



Full wwPDB EM Validation Report ⓘ

Jan 1, 2025 – 10:53 AM EST

PDB ID : 8TVR
EMDB ID : EMD-41649
Title : In situ cryo-EM structure of bacteriophage P22 tail hub protein: tailspike protein complex at 2.8Å resolution
Authors : Iglesias, S.; Cingolani, G.; Feng-Hou, C.
Deposited on : 2023-08-18
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

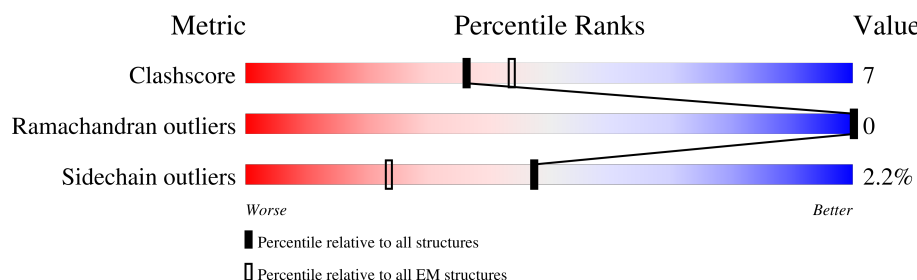
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY









The reported resolution of this entry is 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	667	
1	B	667	
1	C	667	
1	D	667	
1	E	667	
1	F	667	
1	H	667	
1	I	667	

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Mol	Chain	Length	Quality of chain
1	J	667	 15% 82%
1	L	667	 14% 82%
1	M	667	 13% 82%
1	N	667	 15% 82%
1	P	667	 15% 82%
1	Q	667	 15% 82%
1	R	667	 15% 82%
1	V	667	 15% 82%
1	W	667	 14% 82%
1	X	667	 14% 82%
2	G	472	 78% 21%
2	K	472	 74% 25%
2	O	472	 76% 23%
2	S	472	 77% 22%
2	T	472	 79% 21%
2	Y	472	 78% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38532 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 Tail spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	B	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	C	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	D	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	E	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	F	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	H	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	I	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	J	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	L	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	M	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	N	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	P	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	Q	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	R	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	V	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	W	118	Total 913	C 580	N 153	O 179	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	118	Total	C	N	O	S	0	0
			913	580	153	179	1		

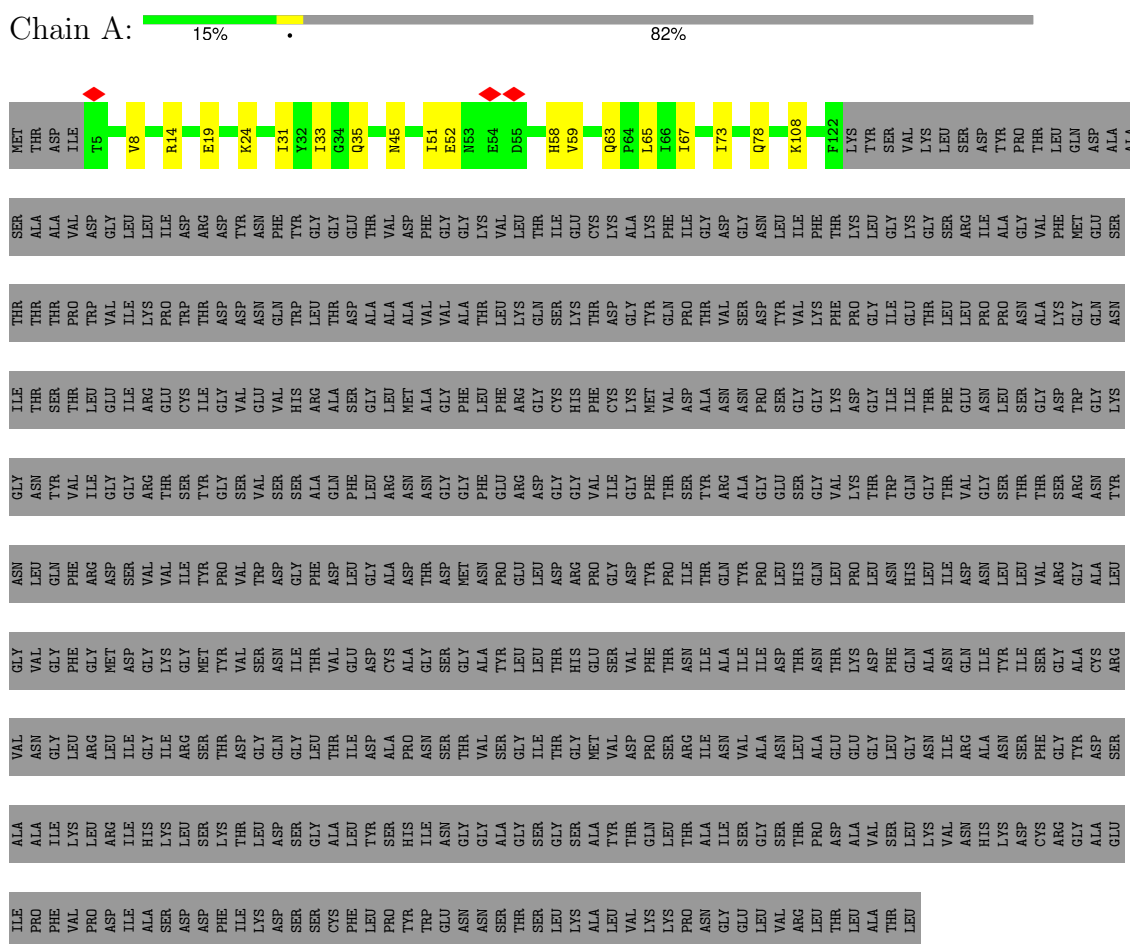
- Molecule 2 is a protein called Packaged DNA stabilization protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	G	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	K	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	O	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	T	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	Y	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		

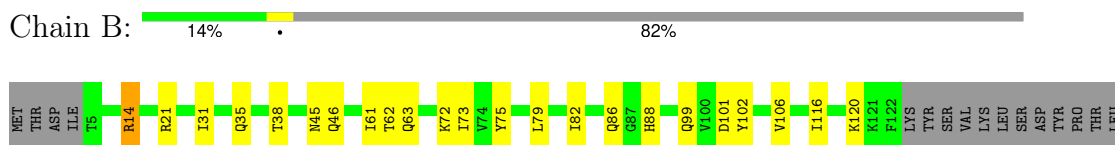
3 Residue-property plots

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: Tail spike protein



• Molecule 1: Tail spike protein



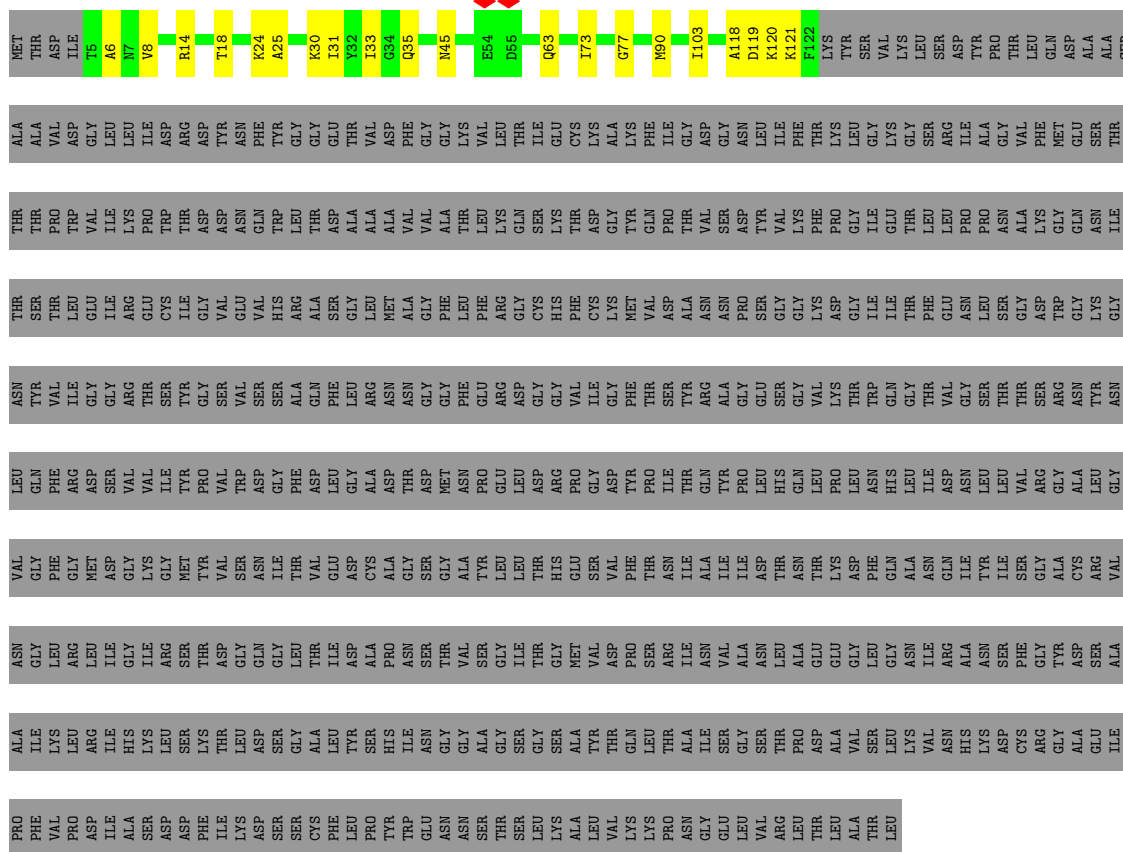
[illegible]

- Molecule 1: Tail spike protein

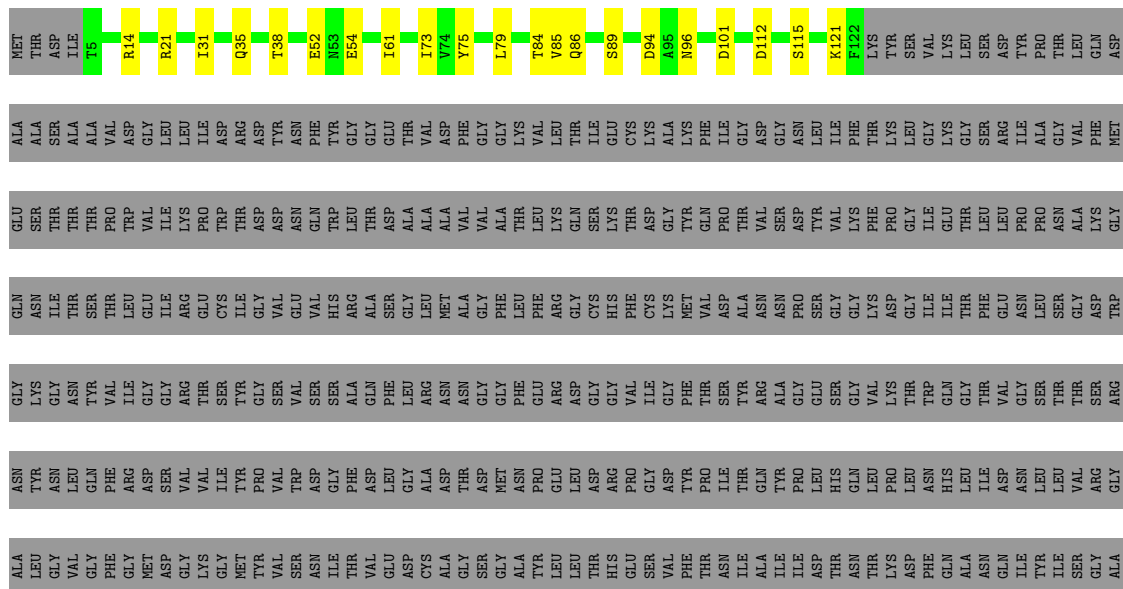
Chain C: 15% . 82%

[illegible]

Chain D: 15% 2% 82%



Chain E: 15% 82%



[illegible]

- Molecule 1: Tail spike protein

Chain F:  15% • 82%

[illegible]

- Molecule 1: Tail spike protein

Chain H:  15% . 82%

[illegible]



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

- Molecule 1: Tail spike protein

Chain M: 13% • 82%

[illegible]

- Molecule 1: Tail spike protein

Chain N: 15% . 82%

IIE	THR	SER
THR	THR	ALA
SER	PRO	ASP
THR	TRP	ILE
LEU	VAL	GLY
GLU	ILE	LEU
ILE	LYS	LEU
ARG	TRP	ILE
GLU	PRO	ASP
CYS	THR	PHE
ILE	ASP	ARG
GLY	THR	ASP
VAL	ASP	TTR
GLU	ASN	ASN
VAL	GLN	PHE
HIS	TRP	GLN
ARG	LEU	GLY
ALA	THR	GLY
SER	ASP	GLU
GLY	ALA	THR
LEU	ALA	VAL
MET	ALA	ASP
ALA	VAL	PHE
GLY	VAL	GLY
PHE	ALA	GLY
LEU	THR	LYS
PHE	LEU	VAL
ARG	LYS	LEU
GLY	GLN	THR
CYS	SER	ILE
HIS	LYS	GLU
PHE	THR	CYS
PHE	ASP	LYS
CYS	ASP	LYS
LYS	GLY	ALA
MET	TYR	LYS
VAL	GLN	PHE
ASP	PRO	ILE
ALA	THR	GLY
ASN	VAL	ASP
ASN	SER	GLY
PRO	ASP	ASN
SER	TYR	LEU
GLY	VAL	ILE
GLY	LYS	PHE
LYS	PHE	THR
ASP	PRO	LYS
GLY	GLY	LEU
ILE	ILE	GLY
ILE	GLU	LYS
THR	THR	GLY
PHE	LEU	SER
GLU	LEU	ARG
ASN	PRO	ILE
LEU	PRO	ALA
SER	ASN	GLY
GLY	LYS	PHE
ASP	THR	MET
TRP	GLY	ASP
GLY	GLN	GLU
VNS	ASN	SER

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

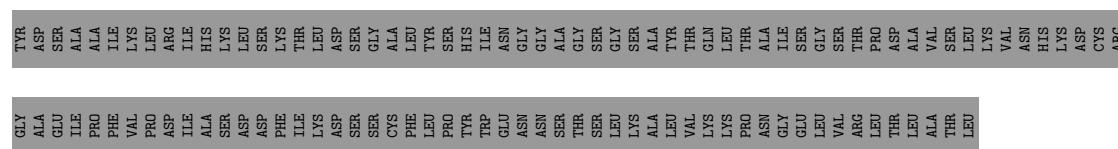
- Molecule 1: Tail spike protein

Chain P:  15% • 82%

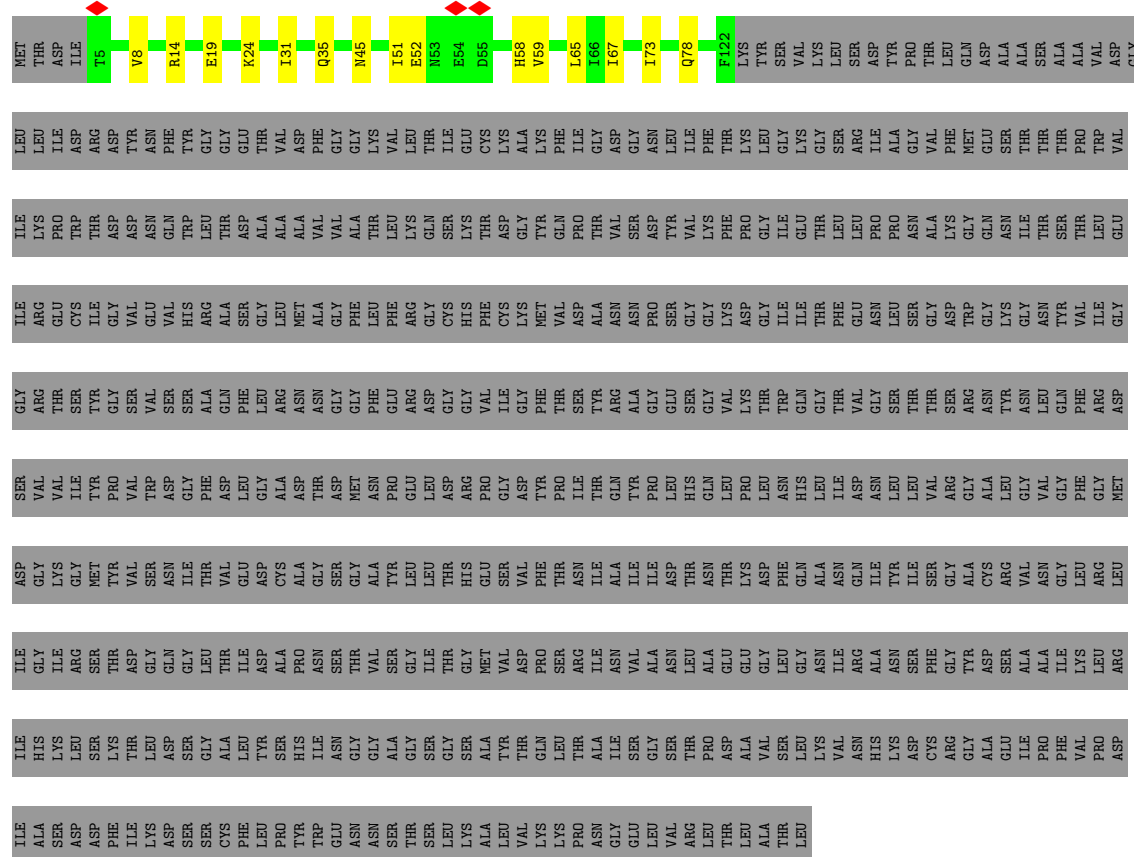
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ILE	ILE	ILE	ILE	ILE	ILE	ILE	MET	ASP	SER	GLY	GLY	VAL	GLY	THR
ALA	ALA	HIS	GLY	VAL	GLY	VAL	GLY	VAL	VAL	ARG	ARG	PRO	LEU	ASP
SER	SER	LYS	ILE	VAL	LYS	VAL	GLY	VAL	VAL	THR	SER	TRP	ASP	T5
ASP	ASP	LEU	SER	ARG	GLY	ILE	MET	ILE	ILE	SER	SER	THR	ARG	A6
PHE	PHE	LYS	SER	THR	THR	THR	THR	PRO	PRO	TYR	GLY	ASP	ARG	H7
ILE	ILE	THR	LEU	ASP	VAL	VAL	VAL	TRP	TRP	SER	VAL	ASP	ASP	V8
LYS	LYS	LEU	LEU	GLY	SER	GLN	ASN	ASP	GLY	SER	VAL	ASN	ASN	R14
ASP	ASP	ASP	SER	GLY	GLY	ILE	ILE	GLY	PHE	SER	VAL	GLN	PHE	E19
SER	SER	GLY	LEU	LEU	THR	THR	THR	PHE	ALA	ALA	ARG	LEU	GLY	K24
CYS	CYS	ALA	THR	THR	THR	THR	VAL	LEU	PHE	GLN	ALA	THR	GLY	A25
PHE	PHE	LEU	ILE	ILE	ILE	ILE	GLU	LEU	ASP	GLY	GLY	ALA	THR	
PRO	PRO	TYR	SER	SER	ALA	SER	CYS	ALA	ARG	ARG	LEU	ALA	VAL	K30
LEU	LEU	HIS	SER	PRO	ASN	ASN	GLY	ALA	ASP	ASN	MET	ALA	ASP	I31
TYR	TYR	ILE	ASN	ASN	ASN	THR	GLY	THR	THR	ASN	ALA	VAL	PHE	
TRP	TRP	ASN	GLY	THR	SER	SER	SER	ASP	ASP	GLY	GLY	VAL	GLY	Q35
GLU	GLU	GLY	THR	VAL	GLY	VAL	GLY	MET	PHE	PHE	PHE	ALA	GLY	
ASN	ASN	GLY	VAL	VAL	ALA	ASN	ALA	ASN	ASN	GLY	THR	LYS	LYS	N45
SER	SER	ALA	SER	ALA	THR	LEU	LYR	PRO	GLU	GLU	PHE	LEU	VAL	
THR	THR	GLY	GLY	GLY	ILE	ILE	LEU	LEU	GLU	ARG	LEU	LYS	LEU	E54
SER	SER	SER	SER	ILE	THR	THR	LEU	ASP	ASP	GLY	GLN	THR	THR	D55
LEU	LEU	GLY	GLY	GLY	GLY	GLY	THR	ASP	GLY	GLY	SER	ILE	ILE	
LYS	LYS	ALA	ALA	MET	GLU	GLU	THR	PRO	VAL	PHE	THR	THR	CYS	I73
ALA	ALA	ALA	VAL	VAL	VAL	VAL	SER	GLY	GLY	GLY	ASP	LYS	LYS	
VAL	VAL	THR	ASP	ASP	THR	THR	VAL	ASP	ASP	THR	GLY	GLY	ALA	G77
LYS	LYS	GLN	THR	PRO	PRO	PRO	PHE	THR	THR	PHE	TYR	TYR	LYS	G78
LYS	LYS	LEU	LEU	SER	SER	SER	THR	ASN	ASN	ILE	ASN	PRO	PHE	M90
PRO	PRO	THR	ALA	ALA	ILE	ILE	ILE	THR	THR	THR	ALA	THR	GLY	
ASN	ASN	ALA	ILE	ASN	ALA	ALA	ILE	THR	ARG	ASN	ASN	VAL	ASP	I103
GLY	GLY	ILE	SER	VAL	VAL	VAL	ILE	TYR	ALA	ALA	ASN	SER	GLY	
GLU	GLU	GLY	GLY	ALA	ALA	ALA	ILE	PRO	GLY	ALA	PRO	ASP	ASN	A118
LEU	LEU	SER	ASN	VAL	ASN	ASN	ILE	LEU	GLU	GLU	PRO	ASP	ASN	D119
VAL	VAL	SER	LEU	ASN	LEU	LEU	THR	LEU	SER	SER	TYR	LEU	LEU	K120
ARG	ARG	THR	THR	HIS	THR	HIS	THR	HIS	SER	SER	GLY	VAL	ILE	K121
LEU	LEU	PRO	ALA	ASN	PRO	ASN	ASN	ASN	GLN	GLY	LYS	PHE	PHE	F122
THR	THR	ASP	GLU	THR	THR	THR	THR	LEU	VAL	VAL	GLY	PHE	THR	
LEU	LEU	ALA	GLU	GLY	GLY	GLY	LYS	PRO	LYS	LYS	ASP	PRO	LYS	LYS
ALA	ALA	VAL	GLY	GLY	GLY	GLY	LEU	LEU	THR	THR	GLY	GLY	LEU	THR
THR	THR	SER	SER	PHE	PHE	PHE	ASN	ASN	ASN	THR	ILE	ILE	GLY	SER
LEU	LEU	LYS	LYS	ASN	ASN	ASN	ALA	HIS	GLN	GLN	ILE	GLY	LYS	VAL
THR	THR	VAL	VAL	ILE	ILE	ILE	ILE	ILE	THR	THR	PHE	LEU	SER	LEU
ASN	ASN	ASN	ASN	ARG	ARG	ARG	GLN	ASP	VAL	VAL	LEU	ARG	ASP	SER
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ILE	ASN	GLY	GLY	GLU	ILE	ILE	THR
LYS	LYS	LYS	ASN	ASN	ASN	ASN	TYR	LEU	LEU	THR	PRO	ILE	ILE	TVR
ASP	ASP	ASP	SER	PHE	SER	SER	ILE	LEU	THR	THR	ASN	GLY	GLY	PRO
CYS	CYS	ARG	GLY	GLY	GLY	GLY	GLY	ARG	ARG	SER	LYS	ALA	PHE	THR
GLY	GLY	TYR	TYR	TYR	ALA	ALA	ALA	GLY	ARG	ARG	GLY	GLY	MET	GLN
ALA	ALA	ASP	ASP	ASP	CYS	CYS	CYS	ALA	ALA	ALA	GLY	GLN	GLU	ASP
GLU	GLU	GLU	GLU	GLU	ARG	ARG	ARG	LEU	LEU	TYR	GLY	GLN	GLU	GLY
SER	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
ALA	ALA	ILE	ALA	ALA	ALA	ALA	VAL	GLY	GLY	ASN	ILE	ILE	THR	ALA
THR	THR	PHE	ILE	ALA	ALA	ALA	ASN	VAL	VAL	ASN	GLY	LYS	PHE	ALA
VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
THR	THR	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
PRO	PRO	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA

- Molecule 1: Tail spike protein

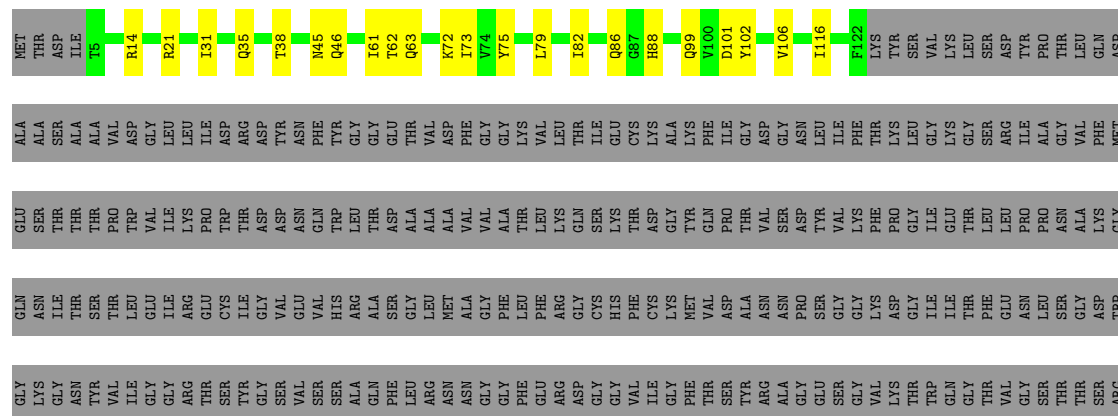
Chain Q: 15% . 82%



- Molecule 1: Tail spike protein



- Molecule 1: Tail spike protein



[illegible]

- Molecule 1: Tail spike protein

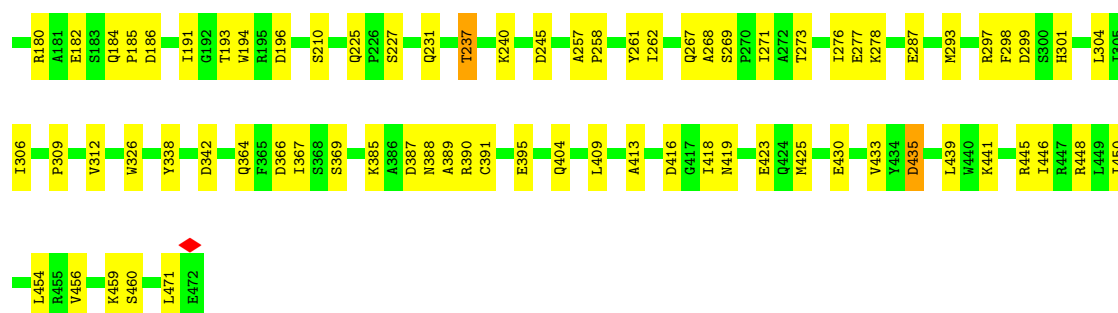
Chain X:  14% 2% 82%

[illegible]

- Molecule 2: Packaged DNA stabilization protein gp10

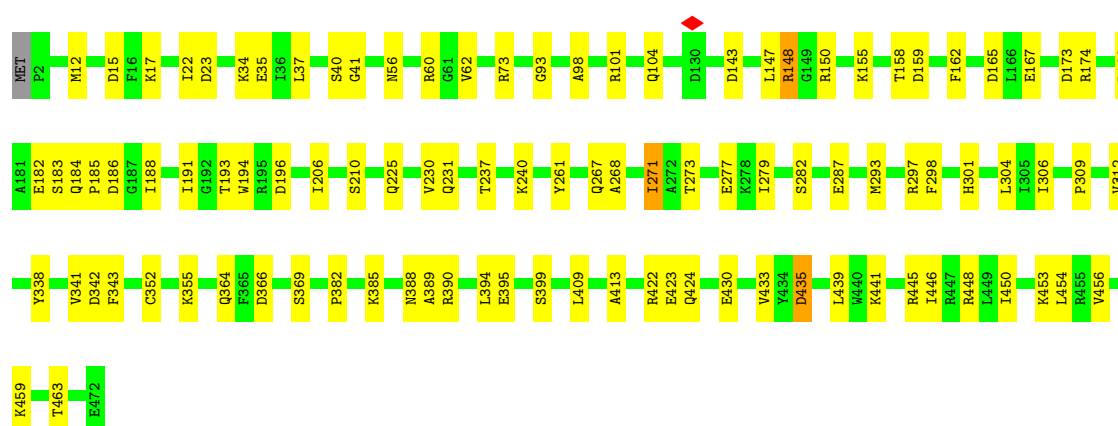
Chain S:  77% 22%

MET	P2	F16	K17	D20	D23	Y24	L25	K34	E35	I36	L37	S40	G41	D54	R60	E63	A67	R73	G93	H99	G100	R101	R116	Y117	D118	V141	R142	D143	L147	R148	G149	R150	W153	S154	K155	T158	D159	D165	D173	P174
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



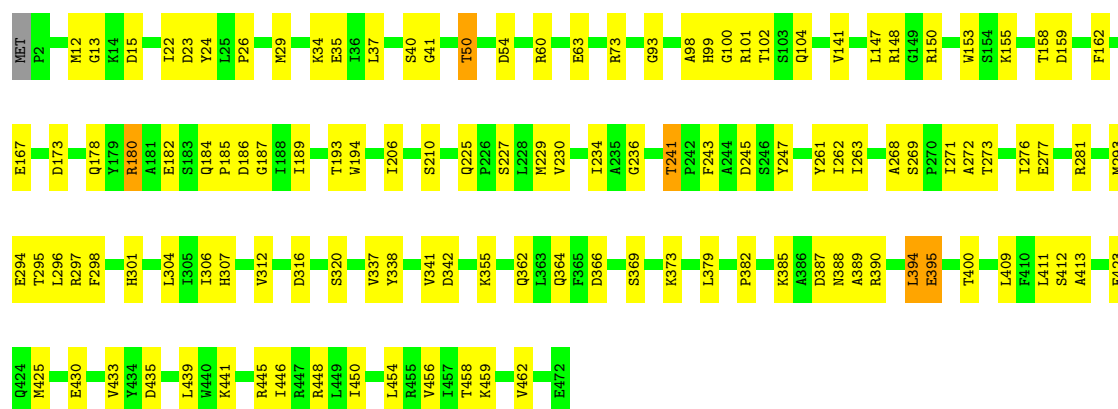
- Molecule 2: Packaged DNA stabilization protein gp10

Chain G: 78% 21% .



- Molecule 2: Packaged DNA stabilization protein gp10

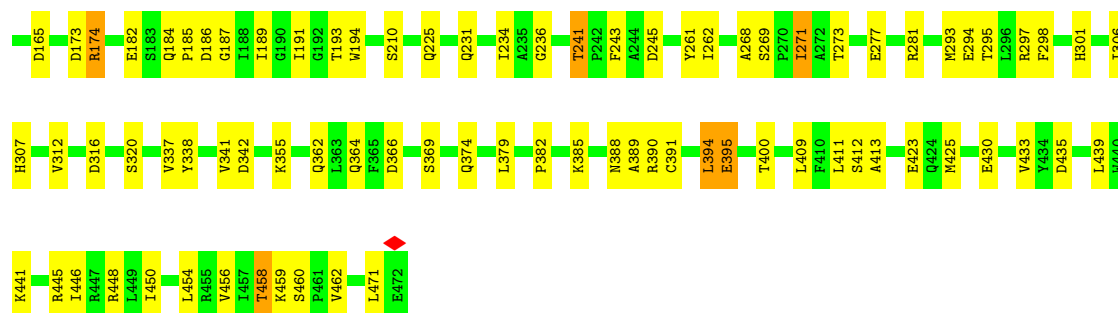
Chain K: 74% 25% .



- Molecule 2: Packaged DNA stabilization protein gp10

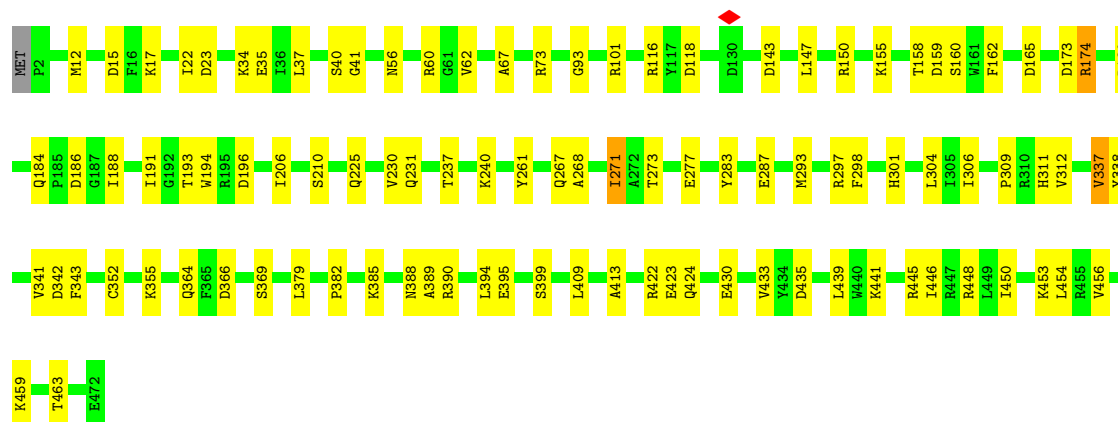
Chain O: 76% 23% .





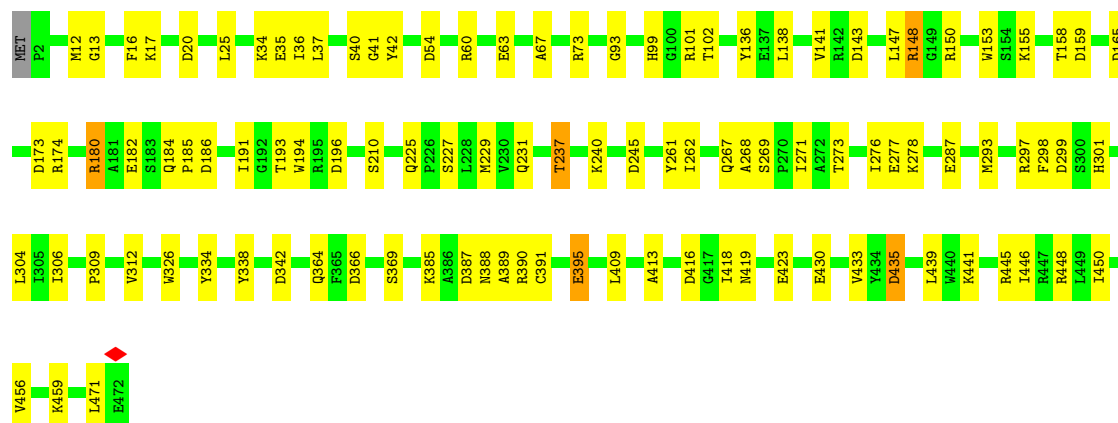
- Molecule 2: Packaged DNA stabilization protein gp10

Chain T: 79% 21%



- Molecule 2: Packaged DNA stabilization protein gp10

Chain Y: 78% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	38155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.08	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	35.452	Depositor
Minimum map value	-27.985	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	512.9599, 512.9599, 512.9599	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.165818, 1.165818, 1.165818	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	0.25	0/931	0.45	0/1270
1	B	0.27	0/931	0.46	0/1270
1	C	0.27	0/931	0.48	0/1270
1	D	0.26	0/931	0.46	0/1270
1	E	0.27	0/931	0.45	0/1270
1	F	0.26	0/931	0.48	0/1270
1	H	0.25	0/931	0.45	0/1270
1	I	0.27	0/931	0.45	0/1270
1	J	0.26	0/931	0.47	0/1270
1	L	0.25	0/931	0.45	0/1270
1	M	0.27	0/931	0.45	0/1270
1	N	0.26	0/931	0.47	0/1270
1	P	0.26	0/931	0.46	0/1270
1	Q	0.27	0/931	0.45	0/1270
1	R	0.26	0/931	0.48	0/1270
1	V	0.25	0/931	0.46	0/1270
1	W	0.27	0/931	0.45	0/1270
1	X	0.26	0/931	0.48	0/1270
2	G	0.26	0/3764	0.53	0/5097
2	K	0.26	0/3764	0.53	0/5097
2	O	0.25	0/3764	0.53	0/5097
2	S	0.26	0/3764	0.53	0/5097
2	T	0.25	0/3764	0.53	0/5097
2	Y	0.26	0/3764	0.53	0/5097
All	All	0.26	0/39342	0.50	0/53442

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 ⓘ

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	913	0	903	12	0
1	B	913	0	903	17	0
1	C	913	0	903	10	0
1	D	913	0	903	12	0
1	E	913	0	903	15	0
1	F	913	0	903	10	0
1	H	913	0	903	18	0
1	I	913	0	903	22	0
1	J	913	0	903	11	0
1	L	913	0	903	18	0
1	M	913	0	903	19	0
1	N	913	0	903	11	0
1	P	913	0	903	12	0
1	Q	913	0	903	13	0
1	R	913	0	903	11	0
1	V	913	0	903	10	0
1	W	913	0	903	15	0
1	X	913	0	903	10	0
2	G	3683	0	3590	66	0
2	K	3683	0	3590	80	0
2	O	3683	0	3590	75	0
2	S	3683	0	3590	68	0
2	T	3683	0	3590	63	0
2	Y	3683	0	3590	66	0
All	All	38532	0	37794	571	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 7.

All (571) 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)
2:G:395:GLU:HG2	2:G:439:LEU:HD13	1.67	0.76
2:T:395:GLU:HG2	2:T:439:LEU:HD13	1.67	0.76
2:S:409:LEU:HD12	2:S:456:VAL:HG22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:262:ILE:HD12	2:S:271:ILE:HG13	1.68	0.76
2:K:395:GLU:HG2	2:K:439:LEU:HD13	1.68	0.75
2:O:395:GLU:HG2	2:O:439:LEU:HD13	1.68	0.75
2:O:73:ARG:NH2	2:O:342:ASP:O	2.20	0.75
2:K:73:ARG:NH2	2:K:342:ASP:O	2.20	0.75
1:W:31:ILE:HD12	1:W:73:ILE:HD11	1.69	0.75
2:K:158:THR:O	2:K:180:ARG:NH2	2.20	0.74
2:O:385:LYS:HB2	2:Y:37:LEU:HD13	1.69	0.73
2:Y:395:GLU:HG2	2:Y:439:LEU:HD13	1.71	0.73
1:B:31:ILE:HD12	1:B:73:ILE:HD11	1.69	0.73
2:Y:262:ILE:HD12	2:Y:271:ILE:HG13	1.70	0.72
2:S:298:PHE:O	2:S:301:HIS:HB2	1.89	0.72
2:G:422:ARG:NH2	2:G:424:GLN:OE1	2.23	0.72
2:T:422:ARG:NH2	2:T:424:GLN:OE1	2.23	0.72
2:S:165:ASP:OD2	2:S:174:ARG:NH1	2.23	0.72
2:O:165:ASP:OD2	2:O:174:ARG:NH1	2.24	0.71
2:Y:298:PHE:O	2:Y:301:HIS:HB2	1.89	0.71
2:O:409:LEU:HD12	2:O:456:VAL:HG22	1.71	0.71
2:O:231:GLN:NE2	2:Y:194:TRP:O	2.24	0.70
2:O:194:TRP:O	2:T:231:GLN:NE2	2.24	0.70
2:O:37:LEU:HD13	2:T:385:LYS:HB2	1.74	0.70
2:G:165:ASP:OD2	2:G:174:ARG:NH1	2.26	0.69
1:I:116:ILE:HD12	1:I:116:ILE:H	1.57	0.69
2:Y:165:ASP:OD2	2:Y:174:ARG:NH1	2.24	0.69
2:G:231:GLN:NE2	2:K:194:TRP:O	2.24	0.69
2:G:385:LYS:HB2	2:K:37:LEU:HD13	1.73	0.69
2:S:73:ARG:NH2	2:S:342:ASP:O	2.26	0.69
2:Y:73:ARG:NH2	2:Y:342:ASP:O	2.26	0.68
2:K:409:LEU:HD12	2:K:456:VAL:HG22	1.75	0.68
2:T:159:ASP:OD1	2:T:184:GLN:NE2	2.26	0.68
2:O:98:ALA:O	2:O:104:GLN:NE2	2.26	0.67
2:K:98:ALA:O	2:K:104:GLN:NE2	2.27	0.67
2:Y:439:LEU:HD21	2:Y:441:LYS:HE2	1.74	0.67
1:H:31:ILE:HG13	1:H:67:ILE:HD11	1.76	0.67
2:K:298:PHE:O	2:K:301:HIS:HB2	1.95	0.67
1:L:31:ILE:HG13	1:L:67:ILE:HD11	1.77	0.67
2:S:186:ASP:OD1	2:T:101:ARG:NH1	2.28	0.66
1:J:18:THR:HA	1:J:25:ALA:HA	1.77	0.66
2:S:159:ASP:OD1	2:S:184:GLN:NE2	2.28	0.66
1:E:31:ILE:HD12	1:E:73:ILE:HD11	1.77	0.66
1:Q:31:ILE:HD12	1:Q:73:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:231:GLN:NE2	2:T:194:TRP:O	2.29	0.66
1:N:18:THR:HA	1:N:25:ALA:HA	1.76	0.66
2:G:150:ARG:NH2	2:G:173:ASP:OD1	2.29	0.65
2:G:194:TRP:O	2:Y:231:GLN:NE2	2.29	0.65
2:G:297:ARG:NH2	2:Y:277:GLU:OE1	2.25	0.65
2:G:186:ASP:OD2	2:K:101:ARG:NH1	2.30	0.65
2:G:159:ASP:OD1	2:G:184:GLN:NE2	2.29	0.65
2:O:389:ALA:HB3	2:O:446:ILE:HD12	1.78	0.65
1:W:14:ARG:HB3	1:W:72:LYS:HD3	1.78	0.65
2:S:101:ARG:NH1	2:K:186:ASP:OD1	2.30	0.65
1:H:28:ASN:HA	1:H:67:ILE:O	1.97	0.65
2:O:298:PHE:O	2:O:301:HIS:HB2	1.95	0.65
2:Y:388:ASN:OD1	2:Y:445:ARG:NH2	2.30	0.65
2:K:159:ASP:OD1	2:K:184:GLN:NE2	2.29	0.64
2:O:159:ASP:OD1	2:O:184:GLN:NE2	2.30	0.64
2:G:23:ASP:OD1	2:K:34:LYS:NZ	2.29	0.64
2:O:34:LYS:NZ	2:T:23:ASP:OD1	2.29	0.64
1:L:28:ASN:HA	1:L:67:ILE:O	1.97	0.64
2:O:458:THR:HG22	2:O:460:SER:H	1.61	0.64
2:O:101:ARG:NH1	2:T:186:ASP:OD2	2.30	0.64
2:S:150:ARG:NH2	2:S:173:ASP:OD1	2.30	0.64
1:B:14:ARG:HB3	1:B:72:LYS:HD3	1.80	0.63
2:Y:150:ARG:NH2	2:Y:173:ASP:OD1	2.30	0.63
2:S:388:ASN:OD1	2:S:445:ARG:NH2	2.30	0.63
2:S:299:ASP:OD1	2:K:281:ARG:NH1	2.32	0.63
2:G:73:ARG:NH2	2:G:342:ASP:O	2.29	0.63
1:J:52:GLU:OE2	1:J:58:HIS:NE2	2.32	0.63
2:K:409:LEU:HD11	2:K:454:LEU:HG	1.79	0.63
2:T:409:LEU:HD12	2:T:456:VAL:HG22	1.81	0.63
2:O:281:ARG:NH1	2:Y:299:ASP:OD1	2.32	0.63
2:Y:20:ASP:OD2	2:Y:278:LYS:NZ	2.32	0.63
1:H:31:ILE:HD12	1:H:73:ILE:HD11	1.80	0.62
2:T:150:ARG:NH2	2:T:173:ASP:OD1	2.31	0.62
1:L:31:ILE:HD12	1:L:73:ILE:HD11	1.80	0.62
1:D:33:ILE:O	1:D:63:GLN:NE2	2.32	0.62
1:P:8:VAL:HG11	1:Q:86:GLN:HA	1.81	0.62
2:T:165:ASP:OD2	2:T:174:ARG:NH1	2.33	0.62
2:G:101:ARG:NH1	2:Y:186:ASP:OD1	2.31	0.62
2:S:20:ASP:OD2	2:S:278:LYS:NZ	2.32	0.62
2:S:37:LEU:HD13	2:K:385:LYS:HB2	1.81	0.62
1:D:8:VAL:HG11	1:E:86:GLN:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:277:GLU:OE1	2:T:297:ARG:NH2	2.25	0.62
2:O:186:ASP:OD1	2:Y:101:ARG:NH1	2.31	0.61
2:G:409:LEU:HD12	2:G:456:VAL:HG22	1.82	0.61
2:O:150:ARG:NH2	2:O:173:ASP:OD1	2.34	0.61
1:V:19:GLU:HG3	1:V:24:LYS:HG3	1.82	0.61
1:F:18:THR:HA	1:F:25:ALA:HA	1.83	0.61
1:N:52:GLU:OE1	1:N:58:HIS:NE2	2.33	0.61
2:S:395:GLU:HB2	2:S:439:LEU:HD13	1.83	0.61
2:G:293:MET:HE3	2:G:304:LEU:HD11	1.82	0.61
2:G:155:LYS:HE2	2:G:158:THR:HG21	1.81	0.61
2:G:180:ARG:NH2	2:G:182:GLU:OE2	2.33	0.61
2:O:241:THR:HG21	2:O:294:GLU:HA	1.82	0.61
1:H:19:GLU:HG3	1:H:24:LYS:HG3	1.82	0.61
1:A:8:VAL:HG11	1:B:86:GLN:HA	1.83	0.61
1:H:8:VAL:HG11	1:I:86:GLN:HA	1.82	0.60
2:T:293:MET:HE3	2:T:304:LEU:HD11	1.82	0.60
1:V:8:VAL:HG11	1:W:86:GLN:HA	1.82	0.60
2:Y:364:GLN:NE2	2:Y:366:ASP:OD1	2.31	0.60
1:L:8:VAL:HG11	1:M:86:GLN:HA	1.82	0.60
2:T:160:SER:OG	2:T:180:ARG:NH1	2.34	0.60
2:O:23:ASP:OD1	2:Y:34:LYS:NZ	2.35	0.59
2:T:155:LYS:HE2	2:T:158:THR:HG21	1.84	0.59
2:T:389:ALA:HB3	2:T:446:ILE:HD12	1.85	0.59
2:K:241:THR:HG21	2:K:294:GLU:HA	1.83	0.59
1:M:31:ILE:HD12	1:M:73:ILE:HD11	1.84	0.59
1:I:14:ARG:HG2	1:I:79:LEU:HD13	1.84	0.59
1:I:31:ILE:HD12	1:I:73:ILE:HD11	1.84	0.59
1:M:14:ARG:HG2	1:M:79:LEU:HD13	1.85	0.59
2:K:29:MET:HE1	2:K:462:VAL:HB	1.85	0.59
2:G:364:GLN:NE2	2:G:366:ASP:OD1	2.31	0.59
1:Q:54:GLU:OE1	2:T:453:LYS:NZ	2.26	0.59
1:E:112:ASP:OD2	1:E:115:SER:OG	2.20	0.59
2:O:293:MET:HG2	2:O:306:ILE:HG12	1.84	0.59
1:A:19:GLU:HG3	1:A:24:LYS:HG3	1.84	0.59
2:O:435:ASP:OD1	2:T:448:ARG:NH2	2.28	0.58
2:Y:159:ASP:OD1	2:Y:184:GLN:NE2	2.35	0.58
2:Y:389:ALA:HB3	2:Y:446:ILE:HD12	1.85	0.58
2:K:150:ARG:NH2	2:K:173:ASP:OD1	2.35	0.58
1:N:49:VAL:HG23	1:N:61:ILE:HG13	1.86	0.58
2:S:180:ARG:HG2	2:S:182:GLU:HG2	1.86	0.58
2:T:73:ARG:NH2	2:T:342:ASP:O	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:143:ASP:HB3	2:Y:191:ILE:HG22	1.86	0.57
2:G:12:MET:HB3	2:G:382:PRO:HA	1.86	0.57
2:Y:430:GLU:HB3	2:Y:433:VAL:HB	1.86	0.57
2:S:143:ASP:HB3	2:S:191:ILE:HG22	1.86	0.57
2:K:293:MET:HG2	2:K:306:ILE:HG12	1.84	0.57
2:O:448:ARG:NH2	2:Y:435:ASP:OD1	2.25	0.57
2:T:12:MET:HB3	2:T:382:PRO:HA	1.86	0.57
2:S:389:ALA:HB3	2:S:446:ILE:HD12	1.87	0.57
1:B:116:ILE:HD12	1:B:116:ILE:H	1.69	0.57
2:O:388:ASN:OD1	2:O:445:ARG:NH2	2.34	0.57
1:R:16:ILE:HD11	1:R:72:LYS:HE2	1.87	0.57
1:L:33:ILE:O	1:L:63:GLN:NE2	2.38	0.57
1:R:99:GLN:NE2	2:T:423:GLU:O	2.37	0.57
1:M:116:ILE:H	1:M:116:ILE:HD12	1.69	0.57
1:F:99:GLN:NE2	2:G:423:GLU:O	2.38	0.57
2:G:159:ASP:HB2	2:K:101:ARG:HH12	1.69	0.57
2:K:389:ALA:HB3	2:K:446:ILE:HD12	1.87	0.57
2:S:287:GLU:HB3	2:S:309:PRO:HG3	1.86	0.57
2:S:430:GLU:HB3	2:S:433:VAL:HB	1.85	0.57
2:G:17:LYS:HA	2:G:17:LYS:HE2	1.87	0.57
2:O:430:GLU:HB3	2:O:433:VAL:HB	1.87	0.57
2:Y:158:THR:O	2:Y:180:ARG:NH2	2.38	0.57
2:O:101:ARG:HH12	2:T:159:ASP:HB2	1.70	0.56
2:K:430:GLU:HB3	2:K:433:VAL:HB	1.87	0.56
1:A:33:ILE:O	1:A:63:GLN:NE2	2.39	0.56
2:O:439:LEU:HD21	2:O:441:LYS:HE2	1.87	0.56
2:G:389:ALA:HB3	2:G:446:ILE:HD12	1.86	0.56
1:H:33:ILE:O	1:H:63:GLN:NE2	2.38	0.56
1:W:14:ARG:HG2	1:W:79:LEU:HD13	1.88	0.56
2:K:439:LEU:HD21	2:K:441:LYS:HE2	1.86	0.56
1:J:33:ILE:HG22	1:J:90:MET:HG3	1.87	0.56
1:F:55:ASP:OD1	1:F:55:ASP:N	2.39	0.56
2:K:34:LYS:H	2:K:41:GLY:HA2	1.71	0.56
2:O:29:MET:HE1	2:O:462:VAL:HB	1.87	0.55
1:F:16:ILE:HD11	1:F:72:LYS:HE2	1.87	0.55
2:O:34:LYS:H	2:O:41:GLY:HA2	1.71	0.55
2:S:34:LYS:NZ	2:K:23:ASP:OD1	2.39	0.55
1:N:33:ILE:HG22	1:N:90:MET:HG3	1.87	0.55
2:O:413:ALA:HB1	2:O:450:ILE:HD11	1.88	0.55
1:P:118:ALA:HA	1:P:121:LYS:HG2	1.89	0.55
2:K:369:SER:HB3	2:K:459:LYS:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:17:LYS:HE2	2:T:17:LYS:HA	1.87	0.55
1:D:120:LYS:HD3	1:D:120:LYS:N	2.21	0.55
2:G:409:LEU:HD11	2:G:454:LEU:HG	1.89	0.55
2:T:293:MET:HG2	2:T:306:ILE:HG12	1.88	0.55
1:L:28:ASN:CA	1:L:67:ILE:O	2.55	0.55
1:H:28:ASN:CA	1:H:67:ILE:O	2.54	0.55
2:G:293:MET:HG2	2:G:306:ILE:HG12	1.88	0.54
2:K:388:ASN:OD1	2:K:445:ARG:NH2	2.35	0.54
1:P:120:LYS:HD3	1:P:120:LYS:N	2.22	0.54
2:K:390:ARG:HA	2:K:445:ARG:HA	1.88	0.54
1:B:73:ILE:HG21	1:B:82:ILE:HG13	1.88	0.54
1:D:118:ALA:HA	1:D:121:LYS:HG2	1.89	0.54
1:D:119:ASP:OD1	1:E:121:LYS:NZ	2.41	0.54
2:G:390:ARG:HA	2:G:445:ARG:HA	1.88	0.54
1:W:116:ILE:H	1:W:116:ILE:HD12	1.71	0.54
2:O:50:THR:HG23	2:O:362:GLN:HG3	1.90	0.54
2:O:147:LEU:HB2	2:O:193:THR:HG21	1.89	0.54
2:Y:293:MET:HE3	2:Y:304:LEU:HD11	1.89	0.54
2:S:147:LEU:HB2	2:S:193:THR:HG21	1.89	0.54
2:S:210:SER:OG	2:S:225:GLN:OE1	2.24	0.54
2:G:210:SER:OG	2:G:225:GLN:OE1	2.23	0.54
2:O:294:GLU:OE2	2:O:307:HIS:NE2	2.40	0.54
2:T:390:ARG:HA	2:T:445:ARG:HA	1.89	0.54
2:K:413:ALA:HB1	2:K:450:ILE:HD11	1.88	0.54
1:R:55:ASP:OD1	1:R:55:ASP:N	2.38	0.54
1:A:31:ILE:HB	1:A:65:LEU:HB2	1.89	0.54
1:V:31:ILE:HB	1:V:65:LEU:HB2	1.89	0.54
2:Y:180:ARG:HG2	2:Y:182:GLU:HG2	1.90	0.54
2:O:369:SER:HB3	2:O:459:LYS:HG2	1.90	0.54
1:W:73:ILE:HG21	1:W:82:ILE:HG13	1.89	0.54
2:Y:147:LEU:HB2	2:Y:193:THR:HG21	1.89	0.54
1:R:18:THR:HA	1:R:25:ALA:HA	1.89	0.54
2:Y:369:SER:HB3	2:Y:459:LYS:HG2	1.91	0.53
2:S:369:SER:HB3	2:S:459:LYS:HG2	1.91	0.53
2:T:409:LEU:HD11	2:T:454:LEU:HG	1.89	0.53
2:K:155:LYS:HE2	2:K:158:THR:HG21	1.91	0.53
2:O:155:LYS:HE2	2:O:158:THR:HG21	1.90	0.53
2:S:439:LEU:HD21	2:S:441:LYS:HE2	1.90	0.53
2:S:194:TRP:NE1	2:S:245:ASP:O	2.35	0.53
1:B:14:ARG:HG2	1:B:79:LEU:HD13	1.90	0.52
2:S:293:MET:HE3	2:S:304:LEU:HD11	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:37:LEU:HD13	2:Y:385:LYS:HB2	1.90	0.52
2:G:148:ARG:HA	2:Y:182:GLU:O	2.08	0.52
2:K:50:THR:HG23	2:K:362:GLN:HG3	1.91	0.52
1:V:51:ILE:HG12	1:V:59:VAL:HB	1.91	0.52
2:T:210:SER:OG	2:T:225:GLN:OE1	2.24	0.52
2:T:364:GLN:NE2	2:T:366:ASP:OD1	2.31	0.52
1:X:33:ILE:HG22	1:X:90:MET:HG3	1.91	0.52
1:R:33:ILE:HG22	1:R:90:MET:HG3	1.90	0.52
2:S:385:LYS:HB2	2:T:37:LEU:HD13	1.91	0.52
1:F:33:ILE:HG22	1:F:90:MET:HG3	1.91	0.52
1:C:31:ILE:HB	1:C:65:LEU:HB2	1.92	0.52
1:J:49:VAL:HG23	1:J:61:ILE:HG13	1.92	0.52
1:M:55:ASP:OD1	1:M:57:SER:OG	2.22	0.52
1:A:31:ILE:HG13	1:A:67:ILE:HD11	1.92	0.52
1:A:51:ILE:HG12	1:A:59:VAL:HB	1.92	0.52
2:S:435:ASP:OD1	2:K:448:ARG:NH2	2.26	0.52
2:Y:210:SER:OG	2:Y:225:GLN:OE1	2.27	0.52
2:G:35:GLU:HA	2:G:40:SER:HA	1.93	0.51
2:S:404:GLN:OE1	2:S:460:SER:OG	2.26	0.51
1:X:31:ILE:HB	1:X:65:LEU:HB2	1.93	0.51
2:T:369:SER:HB3	2:T:459:LYS:HG2	1.93	0.51
1:D:31:ILE:HD12	1:D:73:ILE:HD11	1.93	0.51
2:K:294:GLU:OE2	2:K:307:HIS:NE2	2.40	0.51
1:P:31:ILE:HD12	1:P:73:ILE:HD11	1.92	0.51
1:M:14:ARG:HB3	1:M:72:LYS:HD3	1.92	0.51
2:K:147:LEU:HB2	2:K:193:THR:HG21	1.93	0.51
2:K:364:GLN:NE2	2:K:366:ASP:OD1	2.28	0.51
1:V:78:GLN:HA	1:W:21:ARG:HH22	1.76	0.51
2:G:101:ARG:NH2	2:Y:185:PRO:O	2.44	0.51
2:T:34:LYS:H	2:T:41:GLY:HA2	1.76	0.51
2:S:390:ARG:HA	2:S:445:ARG:HA	1.92	0.51
2:O:262:ILE:HD12	2:O:271:ILE:HG13	1.93	0.51
2:O:390:ARG:HA	2:O:445:ARG:HA	1.93	0.51
1:A:78:GLN:HA	1:B:21:ARG:HH22	1.76	0.51
2:G:369:SER:HB3	2:G:459:LYS:HG2	1.93	0.51
2:G:448:ARG:NH2	2:K:435:ASP:OD1	2.28	0.51
2:Y:63:GLU:OE1	2:Y:99:HIS:ND1	2.44	0.51
1:C:31:ILE:HG13	1:C:67:ILE:HD11	1.93	0.50
1:I:14:ARG:HB3	1:I:72:LYS:HD3	1.94	0.50
2:T:439:LEU:HD21	2:T:441:LYS:HE2	1.92	0.50
1:V:31:ILE:HG13	1:V:67:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:390:ARG:HA	2:Y:445:ARG:HA	1.93	0.50
2:S:237:THR:O	2:S:240:LYS:NZ	2.45	0.50
2:K:312:VAL:HG21	2:K:338:TYR:HB3	1.94	0.50
2:Y:194:TRP:NE1	2:Y:245:ASP:O	2.35	0.50
2:G:60:ARG:HD2	2:G:93:GLY:O	2.12	0.50
1:X:31:ILE:HG13	1:X:67:ILE:HD11	1.93	0.50
2:G:439:LEU:HD21	2:G:441:LYS:HE2	1.93	0.50
1:P:14:ARG:NH1	1:Q:101:ASP:OD1	2.44	0.50
2:T:60:ARG:HD2	2:T:93:GLY:O	2.12	0.50
2:G:183:SER:HB2	2:K:148:ARG:NH1	2.27	0.50
1:D:14:ARG:NH1	1:E:101:ASP:OD1	2.45	0.49
1:J:47:ILE:HD11	1:J:88:HIS:HB3	1.94	0.49
1:N:47:ILE:HD11	1:N:88:HIS:HB3	1.94	0.49
2:G:34:LYS:H	2:G:41:GLY:HA2	1.76	0.49
1:D:90:MET:HE3	1:D:103:ILE:HD13	1.94	0.49
1:P:19:GLU:HG3	1:P:24:LYS:HG3	1.94	0.49
2:Y:136:TYR:HB2	2:Y:138:LEU:HD13	1.93	0.49
1:I:73:ILE:HG21	1:I:82:ILE:HG13	1.94	0.49
2:K:316:ASP:O	2:K:320:SER:OG	2.30	0.49
2:O:194:TRP:NE1	2:O:245:ASP:O	2.39	0.49
2:Y:237:THR:O	2:Y:240:LYS:NZ	2.45	0.49
2:S:413:ALA:HB1	2:S:450:ILE:HD11	1.95	0.49
1:P:90:MET:HE3	1:P:103:ILE:HD13	1.95	0.49
2:T:143:ASP:HB3	2:T:191:ILE:HG22	1.95	0.49
2:T:298:PHE:O	2:T:301:HIS:HB2	2.12	0.49
2:K:13:GLY:HA3	2:K:24:TYR:CZ	2.48	0.49
2:O:312:VAL:HG21	2:O:338:TYR:HB3	1.94	0.48
1:R:30:LYS:HB2	1:R:30:LYS:HE2	1.58	0.48
2:K:15:ASP:HB2	2:K:22:ILE:HD13	1.95	0.48
2:K:261:TYR:HB3	2:K:268:ALA:HB1	1.94	0.48
2:G:298:PHE:O	2:G:301:HIS:HB2	2.12	0.48
2:O:261:TYR:HB3	2:O:268:ALA:HB1	1.95	0.48
1:L:18:THR:HA	1:L:25:ALA:HA	1.94	0.48
1:V:31:ILE:HD12	1:V:73:ILE:HD11	1.96	0.48
2:Y:12:MET:HG3	2:Y:13:GLY:N	2.28	0.48
2:Y:17:LYS:HE2	2:Y:17:LYS:HA	1.96	0.48
2:G:182:GLU:O	2:K:148:ARG:HA	2.14	0.48
1:I:117:GLU:O	1:I:121:LYS:HB2	2.14	0.48
2:T:62:VAL:HG23	2:T:73:ARG:HG2	1.96	0.48
2:S:63:GLU:OE2	2:S:99:HIS:ND1	2.46	0.48
2:O:13:GLY:HA3	2:O:24:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:17:LYS:HA	2:S:17:LYS:HE2	1.96	0.48
2:S:23:ASP:OD1	2:T:34:LYS:NZ	2.47	0.48
1:M:73:ILE:HG21	1:M:82:ILE:HG13	1.95	0.48
2:T:388:ASN:OD1	2:T:445:ARG:NH1	2.47	0.48
2:Y:413:ALA:HB1	2:Y:450:ILE:HD11	1.96	0.48
1:A:31:ILE:HD12	1:A:73:ILE:HD11	1.96	0.47
2:Y:261:TYR:HB3	2:Y:268:ALA:HB1	1.97	0.47
1:A:108:LYS:HD2	1:C:112:ASP:OD2	2.13	0.47
2:S:409:LEU:O	2:S:425:MET:HA	2.14	0.47
2:G:143:ASP:HB3	2:G:191:ILE:HG22	1.95	0.47
2:T:312:VAL:HG21	2:T:338:TYR:HB3	1.96	0.47
2:S:297:ARG:NH2	2:K:277:GLU:OE1	2.33	0.47
2:K:35:GLU:HA	2:K:40:SER:HA	1.97	0.47
1:M:117:GLU:O	1:M:121:LYS:HB2	2.15	0.47
2:O:15:ASP:HB2	2:O:22:ILE:HD13	1.95	0.47
2:S:293:MET:HG2	2:S:306:ILE:HG12	1.96	0.47
2:K:63:GLU:OE2	2:K:99:HIS:ND1	2.46	0.47
2:S:312:VAL:HG21	2:S:338:TYR:HB3	1.97	0.47
2:K:12:MET:HB3	2:K:382:PRO:HA	1.96	0.47
2:O:12:MET:HB3	2:O:382:PRO:HA	1.96	0.47
1:Q:35:GLN:O	1:Q:38:THR:HG22	2.15	0.47
2:T:261:TYR:HB3	2:T:268:ALA:HB1	1.96	0.47
2:Y:293:MET:HG2	2:Y:306:ILE:HG12	1.95	0.47
2:G:312:VAL:HG21	2:G:338:TYR:HB3	1.95	0.47
2:G:388:ASN:OD1	2:G:445:ARG:NH1	2.48	0.47
2:O:316:ASP:O	2:O:320:SER:OG	2.30	0.47
1:V:35:GLN:HG2	1:V:45:ASN:O	2.15	0.47
2:S:16:PHE:HB3	2:S:418:ILE:HD13	1.97	0.47
2:Y:391:CYS:HB3	2:Y:471:LEU:HD23	1.97	0.47
1:D:18:THR:HA	1:D:25:ALA:HA	1.97	0.47
1:E:35:GLN:O	1:E:89:SER:OG	2.24	0.47
2:G:341:VAL:HB	2:G:355:LYS:HE3	1.97	0.46
2:S:261:TYR:HB3	2:S:268:ALA:HB1	1.97	0.46
2:S:34:LYS:O	2:S:41:GLY:N	2.49	0.46
2:O:35:GLU:HA	2:O:40:SER:HA	1.97	0.46
2:Y:312:VAL:HG21	2:Y:338:TYR:HB3	1.97	0.46
2:G:62:VAL:HG23	2:G:73:ARG:HG2	1.97	0.46
2:K:194:TRP:NE1	2:K:245:ASP:O	2.39	0.46
2:Y:155:LYS:HE2	2:Y:158:THR:HG21	1.98	0.46
2:Y:287:GLU:HB3	2:Y:309:PRO:HG3	1.97	0.46
2:G:185:PRO:HB3	2:K:100:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:53:ASN:OD1	1:R:57:SER:OG	2.20	0.46
1:L:19:GLU:HG3	1:L:24:LYS:HG3	1.98	0.46
2:O:341:VAL:HB	2:O:355:LYS:HE3	1.97	0.46
2:K:341:VAL:HB	2:K:355:LYS:HE3	1.97	0.46
1:X:52:GLU:HG3	1:X:58:HIS:NE2	2.31	0.46
1:A:35:GLN:HG2	1:A:45:ASN:O	2.15	0.46
2:K:184:GLN:NE2	2:K:187:GLY:O	2.44	0.46
1:X:85:VAL:HG23	1:X:86:GLN:HG2	1.98	0.46
2:Y:35:GLU:HA	2:Y:40:SER:HA	1.98	0.46
1:A:52:GLU:OE2	1:A:58:HIS:NE2	2.50	0.45
2:G:261:TYR:HB3	2:G:268:ALA:HB1	1.96	0.45
1:J:22:SER:HB2	1:J:24:LYS:NZ	2.31	0.45
1:C:68:ASN:ND2	1:C:69:ALA:H	2.14	0.45
1:E:35:GLN:O	1:E:38:THR:HG22	2.17	0.45
1:J:99:GLN:NE2	2:K:423:GLU:O	2.46	0.45
1:W:35:GLN:O	1:W:38:THR:HG22	2.16	0.45
2:S:158:THR:O	2:S:180:ARG:NH2	2.49	0.45
1:I:55:ASP:OD1	1:I:57:SER:OG	2.23	0.45
2:O:63:GLU:OE2	2:O:99:HIS:ND1	2.47	0.45
2:G:399:SER:HB3	2:G:463:THR:HB	1.97	0.45
2:O:364:GLN:NE2	2:O:366:ASP:OD1	2.28	0.45
1:B:35:GLN:O	1:B:38:THR:HG22	2.17	0.45
1:C:85:VAL:HG23	1:C:86:GLN:HG2	1.98	0.45
2:S:185:PRO:O	2:T:101:ARG:NH2	2.49	0.45
1:H:18:THR:HA	1:H:25:ALA:HA	1.97	0.45
1:X:47:ILE:HD11	1:X:88:HIS:HB3	1.98	0.45
2:Y:16:PHE:HB3	2:Y:418:ILE:HD13	1.97	0.45
2:Y:34:LYS:O	2:Y:41:GLY:N	2.49	0.45
1:E:14:ARG:HD2	1:E:79:LEU:HD13	1.97	0.45
1:E:121:LYS:HB3	1:E:121:LYS:HE2	1.62	0.45
2:S:273:THR:O	2:S:277:GLU:HG3	2.16	0.45
2:S:391:CYS:HB3	2:S:471:LEU:HD23	1.99	0.45
2:K:456:VAL:HG12	2:K:458:THR:HG23	1.99	0.45
2:T:312:VAL:HG23	2:T:337:VAL:HG22	1.99	0.45
1:L:14:ARG:NH1	1:M:101:ASP:OD1	2.49	0.45
1:L:46:GLN:HB3	1:L:63:GLN:HE21	1.81	0.45
2:T:116:ARG:NH1	2:T:118:ASP:OD2	2.49	0.45
1:X:68:ASN:ND2	1:X:69:ALA:H	2.15	0.45
2:G:206:ILE:HB	2:G:230:VAL:HB	1.99	0.45
1:H:14:ARG:NH1	1:I:101:ASP:OD1	2.50	0.45
1:Q:14:ARG:HD2	1:Q:79:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:61:ILE:HD11	1:Q:75:TYR:CE1	2.52	0.45
2:T:15:ASP:HB2	2:T:22:ILE:HD13	1.99	0.45
1:C:52:GLU:HG3	1:C:58:HIS:NE2	2.32	0.44
2:G:413:ALA:HB1	2:G:450:ILE:HD11	1.99	0.44
1:H:46:GLN:HB3	1:H:63:GLN:HE21	1.81	0.44
2:K:141:VAL:HG22	2:K:153:TRP:CD1	2.52	0.44
2:T:399:SER:HB3	2:T:463:THR:HB	1.98	0.44
2:K:262:ILE:HD12	2:K:271:ILE:HG13	1.99	0.44
2:S:116:ARG:NH1	2:S:118:ASP:OD2	2.50	0.44
1:F:30:LYS:HE2	1:F:30:LYS:HB2	1.58	0.44
2:G:435:ASP:OD1	2:Y:448:ARG:NH2	2.44	0.44
1:H:28:ASN:N	1:H:67:ILE:O	2.51	0.44
1:H:77:GLY:O	1:I:21:ARG:NH2	2.51	0.44
1:M:61:ILE:HD11	1:M:75:TYR:CE1	2.52	0.44
1:W:21:ARG:HA	1:W:21:ARG:HD3	1.85	0.44
1:B:61:ILE:HD12	1:B:61:ILE:HA	1.87	0.44
1:L:28:ASN:N	1:L:67:ILE:O	2.50	0.44
1:L:77:GLY:O	1:M:21:ARG:NH2	2.51	0.44
1:N:22:SER:HB2	1:N:24:LYS:NZ	2.31	0.44
2:T:413:ALA:HB1	2:T:450:ILE:HD11	1.98	0.44
1:B:61:ILE:HD11	1:B:75:TYR:CE1	2.53	0.44
2:S:155:LYS:HE2	2:S:158:THR:HG21	2.00	0.44
2:S:364:GLN:NE2	2:S:366:ASP:OD1	2.27	0.44
2:G:277:GLU:OE1	2:K:297:ARG:NH2	2.35	0.44
1:I:61:ILE:HD11	1:I:75:TYR:CE1	2.52	0.44
2:O:184:GLN:NE2	2:O:187:GLY:O	2.44	0.44
2:G:15:ASP:HB2	2:G:22:ILE:HD13	1.99	0.44
2:G:430:GLU:HB3	2:G:433:VAL:HB	1.99	0.44
1:I:35:GLN:O	1:I:38:THR:HG22	2.18	0.44
2:O:391:CYS:HB3	2:O:471:LEU:HD23	1.99	0.44
2:O:409:LEU:O	2:O:425:MET:HA	2.18	0.44
2:T:147:LEU:HB2	2:T:193:THR:HG21	2.00	0.44
1:W:61:ILE:HD11	1:W:75:TYR:CE1	2.53	0.44
2:Y:141:VAL:HG22	2:Y:153:TRP:CD1	2.53	0.44
1:C:99:GLN:NE2	2:S:423:GLU:O	2.51	0.44
2:S:148:ARG:HA	2:K:182:GLU:O	2.18	0.44
2:G:167:GLU:HG3	2:G:174:ARG:HH12	1.82	0.44
2:O:297:ARG:NH2	2:T:277:GLU:OE1	2.35	0.44
2:Y:60:ARG:HD2	2:Y:93:GLY:O	2.18	0.44
2:T:35:GLU:HA	2:T:40:SER:HA	2.00	0.44
2:T:341:VAL:HB	2:T:355:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ILE:HB	1:H:65:LEU:HB2	2.00	0.43
1:H:79:LEU:HD11	1:I:20:SER:HB2	2.00	0.43
2:S:60:ARG:HD2	2:S:93:GLY:O	2.18	0.43
1:F:36:ILE:HA	1:F:89:SER:HB3	1.99	0.43
2:G:271:ILE:HD13	2:G:271:ILE:HA	1.75	0.43
2:O:143:ASP:HB3	2:O:191:ILE:HG22	1.99	0.43
2:T:343:PHE:CD1	2:T:352:CYS:HB3	2.53	0.43
2:T:430:GLU:HB3	2:T:433:VAL:HB	1.99	0.43
1:X:18:THR:HA	1:X:25:ALA:HA	1.99	0.43
1:E:61:ILE:HD11	1:E:75:TYR:CE1	2.54	0.43
2:G:287:GLU:HB3	2:G:309:PRO:HG3	2.00	0.43
1:L:11:SER:HA	1:M:15:PRO:HG2	2.00	0.43
1:X:36:ILE:HD12	2:Y:334:TYR:CE2	2.53	0.43
1:I:31:ILE:HG13	1:I:67:ILE:HD11	2.01	0.43
2:O:141:VAL:HG22	2:O:153:TRP:CD1	2.52	0.43
2:O:243:PHE:HA	2:O:295:THR:HG21	2.00	0.43
2:S:141:VAL:HG22	2:S:153:TRP:CD1	2.53	0.43
2:S:186:ASP:HB3	2:T:67:ALA:HA	2.00	0.43
1:F:74:VAL:HG12	1:F:79:LEU:HD23	2.00	0.43
1:L:79:LEU:HD11	1:M:20:SER:HB2	2.00	0.43
1:R:36:ILE:HA	1:R:89:SER:HB3	2.00	0.43
2:T:155:LYS:HB2	2:T:162:PHE:HE1	1.84	0.43
2:S:67:ALA:HA	2:K:186:ASP:HB3	2.01	0.43
2:G:273:THR:O	2:G:277:GLU:HG3	2.19	0.43
1:P:6:ALA:HB1	1:Q:84:THR:O	2.19	0.43
2:Y:271:ILE:HG22	2:Y:326:TRP:HZ2	1.84	0.43
1:B:99:GLN:NE2	1:B:102:TYR:HB2	2.34	0.43
1:J:30:LYS:HB2	1:J:30:LYS:HE2	1.52	0.43
2:O:182:GLU:O	2:Y:148:ARG:HA	2.19	0.43
1:H:11:SER:HA	1:I:15:PRO:HG2	2.00	0.43
2:K:234:ILE:HD12	2:K:236:GLY:O	2.18	0.43
1:N:99:GLN:NE2	2:O:423:GLU:O	2.46	0.43
2:O:394:LEU:HD13	2:O:411:LEU:HD21	2.00	0.43
1:Q:61:ILE:HD12	1:Q:61:ILE:HA	1.91	0.43
1:R:74:VAL:HG12	1:R:79:LEU:HD23	2.01	0.43
1:X:99:GLN:NE2	2:Y:423:GLU:O	2.50	0.43
1:C:52:GLU:HG3	1:C:58:HIS:CD2	2.54	0.43
2:S:35:GLU:HA	2:S:40:SER:HA	2.01	0.43
2:G:343:PHE:CD1	2:G:352:CYS:HB3	2.53	0.43
1:I:61:ILE:HD12	1:I:61:ILE:HA	1.89	0.43
2:K:26:PRO:HB2	2:K:29:MET:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:155:LYS:HB2	2:K:162:PHE:HE1	1.84	0.43
2:O:234:ILE:HD12	2:O:236:GLY:O	2.18	0.43
2:Y:416:ASP:OD2	2:Y:419:ASN:ND2	2.51	0.43
1:E:54:GLU:OE1	2:G:453:LYS:NZ	2.30	0.43
2:G:155:LYS:HB2	2:G:162:PHE:HE1	1.84	0.43
2:K:243:PHE:HA	2:K:295:THR:HG21	2.01	0.43
1:L:31:ILE:HB	1:L:65:LEU:HB2	2.00	0.43
2:O:409:LEU:HD21	2:O:454:LEU:HD12	2.00	0.43
2:T:287:GLU:HB3	2:T:309:PRO:HG3	1.99	0.43
1:W:99:GLN:NE2	1:W:102:TYR:HB2	2.34	0.43
2:G:159:ASP:HA	2:G:188:ILE:HB	2.00	0.42
2:G:185:PRO:O	2:G:186:ASP:HB2	2.19	0.42
2:K:162:PHE:CE2	2:K:178:GLN:HG3	2.54	0.42
1:M:35:GLN:O	1:M:38:THR:HG22	2.18	0.42
1:B:46:GLN:CD	1:B:63:GLN:HG2	2.40	0.42
1:M:31:ILE:HG13	1:M:67:ILE:HD11	2.00	0.42
2:O:26:PRO:HB2	2:O:29:MET:HB2	2.01	0.42
2:O:155:LYS:HB2	2:O:162:PHE:HE1	1.84	0.42
2:T:237:THR:O	2:T:240:LYS:NZ	2.53	0.42
2:T:271:ILE:HD13	2:T:271:ILE:HA	1.75	0.42
2:S:271:ILE:HG22	2:S:326:TRP:HZ2	1.84	0.42
2:S:416:ASP:OD2	2:S:419:ASN:ND2	2.52	0.42
2:O:400:THR:OG1	2:O:433:VAL:O	2.26	0.42
2:S:25:LEU:HD11	2:S:276:ILE:HD11	2.01	0.42
2:T:273:THR:O	2:T:277:GLU:HG3	2.19	0.42
2:Y:409:LEU:HD13	2:Y:456:VAL:HG22	2.00	0.42
2:K:26:PRO:HB3	2:K:379:LEU:HD23	2.02	0.42
2:K:394:LEU:HD13	2:K:411:LEU:HD21	2.01	0.42
2:Y:273:THR:O	2:Y:277:GLU:HG3	2.18	0.42
2:O:412:SER:HB3	2:O:423:GLU:HG3	2.02	0.42
1:V:14:ARG:NH1	1:W:101:ASP:OD1	2.52	0.42
2:K:206:ILE:HB	2:K:230:VAL:HB	2.02	0.42
2:T:159:ASP:HA	2:T:188:ILE:HB	2.02	0.42
2:T:283:TYR:OH	2:T:311:HIS:ND1	2.33	0.42
2:G:147:LEU:HB2	2:G:193:THR:HG21	2.01	0.42
2:O:60:ARG:HD2	2:O:93:GLY:O	2.19	0.42
2:O:273:THR:O	2:O:277:GLU:HG3	2.20	0.42
1:B:88:HIS:CE1	1:B:106:VAL:HG21	2.55	0.42
1:C:18:THR:HA	1:C:25:ALA:HA	2.00	0.42
2:S:387:ASP:OD1	2:S:448:ARG:HA	2.20	0.42
1:I:88:HIS:CE1	1:I:106:VAL:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:296:LEU:HD23	2:K:296:LEU:HA	1.90	0.42
2:O:185:PRO:O	2:Y:101:ARG:NH2	2.53	0.42
1:V:52:GLU:OE2	1:V:58:HIS:NE2	2.52	0.42
2:S:101:ARG:NH2	2:K:185:PRO:O	2.52	0.42
1:D:6:ALA:HB1	1:E:84:THR:O	2.19	0.42
1:I:38:THR:O	1:I:102:TYR:OH	2.27	0.42
2:K:273:THR:O	2:K:277:GLU:HG3	2.20	0.42
1:M:10:VAL:HB	1:N:82:ILE:HB	2.02	0.42
2:O:210:SER:OG	2:O:225:GLN:OE1	2.37	0.42
1:W:88:HIS:CE1	1:W:106:VAL:HG21	2.54	0.42
1:E:94:ASP:HB3	1:E:96:ASN:OD1	2.20	0.41
2:K:189:ILE:H	2:K:189:ILE:HG12	1.68	0.41
1:P:77:GLY:O	1:Q:21:ARG:NH2	2.54	0.41
1:W:46:GLN:CD	1:W:63:GLN:HG2	2.40	0.41
1:C:33:ILE:HG22	1:C:90:MET:HG3	2.02	0.41
2:S:409:LEU:HD11	2:S:454:LEU:HG	2.01	0.41
2:G:237:THR:O	2:G:240:LYS:NZ	2.53	0.41
2:K:210:SER:OG	2:K:225:GLN:OE1	2.34	0.41
1:M:88:HIS:CE1	1:M:106:VAL:HG21	2.55	0.41
2:G:98:ALA:O	2:G:104:GLN:NE2	2.53	0.41
2:K:409:LEU:O	2:K:425:MET:HA	2.21	0.41
1:Q:94:ASP:HB3	1:Q:96:ASN:OD1	2.20	0.41
2:Y:25:LEU:HD11	2:Y:276:ILE:HD11	2.02	0.41
1:H:6:ALA:HB1	1:I:84:THR:O	2.20	0.41
2:K:60:ARG:HD2	2:K:93:GLY:O	2.20	0.41
1:A:14:ARG:NH1	1:B:101:ASP:OD1	2.53	0.41
2:S:34:LYS:H	2:S:41:GLY:HA2	1.85	0.41
1:F:53:ASN:OD1	1:F:57:SER:OG	2.20	0.41
1:N:61:ILE:HD11	1:N:82:ILE:HD12	2.02	0.41
2:O:277:GLU:OE1	2:Y:297:ARG:NH2	2.33	0.41
2:T:379:LEU:HD23	2:T:379:LEU:HA	1.92	0.41
1:W:38:THR:HG21	1:W:45:ASN:HB3	2.01	0.41
1:D:77:GLY:O	1:E:21:ARG:NH2	2.54	0.41
2:G:279:ILE:O	2:G:282:SER:OG	2.30	0.41
1:L:82:ILE:HB	1:N:10:VAL:HB	2.02	0.41
1:I:10:VAL:HB	1:J:82:ILE:HB	2.02	0.41
2:K:412:SER:HB3	2:K:423:GLU:HG3	2.02	0.41
1:L:26:VAL:HG12	1:L:29:GLY:HA3	2.02	0.41
2:O:186:ASP:HB3	2:Y:67:ALA:HA	2.02	0.41
2:O:189:ILE:H	2:O:189:ILE:HG12	1.68	0.41
2:T:206:ILE:HB	2:T:230:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:THR:HG21	1:B:45:ASN:HB3	2.02	0.41
1:F:49:VAL:HG23	1:F:61:ILE:HG13	2.03	0.41
1:J:61:ILE:HD11	1:J:82:ILE:HD12	2.02	0.41
2:K:272:ALA:HB1	2:K:276:ILE:HB	2.03	0.41
1:L:90:MET:SD	1:L:92:ILE:HD11	2.61	0.41
1:M:105:ASN:ND2	1:M:108:LYS:HE3	2.36	0.41
1:N:30:LYS:HE2	1:N:30:LYS:HB2	1.52	0.41
1:P:25:ALA:HB2	1:Q:23:PHE:CD1	2.56	0.41
1:P:78:GLN:HA	1:Q:21:ARG:HH22	1.86	0.41
1:R:49:VAL:HG23	1:R:61:ILE:HG13	2.03	0.41
2:S:364:GLN:HB3	2:S:367:ILE:HG12	2.02	0.41
2:O:374:GLN:HB3	2:O:459:LYS:HG3	2.03	0.41
2:Y:36:ILE:HD11	2:Y:42:TYR:CD1	2.56	0.41
1:B:116:ILE:HG22	1:B:120:LYS:HE3	2.02	0.40
2:S:257:ALA:HA	2:S:258:PRO:HD3	1.95	0.40
1:D:35:GLN:HG2	1:D:45:ASN:O	2.21	0.40
2:O:101:ARG:HE	2:O:101:ARG:HB2	1.59	0.40
1:R:31:ILE:HB	1:R:65:LEU:HB2	2.04	0.40
2:S:99:HIS:NE2	2:K:185:PRO:HG2	2.36	0.40
1:E:84:THR:OG1	1:E:85:VAL:N	2.55	0.40
1:H:82:ILE:HB	1:J:10:VAL:HB	2.02	0.40
1:H:90:MET:SD	1:H:92:ILE:HD11	2.61	0.40
1:I:94:ASP:HB3	1:I:96:ASN:OD1	2.21	0.40
2:K:271:ILE:HD13	2:K:271:ILE:HA	1.93	0.40
2:K:293:MET:HE3	2:K:304:LEU:HD11	2.03	0.40
2:K:400:THR:OG1	2:K:433:VAL:O	2.26	0.40
1:M:94:ASP:HB3	1:M:96:ASN:OD1	2.21	0.40
1:P:35:GLN:HG2	1:P:45:ASN:O	2.20	0.40
2:Y:387:ASP:OD1	2:Y:448:ARG:HA	2.20	0.40
1:I:105:ASN:ND2	1:I:108:LYS:HE3	2.36	0.40
2:O:409:LEU:HD11	2:O:454:LEU:HG	2.03	0.40
1:B:21:ARG:HD3	1:B:21:ARG:HA	1.85	0.40
2:Y:34:LYS:H	2:Y:41:GLY:HA2	1.86	0.40
2:K:247:TYR:HB2	2:K:263:ILE:HD12	2.04	0.40
2:O:26:PRO:HB3	2:O:379:LEU:HD23	2.02	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	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	B	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	C	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	D	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	E	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	F	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	H	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	I	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	J	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	L	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	M	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	N	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	P	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	Q	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	R	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	V	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	W	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	X	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
2	G	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
2	K	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
2	O	469/472 (99%)	439 (94%)	30 (6%)	0	100	100
2	S	469/472 (99%)	437 (93%)	32 (7%)	0	100	100
2	T	469/472 (99%)	439 (94%)	30 (6%)	0	100	100
2	Y	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
All	All	4902/14838 (33%)	4662 (95%)	240 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	101/548 (18%)	101 (100%)	0	100	100
1	B	101/548 (18%)	99 (98%)	2 (2%)	50	81
1	C	101/548 (18%)	98 (97%)	3 (3%)	36	70
1	D	101/548 (18%)	99 (98%)	2 (2%)	50	81
1	E	101/548 (18%)	100 (99%)	1 (1%)	73	91
1	F	101/548 (18%)	97 (96%)	4 (4%)	27	60
1	H	101/548 (18%)	101 (100%)	0	100	100
1	I	101/548 (18%)	98 (97%)	3 (3%)	36	70
1	J	101/548 (18%)	99 (98%)	2 (2%)	50	81
1	L	101/548 (18%)	101 (100%)	0	100	100
1	M	101/548 (18%)	98 (97%)	3 (3%)	36	70
1	N	101/548 (18%)	98 (97%)	3 (3%)	36	70
1	P	101/548 (18%)	100 (99%)	1 (1%)	73	91
1	Q	101/548 (18%)	101 (100%)	0	100	100
1	R	101/548 (18%)	99 (98%)	2 (2%)	50	81
1	V	101/548 (18%)	101 (100%)	0	100	100
1	W	101/548 (18%)	100 (99%)	1 (1%)	73	91
1	X	101/548 (18%)	96 (95%)	5 (5%)	20	51
2	G	394/395 (100%)	387 (98%)	7 (2%)	54	83
2	K	394/395 (100%)	380 (96%)	14 (4%)	30	64
2	O	394/395 (100%)	383 (97%)	11 (3%)	38	72
2	S	394/395 (100%)	386 (98%)	8 (2%)	50	81
2	T	394/395 (100%)	386 (98%)	8 (2%)	50	81
2	Y	394/395 (100%)	382 (97%)	12 (3%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4182/12234 (34%)	4090 (98%)	92 (2%)	47 79

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	ARG
1	B	62	THR
1	C	57	SER
1	C	106	VAL
1	C	112	ASP
2	S	54	ASP
2	S	148	ARG
2	S	196	ASP
2	S	227	SER
2	S	237	THR
2	S	267	GLN
2	S	269	SER
2	S	435	ASP
1	D	24	LYS
1	D	30	LYS
1	E	52	GLU
1	F	24	LYS
1	F	84	THR
1	F	106	VAL
1	F	112	ASP
2	G	56	ASN
2	G	148	ARG
2	G	196	ASP
2	G	267	GLN
2	G	271	ILE
2	G	394	LEU
2	G	435	ASP
1	I	54	GLU
1	I	55	ASP
1	I	98	SER
1	J	20	SER
1	J	84	THR
2	K	50	THR
2	K	54	ASP
2	K	102	THR
2	K	167	GLU
2	K	180	ARG

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Mol	Chain	Res	Type
2	K	227	SER
2	K	229	MET
2	K	241	THR
2	K	269	SER
2	K	337	VAL
2	K	373	LYS
2	K	387	ASP
2	K	394	LEU
2	K	395	GLU
1	M	54	GLU
1	M	55	ASP
1	M	98	SER
1	N	20	SER
1	N	84	THR
1	N	94	ASP
2	O	50	THR
2	O	54	ASP
2	O	102	THR
2	O	174	ARG
2	O	241	THR
2	O	269	SER
2	O	271	ILE
2	O	337	VAL
2	O	394	LEU
2	O	395	GLU
2	O	458	THR
1	P	30	LYS
1	R	84	THR
1	R	112	ASP
2	T	56	ASN
2	T	174	ARG
2	T	196	ASP
2	T	267	GLN
2	T	271	ILE
2	T	337	VAL
2	T	394	LEU
2	T	435	ASP
1	W	62	THR
1	X	57	SER
1	X	84	THR
1	X	106	VAL
1	X	108	LYS

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Mol	Chain	Res	Type
1	X	112	ASP
2	Y	54	ASP
2	Y	102	THR
2	Y	148	ARG
2	Y	180	ARG
2	Y	196	ASP
2	Y	227	SER
2	Y	229	MET
2	Y	237	THR
2	Y	267	GLN
2	Y	269	SER
2	Y	395	GLU
2	Y	435	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	63	GLN
1	D	46	GLN
1	D	63	GLN
1	H	46	GLN
1	H	63	GLN
1	L	46	GLN
1	L	63	GLN
1	P	46	GLN
1	V	46	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

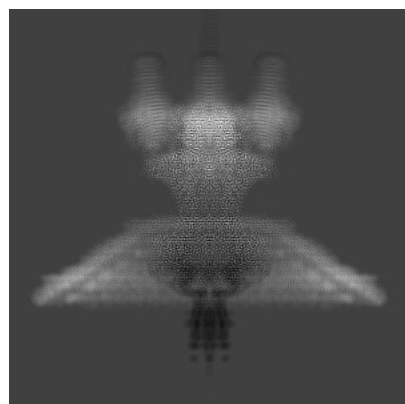
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41649. These allow visual inspection of the internal detail of the map and identification of artifacts.

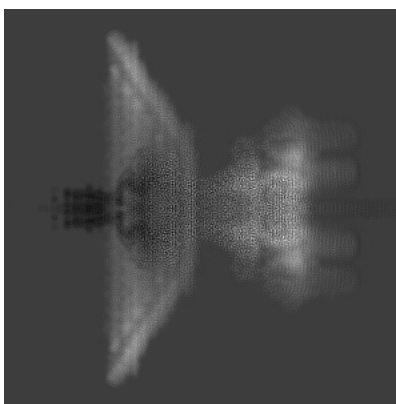
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

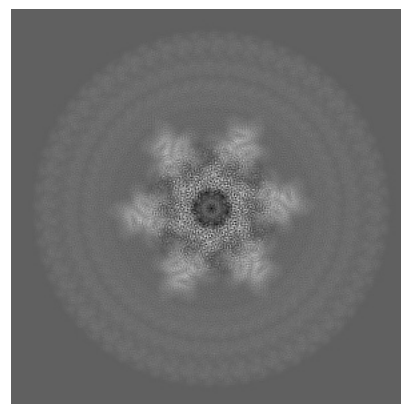
6.1.1 Primary map



X

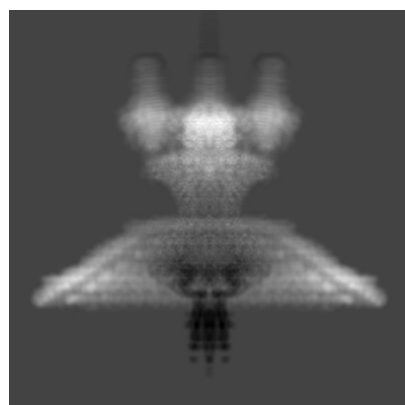


Y

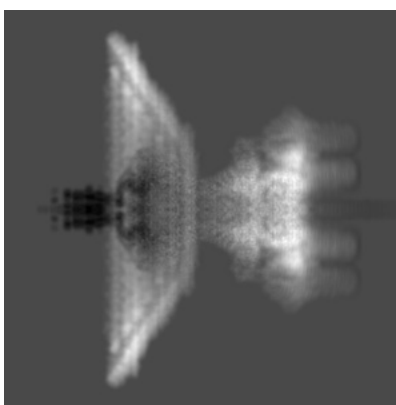


Z

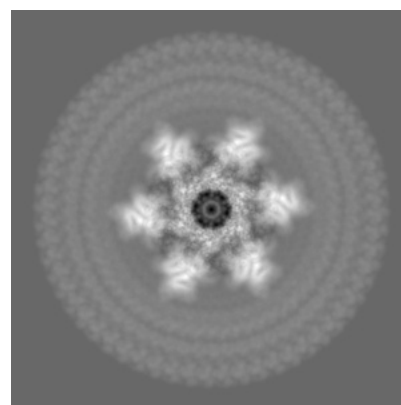
6.1.2 Raw map



X



Y



Z

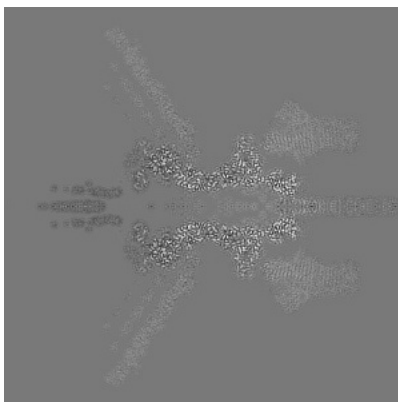
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

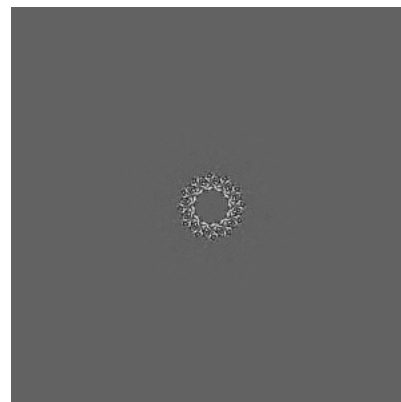
6.2.1 Primary map



X Index: 220

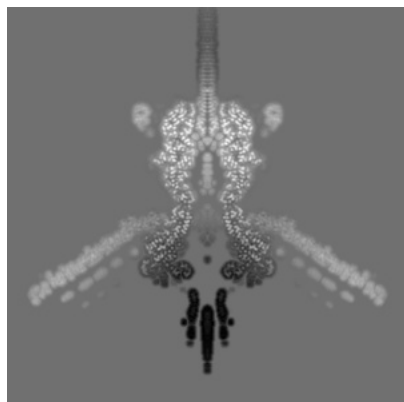


Y Index: 220

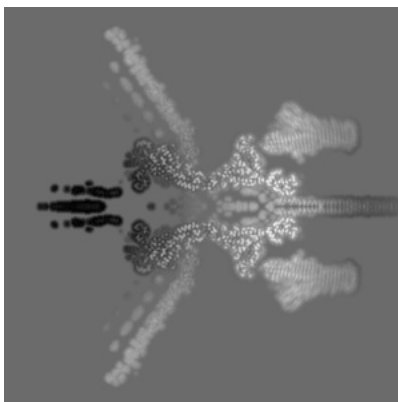


Z Index: 220

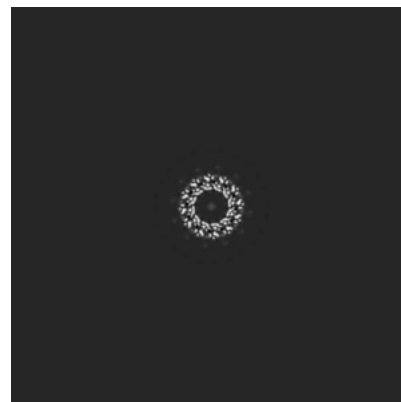
6.2.2 Raw map



X Index: 220



Y Index: 220

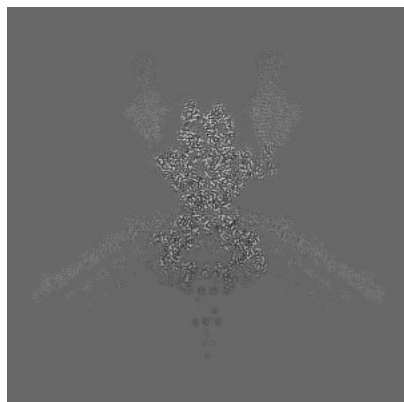


Z Index: 220

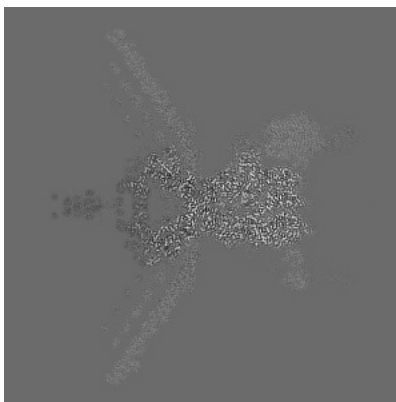
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

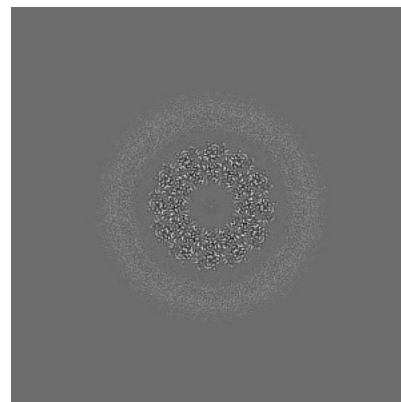
6.3.1 Primary map



X Index: 244



Y Index: 241

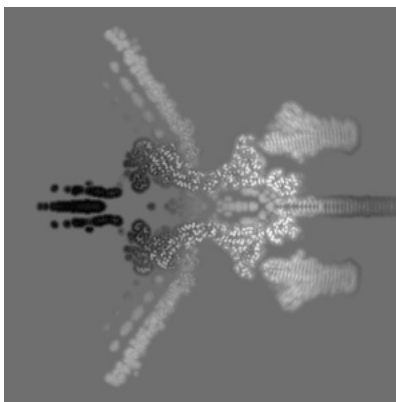


Z Index: 182

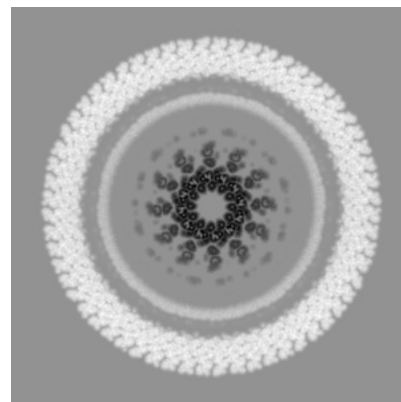
6.3.2 Raw map



X Index: 236



Y Index: 221

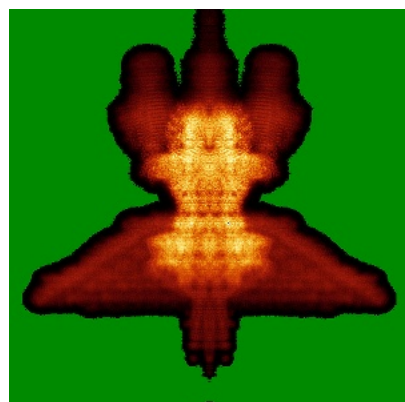


Z Index: 143

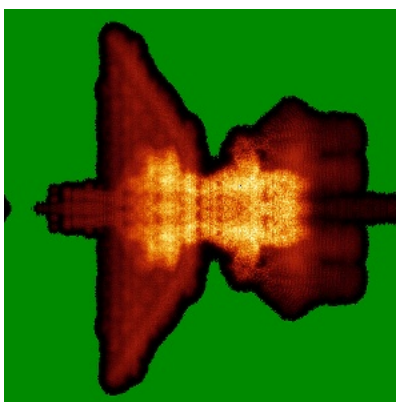
The images above show the largest variance slices of the map in three orthogonal directions.

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

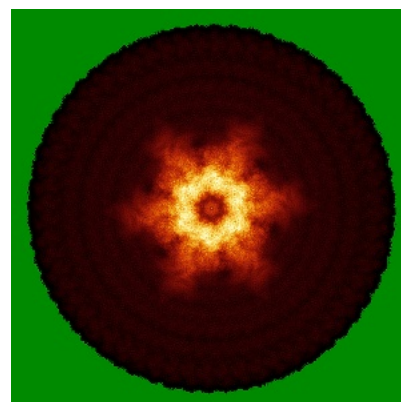
6.4.1 Primary map



X

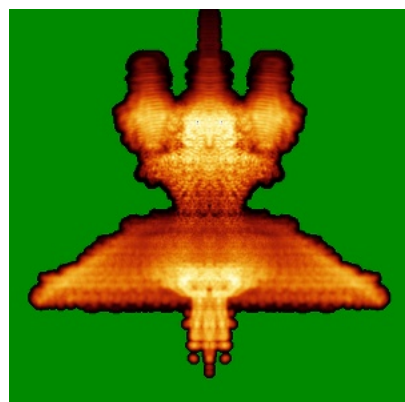


Y

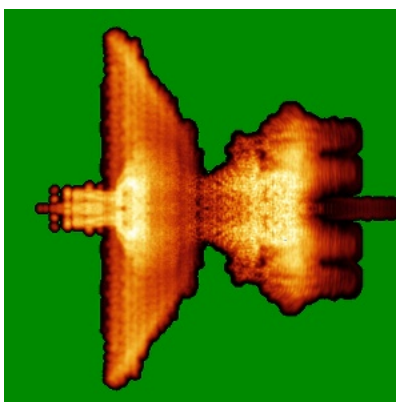


Z

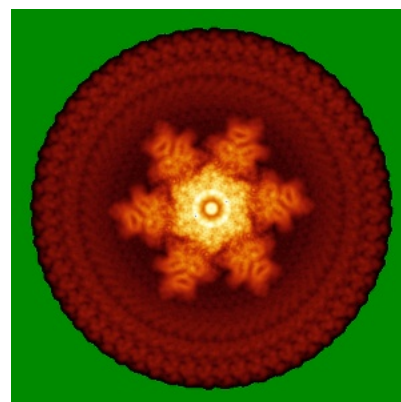
6.4.2 Raw map



X



Y

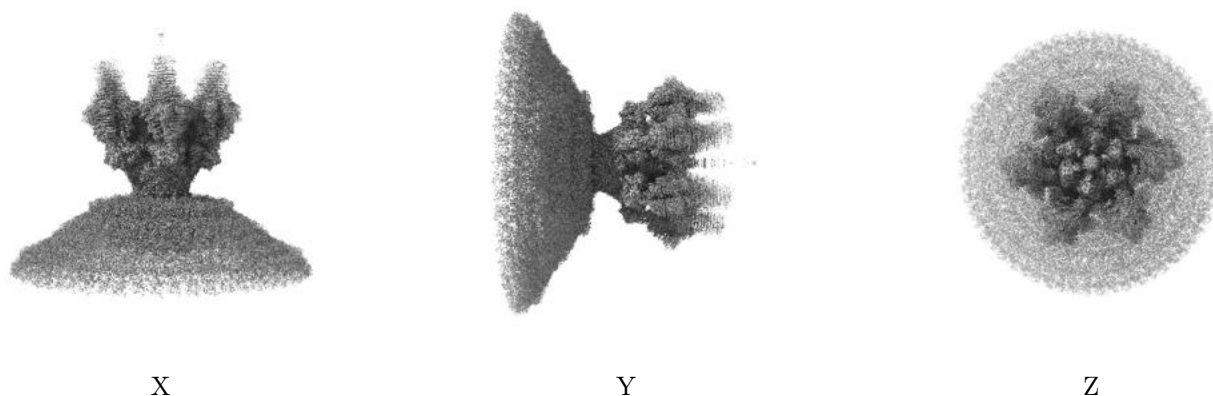


Z

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.

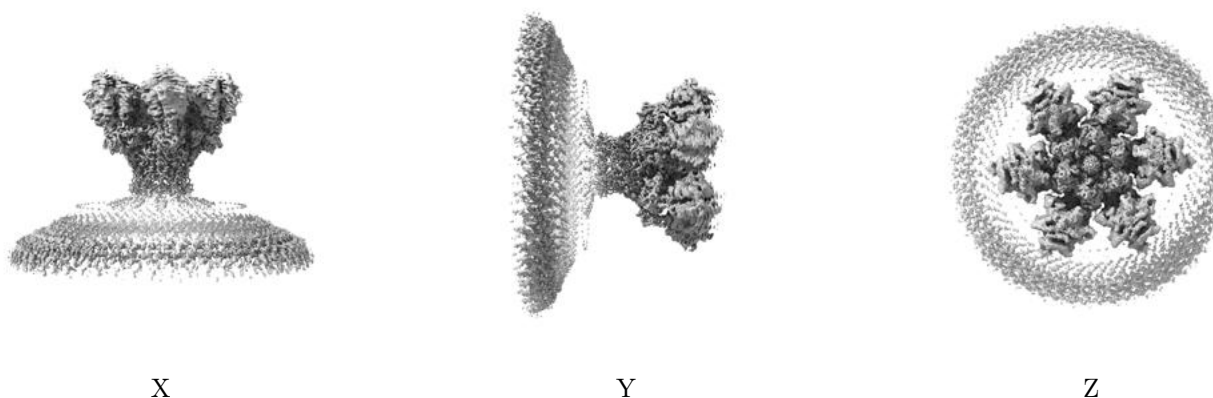
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. 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.

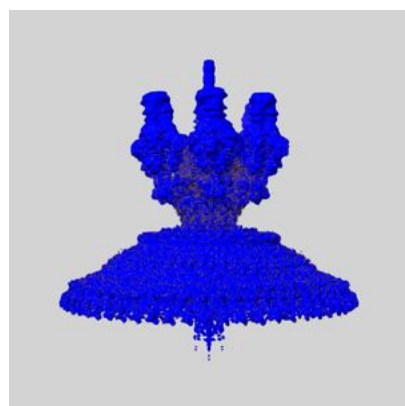
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

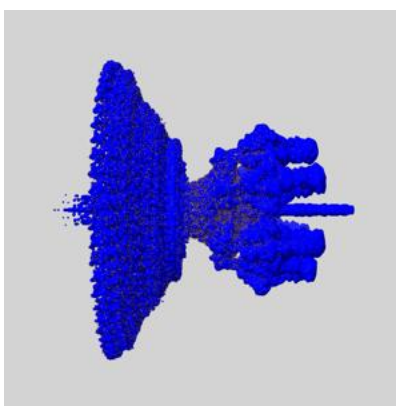
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

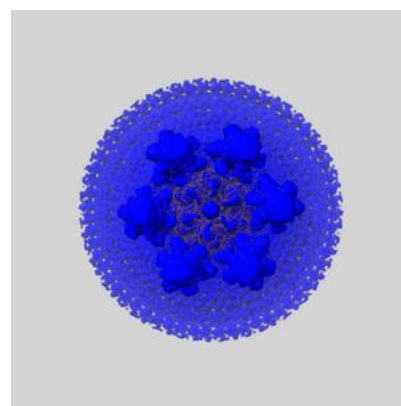
6.6.1 emd_41649_msk_1.map [i](#)



X



Y

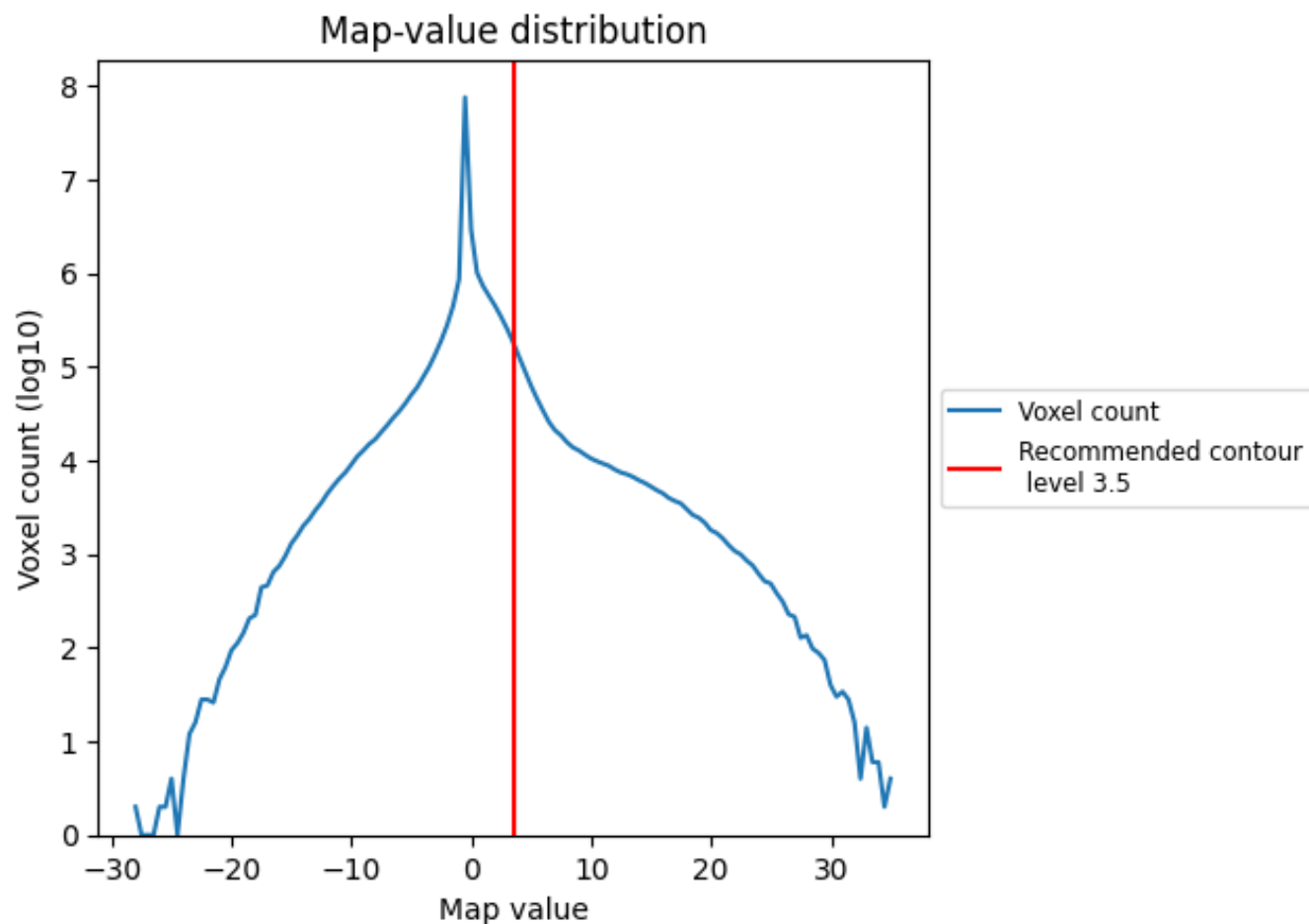


Z

7 Map analysis [i](#)

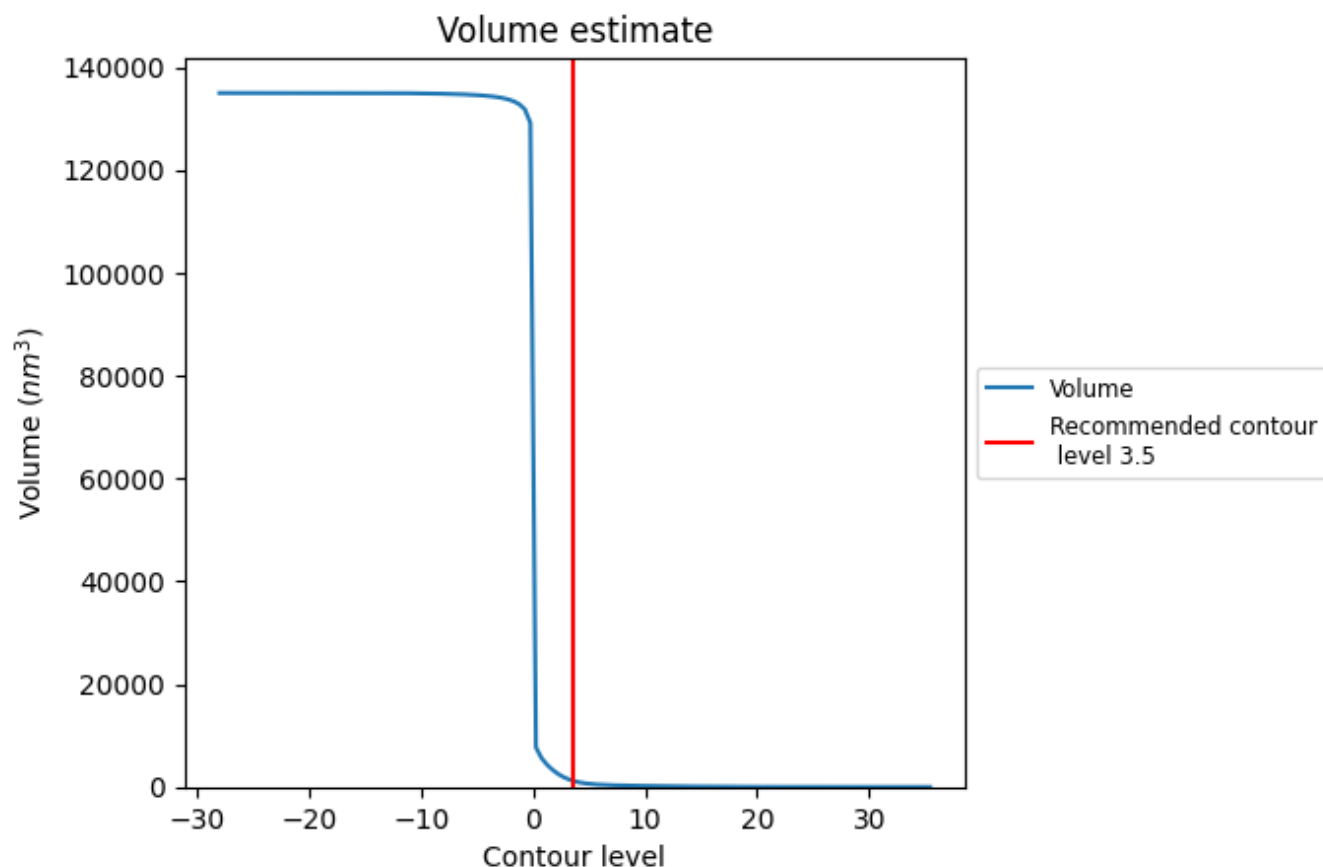
This section contains the results of statistical analysis of the map.

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.

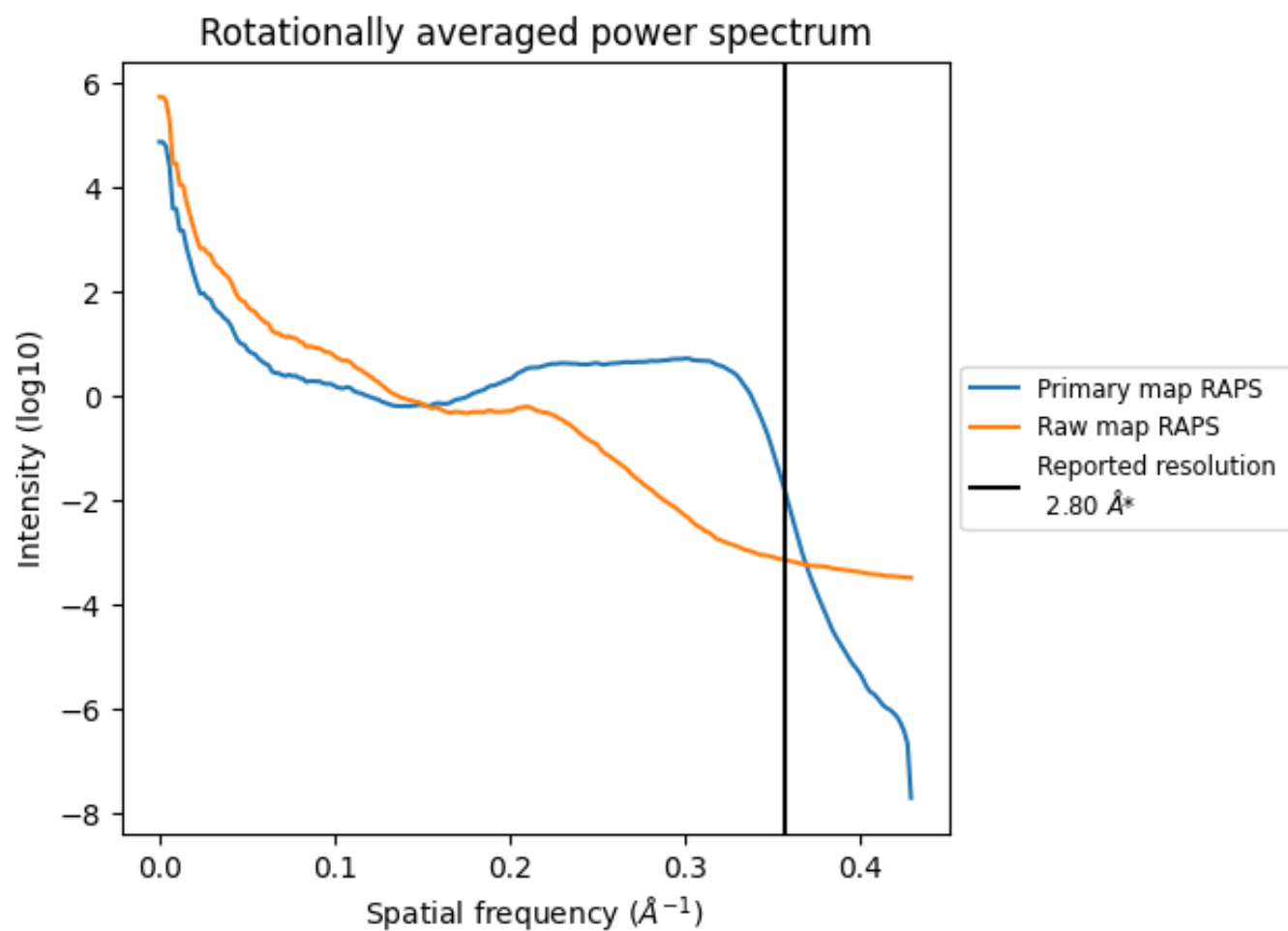
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1261 nm³; this corresponds to an approximate mass of 1139 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 ⓘ

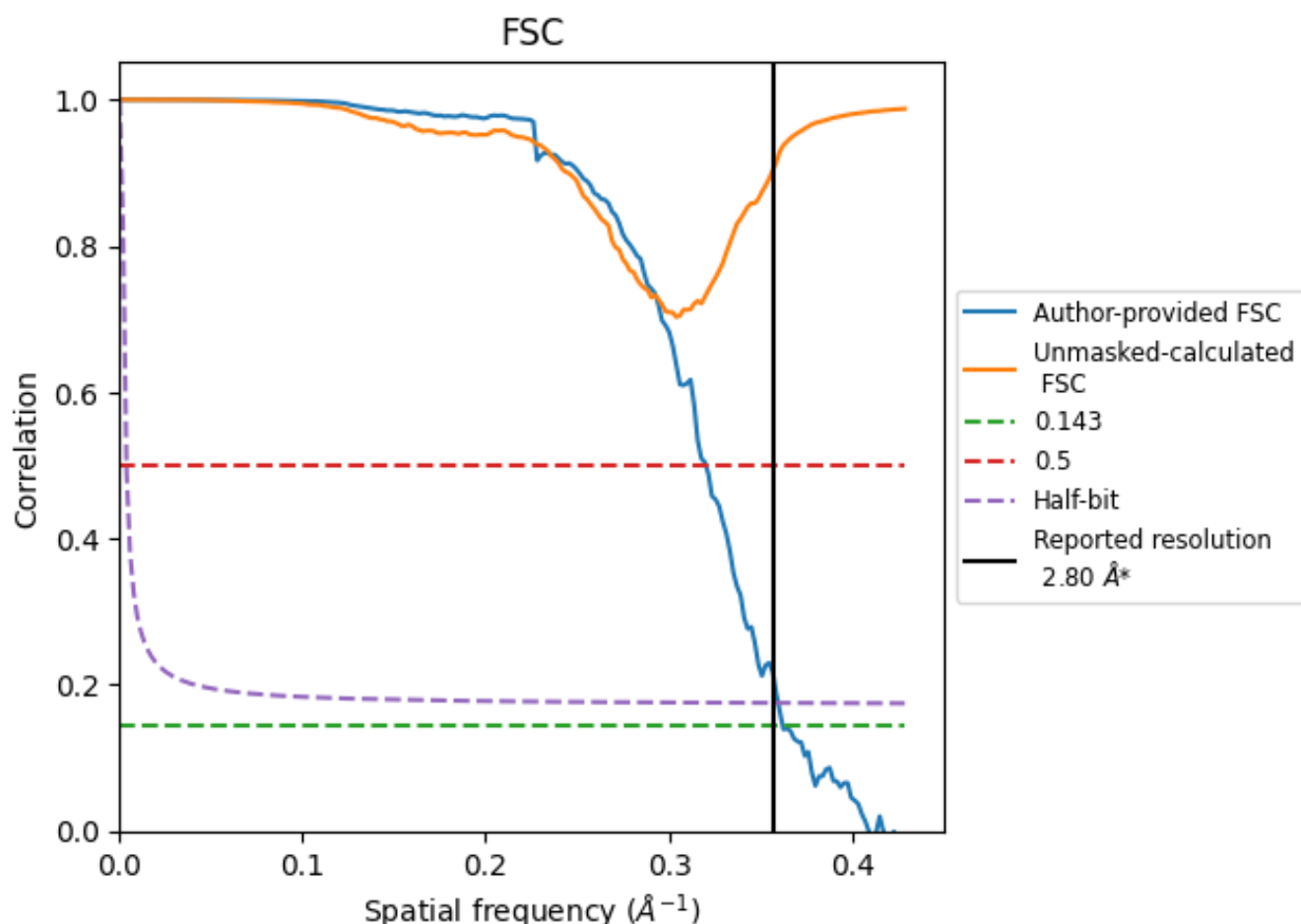


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

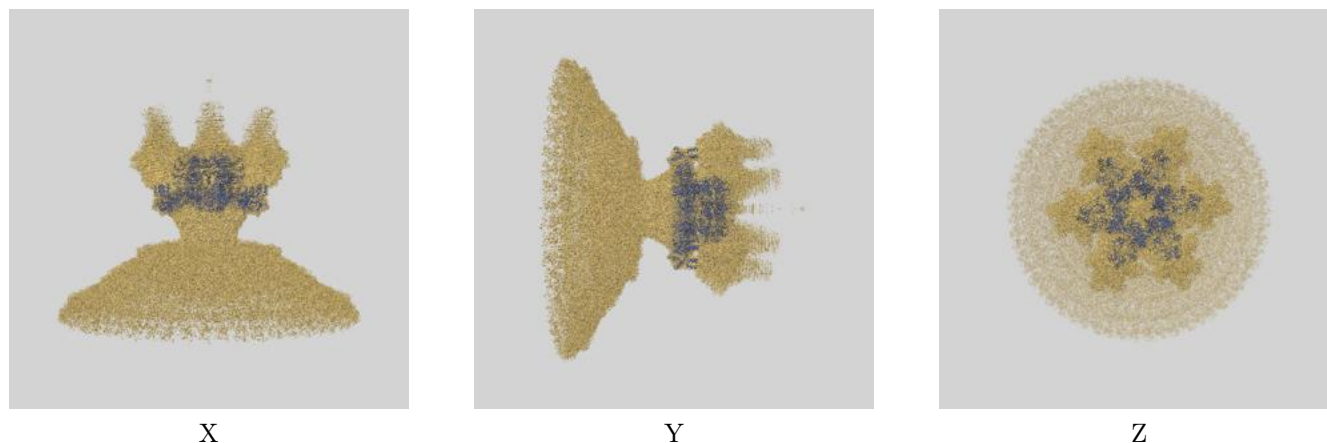
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.12	2.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

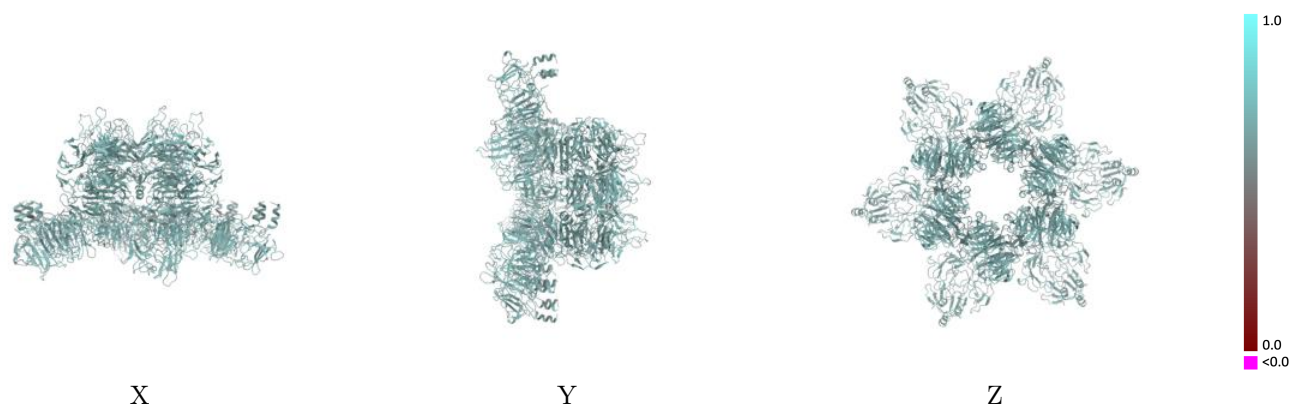
This section contains information regarding the fit between EMDB map EMD-41649 and PDB model 8TVR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



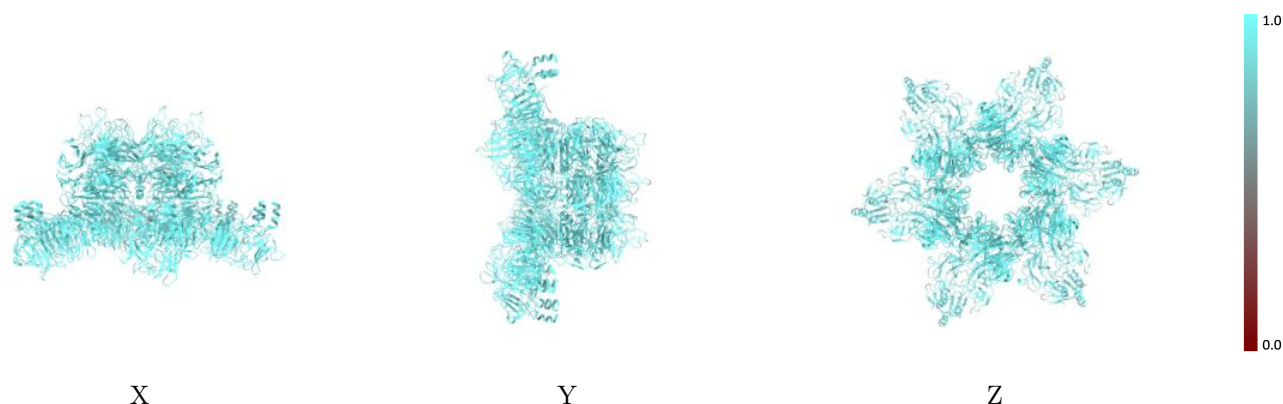
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



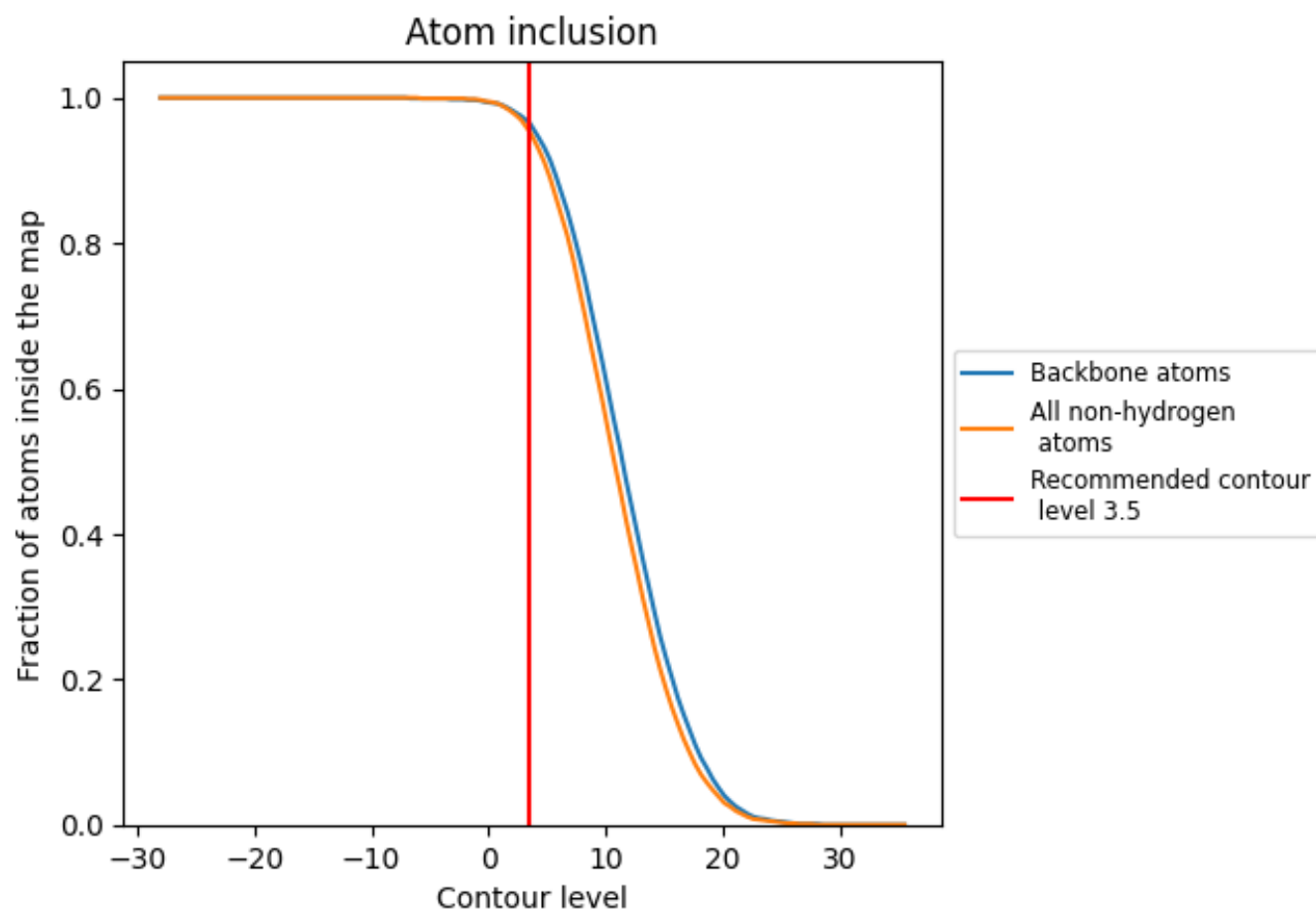
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.6270
A	 0.8980	 0.6060
B	 0.9520	 0.6230
C	 0.9510	 0.6290
D	 0.8940	 0.6060
E	 0.9520	 0.6250
F	 0.9530	 0.6280
G	 0.9680	 0.6320
H	 0.8990	 0.6080
I	 0.9470	 0.6270
J	 0.9530	 0.6280
K	 0.9690	 0.6340
L	 0.8990	 0.6070
M	 0.9490	 0.6260
N	 0.9520	 0.6300
O	 0.9670	 0.6340
P	 0.8910	 0.6080
Q	 0.9510	 0.6230
R	 0.9510	 0.6310
S	 0.9670	 0.6330
T	 0.9680	 0.6310
V	 0.8980	 0.6070
W	 0.9500	 0.6230
X	 0.9480	 0.6280
Y	 0.9680	 0.6330

