



## Full wwPDB EM Validation Report ⓘ

May 28, 2024 – 12:30 PM EDT

PDB ID : 8U7I  
EMDB ID : EMD-41983  
Title : Structure of the phage immune evasion protein Gad1 bound to the Gabija GajAB complex  
Authors : Antine, S.P.; Johnson, A.G.; Mooney, S.E.; Mayer, M.L.; Kranzusch, P.J.  
Deposited on : 2023-09-15  
Resolution : 2.57 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](mailto: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>.

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

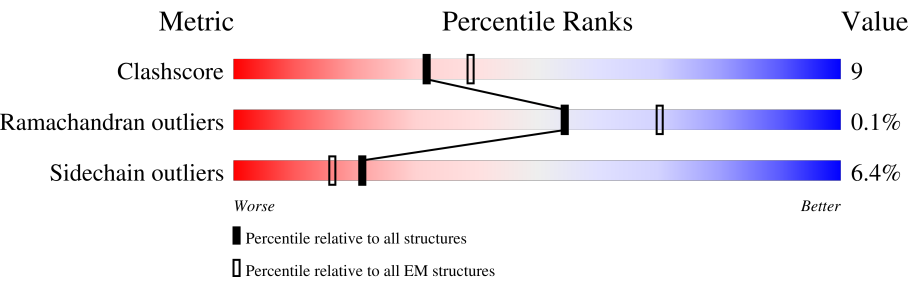
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.57 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	675	<div><div></div><div>74%18%7%</div></div>
1	B	675	<div><div></div><div>77%15%7%</div></div>
1	C	675	<div><div></div><div>75%17%7%</div></div>
1	D	675	<div><div></div><div>76%16%7%</div></div>
2	E	494	<div><div>9%</div><div>39%18%42%</div></div>
2	F	494	<div><div>10%</div><div>41%15%42%</div></div>
2	G	494	<div><div>11%</div><div>41%16%42%</div></div>
2	H	494	<div><div>11%</div><div>42%15%42%</div></div>

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Mol	Chain	Length	Quality of chain
3	I	295	<div><div><div></div><div></div><div></div></div><div>32%19%•45%</div></div>
3	J	295	<div><div><div></div><div></div><div></div></div><div>33%20%•45%</div></div>
3	K	295	<div><div><div></div><div></div><div></div></div><div>34%19%•45%</div></div>
3	L	295	<div><div><div></div><div></div><div></div></div><div>29%23%•45%</div></div>
3	M	295	<div><div><div></div><div></div><div></div></div><div>27%11%•61%</div></div>
3	N	295	<div><div><div></div><div></div><div></div></div><div>25%12%•61%</div></div>
3	O	295	<div><div><div></div><div></div><div></div></div><div>25%12%•61%</div></div>
3	P	295	<div><div><div></div><div></div><div></div></div><div>23%14%•61%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38864 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 Endonuclease GajA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	626	Total	C	N	O	S	0	0
			5111	3268	849	977	17		
1	B	626	Total	C	N	O	S	0	0
			5111	3268	849	977	17		
1	C	626	Total	C	N	O	S	0	0
			5111	3268	849	977	17		
1	D	626	Total	C	N	O	S	0	0
			5111	3268	849	977	17		

There are 392 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-96	MET	-	expression tag	UNP J8H9C1
A	-95	GLY	-	expression tag	UNP J8H9C1
A	-94	SER	-	expression tag	UNP J8H9C1
A	-93	SER	-	expression tag	UNP J8H9C1
A	-92	HIS	-	expression tag	UNP J8H9C1
A	-91	HIS	-	expression tag	UNP J8H9C1
A	-90	HIS	-	expression tag	UNP J8H9C1
A	-89	HIS	-	expression tag	UNP J8H9C1
A	-88	HIS	-	expression tag	UNP J8H9C1
A	-87	HIS	-	expression tag	UNP J8H9C1
A	-86	GLY	-	expression tag	UNP J8H9C1
A	-85	SER	-	expression tag	UNP J8H9C1
A	-84	GLY	-	expression tag	UNP J8H9C1
A	-83	VAL	-	expression tag	UNP J8H9C1
A	-82	LYS	-	expression tag	UNP J8H9C1
A	-81	THR	-	expression tag	UNP J8H9C1
A	-80	GLU	-	expression tag	UNP J8H9C1
A	-79	ASN	-	expression tag	UNP J8H9C1
A	-78	ASN	-	expression tag	UNP J8H9C1
A	-77	ASP	-	expression tag	UNP J8H9C1
A	-76	HIS	-	expression tag	UNP J8H9C1
A	-75	ILE	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-74	ASN	-	expression tag	UNP J8H9C1
A	-73	LEU	-	expression tag	UNP J8H9C1
A	-72	LYS	-	expression tag	UNP J8H9C1
A	-71	VAL	-	expression tag	UNP J8H9C1
A	-70	ALA	-	expression tag	UNP J8H9C1
A	-69	GLY	-	expression tag	UNP J8H9C1
A	-68	GLN	-	expression tag	UNP J8H9C1
A	-67	ASP	-	expression tag	UNP J8H9C1
A	-66	GLY	-	expression tag	UNP J8H9C1
A	-65	SER	-	expression tag	UNP J8H9C1
A	-64	VAL	-	expression tag	UNP J8H9C1
A	-63	VAL	-	expression tag	UNP J8H9C1
A	-62	GLN	-	expression tag	UNP J8H9C1
A	-61	PHE	-	expression tag	UNP J8H9C1
A	-60	LYS	-	expression tag	UNP J8H9C1
A	-59	ILE	-	expression tag	UNP J8H9C1
A	-58	LYS	-	expression tag	UNP J8H9C1
A	-57	ARG	-	expression tag	UNP J8H9C1
A	-56	HIS	-	expression tag	UNP J8H9C1
A	-55	THR	-	expression tag	UNP J8H9C1
A	-54	PRO	-	expression tag	UNP J8H9C1
A	-53	LEU	-	expression tag	UNP J8H9C1
A	-52	SER	-	expression tag	UNP J8H9C1
A	-51	LYS	-	expression tag	UNP J8H9C1
A	-50	LEU	-	expression tag	UNP J8H9C1
A	-49	MET	-	expression tag	UNP J8H9C1
A	-48	LYS	-	expression tag	UNP J8H9C1
A	-47	ALA	-	expression tag	UNP J8H9C1
A	-46	TYR	-	expression tag	UNP J8H9C1
A	-45	CYS	-	expression tag	UNP J8H9C1
A	-44	GLU	-	expression tag	UNP J8H9C1
A	-43	ARG	-	expression tag	UNP J8H9C1
A	-42	GLN	-	expression tag	UNP J8H9C1
A	-41	GLY	-	expression tag	UNP J8H9C1
A	-40	LEU	-	expression tag	UNP J8H9C1
A	-39	SER	-	expression tag	UNP J8H9C1
A	-38	MET	-	expression tag	UNP J8H9C1
A	-37	ARG	-	expression tag	UNP J8H9C1
A	-36	GLN	-	expression tag	UNP J8H9C1
A	-35	ILE	-	expression tag	UNP J8H9C1
A	-34	ARG	-	expression tag	UNP J8H9C1
A	-33	PHE	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	ARG	-	expression tag	UNP J8H9C1
A	-31	PHE	-	expression tag	UNP J8H9C1
A	-30	ASP	-	expression tag	UNP J8H9C1
A	-29	GLY	-	expression tag	UNP J8H9C1
A	-28	GLN	-	expression tag	UNP J8H9C1
A	-27	PRO	-	expression tag	UNP J8H9C1
A	-26	ILE	-	expression tag	UNP J8H9C1
A	-25	ASN	-	expression tag	UNP J8H9C1
A	-24	GLU	-	expression tag	UNP J8H9C1
A	-23	THR	-	expression tag	UNP J8H9C1
A	-22	ASP	-	expression tag	UNP J8H9C1
A	-21	THR	-	expression tag	UNP J8H9C1
A	-20	PRO	-	expression tag	UNP J8H9C1
A	-19	ALA	-	expression tag	UNP J8H9C1
A	-18	GLN	-	expression tag	UNP J8H9C1
A	-17	LEU	-	expression tag	UNP J8H9C1
A	-16	GLU	-	expression tag	UNP J8H9C1
A	-15	MET	-	expression tag	UNP J8H9C1
A	-14	GLU	-	expression tag	UNP J8H9C1
A	-13	ASP	-	expression tag	UNP J8H9C1
A	-12	GLU	-	expression tag	UNP J8H9C1
A	-11	ASP	-	expression tag	UNP J8H9C1
A	-10	THR	-	expression tag	UNP J8H9C1
A	-9	ILE	-	expression tag	UNP J8H9C1
A	-8	ASP	-	expression tag	UNP J8H9C1
A	-7	VAL	-	expression tag	UNP J8H9C1
A	-6	PHE	-	expression tag	UNP J8H9C1
A	-5	GLN	-	expression tag	UNP J8H9C1
A	-4	GLN	-	expression tag	UNP J8H9C1
A	-3	GLN	-	expression tag	UNP J8H9C1
A	-2	THR	-	expression tag	UNP J8H9C1
A	-1	GLY	-	expression tag	UNP J8H9C1
A	0	GLY	-	expression tag	UNP J8H9C1
A	1	SER	-	expression tag	UNP J8H9C1
B	-96	MET	-	expression tag	UNP J8H9C1
B	-95	GLY	-	expression tag	UNP J8H9C1
B	-94	SER	-	expression tag	UNP J8H9C1
B	-93	SER	-	expression tag	UNP J8H9C1
B	-92	HIS	-	expression tag	UNP J8H9C1
B	-91	HIS	-	expression tag	UNP J8H9C1
B	-90	HIS	-	expression tag	UNP J8H9C1
B	-89	HIS	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-88	HIS	-	expression tag	UNP J8H9C1
B	-87	HIS	-	expression tag	UNP J8H9C1
B	-86	GLY	-	expression tag	UNP J8H9C1
B	-85	SER	-	expression tag	UNP J8H9C1
B	-84	GLY	-	expression tag	UNP J8H9C1
B	-83	VAL	-	expression tag	UNP J8H9C1
B	-82	LYS	-	expression tag	UNP J8H9C1
B	-81	THR	-	expression tag	UNP J8H9C1
B	-80	GLU	-	expression tag	UNP J8H9C1
B	-79	ASN	-	expression tag	UNP J8H9C1
B	-78	ASN	-	expression tag	UNP J8H9C1
B	-77	ASP	-	expression tag	UNP J8H9C1
B	-76	HIS	-	expression tag	UNP J8H9C1
B	-75	ILE	-	expression tag	UNP J8H9C1
B	-74	ASN	-	expression tag	UNP J8H9C1
B	-73	LEU	-	expression tag	UNP J8H9C1
B	-72	LYS	-	expression tag	UNP J8H9C1
B	-71	VAL	-	expression tag	UNP J8H9C1
B	-70	ALA	-	expression tag	UNP J8H9C1
B	-69	GLY	-	expression tag	UNP J8H9C1
B	-68	GLN	-	expression tag	UNP J8H9C1
B	-67	ASP	-	expression tag	UNP J8H9C1
B	-66	GLY	-	expression tag	UNP J8H9C1
B	-65	SER	-	expression tag	UNP J8H9C1
B	-64	VAL	-	expression tag	UNP J8H9C1
B	-63	VAL	-	expression tag	UNP J8H9C1
B	-62	GLN	-	expression tag	UNP J8H9C1
B	-61	PHE	-	expression tag	UNP J8H9C1
B	-60	LYS	-	expression tag	UNP J8H9C1
B	-59	ILE	-	expression tag	UNP J8H9C1
B	-58	LYS	-	expression tag	UNP J8H9C1
B	-57	ARG	-	expression tag	UNP J8H9C1
B	-56	HIS	-	expression tag	UNP J8H9C1
B	-55	THR	-	expression tag	UNP J8H9C1
B	-54	PRO	-	expression tag	UNP J8H9C1
B	-53	LEU	-	expression tag	UNP J8H9C1
B	-52	SER	-	expression tag	UNP J8H9C1
B	-51	LYS	-	expression tag	UNP J8H9C1
B	-50	LEU	-	expression tag	UNP J8H9C1
B	-49	MET	-	expression tag	UNP J8H9C1
B	-48	LYS	-	expression tag	UNP J8H9C1
B	-47	ALA	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-46	TYR	-	expression tag	UNP J8H9C1
B	-45	CYS	-	expression tag	UNP J8H9C1
B	-44	GLU	-	expression tag	UNP J8H9C1
B	-43	ARG	-	expression tag	UNP J8H9C1
B	-42	GLN	-	expression tag	UNP J8H9C1
B	-41	GLY	-	expression tag	UNP J8H9C1
B	-40	LEU	-	expression tag	UNP J8H9C1
B	-39	SER	-	expression tag	UNP J8H9C1
B	-38	MET	-	expression tag	UNP J8H9C1
B	-37	ARG	-	expression tag	UNP J8H9C1
B	-36	GLN	-	expression tag	UNP J8H9C1
B	-35	ILE	-	expression tag	UNP J8H9C1
B	-34	ARG	-	expression tag	UNP J8H9C1
B	-33	PHE	-	expression tag	UNP J8H9C1
B	-32	ARG	-	expression tag	UNP J8H9C1
B	-31	PHE	-	expression tag	UNP J8H9C1
B	-30	ASP	-	expression tag	UNP J8H9C1
B	-29	GLY	-	expression tag	UNP J8H9C1
B	-28	GLN	-	expression tag	UNP J8H9C1
B	-27	PRO	-	expression tag	UNP J8H9C1
B	-26	ILE	-	expression tag	UNP J8H9C1
B	-25	ASN	-	expression tag	UNP J8H9C1
B	-24	GLU	-	expression tag	UNP J8H9C1
B	-23	THR	-	expression tag	UNP J8H9C1
B	-22	ASP	-	expression tag	UNP J8H9C1
B	-21	THR	-	expression tag	UNP J8H9C1
B	-20	PRO	-	expression tag	UNP J8H9C1
B	-19	ALA	-	expression tag	UNP J8H9C1
B	-18	GLN	-	expression tag	UNP J8H9C1
B	-17	LEU	-	expression tag	UNP J8H9C1
B	-16	GLU	-	expression tag	UNP J8H9C1
B	-15	MET	-	expression tag	UNP J8H9C1
B	-14	GLU	-	expression tag	UNP J8H9C1
B	-13	ASP	-	expression tag	UNP J8H9C1
B	-12	GLU	-	expression tag	UNP J8H9C1
B	-11	ASP	-	expression tag	UNP J8H9C1
B	-10	THR	-	expression tag	UNP J8H9C1
B	-9	ILE	-	expression tag	UNP J8H9C1
B	-8	ASP	-	expression tag	UNP J8H9C1
B	-7	VAL	-	expression tag	UNP J8H9C1
B	-6	PHE	-	expression tag	UNP J8H9C1
B	-5	GLN	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLN	-	expression tag	UNP J8H9C1
B	-3	GLN	-	expression tag	UNP J8H9C1
B	-2	THR	-	expression tag	UNP J8H9C1
B	-1	GLY	-	expression tag	UNP J8H9C1
B	0	GLY	-	expression tag	UNP J8H9C1
B	1	SER	-	expression tag	UNP J8H9C1
C	-96	MET	-	expression tag	UNP J8H9C1
C	-95	GLY	-	expression tag	UNP J8H9C1
C	-94	SER	-	expression tag	UNP J8H9C1
C	-93	SER	-	expression tag	UNP J8H9C1
C	-92	HIS	-	expression tag	UNP J8H9C1
C	-91	HIS	-	expression tag	UNP J8H9C1
C	-90	HIS	-	expression tag	UNP J8H9C1
C	-89	HIS	-	expression tag	UNP J8H9C1
C	-88	HIS	-	expression tag	UNP J8H9C1
C	-87	HIS	-	expression tag	UNP J8H9C1
C	-86	GLY	-	expression tag	UNP J8H9C1
C	-85	SER	-	expression tag	UNP J8H9C1
C	-84	GLY	-	expression tag	UNP J8H9C1
C	-83	VAL	-	expression tag	UNP J8H9C1
C	-82	LYS	-	expression tag	UNP J8H9C1
C	-81	THR	-	expression tag	UNP J8H9C1
C	-80	GLU	-	expression tag	UNP J8H9C1
C	-79	ASN	-	expression tag	UNP J8H9C1
C	-78	ASN	-	expression tag	UNP J8H9C1
C	-77	ASP	-	expression tag	UNP J8H9C1
C	-76	HIS	-	expression tag	UNP J8H9C1
C	-75	ILE	-	expression tag	UNP J8H9C1
C	-74	ASN	-	expression tag	UNP J8H9C1
C	-73	LEU	-	expression tag	UNP J8H9C1
C	-72	LYS	-	expression tag	UNP J8H9C1
C	-71	VAL	-	expression tag	UNP J8H9C1
C	-70	ALA	-	expression tag	UNP J8H9C1
C	-69	GLY	-	expression tag	UNP J8H9C1
C	-68	GLN	-	expression tag	UNP J8H9C1
C	-67	ASP	-	expression tag	UNP J8H9C1
C	-66	GLY	-	expression tag	UNP J8H9C1
C	-65	SER	-	expression tag	UNP J8H9C1
C	-64	VAL	-	expression tag	UNP J8H9C1
C	-63	VAL	-	expression tag	UNP J8H9C1
C	-62	GLN	-	expression tag	UNP J8H9C1
C	-61	PHE	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-60	LYS	-	expression tag	UNP J8H9C1
C	-59	ILE	-	expression tag	UNP J8H9C1
C	-58	LYS	-	expression tag	UNP J8H9C1
C	-57	ARG	-	expression tag	UNP J8H9C1
C	-56	HIS	-	expression tag	UNP J8H9C1
C	-55	THR	-	expression tag	UNP J8H9C1
C	-54	PRO	-	expression tag	UNP J8H9C1
C	-53	LEU	-	expression tag	UNP J8H9C1
C	-52	SER	-	expression tag	UNP J8H9C1
C	-51	LYS	-	expression tag	UNP J8H9C1
C	-50	LEU	-	expression tag	UNP J8H9C1
C	-49	MET	-	expression tag	UNP J8H9C1
C	-48	LYS	-	expression tag	UNP J8H9C1
C	-47	ALA	-	expression tag	UNP J8H9C1
C	-46	TYR	-	expression tag	UNP J8H9C1
C	-45	CYS	-	expression tag	UNP J8H9C1
C	-44	GLU	-	expression tag	UNP J8H9C1
C	-43	ARG	-	expression tag	UNP J8H9C1
C	-42	GLN	-	expression tag	UNP J8H9C1
C	-41	GLY	-	expression tag	UNP J8H9C1
C	-40	LEU	-	expression tag	UNP J8H9C1
C	-39	SER	-	expression tag	UNP J8H9C1
C	-38	MET	-	expression tag	UNP J8H9C1
C	-37	ARG	-	expression tag	UNP J8H9C1
C	-36	GLN	-	expression tag	UNP J8H9C1
C	-35	ILE	-	expression tag	UNP J8H9C1
C	-34	ARG	-	expression tag	UNP J8H9C1
C	-33	PHE	-	expression tag	UNP J8H9C1
C	-32	ARG	-	expression tag	UNP J8H9C1
C	-31	PHE	-	expression tag	UNP J8H9C1
C	-30	ASP	-	expression tag	UNP J8H9C1
C	-29	GLY	-	expression tag	UNP J8H9C1
C	-28	GLN	-	expression tag	UNP J8H9C1
C	-27	PRO	-	expression tag	UNP J8H9C1
C	-26	ILE	-	expression tag	UNP J8H9C1
C	-25	ASN	-	expression tag	UNP J8H9C1
C	-24	GLU	-	expression tag	UNP J8H9C1
C	-23	THR	-	expression tag	UNP J8H9C1
C	-22	ASP	-	expression tag	UNP J8H9C1
C	-21	THR	-	expression tag	UNP J8H9C1
C	-20	PRO	-	expression tag	UNP J8H9C1
C	-19	ALA	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLN	-	expression tag	UNP J8H9C1
C	-17	LEU	-	expression tag	UNP J8H9C1
C	-16	GLU	-	expression tag	UNP J8H9C1
C	-15	MET	-	expression tag	UNP J8H9C1
C	-14	GLU	-	expression tag	UNP J8H9C1
C	-13	ASP	-	expression tag	UNP J8H9C1
C	-12	GLU	-	expression tag	UNP J8H9C1
C	-11	ASP	-	expression tag	UNP J8H9C1
C	-10	THR	-	expression tag	UNP J8H9C1
C	-9	ILE	-	expression tag	UNP J8H9C1
C	-8	ASP	-	expression tag	UNP J8H9C1
C	-7	VAL	-	expression tag	UNP J8H9C1
C	-6	PHE	-	expression tag	UNP J8H9C1
C	-5	GLN	-	expression tag	UNP J8H9C1
C	-4	GLN	-	expression tag	UNP J8H9C1
C	-3	GLN	-	expression tag	UNP J8H9C1
C	-2	THR	-	expression tag	UNP J8H9C1
C	-1	GLY	-	expression tag	UNP J8H9C1
C	0	GLY	-	expression tag	UNP J8H9C1
C	1	SER	-	expression tag	UNP J8H9C1
D	-96	MET	-	expression tag	UNP J8H9C1
D	-95	GLY	-	expression tag	UNP J8H9C1
D	-94	SER	-	expression tag	UNP J8H9C1
D	-93	SER	-	expression tag	UNP J8H9C1
D	-92	HIS	-	expression tag	UNP J8H9C1
D	-91	HIS	-	expression tag	UNP J8H9C1
D	-90	HIS	-	expression tag	UNP J8H9C1
D	-89	HIS	-	expression tag	UNP J8H9C1
D	-88	HIS	-	expression tag	UNP J8H9C1
D	-87	HIS	-	expression tag	UNP J8H9C1
D	-86	GLY	-	expression tag	UNP J8H9C1
D	-85	SER	-	expression tag	UNP J8H9C1
D	-84	GLY	-	expression tag	UNP J8H9C1
D	-83	VAL	-	expression tag	UNP J8H9C1
D	-82	LYS	-	expression tag	UNP J8H9C1
D	-81	THR	-	expression tag	UNP J8H9C1
D	-80	GLU	-	expression tag	UNP J8H9C1
D	-79	ASN	-	expression tag	UNP J8H9C1
D	-78	ASN	-	expression tag	UNP J8H9C1
D	-77	ASP	-	expression tag	UNP J8H9C1
D	-76	HIS	-	expression tag	UNP J8H9C1
D	-75	ILE	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-74	ASN	-	expression tag	UNP J8H9C1
D	-73	LEU	-	expression tag	UNP J8H9C1
D	-72	LYS	-	expression tag	UNP J8H9C1
D	-71	VAL	-	expression tag	UNP J8H9C1
D	-70	ALA	-	expression tag	UNP J8H9C1
D	-69	GLY	-	expression tag	UNP J8H9C1
D	-68	GLN	-	expression tag	UNP J8H9C1
D	-67	ASP	-	expression tag	UNP J8H9C1
D	-66	GLY	-	expression tag	UNP J8H9C1
D	-65	SER	-	expression tag	UNP J8H9C1
D	-64	VAL	-	expression tag	UNP J8H9C1
D	-63	VAL	-	expression tag	UNP J8H9C1
D	-62	GLN	-	expression tag	UNP J8H9C1
D	-61	PHE	-	expression tag	UNP J8H9C1
D	-60	LYS	-	expression tag	UNP J8H9C1
D	-59	ILE	-	expression tag	UNP J8H9C1
D	-58	LYS	-	expression tag	UNP J8H9C1
D	-57	ARG	-	expression tag	UNP J8H9C1
D	-56	HIS	-	expression tag	UNP J8H9C1
D	-55	THR	-	expression tag	UNP J8H9C1
D	-54	PRO	-	expression tag	UNP J8H9C1
D	-53	LEU	-	expression tag	UNP J8H9C1
D	-52	SER	-	expression tag	UNP J8H9C1
D	-51	LYS	-	expression tag	UNP J8H9C1
D	-50	LEU	-	expression tag	UNP J8H9C1
D	-49	MET	-	expression tag	UNP J8H9C1
D	-48	LYS	-	expression tag	UNP J8H9C1
D	-47	ALA	-	expression tag	UNP J8H9C1
D	-46	TYR	-	expression tag	UNP J8H9C1
D	-45	CYS	-	expression tag	UNP J8H9C1
D	-44	GLU	-	expression tag	UNP J8H9C1
D	-43	ARG	-	expression tag	UNP J8H9C1
D	-42	GLN	-	expression tag	UNP J8H9C1
D	-41	GLY	-	expression tag	UNP J8H9C1
D	-40	LEU	-	expression tag	UNP J8H9C1
D	-39	SER	-	expression tag	UNP J8H9C1
D	-38	MET	-	expression tag	UNP J8H9C1
D	-37	ARG	-	expression tag	UNP J8H9C1
D	-36	GLN	-	expression tag	UNP J8H9C1
D	-35	ILE	-	expression tag	UNP J8H9C1
D	-34	ARG	-	expression tag	UNP J8H9C1
D	-33	PHE	-	expression tag	UNP J8H9C1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-32	ARG	-	expression tag	UNP J8H9C1
D	-31	PHE	-	expression tag	UNP J8H9C1
D	-30	ASP	-	expression tag	UNP J8H9C1
D	-29	GLY	-	expression tag	UNP J8H9C1
D	-28	GLN	-	expression tag	UNP J8H9C1
D	-27	PRO	-	expression tag	UNP J8H9C1
D	-26	ILE	-	expression tag	UNP J8H9C1
D	-25	ASN	-	expression tag	UNP J8H9C1
D	-24	GLU	-	expression tag	UNP J8H9C1
D	-23	THR	-	expression tag	UNP J8H9C1
D	-22	ASP	-	expression tag	UNP J8H9C1
D	-21	THR	-	expression tag	UNP J8H9C1
D	-20	PRO	-	expression tag	UNP J8H9C1
D	-19	ALA	-	expression tag	UNP J8H9C1
D	-18	GLN	-	expression tag	UNP J8H9C1
D	-17	LEU	-	expression tag	UNP J8H9C1
D	-16	GLU	-	expression tag	UNP J8H9C1
D	-15	MET	-	expression tag	UNP J8H9C1
D	-14	GLU	-	expression tag	UNP J8H9C1
D	-13	ASP	-	expression tag	UNP J8H9C1
D	-12	GLU	-	expression tag	UNP J8H9C1
D	-11	ASP	-	expression tag	UNP J8H9C1
D	-10	THR	-	expression tag	UNP J8H9C1
D	-9	ILE	-	expression tag	UNP J8H9C1
D	-8	ASP	-	expression tag	UNP J8H9C1
D	-7	VAL	-	expression tag	UNP J8H9C1
D	-6	PHE	-	expression tag	UNP J8H9C1
D	-5	GLN	-	expression tag	UNP J8H9C1
D	-4	GLN	-	expression tag	UNP J8H9C1
D	-3	GLN	-	expression tag	UNP J8H9C1
D	-2	THR	-	expression tag	UNP J8H9C1
D	-1	GLY	-	expression tag	UNP J8H9C1
D	0	GLY	-	expression tag	UNP J8H9C1
D	1	SER	-	expression tag	UNP J8H9C1

- Molecule 2 is a protein called Gabija protein GajB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	288	Total	C	N	O	S	0	0
			2326	1502	381	441	2		
2	F	288	Total	C	N	O	S	0	0
			2326	1502	381	441	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	288	Total	C	N	O	S	0	0
			2326	1502	381	441	2		
2	H	288	Total	C	N	O	S	0	0
			2326	1502	381	441	2		

- Molecule 3 is a protein called Gabija Anti-Defense 1.

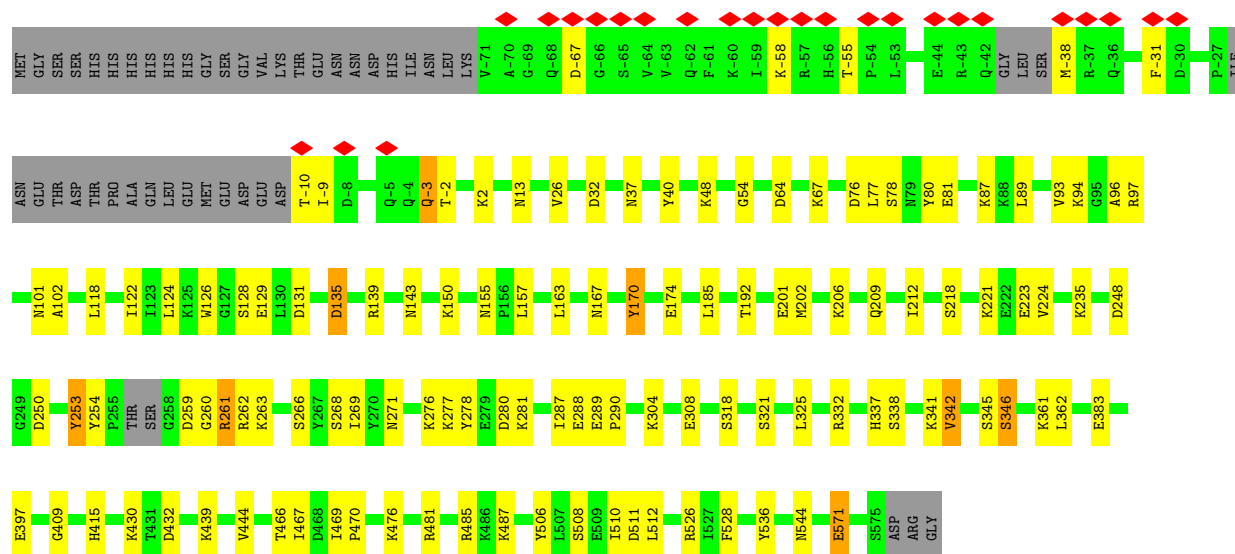
Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	162	Total	C	N	O	S	0	0
			1346	867	231	240	8		
3	J	162	Total	C	N	O	S	0	0
			1346	867	231	240	8		
3	K	162	Total	C	N	O	S	0	0
			1346	867	231	240	8		
3	L	162	Total	C	N	O	S	0	0
			1346	867	231	240	8		
3	M	114	Total	C	N	O	S	0	0
			933	602	152	172	7		
3	N	114	Total	C	N	O	S	0	0
			933	602	152	172	7		
3	O	114	Total	C	N	O	S	0	0
			933	602	152	172	7		
3	P	114	Total	C	N	O	S	0	0
			933	602	152	172	7		





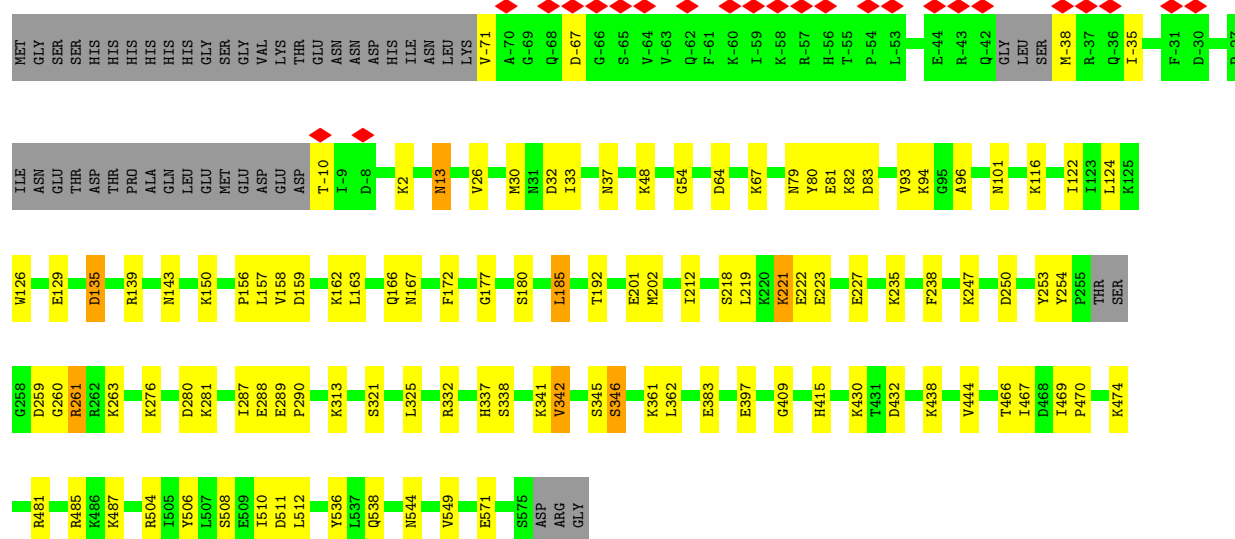
• Molecule 1: Endonuclease GajA

Chain C: 75% 17% 7%



• Molecule 1: Endonuclease GajA

Chain D: 76% 16% 7%



• Molecule 2: Gabija protein GajB

Chain E: 9% 39% 18% 42%







ILE MET ASP ASN LYS LYS TVR SER ASP TYR ILE GLU THR LEU MET LYS GLU LEU LYS ILE ILE ILE ILE SER ILE

### • Molecule 3: Gabija Anti-Defense 1

Chain I: 32% 19% 45%

MET LYS LEU LYS ILE GLY ILE LYS THR SER ASP TYR ILE GLU CYS PHE LEU THR LEU MET LYS GLU LEU LYS ILE ILE ILE ILE SER ILE

PRO ALA LYS LYS ILE ASN HIS ARG TYR GLU ASN LEU LYS LEU VAL GLY PHE GLN ASP SER PHE GLY THR PRO LYS VAL ILE HIS SER GLN ALA

MET ASN VAL ILE GLU ASN HIS ARG TYR GLU ASN LEU LYS LEU VAL GLY PHE GLN ASP SER PHE GLY THR PRO LYS VAL ILE HIS SER GLN ALA

V210 D211 N213 A214 M215 Y216 K217 R218 R219 K222 L223 R226 F227 Q228 V233 K237 K241 A242 Q244 I248 S253 G254 K255 D256 V257 E258 D259 S262 L268 D269 D270 L271 E277 P278 L279 V280 E281 C282 K283 C284 C285 R288 G289 V290 I291 N292 N293

GLU ASN

### • Molecule 3: Gabija Anti-Defense 1

Chain J: 33% 20% 45%

MET LYS LEU LYS ILE GLY ILE LYS THR SER ASP TYR ILE GLU CYS PHE LEU VAL GLY PHE GLN ASP SER PHE GLY THR PRO LYS VAL ILE HIS SER GLN ALA

PRO ALA LYS LYS ILE ASN HIS ARG TYR GLU ASN LEU LYS LEU VAL GLY PHE GLN ASP SER PHE GLY THR PRO LYS VAL ILE HIS SER GLN ALA

MET ASN VAL ILE GLU ASN HIS ARG TYR GLU ASN LEU LYS LEU VAL GLY PHE GLN ASP SER PHE GLY THR PRO LYS VAL ILE HIS SER GLN ALA

E207 Y208 L212 M215 Y216 K217 R219 K222 L223 R226 F227 Q228 T229 K230 R231 E232 K241 V249 F252 S253 D256 V257 L260 L268 D269 D270 P278 E281 C282 K283 C284 C285 K286 G287 R288 L292 N293 GLU ASN

### • Molecule 3: Gabija Anti-Defense 1

Chain K: 34% 19% 45%

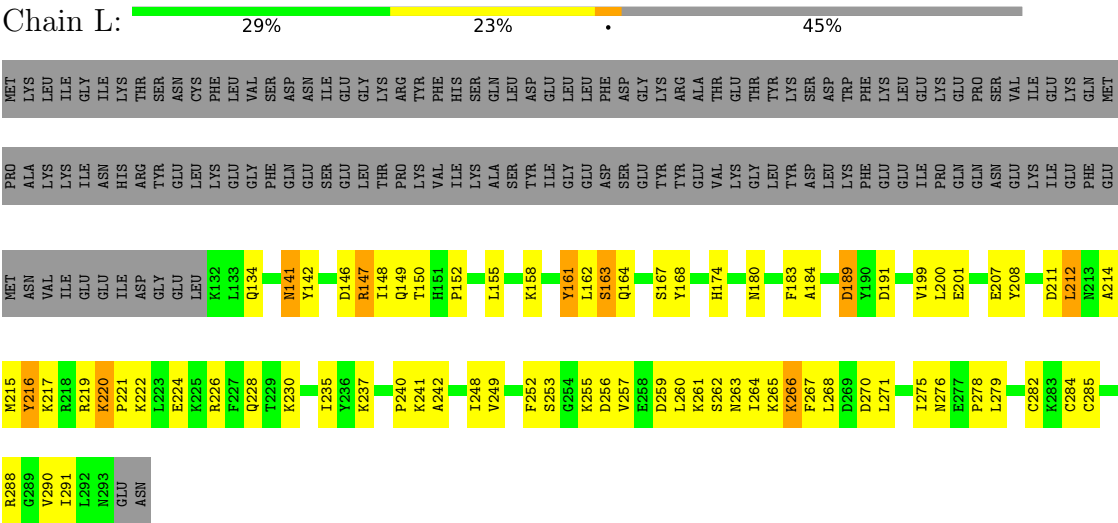
MET LYS LEU LYS ILE GLY ILE LYS THR SER ASP TYR ILE GLU CYS PHE LEU VAL GLY PHE GLN ASP SER PHE GLY THR PRO LYS VAL ILE HIS SER GLN ALA

PRO ALA LYS LYS ILE ASN HIS ARG TYR GLU ASN LEU LYS LEU VAL GLY PHE GLN ASP SER PHE GLY THR PRO LYS VAL ILE HIS SER GLN ALA

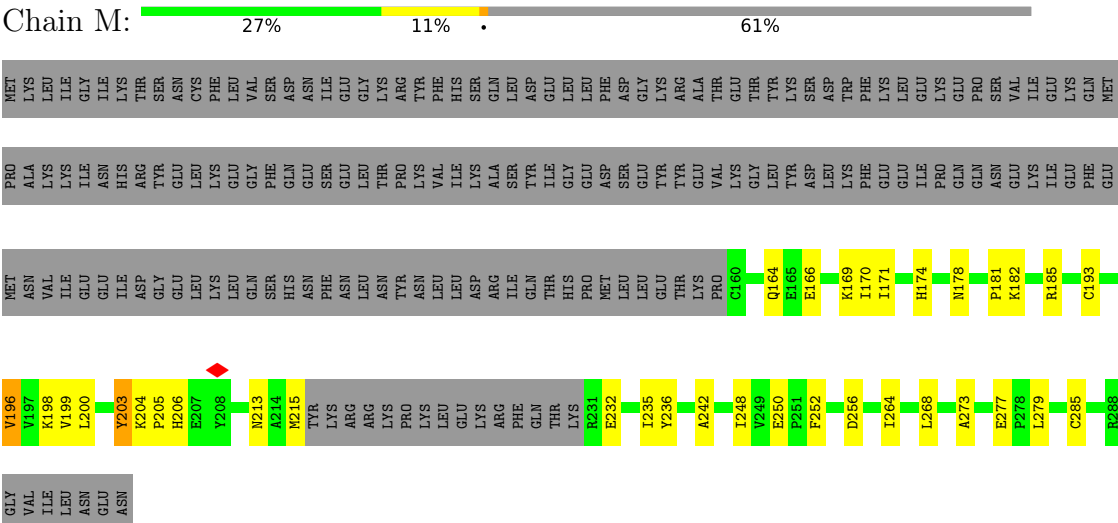
MET ASN VAL ILE GLU ASN HIS ARG TYR GLU ASN LEU LYS LEU VAL GLY PHE GLN ASP SER PHE GLY THR PRO LYS VAL ILE HIS SER GLN ALA

L212 N213 A214 M215 Y216 K217 R218 R219 K222 K225 R226 F227 Q228 T229 K230 R231 E232 K241 V249 F252 S253 D256 V257 L260 L268 D269 D270 P278 E277 L279 C282 K283 C284 C285 K286 G287 R288 L292 N293 GLU ASN

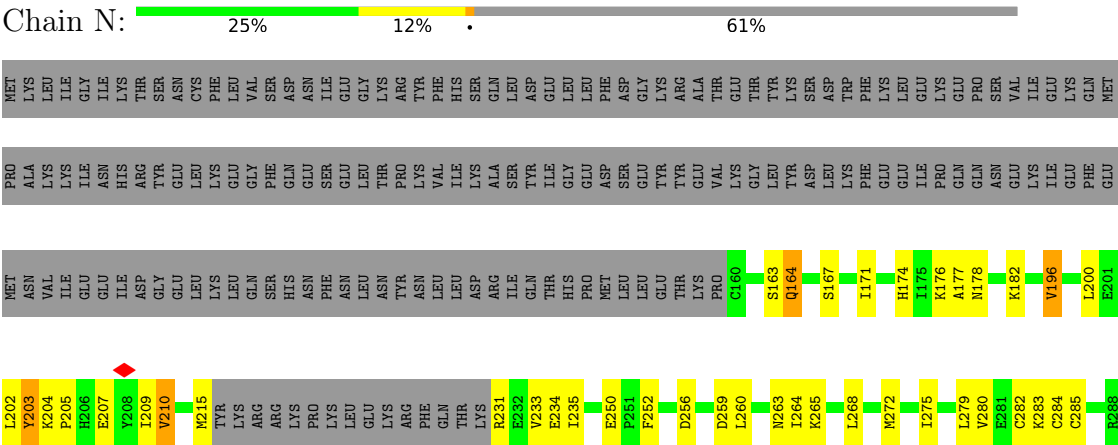
• Molecule 3: Gabija Anti-Defense 1



• Molecule 3: Gabija Anti-Defense 1



• Molecule 3: Gabija Anti-Defense 1



I275		V280		K283	C284	C285		R288	GLY	VAL	ILE	LEU	ASN	GLU	ASN
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	351193	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	41.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.269	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.028	Depositor
Map size ( $\text{\AA}$ )	311.5, 311.5, 311.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.89, 0.89, 0.89	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	0.30	0/5196	0.45	0/6968
1	B	0.30	0/5196	0.46	0/6968
1	C	0.30	0/5196	0.45	0/6968
1	D	0.30	0/5196	0.46	0/6968
2	E	0.27	0/2365	0.47	0/3179
2	F	0.28	0/2365	0.50	1/3179 (0.0%)
2	G	0.26	0/2365	0.45	0/3179
2	H	0.26	0/2365	0.48	1/3179 (0.0%)
3	I	0.28	0/1374	0.57	0/1849
3	J	0.28	0/1374	0.48	0/1849
3	K	0.29	0/1374	0.58	1/1849 (0.1%)
3	L	0.29	0/1374	0.55	0/1849
3	M	0.31	0/951	0.58	0/1280
3	N	0.33	0/951	0.63	0/1280
3	O	0.34	0/951	0.63	0/1280
3	P	0.32	0/951	0.58	0/1280
All	All	0.29	0/39544	0.49	3/53104 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	129	PRO	CA-N-CD	-6.12	102.93	111.50
3	K	270	ASP	CB-CG-OD2	5.67	123.41	118.30
2	H	326	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	5111	0	5155	78	0
1	B	5111	0	5155	66	0
1	C	5111	0	5155	71	0
1	D	5111	0	5155	75	0
2	E	2326	0	2331	60	0
2	F	2326	0	2331	57	0
2	G	2326	0	2331	54	0
2	H	2326	0	2331	55	0
3	I	1346	0	1388	44	0
3	J	1346	0	1388	38	0
3	K	1346	0	1388	45	0
3	L	1346	0	1388	50	0
3	M	933	0	946	26	0
3	N	933	0	946	34	0
3	O	933	0	946	27	0
3	P	933	0	946	32	0
All	All	38864	0	39280	740	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (740) 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)
3:O:182:LYS:HD3	3:O:204:LYS:HB3	1.53	0.88
3:L:263:ASN:HA	3:L:266:LYS:HE3	1.57	0.85
3:O:198:LYS:HB2	3:O:235:ILE:HD11	1.63	0.80
3:M:185:ARG:HH22	3:N:177:ALA:HA	1.45	0.80
2:E:112:LYS:HA	2:E:115:GLN:HE22	1.46	0.79
1:A:13:ASN:HB3	1:A:342:VAL:HG21	1.65	0.79
2:E:129:PRO:HB3	2:E:200:ARG:HG2	1.66	0.78
1:B:162:LYS:O	1:B:162:LYS:NZ	2.18	0.74
2:F:28:VAL:HG21	2:F:60:ARG:HD3	1.70	0.73
1:D:397:GLU:OE1	1:D:397:GLU:N	2.19	0.72
3:K:164:GLN:NE2	3:K:249:VAL:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:229:THR:HG23	3:J:230:LYS:HG3	1.71	0.72
3:N:182:LYS:HB2	3:N:204:LYS:HD3	1.71	0.71
2:G:5:GLN:N	2:G:5:GLN:OE1	2.22	0.71
2:E:5:GLN:N	2:E:5:GLN:OE1	2.23	0.71
1:B:383:GLU:HG3	1:B:512:LEU:HD22	1.73	0.70
3:M:232:GLU:N	3:M:232:GLU:OE1	2.24	0.70
3:O:203:TYR:CD1	3:O:205:PRO:HD2	2.26	0.70
2:E:115:GLN:OE1	2:E:115:GLN:N	2.24	0.70
3:K:200:LEU:HA	3:K:279:LEU:HD13	1.74	0.70
1:A:383:GLU:HG3	1:A:512:LEU:HD22	1.75	0.69
1:D:511:ASP:OD2	1:D:538:GLN:NE2	2.25	0.69
1:D:383:GLU:HG3	1:D:512:LEU:HD22	1.74	0.69
1:A:511:ASP:OD2	1:A:538:GLN:NE2	2.25	0.69
1:C:13:ASN:HB3	1:C:342:VAL:HG21	1.74	0.69
2:H:161:ILE:HB	2:H:188:ILE:HG22	1.75	0.69
3:L:211:ASP:HB3	3:L:214:ALA:HB2	1.75	0.68
2:E:51:ASN:OD1	2:E:55:LYS:NZ	2.26	0.68
2:F:5:GLN:OE1	2:F:5:GLN:N	2.25	0.68
2:H:14:LEU:HD23	2:H:188:ILE:HD11	1.74	0.68
1:B:-4:GLN:NE2	1:B:103:ASP:OD2	2.22	0.68
1:C:383:GLU:HG3	1:C:512:LEU:HD22	1.76	0.68
1:C:170:TYR:OH	1:C:276:LYS:O	2.10	0.68
1:D:2:LYS:NZ	1:D:83:ASP:OD2	2.27	0.68
2:E:97:ASN:ND2	2:F:97:ASN:O	2.26	0.68
3:M:185:ARG:HE	3:M:199:VAL:HG11	1.60	0.67
2:G:121:ASN:HB3	2:H:122:ILE:HG12	1.77	0.67
1:B:511:ASP:OD2	1:B:538:GLN:NE2	2.27	0.67
1:B:65:THR:HG23	1:B:113:TYR:HB3	1.76	0.67
1:D:13:ASN:OD1	1:D:13:ASN:N	2.27	0.67
2:H:126:TYR:HD2	2:H:133:PHE:HB2	1.60	0.67
3:O:166:GLU:OE2	3:O:166:GLU:N	2.25	0.67
3:L:266:LYS:HD2	3:L:267:PHE:N	2.09	0.67
2:E:393:ASP:HB3	2:E:396:GLU:HB2	1.75	0.66
2:F:120:GLN:HE21	2:F:122:ILE:HG22	1.61	0.66
1:D:223:GLU:OE2	3:I:241:LYS:NZ	2.29	0.66
1:C:13:ASN:OD1	1:C:37:ASN:ND2	2.29	0.66
3:I:285:CYS:HB3	3:I:288:ARG:HE	1.59	0.66
3:I:270:ASP:OD1	3:I:271:LEU:N	2.29	0.65
3:K:272:MET:HE3	3:K:272:MET:O	1.97	0.65
2:G:120:GLN:HG3	2:G:122:ILE:H	1.62	0.65
3:N:174:HIS:CE1	3:N:268:LEU:HD21	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ILE:HD12	1:A:551:ASN:HB2	1.79	0.65
3:P:200:LEU:HD11	3:P:233:VAL:HG12	1.79	0.65
2:F:74:ASP:OD2	2:F:75:GLY:N	2.30	0.64
1:C:287:ILE:HG22	1:C:290:PRO:HG3	1.80	0.64
2:F:51:ASN:HB3	2:F:346:ALA:HA	1.79	0.64
1:A:176:GLN:OE1	3:I:226:ARG:NH2	2.30	0.64
2:G:329:GLU:HG3	2:G:347:GLU:HG3	1.80	0.64
1:B:287:ILE:HG22	1:B:290:PRO:HG3	1.79	0.64
3:M:166:GLU:OE2	3:M:166:GLU:N	2.24	0.64
2:H:323:ASN:OD1	2:H:323:ASN:N	2.28	0.63
3:M:196:VAL:HG22	3:M:235:ILE:HD11	1.80	0.63
2:F:102:TYR:O	2:F:106:GLN:NE2	2.32	0.63
1:A:172:PHE:HD2	1:A:238:PHE:HE1	1.45	0.63
1:C:250:ASP:OD2	1:C:254:TYR:OH	2.16	0.63
1:D:235:LYS:HD3	3:J:218:ARG:HH21	1.63	0.63
2:H:332:LYS:NZ	2:H:343:ASP:OD2	2.32	0.62
2:H:74:ASP:OD2	2:H:75:GLY:N	2.33	0.62
3:I:203:TYR:OH	3:I:281:GLU:O	2.15	0.62
2:E:14:LEU:HB2	2:E:219:LYS:HA	1.81	0.62
3:L:147:ARG:HH11	3:L:148:ILE:HG12	1.64	0.62
1:D:287:ILE:HG22	1:D:290:PRO:HG3	1.80	0.62
1:A:287:ILE:HG22	1:A:290:PRO:HG3	1.81	0.62
2:H:75:GLY:O	2:H:79:SER:OG	2.18	0.62
3:L:270:ASP:OD2	3:L:271:LEU:N	2.32	0.62
1:A:340:GLU:OE2	1:A:340:GLU:N	2.26	0.62
1:A:432:ASP:HB2	1:A:511:ASP:HA	1.82	0.61
3:N:203:TYR:HD2	3:N:205:PRO:HD2	1.65	0.61
2:F:5:GLN:HA	2:F:8:LYS:HZ3	1.65	0.61
3:J:285:CYS:HB3	3:J:288:ARG:HG2	1.81	0.61
2:H:112:LYS:HA	2:H:115:GLN:HG3	1.82	0.61
3:J:206:HIS:HB3	3:J:228:GLN:HG3	1.82	0.61
2:F:329:GLU:HG3	2:F:347:GLU:HG3	1.82	0.61
1:B:487:LYS:HE3	1:B:510:ILE:HD11	1.82	0.61
1:D:13:ASN:HD21	1:D:33:ILE:HG22	1.66	0.61
2:E:17:ALA:O	2:E:23:LYS:NZ	2.34	0.61
3:N:182:LYS:HD3	3:N:204:LYS:HG2	1.81	0.61
1:A:163:LEU:O	1:A:167:ASN:ND2	2.33	0.61
1:D:64:ASP:HB3	1:D:67:LYS:HE2	1.83	0.61
2:F:83:ARG:NH2	2:F:98:PHE:O	2.34	0.61
1:B:212:ILE:HD11	1:C:269:ILE:HG13	1.83	0.60
1:C:155:ASN:ND2	1:C:157:LEU:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLY:O	3:J:226:ARG:NH1	2.34	0.60
3:M:178:ASN:HD21	3:N:205:PRO:HA	1.65	0.60
2:G:206:ASN:OD1	2:G:207:PHE:N	2.35	0.60
1:B:432:ASP:HB2	1:B:511:ASP:HA	1.84	0.60
1:D:156:PRO:HG2	1:D:157:LEU:HD22	1.84	0.60
3:O:272:MET:O	3:O:276:ASN:ND2	2.35	0.60
1:C:223:GLU:OE2	3:K:241:LYS:NZ	2.25	0.59
1:A:414:ASN:OD1	1:A:455:ASN:ND2	2.34	0.59
2:E:164:TYR:OH	2:E:172:HIS:ND1	2.33	0.59
3:L:180:ASN:HD21	3:L:183:PHE:HB2	1.68	0.59
3:P:198:LYS:HB2	3:P:235:ILE:HD11	1.83	0.59
3:M:185:ARG:NH1	3:N:176:LYS:O	2.35	0.59
2:F:5:GLN:HA	2:F:8:LYS:NZ	2.17	0.59
3:K:185:ARG:HH21	3:K:187:THR:HG22	1.68	0.59
2:G:4:GLU:OE1	2:G:8:LYS:NZ	2.30	0.59
1:A:246:LYS:NZ	1:A:250:ASP:O	2.34	0.59
3:L:279:LEU:HD22	3:L:290:VAL:HG23	1.83	0.59
2:E:38:ASN:OD1	2:E:66:ARG:NH2	2.36	0.59
1:B:527:ILE:HD12	1:B:551:ASN:HB2	1.83	0.58
1:C:64:ASP:HB3	1:C:67:LYS:HE2	1.84	0.58
3:O:232:GLU:OE1	3:O:232:GLU:N	2.34	0.58
2:F:38:ASN:OD1	2:F:66:ARG:NH2	2.36	0.58
3:I:144:LEU:HD12	3:I:145:LEU:HD12	1.86	0.58
1:A:-3:GLN:NE2	1:A:78:SER:O	2.37	0.58
3:K:213:ASN:HD22	3:K:219:ARG:HG3	1.69	0.58
1:D:260:GLY:HA2	1:D:263:LYS:HG3	1.85	0.58
3:K:163:SER:HB3	3:K:166:GLU:HB3	1.84	0.58
2:H:14:LEU:HD12	2:H:219:LYS:HB3	1.85	0.58
2:H:38:ASN:OD1	2:H:66:ARG:NH2	2.36	0.58
3:M:203:TYR:CD2	3:M:205:PRO:HD2	2.38	0.58
1:C:-3:GLN:NE2	1:C:81:GLU:OE2	2.36	0.58
3:I:146:ASP:O	3:I:149:GLN:NE2	2.35	0.58
3:J:136:HIS:O	3:J:136:HIS:ND1	2.36	0.58
1:A:269:ILE:HG13	1:D:212:ILE:HD11	1.85	0.58
2:F:382:ILE:HD12	2:F:383:ASN:N	2.18	0.58
1:D:444:VAL:HA	1:D:466:THR:HA	1.86	0.58
1:A:337:HIS:NE2	1:A:345:SER:OG	2.32	0.57
2:G:93:ASP:N	2:G:93:ASP:OD1	2.36	0.57
2:G:97:ASN:O	2:H:97:ASN:ND2	2.36	0.57
2:F:104:ASP:OD2	2:F:355:ARG:NH2	2.37	0.57
2:G:38:ASN:OD1	2:G:66:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:209:ILE:HG12	3:I:223:LEU:HD12	1.85	0.57
1:A:255:PRO:O	1:A:262:ARG:NH1	2.37	0.57
1:A:536:TYR:O	1:A:544:ASN:ND2	2.37	0.57
2:E:161:ILE:HB	2:E:188:ILE:HG22	1.87	0.57
3:L:168:TYR:HB2	3:L:249:VAL:HG11	1.85	0.57
1:C:163:LEU:O	1:C:167:ASN:ND2	2.36	0.57
1:C:536:TYR:O	1:C:544:ASN:ND2	2.38	0.57
2:F:101:GLU:OE2	2:F:105:ASN:ND2	2.31	0.57
1:B:192:THR:OG1	3:K:217:LYS:NZ	2.38	0.57
1:B:-35:ILE:HD11	1:B:-7:VAL:HB	1.88	0.56
1:D:81:GLU:OE2	1:D:82:LYS:NZ	2.38	0.56
3:J:168:TYR:HB2	3:J:249:VAL:HG11	1.87	0.56
3:L:189:ASP:OD1	3:L:189:ASP:N	2.38	0.56
1:D:280:ASP:OD1	1:D:280:ASP:N	2.38	0.56
2:G:131:LYS:HB3	2:G:136:GLN:HE22	1.71	0.56
3:J:288:ARG:HH22	3:N:280:VAL:HB	1.71	0.56
2:G:181:GLN:N	2:G:181:GLN:OE1	2.39	0.56
1:C:487:LYS:HE2	1:C:510:ILE:HD11	1.88	0.56
2:E:218:ASN:HB3	2:E:220:TYR:HE1	1.71	0.56
3:I:134:GLN:HB2	3:I:136:HIS:HD2	1.70	0.56
3:L:260:LEU:O	3:L:264:ILE:HG12	2.06	0.56
3:N:196:VAL:HG22	3:N:235:ILE:HD11	1.87	0.56
3:O:185:ARG:HH22	3:P:177:ALA:HA	1.71	0.56
1:D:487:LYS:HE2	1:D:510:ILE:HD11	1.88	0.55
2:G:323:ASN:OD1	2:G:323:ASN:N	2.29	0.55
3:L:241:LYS:HG2	3:L:242:ALA:H	1.71	0.55
2:H:327:LEU:HD23	2:H:327:LEU:H	1.70	0.55
3:J:281:GLU:HB3	3:J:287:GLY:HA2	1.88	0.55
3:K:255:LYS:N	3:K:259:ASP:OD2	2.38	0.55
3:L:285:CYS:HB3	3:L:288:ARG:HB3	1.89	0.55
1:B:64:ASP:HB3	1:B:67:LYS:HE2	1.88	0.55
3:L:174:HIS:CD2	3:L:268:LEU:HD13	2.41	0.55
1:A:192:THR:OG1	3:I:217:LYS:NZ	2.39	0.55
2:G:343:ASP:OD1	2:G:343:ASP:N	2.38	0.55
3:I:189:ASP:OD2	3:I:189:ASP:N	2.40	0.55
3:K:168:TYR:HB2	3:K:249:VAL:HG11	1.89	0.55
1:B:542:LEU:HD13	1:D:409:GLY:HA3	1.88	0.55
2:G:97:ASN:ND2	2:H:97:ASN:O	2.40	0.55
3:L:201:GLU:HB3	3:L:230:LYS:HG2	1.88	0.55
3:N:280:VAL:HG12	3:N:282:CYS:H	1.71	0.55
3:P:170:ILE:HD12	3:P:264:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:15:VAL:HB	2:E:189:VAL:HG22	1.88	0.55
2:F:206:ASN:OD1	2:F:207:PHE:N	2.40	0.55
3:M:182:LYS:HA	3:M:204:LYS:HG3	1.89	0.55
1:A:280:ASP:N	1:A:280:ASP:OD1	2.40	0.54
1:D:221:LYS:HE2	1:D:221:LYS:N	2.23	0.54
3:P:256:ASP:OD2	3:P:257:VAL:N	2.39	0.54
1:B:247:LYS:HG2	1:B:254:TYR:HE2	1.72	0.54
1:C:467:ILE:HD11	1:C:485:ARG:HG2	1.89	0.54
3:M:171:ILE:HG22	3:M:268:LEU:HD21	1.90	0.54
2:F:179:LYS:HD3	2:F:186:LEU:HD12	1.88	0.54
2:H:17:ALA:HB3	2:H:23:LYS:HB3	1.89	0.54
3:I:216:TYR:HB2	3:I:219:ARG:HD3	1.89	0.54
3:L:255:LYS:N	3:L:259:ASP:OD2	2.40	0.54
2:E:78:GLU:OE2	2:E:134:LYS:NZ	2.37	0.54
1:C:192:THR:OG1	3:L:217:LYS:NZ	2.40	0.54
1:B:504:ARG:HD3	1:B:571:GLU:HG2	1.90	0.54
3:K:199:VAL:HG22	3:K:232:GLU:HG2	1.90	0.54
1:B:162:LYS:NZ	1:B:166:GLN:OE1	2.39	0.54
1:C:397:GLU:HG3	1:D:221:LYS:HE3	1.89	0.54
1:B:170:TYR:OH	1:B:276:LYS:O	2.26	0.53
2:F:52:LYS:HB3	2:F:346:ALA:HB1	1.89	0.53
2:F:93:ASP:OD1	2:F:93:ASP:N	2.41	0.53
3:I:169:LYS:NZ	3:I:173:ASN:OD1	2.35	0.53
2:G:15:VAL:HB	2:G:189:VAL:HG22	1.90	0.53
1:D:467:ILE:HD11	1:D:485:ARG:HG2	1.89	0.53
2:F:50:THR:HG22	2:F:53:ALA:H	1.74	0.53
3:I:140:LEU:HD21	3:I:257:VAL:HG22	1.91	0.53
1:D:163:LEU:O	1:D:167:ASN:ND2	2.35	0.53
2:H:6:ILE:HG13	2:H:220:TYR:HD2	1.74	0.53
3:P:283:LYS:HE3	3:P:284:CYS:HB3	1.91	0.53
1:D:504:ARG:HD3	1:D:571:GLU:HG2	1.91	0.53
3:K:211:ASP:HB3	3:K:214:ALA:HB2	1.91	0.53
3:L:275:ILE:HD12	3:L:275:ILE:H	1.73	0.53
1:D:94:LYS:HG3	2:H:151:TYR:CZ	2.44	0.53
3:J:140:LEU:HD22	3:J:257:VAL:HG22	1.91	0.53
3:O:163:SER:OG	3:O:164:GLN:N	2.39	0.53
1:B:536:TYR:O	1:B:544:ASN:ND2	2.41	0.53
1:A:223:GLU:OE2	3:J:241:LYS:NZ	2.42	0.53
1:D:536:TYR:O	1:D:544:ASN:ND2	2.42	0.53
3:L:271:LEU:O	3:L:275:ILE:HD12	2.08	0.53
2:E:74:ASP:OD2	2:E:75:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASN:HB3	1:B:342:VAL:HG21	1.91	0.52
1:C:94:LYS:HG3	2:G:151:TYR:CZ	2.44	0.52
2:E:150:GLN:O	2:E:154:SER:OG	2.27	0.52
2:H:104:ASP:OD1	2:H:355:ARG:NH2	2.43	0.52
3:K:136:HIS:O	3:K:136:HIS:ND1	2.42	0.52
1:D:341:LYS:HA	1:D:341:LYS:HE2	1.91	0.52
2:E:376:LEU:HA	2:E:379:GLN:HE21	1.74	0.52
2:F:180:ASP:OD1	2:F:181:GLN:N	2.42	0.52
1:B:150:LYS:HB2	1:B:281:LYS:HD3	1.91	0.52
2:E:206:ASN:OD1	2:E:207:PHE:N	2.42	0.52
2:F:343:ASP:N	2:F:343:ASP:OD1	2.43	0.52
3:I:208:TYR:CE1	3:I:226:ARG:HB2	2.45	0.52
3:N:204:LYS:HG3	3:N:205:PRO:HD3	1.90	0.52
1:A:185:LEU:HD21	3:I:215:MET:HG3	1.90	0.52
2:H:23:LYS:NZ	2:H:163:GLU:OE2	2.42	0.52
2:H:341:ILE:HD12	2:H:344:LEU:HD21	1.92	0.52
3:K:226:ARG:HH11	3:K:226:ARG:HB3	1.74	0.52
3:O:210:VAL:HA	3:P:261:LYS:HZ1	1.75	0.52
2:E:355:ARG:HD2	2:F:118:LYS:HG2	1.90	0.52
2:E:98:PHE:HB2	2:E:122:ILE:HA	1.92	0.52
1:D:192:THR:OG1	3:J:217:LYS:NZ	2.42	0.52
3:I:255:LYS:N	3:I:259:ASP:OD2	2.42	0.52
3:M:166:GLU:HA	3:M:169:LYS:HB2	1.92	0.52
1:A:94:LYS:HG3	2:E:151:TYR:CZ	2.45	0.52
1:A:504:ARG:HD3	1:A:571:GLU:HG2	1.91	0.52
1:B:94:LYS:HG3	2:F:151:TYR:CZ	2.45	0.52
2:H:206:ASN:OD1	2:H:207:PHE:N	2.43	0.52
1:D:506:TYR:OH	1:D:571:GLU:OE1	2.28	0.51
3:K:285:CYS:SG	3:K:288:ARG:HD2	2.51	0.51
3:I:207:GLU:HG3	3:I:227:PHE:CE1	2.44	0.51
1:C:506:TYR:OH	1:C:571:GLU:OE1	2.27	0.51
2:F:3:ARG:O	2:F:7:ILE:HD13	2.10	0.51
3:M:196:VAL:HG13	3:M:236:TYR:HB3	1.92	0.51
1:B:467:ILE:HD11	1:B:485:ARG:HG2	1.92	0.51
1:C:260:GLY:HA2	1:C:263:LYS:HG3	1.92	0.51
1:D:332:ARG:NH1	1:D:346:SER:OG	2.41	0.51
1:D:337:HIS:NE2	1:D:345:SER:OG	2.36	0.51
2:G:14:LEU:HB3	2:G:219:LYS:HA	1.92	0.51
3:I:242:ALA:HA	3:I:248:ILE:HD11	1.92	0.51
2:F:382:ILE:HD12	2:F:383:ASN:H	1.73	0.51
2:E:109:SER:O	2:E:113:GLY:N	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:GLU:OE2	2:H:134:LYS:NZ	2.38	0.51
3:L:262:SER:HA	3:L:265:LYS:HG2	1.92	0.51
3:P:284:CYS:SG	3:P:285:CYS:N	2.83	0.51
3:O:181:PRO:HG2	3:P:179:ILE:O	2.11	0.51
1:A:506:TYR:OH	1:A:571:GLU:OE1	2.28	0.51
2:G:326:LEU:HD12	2:G:327:LEU:HD22	1.92	0.51
1:D:13:ASN:HB2	1:D:342:VAL:HG21	1.92	0.51
3:K:206:HIS:HB3	3:K:228:GLN:HG3	1.93	0.51
2:E:50:THR:HG22	2:E:52:LYS:H	1.76	0.51
3:P:174:HIS:ND1	3:P:268:LEU:HD13	2.26	0.51
1:D:185:LEU:HD11	3:J:215:MET:HG3	1.93	0.50
2:H:24:THR:HG22	2:H:60:ARG:HH21	1.75	0.50
3:L:134:GLN:HG2	3:L:257:VAL:HG11	1.91	0.50
1:A:487:LYS:HE2	1:A:510:ILE:HD11	1.93	0.50
3:J:189:ASP:OD2	3:J:189:ASP:N	2.38	0.50
3:M:174:HIS:CG	3:M:268:LEU:HD13	2.46	0.50
3:N:164:GLN:O	3:N:167:SER:OG	2.28	0.50
1:D:101:ASN:ND2	1:D:129:GLU:OE2	2.45	0.50
1:D:166:GLN:N	1:D:166:GLN:OE1	2.44	0.50
3:P:252:PHE:HB3	3:P:260:LEU:HD11	1.93	0.50
2:G:169:LYS:HA	2:G:206:ASN:HD22	1.77	0.50
2:H:53:ALA:HA	2:H:56:GLU:HG2	1.93	0.50
3:K:226:ARG:HB3	3:K:226:ARG:NH1	2.25	0.50
1:D:250:ASP:OD2	1:D:254:TYR:OH	2.25	0.50
3:I:279:LEU:HB3	3:I:290:VAL:HG21	1.94	0.50
3:L:141:ASN:HB2	3:L:161:TYR:CE2	2.46	0.50
3:I:209:ILE:HD11	3:I:223:LEU:HB3	1.93	0.50
2:E:78:GLU:HA	2:E:82:ILE:HB	1.93	0.50
2:F:150:GLN:O	2:F:154:SER:OG	2.26	0.49
1:A:362:LEU:HD21	1:A:415:HIS:CD2	2.47	0.49
1:B:229:LYS:HG3	1:C:253:TYR:HE1	1.77	0.49
3:L:216:TYR:HB2	3:L:219:ARG:HD3	1.94	0.49
3:L:262:SER:O	3:L:266:LYS:HG3	2.12	0.49
1:A:250:ASP:OD2	1:A:254:TYR:OH	2.28	0.49
1:A:332:ARG:HD2	1:A:346:SER:OG	2.12	0.49
1:B:-71:VAL:HA	1:B:-9:ILE:H	1.76	0.49
1:C:201:GLU:HA	1:C:201:GLU:OE1	2.13	0.49
2:E:133:PHE:HA	2:E:136:GLN:HE21	1.77	0.49
2:E:329:GLU:H	2:E:329:GLU:CD	2.14	0.49
3:O:209:ILE:O	3:P:261:LYS:NZ	2.45	0.49
2:E:343:ASP:OD1	2:E:343:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:HB2	1:A:281:LYS:HD3	1.94	0.49
2:F:377:ILE:O	2:F:381:LEU:HD13	2.11	0.49
2:H:5:GLN:OE1	2:H:5:GLN:HA	2.13	0.49
3:K:142:TYR:CE1	3:K:160:CYS:HB3	2.48	0.49
2:H:329:GLU:O	2:H:332:LYS:HG3	2.12	0.49
2:H:330:VAL:HG21	2:H:364:ILE:HD12	1.93	0.49
1:C:341:LYS:HE2	1:C:341:LYS:HA	1.94	0.49
1:D:261:ARG:HG2	1:D:261:ARG:HH11	1.77	0.49
3:K:212:LEU:HB2	3:K:222:LYS:NZ	2.28	0.49
1:B:280:ASP:OD1	1:B:280:ASP:N	2.44	0.49
3:I:211:ASP:HB2	3:I:214:ALA:HB2	1.94	0.49
3:K:183:PHE:HA	3:K:279:LEU:HD21	1.95	0.49
2:G:329:GLU:O	2:G:332:LYS:HG3	2.13	0.49
1:C:-31:PHE:HB2	1:C:-9:ILE:HG22	1.95	0.49
1:D:159:ASP:HB3	1:D:162:LYS:HB3	1.95	0.49
1:D:150:LYS:HB2	1:D:281:LYS:HD3	1.95	0.48
2:F:126:TYR:HD2	2:F:131:LYS:HG3	1.78	0.48
2:F:129:PRO:HD3	2:F:200:ARG:NH1	2.28	0.48
3:L:216:TYR:CB	3:L:219:ARG:HD3	2.43	0.48
1:B:13:ASN:OD1	1:B:13:ASN:N	2.45	0.48
1:D:332:ARG:HD2	1:D:346:SER:OG	2.13	0.48
3:J:147:ARG:HD3	3:J:147:ARG:C	2.32	0.48
2:E:14:LEU:HG	2:E:217:PHE:HD2	1.79	0.48
2:H:158:LYS:HE3	2:H:187:PHE:HB2	1.95	0.48
3:L:256:ASP:O	3:L:260:LEU:N	2.34	0.48
1:C:332:ARG:HD2	1:C:346:SER:OG	2.13	0.48
2:G:159:ILE:HB	2:G:186:LEU:HD23	1.95	0.48
2:H:343:ASP:OD1	2:H:343:ASP:N	2.36	0.48
3:O:185:ARG:NH1	3:P:176:LYS:O	2.36	0.48
2:G:98:PHE:HB2	2:G:122:ILE:HA	1.95	0.48
2:H:362:LYS:HA	2:H:365:ASN:HD21	1.78	0.48
3:I:146:ASP:O	3:I:158:LYS:NZ	2.46	0.48
3:L:212:LEU:HD21	3:L:224:GLU:HB2	1.96	0.48
1:C:26:VAL:HG11	1:C:325:LEU:HD21	1.95	0.48
3:J:161:TYR:HA	3:J:253:SER:HA	1.95	0.48
3:J:175:ILE:HG22	3:J:186:ILE:HD11	1.96	0.48
1:A:64:ASP:HB3	1:A:67:LYS:HE2	1.95	0.48
1:B:93:VAL:HG13	1:B:96:ALA:HB3	1.96	0.48
2:F:325:THR:HA	2:F:328:LYS:HD2	1.95	0.48
2:H:135:PHE:CZ	2:H:171:MET:HG2	2.49	0.48
3:I:216:TYR:HB2	3:I:219:ARG:CD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:284:CYS:SG	3:K:285:CYS:N	2.87	0.48
3:M:203:TYR:HD2	3:M:205:PRO:HD2	1.79	0.48
2:G:106:GLN:HG3	2:G:125:THR:HG23	1.95	0.48
3:L:201:GLU:HA	3:L:230:LYS:HA	1.95	0.48
1:B:33:ILE:HD11	1:D:259:ASP:HB2	1.96	0.48
1:B:469:ILE:O	1:B:469:ILE:HD12	2.14	0.48
1:D:26:VAL:HG11	1:D:325:LEU:HD21	1.96	0.48
3:I:163:SER:O	3:I:167:SER:OG	2.32	0.48
3:K:141:ASN:HD22	3:K:161:TYR:HE2	1.60	0.48
3:K:147:ARG:HD3	3:K:147:ARG:C	2.35	0.48
1:B:474:LYS:O	1:D:474:LYS:NZ	2.47	0.47
3:O:264:ILE:HG21	3:P:209:ILE:HG12	1.96	0.47
1:B:225:SER:OG	1:C:248:ASP:OD1	2.33	0.47
1:B:506:TYR:OH	1:B:571:GLU:OE1	2.30	0.47
3:N:174:HIS:CG	3:N:268:LEU:HD11	2.49	0.47
1:A:209:GLN:HA	1:A:212:ILE:HG22	1.96	0.47
2:E:4:GLU:OE1	2:E:8:LYS:NZ	2.36	0.47
3:N:284:CYS:SG	3:N:285:CYS:N	2.87	0.47
1:A:469:ILE:HD12	1:A:469:ILE:O	2.14	0.47
1:C:280:ASP:OD1	1:C:280:ASP:N	2.46	0.47
2:E:116:VAL:C	2:E:120:GLN:HE21	2.18	0.47
3:J:142:TYR:CE1	3:J:160:CYS:HB3	2.50	0.47
3:O:235:ILE:N	3:O:235:ILE:HD12	2.29	0.47
1:B:167:ASN:O	1:B:171:ILE:HG13	2.15	0.47
1:B:202:MET:HE1	1:C:185:LEU:HD13	1.96	0.47
1:C:209:GLN:HA	1:C:212:ILE:HG22	1.96	0.47
2:E:53:ALA:HA	2:E:56:GLU:HG2	1.97	0.47
2:F:73:ASN:OD1	2:F:73:ASN:N	2.39	0.47
3:O:167:SER:O	3:O:171:ILE:HG13	2.15	0.47
1:A:93:VAL:HG13	1:A:96:ALA:HB3	1.96	0.47
1:C:362:LEU:HD21	1:C:415:HIS:CD2	2.50	0.47
1:D:93:VAL:HG13	1:D:96:ALA:HB3	1.96	0.47
1:D:432:ASP:HA	1:D:508:SER:HB2	1.95	0.47
3:K:212:LEU:HB2	3:K:222:LYS:HZ3	1.80	0.47
3:N:252:PHE:HB3	3:N:260:LEU:HD11	1.97	0.47
3:P:166:GLU:O	3:P:170:ILE:HG12	2.14	0.47
1:A:444:VAL:HA	1:A:466:THR:HA	1.97	0.47
1:B:524:MET:HG2	1:B:533:PRO:HB2	1.97	0.47
2:E:98:PHE:CD2	2:E:123:LEU:HB2	2.50	0.47
2:F:36:LYS:HB2	2:F:36:LYS:HE2	1.72	0.47
3:J:163:SER:O	3:J:167:SER:OG	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:179:ILE:HD12	3:J:186:ILE:HG13	1.96	0.47
3:J:216:TYR:HB2	3:J:219:ARG:HG2	1.97	0.47
3:K:162:LEU:HD12	3:K:162:LEU:HA	1.75	0.47
3:L:241:LYS:NZ	3:L:241:LYS:HB2	2.30	0.47
1:A:54:GLY:HA2	1:A:122:ILE:HD12	1.97	0.47
1:B:26:VAL:HG11	1:B:325:LEU:HD21	1.97	0.47
1:B:159:ASP:HB3	1:B:162:LYS:HB3	1.95	0.47
2:G:112:LYS:HA	2:G:115:GLN:HG3	1.95	0.47
3:O:265:LYS:HB2	3:O:265:LYS:HE2	1.57	0.47
1:D:54:GLY:HA2	1:D:122:ILE:HD12	1.97	0.47
1:D:469:ILE:HD12	1:D:469:ILE:O	2.15	0.47
2:E:178:LEU:HD23	2:E:182:LEU:HD12	1.96	0.47
3:L:184:ALA:HA	3:L:199:VAL:HG23	1.97	0.47
1:C:3:GLN:HA	1:C:78:SER:HB2	1.97	0.47
1:C:150:LYS:HB2	1:C:281:LYS:HD3	1.97	0.47
1:C:332:ARG:NH1	1:C:346:SER:OG	2.41	0.47
3:I:174:HIS:CG	3:I:268:LEU:HD13	2.50	0.47
3:I:282:CYS:HB3	3:M:285:CYS:HB3	1.49	0.47
1:A:332:ARG:NH1	1:A:346:SER:OG	2.40	0.46
2:G:204:PRO:O	2:G:208:ASN:ND2	2.39	0.46
2:G:362:LYS:HA	2:G:365:ASN:ND2	2.30	0.46
3:J:163:SER:HB3	3:J:166:GLU:HB3	1.96	0.46
3:M:264:ILE:HD11	3:N:209:ILE:CG2	2.45	0.46
3:N:209:ILE:HD12	3:N:210:VAL:N	2.30	0.46
3:O:200:LEU:HD11	3:O:233:VAL:HG12	1.97	0.46
1:B:304:LYS:HG3	1:B:308:GLU:HG3	1.98	0.46
1:C:48:LYS:HB3	1:C:48:LYS:HE2	1.78	0.46
1:C:432:ASP:HA	1:C:508:SER:HB2	1.97	0.46
2:F:164:TYR:OH	2:F:172:HIS:ND1	2.37	0.46
2:F:378:ASN:O	2:F:382:ILE:HG13	2.14	0.46
2:G:78:GLU:HA	2:G:82:ILE:HB	1.97	0.46
3:K:189:ASP:OD2	3:K:189:ASP:N	2.42	0.46
3:L:147:ARG:HD3	3:L:147:ARG:C	2.36	0.46
1:A:527:ILE:HD11	1:A:548:LEU:HD12	1.98	0.46
1:C:444:VAL:HA	1:C:466:THR:HA	1.97	0.46
2:E:14:LEU:HD11	2:E:217:PHE:HB3	1.98	0.46
2:H:121:ASN:C	2:H:122:ILE:HD12	2.35	0.46
1:A:397:GLU:OE1	1:A:397:GLU:N	2.45	0.46
1:B:185:LEU:HD23	3:K:214:ALA:HB3	1.97	0.46
2:E:135:PHE:CE2	2:E:171:MET:HG2	2.51	0.46
2:G:36:LYS:HE2	2:G:36:LYS:HB2	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:146:ASP:O	3:K:149:GLN:NE2	2.48	0.46
3:K:216:TYR:HB2	3:K:219:ARG:CD	2.46	0.46
1:D:162:LYS:HD3	1:D:162:LYS:C	2.36	0.46
3:P:272:MET:O	3:P:275:ILE:HG13	2.16	0.46
1:B:49:GLU:OE1	1:B:52:LYS:NZ	2.42	0.46
2:F:57:ILE:O	2:F:61:LEU:HD22	2.16	0.46
3:L:257:VAL:HG12	3:L:261:LYS:NZ	2.31	0.46
1:A:185:LEU:HD13	1:D:202:MET:HE1	1.98	0.46
1:D:172:PHE:HD2	1:D:238:PHE:HE1	1.64	0.46
1:D:201:GLU:HA	1:D:201:GLU:OE1	2.16	0.46
2:E:377:ILE:O	2:E:381:LEU:HD13	2.15	0.46
3:L:183:PHE:CZ	3:L:278:PRO:HB3	2.51	0.46
1:A:5:ASN:ND2	1:A:18:ASN:OD1	2.49	0.46
1:B:172:PHE:HD2	1:B:238:PHE:HE1	1.62	0.46
2:E:6:ILE:HG22	2:E:220:TYR:CD2	2.51	0.46
2:E:159:ILE:HB	2:E:186:LEU:HD23	1.97	0.46
2:G:121:ASN:O	2:G:121:ASN:ND2	2.49	0.46
3:L:146:ASP:HB2	3:L:158:LYS:NZ	2.31	0.46
2:E:126:TYR:HD1	2:E:131:LYS:HG3	1.81	0.46
3:K:285:CYS:HB2	3:O:282:CYS:O	2.16	0.46
3:L:147:ARG:HA	3:L:155:LEU:HD21	1.96	0.46
3:M:206:HIS:CE1	3:N:265:LYS:HG3	2.51	0.46
1:A:48:LYS:HB3	1:A:48:LYS:HE2	1.77	0.46
2:F:168:ASP:OD1	2:F:169:LYS:N	2.48	0.46
3:N:252:PHE:CG	3:N:264:ILE:HD11	2.51	0.46
1:A:35:ILE:HA	1:A:6:PHE:O	2.16	0.45
1:A:26:VAL:HG11	1:A:325:LEU:HD21	1.98	0.45
2:F:2:SER:N	2:F:5:GLN:HE22	2.15	0.45
2:G:107:PHE:HE2	2:G:124:GLY:HA3	1.81	0.45
1:A:216:TYR:OH	1:D:261:ARG:HD3	2.16	0.45
1:C:77:LEU:HD21	1:C:89:LEU:HD23	1.98	0.45
2:H:204:PRO:O	2:H:208:ASN:ND2	2.38	0.45
1:A:523:SER:O	1:A:527:ILE:HG23	2.16	0.45
1:D:13:ASN:OD1	1:D:37:ASN:ND2	2.48	0.45
1:D:362:LEU:HD21	1:D:415:HIS:CD2	2.52	0.45
3:M:204:LYS:HA	3:M:204:LYS:HD3	1.67	0.45
1:A:2:LYS:O	1:A:76:ASP:N	2.46	0.45
1:C:97:ARG:NH2	1:C:102:ALA:O	2.49	0.45
2:F:97:ASN:OD1	2:F:121:ASN:ND2	2.37	0.45
3:J:146:ASP:O	3:J:150:THR:HG22	2.16	0.45
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-58:LYS:HB2	1:C:-55:THR:OG1	2.16	0.45
1:C:170:TYR:CE2	1:C:277:LYS:HD3	2.51	0.45
2:H:74:ASP:OD1	2:H:102:TYR:OH	2.34	0.45
2:E:48:THR:HA	2:E:162:ASP:OD1	2.17	0.45
2:F:380:VAL:HA	2:F:383:ASN:HD21	1.82	0.45
2:G:106:GLN:HB3	2:G:127:SER:OG	2.16	0.45
3:L:142:TYR:CE2	3:L:155:LEU:HB3	2.52	0.45
1:C:54:GLY:HA2	1:C:122:ILE:HD12	1.98	0.45
1:C:93:VAL:HG13	1:C:96:ALA:HB3	1.99	0.45
2:G:164:TYR:OH	2:G:172:HIS:ND1	2.44	0.45
1:C:469:ILE:HD12	1:C:469:ILE:O	2.16	0.45
2:G:161:ILE:HB	2:G:188:ILE:HG22	1.98	0.45
3:I:279:LEU:HB3	3:I:290:VAL:CG2	2.47	0.45
3:M:252:PHE:CD1	3:M:264:ILE:HG22	2.52	0.45
3:N:235:ILE:HD13	3:N:275:ILE:HG12	1.98	0.45
2:F:72:THR:HG21	2:F:350:GLY:HA2	1.99	0.45
3:K:216:TYR:HB2	3:K:219:ARG:HD3	1.99	0.45
3:K:284:CYS:SG	3:O:284:CYS:N	2.85	0.45
3:L:180:ASN:ND2	3:L:276:ASN:OD1	2.35	0.45
3:L:220:LYS:HD3	3:L:221:PRO:HD2	1.99	0.45
1:A:131:ASP:N	1:A:131:ASP:OD1	2.51	0.44
1:A:229:LYS:HG3	1:D:253:TYR:HE1	1.82	0.44
1:C:139:ARG:NH1	1:D:135:ASP:OD2	2.49	0.44
1:C:202:MET:O	1:C:206:LYS:HB2	2.17	0.44
1:C:337:HIS:NE2	1:C:345:SER:OG	2.35	0.44
2:E:107:PHE:HB2	2:E:126:TYR:CE2	2.52	0.44
2:E:132:ASN:N	2:E:170:ASP:OD2	2.45	0.44
1:D:430:LYS:NZ	1:D:508:SER:OG	2.44	0.44
3:I:211:ASP:OD1	3:I:223:LEU:HD13	2.17	0.44
3:K:179:ILE:HG22	3:K:275:ILE:HG21	1.98	0.44
3:K:278:PRO:HB2	3:K:293:ASN:H	1.83	0.44
1:B:469:ILE:HG22	1:B:481:ARG:HG2	1.99	0.44
2:F:222:LEU:HD22	2:F:226:PHE:CZ	2.52	0.44
3:M:166:GLU:O	3:M:170:ILE:HG13	2.18	0.44
3:O:177:ALA:HA	3:P:185:ARG:HH22	1.83	0.44
3:P:193:CYS:HB2	3:P:246:TYR:CE2	2.52	0.44
2:E:130:LYS:HA	2:E:130:LYS:HD3	1.81	0.44
2:G:57:ILE:O	2:G:61:LEU:HD22	2.17	0.44
3:J:222:LYS:O	3:J:222:LYS:NZ	2.31	0.44
3:N:200:LEU:HD11	3:N:233:VAL:HG12	2.00	0.44
1:A:177:GLY:O	3:I:226:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASP:OD1	1:B:131:ASP:N	2.50	0.44
2:H:23:LYS:HD2	2:H:189:VAL:HG11	2.00	0.44
3:J:199:VAL:HG22	3:J:232:GLU:HG2	1.98	0.44
3:N:283:LYS:HB3	3:N:284:CYS:H	1.51	0.44
1:A:-58:LYS:HA	1:A:-58:LYS:HD3	1.89	0.44
1:C:124:LEU:HD12	1:C:143:ASN:HD21	1.83	0.44
2:H:334:VAL:HG22	2:H:368:LEU:HD23	1.99	0.44
3:N:182:LYS:HE2	3:N:203:TYR:HA	2.00	0.44
1:B:124:LEU:HD12	1:B:143:ASN:HD21	1.83	0.44
1:B:185:LEU:HD21	3:K:215:MET:HG3	2.00	0.44
2:G:324:ALA:HA	2:G:327:LEU:HD23	1.98	0.44
2:H:326:LEU:HD12	2:H:327:LEU:N	2.33	0.44
2:H:363:ILE:HD11	2:H:383:ASN:OD1	2.18	0.44
3:I:147:ARG:C	3:I:147:ARG:HD2	2.38	0.44
1:D:432:ASP:HB2	1:D:511:ASP:HA	2.00	0.44
2:E:55:LYS:HZ1	2:E:346:ALA:HB1	1.83	0.44
2:F:15:VAL:HB	2:F:189:VAL:HG22	1.98	0.44
2:F:135:PHE:CE2	2:F:171:MET:HG2	2.53	0.44
3:J:288:ARG:HB3	3:N:231:ARG:NH2	2.33	0.44
3:L:282:CYS:SG	3:L:285:CYS:HB2	2.57	0.44
3:N:256:ASP:OD2	3:N:259:ASP:N	2.30	0.44
3:K:186:ILE:HD11	3:K:189:ASP:HB3	2.00	0.44
3:P:199:VAL:HG12	3:P:201:GLU:HB3	1.99	0.44
1:A:124:LEU:HD12	1:A:143:ASN:HD21	1.83	0.43
1:B:201:GLU:OE2	1:B:201:GLU:HA	2.18	0.43
2:G:165:GLN:NE2	2:G:191:ASP:HB3	2.33	0.43
3:K:282:CYS:HB3	3:K:285:CYS:H	1.82	0.43
1:B:-32:ARG:NH2	1:B:20:ASN:OD1	2.50	0.43
1:B:229:LYS:HG3	1:C:253:TYR:CE1	2.53	0.43
2:E:214:SER:OG	2:E:216:ASP:OD1	2.35	0.43
3:I:155:LEU:HD23	3:I:158:LYS:HD3	1.98	0.43
3:J:144:LEU:HD23	3:J:145:LEU:H	1.83	0.43
3:L:174:HIS:CE1	3:L:268:LEU:HB3	2.54	0.43
3:O:182:LYS:HE3	3:O:183:PHE:CE1	2.53	0.43
2:H:167:SER:HB2	2:H:171:MET:HE2	1.99	0.43
3:J:278:PRO:HG2	3:J:292:LEU:HG	1.99	0.43
1:A:220:LYS:HG2	1:A:222:GLU:HB2	1.99	0.43
1:B:281:LYS:HB3	1:B:281:LYS:HE2	1.77	0.43
2:E:126:TYR:CZ	2:E:133:PHE:HB2	2.52	0.43
2:E:387:LYS:HD3	2:E:387:LYS:HA	1.92	0.43
2:F:357:ILE:HA	2:F:360:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:135:PHE:CE2	2:H:171:MET:HG2	2.54	0.43
3:J:174:HIS:CD2	3:J:268:LEU:HD23	2.54	0.43
3:N:204:LYS:HG3	3:N:205:PRO:CD	2.48	0.43
1:A:162:LYS:HD2	1:A:162:LYS:O	2.18	0.43
3:N:202:LEU:HD12	3:N:202:LEU:HA	1.90	0.43
1:A:276:LYS:HE2	1:A:276:LYS:HB3	1.86	0.43
1:A:431:THR:OG1	1:A:432:ASP:N	2.52	0.43
1:B:13:ASN:HD21	1:B:33:ILE:HG22	1.84	0.43
3:K:136:HIS:ND1	3:K:138:PHE:O	2.52	0.43
1:A:397:GLU:HB2	1:A:400:LEU:HD22	2.01	0.43
1:B:362:LEU:HD21	1:B:415:HIS:NE2	2.33	0.43
1:C:259:ASP:HA	1:C:262:ARG:HG3	2.01	0.43
2:F:327:LEU:HD12	2:F:327:LEU:H	1.82	0.43
2:H:12:ASN:HB3	2:H:217:PHE:CZ	2.54	0.43
2:H:52:LYS:HB3	2:H:52:LYS:HE3	1.83	0.43
3:M:273:ALA:O	3:M:277:GLU:HB3	2.19	0.43
1:B:-34:ARG:HB3	1:B:-6:PHE:HB3	2.01	0.43
1:C:288:GLU:HG3	1:C:289:GLU:HG2	2.01	0.43
2:H:50:THR:HG22	2:H:52:LYS:H	1.84	0.43
1:A:172:PHE:HD2	1:A:238:PHE:CE1	2.31	0.43
1:A:439:LYS:HD2	1:C:528:PHE:O	2.18	0.43
1:D:362:LEU:HD21	1:D:415:HIS:NE2	2.34	0.43
2:E:26:ILE:HD13	2:E:26:ILE:HA	1.85	0.43
2:G:2:SER:N	2:G:5:GLN:HE22	2.16	0.43
2:G:223:THR:OG1	2:G:225:ASN:O	2.29	0.43
3:L:241:LYS:HG2	3:L:242:ALA:N	2.34	0.43
3:N:167:SER:O	3:N:171:ILE:HG13	2.18	0.43
1:A:-49:MET:HG2	1:A:-33:PHE:CD2	2.54	0.43
1:A:129:GLU:HB3	1:A:131:ASP:OD1	2.19	0.43
1:B:362:LEU:HD21	1:B:415:HIS:CD2	2.54	0.43
1:C:304:LYS:HG3	1:C:308:GLU:HG3	2.01	0.43
2:H:364:ILE:HD13	2:H:364:ILE:HA	1.90	0.43
3:M:181:PRO:HB2	3:N:177:ALA:O	2.19	0.43
3:P:261:LYS:HA	3:P:264:ILE:HG22	2.00	0.43
1:A:430:LYS:NZ	1:A:508:SER:OG	2.48	0.42
1:A:542:LEU:HD13	1:C:409:GLY:HA3	2.00	0.42
2:G:52:LYS:HA	2:G:55:LYS:HE2	2.01	0.42
3:J:212:LEU:HD23	3:J:222:LYS:HZ1	1.84	0.42
3:K:282:CYS:HB2	3:K:285:CYS:HB3	2.00	0.42
1:D:48:LYS:HE2	1:D:48:LYS:HB3	1.69	0.42
2:F:24:THR:OG1	2:F:60:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:169:LYS:HE3	3:P:169:LYS:HB2	1.88	0.42
1:D:162:LYS:HD3	1:D:162:LYS:O	2.19	0.42
2:E:98:PHE:H	2:E:98:PHE:HD1	1.68	0.42
3:P:167:SER:O	3:P:171:ILE:HG13	2.19	0.42
1:A:79:ASN:OD1	1:A:79:ASN:N	2.49	0.42
1:A:247:LYS:NZ	1:D:222:GLU:OE2	2.52	0.42
1:A:442:LYS:HA	1:A:442:LYS:HD3	1.74	0.42
2:F:27:LEU:HD23	2:F:27:LEU:HA	1.85	0.42
2:G:20:GLY:HA2	2:G:23:LYS:HG3	2.02	0.42
3:L:282:CYS:HB3	3:L:291:ILE:HG13	2.01	0.42
3:M:198:LYS:NZ	3:M:277:GLU:O	2.48	0.42
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.78	0.42
1:A:447:LEU:HD21	1:A:465:ILE:HG12	2.01	0.42
1:D:124:LEU:HD12	1:D:143:ASN:HD21	1.84	0.42
2:G:74:ASP:OD1	2:G:74:ASP:N	2.50	0.42
2:H:9:ASP:O	2:H:30:LYS:NZ	2.46	0.42
3:I:207:GLU:HG3	3:I:227:PHE:HE1	1.82	0.42
3:J:184:ALA:HA	3:J:199:VAL:HG23	2.01	0.42
3:L:163:SER:O	3:L:167:SER:OG	2.31	0.42
2:F:120:GLN:HE21	2:F:122:ILE:CG2	2.32	0.42
3:I:146:ASP:OD2	3:I:158:LYS:NZ	2.52	0.42
3:I:151:HIS:HB3	3:I:154:LEU:HB2	2.00	0.42
3:K:282:CYS:CB	3:K:285:CYS:HB3	2.50	0.42
3:N:231:ARG:HH11	3:N:233:VAL:HB	1.84	0.42
1:C:101:ASN:HB2	1:C:128:SER:HB2	2.01	0.42
1:D:247:LYS:HB3	1:D:247:LYS:HE3	1.76	0.42
3:M:185:ARG:HH12	3:N:176:LYS:C	2.22	0.42
3:M:242:ALA:N	3:M:248:ILE:HD11	2.35	0.42
3:N:202:LEU:HB3	3:N:207:GLU:OE2	2.19	0.42
1:C:135:ASP:OD2	1:D:139:ARG:NH1	2.52	0.42
1:D:438:LYS:HE2	1:D:438:LYS:HB2	1.92	0.42
2:E:52:LYS:HE3	2:E:52:LYS:HB3	1.86	0.42
2:F:126:TYR:CD2	2:F:131:LYS:HG3	2.54	0.42
2:F:130:LYS:HA	2:F:130:LYS:HD3	1.83	0.42
3:K:256:ASP:H	3:K:259:ASP:HB3	1.84	0.42
3:O:280:VAL:HG12	3:O:282:CYS:H	1.85	0.42
1:A:135:ASP:OD2	1:B:139:ARG:NH1	2.52	0.42
1:C:185:LEU:HA	1:C:185:LEU:HD12	1.86	0.42
1:C:261:ARG:HB3	1:C:261:ARG:CZ	2.50	0.42
1:D:288:GLU:HG3	1:D:289:GLU:HG2	2.01	0.42
2:E:352:LEU:HD12	2:E:357:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:23:LYS:NZ	2:G:191:ASP:HB2	2.35	0.42
2:H:126:TYR:HD1	2:H:128:ASN:H	1.67	0.42
3:J:136:HIS:ND1	3:J:138:PHE:O	2.53	0.42
1:A:542:LEU:HD23	1:A:542:LEU:HA	1.85	0.42
1:C:2:LYS:O	1:C:76:ASP:N	2.46	0.42
1:C:432:ASP:HB2	1:C:511:ASP:HA	2.02	0.42
2:G:24:THR:HG22	2:G:60:ARG:NH1	2.35	0.42
3:K:158:LYS:HB2	3:K:158:LYS:HE3	1.97	0.42
1:A:-4:GLN:NE2	1:A:103:ASP:OD2	2.37	0.41
1:B:5:ASN:OD1	1:B:18:ASN:ND2	2.53	0.41
1:D:162:LYS:HD3	1:D:166:GLN:HE22	1.85	0.41
3:L:212:LEU:HB2	3:L:222:LYS:NZ	2.35	0.41
1:A:288:GLU:HG3	1:A:289:GLU:HG2	2.02	0.41
1:C:87:LYS:HE2	2:G:153:PHE:HE2	1.84	0.41
3:P:175:ILE:O	3:P:179:ILE:HB	2.20	0.41
2:E:341:ILE:HD12	2:E:344:LEU:HD21	2.01	0.41
3:I:198:LYS:HB3	3:I:233:VAL:HG22	2.01	0.41
3:J:204:LYS:HD3	3:J:283:LYS:HE2	2.01	0.41
3:K:228:GLN:HE22	3:K:231:ARG:HB2	1.85	0.41
3:L:162:LEU:HB2	3:L:252:PHE:HB2	2.02	0.41
3:L:242:ALA:HA	3:L:248:ILE:HD11	2.01	0.41
3:O:210:VAL:HA	3:P:261:LYS:NZ	2.35	0.41
1:A:470:PRO:HD3	1:A:481:ARG:HH12	1.85	0.41
3:I:280:VAL:O	3:I:291:ILE:N	2.48	0.41
3:P:179:ILE:HD12	3:P:179:ILE:HA	1.84	0.41
1:C:362:LEU:HD21	1:C:415:HIS:NE2	2.35	0.41
1:C:470:PRO:HD3	1:C:481:ARG:HH12	1.85	0.41
2:G:98:PHE:HB3	2:G:121:ASN:HD22	1.85	0.41
2:G:98:PHE:CD1	2:G:123:LEU:HB2	2.55	0.41
3:I:133:LEU:HD12	3:I:133:LEU:HA	1.83	0.41
3:L:191:ASP:N	3:L:191:ASP:OD1	2.53	0.41
1:A:260:GLY:HA2	1:A:263:LYS:NZ	2.35	0.41
1:B:2:LYS:O	1:B:76:ASP:N	2.45	0.41
1:B:247:LYS:HD2	1:C:224:VAL:HG12	2.03	0.41
2:G:55:LYS:HE2	2:G:55:LYS:HB2	1.84	0.41
2:H:49:PHE:HZ	2:H:167:SER:HA	1.86	0.41
2:F:50:THR:CG2	2:F:52:LYS:HG3	2.51	0.41
3:I:137:ASN:OD1	3:I:138:PHE:N	2.54	0.41
3:O:161:TYR:N	3:O:161:TYR:CD2	2.89	0.41
3:O:185:ARG:HH12	3:P:176:LYS:C	2.21	0.41
3:O:256:ASP:OD2	3:O:256:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:265:LYS:HE2	3:P:265:LYS:HB2	1.74	0.41
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.81	0.41
2:E:5:GLN:HG2	2:E:220:TYR:HE2	1.86	0.41
2:G:374:GLN:O	2:G:378:ASN:ND2	2.50	0.41
3:P:198:LYS:HB2	3:P:235:ILE:CD1	2.50	0.41
1:A:93:VAL:HG11	1:A:97:ARG:HG3	2.03	0.41
1:B:48:LYS:HB3	1:B:48:LYS:HE2	1.77	0.41
1:B:431:THR:OG1	1:B:432:ASP:N	2.54	0.41
1:C:268:SER:HA	1:C:271:ASN:HB2	2.03	0.41
1:C:281:LYS:HE2	1:C:281:LYS:HB3	1.74	0.41
1:D:79:ASN:OD1	1:D:79:ASN:N	2.54	0.41
1:D:227:GLU:OE2	3:I:244:GLN:NE2	2.52	0.41
2:E:2:SER:N	2:E:5:GLN:HE22	2.19	0.41
2:E:39:LYS:HB3	2:E:39:LYS:HE3	1.78	0.41
2:G:102:TYR:O	2:G:125:THR:HG21	2.21	0.41
2:G:179:LYS:HD3	2:G:186:LEU:HD12	2.03	0.41
2:H:44:ILE:HG13	2:H:68:ASN:OD1	2.21	0.41
3:I:162:LEU:HD12	3:I:162:LEU:HA	1.76	0.41
3:J:162:LEU:N	3:J:252:PHE:O	2.46	0.41
3:J:284:CYS:SG	3:N:283:LYS:HB3	2.61	0.41
3:L:152:PRO:HA	3:L:155:LEU:HB2	2.02	0.41
3:L:288:ARG:NH2	3:P:280:VAL:HB	2.36	0.41
3:M:170:ILE:HD12	3:M:171:ILE:N	2.35	0.41
1:C:476:LYS:HE2	1:C:476:LYS:HB3	1.73	0.41
1:D:276:LYS:HB3	1:D:276:LYS:HE2	1.85	0.41
2:E:126:TYR:CE2	2:E:133:PHE:HB2	2.56	0.41
2:H:25:THR:HA	2:H:60:ARG:HH22	1.86	0.41
3:J:147:ARG:HD3	3:J:148:ILE:N	2.36	0.41
3:L:240:PRO:HA	3:L:249:VAL:HG12	2.03	0.41
3:N:171:ILE:HG13	3:N:171:ILE:H	1.63	0.41
1:A:281:LYS:HE2	1:A:281:LYS:HB3	1.74	0.40
2:F:15:VAL:HG12	2:F:17:ALA:H	1.86	0.40
2:F:129:PRO:HD3	2:F:200:ARG:HH11	1.86	0.40
2:H:133:PHE:HA	2:H:136:GLN:NE2	2.36	0.40
3:K:198:LYS:NZ	3:K:277:GLU:HB3	2.36	0.40
3:L:207:GLU:OE1	3:L:208:TYR:N	2.55	0.40
1:A:201:GLU:HA	1:A:201:GLU:OE1	2.21	0.40
1:B:13:ASN:HD21	1:B:33:ILE:CG2	2.35	0.40
1:B:129:GLU:HB3	1:B:131:ASP:OD1	2.20	0.40
1:C:430:LYS:NZ	1:C:508:SER:OG	2.43	0.40
1:D:-35:ILE:H	1:D:-35:ILE:HG13	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:169:LYS:HE3	3:I:169:LYS:HB3	1.93	0.40
3:J:202:LEU:HD12	3:J:228:GLN:NE2	2.36	0.40
3:J:252:PHE:HB3	3:J:260:LEU:HD11	2.03	0.40
3:O:176:LYS:C	3:P:185:ARG:HH12	2.25	0.40
1:A:527:ILE:O	1:C:439:LYS:NZ	2.50	0.40
1:B:103:ASP:OD1	1:B:103:ASP:N	2.40	0.40
1:C:278:TYR:HB3	1:C:281:LYS:HG3	2.04	0.40
1:D:221:LYS:HE2	1:D:221:LYS:H	1.86	0.40
2:E:93:ASP:OD1	2:E:93:ASP:N	2.52	0.40
2:F:159:ILE:HB	2:F:186:LEU:HD23	2.02	0.40
2:F:344:LEU:O	2:F:344:LEU:HD12	2.20	0.40
2:G:44:ILE:HG13	2:G:68:ASN:OD1	2.21	0.40
2:G:48:THR:O	2:G:72:THR:HA	2.21	0.40
2:G:150:GLN:O	2:G:154:SER:OG	2.31	0.40
2:H:15:VAL:HG12	2:H:189:VAL:HG13	2.03	0.40
2:H:329:GLU:HG3	2:H:347:GLU:HG3	2.03	0.40
3:I:212:LEU:HB2	3:I:222:LYS:HZ1	1.86	0.40
3:K:207:GLU:OE2	3:K:225:LYS:NZ	2.41	0.40
3:P:188:SER:HB3	3:P:195:THR:HB	2.03	0.40
1:A:77:LEU:HD21	1:A:89:LEU:HD23	2.03	0.40
1:B:-61:PHE:CG	1:B:-50:LEU:HD11	2.56	0.40
1:C:129:GLU:HB3	1:C:131:ASP:OD1	2.22	0.40
2:E:362:LYS:HA	2:E:365:ASN:HD21	1.85	0.40
2:G:121:ASN:HB3	2:H:122:ILE:CG1	2.49	0.40
2:H:152:ILE:HD13	2:H:152:ILE:HA	1.98	0.40
3:I:174:HIS:CE1	3:I:268:LEU:HB3	2.57	0.40
1:B:45:LEU:HD11	1:B:107:ILE:HG22	2.04	0.40
1:D:470:PRO:HD3	1:D:481:ARG:HH12	1.87	0.40
2:E:107:PHE:HB2	2:E:126:TYR:HE2	1.86	0.40
2:F:98:PHE:CD2	2:F:123:LEU:HB2	2.57	0.40
2:H:327:LEU:HA	2:H:330:VAL:HG12	2.04	0.40
3:P:187:THR:OG1	3:P:188:SER:N	2.54	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	618/675 (92%)	602 (97%)	15 (2%)	1 (0%)	47	69
1	B	618/675 (92%)	602 (97%)	15 (2%)	1 (0%)	47	69
1	C	618/675 (92%)	602 (97%)	15 (2%)	1 (0%)	47	69
1	D	618/675 (92%)	600 (97%)	17 (3%)	1 (0%)	47	69
2	E	276/494 (56%)	271 (98%)	5 (2%)	0	100	100
2	F	276/494 (56%)	272 (99%)	4 (1%)	0	100	100
2	G	276/494 (56%)	271 (98%)	5 (2%)	0	100	100
2	H	276/494 (56%)	271 (98%)	5 (2%)	0	100	100
3	I	160/295 (54%)	155 (97%)	5 (3%)	0	100	100
3	J	160/295 (54%)	156 (98%)	4 (2%)	0	100	100
3	K	160/295 (54%)	153 (96%)	7 (4%)	0	100	100
3	L	160/295 (54%)	155 (97%)	5 (3%)	0	100	100
3	M	110/295 (37%)	104 (94%)	6 (6%)	0	100	100
3	N	110/295 (37%)	102 (93%)	8 (7%)	0	100	100
3	O	110/295 (37%)	102 (93%)	8 (7%)	0	100	100
3	P	110/295 (37%)	101 (92%)	9 (8%)	0	100	100
All	All	4656/7036 (66%)	4519 (97%)	133 (3%)	4 (0%)	54	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	VAL
1	B	342	VAL
1	C	342	VAL
1	D	342	VAL

### 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	571/614 (93%)	552 (97%)	19 (3%)	38	61
1	B	571/614 (93%)	550 (96%)	21 (4%)	34	57
1	C	571/614 (93%)	545 (95%)	26 (5%)	27	49
1	D	571/614 (93%)	548 (96%)	23 (4%)	31	55
2	E	253/448 (56%)	241 (95%)	12 (5%)	26	48
2	F	253/448 (56%)	237 (94%)	16 (6%)	18	35
2	G	253/448 (56%)	236 (93%)	17 (7%)	16	31
2	H	253/448 (56%)	238 (94%)	15 (6%)	19	37
3	I	153/276 (55%)	129 (84%)	24 (16%)	2	4
3	J	153/276 (55%)	138 (90%)	15 (10%)	8	14
3	K	153/276 (55%)	138 (90%)	15 (10%)	8	14
3	L	153/276 (55%)	133 (87%)	20 (13%)	4	7
3	M	106/276 (38%)	96 (91%)	10 (9%)	8	16
3	N	106/276 (38%)	94 (89%)	12 (11%)	6	10
3	O	106/276 (38%)	89 (84%)	17 (16%)	2	4
3	P	106/276 (38%)	90 (85%)	16 (15%)	3	4
All	All	4332/6456 (67%)	4054 (94%)	278 (6%)	21	34

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-71	VAL
1	A	-65	SER
1	A	32	ASP
1	A	80	TYR
1	A	116	LYS
1	A	118	LEU
1	A	126	TRP
1	A	166	GLN
1	A	170	TYR
1	A	197	GLN
1	A	218	SER
1	A	221	LYS
1	A	261	ARG
1	A	321	SER
1	A	338	SER

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Mol	Chain	Res	Type
1	A	346	SER
1	A	361	LYS
1	A	459	ARG
1	A	571	GLU
1	B	-38	MET
1	B	-30	ASP
1	B	13	ASN
1	B	30	MET
1	B	32	ASP
1	B	65	THR
1	B	80	TYR
1	B	116	LYS
1	B	126	TRP
1	B	157	LEU
1	B	170	TYR
1	B	218	SER
1	B	221	LYS
1	B	251	SER
1	B	261	ARG
1	B	313	LYS
1	B	321	SER
1	B	338	SER
1	B	346	SER
1	B	361	LYS
1	B	485	ARG
1	C	-67	ASP
1	C	-38	MET
1	C	-10	THR
1	C	-3	GLN
1	C	-2	THR
1	C	32	ASP
1	C	40	TYR
1	C	80	TYR
1	C	118	LEU
1	C	126	TRP
1	C	135	ASP
1	C	170	TYR
1	C	174	GLU
1	C	218	SER
1	C	221	LYS
1	C	235	LYS
1	C	253	TYR

*Continued on next page...*

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Mol	Chain	Res	Type
1	C	261	ARG
1	C	266	SER
1	C	318	SER
1	C	321	SER
1	C	338	SER
1	C	346	SER
1	C	361	LYS
1	C	526	ARG
1	C	571	GLU
1	D	-71	VAL
1	D	-67	ASP
1	D	-38	MET
1	D	-10	THR
1	D	13	ASN
1	D	30	MET
1	D	32	ASP
1	D	80	TYR
1	D	116	LYS
1	D	126	TRP
1	D	135	ASP
1	D	158	VAL
1	D	180	SER
1	D	185	LEU
1	D	218	SER
1	D	221	LYS
1	D	261	ARG
1	D	313	LYS
1	D	321	SER
1	D	338	SER
1	D	346	SER
1	D	361	LYS
1	D	549	VAL
2	E	6	ILE
2	E	29	SER
2	E	36	LYS
2	E	52	LYS
2	E	79	SER
2	E	102	TYR
2	E	126	TYR
2	E	154	SER
2	E	332	LYS
2	E	358	LYS

*Continued on next page...*

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Mol	Chain	Res	Type
2	E	379	GLN
2	E	400	PHE
2	F	8	LYS
2	F	24	THR
2	F	52	LYS
2	F	73	ASN
2	F	79	SER
2	F	109	SER
2	F	115	GLN
2	F	121	ASN
2	F	126	TYR
2	F	154	SER
2	F	200	ARG
2	F	217	PHE
2	F	226	PHE
2	F	354	SER
2	F	360	ILE
2	F	362	LYS
2	G	25	THR
2	G	36	LYS
2	G	74	ASP
2	G	111	ASP
2	G	115	GLN
2	G	121	ASN
2	G	127	SER
2	G	176	MET
2	G	217	PHE
2	G	221	HIS
2	G	226	PHE
2	G	323	ASN
2	G	326	LEU
2	G	328	LYS
2	G	332	LYS
2	G	353	SER
2	G	400	PHE
2	H	7	ILE
2	H	52	LYS
2	H	93	ASP
2	H	107	PHE
2	H	115	GLN
2	H	176	MET
2	H	215	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	217	PHE
2	H	323	ASN
2	H	326	LEU
2	H	332	LYS
2	H	344	LEU
2	H	354	SER
2	H	381	LEU
2	H	400	PHE
3	I	136	HIS
3	I	140	LEU
3	I	141	ASN
3	I	144	LEU
3	I	146	ASP
3	I	147	ARG
3	I	153	MET
3	I	167	SER
3	I	185	ARG
3	I	189	ASP
3	I	191	ASP
3	I	203	TYR
3	I	215	MET
3	I	216	TYR
3	I	219	ARG
3	I	222	LYS
3	I	228	GLN
3	I	237	LYS
3	I	253	SER
3	I	256	ASP
3	I	262	SER
3	I	277	GLU
3	I	283	LYS
3	I	288	ARG
3	J	147	ARG
3	J	149	GLN
3	J	164	GLN
3	J	167	SER
3	J	189	ASP
3	J	191	ASP
3	J	200	LEU
3	J	203	TYR
3	J	208	TYR
3	J	216	TYR

*Continued on next page...*



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Mol	Chain	Res	Type
3	J	224	GLU
3	J	256	ASP
3	J	270	ASP
3	J	282	CYS
3	J	284	CYS
3	K	133	LEU
3	K	141	ASN
3	K	146	ASP
3	K	147	ARG
3	K	153	MET
3	K	161	TYR
3	K	196	VAL
3	K	215	MET
3	K	216	TYR
3	K	218	ARG
3	K	219	ARG
3	K	228	GLN
3	K	229	THR
3	K	253	SER
3	K	292	LEU
3	L	141	ASN
3	L	147	ARG
3	L	149	GLN
3	L	150	THR
3	L	161	TYR
3	L	163	SER
3	L	164	GLN
3	L	189	ASP
3	L	200	LEU
3	L	212	LEU
3	L	215	MET
3	L	216	TYR
3	L	220	LYS
3	L	226	ARG
3	L	228	GLN
3	L	235	ILE
3	L	237	LYS
3	L	253	SER
3	L	266	LYS
3	L	284	CYS
3	M	164	GLN
3	M	193	CYS

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Mol	Chain	Res	Type
3	M	196	VAL
3	M	200	LEU
3	M	203	TYR
3	M	213	ASN
3	M	215	MET
3	M	250	GLU
3	M	256	ASP
3	M	279	LEU
3	N	163	SER
3	N	164	GLN
3	N	178	ASN
3	N	196	VAL
3	N	203	TYR
3	N	210	VAL
3	N	215	MET
3	N	234	GLU
3	N	250	GLU
3	N	263	ASN
3	N	272	MET
3	N	279	LEU
3	O	163	SER
3	O	164	GLN
3	O	203	TYR
3	O	209	ILE
3	O	211	ASP
3	O	213	ASN
3	O	215	MET
3	O	234	GLU
3	O	250	GLU
3	O	253	SER
3	O	256	ASP
3	O	258	GLU
3	O	263	ASN
3	O	266	LYS
3	O	270	ASP
3	O	279	LEU
3	O	282	CYS
3	P	161	TYR
3	P	163	SER
3	P	166	GLU
3	P	167	SER
3	P	178	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
3	P	185	ARG
3	P	196	VAL
3	P	198	LYS
3	P	200	LEU
3	P	204	LYS
3	P	208	TYR
3	P	215	MET
3	P	234	GLU
3	P	250	GLU
3	P	263	ASN
3	P	285	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	136	GLN
3	I	174	HIS
3	K	164	GLN
3	K	178	ASN
3	K	276	ASN
3	N	174	HIS
3	N	178	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

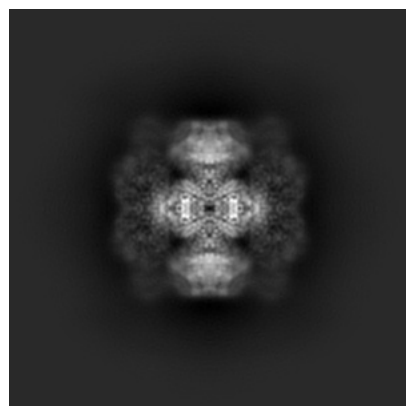
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41983. These allow visual inspection of the internal detail of the map and identification of artifacts.

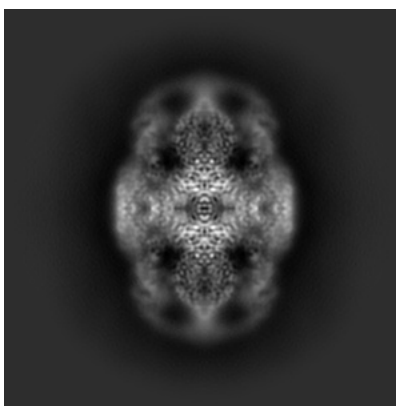
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

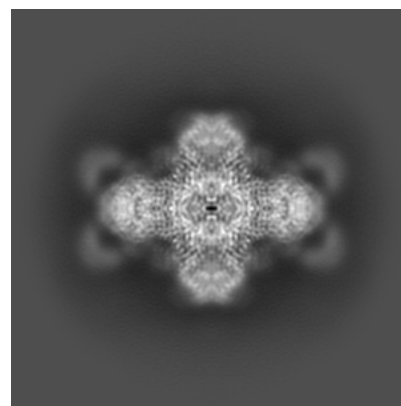
#### 6.1.1 Primary map



X

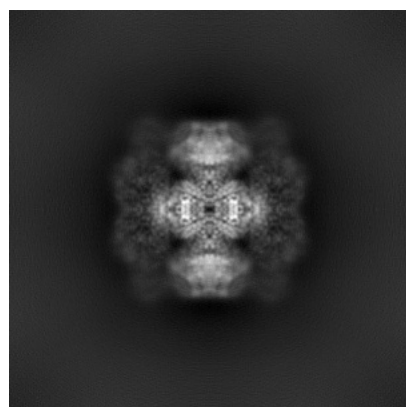


Y

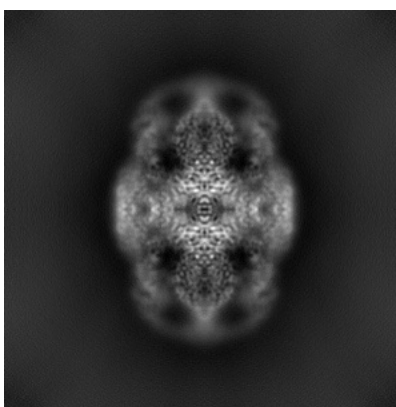


Z

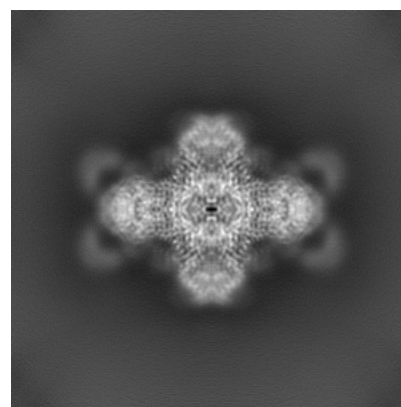
#### 6.1.2 Raw map



X



Y

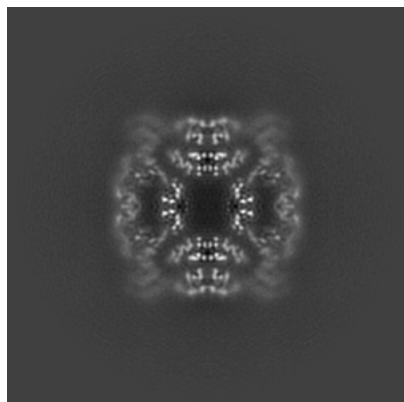


Z

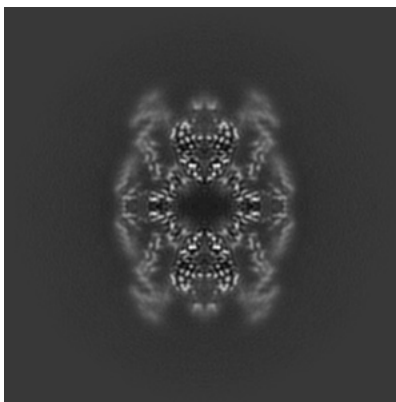
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

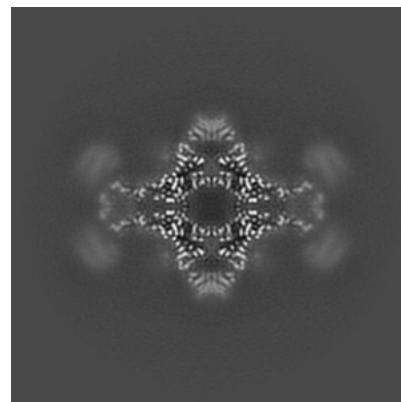
### 6.2.1 Primary map



X Index: 175

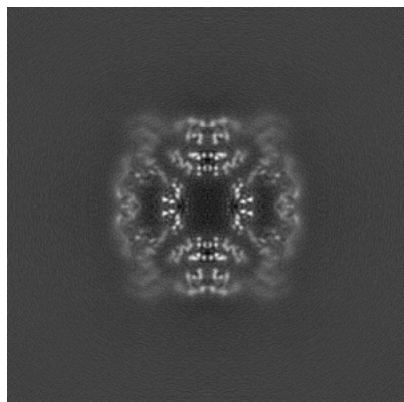


Y Index: 175

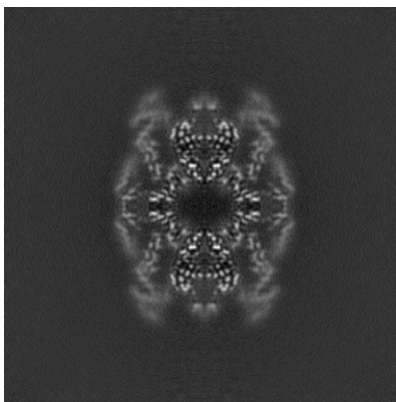


Z Index: 175

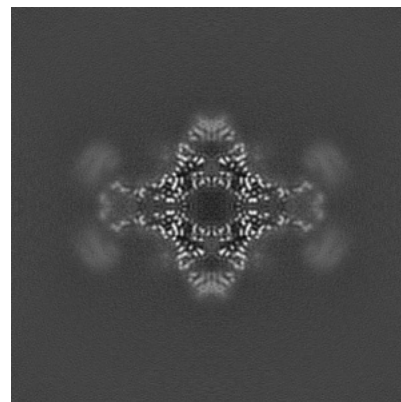
### 6.2.2 Raw map



X Index: 175



Y Index: 175

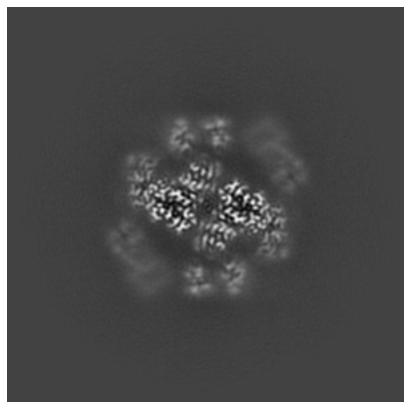


Z Index: 175

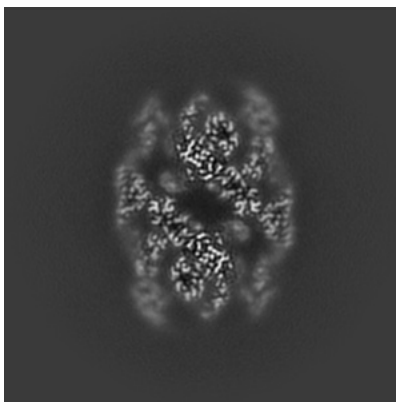
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

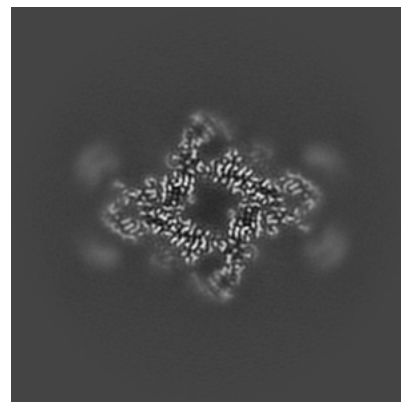
### 6.3.1 Primary map



X Index: 196

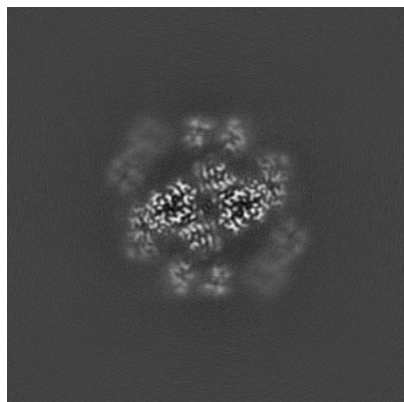


Y Index: 167

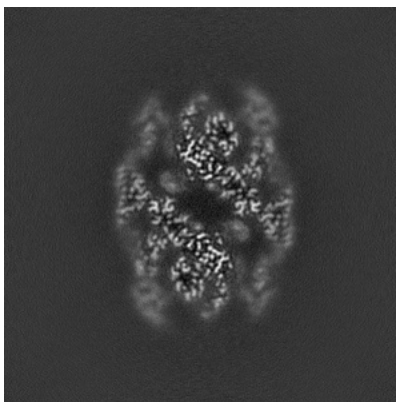


Z Index: 182

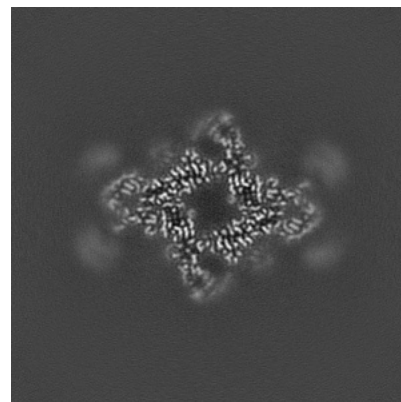
### 6.3.2 Raw map



X Index: 154



Y Index: 167

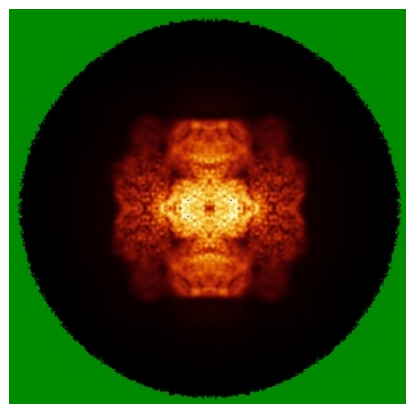


Z Index: 168

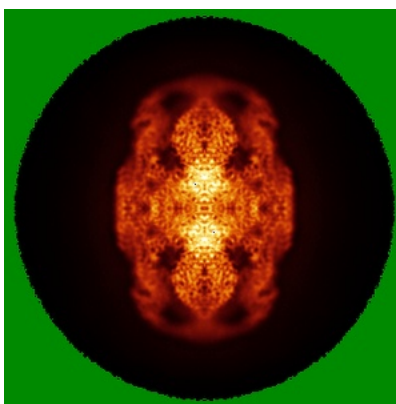
The images above show the largest variance slices of the map in three orthogonal directions.

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

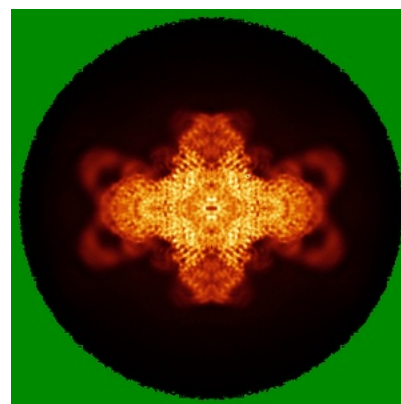
### 6.4.1 Primary map



X

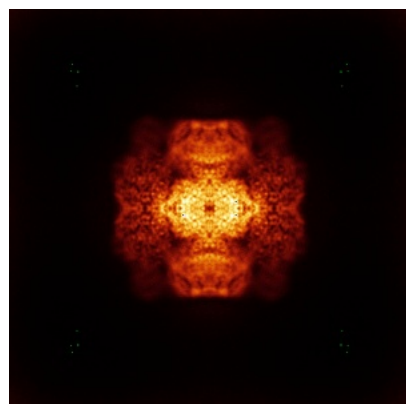


Y

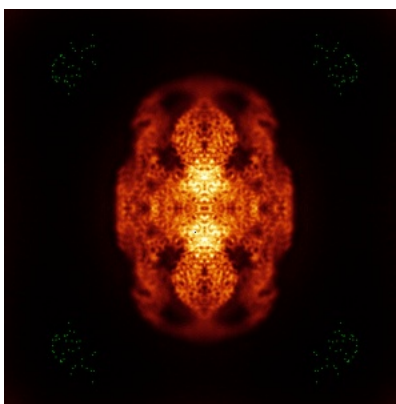


Z

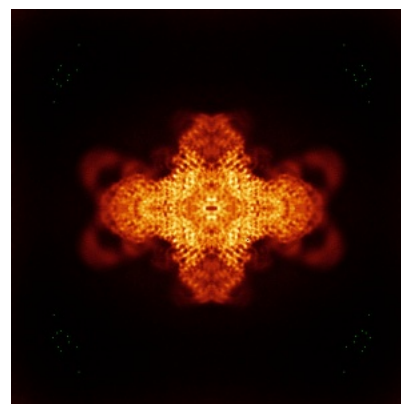
### 6.4.2 Raw map



X



Y



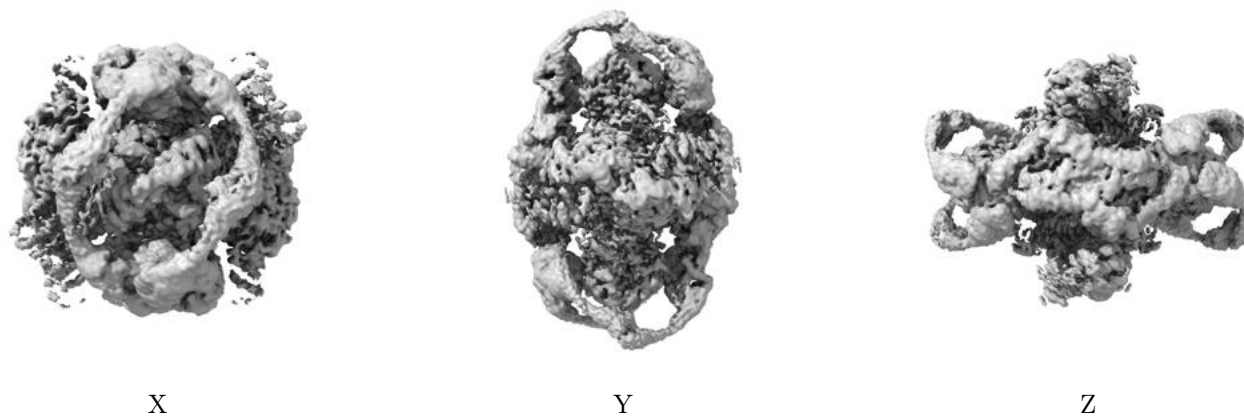
Z

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



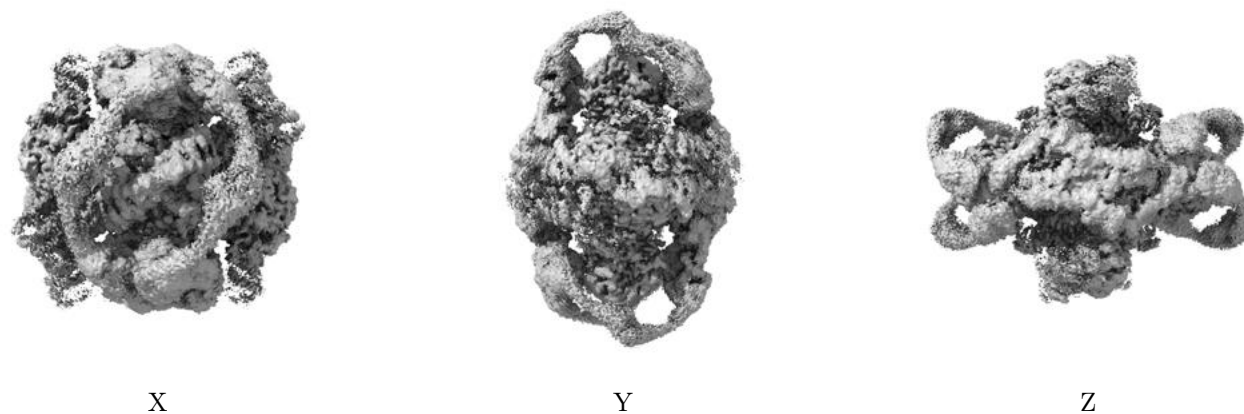
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

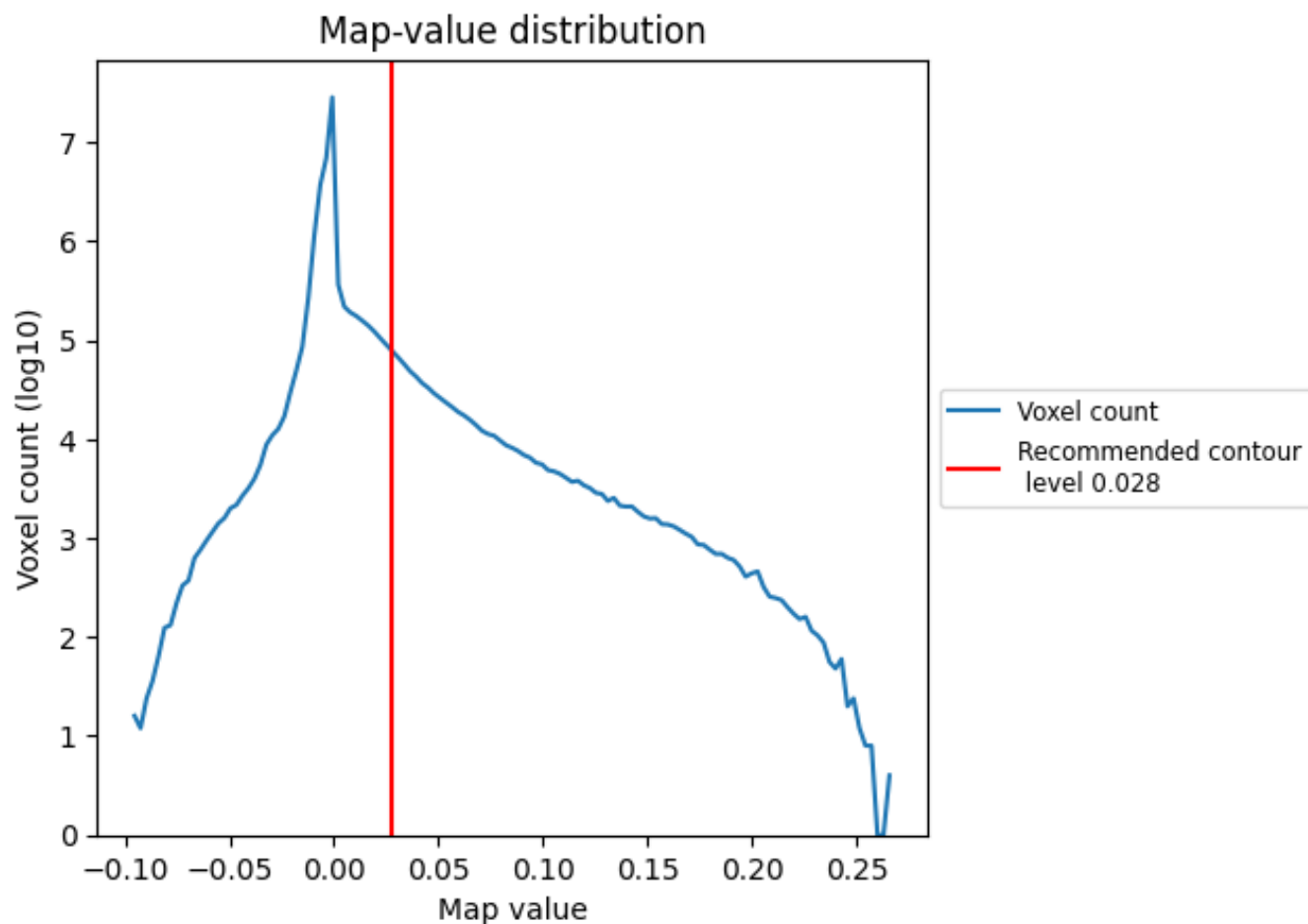
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

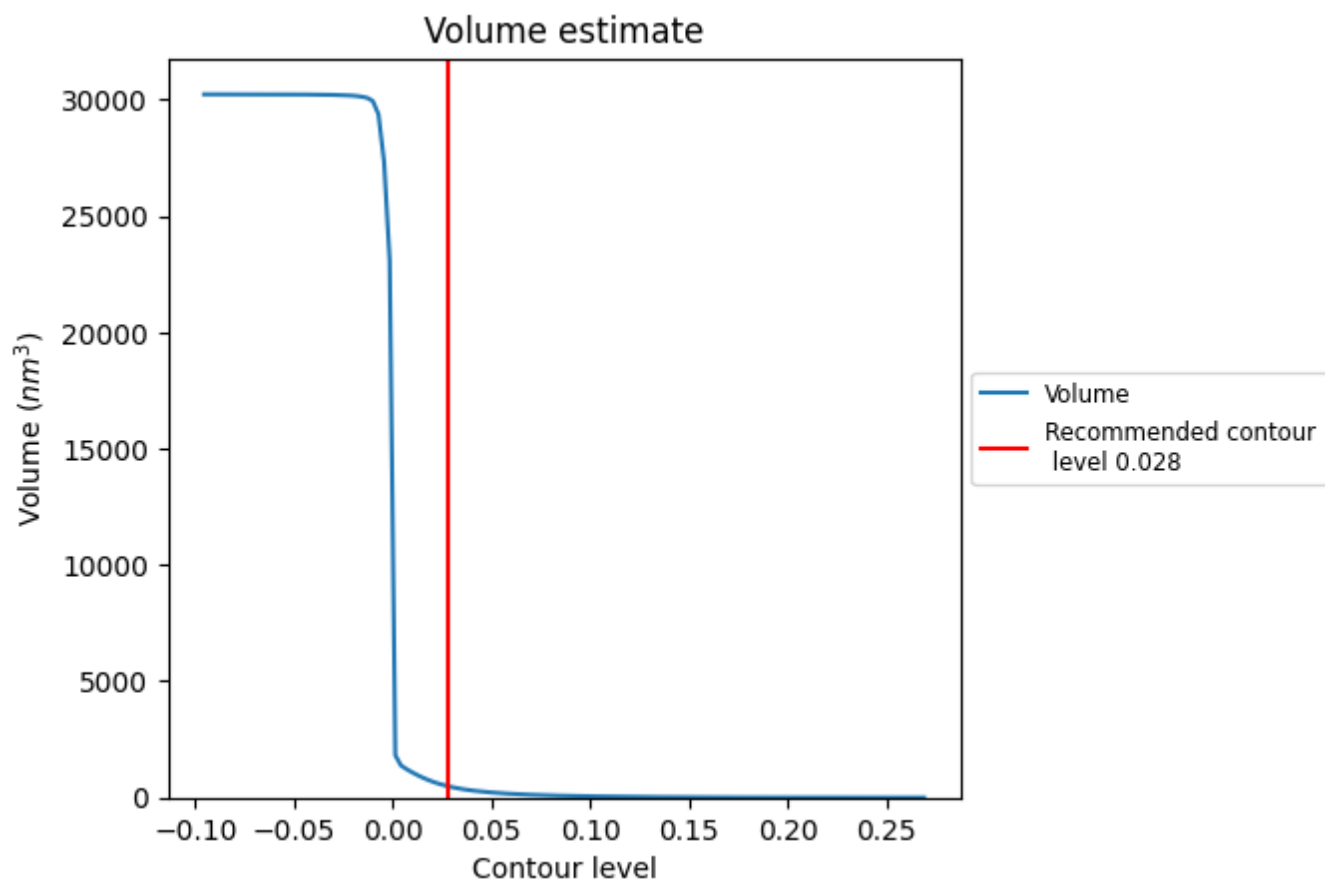
This section contains the results of statistical analysis of the map.

### 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.

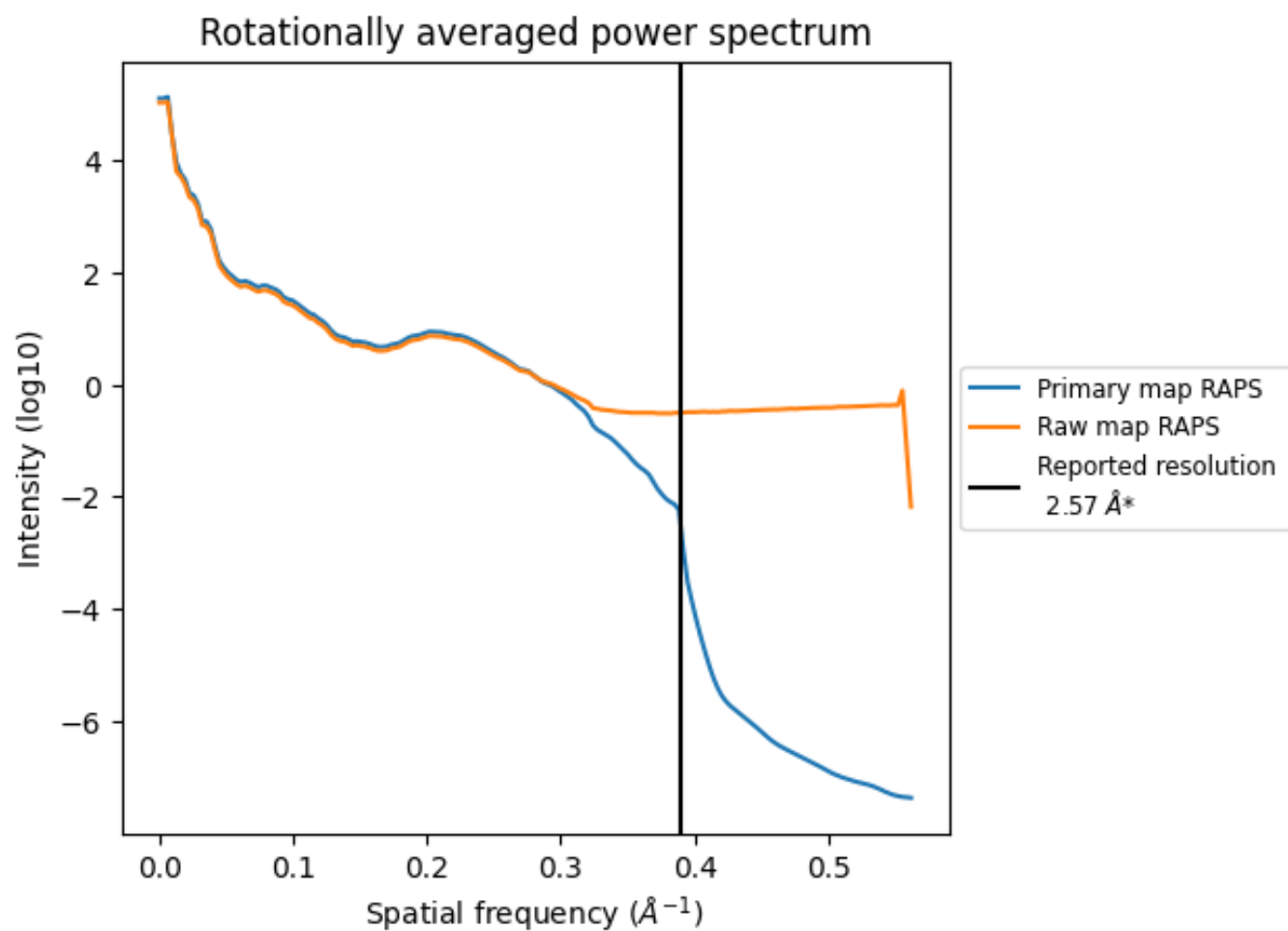
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 487  $\text{nm}^3$ ; this corresponds to an approximate mass of 440 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 ⓘ

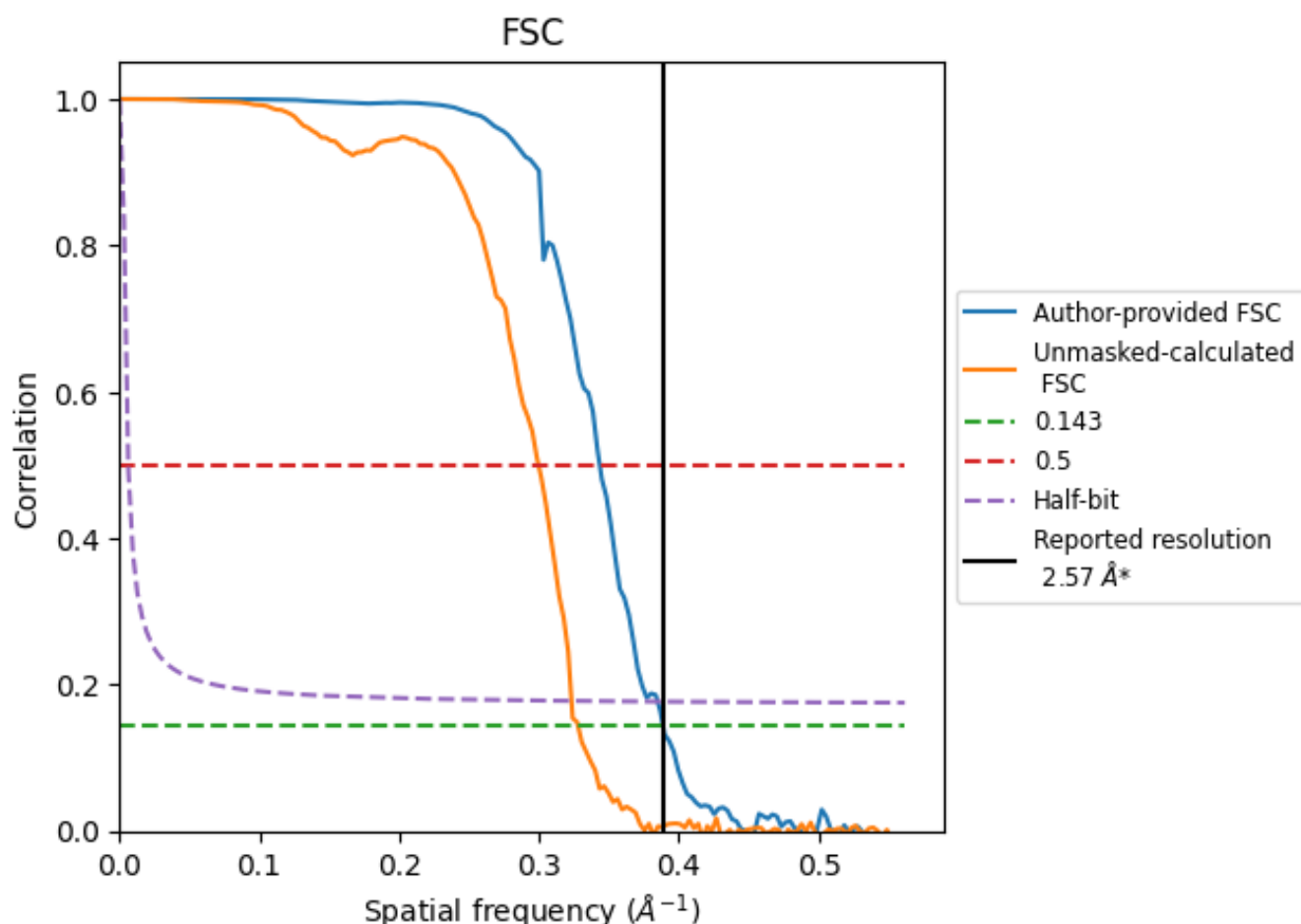


\*Reported resolution corresponds to spatial frequency of 0.389  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.389  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

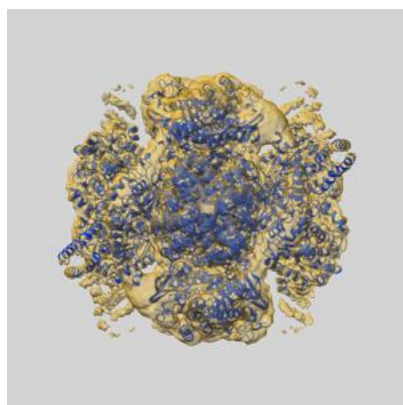
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.57	2.91	2.60
Unmasked-calculated*	3.05	3.34	3.09

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.05 differs from the reported value 2.57 by more than 10 %

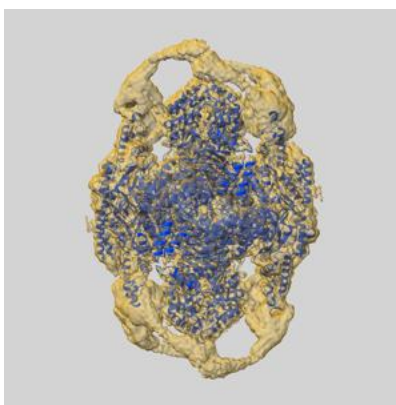
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41983 and PDB model 8U7I. Per-residue inclusion information can be found in section 3 on page 15.

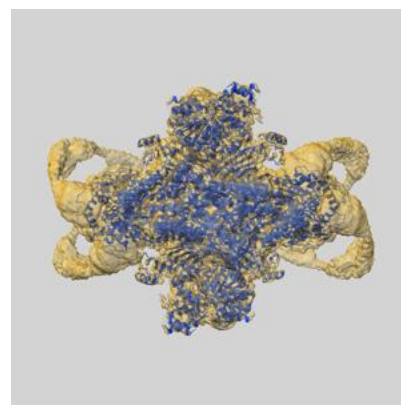
### 9.1 Map-model overlay [i](#)



X



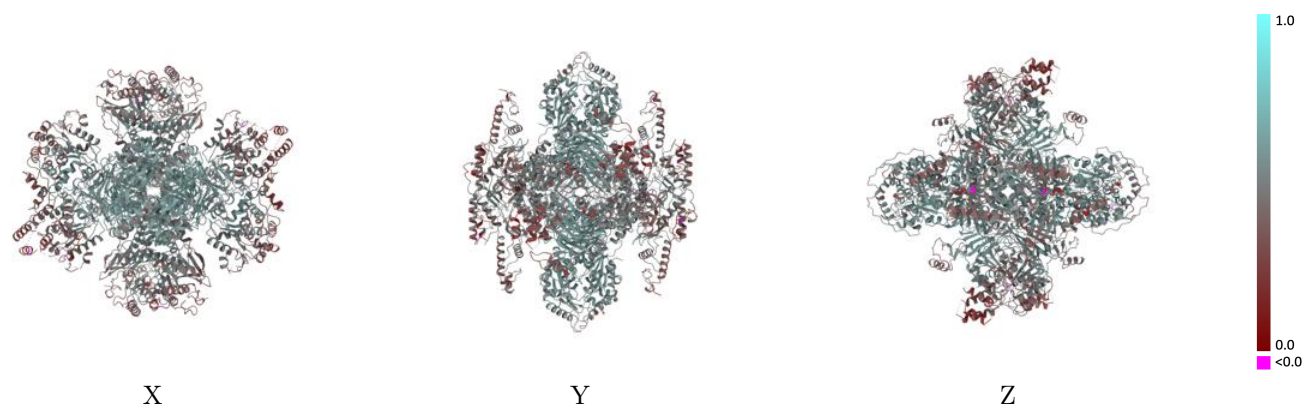
Y



Z

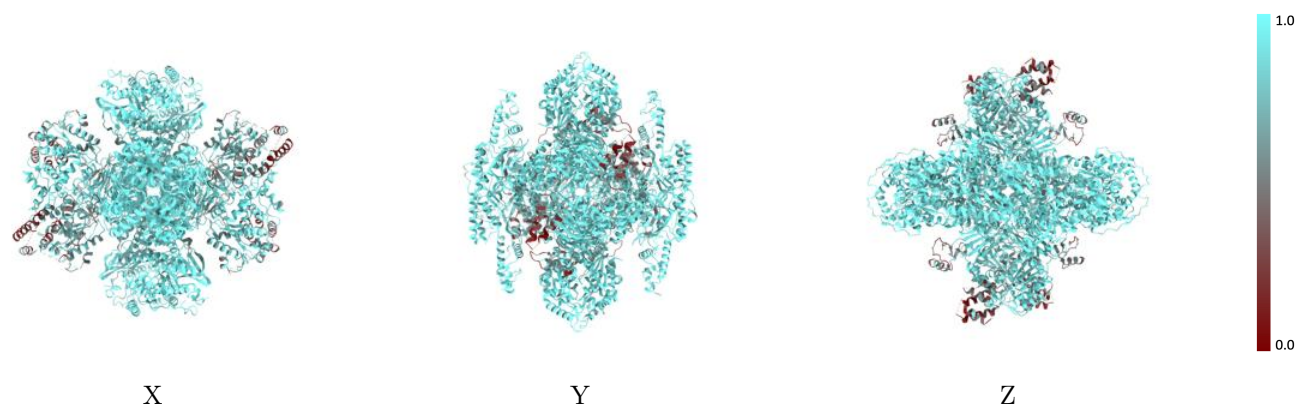
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

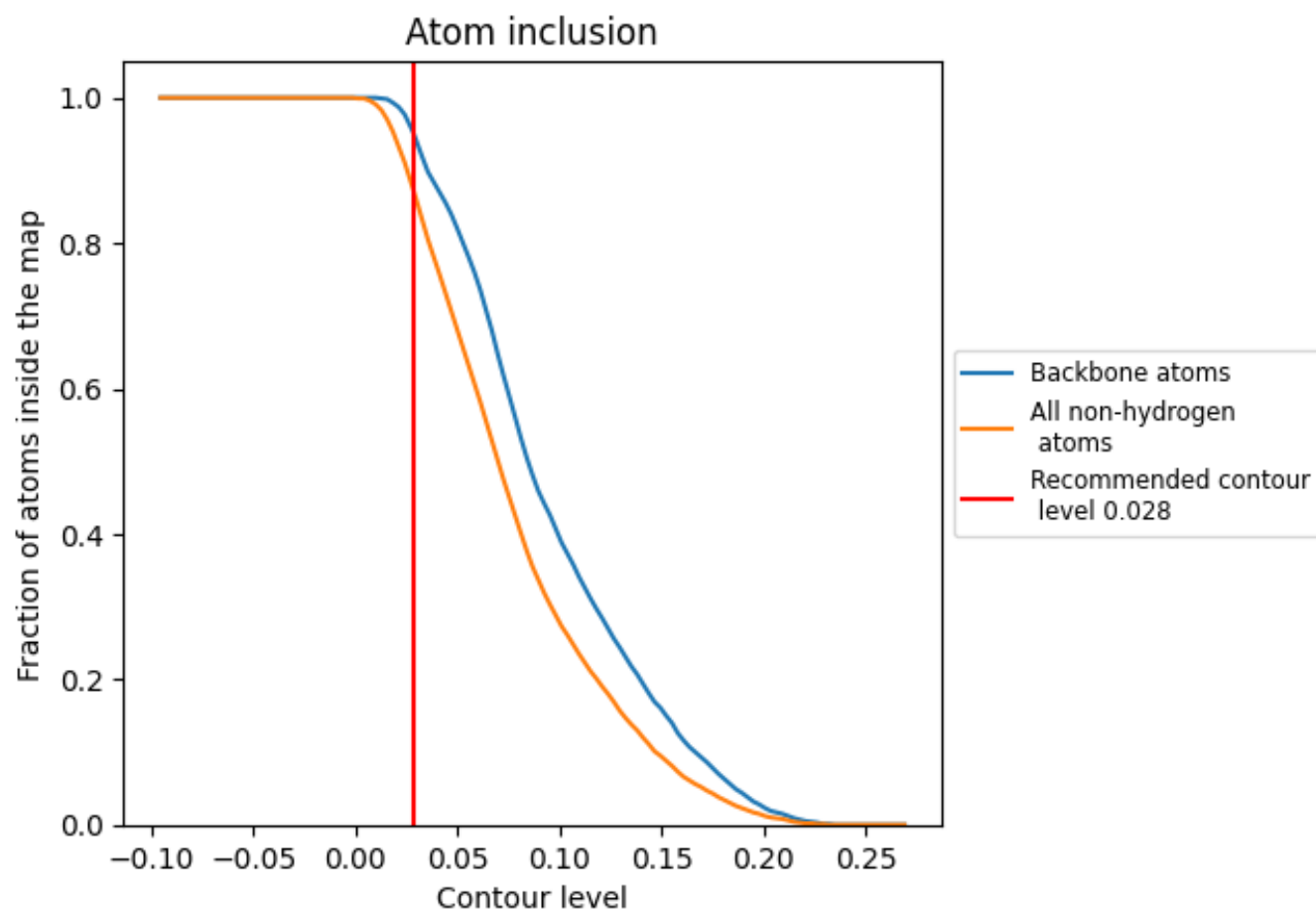
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).



## 9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8760</div>	<div><div></div>0.4910</div>
A	<div><div></div>0.9100</div>	<div><div></div>0.5540</div>
B	<div><div></div>0.9080</div>	<div><div></div>0.5530</div>
C	<div><div></div>0.9110</div>	<div><div></div>0.5540</div>
D	<div><div></div>0.9100</div>	<div><div></div>0.5550</div>
E	<div><div></div>0.7440</div>	<div><div></div>0.4210</div>
F	<div><div></div>0.7500</div>	<div><div></div>0.4260</div>
G	<div><div></div>0.7460</div>	<div><div></div>0.4240</div>
H	<div><div></div>0.7400</div>	<div><div></div>0.4190</div>
I	<div><div></div>0.9390</div>	<div><div></div>0.4240</div>
J	<div><div></div>0.9390</div>	<div><div></div>0.4250</div>
K	<div><div></div>0.9360</div>	<div><div></div>0.4120</div>
L	<div><div></div>0.9410</div>	<div><div></div>0.4210</div>
M	<div><div></div>0.9280</div>	<div><div></div>0.4080</div>
N	<div><div></div>0.9320</div>	<div><div></div>0.4170</div>
O	<div><div></div>0.9360</div>	<div><div></div>0.4210</div>
P	<div><div></div>0.9350</div>	<div><div></div>0.4190</div>

1.0

0.0

<0.0