



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:34 PM UTC

PDB ID : 8RT6 / pdb_00008rt6
EMDB ID : EMD-19480
Title : Conformation-A of the full-length outer membrane core complex (TrwH/VirB7, TrwF/VirB9, TrwE/VirB10CTD) from the fully-assembled R388 type IV secretion system determined by cryo-EM.
Authors : Mace, K.; Waksman, G.
Deposited on : 2024-01-25
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

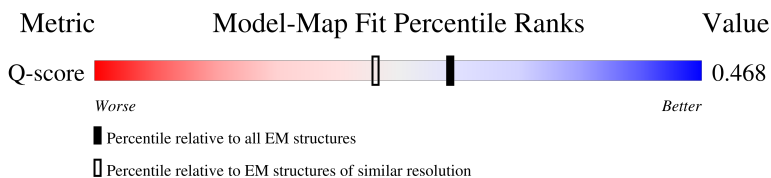
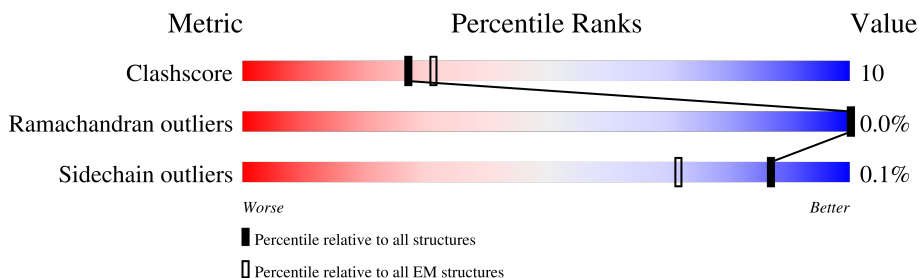
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.18 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14470 (2.68 - 3.68)

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	395	
1	D	395	
1	G	395	
1	J	395	

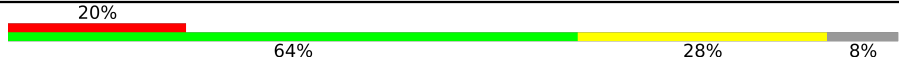


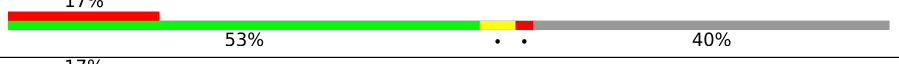

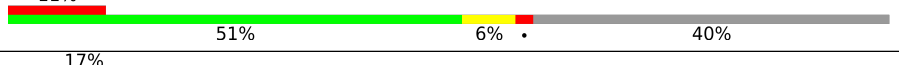
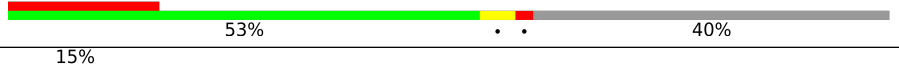
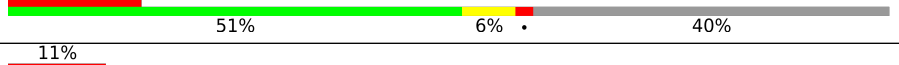
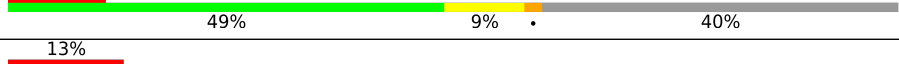


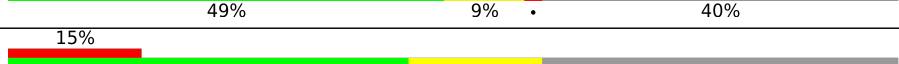
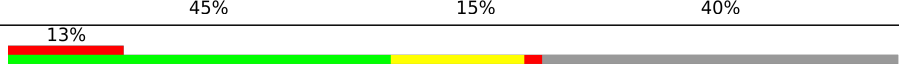

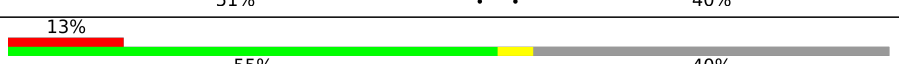
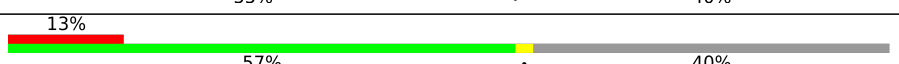
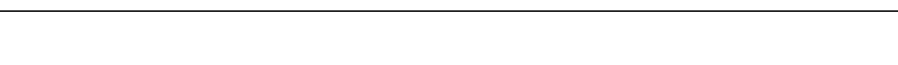
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Mol	Chain	Length	Quality of chain
1	M	395	9% 45% 11% 44%
1	P	395	8% 47% 9% 44%
1	S	395	8% 48% 8% 44%
1	V	395	9% 46% 10% 44%
1	Y	395	9% 46% 10% 44%
1	b	395	8% 45% 11% 44%
1	e	395	10% 46% 10% 44%
1	h	395	9% 45% 11% 44%
1	k	395	8% 49% 7% 44%
1	n	395	7% 47% 9% 44%
1	u	395	5% 95%
1	y	395	95%
2	B	266	25% 67% 26% 8%
2	E	266	18% 65% 27% 8%
2	H	266	18% 66% 26% 8%
2	K	266	17% 74% 18% 8%
2	N	266	14% 71% 21% 8%
2	Q	266	21% 67% 26% 8%
2	T	266	22% 73% 19% 8%
2	W	266	32% 68% 24% 8%
2	Z	266	27% 63% 29% 8%
2	c	266	20% 60% 32% 8%
2	f	266	18% 64% 29% 8%
2	i	266	16% 68% 24% 8%
2	l	266	17% 68% 25% 8%

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Mol	Chain	Length	Quality of chain
2	o	266	
2	v	266	
2	z	266	
3	C	47	
3	F	47	
3	I	47	
3	L	47	
3	O	47	
3	R	47	
3	U	47	
3	X	47	
3	a	47	
3	d	47	
3	g	47	
3	j	47	
3	m	47	
3	p	47	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 55802 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 TrwE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	221	1670	1038	306	319	7	0	0
1	D	221	1670	1038	306	319	7	0	0
1	G	221	1670	1038	306	319	7	0	0
1	J	221	1670	1038	306	319	7	0	0
1	M	221	1670	1038	306	319	7	0	0
1	P	221	1670	1038	306	319	7	0	0
1	S	221	1670	1038	306	319	7	0	0
1	V	221	1670	1038	306	319	7	0	0
1	Y	221	1670	1038	306	319	7	0	0
1	b	221	1670	1038	306	319	7	0	0
1	e	221	1670	1038	306	319	7	0	0
1	h	221	1670	1038	306	319	7	0	0
1	k	221	1670	1038	306	319	7	0	0
1	n	221	1670	1038	306	319	7	0	0
1	u	19	149	92	29	27	1	0	0
1	y	19	149	92	29	27	1	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ASP	ASN	conflict	UNP O50337
D	335	ASP	ASN	conflict	UNP O50337
G	335	ASP	ASN	conflict	UNP O50337
J	335	ASP	ASN	conflict	UNP O50337
M	335	ASP	ASN	conflict	UNP O50337
P	335	ASP	ASN	conflict	UNP O50337
S	335	ASP	ASN	conflict	UNP O50337
V	335	ASP	ASN	conflict	UNP O50337
Y	335	ASP	ASN	conflict	UNP O50337
b	335	ASP	ASN	conflict	UNP O50337
e	335	ASP	ASN	conflict	UNP O50337
h	335	ASP	ASN	conflict	UNP O50337
k	335	ASP	ASN	conflict	UNP O50337
n	335	ASP	ASN	conflict	UNP O50337
u	335	ASP	ASN	conflict	UNP O50337
y	335	ASP	ASN	conflict	UNP O50337

- Molecule 2 is a protein called TrwF protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	246	1955	1226	356	367	6	0	0
2	E	246	1955	1226	356	367	6	0	0
2	H	246	1955	1226	356	367	6	0	0
2	K	246	1955	1226	356	367	6	0	0
2	N	246	1955	1226	356	367	6	0	0
2	Q	246	1955	1226	356	367	6	0	0
2	T	246	1955	1226	356	367	6	0	0
2	W	246	1955	1226	356	367	6	0	0
2	Z	246	1955	1226	356	367	6	0	0
2	c	246	1955	1226	356	367	6	0	0
2	f	246	1955	1226	356	367	6	0	0
2	i	246	1955	1226	356	367	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	246	Total	C	N	O	S	0	0
			1955	1226	356	367	6		
2	o	246	Total	C	N	O	S	0	0
			1955	1226	356	367	6		
2	v	108	Total	C	N	O	S	0	0
			886	560	161	162	3		
2	z	108	Total	C	N	O	S	0	0
			886	560	161	162	3		

There are 304 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	ASP	ILE	conflict	UNP O50336
B	72	SER	PRO	conflict	UNP O50336
B	73	GLU	LYS	conflict	UNP O50336
B	74	ALA	PRO	conflict	UNP O50336
B	75	TYR	MET	conflict	UNP O50336
B	76	ALA	PRO	conflict	UNP O50336
B	77	PHE	LEU	conflict	UNP O50336
B	78	ALA	PRO	conflict	UNP O50336
B	79	ARG	GLY	conflict	UNP O50336
B	80	LYS	ARG	conflict	UNP O50336
B	81	GLY	ALA	conflict	UNP O50336
B	82	ARG	GLY	conflict	UNP O50336
B	83	HIS	ILE	conflict	UNP O50336
B	84	ILE	PHE	conflict	UNP O50336
B	85	PHE	LEU	conflict	UNP O50336
B	86	ILE	SER	conflict	UNP O50336
B	87	LYS	SER	conflict	UNP O50336
B	88	PRO	ARG	conflict	UNP O50336
B	89	GLN	THR	conflict	UNP O50336
E	71	ASP	ILE	conflict	UNP O50336
E	72	SER	PRO	conflict	UNP O50336
E	73	GLU	LYS	conflict	UNP O50336
E	74	ALA	PRO	conflict	UNP O50336
E	75	TYR	MET	conflict	UNP O50336
E	76	ALA	PRO	conflict	UNP O50336
E	77	PHE	LEU	conflict	UNP O50336
E	78	ALA	PRO	conflict	UNP O50336
E	79	ARG	GLY	conflict	UNP O50336
E	80	LYS	ARG	conflict	UNP O50336
E	81	GLY	ALA	conflict	UNP O50336
E	82	ARG	GLY	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
E	83	HIS	ILE	conflict	UNP O50336
E	84	ILE	PHE	conflict	UNP O50336
E	85	PHE	LEU	conflict	UNP O50336
E	86	ILE	SER	conflict	UNP O50336
E	87	LYS	SER	conflict	UNP O50336
E	88	PRO	ARG	conflict	UNP O50336
E	89	GLN	THR	conflict	UNP O50336
H	71	ASP	ILE	conflict	UNP O50336
H	72	SER	PRO	conflict	UNP O50336
H	73	GLU	LYS	conflict	UNP O50336
H	74	ALA	PRO	conflict	UNP O50336
H	75	TYR	MET	conflict	UNP O50336
H	76	ALA	PRO	conflict	UNP O50336
H	77	PHE	LEU	conflict	UNP O50336
H	78	ALA	PRO	conflict	UNP O50336
H	79	ARG	GLY	conflict	UNP O50336
H	80	LYS	ARG	conflict	UNP O50336
H	81	GLY	ALA	conflict	UNP O50336
H	82	ARG	GLY	conflict	UNP O50336
H	83	HIS	ILE	conflict	UNP O50336
H	84	ILE	PHE	conflict	UNP O50336
H	85	PHE	LEU	conflict	UNP O50336
H	86	ILE	SER	conflict	UNP O50336
H	87	LYS	SER	conflict	UNP O50336
H	88	PRO	ARG	conflict	UNP O50336
H	89	GLN	THR	conflict	UNP O50336
K	71	ASP	ILE	conflict	UNP O50336
K	72	SER	PRO	conflict	UNP O50336
K	73	GLU	LYS	conflict	UNP O50336
K	74	ALA	PRO	conflict	UNP O50336
K	75	TYR	MET	conflict	UNP O50336
K	76	ALA	PRO	conflict	UNP O50336
K	77	PHE	LEU	conflict	UNP O50336
K	78	ALA	PRO	conflict	UNP O50336
K	79	ARG	GLY	conflict	UNP O50336
K	80	LYS	ARG	conflict	UNP O50336
K	81	GLY	ALA	conflict	UNP O50336
K	82	ARG	GLY	conflict	UNP O50336
K	83	HIS	ILE	conflict	UNP O50336
K	84	ILE	PHE	conflict	UNP O50336
K	85	PHE	LEU	conflict	UNP O50336
K	86	ILE	SER	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
K	87	LYS	SER	conflict	UNP O50336
K	88	PRO	ARG	conflict	UNP O50336
K	89	GLN	THR	conflict	UNP O50336
N	71	ASP	ILE	conflict	UNP O50336
N	72	SER	PRO	conflict	UNP O50336
N	73	GLU	LYS	conflict	UNP O50336
N	74	ALA	PRO	conflict	UNP O50336
N	75	TYR	MET	conflict	UNP O50336
N	76	ALA	PRO	conflict	UNP O50336
N	77	PHE	LEU	conflict	UNP O50336
N	78	ALA	PRO	conflict	UNP O50336
N	79	ARG	GLY	conflict	UNP O50336
N	80	LYS	ARG	conflict	UNP O50336
N	81	GLY	ALA	conflict	UNP O50336
N	82	ARG	GLY	conflict	UNP O50336
N	83	HIS	ILE	conflict	UNP O50336
N	84	ILE	PHE	conflict	UNP O50336
N	85	PHE	LEU	conflict	UNP O50336
N	86	ILE	SER	conflict	UNP O50336
N	87	LYS	SER	conflict	UNP O50336
N	88	PRO	ARG	conflict	UNP O50336
N	89	GLN	THR	conflict	UNP O50336
Q	71	ASP	ILE	conflict	UNP O50336
Q	72	SER	PRO	conflict	UNP O50336
Q	73	GLU	LYS	conflict	UNP O50336
Q	74	ALA	PRO	conflict	UNP O50336
Q	75	TYR	MET	conflict	UNP O50336
Q	76	ALA	PRO	conflict	UNP O50336
Q	77	PHE	LEU	conflict	UNP O50336
Q	78	ALA	PRO	conflict	UNP O50336
Q	79	ARG	GLY	conflict	UNP O50336
Q	80	LYS	ARG	conflict	UNP O50336
Q	81	GLY	ALA	conflict	UNP O50336
Q	82	ARG	GLY	conflict	UNP O50336
Q	83	HIS	ILE	conflict	UNP O50336
Q	84	ILE	PHE	conflict	UNP O50336
Q	85	PHE	LEU	conflict	UNP O50336
Q	86	ILE	SER	conflict	UNP O50336
Q	87	LYS	SER	conflict	UNP O50336
Q	88	PRO	ARG	conflict	UNP O50336
Q	89	GLN	THR	conflict	UNP O50336
T	71	ASP	ILE	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
T	72	SER	PRO	conflict	UNP O50336
T	73	GLU	LYS	conflict	UNP O50336
T	74	ALA	PRO	conflict	UNP O50336
T	75	TYR	MET	conflict	UNP O50336
T	76	ALA	PRO	conflict	UNP O50336
T	77	PHE	LEU	conflict	UNP O50336
T	78	ALA	PRO	conflict	UNP O50336
T	79	ARG	GLY	conflict	UNP O50336
T	80	LYS	ARG	conflict	UNP O50336
T	81	GLY	ALA	conflict	UNP O50336
T	82	ARG	GLY	conflict	UNP O50336
T	83	HIS	ILE	conflict	UNP O50336
T	84	ILE	PHE	conflict	UNP O50336
T	85	PHE	LEU	conflict	UNP O50336
T	86	ILE	SER	conflict	UNP O50336
T	87	LYS	SER	conflict	UNP O50336
T	88	PRO	ARG	conflict	UNP O50336
T	89	GLN	THR	conflict	UNP O50336
W	71	ASP	ILE	conflict	UNP O50336
W	72	SER	PRO	conflict	UNP O50336
W	73	GLU	LYS	conflict	UNP O50336
W	74	ALA	PRO	conflict	UNP O50336
W	75	TYR	MET	conflict	UNP O50336
W	76	ALA	PRO	conflict	UNP O50336
W	77	PHE	LEU	conflict	UNP O50336
W	78	ALA	PRO	conflict	UNP O50336
W	79	ARG	GLY	conflict	UNP O50336
W	80	LYS	ARG	conflict	UNP O50336
W	81	GLY	ALA	conflict	UNP O50336
W	82	ARG	GLY	conflict	UNP O50336
W	83	HIS	ILE	conflict	UNP O50336
W	84	ILE	PHE	conflict	UNP O50336
W	85	PHE	LEU	conflict	UNP O50336
W	86	ILE	SER	conflict	UNP O50336
W	87	LYS	SER	conflict	UNP O50336
W	88	PRO	ARG	conflict	UNP O50336
W	89	GLN	THR	conflict	UNP O50336
Z	71	ASP	ILE	conflict	UNP O50336
Z	72	SER	PRO	conflict	UNP O50336
Z	73	GLU	LYS	conflict	UNP O50336
Z	74	ALA	PRO	conflict	UNP O50336
Z	75	TYR	MET	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	76	ALA	PRO	conflict	UNP O50336
Z	77	PHE	LEU	conflict	UNP O50336
Z	78	ALA	PRO	conflict	UNP O50336
Z	79	ARG	GLY	conflict	UNP O50336
Z	80	LYS	ARG	conflict	UNP O50336
Z	81	GLY	ALA	conflict	UNP O50336
Z	82	ARG	GLY	conflict	UNP O50336
Z	83	HIS	ILE	conflict	UNP O50336
Z	84	ILE	PHE	conflict	UNP O50336
Z	85	PHE	LEU	conflict	UNP O50336
Z	86	ILE	SER	conflict	UNP O50336
Z	87	LYS	SER	conflict	UNP O50336
Z	88	PRO	ARG	conflict	UNP O50336
Z	89	GLN	THR	conflict	UNP O50336
c	71	ASP	ILE	conflict	UNP O50336
c	72	SER	PRO	conflict	UNP O50336
c	73	GLU	LYS	conflict	UNP O50336
c	74	ALA	PRO	conflict	UNP O50336
c	75	TYR	MET	conflict	UNP O50336
c	76	ALA	PRO	conflict	UNP O50336
c	77	PHE	LEU	conflict	UNP O50336
c	78	ALA	PRO	conflict	UNP O50336
c	79	ARG	GLY	conflict	UNP O50336
c	80	LYS	ARG	conflict	UNP O50336
c	81	GLY	ALA	conflict	UNP O50336
c	82	ARG	GLY	conflict	UNP O50336
c	83	HIS	ILE	conflict	UNP O50336
c	84	ILE	PHE	conflict	UNP O50336
c	85	PHE	LEU	conflict	UNP O50336
c	86	ILE	SER	conflict	UNP O50336
c	87	LYS	SER	conflict	UNP O50336
c	88	PRO	ARG	conflict	UNP O50336
c	89	GLN	THR	conflict	UNP O50336
f	71	ASP	ILE	conflict	UNP O50336
f	72	SER	PRO	conflict	UNP O50336
f	73	GLU	LYS	conflict	UNP O50336
f	74	ALA	PRO	conflict	UNP O50336
f	75	TYR	MET	conflict	UNP O50336
f	76	ALA	PRO	conflict	UNP O50336
f	77	PHE	LEU	conflict	UNP O50336
f	78	ALA	PRO	conflict	UNP O50336
f	79	ARG	GLY	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
f	80	LYS	ARG	conflict	UNP O50336
f	81	GLY	ALA	conflict	UNP O50336
f	82	ARG	GLY	conflict	UNP O50336
f	83	HIS	ILE	conflict	UNP O50336
f	84	ILE	PHE	conflict	UNP O50336
f	85	PHE	LEU	conflict	UNP O50336
f	86	ILE	SER	conflict	UNP O50336
f	87	LYS	SER	conflict	UNP O50336
f	88	PRO	ARG	conflict	UNP O50336
f	89	GLN	THR	conflict	UNP O50336
i	71	ASP	ILE	conflict	UNP O50336
i	72	SER	PRO	conflict	UNP O50336
i	73	GLU	LYS	conflict	UNP O50336
i	74	ALA	PRO	conflict	UNP O50336
i	75	TYR	MET	conflict	UNP O50336
i	76	ALA	PRO	conflict	UNP O50336
i	77	PHE	LEU	conflict	UNP O50336
i	78	ALA	PRO	conflict	UNP O50336
i	79	ARG	GLY	conflict	UNP O50336
i	80	LYS	ARG	conflict	UNP O50336
i	81	GLY	ALA	conflict	UNP O50336
i	82	ARG	GLY	conflict	UNP O50336
i	83	HIS	ILE	conflict	UNP O50336
i	84	ILE	PHE	conflict	UNP O50336
i	85	PHE	LEU	conflict	UNP O50336
i	86	ILE	SER	conflict	UNP O50336
i	87	LYS	SER	conflict	UNP O50336
i	88	PRO	ARG	conflict	UNP O50336
i	89	GLN	THR	conflict	UNP O50336
l	71	ASP	ILE	conflict	UNP O50336
l	72	SER	PRO	conflict	UNP O50336
l	73	GLU	LYS	conflict	UNP O50336
l	74	ALA	PRO	conflict	UNP O50336
l	75	TYR	MET	conflict	UNP O50336
l	76	ALA	PRO	conflict	UNP O50336
l	77	PHE	LEU	conflict	UNP O50336
l	78	ALA	PRO	conflict	UNP O50336
l	79	ARG	GLY	conflict	UNP O50336
l	80	LYS	ARG	conflict	UNP O50336
l	81	GLY	ALA	conflict	UNP O50336
l	82	ARG	GLY	conflict	UNP O50336
l	83	HIS	ILE	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
l	84	ILE	PHE	conflict	UNP O50336
l	85	PHE	LEU	conflict	UNP O50336
l	86	ILE	SER	conflict	UNP O50336
l	87	LYS	SER	conflict	UNP O50336
l	88	PRO	ARG	conflict	UNP O50336
l	89	GLN	THR	conflict	UNP O50336
o	71	ASP	ILE	conflict	UNP O50336
o	72	SER	PRO	conflict	UNP O50336
o	73	GLU	LYS	conflict	UNP O50336
o	74	ALA	PRO	conflict	UNP O50336
o	75	TYR	MET	conflict	UNP O50336
o	76	ALA	PRO	conflict	UNP O50336
o	77	PHE	LEU	conflict	UNP O50336
o	78	ALA	PRO	conflict	UNP O50336
o	79	ARG	GLY	conflict	UNP O50336
o	80	LYS	ARG	conflict	UNP O50336
o	81	GLY	ALA	conflict	UNP O50336
o	82	ARG	GLY	conflict	UNP O50336
o	83	HIS	ILE	conflict	UNP O50336
o	84	ILE	PHE	conflict	UNP O50336
o	85	PHE	LEU	conflict	UNP O50336
o	86	ILE	SER	conflict	UNP O50336
o	87	LYS	SER	conflict	UNP O50336
o	88	PRO	ARG	conflict	UNP O50336
o	89	GLN	THR	conflict	UNP O50336
v	71	ASP	ILE	conflict	UNP O50336
v	72	SER	PRO	conflict	UNP O50336
v	73	GLU	LYS	conflict	UNP O50336
v	74	ALA	PRO	conflict	UNP O50336
v	75	TYR	MET	conflict	UNP O50336
v	76	ALA	PRO	conflict	UNP O50336
v	77	PHE	LEU	conflict	UNP O50336
v	78	ALA	PRO	conflict	UNP O50336
v	79	ARG	GLY	conflict	UNP O50336
v	80	LYS	ARG	conflict	UNP O50336
v	81	GLY	ALA	conflict	UNP O50336
v	82	ARG	GLY	conflict	UNP O50336
v	83	HIS	ILE	conflict	UNP O50336
v	84	ILE	PHE	conflict	UNP O50336
v	85	PHE	LEU	conflict	UNP O50336
v	86	ILE	SER	conflict	UNP O50336
v	87	LYS	SER	conflict	UNP O50336

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Chain	Residue	Modelled	Actual	Comment	Reference
v	88	PRO	ARG	conflict	UNP O50336
v	89	GLN	THR	conflict	UNP O50336
z	71	ASP	ILE	conflict	UNP O50336
z	72	SER	PRO	conflict	UNP O50336
z	73	GLU	LYS	conflict	UNP O50336
z	74	ALA	PRO	conflict	UNP O50336
z	75	TYR	MET	conflict	UNP O50336
z	76	ALA	PRO	conflict	UNP O50336
z	77	PHE	LEU	conflict	UNP O50336
z	78	ALA	PRO	conflict	UNP O50336
z	79	ARG	GLY	conflict	UNP O50336
z	80	LYS	ARG	conflict	UNP O50336
z	81	GLY	ALA	conflict	UNP O50336
z	82	ARG	GLY	conflict	UNP O50336
z	83	HIS	ILE	conflict	UNP O50336
z	84	ILE	PHE	conflict	UNP O50336
z	85	PHE	LEU	conflict	UNP O50336
z	86	ILE	SER	conflict	UNP O50336
z	87	LYS	SER	conflict	UNP O50336
z	88	PRO	ARG	conflict	UNP O50336
z	89	GLN	THR	conflict	UNP O50336

- Molecule 3 is a protein called TrwH protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	F	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	I	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	L	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	O	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	R	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	U	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	X	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	a	28	Total	C	N	O	S	0	0
			213	133	38	41	1		

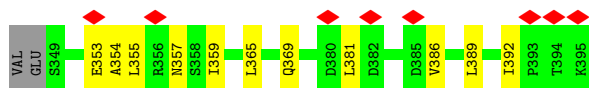
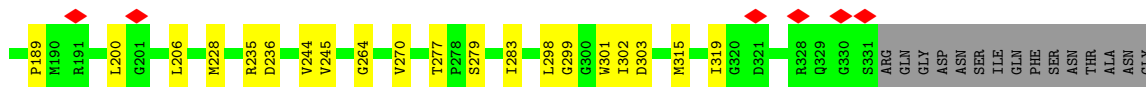
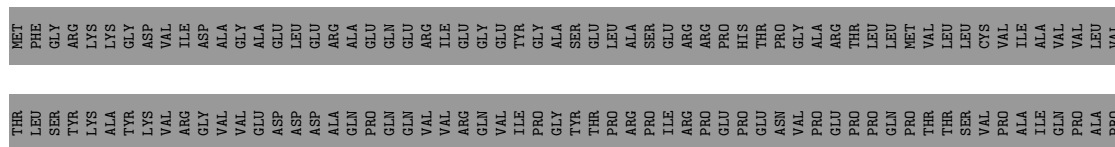
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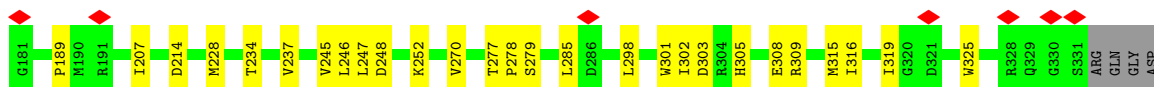
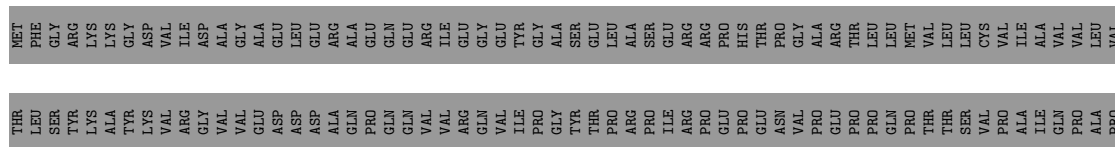
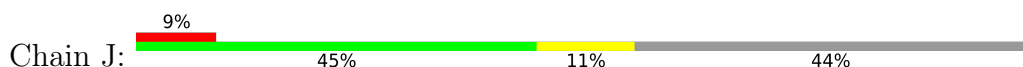
Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	g	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	j	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	m	28	Total	C	N	O	S	0	0
			213	133	38	41	1		
3	p	28	Total	C	N	O	S	0	0
			213	133	38	41	1		



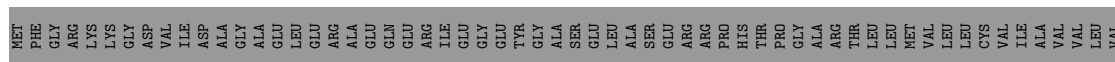
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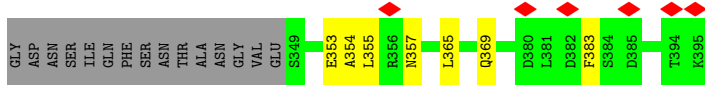


• Molecule 1: TrwE protein

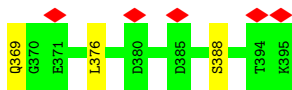
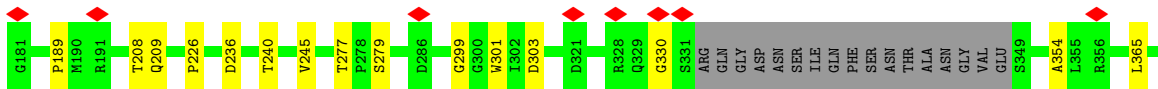
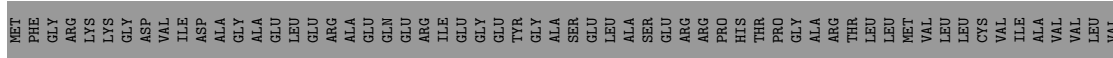


• Molecule 1: TrwE protein

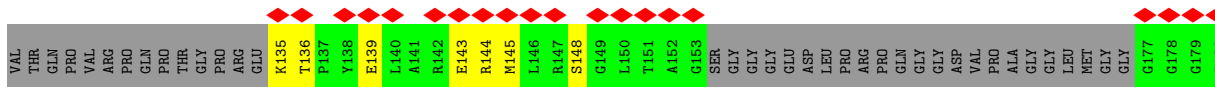
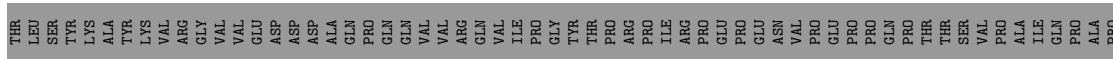
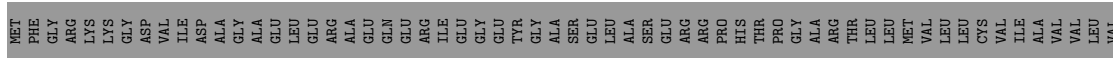




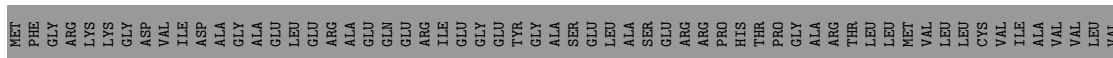
• Molecule 1: TrwE protein

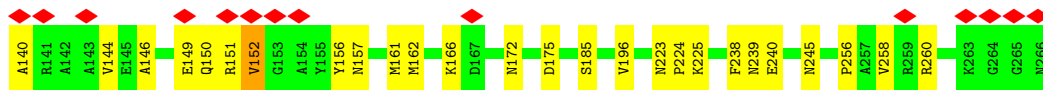


• Molecule 1: TrwE protein

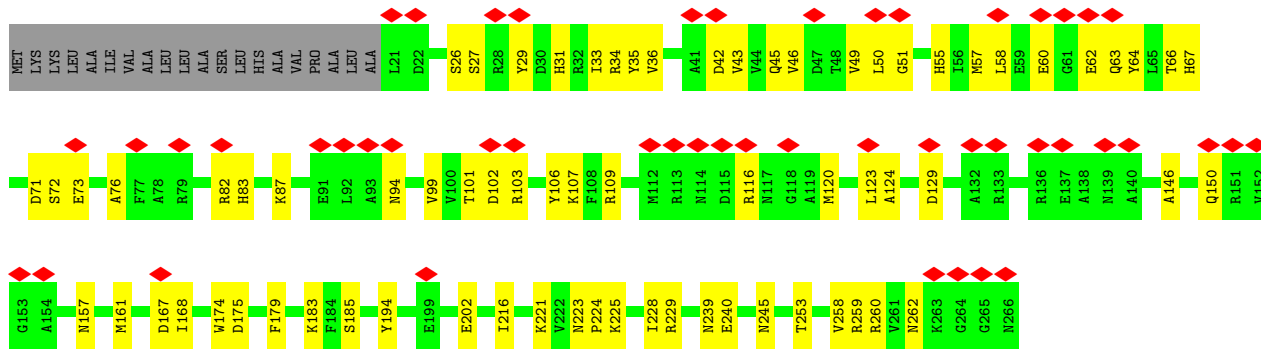


• Molecule 1: TrwE protein

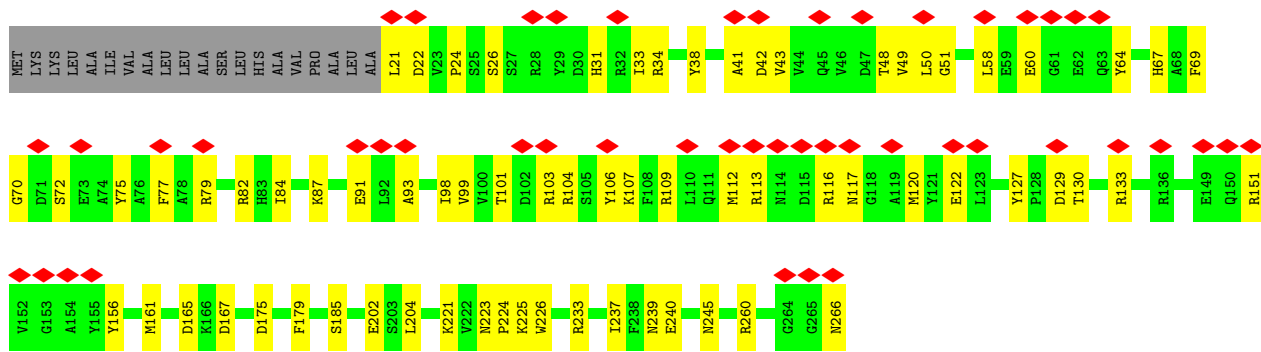




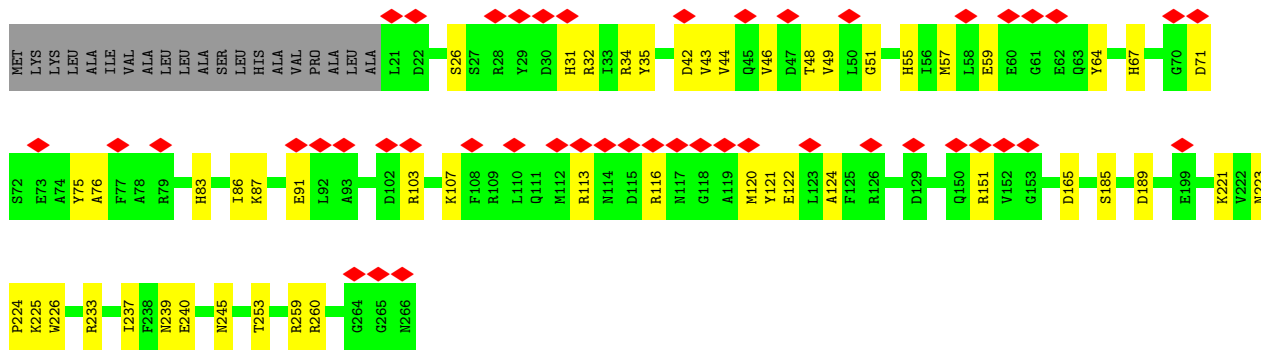
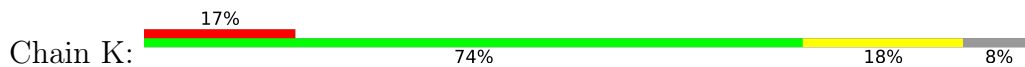
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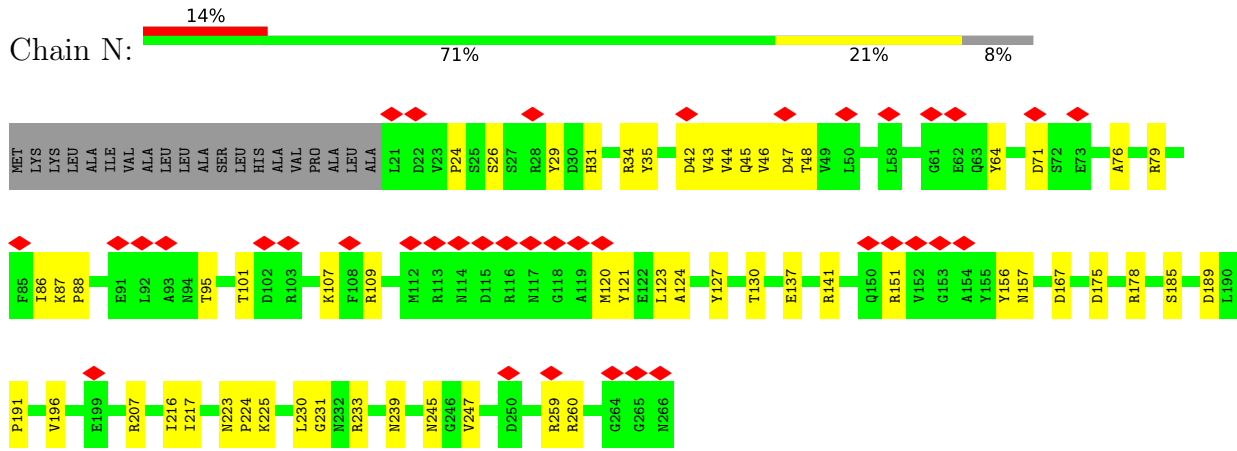
• Molecule 2: TrwF protein



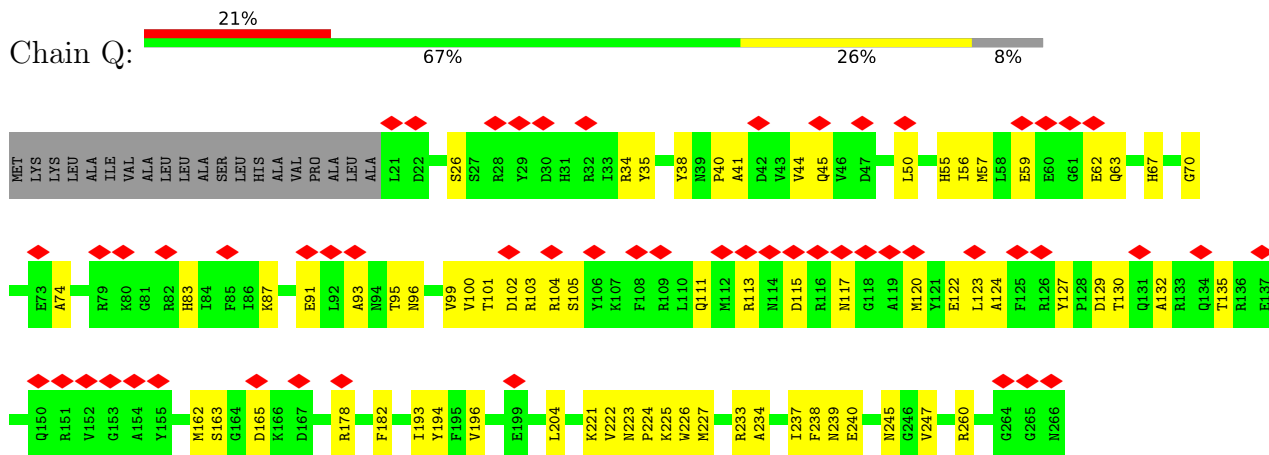
• Molecule 2: TrwF protein



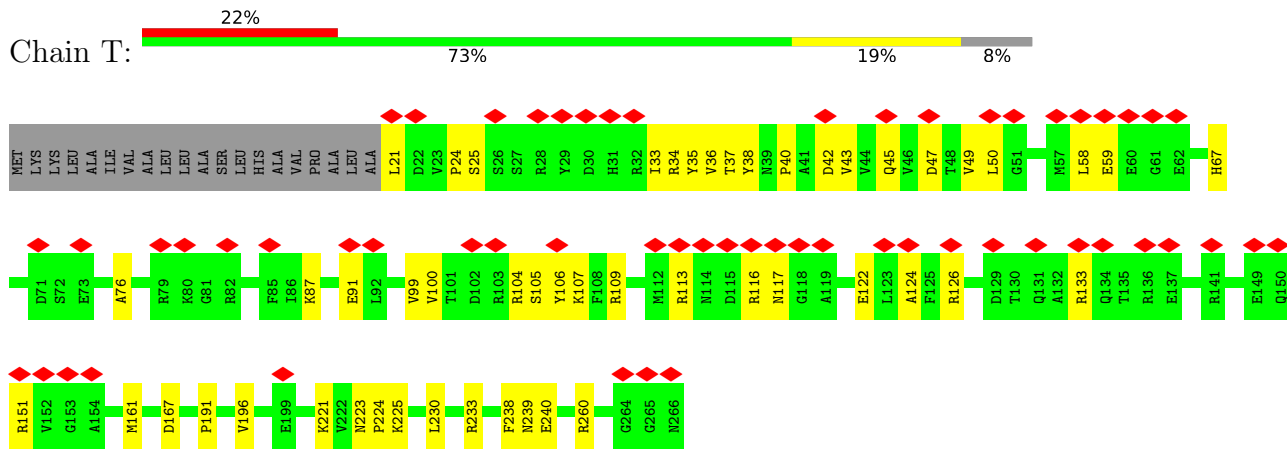
• Molecule 2: TrwF protein



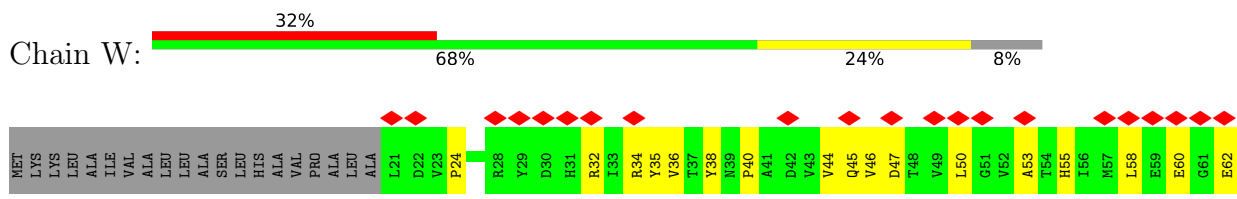
• Molecule 2: TrwF protein

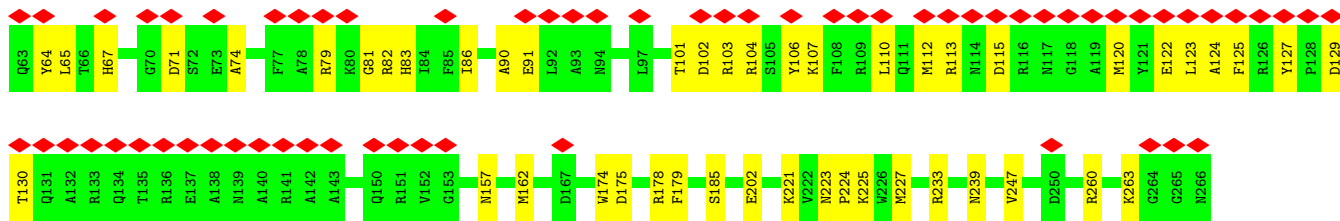


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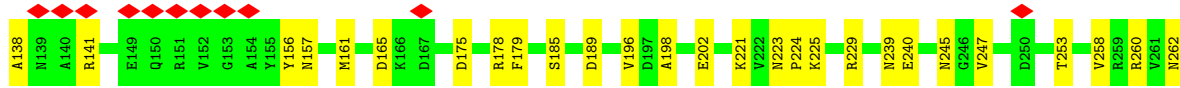
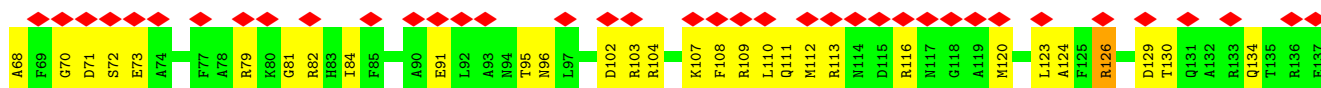
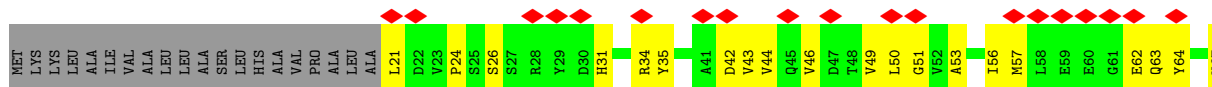


• Molecule 2: TrwF protein

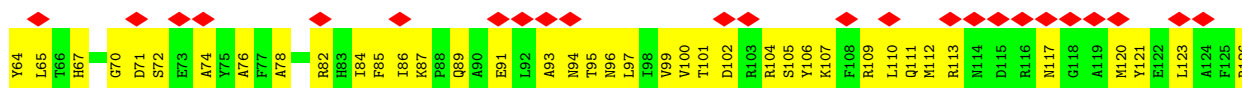
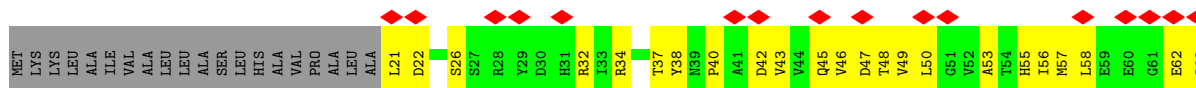




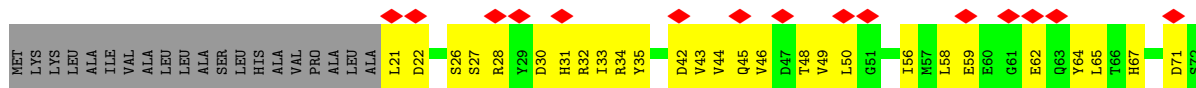
• Molecule 2: TrwF protein

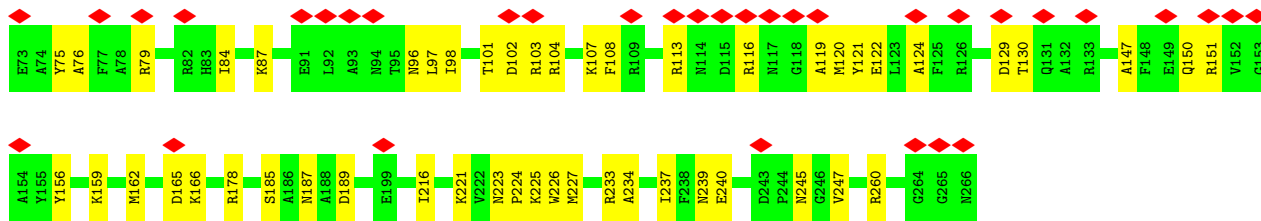


• Molecule 2: TrwF protein

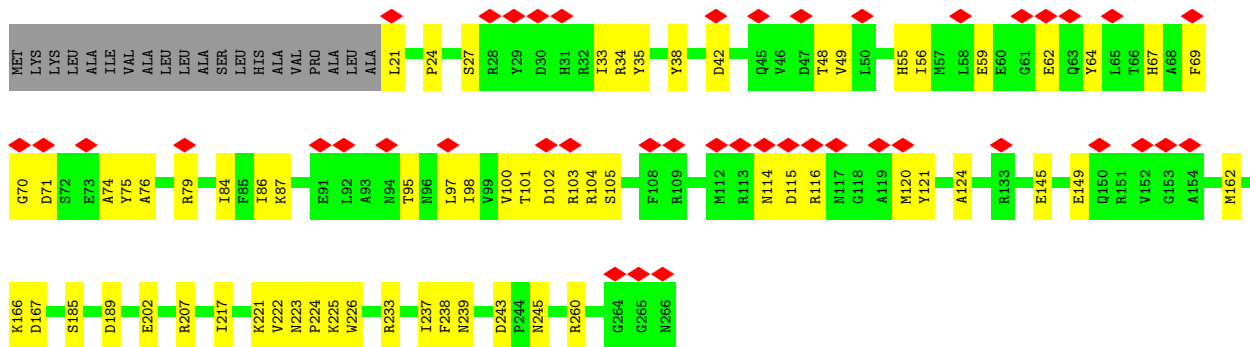


• Molecule 2: TrwF protein

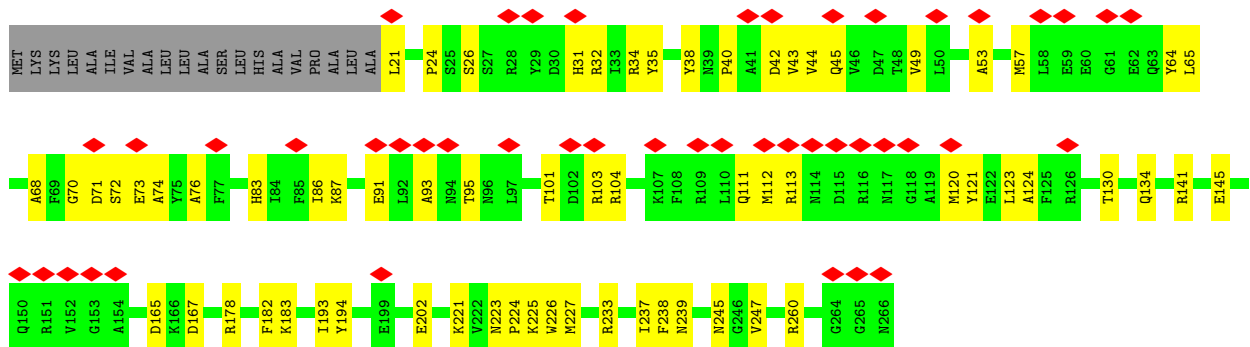




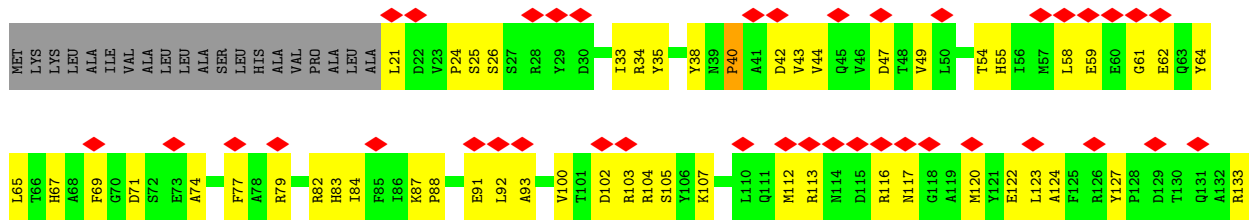
• Molecule 2: TrwF protein

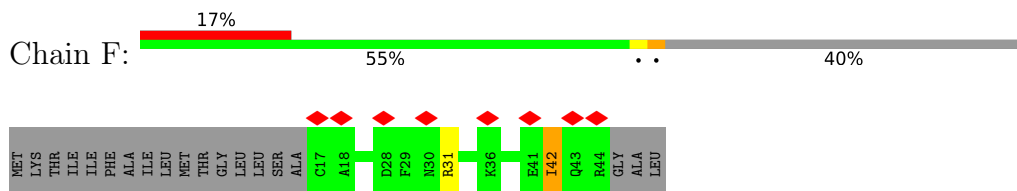


• Molecule 2: TrwF protein

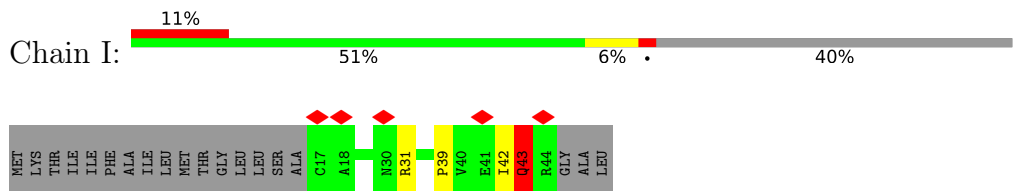


• Molecule 2: TrwF protein

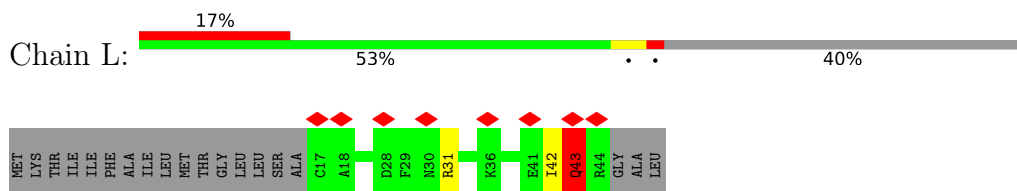




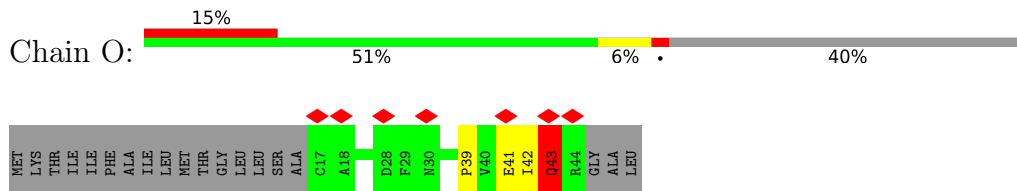
• Molecule 3: TrwH protein



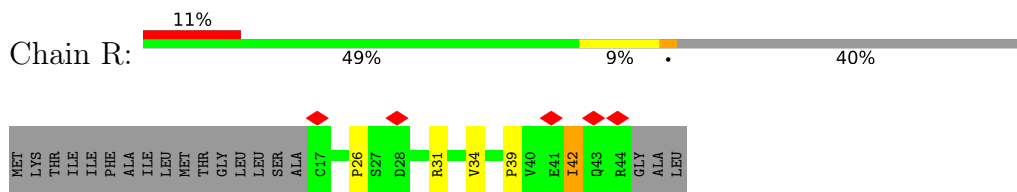
• Molecule 3: TrwH protein



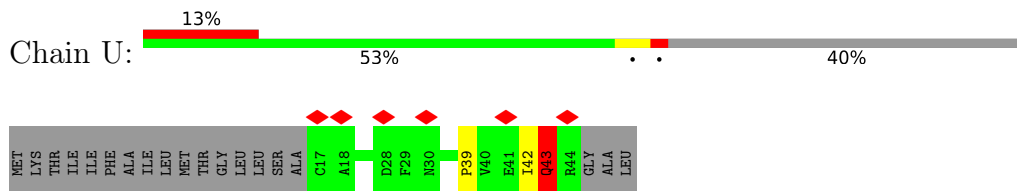
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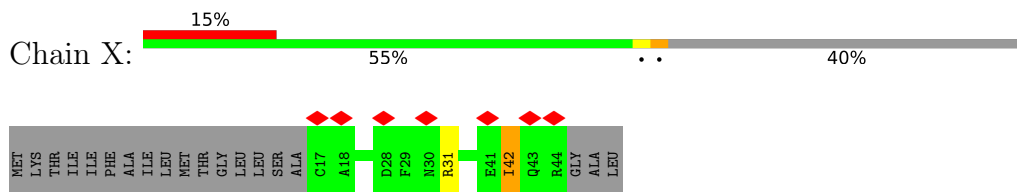
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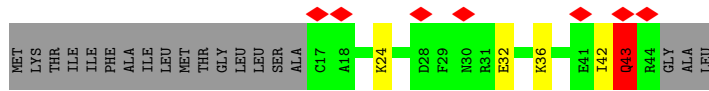
• Molecule 3: TrwH protein



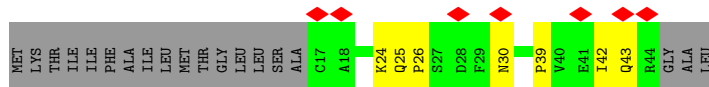
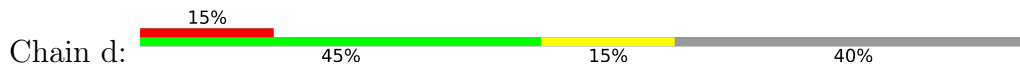
• Molecule 3: TrwH protein



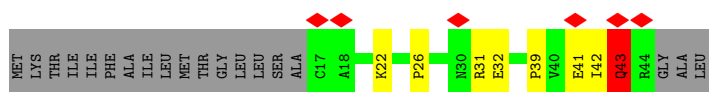
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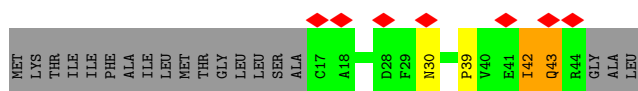
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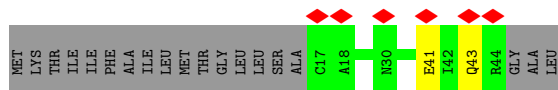
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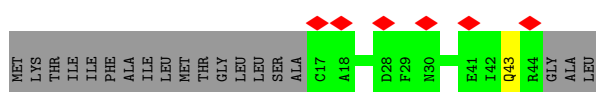
• Molecule 3: TrwH protein



• Molecule 3: TrwH protein



• Molecule 3: TrwH protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	296445	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 ($e^-/\text{\AA}^2$)	57.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.059	Depositor
Minimum map value	-0.260	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	320.1, 320.1, 320.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	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	0.53	0/1696	0.53	2/2290 (0.1%)
1	D	0.52	0/1696	0.47	0/2290
1	G	0.53	0/1696	0.47	0/2290
1	J	0.54	0/1696	0.48	0/2290
1	M	0.54	0/1696	0.49	0/2290
1	P	0.53	0/1696	0.49	0/2290
1	S	0.53	0/1696	0.49	0/2290
1	V	0.52	0/1696	0.47	0/2290
1	Y	0.52	0/1696	0.47	0/2290
1	b	0.53	0/1696	0.49	0/2290
1	e	0.54	0/1696	0.48	0/2290
1	h	0.54	0/1696	0.49	0/2290
1	k	0.52	0/1696	0.48	0/2290
1	n	0.52	0/1696	0.46	0/2290
1	u	0.18	0/150	0.44	0/199
1	y	0.16	0/150	0.40	0/199
2	B	0.36	0/1999	0.50	2/2712 (0.1%)
2	E	0.35	0/1999	0.42	0/2712
2	H	0.35	0/1999	0.41	0/2712
2	K	0.36	0/1999	0.44	0/2712
2	N	0.36	0/1999	0.42	0/2712
2	Q	0.36	0/1999	0.41	0/2712
2	T	0.36	0/1999	0.42	0/2712
2	W	0.36	0/1999	0.43	0/2712
2	Z	0.36	0/1999	0.42	2/2712 (0.1%)
2	c	0.36	0/1999	0.41	0/2712
2	f	0.36	0/1999	0.44	0/2712
2	i	0.36	0/1999	0.44	0/2712
2	l	0.37	0/1999	0.47	1/2712 (0.0%)
2	o	0.35	0/1999	0.45	1/2712 (0.0%)
2	v	0.20	0/906	0.40	0/1226
2	z	0.21	0/906	0.40	0/1226
3	C	0.36	0/218	1.14	1/297 (0.3%)
3	F	0.37	0/218	0.54	1/297 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	I	0.36	0/218	1.24	1/297 (0.3%)
3	L	0.37	0/218	0.69	2/297 (0.7%)
3	O	0.35	0/218	0.73	1/297 (0.3%)
3	R	0.35	0/218	0.57	1/297 (0.3%)
3	U	0.38	0/218	1.37	1/297 (0.3%)
3	X	0.35	0/218	0.53	1/297 (0.3%)
3	a	0.36	0/218	1.39	1/297 (0.3%)
3	d	0.42	0/218	0.51	0/297
3	g	0.34	0/218	0.90	1/297 (0.3%)
3	j	0.34	0/218	1.22	2/297 (0.7%)
3	m	0.37	0/218	0.52	0/297
3	p	0.34	0/218	0.55	0/297
All	All	0.43	0/56894	0.49	21/77036 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	I	0	1
3	L	0	1
3	O	0	1
3	U	0	1
3	a	0	1
3	g	0	1
3	j	0	1
3	m	0	1
3	p	0	1
All	All	0	10

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	43	GLN	O-C-N	-22.44	96.21	122.91
3	U	43	GLN	O-C-N	-22.07	97.73	122.67
3	I	43	GLN	O-C-N	-20.11	98.45	122.58
3	j	43	GLN	O-C-N	-19.24	96.63	122.41
3	C	43	GLN	O-C-N	-18.09	101.39	122.91
3	g	43	GLN	O-C-N	-12.93	107.06	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	43	GLN	O-C-N	-9.94	111.44	122.67
2	l	40	PRO	CA-N-CD	-9.15	99.19	112.00
3	L	43	GLN	O-C-N	-7.57	112.27	122.41
1	A	276	GLU	CA-C-N	7.10	131.46	120.60
1	A	276	GLU	C-N-CA	7.10	131.46	120.60
3	R	42	ILE	N-CA-C	-6.26	106.41	112.29
3	F	42	ILE	N-CA-C	-6.03	105.87	112.80
3	X	42	ILE	N-CA-C	-5.88	106.04	112.80
3	L	42	ILE	N-CA-C	-5.43	106.55	112.80
2	o	40	PRO	CA-N-CD	-5.30	104.58	112.00
3	j	42	ILE	N-CA-C	-5.10	106.93	112.80
2	B	150	GLN	CA-C-N	5.03	131.14	121.54
2	B	150	GLN	C-N-CA	5.03	131.14	121.54
2	Z	126	ARG	CA-C-N	-5.01	114.33	122.65
2	Z	126	ARG	C-N-CA	-5.01	114.33	122.65

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	43	GLN	Mainchain
3	I	43	GLN	Mainchain
3	L	43	GLN	Mainchain
3	O	43	GLN	Mainchain
3	U	43	GLN	Mainchain
3	a	43	GLN	Mainchain
3	g	43	GLN	Mainchain
3	j	43	GLN	Mainchain
3	m	43	GLN	Mainchain
3	p	43	GLN	Mainchain

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1670	0	1661	32	0
1	D	1670	0	1661	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1670	0	1661	35	0
1	J	1670	0	1661	33	0
1	M	1670	0	1661	36	0
1	P	1670	0	1661	26	0
1	S	1670	0	1661	25	0
1	V	1670	0	1661	34	0
1	Y	1670	0	1661	31	0
1	b	1670	0	1661	33	0
1	e	1670	0	1661	34	0
1	h	1670	0	1661	32	0
1	k	1670	0	1661	23	0
1	n	1670	0	1661	30	0
1	u	149	0	156	6	0
1	y	149	0	156	6	0
2	B	1955	0	1891	53	0
2	E	1955	0	1891	58	0
2	H	1955	0	1891	60	0
2	K	1955	0	1891	43	0
2	N	1955	0	1891	48	0
2	Q	1955	0	1891	57	0
2	T	1955	0	1891	36	0
2	W	1955	0	1891	48	0
2	Z	1955	0	1891	67	0
2	c	1955	0	1891	73	0
2	f	1955	0	1891	67	0
2	i	1955	0	1891	50	0
2	l	1955	0	1891	50	0
2	o	1955	0	1891	63	0
2	v	886	0	863	29	0
2	z	886	0	863	34	0
3	C	213	0	211	3	0
3	F	213	0	211	2	0
3	I	213	0	211	4	0
3	L	213	0	211	2	0
3	O	213	0	211	2	0
3	R	213	0	211	6	0
3	U	213	0	211	2	0
3	X	213	0	211	2	0
3	a	213	0	211	3	0
3	d	213	0	211	7	0
3	g	213	0	211	10	0
3	j	213	0	211	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	m	213	0	211	1	0
3	p	213	0	211	0	0
All	All	55802	0	54720	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1080) 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:o:34:ARG:NH1	2:o:120:MET:SD	2.37	0.96
2:N:34:ARG:HH21	2:N:120:MET:HB2	1.32	0.94
2:H:33:ILE:HD11	2:K:107:LYS:HE3	1.51	0.93
2:o:24:PRO:HB2	2:o:34:ARG:HG2	1.55	0.87
2:H:106:TYR:HH	2:H:127:TYR:HH	1.21	0.86
1:G:392:ILE:HD11	2:K:259:ARG:HB2	1.60	0.83
2:E:62:GLU:HG2	2:E:101:THR:HG21	1.62	0.81
1:D:235:ARG:HD3	2:H:221:LYS:HD3	1.61	0.80
2:Q:240:GLU:OE2	3:R:31:ARG:NH2	2.15	0.80
2:T:45:GLN:OE1	2:T:109:ARG:NH1	2.13	0.80
2:Z:21:LEU:N	2:Z:42:ASP:OD1	2.14	0.80
2:o:55:HIS:HB3	2:o:122:GLU:HG2	1.64	0.79
1:G:235:ARG:HD3	2:K:221:LYS:HD3	1.64	0.78
2:B:107:LYS:NZ	2:o:122:GLU:OE2	2.16	0.78
2:z:64:TYR:OH	2:z:67:HIS:ND1	2.16	0.78
2:W:50:LEU:HB2	2:W:112:MET:HE1	1.64	0.77
1:V:235:ARG:HD3	2:Z:221:LYS:HD3	1.67	0.76
2:f:64:TYR:HH	2:f:67:HIS:HD1	1.33	0.76
2:K:49:VAL:HG12	2:K:113:ARG:HB2	1.66	0.76
1:A:142:ARG:NH2	2:o:91:GLU:OE1	2.18	0.76
2:T:161:MET:HG3	2:T:240:GLU:HG3	1.68	0.76
2:f:103:ARG:HG3	2:f:104:ARG:HG2	1.66	0.76
2:i:34:ARG:HD2	2:i:120:MET:HE1	1.67	0.76
2:Q:34:ARG:HD2	2:Q:120:MET:HE2	1.68	0.75
1:e:235:ARG:HD3	2:i:221:LYS:HD3	1.66	0.75
2:B:49:VAL:HG12	2:B:113:ARG:HB2	1.67	0.75
1:h:177:GLY:HA3	1:k:189:PRO:HG2	1.69	0.75
2:Z:62:GLU:OE1	2:Z:104:ARG:NH1	2.20	0.75
2:W:91:GLU:OE2	1:u:142:ARG:NH2	2.21	0.74
1:b:277:THR:HG22	1:b:279:SER:H	1.54	0.73
2:N:24:PRO:HB2	2:N:34:ARG:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:87:LYS:NZ	1:S:145:MET:O	2.19	0.73
2:c:151:ARG:NH2	3:d:43:GLN:OE1	2.22	0.73
2:Q:227:MET:HE1	3:R:26:PRO:HD3	1.70	0.73
2:E:87:LYS:NZ	1:G:148:SER:O	2.20	0.72
2:T:24:PRO:HB3	2:T:36:VAL:HB	1.72	0.72
1:S:235:ARG:HD3	2:W:221:LYS:HD3	1.70	0.72
2:o:59:GLU:OE1	2:o:104:ARG:NH1	2.23	0.72
2:E:262:ASN:OD1	1:n:199:ARG:NH2	2.23	0.71
2:i:59:GLU:OE2	2:i:104:ARG:NH2	2.23	0.71
2:Q:26:SER:HA	2:Q:34:ARG:HG2	1.72	0.70
2:f:64:TYR:HA	2:f:101:THR:HG22	1.74	0.70
1:A:235:ARG:HD3	2:E:221:LYS:HD3	1.74	0.70
1:A:392:ILE:HD11	2:E:259:ARG:HB3	1.74	0.69
1:G:299:GLY:HA2	1:G:365:LEU:HD11	1.74	0.69
2:H:49:VAL:HG12	2:H:113:ARG:HB2	1.73	0.69
1:b:235:ARG:HD3	2:f:221:LYS:HD2	1.73	0.69
1:k:369:GLN:NE2	2:l:202:GLU:OE1	2.25	0.69
1:D:277:THR:HG22	1:D:279:SER:H	1.58	0.69
3:d:39:PRO:HD2	3:d:42:ILE:HD12	1.73	0.69
2:v:24:PRO:HB2	2:v:34:ARG:HB3	1.74	0.69
2:Z:70:GLY:HA3	2:Z:95:THR:HB	1.75	0.69
2:K:151:ARG:NH2	3:L:43:GLN:OE1	2.25	0.68
2:B:94:ASN:O	2:o:116:ARG:NH2	2.26	0.68
2:K:59:GLU:OE1	2:K:103:ARG:NH1	2.26	0.68
2:l:64:TYR:HA	2:l:101:THR:HG22	1.73	0.68
2:E:49:VAL:HB	2:E:116:ARG:HA	1.76	0.68
1:G:315:MET:HE3	1:G:319:ILE:HD12	1.76	0.68
1:u:144:ARG:NH1	2:v:91:GLU:O	2.27	0.68
2:B:157:ASN:HB3	2:B:175:ASP:OD1	1.93	0.68
2:v:64:TYR:HA	2:v:101:THR:HG22	1.75	0.68
2:K:57:MET:SD	2:K:83:HIS:ND1	2.68	0.67
1:D:148:SER:OG	2:E:71:ASP:OD1	2.11	0.67
2:E:94:ASN:O	2:z:116:ARG:NH2	2.27	0.67
2:c:151:ARG:NH1	2:c:156:TYR:OH	2.27	0.67
2:K:64:TYR:OH	2:K:67:HIS:ND1	2.27	0.67
1:b:245:VAL:O	2:f:260:ARG:NH2	2.27	0.67
2:E:253:THR:OG1	2:E:258:VAL:O	2.13	0.67
1:V:245:VAL:O	2:Z:260:ARG:NH2	2.27	0.67
2:N:43:VAL:HG12	2:N:107:LYS:HB3	1.75	0.67
2:z:113:ARG:NH2	2:z:115:ASP:OD1	2.28	0.67
2:c:64:TYR:OH	2:c:67:HIS:ND1	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:162:MET:HE3	2:f:166:LYS:HD2	1.75	0.66
2:W:60:GLU:O	2:W:103:ARG:NH2	2.28	0.66
1:M:235:ARG:HD3	2:Q:221:LYS:HD3	1.75	0.66
2:l:32:ARG:HD3	2:l:121:TYR:CE2	2.31	0.66
1:G:245:VAL:O	2:K:260:ARG:NH2	2.29	0.66
1:k:152:ALA:HB2	2:l:72:SER:HB2	1.77	0.66
2:K:34:ARG:HE	2:K:120:MET:HG3	1.59	0.66
1:V:177:GLY:HA3	1:Y:189:PRO:HG2	1.78	0.66
2:f:49:VAL:HG12	2:f:113:ARG:HB2	1.77	0.66
1:J:177:GLY:HA3	1:M:189:PRO:HG2	1.79	0.65
1:y:144:ARG:NH1	2:z:91:GLU:O	2.30	0.65
1:M:355:LEU:O	1:M:359:ILE:HB	1.96	0.65
2:W:64:TYR:OH	2:W:67:HIS:ND1	2.26	0.65
2:c:49:VAL:HG12	2:c:113:ARG:HB2	1.79	0.65
2:Z:185:SER:HB2	2:c:245:ASN:HA	1.79	0.65
2:o:161:MET:HG2	2:o:240:GLU:HG3	1.79	0.65
2:N:87:LYS:NZ	1:P:145:MET:O	2.30	0.65
2:l:32:ARG:HH21	2:o:21:LEU:HD21	1.62	0.65
2:N:157:ASN:HB3	2:N:175:ASP:OD2	1.97	0.64
2:c:34:ARG:HD2	2:c:120:MET:HG3	1.79	0.64
1:e:277:THR:HG22	1:e:279:SER:H	1.63	0.64
2:H:151:ARG:NH2	3:I:43:GLN:OE1	2.29	0.64
2:Z:56:ILE:HB	2:Z:84:ILE:HB	1.79	0.64
1:b:136:THR:HG23	1:b:139:GLU:H	1.62	0.64
2:H:24:PRO:HB2	2:H:34:ARG:HB3	1.79	0.64
2:T:37:THR:HG22	2:T:126:ARG:HB2	1.80	0.64
2:T:167:ASP:OD2	2:T:233:ARG:NE	2.30	0.64
3:j:39:PRO:HD2	3:j:42:ILE:HD12	1.79	0.64
2:i:207:ARG:NH1	2:i:217:ILE:HD13	2.11	0.64
2:z:58:LEU:HB2	2:z:82:ARG:HB2	1.79	0.64
1:M:177:GLY:HA3	1:P:189:PRO:HG2	1.79	0.64
2:T:21:LEU:N	2:T:42:ASP:OD1	2.30	0.64
2:E:183:LYS:HG3	2:E:216:ILE:HG12	1.79	0.64
1:G:144:ARG:NH1	2:H:91:GLU:O	2.30	0.64
1:k:245:VAL:O	2:o:260:ARG:NH2	2.31	0.64
1:P:245:VAL:O	2:T:260:ARG:NH2	2.31	0.64
2:f:21:LEU:HD22	2:f:45:GLN:HB2	1.80	0.64
1:n:277:THR:HG22	1:n:279:SER:H	1.61	0.64
2:N:45:GLN:OE1	2:N:109:ARG:NH1	2.28	0.64
2:l:183:LYS:NZ	3:m:41:GLU:OE1	2.30	0.64
2:W:157:ASN:HB3	2:W:175:ASP:OD1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:245:VAL:O	2:Q:260:ARG:NH2	2.31	0.63
2:Q:100:VAL:HG23	2:Q:105:SER:HB2	1.79	0.63
2:o:88:PRO:HB3	2:o:112:MET:HE1	1.79	0.63
2:o:196:VAL:HG11	2:o:225:LYS:HD3	1.80	0.63
2:K:26:SER:OG	2:K:34:ARG:NH1	2.31	0.63
2:o:157:ASN:HB3	2:o:175:ASP:OD1	1.99	0.63
2:B:58:LEU:HD22	2:B:106:TYR:HE2	1.63	0.63
2:E:240:GLU:OE2	3:F:31:ARG:NH1	2.32	0.63
2:E:223:ASN:ND2	2:E:225:LYS:O	2.30	0.63
1:n:355:LEU:O	1:n:359:ILE:HB	1.99	0.63
2:Z:31:HIS:O	2:Z:34:ARG:NE	2.32	0.62
2:Z:34:ARG:HD3	2:Z:120:MET:HG3	1.81	0.62
2:v:113:ARG:NH1	2:v:115:ASP:OD1	2.31	0.62
1:D:369:GLN:NE2	2:E:202:GLU:OE1	2.31	0.62
1:M:353:GLU:O	1:M:357:ASN:ND2	2.27	0.62
2:c:64:TYR:HA	2:c:101:THR:HG22	1.80	0.62
1:M:144:ARG:NH2	2:N:71:ASP:OD2	2.31	0.62
2:l:35:TYR:HD2	2:l:124:ALA:HB3	1.64	0.62
2:o:38:TYR:CE2	2:o:40:PRO:HD3	2.34	0.62
1:V:270:VAL:HG21	1:V:298:LEU:HD22	1.81	0.62
2:v:43:VAL:HG12	2:v:107:LYS:HD2	1.81	0.62
3:O:39:PRO:HD2	3:O:42:ILE:HD12	1.82	0.62
1:D:207:ILE:HG13	1:D:246:LEU:HD12	1.81	0.61
1:Y:141:ALA:O	1:Y:145:MET:HG2	2.00	0.61
3:C:39:PRO:HD2	3:C:42:ILE:HD12	1.82	0.61
2:f:32:ARG:HD2	2:f:121:TYR:CE2	2.35	0.61
2:f:165:ASP:OD1	2:f:233:ARG:NH1	2.33	0.61
3:a:32:GLU:OE1	3:a:36:LYS:NZ	2.29	0.61
2:c:58:LEU:O	2:c:82:ARG:NH1	2.33	0.61
2:c:223:ASN:ND2	2:c:225:LYS:O	2.33	0.61
2:f:97:LEU:HB3	2:f:108:PHE:HB2	1.82	0.61
2:z:62:GLU:HG3	2:z:103:ARG:HG3	1.82	0.61
1:Y:207:ILE:HG13	1:Y:246:LEU:HD12	1.82	0.61
1:b:141:ALA:O	1:b:145:MET:HG2	2.00	0.61
1:n:369:GLN:NE2	2:o:202:GLU:OE1	2.33	0.61
2:z:49:VAL:HG12	2:z:113:ARG:HB3	1.83	0.61
2:f:185:SER:HB2	2:i:245:ASN:HA	1.82	0.61
1:h:204:ASP:OD2	1:h:243:ARG:NH1	2.33	0.61
1:Y:177:GLY:HA3	1:b:189:PRO:HG2	1.83	0.60
2:Z:109:ARG:HD2	2:v:32:ARG:HH12	1.65	0.60
2:E:66:THR:HG23	2:z:80:LYS:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:144:ARG:NH1	2:c:91:GLU:O	2.34	0.60
2:c:121:TYR:CE1	2:f:96:ASN:HB2	2.36	0.60
2:K:87:LYS:NZ	1:M:145:MET:O	2.34	0.60
2:B:59:GLU:C	2:B:82:ARG:HE	2.09	0.60
1:P:144:ARG:NH1	2:Q:91:GLU:O	2.35	0.60
2:T:196:VAL:HG11	2:T:225:LYS:HD3	1.84	0.60
2:o:65:LEU:HB3	2:o:100:VAL:HG13	1.83	0.60
1:D:145:MET:O	2:z:87:LYS:NZ	2.32	0.60
2:K:51:GLY:HA3	2:K:116:ARG:HH21	1.66	0.60
2:Z:103:ARG:HG3	2:Z:104:ARG:HG2	1.84	0.60
2:B:49:VAL:HB	2:B:116:ARG:HA	1.84	0.60
1:G:277:THR:HG22	1:G:279:SER:H	1.66	0.60
2:Q:44:VAL:HG11	2:Q:123:LEU:HD21	1.84	0.60
2:f:166:LYS:NZ	3:g:32:GLU:OE2	2.34	0.60
1:G:177:GLY:HA3	1:J:189:PRO:HG2	1.83	0.60
1:J:245:VAL:O	2:N:260:ARG:NH2	2.35	0.60
1:b:149:GLY:O	2:c:72:SER:OG	2.14	0.59
1:h:369:GLN:NE2	2:i:202:GLU:OE1	2.34	0.59
2:i:64:TYR:HA	2:i:101:THR:HG22	1.84	0.59
2:E:46:VAL:HA	2:E:120:MET:HE1	1.84	0.59
1:V:353:GLU:OE2	1:V:356:ARG:NH1	2.35	0.59
2:f:48:THR:OG1	2:f:75:TYR:OH	2.19	0.59
1:k:376:LEU:HD22	1:n:228:MET:HB2	1.83	0.59
2:z:46:VAL:HA	2:z:120:MET:HE1	1.84	0.59
2:f:227:MET:HE1	3:g:26:PRO:HD3	1.85	0.59
2:l:44:VAL:HG11	2:l:123:LEU:HD21	1.84	0.59
2:c:78:ALA:HB3	2:c:85:PHE:HB2	1.83	0.59
1:P:136:THR:HG23	1:P:139:GLU:H	1.67	0.59
2:o:113:ARG:NE	2:o:117:ASN:O	2.36	0.59
1:A:144:ARG:NH2	2:B:71:ASP:OD1	2.36	0.59
2:T:76:ALA:HB3	2:T:87:LYS:HB3	1.84	0.59
2:c:157:ASN:HB3	2:c:175:ASP:OD1	2.03	0.59
1:J:277:THR:HG22	1:J:279:SER:H	1.67	0.59
2:Z:224:PRO:HA	2:Z:239:ASN:HB3	1.84	0.59
1:Y:299:GLY:HA2	1:Y:365:LEU:HD11	1.85	0.58
2:K:48:THR:OG1	2:K:75:TYR:OH	2.19	0.58
2:N:185:SER:HB2	2:Q:245:ASN:HA	1.84	0.58
2:Q:62:GLU:OE1	2:Q:104:ARG:NH1	2.35	0.58
2:Z:116:ARG:NH2	2:c:94:ASN:O	2.36	0.58
2:i:207:ARG:HD2	2:i:217:ILE:HG23	1.84	0.58
2:v:21:LEU:N	2:v:42:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:60:GLU:O	2:z:103:ARG:NH2	2.31	0.58
2:Q:196:VAL:HG11	2:Q:225:LYS:HD3	1.86	0.58
2:c:224:PRO:HA	2:c:239:ASN:HB3	1.85	0.58
2:T:224:PRO:HA	2:T:239:ASN:HB3	1.86	0.58
2:Z:50:LEU:HB2	2:Z:112:MET:HE1	1.84	0.58
2:Z:109:ARG:NH2	2:Z:111:GLN:OE1	2.37	0.58
2:c:50:LEU:HG	1:e:145:MET:HE3	1.84	0.58
1:k:143:GLU:O	1:k:147:ARG:HG3	2.04	0.58
1:Y:148:SER:HB3	2:Z:73:GLU:HB2	1.86	0.58
2:c:100:VAL:HG12	2:c:105:SER:HB2	1.84	0.58
2:v:113:ARG:HH11	2:v:117:ASN:H	1.50	0.58
2:Z:34:ARG:HG2	2:Z:120:MET:HE2	1.85	0.58
3:g:39:PRO:HD2	3:g:42:ILE:HD12	1.86	0.58
2:o:224:PRO:HA	2:o:239:ASN:HB3	1.85	0.58
1:e:245:VAL:O	2:i:260:ARG:NH2	2.33	0.58
1:e:353:GLU:O	1:e:357:ASN:ND2	2.33	0.58
2:f:226:TRP:HB2	2:f:237:ILE:HB	1.86	0.58
1:b:355:LEU:O	1:b:359:ILE:HB	2.04	0.58
2:f:34:ARG:HD2	2:f:120:MET:SD	2.44	0.58
2:B:223:ASN:ND2	2:B:225:LYS:O	2.34	0.57
1:J:301:TRP:CZ3	1:J:303:ASP:HB2	2.39	0.57
2:N:35:TYR:HD2	2:N:124:ALA:HB3	1.69	0.57
2:Q:224:PRO:HA	2:Q:239:ASN:HB3	1.85	0.57
1:b:299:GLY:HA2	1:b:365:LEU:HD11	1.87	0.57
2:B:87:LYS:NZ	1:y:145:MET:O	2.25	0.57
1:P:353:GLU:O	1:P:357:ASN:ND2	2.35	0.57
1:Y:144:ARG:NH1	2:Z:91:GLU:O	2.38	0.57
2:N:121:TYR:CE2	2:Q:96:ASN:HB2	2.39	0.57
2:l:34:ARG:HD2	2:l:120:MET:HG3	1.87	0.57
2:K:35:TYR:HD2	2:K:124:ALA:HB3	1.68	0.57
1:S:384:SER:O	2:W:263:LYS:NZ	2.32	0.57
2:l:76:ALA:HB3	2:l:87:LYS:HB3	1.87	0.57
1:J:139:GLU:O	1:J:143:GLU:HG2	2.04	0.57
1:S:177:GLY:HA3	1:V:189:PRO:HG2	1.86	0.57
2:Z:178:ARG:HH21	2:Z:247:VAL:HG13	1.70	0.57
1:D:299:GLY:HA2	1:D:365:LEU:HD11	1.87	0.57
2:N:45:GLN:NE2	2:N:47:ASP:OD1	2.36	0.57
2:z:79:ARG:NH2	2:z:81:GLY:O	2.37	0.57
1:A:148:SER:O	2:o:87:LYS:NZ	2.37	0.57
2:B:62:GLU:HA	2:B:103:ARG:HH22	1.70	0.57
1:b:152:ALA:HB2	2:c:72:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:162:MET:HE3	2:i:166:LYS:HD2	1.87	0.57
2:c:70:GLY:HA3	2:c:95:THR:HB	1.87	0.57
2:K:165:ASP:OD1	2:K:233:ARG:NH1	2.38	0.56
2:T:151:ARG:NH2	3:U:43:GLN:OE1	2.38	0.56
2:f:50:LEU:HD11	1:h:146:LEU:HD12	1.85	0.56
2:E:101:THR:HG22	2:E:102:ASP:H	1.70	0.56
2:K:226:TRP:HB2	2:K:237:ILE:HB	1.86	0.56
2:W:34:ARG:HD2	2:W:120:MET:HE2	1.86	0.56
1:b:139:GLU:O	1:b:143:GLU:HG2	2.03	0.56
2:o:105:SER:O	2:o:107:LYS:NZ	2.22	0.56
2:H:34:ARG:HD2	2:H:120:MET:HE2	1.87	0.56
2:H:60:GLU:O	2:H:103:ARG:NH2	2.38	0.56
2:H:161:MET:HG2	2:H:240:GLU:HG3	1.87	0.56
1:P:177:GLY:HA3	1:S:189:PRO:HG2	1.87	0.56
2:Q:35:TYR:HD2	2:Q:124:ALA:HB3	1.70	0.56
2:T:87:LYS:HB2	1:V:150:LEU:HD21	1.87	0.56
1:e:214:ASP:OD2	1:e:234:THR:OG1	2.23	0.56
2:i:56:ILE:HB	2:i:84:ILE:HB	1.87	0.56
1:k:144:ARG:NH1	2:l:91:GLU:O	2.37	0.56
2:i:167:ASP:OD2	2:i:233:ARG:NE	2.37	0.56
1:D:353:GLU:O	1:D:357:ASN:ND2	2.31	0.56
2:K:49:VAL:HB	2:K:116:ARG:HA	1.86	0.56
1:S:355:LEU:O	1:S:359:ILE:HB	2.06	0.56
1:b:353:GLU:O	1:b:357:ASN:ND2	2.28	0.56
2:v:38:TYR:HE2	2:v:40:PRO:HG3	1.70	0.56
2:z:35:TYR:HD2	2:z:124:ALA:HB3	1.71	0.56
2:W:44:VAL:HG11	2:W:123:LEU:HD21	1.87	0.56
2:z:62:GLU:OE1	2:z:104:ARG:NH2	2.39	0.56
1:A:354:ALA:HB2	1:n:355:LEU:HD21	1.87	0.56
2:H:64:TYR:HA	2:H:101:THR:HG22	1.87	0.56
2:H:223:ASN:ND2	2:H:225:LYS:O	2.39	0.56
2:Z:49:VAL:HG12	2:Z:113:ARG:HB2	1.87	0.56
2:f:26:SER:HB3	2:f:31:HIS:HA	1.86	0.56
2:f:240:GLU:OE1	3:g:31:ARG:NH1	2.38	0.56
2:B:69:PHE:HZ	2:B:77:PHE:HB2	1.71	0.56
2:Z:63:GLN:HB3	2:Z:102:ASP:OD2	2.06	0.56
2:c:62:GLU:OE1	2:c:101:THR:OG1	2.14	0.56
1:e:136:THR:HG23	1:e:139:GLU:H	1.70	0.56
2:f:121:TYR:HB3	2:i:98:ILE:HD11	1.88	0.56
1:n:190:MET:HE3	1:n:192:LEU:HD11	1.88	0.56
2:K:32:ARG:HB3	2:K:121:TYR:HD2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:104:ARG:HH22	2:f:130:THR:HG23	1.71	0.56
2:o:35:TYR:HD2	2:o:124:ALA:HB3	1.71	0.56
2:z:34:ARG:HD2	2:z:120:MET:HG3	1.86	0.56
1:e:141:ALA:O	1:e:145:MET:HG3	2.06	0.55
2:Q:63:GLN:O	2:Q:101:THR:OG1	2.21	0.55
1:Y:208:THR:HG23	1:Y:240:THR:HG21	1.87	0.55
2:f:129:ASP:OD1	2:f:130:THR:N	2.39	0.55
2:B:100:VAL:HG12	2:B:105:SER:HB2	1.89	0.55
1:b:177:GLY:HA3	1:e:189:PRO:HG2	1.88	0.55
1:h:277:THR:HG22	1:h:279:SER:H	1.71	0.55
2:i:21:LEU:N	2:i:42:ASP:OD1	2.39	0.55
2:Q:59:GLU:OE1	2:Q:103:ARG:NH2	2.40	0.55
2:f:46:VAL:HG23	2:f:120:MET:HE1	1.88	0.55
2:v:74:ALA:HB1	2:v:93:ALA:HB1	1.89	0.55
1:A:355:LEU:O	1:A:359:ILE:HB	2.07	0.55
1:k:277:THR:HG22	1:k:279:SER:H	1.72	0.55
2:v:21:LEU:HD22	2:v:45:GLN:HB2	1.88	0.55
2:E:26:SER:HB3	2:E:31:HIS:HA	1.89	0.55
2:K:46:VAL:HG23	2:K:120:MET:SD	2.47	0.55
2:N:26:SER:HB3	2:N:31:HIS:HA	1.89	0.55
2:W:62:GLU:OE1	2:W:104:ARG:NH1	2.40	0.55
1:k:208:THR:HG23	1:k:240:THR:HG21	1.89	0.55
2:o:225:LYS:HE2	2:o:238:PHE:CE1	2.42	0.55
1:S:208:THR:HG23	1:S:240:THR:HG21	1.88	0.55
2:Z:109:ARG:HD2	2:v:32:ARG:NH1	2.22	0.55
1:k:136:THR:HG23	1:k:139:GLU:H	1.72	0.55
2:B:36:VAL:O	2:B:126:ARG:N	2.38	0.55
1:D:204:ASP:OD2	1:D:243:ARG:NH1	2.35	0.55
2:Q:165:ASP:OD1	2:Q:233:ARG:NH1	2.40	0.55
2:c:121:TYR:HE1	2:f:96:ASN:HB2	1.70	0.55
2:N:223:ASN:ND2	2:N:225:LYS:O	2.40	0.54
1:Y:150:LEU:HD22	2:Z:68:ALA:HB1	1.88	0.54
2:i:48:THR:HG21	2:i:75:TYR:HE2	1.72	0.54
1:Y:136:THR:HG23	1:Y:139:GLU:H	1.72	0.54
2:E:36:VAL:HG23	2:E:123:LEU:HD11	1.89	0.54
2:i:87:LYS:NZ	2:l:70:GLY:O	2.32	0.54
2:H:26:SER:HB2	2:H:31:HIS:HA	1.89	0.54
2:N:26:SER:HA	2:N:34:ARG:HG3	1.89	0.54
1:P:355:LEU:O	1:P:359:ILE:HB	2.08	0.54
2:Q:129:ASP:OD1	2:Q:130:THR:N	2.41	0.54
2:Z:35:TYR:HD1	2:Z:124:ALA:HB3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:145:MET:HA	2:i:71:ASP:OD1	2.07	0.54
2:l:71:ASP:HB2	2:l:95:THR:HG21	1.89	0.54
2:l:202:GLU:OE2	2:l:227:MET:HG2	2.08	0.54
1:u:139:GLU:O	1:u:143:GLU:HG2	2.06	0.54
2:H:122:GLU:HG3	2:K:107:LYS:HD3	1.89	0.54
2:o:64:TYR:OH	2:o:67:HIS:ND1	2.22	0.54
1:A:299:GLY:HA2	1:A:365:LEU:HD11	1.90	0.54
2:N:44:VAL:HG22	2:N:107:LYS:O	2.07	0.54
2:o:49:VAL:HG12	2:o:113:ARG:HB2	1.89	0.54
1:Y:245:VAL:O	2:c:260:ARG:NH2	2.40	0.54
2:v:21:LEU:HD21	2:v:109:ARG:HD3	1.89	0.54
2:K:31:HIS:CE1	2:K:32:ARG:HH21	2.25	0.54
2:N:34:ARG:NH2	2:N:120:MET:HB2	2.13	0.54
2:B:64:TYR:HA	2:B:101:THR:HG22	1.90	0.54
2:i:49:VAL:HB	2:i:116:ARG:HA	1.89	0.54
2:l:74:ALA:HB1	2:l:93:ALA:HB1	1.89	0.53
1:A:315:MET:HE2	1:n:306:PHE:CZ	2.43	0.53
2:E:146:ALA:O	2:E:150:GLN:HB2	2.07	0.53
1:J:207:ILE:HG13	1:J:246:LEU:HD12	1.91	0.53
1:V:369:GLN:NE2	2:W:202:GLU:OE2	2.41	0.53
1:h:245:VAL:O	2:l:260:ARG:NH2	2.38	0.53
2:i:35:TYR:HD2	2:i:124:ALA:HB3	1.73	0.53
2:i:145:GLU:O	2:i:149:GLU:HG2	2.08	0.53
2:H:58:LEU:O	2:H:82:ARG:NH2	2.41	0.53
2:c:106:TYR:C	2:c:107:LYS:HD3	2.33	0.53
2:o:38:TYR:CE2	2:o:104:ARG:HD3	2.43	0.53
1:A:225:GLN:NE2	1:n:267:ARG:O	2.34	0.53
2:Q:55:HIS:HB3	2:Q:122:GLU:HG2	1.91	0.53
2:Z:165:ASP:CG	3:a:24:LYS:HZ3	2.15	0.53
2:i:70:GLY:HA3	2:i:95:THR:HB	1.90	0.53
2:v:44:VAL:HG11	2:v:123:LEU:HD21	1.91	0.53
2:B:122:GLU:HG3	2:z:107:LYS:HD3	1.91	0.53
1:h:139:GLU:O	1:h:143:GLU:HG2	2.09	0.53
2:i:62:GLU:OE1	2:i:104:ARG:NH1	2.41	0.53
2:E:51:GLY:HA3	2:E:116:ARG:HH21	1.74	0.53
2:H:130:THR:HA	2:H:133:ARG:HG2	1.90	0.53
2:Q:225:LYS:HE2	2:Q:238:PHE:CE1	2.43	0.53
2:W:58:LEU:O	2:W:82:ARG:NH2	2.42	0.53
2:o:21:LEU:N	2:o:42:ASP:OD1	2.41	0.53
2:N:64:TYR:HA	2:N:101:THR:HG22	1.91	0.53
2:i:223:ASN:ND2	2:i:225:LYS:O	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:MET:HE1	1:G:228:MET:HE2	1.91	0.53
2:B:83:HIS:CE1	2:z:100:VAL:HG11	2.44	0.53
2:H:185:SER:HB2	2:K:245:ASN:HA	1.91	0.53
2:N:46:VAL:HA	2:N:120:MET:HE1	1.90	0.53
2:W:224:PRO:HA	2:W:239:ASN:HB3	1.90	0.53
2:i:24:PRO:HB2	2:i:34:ARG:HG3	1.90	0.53
2:l:38:TYR:CZ	2:l:104:ARG:HD3	2.43	0.53
1:n:299:GLY:HA2	1:n:365:LEU:HD11	1.91	0.53
2:E:55:HIS:HB2	2:H:98:ILE:HD13	1.90	0.52
1:M:136:THR:HG23	1:M:139:GLU:H	1.74	0.52
2:N:224:PRO:HA	2:N:239:ASN:HB3	1.91	0.52
2:Z:26:SER:HB3	2:Z:31:HIS:HA	1.91	0.52
2:Z:104:ARG:HG3	2:Z:104:ARG:HH11	1.74	0.52
2:f:59:GLU:OE2	2:f:104:ARG:NH1	2.42	0.52
1:n:144:ARG:NH1	2:o:92:LEU:O	2.42	0.52
1:D:374:ASN:HD22	2:H:204:LEU:HD12	1.74	0.52
2:E:101:THR:HG22	2:E:102:ASP:N	2.24	0.52
2:Z:64:TYR:OH	2:Z:67:HIS:ND1	2.32	0.52
1:k:139:GLU:O	1:k:143:GLU:HG2	2.08	0.52
2:B:156:TYR:CD2	3:C:42:ILE:HG23	2.45	0.52
2:K:224:PRO:HA	2:K:239:ASN:HB3	1.91	0.52
2:T:24:PRO:HB2	2:T:34:ARG:HG2	1.90	0.52
2:c:45:GLN:NE2	2:c:47:ASP:OD2	2.34	0.52
2:f:43:VAL:HG12	2:f:107:LYS:HB3	1.91	0.52
2:l:21:LEU:HD22	2:l:45:GLN:HB2	1.90	0.52
2:H:99:VAL:HG13	2:H:106:TYR:HB2	1.91	0.52
2:K:185:SER:HB2	2:N:245:ASN:HA	1.91	0.52
2:Q:226:TRP:HB2	2:Q:237:ILE:HB	1.91	0.52
1:P:248:ASP:HB2	1:P:278:PRO:HD2	1.92	0.52
2:T:50:LEU:HG	1:V:145:MET:HE3	1.92	0.52
1:Y:152:ALA:HB2	2:Z:72:SER:HB3	1.92	0.52
2:T:47:ASP:HB2	2:T:113:ARG:HG3	1.91	0.52
2:Z:175:ASP:HB2	2:Z:179:PHE:O	2.09	0.52
1:D:374:ASN:ND2	2:H:204:LEU:HD12	2.25	0.52
2:E:87:LYS:HE3	2:H:70:GLY:O	2.10	0.52
1:P:190:MET:HE1	1:V:228:MET:HE2	1.92	0.52
1:V:145:MET:HG2	2:W:71:ASP:OD2	2.10	0.52
1:V:299:GLY:HA2	1:V:365:LEU:HD11	1.92	0.52
2:W:202:GLU:OE1	2:W:227:MET:HG2	2.09	0.52
2:Z:64:TYR:HB3	2:Z:79:ARG:HH21	1.74	0.52
1:k:147:ARG:NH2	2:l:73:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:GLU:O	1:G:143:GLU:HG2	2.09	0.52
2:W:35:TYR:HD2	2:W:124:ALA:HB3	1.75	0.52
2:W:129:ASP:OD1	2:W:130:THR:N	2.43	0.52
2:c:22:ASP:N	2:c:43:VAL:O	2.31	0.52
2:i:102:ASP:OD2	2:i:103:ARG:N	2.43	0.52
2:H:226:TRP:HB2	2:H:237:ILE:HB	1.91	0.52
1:y:139:GLU:O	1:y:143:GLU:HG2	2.10	0.52
2:N:167:ASP:OD1	2:N:233:ARG:NE	2.43	0.52
2:c:74:ALA:O	2:c:89:GLN:N	2.35	0.52
3:U:39:PRO:HD2	3:U:42:ILE:HD12	1.93	0.51
2:c:165:ASP:OD2	3:d:24:LYS:NZ	2.36	0.51
2:H:48:THR:OG1	2:H:75:TYR:OH	2.29	0.51
1:J:136:THR:HG23	1:J:139:GLU:H	1.74	0.51
1:S:199:ARG:NH2	2:Z:262:ASN:OD1	2.42	0.51
1:V:190:MET:HE1	1:b:228:MET:HE2	1.93	0.51
2:Z:42:ASP:OD1	2:Z:43:VAL:N	2.41	0.51
2:o:42:ASP:OD1	2:o:43:VAL:N	2.44	0.51
2:H:31:HIS:O	2:H:34:ARG:NH1	2.44	0.51
1:M:270:VAL:HG21	1:M:298:LEU:HD22	1.93	0.51
2:W:223:ASN:ND2	2:W:225:LYS:O	2.39	0.51
2:c:53:ALA:H	2:f:96:ASN:HD21	1.59	0.51
1:e:376:LEU:HD22	1:h:228:MET:HB2	1.92	0.51
2:l:224:PRO:HA	2:l:239:ASN:HB3	1.92	0.51
1:M:248:ASP:HB2	1:M:278:PRO:HD2	1.92	0.51
2:T:225:LYS:HE2	2:T:238:PHE:CE1	2.46	0.51
2:c:167:ASP:OD1	2:c:233:ARG:NE	2.43	0.51
2:c:178:ARG:HG3	2:c:178:ARG:HH11	1.76	0.51
2:B:59:GLU:HG2	2:B:62:GLU:OE1	2.10	0.51
1:D:305:HIS:O	1:D:309:ARG:HG3	2.11	0.51
1:n:136:THR:HG23	1:n:139:GLU:H	1.75	0.51
2:E:45:GLN:OE1	2:E:109:ARG:NH2	2.42	0.51
1:M:207:ILE:HG13	1:M:246:LEU:HD12	1.91	0.51
2:W:86:ILE:HD12	2:W:110:LEU:HD21	1.91	0.51
2:Z:44:VAL:HG11	2:Z:123:LEU:HD21	1.93	0.51
2:i:114:ASN:OD1	2:i:115:ASP:N	2.43	0.51
1:A:237:VAL:HB	1:A:247:LEU:HB2	1.93	0.51
2:W:38:TYR:HE2	2:W:40:PRO:HG3	1.76	0.51
2:Z:49:VAL:HB	2:Z:116:ARG:HA	1.92	0.51
2:c:87:LYS:NZ	1:e:148:SER:O	2.31	0.51
2:N:64:TYR:HB3	2:N:79:ARG:HH11	1.76	0.51
2:Z:56:ILE:N	2:Z:84:ILE:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:37:THR:HG22	2:c:126:ARG:HD2	1.93	0.51
2:c:53:ALA:H	2:f:96:ASN:ND2	2.09	0.51
2:v:69:PHE:HE2	2:v:77:PHE:HB2	1.76	0.51
1:G:270:VAL:HG21	1:G:298:LEU:HD22	1.93	0.51
1:Y:143:GLU:O	1:Y:147:ARG:HG3	2.10	0.51
2:Z:202:GLU:OE2	2:Z:229:ARG:NH2	2.39	0.51
1:D:139:GLU:O	1:D:143:GLU:HG2	2.11	0.50
2:E:202:GLU:OE2	2:E:229:ARG:NH2	2.34	0.50
1:J:355:LEU:O	1:J:359:ILE:HB	2.12	0.50
1:A:272:TRP:HE1	1:A:289:GLY:HA3	1.76	0.50
1:D:142:ARG:HH21	2:z:91:GLU:CD	2.20	0.50
2:E:34:ARG:CD	2:E:120:MET:HG2	2.41	0.50
2:Q:122:GLU:OE1	2:T:107:LYS:HE3	2.12	0.50
2:o:145:GLU:O	2:o:149:GLU:HG2	2.11	0.50
2:o:175:ASP:HB2	2:o:179:PHE:O	2.11	0.50
2:T:35:TYR:HD1	2:T:124:ALA:HB3	1.76	0.50
1:b:198:GLY:O	1:e:386:VAL:HG11	2.12	0.50
2:f:227:MET:HE1	3:g:26:PRO:HG3	1.94	0.50
2:H:129:ASP:OD1	2:H:129:ASP:N	2.42	0.50
2:Z:157:ASN:HB3	2:Z:175:ASP:OD2	2.12	0.50
2:N:46:VAL:HG12	2:N:48:THR:HG23	1.93	0.50
2:i:27:SER:OG	2:i:33:ILE:O	2.19	0.50
2:B:65:LEU:HB2	2:B:100:VAL:HG23	1.94	0.50
1:D:245:VAL:O	2:H:260:ARG:NH2	2.41	0.50
2:T:91:GLU:OE1	1:V:142:ARG:NH2	2.44	0.50
1:V:139:GLU:O	1:V:143:GLU:HG2	2.12	0.50
1:Y:277:THR:HG22	1:Y:279:SER:H	1.77	0.50
2:c:136:ARG:HG3	2:c:136:ARG:HH11	1.75	0.50
2:z:26:SER:HB3	2:z:31:HIS:HA	1.92	0.50
2:z:45:GLN:OE1	2:z:109:ARG:NH2	2.44	0.50
2:Q:113:ARG:NE	2:Q:117:ASN:O	2.45	0.50
1:e:272:TRP:CD1	1:e:375:ILE:HG12	2.46	0.50
1:V:143:GLU:O	1:V:147:ARG:HG3	2.12	0.50
2:W:185:SER:HB2	2:Z:245:ASN:HA	1.94	0.50
2:f:187:ASN:ND2	2:i:243:ASP:O	2.44	0.50
2:z:42:ASP:OD1	2:z:43:VAL:N	2.45	0.50
1:A:378:ALA:HA	1:D:228:MET:HE1	1.93	0.49
2:c:50:LEU:HD11	1:e:146:LEU:HD12	1.93	0.49
2:f:178:ARG:HH21	2:f:247:VAL:HG23	1.77	0.49
1:h:207:ILE:HG13	1:h:246:LEU:HD12	1.94	0.49
2:c:97:LEU:HB2	2:c:110:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:185:SER:HB2	2:l:245:ASN:HA	1.94	0.49
1:A:376:LEU:HD22	1:D:228:MET:HB2	1.94	0.49
2:B:146:ALA:HA	2:B:149:GLU:OE1	2.12	0.49
1:P:312:GLY:O	1:P:316:ILE:HG12	2.11	0.49
2:T:191:PRO:HB3	2:T:230:LEU:HB2	1.94	0.49
2:W:46:VAL:HG13	2:W:120:MET:SD	2.53	0.49
2:W:55:HIS:NE2	2:W:83:HIS:HB3	2.27	0.49
1:h:299:GLY:HA2	1:h:365:LEU:HD11	1.94	0.49
2:i:189:ASP:OD1	2:l:221:LYS:NZ	2.44	0.49
1:G:244:VAL:HG22	2:K:253:THR:HG22	1.93	0.49
2:H:224:PRO:HA	2:H:239:ASN:HB3	1.94	0.49
1:S:312:GLY:O	1:S:316:ILE:HG12	2.12	0.49
1:A:353:GLU:OE1	1:A:356:ARG:NH1	2.45	0.49
2:E:42:ASP:OD1	2:E:43:VAL:N	2.43	0.49
2:H:42:ASP:OD1	2:H:43:VAL:N	2.42	0.49
2:H:165:ASP:OD1	2:H:233:ARG:NH1	2.46	0.49
2:N:196:VAL:HG11	2:N:225:LYS:HD3	1.95	0.49
2:W:79:ARG:NH1	2:W:81:GLY:O	2.45	0.49
1:b:302:ILE:HD11	1:b:365:LEU:HD12	1.94	0.49
1:b:306:PHE:CZ	1:e:315:MET:HE2	2.47	0.49
2:i:38:TYR:CE2	2:i:104:ARG:HD3	2.47	0.49
2:o:61:GLY:O	2:o:103:ARG:NH2	2.46	0.49
1:M:185:GLU:OE2	1:M:188:GLN:NE2	2.45	0.49
2:Z:126:ARG:HG3	2:Z:126:ARG:HH11	1.77	0.49
1:J:141:ALA:O	1:J:145:MET:HG3	2.13	0.49
2:N:34:ARG:HH21	2:N:120:MET:CB	2.16	0.49
3:R:39:PRO:HD2	3:R:42:ILE:HD12	1.95	0.49
1:S:204:ASP:OD1	1:S:241:SER:OG	2.31	0.49
1:S:270:VAL:HG21	1:S:298:LEU:HD22	1.95	0.49
2:Z:161:MET:HG2	2:Z:240:GLU:HG3	1.94	0.49
2:l:24:PRO:HB2	2:l:34:ARG:HD3	1.95	0.49
2:v:59:GLU:OE1	2:v:104:ARG:NH2	2.46	0.49
2:v:75:TYR:HA	2:v:87:LYS:O	2.13	0.49
2:B:38:TYR:CZ	2:B:104:ARG:HD3	2.48	0.49
2:B:185:SER:HB2	2:E:245:ASN:HA	1.95	0.49
1:D:177:GLY:HA3	1:G:189:PRO:HG2	1.94	0.49
2:H:240:GLU:OE2	3:I:31:ARG:NH1	2.46	0.49
1:M:200:LEU:HD22	1:M:206:LEU:HD21	1.95	0.49
2:i:224:PRO:HA	2:i:239:ASN:HB3	1.95	0.49
1:A:198:GLY:O	1:D:386:VAL:HG11	2.12	0.49
2:E:50:LEU:O	2:E:116:ARG:NE	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:248:ASP:HB2	1:J:278:PRO:HD2	1.95	0.49
1:P:235:ARG:HD3	2:T:221:LYS:HE3	1.94	0.49
2:Z:24:PRO:HB2	2:Z:34:ARG:HB3	1.94	0.49
1:b:204:ASP:OD2	1:b:243:ARG:NH1	2.31	0.49
1:n:191:ARG:HG3	1:n:191:ARG:HH11	1.77	0.49
2:H:64:TYR:OH	2:H:67:HIS:ND1	2.46	0.49
2:c:76:ALA:O	2:c:86:ILE:HA	2.13	0.49
2:i:100:VAL:HG23	2:i:105:SER:HB3	1.94	0.49
2:l:103:ARG:HD2	2:l:104:ARG:HH22	1.78	0.49
2:z:58:LEU:HD12	2:z:82:ARG:HA	1.94	0.49
1:J:302:ILE:HD11	1:J:365:LEU:HD12	1.95	0.48
2:N:207:ARG:HD2	2:N:217:ILE:CG2	2.43	0.48
2:T:113:ARG:NE	2:T:117:ASN:O	2.46	0.48
2:W:55:HIS:CE1	2:v:100:VAL:HG11	2.48	0.48
2:c:55:HIS:HB2	2:f:98:ILE:HG21	1.95	0.48
2:B:245:ASN:HA	2:o:185:SER:HB2	1.93	0.48
1:G:141:ALA:O	1:G:145:MET:HG3	2.12	0.48
1:M:285:LEU:HD12	1:M:285:LEU:O	2.13	0.48
2:i:38:TYR:OH	2:i:104:ARG:HB2	2.12	0.48
2:i:207:ARG:HD2	2:i:217:ILE:CG2	2.43	0.48
1:A:248:ASP:HB2	1:A:278:PRO:HD2	1.95	0.48
1:A:270:VAL:HG21	1:A:298:LEU:HD22	1.95	0.48
2:H:79:ARG:HG3	2:H:84:ILE:HG13	1.94	0.48
1:M:139:GLU:O	1:M:143:GLU:HG2	2.12	0.48
2:Q:223:ASN:ND2	2:Q:225:LYS:O	2.46	0.48
2:c:185:SER:HB2	2:f:245:ASN:HA	1.95	0.48
2:f:22:ASP:HB2	2:f:44:VAL:HG12	1.96	0.48
2:f:33:ILE:HD12	2:f:122:GLU:OE2	2.13	0.48
2:o:100:VAL:HG23	2:o:105:SER:HB2	1.96	0.48
2:K:91:GLU:HG2	1:M:146:LEU:HD21	1.94	0.48
2:N:87:LYS:HE3	2:Q:70:GLY:O	2.13	0.48
2:W:174:TRP:CD1	3:X:42:ILE:HD11	2.49	0.48
1:k:150:LEU:HD22	2:l:68:ALA:HB1	1.96	0.48
2:l:49:VAL:HG12	2:l:113:ARG:HB2	1.95	0.48
2:H:103:ARG:HE	2:H:104:ARG:HH22	1.62	0.48
1:V:355:LEU:O	1:V:359:ILE:HB	2.12	0.48
1:h:213:LEU:HG	1:h:237:VAL:HG21	1.96	0.48
2:o:223:ASN:ND2	2:o:225:LYS:O	2.47	0.48
2:v:79:ARG:HH11	2:v:79:ARG:HG2	1.77	0.48
1:G:302:ILE:HD11	1:G:365:LEU:HD12	1.95	0.48
1:S:245:VAL:O	2:W:260:ARG:NH2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:121:TYR:HD1	2:f:98:ILE:HD11	1.77	0.48
2:f:227:MET:HE2	2:f:234:ALA:HB1	1.96	0.48
1:G:200:LEU:HD22	1:G:206:LEU:HD21	1.94	0.48
2:H:91:GLU:HG2	1:J:146:LEU:HD21	1.95	0.48
1:P:207:ILE:HG13	1:P:246:LEU:HD12	1.95	0.48
1:b:270:VAL:HG21	1:b:298:LEU:HD22	1.94	0.48
1:e:139:GLU:O	1:e:143:GLU:HG2	2.13	0.48
2:f:224:PRO:HA	2:f:239:ASN:HB3	1.96	0.48
2:i:79:ARG:HG3	2:i:84:ILE:HD13	1.95	0.48
2:l:83:HIS:CD2	2:o:100:VAL:HG21	2.49	0.48
2:B:24:PRO:HB2	2:B:34:ARG:HB3	1.95	0.48
1:J:270:VAL:HG21	1:J:298:LEU:HD22	1.96	0.48
1:M:143:GLU:O	1:M:147:ARG:HG3	2.13	0.48
2:T:105:SER:O	2:T:107:LYS:NZ	2.28	0.48
2:N:127:TYR:HB2	2:N:130:THR:HG22	1.94	0.48
1:S:136:THR:HG23	1:S:139:GLU:H	1.79	0.48
1:S:139:GLU:O	1:S:143:GLU:HG2	2.13	0.48
2:f:32:ARG:HD2	2:f:121:TYR:CZ	2.49	0.48
1:u:143:GLU:O	1:u:147:ARG:HG3	2.13	0.48
1:G:301:TRP:CZ3	1:G:303:ASP:HB2	2.49	0.48
2:N:207:ARG:HD2	2:N:217:ILE:HG23	1.96	0.48
2:l:42:ASP:OD1	2:l:43:VAL:N	2.43	0.48
2:o:59:GLU:HB2	2:o:62:GLU:HB2	1.96	0.48
1:u:136:THR:HG23	1:u:139:GLU:H	1.78	0.48
2:K:91:GLU:CD	1:M:142:ARG:HH21	2.21	0.47
1:P:236:ASP:HB3	1:P:245:VAL:HG13	1.95	0.47
1:V:190:MET:HE2	1:V:190:MET:HB3	1.77	0.47
2:Z:138:ALA:HA	2:Z:141:ARG:HH21	1.79	0.47
2:N:178:ARG:NH2	2:N:247:VAL:HG13	2.29	0.47
1:k:388:SER:HB3	2:o:263:LYS:HE3	1.96	0.47
2:E:34:ARG:HD2	2:E:120:MET:HG2	1.95	0.47
2:E:157:ASN:HB3	2:E:175:ASP:OD1	2.15	0.47
2:N:76:ALA:O	2:N:86:ILE:HA	2.13	0.47
2:W:62:GLU:OE2	2:W:101:THR:OG1	2.25	0.47
2:v:114:ASN:OD1	2:v:115:ASP:N	2.47	0.47
1:b:234:THR:HB	2:c:189:ASP:HB3	1.97	0.47
1:e:234:THR:HB	2:f:189:ASP:HB3	1.97	0.47
2:W:127:TYR:HB2	2:W:130:THR:HG22	1.96	0.47
1:Y:198:GLY:O	1:b:386:VAL:HG11	2.14	0.47
2:f:49:VAL:HB	2:f:116:ARG:HA	1.96	0.47
2:l:38:TYR:CE2	2:l:104:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:SER:N	2:E:33:ILE:O	2.42	0.47
2:T:67:HIS:HA	2:T:99:VAL:HA	1.96	0.47
2:T:133:ARG:HB3	2:T:133:ARG:NH1	2.30	0.47
2:Z:51:GLY:HA3	2:Z:116:ARG:NH2	2.30	0.47
3:d:25:GLN:OE1	3:d:26:PRO:HD2	2.15	0.47
2:l:112:MET:HE3	2:l:112:MET:HB3	1.82	0.47
1:n:145:MET:O	1:n:148:SER:OG	2.32	0.47
2:B:26:SER:HA	2:B:34:ARG:HA	1.96	0.47
2:B:44:VAL:HG11	2:B:123:LEU:HD21	1.96	0.47
1:D:143:GLU:O	1:D:147:ARG:HG3	2.14	0.47
2:H:91:GLU:CD	1:J:142:ARG:HH21	2.22	0.47
1:J:252:LYS:HB3	1:J:252:LYS:HE2	1.66	0.47
1:J:315:MET:HE3	1:J:319:ILE:HD12	1.96	0.47
2:N:151:ARG:NH2	2:N:156:TYR:OH	2.37	0.47
1:P:267:ARG:O	1:S:225:GLN:NE2	2.37	0.47
2:Q:56:ILE:HG12	2:Q:123:LEU:HB3	1.96	0.47
2:W:178:ARG:HH21	2:W:247:VAL:HG13	1.79	0.47
2:Z:91:GLU:HG2	1:b:146:LEU:HD21	1.96	0.47
2:c:38:TYR:HE2	2:c:40:PRO:HG3	1.80	0.47
2:c:46:VAL:HG12	2:c:48:THR:HG23	1.96	0.47
1:e:145:MET:HA	2:f:71:ASP:OD1	2.15	0.47
2:o:35:TYR:CD2	2:o:124:ALA:HB3	2.50	0.47
1:e:207:ILE:HG13	1:e:246:LEU:HD12	1.97	0.47
1:n:135:LYS:HA	1:n:135:LYS:HD3	1.76	0.47
2:o:24:PRO:HB2	2:o:34:ARG:CG	2.38	0.47
2:o:79:ARG:HG3	2:o:84:ILE:HG12	1.96	0.47
2:B:34:ARG:HG3	2:B:34:ARG:HH11	1.79	0.47
2:W:24:PRO:HB2	2:W:34:ARG:HD3	1.95	0.47
2:W:55:HIS:HB3	2:W:122:GLU:HG3	1.97	0.47
2:W:113:ARG:HH11	2:W:115:ASP:CG	2.22	0.47
2:Z:53:ALA:H	2:c:96:ASN:ND2	2.13	0.47
2:c:55:HIS:CE1	2:c:57:MET:HE2	2.49	0.47
1:h:200:LEU:HD22	1:h:206:LEU:HD21	1.96	0.47
2:H:43:VAL:HG12	2:H:107:LYS:HB3	1.97	0.47
2:H:113:ARG:NH1	2:H:117:ASN:O	2.47	0.47
2:N:87:LYS:HG2	2:N:88:PRO:HD2	1.98	0.47
1:P:277:THR:HG22	1:P:279:SER:H	1.78	0.47
1:Y:376:LEU:HD22	1:b:228:MET:HB2	1.96	0.47
2:B:144:VAL:HG13	2:B:258:VAL:HG11	1.96	0.46
1:S:376:LEU:HD22	1:V:228:MET:HB2	1.97	0.46
1:e:314:ILE:HD11	1:h:315:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:49:VAL:HG12	2:v:113:ARG:HB3	1.97	0.46
2:B:115:ASP:OD1	2:B:115:ASP:N	2.45	0.46
2:E:35:TYR:HD2	2:E:124:ALA:HB3	1.79	0.46
1:G:353:GLU:O	1:G:357:ASN:ND2	2.46	0.46
1:M:204:ASP:OD2	1:M:243:ARG:NH1	2.38	0.46
2:Z:223:ASN:ND2	2:Z:225:LYS:O	2.47	0.46
1:b:218:GLU:HG3	1:b:219:THR:N	2.30	0.46
2:o:59:GLU:HG3	2:o:127:TYR:CZ	2.50	0.46
1:A:244:VAL:HG22	2:E:253:THR:HG22	1.97	0.46
1:G:136:THR:HG23	1:G:139:GLU:H	1.78	0.46
1:k:236:ASP:HB3	1:k:245:VAL:HG13	1.98	0.46
2:B:57:MET:HE1	2:B:83:HIS:CE1	2.50	0.46
2:H:69:PHE:CE2	2:H:77:PHE:HB2	2.50	0.46
2:T:58:LEU:HD22	2:T:106:TYR:CE2	2.49	0.46
2:c:93:ALA:HB3	2:c:112:MET:HE3	1.97	0.46
1:J:135:LYS:HA	1:J:135:LYS:HD3	1.72	0.46
2:Z:79:ARG:NH1	2:Z:81:GLY:H	2.14	0.46
2:Z:91:GLU:OE2	1:b:142:ARG:NH2	2.48	0.46
2:c:156:TYR:CD2	3:d:42:ILE:HG23	2.50	0.46
2:f:27:SER:OG	2:f:30:ASP:O	2.31	0.46
1:A:245:VAL:O	2:E:260:ARG:NH2	2.48	0.46
2:B:80:LYS:HE2	2:B:80:LYS:HB2	1.71	0.46
1:D:146:LEU:HD12	2:z:50:LEU:HD11	1.98	0.46
1:D:148:SER:HB3	2:E:73:GLU:HG3	1.98	0.46
2:E:57:MET:HG2	2:E:83:HIS:ND1	2.31	0.46
2:K:223:ASN:ND2	2:K:225:LYS:O	2.49	0.46
2:Q:70:GLY:HA3	2:Q:95:THR:HB	1.96	0.46
2:f:28:ARG:HB3	2:f:28:ARG:NH1	2.31	0.46
2:B:172:ASN:HB3	3:C:39:PRO:HG3	1.98	0.46
2:Q:67:HIS:HA	2:Q:99:VAL:HA	1.98	0.46
2:l:87:LYS:NZ	1:n:148:SER:O	2.41	0.46
1:M:302:ILE:HD11	1:M:365:LEU:HD12	1.96	0.46
2:f:156:TYR:CD2	3:g:42:ILE:HG23	2.51	0.46
1:h:248:ASP:HB2	1:h:278:PRO:HD2	1.96	0.46
2:i:69:PHE:CE1	2:i:97:LEU:HD13	2.51	0.46
1:k:299:GLY:HA2	1:k:365:LEU:HD11	1.97	0.46
2:E:175:ASP:HB2	2:E:179:PHE:O	2.16	0.46
2:Z:35:TYR:CD1	2:Z:124:ALA:HB3	2.50	0.46
2:i:62:GLU:HG3	2:i:103:ARG:HG3	1.98	0.46
2:o:25:SER:C	2:o:34:ARG:HG3	2.41	0.46
2:E:58:LEU:HD22	2:E:106:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:49:VAL:HB	2:T:116:ARG:HA	1.98	0.46
1:V:208:THR:HG23	1:V:240:THR:HG21	1.97	0.46
1:e:355:LEU:O	1:e:359:ILE:HB	2.15	0.46
2:f:151:ARG:NH2	3:g:43:GLN:OE1	2.40	0.46
2:o:44:VAL:HG11	2:o:123:LEU:HD21	1.97	0.46
1:M:374:ASN:ND2	2:Q:204:LEU:HD12	2.31	0.45
1:V:135:LYS:HA	1:V:135:LYS:HD3	1.71	0.45
2:i:226:TRP:HB2	2:i:237:ILE:HB	1.98	0.45
2:o:59:GLU:OE2	2:o:103:ARG:NH1	2.49	0.45
1:D:355:LEU:O	1:D:359:ILE:HB	2.16	0.45
2:H:104:ARG:NE	2:H:127:TYR:HE2	2.13	0.45
2:K:32:ARG:HB3	2:K:121:TYR:CD2	2.50	0.45
2:Z:129:ASP:OD1	2:Z:129:ASP:N	2.47	0.45
2:l:45:GLN:NE2	2:l:111:GLN:OE1	2.49	0.45
2:z:35:TYR:CD2	2:z:124:ALA:HB3	2.49	0.45
2:B:151:ARG:O	2:B:152:VAL:HG23	2.15	0.45
2:c:38:TYR:CZ	2:c:104:ARG:HD3	2.51	0.45
2:l:165:ASP:OD1	2:l:233:ARG:NH1	2.49	0.45
1:n:144:ARG:NH2	2:o:74:ALA:HB2	2.31	0.45
1:G:359:ILE:HG21	1:J:357:ASN:OD1	2.17	0.45
1:S:302:ILE:HD11	1:S:365:LEU:HD12	1.97	0.45
2:H:21:LEU:HD21	2:H:109:ARG:HD2	1.98	0.45
1:n:247:LEU:HD13	1:n:275:ILE:HD13	1.99	0.45
2:E:161:MET:HG2	2:E:240:GLU:HG3	1.99	0.45
2:E:185:SER:HB2	2:H:245:ASN:HA	1.98	0.45
2:H:93:ALA:HB3	2:H:112:MET:HB2	1.98	0.45
2:N:120:MET:SD	2:N:123:LEU:HB2	2.56	0.45
1:S:182:GLU:O	1:S:186:LYS:HG3	2.16	0.45
1:V:144:ARG:NH1	2:W:91:GLU:O	2.50	0.45
2:l:57:MET:SD	2:l:124:ALA:HA	2.56	0.45
2:H:38:TYR:CE2	2:H:104:ARG:HD3	2.52	0.45
1:J:237:VAL:HB	1:J:247:LEU:HB2	1.99	0.45
2:o:102:ASP:OD1	2:o:103:ARG:N	2.49	0.45
2:H:91:GLU:OE2	1:J:142:ARG:NH2	2.50	0.45
2:K:76:ALA:O	2:K:86:ILE:HA	2.16	0.45
2:W:175:ASP:HB2	2:W:179:PHE:O	2.17	0.45
1:Y:139:GLU:O	1:Y:143:GLU:HG2	2.16	0.45
2:c:129:ASP:OD1	2:c:129:ASP:N	2.47	0.45
1:e:246:LEU:HD13	1:e:383:PHE:CD1	2.52	0.45
2:f:79:ARG:HG3	2:f:84:ILE:HG12	1.97	0.45
1:h:285:LEU:HD12	1:h:285:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:207:ILE:HG13	1:V:246:LEU:HD12	1.98	0.45
2:f:147:ALA:O	2:f:150:GLN:HG2	2.17	0.45
2:E:224:PRO:HA	2:E:239:ASN:HB3	1.98	0.45
2:H:69:PHE:HE2	2:H:77:PHE:HB2	1.81	0.45
2:H:87:LYS:HB2	1:J:150:LEU:HD21	1.98	0.45
1:e:209:GLN:O	1:h:252:LYS:HE3	2.17	0.45
2:f:42:ASP:OD1	2:f:43:VAL:N	2.50	0.45
2:f:56:ILE:HB	2:f:84:ILE:HB	1.98	0.45
1:h:353:GLU:O	1:h:357:ASN:ND2	2.45	0.45
2:o:93:ALA:HB3	2:o:112:MET:HE2	1.98	0.45
2:v:113:ARG:HH11	2:v:117:ASN:N	2.15	0.45
2:B:196:VAL:HG11	2:B:225:LYS:HD3	2.00	0.44
1:D:369:GLN:HG3	2:E:194:TYR:CZ	2.52	0.44
1:P:190:MET:HB3	1:P:190:MET:HE2	1.81	0.44
2:Q:74:ALA:HB1	2:Q:93:ALA:HB1	1.98	0.44
2:Q:227:MET:HE3	2:Q:234:ALA:HB1	1.98	0.44
2:T:59:GLU:OE1	2:T:104:ARG:NH1	2.50	0.44
1:Y:248:ASP:HB2	1:Y:278:PRO:HD2	1.98	0.44
2:Z:57:MET:HG2	2:Z:82:ARG:NH2	2.32	0.44
2:f:35:TYR:HD2	2:f:124:ALA:HB3	1.82	0.44
1:h:272:TRP:HE1	1:h:289:GLY:HA3	1.83	0.44
1:D:315:MET:HE3	1:D:315:MET:HB3	1.86	0.44
1:P:189:PRO:HB3	1:V:286:ASP:OD2	2.17	0.44
2:Q:59:GLU:HB2	2:Q:127:TYR:CZ	2.52	0.44
2:W:46:VAL:HB	2:W:110:LEU:HD12	1.99	0.44
1:Y:246:LEU:HD13	1:Y:383:PHE:CD1	2.53	0.44
2:c:21:LEU:N	2:c:42:ASP:OD1	2.49	0.44
2:c:189:ASP:OD2	2:f:221:LYS:HE2	2.17	0.44
2:f:227:MET:HE1	3:g:26:PRO:CD	2.47	0.44
2:B:58:LEU:HD21	2:B:84:ILE:HD12	1.98	0.44
1:G:135:LYS:HA	1:G:135:LYS:HD3	1.70	0.44
1:J:376:LEU:HD22	1:M:228:MET:HB2	1.98	0.44
1:b:315:MET:HB3	1:b:315:MET:HE3	1.68	0.44
2:B:140:ALA:O	2:B:144:VAL:HG23	2.17	0.44
2:E:167:ASP:OD2	2:E:168:ILE:HG23	2.17	0.44
1:G:355:LEU:O	1:G:359:ILE:HB	2.18	0.44
1:J:145:MET:HG2	2:K:71:ASP:OD2	2.18	0.44
1:J:285:LEU:HD12	1:J:285:LEU:O	2.17	0.44
2:N:71:ASP:HB2	2:N:95:THR:HG21	1.99	0.44
2:Q:38:TYR:HE2	2:Q:40:PRO:HG3	1.81	0.44
2:T:25:SER:O	2:T:34:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:43:VAL:HG12	2:T:107:LYS:HB3	1.99	0.44
1:V:141:ALA:O	1:V:145:MET:HG3	2.18	0.44
2:B:152:VAL:HG21	2:B:256:PRO:HG2	1.99	0.44
2:E:76:ALA:HB3	2:E:87:LYS:HB3	1.99	0.44
1:J:214:ASP:OD2	1:J:234:THR:OG1	2.34	0.44
2:Q:221:LYS:HG3	2:Q:222:VAL:N	2.32	0.44
2:W:58:LEU:HD22	2:W:106:TYR:CE2	2.52	0.44
2:f:26:SER:HA	2:f:34:ARG:HG2	1.99	0.44
2:l:167:ASP:OD1	2:l:233:ARG:NE	2.50	0.44
2:z:58:LEU:HD22	2:z:106:TYR:CE2	2.53	0.44
1:M:374:ASN:HD22	2:Q:204:LEU:HD12	1.81	0.44
1:P:143:GLU:O	1:P:147:ARG:HG3	2.17	0.44
2:Q:57:MET:SD	2:Q:83:HIS:ND1	2.91	0.44
2:Q:223:ASN:OD1	2:Q:224:PRO:HD2	2.18	0.44
2:T:223:ASN:ND2	2:T:225:LYS:O	2.51	0.44
1:Y:135:LYS:HA	1:Y:135:LYS:HD3	1.74	0.44
1:e:228:MET:HE2	1:e:228:MET:HB3	1.81	0.44
1:k:140:LEU:HD23	1:k:140:LEU:HA	1.84	0.44
1:P:198:GLY:O	1:S:386:VAL:HG11	2.18	0.44
2:W:45:GLN:NE2	2:W:47:ASP:OD1	2.50	0.44
1:b:190:MET:HE3	1:b:192:LEU:HD11	2.00	0.44
1:e:355:LEU:HD21	1:h:354:ALA:HB2	2.00	0.44
1:y:141:ALA:O	1:y:145:MET:HG2	2.18	0.44
2:B:107:LYS:HD3	2:o:33:ILE:HD11	2.00	0.44
2:c:127:TYR:HB3	2:c:129:ASP:OD1	2.17	0.44
1:n:139:GLU:O	1:n:143:GLU:HG2	2.17	0.44
2:K:55:HIS:HD1	2:K:122:GLU:HG2	1.82	0.44
1:b:285:LEU:HD12	1:b:285:LEU:O	2.18	0.44
2:z:64:TYR:HE1	2:z:99:VAL:HG23	1.83	0.44
2:B:34:ARG:HD2	2:B:120:MET:HE2	2.00	0.43
2:l:71:ASP:CB	2:l:95:THR:HG21	2.48	0.43
1:y:143:GLU:O	1:y:147:ARG:HG3	2.17	0.43
2:z:69:PHE:HE2	2:z:77:PHE:HB2	1.83	0.43
2:B:224:PRO:HA	2:B:239:ASN:HB3	1.99	0.43
2:H:167:ASP:OD2	2:H:233:ARG:NE	2.51	0.43
3:I:39:PRO:HD2	3:I:42:ILE:HD12	1.99	0.43
1:M:370:GLY:O	2:N:231:GLY:N	2.43	0.43
2:Q:62:GLU:OE2	2:Q:101:THR:HG21	2.18	0.43
2:T:33:ILE:HD12	2:T:122:GLU:CD	2.43	0.43
1:V:200:LEU:HD22	1:V:206:LEU:HD21	1.99	0.43
2:Z:253:THR:OG1	2:Z:258:VAL:O	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:LEU:HD13	1:D:383:PHE:CD1	2.54	0.43
2:E:29:TYR:HB2	2:H:41:ALA:O	2.18	0.43
2:H:22:ASP:N	2:H:43:VAL:O	2.35	0.43
2:K:34:ARG:HD2	2:K:120:MET:HE2	1.98	0.43
1:M:236:ASP:HB3	1:M:245:VAL:HG13	2.00	0.43
2:Q:26:SER:OG	2:Q:34:ARG:NE	2.51	0.43
2:Q:162:MET:HB3	3:R:34:VAL:HG22	2.00	0.43
1:V:248:ASP:HB2	1:V:278:PRO:HD2	1.99	0.43
2:E:87:LYS:HB2	1:G:150:LEU:HD21	1.99	0.43
2:H:51:GLY:HA3	2:H:116:ARG:NH2	2.33	0.43
2:Q:113:ARG:NH1	2:Q:115:ASP:OD1	2.51	0.43
1:S:285:LEU:O	1:S:285:LEU:HD12	2.18	0.43
1:V:194:GLY:HA2	1:Y:379:ARG:HB2	2.00	0.43
2:Z:156:TYR:CD2	3:a:42:ILE:HG23	2.53	0.43
3:d:30:ASN:OD1	3:d:30:ASN:N	2.50	0.43
2:i:62:GLU:OE2	2:i:101:THR:OG1	2.31	0.43
1:n:145:MET:HA	2:o:71:ASP:OD1	2.19	0.43
2:E:62:GLU:HG3	2:E:103:ARG:HD2	1.99	0.43
2:W:233:ARG:HD2	2:Z:198:ALA:HB3	2.00	0.43
1:Y:145:MET:HA	2:Z:71:ASP:OD2	2.19	0.43
2:c:99:VAL:CG1	2:c:106:TYR:HB2	2.49	0.43
1:P:137:PRO:HA	1:P:140:LEU:HB2	2.01	0.43
2:Q:50:LEU:HG	1:S:145:MET:SD	2.58	0.43
2:Q:57:MET:HE3	2:Q:57:MET:HA	2.00	0.43
1:Y:272:TRP:CD1	1:Y:375:ILE:HG12	2.53	0.43
2:i:87:LYS:HE3	2:i:87:LYS:HB2	1.76	0.43
1:n:302:ILE:HD11	1:n:365:LEU:HD12	2.00	0.43
2:o:69:PHE:CZ	2:o:77:PHE:HB2	2.54	0.43
2:z:59:GLU:OE1	2:z:103:ARG:NH1	2.51	0.43
1:G:152:ALA:HB2	2:H:72:SER:HB3	2.01	0.43
1:J:234:THR:HB	2:K:189:ASP:HB3	1.99	0.43
2:T:122:GLU:OE2	2:W:107:LYS:HD3	2.18	0.43
2:W:38:TYR:CZ	2:W:104:ARG:HD3	2.54	0.43
2:W:65:LEU:HD11	2:W:102:ASP:OD1	2.19	0.43
1:e:140:LEU:HD23	1:e:140:LEU:HA	1.83	0.43
1:h:246:LEU:HD13	1:h:383:PHE:CD1	2.54	0.43
2:i:64:TYR:OH	2:i:67:HIS:ND1	2.52	0.43
2:i:221:LYS:HG3	2:i:222:VAL:N	2.34	0.43
2:v:116:ARG:O	2:v:116:ARG:HG3	2.18	0.43
2:B:260:ARG:NH2	1:n:245:VAL:O	2.45	0.43
1:G:355:LEU:HD12	1:G:355:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:235:ARG:CD	2:Q:221:LYS:HD3	2.47	0.43
2:N:42:ASP:OD1	2:N:43:VAL:N	2.52	0.43
1:h:355:LEU:HD21	1:k:354:ALA:HB2	1.99	0.43
1:D:198:GLY:O	1:G:386:VAL:HG11	2.19	0.43
1:M:355:LEU:HD12	1:M:355:LEU:HA	1.81	0.43
2:N:207:ARG:NH1	2:N:217:ILE:HD13	2.34	0.43
2:f:223:ASN:ND2	2:f:225:LYS:O	2.47	0.43
1:h:247:LEU:HD13	1:h:275:ILE:HD13	2.00	0.43
2:i:76:ALA:O	2:i:86:ILE:HA	2.18	0.43
2:i:223:ASN:OD1	2:i:224:PRO:HD2	2.18	0.43
1:n:213:LEU:HG	1:n:237:VAL:HG21	2.01	0.43
1:n:285:LEU:HD12	1:n:285:LEU:O	2.19	0.43
2:H:50:LEU:HB2	2:H:112:MET:HE3	2.00	0.43
2:Q:45:GLN:NE2	2:Q:111:GLN:OE1	2.51	0.43
2:T:223:ASN:OD1	2:T:224:PRO:HD2	2.19	0.43
1:Y:355:LEU:HD12	1:Y:355:LEU:HA	1.81	0.43
1:b:135:LYS:HD3	1:b:135:LYS:HA	1.74	0.43
2:c:172:ASN:HB3	3:d:39:PRO:HG3	2.00	0.43
2:i:225:LYS:HE2	2:i:238:PHE:CE1	2.54	0.43
1:A:355:LEU:HD12	1:A:355:LEU:HA	1.83	0.42
2:B:225:LYS:HG3	2:B:238:PHE:CD1	2.53	0.42
2:N:137:GLU:O	2:N:141:ARG:HG3	2.19	0.42
1:P:228:MET:HE3	1:P:228:MET:HB3	1.92	0.42
2:Q:163:SER:HB3	3:R:31:ARG:HG2	2.01	0.42
2:c:109:ARG:NH2	2:c:111:GLN:OE1	2.52	0.42
2:B:162:MET:HE3	2:B:166:LYS:HD2	2.00	0.42
2:E:63:GLN:O	2:E:101:THR:HG23	2.19	0.42
2:c:21:LEU:HD22	2:c:45:GLN:HB2	2.01	0.42
2:f:49:VAL:HG22	2:f:119:ALA:HB2	2.01	0.42
2:f:216:ILE:HD11	3:g:41:GLU:HG2	2.01	0.42
2:o:55:HIS:CE1	2:o:83:HIS:HD1	2.37	0.42
2:o:58:LEU:HB2	2:o:82:ARG:HB2	2.01	0.42
1:A:201:GLY:HA2	2:H:266:ASN:OD1	2.19	0.42
1:D:141:ALA:O	1:D:145:MET:HG2	2.19	0.42
1:D:355:LEU:HD21	1:G:354:ALA:HB2	2.01	0.42
2:E:43:VAL:HG12	2:E:107:LYS:HB3	2.00	0.42
1:J:316:ILE:HD13	1:J:316:ILE:HA	1.88	0.42
1:M:234:THR:HB	2:N:189:ASP:HB3	2.00	0.42
2:T:38:TYR:HE2	2:T:40:PRO:HG3	1.85	0.42
1:e:135:LYS:HD3	1:e:135:LYS:HA	1.73	0.42
3:j:30:ASN:OD1	3:j:30:ASN:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:115:ASP:OD1	2:z:115:ASP:N	2.47	0.42
1:D:272:TRP:HE1	1:D:289:GLY:HA3	1.85	0.42
2:E:129:ASP:OD2	2:E:129:ASP:N	2.51	0.42
2:Z:70:GLY:N	2:Z:96:ASN:O	2.51	0.42
1:h:136:THR:HG23	1:h:139:GLU:H	1.83	0.42
1:A:290:THR:HG22	1:A:296:ALA:HA	2.00	0.42
2:B:46:VAL:HG13	2:B:120:MET:SD	2.60	0.42
2:E:150:GLN:O	2:E:150:GLN:HG2	2.20	0.42
2:K:223:ASN:OD1	2:K:224:PRO:HD2	2.19	0.42
1:M:277:THR:HG22	1:M:279:SER:H	1.83	0.42
2:Q:62:GLU:HG3	2:Q:103:ARG:HG3	2.01	0.42
2:Q:194:TYR:HB2	2:Q:227:MET:HB3	2.01	0.42
1:Y:329:GLN:O	1:Y:329:GLN:HG2	2.19	0.42
1:b:182:GLU:HG2	1:k:226:PRO:HG3	2.02	0.42
2:i:34:ARG:CD	2:i:120:MET:HE1	2.44	0.42
1:u:140:LEU:HD23	1:u:140:LEU:HA	1.91	0.42
1:D:309:ARG:HD2	1:D:359:ILE:O	2.20	0.42
1:G:264:GLY:HA2	1:J:308:GLU:OE1	2.20	0.42
2:W:122:GLU:OE1	2:v:107:LYS:HD3	2.20	0.42
2:c:56:ILE:HB	2:c:84:ILE:HG13	2.01	0.42
1:k:369:GLN:HB2	2:l:194:TYR:OH	2.20	0.42
2:H:156:TYR:CD2	3:I:42:ILE:HG23	2.54	0.42
1:P:355:LEU:HD12	1:P:355:LEU:HA	1.89	0.42
2:c:250:ASP:OD2	2:c:250:ASP:N	2.53	0.42
2:f:64:TYR:OH	2:f:67:HIS:ND1	2.35	0.42
2:i:55:HIS:N	2:i:121:TYR:O	2.30	0.42
2:l:182:PHE:CD2	2:l:193:ILE:HD13	2.55	0.42
2:B:56:ILE:HD13	2:B:108:PHE:CE1	2.55	0.42
1:D:152:ALA:HB2	2:E:72:SER:HB3	2.00	0.42
2:E:60:GLU:OE2	2:E:82:ARG:NH2	2.53	0.42
2:Q:101:THR:HG23	2:Q:103:ARG:H	1.84	0.42
1:V:302:ILE:HD11	1:V:365:LEU:HD12	2.00	0.42
2:Z:53:ALA:H	2:c:96:ASN:HD21	1.68	0.42
2:Z:130:THR:O	2:Z:134:GLN:HG2	2.20	0.42
2:z:113:ARG:NH2	2:z:117:ASN:H	2.17	0.42
1:P:204:ASP:OD2	1:P:241:SER:OG	2.30	0.42
1:S:299:GLY:HA2	1:S:365:LEU:HD11	2.01	0.42
2:c:58:LEU:HD22	2:c:106:TYR:CE2	2.55	0.42
2:f:33:ILE:HD12	2:f:122:GLU:CD	2.44	0.42
1:h:238:TYR:OH	2:l:178:ARG:HD3	2.19	0.42
2:l:26:SER:HB3	2:l:31:HIS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:38:TYR:OH	2:l:104:ARG:HB2	2.20	0.42
2:l:223:ASN:ND2	2:l:225:LYS:O	2.52	0.42
2:o:25:SER:N	2:o:35:TYR:O	2.48	0.42
2:o:47:ASP:H	2:o:120:MET:HE2	1.84	0.42
2:o:176:ASP:OD1	2:o:176:ASP:N	2.51	0.42
2:E:168:ILE:HD12	2:E:228:ILE:HG22	2.01	0.42
1:G:236:ASP:HB3	1:G:245:VAL:HG13	2.00	0.42
2:K:44:VAL:HG22	2:K:107:LYS:O	2.19	0.42
1:M:299:GLY:HA2	1:M:365:LEU:HD11	2.01	0.42
2:W:36:VAL:O	2:W:125:PHE:HA	2.20	0.42
1:e:305:HIS:O	1:e:309:ARG:HG3	2.20	0.42
2:f:62:GLU:HG3	2:f:103:ARG:HD2	2.01	0.42
1:h:189:PRO:HB3	1:n:286:ASP:OD2	2.20	0.42
1:G:369:GLN:NE2	2:H:202:GLU:OE1	2.53	0.41
1:J:228:MET:HE2	1:J:228:MET:HB3	1.75	0.41
1:P:247:LEU:HD13	1:P:275:ILE:HD13	2.02	0.41
1:P:285:LEU:HD12	1:P:285:LEU:O	2.20	0.41
2:Q:178:ARG:HH21	2:Q:247:VAL:HG23	1.85	0.41
2:T:100:VAL:HG23	2:T:105:SER:HB2	2.02	0.41
2:W:74:ALA:HA	2:W:90:ALA:HB3	2.02	0.41
2:c:63:GLN:HB3	2:c:102:ASP:OD2	2.20	0.41
2:f:159:LYS:HB3	2:f:159:LYS:HE3	1.66	0.41
1:Y:355:LEU:HD21	1:b:354:ALA:HB2	2.02	0.41
2:Z:108:PHE:HE1	2:Z:123:LEU:HD23	1.85	0.41
2:o:133:ARG:O	2:o:137:GLU:HG2	2.20	0.41
2:K:76:ALA:N	2:K:87:LYS:O	2.39	0.41
1:V:246:LEU:HD13	1:V:383:PHE:CD1	2.55	0.41
1:n:305:HIS:O	1:n:309:ARG:HG3	2.20	0.41
2:o:54:THR:HG22	2:o:120:MET:HB3	2.03	0.41
2:o:140:ALA:O	2:o:144:VAL:HG23	2.20	0.41
2:v:93:ALA:H	2:v:112:MET:HG3	1.85	0.41
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.90	0.41
2:B:26:SER:HB3	2:B:31:HIS:HA	2.02	0.41
2:B:43:VAL:HA	2:B:107:LYS:HB2	2.03	0.41
2:E:67:HIS:HA	2:E:99:VAL:HA	2.02	0.41
1:J:305:HIS:O	1:J:309:ARG:HG3	2.20	0.41
2:Q:182:PHE:CD2	2:Q:193:ILE:HD13	2.55	0.41
2:Q:227:MET:HE1	3:R:26:PRO:CD	2.44	0.41
2:c:133:ARG:HA	2:c:136:ARG:NH1	2.36	0.41
2:l:226:TRP:HB2	2:l:237:ILE:HB	2.01	0.41
1:A:327:SER:HA	1:n:325:TRP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:THR:O	2:B:112:MET:HA	2.20	0.41
1:h:144:ARG:NH2	2:i:74:ALA:HB2	2.36	0.41
2:z:59:GLU:C	2:z:82:ARG:HE	2.29	0.41
1:A:382:ASP:OD1	1:A:384:SER:OG	2.33	0.41
2:B:31:HIS:O	2:B:34:ARG:NH1	2.53	0.41
1:G:244:VAL:CG2	1:G:389:LEU:HD21	2.51	0.41
2:H:122:GLU:CG	2:K:107:LYS:HD3	2.51	0.41
2:K:31:HIS:CE1	2:K:32:ARG:NH2	2.88	0.41
2:N:191:PRO:HB3	2:N:230:LEU:HB2	2.02	0.41
1:e:236:ASP:HB3	1:e:245:VAL:HG13	2.03	0.41
1:k:209:GLN:O	1:n:252:LYS:HE3	2.20	0.41
1:A:329:GLN:O	1:A:329:GLN:HG2	2.21	0.41
2:Q:102:ASP:OD1	2:Q:103:ARG:HG2	2.21	0.41
2:c:56:ILE:HG12	2:c:123:LEU:HB3	2.03	0.41
2:c:65:LEU:HD11	2:c:102:ASP:OD1	2.21	0.41
2:c:71:ASP:HB2	2:c:74:ALA:HB3	2.03	0.41
2:f:87:LYS:HE3	1:h:148:SER:O	2.21	0.41
1:h:302:ILE:HD11	1:h:365:LEU:HD12	2.01	0.41
1:h:325:TRP:HE1	1:k:330:GLY:HA2	1.86	0.41
2:l:225:LYS:HE2	2:l:238:PHE:CE1	2.56	0.41
1:n:236:ASP:HB3	1:n:245:VAL:HG13	2.02	0.41
1:G:283:ILE:CD1	1:G:381:LEU:HB3	2.51	0.41
2:K:34:ARG:CD	2:K:120:MET:HE2	2.51	0.41
1:S:135:LYS:HA	1:S:139:GLU:OE2	2.21	0.41
1:V:388:SER:HB3	2:Z:263:LYS:HE3	2.02	0.41
1:Y:305:HIS:O	1:Y:309:ARG:HG3	2.20	0.41
2:Z:107:LYS:NZ	2:v:33:ILE:HD12	2.36	0.41
2:f:76:ALA:HB3	2:f:87:LYS:HB3	2.03	0.41
1:k:301:TRP:CZ3	1:k:303:ASP:HB2	2.55	0.41
2:l:141:ARG:O	2:l:145:GLU:HG2	2.21	0.41
1:A:301:TRP:CZ3	1:A:303:ASP:HB2	2.56	0.41
1:D:150:LEU:HD21	2:z:87:LYS:HB2	2.02	0.41
2:E:64:TYR:HE2	2:E:99:VAL:HG23	1.85	0.41
1:J:392:ILE:HD11	2:N:259:ARG:HG2	2.03	0.41
2:N:42:ASP:O	2:N:107:LYS:HE2	2.20	0.41
2:N:87:LYS:HD3	2:N:88:PRO:O	2.20	0.41
1:Y:234:THR:HB	2:Z:189:ASP:HB3	2.03	0.41
2:Z:107:LYS:HZ3	2:v:122:GLU:HB3	1.86	0.41
2:Z:196:VAL:HG11	2:Z:225:LYS:HD3	2.02	0.41
2:c:32:ARG:HG2	2:c:121:TYR:CD2	2.56	0.41
2:c:76:ALA:N	2:c:87:LYS:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:184:ALA:HB2	1:h:190:MET:SD	2.61	0.41
1:e:247:LEU:HD13	1:e:275:ILE:HD13	2.03	0.41
1:h:246:LEU:HD23	1:h:246:LEU:HA	1.86	0.41
2:l:76:ALA:O	2:l:86:ILE:HA	2.21	0.41
2:v:46:VAL:HG13	2:v:120:MET:CE	2.51	0.41
2:z:49:VAL:HB	2:z:116:ARG:HA	2.02	0.41
1:D:200:LEU:HD22	1:D:206:LEU:HD21	2.03	0.41
2:H:175:ASP:HB2	2:H:179:PHE:O	2.21	0.41
1:J:325:TRP:HE1	1:M:330:GLY:HA2	1.85	0.41
1:M:181:GLY:O	1:M:185:GLU:HB2	2.21	0.41
1:M:315:MET:HE2	1:M:315:MET:HB3	1.91	0.41
1:S:198:GLY:O	1:V:386:VAL:HG11	2.21	0.41
1:S:252:LYS:HB3	1:S:252:LYS:HE2	1.92	0.41
1:Y:301:TRP:CZ3	1:Y:303:ASP:HB2	2.56	0.41
3:g:22:LYS:HB3	3:g:22:LYS:HE3	1.92	0.41
2:i:24:PRO:HB2	2:i:34:ARG:CG	2.51	0.41
2:l:130:THR:O	2:l:134:GLN:HG3	2.21	0.41
2:o:133:ARG:HA	2:o:136:ARG:CZ	2.51	0.41
2:B:161:MET:HG2	2:B:240:GLU:HG3	2.03	0.40
1:D:285:LEU:HD12	1:D:285:LEU:O	2.22	0.40
2:E:174:TRP:CD1	3:F:42:ILE:HD11	2.56	0.40
1:M:140:LEU:HD23	1:M:140:LEU:HA	1.84	0.40
2:N:216:ILE:HD11	3:O:41:GLU:HG2	2.03	0.40
2:W:53:ALA:H	2:v:96:ASN:HD21	1.69	0.40
1:Y:190:MET:HE2	1:Y:190:MET:HB3	1.83	0.40
2:f:65:LEU:HD11	2:f:102:ASP:OD1	2.20	0.40
1:n:234:THR:HB	2:o:189:ASP:HB3	2.03	0.40
1:A:139:GLU:O	1:A:143:GLU:HG2	2.21	0.40
2:B:94:ASN:HB2	2:o:116:ARG:HH22	1.86	0.40
1:G:140:LEU:HD23	1:G:140:LEU:HA	1.91	0.40
2:K:240:GLU:OE1	3:L:31:ARG:NH1	2.54	0.40
2:Z:223:ASN:OD1	2:Z:224:PRO:HD2	2.21	0.40
2:c:113:ARG:NE	2:c:117:ASN:O	2.54	0.40
2:z:80:LYS:HB3	2:z:80:LYS:HE3	1.97	0.40
1:A:232:HIS:HA	1:A:251:SER:O	2.22	0.40
2:B:57:MET:SD	2:B:82:ARG:NH1	2.95	0.40
1:G:143:GLU:O	1:G:147:ARG:HG3	2.22	0.40
2:H:51:GLY:HA3	2:H:116:ARG:HH21	1.86	0.40
2:N:223:ASN:OD1	2:N:224:PRO:HD2	2.22	0.40
1:V:301:TRP:CZ3	1:V:303:ASP:HB2	2.56	0.40
2:c:38:TYR:CE1	2:c:104:ARG:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:309:ARG:HD2	1:e:359:ILE:O	2.21	0.40
2:l:53:ALA:HB2	2:o:69:PHE:O	2.21	0.40
1:M:213:LEU:HG	1:M:237:VAL:HG21	2.02	0.40
1:V:136:THR:HG23	1:V:139:GLU:H	1.86	0.40
2:W:162:MET:O	3:X:31:ARG:HA	2.22	0.40
2:Z:46:VAL:HB	2:Z:110:LEU:HD23	2.04	0.40
1:b:376:LEU:HD22	1:e:228:MET:HB2	2.02	0.40
2:c:26:SER:HA	2:c:34:ARG:HA	2.03	0.40
2:c:136:ARG:HG3	2:c:136:ARG:NH1	2.37	0.40
2:c:196:VAL:HG22	2:c:202:GLU:HG3	2.04	0.40
1:e:315:MET:SD	1:e:319:ILE:HD12	2.62	0.40
2:f:58:LEU:HB3	2:f:62:GLU:OE1	2.22	0.40
1:y:142:ARG:HA	1:y:145:MET:HG2	2.02	0.40
1:A:315:MET:SD	1:A:319:ILE:HD12	2.62	0.40
1:D:190:MET:HE2	1:D:190:MET:HB3	1.97	0.40
2:H:223:ASN:OD1	2:H:224:PRO:HD2	2.22	0.40
2:K:42:ASP:OD1	2:K:43:VAL:N	2.54	0.40
2:N:29:TYR:HB2	2:Q:41:ALA:O	2.21	0.40
2:Q:132:ALA:HA	2:Q:135:THR:HG22	2.03	0.40
2:W:32:ARG:HA	2:W:34:ARG:HH12	1.86	0.40
1:Y:208:THR:CG2	1:Y:240:THR:HG21	2.51	0.40
2:l:65:LEU:HD23	2:l:101:THR:HA	2.03	0.40
2:l:178:ARG:NH2	2:l:247:VAL:HG13	2.36	0.40
2:o:26:SER:HA	2:o:34:ARG:HA	2.04	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	215/395 (54%)	213 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	215/395 (54%)	210 (98%)	5 (2%)	0	100	100
1	G	215/395 (54%)	210 (98%)	5 (2%)	0	100	100
1	J	215/395 (54%)	212 (99%)	3 (1%)	0	100	100
1	M	215/395 (54%)	210 (98%)	5 (2%)	0	100	100
1	P	215/395 (54%)	210 (98%)	5 (2%)	0	100	100
1	S	215/395 (54%)	212 (99%)	3 (1%)	0	100	100
1	V	215/395 (54%)	208 (97%)	7 (3%)	0	100	100
1	Y	215/395 (54%)	211 (98%)	4 (2%)	0	100	100
1	b	215/395 (54%)	211 (98%)	4 (2%)	0	100	100
1	e	215/395 (54%)	209 (97%)	6 (3%)	0	100	100
1	h	215/395 (54%)	210 (98%)	5 (2%)	0	100	100
1	k	215/395 (54%)	209 (97%)	6 (3%)	0	100	100
1	n	215/395 (54%)	212 (99%)	3 (1%)	0	100	100
1	u	17/395 (4%)	17 (100%)	0	0	100	100
1	y	17/395 (4%)	17 (100%)	0	0	100	100
2	B	244/266 (92%)	229 (94%)	14 (6%)	1 (0%)	30	60
2	E	244/266 (92%)	236 (97%)	8 (3%)	0	100	100
2	H	244/266 (92%)	232 (95%)	12 (5%)	0	100	100
2	K	244/266 (92%)	232 (95%)	12 (5%)	0	100	100
2	N	244/266 (92%)	235 (96%)	9 (4%)	0	100	100
2	Q	244/266 (92%)	237 (97%)	7 (3%)	0	100	100
2	T	244/266 (92%)	235 (96%)	9 (4%)	0	100	100
2	W	244/266 (92%)	234 (96%)	10 (4%)	0	100	100
2	Z	244/266 (92%)	233 (96%)	11 (4%)	0	100	100
2	c	244/266 (92%)	235 (96%)	9 (4%)	0	100	100
2	f	244/266 (92%)	234 (96%)	10 (4%)	0	100	100
2	i	244/266 (92%)	236 (97%)	8 (3%)	0	100	100
2	l	244/266 (92%)	232 (95%)	12 (5%)	0	100	100
2	o	244/266 (92%)	236 (97%)	8 (3%)	0	100	100
2	v	106/266 (40%)	102 (96%)	4 (4%)	0	100	100
2	z	106/266 (40%)	103 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	26/47 (55%)	26 (100%)	0	0	100	100
3	F	26/47 (55%)	26 (100%)	0	0	100	100
3	I	26/47 (55%)	26 (100%)	0	0	100	100
3	L	26/47 (55%)	25 (96%)	1 (4%)	0	100	100
3	O	26/47 (55%)	25 (96%)	1 (4%)	0	100	100
3	R	26/47 (55%)	25 (96%)	1 (4%)	0	100	100
3	U	26/47 (55%)	26 (100%)	0	0	100	100
3	X	26/47 (55%)	25 (96%)	1 (4%)	0	100	100
3	a	26/47 (55%)	26 (100%)	0	0	100	100
3	d	26/47 (55%)	26 (100%)	0	0	100	100
3	g	26/47 (55%)	26 (100%)	0	0	100	100
3	j	26/47 (55%)	26 (100%)	0	0	100	100
3	m	26/47 (55%)	26 (100%)	0	0	100	100
3	p	26/47 (55%)	26 (100%)	0	0	100	100
All	All	7036/11234 (63%)	6822 (97%)	213 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	VAL

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	176/318 (55%)	176 (100%)	0	100	100
1	D	176/318 (55%)	176 (100%)	0	100	100
1	G	176/318 (55%)	176 (100%)	0	100	100
1	J	176/318 (55%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	176/318 (55%)	176 (100%)	0	100	100
1	P	176/318 (55%)	176 (100%)	0	100	100
1	S	176/318 (55%)	176 (100%)	0	100	100
1	V	176/318 (55%)	176 (100%)	0	100	100
1	Y	176/318 (55%)	176 (100%)	0	100	100
1	b	176/318 (55%)	176 (100%)	0	100	100
1	e	176/318 (55%)	176 (100%)	0	100	100
1	h	176/318 (55%)	176 (100%)	0	100	100
1	k	176/318 (55%)	176 (100%)	0	100	100
1	n	176/318 (55%)	175 (99%)	1 (1%)	78	82
1	u	15/318 (5%)	15 (100%)	0	100	100
1	y	15/318 (5%)	15 (100%)	0	100	100
2	B	202/216 (94%)	202 (100%)	0	100	100
2	E	202/216 (94%)	202 (100%)	0	100	100
2	H	202/216 (94%)	202 (100%)	0	100	100
2	K	202/216 (94%)	202 (100%)	0	100	100
2	N	202/216 (94%)	202 (100%)	0	100	100
2	Q	202/216 (94%)	202 (100%)	0	100	100
2	T	202/216 (94%)	202 (100%)	0	100	100
2	W	202/216 (94%)	202 (100%)	0	100	100
2	Z	202/216 (94%)	202 (100%)	0	100	100
2	c	202/216 (94%)	202 (100%)	0	100	100
2	f	202/216 (94%)	202 (100%)	0	100	100
2	i	202/216 (94%)	202 (100%)	0	100	100
2	l	202/216 (94%)	202 (100%)	0	100	100
2	o	202/216 (94%)	202 (100%)	0	100	100
2	v	93/216 (43%)	93 (100%)	0	100	100
2	z	93/216 (43%)	93 (100%)	0	100	100
3	C	25/40 (62%)	24 (96%)	1 (4%)	28	58
3	F	25/40 (62%)	25 (100%)	0	100	100
3	I	25/40 (62%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	25/40 (62%)	25 (100%)	0	100	100
3	O	25/40 (62%)	24 (96%)	1 (4%)	28	58
3	R	25/40 (62%)	25 (100%)	0	100	100
3	U	25/40 (62%)	25 (100%)	0	100	100
3	X	25/40 (62%)	25 (100%)	0	100	100
3	a	25/40 (62%)	24 (96%)	1 (4%)	28	58
3	d	25/40 (62%)	25 (100%)	0	100	100
3	g	25/40 (62%)	25 (100%)	0	100	100
3	j	25/40 (62%)	25 (100%)	0	100	100
3	m	25/40 (62%)	25 (100%)	0	100	100
3	p	25/40 (62%)	25 (100%)	0	100	100
All	All	5858/9104 (64%)	5854 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	43	GLN
3	O	43	GLN
3	a	43	GLN
1	n	374	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	271	GLN
1	A	357	ASN
1	A	360	ASN
1	A	374	ASN
2	B	83	HIS
1	D	232	HIS
1	D	271	GLN
1	D	374	ASN
2	E	214	ASN
1	G	212	GLN
1	G	232	HIS
1	G	271	GLN

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Mol	Chain	Res	Type
1	G	374	ASN
2	H	31	HIS
2	H	39	ASN
2	K	31	HIS
2	K	172	ASN
2	N	39	ASN
2	N	94	ASN
1	P	271	GLN
1	P	360	ASN
2	Q	31	HIS
2	T	232	ASN
1	V	360	ASN
2	W	55	HIS
2	W	83	HIS
1	Y	271	GLN
2	c	94	ASN
2	c	172	ASN
1	e	284	ASN
1	e	374	ASN
2	f	31	HIS
2	f	45	GLN
2	f	89	GLN
2	f	117	ASN
1	h	232	HIS
2	i	201	ASN
2	l	39	ASN
2	l	150	GLN
2	l	172	ASN
1	n	271	GLN
1	n	284	ASN
2	o	39	ASN
2	z	94	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

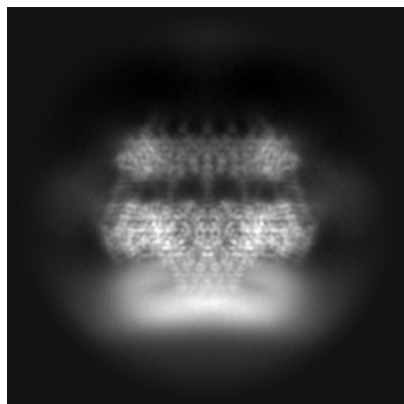
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19480. These allow visual inspection of the internal detail of the map and identification of artifacts.

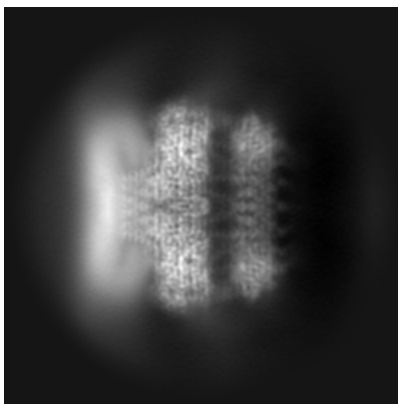
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

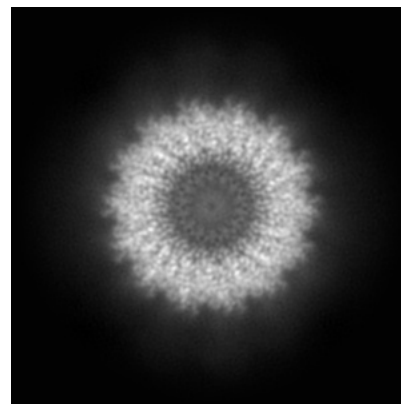
6.1.1 Primary map



X

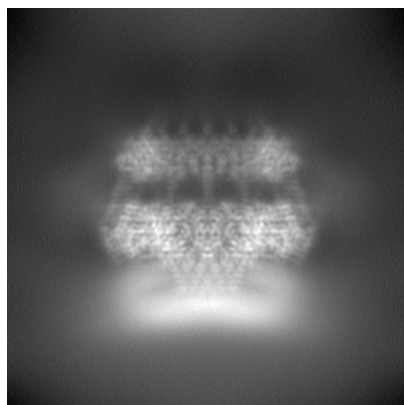


Y

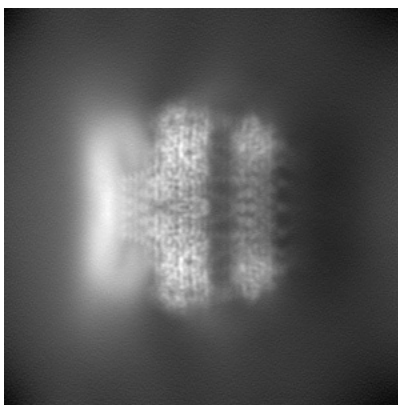


Z

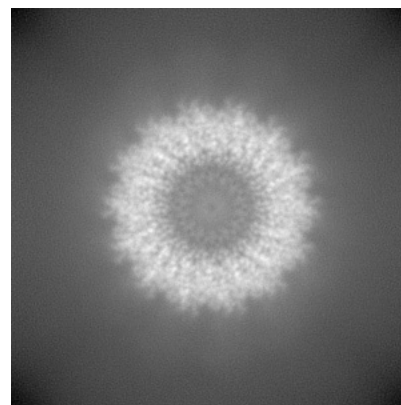
6.1.2 Raw map



X



Y

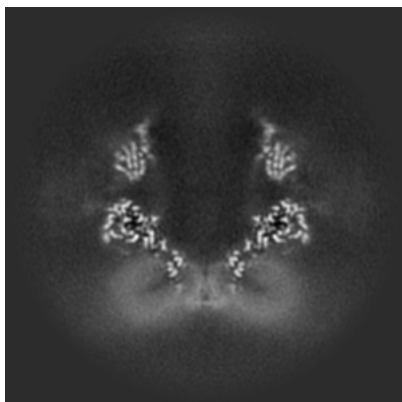


Z

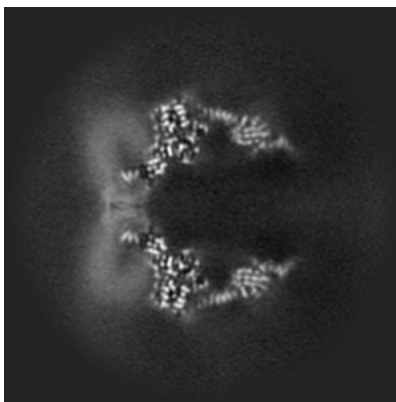
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

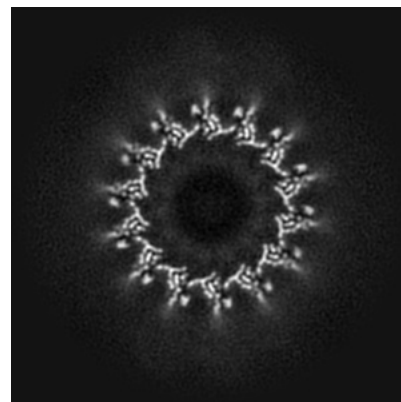
6.2.1 Primary map



X Index: 150

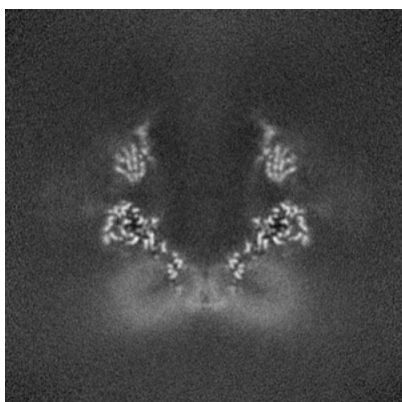


Y Index: 150

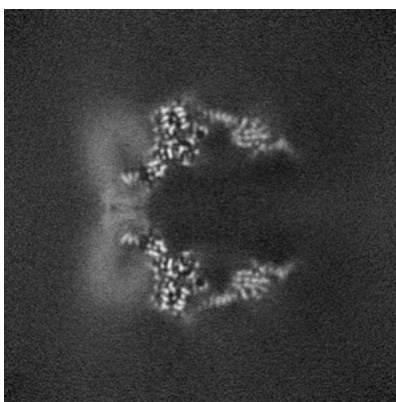


Z Index: 150

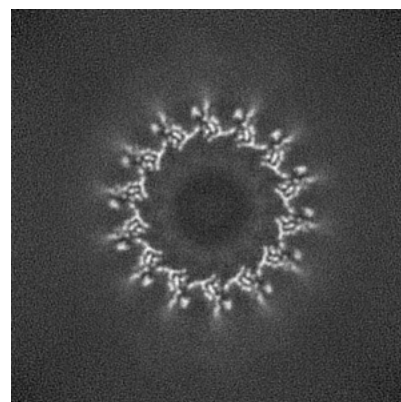
6.2.2 Raw map



X Index: 150



Y Index: 150

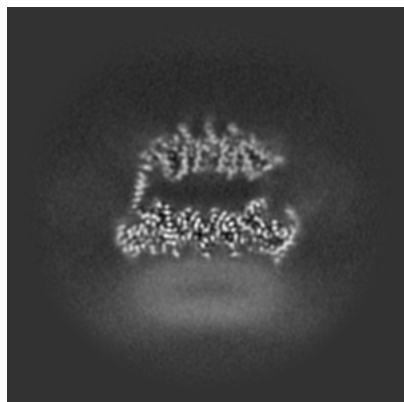


Z Index: 150

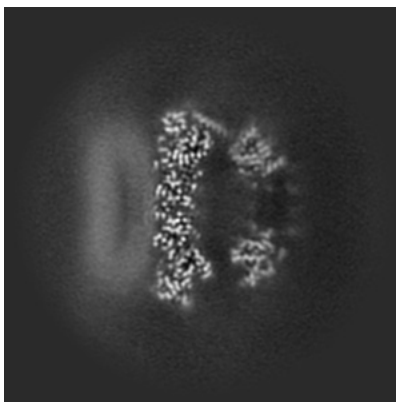
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

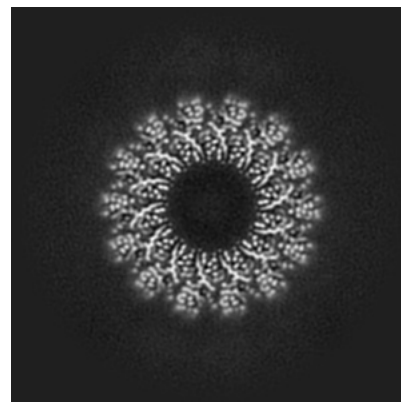
6.3.1 Primary map



X Index: 104

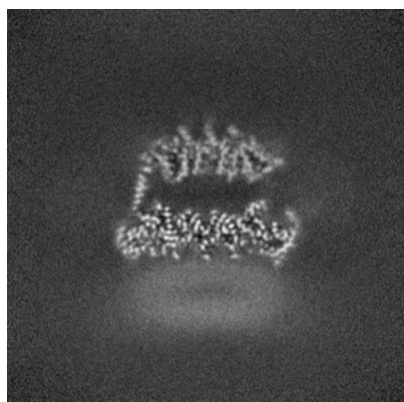


Y Index: 113

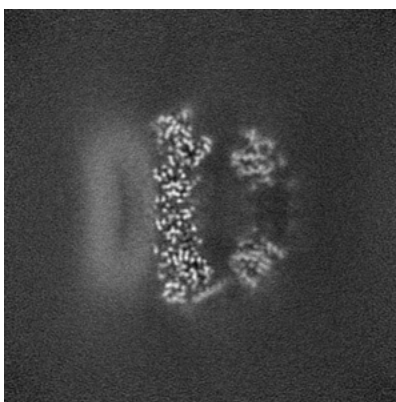


Z Index: 132

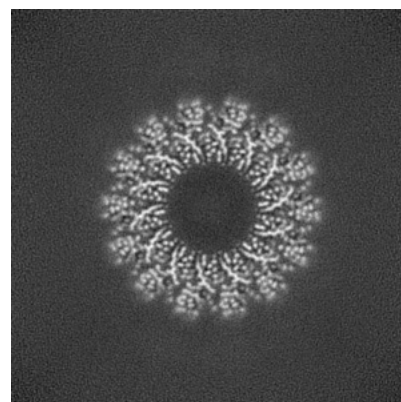
6.3.2 Raw map



X Index: 104



Y Index: 187

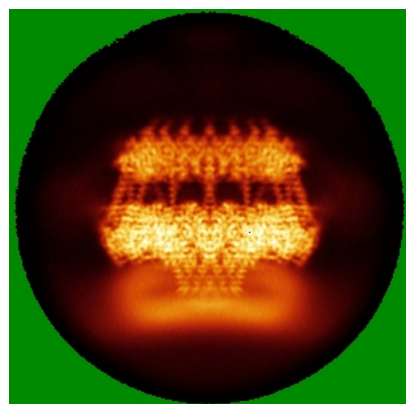


Z Index: 132

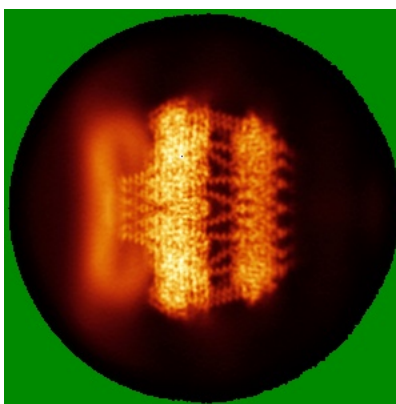
The images above show the largest variance slices of the map in three orthogonal directions.

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

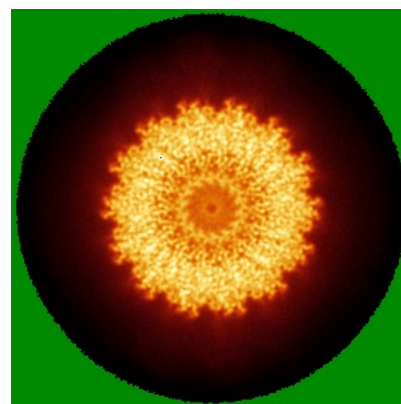
6.4.1 Primary map



X

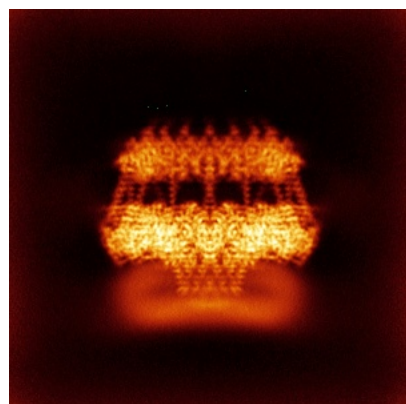


Y

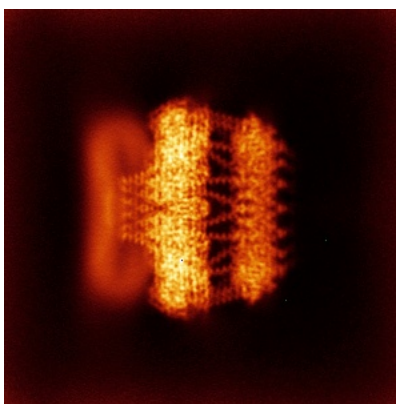


Z

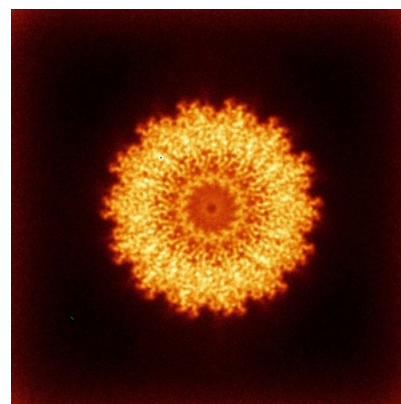
6.4.2 Raw map



X



Y

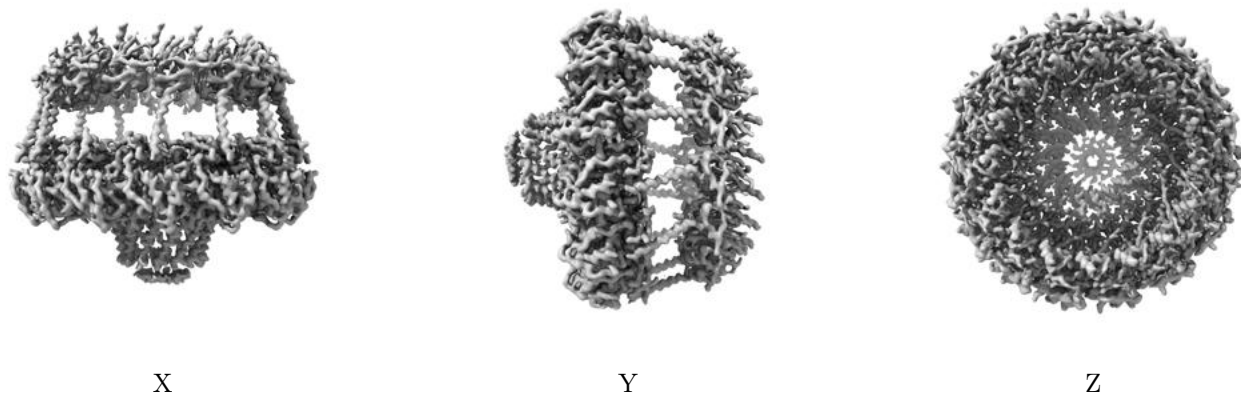


Z

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

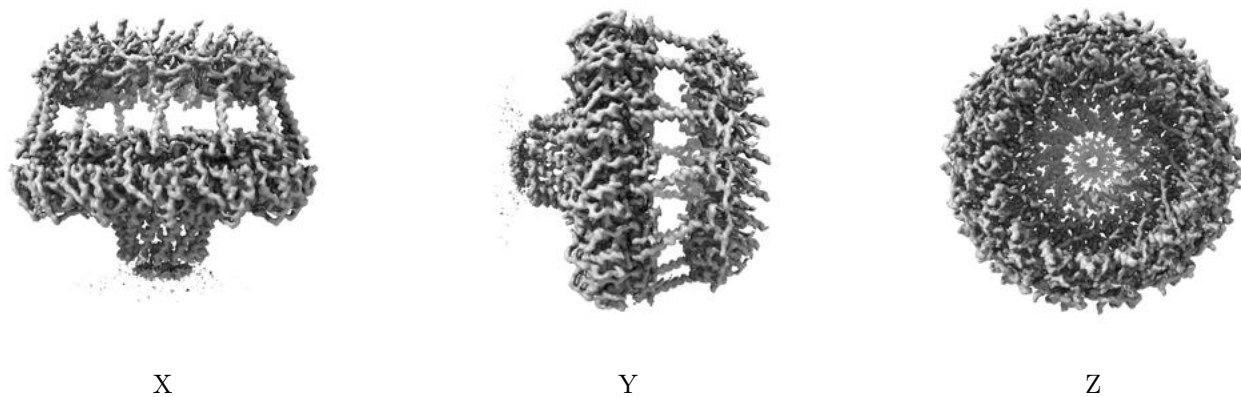
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

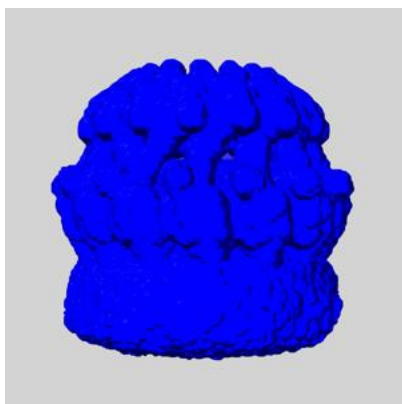
6.6 Mask visualisation [i](#)

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

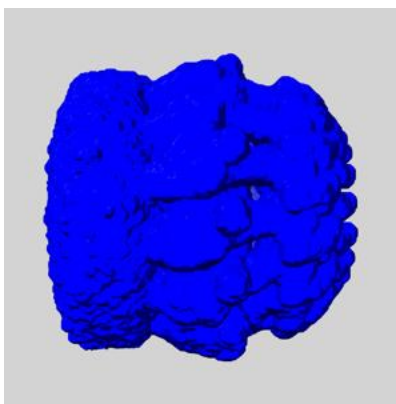
A mask typically either:

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

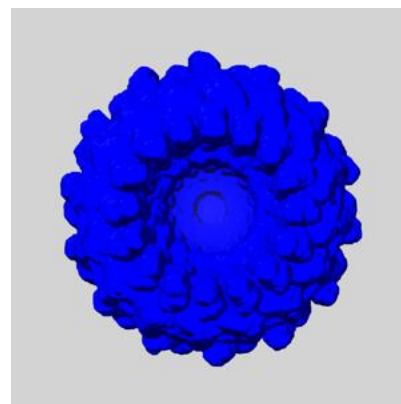
6.6.1 emd_19480_msk_1.map [i](#)



X



Y

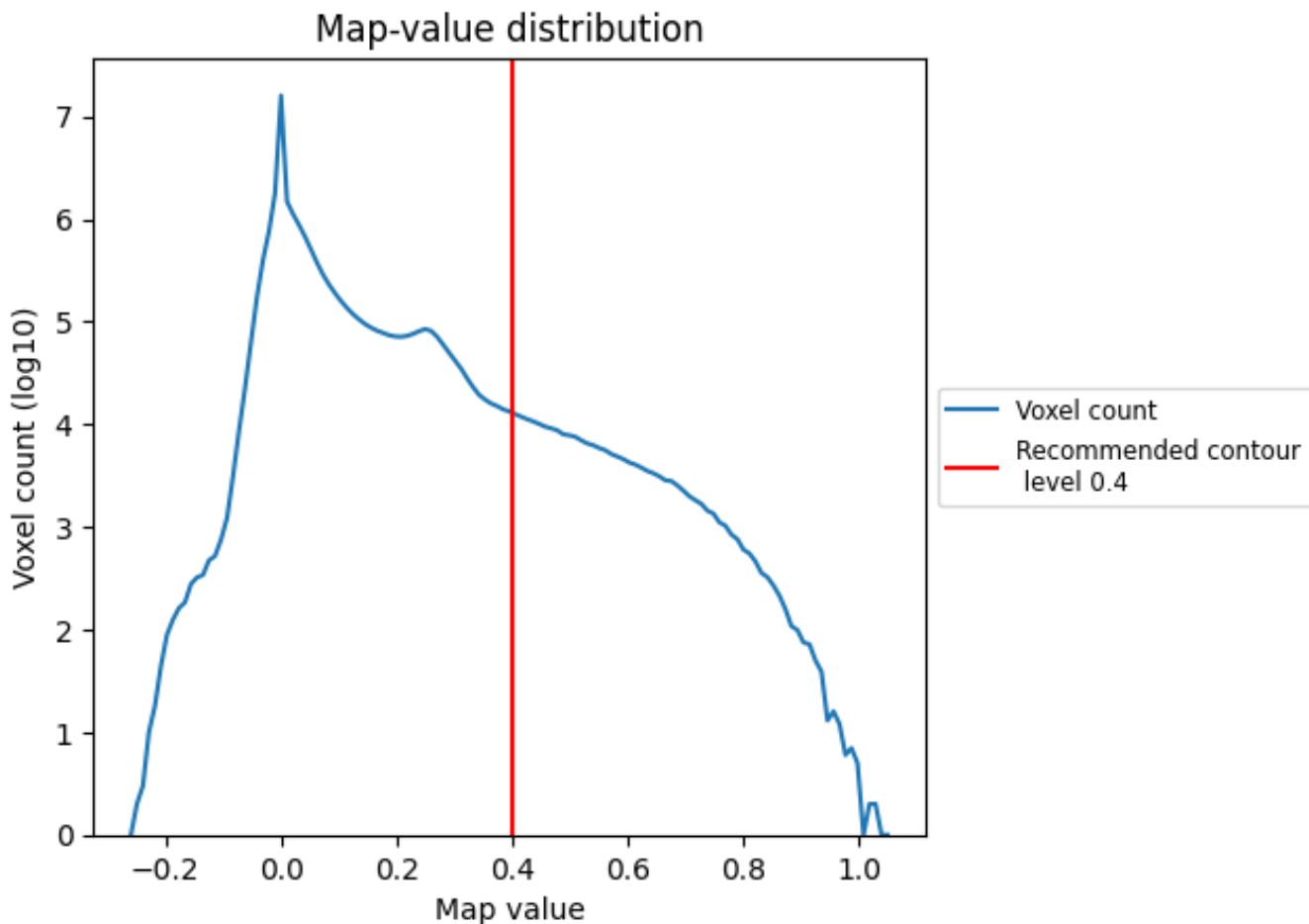


Z

7 Map analysis [i](#)

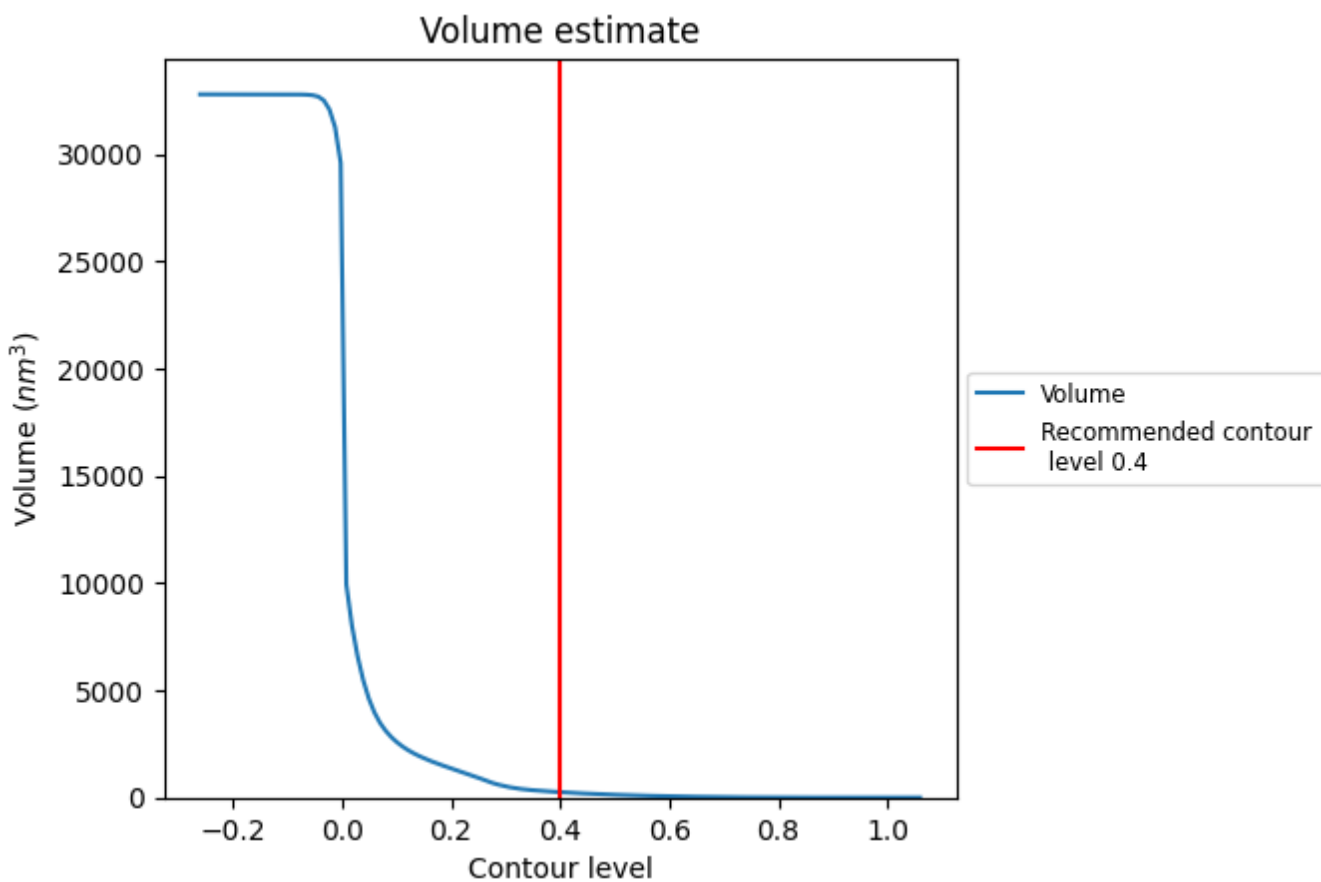
This section contains the results of statistical analysis of the map.

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.

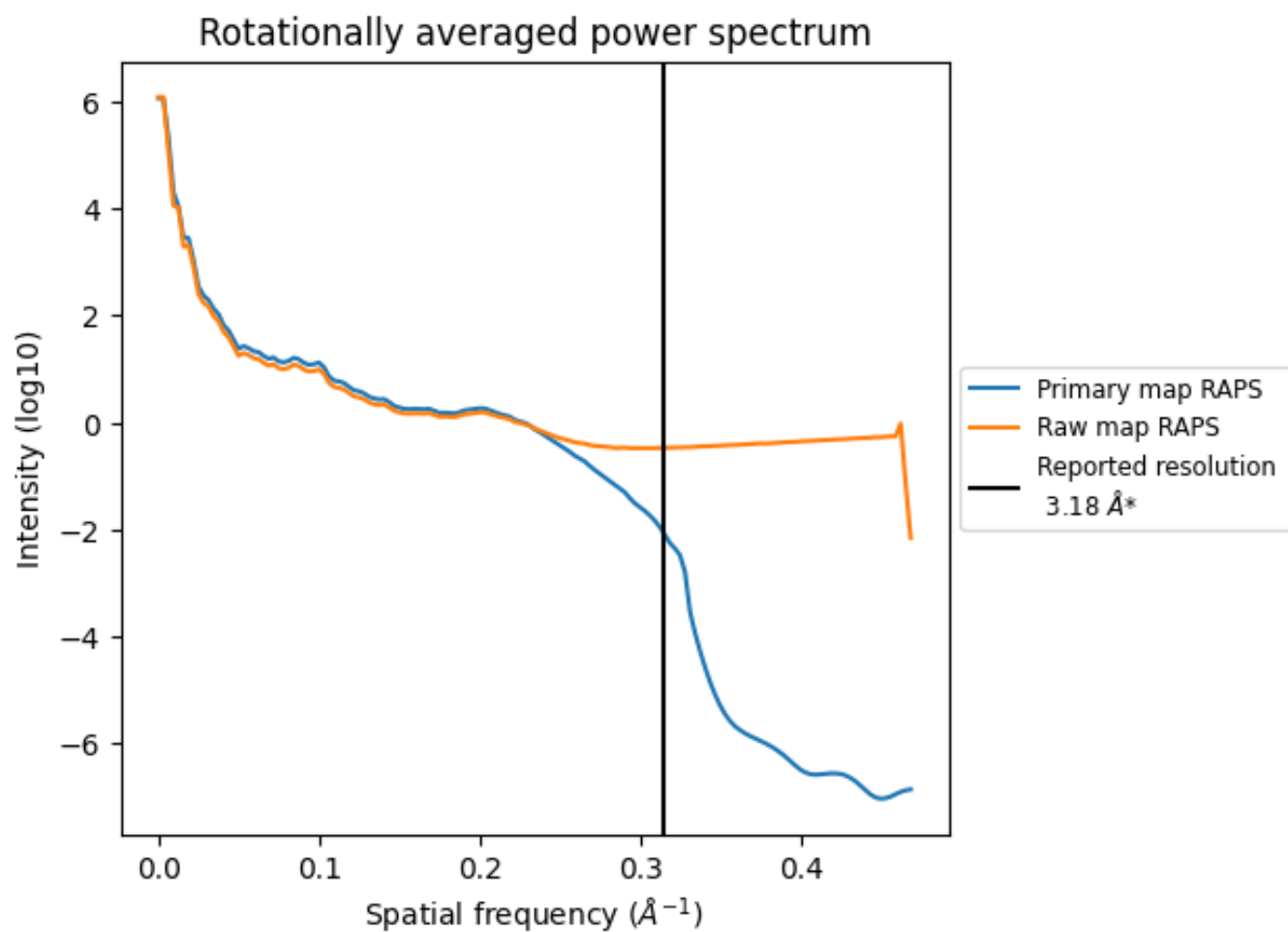
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 nm³; this corresponds to an approximate mass of 227 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 i

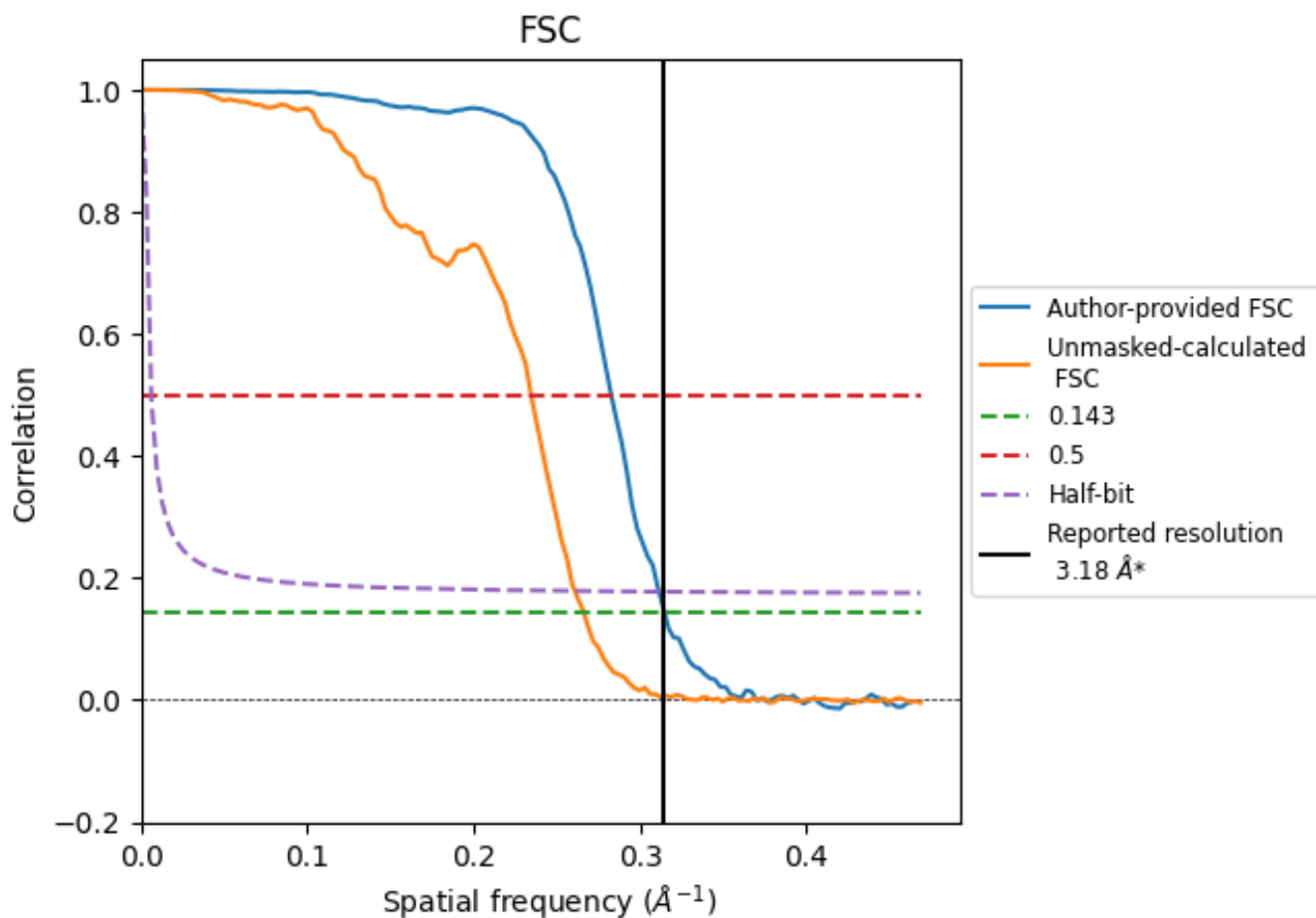


*Reported resolution corresponds to spatial frequency of 0.314 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.314\AA^{-1}

8.2 Resolution estimates [i](#)

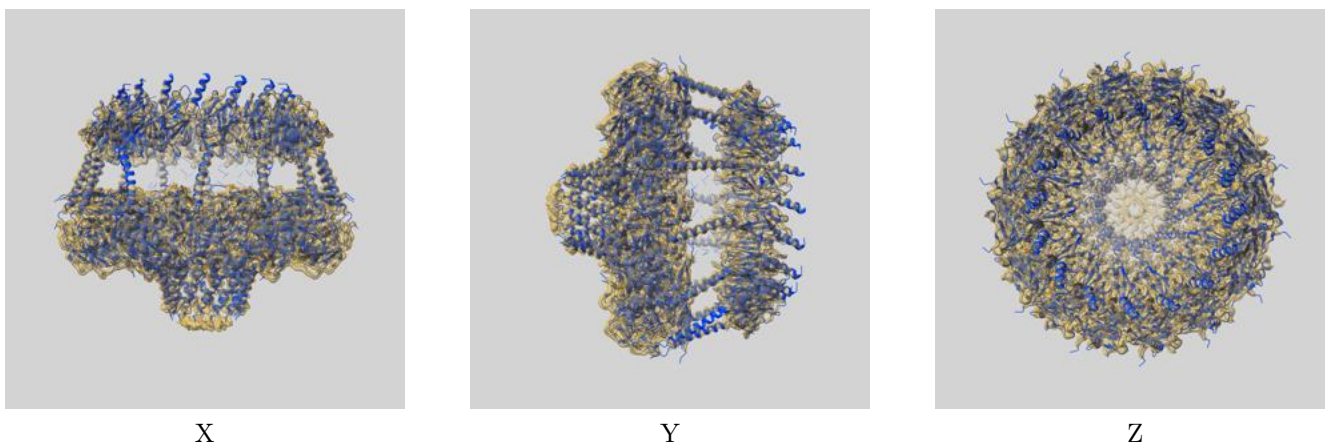
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.54	3.21
Unmasked-calculated*	3.76	4.26	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.18 by more than 10 %

9 Map-model fit [i](#)

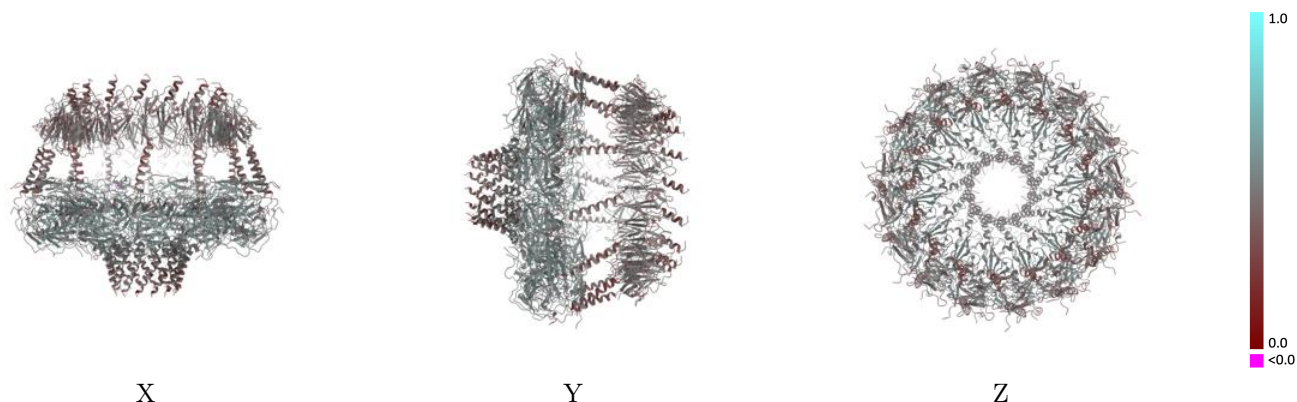
This section contains information regarding the fit between EMDB map EMD-19480 and PDB model 8RT6. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



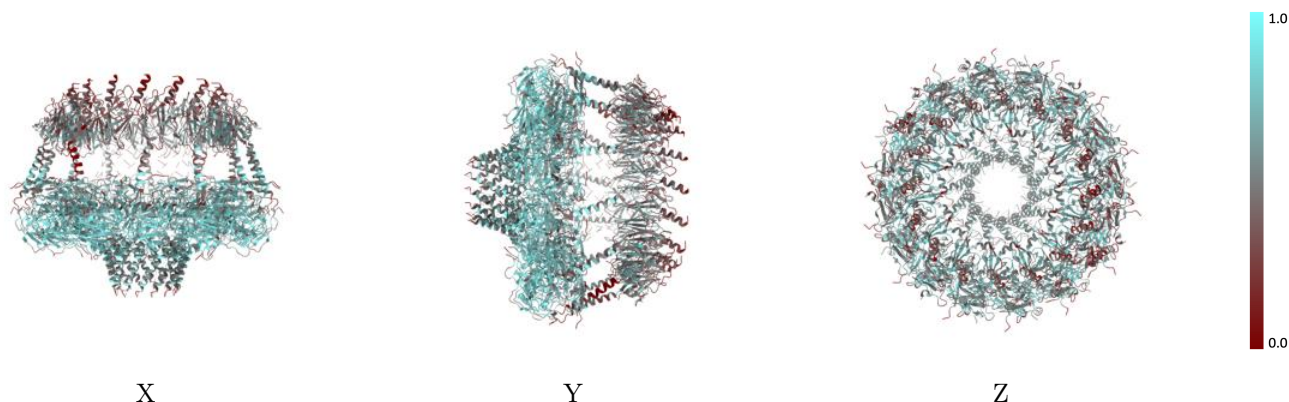
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



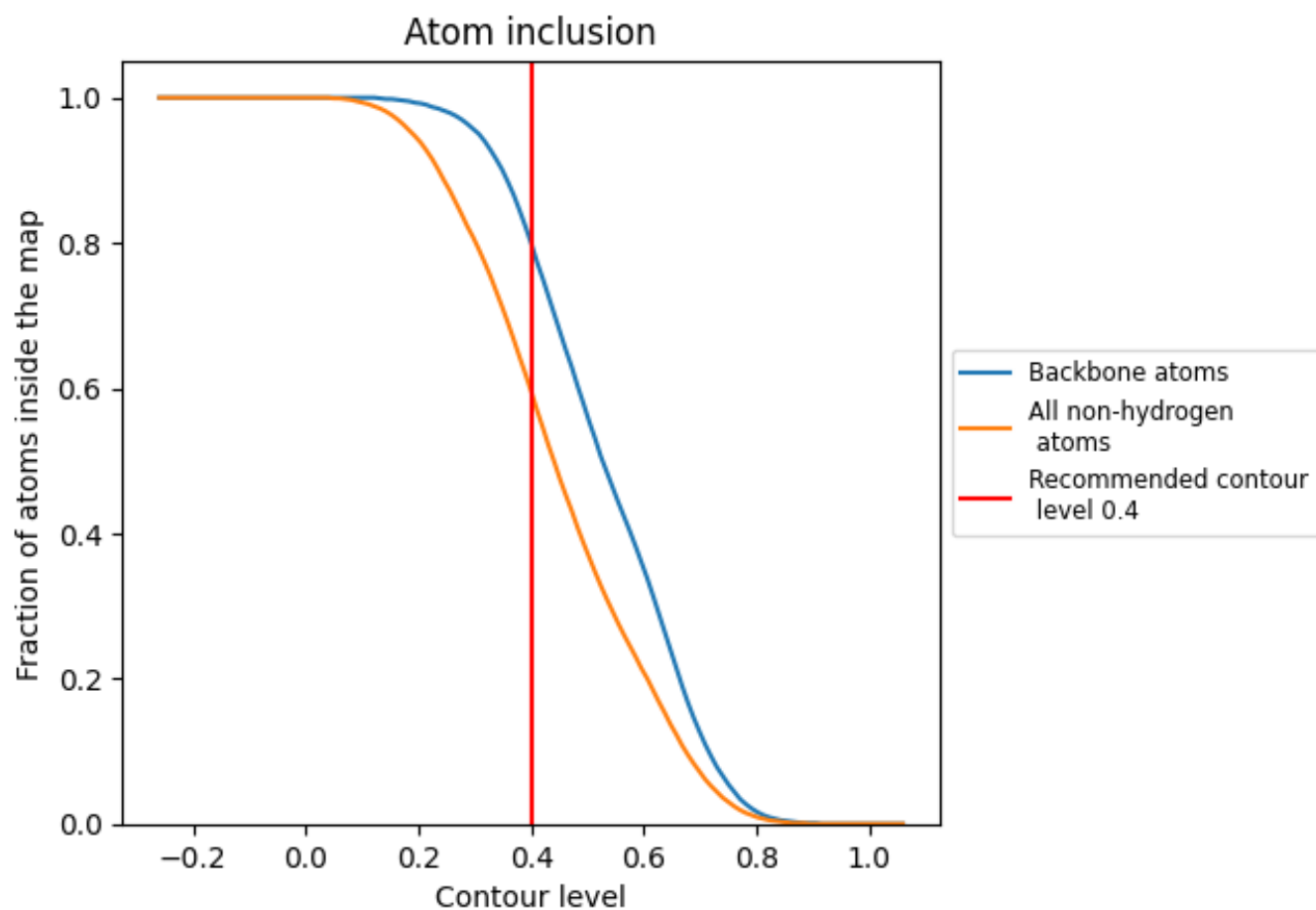
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 60% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5950	 0.4680
A	 0.6420	 0.4940
B	 0.5460	 0.4480
C	 0.5690	 0.4690
D	 0.6400	 0.4940
E	 0.5860	 0.4570
F	 0.5540	 0.4690
G	 0.6340	 0.4910
H	 0.6020	 0.4630
I	 0.5690	 0.4570
J	 0.6400	 0.4890
K	 0.6050	 0.4550
L	 0.5540	 0.4580
M	 0.6350	 0.4930
N	 0.6050	 0.4540
O	 0.5540	 0.4590
P	 0.6350	 0.4900
Q	 0.5810	 0.4550
R	 0.5740	 0.4680
S	 0.6330	 0.4930
T	 0.5690	 0.4520
U	 0.5970	 0.4700
V	 0.6360	 0.4930
W	 0.5200	 0.4380
X	 0.5780	 0.4690
Y	 0.6270	 0.4930
Z	 0.5450	 0.4470
a	 0.5780	 0.4640
b	 0.6370	 0.4880
c	 0.5800	 0.4510
d	 0.5640	 0.4680
e	 0.6360	 0.4850
f	 0.5890	 0.4530
g	 0.5590	 0.4520
h	 0.6360	 0.4930



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Chain	Atom inclusion	Q-score
i	 0.5920	 0.4530
j	 0.5450	 0.4660
k	 0.6350	 0.4910
l	 0.5860	 0.4570
m	 0.5590	 0.4630
n	 0.6420	 0.4920
o	 0.5850	 0.4580
p	 0.5880	 0.4710
u	 0.2040	 0.3530
v	 0.3570	 0.4010
y	 0.2750	 0.3790
z	 0.4560	 0.4260