PRO:HB2	3:E:291:PRO:HD3	1.94	0.50
4:H:92:PHE:HB3	4:H:93:LEU:HD12	1.94	0.50
1:B:197:ARG:HE	1:B:200:ILE:HD12	1.76	0.50
1:A:92:ARG:HA	1:A:95:ARG:HB3	1.93	0.50
3:D:132:GLU:OE2	3:D:136:LYS:NZ	2.44	0.50
3:D:236:LEU:HD11	3:D:257:VAL:HG12	1.93	0.50
3:N:166:LEU:HB2	3:N:198:LEU:HD21	1.94	0.50
3:N:266:CYS:O	3:N:268:ARG:HD3	2.11	0.50
3:D:10:LEU:HD22	3:D:106:ARG:HB2	1.94	0.49
3:L:13:TRP:O	3:L:17:LEU:HD12	2.11	0.49
3:M:176:THR:HG22	3:M:178:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:28:VAL:HG11	3:I:142:VAL:HG13	1.94	0.49
3:M:31:LEU:HA	3:M:34:LYS:NZ	2.27	0.49
3:N:54:VAL:HG13	3:N:81:LEU:HD23	1.94	0.49
3:N:76:PRO:O	3:N:110:ARG:NH1	2.45	0.49
3:N:176:THR:HG22	3:N:178:ASP:H	1.77	0.49
3:M:97:VAL:O	3:M:101:VAL:HG22	2.12	0.49
3:E:116:GLY:H	3:E:119:GLU:CD	2.20	0.49
3:E:246:GLU:N	3:E:246:GLU:OE1	2.46	0.49
3:D:152:TYR:O	3:D:185:ARG:NH1	2.45	0.49
3:E:37:GLU:O	3:E:41:LYS:HG2	2.13	0.49
3:N:121:ARG:O	3:N:125:GLN:NE2	2.43	0.49
2:G:155:ASP:O	2:G:159:LYS:N	2.44	0.49
2:G:236:SER:HB2	2:G:288:GLN:HG2	1.94	0.49
4:H:21:ALA:O	4:H:24:SER:O	2.31	0.49
3:K:112:THR:O	3:K:112:THR:OG1	2.30	0.49
1:A:182:GLU:O	1:A:186:ILE:HG23	2.13	0.49
4:H:7:GLN:HG2	4:H:8:SER:H	1.78	0.49
3:M:48:VAL:HG12	3:M:52:VAL:HG21	1.95	0.49
2:C:174:LYS:HD3	2:C:191:GLY:HA3	1.95	0.49
3:E:200:TRP:CD2	3:E:216:ALA:HB3	2.48	0.49
3:I:23:LEU:HD13	3:I:98:THR:HG21	1.95	0.48
3:K:119:GLU:OE1	3:K:119:GLU:N	2.46	0.48
1:B:137:GLU:OE1	3:L:268:ARG:NH2	2.38	0.48
1:A:194:GLN:HB3	1:A:198:GLU:HG2	1.96	0.48
4:F:145:PHE:HD1	4:F:149:GLU:HG3	1.78	0.48
3:D:44:ASN:HB2	3:D:181:ARG:HA	1.96	0.48
4:F:100:LEU:HA	4:F:103:LEU:HD12	1.94	0.48
2:G:70:THR:HG23	4:H:132:PRO:HD3	1.94	0.48
3:N:86:TYR:HB2	3:N:119:GLU:OE2	2.14	0.48
2:G:75:CYS:SG	2:G:76:LYS:N	2.85	0.48
3:I:51:PRO:HA	3:I:278:LEU:O	2.13	0.48
3:N:126:VAL:HG23	3:N:127:TYR:HD1	1.78	0.48
2:G:355:SER:OG	2:G:356:GLN:N	2.45	0.48
3:I:10:LEU:HD23	3:I:106:ARG:HB2	1.96	0.48
1:B:121:GLN:NE2	3:E:122:GLN:OE1	2.47	0.48
2:C:116:ILE:HG21	2:C:691:PHE:HZ	1.78	0.48
3:D:202:ASP:OD1	3:D:239:ARG:NH2	2.47	0.48
3:E:25:GLU:OE1	3:E:25:GLU:N	2.47	0.48
3:N:37:GLU:HG3	3:N:38:ILE:HD13	1.96	0.48
3:N:172:PRO:HB3	3:N:209:TRP:CZ3	2.47	0.48
2:C:109:TYR:HB2	2:C:113:GLY:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:244:MET:HB2	2:C:265:LEU:HD21	1.95	0.47
4:H:149:GLU:HA	4:H:152:GLN:HG3	1.96	0.47
4:H:55:LEU:O	4:H:59:ILE:HG12	2.15	0.47
3:M:117:ASN:HA	3:M:199:LEU:HD23	1.96	0.47
4:F:5:LYS:HA	4:F:15:GLU:HA	1.95	0.47
2:C:676:THR:O	2:C:679:HIS:ND1	2.47	0.47
3:M:96:THR:O	3:M:100:LEU:HG	2.14	0.47
3:D:49:ARG:HA	3:D:49:ARG:HD3	1.75	0.47
3:J:237:VAL:HB	3:J:256:VAL:HG22	1.96	0.47
3:K:264:ASN:N	3:K:271:ASN:OD1	2.47	0.47
3:N:53:THR:HG23	3:N:277:GLU:OE1	2.15	0.47
3:N:202:ASP:OD2	3:N:214:ARG:NE	2.48	0.47
1:A:192:LEU:HD12	1:B:192:LEU:HD12	1.97	0.47
2:G:144:CYS:HB2	2:G:194:ARG:HH11	1.78	0.47
2:G:318:HIS:HB2	2:G:321:PRO:HD2	1.97	0.47
3:M:17:LEU:HD11	3:M:23:LEU:HG	1.97	0.47
2:C:692:GLY:HA2	2:C:708:ASN:HB2	1.97	0.47
2:G:96:ALA:O	2:G:100:GLY:N	2.48	0.47
3:K:124:THR:HB	3:K:129:PHE:HB3	1.97	0.47
3:K:225:SER:O	3:K:229:ASN:HB2	2.15	0.47
3:N:95:GLU:HA	3:N:98:THR:HG22	1.96	0.47
2:G:244:MET:HG2	2:G:265:LEU:HD11	1.96	0.47
3:I:38:ILE:HD12	3:I:105:VAL:HG22	1.97	0.47
3:I:261:SER:O	3:I:261:SER:OG	2.31	0.47
3:J:124:THR:HB	3:J:129:PHE:HB3	1.97	0.47
3:K:202:ASP:N	3:K:202:ASP:OD1	2.48	0.47
2:G:236:SER:OG	2:G:286:GLN:NE2	2.48	0.47
3:I:124:THR:HB	3:I:129:PHE:HB3	1.97	0.47
3:K:32:CYS:O	3:K:36:LYS:HG2	2.15	0.47
3:E:67:GLU:HG2	3:E:289:PHE:HD2	1.79	0.46
2:G:281:HIS:HB3	2:G:309:PHE:HE2	1.79	0.46
3:L:158:LEU:HD21	3:L:177:LEU:HD13	1.97	0.46
3:M:276:MET:HE1	3:M:278:LEU:HG	1.97	0.46
3:D:159:VAL:HB	3:D:163:ILE:HB	1.98	0.46
2:G:65:TYR:OH	2:G:684:GLY:O	2.34	0.46
3:K:119:GLU:HB3	3:K:150:PHE:CD2	2.51	0.46
3:L:66:MET:HE3	3:L:66:MET:HA	1.97	0.46
2:C:59:LEU:HD21	2:C:78:TRP:HE1	1.81	0.46
2:C:643:PRO:HA	2:C:674:PRO:HA	1.97	0.46
3:E:114:LEU:HD21	3:E:157:ALA:HB2	1.98	0.46
2:G:283:ARG:NH1	2:G:311:ASP:OD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLU:OE1	1:B:127:LYS:NZ	2.39	0.46
1:B:135:GLU:HG3	3:I:89:ARG:HH22	1.79	0.46
2:C:113:GLY:HA3	2:C:707:THR:HG21	1.97	0.46
3:D:51:PRO:HA	3:D:278:LEU:O	2.15	0.46
3:D:67:GLU:HB2	3:D:292:ALA:HB2	1.98	0.46
4:F:100:LEU:O	4:F:104:ILE:HG13	2.15	0.46
3:M:53:THR:HA	3:M:276:MET:O	2.16	0.46
3:N:202:ASP:CG	3:N:214:ARG:HE	2.24	0.46
2:C:201:HIS:NE2	3:D:91:TYR:HA	2.30	0.46
3:L:133:CYS:SG	3:L:143:TRP:HB2	2.56	0.46
3:M:200:TRP:HB2	3:M:216:ALA:HB3	1.98	0.46
2:G:56:GLU:HG3	2:G:81:LEU:HD22	1.97	0.46
3:I:248:TYR:HA	3:I:258:THR:O	2.16	0.46
3:J:155:LEU:HD21	3:J:195:MET:HE3	1.97	0.46
3:J:274:ALA:HA	3:J:287:LEU:O	2.16	0.46
1:A:96:LYS:O	1:A:100:THR:HG23	2.16	0.45
2:C:117:THR:O	2:C:708:ASN:ND2	2.48	0.45
2:G:62:LEU:HA	4:H:128:LYS:HD3	1.98	0.45
4:H:123:VAL:O	4:H:127:ILE:HG23	2.16	0.45
3:I:31:LEU:HD12	3:I:101:VAL:HG23	1.98	0.45
3:K:35:ALA:O	3:K:39:LEU:HD12	2.15	0.45
3:K:38:ILE:HD12	3:K:38:ILE:H	1.81	0.45
3:M:17:LEU:HD23	3:M:99:LEU:HA	1.99	0.45
2:C:213:TYR:OH	2:C:218:ASN:OD1	2.25	0.45
3:I:260:PHE:HE1	3:I:262:ALA:HB3	1.82	0.45
3:M:38:ILE:HD11	3:M:108:ARG:HB2	1.99	0.45
3:K:246:GLU:OE1	3:K:246:GLU:N	2.48	0.45
3:M:162:GLN:HG3	3:M:235:THR:HG22	1.98	0.45
4:F:4:ILE:O	4:F:6:LEU:HD22	2.17	0.45
4:F:134:GLU:O	4:F:138:THR:HG22	2.16	0.45
4:H:128:LYS:HB2	4:H:128:LYS:HE2	1.40	0.45
4:H:131:THR:HB	4:H:134:GLU:HB3	1.98	0.45
2:C:140:THR:HG22	2:C:141:GLN:H	1.82	0.45
2:C:251:LEU:HD13	2:C:257:SER:HB3	1.98	0.45
3:I:54:VAL:HB	3:I:276:MET:HB3	1.98	0.45
3:I:122:GLN:H	3:I:122:GLN:HG2	1.54	0.45
3:K:83:MET:O	3:K:167:HIS:ND1	2.49	0.45
3:N:13:TRP:HB3	3:N:23:LEU:HD11	1.98	0.45
1:A:96:LYS:NZ	3:K:245:MET:HB2	2.32	0.45
3:D:29:LYS:O	3:D:33:GLU:HG2	2.17	0.45
3:J:204:ASP:O	3:J:252:HIS:NE2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:261:SER:O	3:L:261:SER:OG	2.29	0.45
3:M:54:VAL:HG22	3:M:81:LEU:HB3	1.99	0.45
2:C:124:ALA:HA	2:C:134:TYR:O	2.16	0.45
2:G:292:ASP:HB3	2:G:295:THR:HG22	1.99	0.45
3:N:174:ILE:HG23	3:N:179:HIS:HB2	1.99	0.45
3:D:85:ASP:OD1	3:D:85:ASP:N	2.45	0.45
2:G:244:MET:HG3	2:G:263:LEU:HD23	1.98	0.45
4:F:130:LYS:HD3	4:F:134:GLU:HG3	1.98	0.45
3:N:141:ASN:N	3:N:141:ASN:OD1	2.48	0.45
3:E:114:LEU:HD23	3:E:154:PRO:HG2	1.99	0.44
3:N:126:VAL:HG23	3:N:127:TYR:CD1	2.53	0.44
1:B:110:GLU:OE1	3:E:214:ARG:NH1	2.50	0.44
2:C:72:ALA:O	4:F:153:VAL:HG11	2.18	0.44
4:H:124:ALA:O	4:H:125:ASN:C	2.60	0.44
3:K:131:ASP:O	3:K:135:ARG:HG3	2.18	0.44
3:J:36:LYS:HB2	3:J:36:LYS:HE3	1.77	0.44
3:L:55:CYS:O	3:L:83:MET:HG2	2.18	0.44
3:M:61:GLN:NE2	3:M:264:ASN:O	2.51	0.44
3:N:59:HIS:HD2	3:N:88:ASP:CB	2.25	0.44
2:C:642:LYS:HD3	2:C:643:PRO:HD2	1.98	0.44
3:N:169:GLY:HA3	3:N:220:PHE:CZ	2.52	0.44
2:C:200:LEU:HD12	2:C:200:LEU:HA	1.84	0.44
4:F:132:PRO:O	4:F:136:ARG:HG2	2.17	0.44
2:G:243:LYS:HA	2:G:263:LEU:O	2.16	0.44
3:I:29:LYS:HE2	3:I:145:TYR:CE2	2.53	0.44
3:I:37:GLU:HA	3:I:40:THR:HG22	2.00	0.44
3:M:117:ASN:HB2	3:M:200:TRP:NE1	2.32	0.44
3:N:174:ILE:HD13	3:N:180:ILE:HG12	1.99	0.44
4:H:97:GLN:NE2	4:H:101:PHE:HZ	2.16	0.44
4:H:157:ASN:C	4:H:158:GLN:HG3	2.43	0.44
3:I:173:SER:O	3:I:174:ILE:HD13	2.18	0.44
2:C:189:PHE:HD1	2:C:210:ILE:HG22	1.83	0.44
2:C:355:SER:OG	2:C:356:GLN:N	2.51	0.44
4:H:54:ILE:O	4:H:58:VAL:HG13	2.18	0.44
3:M:277:GLU:HB2	3:M:285:SER:O	2.17	0.44
2:G:156:LEU:HD11	2:G:689:ILE:HD11	1.99	0.44
3:I:20:CYS:HA	3:I:62:PHE:HE2	1.82	0.44
3:I:264:ASN:N	3:I:271:ASN:OD1	2.51	0.44
3:D:274:ALA:HA	3:D:288:GLN:HA	1.98	0.43
4:H:4:ILE:HG22	4:H:16:VAL:HB	1.99	0.43
4:H:131:THR:HB	4:H:134:GLU:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:264:ASN:HA	3:M:270:GLY:HA2	1.99	0.43
3:N:141:ASN:HB2	3:N:145:TYR:CZ	2.52	0.43
2:G:302:CYS:SG	2:G:303:GLY:N	2.90	0.43
3:K:61:GLN:HG2	3:K:267:TYR:HE1	1.82	0.43
2:G:104:TRP:NE1	2:G:670:VAL:O	2.51	0.43
3:J:159:VAL:HB	3:J:163:ILE:HB	2.00	0.43
3:K:45:VAL:HG21	3:K:177:LEU:HD11	2.01	0.43
3:K:199:LEU:HD23	3:K:199:LEU:HA	1.88	0.43
3:L:37:GLU:HA	3:L:40:THR:HG22	2.00	0.43
3:M:41:LYS:HZ1	3:M:108:ARG:HD3	1.83	0.43
3:M:49:ARG:HA	3:M:49:ARG:HD3	1.84	0.43
3:N:174:ILE:HD11	3:N:183:LEU:HD11	2.00	0.43
3:E:172:PRO:HD3	3:E:209:TRP:CZ3	2.54	0.43
4:H:115:LEU:HD23	4:H:115:LEU:HA	1.74	0.43
3:I:178:ASP:OD1	3:I:178:ASP:N	2.51	0.43
3:L:174:ILE:HD12	3:L:180:ILE:HG13	1.98	0.43
1:A:194:GLN:O	1:A:197:ARG:N	2.51	0.43
1:B:128:GLU:HG3	3:I:245:MET:HG2	1.99	0.43
2:C:259:ASP:HB2	2:C:272:LYS:HE3	2.01	0.43
3:D:283:LYS:HD2	3:D:283:LYS:HA	1.90	0.43
4:H:30:MET:SD	4:H:31:LEU:HG	2.59	0.43
3:K:49:ARG:HE	3:K:51:PRO:HG2	1.83	0.43
3:K:144:LYS:HD3	3:K:144:LYS:N	2.34	0.43
2:C:67:GLU:OE1	2:C:67:GLU:N	2.51	0.43
3:E:279:ASP:OD1	3:E:283:LYS:N	2.43	0.43
2:G:284:GLY:N	2:G:302:CYS:O	2.52	0.43
4:H:95:VAL:HG22	4:H:96:ASP:H	1.83	0.43
3:K:68:LEU:HD13	3:K:275:ILE:HG21	2.01	0.43
3:L:156:THR:HG22	3:L:166:LEU:HB3	2.01	0.43
2:C:59:LEU:HD23	2:C:59:LEU:HA	1.85	0.43
3:D:130:TYR:O	3:D:134:LEU:HB2	2.18	0.43
4:F:27:ILE:HA	4:F:30:MET:HE3	2.00	0.43
4:F:67:ASP:OD2	4:F:67:ASP:N	2.48	0.43
3:I:252:HIS:HB2	3:I:256:VAL:HG22	2.00	0.43
3:J:118:HIS:HA	3:J:123:ILE:HG21	2.01	0.43
3:N:6:PHE:HA	3:N:9:GLU:HG3	2.00	0.43
1:B:132:VAL:HG22	3:I:243:LEU:HB3	2.00	0.43
3:D:118:HIS:HA	3:D:123:ILE:HG21	2.00	0.43
3:N:263:PRO:HB2	3:N:291:PRO:HD3	2.01	0.43
1:A:194:GLN:HA	1:A:197:ARG:HB2	2.01	0.43
3:D:205:ASP:OD1	3:D:205:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:11:ASP:O	3:L:15:GLU:HG2	2.19	0.43
3:N:118:HIS:ND1	3:N:123:ILE:HG21	2.34	0.42
2:C:646:MET:HE2	2:C:646:MET:HB3	1.84	0.42
3:I:232:ASN:HB2	3:I:234:LEU:HD23	2.01	0.42
3:L:119:GLU:HB3	3:L:150:PHE:CG	2.55	0.42
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.78	0.42
2:C:65:TYR:OH	2:C:687:GLU:OE2	2.29	0.42
3:D:17:LEU:HD21	3:D:23:LEU:HG	1.99	0.42
4:F:20:ILE:HG21	4:F:59:ILE:HG23	2.02	0.42
4:F:55:LEU:HA	4:F:58:VAL:HG12	2.00	0.42
2:G:281:HIS:ND1	2:G:282:PRO:HD2	2.34	0.42
3:N:13:TRP:NE1	3:N:27:GLN:OE1	2.52	0.42
3:N:36:LYS:HE3	3:N:36:LYS:HB3	1.90	0.42
3:N:68:LEU:HA	3:N:71:ILE:HG22	2.01	0.42
1:A:194:GLN:O	1:A:195:LEU:C	2.57	0.42
1:B:136:LYS:HD2	3:I:213:PRO:HG2	2.00	0.42
1:B:197:ARG:NE	1:B:200:ILE:HD12	2.33	0.42
2:C:315:LEU:HD13	2:C:324:TRP:CE2	2.55	0.42
3:D:83:MET:SD	3:D:165:CYS:HB3	2.59	0.42
2:G:331:ASN:HB2	2:G:662:TRP:HB2	2.00	0.42
3:J:132:GLU:OE2	3:J:135:ARG:NH2	2.52	0.42
3:K:170:LEU:HD22	3:K:170:LEU:H	1.84	0.42
3:N:53:THR:HB	3:N:80:TYR:HA	2.01	0.42
3:N:117:ASN:HB2	3:N:200:TRP:NE1	2.34	0.42
3:K:10:LEU:HD23	3:K:10:LEU:HA	1.82	0.42
3:K:273:ALA:O	3:K:288:GLN:HA	2.20	0.42
3:N:97:VAL:O	3:N:101:VAL:HG23	2.18	0.42
3:E:54:VAL:HB	3:E:276:MET:HB3	2.01	0.42
3:E:246:GLU:HA	3:E:272:GLN:HB3	2.02	0.42
4:F:63:THR:HA	4:F:66:LYS:HG2	2.01	0.42
2:G:244:MET:O	2:G:262:VAL:HA	2.20	0.42
3:K:44:ASN:ND2	3:K:180:ILE:O	2.52	0.42
3:K:119:GLU:HB3	3:K:150:PHE:CG	2.54	0.42
3:M:108:ARG:O	3:M:108:ARG:NH1	2.52	0.42
3:N:229:ASN:HD22	3:N:255:ASN:HD22	1.67	0.42
1:B:166:GLU:O	1:B:170:GLN:HG2	2.19	0.42
2:C:109:TYR:OH	2:C:159:LYS:O	2.30	0.42
4:F:115:LEU:HD23	4:F:115:LEU:HA	1.86	0.42
3:I:59:HIS:CE1	3:I:85:ASP:HB3	2.54	0.42
3:L:273:ALA:O	3:L:288:GLN:HA	2.19	0.42
3:M:93:SER:O	3:M:97:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:153:VAL:O	4:F:156:GLU:HB2	2.20	0.42
3:K:39:LEU:HD23	3:K:153:LEU:HD23	2.01	0.42
3:N:49:ARG:HG2	3:N:51:PRO:HD3	2.00	0.42
3:J:264:ASN:HB2	3:J:291:PRO:HG3	2.01	0.42
3:K:143:TRP:O	3:K:147:THR:HG22	2.19	0.42
3:K:203:PRO:HD3	3:K:239:ARG:CZ	2.50	0.42
3:K:260:PHE:CE1	3:K:262:ALA:HB3	2.55	0.42
1:B:203:GLU:OE1	3:M:269:CYS:HB2	2.20	0.41
2:C:63:SER:H	4:F:128:LYS:HZ1	1.66	0.41
2:C:67:GLU:HG2	4:F:128:LYS:HZ3	1.85	0.41
3:E:38:ILE:HD12	3:E:38:ILE:H	1.85	0.41
3:J:250:TRP:CE3	3:J:254:ARG:HG2	2.55	0.41
3:M:36:LYS:O	3:M:40:THR:HG22	2.20	0.41
3:N:223:ASP:OD1	3:N:223:ASP:N	2.51	0.41
3:E:52:VAL:HG23	3:E:278:LEU:HB2	2.02	0.41
2:G:258:ASN:HD22	2:G:282:PRO:HD3	1.85	0.41
3:I:164:PHE:CE2	3:I:166:LEU:HD13	2.55	0.41
3:K:67:GLU:O	3:K:71:ILE:HG22	2.20	0.41
3:K:92:TYR:O	3:K:96:THR:HG23	2.20	0.41
3:L:73:GLY:O	3:L:80:TYR:OH	2.35	0.41
3:N:53:THR:O	3:N:81:LEU:N	2.53	0.41
3:I:27:GLN:H	3:I:27:GLN:HG3	1.52	0.41
3:J:122:GLN:H	3:J:122:GLN:HG3	1.72	0.41
3:J:243:LEU:HD22	3:J:265:TYR:HD2	1.85	0.41
3:K:185:ARG:H	3:K:185:ARG:HG2	1.64	0.41
3:M:31:LEU:HA	3:M:34:LYS:HZ2	1.84	0.41
3:N:131:ASP:HB3	3:N:135:ARG:NH2	2.35	0.41
3:E:57:ASP:N	3:E:57:ASP:OD1	2.52	0.41
4:F:25:VAL:HA	4:F:28:LYS:CG	2.50	0.41
3:M:30:SER:O	3:M:34:LYS:HG3	2.20	0.41
3:M:114:LEU:HD21	3:M:157:ALA:HB2	2.01	0.41
3:D:108:ARG:HG2	3:D:109:GLU:HG3	2.02	0.41
3:E:112:THR:O	3:E:112:THR:OG1	2.37	0.41
4:H:17:ASP:OD1	4:H:18:VAL:N	2.52	0.41
3:M:249:ASN:O	3:M:257:VAL:HA	2.21	0.41
3:N:77:ASP:N	3:N:77:ASP:OD1	2.52	0.41
3:N:169:GLY:HA3	3:N:220:PHE:CE2	2.54	0.41
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.90	0.41
1:B:193:GLU:OE1	1:B:196:ARG:HD2	2.21	0.41
1:B:215:ASN:OD1	3:M:215:GLY:HA2	2.21	0.41
3:D:84:GLY:HA2	3:D:167:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:345:CYS:O	2:G:351:VAL:HA	2.20	0.41
3:J:122:GLN:NE2	3:J:188:GLU:OE2	2.44	0.41
3:L:159:VAL:HG21	3:L:278:LEU:HD12	2.02	0.41
3:N:61:GLN:HB3	3:N:64:ASP:HB2	2.02	0.41
2:C:63:SER:H	4:F:128:LYS:HZ2	1.68	0.41
2:C:346:ARG:NH1	2:C:348:GLY:O	2.53	0.41
4:F:5:LYS:O	4:F:6:LEU:HD13	2.21	0.41
3:K:26:SER:O	3:K:30:SER:OG	2.36	0.41
3:K:31:LEU:HD12	3:K:31:LEU:HA	1.89	0.41
3:K:279:ASP:OD1	3:K:283:LYS:N	2.48	0.41
1:A:125:LYS:O	1:A:129:THR:HG23	2.21	0.41
2:C:190:GLY:HA3	2:C:235:HIS:HE1	1.86	0.41
2:C:190:GLY:HA3	2:C:235:HIS:CE1	2.56	0.41
3:E:190:PRO:O	3:E:196:CYS:HB2	2.21	0.41
3:L:260:PHE:CE1	3:L:262:ALA:HB3	2.55	0.41
3:M:234:LEU:HD21	3:M:237:VAL:HG23	2.02	0.41
3:M:260:PHE:CE2	3:M:262:ALA:HB3	2.56	0.41
1:B:212:ALA:HA	1:B:215:ASN:HB3	2.02	0.41
2:C:356:GLN:O	2:C:647:TYR:OH	2.33	0.41
3:D:115:ARG:HG2	3:D:119:GLU:HG3	2.02	0.41
3:D:307:TYR:HD2	3:D:309:MLL:HD23	1.86	0.41
4:F:24:SER:HB3	4:F:27:ILE:HB	2.02	0.41
4:H:144:ASP:OD1	4:H:145:PHE:N	2.54	0.41
3:I:109:GLU:OE1	3:I:109:GLU:N	2.53	0.41
3:L:52:VAL:HG22	3:L:53:THR:H	1.86	0.41
3:L:131:ASP:OD1	3:L:131:ASP:N	2.53	0.41
3:M:16:GLN:NE2	3:M:23:LEU:HD23	2.35	0.41
3:M:189:VAL:HA	3:M:195:MET:HE3	2.02	0.41
3:N:99:LEU:HD12	3:N:100:LEU:HG	2.03	0.41
3:N:181:ARG:HH11	3:N:181:ARG:HA	1.85	0.41
2:C:136:PHE:HB2	2:C:151:LEU:HD12	2.02	0.41
2:C:314:LEU:HD13	2:C:327:LEU:HD11	2.03	0.41
4:F:6:LEU:CD1	4:F:45:VAL:H	2.33	0.41
2:G:140:THR:HG22	2:G:141:GLN:H	1.87	0.41
2:G:190:GLY:HA3	2:G:235:HIS:HE1	1.86	0.41
4:H:27:ILE:H	4:H:27:ILE:HG13	1.67	0.41
3:L:25:GLU:O	3:L:29:LYS:HG2	2.21	0.41
3:M:175:ASP:H	3:M:179:HIS:CE1	2.39	0.41
3:N:13:TRP:HZ3	3:N:31:LEU:HB2	1.86	0.41
2:C:189:PHE:CD1	2:C:210:ILE:HG22	2.55	0.40
3:D:209:TRP:CZ3	3:D:220:PHE:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:7:GLN:HB2	4:F:46:PRO:HA	2.03	0.40
3:M:178:ASP:HA	3:M:181:ARG:HB2	2.03	0.40
1:A:112:ILE:HD13	1:A:112:ILE:HA	1.91	0.40
3:D:117:ASN:OD1	3:D:117:ASN:N	2.55	0.40
3:J:243:LEU:HD11	3:J:271:ASN:HD22	1.85	0.40
3:K:30:SER:HA	3:K:33:GLU:OE2	2.21	0.40
3:M:16:GLN:HA	3:M:21:LYS:HZ3	1.86	0.40
1:A:185:THR:O	1:A:186:ILE:C	2.65	0.40
3:E:30:SER:O	3:E:34:LYS:HG2	2.21	0.40
3:E:49:ARG:HG3	3:E:51:PRO:HD2	2.03	0.40
4:F:30:MET:HA	4:F:33:ASP:HB2	2.02	0.40
3:I:243:LEU:HD13	3:I:265:TYR:HD2	1.87	0.40
4:F:96:ASP:OD1	4:F:96:ASP:N	2.54	0.40
2:G:314:LEU:HB2	2:G:327:LEU:HD11	2.02	0.40
3:I:149:LEU:HD23	3:I:149:LEU:HA	1.95	0.40
3:K:190:PRO:O	3:K:196:CYS:HB2	2.22	0.40
3:L:88:ASP:HB2	3:L:118:HIS:ND1	2.36	0.40
3:M:54:VAL:HG13	3:M:81:LEU:HD22	2.03	0.40
3:N:59:HIS:CD2	3:N:88:ASP:CB	3.02	0.40
1:A:186:ILE:O	1:A:187:SER:C	2.64	0.40
3:E:39:LEU:O	3:E:42:GLU:HB3	2.22	0.40
3:J:29:LYS:HB2	3:J:145:TYR:CE2	2.56	0.40
3:K:115:ARG:NH2	3:K:151:ASP:HA	2.36	0.40
3:K:277:GLU:CB	3:K:285:SER:O	2.70	0.40
3:M:77:ASP:O	3:M:110:ARG:NH2	2.52	0.40
3:N:195:MET:HE2	3:N:195:MET:HB3	2.01	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	132/490 (27%)	131 (99%)	1 (1%)	0	100	100
1	B	129/490 (26%)	126 (98%)	3 (2%)	0	100	100
2	C	376/691 (54%)	341 (91%)	34 (9%)	1 (0%)	36	68
2	G	377/691 (55%)	345 (92%)	32 (8%)	0	100	100
3	D	292/336 (87%)	274 (94%)	18 (6%)	0	100	100
3	E	289/336 (86%)	267 (92%)	22 (8%)	0	100	100
3	I	289/336 (86%)	266 (92%)	23 (8%)	0	100	100
3	J	290/336 (86%)	276 (95%)	14 (5%)	0	100	100
3	K	289/336 (86%)	264 (91%)	25 (9%)	0	100	100
3	L	289/336 (86%)	268 (93%)	21 (7%)	0	100	100
3	M	289/336 (86%)	268 (93%)	21 (7%)	0	100	100
3	N	289/336 (86%)	264 (91%)	25 (9%)	0	100	100
4	F	130/151 (86%)	116 (89%)	14 (11%)	0	100	100
4	H	130/151 (86%)	114 (88%)	16 (12%)	0	100	100
All	All	3590/5352 (67%)	3320 (92%)	269 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	199	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/437 (29%)	123 (98%)	3 (2%)	43	70
1	B	124/437 (28%)	124 (100%)	0	100	100
2	C	329/580 (57%)	325 (99%)	4 (1%)	63	79
2	G	330/580 (57%)	328 (99%)	2 (1%)	78	84
3	D	260/297 (88%)	258 (99%)	2 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	255/297 (86%)	253 (99%)	2 (1%)	73	82
3	I	255/297 (86%)	254 (100%)	1 (0%)	84	86
3	J	257/297 (86%)	256 (100%)	1 (0%)	84	86
3	K	255/297 (86%)	253 (99%)	2 (1%)	73	82
3	L	255/297 (86%)	254 (100%)	1 (0%)	84	86
3	M	255/297 (86%)	251 (98%)	4 (2%)	55	75
3	N	255/297 (86%)	252 (99%)	3 (1%)	63	79
4	F	125/135 (93%)	114 (91%)	11 (9%)	9	35
4	H	125/135 (93%)	116 (93%)	9 (7%)	13	44
All	All	3206/4680 (68%)	3161 (99%)	45 (1%)	57	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	195	LEU
1	A	201	ASP
2	C	74	VAL
2	C	111	TYR
2	C	202	GLN
2	C	263	LEU
3	D	85	ASP
3	D	86	TYR
3	E	21	LYS
3	E	97	VAL
4	F	16	VAL
4	F	30	MET
4	F	43	ASP
4	F	44	PRO
4	F	47	LEU
4	F	85	ILE
4	F	93	LEU
4	F	104	ILE
4	F	117	ASP
4	F	144	ASP
4	F	153	VAL
2	G	288	GLN
2	G	334	HIS
4	H	25	VAL

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Mol	Chain	Res	Type
4	H	50	VAL
4	H	62	CYS
4	H	112	ILE
4	H	113	LYS
4	H	127	ILE
4	H	128	LYS
4	H	130	LYS
4	H	145	PHE
3	I	280	ASP
3	J	12	GLN
3	K	33	GLU
3	K	134	LEU
3	L	253	ASP
3	M	83	MET
3	M	87	VAL
3	M	88	ASP
3	M	153	LEU
3	N	92	TYR
3	N	224	ILE
3	N	245	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	B	170	GLN
2	C	66	GLN
3	E	162	GLN
4	F	60	GLN
2	G	145	ASN
2	G	202	GLN
2	G	318	HIS
4	H	97	GLN
4	H	108	ASN
4	H	125	ASN
3	I	255	ASN
3	J	162	GLN
3	J	179	HIS
3	K	61	GLN
3	K	118	HIS
3	K	229	ASN
3	L	16	GLN

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Mol	Chain	Res	Type
3	L	18	ASN
3	L	63	HIS
3	L	125	GLN
3	L	271	ASN
3	M	46	GLN
3	M	125	GLN
3	M	230	HIS
3	M	255	ASN
3	N	61	GLN
3	N	162	GLN
3	N	191	HIS
3	N	229	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MLL	J	309	3	8,9,9	0.52	0	9,11,11	0.57	0
3	MLL	D	309	3	8,9,9	0.53	0	9,11,11	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLL	J	309	3	-	8/10/10/10	-
3	MLL	D	309	3	-	8/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	309	MLL	N-CA-CB-CG
3	D	309	MLL	C-CA-CB-CG
3	D	309	MLL	OXT-C-CA-N
3	D	309	MLL	O-C-CA-CB
3	D	309	MLL	OXT-C-CA-CB
3	J	309	MLL	CA-C-OXT-C10
3	D	309	MLL	CA-C-OXT-C10
3	D	309	MLL	O-C-OXT-C10
3	J	309	MLL	O-C-OXT-C10
3	J	309	MLL	CA-CB-CG-CD1
3	J	309	MLL	CA-CB-CG-CD2
3	D	309	MLL	O-C-CA-N
3	J	309	MLL	OXT-C-CA-N
3	J	309	MLL	O-C-CA-CB
3	J	309	MLL	OXT-C-CA-CB
3	J	309	MLL	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	309	MLL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

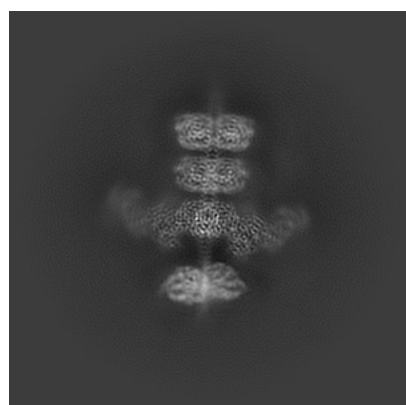
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49966. These allow visual inspection of the internal detail of the map and identification of artifacts.

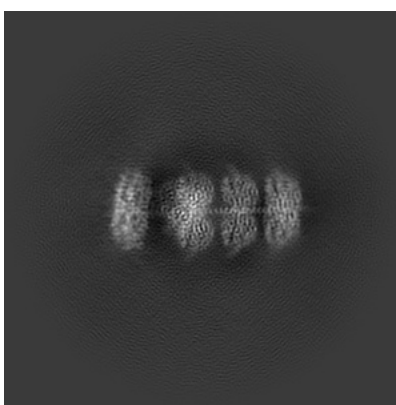
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

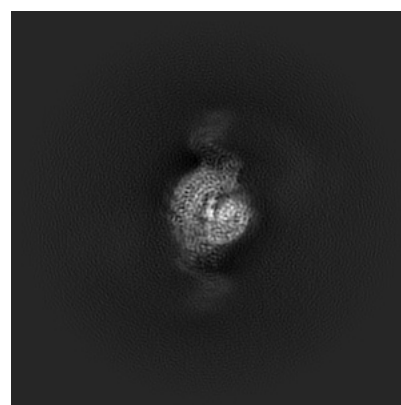
6.1.1 Primary map



X



Y

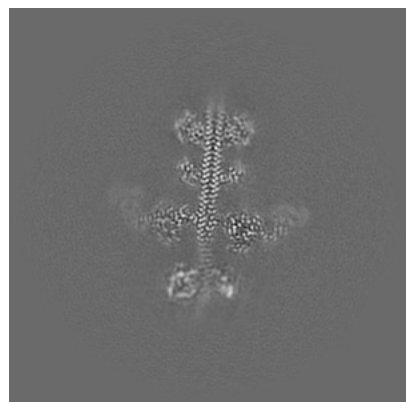


Z

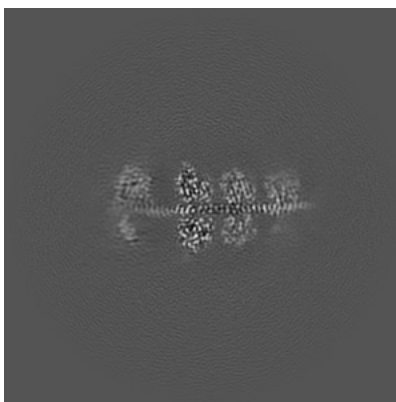
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

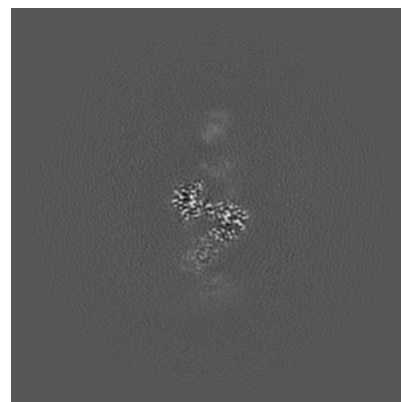
6.2.1 Primary map



X Index: 240



Y Index: 240

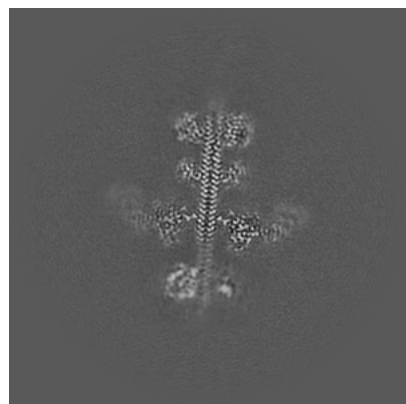


Z Index: 240

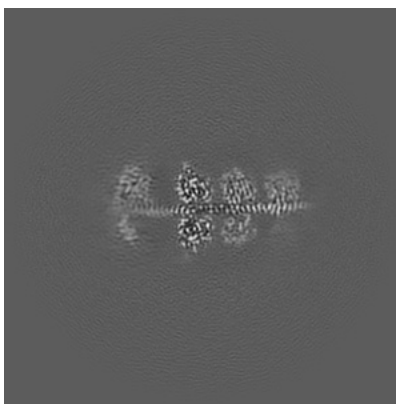
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

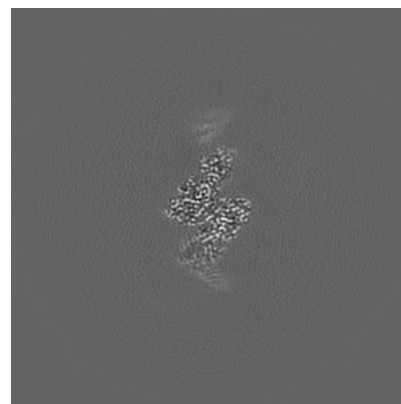
6.3.1 Primary map



X Index: 238



Y Index: 239

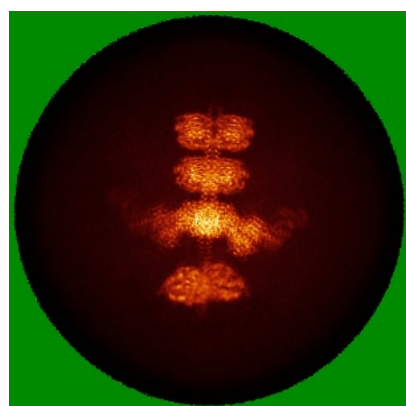


Z Index: 224

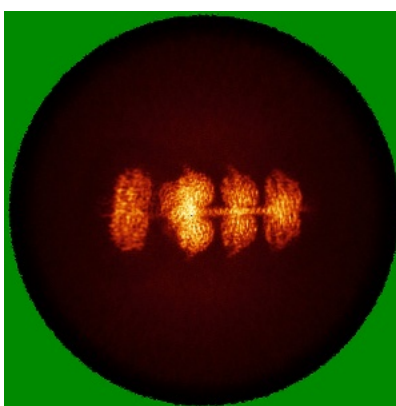
The images above show the largest variance slices of the map in three orthogonal directions.

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

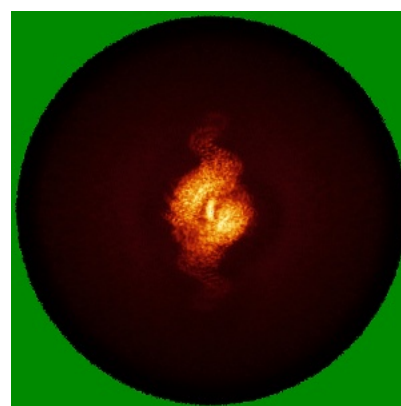
6.4.1 Primary map



X



Y

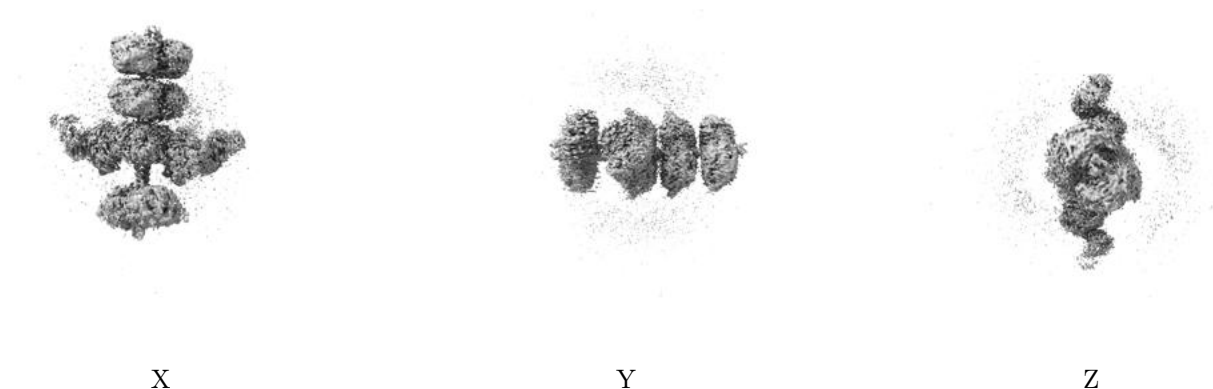


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

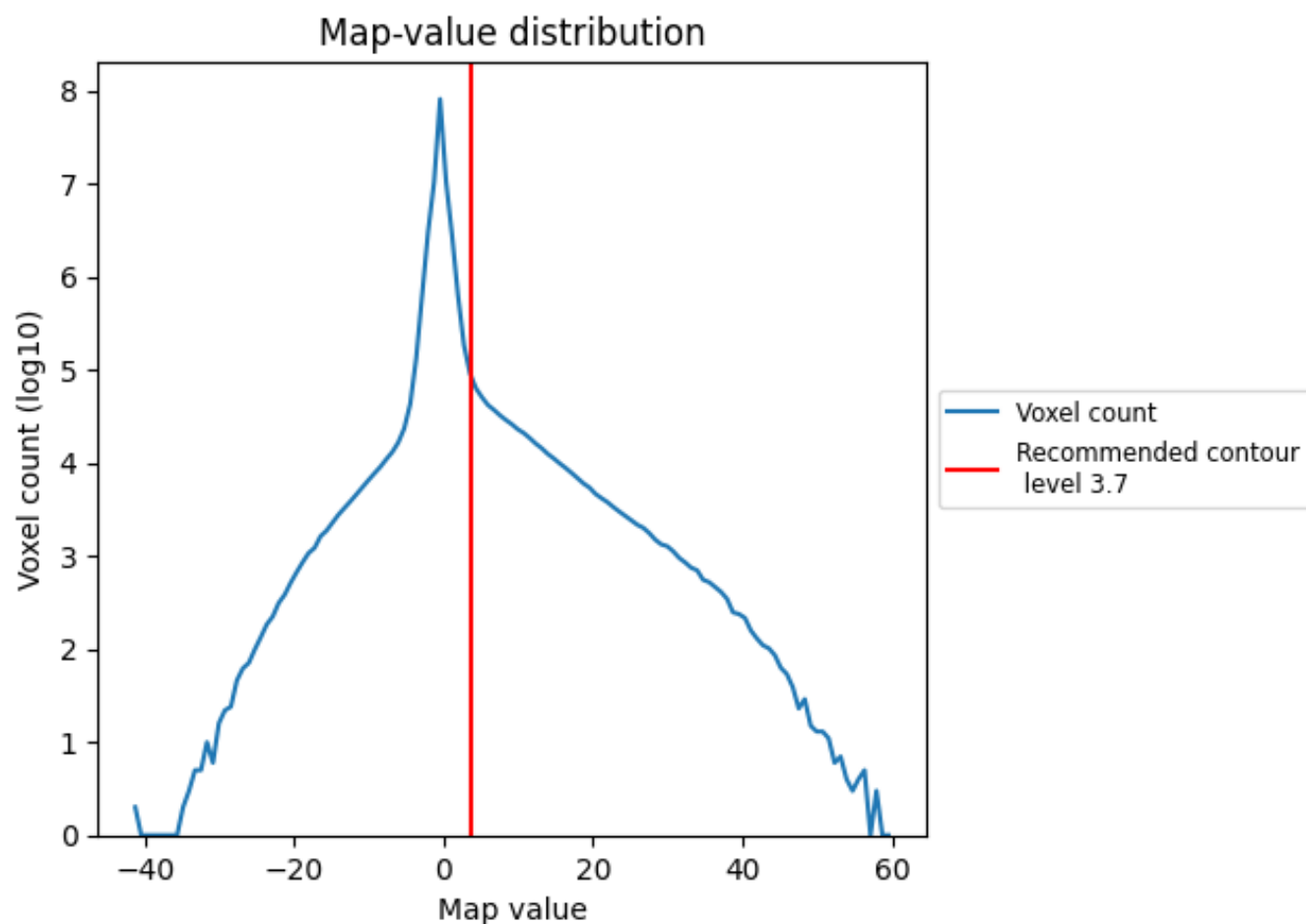
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

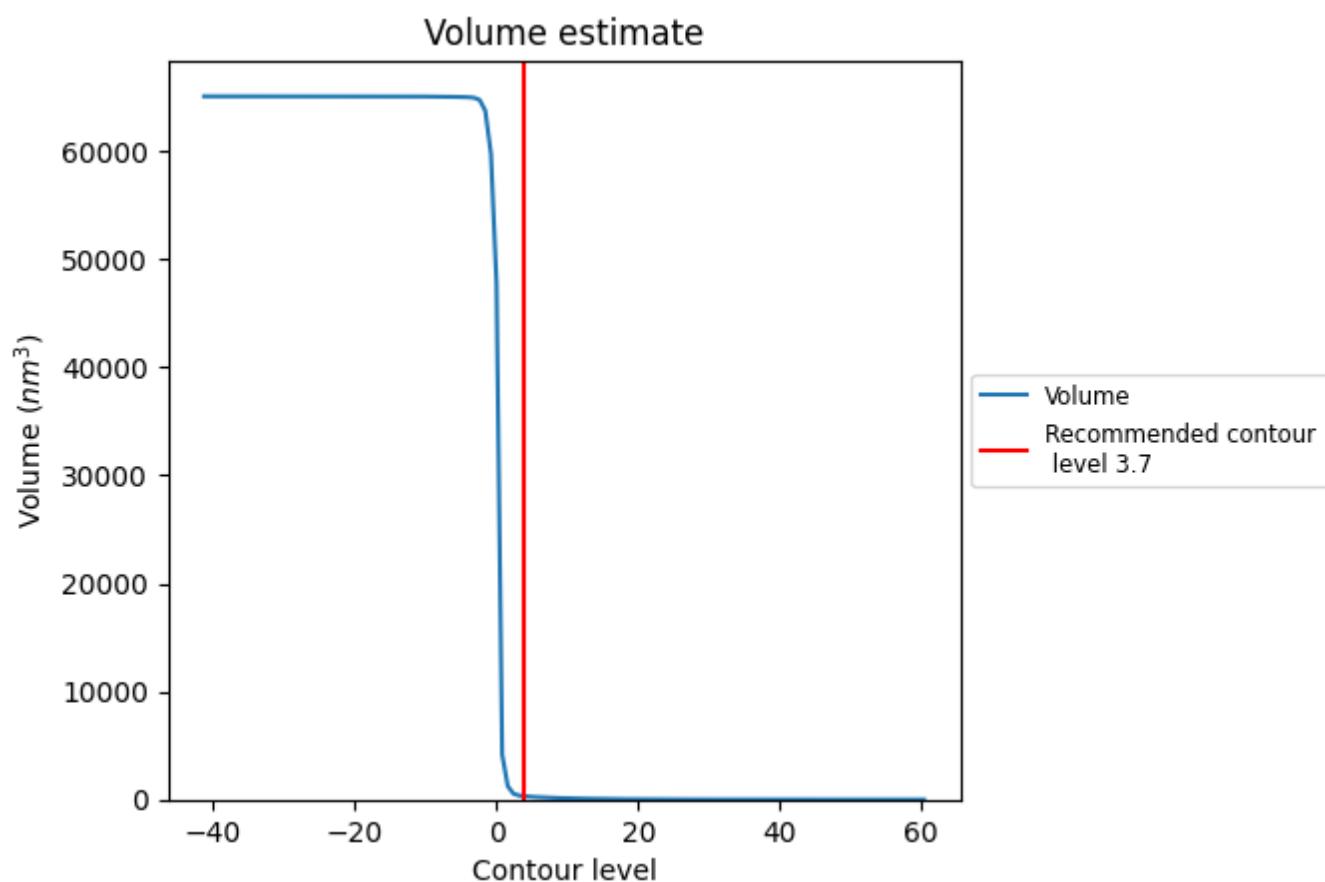
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

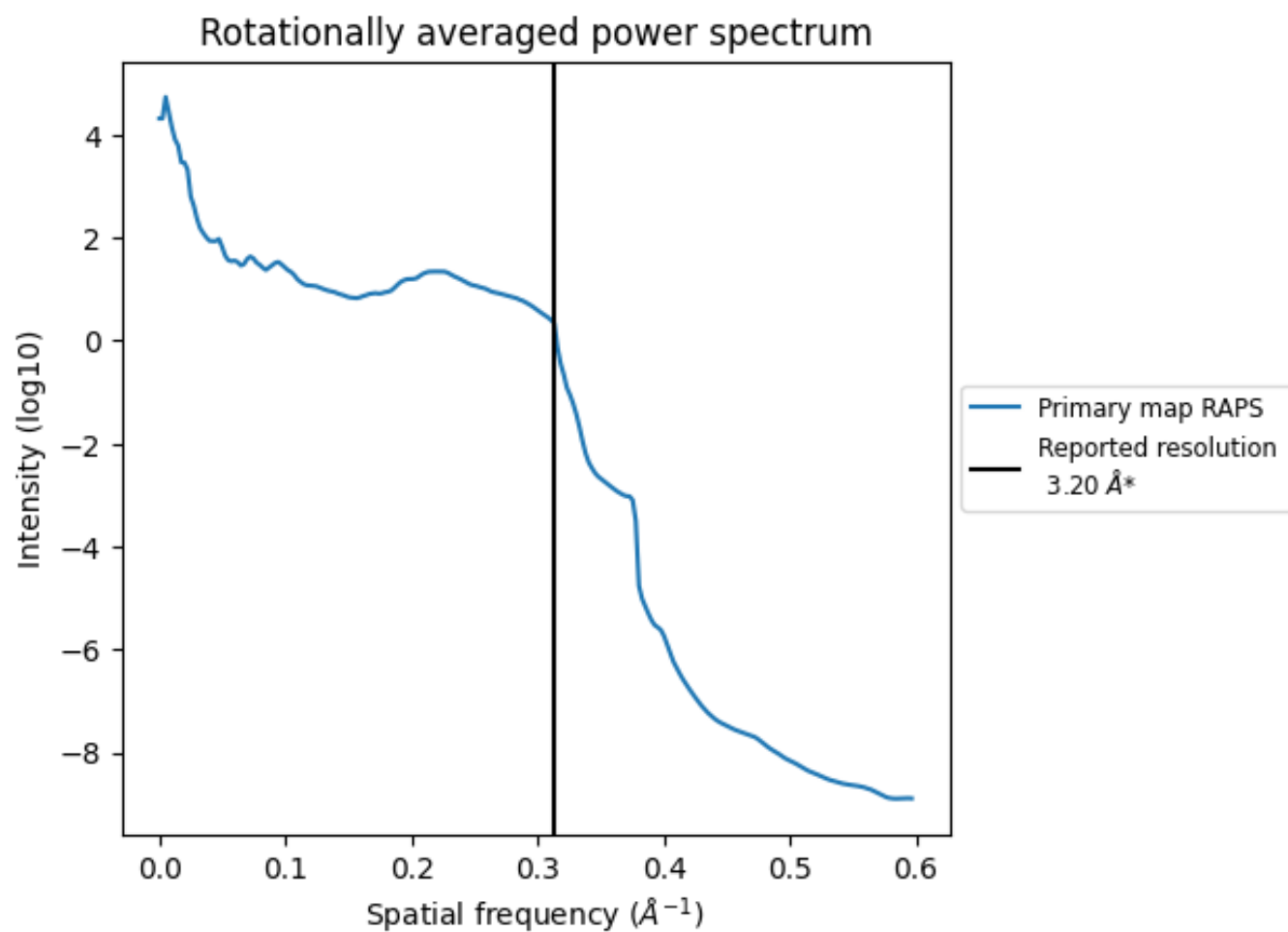
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm³; this corresponds to an approximate mass of 297 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 0.312 Å⁻¹

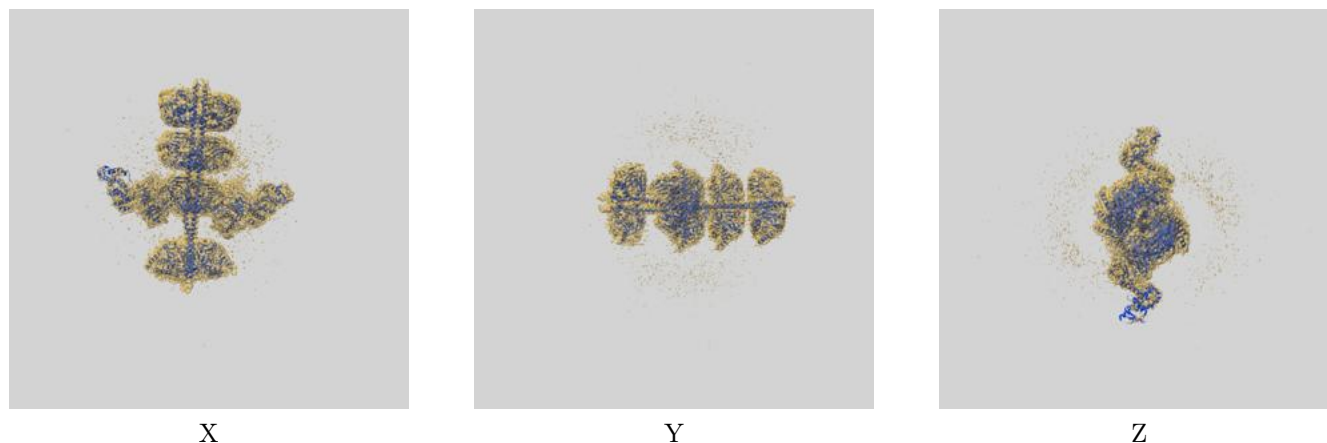
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

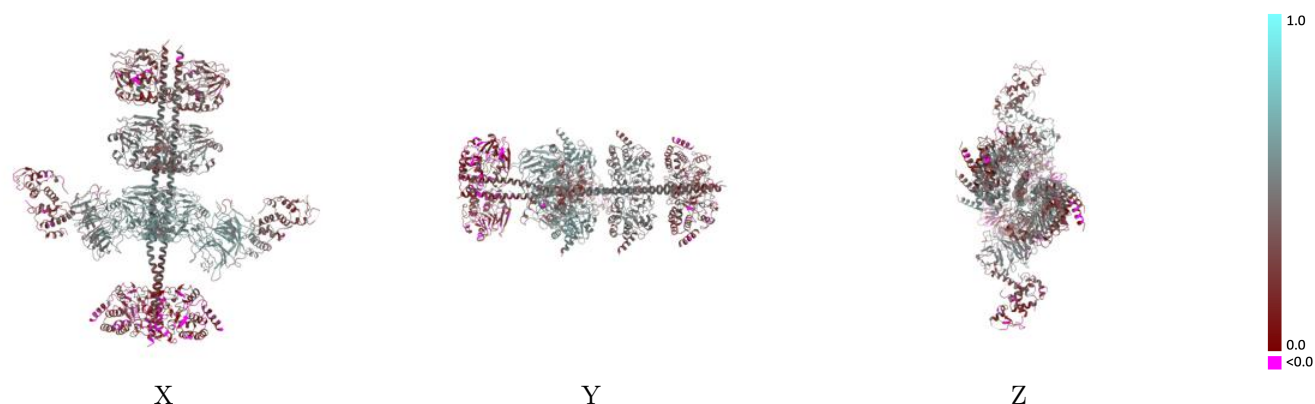
This section contains information regarding the fit between EMDB map EMD-49966 and PDB model 9O04. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



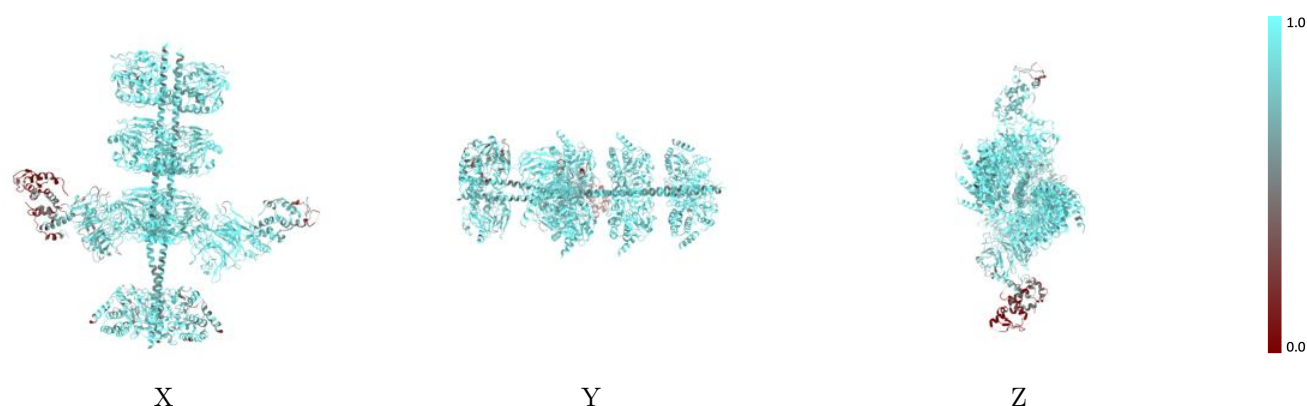
The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



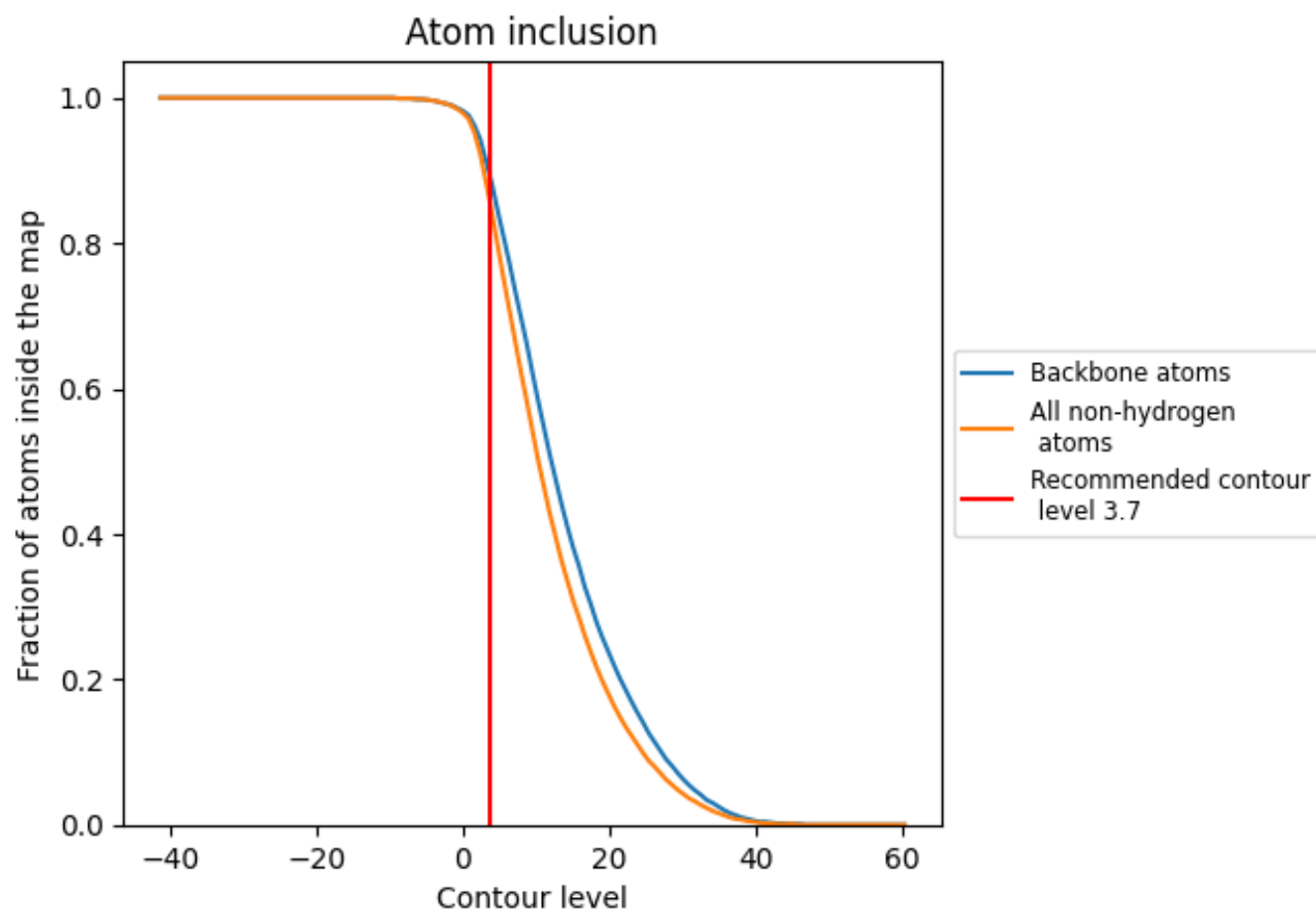
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.3960
A	 0.8570	 0.4050
B	 0.8200	 0.3730
C	 0.9200	 0.5200
D	 0.9460	 0.5610
E	 0.9100	 0.3260
F	 0.6920	 0.3400
G	 0.7780	 0.4370
H	 0.2430	 0.2530
I	 0.9370	 0.4440
J	 0.9530	 0.5620
K	 0.9020	 0.3190
L	 0.9410	 0.4600
M	 0.8720	 0.1950
N	 0.7930	 0.1780

