



Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 07:23 am BST

PDB ID : 9TRE / pdb_00009tre
EMDB ID : EMD-56176
Title : Bacterial antiviral defense protein PD-T7-3 (H122A) in complex with a fragment of RNA
Authors : Puteikiene, R.; Sasnauskas, G.
Deposited on : 2025-12-23
Resolution : 3.08 Å(reported)
Based on initial model : .

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:

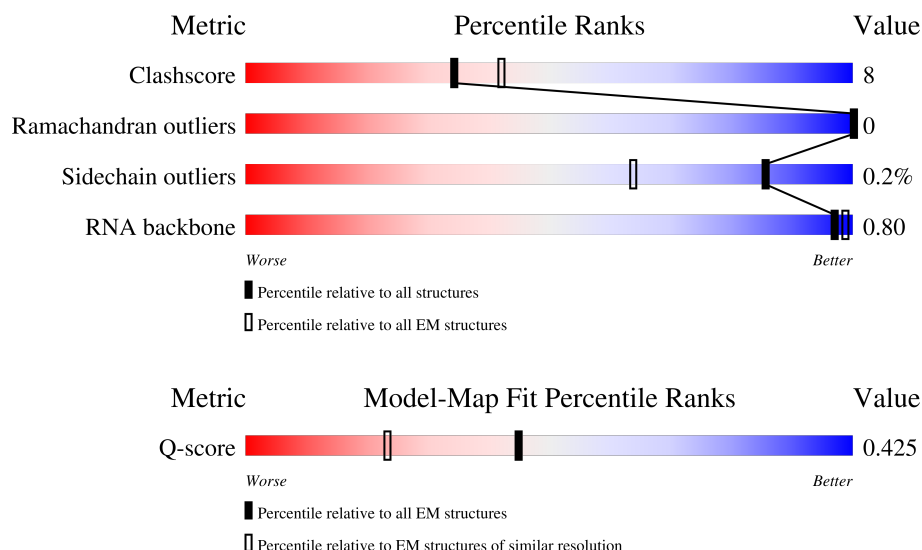
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.08 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.



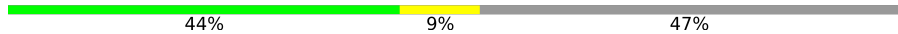
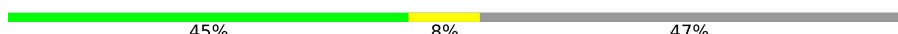
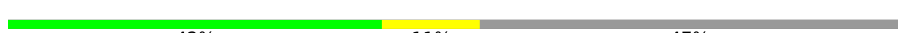
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14000 (2.58 - 3.58)

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	465	
1	B	465	
1	C	465	

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Mol	Chain	Length	Quality of chain
1	D	465	
1	E	465	
1	F	465	
1	G	465	
1	H	465	
1	I	465	
1	J	465	
1	K	465	
1	L	465	
2	M	7	
3	N	7	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34426 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 Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30, HEPN active site mutant H122A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	445	Total	C	N	O	S	0	0
			3567	2295	615	645	12		
1	B	435	Total	C	N	O	S	0	0
			3248	2113	563	561	11		
1	C	444	Total	C	N	O	S	0	0
			3492	2253	607	620	12		
1	D	445	Total	C	N	O	S	0	0
			3563	2293	615	643	12		
1	E	246	Total	C	N	O	S	0	0
			1910	1244	327	332	7		
1	F	347	Total	C	N	O	S	0	0
			2688	1736	464	479	9		
1	G	445	Total	C	N	O	S	0	0
			3567	2295	615	645	12		
1	H	246	Total	C	N	O	S	0	0
			1902	1241	325	329	7		
1	I	321	Total	C	N	O	S	0	0
			2519	1630	430	451	8		
1	J	445	Total	C	N	O	S	0	0
			3544	2277	609	646	12		
1	K	246	Total	C	N	O	S	0	0
			1902	1243	326	326	7		
1	L	288	Total	C	N	O	S	0	0
			2233	1441	381	403	8		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	ALA	HIS	engineered mutation	UNP Q858S9
A	456	PHE	-	expression tag	UNP Q858S9
A	457	GLU	-	expression tag	UNP Q858S9
A	458	SER	-	expression tag	UNP Q858S9
A	459	GLY	-	expression tag	UNP Q858S9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	460	HIS	-	expression tag	UNP Q858S9
A	461	HIS	-	expression tag	UNP Q858S9
A	462	HIS	-	expression tag	UNP Q858S9
A	463	HIS	-	expression tag	UNP Q858S9
A	464	HIS	-	expression tag	UNP Q858S9
A	465	HIS	-	expression tag	UNP Q858S9
B	122	ALA	HIS	engineered mutation	UNP Q858S9
B	456	PHE	-	expression tag	UNP Q858S9
B	457	GLU	-	expression tag	UNP Q858S9
B	458	SER	-	expression tag	UNP Q858S9
B	459	GLY	-	expression tag	UNP Q858S9
B	460	HIS	-	expression tag	UNP Q858S9
B	461	HIS	-	expression tag	UNP Q858S9
B	462	HIS	-	expression tag	UNP Q858S9
B	463	HIS	-	expression tag	UNP Q858S9
B	464	HIS	-	expression tag	UNP Q858S9
B	465	HIS	-	expression tag	UNP Q858S9
C	122	ALA	HIS	engineered mutation	UNP Q858S9
C	456	PHE	-	expression tag	UNP Q858S9
C	457	GLU	-	expression tag	UNP Q858S9
C	458	SER	-	expression tag	UNP Q858S9
C	459	GLY	-	expression tag	UNP Q858S9
C	460	HIS	-	expression tag	UNP Q858S9
C	461	HIS	-	expression tag	UNP Q858S9
C	462	HIS	-	expression tag	UNP Q858S9
C	463	HIS	-	expression tag	UNP Q858S9
C	464	HIS	-	expression tag	UNP Q858S9
C	465	HIS	-	expression tag	UNP Q858S9
D	122	ALA	HIS	engineered mutation	UNP Q858S9
D	456	PHE	-	expression tag	UNP Q858S9
D	457	GLU	-	expression tag	UNP Q858S9
D	458	SER	-	expression tag	UNP Q858S9
D	459	GLY	-	expression tag	UNP Q858S9
D	460	HIS	-	expression tag	UNP Q858S9
D	461	HIS	-	expression tag	UNP Q858S9
D	462	HIS	-	expression tag	UNP Q858S9
D	463	HIS	-	expression tag	UNP Q858S9
D	464	HIS	-	expression tag	UNP Q858S9
D	465	HIS	-	expression tag	UNP Q858S9
E	122	ALA	HIS	engineered mutation	UNP Q858S9
E	456	PHE	-	expression tag	UNP Q858S9
E	457	GLU	-	expression tag	UNP Q858S9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	458	SER	-	expression tag	UNP Q858S9
E	459	GLY	-	expression tag	UNP Q858S9
E	460	HIS	-	expression tag	UNP Q858S9
E	461	HIS	-	expression tag	UNP Q858S9
E	462	HIS	-	expression tag	UNP Q858S9
E	463	HIS	-	expression tag	UNP Q858S9
E	464	HIS	-	expression tag	UNP Q858S9
E	465	HIS	-	expression tag	UNP Q858S9
F	122	ALA	HIS	engineered mutation	UNP Q858S9
F	456	PHE	-	expression tag	UNP Q858S9
F	457	GLU	-	expression tag	UNP Q858S9
F	458	SER	-	expression tag	UNP Q858S9
F	459	GLY	-	expression tag	UNP Q858S9
F	460	HIS	-	expression tag	UNP Q858S9
F	461	HIS	-	expression tag	UNP Q858S9
F	462	HIS	-	expression tag	UNP Q858S9
F	463	HIS	-	expression tag	UNP Q858S9
F	464	HIS	-	expression tag	UNP Q858S9
F	465	HIS	-	expression tag	UNP Q858S9
G	122	ALA	HIS	engineered mutation	UNP Q858S9
G	456	PHE	-	expression tag	UNP Q858S9
G	457	GLU	-	expression tag	UNP Q858S9
G	458	SER	-	expression tag	UNP Q858S9
G	459	GLY	-	expression tag	UNP Q858S9
G	460	HIS	-	expression tag	UNP Q858S9
G	461	HIS	-	expression tag	UNP Q858S9
G	462	HIS	-	expression tag	UNP Q858S9
G	463	HIS	-	expression tag	UNP Q858S9
G	464	HIS	-	expression tag	UNP Q858S9
G	465	HIS	-	expression tag	UNP Q858S9
H	122	ALA	HIS	engineered mutation	UNP Q858S9
H	456	PHE	-	expression tag	UNP Q858S9
H	457	GLU	-	expression tag	UNP Q858S9
H	458	SER	-	expression tag	UNP Q858S9
H	459	GLY	-	expression tag	UNP Q858S9
H	460	HIS	-	expression tag	UNP Q858S9
H	461	HIS	-	expression tag	UNP Q858S9
H	462	HIS	-	expression tag	UNP Q858S9
H	463	HIS	-	expression tag	UNP Q858S9
H	464	HIS	-	expression tag	UNP Q858S9
H	465	HIS	-	expression tag	UNP Q858S9
I	122	ALA	HIS	engineered mutation	UNP Q858S9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	456	PHE	-	expression tag	UNP Q858S9
I	457	GLU	-	expression tag	UNP Q858S9
I	458	SER	-	expression tag	UNP Q858S9
I	459	GLY	-	expression tag	UNP Q858S9
I	460	HIS	-	expression tag	UNP Q858S9
I	461	HIS	-	expression tag	UNP Q858S9
I	462	HIS	-	expression tag	UNP Q858S9
I	463	HIS	-	expression tag	UNP Q858S9
I	464	HIS	-	expression tag	UNP Q858S9
I	465	HIS	-	expression tag	UNP Q858S9
J	122	ALA	HIS	engineered mutation	UNP Q858S9
J	456	PHE	-	expression tag	UNP Q858S9
J	457	GLU	-	expression tag	UNP Q858S9
J	458	SER	-	expression tag	UNP Q858S9
J	459	GLY	-	expression tag	UNP Q858S9
J	460	HIS	-	expression tag	UNP Q858S9
J	461	HIS	-	expression tag	UNP Q858S9
J	462	HIS	-	expression tag	UNP Q858S9
J	463	HIS	-	expression tag	UNP Q858S9
J	464	HIS	-	expression tag	UNP Q858S9
J	465	HIS	-	expression tag	UNP Q858S9
K	122	ALA	HIS	engineered mutation	UNP Q858S9
K	456	PHE	-	expression tag	UNP Q858S9
K	457	GLU	-	expression tag	UNP Q858S9
K	458	SER	-	expression tag	UNP Q858S9
K	459	GLY	-	expression tag	UNP Q858S9
K	460	HIS	-	expression tag	UNP Q858S9
K	461	HIS	-	expression tag	UNP Q858S9
K	462	HIS	-	expression tag	UNP Q858S9
K	463	HIS	-	expression tag	UNP Q858S9
K	464	HIS	-	expression tag	UNP Q858S9
K	465	HIS	-	expression tag	UNP Q858S9
L	122	ALA	HIS	engineered mutation	UNP Q858S9
L	456	PHE	-	expression tag	UNP Q858S9
L	457	GLU	-	expression tag	UNP Q858S9
L	458	SER	-	expression tag	UNP Q858S9
L	459	GLY	-	expression tag	UNP Q858S9
L	460	HIS	-	expression tag	UNP Q858S9
L	461	HIS	-	expression tag	UNP Q858S9
L	462	HIS	-	expression tag	UNP Q858S9
L	463	HIS	-	expression tag	UNP Q858S9
L	464	HIS	-	expression tag	UNP Q858S9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	465	HIS	-	expression tag	UNP Q858S9

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	7	Total	C	N	O	P	0	0
			151	70	35	40	6		

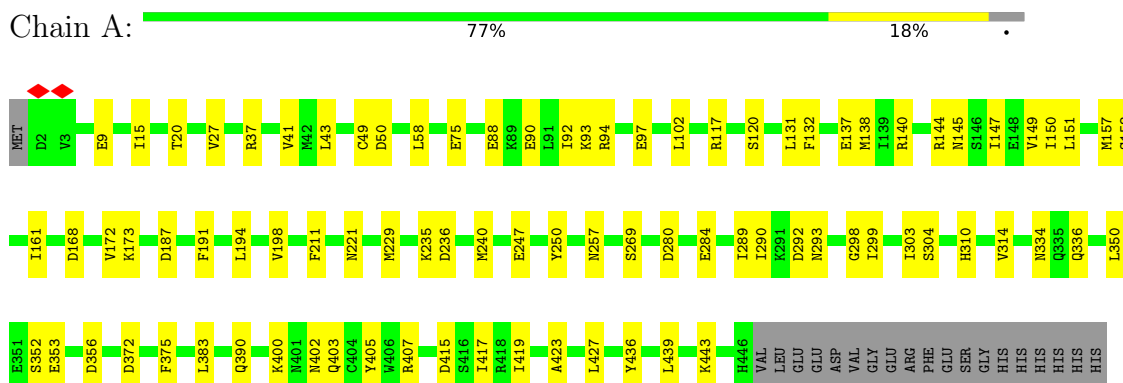
- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	7	Total	C	N	O	P	0	0
			140	63	14	56	7		

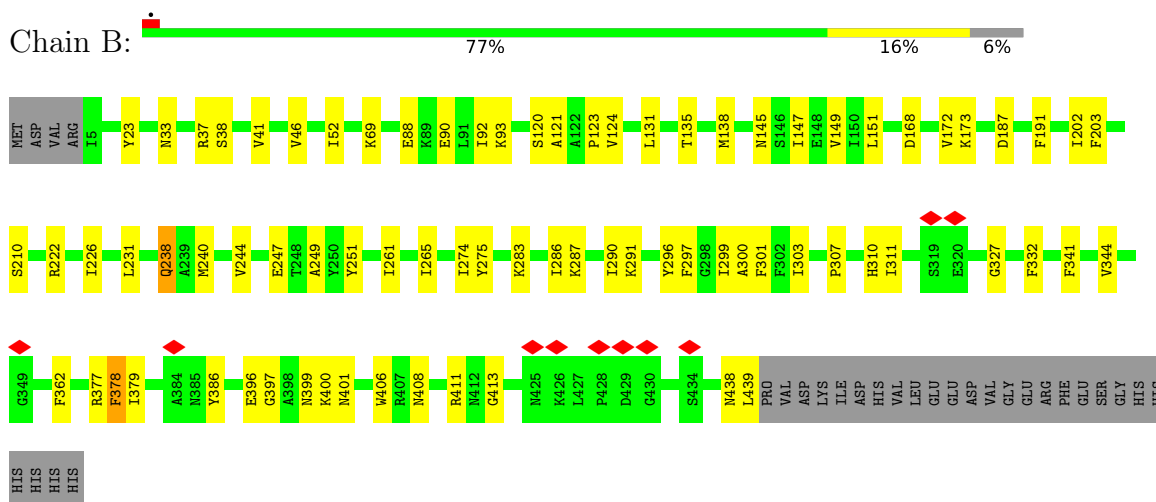
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30, HEPN active site mutant H122A

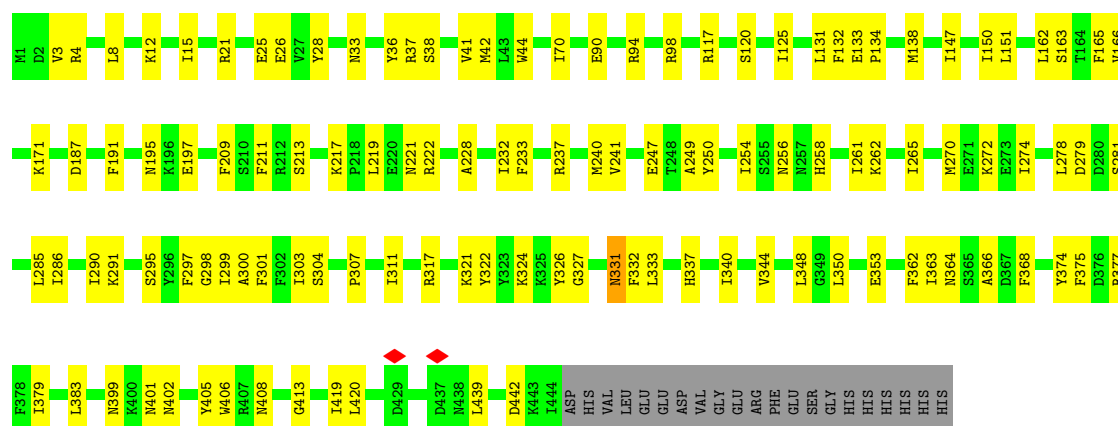


- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30, HEPN active site mutant H122A

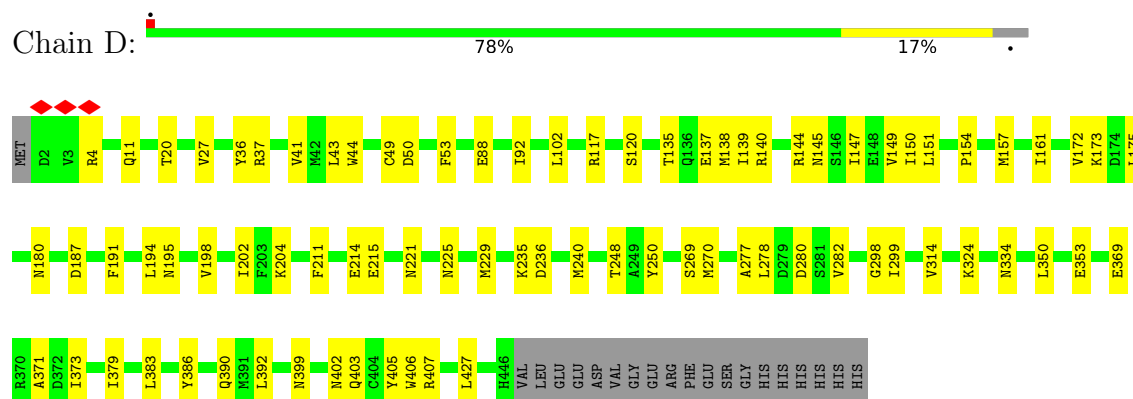


- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30, HEPN active site mutant H122A

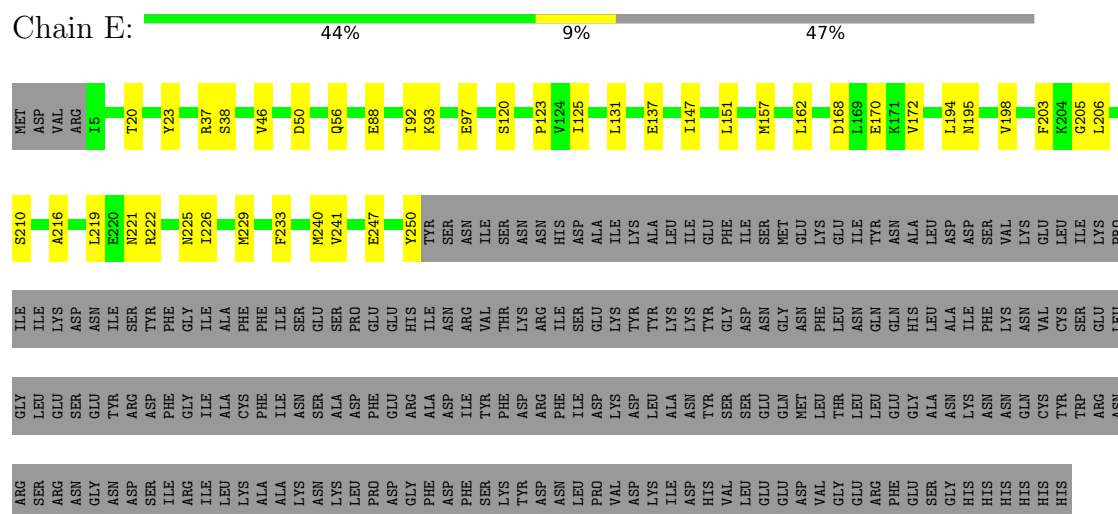




- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30, HEPN active site mutant H122A



- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30, HEPN active site mutant H122A



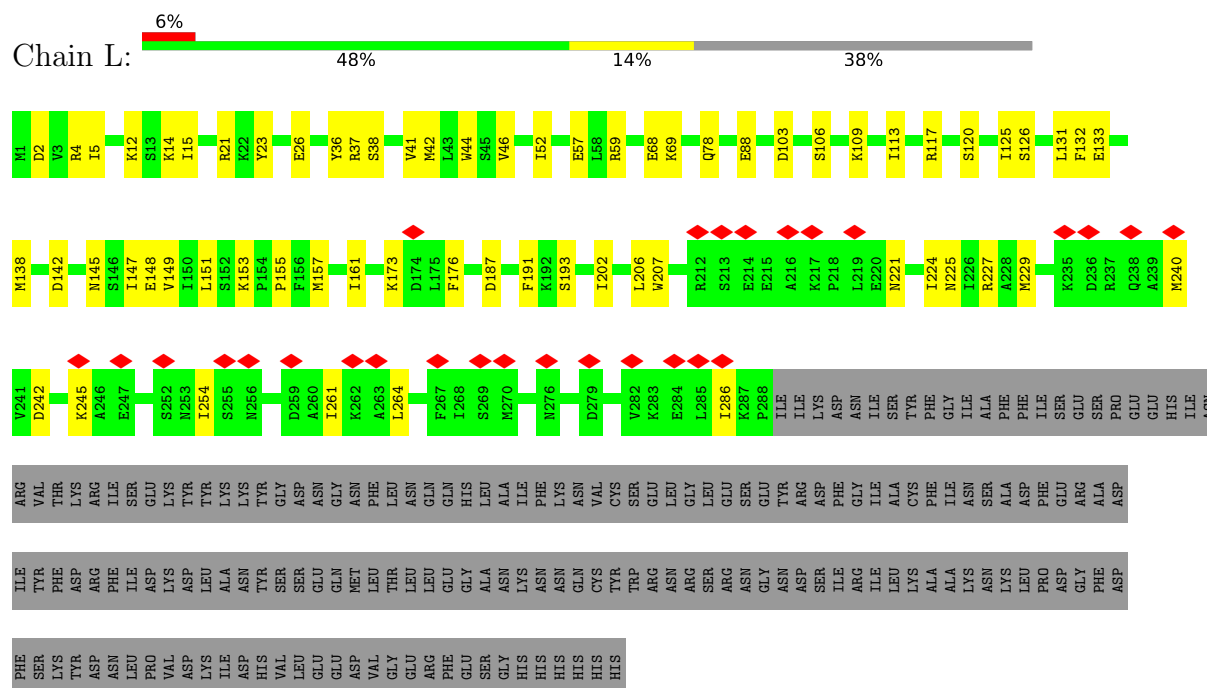
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30, HEPN active site mutant H122A



WORLD WIDE
PDB
PROTEIN DATA BANK



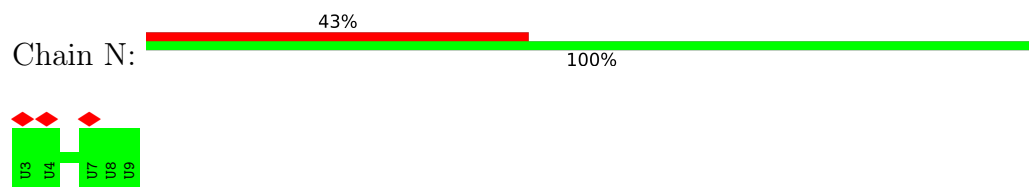
- Molecule 1: Bacterial antiviral defense protein PD-T7-3 from Escherichia coli strain ECOR30, HEPN active site mutant H122A



- Molecule 2: RNA



- Molecule 3: RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.762	Depositor
Minimum map value	-0.182	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/3640	0.23	0/4912
1	B	0.11	0/3317	0.27	0/4502
1	C	0.11	0/3564	0.30	0/4819
1	D	0.11	0/3636	0.23	0/4907
1	E	0.11	0/1949	0.25	0/2641
1	F	0.10	0/2740	0.24	0/3711
1	G	0.11	0/3640	0.23	0/4912
1	H	0.13	0/1941	0.26	0/2631
1	I	0.11	0/2567	0.27	0/3475
1	J	0.12	0/3616	0.24	0/4884
1	K	0.12	0/1941	0.27	0/2630
1	L	0.10	0/2275	0.24	0/3085
2	M	0.05	0/171	0.09	0/265
3	N	0.04	0/153	0.07	0/234
All	All	0.11	0/35150	0.25	0/47608

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3567	0	3529	57	0
1	B	3248	0	3065	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3492	0	3425	85	0
1	D	3563	0	3525	54	0
1	E	1910	0	1894	28	0
1	F	2688	0	2638	50	0
1	G	3567	0	3529	49	0
1	H	1902	0	1885	29	0
1	I	2519	0	2507	45	0
1	J	3544	0	3478	57	0
1	K	1902	0	1894	37	0
1	L	2233	0	2197	48	0
2	M	151	0	79	5	0
3	N	140	0	71	0	0
All	All	34426	0	33716	555	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 8.

All (555) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161:ILE:HD11	1:L:202:ILE:HD11	1.55	0.88
1:B:397:GLY:HA2	1:B:400:LYS:HE3	1.66	0.78
1:J:278:LEU:HD23	1:J:282:VAL:HG11	1.64	0.77
1:B:38:SER:HB3	1:I:38:SER:HB3	1.68	0.76
1:F:38:SER:HB3	1:K:38:SER:HB3	1.70	0.73
1:E:38:SER:HB3	1:L:38:SER:HB3	1.71	0.73
1:C:38:SER:HB3	1:H:38:SER:HB2	1.71	0.71
1:B:261:ILE:HG23	1:B:286:ILE:HG22	1.73	0.71
1:L:207:TRP:HA	1:L:229:MET:CE	2.21	0.70
1:F:162:LEU:HD21	1:F:205:GLY:HA3	1.74	0.70
1:D:278:LEU:HD23	1:D:282:VAL:HG11	1.75	0.69
1:G:149:VAL:HG12	1:G:150:ILE:HG12	1.74	0.68
1:G:278:LEU:HD13	1:G:282:VAL:HG11	1.76	0.68
1:J:149:VAL:HG12	1:J:150:ILE:HG12	1.76	0.68
1:D:149:VAL:HG12	1:D:150:ILE:HG12	1.75	0.68
1:C:211:PHE:HB3	1:C:254:ILE:HG23	1.75	0.67
1:L:157:MET:HE2	1:L:193:SER:HB2	1.76	0.67
1:C:125:ILE:HD12	1:C:125:ILE:H	1.60	0.67
1:C:326:TYR:H	1:C:366:ALA:HB2	1.59	0.66
1:B:261:ILE:HD12	1:B:261:ILE:H	1.61	0.66
1:J:355:ARG:HG2	1:J:382:ASP:OD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLU:OE1	1:A:9:GLU:N	2.26	0.66
1:A:149:VAL:HG12	1:A:150:ILE:HG12	1.77	0.65
1:L:207:TRP:HA	1:L:229:MET:HE1	1.78	0.65
1:I:212:ARG:HD2	1:I:253:ASN:HB3	1.78	0.65
1:E:137:GLU:HG2	1:J:140:ARG:HD2	1.78	0.65
1:A:292:ASP:OD1	1:A:293:ASN:ND2	2.30	0.65
1:H:147:ILE:HA	1:H:151:LEU:HB2	1.79	0.65
1:B:399:ASN:HB3	1:B:438:ASN:HB3	1.80	0.64
1:C:232:ILE:HG22	1:C:240:MET:HE3	1.78	0.64
1:C:261:ILE:O	1:C:265:ILE:HG12	1.97	0.64
1:B:261:ILE:O	1:B:265:ILE:HG13	1.98	0.64
1:E:147:ILE:HA	1:E:151:LEU:HB2	1.79	0.63
1:J:382:ASP:OD1	1:J:382:ASP:O	2.17	0.63
1:J:184:LYS:O	1:J:188:VAL:HG12	1.98	0.63
1:B:145:ASN:O	1:B:149:VAL:HB	1.99	0.62
1:D:41:VAL:HA	1:D:117:ARG:HG3	1.81	0.62
1:D:157:MET:HA	1:D:161:ILE:HD11	1.81	0.62
1:I:187:ASP:HA	1:I:191:PHE:HB2	1.81	0.62
1:J:7:SER:HB2	1:J:10:SER:HB3	1.81	0.62
1:C:383:LEU:HD21	1:C:419:ILE:HD13	1.81	0.62
1:I:15:ILE:O	1:I:21:ARG:NH2	2.31	0.62
1:K:147:ILE:HA	1:K:151:LEU:HB2	1.82	0.62
1:B:135:THR:H	1:B:138:MET:HE3	1.63	0.62
1:F:268:ILE:HD11	1:F:274:ILE:HB	1.82	0.61
1:E:93:LYS:O	1:E:97:GLU:HG3	1.99	0.61
1:I:37:ARG:HG2	1:I:120:SER:HB3	1.82	0.61
1:L:37:ARG:HH21	1:L:133:GLU:HB2	1.65	0.61
1:L:221:ASN:O	1:L:225:ASN:ND2	2.33	0.61
1:C:4:ARG:NH1	1:C:36:TYR:OH	2.33	0.61
1:G:382:ASP:OD1	1:G:385:ASN:ND2	2.34	0.61
1:E:203:PHE:HZ	1:E:233:PHE:HE1	1.48	0.61
1:F:157:MET:HE2	1:F:193:SER:HB2	1.81	0.61
1:A:132:PHE:HZ	1:A:138:MET:HE1	1.66	0.61
1:E:194:LEU:HD22	1:E:198:VAL:HG21	1.82	0.61
1:J:58:LEU:HD11	1:J:158:SER:HB2	1.83	0.61
1:A:37:ARG:HG3	1:A:120:SER:HB3	1.82	0.61
1:E:37:ARG:HG2	1:E:120:SER:HB3	1.82	0.60
1:F:15:ILE:O	1:F:21:ARG:NH2	2.34	0.60
1:C:37:ARG:HH21	1:C:133:GLU:HB2	1.66	0.60
1:I:4:ARG:NH1	1:I:36:TYR:OH	2.34	0.60
1:B:222:ARG:HG2	1:B:226:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLU:HB2	1:C:42:MET:HE2	1.83	0.60
1:L:161:ILE:CD1	1:L:202:ILE:HD11	2.30	0.60
1:C:15:ILE:O	1:C:21:ARG:NH2	2.35	0.60
1:I:278:LEU:HD13	1:I:282:VAL:HG11	1.83	0.60
1:I:93:LYS:O	1:I:97:GLU:HG2	2.02	0.60
1:C:147:ILE:HA	1:C:151:LEU:HB2	1.83	0.60
1:F:301:PHE:HE2	1:F:344:VAL:HG11	1.65	0.60
1:L:147:ILE:HA	1:L:151:LEU:HB2	1.82	0.59
1:J:379:ILE:O	1:J:383:LEU:HB2	2.02	0.59
1:K:37:ARG:HG2	1:K:120:SER:HB3	1.85	0.59
1:B:238:GLN:CD	1:B:238:GLN:H	2.10	0.59
1:B:300:ALA:O	1:B:310:HIS:NE2	2.35	0.59
1:C:299:ILE:HD11	1:C:337:HIS:HB3	1.84	0.59
1:C:274:ILE:O	1:C:278:LEU:HD22	2.03	0.59
1:G:58:LEU:HD11	1:G:158:SER:HB2	1.84	0.59
1:A:423:ALA:O	1:A:427:LEU:HD12	2.02	0.59
1:H:37:ARG:HG2	1:H:120:SER:HB3	1.85	0.59
1:I:272:LYS:HD3	1:I:275:TYR:HB3	1.83	0.59
1:B:37:ARG:HG2	1:B:120:SER:HB3	1.84	0.59
1:J:215:GLU:O	1:J:219:LEU:HD22	2.03	0.58
1:L:15:ILE:O	1:L:21:ARG:NH2	2.30	0.58
1:K:154:PRO:HD2	1:K:157:MET:HE3	1.86	0.58
1:J:247:GLU:HG2	1:J:250:TYR:HB3	1.85	0.58
1:B:400:LYS:HZ2	1:B:401:ASN:HB2	1.69	0.57
1:L:37:ARG:HG2	1:L:120:SER:HB3	1.85	0.57
1:F:4:ARG:NH1	1:F:36:TYR:OH	2.37	0.57
1:L:261:ILE:HG23	1:L:286:ILE:HG22	1.86	0.57
1:F:44:TRP:CD1	1:F:117:ARG:HD2	2.40	0.57
1:A:402:ASN:ND2	1:A:403:GLN:OE1	2.36	0.57
1:C:408:ASN:O	1:C:413:GLY:N	2.37	0.57
1:A:145:ASN:O	1:A:149:VAL:HB	2.04	0.57
1:A:280:ASP:O	1:A:284:GLU:HG2	2.05	0.57
1:C:217:LYS:O	1:C:221:ASN:ND2	2.36	0.57
1:K:93:LYS:O	1:K:97:GLU:HG3	2.03	0.57
1:C:98:ARG:NH1	2:M:4:A:O2'	2.37	0.57
1:K:23:TYR:HB3	1:K:46:VAL:HG22	1.87	0.56
1:H:93:LYS:O	1:H:97:GLU:HG3	2.04	0.56
1:L:132:PHE:HZ	1:L:138:MET:HE1	1.69	0.56
1:L:207:TRP:N	1:L:229:MET:HE2	2.20	0.56
1:C:209:PHE:O	1:C:213:SER:OG	2.22	0.56
1:I:290:ILE:HB	1:I:297:PHE:HD1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:TYR:HB3	1:H:46:VAL:HG22	1.88	0.56
1:H:44:TRP:CD1	1:H:117:ARG:HD2	2.41	0.56
1:F:150:ILE:HG22	1:F:151:LEU:HD23	1.88	0.56
1:K:186:LEU:HD12	1:K:231:LEU:HD12	1.88	0.56
1:F:325:LYS:O	1:F:331:ASN:ND2	2.39	0.56
1:I:191:PHE:HB3	1:I:235:LYS:HE2	1.88	0.56
1:B:147:ILE:HA	1:B:151:LEU:HB2	1.88	0.56
1:J:147:ILE:HA	1:J:151:LEU:HB2	1.88	0.56
1:D:371:ALA:HB3	1:D:407:ARG:HD3	1.88	0.56
1:I:176:PHE:O	1:I:227:ARG:NH2	2.38	0.56
1:E:137:GLU:OE1	1:J:144:ARG:HD3	2.06	0.55
1:D:144:ARG:HD3	1:K:137:GLU:OE1	2.06	0.55
1:E:225:ASN:O	1:E:229:MET:HG2	2.07	0.55
1:J:20:THR:HG21	1:J:50:ASP:OD2	2.06	0.55
1:D:20:THR:HG21	1:D:50:ASP:OD2	2.06	0.55
1:B:23:TYR:HH	1:I:130:THR:HG1	1.53	0.55
1:B:327:GLY:HA2	1:B:332:PHE:HB2	1.88	0.55
1:C:258:HIS:O	1:C:262:LYS:HG3	2.06	0.55
1:H:222:ARG:O	1:H:226:ILE:HG12	2.06	0.54
1:J:187:ASP:HA	1:J:191:PHE:HB2	1.90	0.54
1:D:204:LYS:HG3	1:D:250:TYR:CE1	2.42	0.54
1:A:352:SER:OG	1:A:353:GLU:OE1	2.26	0.54
1:C:281:SER:O	1:C:285:LEU:HD12	2.07	0.54
1:C:33:ASN:OD1	1:H:33:ASN:ND2	2.40	0.54
1:C:274:ILE:HD12	1:C:274:ILE:H	1.72	0.54
1:C:12:LYS:NZ	1:C:25:GLU:OE2	2.40	0.54
1:C:399:ASN:HD21	1:C:439:LEU:HD22	1.73	0.54
1:G:147:ILE:HA	1:G:151:LEU:HB2	1.90	0.54
1:I:130:THR:OG1	1:I:131:LEU:N	2.41	0.54
1:A:173:LYS:NZ	1:A:221:ASN:OD1	2.36	0.53
1:C:374:TYR:HE1	1:C:377:ARG:HH21	1.57	0.53
1:D:140:ARG:HD2	1:K:137:GLU:HG2	1.89	0.53
1:C:362:PHE:CE2	1:C:379:ILE:HG12	2.42	0.53
1:B:362:PHE:CD2	1:B:379:ILE:HG13	2.43	0.53
1:D:386:TYR:HD2	1:D:390:GLN:HB3	1.73	0.53
1:F:311:ILE:HD12	1:F:312:ASN:N	2.23	0.53
1:C:41:VAL:HA	1:C:117:ARG:HD3	1.91	0.53
1:C:90:GLU:O	1:C:94:ARG:HG2	2.08	0.53
1:G:3:VAL:HG23	1:G:4:ARG:HG3	1.90	0.53
1:I:41:VAL:HA	1:I:117:ARG:HD3	1.90	0.53
1:A:372:ASP:OD1	1:A:407:ARG:NE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ASP:OD1	1:C:442:ASP:N	2.42	0.53
1:G:11:GLN:HB3	1:G:147:ILE:HG21	1.89	0.53
1:H:203:PHE:HD2	1:H:240:MET:SD	2.31	0.53
1:A:144:ARG:HD3	1:H:137:GLU:OE2	2.09	0.53
1:D:211:PHE:CE2	1:D:229:MET:HE1	2.43	0.53
1:L:207:TRP:HA	1:L:229:MET:HE2	1.90	0.53
1:A:257:ASN:OD1	1:C:171:LYS:NZ	2.31	0.53
1:A:417:ILE:HD12	1:A:443:LYS:HB3	1.91	0.53
1:C:270:MET:HA	1:C:270:MET:HE2	1.91	0.53
1:D:145:ASN:O	1:D:149:VAL:HB	2.09	0.53
1:I:94:ARG:HD3	1:I:98:ARG:HH21	1.72	0.53
1:B:377:ARG:HD2	1:B:378:PHE:CE2	2.44	0.52
1:E:123:PRO:O	1:L:78:GLN:NE2	2.38	0.52
1:E:125:ILE:HG12	1:L:52:ILE:HD13	1.90	0.52
1:E:162:LEU:HD21	1:E:205:GLY:HA3	1.90	0.52
1:G:353:GLU:N	1:G:353:GLU:OE1	2.42	0.52
1:G:391:MET:O	1:G:395:LEU:HG	2.10	0.52
1:I:150:ILE:HG22	1:I:151:LEU:HD12	1.90	0.52
1:C:272:LYS:NZ	1:C:304:SER:O	2.36	0.52
1:J:154:PRO:HD2	1:J:157:MET:HG2	1.91	0.52
1:L:103:ASP:H	1:L:106:SER:HB2	1.75	0.52
1:L:44:TRP:CD1	1:L:117:ARG:HG2	2.45	0.52
1:C:247:GLU:OE1	1:C:250:TYR:N	2.41	0.52
1:D:280:ASP:HB2	1:F:188:VAL:HG11	1.91	0.51
1:D:135:THR:H	1:D:138:MET:HE3	1.76	0.51
1:F:309:GLU:HA	1:F:312:ASN:HD21	1.74	0.51
1:A:157:MET:HA	1:A:161:ILE:HD11	1.91	0.51
1:G:386:TYR:HB2	1:G:391:MET:HE2	1.92	0.51
1:A:132:PHE:CZ	1:A:138:MET:HE1	2.45	0.51
1:L:4:ARG:NH1	1:L:36:TYR:OH	2.44	0.51
1:C:187:ASP:HA	1:C:191:PHE:HB2	1.92	0.51
1:C:272:LYS:NZ	1:C:301:PHE:O	2.43	0.51
1:D:173:LYS:NZ	1:D:221:ASN:OD1	2.38	0.50
1:E:20:THR:HG21	1:E:50:ASP:OD2	2.10	0.50
1:B:275:TYR:CE1	1:B:283:LYS:HG2	2.46	0.50
1:C:41:VAL:HG11	1:H:41:VAL:HG11	1.94	0.50
1:C:301:PHE:HE2	1:C:344:VAL:HG11	1.75	0.50
1:D:102:LEU:HD21	1:D:150:ILE:HD11	1.92	0.50
1:L:59:ARG:HG3	1:L:68:GLU:HG2	1.93	0.50
1:L:206:LEU:C	1:L:229:MET:HE2	2.36	0.50
1:A:102:LEU:HD21	1:A:150:ILE:HD11	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:GLY:HA2	1:F:332:PHE:HB3	1.92	0.50
1:C:363:ILE:O	1:C:401:ASN:ND2	2.44	0.50
1:F:41:VAL:HG11	1:K:41:VAL:HG11	1.94	0.50
1:A:58:LEU:HD11	1:A:158:SER:OG	2.12	0.50
1:C:368:PHE:HE1	1:C:406:TRP:HB3	1.76	0.50
1:F:81:ASP:N	1:F:81:ASP:OD1	2.42	0.50
1:F:290:ILE:HB	1:F:297:PHE:HD1	1.76	0.50
1:J:188:VAL:HG11	1:K:174:ASP:HB2	1.94	0.50
1:L:207:TRP:CA	1:L:229:MET:HE2	2.42	0.50
1:D:225:ASN:O	1:D:229:MET:HG3	2.12	0.50
1:D:350:LEU:HB3	1:D:353:GLU:HB2	1.94	0.50
1:J:191:PHE:HB3	1:J:235:LYS:HE3	1.94	0.50
1:L:26:GLU:HB2	1:L:42:MET:HE2	1.93	0.50
1:L:173:LYS:HA	1:L:224:ILE:HD13	1.93	0.50
1:K:223:GLU:O	1:K:227:ARG:HG3	2.12	0.49
1:G:20:THR:HG21	1:G:50:ASP:OD2	2.12	0.49
1:I:162:LEU:HD21	1:I:205:GLY:HA3	1.94	0.49
1:F:78:GLN:NE2	1:K:123:PRO:O	2.41	0.49
1:B:299:ILE:HA	1:B:341:PHE:HE1	1.76	0.49
1:J:173:LYS:NZ	1:J:221:ASN:OD1	2.39	0.49
1:A:140:ARG:HD2	1:H:137:GLU:HG2	1.94	0.49
1:C:295:SER:HA	1:C:333:LEU:HD12	1.93	0.49
1:D:369:GLU:O	1:D:373:ILE:HG22	2.13	0.49
1:G:9:GLU:CD	1:G:9:GLU:H	2.20	0.49
1:C:297:PHE:CE2	1:C:317:ARG:HD3	2.48	0.49
1:D:27:VAL:HG11	1:D:43:LEU:HD13	1.94	0.49
2:M:6:A:H2'	2:M:7:A:H8	1.77	0.49
1:K:225:ASN:O	1:K:229:MET:HG2	2.12	0.49
1:B:124:VAL:HA	1:I:78:GLN:HE22	1.77	0.48
1:D:187:ASP:HA	1:D:191:PHE:HB2	1.95	0.48
1:F:272:LYS:HZ2	1:F:275:TYR:HB3	1.77	0.48
1:K:247:GLU:HG3	1:K:250:TYR:HB2	1.95	0.48
1:H:203:PHE:HE1	1:H:207:TRP:HE3	1.59	0.48
1:C:237:ARG:HG2	1:C:237:ARG:HH11	1.79	0.48
1:K:227:ARG:O	1:K:231:LEU:HG	2.12	0.48
1:A:20:THR:HG21	1:A:50:ASP:OD2	2.14	0.48
1:A:49:CYS:SG	1:G:131:LEU:HG	2.53	0.48
1:H:69:LYS:HE2	1:H:69:LYS:HA	1.95	0.48
1:L:23:TYR:HB3	1:L:46:VAL:HG22	1.96	0.48
1:A:137:GLU:OE2	1:H:140:ARG:NH1	2.46	0.48
1:B:23:TYR:HB3	1:B:46:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HG	1:G:49:CYS:SG	2.53	0.48
1:B:203:PHE:HB2	1:B:240:MET:HE1	1.94	0.48
1:I:44:TRP:CD1	1:I:117:ARG:HG2	2.47	0.48
1:J:295:SER:HA	1:J:333:LEU:HD23	1.95	0.48
1:E:88:GLU:O	1:E:92:ILE:HG12	2.14	0.48
1:A:289:ILE:O	1:A:293:ASN:ND2	2.27	0.48
1:B:377:ARG:HD2	1:B:378:PHE:CD2	2.49	0.48
1:E:247:GLU:CD	1:E:250:TYR:H	2.22	0.48
1:A:383:LEU:HD11	1:A:419:ILE:HD13	1.95	0.47
1:C:219:LEU:HD22	1:C:222:ARG:HH22	1.78	0.47
1:B:41:VAL:HG11	1:I:41:VAL:HG11	1.97	0.47
1:D:4:ARG:NH1	1:K:133:GLU:OE2	2.47	0.47
1:C:348:LEU:HB2	1:C:350:LEU:HD12	1.97	0.47
1:G:245:LYS:HG2	1:G:277:ALA:HB2	1.97	0.47
1:J:298:GLY:HA2	1:J:314:VAL:HG21	1.96	0.47
1:D:53:PHE:HE1	1:J:130:THR:HG21	1.78	0.47
1:G:102:LEU:HD21	1:G:150:ILE:HD11	1.97	0.47
1:C:44:TRP:CD1	1:C:117:ARG:HG2	2.50	0.47
1:C:237:ARG:NH1	1:C:241:VAL:HG21	2.29	0.47
1:F:21:ARG:O	1:F:25:GLU:HG2	2.15	0.47
1:J:363:ILE:HD12	1:J:397:GLY:HA3	1.96	0.47
1:L:148:GLU:HG3	1:L:149:VAL:HG13	1.97	0.47
1:G:242:ASP:OD1	1:G:242:ASP:N	2.48	0.47
1:G:370:ARG:HA	1:G:373:ILE:HG22	1.97	0.47
1:A:147:ILE:HA	1:A:151:LEU:HB2	1.96	0.47
1:C:327:GLY:H	1:C:332:PHE:HB3	1.80	0.47
1:J:269:SER:HB2	1:J:299:ILE:O	2.14	0.47
1:L:254:ILE:HD13	1:L:264:LEU:HD13	1.96	0.47
1:E:203:PHE:HZ	1:E:233:PHE:CE1	2.30	0.47
1:F:301:PHE:CE2	1:F:344:VAL:HG11	2.47	0.47
1:I:276:ASN:OD1	1:I:277:ALA:N	2.49	0.47
1:A:415:ASP:O	1:A:419:ILE:HG12	2.14	0.46
1:C:350:LEU:HB3	1:C:353:GLU:HB2	1.97	0.46
1:B:408:ASN:O	1:B:413:GLY:N	2.41	0.46
1:C:299:ILE:HD12	1:C:340:ILE:HB	1.96	0.46
1:B:379:ILE:HG23	1:B:386:TYR:HE2	1.81	0.46
1:C:163:SER:O	1:C:166:VAL:HG22	2.15	0.46
1:J:131:LEU:HD23	1:J:131:LEU:HA	1.77	0.46
1:K:8:LEU:HD13	1:K:143:ILE:HG21	1.96	0.46
1:K:187:ASP:HA	1:K:191:PHE:HB2	1.97	0.46
1:A:436:TYR:HB3	1:A:439:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:LEU:HD23	1:I:71:LEU:HA	1.78	0.46
1:J:245:LYS:HA	1:J:277:ALA:HB1	1.97	0.46
1:K:44:TRP:CD1	1:K:117:ARG:HD2	2.50	0.46
1:F:33:ASN:ND2	1:K:33:ASN:OD1	2.48	0.46
1:F:304:SER:HB2	1:F:310:HIS:HB2	1.97	0.46
1:F:334:ASN:OD1	1:F:335:GLN:N	2.43	0.46
1:H:203:PHE:HD1	1:H:203:PHE:O	1.99	0.46
1:A:247:GLU:HG2	1:A:250:TYR:HB3	1.98	0.46
1:C:195:ASN:OD1	1:C:195:ASN:N	2.42	0.46
1:C:307:PRO:O	1:C:311:ILE:HG12	2.16	0.46
1:J:368:PHE:HE1	1:J:403:GLN:HA	1.81	0.46
1:C:326:TYR:HE1	1:C:374:TYR:HE2	1.62	0.46
1:H:150:ILE:HG23	1:H:151:LEU:HD23	1.98	0.46
1:D:248:THR:HG22	1:D:277:ALA:O	2.16	0.46
1:D:383:LEU:HD12	1:D:383:LEU:HA	1.81	0.46
1:G:256:ASN:HB2	1:I:171:LYS:HE2	1.98	0.46
1:I:12:LYS:HE2	1:I:21:ARG:HG2	1.98	0.46
1:I:162:LEU:O	1:I:165:PHE:HB3	2.16	0.46
1:I:209:PHE:O	1:I:213:SER:OG	2.34	0.46
1:A:290:ILE:HD12	1:A:303:ILE:HD13	1.98	0.46
1:F:295:SER:HA	1:F:333:LEU:HD13	1.98	0.46
1:L:149:VAL:O	1:L:153:LYS:HE2	2.16	0.46
1:C:301:PHE:CD1	1:C:301:PHE:N	2.84	0.45
1:G:245:LYS:HA	1:G:277:ALA:HB1	1.98	0.45
1:A:191:PHE:HB3	1:A:235:LYS:HE3	1.98	0.45
1:C:326:TYR:CE1	1:C:374:TYR:HE2	2.34	0.45
1:D:298:GLY:HA2	1:D:314:VAL:HG21	1.98	0.45
1:A:269:SER:HB2	1:A:299:ILE:O	2.15	0.45
1:C:8:LEU:HB3	1:C:28:TYR:CD2	2.51	0.45
1:C:131:LEU:HD23	1:C:131:LEU:HA	1.81	0.45
1:D:204:LYS:HE3	1:D:204:LYS:HB2	1.68	0.45
1:F:37:ARG:HG2	1:F:120:SER:HB3	1.98	0.45
1:G:179:ASP:HA	1:G:227:ARG:HH21	1.81	0.45
1:G:298:GLY:HA2	1:G:314:VAL:HG21	1.98	0.45
1:B:93:LYS:HB3	1:B:93:LYS:HE2	1.73	0.45
1:D:154:PRO:HD2	1:D:157:MET:HG3	1.97	0.45
1:G:168:ASP:O	1:G:172:VAL:HG22	2.16	0.45
1:B:123:PRO:O	1:I:78:GLN:NE2	2.43	0.45
1:H:88:GLU:O	1:H:92:ILE:HG12	2.15	0.45
1:J:217:LYS:HA	1:J:220:GLU:HG2	1.99	0.45
1:G:131:LEU:HD23	1:G:131:LEU:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LYS:HD2	1:B:401:ASN:N	2.31	0.45
1:F:149:VAL:HG23	1:F:150:ILE:HG12	1.99	0.45
1:I:23:TYR:HB3	1:I:46:VAL:HG22	1.98	0.45
1:J:399:ASN:O	1:J:438:ASN:ND2	2.50	0.45
1:D:405:TYR:HE1	1:D:406:TRP:HE3	1.65	0.45
1:J:219:LEU:HD12	1:J:222:ARG:HH21	1.80	0.45
1:K:206:LEU:C	1:K:229:MET:HE1	2.42	0.45
1:A:157:MET:SD	1:A:198:VAL:HG21	2.57	0.45
1:A:356:ASP:OD1	1:A:390:GLN:NE2	2.50	0.45
1:B:88:GLU:O	1:B:92:ILE:HG12	2.17	0.45
1:B:439:LEU:HD12	1:B:439:LEU:H	1.82	0.44
1:D:269:SER:HB2	1:D:299:ILE:O	2.17	0.44
1:F:102:LEU:HD21	1:F:150:ILE:HD11	1.98	0.44
1:G:50:ASP:OD1	1:G:54:LYS:NZ	2.43	0.44
1:J:195:ASN:N	1:J:195:ASN:OD1	2.47	0.44
2:M:6:A:H2'	2:M:7:A:C8	2.51	0.44
1:C:150:ILE:HG23	1:C:151:LEU:HD23	2.00	0.44
1:D:88:GLU:O	1:D:92:ILE:HG12	2.17	0.44
1:E:195:ASN:OD1	1:E:198:VAL:HG22	2.18	0.44
1:F:131:LEU:HD23	1:F:131:LEU:HA	1.89	0.44
1:G:149:VAL:O	1:G:153:LYS:HD2	2.17	0.44
1:G:154:PRO:HD2	1:G:157:MET:HG3	1.99	0.44
1:J:204:LYS:HG3	1:J:250:TYR:CE2	2.51	0.44
1:A:168:ASP:O	1:A:172:VAL:HG22	2.17	0.44
1:B:33:ASN:OD1	1:I:33:ASN:ND2	2.50	0.44
1:C:322:TYR:O	1:C:364:ASN:HB3	2.17	0.44
1:A:375:PHE:HE1	1:A:419:ILE:HD11	1.82	0.44
1:F:8:LEU:HB3	1:F:28:TYR:CD2	2.51	0.44
1:G:37:ARG:HG2	1:G:120:SER:HB3	1.99	0.44
1:G:89:LYS:HE3	1:G:114:GLN:HE22	1.83	0.44
1:G:194:LEU:HD23	1:G:194:LEU:HA	1.85	0.44
1:J:88:GLU:O	1:J:92:ILE:HG12	2.17	0.44
1:B:231:LEU:HD13	1:B:231:LEU:HA	1.86	0.44
1:B:396:GLU:O	1:B:400:LYS:HG3	2.18	0.44
1:D:137:GLU:OE2	1:K:140:ARG:NH1	2.51	0.44
1:F:103:ASP:H	1:F:106:SER:HB2	1.82	0.44
1:F:161:ILE:HD11	1:F:190:TYR:HE1	1.81	0.44
1:H:175:LEU:HD12	1:H:175:LEU:HA	1.86	0.44
1:L:125:ILE:HG13	1:L:126:SER:N	2.32	0.44
1:D:191:PHE:HB3	1:D:235:LYS:HE3	1.99	0.44
1:J:261:ILE:HD13	1:J:285:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:PHE:CE1	1:K:207:TRP:HE3	2.35	0.44
1:D:214:GLU:N	1:D:214:GLU:OE1	2.51	0.44
1:J:157:MET:SD	1:J:161:ILE:HD11	2.58	0.44
1:J:204:LYS:HG3	1:J:250:TYR:CZ	2.53	0.44
1:K:145:ASN:O	1:K:149:VAL:HB	2.18	0.44
1:L:131:LEU:HD23	1:L:131:LEU:HA	1.85	0.44
1:E:240:MET:HG3	1:E:241:VAL:N	2.33	0.44
1:G:175:LEU:HD21	1:H:178:SER:HB3	2.00	0.44
1:I:37:ARG:HH21	1:I:133:GLU:HB2	1.83	0.44
1:J:50:ASP:OD1	1:J:54:LYS:NZ	2.47	0.44
1:A:15:ILE:HG12	1:A:151:LEU:HB3	1.99	0.43
1:L:242:ASP:HA	1:L:245:LYS:HG2	2.00	0.43
1:B:69:LYS:HB3	1:B:69:LYS:HE3	1.80	0.43
1:C:228:ALA:O	1:C:232:ILE:HG13	2.19	0.43
1:D:11:GLN:HB3	1:D:147:ILE:HG21	1.99	0.43
1:D:147:ILE:HA	1:D:151:LEU:HB2	1.99	0.43
1:E:56:GLN:NE2	1:L:125:ILE:O	2.51	0.43
1:L:187:ASP:HA	1:L:191:PHE:HB2	2.00	0.43
1:A:75:GLU:HG2	1:G:125:ILE:HD12	2.00	0.43
1:A:117:ARG:HH12	1:G:117:ARG:HH12	1.66	0.43
1:B:296:TYR:CD1	1:B:299:ILE:HD11	2.54	0.43
1:C:37:ARG:HG2	1:C:120:SER:HB3	2.00	0.43
1:C:70:ILE:HD11	1:C:98:ARG:HB2	2.01	0.43
1:C:134:PRO:HB3	1:C:138:MET:HE2	1.99	0.43
1:D:198:VAL:O	1:D:202:ILE:HG13	2.17	0.43
1:D:324:LYS:HE3	1:D:403:GLN:HG2	2.00	0.43
1:K:226:ILE:HA	1:K:229:MET:HG2	2.00	0.43
1:J:370:ARG:HA	1:J:373:ILE:HG22	2.01	0.43
1:L:2:ASP:HB3	1:L:5:ILE:HG12	1.99	0.43
1:L:206:LEU:O	1:L:229:MET:CE	2.67	0.43
1:D:44:TRP:CD1	1:D:117:ARG:HD3	2.53	0.43
1:F:20:THR:HG21	1:F:50:ASP:OD2	2.19	0.43
1:F:268:ILE:HD12	1:F:268:ILE:HA	1.82	0.43
1:I:147:ILE:HA	1:I:151:LEU:HB2	1.99	0.43
1:B:247:GLU:OE2	1:B:249:ALA:N	2.52	0.43
1:D:137:GLU:OE1	1:K:144:ARG:NH1	2.49	0.43
1:F:117:ARG:HH21	1:K:117:ARG:HH22	1.65	0.43
1:G:9:GLU:CD	1:G:9:GLU:N	2.77	0.43
1:H:124:VAL:HG12	1:H:127:ASP:H	1.83	0.43
1:K:109:LYS:HD3	1:K:145:ASN:HB3	2.00	0.43
1:G:188:VAL:HG21	1:H:174:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:PHE:HZ	1:G:313:ARG:HH21	1.66	0.43
1:K:207:TRP:CE2	1:K:211:PHE:HD2	2.37	0.43
1:K:228:ALA:O	1:K:232:ILE:HG13	2.19	0.43
1:C:279:ASP:OD1	1:C:279:ASP:C	2.62	0.43
1:D:194:LEU:HD23	1:D:194:LEU:HA	1.83	0.43
1:L:57:GLU:HG2	1:L:155:PRO:HG3	2.00	0.43
1:A:336:GLN:H	1:A:336:GLN:CD	2.27	0.43
1:B:168:ASP:O	1:B:172:VAL:HG22	2.18	0.43
1:B:303:ILE:HB	1:B:310:HIS:NE2	2.33	0.43
1:C:233:PHE:CE1	1:C:237:ARG:HG3	2.54	0.43
1:L:14:LYS:HB2	1:L:14:LYS:HE2	1.89	0.43
1:B:121:ALA:HB1	1:I:117:ARG:NH2	2.34	0.43
1:B:131:LEU:HD12	1:B:131:LEU:HA	1.89	0.43
1:C:327:GLY:N	1:C:332:PHE:HB3	2.34	0.43
1:E:23:TYR:HB3	1:E:46:VAL:HG22	2.00	0.43
1:E:168:ASP:O	1:E:172:VAL:HG22	2.19	0.43
1:F:158:SER:O	1:F:161:ILE:HG22	2.18	0.43
1:G:363:ILE:HD12	1:G:397:GLY:HA3	2.01	0.43
1:I:132:PHE:HZ	1:I:138:MET:HE1	1.83	0.43
1:I:183:LYS:HB2	1:I:231:LEU:HD22	1.99	0.43
1:I:280:ASP:OD1	1:I:280:ASP:N	2.50	0.43
1:K:88:GLU:O	1:K:92:ILE:HG12	2.17	0.43
1:B:187:ASP:HA	1:B:191:PHE:HB2	2.00	0.42
1:H:236:ASP:O	1:H:240:MET:HE3	2.19	0.42
1:L:176:PHE:O	1:L:227:ARG:NH2	2.51	0.42
1:A:236:ASP:O	1:A:240:MET:HG2	2.18	0.42
1:D:37:ARG:HG2	1:D:120:SER:HB3	2.01	0.42
1:L:206:LEU:C	1:L:229:MET:CE	2.92	0.42
1:C:117:ARG:NH2	1:H:121:ALA:HB1	2.34	0.42
1:C:162:LEU:O	1:C:165:PHE:HB3	2.20	0.42
1:C:402:ASN:HA	1:C:405:TYR:CZ	2.54	0.42
1:F:117:ARG:HH22	1:K:121:ALA:HB1	1.84	0.42
1:G:195:ASN:OD1	1:G:195:ASN:N	2.48	0.42
1:G:396:GLU:O	1:G:400:LYS:HG3	2.19	0.42
1:I:102:LEU:HD21	1:I:150:ILE:HD11	2.01	0.42
1:I:134:PRO:HB3	1:I:138:MET:HE2	2.01	0.42
1:J:215:GLU:O	1:J:218:PRO:HD2	2.19	0.42
1:A:350:LEU:HB3	1:A:353:GLU:HB2	2.01	0.42
1:C:291:LYS:HE3	1:C:291:LYS:HB3	1.83	0.42
1:F:275:TYR:CD2	1:F:302:PHE:HD2	2.38	0.42
1:G:41:VAL:HA	1:G:117:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:LYS:HB2	1:J:250:TYR:OH	2.20	0.42
1:L:240:MET:HE2	1:L:240:MET:HB2	1.93	0.42
1:C:324:LYS:HE2	1:C:324:LYS:HB3	1.82	0.42
1:E:170:GLU:OE2	1:E:221:ASN:ND2	2.52	0.42
1:B:301:PHE:CE2	1:B:344:VAL:HG11	2.55	0.42
1:D:402:ASN:HA	1:D:405:TYR:CZ	2.55	0.42
1:E:210:SER:O	1:E:222:ARG:NH2	2.53	0.42
1:F:18:ARG:HG3	1:F:19:ARG:N	2.34	0.42
1:I:109:LYS:HD3	1:I:145:ASN:HB3	2.02	0.42
1:E:157:MET:HE2	1:E:157:MET:HB3	1.96	0.42
1:J:356:ASP:OD1	1:J:390:GLN:NE2	2.52	0.42
1:A:211:PHE:CE2	1:A:229:MET:HE1	2.54	0.42
1:B:90:GLU:OE1	1:B:93:LYS:NZ	2.40	0.42
1:H:145:ASN:O	1:H:149:VAL:HB	2.20	0.42
1:J:73:GLU:OE1	1:J:98:ARG:NH1	2.49	0.42
1:L:69:LYS:HE2	1:L:69:LYS:HB2	1.88	0.42
1:B:290:ILE:O	1:B:297:PHE:HB2	2.20	0.42
1:F:44:TRP:HZ3	1:F:110:VAL:HG13	1.85	0.42
1:F:257:ASN:O	1:F:261:ILE:HG12	2.20	0.42
1:G:6:PHE:CE1	1:G:11:GLN:HG3	2.55	0.42
1:G:135:THR:OG1	1:G:138:MET:HG3	2.20	0.42
1:G:324:LYS:NZ	1:G:401:ASN:HA	2.35	0.42
1:J:386:TYR:HD1	1:J:390:GLN:HB3	1.85	0.42
1:L:46:VAL:HG12	1:L:151:LEU:HD11	2.01	0.42
1:C:197:GLU:H	1:C:197:GLU:CD	2.26	0.42
1:E:131:LEU:HD12	1:E:131:LEU:HA	1.92	0.42
1:F:162:LEU:O	1:F:165:PHE:HB3	2.20	0.42
1:C:247:GLU:OE1	1:C:249:ALA:N	2.53	0.41
1:L:44:TRP:NE1	1:L:88:GLU:OE1	2.50	0.41
1:D:334:ASN:OD1	1:D:334:ASN:N	2.53	0.41
1:F:159:GLN:H	1:F:159:GLN:HG3	1.69	0.41
1:F:247:GLU:OE1	1:F:249:ALA:N	2.52	0.41
1:G:269:SER:HB2	1:G:299:ILE:O	2.20	0.41
1:H:168:ASP:O	1:H:172:VAL:HG22	2.20	0.41
1:K:191:PHE:CZ	1:K:232:ILE:HG12	2.55	0.41
1:C:286:ILE:O	1:C:290:ILE:HG22	2.20	0.41
1:C:321:LYS:HD3	1:C:321:LYS:HA	1.78	0.41
1:H:162:LEU:HD21	1:H:205:GLY:HA3	2.02	0.41
1:H:203:PHE:C	1:H:203:PHE:CD1	2.99	0.41
1:J:392:LEU:HD23	1:J:392:LEU:HA	1.89	0.41
1:K:124:VAL:HG12	1:K:127:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:O	1:A:97:GLU:HG2	2.20	0.41
1:C:132:PHE:HZ	1:C:138:MET:HE1	1.84	0.41
1:C:326:TYR:HA	1:C:331:ASN:HD22	1.85	0.41
1:C:362:PHE:HZ	1:C:375:PHE:N	2.18	0.41
1:C:420:LEU:HA	1:C:420:LEU:HD23	1.84	0.41
1:F:134:PRO:HB3	1:F:138:MET:HE2	2.03	0.41
1:I:199:LEU:HD23	1:I:199:LEU:HA	1.90	0.41
1:J:16:TYR:CE1	1:J:192:LYS:HE2	2.56	0.41
1:A:27:VAL:HG11	1:A:43:LEU:HD13	2.02	0.41
1:B:244:VAL:HA	1:B:251:TYR:HE2	1.86	0.41
1:C:3:VAL:HG22	1:D:270:MET:HE1	2.01	0.41
1:I:8:LEU:HB3	1:I:28:TYR:CD2	2.55	0.41
1:J:290:ILE:HD12	1:J:303:ILE:HD13	2.02	0.41
1:J:402:ASN:ND2	1:J:405:TYR:OH	2.53	0.41
1:A:353:GLU:OE1	1:A:353:GLU:N	2.54	0.41
1:B:287:LYS:O	1:B:290:ILE:HG12	2.20	0.41
1:F:37:ARG:HH21	1:F:133:GLU:HB2	1.85	0.41
1:J:383:LEU:HA	1:J:386:TYR:CD2	2.56	0.41
1:K:194:LEU:HG	1:K:198:VAL:HG11	2.02	0.41
2:M:4:A:H2'	2:M:5:A:C8	2.56	0.41
1:B:173:LYS:H	1:B:173:LYS:HG2	1.69	0.41
1:C:301:PHE:N	1:C:301:PHE:HD1	2.19	0.41
1:D:157:MET:SD	1:D:198:VAL:HG21	2.61	0.41
1:D:215:GLU:N	1:D:215:GLU:OE1	2.54	0.41
1:I:261:ILE:HG23	1:I:286:ILE:HG12	2.01	0.41
1:J:391:MET:HG2	1:J:423:ALA:HA	2.02	0.41
1:L:109:LYS:HD3	1:L:145:ASN:HB3	2.03	0.41
1:A:334:ASN:OD1	1:A:334:ASN:N	2.54	0.41
1:D:236:ASP:O	1:D:240:MET:HG2	2.20	0.41
1:F:73:GLU:OE1	1:F:98:ARG:NH2	2.54	0.41
1:F:311:ILE:HG22	1:F:341:PHE:HE1	1.86	0.41
1:G:402:ASN:HA	1:G:405:TYR:CZ	2.56	0.41
1:L:41:VAL:HA	1:L:117:ARG:HD3	2.03	0.41
1:L:113:ILE:HG12	1:L:142:ASP:HB3	2.03	0.41
1:A:187:ASP:HA	1:A:191:PHE:HB2	2.01	0.41
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.86	0.41
1:B:244:VAL:HG21	1:B:274:ILE:HD12	2.03	0.41
1:B:287:LYS:O	1:B:291:LYS:HG2	2.20	0.41
1:B:307:PRO:O	1:B:311:ILE:HG13	2.21	0.41
1:C:232:ILE:HG22	1:C:240:MET:CE	2.49	0.41
1:C:247:GLU:CD	1:C:247:GLU:C	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:VAL:HA	1:D:175:LEU:HD13	2.02	0.41
1:D:195:ASN:N	1:D:195:ASN:OD1	2.51	0.41
1:D:379:ILE:HG23	1:D:383:LEU:HD13	2.02	0.41
1:E:226:ILE:HA	1:E:229:MET:HG2	2.03	0.41
1:F:57:GLU:HG2	1:F:155:PRO:HG3	2.03	0.41
1:G:106:SER:HB3	1:G:149:VAL:HG13	2.02	0.41
1:J:18:ARG:H	1:J:18:ARG:HG3	1.61	0.41
1:K:168:ASP:O	1:K:172:VAL:HG22	2.21	0.41
1:A:400:LYS:HB3	1:A:400:LYS:HE3	1.71	0.41
1:D:392:LEU:HG	1:D:427:LEU:HD21	2.03	0.41
1:A:402:ASN:HA	1:A:405:TYR:CE2	2.56	0.40
1:C:298:GLY:O	1:C:301:PHE:HE1	2.03	0.40
1:D:36:TYR:CD1	1:D:139:ILE:HG21	2.57	0.40
1:D:49:CYS:SG	1:J:131:LEU:HG	2.61	0.40
1:E:216:ALA:O	1:E:219:LEU:HG	2.21	0.40
1:G:211:PHE:CE2	1:G:229:MET:HE1	2.55	0.40
1:H:74:ILE:HG13	1:H:91:LEU:HB2	2.02	0.40
1:I:55:LEU:HD21	1:I:99:THR:HG21	2.03	0.40
1:A:88:GLU:O	1:A:92:ILE:HG12	2.20	0.40
1:A:90:GLU:OE1	1:A:94:ARG:NH1	2.52	0.40
1:A:298:GLY:HA2	1:A:314:VAL:HG21	2.03	0.40
1:B:202:ILE:HD13	1:B:202:ILE:HA	1.90	0.40
1:G:264:LEU:O	1:G:268:ILE:HG12	2.21	0.40
1:G:295:SER:OG	1:G:337:HIS:ND1	2.45	0.40
1:A:304:SER:HB2	1:A:310:HIS:HB2	2.03	0.40
1:B:23:TYR:OH	1:I:130:THR:OG1	2.27	0.40
1:B:210:SER:O	1:B:222:ARG:NH1	2.54	0.40
1:E:206:LEU:C	1:E:229:MET:HE1	2.47	0.40
1:J:204:LYS:HE3	1:J:204:LYS:HB2	1.88	0.40
1:L:12:LYS:HE2	1:L:21:ARG:HG2	2.02	0.40
2:M:7:A:H2'	2:M:8:A:C8	2.56	0.40
1:B:52:ILE:HD13	1:B:52:ILE:HA	1.87	0.40
1:B:406:TRP:CD1	1:B:411:ARG:HD3	2.57	0.40
1:C:300:ALA:O	1:C:303:ILE:HG22	2.22	0.40
1:F:235:LYS:HE3	1:F:235:LYS:HB3	1.90	0.40
1:J:173:LYS:HB3	1:J:173:LYS:HE2	1.87	0.40
1:A:41:VAL:HA	1:A:117:ARG:HG3	2.04	0.40
1:I:20:THR:HG21	1:I:50:ASP:OD2	2.22	0.40
1:J:3:VAL:HG23	1:J:4:ARG:HG3	2.04	0.40
1:J:236:ASP:O	1:J:240:MET:HG2	2.21	0.40
1:J:373:ILE:HD12	1:J:373:ILE:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:383:LEU:HA	1:J:386:TYR:CE2	2.56	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	443/465 (95%)	435 (98%)	8 (2%)	0	100	100
1	B	433/465 (93%)	419 (97%)	14 (3%)	0	100	100
1	C	442/465 (95%)	431 (98%)	11 (2%)	0	100	100
1	D	443/465 (95%)	432 (98%)	11 (2%)	0	100	100
1	E	244/465 (52%)	236 (97%)	8 (3%)	0	100	100
1	F	345/465 (74%)	336 (97%)	9 (3%)	0	100	100
1	G	443/465 (95%)	434 (98%)	9 (2%)	0	100	100
1	H	244/465 (52%)	237 (97%)	7 (3%)	0	100	100
1	I	319/465 (69%)	313 (98%)	6 (2%)	0	100	100
1	J	443/465 (95%)	434 (98%)	9 (2%)	0	100	100
1	K	244/465 (52%)	239 (98%)	5 (2%)	0	100	100
1	L	286/465 (62%)	279 (98%)	7 (2%)	0	100	100
All	All	4329/5580 (78%)	4225 (98%)	104 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/426 (89%)	378 (100%)	0	100	100
1	B	302/426 (71%)	300 (99%)	2 (1%)	76	80
1	C	359/426 (84%)	357 (99%)	2 (1%)	78	81
1	D	377/426 (88%)	375 (100%)	2 (0%)	81	83
1	E	195/426 (46%)	195 (100%)	0	100	100
1	F	276/426 (65%)	276 (100%)	0	100	100
1	G	378/426 (89%)	378 (100%)	0	100	100
1	H	193/426 (45%)	193 (100%)	0	100	100
1	I	264/426 (62%)	264 (100%)	0	100	100
1	J	373/426 (88%)	372 (100%)	1 (0%)	86	85
1	K	193/426 (45%)	193 (100%)	0	100	100
1	L	231/426 (54%)	231 (100%)	0	100	100
All	All	3519/5112 (69%)	3512 (100%)	7 (0%)	85	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	238	GLN
1	B	378	PHE
1	C	256	ASN
1	C	331	ASN
1	D	180	ASN
1	D	399	ASN
1	J	399	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	C	256	ASN
1	C	257	ASN
1	F	33	ASN
1	G	257	ASN

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Mol	Chain	Res	Type
1	G	364	ASN
1	I	136	GLN
1	I	221	ASN
1	I	257	ASN
1	J	276	ASN
1	J	293	ASN
1	J	399	ASN
1	K	62	HIS
1	L	63	ASN
1	L	225	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	M	6/7 (85%)	0	0
3	N	6/7 (85%)	0	0
All	All	12/14 (85%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

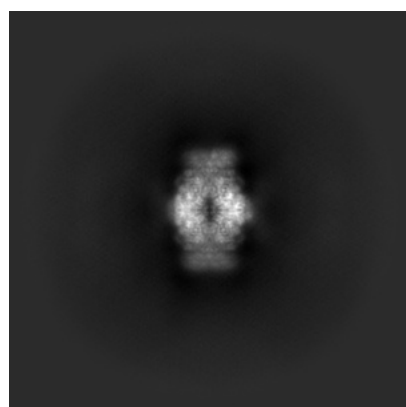
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56176. These allow visual inspection of the internal detail of the map and identification of artifacts.

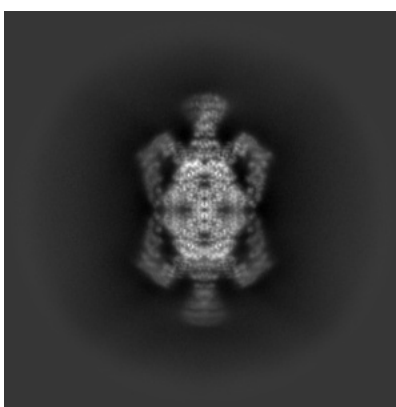
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

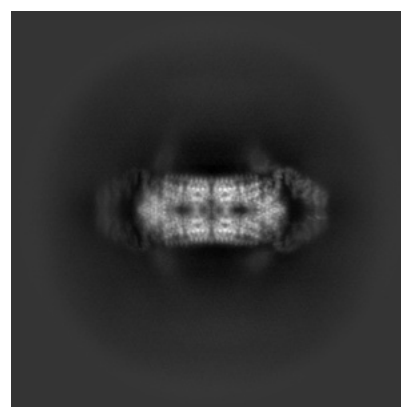
6.1.1 Primary map



X



Y

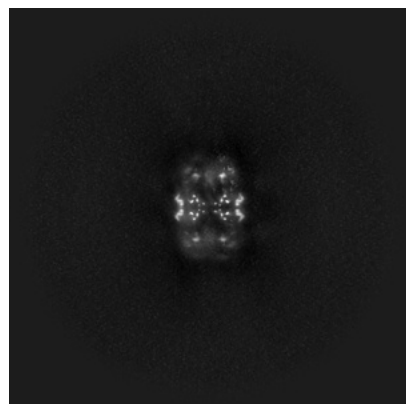


Z

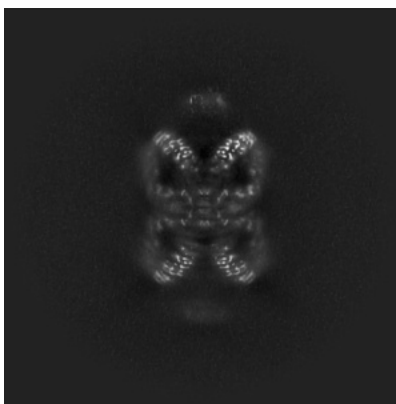
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

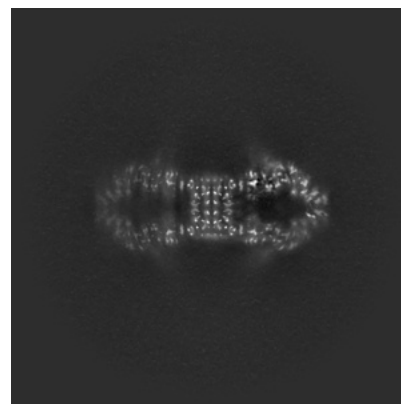
6.2.1 Primary map



X Index: 200



Y Index: 200

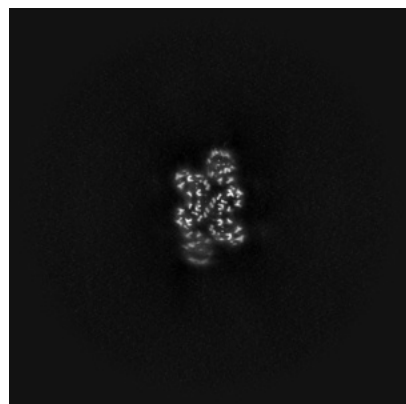


Z Index: 200

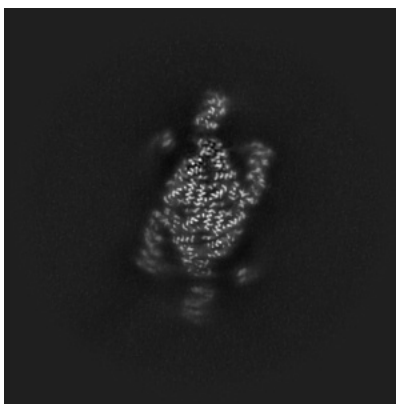
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

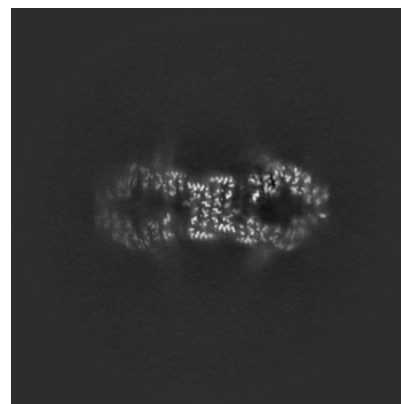
6.3.1 Primary map



X Index: 215



Y Index: 220

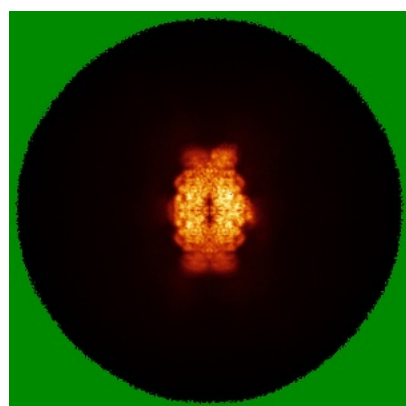


Z Index: 203

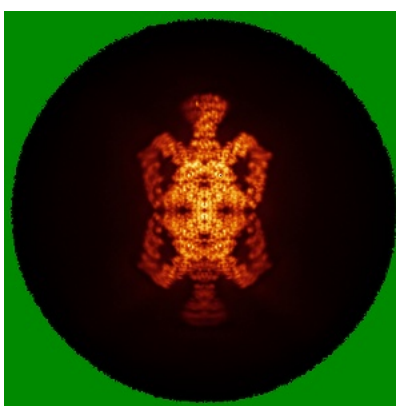
The images above show the largest variance slices of the map in three orthogonal directions.

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

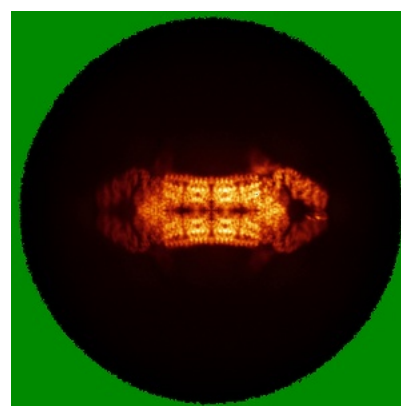
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

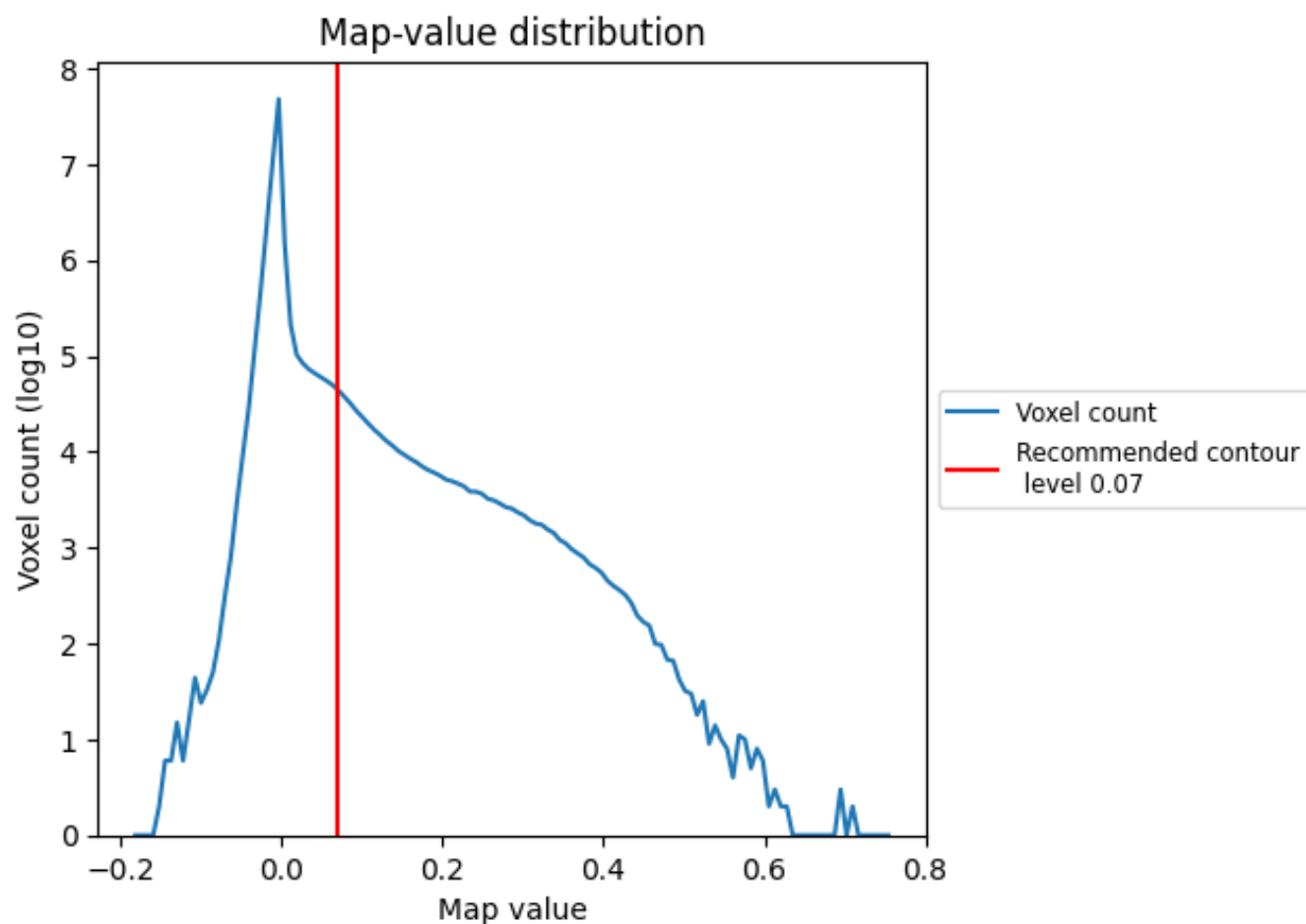
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

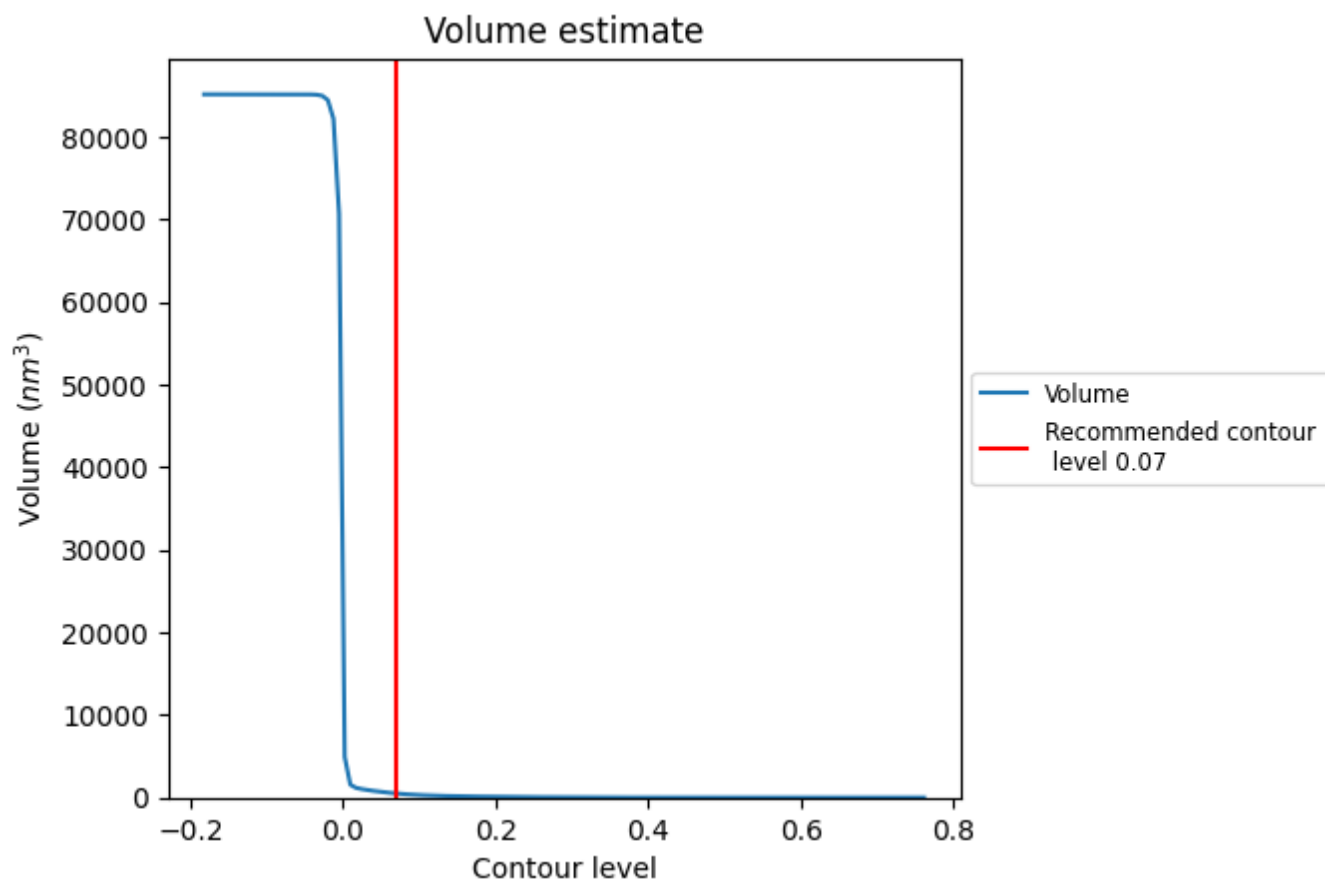
This section contains the results of statistical analysis of the map.

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.

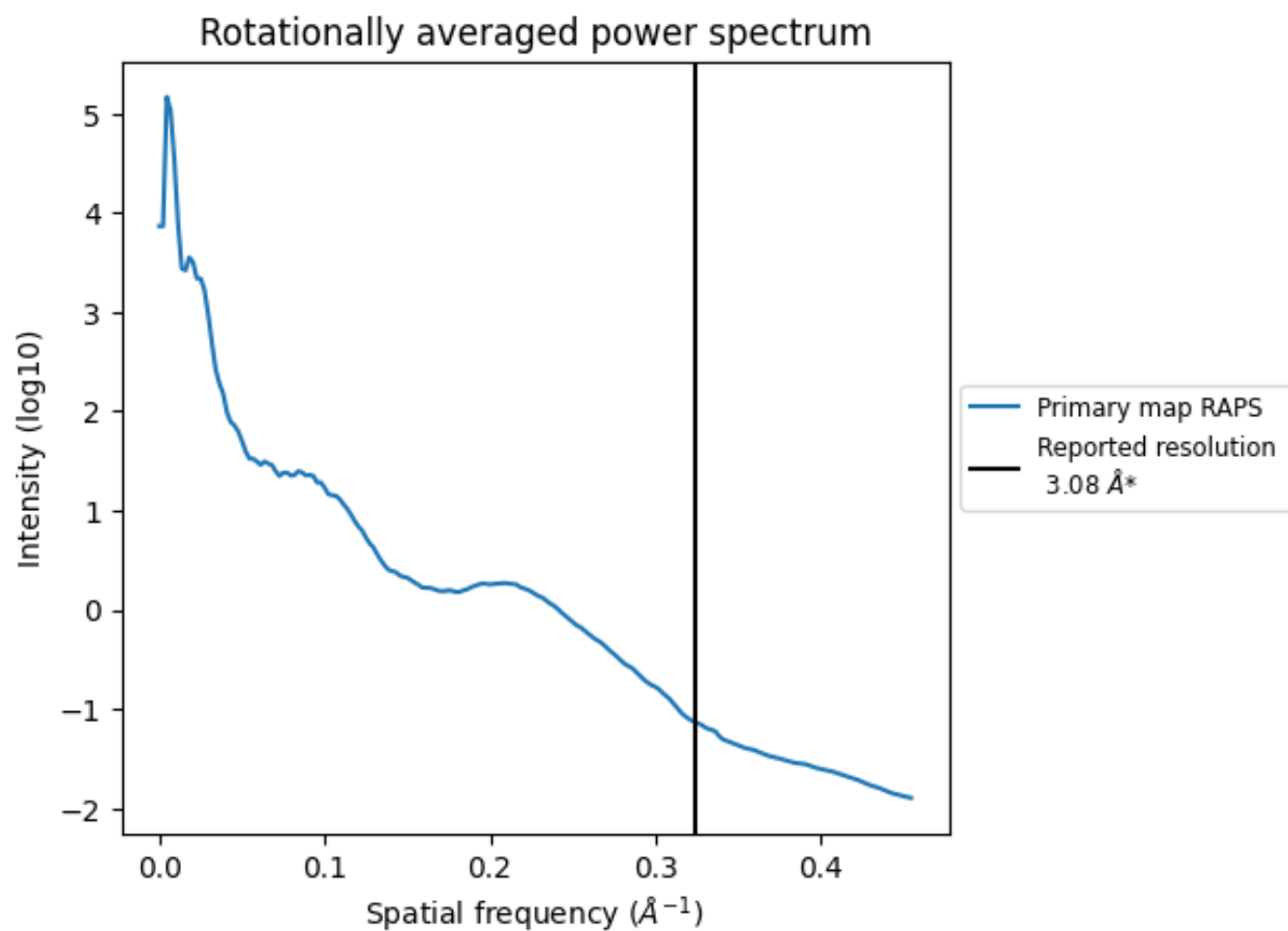
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 494 nm^3 ; this corresponds to an approximate mass of 446 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 0.325 $\text{\AA}^{-1}$

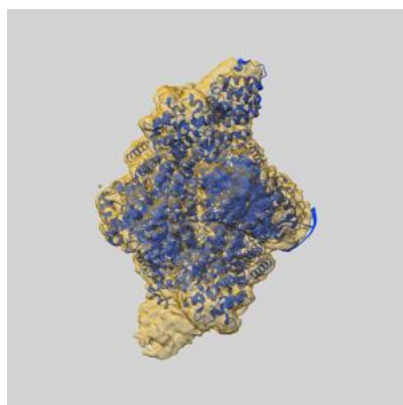
8 Fourier-Shell correlation

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

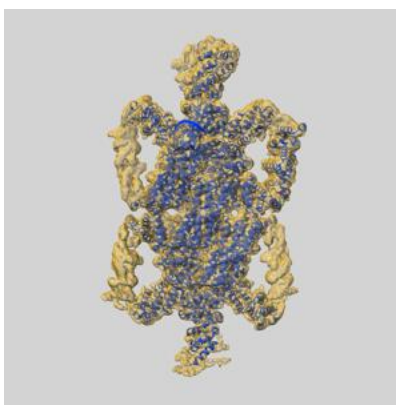
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56176 and PDB model 9TRE. Per-residue inclusion information can be found in section [3](#) on page [9](#).

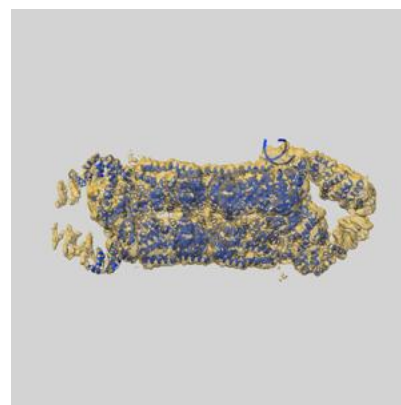
9.1 Map-model overlay [i](#)



X



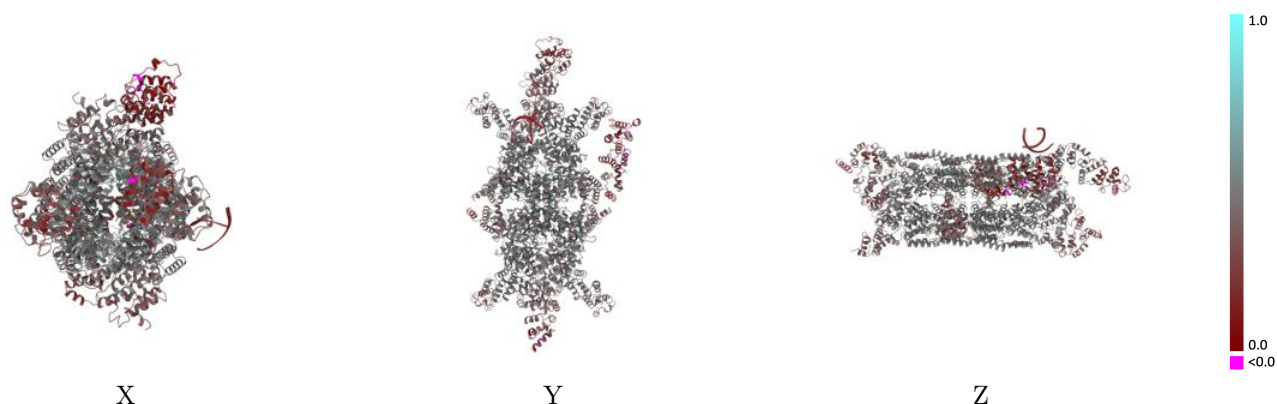
Y



Z

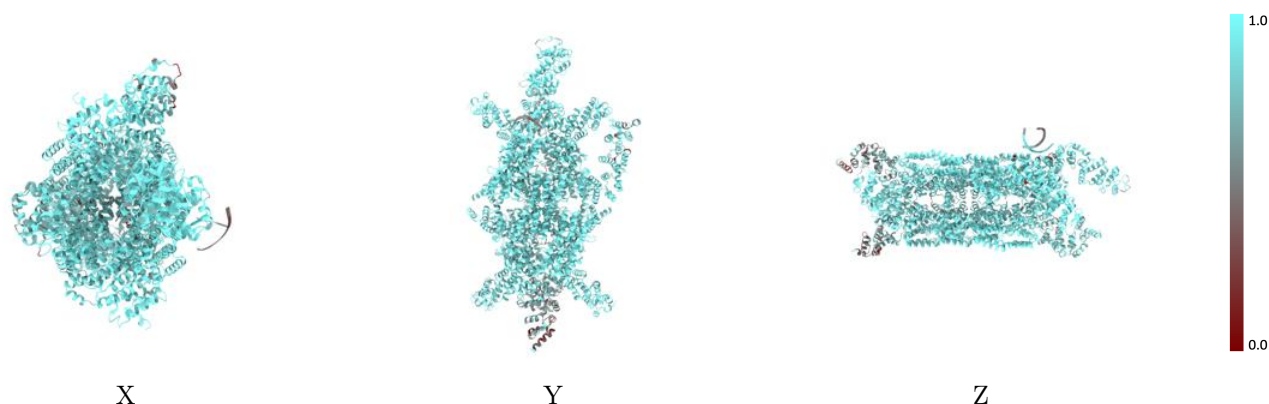
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



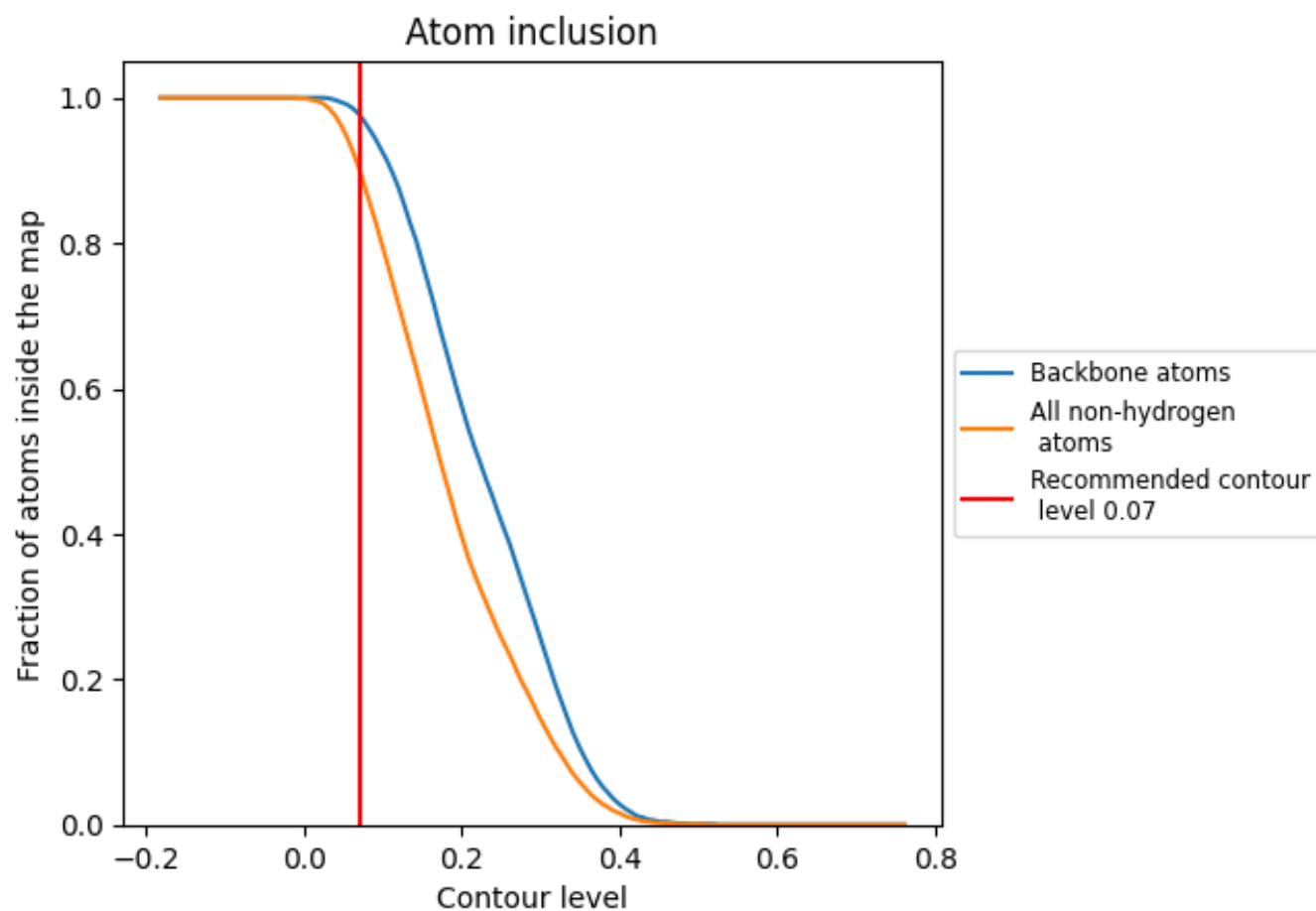
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 90% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.4250
A	 0.9380	 0.4710
B	 0.9350	 0.3450
C	 0.9420	 0.4010
D	 0.9290	 0.4560
E	 0.9410	 0.4280
F	 0.8680	 0.4130
G	 0.9150	 0.4530
H	 0.9210	 0.4390
I	 0.7640	 0.4070
J	 0.9180	 0.4520
K	 0.9330	 0.4290
L	 0.7900	 0.4230
M	 0.9200	 0.1800
N	 0.5140	 0.1210

