



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:04 AM UTC

PDB ID : 9JG6 / pdb_00009jg6
EMDB ID : EMD-61457
Title : The tail-complex structure of phage P22
Authors : Liu, H.R.; Xiao, H.
Deposited on : 2024-09-06
Resolution : 3.21 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

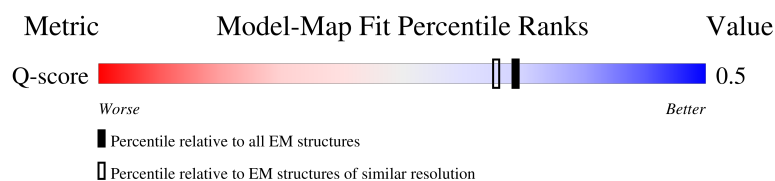
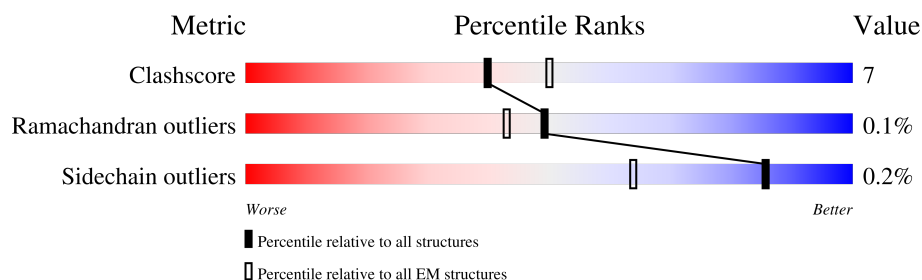
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 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.



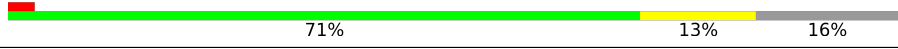
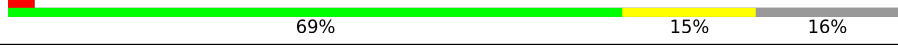
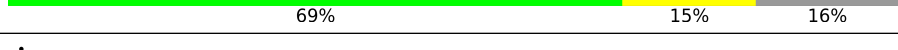
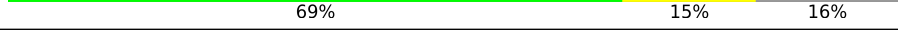
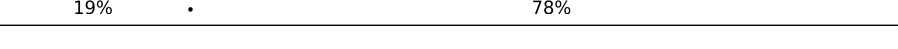
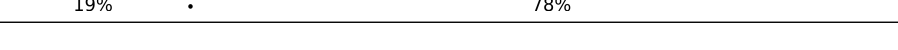
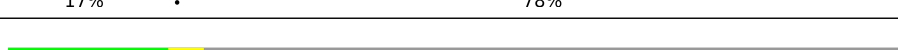
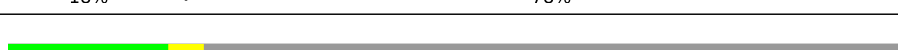
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14613 (2.71 - 3.71)

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	725	 71% 13% 16%
1	B	725	 68% 16% 16%
1	C	725	 69% 14% 16%
1	D	725	 70% 14% 16%

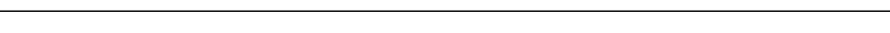
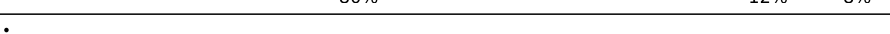
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Mol	Chain	Length	Quality of chain
1	E	725	
1	F	725	
1	G	725	
1	H	725	
1	I	725	
1	J	725	
1	K	725	
1	L	725	
2	M	667	
2	N	667	
2	O	667	
2	P	667	
2	Q	667	
2	R	667	
2	S	667	
2	T	667	
2	U	667	
2	V	667	
2	W	667	
2	X	667	
2	Y	667	
2	Z	667	
2	s	667	
2	v	667	
2	w	667	

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Mol	Chain	Length	Quality of chain
2	x	667	
3	a	472	
3	b	472	
3	c	472	
3	d	472	
3	e	472	
3	f	472	
4	g	166	
4	h	166	
4	i	166	
4	j	166	
4	k	166	
4	l	166	
4	m	166	
4	n	166	
4	o	166	
4	p	166	
4	q	166	
4	r	166	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 115680 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	B	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	C	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	D	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	E	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	F	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	G	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	H	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	I	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	J	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	K	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		
1	L	608	Total	C	N	O	S	0	0
			4908	3090	840	957	21		

- Molecule 2 is a protein called Endorhamnosidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		
2	N	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		
2	O	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	Q	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	R	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	S	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	T	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	U	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	V	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	W	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	X	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	Y	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	Z	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		
2	s	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		
2	v	149	Total	C	N	O	S	0	0
			1161	740	191	229	1		
2	w	149	Total	C	N	O	S	0	0
			1148	727	190	230	1		
2	x	147	Total	C	N	O	S	0	0
			1129	717	185	226	1		

- Molecule 3 is a protein called Phage stabilisation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		
3	b	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		
3	c	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		
3	d	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		
3	f	470	Total	C	N	O	S	0	0
			3676	2320	630	708	18		

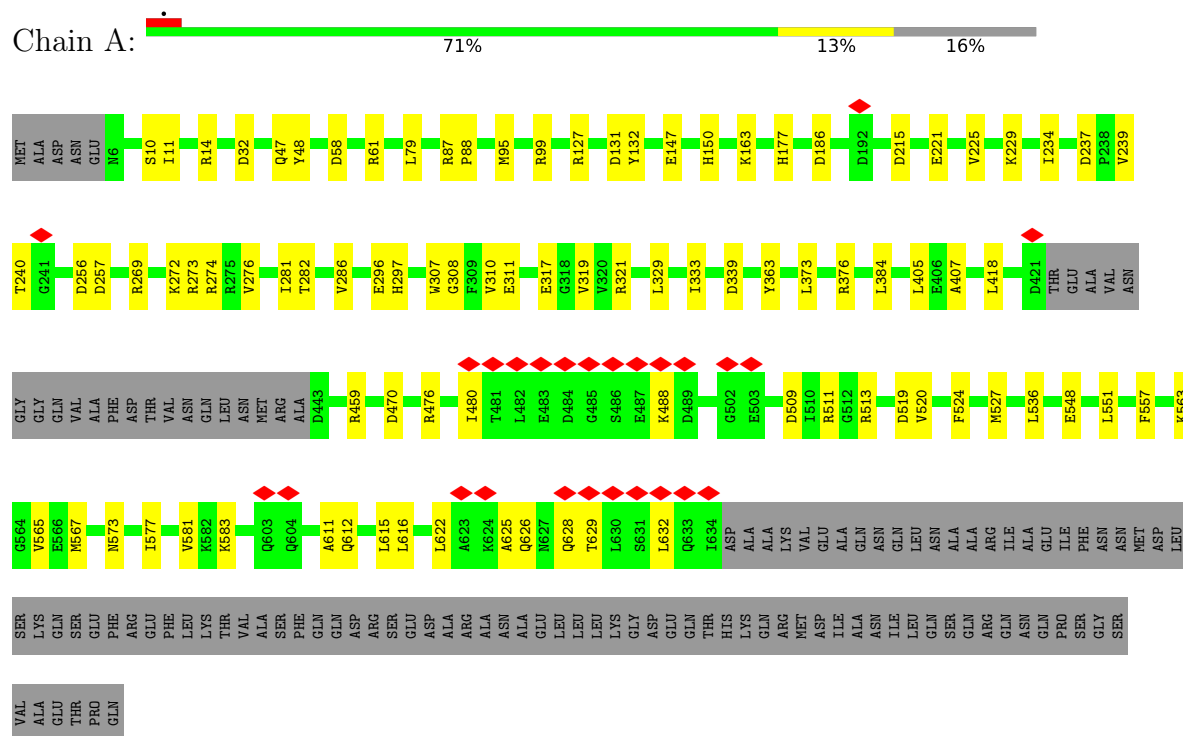
- Molecule 4 is a protein called P22 tail accessory factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	h	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	i	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	j	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	k	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	l	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	m	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	n	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	o	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	p	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	q	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		
4	r	153	Total	C	N	O	S	0	0
			1175	736	202	231	6		

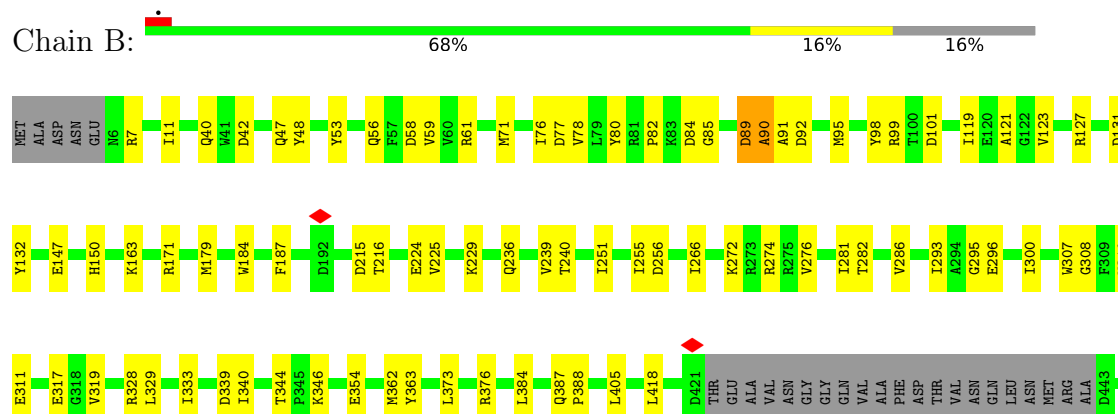
3 Residue-property plots

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

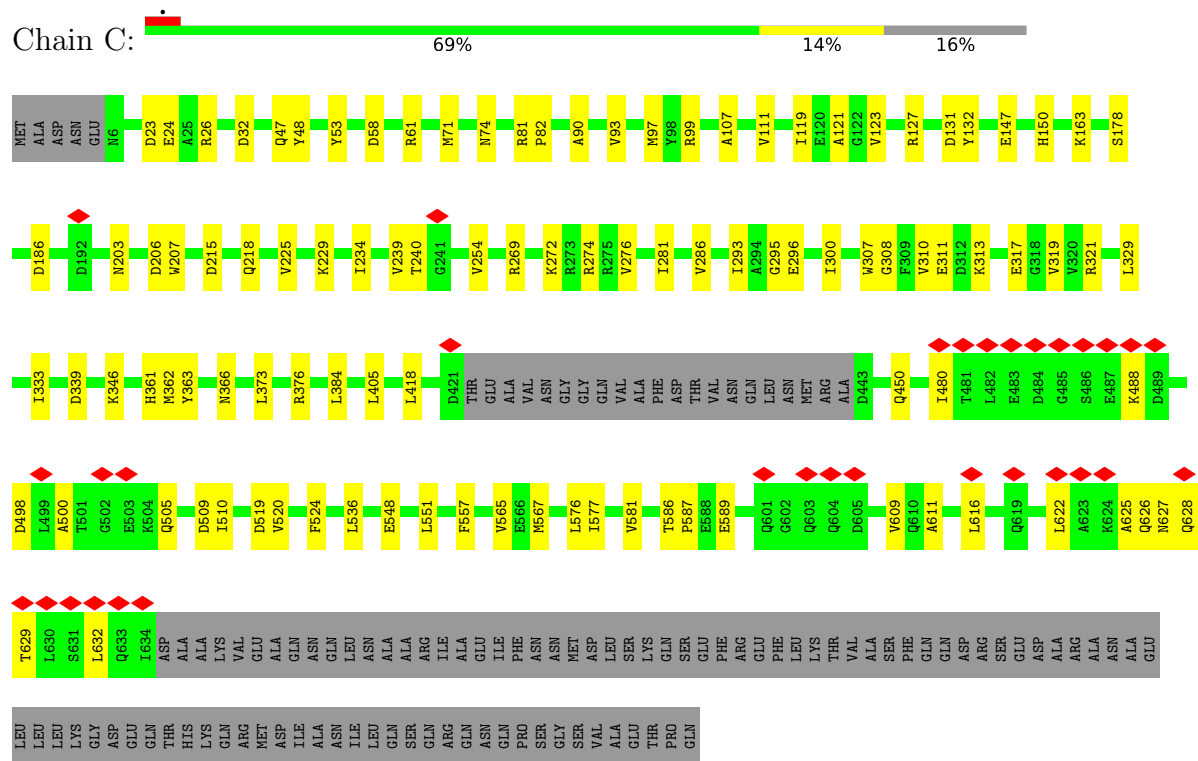
• Molecule 1: Portal protein



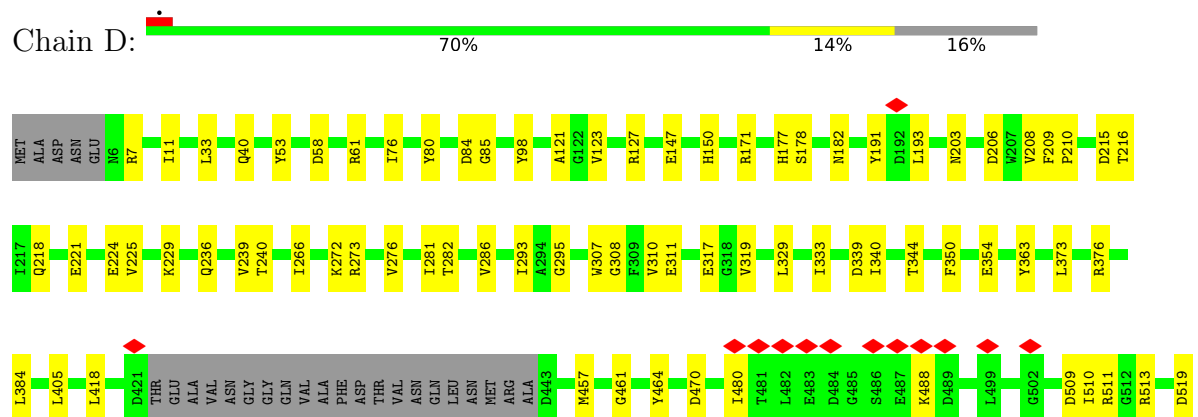
• Molecule 1: Portal protein

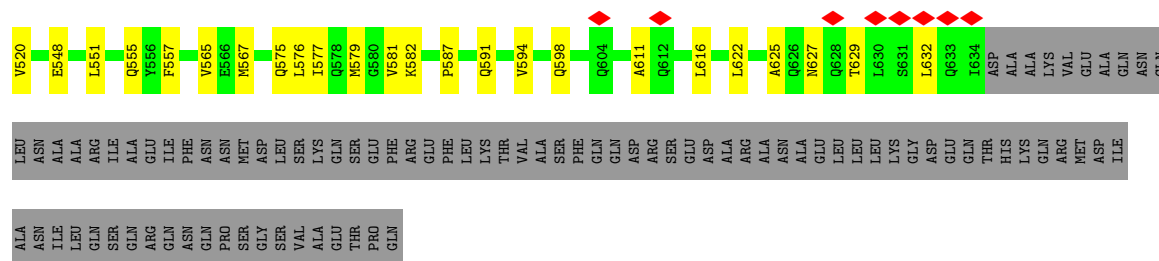


- Molecule 1: Portal protein

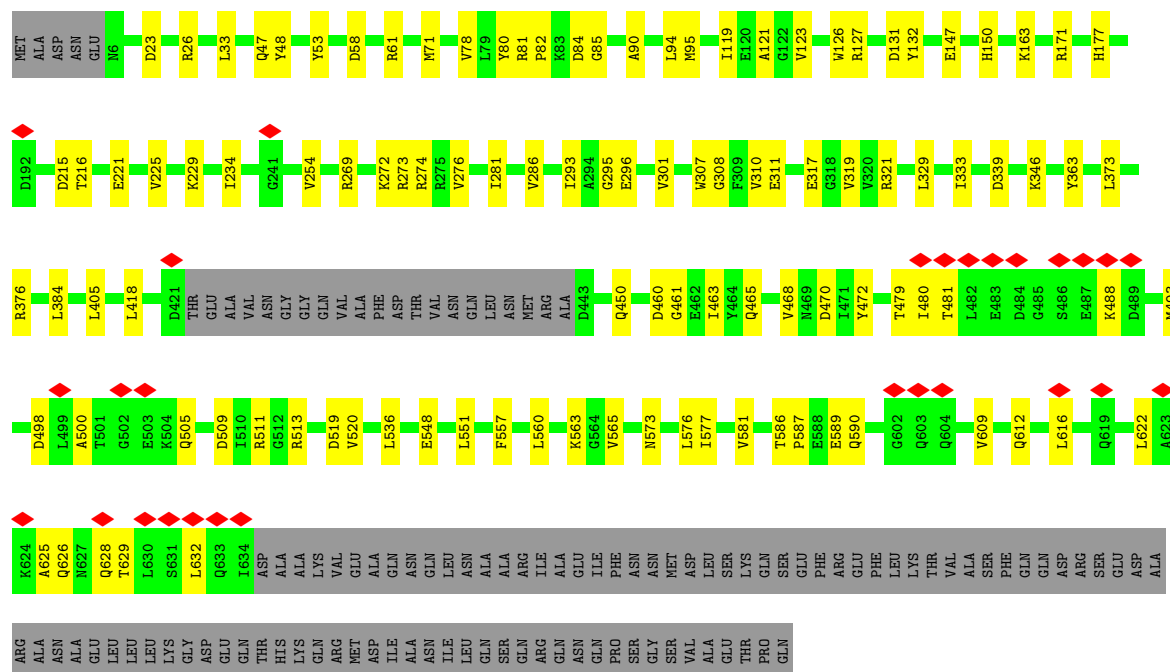


- Molecule 1: Portal protein

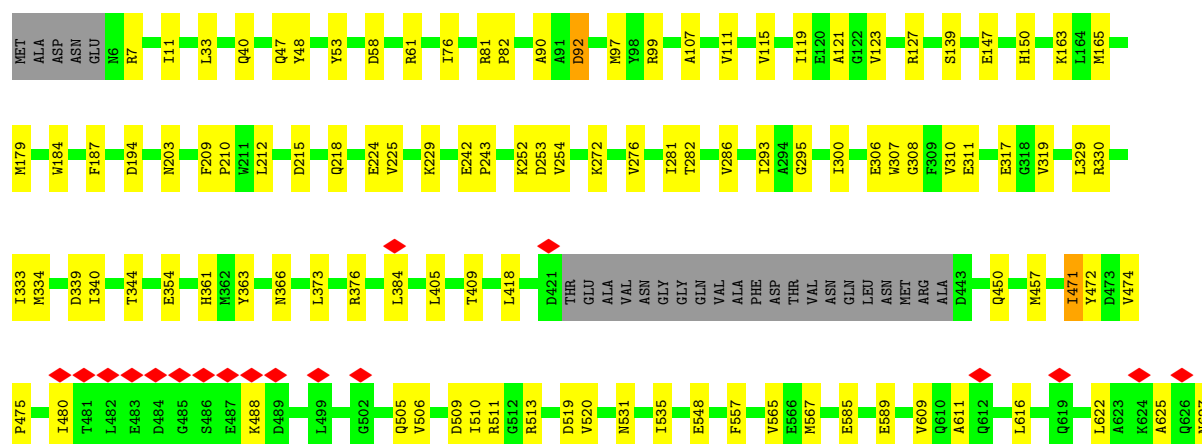




• Molecule 1: Portal protein



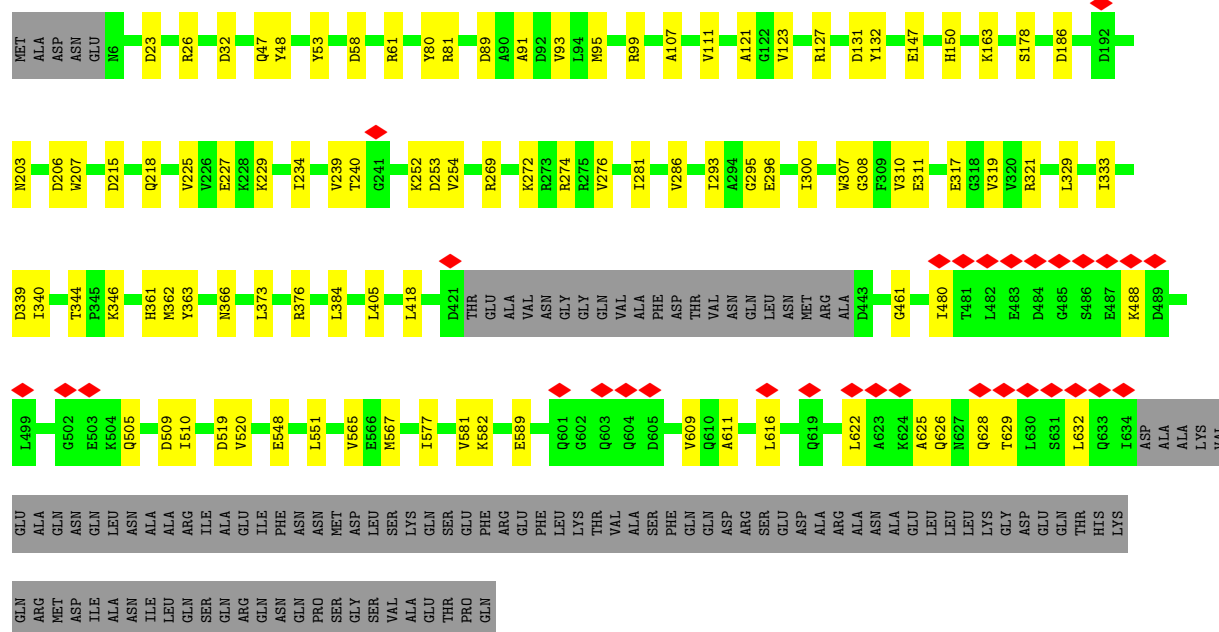
• Molecule 1: Portal protein



LEU
LEU
LEU
LYS
GLY
ASP
GLU
GLN
THR
HIS
LYS
GLN
ARG
MET
ASP
TLE
ALA
ASN
TLE
LEU
GLN
SER
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GLY
SER
SER
VAL
ALA
GLU
THR
PRO
GLN

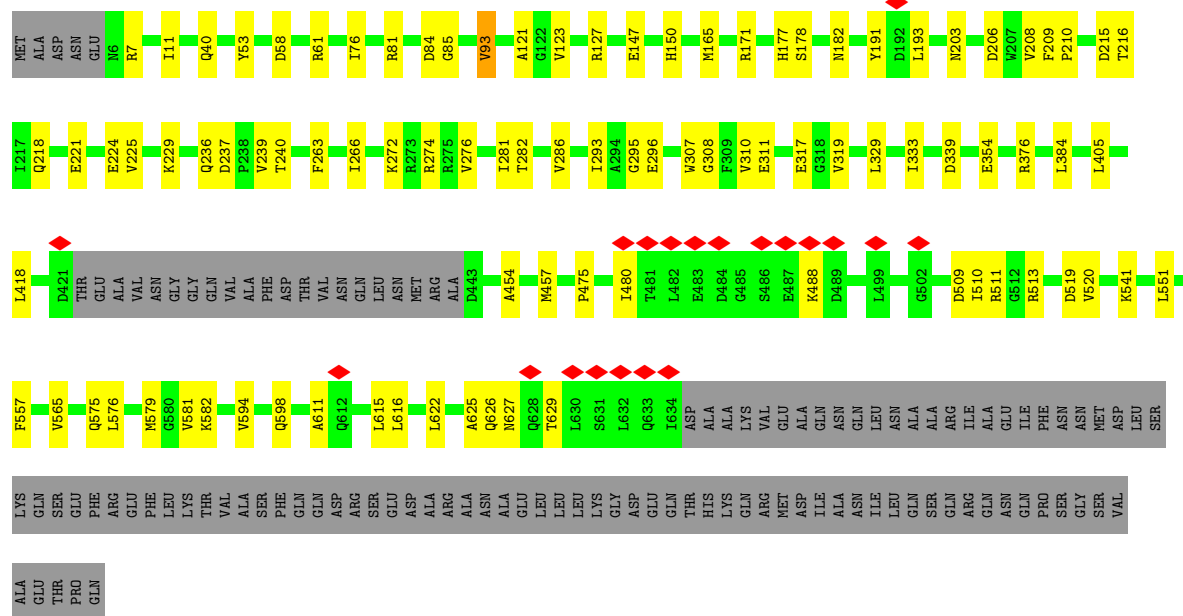
• Molecule 1: Portal protein

Chain I:



• Molecule 1: Portal protein

Chain J:



• Molecule 1: Portal protein

- Molecule 1: Portal protein

- Molecule 2: Endorhamnosidase





[illegible]

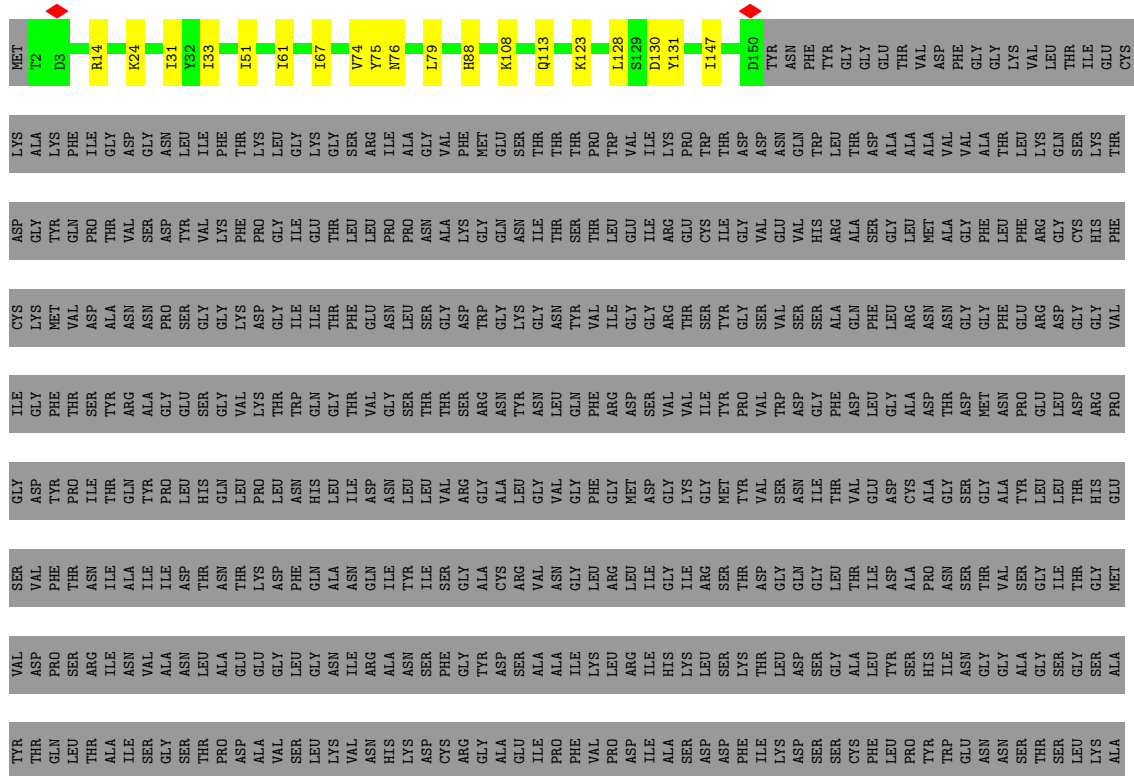
- Molecule 2: Endorhamnosidase

[illegible]

- Molecule 2: Endorhamnosidase

[illegible]





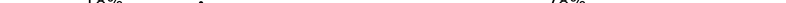
[illegible]

- Molecule 2: Endorhamnosidase

Chain s: 17% 1% 78%

LYS	LEU	GLY	SER	TRP	VAL	GLU	ASN	ASN	MET
ASP	ASP	GLN	ASN	GLY	SER	VAL	GLN	PHE	T2
SER	SER	GLY	ILE	ASP	HIS	THR	TRP	THR	V9
CYS	ALA	THR	VAL	ASP	ALA	ARG	LEU	GLY	
PHE	LEU	ILE	GLU	LEU	PHE	ALA	THR	GLY	R14
PRO	TYR	ASP	CYS	GLY	LEU	GLY	ALA	THR	
LEU	SER	ALA	ASP	ALA	ARG	LEU	ALA	VAL	Q36
TYR	HIS	PRO	ALA	ASP	ASN	MET	ALA	ASP	
TRP	ILE	ASN	GLY	THR	ASN	ALA	VAL	PHE	P43
GLU	ASN	SER	SER	ASP	GLY	GLY	VAL	GLY	
ASN	GLY	THR	ALA	MET	GLY	PHE	ALA	GLY	Q46
ASN	GLY	VAL	ALA	ASN	PHE	LEU	THR	LYS	
SER	ALA	SER	TYR	PRO	GLU	PHE	LEU	VAL	I51
THR	GLY	GLY	LEU	GLU	ARG	ARG	LYS	LEU	
SER	SER	ILE	LEU	LEU	ASP	THR	GLN	THR	H58
LEU	GLY	THR	THR	ASP	GLY	CYS	SER	ILE	
LYS	SER	GLY	HIS	ARG	GLY	HIS	LYS	GLU	N68
ALA	ALA	MET	GLU	PRO	VAL	PHE	THR	CYS	
LEU	TYR	VAL	SER	GLY	ILE	PHE	ASP	LYS	V74
VAL	THR	ASP	GLU	ASP	GLY	LYS	GLY	ALA	
LYS	GLN	PRO	PHE	TYR	PHE	THR	MET	LYS	N76
LYS	LEU	SER	THR	PRO	THR	VAL	GLN	PHE	G77
PRO	THR	ARG	ASN	ILE	SER	ASP	PRO	ILE	Q78
ASN	ALA	ILE	ILE	THR	TYR	ALA	THR	GLY	L79
GLY	ILE	ASN	ALA	GLN	ARG	ASN	VAL	ASP	V80
GLU	SER	VAL	ILE	TYR	ALA	THR	SER	GLY	K81
LEU	GLY	ALA	ILE	GLY	GLY	PRO	ASN	ASN	I82
VAL	SER	ASN	ASP	LEU	GLU	SER	TYR	LEU	V83
ARG	THR	LEU	THR	HIS	SER	GLY	VAL	ILE	T84
LEU	PRO	ALA	ASN	GLN	GLY	GLY	LYS	PHE	V85
THR	ASP	GLU	THR	LEU	VAL	THR	PHE	THR	Q86
LEU	ALA	GLU	LYS	PRO	THR	ASP	PRO	LYS	
ALA	VAL	GLY	ASP	LEU	THR	ILE	GLY	LEU	S89
THR	SER	LEU	PHE	ASN	TRP	ILE	ILE	GLY	
LEU	LEU	GLY	GLN	HIS	GLN	ILE	GLY	LYS	D94
LYS	LYS	ASN	ALA	LEU	GLY	THR	THR	GLY	A95
VAL	VAL	ILE	ASN	ILE	THR	PHE	LEU	SER	
ASN	ASN	ARG	ASN	ASN	VAL	GLU	LEU	ARG	D101
HIS	HIS	ALA	ILE	LEU	GLY	ASN	PRO	ILE	Y102
LYS	ASP	ASN	TYR	ASN	SER	LEU	PRO	ALA	
ASP	ASP	SER	ILE	LEU	THR	SER	ASN	GLY	E117
CYS	CYS	PHE	SER	VAL	THR	GLY	ALA	VAL	
ARG	ARG	GLY	GLY	ARG	SER	ASP	LYS	PHE	K121
GLY	GLY	TYR	ALA	GLY	ARG	TRP	GLY	MET	F122
ALA	ALA	ASP	CYS	ALA	ASN	GLY	GLN	GLU	K123
GLU	GLU	SER	ARG	LEU	TYR	LYS	ASN	SER	
ILE	ILE	ALA	VAL	GLY	ASN	GLY	ILE	THR	K127
PRO	PRO	ALA	ASN	VAL	GLN	ASN	THR	THR	T133
PHE	VAL	ILE	GLY	PHE	THR	VAL	THR	PRO	
VAL	VAL	LYS	LEU	GLY	ARG	ILE	LEU	TRP	D136
ASP	ASP	LEU	ARG	MET	ASP	ASP	GLU	VAL	A137
ILE	ILE	ILE	ILE	ASP	SER	GLY	ILE	ILE	
ALA	ALA	HIS	GLY	GLY	VAL	THR	ARG	LYS	L146
SER	SER	LYS	ILE	LYS	VAL	THR	GLU	PRO	I147
ASP	ASP	LEU	SER	GLY	ILE	THR	CYS	TRP	D148
ASP	ASP	SER	ARG	MET	TYR	TYR	ILE	THR	ARG
PHE	PHE	LYS	THR	TYR	PRO	GLY	GLY	ASP	ASP

- Molecule 2: Endorhamnosidase

Chain v:  18% . 78%

[illegible]

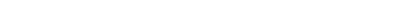
[illegible]

- Molecule 2: Endorhamnosidase

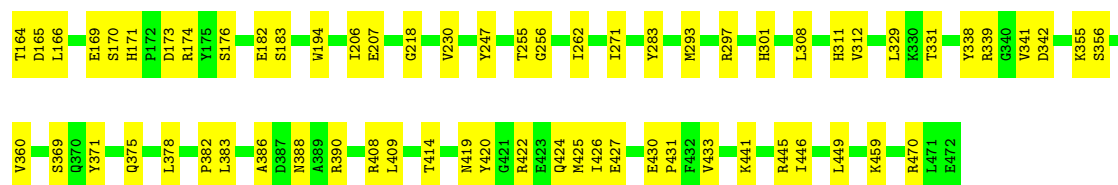
Chain w: 20% 78%

[illegible]

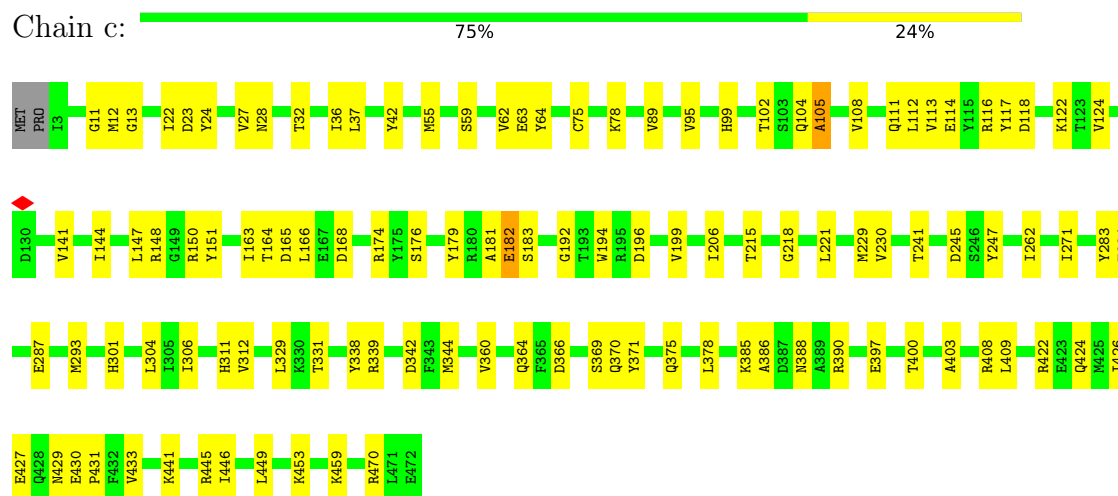
- Molecule 2: Endorhamnosidase

Chain x:  18% . 78%

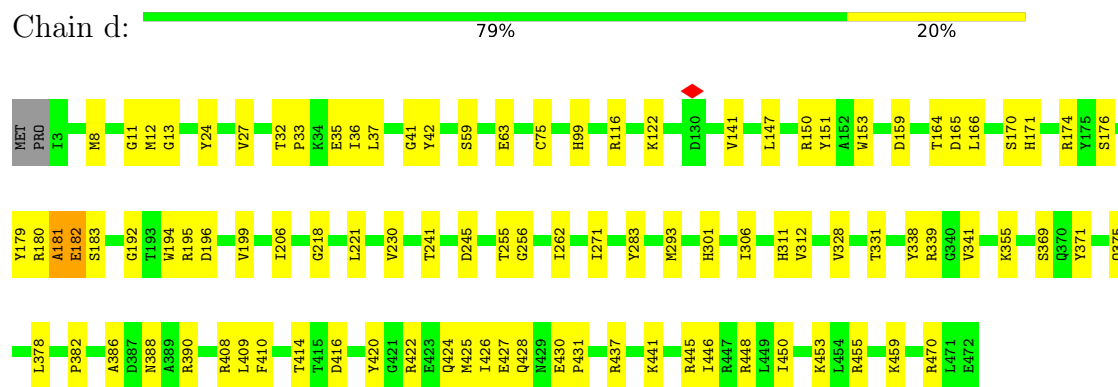




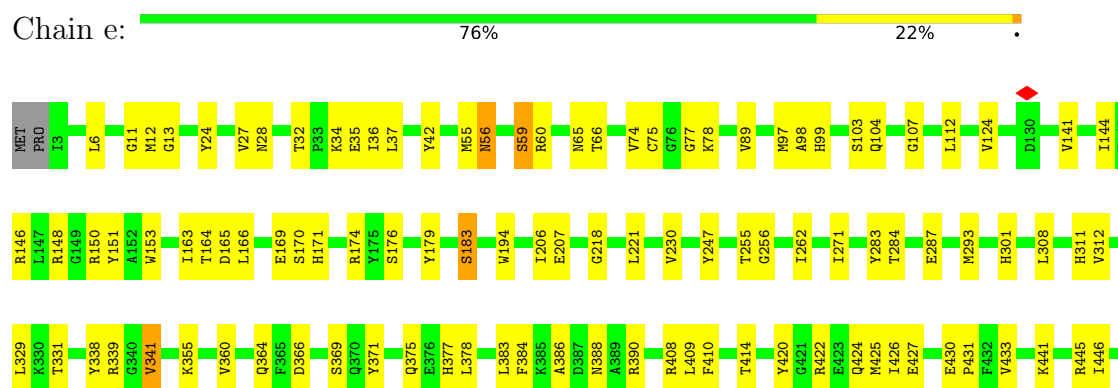
• Molecule 3: Phage stabilisation protein



• Molecule 3: Phage stabilisation protein



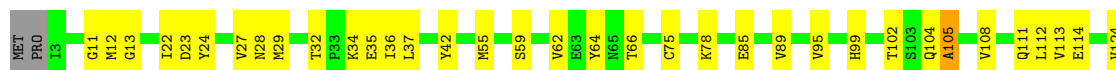
• Molecule 3: Phage stabilisation protein





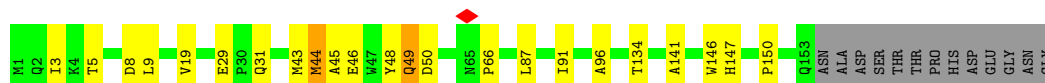
• Molecule 3: Phage stabilisation protein

Chain f: 77% 23%



• Molecule 4: P22 tail accessory factor

Chain g: 78% 13% 8%



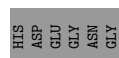
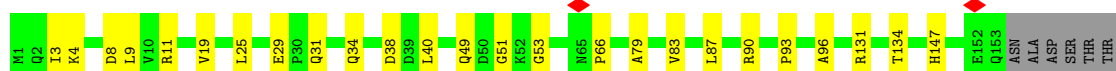
• Molecule 4: P22 tail accessory factor

Chain h: 81% 10% 8%



• Molecule 4: P22 tail accessory factor

Chain i: 77% 15% 8%

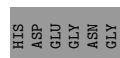
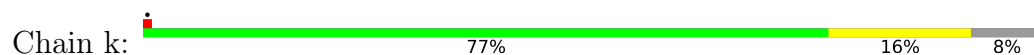


• Molecule 4: P22 tail accessory factor

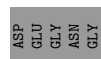
Chain j: 81% 11% 8%



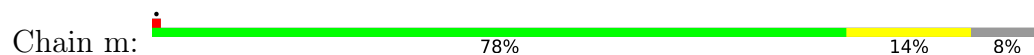
- Molecule 4: P22 tail accessory factor



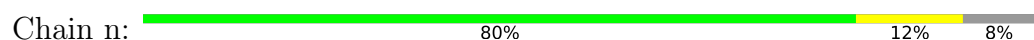
- Molecule 4: P22 tail accessory factor



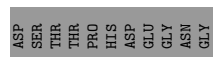
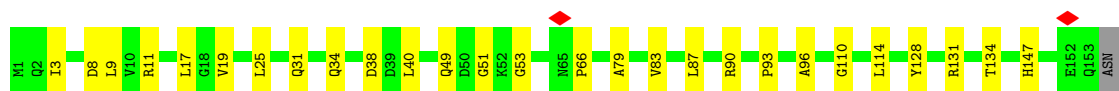
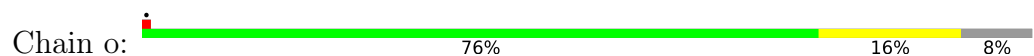
- Molecule 4: P22 tail accessory factor



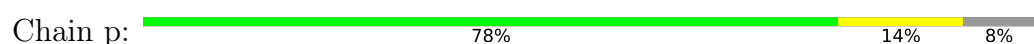
- Molecule 4: P22 tail accessory factor

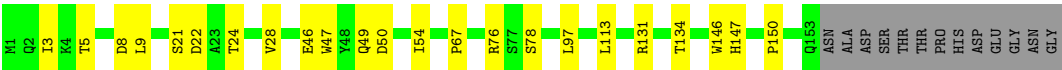


- Molecule 4: P22 tail accessory factor

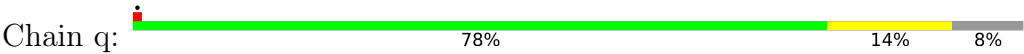


- Molecule 4: P22 tail accessory factor

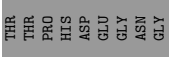




● Molecule 4: P22 tail accessory factor



● Molecule 4: P22 tail accessory factor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82501	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.704	Depositor
Minimum map value	-16.371	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.237	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/5009	0.33	0/6794
1	B	0.18	0/5009	0.35	1/6794 (0.0%)
1	C	0.15	0/5009	0.33	0/6794
1	D	0.14	0/5009	0.33	0/6794
1	E	0.15	0/5009	0.35	0/6794
1	F	0.20	0/5009	0.36	0/6794
1	G	0.16	0/5009	0.33	0/6794
1	H	0.17	0/5009	0.36	0/6794
1	I	0.19	0/5009	0.34	0/6794
1	J	0.17	0/5009	0.34	0/6794
1	K	0.21	0/5009	0.38	2/6794 (0.0%)
1	L	0.20	0/5009	0.36	0/6794
2	M	0.26	0/1150	0.44	0/1570
2	N	0.26	0/1150	0.49	2/1570 (0.1%)
2	O	0.27	0/1150	0.47	0/1570
2	P	0.15	0/1185	0.36	0/1616
2	Q	0.15	0/1185	0.36	0/1616
2	R	0.14	0/1185	0.36	0/1616
2	S	0.14	0/1185	0.36	0/1616
2	T	0.15	0/1185	0.37	0/1616
2	U	0.13	0/1169	0.31	0/1595
2	V	0.13	0/1169	0.33	0/1595
2	W	0.14	0/1169	0.31	0/1595
2	X	0.23	0/1169	0.36	0/1595
2	Y	0.14	0/1169	0.34	0/1595
2	Z	0.35	1/1150 (0.1%)	0.50	0/1570
2	s	0.31	0/1150	0.49	0/1570
2	v	0.14	0/1185	0.36	0/1616
2	w	0.14	0/1169	0.32	0/1595
2	x	0.27	0/1150	0.47	0/1570
3	a	0.21	0/3756	0.46	2/5086 (0.0%)
3	b	0.23	0/3756	0.44	0/5086
3	c	0.25	0/3756	0.45	2/5086 (0.0%)
3	d	0.20	0/3756	0.44	2/5086 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	0.24	0/3756	0.46	3/5086 (0.1%)
3	f	0.23	0/3756	0.44	0/5086
4	g	0.58	4/1200 (0.3%)	0.62	3/1626 (0.2%)
4	h	0.24	0/1200	0.43	0/1626
4	i	0.24	0/1200	0.40	0/1626
4	j	0.25	0/1200	0.45	0/1626
4	k	0.27	0/1200	0.43	0/1626
4	l	0.26	0/1200	0.43	0/1626
4	m	0.26	0/1200	0.44	0/1626
4	n	0.29	0/1200	0.44	0/1626
4	o	0.25	0/1200	0.41	0/1626
4	p	0.32	0/1200	0.50	0/1626
4	q	0.28	0/1200	0.41	0/1626
4	r	0.32	0/1200	0.53	2/1626 (0.1%)
All	All	0.21	5/118068 (0.0%)	0.39	19/160242 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	g	48	TYR	CA-C	-8.07	1.43	1.53
2	Z	79	LEU	CA-C	-7.30	1.44	1.52
4	g	45	ALA	CA-C	-6.79	1.43	1.52
4	g	49	GLN	CA-C	-6.18	1.46	1.53
4	g	46	GLU	N-CA	-5.11	1.39	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	g	46	GLU	N-CA-C	-11.22	99.59	113.28
3	e	56	ASN	N-CA-C	7.46	119.49	111.36
4	r	64	GLU	N-CA-C	-7.38	102.93	112.23
1	K	90	ALA	N-CA-C	-6.74	106.26	114.75
3	c	182	GLU	N-CA-C	6.68	123.22	113.40
3	d	182	GLU	N-CA-C	6.14	122.84	113.51
3	a	182	GLU	N-CA-C	6.09	122.84	113.28
1	B	90	ALA	N-CA-C	-5.93	107.86	114.62
3	c	183	SER	N-CA-C	-5.89	104.55	110.97
3	a	183	SER	N-CA-C	-5.84	104.82	111.07
4	g	46	GLU	CA-C-N	-5.79	111.41	122.53
4	g	46	GLU	C-N-CA	-5.79	111.41	122.53
3	d	183	SER	N-CA-C	-5.50	105.18	111.07
1	K	94	LEU	N-CA-C	-5.18	106.47	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	r	62	ASP	N-CA-C	5.10	119.58	112.90
3	e	183	SER	CA-C-N	5.10	133.23	123.65
3	e	183	SER	C-N-CA	5.10	133.23	123.65
2	N	78	GLN	CA-C-N	5.09	132.00	121.32
2	N	78	GLN	C-N-CA	5.09	132.00	121.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4908	0	4770	72	0
1	B	4908	0	4770	90	0
1	C	4908	0	4770	82	0
1	D	4908	0	4770	77	0
1	E	4908	0	4770	79	0
1	F	4908	0	4770	82	0
1	G	4908	0	4770	76	0
1	H	4908	0	4770	81	0
1	I	4908	0	4770	76	0
1	J	4908	0	4770	71	0
1	K	4908	0	4770	81	0
1	L	4908	0	4770	80	0
2	M	1129	0	1118	17	0
2	N	1129	0	1118	18	0
2	O	1129	0	1118	21	0
2	P	1161	0	1139	19	0
2	Q	1161	0	1139	19	0
2	R	1161	0	1139	15	0
2	S	1161	0	1139	21	0
2	T	1161	0	1139	22	0
2	U	1148	0	1135	12	0
2	V	1148	0	1135	16	0
2	W	1148	0	1135	15	0
2	X	1148	0	1135	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	1148	0	1135	17	0
2	Z	1129	0	1118	19	0
2	s	1129	0	1118	21	0
2	v	1161	0	1139	19	0
2	w	1148	0	1135	13	0
2	x	1129	0	1118	19	0
3	a	3676	0	3582	71	0
3	b	3676	0	3582	65	0
3	c	3676	0	3582	70	0
3	d	3676	0	3582	74	0
3	e	3676	0	3582	71	0
3	f	3676	0	3582	68	0
4	g	1175	0	1141	15	0
4	h	1175	0	1141	15	0
4	i	1175	0	1141	19	0
4	j	1175	0	1141	16	0
4	k	1175	0	1141	19	0
4	l	1175	0	1141	22	0
4	m	1175	0	1141	16	0
4	n	1175	0	1141	16	0
4	o	1175	0	1141	21	0
4	p	1175	0	1141	16	0
4	q	1175	0	1141	17	0
4	r	1175	0	1141	25	0
All	All	115680	0	112776	1615	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1615) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TRP:HE1	1:L:150:HIS:HE1	1.22	0.87
1:B:150:HIS:HE1	1:C:307:TRP:HE1	1.24	0.86
1:H:150:HIS:HE1	1:I:307:TRP:HE1	1.24	0.86
1:F:150:HIS:HE1	1:G:307:TRP:HE1	1.22	0.85
3:c:116:ARG:HD2	3:c:122:LYS:HG3	1.59	0.85
2:s:94:ASP:OD1	2:s:95:ALA:N	2.09	0.85
1:J:150:HIS:HE1	1:K:307:TRP:HE1	1.25	0.84
2:O:94:ASP:OD1	2:O:95:ALA:N	2.09	0.84
1:I:150:HIS:HE1	1:J:307:TRP:HE1	1.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:HIS:HE1	1:D:307:TRP:HE1	1.28	0.81
1:A:150:HIS:HE1	1:B:307:TRP:HE1	1.29	0.78
1:G:150:HIS:HE1	1:H:307:TRP:HE1	1.31	0.76
2:Z:94:ASP:OD1	2:Z:95:ALA:N	2.19	0.75
2:N:94:ASP:OD1	2:N:95:ALA:N	2.18	0.74
4:n:146:TRP:HZ2	4:n:150:PRO:HD3	1.52	0.74
1:C:567:MET:SD	1:D:555:GLN:NE2	2.62	0.72
2:M:9:VAL:HG12	2:R:83:VAL:HG22	1.72	0.72
2:P:42:ASN:O	2:P:46:GLN:NE2	2.23	0.71
3:e:107:GLY:HA3	3:e:144:ILE:HD11	1.73	0.71
2:v:40:PRO:O	2:v:46:GLN:NE2	2.24	0.70
2:v:83:VAL:HG22	2:x:9:VAL:HG12	1.72	0.70
1:D:150:HIS:HE1	1:E:307:TRP:HE1	1.39	0.70
3:c:331:THR:HG22	3:c:370:GLN:HE22	1.56	0.70
2:N:9:VAL:HG12	2:S:83:VAL:HG22	1.73	0.70
3:b:107:GLY:HA3	3:b:144:ILE:HD11	1.73	0.70
2:S:42:ASN:O	2:S:46:GLN:NE2	2.23	0.69
3:f:331:THR:HG22	3:f:370:GLN:HE22	1.56	0.69
1:I:95:MET:HE2	1:I:99:ARG:HH11	1.57	0.69
2:P:83:VAL:HG22	2:Z:9:VAL:HG12	1.73	0.69
1:I:567:MET:HE1	1:J:576:LEU:HD13	1.74	0.69
2:O:9:VAL:HG12	2:T:83:VAL:HG22	1.75	0.68
2:Q:42:ASN:O	2:Q:46:GLN:NE2	2.26	0.68
3:e:59:SER:HA	3:e:75:CYS:HA	1.74	0.68
1:B:82:PRO:HB3	1:B:90:ALA:HB3	1.75	0.68
1:E:150:HIS:HE1	1:F:307:TRP:HE1	1.43	0.67
1:E:587:PRO:HA	1:E:590:GLN:NE2	2.10	0.67
1:H:616:LEU:HD22	1:I:622:LEU:HD11	1.75	0.67
1:K:587:PRO:HA	1:K:590:GLN:NE2	2.10	0.67
2:U:78:GLN:NE2	4:j:25:LEU:O	2.27	0.67
3:a:258:PRO:HB3	3:a:288:MET:HE1	1.77	0.66
2:R:40:PRO:O	2:R:46:GLN:NE2	2.28	0.66
2:T:42:ASN:O	2:T:46:GLN:NE2	2.23	0.66
1:J:203:ASN:OD1	1:J:218:GLN:NE2	2.28	0.66
1:D:203:ASN:OD1	1:D:218:GLN:NE2	2.28	0.66
1:B:616:LEU:HD22	1:C:622:LEU:HD11	1.75	0.66
1:C:229:LYS:HA	1:C:272:LYS:HA	1.77	0.66
3:b:255:THR:HG22	3:b:256:GLY:H	1.58	0.66
4:r:146:TRP:HZ2	4:r:150:PRO:HD3	1.61	0.65
1:K:150:HIS:HE1	1:L:307:TRP:HE1	1.42	0.65
1:B:95:MET:HE2	1:B:99:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:123:LYS:NZ	2:Q:143:ASP:OD2	2.29	0.65
2:S:125:SER:HB3	2:X:123:LYS:HB2	1.78	0.65
3:b:59:SER:HA	3:b:75:CYS:HA	1.77	0.65
2:P:125:SER:HB3	2:U:123:LYS:HB2	1.78	0.65
1:A:407:ALA:HB1	1:L:334:MET:HE1	1.78	0.65
1:I:229:LYS:HA	1:I:272:LYS:HA	1.78	0.65
3:c:331:THR:O	3:c:375:GLN:NE2	2.27	0.65
2:Q:40:PRO:O	2:Q:46:GLN:NE2	2.27	0.65
3:f:331:THR:O	3:f:375:GLN:NE2	2.27	0.65
1:I:186:ASP:OD2	1:J:171:ARG:NH1	2.29	0.65
3:b:27:VAL:HB	3:b:378:LEU:HB2	1.77	0.65
1:A:229:LYS:HA	1:A:272:LYS:HA	1.78	0.65
2:Q:83:VAL:HG22	2:s:9:VAL:HG12	1.79	0.65
4:k:40:LEU:HD13	4:k:87:LEU:HD22	1.79	0.65
2:X:108:LYS:O	2:X:113:GLN:NE2	2.31	0.64
4:r:62:ASP:O	4:r:63:ASP:HB2	1.95	0.64
2:P:40:PRO:O	2:P:46:GLN:NE2	2.26	0.64
1:K:229:LYS:HA	1:K:272:LYS:HA	1.79	0.64
1:C:186:ASP:OD2	1:D:171:ARG:NH1	2.30	0.64
2:N:14:ARG:NH1	2:S:101:ASP:OD2	2.31	0.64
3:d:165:ASP:OD2	3:d:174:ARG:NH1	2.31	0.64
3:e:27:VAL:HB	3:e:378:LEU:HB2	1.79	0.64
1:I:609:VAL:HG13	1:J:615:LEU:HD12	1.79	0.64
3:b:176:SER:HB3	3:b:218:GLY:HA2	1.78	0.64
2:U:108:LYS:O	2:U:113:GLN:NE2	2.30	0.64
3:b:408:ARG:HE	3:b:425:MET:HE2	1.63	0.64
1:G:229:LYS:HA	1:G:272:LYS:HA	1.78	0.64
3:a:59:SER:HA	3:a:75:CYS:HA	1.79	0.64
3:c:59:SER:HA	3:c:75:CYS:HA	1.78	0.64
1:F:229:LYS:HA	1:F:272:LYS:HA	1.80	0.64
3:d:159:ASP:HB3	3:d:180:ARG:HG3	1.79	0.64
4:r:40:LEU:HD13	4:r:87:LEU:HD22	1.79	0.64
3:d:59:SER:HA	3:d:75:CYS:HA	1.79	0.63
3:c:165:ASP:OD2	3:c:174:ARG:NH1	2.32	0.63
3:a:165:ASP:OD2	3:a:174:ARG:NH1	2.31	0.63
2:V:108:LYS:O	2:V:113:GLN:NE2	2.32	0.63
2:W:108:LYS:O	2:W:113:GLN:NE2	2.32	0.63
1:D:319:VAL:HG22	1:D:418:LEU:HD11	1.80	0.63
4:l:146:TRP:HZ2	4:l:150:PRO:HD3	1.62	0.63
1:C:319:VAL:HG22	1:C:418:LEU:HD11	1.81	0.63
1:E:229:LYS:HA	1:E:272:LYS:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:319:VAL:HG22	1:J:418:LEU:HD11	1.80	0.63
3:b:55:MET:HE3	3:b:360:VAL:HG11	1.79	0.63
3:d:147:LEU:HD11	3:d:196:ASP:HA	1.80	0.63
3:f:165:ASP:OD2	3:f:174:ARG:NH1	2.31	0.63
1:E:587:PRO:HA	1:E:590:GLN:HE22	1.64	0.63
4:l:40:LEU:HD13	4:l:87:LEU:HD22	1.80	0.63
3:e:165:ASP:OD2	3:e:174:ARG:NH1	2.32	0.63
3:c:422:ARG:NH2	3:c:424:GLN:OE1	2.32	0.62
3:d:255:THR:HG22	3:d:256:GLY:H	1.64	0.62
1:H:95:MET:HE2	1:H:99:ARG:HH11	1.62	0.62
3:e:55:MET:HE3	3:e:360:VAL:HG11	1.80	0.62
3:a:147:LEU:HD11	3:a:196:ASP:HA	1.80	0.62
4:q:40:LEU:HD13	4:q:87:LEU:HD22	1.79	0.62
2:w:108:LYS:O	2:w:113:GLN:NE2	2.32	0.62
3:f:422:ARG:NH2	3:f:424:GLN:OE1	2.33	0.62
4:p:146:TRP:HZ2	4:p:150:PRO:HD3	1.62	0.62
1:I:319:VAL:HG22	1:I:418:LEU:HD11	1.80	0.62
2:S:40:PRO:O	2:S:46:GLN:NE2	2.26	0.62
1:F:127:ARG:NH1	1:F:147:GLU:OE1	2.33	0.62
2:P:55:ASP:OD1	2:P:56:GLY:N	2.32	0.62
3:f:36:ILE:HG22	3:f:37:LEU:H	1.65	0.62
1:C:567:MET:HE1	1:D:576:LEU:HD13	1.80	0.62
1:D:229:LYS:HA	1:D:272:LYS:HA	1.81	0.62
1:L:229:LYS:HA	1:L:272:LYS:HA	1.80	0.62
3:a:63:GLU:OE2	3:a:99:HIS:ND1	2.32	0.62
3:f:27:VAL:HB	3:f:378:LEU:HB2	1.82	0.62
1:D:40:GLN:NE2	1:D:58:ASP:OD1	2.29	0.62
1:K:94:LEU:HD11	1:K:465:GLN:HG3	1.80	0.62
1:J:551:LEU:HD11	1:J:581:VAL:HG21	1.82	0.61
1:L:127:ARG:NH1	1:L:147:GLU:OE1	2.33	0.61
3:b:165:ASP:OD2	3:b:174:ARG:NH1	2.32	0.61
3:c:27:VAL:HB	3:c:378:LEU:HB2	1.81	0.61
1:E:560:LEU:HD22	1:E:565:VAL:HG11	1.83	0.61
1:L:203:ASN:OD1	1:L:218:GLN:NE2	2.33	0.61
2:M:101:ASP:OD1	2:M:102:TYR:N	2.34	0.61
2:P:101:ASP:OD2	2:Z:14:ARG:NH1	2.33	0.61
4:g:146:TRP:HZ2	4:g:150:PRO:HD3	1.64	0.61
2:Y:108:LYS:O	2:Y:113:GLN:NE2	2.32	0.61
1:C:203:ASN:OD1	1:C:218:GLN:NE2	2.33	0.61
1:F:334:MET:HE1	1:G:407:ALA:HB1	1.82	0.61
1:B:61:ARG:NH2	1:C:317:GLU:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:ASN:OD1	1:I:218:GLN:NE2	2.33	0.61
3:a:176:SER:HB3	3:a:218:GLY:HA2	1.82	0.61
4:o:40:LEU:HD13	4:o:87:LEU:HD22	1.82	0.61
1:K:91:ALA:O	1:K:95:MET:HB2	2.01	0.61
1:D:567:MET:HE1	1:E:576:LEU:HD13	1.82	0.61
1:D:594:VAL:O	1:D:598:GLN:HG3	2.01	0.61
1:H:61:ARG:NH2	1:I:317:GLU:OE1	2.34	0.61
1:H:215:ASP:OD1	1:H:216:THR:N	2.33	0.61
2:x:101:ASP:OD1	2:x:102:TYR:N	2.33	0.61
1:H:376:ARG:HH11	1:I:384:LEU:HD23	1.65	0.60
1:B:215:ASP:OD1	1:B:216:THR:N	2.33	0.60
1:H:142:GLN:HG2	1:H:471:ILE:HD11	1.82	0.60
1:J:229:LYS:HA	1:J:272:LYS:HA	1.82	0.60
1:J:594:VAL:O	1:J:598:GLN:HG3	2.02	0.60
4:i:40:LEU:HD13	4:i:87:LEU:HD22	1.82	0.60
3:a:470:ARG:HH12	4:g:96:ALA:HB3	1.66	0.60
3:d:180:ARG:HG2	3:d:182:GLU:HG3	1.83	0.60
2:P:132:PRO:O	2:P:149:ARG:NH2	2.35	0.60
3:b:331:THR:O	3:b:375:GLN:NE2	2.32	0.60
3:b:422:ARG:NH2	3:b:424:GLN:OE1	2.35	0.60
1:F:203:ASN:OD1	1:F:218:GLN:NE2	2.33	0.60
3:e:255:THR:HG22	3:e:256:GLY:H	1.67	0.60
1:F:319:VAL:HG22	1:F:418:LEU:HD11	1.82	0.60
1:L:319:VAL:HG22	1:L:418:LEU:HD11	1.82	0.60
2:v:46:GLN:NE2	2:v:63:GLN:OE1	2.34	0.60
1:B:376:ARG:HH11	1:C:384:LEU:HD23	1.65	0.60
1:E:126:TRP:NE1	1:E:460:ASP:OD2	2.30	0.60
2:Z:75:TYR:HB2	2:Z:79:LEU:HD22	1.84	0.60
3:a:422:ARG:NH2	3:a:424:GLN:OE1	2.35	0.60
1:K:560:LEU:HD22	1:K:565:VAL:HG11	1.83	0.60
1:K:587:PRO:HA	1:K:590:GLN:HE22	1.66	0.60
3:b:408:ARG:HA	3:b:427:GLU:HA	1.82	0.60
3:e:364:GLN:NE2	3:e:366:ASP:OD1	2.33	0.60
1:J:61:ARG:NH2	1:K:317:GLU:OE2	2.35	0.59
2:Z:93:TYR:OH	3:b:408:ARG:NH2	2.35	0.59
3:d:470:ARG:HH12	4:m:96:ALA:HB3	1.66	0.59
1:C:239:VAL:HG12	1:C:240:THR:HG23	1.85	0.59
2:O:101:ASP:OD2	2:Y:14:ARG:NH1	2.35	0.59
3:a:27:VAL:HG12	3:a:378:LEU:HB2	1.84	0.59
2:v:14:ARG:NH1	2:w:101:ASP:OD1	2.35	0.59
1:J:127:ARG:NH1	1:J:147:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:46:GLN:NE2	2:R:63:GLN:OE1	2.35	0.59
2:T:34:GLY:HA3	2:T:40:PRO:HB3	1.82	0.59
2:V:14:ARG:NH1	2:s:101:ASP:OD2	2.35	0.59
3:a:410:PHE:HB2	3:a:455:ARG:HB2	1.84	0.59
3:c:78:LYS:HA	3:c:89:VAL:HG12	1.84	0.59
3:d:422:ARG:NH2	3:d:424:GLN:OE1	2.36	0.59
1:D:61:ARG:NH2	1:E:317:GLU:OE2	2.35	0.59
3:e:408:ARG:HE	3:e:425:MET:HE2	1.66	0.59
2:w:130:ASP:OD1	2:w:131:TYR:N	2.36	0.59
4:h:25:LEU:O	2:w:78:GLN:NE2	2.31	0.59
1:D:127:ARG:NH1	1:D:147:GLU:OE1	2.34	0.59
2:N:85:VAL:HG13	2:N:86:GLN:HG3	1.85	0.59
3:b:112:LEU:HD23	3:b:124:VAL:HG21	1.85	0.59
3:e:112:LEU:HD23	3:e:124:VAL:HG21	1.85	0.59
3:e:422:ARG:NH2	3:e:424:GLN:OE1	2.34	0.59
2:v:34:GLY:HA3	2:v:40:PRO:HB3	1.85	0.59
1:L:209:PHE:CD1	1:L:210:PRO:HD2	2.38	0.59
2:X:24:LYS:HD3	4:p:67:PRO:HG2	1.85	0.59
3:d:181:ALA:O	3:d:182:GLU:HB2	2.02	0.59
2:R:14:ARG:NH1	2:W:101:ASP:OD1	2.36	0.59
3:a:369:SER:HB3	3:a:459:LYS:HB2	1.85	0.59
3:d:331:THR:HG23	3:d:338:TYR:HA	1.84	0.58
3:d:339:ARG:HD3	3:d:371:TYR:HE2	1.68	0.58
1:D:376:ARG:HH11	1:E:384:LEU:HD23	1.68	0.58
1:F:209:PHE:CD1	1:F:210:PRO:HD2	2.38	0.58
1:J:236:GLN:HB2	1:J:266:ILE:HD11	1.85	0.58
2:M:43:PRO:HA	2:M:46:GLN:NE2	2.19	0.58
2:S:132:PRO:O	2:S:149:ARG:NH2	2.36	0.58
3:e:176:SER:HB3	3:e:218:GLY:HA2	1.85	0.58
1:H:229:LYS:HA	1:H:272:LYS:HA	1.84	0.58
1:E:215:ASP:OD1	1:E:216:THR:N	2.36	0.58
3:c:55:MET:HE3	3:c:360:VAL:HG11	1.85	0.58
2:x:43:PRO:HA	2:x:46:GLN:HG3	1.85	0.58
1:B:179:MET:HE1	1:B:187:PHE:HB2	1.86	0.58
1:G:178:SER:OG	1:G:215:ASP:OD2	2.22	0.58
2:Z:85:VAL:HG13	2:Z:86:GLN:HG3	1.85	0.58
3:f:55:MET:HE3	3:f:360:VAL:HG11	1.86	0.58
1:I:239:VAL:HG12	1:I:240:THR:HG23	1.85	0.58
3:f:78:LYS:HA	3:f:89:VAL:HG12	1.83	0.58
1:B:229:LYS:HA	1:B:272:LYS:HA	1.84	0.58
3:a:181:ALA:O	3:a:182:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:255:THR:HG22	3:a:256:GLY:H	1.68	0.58
3:b:386:ALA:HB3	3:b:446:ILE:HD11	1.86	0.58
2:s:75:TYR:HB2	2:s:79:LEU:HD22	1.85	0.58
3:b:36:ILE:HG22	3:b:37:LEU:H	1.69	0.58
3:d:331:THR:O	3:d:375:GLN:NE2	2.35	0.58
3:c:293:MET:HE3	3:c:306:ILE:HG12	1.85	0.58
3:c:400:THR:OG1	3:c:433:VAL:O	2.22	0.58
1:A:551:LEU:HD11	1:A:581:VAL:HG21	1.86	0.57
3:b:470:ARG:HH12	4:i:96:ALA:HB3	1.69	0.57
4:g:66:PRO:HG2	2:x:28:ASN:ND2	2.19	0.57
1:I:317:GLU:HG3	1:I:321:ARG:HG3	1.86	0.57
3:e:386:ALA:HB3	3:e:446:ILE:HD11	1.84	0.57
1:K:82:PRO:HB3	1:K:90:ALA:HB3	1.86	0.57
2:R:51:ILE:HG12	2:R:61:ILE:HG13	1.86	0.57
3:d:27:VAL:HG12	3:d:378:LEU:HB2	1.85	0.57
1:I:567:MET:HE2	1:J:582:LYS:HG3	1.87	0.57
2:T:40:PRO:O	2:T:46:GLN:NE2	2.35	0.57
3:e:331:THR:O	3:e:375:GLN:NE2	2.35	0.57
3:d:369:SER:HB3	3:d:459:LYS:HB2	1.86	0.57
1:H:179:MET:HE1	1:H:187:PHE:HB2	1.86	0.57
1:K:150:HIS:CE1	1:L:307:TRP:HE1	2.21	0.57
3:a:331:THR:HG23	3:a:338:TYR:HA	1.86	0.57
1:C:317:GLU:HG3	1:C:321:ARG:HG3	1.86	0.57
1:E:150:HIS:CE1	1:F:307:TRP:HE1	2.21	0.57
1:G:551:LEU:HD11	1:G:581:VAL:HG21	1.86	0.57
4:p:5:THR:OG1	4:p:8:ASP:OD1	2.21	0.57
1:A:615:LEU:HD12	1:L:609:VAL:HG13	1.87	0.57
1:J:376:ARG:HH11	1:K:384:LEU:HD23	1.69	0.57
1:K:215:ASP:OD1	1:K:216:THR:N	2.36	0.57
2:W:130:ASP:OD1	2:W:131:TYR:N	2.37	0.57
1:C:131:ASP:OD1	1:C:132:TYR:N	2.38	0.57
1:C:363:TYR:OH	1:C:373:LEU:O	2.20	0.57
1:D:215:ASP:OD1	1:D:216:THR:N	2.38	0.57
3:c:283:TYR:OH	3:c:311:HIS:ND1	2.34	0.57
3:d:116:ARG:HE	3:d:122:LYS:HD2	1.68	0.57
3:f:400:THR:OG1	3:f:433:VAL:O	2.23	0.57
2:v:132:PRO:O	2:v:149:ARG:NH2	2.38	0.57
3:d:36:ILE:HG22	3:d:37:LEU:H	1.70	0.57
3:f:181:ALA:O	3:f:182:GLU:HG2	2.04	0.57
2:Q:132:PRO:O	2:Q:149:ARG:NH2	2.37	0.56
2:Z:73:ILE:HD13	2:Z:82:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:180:ARG:HB2	3:d:180:ARG:CZ	2.34	0.56
3:d:386:ALA:HB3	3:d:446:ILE:HD11	1.87	0.56
4:n:146:TRP:CZ2	4:n:150:PRO:HD3	2.38	0.56
1:B:42:ASP:OD2	1:B:328:ARG:NH2	2.35	0.56
1:D:333:ILE:HG21	1:D:405:LEU:HB2	1.86	0.56
1:J:40:GLN:NE2	1:J:58:ASP:OD1	2.29	0.56
3:b:151:TYR:H	3:b:164:THR:HB	1.70	0.56
3:e:470:ARG:HH12	4:o:96:ALA:HB3	1.69	0.56
1:A:563:LYS:HB3	1:B:92:ASP:OD2	2.05	0.56
1:C:74:ASN:HB2	1:C:450:GLN:HE22	1.70	0.56
1:C:81:ARG:NH1	1:C:519:ASP:OD2	2.37	0.56
1:G:150:HIS:CE1	1:H:307:TRP:HE1	2.19	0.56
1:H:42:ASP:OD2	1:H:328:ARG:NH2	2.36	0.56
1:J:333:ILE:HG21	1:J:405:LEU:HB2	1.87	0.56
2:S:34:GLY:HA3	2:S:40:PRO:HB3	1.87	0.56
2:T:132:PRO:O	2:T:149:ARG:NH2	2.37	0.56
3:a:36:ILE:HG22	3:a:37:LEU:H	1.70	0.56
3:e:36:ILE:HG22	3:e:37:LEU:H	1.69	0.56
4:k:49:GLN:NE2	4:l:113:LEU:HD23	2.19	0.56
4:q:49:GLN:NE2	4:r:113:LEU:HD23	2.21	0.56
2:N:78:GLN:HE22	2:S:20:SER:HB2	1.69	0.56
3:e:408:ARG:HA	3:e:427:GLU:HA	1.88	0.56
3:f:331:THR:HG23	3:f:338:TYR:HA	1.88	0.56
4:r:134:THR:OG1	4:r:147:HIS:O	2.21	0.56
3:a:386:ALA:HB3	3:a:446:ILE:HD11	1.86	0.56
2:v:51:ILE:HG12	2:v:61:ILE:HG13	1.88	0.56
1:B:236:GLN:HB2	1:B:266:ILE:HD11	1.87	0.56
1:J:11:ILE:HG21	1:J:281:ILE:HG21	1.87	0.56
1:L:40:GLN:NE2	1:L:58:ASP:OD1	2.36	0.56
3:c:176:SER:HB3	3:c:218:GLY:HA2	1.88	0.56
1:D:11:ILE:HG21	1:D:281:ILE:HG21	1.88	0.56
2:M:28:ASN:ND2	4:m:66:PRO:HG2	2.20	0.56
2:P:34:GLY:HA3	2:P:40:PRO:HB3	1.86	0.56
3:f:293:MET:HE3	3:f:306:ILE:HG12	1.86	0.56
1:I:81:ARG:NH1	1:I:519:ASP:OD2	2.39	0.56
2:T:94:ASP:OD1	2:T:95:ALA:N	2.36	0.56
1:D:236:GLN:HB2	1:D:266:ILE:HD11	1.88	0.56
3:c:181:ALA:O	3:c:182:GLU:HB2	2.05	0.56
3:d:408:ARG:HA	3:d:427:GLU:HA	1.86	0.56
2:Q:33:ILE:HG21	2:Q:84:THR:HG21	1.88	0.56
2:U:24:LYS:HD3	4:j:67:PRO:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:130:ASP:OD1	2:V:131:TYR:N	2.39	0.56
3:b:338:TYR:O	3:b:355:LYS:HD2	2.06	0.56
3:f:364:GLN:NE2	3:f:366:ASP:OD1	2.35	0.56
1:J:281:ILE:HG22	1:J:286:VAL:HG12	1.88	0.55
2:Y:130:ASP:OD1	2:Y:131:TYR:N	2.39	0.55
4:g:146:TRP:CZ2	4:g:150:PRO:HD3	2.40	0.55
1:J:182:ASN:OD1	1:K:171:ARG:NH2	2.39	0.55
1:K:557:PHE:HE2	1:L:548:GLU:HG2	1.71	0.55
3:a:339:ARG:HD3	3:a:371:TYR:HE2	1.71	0.55
1:H:236:GLN:HB2	1:H:266:ILE:HD11	1.88	0.55
1:I:131:ASP:OD1	1:I:132:TYR:N	2.37	0.55
1:I:363:TYR:OH	1:I:373:LEU:O	2.21	0.55
1:K:81:ARG:NH1	1:K:519:ASP:OD2	2.39	0.55
3:a:408:ARG:HA	3:a:427:GLU:HA	1.89	0.55
3:f:176:SER:HB3	3:f:218:GLY:HA2	1.88	0.55
4:g:5:THR:OG1	4:g:8:ASP:OD2	2.25	0.55
1:D:182:ASN:OD1	1:E:171:ARG:NH2	2.39	0.55
1:E:557:PHE:HE2	1:F:548:GLU:HG2	1.72	0.55
1:G:186:ASP:OD2	1:H:171:ARG:NH1	2.39	0.55
3:a:8:MET:HE3	3:a:379:LEU:HD13	1.88	0.55
1:E:81:ARG:NH1	1:E:519:ASP:OD2	2.39	0.55
1:J:215:ASP:OD1	1:J:216:THR:N	2.38	0.55
3:d:390:ARG:HD3	4:n:97:LEU:HD21	1.88	0.55
2:v:33:ILE:HG21	2:v:84:THR:HG21	1.88	0.55
1:B:509:ASP:OD1	1:B:510:ILE:N	2.39	0.55
2:S:33:ILE:HG21	2:S:84:THR:HG21	1.89	0.55
3:f:78:LYS:HE2	3:f:85:GLU:OE2	2.07	0.55
2:s:85:VAL:O	2:s:86:GLN:HG2	2.07	0.55
1:E:551:LEU:HD11	1:E:581:VAL:HG21	1.89	0.55
2:V:78:GLN:NE2	4:l:25:LEU:O	2.32	0.55
4:l:134:THR:OG1	4:l:147:HIS:O	2.20	0.55
2:N:93:TYR:OH	3:e:408:ARG:NH2	2.40	0.55
1:A:239:VAL:HG12	1:A:240:THR:HG23	1.88	0.55
1:F:293:ILE:HG22	1:F:295:GLY:H	1.71	0.55
2:Q:94:ASP:OD1	2:Q:95:ALA:N	2.36	0.55
2:X:130:ASP:OD1	2:X:131:TYR:N	2.40	0.55
3:a:11:GLY:O	3:a:24:TYR:N	2.38	0.55
4:n:134:THR:OG1	4:n:147:HIS:O	2.24	0.55
1:B:551:LEU:HD11	1:B:581:VAL:HG21	1.87	0.54
1:L:179:MET:HE1	1:L:187:PHE:HB2	1.89	0.54
3:a:390:ARG:HD3	4:h:97:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:176:SER:HB3	3:d:218:GLY:HA2	1.88	0.54
1:F:11:ILE:HG21	1:F:281:ILE:HG21	1.88	0.54
1:H:557:PHE:HE2	1:I:548:GLU:HG2	1.71	0.54
1:L:363:TYR:OH	1:L:373:LEU:O	2.26	0.54
2:R:132:PRO:O	2:R:149:ARG:NH2	2.40	0.54
3:a:388:ASN:OD1	3:a:445:ARG:NH1	2.40	0.54
1:B:519:ASP:OD1	1:B:520:VAL:N	2.40	0.54
1:H:82:PRO:HB3	1:H:90:ALA:HB3	1.88	0.54
1:L:310:VAL:HG13	1:L:311:GLU:H	1.72	0.54
3:e:146:ARG:NH1	3:e:169:GLU:OE2	2.36	0.54
1:D:551:LEU:HD11	1:D:581:VAL:HG21	1.90	0.54
1:E:254:VAL:HG21	1:E:505:GLN:HG2	1.89	0.54
1:F:609:VAL:HG13	1:G:615:LEU:HD12	1.89	0.54
1:K:281:ILE:HG22	1:K:286:VAL:HG12	1.89	0.54
1:L:215:ASP:OD1	1:L:215:ASP:N	2.41	0.54
2:N:46:GLN:HB3	2:N:63:GLN:HE21	1.72	0.54
3:e:151:TYR:H	3:e:164:THR:HB	1.73	0.54
4:l:146:TRP:CZ2	4:l:150:PRO:HD3	2.42	0.54
2:s:127:LYS:HA	2:s:146:LEU:HB3	1.88	0.54
1:C:225:VAL:HG22	1:C:276:VAL:HG22	1.90	0.54
3:f:470:ARG:HH12	4:q:96:ALA:HB3	1.73	0.54
4:r:146:TRP:CZ2	4:r:150:PRO:HD3	2.42	0.54
1:F:81:ARG:NH1	1:F:519:ASP:OD2	2.38	0.54
2:R:34:GLY:HA3	2:R:40:PRO:HB3	1.90	0.54
1:C:150:HIS:CE1	1:D:307:TRP:HE1	2.18	0.54
2:O:85:VAL:O	2:O:86:GLN:HG2	2.07	0.54
2:T:33:ILE:HG21	2:T:84:THR:HG21	1.90	0.54
4:h:134:THR:OG1	4:h:147:HIS:O	2.22	0.54
1:F:40:GLN:NE2	1:F:58:ASP:OD1	2.37	0.54
1:I:362:MET:HE1	1:I:373:LEU:HD12	1.90	0.54
1:I:480:ILE:HB	1:I:488:LYS:HD2	1.89	0.54
2:Y:78:GLN:NE2	4:r:25:LEU:O	2.30	0.54
3:b:146:ARG:NH1	3:b:169:GLU:OE2	2.36	0.54
3:d:27:VAL:HG23	3:d:328:VAL:HG13	1.90	0.54
3:d:341:VAL:HG23	3:d:355:LYS:HB3	1.89	0.54
3:e:331:THR:HG23	3:e:338:TYR:HA	1.90	0.54
3:f:64:TYR:HB2	3:f:344:MET:HE2	1.89	0.54
4:h:141:ALA:HB1	4:h:146:TRP:HE3	1.73	0.54
1:D:616:LEU:HD22	1:E:622:LEU:HD11	1.90	0.54
1:F:179:MET:HE1	1:F:187:PHE:HB2	1.89	0.54
1:F:310:VAL:HG13	1:F:311:GLU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:509:ASP:OD1	1:H:510:ILE:N	2.40	0.54
2:U:130:ASP:OD1	2:U:131:TYR:N	2.40	0.54
1:A:376:ARG:HH11	1:B:384:LEU:HD23	1.73	0.53
1:F:361:HIS:O	1:F:366:ASN:ND2	2.40	0.53
1:L:293:ILE:HG22	1:L:295:GLY:H	1.73	0.53
1:A:626:GLN:O	1:A:629:THR:OG1	2.24	0.53
1:D:225:VAL:HG22	1:D:276:VAL:HG22	1.90	0.53
1:F:509:ASP:OD1	1:F:511:ARG:N	2.41	0.53
1:K:254:VAL:HG21	1:K:505:GLN:HG2	1.89	0.53
2:N:101:ASP:OD2	2:X:14:ARG:NH1	2.41	0.53
3:d:388:ASN:OD1	3:d:445:ARG:NH1	2.41	0.53
1:A:99:ARG:NH1	1:A:524:PHE:HB2	2.23	0.53
1:C:480:ILE:HB	1:C:488:LYS:HD2	1.89	0.53
1:E:281:ILE:HG22	1:E:286:VAL:HG12	1.89	0.53
1:G:333:ILE:HG21	1:G:405:LEU:HB2	1.89	0.53
2:X:33:ILE:HG23	2:X:88:HIS:HB2	1.90	0.53
3:c:386:ALA:HB3	3:c:446:ILE:HD11	1.90	0.53
1:L:225:VAL:HG22	1:L:276:VAL:HG22	1.90	0.53
3:c:470:ARG:HH12	4:k:96:ALA:HB3	1.74	0.53
4:p:146:TRP:CZ2	4:p:150:PRO:HD3	2.42	0.53
4:l:3:ILE:HG22	4:l:9:LEU:HD12	1.91	0.53
1:C:333:ILE:HG21	1:C:405:LEU:HB2	1.90	0.53
1:D:519:ASP:OD1	1:D:520:VAL:N	2.40	0.53
1:F:363:TYR:OH	1:F:373:LEU:O	2.26	0.53
3:b:78:LYS:HA	3:b:89:VAL:HG12	1.89	0.53
3:e:341:VAL:HG22	3:e:355:LYS:HE3	1.90	0.53
1:B:333:ILE:HG21	1:B:405:LEU:HB2	1.91	0.53
1:F:215:ASP:N	1:F:215:ASP:OD1	2.41	0.53
3:a:27:VAL:HG23	3:a:328:VAL:HG13	1.90	0.53
3:e:65:ASN:OD1	3:e:99:HIS:ND1	2.42	0.53
1:I:361:HIS:O	1:I:366:ASN:ND2	2.39	0.53
1:J:310:VAL:HG13	1:J:311:GLU:H	1.73	0.53
3:a:151:TYR:H	3:a:164:THR:HB	1.73	0.53
3:d:151:TYR:H	3:d:164:THR:HB	1.73	0.53
1:A:281:ILE:HG22	1:A:286:VAL:HG12	1.91	0.53
1:B:557:PHE:HE2	1:C:548:GLU:HG2	1.73	0.53
1:D:281:ILE:HG22	1:D:286:VAL:HG12	1.90	0.53
1:E:329:LEU:O	1:E:333:ILE:HG12	2.09	0.53
1:G:281:ILE:HG22	1:G:286:VAL:HG12	1.91	0.53
3:c:331:THR:HG23	3:c:338:TYR:HA	1.89	0.53
1:A:480:ILE:HB	1:A:488:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:VAL:HG12	1:G:240:THR:HG23	1.90	0.53
1:K:616:LEU:HD22	1:L:622:LEU:HD11	1.91	0.53
2:S:53:ASN:OD1	2:S:57:SER:OG	2.26	0.53
3:e:56:ASN:ND2	3:e:77:GLY:HA3	2.23	0.53
1:E:376:ARG:NH2	1:F:354:GLU:OE2	2.35	0.52
1:G:376:ARG:HH11	1:H:384:LEU:HD23	1.73	0.52
1:H:609:VAL:HB	1:I:611:ALA:HB1	1.92	0.52
1:J:225:VAL:HG22	1:J:276:VAL:HG22	1.91	0.52
2:M:68:ASN:HB3	2:M:74:VAL:HB	1.90	0.52
3:b:65:ASN:OD1	3:b:99:HIS:ND1	2.42	0.52
3:c:64:TYR:HB2	3:c:344:MET:HE2	1.92	0.52
3:d:32:THR:HG22	3:d:301:HIS:NE2	2.24	0.52
1:C:362:MET:HE1	1:C:373:LEU:HD12	1.90	0.52
2:P:53:ASN:OD1	2:P:57:SER:OG	2.27	0.52
3:e:170:SER:O	3:e:171:HIS:ND1	2.43	0.52
3:e:283:TYR:OH	3:e:311:HIS:ND1	2.32	0.52
1:A:225:VAL:HG22	1:A:276:VAL:HG22	1.92	0.52
1:C:519:ASP:OD1	1:C:520:VAL:N	2.42	0.52
1:C:616:LEU:HD22	1:D:622:LEU:HD11	1.91	0.52
1:E:480:ILE:HB	1:E:488:LYS:HD2	1.91	0.52
1:K:225:VAL:HG22	1:K:276:VAL:HG22	1.92	0.52
3:c:32:THR:HG22	3:c:301:HIS:CE1	2.44	0.52
3:d:165:ASP:OD1	3:d:166:LEU:N	2.40	0.52
1:A:150:HIS:CE1	1:B:307:TRP:HE1	2.18	0.52
1:E:225:VAL:HG22	1:E:276:VAL:HG22	1.91	0.52
1:I:616:LEU:HD22	1:J:622:LEU:HD11	1.92	0.52
1:J:616:LEU:HD22	1:K:622:LEU:HD11	1.91	0.52
2:P:101:ASP:OD1	2:P:102:TYR:N	2.43	0.52
2:W:78:GLN:NE2	4:n:25:LEU:O	2.32	0.52
3:f:283:TYR:OH	3:f:311:HIS:ND1	2.34	0.52
2:x:68:ASN:HB3	2:x:74:VAL:HB	1.91	0.52
1:K:480:ILE:HB	1:K:488:LYS:HD2	1.90	0.52
3:a:194:TRP:NE1	3:a:245:ASP:O	2.42	0.52
3:d:408:ARG:HD3	3:d:425:MET:HE2	1.90	0.52
1:I:23:ASP:OD1	1:I:26:ARG:NH2	2.43	0.52
1:I:225:VAL:HG22	1:I:276:VAL:HG22	1.91	0.52
2:U:33:ILE:HG23	2:U:88:HIS:HB2	1.90	0.52
1:A:384:LEU:HD23	1:L:376:ARG:HH11	1.74	0.52
1:B:310:VAL:HG13	1:B:311:GLU:H	1.75	0.52
1:C:361:HIS:O	1:C:366:ASN:ND2	2.42	0.52
1:F:225:VAL:HG22	1:F:276:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:3:ILE:HG22	4:g:9:LEU:HD12	1.91	0.52
4:g:134:THR:OG1	4:g:147:HIS:O	2.25	0.52
4:m:141:ALA:HB1	4:m:146:TRP:HE3	1.75	0.52
2:N:78:GLN:NE2	2:S:20:SER:HB2	2.25	0.52
2:U:94:ASP:OD1	2:U:95:ALA:N	2.41	0.52
2:V:9:VAL:HG22	2:s:83:VAL:HG12	1.91	0.52
3:a:32:THR:HG22	3:a:301:HIS:NE2	2.25	0.52
3:c:408:ARG:HA	3:c:427:GLU:HA	1.92	0.52
4:o:31:GLN:NE2	4:p:22:ASP:OD2	2.42	0.52
1:C:23:ASP:OD1	1:C:26:ARG:NH2	2.43	0.52
1:C:329:LEU:O	1:C:333:ILE:HG12	2.10	0.52
1:C:586:THR:OG1	1:C:587:PRO:HD2	2.10	0.52
1:K:329:LEU:O	1:K:333:ILE:HG12	2.10	0.52
2:Q:34:GLY:HA3	2:Q:40:PRO:HB3	1.90	0.52
3:c:151:TYR:H	3:c:164:THR:HB	1.75	0.52
3:d:159:ASP:HB3	3:d:180:ARG:CG	2.40	0.52
3:e:11:GLY:O	3:e:24:TYR:N	2.40	0.52
3:f:32:THR:HG22	3:f:301:HIS:CE1	2.45	0.52
4:p:76:ARG:NH1	4:p:78:SER:OG	2.43	0.52
1:F:376:ARG:HH11	1:G:384:LEU:HD23	1.74	0.52
1:K:333:ILE:HG21	1:K:405:LEU:HB2	1.90	0.52
1:K:551:LEU:HD11	1:K:581:VAL:HG21	1.92	0.52
3:a:341:VAL:HG23	3:a:355:LYS:HB3	1.91	0.52
3:f:179:TYR:OH	3:f:221:LEU:HB2	2.10	0.52
3:f:386:ALA:HB3	3:f:446:ILE:HD11	1.90	0.52
1:G:480:ILE:HB	1:G:488:LYS:HD2	1.92	0.51
2:O:83:VAL:HG12	2:Y:9:VAL:HG22	1.91	0.51
3:b:341:VAL:HG22	3:b:355:LYS:CE	2.40	0.51
3:f:104:GLN:O	3:f:105:ALA:HB3	2.09	0.51
3:f:151:TYR:H	3:f:164:THR:HB	1.75	0.51
1:A:150:HIS:CD2	1:B:163:LYS:HG3	2.46	0.51
1:J:7:ARG:NH2	1:J:224:GLU:OE2	2.35	0.51
1:L:330:ARG:NH1	1:L:409:THR:OG1	2.42	0.51
3:e:183:SER:OG	3:e:207:GLU:OE1	2.29	0.51
4:m:5:THR:OG1	4:m:8:ASP:OD2	2.26	0.51
1:D:7:ARG:NH2	1:D:224:GLU:OE2	2.35	0.51
1:L:81:ARG:NH1	1:L:519:ASP:OD2	2.38	0.51
2:V:125:SER:OG	2:s:123:LYS:HB3	2.10	0.51
3:a:165:ASP:OD1	3:a:166:LEU:N	2.40	0.51
3:b:183:SER:OG	3:b:207:GLU:OE1	2.29	0.51
3:c:63:GLU:CD	3:c:99:HIS:HD1	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:339:ARG:HD3	3:e:371:TYR:HE2	1.76	0.51
1:E:333:ILE:HG21	1:E:405:LEU:HB2	1.91	0.51
1:E:468:VAL:HG13	1:E:472:TYR:HD2	1.75	0.51
1:K:376:ARG:NH2	1:L:354:GLU:OE2	2.36	0.51
2:T:125:SER:OG	2:Y:123:LYS:NZ	2.40	0.51
3:d:312:VAL:HG21	3:d:338:TYR:H	1.76	0.51
1:C:551:LEU:HD11	1:C:581:VAL:HG21	1.92	0.51
3:a:383:LEU:HD23	3:a:449:LEU:HD13	1.91	0.51
3:b:341:VAL:HG22	3:b:355:LYS:HE3	1.91	0.51
3:d:194:TRP:NE1	3:d:245:ASP:O	2.44	0.51
1:G:81:ARG:NH1	1:G:519:ASP:OD2	2.44	0.51
1:I:333:ILE:HG21	1:I:405:LEU:HB2	1.90	0.51
3:a:448:ARG:HD3	4:i:25:LEU:HD12	1.92	0.51
3:c:116:ARG:HD2	3:c:122:LYS:CG	2.38	0.51
3:e:255:THR:HG22	3:e:256:GLY:N	2.26	0.51
1:H:333:ILE:HG21	1:H:405:LEU:HB2	1.91	0.51
1:K:626:GLN:O	1:K:629:THR:OG1	2.24	0.51
2:R:33:ILE:HG21	2:R:84:THR:HG21	1.92	0.51
3:b:170:SER:O	3:b:171:HIS:ND1	2.43	0.51
3:e:283:TYR:HE2	3:e:308:LEU:HD13	1.75	0.51
4:j:3:ILE:HG22	4:j:9:LEU:HD12	1.92	0.51
1:E:616:LEU:HD22	1:F:622:LEU:HD11	1.92	0.51
3:f:408:ARG:HA	3:f:427:GLU:HA	1.92	0.51
1:F:471:ILE:HG22	1:F:472:TYR:CD1	2.45	0.51
2:U:14:ARG:NH1	2:Z:101:ASP:OD2	2.44	0.51
3:b:36:ILE:HD11	3:b:42:TYR:HD1	1.76	0.51
4:h:146:TRP:CZ2	4:h:150:PRO:HD3	2.46	0.51
4:k:3:ILE:HG22	4:k:9:LEU:HD12	1.93	0.51
4:m:3:ILE:HG22	4:m:9:LEU:HD12	1.91	0.51
1:B:609:VAL:HB	1:C:611:ALA:HB1	1.93	0.51
1:F:165:MET:HA	1:F:307:TRP:CZ3	2.46	0.51
1:H:519:ASP:OD1	1:H:520:VAL:N	2.41	0.51
3:b:13:GLY:HA3	3:b:24:TYR:CE2	2.45	0.51
3:c:165:ASP:OD1	3:c:166:LEU:N	2.43	0.51
3:d:255:THR:HG22	3:d:256:GLY:N	2.26	0.51
4:r:3:ILE:HG22	4:r:9:LEU:HD12	1.92	0.51
1:A:234:ILE:HD11	1:A:269:ARG:HG3	1.93	0.50
1:A:333:ILE:HG21	1:A:405:LEU:HB2	1.93	0.50
1:B:329:LEU:O	1:B:333:ILE:HG12	2.11	0.50
1:D:310:VAL:HG13	1:D:311:GLU:H	1.75	0.50
1:I:150:HIS:CE1	1:J:307:TRP:HE1	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:206:ASP:OD1	1:I:207:TRP:N	2.43	0.50
1:K:126:TRP:NE1	1:K:460:ASP:OD2	2.31	0.50
1:K:319:VAL:HG22	1:K:418:LEU:HD11	1.94	0.50
3:b:11:GLY:O	3:b:24:TYR:N	2.41	0.50
3:d:63:GLU:OE2	3:d:99:HIS:ND1	2.43	0.50
1:D:239:VAL:HG12	1:D:240:THR:HG23	1.93	0.50
1:F:330:ARG:NH1	1:F:409:THR:OG1	2.44	0.50
1:I:551:LEU:HD11	1:I:581:VAL:HG21	1.93	0.50
1:J:239:VAL:HG12	1:J:240:THR:HG23	1.93	0.50
1:K:80:TYR:OH	1:K:461:GLY:O	2.29	0.50
1:K:93:VAL:HG21	1:K:475:PRO:HD2	1.93	0.50
1:K:468:VAL:HG13	1:K:472:TYR:HD2	1.75	0.50
2:N:78:GLN:HE22	2:S:20:SER:CB	2.25	0.50
2:Y:33:ILE:HG23	2:Y:88:HIS:HB2	1.94	0.50
3:c:388:ASN:OD1	3:c:445:ARG:NH1	2.44	0.50
3:d:35:GLU:O	3:d:35:GLU:HG3	2.10	0.50
1:A:215:ASP:N	1:A:215:ASP:OD1	2.44	0.50
1:A:616:LEU:HD22	1:B:622:LEU:HD11	1.93	0.50
1:G:150:HIS:CD2	1:H:163:LYS:HG3	2.46	0.50
1:B:77:ASP:OD1	1:B:78:VAL:N	2.36	0.50
1:B:225:VAL:HG22	1:B:276:VAL:HG22	1.94	0.50
1:B:626:GLN:O	1:B:629:THR:OG1	2.27	0.50
1:J:339:ASP:OD1	4:k:128:TYR:OH	2.25	0.50
1:L:333:ILE:HG21	1:L:405:LEU:HB2	1.93	0.50
2:P:33:ILE:HG21	2:P:84:THR:HG21	1.92	0.50
3:b:339:ARG:HD3	3:b:371:TYR:HE2	1.76	0.50
3:c:36:ILE:HG22	3:c:37:LEU:H	1.76	0.50
3:d:179:TYR:OH	3:d:221:LEU:HB2	2.11	0.50
2:w:33:ILE:HG23	2:w:88:HIS:HB2	1.93	0.50
1:D:53:TYR:O	4:p:131:ARG:NH1	2.45	0.50
1:D:480:ILE:HB	1:D:488:LYS:HD2	1.94	0.50
1:F:281:ILE:HG22	1:F:286:VAL:HG12	1.92	0.50
1:G:177:HIS:NE2	1:G:221:GLU:OE1	2.34	0.50
1:H:225:VAL:HG22	1:H:276:VAL:HG22	1.93	0.50
1:J:509:ASP:OD1	1:J:511:ARG:N	2.40	0.50
2:N:28:ASN:ND2	4:o:66:PRO:HG2	2.26	0.50
3:c:179:TYR:OH	3:c:221:LEU:HB2	2.11	0.50
4:o:49:GLN:HE21	4:p:113:LEU:HD23	1.77	0.50
1:B:53:TYR:O	4:n:131:ARG:NH1	2.45	0.50
1:F:329:LEU:O	1:F:333:ILE:HG12	2.12	0.50
1:G:225:VAL:HG22	1:G:276:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:616:LEU:HD22	1:G:622:LEU:HD11	1.94	0.50
1:G:91:ALA:O	1:G:95:MET:HB2	2.12	0.50
1:H:310:VAL:HG13	1:H:311:GLU:H	1.77	0.50
1:I:329:LEU:O	1:I:333:ILE:HG12	2.11	0.50
2:W:33:ILE:HG23	2:W:88:HIS:HB2	1.93	0.50
3:a:312:VAL:HG21	3:a:338:TYR:H	1.76	0.50
4:q:46:GLU:O	4:q:49:GLN:HG2	2.11	0.50
1:F:333:ILE:HG21	1:F:405:LEU:HB2	1.93	0.50
1:H:53:TYR:O	4:h:131:ARG:NH1	2.45	0.50
1:H:340:ILE:O	1:H:344:THR:OG1	2.24	0.50
1:J:480:ILE:HB	1:J:488:LYS:HD2	1.94	0.50
1:L:165:MET:HA	1:L:307:TRP:CZ3	2.47	0.50
1:L:329:LEU:O	1:L:333:ILE:HG12	2.12	0.50
3:a:408:ARG:HH12	2:x:93:TYR:HH	1.57	0.50
4:m:1:MET:O	4:m:1:MET:HE3	2.12	0.50
1:L:480:ILE:HB	1:L:488:LYS:HD2	1.94	0.50
3:a:409:LEU:N	3:a:426:ILE:O	2.39	0.50
3:d:448:ARG:HD3	4:o:25:LEU:HD12	1.93	0.50
1:G:616:LEU:HD22	1:H:622:LEU:HD11	1.93	0.49
1:G:626:GLN:O	1:G:629:THR:OG1	2.23	0.49
1:H:329:LEU:O	1:H:333:ILE:HG12	2.12	0.49
2:S:101:ASP:OD1	2:S:102:TYR:N	2.45	0.49
3:b:165:ASP:OD1	3:b:166:LEU:N	2.45	0.49
3:c:262:ILE:HD12	3:c:271:ILE:HG21	1.93	0.49
3:f:388:ASN:OD1	3:f:445:ARG:NH1	2.45	0.49
1:A:317:GLU:OE1	1:L:61:ARG:NH2	2.45	0.49
1:D:150:HIS:CE1	1:E:307:TRP:HE1	2.24	0.49
1:K:150:HIS:CD2	1:L:163:LYS:HG3	2.47	0.49
3:d:170:SER:O	3:d:171:HIS:ND1	2.45	0.49
4:p:46:GLU:O	4:p:46:GLU:HG2	2.11	0.49
1:A:329:LEU:O	1:A:333:ILE:HG12	2.13	0.49
1:C:376:ARG:NH2	1:D:354:GLU:OE2	2.41	0.49
1:E:23:ASP:OD1	1:E:26:ARG:NH2	2.45	0.49
1:G:215:ASP:OD1	1:G:215:ASP:N	2.44	0.49
2:T:42:ASN:O	2:T:42:ASN:ND2	2.39	0.49
2:T:42:ASN:C	2:T:42:ASN:HD22	2.13	0.49
2:U:128:LEU:HD12	2:U:147:ILE:HA	1.93	0.49
4:i:134:THR:OG1	4:i:147:HIS:O	2.22	0.49
4:o:134:THR:OG1	4:o:147:HIS:O	2.22	0.49
1:A:319:VAL:HG22	1:A:418:LEU:HD11	1.93	0.49
1:E:61:ARG:NH2	1:F:317:GLU:OE1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:VAL:HG22	1:E:418:LEU:HD11	1.94	0.49
3:a:116:ARG:HE	3:a:122:LYS:HD2	1.78	0.49
4:p:3:ILE:HG22	4:p:9:LEU:HD12	1.94	0.49
1:E:626:GLN:O	1:E:629:THR:OG1	2.24	0.49
1:F:519:ASP:OD1	1:F:520:VAL:N	2.42	0.49
1:I:215:ASP:N	1:I:215:ASP:OD1	2.45	0.49
3:d:410:PHE:HB2	3:d:455:ARG:HB2	1.93	0.49
1:A:186:ASP:OD2	1:B:171:ARG:NH1	2.46	0.49
1:G:131:ASP:OD1	1:G:132:TYR:N	2.46	0.49
1:K:23:ASP:OD1	1:K:26:ARG:NH2	2.46	0.49
3:c:36:ILE:HD11	3:c:42:TYR:CD1	2.48	0.49
3:e:338:TYR:O	3:e:355:LYS:HD2	2.12	0.49
4:k:134:THR:OG1	4:k:147:HIS:O	2.26	0.49
2:S:94:ASP:OD1	2:S:95:ALA:N	2.40	0.49
2:V:94:ASP:OD1	2:V:95:ALA:N	2.46	0.49
3:a:262:ILE:HD12	3:a:271:ILE:HG21	1.93	0.49
4:k:8:ASP:OD1	4:k:11:ARG:NH1	2.45	0.49
4:m:134:THR:OG1	4:m:147:HIS:O	2.24	0.49
4:q:79:ALA:O	4:q:83:VAL:HG23	2.13	0.49
2:Q:55:ASP:OD1	2:Q:56:GLY:N	2.46	0.49
3:e:66:THR:H	3:e:99:HIS:CE1	2.31	0.49
3:e:414:THR:HG23	3:e:420:TYR:CD2	2.48	0.49
3:f:105:ALA:HA	3:f:114:GLU:HA	1.95	0.49
3:f:182:GLU:O	3:f:182:GLU:HG3	2.12	0.49
2:w:31:ILE:HB	2:w:65:LEU:HB2	1.95	0.49
1:A:177:HIS:NE2	1:A:221:GLU:OE1	2.36	0.49
1:L:58:ASP:OD2	1:L:61:ARG:HB2	2.13	0.49
3:a:293:MET:HG2	3:a:306:ILE:HG12	1.95	0.49
3:f:262:ILE:HD12	3:f:271:ILE:HG21	1.94	0.49
4:o:8:ASP:OD1	4:o:11:ARG:NH1	2.45	0.49
1:B:80:TYR:OH	1:B:461:GLY:O	2.29	0.49
1:D:340:ILE:O	1:D:344:THR:OG1	2.27	0.49
1:G:254:VAL:HG22	1:G:257:ASP:HB2	1.93	0.49
1:G:319:VAL:HG22	1:G:418:LEU:HD11	1.94	0.49
1:H:551:LEU:HD11	1:H:581:VAL:HG21	1.95	0.49
1:I:61:ARG:NH2	1:J:317:GLU:OE1	2.45	0.49
1:L:509:ASP:OD1	1:L:511:ARG:N	2.42	0.49
2:N:136:ASP:OD1	2:N:137:ALA:N	2.46	0.49
2:V:94:ASP:OD2	4:l:66:PRO:HB3	2.13	0.49
3:a:170:SER:O	3:a:171:HIS:ND1	2.45	0.49
3:b:414:THR:HG23	3:b:420:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASP:OD1	1:C:207:TRP:N	2.45	0.48
1:G:376:ARG:NH1	1:H:384:LEU:HD23	2.28	0.48
1:H:80:TYR:OH	1:H:461:GLY:O	2.29	0.48
3:b:66:THR:H	3:b:99:HIS:CE1	2.32	0.48
3:b:369:SER:HB3	3:b:459:LYS:HB2	1.94	0.48
2:x:136:ASP:OD1	2:x:136:ASP:N	2.45	0.48
1:A:622:LEU:HD11	1:L:616:LEU:HD22	1.94	0.48
1:B:7:ARG:NH2	1:B:224:GLU:OE2	2.37	0.48
1:C:281:ILE:HG22	1:C:286:VAL:HG12	1.94	0.48
1:D:577:ILE:HG12	1:D:582:LYS:HB2	1.94	0.48
2:Q:49:VAL:HG23	2:Q:61:ILE:HB	1.94	0.48
2:T:51:ILE:HD12	2:T:80:VAL:HB	1.94	0.48
2:X:14:ARG:HH11	2:X:79:LEU:HD23	1.78	0.48
2:Y:72:LYS:HD3	2:Y:79:LEU:HD21	1.94	0.48
3:a:283:TYR:OH	3:a:311:HIS:ND1	2.37	0.48
3:b:341:VAL:CG2	3:b:355:LYS:HB3	2.43	0.48
3:c:104:GLN:O	3:c:105:ALA:HB3	2.13	0.48
3:d:141:VAL:HG13	3:d:153:TRP:HB2	1.95	0.48
3:d:262:ILE:HD12	3:d:271:ILE:HG21	1.94	0.48
1:A:509:ASP:OD1	1:A:511:ARG:N	2.44	0.48
1:C:626:GLN:O	1:C:629:THR:OG1	2.25	0.48
1:J:178:SER:OG	1:J:215:ASP:OD2	2.26	0.48
2:M:43:PRO:HA	2:M:46:GLN:HE21	1.77	0.48
2:Q:101:ASP:OD2	2:s:14:ARG:NH1	2.46	0.48
2:Y:94:ASP:OD1	2:Y:95:ALA:N	2.45	0.48
2:Z:136:ASP:OD1	2:Z:137:ALA:N	2.46	0.48
3:a:195:ARG:NH1	3:f:229:MET:O	2.43	0.48
3:e:312:VAL:HG21	3:e:338:TYR:H	1.78	0.48
1:J:209:PHE:CG	1:J:210:PRO:HD2	2.48	0.48
3:d:293:MET:HG2	3:d:306:ILE:HG12	1.94	0.48
2:w:105:ASN:HB3	2:w:108:LYS:HG2	1.96	0.48
1:D:150:HIS:CD2	1:E:163:LYS:HG3	2.48	0.48
1:J:519:ASP:OD1	1:J:520:VAL:N	2.41	0.48
2:M:101:ASP:OD2	2:W:14:ARG:NH1	2.47	0.48
2:V:24:LYS:HZ1	4:l:65:ASN:HB3	1.78	0.48
2:X:31:ILE:HD11	2:X:67:ILE:HD11	1.96	0.48
3:b:331:THR:HG23	3:b:338:TYR:HA	1.94	0.48
3:e:13:GLY:HA3	3:e:24:TYR:CE2	2.48	0.48
3:e:390:ARG:HD3	4:p:97:LEU:HD21	1.96	0.48
3:f:165:ASP:OD1	3:f:166:LEU:N	2.43	0.48
1:E:80:TYR:OH	1:E:461:GLY:O	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:VAL:HG13	1:E:311:GLU:H	1.79	0.48
1:E:363:TYR:OH	1:E:373:LEU:O	2.30	0.48
1:F:58:ASP:OD2	1:F:61:ARG:HB2	2.13	0.48
1:I:281:ILE:HG22	1:I:286:VAL:HG12	1.96	0.48
1:J:53:TYR:O	4:j:131:ARG:NH1	2.46	0.48
1:K:310:VAL:HG13	1:K:311:GLU:H	1.78	0.48
3:c:11:GLY:O	3:c:24:TYR:N	2.39	0.48
3:e:206:ILE:HB	3:e:230:VAL:HB	1.96	0.48
3:f:59:SER:HA	3:f:75:CYS:HA	1.96	0.48
3:f:165:ASP:HB3	3:f:168:ASP:O	2.14	0.48
4:r:62:ASP:O	4:r:63:ASP:CB	2.62	0.48
4:r:79:ALA:O	4:r:83:VAL:HG23	2.13	0.48
1:B:58:ASP:OD1	1:B:59:VAL:N	2.46	0.48
1:F:480:ILE:HB	1:F:488:LYS:HD2	1.96	0.48
1:G:329:LEU:O	1:G:333:ILE:HG12	2.14	0.48
1:I:252:LYS:HG3	1:I:253:ASP:OD1	2.14	0.48
1:I:274:ARG:HB2	1:I:296:GLU:HG2	1.96	0.48
1:K:61:ARG:NH2	1:L:317:GLU:OE1	2.41	0.48
2:P:94:ASP:OD1	2:P:95:ALA:N	2.41	0.48
3:c:409:LEU:N	3:c:426:ILE:O	2.41	0.48
3:d:36:ILE:HD11	3:d:42:TYR:HD1	1.79	0.48
3:f:194:TRP:NE1	3:f:245:ASP:O	2.45	0.48
3:f:339:ARG:HD3	3:f:371:TYR:HE2	1.79	0.48
3:f:369:SER:HB3	3:f:459:LYS:HB2	1.95	0.48
4:k:79:ALA:O	4:k:83:VAL:HG23	2.13	0.48
4:l:79:ALA:O	4:l:83:VAL:HG23	2.14	0.48
2:v:101:ASP:OD2	2:x:14:ARG:NH1	2.46	0.48
1:G:32:ASP:OD2	1:G:321:ARG:HG2	2.14	0.48
1:I:310:VAL:HG13	1:I:311:GLU:H	1.79	0.48
2:T:123:LYS:O	2:Y:122:PHE:HD1	1.96	0.48
3:a:255:THR:HG22	3:a:256:GLY:N	2.28	0.48
3:c:165:ASP:HB3	3:c:168:ASP:O	2.13	0.48
3:e:36:ILE:HD11	3:e:42:TYR:HD1	1.77	0.48
1:J:274:ARG:NH1	1:J:296:GLU:OE2	2.47	0.48
2:S:55:ASP:OD1	2:S:56:GLY:N	2.47	0.48
3:c:364:GLN:NE2	3:c:366:ASP:OD1	2.39	0.48
1:A:519:ASP:OD1	1:A:520:VAL:N	2.47	0.48
4:m:146:TRP:CZ2	4:m:150:PRO:HD3	2.49	0.48
2:x:94:ASP:OD1	2:x:95:ALA:N	2.44	0.48
1:A:376:ARG:NH1	1:B:384:LEU:HD23	2.28	0.47
1:C:376:ARG:NH1	1:D:384:LEU:HD23	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ILE:HG22	1:D:457:MET:HG3	1.95	0.47
1:D:209:PHE:CG	1:D:210:PRO:HD2	2.48	0.47
1:H:58:ASP:OD1	1:H:59:VAL:N	2.47	0.47
1:J:626:GLN:O	1:J:629:THR:OG1	2.28	0.47
2:M:123:LYS:HB3	2:W:125:SER:OG	2.14	0.47
2:T:50:TYR:HE1	2:T:60:GLN:HG2	1.79	0.47
2:V:72:LYS:HD3	2:V:79:LEU:HD21	1.94	0.47
3:a:13:GLY:HA3	3:a:24:TYR:CE2	2.49	0.47
3:b:409:LEU:N	3:b:426:ILE:O	2.40	0.47
4:o:51:GLY:C	4:o:53:GLY:H	2.21	0.47
1:D:557:PHE:HE2	1:E:548:GLU:HG2	1.78	0.47
3:e:470:ARG:NH1	4:o:96:ALA:HB3	2.30	0.47
4:i:51:GLY:C	4:i:53:GLY:H	2.22	0.47
4:j:146:TRP:CZ2	4:j:150:PRO:HD3	2.48	0.47
4:m:29:GLU:OE1	4:m:31:GLN:N	2.47	0.47
2:Z:68:ASN:HB3	2:Z:74:VAL:HB	1.96	0.47
3:b:470:ARG:NH1	4:i:96:ALA:HB3	2.29	0.47
3:c:194:TRP:NE1	3:c:245:ASP:O	2.45	0.47
2:s:68:ASN:HB3	2:s:74:VAL:HB	1.97	0.47
1:A:256:ASP:OD1	1:A:257:ASP:N	2.47	0.47
1:H:480:ILE:HB	1:H:488:LYS:HD2	1.96	0.47
1:I:376:ARG:NH1	1:J:384:LEU:HD23	2.29	0.47
1:D:509:ASP:OD1	1:D:511:ARG:N	2.41	0.47
2:Y:94:ASP:OD2	4:r:66:PRO:HB3	2.14	0.47
3:b:430:GLU:HB3	3:b:433:VAL:HB	1.97	0.47
3:f:29:MET:HE2	3:f:29:MET:HB3	1.83	0.47
4:i:8:ASP:OD1	4:i:11:ARG:NH1	2.47	0.47
4:j:76:ARG:HH11	4:j:78:SER:HG	1.63	0.47
1:A:274:ARG:HB2	1:A:296:GLU:HG2	1.96	0.47
2:Q:101:ASP:OD1	2:Q:102:TYR:N	2.47	0.47
2:T:55:ASP:OD1	2:T:56:GLY:N	2.48	0.47
2:V:33:ILE:HG23	2:V:88:HIS:HB2	1.97	0.47
3:b:390:ARG:HD3	4:j:97:LEU:HD21	1.96	0.47
3:c:339:ARG:HD3	3:c:371:TYR:HE2	1.79	0.47
3:d:437:ARG:HD2	4:m:26:THR:HG22	1.95	0.47
4:j:134:THR:OG1	4:j:147:HIS:O	2.26	0.47
4:j:141:ALA:HB1	4:j:146:TRP:HE3	1.80	0.47
4:k:28:VAL:HG11	4:k:33:MET:HE2	1.97	0.47
1:C:310:VAL:HG13	1:C:311:GLU:H	1.79	0.47
1:D:310:VAL:HG13	1:D:311:GLU:N	2.29	0.47
1:F:61:ARG:NH2	1:G:317:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:ALA:O	1:F:123:VAL:N	2.47	0.47
1:G:557:PHE:HE2	1:H:548:GLU:HG2	1.78	0.47
1:J:282:THR:O	1:J:282:THR:HG22	2.14	0.47
1:J:310:VAL:HG13	1:J:311:GLU:N	2.29	0.47
1:J:339:ASP:OD2	4:j:131:ARG:NH2	2.30	0.47
1:J:557:PHE:HE2	1:K:548:GLU:HG2	1.79	0.47
2:O:14:ARG:NH1	2:T:101:ASP:OD2	2.48	0.47
2:U:51:ILE:HD12	2:U:61:ILE:HG21	1.97	0.47
3:a:141:VAL:HG13	3:a:153:TRP:HB2	1.96	0.47
3:a:206:ILE:HB	3:a:230:VAL:HB	1.95	0.47
3:b:283:TYR:OH	3:b:311:HIS:ND1	2.32	0.47
3:c:13:GLY:HA3	3:c:24:TYR:CE2	2.50	0.47
3:c:312:VAL:HG21	3:c:338:TYR:H	1.80	0.47
4:k:49:GLN:HE21	4:l:113:LEU:HD23	1.78	0.47
1:B:11:ILE:HG21	1:B:281:ILE:HG21	1.97	0.47
1:B:376:ARG:NH1	1:C:384:LEU:HD23	2.30	0.47
1:H:376:ARG:NH1	1:I:384:LEU:HD23	2.30	0.47
1:I:626:GLN:O	1:I:629:THR:OG1	2.25	0.47
1:K:509:ASP:OD1	1:K:511:ARG:N	2.43	0.47
2:W:78:GLN:NE2	4:n:26:THR:HA	2.30	0.47
3:d:409:LEU:N	3:d:426:ILE:O	2.38	0.47
3:f:13:GLY:HA3	3:f:24:TYR:CE2	2.49	0.47
4:l:49:GLN:O	4:l:50:ASP:HB2	2.14	0.47
4:n:49:GLN:O	4:n:50:ASP:HB2	2.14	0.47
1:B:567:MET:HE1	1:C:576:LEU:HD13	1.97	0.47
1:D:282:THR:HG22	1:D:282:THR:O	2.14	0.47
2:X:51:ILE:HD12	2:X:61:ILE:HG21	1.97	0.47
3:a:378:LEU:HD22	3:a:453:LYS:HE2	1.97	0.47
3:b:441:LYS:HE2	4:i:19:VAL:HG13	1.97	0.47
3:e:262:ILE:HD12	3:e:271:ILE:HG21	1.97	0.47
4:o:34:GLN:NE2	4:o:38:ASP:OD2	2.46	0.47
1:A:32:ASP:OD2	1:A:321:ARG:HG2	2.14	0.47
1:A:567:MET:HG3	1:B:581:VAL:HG12	1.96	0.47
1:B:480:ILE:HB	1:B:488:LYS:HD2	1.96	0.47
1:D:150:HIS:HE1	1:E:307:TRP:NE1	2.09	0.47
1:F:282:THR:O	1:F:282:THR:HG22	2.15	0.47
1:H:310:VAL:HG13	1:H:311:GLU:N	2.30	0.47
1:I:293:ILE:HG22	1:I:295:GLY:H	1.80	0.47
1:K:89:ASP:CG	1:K:89:ASP:O	2.58	0.47
2:O:68:ASN:HB3	2:O:74:VAL:HB	1.96	0.47
2:U:31:ILE:HD11	2:U:67:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:128:LEU:HD12	2:X:147:ILE:HA	1.97	0.47
2:Z:28:ASN:ND2	4:i:66:PRO:HG2	2.30	0.47
3:a:36:ILE:HD11	3:a:42:TYR:HD1	1.79	0.47
3:a:241:THR:O	3:a:242:PRO:C	2.56	0.47
3:d:13:GLY:HA3	3:d:24:TYR:CE2	2.51	0.47
4:i:90:ARG:O	4:i:93:PRO:HD2	2.15	0.47
4:o:3:ILE:HG22	4:o:9:LEU:HD12	1.97	0.47
1:A:131:ASP:OD1	1:A:132:TYR:N	2.46	0.46
1:K:47:GLN:HG2	1:K:48:TYR:H	1.80	0.46
2:P:61:ILE:HG22	2:P:62:THR:O	2.15	0.46
3:e:409:LEU:N	3:e:426:ILE:O	2.33	0.46
4:h:79:ALA:O	4:h:83:VAL:HG23	2.15	0.46
4:q:49:GLN:HE21	4:r:113:LEU:HD23	1.79	0.46
1:A:61:ARG:NH2	1:B:317:GLU:OE2	2.47	0.46
1:A:557:PHE:HE2	1:B:548:GLU:HG2	1.79	0.46
1:B:282:THR:HG22	1:B:282:THR:O	2.15	0.46
1:E:150:HIS:CD2	1:F:163:LYS:HG3	2.50	0.46
1:E:519:ASP:OD1	1:E:520:VAL:N	2.43	0.46
1:G:509:ASP:OD1	1:G:511:ARG:N	2.43	0.46
1:I:339:ASP:OD2	4:i:131:ARG:NH2	2.29	0.46
1:I:376:ARG:HH11	1:J:384:LEU:HD23	1.80	0.46
1:J:329:LEU:O	1:J:333:ILE:HG12	2.15	0.46
2:T:101:ASP:OD1	2:T:102:TYR:N	2.48	0.46
3:a:179:TYR:OH	3:a:221:LEU:HB2	2.15	0.46
3:f:95:VAL:HG11	3:f:108:VAL:HG12	1.98	0.46
1:C:557:PHE:HE2	1:D:548:GLU:HG2	1.80	0.46
1:D:178:SER:OG	1:D:215:ASP:OD2	2.27	0.46
1:H:7:ARG:NH2	1:H:224:GLU:OE2	2.36	0.46
1:I:519:ASP:OD1	1:I:520:VAL:N	2.44	0.46
1:K:84:ASP:OD1	1:K:85:GLY:N	2.48	0.46
1:K:228:LYS:HE2	1:K:228:LYS:HB2	1.80	0.46
2:Q:51:ILE:HD12	2:Q:80:VAL:HB	1.96	0.46
2:Z:21:ARG:HG3	2:Z:21:ARG:HH11	1.80	0.46
3:c:369:SER:HB3	3:c:459:LYS:HB2	1.96	0.46
3:e:12:MET:HE1	3:f:35:GLU:O	2.15	0.46
3:e:32:THR:HG22	3:e:301:HIS:NE2	2.31	0.46
3:e:165:ASP:OD1	3:e:166:LEU:N	2.46	0.46
4:h:26:THR:HA	2:w:78:GLN:NE2	2.30	0.46
1:A:310:VAL:HG13	1:A:311:GLU:H	1.79	0.46
1:C:254:VAL:HG21	1:C:505:GLN:HG2	1.97	0.46
1:G:310:VAL:HG13	1:G:311:GLU:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:ARG:HH21	1:H:524:PHE:HB2	1.80	0.46
1:J:93:VAL:HG21	1:J:475:PRO:HD2	1.97	0.46
3:b:312:VAL:HG21	3:b:338:TYR:H	1.79	0.46
4:g:43:MET:HE3	4:g:44:MET:HE3	1.97	0.46
4:g:141:ALA:HB1	4:g:146:TRP:HE3	1.81	0.46
4:n:79:ALA:O	4:n:83:VAL:HG23	2.15	0.46
1:B:363:TYR:OH	1:B:373:LEU:O	2.30	0.46
1:E:131:ASP:OD1	1:E:132:TYR:N	2.47	0.46
1:H:11:ILE:HG21	1:H:281:ILE:HG21	1.96	0.46
1:J:541:LYS:HE3	1:J:541:LYS:HB2	1.68	0.46
3:c:37:LEU:HD12	3:c:397:GLU:OE2	2.15	0.46
2:s:35:GLN:O	2:s:89:SER:OG	2.28	0.46
1:A:565:VAL:HG13	1:A:565:VAL:O	2.16	0.46
1:B:131:ASP:OD1	1:B:132:TYR:N	2.47	0.46
1:B:339:ASP:OD2	4:n:131:ARG:NH2	2.30	0.46
1:D:575:GLN:O	1:D:579:MET:HG3	2.16	0.46
1:E:47:GLN:HG2	1:E:48:TYR:H	1.80	0.46
1:H:363:TYR:OH	1:H:373:LEU:O	2.29	0.46
2:M:127:LYS:HA	2:M:146:LEU:HB3	1.97	0.46
2:Y:51:ILE:HD11	2:Y:61:ILE:HD13	1.96	0.46
3:b:28:ASN:HA	3:b:329:LEU:HD23	1.96	0.46
3:c:192:GLY:O	3:c:199:VAL:N	2.49	0.46
3:d:430:GLU:HG2	3:d:431:PRO:HD2	1.96	0.46
3:e:369:SER:HB3	3:e:459:LYS:HB2	1.96	0.46
1:B:310:VAL:HG13	1:B:311:GLU:N	2.29	0.46
1:C:99:ARG:NH1	1:C:524:PHE:HB2	2.30	0.46
1:H:282:THR:O	1:H:282:THR:HG22	2.15	0.46
1:J:509:ASP:OD1	1:J:510:ILE:N	2.49	0.46
1:L:121:ALA:O	1:L:123:VAL:N	2.47	0.46
1:L:519:ASP:OD1	1:L:520:VAL:N	2.42	0.46
3:b:283:TYR:HE2	3:b:308:LEU:HD13	1.81	0.46
4:g:29:GLU:OE1	4:g:31:GLN:N	2.49	0.46
4:o:90:ARG:O	4:o:93:PRO:HD2	2.15	0.46
1:C:293:ILE:HG22	1:C:295:GLY:H	1.81	0.46
1:H:339:ASP:OD2	4:h:131:ARG:NH2	2.30	0.46
1:J:206:ASP:HB3	1:J:208:VAL:HG13	1.98	0.46
1:K:274:ARG:HB2	1:K:296:GLU:HG2	1.97	0.46
3:b:98:ALA:HB3	3:b:144:ILE:HG22	1.97	0.46
3:c:36:ILE:HG22	3:c:37:LEU:N	2.31	0.46
3:e:441:LYS:HE2	4:o:19:VAL:HG13	1.98	0.46
3:f:206:ILE:HB	3:f:230:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:49:GLN:O	4:g:50:ASP:HB2	2.15	0.46
1:A:339:ASP:OD1	4:n:128:TYR:OH	2.27	0.46
1:D:509:ASP:OD1	1:D:510:ILE:N	2.49	0.46
1:D:565:VAL:O	1:D:565:VAL:HG13	2.16	0.46
1:F:7:ARG:NH2	1:F:224:GLU:OE2	2.35	0.46
1:F:376:ARG:NH1	1:G:384:LEU:HD23	2.31	0.46
1:J:565:VAL:O	1:J:565:VAL:HG13	2.16	0.46
1:K:363:TYR:OH	1:K:373:LEU:O	2.29	0.46
1:L:194:ASP:OD1	1:L:194:ASP:N	2.49	0.46
1:L:565:VAL:O	1:L:565:VAL:HG13	2.16	0.46
3:d:11:GLY:O	3:d:24:TYR:N	2.42	0.46
3:d:470:ARG:NH1	4:m:96:ALA:HB3	2.31	0.46
3:f:147:LEU:HD11	3:f:196:ASP:HA	1.97	0.46
2:w:14:ARG:NH1	2:x:101:ASP:OD2	2.49	0.46
1:A:11:ILE:HG21	1:A:281:ILE:HG21	1.97	0.46
1:B:76:ILE:HG23	1:B:520:VAL:HG13	1.97	0.46
1:D:121:ALA:O	1:D:123:VAL:N	2.48	0.46
1:G:587:PRO:HA	1:G:590:GLN:NE2	2.31	0.46
1:H:627:ASN:HB3	1:I:632:LEU:HD11	1.97	0.46
1:J:150:HIS:CD2	1:K:163:LYS:HG3	2.51	0.46
1:K:376:ARG:NH1	1:L:384:LEU:HD23	2.31	0.46
2:Q:128:LEU:HD22	2:Q:147:ILE:HD13	1.98	0.46
3:a:414:THR:HG23	3:a:420:TYR:CD2	2.51	0.46
3:e:28:ASN:HA	3:e:329:LEU:HD23	1.97	0.46
3:e:383:LEU:HD13	3:e:449:LEU:HD13	1.98	0.46
4:r:87:LEU:O	4:r:91:ILE:HG13	2.16	0.46
1:A:310:VAL:HG13	1:A:311:GLU:N	2.31	0.45
1:A:384:LEU:HD23	1:L:376:ARG:NH1	2.31	0.45
1:A:622:LEU:HD11	1:L:616:LEU:HB3	1.98	0.45
1:B:274:ARG:HB2	1:B:296:GLU:HG2	1.98	0.45
1:G:310:VAL:HG13	1:G:311:GLU:N	2.31	0.45
2:Y:24:LYS:HB2	2:Y:24:LYS:HE3	1.72	0.45
3:b:262:ILE:HD12	3:b:271:ILE:HG21	1.96	0.45
3:f:409:LEU:N	3:f:426:ILE:O	2.41	0.45
4:k:90:ARG:O	4:k:93:PRO:HD2	2.16	0.45
1:D:329:LEU:O	1:D:333:ILE:HG12	2.16	0.45
1:E:339:ASP:OD1	4:r:128:TYR:OH	2.27	0.45
1:E:376:ARG:HH11	1:F:384:LEU:HD23	1.80	0.45
3:e:98:ALA:HB3	3:e:144:ILE:HG22	1.97	0.45
3:f:312:VAL:HG21	3:f:338:TYR:H	1.80	0.45
1:B:239:VAL:HG12	1:B:240:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLN:HG2	1:C:48:TYR:H	1.82	0.45
1:C:376:ARG:HH11	1:D:384:LEU:HD23	1.80	0.45
1:E:586:THR:OG1	1:E:589:GLU:HG3	2.16	0.45
1:F:340:ILE:O	1:F:344:THR:OG1	2.28	0.45
1:J:627:ASN:HB3	1:K:632:LEU:HD11	1.98	0.45
1:K:519:ASP:OD1	1:K:520:VAL:N	2.44	0.45
1:L:7:ARG:NH2	1:L:224:GLU:OE2	2.36	0.45
2:M:14:ARG:NH1	2:R:101:ASP:OD2	2.49	0.45
2:T:49:VAL:HG23	2:T:61:ILE:HB	1.99	0.45
2:V:31:ILE:HD11	2:V:67:ILE:HD11	1.98	0.45
3:a:37:LEU:HD23	3:f:385:LYS:HB2	1.98	0.45
3:b:206:ILE:HB	3:b:230:VAL:HB	1.97	0.45
4:o:51:GLY:C	4:o:53:GLY:N	2.73	0.45
1:A:237:ASP:OD2	1:A:476:ARG:NH1	2.48	0.45
1:G:519:ASP:OD1	1:G:520:VAL:N	2.47	0.45
1:H:142:GLN:HG2	1:H:471:ILE:CD1	2.47	0.45
2:R:55:ASP:OD1	2:R:56:GLY:N	2.50	0.45
2:R:68:ASN:HD21	2:W:21:ARG:HH21	1.63	0.45
3:d:206:ILE:HB	3:d:230:VAL:HB	1.97	0.45
3:d:414:THR:HG23	3:d:420:TYR:CD2	2.51	0.45
1:C:215:ASP:OD1	1:C:215:ASP:N	2.45	0.45
1:C:310:VAL:HG13	1:C:311:GLU:N	2.31	0.45
1:E:376:ARG:NH1	1:F:384:LEU:HD23	2.31	0.45
1:F:565:VAL:HG13	1:F:565:VAL:O	2.16	0.45
1:G:234:ILE:HD11	1:G:269:ARG:HG3	1.98	0.45
1:I:310:VAL:HG13	1:I:311:GLU:N	2.31	0.45
1:K:310:VAL:HG13	1:K:311:GLU:N	2.31	0.45
1:K:376:ARG:HH11	1:L:384:LEU:HD23	1.80	0.45
3:c:111:GLN:HG3	3:c:113:VAL:HG23	1.98	0.45
3:e:430:GLU:HB3	3:e:433:VAL:HB	1.97	0.45
4:q:8:ASP:OD1	4:q:11:ARG:NH1	2.50	0.45
1:B:627:ASN:HB3	1:C:632:LEU:HD11	1.99	0.45
1:E:310:VAL:HG13	1:E:311:GLU:N	2.32	0.45
1:F:616:LEU:HB3	1:G:622:LEU:HD11	1.98	0.45
1:H:121:ALA:O	1:H:123:VAL:N	2.47	0.45
1:L:11:ILE:HG21	1:L:281:ILE:HG21	1.99	0.45
1:L:97:MET:HE2	1:L:139:SER:HB3	1.99	0.45
2:O:133:THR:OG1	2:O:136:ASP:OD2	2.30	0.45
2:S:61:ILE:HG22	2:S:62:THR:O	2.16	0.45
3:a:182:GLU:O	3:b:148:ARG:HA	2.17	0.45
3:b:147:LEU:HD12	3:b:147:LEU:HA	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:430:GLU:HG2	3:b:431:PRO:HD2	1.99	0.45
4:i:3:ILE:HG22	4:i:9:LEU:HD12	1.97	0.45
1:A:615:LEU:CD1	1:L:609:VAL:HG13	2.47	0.45
1:H:76:ILE:HG23	1:H:520:VAL:HG13	1.99	0.45
1:J:237:ASP:HA	1:J:263:PHE:HE1	1.81	0.45
1:J:376:ARG:NH1	1:K:384:LEU:HD23	2.32	0.45
2:U:119:ASP:OD1	2:Z:114:TYR:OH	2.32	0.45
3:a:35:GLU:O	3:a:35:GLU:HG3	2.16	0.45
3:b:383:LEU:HD13	3:b:449:LEU:HD13	1.97	0.45
3:d:36:ILE:HD11	3:d:42:TYR:CD1	2.52	0.45
3:e:12:MET:HE2	3:f:34:LYS:HZ3	1.81	0.45
3:e:59:SER:C	3:e:60:ARG:HG3	2.41	0.45
3:e:103:SER:HG	3:e:151:TYR:HH	1.56	0.45
4:i:49:GLN:HE21	4:j:113:LEU:HD23	1.80	0.45
2:v:55:ASP:OD1	2:v:56:GLY:N	2.50	0.45
1:E:509:ASP:OD1	1:E:511:ARG:N	2.44	0.45
1:H:95:MET:HE3	1:H:95:MET:HA	1.99	0.45
1:H:274:ARG:HB2	1:H:296:GLU:HG2	1.98	0.45
1:I:58:ASP:OD2	1:I:61:ARG:HB2	2.16	0.45
1:J:76:ILE:HG22	1:J:457:MET:HG3	1.98	0.45
2:M:39:ASP:OD1	3:d:425:MET:HE1	2.17	0.45
3:b:32:THR:HG22	3:b:301:HIS:NE2	2.32	0.45
4:g:43:MET:HE2	4:g:43:MET:HB3	1.90	0.45
1:B:150:HIS:CD2	1:C:163:LYS:HG3	2.52	0.45
1:B:387:GLN:HB2	1:B:388:PRO:HD3	1.99	0.45
1:C:178:SER:OG	1:C:215:ASP:OD2	2.22	0.45
1:D:206:ASP:HB3	1:D:208:VAL:HG13	1.98	0.45
1:D:339:ASP:OD2	4:p:131:ARG:NH2	2.30	0.45
1:E:493:MET:HE3	1:E:493:MET:HB2	1.85	0.45
1:F:252:LYS:HG3	1:F:253:ASP:OD1	2.17	0.45
1:F:609:VAL:HG13	1:G:615:LEU:CD1	2.46	0.45
1:G:11:ILE:HG21	1:G:281:ILE:HG21	1.99	0.45
1:L:310:VAL:HG13	1:L:311:GLU:N	2.31	0.45
3:c:105:ALA:HA	3:c:114:GLU:HA	1.98	0.45
3:c:206:ILE:HB	3:c:230:VAL:HB	1.99	0.45
3:f:111:GLN:HG3	3:f:113:VAL:HG23	1.99	0.45
3:f:390:ARG:HD3	4:r:97:LEU:HD21	1.99	0.45
4:r:49:GLN:O	4:r:50:ASP:HB2	2.16	0.45
1:B:91:ALA:O	1:B:95:MET:HB2	2.17	0.45
1:E:293:ILE:HG22	1:E:295:GLY:H	1.81	0.45
1:G:256:ASP:OD1	1:G:257:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:101:ASP:OD1	2:O:102:TYR:N	2.50	0.45
2:T:128:LEU:HD22	2:T:147:ILE:HD13	1.98	0.45
3:d:33:PRO:HA	3:d:41:GLY:HA2	1.99	0.45
1:A:47:GLN:HG2	1:A:48:TYR:H	1.83	0.44
1:D:376:ARG:NH1	1:E:384:LEU:HD23	2.30	0.44
1:L:281:ILE:HG22	1:L:286:VAL:HG12	1.99	0.44
2:Z:126:VAL:HB	2:Z:131:TYR:HE2	1.82	0.44
3:a:430:GLU:HB3	3:a:433:VAL:HB	1.99	0.44
3:b:388:ASN:OD1	3:b:445:ARG:NH1	2.50	0.44
3:d:283:TYR:OH	3:d:311:HIS:ND1	2.38	0.44
4:l:87:LEU:O	4:l:91:ILE:HG13	2.17	0.44
1:C:93:VAL:HG22	1:C:97:MET:HE3	1.99	0.44
1:D:627:ASN:HB3	1:E:632:LEU:HD11	1.99	0.44
1:E:177:HIS:NE2	1:E:221:GLU:OE1	2.37	0.44
1:E:273:ARG:NH2	1:E:470:ASP:OD2	2.50	0.44
1:F:76:ILE:HG22	1:F:457:MET:HG3	1.99	0.44
1:G:79:LEU:N	1:G:519:ASP:O	2.41	0.44
1:G:376:ARG:NH2	1:H:354:GLU:OE2	2.44	0.44
1:H:150:HIS:CD2	1:I:163:LYS:HG3	2.52	0.44
1:I:234:ILE:HD11	1:I:269:ARG:HD3	2.00	0.44
1:J:509:ASP:O	1:J:513:ARG:HG3	2.17	0.44
2:Z:51:ILE:O	2:Z:58:HIS:HA	2.17	0.44
3:c:229:MET:O	3:d:195:ARG:NH1	2.46	0.44
3:d:409:LEU:HB2	3:d:428:GLN:HG2	1.99	0.44
3:e:179:TYR:OH	3:e:221:LEU:HB2	2.18	0.44
4:q:90:ARG:O	4:q:93:PRO:HD2	2.17	0.44
1:A:58:ASP:OD2	1:A:61:ARG:HB2	2.17	0.44
1:A:339:ASP:OD2	4:m:131:ARG:NH2	2.31	0.44
1:C:577:ILE:HD13	1:C:589:GLU:HB3	1.98	0.44
1:D:293:ILE:HG22	1:D:295:GLY:H	1.81	0.44
1:E:274:ARG:HB2	1:E:296:GLU:HG2	1.98	0.44
1:E:609:VAL:HB	1:F:611:ALA:HB1	1.99	0.44
1:F:99:ARG:HA	1:F:99:ARG:HD3	1.80	0.44
1:H:387:GLN:HB2	1:H:388:PRO:HD3	2.00	0.44
1:H:626:GLN:O	1:H:629:THR:OG1	2.27	0.44
1:I:47:GLN:HG2	1:I:48:TYR:H	1.82	0.44
1:I:80:TYR:OH	1:I:461:GLY:O	2.35	0.44
1:I:121:ALA:O	1:I:123:VAL:N	2.48	0.44
1:I:376:ARG:NH2	1:J:354:GLU:OE2	2.41	0.44
1:L:179:MET:HE2	1:L:184:TRP:HA	1.99	0.44
2:N:68:ASN:HB3	2:N:74:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:441:LYS:HE2	4:g:19:VAL:HG13	1.99	0.44
3:f:112:LEU:HD23	3:f:124:VAL:HG21	1.98	0.44
4:k:29:GLU:OE1	4:k:31:GLN:N	2.51	0.44
1:B:95:MET:HA	1:B:95:MET:HE3	1.99	0.44
1:B:99:ARG:HH21	1:B:524:PHE:HB2	1.83	0.44
1:B:121:ALA:O	1:B:123:VAL:N	2.47	0.44
1:C:58:ASP:OD2	1:C:61:ARG:HB2	2.17	0.44
1:F:474:VAL:HA	1:F:475:PRO:HD3	1.81	0.44
1:G:121:ALA:O	1:G:123:VAL:N	2.50	0.44
1:J:293:ILE:HG22	1:J:295:GLY:H	1.83	0.44
2:O:49:VAL:HG13	2:O:84:THR:HG22	2.00	0.44
2:O:126:VAL:HB	2:O:131:TYR:HE2	1.83	0.44
2:O:127:LYS:HA	2:O:146:LEU:HB3	1.99	0.44
2:P:73:ILE:HG21	2:P:82:ILE:HD12	1.99	0.44
2:Y:31:ILE:HD11	2:Y:67:ILE:HD11	1.98	0.44
3:f:36:ILE:HD11	3:f:42:TYR:HD1	1.83	0.44
4:h:3:ILE:HG22	4:h:9:LEU:HD12	1.99	0.44
4:r:90:ARG:O	4:r:93:PRO:HD2	2.18	0.44
1:B:101:ASP:OD2	1:B:464:TYR:OH	2.24	0.44
1:C:121:ALA:O	1:C:123:VAL:N	2.49	0.44
1:E:509:ASP:O	1:E:513:ARG:HG3	2.18	0.44
1:G:509:ASP:O	1:G:513:ARG:HG3	2.17	0.44
1:H:319:VAL:HG22	1:H:418:LEU:HD11	2.00	0.44
1:I:254:VAL:HG12	1:I:254:VAL:O	2.18	0.44
1:K:307:TRP:CG	1:K:308:GLY:N	2.86	0.44
1:K:609:VAL:HB	1:L:611:ALA:HB1	1.99	0.44
1:L:53:TYR:O	4:l:131:ARG:NH1	2.50	0.44
2:Z:79:LEU:HD12	2:Z:79:LEU:HA	1.57	0.44
3:a:36:ILE:HD11	3:a:42:TYR:CD1	2.52	0.44
3:c:62:VAL:HG11	3:c:342:ASP:HB3	1.99	0.44
4:h:49:GLN:O	4:h:50:ASP:HB2	2.17	0.44
4:i:51:GLY:C	4:i:53:GLY:N	2.74	0.44
4:q:134:THR:OG1	4:q:147:HIS:O	2.26	0.44
1:B:98:TYR:HD1	1:B:464:TYR:CD2	2.36	0.44
1:G:282:THR:HG22	1:G:282:THR:O	2.17	0.44
1:G:363:TYR:OH	1:G:373:LEU:O	2.26	0.44
1:H:10:SER:O	1:H:14:ARG:HG3	2.17	0.44
1:I:254:VAL:HG21	1:I:505:GLN:HG2	1.98	0.44
1:I:509:ASP:OD1	1:I:510:ILE:N	2.50	0.44
1:L:626:GLN:O	1:L:629:THR:OG1	2.27	0.44
2:T:51:ILE:O	2:T:58:HIS:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:75:TYR:O	2:X:76:ASN:HB2	2.17	0.44
3:c:390:ARG:HD3	4:l:97:LEU:HD21	1.99	0.44
3:f:378:LEU:HD22	3:f:453:LYS:HE2	1.99	0.44
4:p:134:THR:OG1	4:p:147:HIS:O	2.27	0.44
1:A:282:THR:O	1:A:282:THR:HG22	2.16	0.44
1:B:319:VAL:HG22	1:B:418:LEU:HD11	1.99	0.44
1:C:509:ASP:OD1	1:C:510:ILE:N	2.50	0.44
1:E:84:ASP:OD1	1:E:85:GLY:N	2.51	0.44
1:F:339:ASP:OD2	4:r:131:ARG:NH2	2.29	0.44
1:H:293:ILE:HG22	1:H:295:GLY:H	1.82	0.44
1:J:81:ARG:NH1	1:J:519:ASP:OD2	2.50	0.44
1:J:177:HIS:NE2	1:J:221:GLU:OE1	2.43	0.44
1:J:191:TYR:HB2	1:J:193:LEU:HD13	2.00	0.44
2:P:49:VAL:HG23	2:P:61:ILE:HB	2.00	0.44
2:S:73:ILE:HG21	2:S:82:ILE:HD12	1.99	0.44
3:f:436:LYS:HB2	3:f:436:LYS:HE3	1.65	0.44
2:x:85:VAL:O	2:x:86:GLN:HG2	2.18	0.44
2:x:127:LYS:HA	2:x:146:LEU:HB3	1.99	0.44
1:B:293:ILE:HG22	1:B:295:GLY:H	1.82	0.44
1:C:61:ARG:NH2	1:D:317:GLU:OE1	2.51	0.44
1:G:47:GLN:HG2	1:G:48:TYR:H	1.83	0.44
1:I:307:TRP:CG	1:I:308:GLY:N	2.86	0.44
1:K:625:ALA:O	1:K:629:THR:HG23	2.18	0.44
2:W:49:VAL:HA	2:W:84:THR:HG22	2.00	0.44
3:e:430:GLU:HG2	3:e:431:PRO:HD2	1.99	0.44
4:j:76:ARG:NH1	4:j:78:SER:OG	2.49	0.44
2:w:49:VAL:HA	2:w:84:THR:HG22	2.00	0.44
1:A:509:ASP:O	1:A:513:ARG:HG3	2.18	0.44
1:B:509:ASP:O	1:B:513:ARG:HG3	2.18	0.44
1:C:127:ARG:HG3	1:C:147:GLU:HB2	1.98	0.44
1:F:310:VAL:HG13	1:F:311:GLU:N	2.31	0.44
1:F:509:ASP:O	1:F:513:ARG:HG3	2.18	0.44
1:G:150:HIS:HE1	1:H:307:TRP:NE1	2.08	0.44
1:I:127:ARG:HG3	1:I:147:GLU:HB2	1.98	0.44
1:L:254:VAL:HG21	1:L:505:GLN:HG2	1.99	0.44
2:Y:78:GLN:NE2	4:r:26:THR:HA	2.33	0.44
3:a:105:ALA:HB1	3:a:112:LEU:HD11	1.99	0.44
3:c:117:TYR:O	3:c:118:ASP:C	2.61	0.44
3:c:147:LEU:HD11	3:c:196:ASP:HA	2.00	0.44
3:d:182:GLU:O	3:e:148:ARG:HA	2.18	0.44
2:w:14:ARG:NH2	2:x:103:ILE:HG12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:TYR:OH	1:A:373:LEU:O	2.27	0.43
1:C:71:MET:HE3	1:C:119:ILE:HD11	1.99	0.43
1:C:234:ILE:HD11	1:C:269:ARG:HD3	1.99	0.43
1:D:509:ASP:O	1:D:513:ARG:HG3	2.18	0.43
1:E:625:ALA:O	1:E:629:THR:HG23	2.18	0.43
1:F:254:VAL:HG21	1:F:505:GLN:HG2	1.99	0.43
1:G:346:LYS:HA	1:G:346:LYS:HD3	1.86	0.43
1:I:89:ASP:O	1:I:89:ASP:CG	2.61	0.43
1:L:99:ARG:HD3	1:L:99:ARG:HA	1.80	0.43
2:Y:24:LYS:HZ1	4:r:65:ASN:HB3	1.82	0.43
3:a:178:GLN:HE21	3:a:178:GLN:HB2	1.63	0.43
3:c:112:LEU:HD23	3:c:124:VAL:HG21	1.98	0.43
3:d:36:ILE:HG13	3:d:42:TYR:HB3	2.00	0.43
4:k:72:ASP:OD1	4:k:73:HIS:N	2.51	0.43
1:A:376:ARG:NH2	1:B:354:GLU:OE2	2.44	0.43
1:F:179:MET:HE2	1:F:184:TRP:HA	2.00	0.43
1:F:585:GLU:N	1:F:589:GLU:OE1	2.34	0.43
1:H:40:GLN:HG3	1:H:56:GLN:NE2	2.33	0.43
1:K:234:ILE:HD11	1:K:269:ARG:HD3	2.00	0.43
1:K:273:ARG:NH2	1:K:470:ASP:OD2	2.51	0.43
1:L:76:ILE:HG22	1:L:457:MET:HG3	1.99	0.43
3:a:430:GLU:HG2	3:a:431:PRO:HD2	1.99	0.43
3:e:194:TRP:HB2	3:e:247:TYR:HE2	1.83	0.43
1:B:251:ILE:O	1:B:255:ILE:HG13	2.19	0.43
1:B:339:ASP:OD1	4:o:128:TYR:OH	2.25	0.43
1:H:509:ASP:O	1:H:513:ARG:HG3	2.18	0.43
1:K:586:THR:OG1	1:K:589:GLU:HG3	2.17	0.43
1:L:509:ASP:O	1:L:513:ARG:HG3	2.18	0.43
2:V:78:GLN:NE2	4:l:26:THR:HA	2.33	0.43
2:W:105:ASN:HB3	2:W:108:LYS:HG2	1.99	0.43
3:a:470:ARG:NH1	4:g:96:ALA:HB3	2.30	0.43
3:c:95:VAL:HG11	3:c:108:VAL:HG12	2.00	0.43
3:f:12:MET:HA	3:f:23:ASP:HA	2.00	0.43
4:h:146:TRP:HZ2	4:h:150:PRO:HD3	1.82	0.43
4:q:29:GLU:OE1	4:q:31:GLN:N	2.50	0.43
1:E:121:ALA:O	1:E:123:VAL:N	2.49	0.43
1:E:307:TRP:CG	1:E:308:GLY:N	2.85	0.43
1:J:121:ALA:O	1:J:123:VAL:N	2.48	0.43
1:K:585:GLU:N	1:K:589:GLU:OE1	2.40	0.43
3:a:36:ILE:HG13	3:a:42:TYR:HB3	2.00	0.43
3:d:12:MET:H	3:d:382:PRO:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:l:90:ARG:O	4:l:93:PRO:HD2	2.18	0.43
4:n:3:ILE:HG22	4:n:9:LEU:HD12	1.99	0.43
2:s:133:THR:OG1	2:s:136:ASP:OD2	2.31	0.43
2:s:136:ASP:OD1	2:s:137:ALA:N	2.51	0.43
1:A:10:SER:O	1:A:14:ARG:HG3	2.18	0.43
1:B:307:TRP:CG	1:B:308:GLY:N	2.87	0.43
1:D:191:TYR:HB2	1:D:193:LEU:HD13	2.01	0.43
1:D:329:LEU:HD23	1:D:329:LEU:HA	1.89	0.43
1:E:612:GLN:O	1:E:616:LEU:HG	2.19	0.43
1:G:536:LEU:HD23	1:G:536:LEU:HA	1.87	0.43
1:H:281:ILE:HG22	1:H:286:VAL:HG12	2.00	0.43
1:J:307:TRP:CG	1:J:308:GLY:N	2.87	0.43
1:L:252:LYS:HG3	1:L:253:ASP:OD1	2.17	0.43
2:O:51:ILE:HG23	2:O:79:LEU:HD11	1.99	0.43
2:Q:51:ILE:HG12	2:Q:61:ILE:HG13	2.00	0.43
3:a:33:PRO:HA	3:a:41:GLY:HA2	1.99	0.43
3:f:62:VAL:HG11	3:f:342:ASP:HB3	2.01	0.43
4:q:72:ASP:OD1	4:q:73:HIS:N	2.51	0.43
4:r:62:ASP:OD2	4:r:64:GLU:HB2	2.18	0.43
1:B:612:GLN:O	1:B:616:LEU:HG	2.19	0.43
1:C:32:ASP:OD2	1:C:321:ARG:HG2	2.18	0.43
1:C:82:PRO:HB3	1:C:90:ALA:HB3	2.01	0.43
1:E:82:PRO:HB3	1:E:90:ALA:HB3	2.01	0.43
1:G:279:SER:HB3	1:G:290:LYS:H	1.83	0.43
1:H:251:ILE:O	1:H:255:ILE:HG13	2.19	0.43
1:K:131:ASP:OD1	1:K:132:TYR:N	2.47	0.43
1:K:509:ASP:O	1:K:513:ARG:HG3	2.18	0.43
1:L:307:TRP:CG	1:L:308:GLY:N	2.87	0.43
3:f:28:ASN:HA	3:f:329:LEU:HD23	2.00	0.43
2:s:101:ASP:OD1	2:s:102:TYR:N	2.51	0.43
2:v:53:ASN:ND2	2:v:57:SER:OG	2.41	0.43
1:A:87:ARG:HB3	1:A:88:PRO:CD	2.49	0.43
1:C:565:VAL:O	1:C:565:VAL:HG13	2.19	0.43
1:I:32:ASP:OD2	1:I:321:ARG:HG2	2.19	0.43
1:I:227:GLU:OE2	1:I:274:ARG:NH1	2.51	0.43
2:Q:20:SER:HB2	2:s:78:GLN:NE2	2.34	0.43
2:R:47:ILE:HD11	2:R:88:HIS:HB3	2.01	0.43
1:A:625:ALA:O	1:A:629:THR:HG23	2.19	0.43
1:B:40:GLN:NE2	1:B:58:ASP:OD2	2.52	0.43
1:B:47:GLN:HG2	1:B:48:TYR:H	1.84	0.43
1:C:616:LEU:HB3	1:D:622:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:TRP:CG	1:D:308:GLY:N	2.86	0.43
1:E:53:TYR:O	4:q:131:ARG:NH1	2.52	0.43
1:F:567:MET:HE2	1:F:567:MET:HB3	1.87	0.43
1:H:40:GLN:NE2	1:H:58:ASP:OD2	2.52	0.43
1:K:58:ASP:OD2	1:K:61:ARG:HB2	2.19	0.43
1:K:339:ASP:OD2	4:k:131:ARG:NH2	2.31	0.43
3:b:194:TRP:HB2	3:b:247:TYR:HE2	1.84	0.43
3:c:378:LEU:HD22	3:c:453:LYS:HE2	2.00	0.43
3:f:37:LEU:HD12	3:f:397:GLU:OE1	2.18	0.43
4:p:49:GLN:O	4:p:50:ASP:HB2	2.18	0.43
4:q:24:THR:HG22	4:q:26:THR:HG23	2.00	0.43
1:F:97:MET:HE2	1:F:139:SER:HB3	2.00	0.43
1:F:627:ASN:HB3	1:G:632:LEU:HD11	2.01	0.43
1:G:58:ASP:OD2	1:G:61:ARG:HB2	2.18	0.43
1:H:307:TRP:CG	1:H:308:GLY:N	2.86	0.43
1:I:609:VAL:HB	1:J:611:ALA:HB1	1.99	0.43
1:K:612:GLN:O	1:K:616:LEU:HG	2.19	0.43
2:M:103:ILE:HG12	2:W:14:ARG:NH2	2.33	0.43
3:b:62:VAL:HG11	3:b:342:ASP:HB3	2.01	0.43
3:c:28:ASN:HA	3:c:329:LEU:HD23	2.00	0.43
3:c:150:ARG:HD2	3:c:163:ILE:HD11	2.01	0.43
1:A:632:LEU:HD11	1:L:627:ASN:HB3	2.00	0.43
1:C:307:TRP:CG	1:C:308:GLY:N	2.86	0.43
1:C:339:ASP:OD2	4:o:131:ARG:NH2	2.29	0.43
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.87	0.43
1:L:82:PRO:HB3	1:L:90:ALA:HB3	2.00	0.43
3:a:409:LEU:HB2	3:a:428:GLN:HG2	2.00	0.43
3:c:194:TRP:HB2	3:c:247:TYR:HE1	1.84	0.43
3:d:150:ARG:HG2	3:d:164:THR:O	2.19	0.43
2:s:51:ILE:O	2:s:58:HIS:HA	2.19	0.43
1:C:609:VAL:HB	1:D:611:ALA:HB1	1.99	0.42
1:F:82:PRO:HB3	1:F:90:ALA:HB3	2.01	0.42
1:G:307:TRP:CG	1:G:308:GLY:N	2.87	0.42
1:I:340:ILE:O	1:I:344:THR:OG1	2.29	0.42
2:N:51:ILE:O	2:N:58:HIS:HA	2.18	0.42
3:d:36:ILE:HG22	3:d:37:LEU:N	2.34	0.42
3:f:36:ILE:HG22	3:f:37:LEU:N	2.33	0.42
4:l:76:ARG:NH1	4:l:78:SER:OG	2.51	0.42
1:A:307:TRP:CG	1:A:308:GLY:N	2.87	0.42
1:C:363:TYR:HE2	1:D:350:PHE:HE1	1.67	0.42
1:D:273:ARG:NH2	1:D:470:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ASP:OD2	1:E:61:ARG:HB2	2.19	0.42
1:E:536:LEU:HD23	1:E:536:LEU:HA	1.88	0.42
1:G:329:LEU:HD23	1:G:329:LEU:HA	1.92	0.42
1:G:625:ALA:O	1:G:629:THR:HG23	2.19	0.42
1:I:565:VAL:HG13	1:I:565:VAL:O	2.19	0.42
3:a:257:ALA:HB3	3:b:297:ARG:HH11	1.84	0.42
2:v:47:ILE:HD11	2:v:88:HIS:HB3	2.00	0.42
1:B:150:HIS:CE1	1:C:307:TRP:HE1	2.17	0.42
1:B:340:ILE:O	1:B:344:THR:OG1	2.24	0.42
1:C:24:GLU:OE1	1:C:313:LYS:NZ	2.52	0.42
1:F:53:TYR:O	4:r:131:ARG:NH1	2.53	0.42
1:H:47:GLN:HG2	1:H:48:TYR:H	1.84	0.42
1:H:239:VAL:HG12	1:H:240:THR:HG23	2.00	0.42
1:H:256:ASP:OD1	1:H:256:ASP:N	2.52	0.42
1:K:293:ILE:HG22	1:K:295:GLY:H	1.84	0.42
2:M:81:LYS:O	2:M:82:ILE:C	2.62	0.42
2:O:136:ASP:OD1	2:O:137:ALA:N	2.52	0.42
3:c:12:MET:HA	3:c:23:ASP:HA	2.02	0.42
2:v:51:ILE:O	2:v:58:HIS:HA	2.19	0.42
1:E:573:ASN:O	1:E:577:ILE:HG12	2.18	0.42
1:G:252:LYS:HE2	1:G:252:LYS:HB3	1.81	0.42
1:I:346:LYS:HA	1:I:346:LYS:HD3	1.87	0.42
1:I:616:LEU:HB3	1:J:622:LEU:HD11	2.01	0.42
1:I:625:ALA:O	1:I:629:THR:HG23	2.19	0.42
1:J:165:MET:HE3	1:J:165:MET:HB2	1.88	0.42
1:L:107:ALA:O	1:L:111:VAL:HG23	2.19	0.42
1:L:190:LYS:HB2	1:L:190:LYS:HE3	1.92	0.42
1:L:625:ALA:O	1:L:629:THR:HG23	2.20	0.42
2:N:51:ILE:CG2	2:N:79:LEU:HD11	2.49	0.42
3:d:339:ARG:HD3	3:d:371:TYR:CE2	2.51	0.42
4:k:24:THR:HG22	4:k:26:THR:HG23	2.01	0.42
4:r:21:SER:O	4:r:24:THR:HG22	2.19	0.42
2:v:122:PHE:CE1	2:x:122:PHE:HB2	2.55	0.42
1:B:281:ILE:HG22	1:B:286:VAL:HG12	1.99	0.42
1:B:625:ALA:O	1:B:629:THR:HG23	2.19	0.42
1:E:234:ILE:HD11	1:E:269:ARG:HD3	2.00	0.42
1:H:71:MET:SD	1:H:119:ILE:HD11	2.60	0.42
1:L:101:ASP:OD2	1:L:464:TYR:OH	2.27	0.42
2:T:131:TYR:HB2	2:T:137:ALA:HB2	2.01	0.42
3:c:293:MET:HE2	3:c:304:LEU:HD11	2.01	0.42
3:f:354:ASP:OD1	3:f:355:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:109:TYR:CZ	4:m:113:LEU:HD11	2.54	0.42
1:B:40:GLN:HG3	1:B:56:GLN:NE2	2.34	0.42
1:B:95:MET:HE2	1:B:99:ARG:NH1	2.33	0.42
1:C:567:MET:HE2	1:D:582:LYS:HG3	2.01	0.42
1:F:107:ALA:O	1:F:111:VAL:HG23	2.20	0.42
1:H:84:ASP:OD1	1:H:85:GLY:N	2.52	0.42
1:H:362:MET:HE1	1:H:373:LEU:HD12	2.02	0.42
2:Q:51:ILE:O	2:Q:58:HIS:HA	2.20	0.42
2:W:31:ILE:HD11	2:W:67:ILE:HD11	2.01	0.42
4:o:79:ALA:O	4:o:83:VAL:HG23	2.20	0.42
2:v:68:ASN:HD21	2:w:21:ARG:HH21	1.66	0.42
2:v:128:LEU:O	2:v:128:LEU:HD23	2.19	0.42
1:A:563:LYS:HB2	1:B:89:ASP:HB3	2.02	0.42
1:A:611:ALA:HB1	1:L:609:VAL:HB	2.01	0.42
1:B:84:ASP:OD1	1:B:85:GLY:N	2.52	0.42
1:B:179:MET:HE2	1:B:184:TRP:HA	2.02	0.42
1:C:625:ALA:O	1:C:629:THR:HG23	2.19	0.42
1:D:177:HIS:NE2	1:D:221:GLU:OE1	2.43	0.42
1:D:625:ALA:O	1:D:629:THR:HG23	2.19	0.42
1:E:78:VAL:O	1:E:95:MET:HE1	2.20	0.42
1:F:212:LEU:HD23	1:F:212:LEU:HA	1.89	0.42
1:F:509:ASP:OD1	1:F:510:ILE:N	2.53	0.42
1:F:609:VAL:HB	1:G:611:ALA:HB1	2.01	0.42
1:H:131:ASP:OD1	1:H:132:TYR:N	2.45	0.42
1:I:107:ALA:O	1:I:111:VAL:HG23	2.20	0.42
1:L:242:GLU:CD	1:L:243:PRO:HD2	2.45	0.42
3:a:30:LEU:HD23	3:a:30:LEU:HA	1.92	0.42
3:a:150:ARG:HG2	3:a:164:THR:O	2.19	0.42
3:c:403:ALA:HB2	3:c:429:ASN:ND2	2.35	0.42
4:i:34:GLN:NE2	4:i:38:ASP:OD2	2.50	0.42
4:r:73:HIS:ND1	4:r:75:LEU:HB2	2.35	0.42
1:C:329:LEU:HD23	1:C:329:LEU:HA	1.88	0.42
1:E:71:MET:SD	1:E:119:ILE:HD11	2.60	0.42
1:G:575:GLN:O	1:G:579:MET:HG3	2.20	0.42
1:G:612:GLN:O	1:G:616:LEU:HG	2.20	0.42
1:K:24:GLU:OE1	1:K:313:LYS:NZ	2.51	0.42
2:Q:123:LYS:O	2:V:122:PHE:HD1	2.02	0.42
2:S:49:VAL:HG23	2:S:61:ILE:HB	2.02	0.42
3:b:34:LYS:HB3	3:b:36:ILE:HD11	2.02	0.42
3:d:8:MET:HE3	3:d:8:MET:HB2	1.88	0.42
3:e:293:MET:HE2	3:e:293:MET:HB3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:q:3:ILE:HG22	4:q:9:LEU:HD12	2.02	0.42
1:A:573:ASN:O	1:A:577:ILE:HG12	2.20	0.42
1:C:107:ALA:O	1:C:111:VAL:HG23	2.20	0.42
1:E:628:GLN:O	1:E:632:LEU:HG	2.19	0.42
1:F:306:GLU:O	1:F:307:TRP:HB2	2.20	0.42
1:F:307:TRP:CG	1:F:308:GLY:N	2.87	0.42
1:F:557:PHE:HE2	1:G:548:GLU:HG2	1.85	0.42
1:G:297:HIS:HB3	1:G:459:ARG:HH21	1.85	0.42
1:J:616:LEU:HB3	1:K:622:LEU:HD11	2.01	0.42
1:K:150:HIS:HE1	1:L:307:TRP:NE1	2.14	0.42
1:K:364:ASP:OD1	1:K:365:GLY:N	2.53	0.42
1:L:469:ASN:O	1:L:508:ASN:ND2	2.52	0.42
2:R:51:ILE:O	2:R:58:HIS:HA	2.20	0.42
3:e:60:ARG:HB2	3:e:74:VAL:CG2	2.50	0.42
3:e:78:LYS:HA	3:e:89:VAL:HG12	2.01	0.42
2:v:19:GLU:HG2	2:v:26:VAL:HG22	2.01	0.42
1:B:468:VAL:HG13	1:B:472:TYR:CD2	2.55	0.42
1:D:363:TYR:OH	1:D:373:LEU:O	2.32	0.42
1:E:563:LYS:HB3	1:F:92:ASP:OD2	2.20	0.42
1:F:300:ILE:H	1:F:300:ILE:HD12	1.85	0.42
1:G:254:VAL:HG11	1:G:505:GLN:HG2	2.02	0.42
1:K:53:TYR:O	4:k:131:ARG:NH1	2.53	0.42
1:K:329:LEU:HD23	1:K:329:LEU:HA	1.92	0.42
1:L:115:VAL:O	1:L:119:ILE:HG12	2.20	0.42
1:L:591:GLN:HA	1:L:594:VAL:HG22	2.02	0.42
2:O:51:ILE:O	2:O:58:HIS:HA	2.19	0.42
3:a:36:ILE:HG22	3:a:37:LEU:N	2.34	0.42
3:d:378:LEU:HD22	3:d:453:LYS:HE2	2.01	0.42
3:d:441:LYS:HE2	4:m:19:VAL:HG13	2.02	0.42
3:f:192:GLY:O	3:f:199:VAL:N	2.51	0.42
3:f:331:THR:HG22	3:f:370:GLN:NE2	2.30	0.42
4:i:79:ALA:O	4:i:83:VAL:HG23	2.20	0.42
4:r:141:ALA:HB1	4:r:146:TRP:HE3	1.85	0.42
1:B:71:MET:SD	1:B:119:ILE:HD11	2.60	0.41
1:B:468:VAL:HG13	1:B:472:TYR:HD2	1.84	0.41
1:D:84:ASP:OD1	1:D:85:GLY:N	2.53	0.41
1:F:505:GLN:OE1	1:F:506:VAL:N	2.53	0.41
1:F:625:ALA:O	1:F:629:THR:HG23	2.20	0.41
1:H:625:ALA:O	1:H:629:THR:HG23	2.19	0.41
1:I:582:LYS:HE2	1:I:582:LYS:HB3	1.74	0.41
1:J:625:ALA:O	1:J:629:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:94:ASP:OD1	2:M:95:ALA:N	2.44	0.41
3:b:12:MET:H	3:b:382:PRO:HA	1.83	0.41
3:b:293:MET:HE2	3:b:293:MET:HB3	1.91	0.41
4:l:21:SER:O	4:l:24:THR:HG22	2.20	0.41
4:m:87:LEU:O	4:m:91:ILE:HG13	2.20	0.41
4:q:4:LYS:HE3	4:q:4:LYS:HB3	1.94	0.41
2:x:81:LYS:O	2:x:82:ILE:C	2.63	0.41
1:A:628:GLN:O	1:A:632:LEU:HG	2.20	0.41
1:C:628:GLN:O	1:C:632:LEU:HG	2.20	0.41
1:F:115:VAL:O	1:F:119:ILE:HG12	2.20	0.41
1:G:10:SER:O	1:G:14:ARG:HG3	2.19	0.41
1:L:47:GLN:HG2	1:L:48:TYR:H	1.85	0.41
1:L:505:GLN:OE1	1:L:506:VAL:N	2.53	0.41
2:T:42:ASN:C	2:T:42:ASN:ND2	2.77	0.41
3:c:22:ILE:O	3:c:22:ILE:HG13	2.20	0.41
3:e:141:VAL:HG22	3:e:153:TRP:CD1	2.55	0.41
3:f:150:ARG:HD2	3:f:163:ILE:HD11	2.02	0.41
4:k:4:LYS:HE3	4:k:4:LYS:HB3	1.94	0.41
2:s:81:LYS:O	2:s:82:ILE:C	2.63	0.41
1:A:273:ARG:HH22	1:A:470:ASP:CG	2.28	0.41
1:C:627:ASN:HB3	1:D:632:LEU:HD11	2.02	0.41
1:E:301:VAL:HG22	1:E:463:ILE:HD12	2.02	0.41
1:H:91:ALA:O	1:H:95:MET:HB2	2.20	0.41
1:H:179:MET:HE2	1:H:184:TRP:HA	2.03	0.41
2:M:93:TYR:HH	3:d:408:ARG:HH12	1.64	0.41
2:O:43:PRO:HA	2:O:46:GLN:OE1	2.21	0.41
2:O:81:LYS:O	2:O:82:ILE:C	2.62	0.41
2:S:51:ILE:O	2:S:58:HIS:HA	2.21	0.41
2:V:24:LYS:HE3	2:V:24:LYS:HB2	1.72	0.41
3:e:6:LEU:HD22	3:e:384:PHE:CE2	2.55	0.41
4:k:4:LYS:H	4:k:4:LYS:HG2	1.71	0.41
4:n:21:SER:O	4:n:24:THR:HG22	2.20	0.41
1:A:163:LYS:HG3	1:L:150:HIS:CD2	2.56	0.41
1:B:346:LYS:HA	1:B:346:LYS:HD3	1.93	0.41
1:C:300:ILE:HD12	1:C:300:ILE:H	1.85	0.41
1:F:150:HIS:CD2	1:G:163:LYS:HG3	2.56	0.41
1:H:300:ILE:HD12	1:H:300:ILE:H	1.85	0.41
1:H:612:GLN:O	1:H:616:LEU:HG	2.19	0.41
1:K:479:THR:HG22	1:K:481:THR:H	1.85	0.41
3:b:182:GLU:O	3:c:148:ARG:HA	2.20	0.41
3:d:181:ALA:O	3:d:182:GLU:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:87:LEU:O	4:g:91:ILE:HG13	2.21	0.41
4:p:47:TRP:O	4:p:54:ILE:N	2.53	0.41
2:s:117:GLU:O	2:s:121:LYS:HB2	2.21	0.41
1:A:297:HIS:HB3	1:A:459:ARG:HH21	1.85	0.41
1:C:53:TYR:O	4:o:131:ARG:NH1	2.54	0.41
1:H:38:VAL:HG23	1:I:310:VAL:HG21	2.02	0.41
1:I:53:TYR:O	4:i:131:ARG:NH1	2.53	0.41
1:K:317:GLU:HG3	1:K:321:ARG:HG3	2.01	0.41
1:K:339:ASP:OD1	4:l:128:TYR:OH	2.27	0.41
2:P:108:LYS:HG3	2:Z:113:GLN:HG3	2.03	0.41
2:W:123:LYS:HD3	2:W:123:LYS:HA	1.77	0.41
2:Z:81:LYS:O	2:Z:82:ILE:C	2.64	0.41
3:a:6:LEU:HD22	3:a:384:PHE:CE2	2.55	0.41
3:e:150:ARG:HD2	3:e:163:ILE:HD11	2.02	0.41
3:e:388:ASN:OD1	3:e:445:ARG:NH1	2.53	0.41
3:f:36:ILE:HD11	3:f:42:TYR:CD1	2.55	0.41
4:l:1:MET:HG3	4:l:3:ILE:H	1.85	0.41
2:v:123:LYS:HD2	2:x:123:LYS:NZ	2.36	0.41
2:x:51:ILE:CG2	2:x:79:LEU:HD11	2.51	0.41
2:x:53:ASN:ND2	2:x:57:SER:OG	2.43	0.41
1:A:612:GLN:O	1:A:616:LEU:HG	2.20	0.41
1:B:127:ARG:NH1	1:B:147:GLU:OE1	2.54	0.41
1:E:317:GLU:HG3	1:E:321:ARG:HG3	2.02	0.41
1:F:242:GLU:CD	1:F:243:PRO:HD2	2.45	0.41
1:H:473:ASP:OD1	1:H:473:ASP:N	2.54	0.41
1:I:300:ILE:HD12	1:I:300:ILE:H	1.85	0.41
1:J:84:ASP:OD1	1:J:85:GLY:N	2.53	0.41
1:L:509:ASP:OD1	1:L:510:ILE:N	2.53	0.41
2:M:51:ILE:CG2	2:M:79:LEU:HD11	2.51	0.41
2:Q:50:TYR:HE1	2:Q:60:GLN:HG2	1.86	0.41
2:R:19:GLU:HG2	2:R:26:VAL:HG22	2.01	0.41
3:a:453:LYS:C	3:a:454:LEU:HD12	2.46	0.41
3:c:385:LYS:HB2	3:d:37:LEU:HD23	2.03	0.41
3:d:414:THR:O	3:d:450:ILE:HA	2.21	0.41
3:e:410:PHE:HB2	3:e:455:ARG:HB2	2.03	0.41
4:j:21:SER:O	4:j:24:THR:HG22	2.21	0.41
4:n:131:ARG:H	4:n:131:ARG:HG2	1.71	0.41
4:p:21:SER:O	4:p:24:THR:HG22	2.20	0.41
1:B:471:ILE:HG22	1:B:472:TYR:CD1	2.55	0.41
1:C:254:VAL:HG12	1:C:254:VAL:O	2.21	0.41
1:I:628:GLN:O	1:I:632:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:573:ASN:O	1:K:577:ILE:HG12	2.21	0.41
1:K:628:GLN:O	1:K:632:LEU:HG	2.20	0.41
2:W:46:GLN:CD	2:W:63:GLN:HG2	2.46	0.41
3:c:430:GLU:HG2	3:c:431:PRO:HD2	2.02	0.41
3:e:284:THR:HG23	3:e:287:GLU:H	1.86	0.41
3:f:22:ILE:O	3:f:22:ILE:HG13	2.20	0.41
3:f:403:ALA:HB2	3:f:429:ASN:ND2	2.35	0.41
4:h:21:SER:O	4:h:24:THR:HG22	2.21	0.41
2:s:43:PRO:HA	2:s:46:GLN:OE1	2.20	0.41
1:B:256:ASP:OD1	1:B:256:ASP:N	2.52	0.41
1:B:605:ASP:HB3	1:B:608:MET:HG2	2.03	0.41
1:D:80:TYR:OH	1:D:461:GLY:O	2.37	0.41
1:F:194:ASP:OD1	1:F:194:ASP:N	2.50	0.41
1:I:91:ALA:O	1:I:95:MET:HB2	2.21	0.41
1:K:177:HIS:NE2	1:K:221:GLU:OE1	2.37	0.41
2:V:51:ILE:HD11	2:V:61:ILE:HD13	2.03	0.41
3:a:339:ARG:HD3	3:a:371:TYR:CE2	2.54	0.41
3:e:35:GLU:HG3	3:e:35:GLU:O	2.21	0.41
3:e:341:VAL:HG22	3:e:355:LYS:CE	2.49	0.41
3:f:66:THR:H	3:f:99:HIS:CD2	2.39	0.41
4:n:141:ALA:HB1	4:n:146:TRP:HE3	1.86	0.41
1:B:40:GLN:HG3	1:B:56:GLN:HE21	1.85	0.41
1:B:362:MET:HE1	1:B:373:LEU:HD12	2.02	0.41
1:D:587:PRO:O	1:D:591:GLN:HG2	2.20	0.41
1:F:33:LEU:HD23	1:F:33:LEU:HA	1.92	0.41
1:G:212:LEU:HD23	1:G:212:LEU:HA	1.90	0.41
1:G:573:ASN:O	1:G:577:ILE:HG12	2.20	0.41
1:G:628:GLN:O	1:G:632:LEU:HG	2.21	0.41
1:H:605:ASP:HB3	1:H:608:MET:HG2	2.03	0.41
1:K:71:MET:SD	1:K:119:ILE:HD11	2.61	0.41
1:K:615:LEU:HD23	1:K:615:LEU:HA	1.94	0.41
1:L:300:ILE:H	1:L:300:ILE:HD12	1.85	0.41
2:N:113:GLN:HG3	2:S:108:LYS:HG3	2.03	0.41
2:P:51:ILE:O	2:P:58:HIS:HA	2.20	0.41
2:Z:21:ARG:HG3	2:Z:21:ARG:NH1	2.36	0.41
3:a:111:GLN:HG3	3:a:113:VAL:HG23	2.03	0.41
3:b:9:MET:HE3	3:b:9:MET:HB2	1.95	0.41
3:b:414:THR:HG22	3:b:419:ASN:O	2.21	0.41
3:c:141:VAL:HG11	3:c:144:ILE:HD11	2.03	0.41
3:c:449:LEU:HD22	3:d:37:LEU:HD21	2.02	0.41
3:d:410:PHE:CD1	3:d:425:MET:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:416:ASP:OD1	3:d:416:ASP:N	2.47	0.41
3:e:377:HIS:HB2	3:e:456:VAL:HB	2.03	0.41
3:f:441:LYS:HE2	4:q:19:VAL:HG13	2.03	0.41
4:i:4:LYS:HE3	4:i:4:LYS:HB3	1.94	0.41
2:s:74:VAL:O	2:s:77:GLY:O	2.39	0.41
1:G:238:PRO:HD3	1:G:263:PHE:CD1	2.56	0.41
1:H:40:GLN:HG3	1:H:56:GLN:HE21	1.85	0.41
1:I:178:SER:OG	1:I:215:ASP:OD2	2.23	0.41
1:K:300:ILE:H	1:K:300:ILE:HD12	1.86	0.41
1:L:531:ASN:O	1:L:535:ILE:HG12	2.21	0.41
2:O:117:GLU:O	2:O:121:LYS:HB2	2.21	0.41
2:P:52:GLU:OE1	2:P:83:VAL:HG21	2.21	0.41
3:a:403:ALA:HB2	3:a:429:ASN:ND2	2.35	0.41
3:d:192:GLY:O	3:d:199:VAL:N	2.52	0.41
3:d:441:LYS:HD2	3:d:441:LYS:HA	1.95	0.41
3:f:430:GLU:HG2	3:f:431:PRO:HD2	2.02	0.41
4:o:110:GLY:O	4:o:114:LEU:HG	2.21	0.41
1:A:95:MET:HG3	1:A:527:MET:HE1	2.02	0.40
1:B:300:ILE:H	1:B:300:ILE:HD12	1.86	0.40
1:B:505:GLN:OE1	1:B:506:VAL:N	2.54	0.40
1:E:498:ASP:C	1:E:500:ALA:H	2.30	0.40
1:J:575:GLN:O	1:J:579:MET:HG3	2.20	0.40
1:K:93:VAL:HG22	1:K:97:MET:HE2	2.02	0.40
2:O:50:TYR:HB3	2:O:58:HIS:HB3	2.04	0.40
3:c:215:THR:O	3:c:215:THR:HG22	2.21	0.40
4:j:131:ARG:H	4:j:131:ARG:HG2	1.71	0.40
2:v:20:SER:HA	2:x:78:GLN:HE22	1.86	0.40
2:w:46:GLN:CD	2:w:63:GLN:HG2	2.46	0.40
1:A:548:GLU:HG2	1:L:557:PHE:HE2	1.85	0.40
1:E:479:THR:HG22	1:E:481:THR:H	1.86	0.40
1:F:47:GLN:HG2	1:F:48:TYR:H	1.85	0.40
1:F:531:ASN:O	1:F:535:ILE:HG12	2.21	0.40
1:L:40:GLN:HG3	1:L:56:GLN:NE2	2.37	0.40
1:L:75:PRO:HB2	1:L:523:SER:HB3	2.03	0.40
1:L:306:GLU:O	1:L:307:TRP:HB2	2.21	0.40
2:O:23:PHE:CD1	2:Y:25:ALA:HB2	2.56	0.40
2:T:117:GLU:HG2	2:T:121:LYS:HD3	2.02	0.40
3:b:12:MET:HE1	3:c:36:ILE:HA	2.02	0.40
3:b:150:ARG:HD2	3:b:163:ILE:HD11	2.03	0.40
3:b:165:ASP:HB2	3:b:173:ASP:HA	2.04	0.40
3:c:241:THR:O	3:c:247:TYR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:141:VAL:HG11	3:f:144:ILE:HD11	2.04	0.40
4:h:17:LEU:HD23	4:h:17:LEU:HA	1.89	0.40
4:h:49:GLN:CA	4:h:49:GLN:HE21	2.33	0.40
1:A:127:ARG:HG3	1:A:147:GLU:HB2	2.04	0.40
1:C:274:ARG:HB2	1:C:296:GLU:HG2	2.03	0.40
1:G:594:VAL:O	1:G:598:GLN:NE2	2.54	0.40
1:L:339:ASP:OD2	4:l:131:ARG:NH2	2.30	0.40
2:R:51:ILE:HD12	2:R:80:VAL:HB	2.03	0.40
3:a:112:LEU:HD23	3:a:124:VAL:HG21	2.02	0.40
3:e:97:MET:HE3	3:e:104:GLN:HE21	1.87	0.40
4:i:29:GLU:OE1	4:i:31:GLN:N	2.54	0.40
4:j:1:MET:HG3	4:j:3:ILE:H	1.87	0.40
4:o:17:LEU:HD23	4:o:17:LEU:HA	1.90	0.40
4:q:4:LYS:H	4:q:4:LYS:HG2	1.71	0.40
2:s:79:LEU:HA	2:s:79:LEU:HD12	1.67	0.40
1:A:79:LEU:N	1:A:519:ASP:O	2.39	0.40
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.88	0.40
1:C:498:ASP:C	1:C:500:ALA:H	2.29	0.40
1:E:346:LYS:HA	1:E:346:LYS:HD3	1.88	0.40
1:G:101:ASP:OD2	1:G:464:TYR:OH	2.25	0.40
1:G:300:ILE:H	1:G:300:ILE:HD12	1.87	0.40
1:G:363:TYR:HE1	1:H:350:PHE:HE1	1.69	0.40
1:H:237:ASP:HA	1:H:263:PHE:CE1	2.57	0.40
1:I:577:ILE:HD13	1:I:589:GLU:HB3	2.04	0.40
1:J:454:ALA:HB1	1:J:520:VAL:HG21	2.03	0.40
2:M:51:ILE:HG23	2:M:79:LEU:HD11	2.02	0.40
3:c:284:THR:HG23	3:c:287:GLU:H	1.87	0.40
3:c:441:LYS:HE2	4:k:19:VAL:HG13	2.04	0.40
3:e:34:LYS:HB3	3:e:36:ILE:HD11	2.02	0.40
4:m:46:GLU:O	4:m:49:GLN:HG2	2.21	0.40
4:n:90:ARG:O	4:n:93:PRO:HD2	2.21	0.40
1:A:583:LYS:HE3	1:A:583:LYS:HB3	1.91	0.40
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.89	0.40
1:C:346:LYS:HA	1:C:346:LYS:HD3	1.87	0.40
1:D:33:LEU:HD23	1:D:33:LEU:HA	1.90	0.40
1:D:76:ILE:HG23	1:D:520:VAL:HG13	2.04	0.40
1:D:98:TYR:HD2	1:D:464:TYR:CD2	2.39	0.40
1:E:33:LEU:HD23	1:E:33:LEU:HA	1.93	0.40
1:E:94:LEU:HD11	1:E:465:GLN:HG3	2.04	0.40
1:E:127:ARG:HG3	1:E:147:GLU:HB2	2.03	0.40
1:H:245:SER:O	1:H:510:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:121:ALA:O	1:K:123:VAL:N	2.49	0.40
2:N:6:ALA:HB1	2:S:83:VAL:HG11	2.03	0.40
2:N:14:ARG:HH21	2:N:80:VAL:HG22	1.87	0.40
2:O:51:ILE:CG2	2:O:79:LEU:HD11	2.52	0.40
2:P:49:VAL:HG21	2:P:65:LEU:HD21	2.04	0.40
3:f:11:GLY:O	3:f:24:TYR:N	2.37	0.40
4:j:4:LYS:HE3	4:j:4:LYS:HB3	1.95	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	604/725 (83%)	569 (94%)	35 (6%)	0	100	100
1	B	604/725 (83%)	567 (94%)	37 (6%)	0	100	100
1	C	604/725 (83%)	572 (95%)	32 (5%)	0	100	100
1	D	604/725 (83%)	568 (94%)	36 (6%)	0	100	100
1	E	604/725 (83%)	569 (94%)	35 (6%)	0	100	100
1	F	604/725 (83%)	567 (94%)	37 (6%)	0	100	100
1	G	604/725 (83%)	568 (94%)	36 (6%)	0	100	100
1	H	604/725 (83%)	568 (94%)	36 (6%)	0	100	100
1	I	604/725 (83%)	565 (94%)	39 (6%)	0	100	100
1	J	604/725 (83%)	567 (94%)	37 (6%)	0	100	100
1	K	604/725 (83%)	569 (94%)	35 (6%)	0	100	100
1	L	604/725 (83%)	567 (94%)	37 (6%)	0	100	100
2	M	145/667 (22%)	133 (92%)	11 (8%)	1 (1%)	18	52
2	N	145/667 (22%)	134 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	145/667 (22%)	135 (93%)	9 (6%)	1 (1%)	18	52
2	P	147/667 (22%)	140 (95%)	6 (4%)	1 (1%)	18	52
2	Q	147/667 (22%)	138 (94%)	8 (5%)	1 (1%)	18	52
2	R	147/667 (22%)	139 (95%)	8 (5%)	0	100	100
2	S	147/667 (22%)	140 (95%)	7 (5%)	0	100	100
2	T	147/667 (22%)	139 (95%)	8 (5%)	0	100	100
2	U	147/667 (22%)	142 (97%)	5 (3%)	0	100	100
2	V	147/667 (22%)	141 (96%)	6 (4%)	0	100	100
2	W	147/667 (22%)	144 (98%)	3 (2%)	0	100	100
2	X	147/667 (22%)	143 (97%)	4 (3%)	0	100	100
2	Y	147/667 (22%)	141 (96%)	6 (4%)	0	100	100
2	Z	145/667 (22%)	134 (92%)	11 (8%)	0	100	100
2	s	145/667 (22%)	135 (93%)	9 (6%)	1 (1%)	18	52
2	v	147/667 (22%)	140 (95%)	7 (5%)	0	100	100
2	w	147/667 (22%)	143 (97%)	4 (3%)	0	100	100
2	x	145/667 (22%)	135 (93%)	9 (6%)	1 (1%)	18	52
3	a	468/472 (99%)	430 (92%)	38 (8%)	0	100	100
3	b	468/472 (99%)	432 (92%)	35 (8%)	1 (0%)	43	73
3	c	468/472 (99%)	432 (92%)	35 (8%)	1 (0%)	43	73
3	d	468/472 (99%)	431 (92%)	36 (8%)	1 (0%)	43	73
3	e	468/472 (99%)	432 (92%)	36 (8%)	0	100	100
3	f	468/472 (99%)	432 (92%)	35 (8%)	1 (0%)	43	73
4	g	151/166 (91%)	142 (94%)	9 (6%)	0	100	100
4	h	151/166 (91%)	138 (91%)	13 (9%)	0	100	100
4	i	151/166 (91%)	141 (93%)	10 (7%)	0	100	100
4	j	151/166 (91%)	138 (91%)	13 (9%)	0	100	100
4	k	151/166 (91%)	143 (95%)	8 (5%)	0	100	100
4	l	151/166 (91%)	137 (91%)	13 (9%)	1 (1%)	18	52
4	m	151/166 (91%)	143 (95%)	8 (5%)	0	100	100
4	n	151/166 (91%)	139 (92%)	12 (8%)	0	100	100
4	o	151/166 (91%)	140 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	p	151/166 (91%)	138 (91%)	13 (9%)	0	100	100
4	q	151/166 (91%)	142 (94%)	9 (6%)	0	100	100
4	r	151/166 (91%)	138 (91%)	13 (9%)	0	100	100
All	All	14502/25530 (57%)	13580 (94%)	911 (6%)	11 (0%)	49	78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	b	356	SER
3	d	181	ALA
4	l	53	GLY
3	c	105	ALA
3	f	105	ALA
2	x	82	ILE
2	M	82	ILE
2	O	82	ILE
2	s	82	ILE
2	P	147	ILE
2	Q	147	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/630 (85%)	533 (100%)	0	100	100
1	B	533/630 (85%)	531 (100%)	2 (0%)	84	85
1	C	533/630 (85%)	533 (100%)	0	100	100
1	D	533/630 (85%)	533 (100%)	0	100	100
1	E	533/630 (85%)	532 (100%)	1 (0%)	87	88
1	F	533/630 (85%)	530 (99%)	3 (1%)	78	83
1	G	533/630 (85%)	533 (100%)	0	100	100
1	H	533/630 (85%)	532 (100%)	1 (0%)	87	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	533/630 (85%)	532 (100%)	1 (0%)	87	88
1	J	533/630 (85%)	532 (100%)	1 (0%)	87	88
1	K	533/630 (85%)	530 (99%)	3 (1%)	78	83
1	L	533/630 (85%)	529 (99%)	4 (1%)	73	80
2	M	125/548 (23%)	125 (100%)	0	100	100
2	N	125/548 (23%)	125 (100%)	0	100	100
2	O	125/548 (23%)	125 (100%)	0	100	100
2	P	127/548 (23%)	127 (100%)	0	100	100
2	Q	127/548 (23%)	126 (99%)	1 (1%)	73	80
2	R	127/548 (23%)	127 (100%)	0	100	100
2	S	127/548 (23%)	127 (100%)	0	100	100
2	T	127/548 (23%)	125 (98%)	2 (2%)	55	73
2	U	127/548 (23%)	127 (100%)	0	100	100
2	V	127/548 (23%)	127 (100%)	0	100	100
2	W	127/548 (23%)	127 (100%)	0	100	100
2	X	127/548 (23%)	126 (99%)	1 (1%)	73	80
2	Y	127/548 (23%)	127 (100%)	0	100	100
2	Z	125/548 (23%)	125 (100%)	0	100	100
2	s	125/548 (23%)	125 (100%)	0	100	100
2	v	127/548 (23%)	127 (100%)	0	100	100
2	w	127/548 (23%)	127 (100%)	0	100	100
2	x	125/548 (23%)	125 (100%)	0	100	100
3	a	393/395 (100%)	392 (100%)	1 (0%)	86	87
3	b	393/395 (100%)	393 (100%)	0	100	100
3	c	393/395 (100%)	392 (100%)	1 (0%)	86	87
3	d	393/395 (100%)	392 (100%)	1 (0%)	86	87
3	e	393/395 (100%)	391 (100%)	2 (0%)	81	84
3	f	393/395 (100%)	392 (100%)	1 (0%)	86	87
4	g	121/131 (92%)	120 (99%)	1 (1%)	73	80
4	h	121/131 (92%)	120 (99%)	1 (1%)	73	80
4	i	121/131 (92%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	j	121/131 (92%)	120 (99%)	1 (1%)	73	80
4	k	121/131 (92%)	121 (100%)	0	100	100
4	l	121/131 (92%)	121 (100%)	0	100	100
4	m	121/131 (92%)	121 (100%)	0	100	100
4	n	121/131 (92%)	121 (100%)	0	100	100
4	o	121/131 (92%)	121 (100%)	0	100	100
4	p	121/131 (92%)	120 (99%)	1 (1%)	73	80
4	q	121/131 (92%)	121 (100%)	0	100	100
4	r	121/131 (92%)	121 (100%)	0	100	100
All	All	12480/21366 (58%)	12450 (100%)	30 (0%)	85	88

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	89	ASP
1	B	450	GLN
1	E	450	GLN
1	F	92	ASP
1	F	450	GLN
1	F	471	ILE
1	H	450	GLN
1	I	93	VAL
1	J	93	VAL
1	K	93	VAL
1	K	94	LEU
1	K	450	GLN
1	L	92	ASP
1	L	93	VAL
1	L	94	LEU
1	L	450	GLN
2	Q	60	GLN
2	T	42	ASN
2	T	60	GLN
2	X	74	VAL
3	a	241	THR
3	c	102	THR
3	d	241	THR
3	e	59	SER
3	e	341	VAL

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Mol	Chain	Res	Type
3	f	102	THR
4	g	44	MET
4	h	49	GLN
4	j	50	ASP
4	p	28	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	327	GLN
1	A	578	GLN
1	A	603	GLN
1	A	612	GLN
1	B	40	GLN
1	B	182	ASN
1	B	327	GLN
1	B	465	GLN
1	B	530	GLN
1	B	610	GLN
1	C	40	GLN
1	C	291	GLN
1	C	450	GLN
1	C	603	GLN
1	D	327	GLN
1	D	361	HIS
1	D	530	GLN
1	D	578	GLN
1	D	603	GLN
1	E	40	GLN
1	E	327	GLN
1	E	465	GLN
1	E	590	GLN
1	E	603	GLN
1	E	612	GLN
1	F	31	ASN
1	F	150	HIS
1	F	361	HIS
1	F	469	ASN
1	F	603	GLN
1	G	327	GLN
1	G	450	GLN

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Mol	Chain	Res	Type
1	G	578	GLN
1	G	603	GLN
1	G	612	GLN
1	H	40	GLN
1	H	172	HIS
1	H	327	GLN
1	H	465	GLN
1	H	530	GLN
1	H	603	GLN
1	H	610	GLN
1	I	530	GLN
1	I	603	GLN
1	I	612	GLN
1	J	327	GLN
1	J	361	HIS
1	J	530	GLN
1	K	40	GLN
1	K	327	GLN
1	K	361	HIS
1	K	465	GLN
1	K	590	GLN
1	K	603	GLN
1	K	612	GLN
1	L	155	HIS
1	L	361	HIS
1	L	603	GLN
2	M	78	GLN
2	M	99	GLN
2	M	135	GLN
2	N	63	GLN
2	N	78	GLN
2	N	135	GLN
2	O	135	GLN
2	P	63	GLN
2	P	135	GLN
2	Q	63	GLN
2	Q	99	GLN
2	Q	135	GLN
2	R	35	GLN
2	R	135	GLN
2	S	63	GLN
2	S	105	ASN

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Mol	Chain	Res	Type
2	S	135	GLN
2	T	42	ASN
2	T	99	GLN
2	T	135	GLN
2	U	78	GLN
2	U	135	GLN
2	V	135	GLN
2	W	135	GLN
2	X	135	GLN
2	Y	135	GLN
2	Z	135	GLN
3	a	178	GLN
3	a	321	GLN
3	a	419	ASN
3	b	225	GLN
3	b	231	GLN
3	b	307	HIS
3	b	375	GLN
3	c	56	ASN
3	c	225	GLN
3	c	307	HIS
3	d	321	GLN
3	d	375	GLN
3	d	419	ASN
3	e	56	ASN
3	e	231	GLN
3	e	375	GLN
3	f	307	HIS
3	f	321	GLN
4	h	49	GLN
4	i	65	ASN
4	k	49	GLN
4	o	31	GLN
4	o	65	ASN
4	q	49	GLN
2	s	135	GLN
2	v	35	GLN
2	v	135	GLN
2	w	135	GLN
2	x	28	ASN
2	x	53	ASN
2	x	58	HIS

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Mol	Chain	Res	Type
2	x	78	GLN
2	x	88	HIS
2	x	135	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

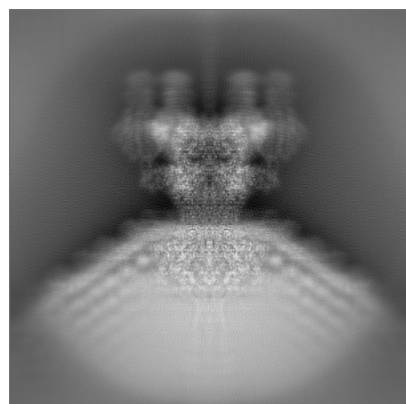
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61457. These allow visual inspection of the internal detail of the map and identification of artifacts.

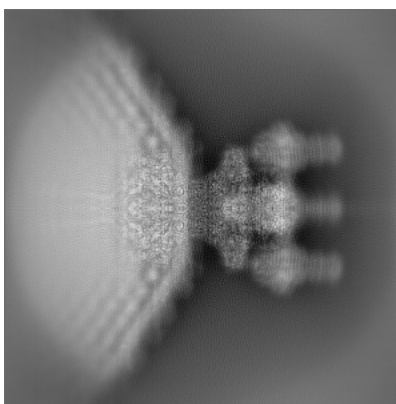
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

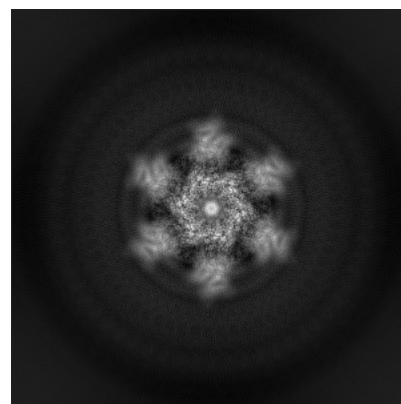
6.1.1 Primary map



X

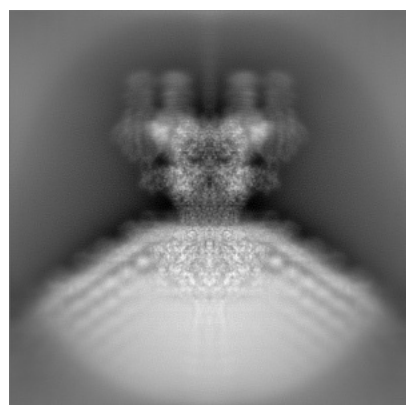


Y

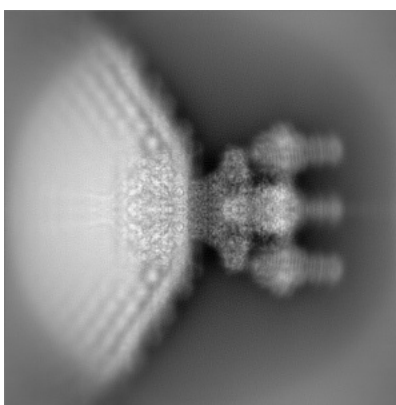


Z

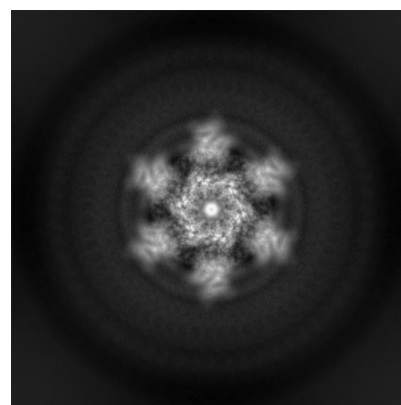
6.1.2 Raw map



X



Y

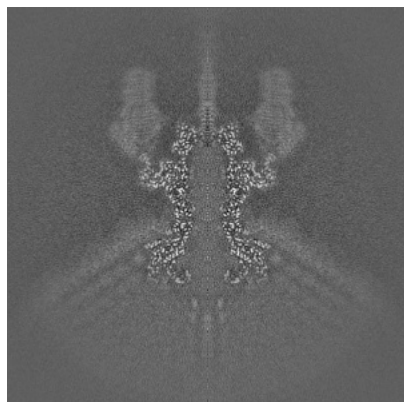


Z

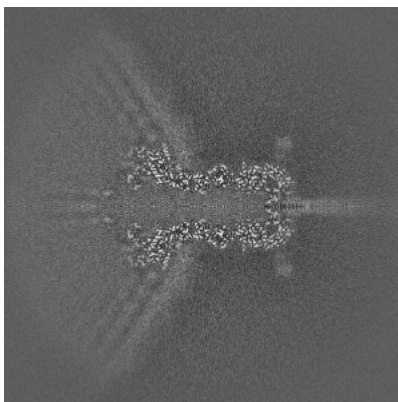
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

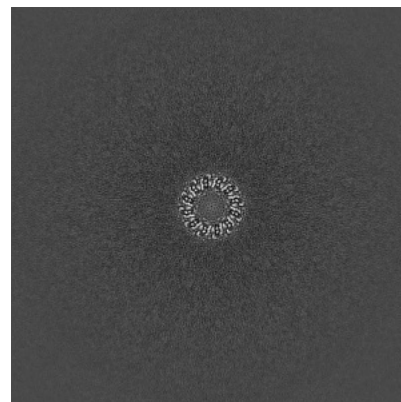
6.2.1 Primary map



X Index: 200

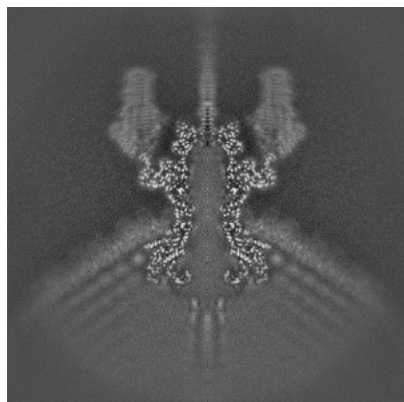


Y Index: 200

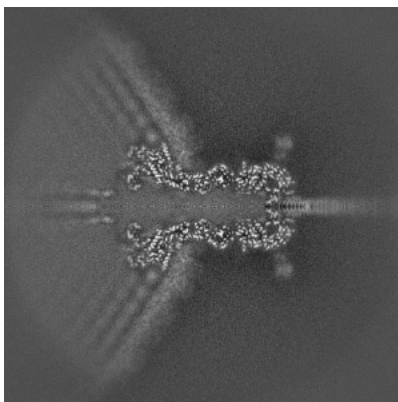


Z Index: 200

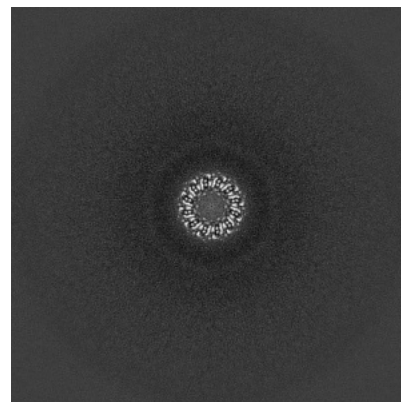
6.2.2 Raw map



X Index: 200



Y Index: 200

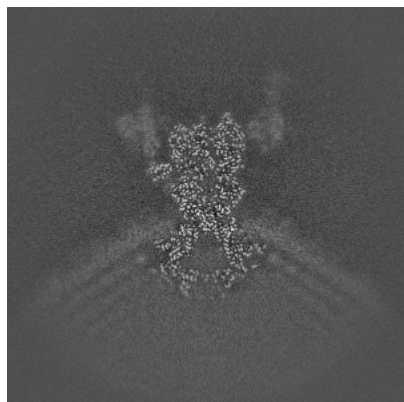


Z Index: 200

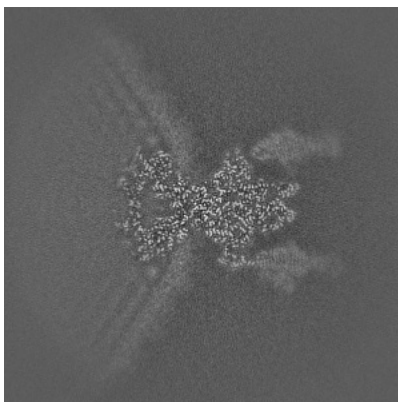
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

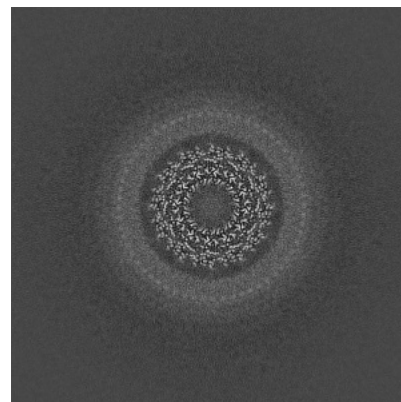
6.3.1 Primary map



X Index: 218

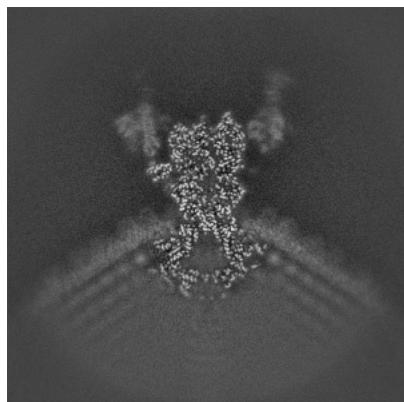


Y Index: 221

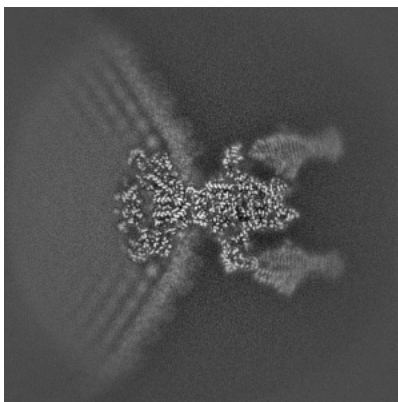


Z Index: 159

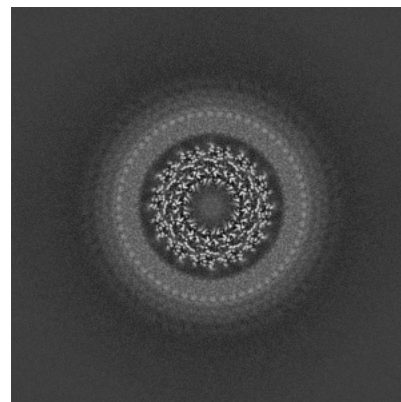
6.3.2 Raw map



X Index: 218



Y Index: 226

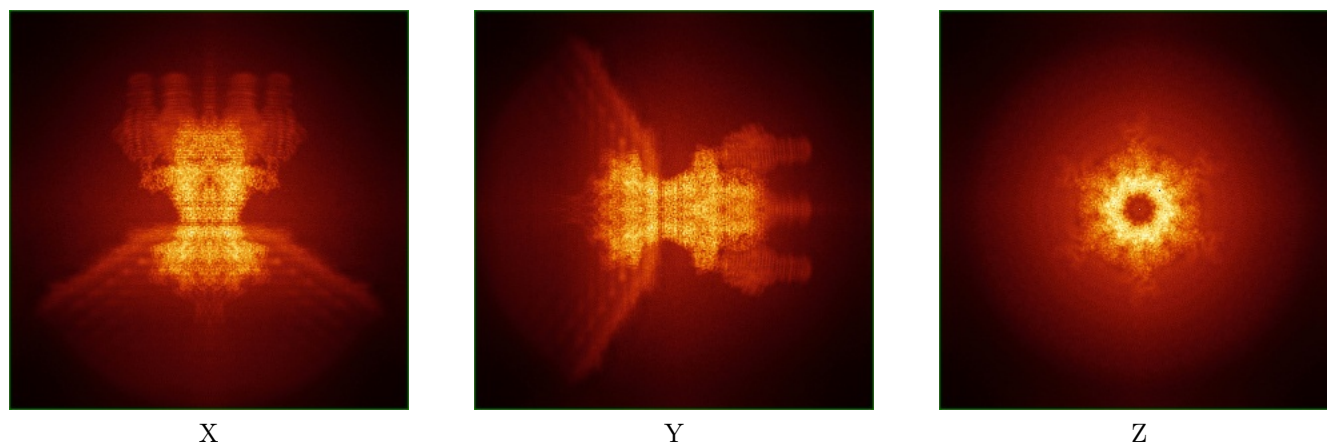


Z Index: 159

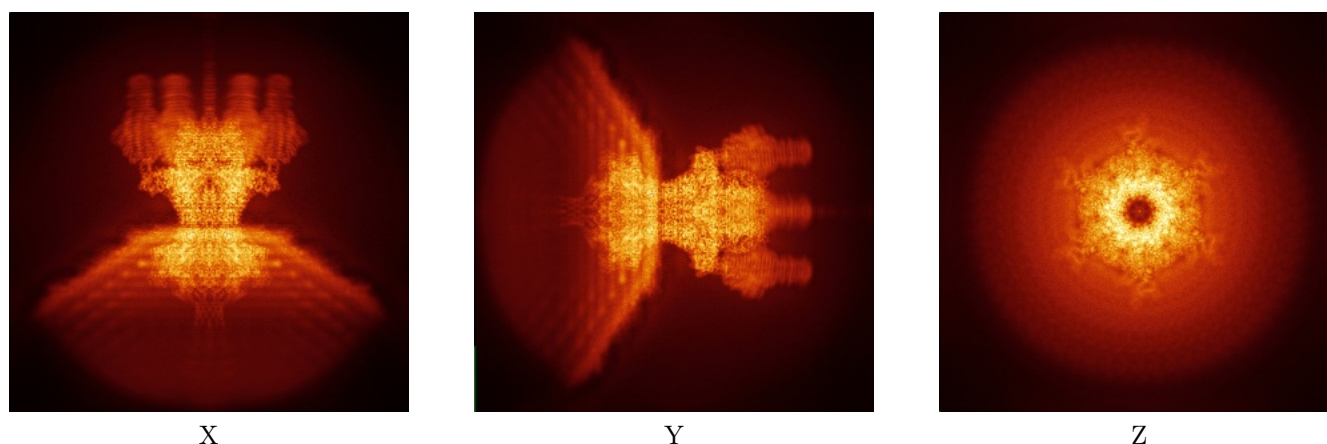
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

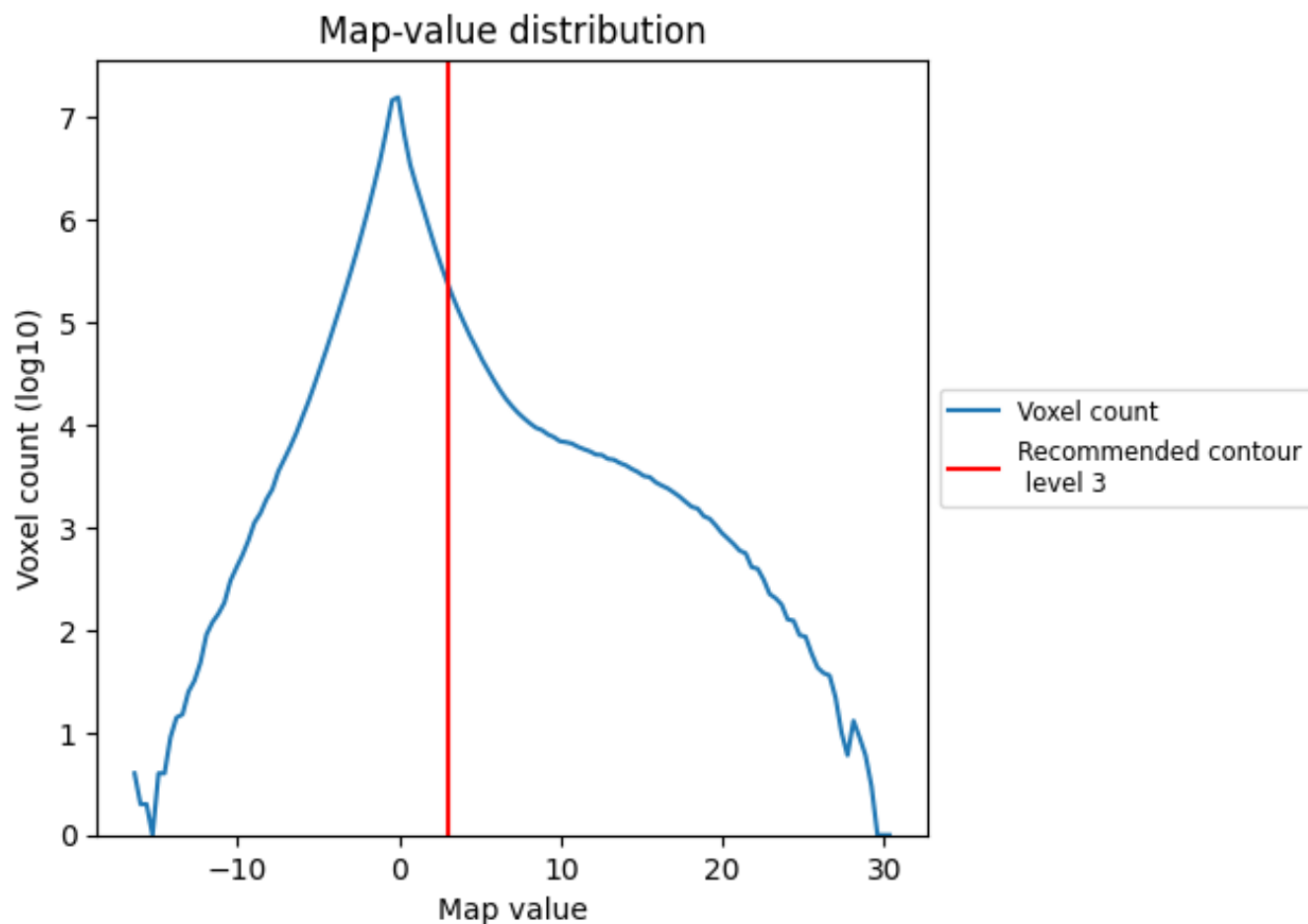
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

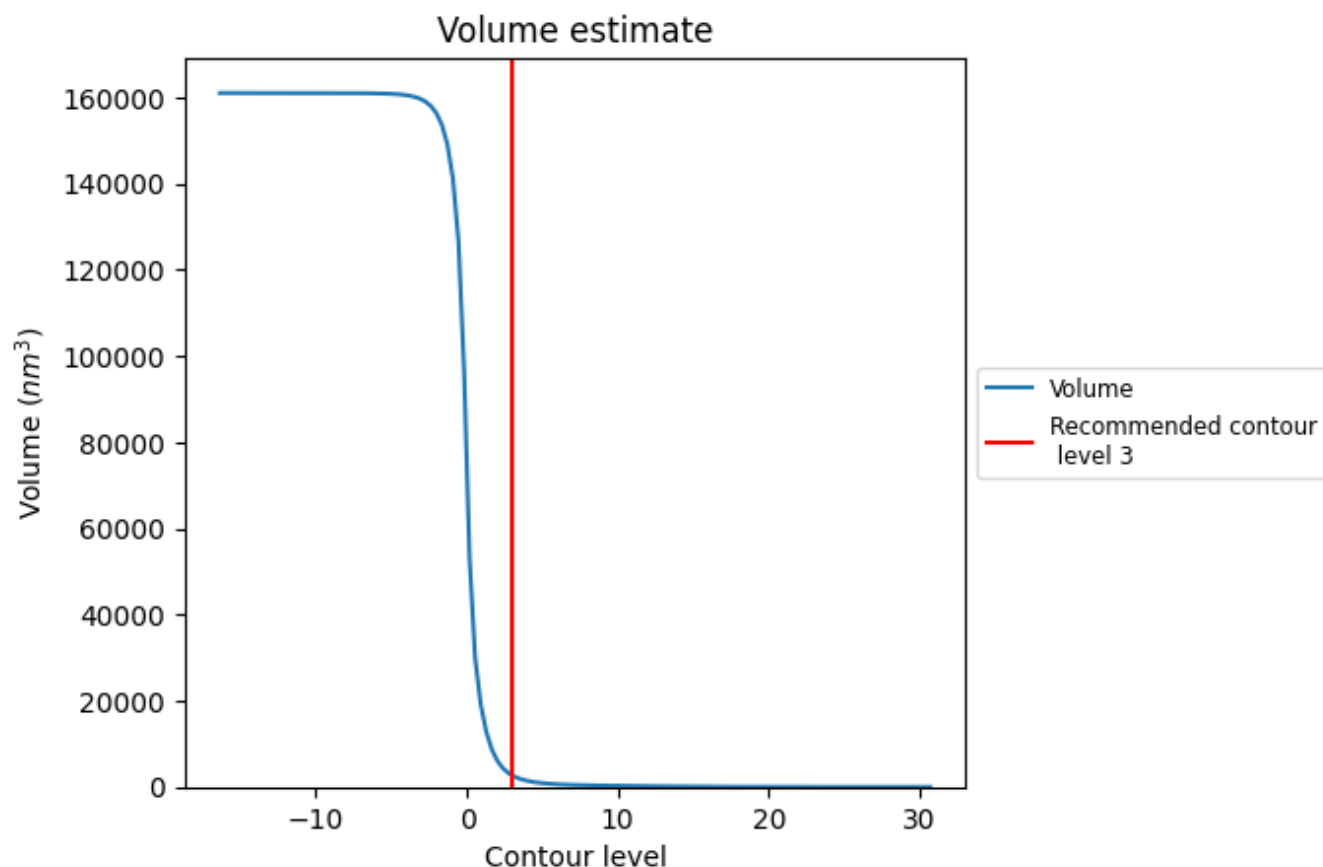
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

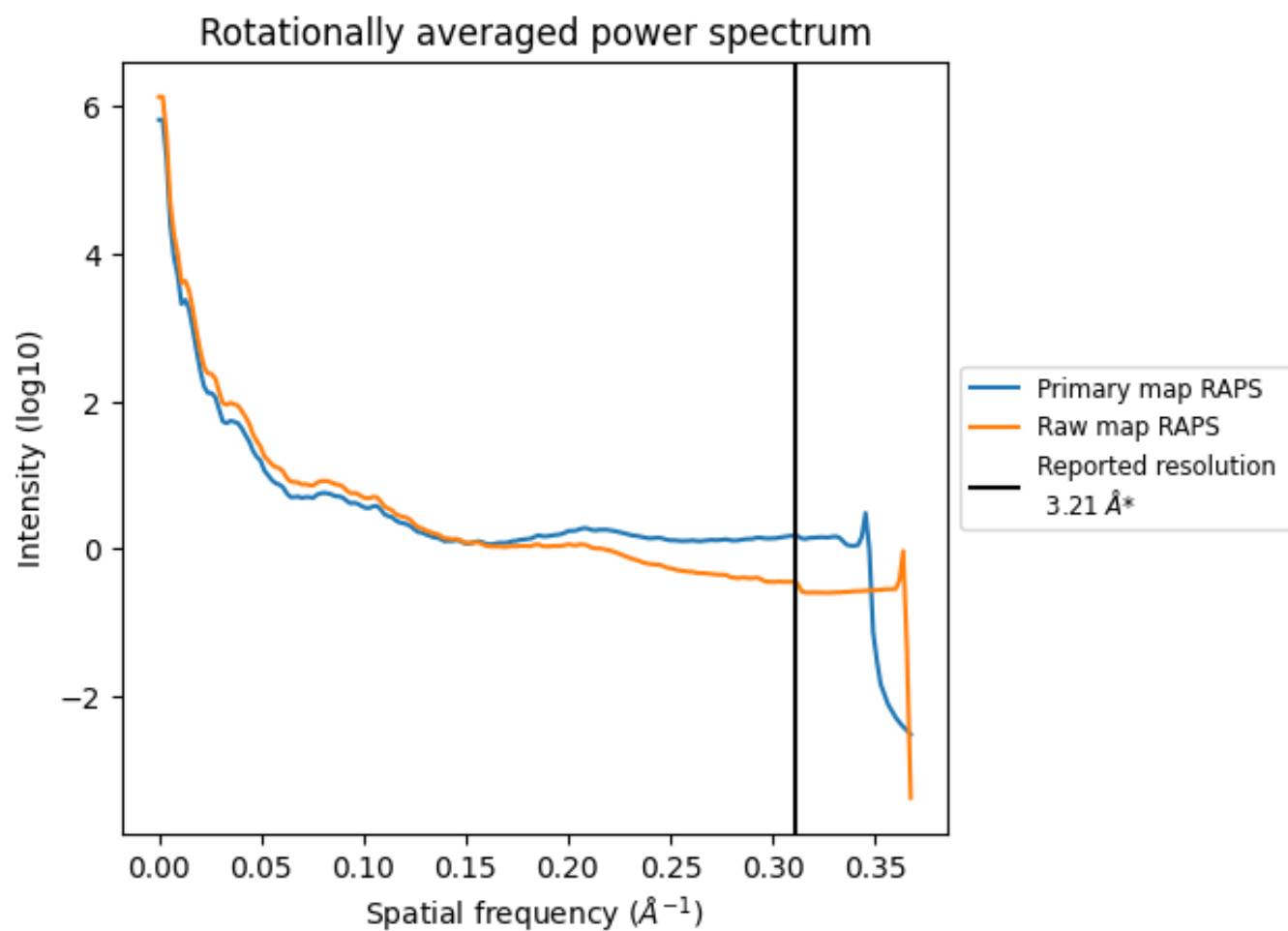
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2711 nm^3 ; this corresponds to an approximate mass of 2449 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

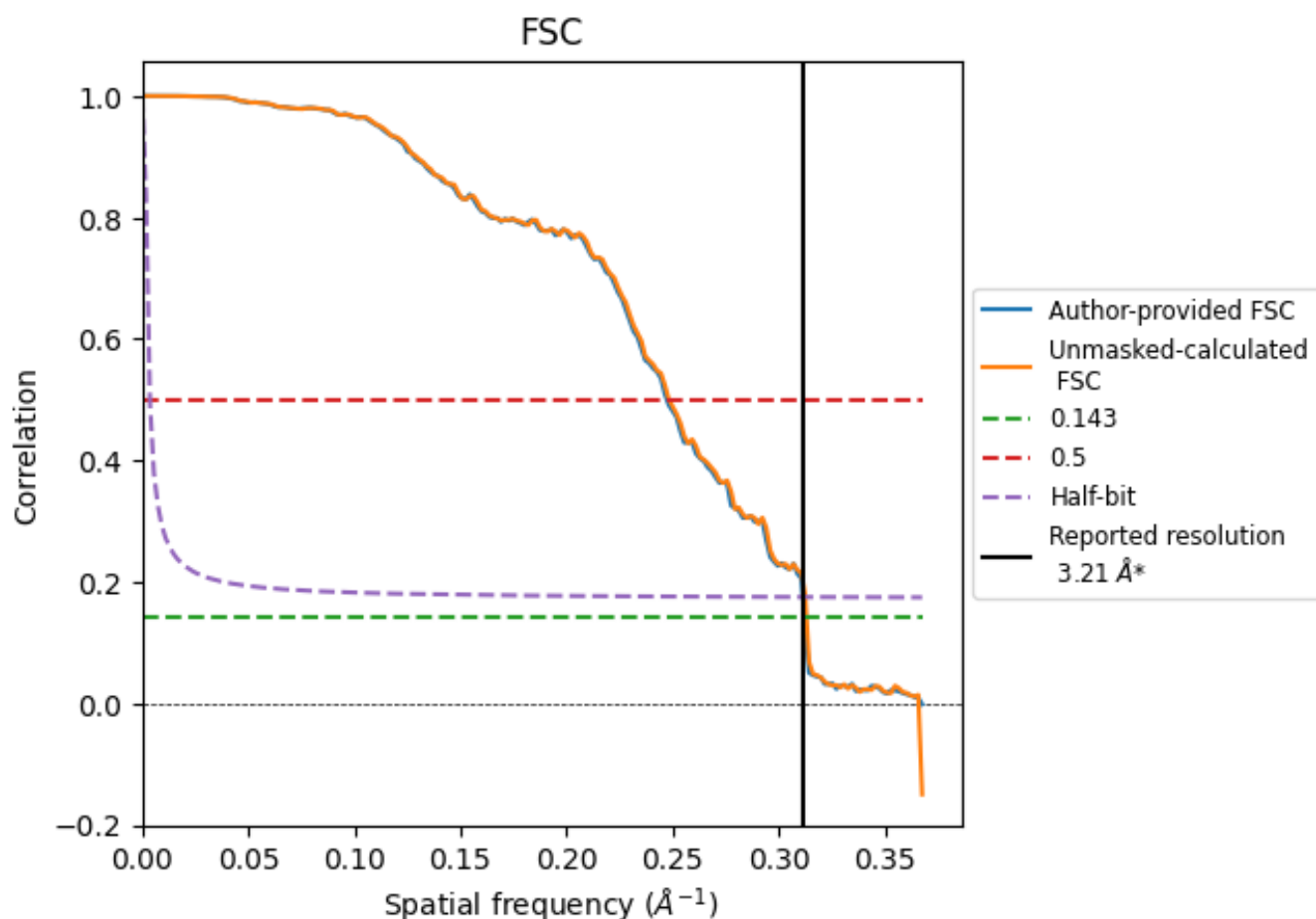


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	4.04	3.21
Unmasked-calculated*	3.19	4.03	3.20

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

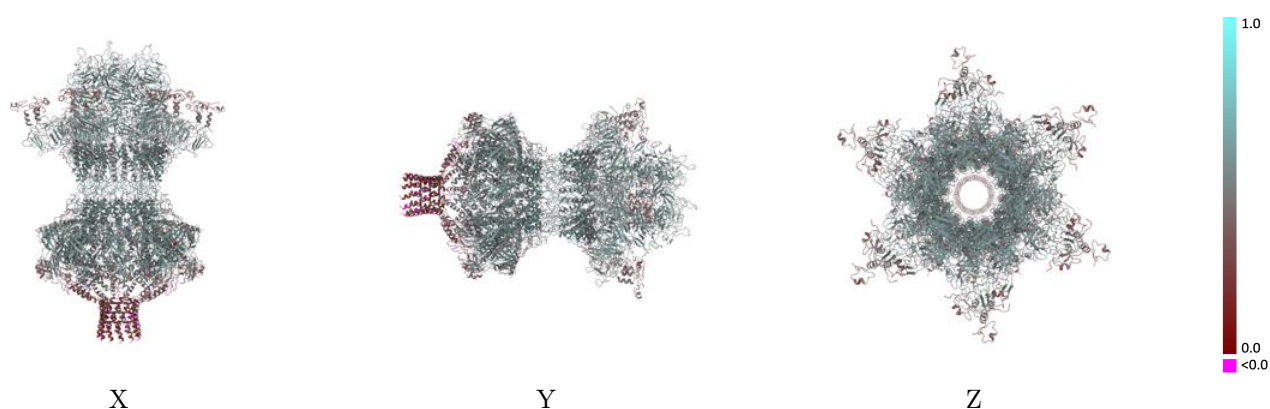
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61457 and PDB model 9JG6. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

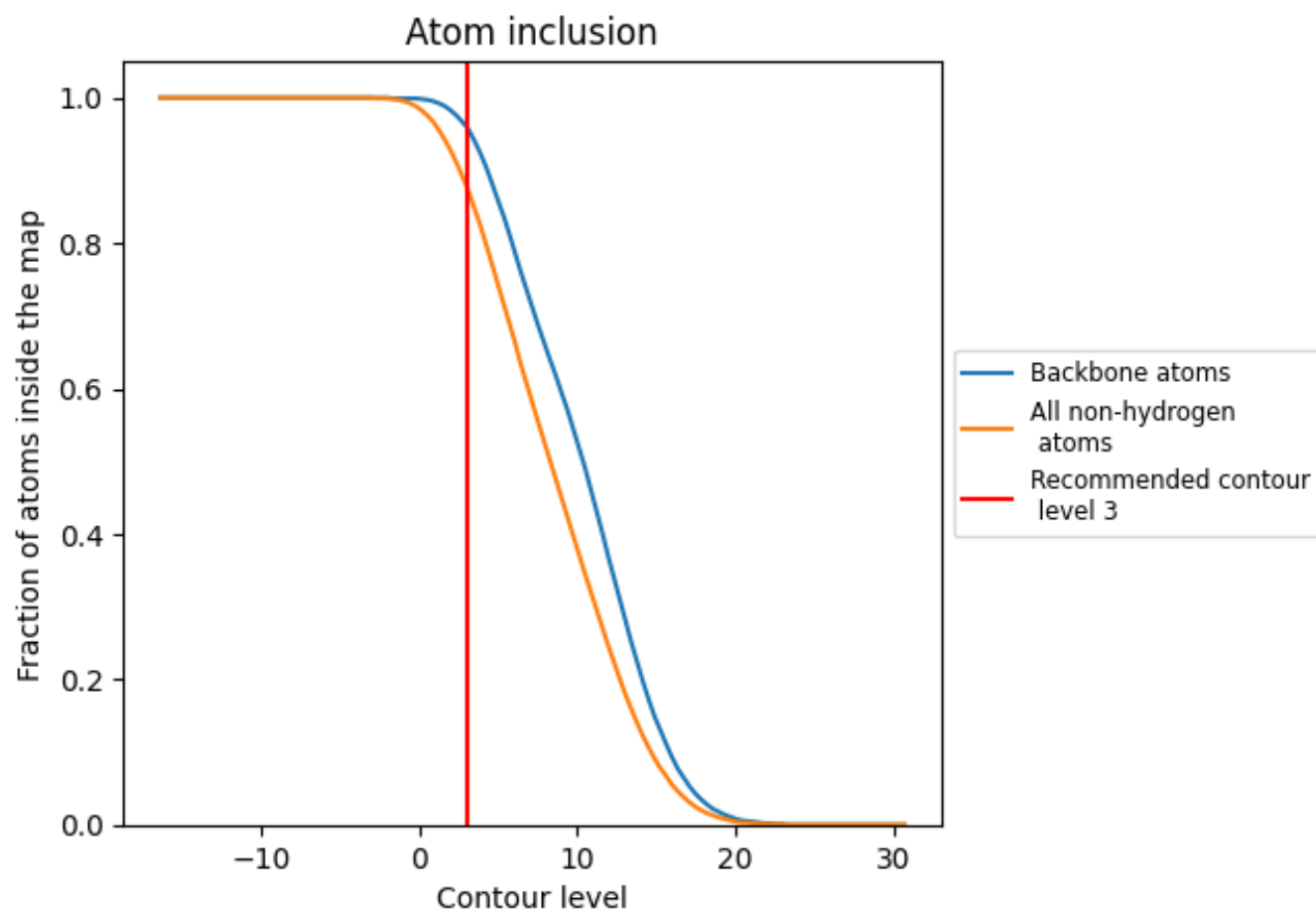


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.5000
A	 0.8420	 0.4860
B	 0.8400	 0.4910
C	 0.8400	 0.4850
D	 0.8440	 0.4880
E	 0.8420	 0.4870
F	 0.8380	 0.4870
G	 0.8440	 0.4850
H	 0.8410	 0.4910
I	 0.8420	 0.4850
J	 0.8460	 0.4910
K	 0.8450	 0.4880
L	 0.8410	 0.4870
M	 0.9190	 0.4780
N	 0.9180	 0.4780
O	 0.9180	 0.4810
P	 0.8950	 0.4530
Q	 0.8950	 0.4510
R	 0.8970	 0.4490
S	 0.8970	 0.4530
T	 0.8990	 0.4550
U	 0.9060	 0.4950
V	 0.9040	 0.4920
W	 0.9070	 0.4920
X	 0.9070	 0.4960
Y	 0.9000	 0.4970
Z	 0.9180	 0.4830
a	 0.9240	 0.5420
b	 0.9250	 0.5420
c	 0.9240	 0.5420
d	 0.9250	 0.5420
e	 0.9240	 0.5410
f	 0.9220	 0.5430
g	 0.9130	 0.5140
h	 0.9150	 0.5240



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Chain	Atom inclusion	Q-score
i	 0.9080	 0.5170
j	 0.9140	 0.5250
k	 0.9070	 0.5160
l	 0.9210	 0.5260
m	 0.9130	 0.5130
n	 0.9160	 0.5210
o	 0.9070	 0.5160
p	 0.9170	 0.5270
q	 0.9080	 0.5110
r	 0.9180	 0.5230
s	 0.9180	 0.4840
v	 0.9010	 0.4540
w	 0.9070	 0.4940
x	 0.9180	 0.4790