



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:27 PM UTC

PDB ID : 8KEC / pdb_00008kec
EMDB ID : EMD-37152
Title : Cyanophage A-1(L) tail fiber
Authors : Yu, R.C.; Li, Q.; Zhou, C.Z.
Deposited on : 2023-08-11
Resolution : 3.90 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

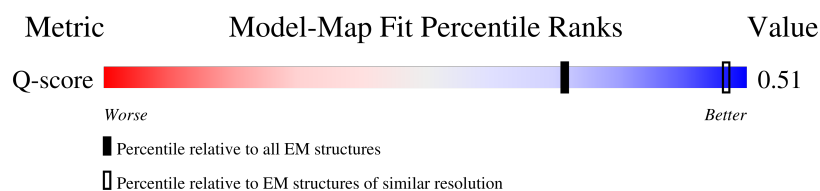
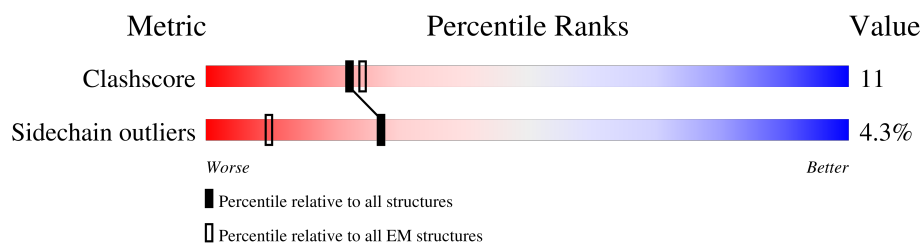
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

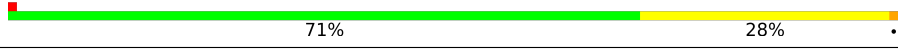
The reported resolution of this entry is 3.90 Å.

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.



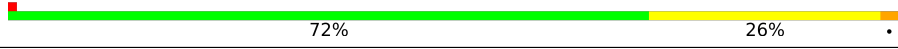
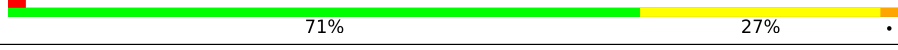
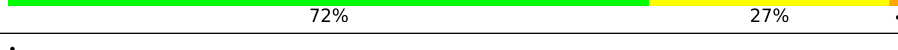
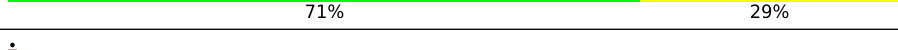
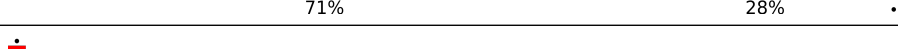
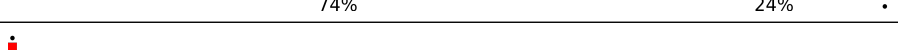
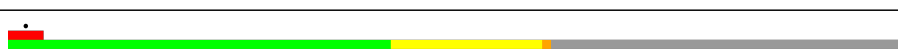
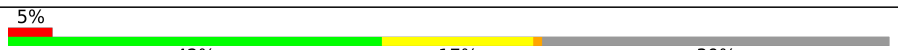
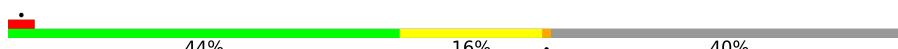
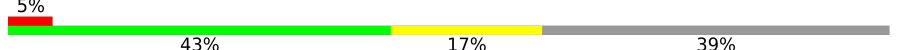
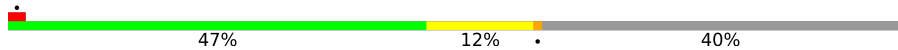
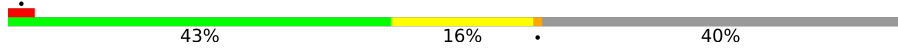
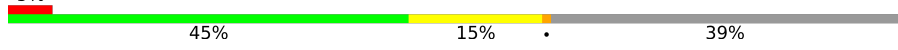
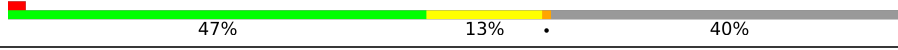
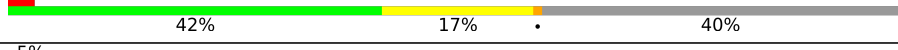
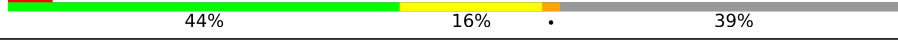
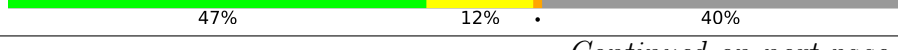
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	379	
1	B	379	
1	C	379	
1	D	379	
1	E	379	

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Mol	Chain	Length	Quality of chain
1	F	379	
1	G	379	
1	H	379	
1	I	379	
1	J	379	
1	K	379	
1	L	379	
1	M	379	
1	N	379	
1	O	379	
1	P	379	
1	Q	379	
1	R	379	
2	a	462	
2	b	462	
2	c	462	
2	d	462	
2	e	462	
2	f	462	
2	g	462	
2	h	462	
2	i	462	
2	j	462	
2	k	462	
2	l	462	

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Mol	Chain	Length	Quality of chain
2	m	462	42%16%40%
2	n	462	5% 43%16%39%
2	o	462	47%12%40%
2	p	462	45%14%40%
2	q	462	6% 44%15%39%
2	r	462	47%13%40%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 87756 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 Long tail fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	B	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	C	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	D	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	E	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	F	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	G	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	H	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	I	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	J	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	K	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	L	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	M	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	N	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	O	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		
1	P	379	Total	C	N	O	S	0	0
			2795	1744	491	558	2		
1	Q	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	378	Total	C	N	O	S	0	0
			2787	1739	490	557	1		

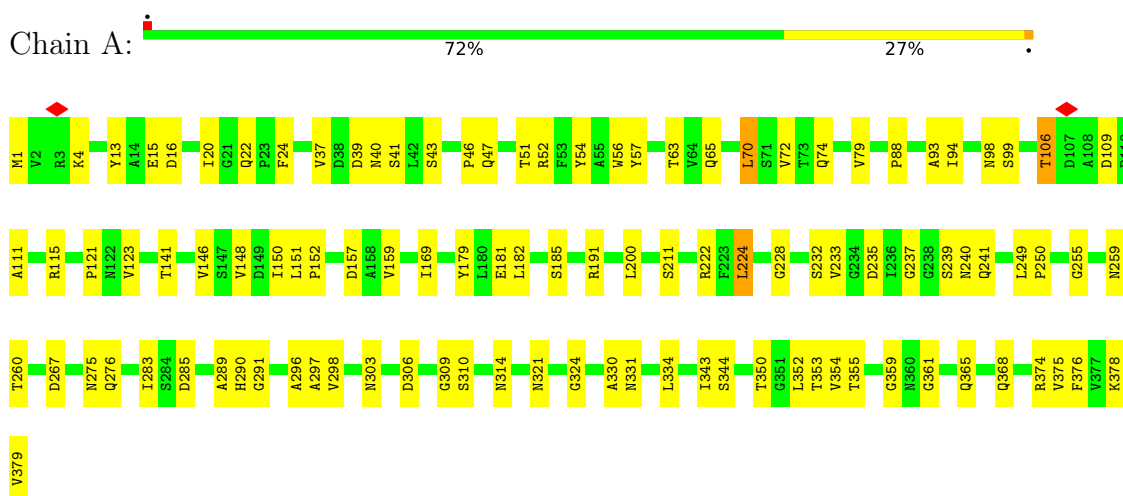
- Molecule 2 is a protein called short tail fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	n	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	i	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	j	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	k	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	l	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	m	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	o	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	p	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	q	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	r	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	a	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	b	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	c	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	d	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	e	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		
2	f	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	g	279	Total	C	N	O	S	0	0
			2083	1328	330	424	1		
2	h	280	Total	C	N	O	S	0	0
			2091	1333	331	425	2		

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.

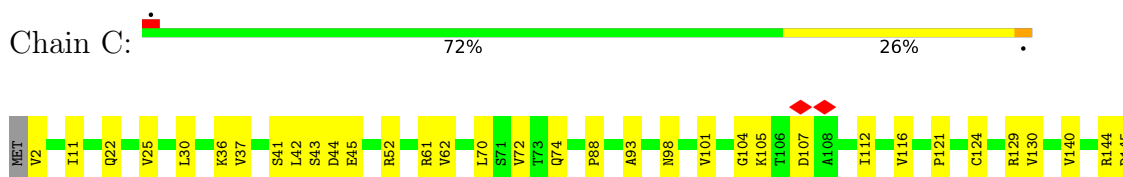
- Molecule 1: Long tail fiber

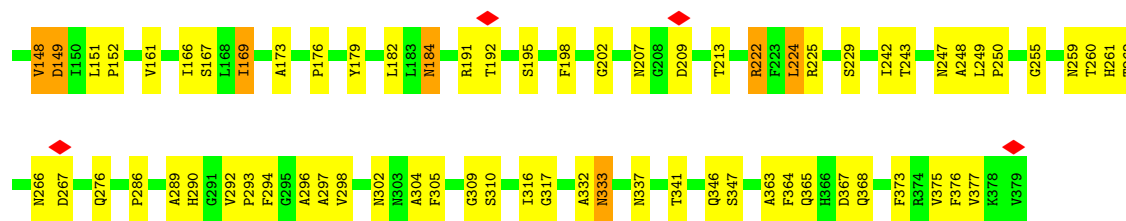


- Molecule 1: Long tail fiber

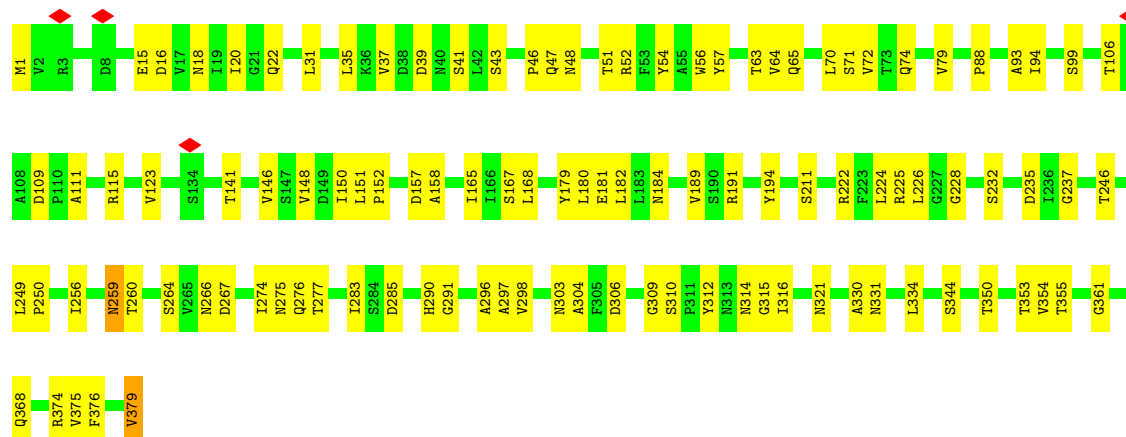


- Molecule 1: Long tail fiber

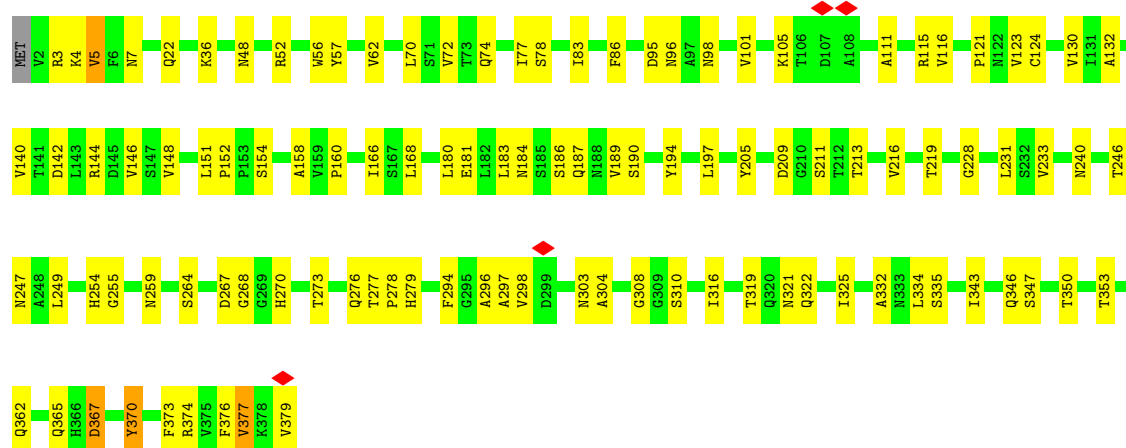




• Molecule 1: Long tail fiber

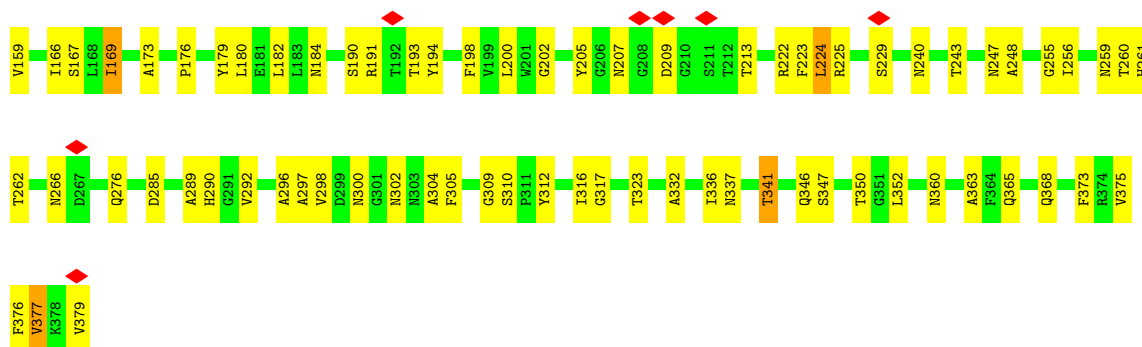


• Molecule 1: Long tail fiber

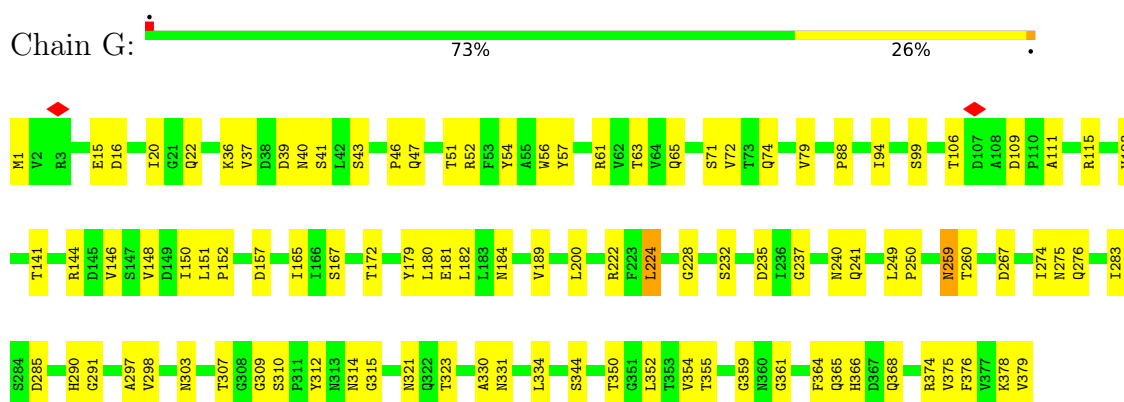


• Molecule 1: Long tail fiber

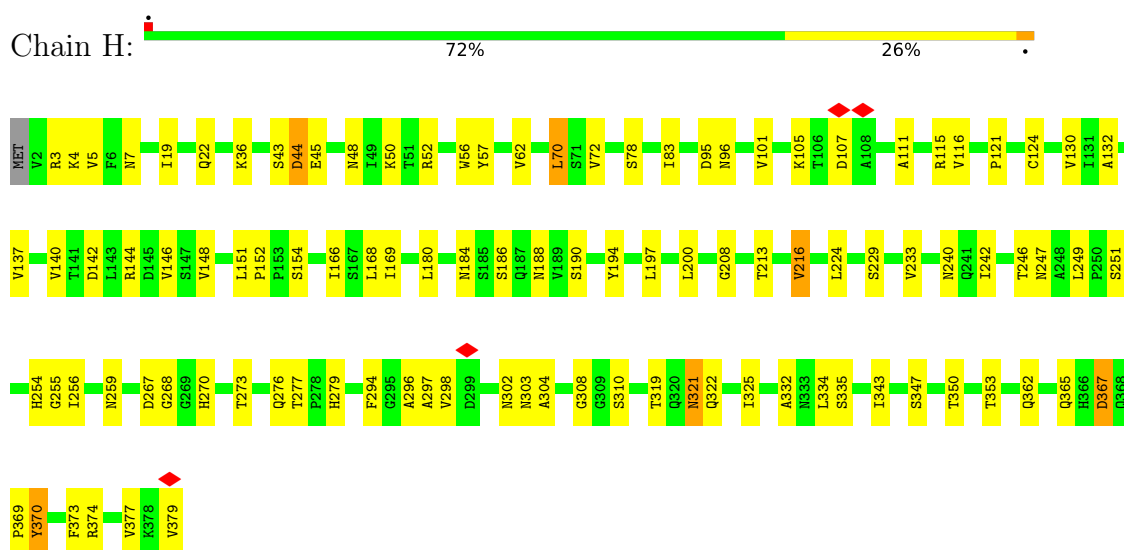




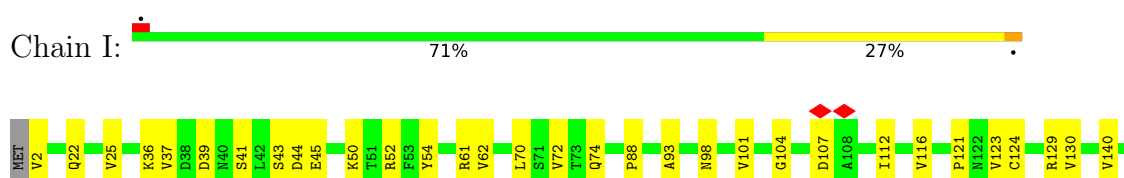
- Molecule 1: Long tail fiber

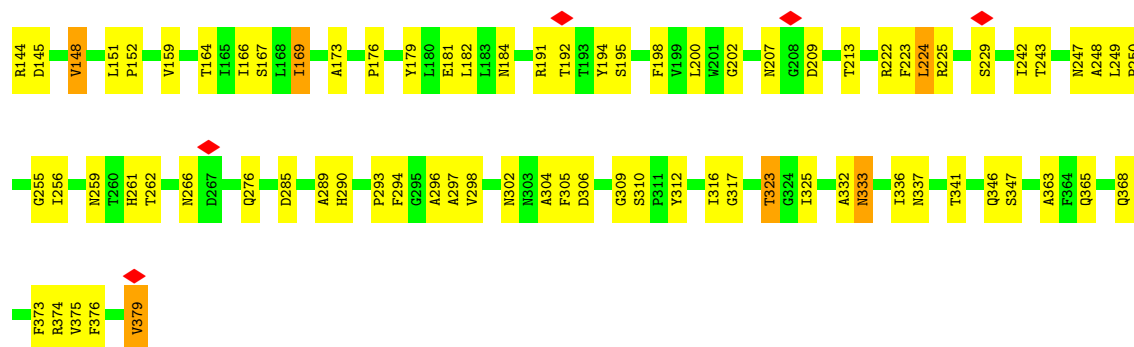


- Molecule 1: Long tail fiber



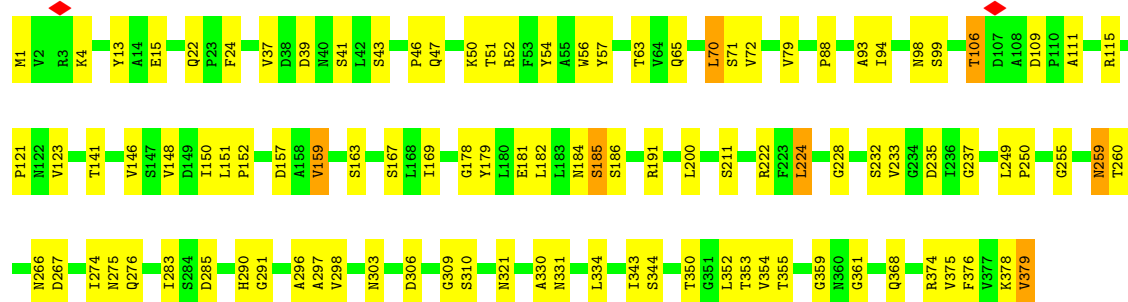
- Molecule 1: Long tail fiber





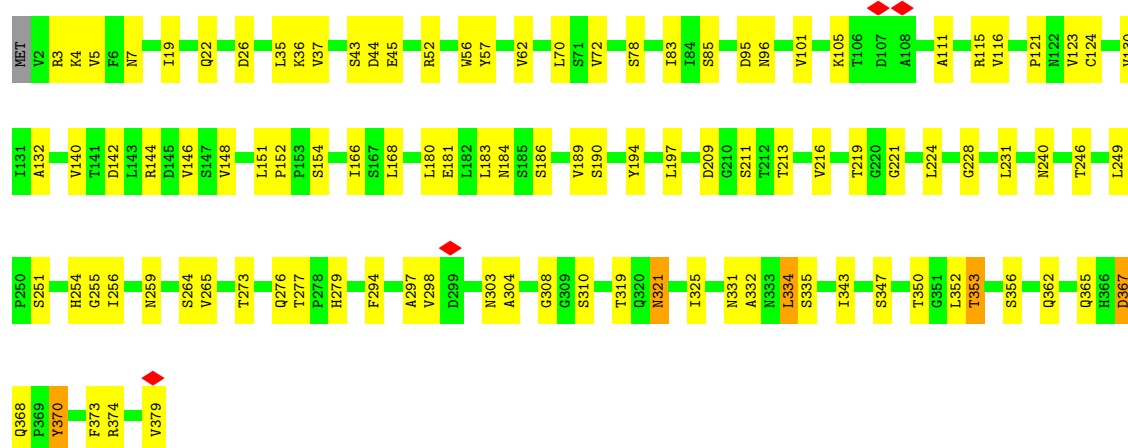
- Molecule 1: Long tail fiber

Chain J: 73% 25% .



- Molecule 1: Long tail fiber

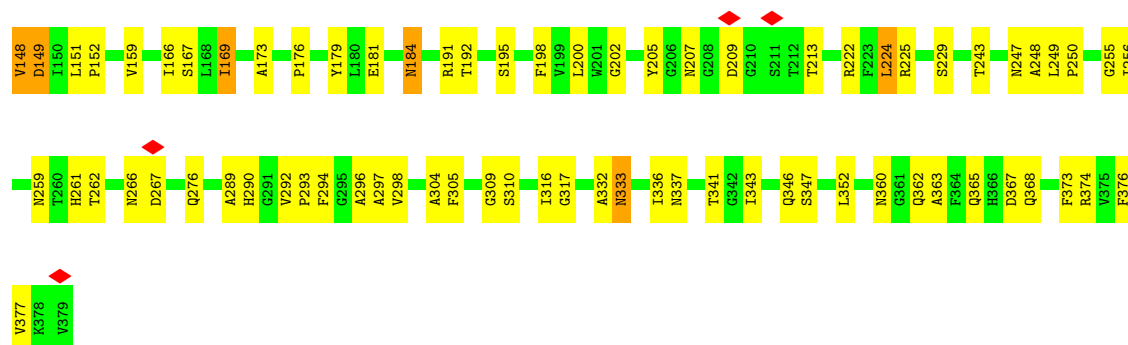
Chain K: 72% 26% .



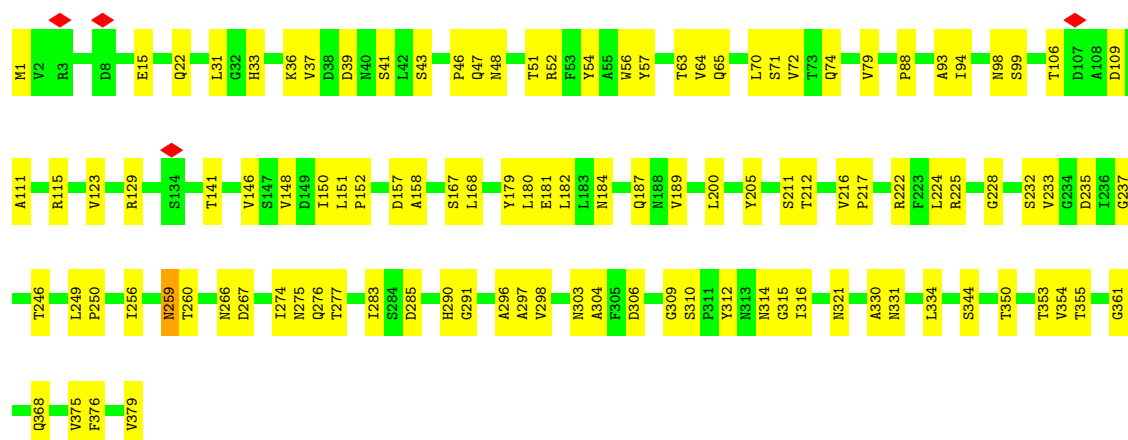
- Molecule 1: Long tail fiber

Chain L: 72% 27% .

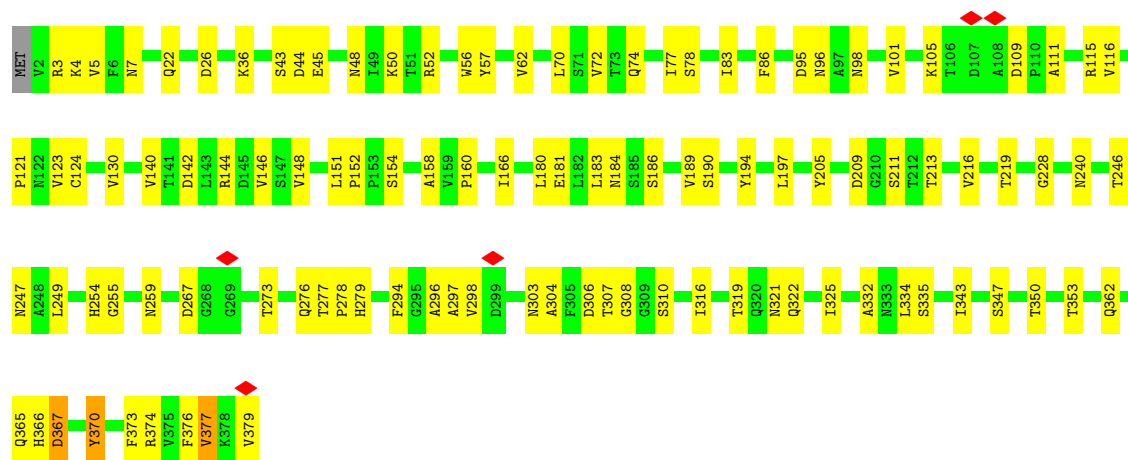




- Molecule 1: Long tail fiber

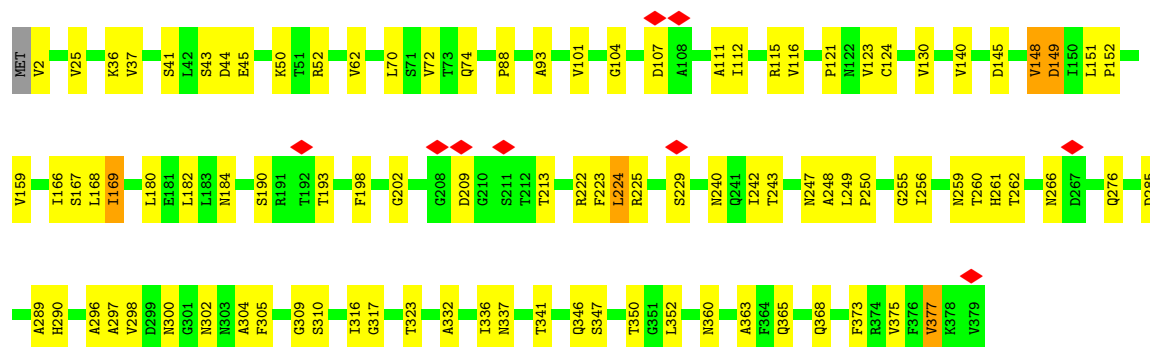


- Molecule 1: Long tail fiber



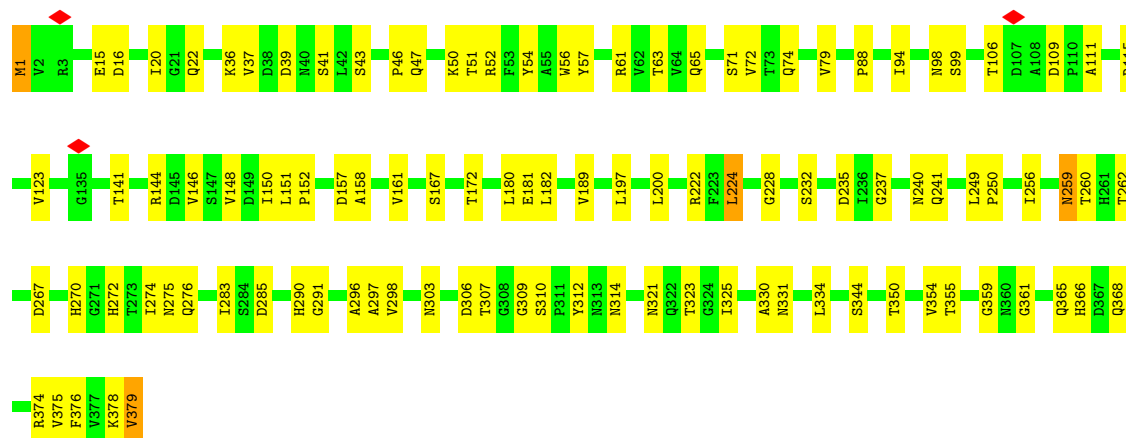
- Molecule 1: Long tail fiber





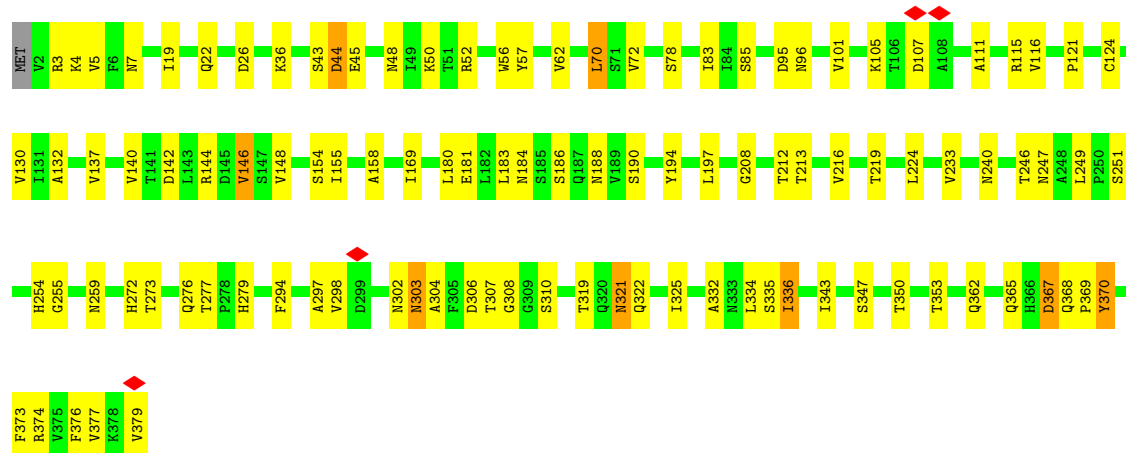
- Molecule 1: Long tail fiber

Chain P: 72% 27%



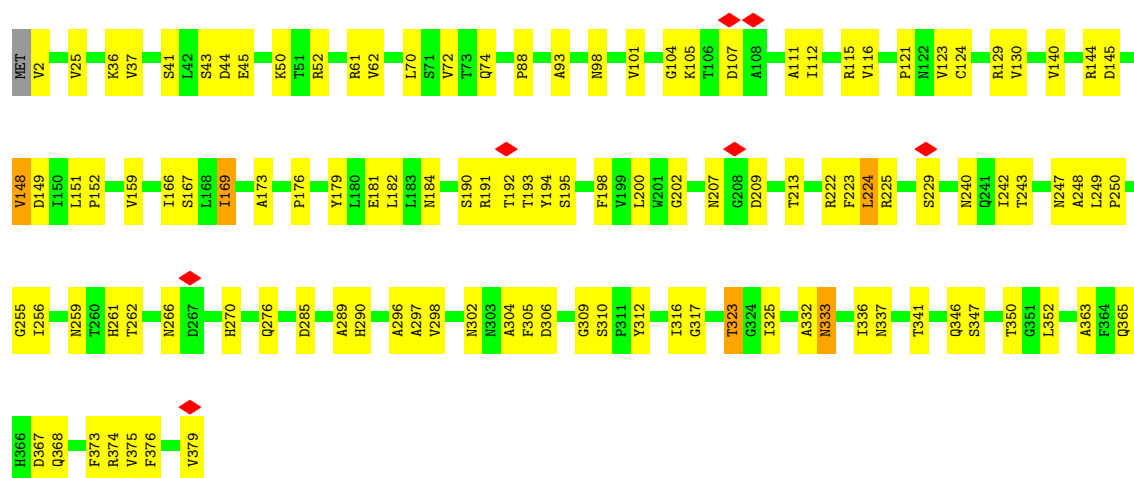
- Molecule 1: Long tail fiber

Chain Q: 72% 26%

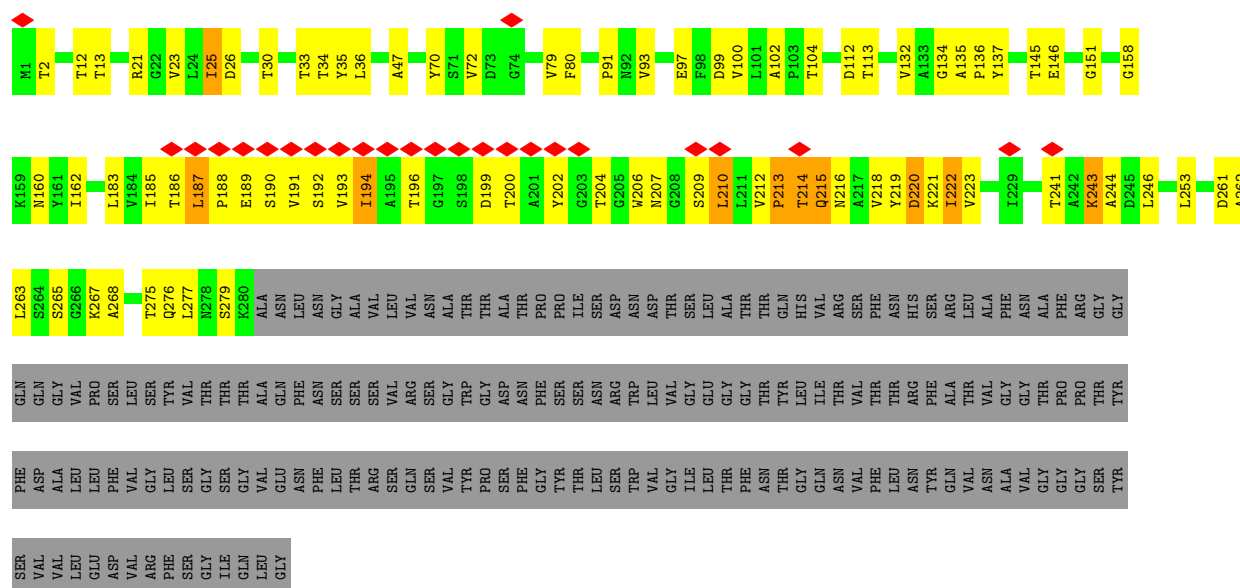
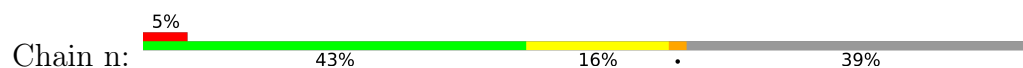


- Molecule 1: Long tail fiber

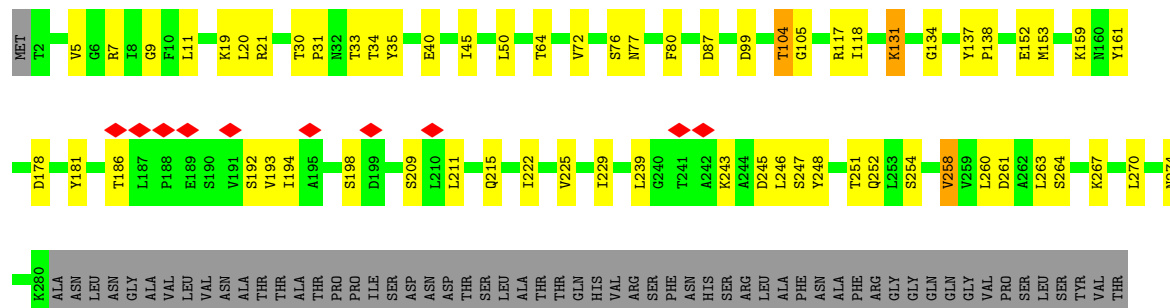
Chain R: 69% 29%



• Molecule 2: short tail fiber



• Molecule 2: short tail fiber

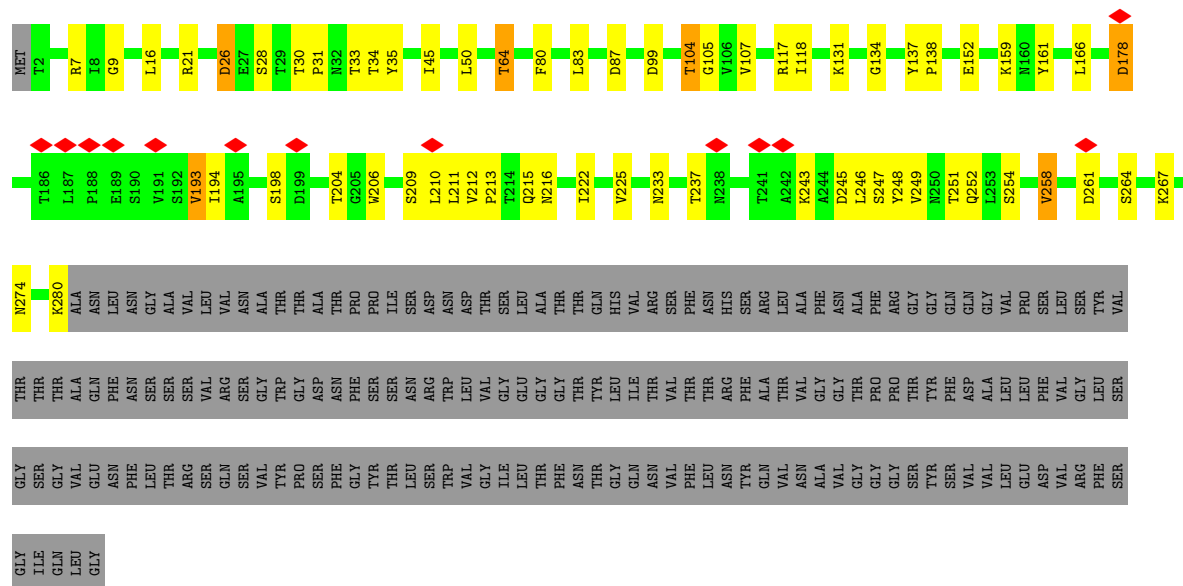




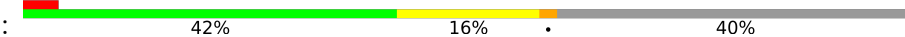
VAL PHE LEU ASN TYR GLN VAL ASN VAL ALA GLY GLY SER TYR VAL VAL LEU GLU ASP VAL ARG PHE SER GLY ILE GLN LEU GLY

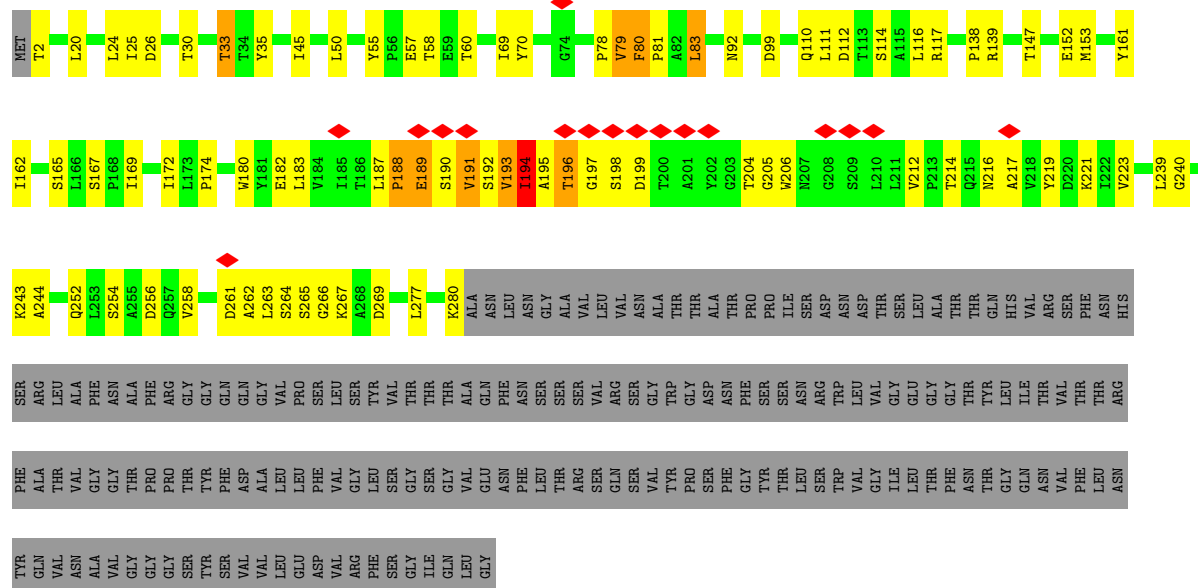
• Molecule 2: short tail fiber

Chain l:  47% 12% 40%



• Molecule 2: short tail fiber

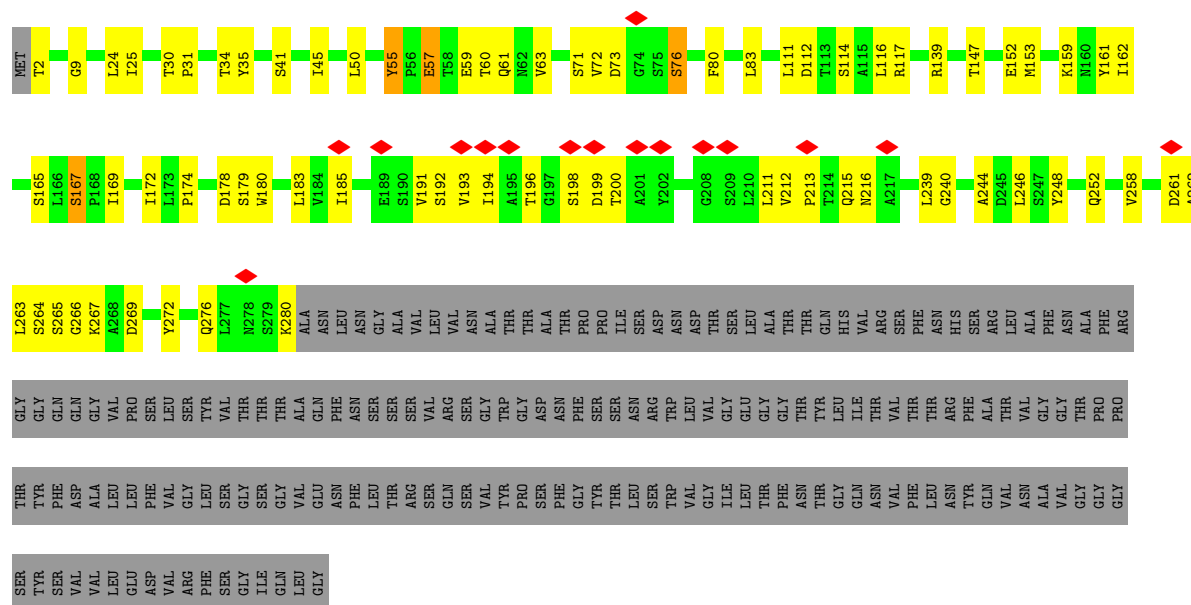
Chain m:  42% 16% 40%



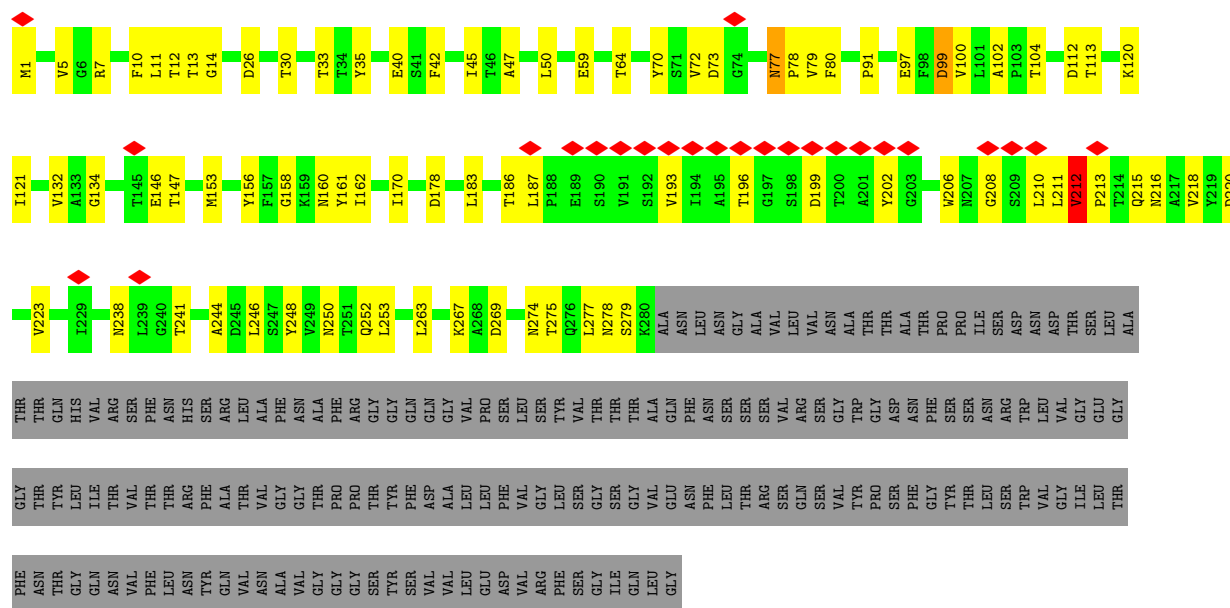
• Molecule 2: short tail fiber

Chain o:  47% 12% 40%





• Molecule 2: short tail fiber



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

TYR
GLN
VAL
ASN
ALA
VAL
GLY
GLY
GLY
SER
TYR
SER
VAL
VAL
LEU
GLU
ASP
VAL
ARG
PHE
SER
GLY
ILE
GLN
LEU
GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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	0/2859	0.30	0/3916
1	B	0.21	0/2851	0.36	0/3906
1	C	0.16	0/2851	0.32	0/3906
1	D	0.17	0/2859	0.30	0/3916
1	E	0.19	0/2851	0.37	0/3906
1	F	0.17	0/2851	0.32	0/3906
1	G	0.17	0/2859	0.30	0/3916
1	H	0.17	0/2851	0.32	0/3906
1	I	0.17	0/2851	0.32	0/3906
1	J	0.18	0/2859	0.32	0/3916
1	K	0.19	0/2851	0.34	0/3906
1	L	0.17	0/2851	0.32	0/3906
1	M	0.17	0/2859	0.31	0/3916
1	N	0.23	0/2851	0.39	0/3906
1	O	0.17	0/2851	0.33	0/3906
1	P	0.17	0/2859	0.30	0/3916
1	Q	0.17	0/2851	0.33	0/3906
1	R	0.17	0/2851	0.33	0/3906
2	a	0.20	0/2122	0.50	4/2914 (0.1%)
2	b	0.22	0/2130	0.57	6/2924 (0.2%)
2	c	0.19	0/2122	0.43	1/2914 (0.0%)
2	d	0.21	0/2122	0.51	3/2914 (0.1%)
2	e	0.22	0/2130	0.55	5/2924 (0.2%)
2	f	0.19	0/2122	0.43	1/2914 (0.0%)
2	g	0.22	0/2122	0.55	7/2914 (0.2%)
2	h	0.23	0/2130	0.55	5/2924 (0.2%)
2	i	0.21	0/2122	0.46	3/2914 (0.1%)
2	j	0.22	0/2122	0.52	1/2914 (0.0%)
2	k	0.22	0/2130	0.55	1/2924 (0.0%)
2	l	0.20	0/2122	0.44	1/2914 (0.0%)
2	m	0.30	1/2122 (0.0%)	0.59	5/2914 (0.2%)
2	n	0.26	0/2130	0.63	3/2924 (0.1%)
2	o	0.22	0/2122	0.46	1/2914 (0.0%)
2	p	0.26	1/2122 (0.0%)	0.54	4/2914 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	q	0.21	0/2130	0.51	3/2924 (0.1%)
2	r	0.21	0/2122	0.47	4/2914 (0.1%)
All	All	0.20	2/89610 (0.0%)	0.42	58/122880 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	p	81	PRO	N-CD	6.02	1.56	1.47
2	m	187	LEU	C-N	5.48	1.38	1.33

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	79	VAL	N-CA-C	-9.85	99.32	110.05
2	e	79	VAL	N-CA-C	-9.82	99.35	110.05
2	g	79	VAL	N-CA-C	-9.36	99.84	110.05
2	b	79	VAL	N-CA-C	-9.26	99.95	110.05
2	h	79	VAL	N-CA-C	-8.43	100.86	110.05
2	p	79	VAL	N-CA-C	-8.42	97.50	109.63
2	n	215	GLN	N-CA-C	8.22	121.86	110.35
2	j	80	PHE	N-CA-C	7.51	126.42	109.81
2	n	214	THR	N-CA-C	-7.25	101.49	111.28
2	b	212	VAL	N-CA-C	7.14	120.91	112.35
2	b	77	ASN	CA-C-N	-6.83	112.73	119.90
2	b	77	ASN	C-N-CA	-6.83	112.73	119.90
2	h	77	ASN	CA-C-N	-6.76	112.80	119.90
2	h	77	ASN	C-N-CA	-6.76	112.80	119.90
2	e	77	ASN	CA-C-N	-6.75	112.82	119.90
2	e	77	ASN	C-N-CA	-6.75	112.82	119.90
2	i	80	PHE	N-CA-C	6.51	124.20	109.81
2	f	80	PHE	N-CA-C	6.43	122.45	113.57
2	a	80	PHE	N-CA-C	6.32	123.77	109.81
2	g	80	PHE	N-CA-C	6.17	123.45	109.81
2	d	55	TYR	CA-C-N	-6.15	113.44	119.78
2	d	55	TYR	C-N-CA	-6.15	113.44	119.78
2	o	80	PHE	N-CA-C	6.12	123.34	109.81
2	k	80	PHE	N-CA-C	6.11	123.30	109.81
2	m	80	PHE	N-CA-C	6.06	123.21	109.81
2	p	55	TYR	CA-C-N	-6.00	113.60	119.78
2	p	55	TYR	C-N-CA	-6.00	113.60	119.78
2	q	80	PHE	N-CA-C	5.98	123.03	109.81
2	n	213	PRO	N-CA-C	5.89	124.61	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	188	PRO	N-CA-C	5.84	119.80	110.21
2	m	191	VAL	CB-CA-C	5.80	119.06	111.81
2	m	79	VAL	N-CA-C	-5.79	101.55	109.37
2	d	80	PHE	N-CA-C	5.76	122.54	109.81
2	c	80	PHE	N-CA-C	5.75	122.52	109.81
2	g	55	TYR	CA-C-N	-5.75	113.77	119.92
2	g	55	TYR	C-N-CA	-5.75	113.77	119.92
2	b	30	THR	N-CA-C	-5.66	102.46	109.64
2	h	80	PHE	N-CA-C	5.63	122.26	109.81
2	b	80	PHE	N-CA-C	5.59	119.14	108.97
2	q	79	VAL	N-CA-C	-5.55	99.24	107.51
2	r	81	PRO	N-CA-C	-5.54	107.59	114.68
2	e	80	PHE	N-CA-C	5.50	121.96	109.81
2	l	80	PHE	N-CA-C	5.43	121.80	109.81
2	a	30	THR	CA-C-N	-5.41	114.22	119.90
2	a	30	THR	C-N-CA	-5.41	114.22	119.90
2	m	194	ILE	N-CA-C	5.35	120.47	109.34
2	i	77	ASN	CA-C-N	-5.31	113.82	119.98
2	i	77	ASN	C-N-CA	-5.31	113.82	119.98
2	q	212	VAL	N-CA-C	5.22	120.16	108.88
2	r	80	PHE	CA-C-N	-5.22	114.99	120.94
2	r	80	PHE	C-N-CA	-5.22	114.99	120.94
2	h	213	PRO	N-CA-C	5.17	123.11	112.47
2	r	80	PHE	N-CA-C	5.15	121.19	109.81
2	g	28	SER	N-CA-C	-5.09	106.33	112.54
2	g	30	THR	CA-C-N	-5.08	114.39	120.13
2	g	30	THR	C-N-CA	-5.08	114.39	120.13
2	p	59	GLU	N-CA-C	5.08	116.67	111.03
2	e	212	VAL	N-CA-C	5.08	119.85	108.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2795	0	2708	92	0
1	B	2787	0	2696	81	0
1	C	2787	0	2696	84	0
1	D	2795	0	2708	101	0
1	E	2787	0	2696	93	0
1	F	2787	0	2696	83	0
1	G	2795	0	2708	94	0
1	H	2787	0	2696	87	0
1	I	2787	0	2696	85	0
1	J	2795	0	2708	100	0
1	K	2787	0	2696	87	0
1	L	2787	0	2696	86	0
1	M	2795	0	2708	108	0
1	N	2787	0	2696	93	0
1	O	2787	0	2696	81	0
1	P	2795	0	2708	102	0
1	Q	2787	0	2696	89	0
1	R	2787	0	2696	96	0
2	a	2083	0	2082	64	0
2	b	2091	0	2094	69	0
2	c	2083	0	2082	62	0
2	d	2083	0	2082	66	0
2	e	2091	0	2094	66	0
2	f	2083	0	2082	48	0
2	g	2083	0	2082	64	0
2	h	2091	0	2094	53	0
2	i	2083	0	2082	54	0
2	j	2083	0	2082	66	0
2	k	2091	0	2094	73	0
2	l	2083	0	2082	61	0
2	m	2083	0	2082	78	0
2	n	2091	0	2094	91	0
2	o	2083	0	2082	54	0
2	p	2083	0	2082	53	0
2	q	2091	0	2094	54	0
2	r	2083	0	2082	49	0
All	All	87756	0	86148	1984	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 11.

All (1984) 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:N:45:GLU:HB2	1:N:48:ASN:OD1	1.34	1.26
1:J:39:ASP:OD1	1:J:50:LYS:HD2	1.43	1.18
2:n:223:VAL:HG11	2:m:221:LYS:NZ	1.58	1.16
2:k:198:SER:HB3	2:k:212:VAL:CG2	1.76	1.15
1:P:39:ASP:OD1	1:P:50:LYS:HD2	1.53	1.08
2:d:30:THR:OG1	2:d:31:PRO:HD3	1.53	1.06
2:g:30:THR:OG1	2:g:31:PRO:HD3	1.54	1.05
2:k:213:PRO:HG3	2:l:212:VAL:CG1	1.89	1.01
2:n:223:VAL:HG11	2:m:221:LYS:HZ3	1.20	0.96
2:n:263:LEU:HD21	2:m:263:LEU:HD21	1.47	0.95
2:n:223:VAL:HG11	2:m:221:LYS:CE	1.95	0.95
2:k:198:SER:HB3	2:k:212:VAL:HG22	1.44	0.94
2:k:198:SER:HB3	2:k:212:VAL:HG21	1.50	0.93
1:P:39:ASP:OD2	1:P:54:TYR:HE2	1.50	0.93
2:k:197:GLY:O	2:k:212:VAL:HG21	1.69	0.92
1:M:129:ARG:NH2	2:n:275:THR:CG2	2.33	0.92
1:J:39:ASP:OD2	1:J:54:TYR:HE2	1.51	0.92
2:n:223:VAL:CG1	2:m:221:LYS:HE2	2.01	0.91
2:n:223:VAL:CG1	2:m:221:LYS:NZ	2.35	0.88
1:J:39:ASP:OD1	1:J:50:LYS:CD	2.22	0.88
1:N:45:GLU:CB	1:N:48:ASN:OD1	2.22	0.87
2:e:202:TYR:HB2	2:e:218:VAL:HG11	1.56	0.86
1:J:39:ASP:OD2	1:J:54:TYR:CE2	2.28	0.85
1:M:290:HIS:HA	1:N:321:ASN:HD21	1.42	0.85
1:P:39:ASP:OD2	1:P:54:TYR:CE2	2.29	0.84
1:D:290:HIS:HA	1:E:321:ASN:HD21	1.42	0.84
2:g:211:LEU:H	2:h:216:ASN:HB2	1.41	0.83
2:n:223:VAL:CG1	2:m:221:LYS:CE	2.56	0.83
1:A:290:HIS:HA	1:B:321:ASN:HD21	1.42	0.82
2:k:213:PRO:HG3	2:l:212:VAL:HG11	1.63	0.81
1:D:297:ALA:H	1:F:310:SER:HB3	1.46	0.80
1:P:290:HIS:HA	1:Q:321:ASN:HD21	1.45	0.80
1:G:314:ASN:OD1	1:G:315:GLY:N	2.14	0.80
2:d:211:LEU:H	2:e:216:ASN:HB2	1.44	0.80
2:d:159:LYS:HA	2:d:159:LYS:HE3	1.64	0.79
1:J:290:HIS:HA	1:K:321:ASN:HD21	1.44	0.79
2:p:211:LEU:H	2:q:216:ASN:HB2	1.47	0.78
1:P:39:ASP:OD1	1:P:50:LYS:CD	2.31	0.78
1:I:45:GLU:N	1:I:45:GLU:OE2	2.18	0.77
1:G:290:HIS:HA	1:H:321:ASN:HD21	1.46	0.77
1:M:98:ASN:ND2	2:n:279:SER:HA	2.00	0.77
2:b:97:GLU:N	2:b:97:GLU:OE2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:97:GLU:OE2	2:e:97:GLU:N	2.17	0.76
1:P:297:ALA:H	1:R:310:SER:HB3	1.48	0.76
2:c:30:THR:HB	2:c:31:PRO:HD2	1.67	0.76
1:R:45:GLU:N	1:R:45:GLU:OE2	2.17	0.76
2:n:223:VAL:HG13	2:m:221:LYS:HE2	1.68	0.76
2:b:7:ARG:HD2	2:c:30:THR:OG1	1.86	0.76
2:n:158:GLY:HA3	2:m:191:VAL:HB	1.68	0.76
2:q:97:GLU:N	2:q:97:GLU:OE2	2.18	0.75
1:O:45:GLU:N	1:O:45:GLU:OE2	2.20	0.75
1:C:45:GLU:N	1:C:45:GLU:OE2	2.20	0.74
1:Q:322:GLN:NE2	1:R:285:ASP:O	2.20	0.74
1:G:297:ALA:H	1:I:310:SER:HB3	1.51	0.74
1:N:74:GLN:OE1	2:n:265:SER:HB2	1.87	0.74
2:k:97:GLU:N	2:k:97:GLU:OE2	2.18	0.74
2:g:159:LYS:HA	2:g:159:LYS:HE3	1.70	0.74
2:n:134:GLY:HA3	2:o:134:GLY:HA3	1.69	0.74
1:M:310:SER:HB3	1:N:297:ALA:H	1.52	0.74
1:P:1:MET:SD	1:P:1:MET:N	2.52	0.74
1:L:45:GLU:N	1:L:45:GLU:OE2	2.20	0.74
1:M:129:ARG:HH22	2:n:275:THR:HG22	1.52	0.74
2:g:194:ILE:HB	2:h:193:VAL:HA	1.69	0.73
2:h:97:GLU:OE2	2:h:97:GLU:N	2.17	0.73
2:i:131:LYS:NZ	2:g:124:ASN:OD1	2.20	0.73
2:j:124:ASN:OD1	2:l:131:LYS:NZ	2.20	0.73
2:p:124:ASN:OD1	2:r:131:LYS:NZ	2.22	0.73
2:a:124:ASN:OD1	2:c:131:LYS:NZ	2.20	0.73
2:p:194:ILE:HB	2:q:193:VAL:HA	1.71	0.73
1:F:45:GLU:N	1:F:45:GLU:OE2	2.21	0.73
1:A:310:SER:HB3	1:B:297:ALA:H	1.54	0.72
2:i:193:VAL:HG13	2:g:193:VAL:HB	1.72	0.72
1:M:297:ALA:H	1:O:310:SER:HB3	1.53	0.72
1:C:130:VAL:HG22	1:C:140:VAL:HG22	1.71	0.72
1:K:130:VAL:HG22	1:K:140:VAL:HG22	1.72	0.72
1:B:130:VAL:HG22	1:B:140:VAL:HG22	1.71	0.72
1:H:322:GLN:NE2	1:I:285:ASP:O	2.21	0.72
2:a:211:LEU:H	2:b:216:ASN:HB2	1.55	0.72
1:H:197:LEU:HB2	1:H:379:VAL:HG23	1.71	0.72
1:G:106:THR:HG23	1:G:109:ASP:H	1.54	0.71
1:L:130:VAL:HG22	1:L:140:VAL:HG22	1.70	0.71
1:M:321:ASN:ND2	1:O:289:ALA:O	2.24	0.71
1:N:197:LEU:HB2	1:N:379:VAL:HG23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:106:THR:HG23	1:P:109:ASP:H	1.54	0.71
1:Q:197:LEU:HB2	1:Q:379:VAL:HG23	1.72	0.71
1:M:298:VAL:HG22	1:O:310:SER:HB2	1.72	0.71
1:P:310:SER:HB3	1:Q:297:ALA:H	1.55	0.71
2:n:188:PRO:HB2	2:n:191:VAL:HG23	1.70	0.71
1:B:362:GLN:NE2	1:C:247:ASN:O	2.24	0.70
1:E:362:GLN:NE2	1:F:247:ASN:O	2.24	0.70
1:K:362:GLN:NE2	1:L:247:ASN:O	2.24	0.70
1:I:130:VAL:HG22	1:I:140:VAL:HG22	1.73	0.70
1:J:297:ALA:H	1:L:310:SER:HB3	1.55	0.70
2:m:204:THR:HB	2:m:221:LYS:HD2	1.73	0.70
1:H:362:GLN:NE2	1:I:247:ASN:O	2.24	0.70
2:e:153:MET:HB2	2:e:162:ILE:HG12	1.74	0.70
1:A:297:ALA:H	1:C:310:SER:HB3	1.55	0.70
1:D:310:SER:HB3	1:E:297:ALA:H	1.54	0.70
2:a:169:ILE:HB	2:a:172:ILE:HD13	1.74	0.70
1:B:197:LEU:HB2	1:B:379:VAL:HG23	1.72	0.70
1:Q:45:GLU:OE1	1:Q:45:GLU:N	2.25	0.70
2:l:251:THR:OG1	2:l:252:GLN:OE1	2.10	0.70
1:H:45:GLU:OE1	1:H:45:GLU:N	2.25	0.69
1:Q:130:VAL:HG22	1:Q:140:VAL:HG22	1.74	0.69
1:M:314:ASN:ND2	1:O:302:ASN:O	2.25	0.69
1:Q:362:GLN:NE2	1:R:247:ASN:O	2.25	0.69
1:E:240:ASN:HB2	1:E:365:GLN:HE22	1.58	0.69
1:N:362:GLN:NE2	1:O:247:ASN:O	2.25	0.69
2:j:211:LEU:H	2:k:216:ASN:HB2	1.57	0.69
1:G:314:ASN:ND2	1:I:302:ASN:O	2.22	0.69
2:n:263:LEU:CD2	2:m:263:LEU:HD21	2.20	0.69
2:j:139:ARG:HG3	2:j:152:GLU:HG2	1.75	0.69
1:E:130:VAL:HG22	1:E:140:VAL:HG22	1.74	0.69
1:H:130:VAL:HG22	1:H:140:VAL:HG22	1.75	0.69
1:A:275:ASN:HB3	1:B:335:SER:HB3	1.74	0.69
2:n:204:THR:HA	2:n:206:TRP:HZ3	1.58	0.68
1:K:197:LEU:HB2	1:K:379:VAL:HG23	1.73	0.68
1:D:314:ASN:ND2	1:F:302:ASN:O	2.25	0.68
1:E:322:GLN:NE2	1:F:285:ASP:O	2.26	0.68
1:R:130:VAL:HG22	1:R:140:VAL:HG22	1.73	0.68
2:h:189:GLU:OE1	2:h:189:GLU:N	2.23	0.68
1:P:275:ASN:HB3	1:Q:335:SER:HB3	1.75	0.68
1:D:298:VAL:HG22	1:F:310:SER:HB2	1.76	0.68
1:D:321:ASN:ND2	1:F:289:ALA:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:SER:HB3	1:H:297:ALA:H	1.58	0.68
1:N:130:VAL:HG22	1:N:140:VAL:HG22	1.75	0.68
2:i:264:SER:O	2:h:267:LYS:NZ	2.27	0.68
1:J:260:THR:HG23	1:L:347:SER:HB2	1.76	0.68
1:J:275:ASN:HB3	1:K:335:SER:HB3	1.76	0.68
1:O:130:VAL:HG22	1:O:140:VAL:HG22	1.75	0.68
1:N:101:VAL:HG22	1:N:116:VAL:HG22	1.77	0.67
1:E:197:LEU:HB2	1:E:379:VAL:HG23	1.74	0.67
1:M:260:THR:HG23	1:O:347:SER:HB2	1.77	0.67
1:Q:240:ASN:HB2	1:Q:365:GLN:HE22	1.59	0.67
2:g:139:ARG:HG3	2:g:152:GLU:HG2	1.77	0.67
1:F:130:VAL:HG22	1:F:140:VAL:HG22	1.75	0.67
1:K:36:LYS:NZ	1:L:44:ASP:OD2	2.27	0.67
1:M:129:ARG:HH21	2:n:275:THR:CG2	2.05	0.67
1:N:350:THR:HG22	1:O:259:ASN:HD21	1.59	0.67
1:M:43:SER:HA	1:O:36:LYS:HG2	1.76	0.67
1:J:298:VAL:HG22	1:L:310:SER:HB2	1.77	0.67
1:M:106:THR:HG23	1:M:109:ASP:H	1.60	0.67
1:A:240:ASN:ND2	1:A:365:GLN:OE1	2.25	0.67
2:j:240:GLY:O	2:l:243:LYS:NZ	2.27	0.67
1:L:198:PHE:O	1:L:202:GLY:N	2.28	0.67
1:B:264:SER:OG	1:C:346:GLN:NE2	2.28	0.67
1:R:302:ASN:OD1	1:R:302:ASN:O	2.11	0.67
2:n:261:ASP:OD1	2:n:262:ALA:N	2.29	0.66
1:A:314:ASN:ND2	1:C:302:ASN:O	2.20	0.66
1:B:36:LYS:NZ	1:C:44:ASP:OD2	2.27	0.66
2:a:116:LEU:HB2	2:b:100:VAL:HG12	1.77	0.66
2:b:267:LYS:NZ	2:c:264:SER:O	2.27	0.66
1:D:43:SER:HA	1:F:36:LYS:HG2	1.76	0.66
1:H:240:ASN:HB2	1:H:365:GLN:HE22	1.60	0.66
2:b:1:MET:H2	2:b:57:GLU:H	1.43	0.66
2:b:153:MET:HB2	2:b:162:ILE:HG12	1.77	0.66
1:F:121:PRO:HG2	1:F:124:CYS:HB3	1.78	0.66
1:G:298:VAL:HG22	1:I:310:SER:HB2	1.77	0.66
1:K:101:VAL:HG22	1:K:116:VAL:HG22	1.77	0.66
2:e:199:ASP:OD1	2:e:215:GLN:NE2	2.28	0.66
1:D:106:THR:HG23	1:D:109:ASP:H	1.59	0.66
1:G:321:ASN:ND2	1:I:289:ALA:O	2.29	0.66
1:C:198:PHE:O	1:C:202:GLY:N	2.28	0.66
1:N:22:GLN:HG2	1:O:2:VAL:HG22	1.78	0.66
1:A:298:VAL:HG22	1:C:310:SER:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:PRO:HG2	1:I:124:CYS:HB3	1.78	0.66
1:N:36:LYS:NZ	1:O:44:ASP:OD2	2.28	0.66
1:P:314:ASN:ND2	1:R:302:ASN:O	2.27	0.66
2:d:194:ILE:HB	2:e:193:VAL:HA	1.78	0.66
1:H:36:LYS:NZ	1:I:44:ASP:OD2	2.29	0.65
1:P:321:ASN:ND2	1:R:289:ALA:O	2.29	0.65
2:n:277:LEU:CD2	2:o:277:LEU:HD21	2.26	0.65
2:d:139:ARG:HG3	2:d:152:GLU:HG2	1.78	0.65
1:A:260:THR:HG23	1:C:347:SER:HB2	1.77	0.65
1:N:240:ASN:HB2	1:N:365:GLN:HE22	1.61	0.65
2:g:24:LEU:HB3	2:g:35:TYR:HB2	1.78	0.65
2:g:30:THR:HG1	2:g:31:PRO:HD3	1.59	0.65
1:G:1:MET:SD	1:G:1:MET:N	2.56	0.65
2:n:244:ALA:H	2:o:246:LEU:HB2	1.61	0.65
2:j:116:LEU:HB2	2:k:100:VAL:HG12	1.79	0.65
2:p:24:LEU:HB3	2:p:35:TYR:HB2	1.78	0.65
2:q:267:LYS:NZ	2:r:264:SER:O	2.28	0.65
1:B:101:VAL:HG22	1:B:116:VAL:HG22	1.78	0.65
1:H:310:SER:HB2	1:I:297:ALA:HB3	1.78	0.65
1:I:62:VAL:HG22	1:I:72:VAL:HG22	1.78	0.65
1:K:240:ASN:HB2	1:K:365:GLN:HE22	1.61	0.65
1:R:62:VAL:HG22	1:R:72:VAL:HG22	1.78	0.65
1:B:240:ASN:HB2	1:B:365:GLN:HE22	1.61	0.65
1:K:294:PHE:HD2	1:L:316:ILE:HG23	1.62	0.65
1:I:198:PHE:O	1:I:202:GLY:N	2.30	0.65
2:i:243:LYS:NZ	2:g:240:GLY:O	2.29	0.65
2:c:198:SER:HB2	2:c:211:LEU:HD12	1.79	0.65
1:D:260:THR:HG23	1:F:347:SER:HB2	1.78	0.65
1:E:101:VAL:HG22	1:E:116:VAL:HG22	1.78	0.65
2:a:159:LYS:HA	2:a:159:LYS:HE3	1.79	0.65
1:N:294:PHE:HD2	1:O:316:ILE:HG23	1.62	0.65
2:k:267:LYS:NZ	2:l:264:SER:O	2.29	0.65
2:d:193:VAL:HG12	2:d:194:ILE:HG23	1.78	0.65
1:O:121:PRO:HG2	1:O:124:CYS:HB3	1.79	0.64
1:P:298:VAL:HG22	1:R:310:SER:HB2	1.78	0.64
2:d:30:THR:HG1	2:d:31:PRO:HD3	1.59	0.64
1:F:198:PHE:O	1:F:202:GLY:N	2.29	0.64
2:j:194:ILE:HB	2:k:193:VAL:HA	1.80	0.64
2:k:153:MET:HB2	2:k:162:ILE:HG12	1.78	0.64
1:J:111:ALA:O	1:J:115:ARG:NH2	2.30	0.64
1:O:243:THR:HG22	1:O:363:ALA:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:240:GLY:O	2:c:243:LYS:NZ	2.29	0.64
1:M:275:ASN:HB3	1:N:335:SER:HB3	1.80	0.64
2:p:116:LEU:HB2	2:q:100:VAL:HG12	1.80	0.64
1:E:22:GLN:HG2	1:F:2:VAL:HG22	1.78	0.64
1:H:22:GLN:HG2	1:I:2:VAL:HG22	1.79	0.64
1:J:43:SER:HA	1:L:36:LYS:HG2	1.79	0.64
1:K:264:SER:OG	1:L:346:GLN:NE2	2.29	0.64
1:M:129:ARG:HH22	2:n:275:THR:CG2	2.06	0.64
1:M:291:GLY:H	1:N:319:THR:HG22	1.63	0.64
1:Q:43:SER:OG	1:Q:48:ASN:ND2	2.30	0.64
2:m:196:THR:HB	2:o:211:LEU:HD22	1.80	0.64
2:n:162:ILE:CD1	2:n:183:LEU:HD22	2.27	0.64
2:b:117:ARG:O	2:b:120:LYS:HG3	1.97	0.64
1:R:198:PHE:O	1:R:202:GLY:N	2.30	0.64
2:i:198:SER:HB2	2:i:211:LEU:HD12	1.80	0.64
2:m:153:MET:HG3	2:m:162:ILE:HG13	1.80	0.64
1:E:36:LYS:NZ	1:F:44:ASP:OD2	2.28	0.64
1:Q:22:GLN:HG2	1:R:2:VAL:HG22	1.79	0.64
1:Q:101:VAL:HG22	1:Q:116:VAL:HG22	1.80	0.64
2:p:240:GLY:O	2:r:243:LYS:NZ	2.28	0.64
1:E:270:HIS:HB3	1:F:341:THR:HA	1.80	0.64
1:Q:310:SER:HB2	1:R:297:ALA:HB3	1.78	0.64
2:n:244:ALA:HB2	2:o:245:ASP:H	1.61	0.64
1:D:291:GLY:H	1:E:319:THR:HG22	1.63	0.64
1:E:294:PHE:HD2	1:F:316:ILE:HG23	1.62	0.63
1:O:198:PHE:O	1:O:202:GLY:N	2.30	0.63
2:j:24:LEU:HB3	2:j:35:TYR:HB2	1.79	0.63
2:l:45:ILE:HG12	2:l:50:LEU:HD23	1.80	0.63
2:e:1:MET:SD	2:e:1:MET:N	2.68	0.63
2:g:116:LEU:HB2	2:h:100:VAL:HG12	1.80	0.63
1:M:334:LEU:HD21	1:N:334:LEU:HG	1.80	0.63
1:A:43:SER:HA	1:C:36:LYS:HG2	1.79	0.63
1:D:275:ASN:HB3	1:E:335:SER:HB3	1.80	0.63
1:G:260:THR:HG23	1:I:347:SER:HB2	1.80	0.63
1:R:121:PRO:HG2	1:R:124:CYS:HB3	1.79	0.63
2:k:213:PRO:HG3	2:l:212:VAL:HG12	1.77	0.63
1:H:294:PHE:HD2	1:I:316:ILE:HG23	1.63	0.63
1:J:106:THR:HG23	1:J:109:ASP:H	1.64	0.63
1:L:346:GLN:OE1	1:L:346:GLN:N	2.32	0.63
2:d:116:LEU:HB2	2:e:100:VAL:HG12	1.81	0.63
1:D:334:LEU:HD21	1:E:334:LEU:HG	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:O	1:A:115:ARG:NH2	2.31	0.63
1:E:350:THR:HG22	1:F:259:ASN:HD21	1.63	0.63
1:G:275:ASN:HB3	1:H:335:SER:HB3	1.80	0.63
1:A:15:GLU:OE2	1:A:15:GLU:N	2.21	0.63
1:E:121:PRO:HG2	1:E:124:CYS:HB3	1.81	0.63
2:i:45:ILE:HG12	2:i:50:LEU:HD23	1.81	0.63
2:b:6:GLY:HA2	2:c:31:PRO:CB	2.28	0.63
2:b:244:ALA:H	2:c:246:LEU:HB2	1.62	0.63
1:M:111:ALA:O	1:M:115:ARG:NH2	2.32	0.63
1:M:310:SER:HB2	1:N:298:VAL:HG12	1.80	0.63
2:n:277:LEU:HD22	2:o:277:LEU:HD11	1.81	0.63
2:p:193:VAL:HB	2:r:193:VAL:HG13	1.80	0.63
2:c:45:ILE:HG12	2:c:50:LEU:HD23	1.78	0.63
1:A:1:MET:SD	1:A:1:MET:N	2.59	0.62
2:n:100:VAL:CG1	2:m:116:LEU:HB2	2.29	0.62
1:A:106:THR:HG23	1:A:109:ASP:H	1.64	0.62
1:G:182:LEU:HB2	1:G:375:VAL:HG13	1.81	0.62
1:J:310:SER:HB3	1:K:297:ALA:H	1.65	0.62
1:K:350:THR:HG22	1:L:259:ASN:HD21	1.62	0.62
1:A:321:ASN:ND2	1:C:289:ALA:O	2.31	0.62
1:B:310:SER:HB2	1:C:297:ALA:HB3	1.81	0.62
2:m:240:GLY:O	2:o:243:LYS:NZ	2.33	0.62
2:d:252:GLN:HB3	2:e:253:LEU:HD21	1.81	0.62
2:h:109:ASN:ND2	2:h:110:GLN:OE1	2.24	0.62
1:K:308:GLY:N	1:L:304:ALA:O	2.32	0.62
1:P:260:THR:HG23	1:R:347:SER:HB2	1.80	0.62
2:r:45:ILE:HG12	2:r:50:LEU:HD23	1.81	0.62
1:N:310:SER:HB2	1:O:297:ALA:HB3	1.81	0.62
2:q:147:THR:HG22	2:q:170:ILE:HB	1.81	0.62
2:b:6:GLY:N	2:c:31:PRO:HB3	2.15	0.62
1:A:290:HIS:ND1	1:B:321:ASN:OD1	2.33	0.62
1:H:308:GLY:N	1:I:304:ALA:O	2.32	0.62
1:L:62:VAL:HG22	1:L:72:VAL:HG22	1.81	0.62
1:P:43:SER:HA	1:R:36:LYS:HG2	1.81	0.62
2:q:153:MET:HB2	2:q:162:ILE:HG12	1.79	0.62
2:a:194:ILE:HB	2:b:193:VAL:HA	1.82	0.62
1:C:62:VAL:HG22	1:C:72:VAL:HG22	1.81	0.62
2:k:198:SER:CB	2:k:212:VAL:HG22	2.24	0.62
2:e:146:GLU:OE2	2:e:146:GLU:N	2.23	0.62
1:J:321:ASN:ND2	1:L:289:ALA:O	2.31	0.62
2:k:117:ARG:O	2:k:120:LYS:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLN:HG2	1:C:2:VAL:HG22	1.81	0.62
1:Q:308:GLY:N	1:R:304:ALA:O	2.32	0.62
2:m:24:LEU:HB3	2:m:35:TYR:HB2	1.81	0.62
1:H:101:VAL:HG22	1:H:116:VAL:HG22	1.80	0.61
1:R:243:THR:HG22	1:R:363:ALA:HA	1.82	0.61
2:j:159:LYS:HA	2:j:159:LYS:HE3	1.80	0.61
2:o:137:TYR:HB2	2:o:152:GLU:HA	1.81	0.61
1:G:43:SER:HA	1:I:36:LYS:HG2	1.81	0.61
1:M:344:SER:HB3	1:O:266:ASN:HB3	1.82	0.61
1:C:104:GLY:O	1:C:112:ILE:HA	2.00	0.61
1:E:310:SER:HB2	1:F:297:ALA:HB3	1.82	0.61
1:J:291:GLY:H	1:K:319:THR:HG22	1.65	0.61
1:K:22:GLN:HG2	1:L:2:VAL:HG22	1.81	0.61
1:L:104:GLY:O	1:L:112:ILE:HA	2.01	0.61
1:O:222:ARG:HB2	1:O:222:ARG:HH11	1.65	0.61
1:Q:36:LYS:NZ	1:R:44:ASP:OD2	2.30	0.61
2:n:268:ALA:HB2	2:o:270:LEU:HD12	1.81	0.61
2:a:252:GLN:HB3	2:b:253:LEU:HD21	1.80	0.61
1:G:310:SER:HB2	1:H:298:VAL:HG12	1.82	0.61
1:J:344:SER:HB3	1:L:266:ASN:HB3	1.82	0.61
1:K:310:SER:HB2	1:L:297:ALA:HB3	1.81	0.61
2:j:33:THR:HG23	2:o:7:ARG:HG3	1.82	0.61
1:C:346:GLN:OE1	1:C:346:GLN:N	2.32	0.61
2:k:244:ALA:H	2:l:246:LEU:HB2	1.64	0.61
2:e:147:THR:HG22	2:e:170:ILE:HB	1.82	0.61
2:f:137:TYR:HB2	2:f:152:GLU:HA	1.81	0.61
1:D:111:ALA:O	1:D:115:ARG:NH2	2.31	0.61
1:G:111:ALA:O	1:G:115:ARG:NH2	2.34	0.61
1:J:290:HIS:ND1	1:K:321:ASN:OD1	2.33	0.61
2:r:198:SER:HB2	2:r:211:LEU:HD12	1.82	0.61
2:d:114:SER:O	2:d:116:LEU:N	2.33	0.61
1:F:62:VAL:HG22	1:F:72:VAL:HG22	1.83	0.61
2:n:162:ILE:HD11	2:n:183:LEU:HD22	1.82	0.61
2:j:114:SER:O	2:j:116:LEU:N	2.34	0.61
2:m:216:ASN:ND2	2:o:209:SER:O	2.34	0.61
1:Q:294:PHE:HD2	1:R:316:ILE:HG23	1.65	0.61
1:D:310:SER:HB2	1:E:298:VAL:HG12	1.82	0.60
1:F:346:GLN:OE1	1:F:346:GLN:N	2.33	0.60
1:P:111:ALA:O	1:P:115:ARG:NH2	2.34	0.60
2:g:30:THR:OG1	2:g:31:PRO:CD	2.40	0.60
1:P:291:GLY:H	1:Q:319:THR:HG22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:308:GLY:N	1:O:304:ALA:O	2.33	0.60
1:P:290:HIS:ND1	1:Q:321:ASN:OD1	2.35	0.60
2:i:19:LYS:HG3	2:i:40:GLU:HG2	1.83	0.60
2:m:114:SER:O	2:m:116:LEU:N	2.34	0.60
2:q:212:VAL:H	2:q:213:PRO:HD2	1.65	0.60
1:P:39:ASP:CG	1:P:50:LYS:HZ3	2.08	0.60
2:j:162:ILE:HD11	2:j:183:LEU:HB2	1.83	0.60
2:m:69:ILE:HG22	2:m:83:LEU:HD12	1.83	0.60
1:B:57:TYR:CZ	1:C:52:ARG:HD3	2.37	0.60
1:O:346:GLN:OE1	1:O:346:GLN:N	2.32	0.60
1:B:308:GLY:N	1:C:304:ALA:O	2.33	0.60
1:J:39:ASP:CG	1:J:50:LYS:HZ3	2.10	0.60
2:a:24:LEU:HB3	2:a:35:TYR:HB2	1.82	0.60
1:A:291:GLY:H	1:B:319:THR:HG22	1.65	0.60
2:n:253:LEU:HD21	2:m:252:GLN:HB3	1.84	0.60
1:R:346:GLN:OE1	1:R:346:GLN:N	2.33	0.60
2:a:193:VAL:HG21	2:c:193:VAL:HG12	1.83	0.60
2:g:59:GLU:HB2	2:g:91:PRO:HA	1.84	0.60
1:B:294:PHE:HD2	1:C:316:ILE:HG23	1.64	0.60
2:b:7:ARG:CD	2:c:30:THR:OG1	2.49	0.60
2:g:114:SER:O	2:g:116:LEU:N	2.34	0.60
1:N:121:PRO:HG2	1:N:124:CYS:HB3	1.82	0.60
2:l:233:ASN:O	2:l:237:THR:HG23	2.02	0.60
2:a:114:SER:O	2:a:116:LEU:N	2.35	0.60
2:d:24:LEU:HB3	2:d:35:TYR:HB2	1.82	0.60
1:B:350:THR:HG22	1:C:259:ASN:HD21	1.66	0.59
1:J:65:GLN:OE1	1:J:71:SER:OG	2.20	0.59
1:F:194:TYR:HD1	1:F:379:VAL:HG11	1.67	0.59
1:G:290:HIS:ND1	1:H:321:ASN:OD1	2.35	0.59
1:K:57:TYR:CZ	1:L:52:ARG:HD3	2.37	0.59
2:n:263:LEU:HD21	2:m:263:LEU:CD2	2.27	0.59
1:E:308:GLY:N	1:F:304:ALA:O	2.33	0.59
1:G:291:GLY:H	1:H:319:THR:HG22	1.66	0.59
2:i:137:TYR:HB2	2:i:152:GLU:HA	1.83	0.59
2:p:114:SER:O	2:p:116:LEU:N	2.35	0.59
1:B:277:THR:OG1	1:C:333:ASN:OD1	2.21	0.59
2:k:208:GLY:O	2:l:215:GLN:NE2	2.28	0.59
2:o:45:ILE:HG12	2:o:50:LEU:HD23	1.83	0.59
2:b:199:ASP:OD1	2:b:215:GLN:NE2	2.34	0.59
1:A:310:SER:HB2	1:B:298:VAL:HG12	1.84	0.59
1:O:104:GLY:O	1:O:112:ILE:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:310:SER:HB2	1:Q:298:VAL:HG12	1.84	0.59
2:j:216:ASN:OD1	2:l:209:SER:N	2.34	0.59
2:q:244:ALA:H	2:r:246:LEU:HB2	1.66	0.59
2:b:6:GLY:HA2	2:c:31:PRO:HB3	1.85	0.59
2:d:162:ILE:HD11	2:d:183:LEU:HB2	1.83	0.59
2:e:267:LYS:NZ	2:f:264:SER:O	2.35	0.59
2:m:162:ILE:HD11	2:m:183:LEU:HB2	1.84	0.59
1:H:277:THR:OG1	1:I:333:ASN:OD1	2.21	0.59
1:I:346:GLN:OE1	1:I:346:GLN:N	2.32	0.59
2:m:191:VAL:HG12	2:o:194:ILE:HG12	1.84	0.59
2:d:30:THR:OG1	2:d:31:PRO:CD	2.40	0.59
2:e:244:ALA:H	2:f:246:LEU:HB2	1.67	0.59
1:C:121:PRO:HG2	1:C:124:CYS:HB3	1.85	0.59
1:O:62:VAL:HG22	1:O:72:VAL:HG22	1.83	0.59
1:P:314:ASN:CG	1:R:302:ASN:OD1	2.46	0.59
1:Q:350:THR:HG22	1:R:259:ASN:HD21	1.68	0.59
2:q:244:ALA:HB2	2:r:245:ASP:H	1.68	0.59
2:a:159:LYS:NZ	2:c:186:THR:OG1	2.33	0.59
2:b:6:GLY:CA	2:c:31:PRO:HB3	2.32	0.59
1:C:192:THR:O	1:C:195:SER:OG	2.21	0.58
2:r:137:TYR:HB2	2:r:152:GLU:HA	1.84	0.58
2:q:73:ASP:OD1	2:q:77:ASN:N	2.36	0.58
2:a:199:ASP:HB3	2:c:210:LEU:HD12	1.85	0.58
1:G:283:ILE:HD11	1:H:325:ILE:HB	1.85	0.58
1:P:65:GLN:OE1	1:P:71:SER:OG	2.20	0.58
1:F:104:GLY:O	1:F:112:ILE:HA	2.02	0.58
1:G:141:THR:HG21	1:H:83:ILE:HG13	1.86	0.58
1:L:243:THR:HG22	1:L:363:ALA:HA	1.86	0.58
1:P:283:ILE:HD11	1:Q:325:ILE:HB	1.86	0.58
1:D:355:THR:OG1	1:F:255:GLY:O	2.22	0.58
2:m:33:THR:HG23	2:r:7:ARG:HG3	1.84	0.58
2:h:73:ASP:OD1	2:h:77:ASN:N	2.36	0.58
1:F:243:THR:HG22	1:F:363:ALA:HA	1.85	0.58
1:K:209:ASP:OD2	1:K:211:SER:OG	2.22	0.58
1:R:104:GLY:O	1:R:112:ILE:HA	2.04	0.58
1:B:209:ASP:OD2	1:B:211:SER:OG	2.22	0.58
1:P:314:ASN:ND2	1:R:302:ASN:OD1	2.37	0.58
1:G:321:ASN:OD1	1:I:290:HIS:ND1	2.37	0.58
1:R:44:ASP:OD1	1:R:50:LYS:NZ	2.37	0.58
1:F:37:VAL:HG13	1:F:41:SER:HB2	1.86	0.57
1:G:334:LEU:HD21	1:H:334:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:224:LEU:HD21	1:L:373:PHE:CE2	2.39	0.57
2:p:212:VAL:HA	2:q:215:GLN:HA	1.86	0.57
2:g:199:ASP:OD1	2:g:215:GLN:N	2.35	0.57
2:h:215:GLN:H	2:h:215:GLN:CD	2.11	0.57
1:C:169:ILE:HG23	1:C:173:ALA:HB3	1.86	0.57
1:G:72:VAL:O	1:G:88:PRO:HA	2.04	0.57
1:I:104:GLY:O	1:I:112:ILE:HA	2.04	0.57
1:K:183:LEU:O	1:K:219:THR:N	2.36	0.57
1:N:57:TYR:CZ	1:O:52:ARG:HD3	2.39	0.57
2:p:45:ILE:HG12	2:p:50:LEU:HD23	1.86	0.57
2:p:169:ILE:HB	2:p:172:ILE:HD12	1.85	0.57
2:p:199:ASP:OD1	2:p:215:GLN:N	2.35	0.57
2:b:215:GLN:H	2:b:215:GLN:CD	2.12	0.57
1:J:15:GLU:OE2	1:J:15:GLU:N	2.20	0.57
2:k:244:ALA:HB2	2:l:245:ASP:H	1.69	0.57
2:b:147:THR:HG22	2:b:170:ILE:HB	1.86	0.57
2:e:215:GLN:H	2:e:215:GLN:CD	2.12	0.57
1:A:224:LEU:HD21	1:C:373:PHE:CE2	2.39	0.57
1:A:283:ILE:HD11	1:B:325:ILE:HB	1.86	0.57
1:M:39:ASP:OD2	1:M:54:TYR:OH	2.20	0.57
2:n:188:PRO:HB2	2:n:191:VAL:CG2	2.34	0.57
2:c:137:TYR:HB2	2:c:152:GLU:HA	1.86	0.57
1:B:370:TYR:CD1	1:C:225:ARG:HD3	2.39	0.57
1:J:321:ASN:OD1	1:L:290:HIS:ND1	2.38	0.57
1:K:277:THR:OG1	1:L:333:ASN:OD1	2.20	0.57
1:L:192:THR:O	1:L:195:SER:OG	2.22	0.57
1:N:322:GLN:NE2	1:O:285:ASP:O	2.25	0.57
1:P:321:ASN:OD1	1:R:290:HIS:ND1	2.38	0.57
2:l:137:TYR:HB2	2:l:152:GLU:HA	1.85	0.57
1:G:47:GLN:O	1:G:52:ARG:NH2	2.37	0.57
1:J:310:SER:HB2	1:K:298:VAL:HG12	1.84	0.57
1:L:121:PRO:HG2	1:L:124:CYS:HB3	1.85	0.57
2:q:215:GLN:CD	2:q:215:GLN:H	2.13	0.57
1:P:334:LEU:HD21	1:Q:334:LEU:HG	1.87	0.57
2:j:193:VAL:HG21	2:l:193:VAL:HG12	1.87	0.57
1:D:39:ASP:OD2	1:D:54:TYR:OH	2.20	0.57
1:P:72:VAL:O	1:P:88:PRO:HA	2.03	0.57
2:n:136:PRO:HA	2:n:151:GLY:O	2.04	0.57
2:i:9:GLY:N	2:d:34:THR:O	2.32	0.57
2:g:193:VAL:HG12	2:g:194:ILE:HG23	1.87	0.57
1:H:111:ALA:O	1:H:115:ARG:NH2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:SER:HA	1:I:262:THR:HG22	1.87	0.57
1:O:37:VAL:HG13	1:O:41:SER:HB2	1.86	0.57
1:Q:277:THR:OG1	1:R:333:ASN:OD1	2.22	0.57
2:i:248:TYR:OH	2:g:250:ASN:OD1	2.23	0.57
2:b:73:ASP:OD1	2:b:77:ASN:N	2.37	0.57
1:E:57:TYR:CZ	1:F:52:ARG:HD3	2.39	0.57
1:H:57:TYR:CZ	1:I:52:ARG:HD3	2.40	0.57
1:M:224:LEU:HD11	1:O:373:PHE:CE2	2.39	0.57
1:Q:373:PHE:CE2	1:R:224:LEU:HD22	2.39	0.57
1:B:373:PHE:CE1	1:C:224:LEU:HD22	2.40	0.56
1:D:344:SER:HB3	1:F:266:ASN:HB3	1.85	0.56
1:H:373:PHE:CE2	1:I:224:LEU:HD22	2.40	0.56
1:K:121:PRO:HG2	1:K:124:CYS:HB3	1.85	0.56
1:K:370:TYR:CD1	1:L:225:ARG:HD3	2.39	0.56
2:p:34:THR:O	2:c:9:GLY:N	2.33	0.56
2:b:6:GLY:CA	2:c:31:PRO:CB	2.82	0.56
1:B:121:PRO:HG2	1:B:124:CYS:HB3	1.86	0.56
1:D:47:GLN:O	1:D:52:ARG:NH2	2.38	0.56
1:D:148:VAL:HG11	1:E:83:ILE:HD12	1.87	0.56
1:D:321:ASN:OD1	1:F:290:HIS:ND1	2.38	0.56
1:G:65:GLN:OE1	1:G:71:SER:OG	2.23	0.56
1:G:150:ILE:HG13	1:H:78:SER:HB3	1.87	0.56
1:H:350:THR:HG22	1:I:259:ASN:HD21	1.69	0.56
1:I:222:ARG:HB2	1:I:222:ARG:HH11	1.70	0.56
1:L:169:ILE:HG23	1:L:173:ALA:HB3	1.87	0.56
2:d:240:GLY:O	2:f:243:LYS:NZ	2.37	0.56
2:f:198:SER:HB2	2:f:211:LEU:HD12	1.87	0.56
1:A:321:ASN:OD1	1:C:290:HIS:ND1	2.38	0.56
1:E:168:LEU:O	1:F:205:TYR:OH	2.20	0.56
1:J:47:GLN:O	1:J:52:ARG:NH2	2.39	0.56
1:K:373:PHE:CE1	1:L:224:LEU:HD22	2.40	0.56
1:M:321:ASN:OD1	1:O:290:HIS:ND1	2.38	0.56
2:n:206:TRP:HE3	2:n:206:TRP:H	1.53	0.56
1:A:47:GLN:O	1:A:52:ARG:NH2	2.39	0.56
1:D:152:PRO:HG2	1:E:123:VAL:HG13	1.88	0.56
1:M:47:GLN:O	1:M:52:ARG:NH2	2.39	0.56
1:M:355:THR:OG1	1:O:255:GLY:O	2.22	0.56
1:N:166:ILE:HD11	1:O:166:ILE:HD11	1.88	0.56
1:P:224:LEU:HD21	1:R:373:PHE:CE2	2.41	0.56
1:Q:121:PRO:HG2	1:Q:124:CYS:HB3	1.88	0.56
1:R:222:ARG:HB2	1:R:222:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:45:ILE:HG12	2:f:50:LEU:HD23	1.86	0.56
1:Q:57:TYR:CZ	1:R:52:ARG:HD3	2.40	0.56
1:E:373:PHE:CE1	1:F:224:LEU:HD22	2.41	0.56
2:n:12:THR:O	2:n:47:ALA:N	2.38	0.56
1:G:151:LEU:HD12	1:G:152:PRO:HD2	1.88	0.56
1:P:36:LYS:HG2	1:Q:43:SER:HA	1.88	0.56
2:a:216:ASN:ND2	2:c:209:SER:O	2.39	0.56
2:a:162:ILE:HD11	2:a:183:LEU:HB2	1.88	0.56
1:B:183:LEU:O	1:B:219:THR:N	2.36	0.56
1:J:283:ILE:HD11	1:K:325:ILE:HB	1.87	0.56
1:P:94:ILE:HB	1:P:99:SER:HB3	1.88	0.56
1:P:150:ILE:HG13	1:Q:78:SER:HB3	1.87	0.56
2:l:104:THR:OG1	2:l:105:GLY:N	2.39	0.56
2:k:40:GLU:OE2	2:k:70:TYR:OH	2.23	0.55
2:p:153:MET:HE3	2:p:160:ASN:HB3	1.89	0.55
2:r:104:THR:OG1	2:r:105:GLY:N	2.39	0.55
2:a:267:LYS:HB3	2:c:267:LYS:HD2	1.87	0.55
1:A:334:LEU:HD21	1:B:334:LEU:HG	1.88	0.55
1:C:243:THR:HG22	1:C:363:ALA:HA	1.88	0.55
1:I:44:ASP:OD1	1:I:50:LYS:NZ	2.39	0.55
1:I:243:THR:HG22	1:I:363:ALA:HA	1.88	0.55
1:P:331:ASN:HB2	1:Q:276:GLN:CD	2.32	0.55
2:m:45:ILE:HG12	2:m:50:LEU:HD23	1.88	0.55
1:A:181:GLU:HG2	1:A:376:PHE:CE1	2.41	0.55
1:D:290:HIS:ND1	1:E:321:ASN:OD1	2.39	0.55
1:K:62:VAL:HG22	1:K:72:VAL:HG22	1.89	0.55
1:B:224:LEU:HB2	1:C:224:LEU:HD12	1.87	0.55
1:G:331:ASN:HB2	1:H:276:GLN:CD	2.32	0.55
1:K:142:ASP:OD2	1:K:144:ARG:NH2	2.39	0.55
1:P:47:GLN:O	1:P:52:ARG:NH2	2.39	0.55
1:J:309:GLY:HA2	1:K:303:ASN:H	1.71	0.55
2:h:212:VAL:H	2:h:213:PRO:HD2	1.70	0.55
1:B:142:ASP:OD2	1:B:144:ARG:NH2	2.38	0.55
1:J:181:GLU:HG2	1:J:376:PHE:CE1	2.42	0.55
1:N:373:PHE:CE1	1:O:224:LEU:HD22	2.41	0.55
2:i:104:THR:OG1	2:i:105:GLY:N	2.38	0.55
1:G:354:VAL:HA	1:H:255:GLY:HA2	1.89	0.55
2:p:267:LYS:HD3	2:q:269:ASP:HA	1.88	0.55
2:a:45:ILE:HG12	2:a:50:LEU:HD23	1.87	0.55
2:c:104:THR:OG1	2:c:105:GLY:N	2.39	0.55
2:f:64:THR:HG1	2:f:107:VAL:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:ASP:OD2	1:E:211:SER:OG	2.23	0.55
1:E:347:SER:HA	1:F:262:THR:HG22	1.89	0.55
1:N:347:SER:HA	1:O:262:THR:HG22	1.88	0.55
1:P:344:SER:HB3	1:R:266:ASN:HB3	1.89	0.55
2:n:25:ILE:HG21	2:m:99:ASP:HB2	1.89	0.55
2:m:216:ASN:OD1	2:o:209:SER:N	2.36	0.55
2:a:216:ASN:OD1	2:c:209:SER:N	2.33	0.55
2:h:199:ASP:OD1	2:h:215:GLN:NE2	2.40	0.55
1:A:344:SER:HB3	1:C:266:ASN:HB3	1.89	0.55
2:q:248:TYR:O	2:q:252:GLN:HG2	2.07	0.55
2:d:45:ILE:HG12	2:d:50:LEU:HD23	1.88	0.55
2:d:193:VAL:HG21	2:f:193:VAL:HG12	1.88	0.55
1:G:224:LEU:HD21	1:I:373:PHE:CE2	2.42	0.55
1:K:186:SER:HA	1:K:216:VAL:O	2.07	0.55
1:M:15:GLU:OE2	1:M:15:GLU:N	2.33	0.55
1:M:148:VAL:HG11	1:N:83:ILE:HD12	1.88	0.55
1:O:149:ASP:OD1	1:O:149:ASP:N	2.40	0.55
1:Q:44:ASP:OD1	1:Q:50:LYS:NZ	2.32	0.55
2:k:147:THR:HG22	2:k:170:ILE:HB	1.88	0.55
2:g:45:ILE:HG12	2:g:50:LEU:HD23	1.87	0.55
1:A:151:LEU:HD12	1:A:152:PRO:HD2	1.89	0.54
1:I:169:ILE:HG23	1:I:173:ALA:HB3	1.89	0.54
1:B:62:VAL:HG22	1:B:72:VAL:HG22	1.89	0.54
2:i:215:GLN:HB2	2:h:206:TRP:CD1	2.43	0.54
2:j:216:ASN:ND2	2:l:209:SER:O	2.39	0.54
2:l:248:TYR:HD2	2:l:252:GLN:HE22	1.56	0.54
2:m:79:VAL:HG12	2:m:81:PRO:HD2	1.89	0.54
2:a:33:THR:HA	2:f:7:ARG:HG3	1.87	0.54
2:h:212:VAL:N	2:h:213:PRO:HD2	2.22	0.54
1:A:141:THR:HG21	1:B:83:ILE:HG13	1.89	0.54
1:G:344:SER:HB3	1:I:266:ASN:HB3	1.89	0.54
1:H:121:PRO:HG2	1:H:124:CYS:HB3	1.88	0.54
1:P:303:ASN:H	1:R:309:GLY:HA2	1.72	0.54
2:i:209:SER:N	2:g:216:ASN:OD1	2.35	0.54
2:f:104:THR:OG1	2:f:105:GLY:N	2.39	0.54
1:B:111:ALA:O	1:B:115:ARG:NH2	2.36	0.54
1:M:65:GLN:OE1	1:M:71:SER:OG	2.24	0.54
1:M:129:ARG:NH2	2:n:275:THR:HG22	2.11	0.54
1:A:276:GLN:OE1	1:C:332:ALA:N	2.39	0.54
1:E:277:THR:HG23	1:E:278:PRO:HD2	1.89	0.54
1:F:44:ASP:OD1	1:F:50:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:334:LEU:HD21	1:K:334:LEU:HG	1.89	0.54
2:n:2:THR:OG1	2:n:91:PRO:O	2.25	0.54
2:j:269:ASP:N	2:j:269:ASP:OD1	2.41	0.54
2:k:248:TYR:O	2:k:252:GLN:HG2	2.07	0.54
2:b:248:TYR:O	2:b:252:GLN:HG2	2.07	0.54
2:d:211:LEU:H	2:e:216:ASN:CB	2.17	0.54
2:d:263:LEU:HD21	2:e:263:LEU:HD22	1.89	0.54
2:g:162:ILE:HD11	2:g:183:LEU:HB2	1.89	0.54
1:C:149:ASP:N	1:C:149:ASP:OD1	2.41	0.54
1:D:15:GLU:OE1	1:D:15:GLU:N	2.35	0.54
1:D:181:GLU:HG2	1:D:376:PHE:CE1	2.42	0.54
1:G:330:ALA:O	1:H:279:HIS:ND1	2.41	0.54
1:Q:347:SER:HA	1:R:262:THR:HG22	1.88	0.54
2:m:269:ASP:N	2:m:269:ASP:OD1	2.41	0.54
2:e:40:GLU:OE2	2:e:70:TYR:OH	2.24	0.54
2:e:73:ASP:OD1	2:e:77:ASN:N	2.40	0.54
1:A:181:GLU:HG2	1:A:376:PHE:HE1	1.73	0.54
1:B:347:SER:HA	1:C:262:THR:HG22	1.89	0.54
1:C:37:VAL:HG13	1:C:41:SER:HB2	1.89	0.54
1:J:1:MET:SD	1:J:1:MET:N	2.66	0.54
1:L:74:GLN:HB3	1:L:88:PRO:HD3	1.89	0.54
1:M:36:LYS:HG2	1:N:43:SER:HA	1.90	0.54
1:M:98:ASN:HD21	2:n:279:SER:HA	1.69	0.54
1:N:277:THR:HG23	1:N:278:PRO:HD2	1.90	0.54
1:Q:186:SER:HA	1:Q:216:VAL:O	2.07	0.54
2:p:162:ILE:HD11	2:p:183:LEU:HB2	1.90	0.54
1:G:181:GLU:HG2	1:G:376:PHE:CE1	2.43	0.54
1:G:259:ASN:ND2	1:G:259:ASN:N	2.56	0.54
1:J:37:VAL:HG13	1:J:41:SER:HB2	1.89	0.54
1:J:151:LEU:HD12	1:J:152:PRO:HD2	1.90	0.54
1:K:347:SER:HA	1:L:262:THR:HG22	1.88	0.54
2:j:199:ASP:OD2	2:j:216:ASN:ND2	2.39	0.54
1:J:249:LEU:HD12	1:J:250:PRO:HD2	1.89	0.54
1:K:224:LEU:HB2	1:L:224:LEU:HD12	1.89	0.54
1:O:44:ASP:OD1	1:O:50:LYS:NZ	2.40	0.54
2:n:223:VAL:CG1	2:m:221:LYS:HZ1	2.19	0.54
2:i:209:SER:O	2:g:216:ASN:ND2	2.41	0.54
2:o:104:THR:OG1	2:o:105:GLY:N	2.39	0.54
1:G:303:ASN:H	1:I:309:GLY:HA2	1.73	0.54
1:M:151:LEU:HD12	1:M:152:PRO:HD2	1.90	0.54
1:M:355:THR:HG22	1:N:254:HIS:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:181:GLU:HG2	1:P:376:PHE:CE1	2.43	0.54
1:B:43:SER:HB2	1:B:45:GLU:HG2	1.90	0.53
1:P:267:ASP:HB3	1:Q:343:ILE:HD13	1.90	0.53
1:Q:111:ALA:O	1:Q:115:ARG:NH2	2.32	0.53
2:n:220:ASP:HA	2:n:223:VAL:HB	1.90	0.53
1:D:276:GLN:OE1	1:F:332:ALA:N	2.41	0.53
1:E:166:ILE:HD11	1:F:166:ILE:HD11	1.90	0.53
1:J:331:ASN:HB2	1:K:276:GLN:CD	2.33	0.53
1:M:283:ILE:HD11	1:N:325:ILE:HB	1.90	0.53
1:P:151:LEU:HD12	1:P:152:PRO:HD2	1.90	0.53
1:R:222:ARG:HB2	1:R:222:ARG:NH1	2.23	0.53
2:l:26:ASP:HB2	2:l:35:TYR:HE2	1.73	0.53
2:d:199:ASP:OD1	2:d:215:GLN:N	2.37	0.53
1:D:94:ILE:HB	1:D:99:SER:HB3	1.89	0.53
1:E:277:THR:CG2	1:E:278:PRO:HD2	2.38	0.53
1:E:370:TYR:CD1	1:F:225:ARG:HD3	2.43	0.53
1:F:149:ASP:N	1:F:149:ASP:OD1	2.40	0.53
1:H:186:SER:HA	1:H:216:VAL:O	2.08	0.53
1:M:141:THR:HG21	1:N:83:ILE:HG13	1.90	0.53
1:M:181:GLU:HG2	1:M:376:PHE:CE1	2.44	0.53
1:M:290:HIS:ND1	1:N:321:ASN:OD1	2.40	0.53
1:G:94:ILE:HB	1:G:99:SER:HB3	1.91	0.53
1:J:150:ILE:HG13	1:K:78:SER:HB3	1.89	0.53
1:Q:43:SER:HB2	1:Q:45:GLU:OE1	2.07	0.53
2:j:219:TYR:O	2:j:223:VAL:HG13	2.09	0.53
2:a:193:VAL:HG12	2:a:194:ILE:HG23	1.89	0.53
1:M:152:PRO:HG2	1:N:123:VAL:HG13	1.89	0.53
1:O:74:GLN:HB3	1:O:88:PRO:HD3	1.90	0.53
2:i:215:GLN:HB2	2:h:206:TRP:NE1	2.24	0.53
2:p:153:MET:HE2	2:r:181:TYR:CE1	2.44	0.53
2:p:216:ASN:ND2	2:r:209:SER:O	2.42	0.53
1:D:151:LEU:HD12	1:D:152:PRO:HD2	1.91	0.53
1:D:228:GLY:C	1:F:184:ASN:HB3	2.34	0.53
1:I:194:TYR:HD1	1:I:379:VAL:HB	1.74	0.53
1:J:141:THR:HG21	1:K:83:ILE:HG13	1.89	0.53
2:n:104:THR:HG21	2:o:118:ILE:HD11	1.91	0.53
1:A:79:VAL:HG22	1:C:151:LEU:HD22	1.90	0.53
2:j:267:LYS:HB3	2:l:267:LYS:HD2	1.91	0.53
2:a:267:LYS:HD3	2:b:269:ASP:HA	1.91	0.53
2:e:208:GLY:O	2:f:215:GLN:NE2	2.25	0.53
1:P:15:GLU:OE2	1:P:15:GLU:N	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:354:VAL:HA	1:Q:255:GLY:HA2	1.89	0.53
1:Q:184:ASN:ND2	1:R:229:SER:H	2.07	0.53
2:n:202:TYR:CD2	2:n:218:VAL:HG21	2.44	0.53
2:p:31:PRO:HB2	2:c:7:ARG:HG3	1.91	0.53
1:B:362:GLN:HE21	1:C:248:ALA:HA	1.74	0.53
1:F:74:GLN:HB3	1:F:88:PRO:HD3	1.90	0.53
1:J:303:ASN:H	1:L:309:GLY:HA2	1.74	0.53
2:j:45:ILE:HG12	2:j:50:LEU:HD23	1.90	0.53
2:d:212:VAL:HG13	2:e:213:PRO:HA	1.89	0.53
1:C:74:GLN:HB3	1:C:88:PRO:HD3	1.90	0.53
1:I:98:ASN:OD1	1:I:129:ARG:NH1	2.42	0.53
1:K:168:LEU:O	1:L:205:TYR:OH	2.20	0.53
2:n:70:TYR:CD1	2:n:80:PHE:HA	2.43	0.53
1:E:142:ASP:OD2	1:E:144:ARG:NH2	2.41	0.52
1:I:222:ARG:HB2	1:I:222:ARG:NH1	2.23	0.52
1:L:149:ASP:OD1	1:L:149:ASP:N	2.41	0.52
2:m:139:ARG:NE	2:m:152:GLU:OE2	2.42	0.52
2:e:134:GLY:HA3	2:f:134:GLY:HA3	1.91	0.52
2:f:233:ASN:O	2:f:237:THR:HG23	2.10	0.52
1:A:309:GLY:HA2	1:B:303:ASN:H	1.75	0.52
1:A:331:ASN:HB2	1:B:276:GLN:CD	2.34	0.52
1:B:228:GLY:H	1:B:231:LEU:HB2	1.74	0.52
1:M:72:VAL:O	1:M:88:PRO:HA	2.09	0.52
2:j:25:ILE:HD12	2:o:99:ASP:HB2	1.92	0.52
2:j:199:ASP:OD1	2:j:215:GLN:N	2.33	0.52
1:D:123:VAL:HG13	1:F:152:PRO:HG2	1.92	0.52
1:D:355:THR:HG22	1:E:254:HIS:H	1.73	0.52
1:G:79:VAL:HG13	1:I:151:LEU:HD21	1.92	0.52
1:H:142:ASP:OD2	1:H:144:ARG:NH2	2.42	0.52
1:K:43:SER:HB2	1:K:45:GLU:HG2	1.91	0.52
1:N:209:ASP:OD2	1:N:211:SER:OG	2.24	0.52
2:n:13:THR:HG22	2:n:72:VAL:HG21	1.91	0.52
1:D:285:ASP:HA	1:E:325:ILE:HG22	1.92	0.52
1:J:79:VAL:HG22	1:L:151:LEU:HD22	1.91	0.52
1:J:232:SER:N	1:J:235:ASP:OD2	2.42	0.52
1:J:276:GLN:OE1	1:L:332:ALA:N	2.39	0.52
1:L:37:VAL:HG13	1:L:41:SER:HB2	1.90	0.52
1:P:141:THR:HG21	1:Q:83:ILE:HG13	1.89	0.52
1:Q:142:ASP:OD2	1:Q:144:ARG:NH2	2.42	0.52
2:m:169:ILE:HB	2:m:172:ILE:HD12	1.91	0.52
1:A:37:VAL:HG13	1:A:41:SER:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:HD11	1:C:166:ILE:HD11	1.91	0.52
1:B:321:ASN:OD1	1:B:321:ASN:N	2.42	0.52
1:D:283:ILE:HD11	1:E:325:ILE:HB	1.91	0.52
1:K:85:SER:O	2:l:274:ASN:ND2	2.38	0.52
1:M:37:VAL:HG13	1:M:41:SER:HB2	1.91	0.52
1:N:277:THR:CG2	1:N:278:PRO:HD2	2.40	0.52
1:R:74:GLN:HB3	1:R:88:PRO:HD3	1.91	0.52
2:n:246:LEU:HA	2:m:244:ALA:HB2	1.92	0.52
2:a:34:THR:O	2:f:9:GLY:N	2.31	0.52
1:D:72:VAL:O	1:D:88:PRO:HA	2.10	0.52
1:J:181:GLU:HG2	1:J:376:PHE:HE1	1.75	0.52
1:L:191:ARG:NH2	1:L:207:ASN:OD1	2.42	0.52
1:M:70:LEU:HD11	1:M:93:ALA:HB2	1.90	0.52
2:n:209:SER:HA	2:o:215:GLN:HE21	1.75	0.52
2:g:57:GLU:HG2	2:g:59:GLU:H	1.74	0.52
1:A:249:LEU:HD12	1:A:250:PRO:HD2	1.91	0.52
1:H:43:SER:OG	1:H:48:ASN:ND2	2.43	0.52
1:N:362:GLN:HE21	1:O:248:ALA:HA	1.73	0.52
1:P:330:ALA:O	1:Q:279:HIS:ND1	2.41	0.52
2:p:267:LYS:HB3	2:r:267:LYS:HD2	1.92	0.52
2:r:146:GLU:N	2:r:146:GLU:OE2	2.42	0.52
1:G:184:ASN:ND2	1:H:229:SER:H	2.08	0.52
1:L:61:ARG:HB2	1:L:144:ARG:HH21	1.74	0.52
1:M:228:GLY:C	1:O:184:ASN:HB3	2.34	0.52
1:Q:190:SER:HA	1:Q:213:THR:HG22	1.92	0.52
2:n:210:LEU:HG	2:o:215:GLN:HE22	1.73	0.52
2:k:198:SER:CB	2:k:212:VAL:CG2	2.69	0.52
2:m:57:GLU:HG3	2:m:92:ASN:HA	1.91	0.52
2:g:165:SER:OG	2:g:167:SER:O	2.24	0.52
1:H:370:TYR:CD1	1:I:225:ARG:HD3	2.45	0.52
1:I:61:ARG:HB2	1:I:144:ARG:HH21	1.74	0.52
1:K:362:GLN:HE21	1:L:248:ALA:HA	1.74	0.52
1:M:79:VAL:HG22	1:O:151:LEU:HD22	1.92	0.52
1:N:111:ALA:O	1:N:115:ARG:NH2	2.35	0.52
1:Q:370:TYR:CD1	1:R:225:ARG:HD3	2.44	0.52
2:n:97:GLU:OE2	2:n:97:GLU:N	2.39	0.52
2:l:198:SER:HB2	2:l:211:LEU:HD12	1.92	0.52
1:A:303:ASN:H	1:C:309:GLY:HA2	1.75	0.52
1:B:186:SER:HA	1:B:216:VAL:O	2.09	0.52
1:R:61:ARG:HB2	1:R:144:ARG:HH21	1.75	0.52
2:n:206:TRP:CG	2:n:206:TRP:O	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:277:LEU:HD21	2:o:277:LEU:HD21	1.91	0.52
2:l:247:SER:O	2:l:251:THR:HG23	2.09	0.52
2:q:109:ASN:ND2	2:q:110:GLN:OE1	2.41	0.52
2:e:45:ILE:HG22	2:e:50:LEU:HD23	1.92	0.52
2:e:202:TYR:HD2	2:e:206:TRP:CD2	2.27	0.52
1:A:150:ILE:HG13	1:B:78:SER:HB3	1.91	0.51
1:G:309:GLY:HA2	1:H:303:ASN:H	1.75	0.51
1:J:39:ASP:OD1	1:J:50:LYS:CE	2.58	0.51
1:M:94:ILE:HB	1:M:99:SER:HB3	1.91	0.51
1:M:285:ASP:HA	1:N:325:ILE:HG22	1.91	0.51
1:R:98:ASN:OD1	1:R:129:ARG:NH1	2.43	0.51
1:D:70:LEU:HD11	1:D:93:ALA:HB2	1.91	0.51
1:E:186:SER:HA	1:E:216:VAL:O	2.10	0.51
1:H:190:SER:HA	1:H:213:THR:HG22	1.91	0.51
1:I:74:GLN:HB3	1:I:88:PRO:HD3	1.91	0.51
1:J:228:GLY:C	1:L:184:ASN:HB3	2.36	0.51
1:D:331:ASN:HB2	1:E:276:GLN:CD	2.35	0.51
1:D:354:VAL:HA	1:E:255:GLY:HA2	1.92	0.51
1:P:355:THR:OG1	1:R:255:GLY:O	2.28	0.51
2:j:112:ASP:O	2:j:117:ARG:NE	2.43	0.51
2:j:191:VAL:HG21	2:k:159:LYS:HD3	1.92	0.51
2:m:57:GLU:OE2	2:m:60:THR:N	2.38	0.51
2:g:169:ILE:HB	2:g:172:ILE:HD12	1.91	0.51
1:D:79:VAL:HG22	1:F:151:LEU:HD22	1.93	0.51
1:P:79:VAL:HG13	1:R:151:LEU:HD21	1.91	0.51
2:d:169:ILE:HB	2:d:172:ILE:HD12	1.93	0.51
1:A:232:SER:N	1:A:235:ASP:OD2	2.44	0.51
1:D:79:VAL:HG13	1:F:151:LEU:HD21	1.92	0.51
1:G:355:THR:OG1	1:I:255:GLY:O	2.29	0.51
1:N:180:LEU:HD21	1:N:189:VAL:HG11	1.93	0.51
2:n:204:THR:HA	2:n:206:TRP:CZ3	2.42	0.51
2:p:112:ASP:O	2:p:117:ARG:NE	2.44	0.51
1:D:141:THR:HG21	1:E:83:ILE:HG13	1.90	0.51
1:D:150:ILE:HG13	1:E:78:SER:HB3	1.92	0.51
1:H:321:ASN:OD1	1:H:321:ASN:N	2.42	0.51
1:M:79:VAL:HG13	1:O:151:LEU:HD21	1.92	0.51
1:M:303:ASN:H	1:O:309:GLY:HA2	1.76	0.51
1:R:192:THR:O	1:R:195:SER:OG	2.29	0.51
1:R:194:TYR:HD1	1:R:379:VAL:HB	1.75	0.51
2:n:253:LEU:HD11	2:m:256:ASP:OD2	2.11	0.51
2:m:25:ILE:HD12	2:r:99:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:247:SER:OG	2:o:248:TYR:N	2.43	0.51
2:q:199:ASP:OD1	2:q:215:GLN:NE2	2.43	0.51
1:G:267:ASP:HB3	1:H:343:ILE:HD13	1.92	0.51
1:J:79:VAL:HG13	1:L:151:LEU:HD21	1.93	0.51
1:M:123:VAL:HG13	1:O:152:PRO:HG2	1.93	0.51
1:M:309:GLY:HA2	1:N:303:ASN:H	1.76	0.51
1:N:142:ASP:OD2	1:N:144:ARG:NH2	2.43	0.51
1:P:180:LEU:HD11	1:P:189:VAL:HG11	1.93	0.51
2:e:186:THR:HG23	2:f:159:LYS:HD2	1.93	0.51
1:D:181:GLU:HG2	1:D:376:PHE:HE1	1.76	0.51
1:D:303:ASN:H	1:F:309:GLY:HA2	1.76	0.51
1:N:45:GLU:OE1	1:N:45:GLU:HA	2.10	0.51
2:j:169:ILE:HB	2:j:172:ILE:HD12	1.93	0.51
2:l:9:GLY:N	2:g:34:THR:O	2.34	0.51
2:a:139:ARG:NH2	2:a:146:GLU:OE1	2.44	0.51
2:b:57:GLU:OE2	2:b:59:GLU:N	2.44	0.51
2:d:216:ASN:ND2	2:f:209:SER:O	2.44	0.51
1:E:95:ASP:OD2	1:E:96:ASN:ND2	2.44	0.51
1:N:183:LEU:O	1:N:219:THR:N	2.42	0.51
1:N:186:SER:HA	1:N:216:VAL:O	2.10	0.51
1:Q:321:ASN:OD1	1:Q:321:ASN:N	2.42	0.51
1:R:101:VAL:HG22	1:R:116:VAL:HG22	1.93	0.51
2:p:70:TYR:HB3	2:p:79:VAL:O	2.10	0.51
1:C:61:ARG:HB2	1:C:144:ARG:HH21	1.75	0.51
1:G:355:THR:HG22	1:H:254:HIS:H	1.76	0.51
1:H:194:TYR:CD1	1:H:379:VAL:HG21	2.46	0.51
1:I:101:VAL:HG22	1:I:116:VAL:HG22	1.92	0.51
1:N:194:TYR:CD1	1:N:379:VAL:HG21	2.46	0.51
2:n:100:VAL:HG12	2:m:116:LEU:HB2	1.93	0.51
2:k:45:ILE:HG22	2:k:50:LEU:HD23	1.93	0.51
2:g:199:ASP:OD2	2:g:216:ASN:ND2	2.44	0.51
1:E:180:LEU:HD21	1:E:189:VAL:HG11	1.92	0.50
1:G:36:LYS:HB3	1:H:43:SER:HB3	1.92	0.50
1:G:54:TYR:OH	1:H:52:ARG:NH2	2.44	0.50
2:h:59:GLU:HB2	2:h:91:PRO:HA	1.92	0.50
1:G:37:VAL:HG13	1:G:41:SER:HB2	1.93	0.50
1:K:111:ALA:O	1:K:115:ARG:NH2	2.36	0.50
1:L:98:ASN:OD1	1:L:129:ARG:NH1	2.44	0.50
1:M:129:ARG:NH2	2:n:275:THR:HG23	2.22	0.50
1:P:355:THR:HG22	1:Q:254:HIS:H	1.76	0.50
1:R:169:ILE:HG23	1:R:173:ALA:HB3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:202:TYR:OH	2:e:211:LEU:HG	2.12	0.50
1:D:37:VAL:HG13	1:D:41:SER:HB2	1.93	0.50
1:K:321:ASN:OD1	1:K:321:ASN:N	2.42	0.50
1:P:285:ASP:HA	1:Q:325:ILE:HG22	1.93	0.50
1:P:297:ALA:HB2	1:R:312:TYR:HD2	1.76	0.50
1:A:355:THR:OG1	1:C:255:GLY:O	2.29	0.50
1:G:232:SER:N	1:G:235:ASP:OD2	2.45	0.50
1:I:43:SER:HB3	1:I:45:GLU:OE2	2.12	0.50
2:r:247:SER:OG	2:r:248:TYR:N	2.45	0.50
1:A:330:ALA:O	1:B:279:HIS:ND1	2.44	0.50
1:A:355:THR:HG22	1:B:254:HIS:H	1.77	0.50
1:H:184:ASN:ND2	1:I:229:SER:H	2.08	0.50
1:K:166:ILE:HD11	1:L:166:ILE:HD11	1.92	0.50
1:M:15:GLU:H	1:M:15:GLU:CD	2.20	0.50
1:N:95:ASP:OD2	1:N:96:ASN:ND2	2.44	0.50
1:P:37:VAL:HG13	1:P:41:SER:HB2	1.93	0.50
2:b:104:THR:HG21	2:c:118:ILE:HD11	1.94	0.50
1:D:267:ASP:HB3	1:E:343:ILE:HD13	1.92	0.50
1:E:190:SER:HA	1:E:213:THR:HG22	1.93	0.50
2:i:118:ILE:HD11	2:h:104:THR:HG21	1.92	0.50
2:d:165:SER:OG	2:d:167:SER:O	2.25	0.50
2:e:248:TYR:O	2:e:252:GLN:HG2	2.11	0.50
2:g:252:GLN:HB3	2:h:253:LEU:HD21	1.93	0.50
1:G:285:ASP:HA	1:H:325:ILE:HG22	1.93	0.50
1:K:273:THR:HB	1:L:337:ASN:HB3	1.94	0.50
1:M:276:GLN:OE1	1:O:332:ALA:N	2.43	0.50
2:l:99:ASP:HB2	2:g:25:ILE:HD12	1.92	0.50
1:D:330:ALA:O	1:E:279:HIS:ND1	2.44	0.50
1:G:228:GLY:C	1:I:184:ASN:HB3	2.36	0.50
1:P:276:GLN:OE1	1:R:332:ALA:N	2.43	0.50
2:k:189:GLU:N	2:k:189:GLU:OE1	2.43	0.50
2:o:245:ASP:N	2:o:245:ASP:OD1	2.45	0.50
2:a:149:LEU:N	2:a:152:GLU:OE1	2.28	0.50
2:d:267:LYS:HB3	2:f:267:LYS:HD2	1.94	0.50
1:A:343:ILE:HG13	1:C:267:ASP:HA	1.94	0.50
1:G:39:ASP:OD1	1:G:40:ASN:N	2.45	0.50
1:J:359:GLY:O	1:K:251:SER:OG	2.27	0.50
1:R:43:SER:HB3	1:R:45:GLU:OE2	2.12	0.50
1:H:224:LEU:HB2	1:I:224:LEU:HD12	1.93	0.49
1:M:331:ASN:HB2	1:N:276:GLN:CD	2.37	0.49
2:a:269:ASP:OD1	2:a:269:ASP:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:269:ASP:OD1	2:d:269:ASP:N	2.41	0.49
2:h:153:MET:HB2	2:h:162:ILE:HG12	1.93	0.49
1:G:297:ALA:HB2	1:I:312:TYR:HD2	1.76	0.49
1:I:192:THR:O	1:I:195:SER:OG	2.28	0.49
1:M:150:ILE:HG13	1:N:78:SER:HB3	1.94	0.49
1:P:334:LEU:HD11	1:R:276:GLN:HG3	1.94	0.49
1:P:359:GLY:O	1:Q:251:SER:OG	2.28	0.49
2:n:21:ARG:NH2	2:m:111:LEU:HG	2.28	0.49
2:i:247:SER:OG	2:i:248:TYR:N	2.45	0.49
2:p:216:ASN:OD1	2:r:209:SER:N	2.39	0.49
2:d:191:VAL:HG13	2:e:158:GLY:HA3	1.94	0.49
1:J:94:ILE:HB	1:J:99:SER:HB3	1.95	0.49
1:K:166:ILE:HA	1:K:374:ARG:O	2.12	0.49
1:N:190:SER:HA	1:N:213:THR:HG22	1.94	0.49
1:O:145:ASP:HB3	1:O:148:VAL:HG13	1.94	0.49
2:k:7:ARG:HG3	2:l:31:PRO:HB2	1.94	0.49
2:k:220:ASP:HA	2:k:223:VAL:HB	1.94	0.49
2:l:21:ARG:HG3	2:l:64:THR:HB	1.95	0.49
2:m:254:SER:O	2:m:258:VAL:HG12	2.12	0.49
2:d:61:GLN:HB2	2:d:63:VAL:HG23	1.94	0.49
2:d:248:TYR:OH	2:e:250:ASN:OD1	2.30	0.49
1:A:70:LEU:HD11	1:A:93:ALA:HB2	1.94	0.49
1:A:79:VAL:HG13	1:C:151:LEU:HD21	1.93	0.49
1:A:228:GLY:C	1:C:184:ASN:HB3	2.38	0.49
1:J:330:ALA:O	1:K:279:HIS:ND1	2.45	0.49
1:L:209:ASP:H	1:L:213:THR:HG1	1.59	0.49
1:P:182:LEU:HB2	1:P:375:VAL:HG13	1.95	0.49
1:P:232:SER:N	1:P:235:ASP:OD2	2.46	0.49
2:j:191:VAL:HA	2:l:194:ILE:HG12	1.94	0.49
2:j:267:LYS:HD3	2:k:269:ASP:HA	1.95	0.49
2:q:104:THR:HG21	2:r:118:ILE:HD11	1.95	0.49
2:a:193:VAL:O	2:b:188:PRO:HD2	2.13	0.49
1:G:15:GLU:OE2	1:G:15:GLU:N	2.25	0.49
1:N:44:ASP:OD1	1:N:50:LYS:NZ	2.36	0.49
1:P:309:GLY:HA2	1:Q:303:ASN:HB3	1.94	0.49
2:d:174:PRO:HA	2:d:180:TRP:CG	2.48	0.49
1:M:354:VAL:HA	1:N:255:GLY:HA2	1.94	0.49
1:N:370:TYR:CD1	1:O:225:ARG:HD3	2.47	0.49
2:o:206:TRP:HA	2:o:209:SER:HB2	1.95	0.49
2:c:247:SER:O	2:c:251:THR:HG23	2.12	0.49
2:e:274:ASN:O	2:e:278:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:SER:HB3	1:C:45:GLU:OE2	2.12	0.49
1:G:249:LEU:HD12	1:G:250:PRO:HD2	1.94	0.49
1:I:296:ALA:HB2	1:I:306:ASP:HA	1.94	0.49
1:L:43:SER:HB3	1:L:45:GLU:OE2	2.13	0.49
1:M:232:SER:N	1:M:235:ASP:OD2	2.46	0.49
1:P:197:LEU:HB2	1:P:379:VAL:HG12	1.94	0.49
1:Q:95:ASP:OD2	1:Q:96:ASN:ND2	2.46	0.49
2:a:25:ILE:HD12	2:f:99:ASP:HB2	1.95	0.49
2:c:30:THR:HB	2:c:31:PRO:CD	2.41	0.49
1:J:70:LEU:HD11	1:J:93:ALA:HB2	1.94	0.49
1:N:184:ASN:ND2	1:O:229:SER:H	2.11	0.49
2:k:159:LYS:HE3	2:k:182:GLU:OE2	2.13	0.49
2:m:174:PRO:HA	2:m:180:TRP:CG	2.48	0.49
2:d:193:VAL:HG11	2:f:193:VAL:HG12	1.94	0.49
1:A:354:VAL:HA	1:B:255:GLY:HA2	1.95	0.49
1:D:309:GLY:HA2	1:E:303:ASN:H	1.77	0.49
1:J:72:VAL:O	1:J:88:PRO:HA	2.12	0.49
1:J:355:THR:HG22	1:K:254:HIS:H	1.78	0.49
1:M:330:ALA:O	1:N:279:HIS:ND1	2.46	0.49
2:n:213:PRO:HB3	2:m:212:VAL:HG13	1.95	0.49
2:i:99:ASP:HB2	2:d:25:ILE:HD12	1.94	0.49
2:i:159:LYS:HD2	2:h:186:THR:HG23	1.94	0.49
2:i:193:VAL:HG22	2:g:193:VAL:HG21	1.95	0.49
2:l:9:GLY:HA3	2:g:35:TYR:CD1	2.48	0.49
2:a:112:ASP:O	2:a:117:ARG:NE	2.46	0.49
2:g:269:ASP:OD1	2:g:269:ASP:N	2.46	0.49
1:A:15:GLU:H	1:A:15:GLU:CD	2.17	0.48
1:B:273:THR:HB	1:C:337:ASN:HB3	1.94	0.48
1:C:179:TYR:HB3	1:C:376:PHE:HB3	1.94	0.48
1:D:22:GLN:HG2	1:E:3:ARG:NH2	2.28	0.48
1:H:95:ASP:OD2	1:H:96:ASN:ND2	2.46	0.48
1:M:168:LEU:O	1:N:205:TYR:OH	2.26	0.48
2:d:213:PRO:HA	2:f:212:VAL:HG13	1.95	0.48
1:A:267:ASP:HB3	1:B:343:ILE:HD13	1.95	0.48
1:D:65:GLN:OE1	1:D:71:SER:OG	2.31	0.48
1:F:191:ARG:NH2	1:F:207:ASN:OD1	2.46	0.48
1:M:259:ASN:OD1	1:M:259:ASN:N	2.45	0.48
2:i:21:ARG:HG3	2:i:64:THR:HB	1.95	0.48
2:q:220:ASP:HA	2:q:223:VAL:HB	1.95	0.48
1:E:184:ASN:ND2	1:F:229:SER:H	2.11	0.48
1:E:362:GLN:HE21	1:F:248:ALA:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:368:GLN:N	1:J:368:GLN:OE1	2.46	0.48
1:L:25:VAL:HG23	1:L:25:VAL:O	2.14	0.48
2:e:220:ASP:HA	2:e:223:VAL:HB	1.96	0.48
1:C:98:ASN:OD1	1:C:129:ARG:NH1	2.46	0.48
1:D:259:ASN:N	1:D:259:ASN:OD1	2.45	0.48
1:J:54:TYR:OH	1:K:52:ARG:NH2	2.45	0.48
1:J:355:THR:OG1	1:L:255:GLY:O	2.30	0.48
1:L:167:SER:OG	1:L:169:ILE:HG12	2.14	0.48
1:M:182:LEU:HB2	1:M:375:VAL:HG13	1.95	0.48
1:Q:273:THR:HB	1:R:337:ASN:HB3	1.96	0.48
2:i:247:SER:O	2:i:251:THR:HG23	2.13	0.48
2:k:7:ARG:HB2	2:l:31:PRO:O	2.14	0.48
2:k:274:ASN:O	2:k:278:ASN:ND2	2.46	0.48
1:A:148:VAL:HG11	1:B:83:ILE:HD12	1.95	0.48
1:E:183:LEU:O	1:E:219:THR:N	2.43	0.48
1:G:74:GLN:HB3	1:G:88:PRO:HD3	1.95	0.48
1:H:273:THR:HB	1:I:337:ASN:HB3	1.96	0.48
1:P:54:TYR:OH	1:Q:52:ARG:NH2	2.44	0.48
1:P:314:ASN:OD1	1:R:302:ASN:OD1	2.32	0.48
2:j:193:VAL:HG12	2:j:194:ILE:HG23	1.94	0.48
2:e:120:LYS:HG3	2:e:121:ILE:N	2.28	0.48
1:C:167:SER:OG	1:C:169:ILE:HG12	2.14	0.48
1:G:276:GLN:OE1	1:I:332:ALA:N	2.44	0.48
2:n:145:THR:OG1	2:n:146:GLU:OE2	2.27	0.48
2:j:174:PRO:HA	2:j:180:TRP:CG	2.49	0.48
2:j:185:ILE:HD12	2:k:153:MET:HE1	1.96	0.48
2:k:104:THR:HG21	2:l:118:ILE:HD11	1.94	0.48
2:k:134:GLY:HA3	2:l:134:GLY:HA3	1.94	0.48
2:l:245:ASP:OD1	2:l:245:ASP:N	2.45	0.48
2:p:187:LEU:HD12	2:p:187:LEU:O	2.14	0.48
1:A:54:TYR:OH	1:B:52:ARG:NH2	2.45	0.48
1:K:4:LYS:HB2	1:K:4:LYS:HE3	1.60	0.48
1:K:56:TRP:CZ2	1:K:146:VAL:HG12	2.48	0.48
1:P:74:GLN:HB3	1:P:88:PRO:HD3	1.95	0.48
1:R:145:ASP:HB3	1:R:148:VAL:HG13	1.95	0.48
1:R:296:ALA:HB2	1:R:306:ASP:HA	1.96	0.48
2:b:112:ASP:OD1	2:b:113:THR:N	2.46	0.48
2:e:7:ARG:HG3	2:f:31:PRO:HB2	1.95	0.48
1:H:43:SER:HB2	1:H:45:GLU:OE1	2.13	0.48
1:I:25:VAL:O	1:I:25:VAL:HG23	2.14	0.48
1:Q:70:LEU:HD21	1:Q:137:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:188:ASN:OD1	1:Q:208:GLY:HA2	2.14	0.48
2:n:112:ASP:OD1	2:n:113:THR:N	2.46	0.48
2:p:219:TYR:O	2:p:223:VAL:HG13	2.13	0.48
2:p:269:ASP:N	2:p:269:ASP:OD1	2.46	0.48
2:e:112:ASP:OD1	2:e:113:THR:N	2.46	0.48
1:D:168:LEU:O	1:E:205:TYR:OH	2.23	0.48
1:D:224:LEU:HD11	1:F:373:PHE:CE2	2.49	0.48
1:J:182:LEU:HB2	1:J:375:VAL:HG13	1.96	0.48
2:n:192:SER:HA	2:m:197:GLY:HA3	1.96	0.48
2:p:57:GLU:HG2	2:p:59:GLU:H	1.79	0.48
2:d:261:ASP:OD1	2:d:262:ALA:N	2.46	0.48
2:g:112:ASP:O	2:g:117:ARG:NE	2.46	0.48
1:E:194:TYR:CD1	1:E:379:VAL:HG21	2.49	0.48
1:G:79:VAL:HG22	1:I:151:LEU:HD22	1.95	0.48
1:G:222:ARG:NH2	1:G:237:GLY:O	2.42	0.48
1:O:101:VAL:HG22	1:O:116:VAL:HG22	1.96	0.48
2:n:36:LEU:HD23	2:n:36:LEU:H	1.79	0.48
2:n:187:LEU:HD22	2:m:193:VAL:HG12	1.95	0.48
2:k:181:TYR:HB2	2:l:138:PRO:HB2	1.96	0.48
2:p:35:TYR:CD1	2:c:9:GLY:HA3	2.49	0.48
2:b:274:ASN:O	2:b:278:ASN:ND2	2.46	0.48
2:f:247:SER:OG	2:f:248:TYR:N	2.47	0.48
2:g:187:LEU:HD12	2:g:187:LEU:O	2.13	0.48
1:A:182:LEU:HB2	1:A:375:VAL:HG13	1.96	0.47
1:D:224:LEU:HD11	1:F:373:PHE:CD2	2.49	0.47
1:F:145:ASP:HB3	1:F:148:VAL:HG13	1.95	0.47
1:I:145:ASP:HB3	1:I:148:VAL:HG13	1.95	0.47
1:J:57:TYR:CZ	1:K:52:ARG:HD2	2.49	0.47
1:K:190:SER:HA	1:K:213:THR:HG22	1.94	0.47
1:O:222:ARG:HB2	1:O:222:ARG:NH1	2.27	0.47
1:Q:362:GLN:HE21	1:R:248:ALA:HA	1.79	0.47
2:n:207:ASN:OD1	2:o:216:ASN:OD1	2.32	0.47
2:g:198:SER:O	2:g:200:THR:N	2.47	0.47
2:h:40:GLU:OE2	2:h:70:TYR:OH	2.27	0.47
1:M:57:TYR:CZ	1:N:52:ARG:HD2	2.49	0.47
1:M:225:ARG:HA	1:O:223:PHE:HA	1.96	0.47
1:P:57:TYR:CZ	1:Q:52:ARG:HD2	2.48	0.47
1:R:25:VAL:HG23	1:R:25:VAL:O	2.14	0.47
2:a:174:PRO:HA	2:a:180:TRP:CG	2.49	0.47
2:e:5:VAL:C	2:e:50:LEU:HD12	2.39	0.47
1:F:222:ARG:NH1	1:F:222:ARG:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:368:GLN:OE1	1:G:368:GLN:N	2.48	0.47
1:N:4:LYS:HB2	1:N:4:LYS:HE3	1.60	0.47
1:P:56:TRP:CZ2	1:P:146:VAL:HG12	2.50	0.47
2:l:7:ARG:HB2	2:g:33:THR:HG23	1.96	0.47
2:m:267:LYS:HB3	2:o:267:LYS:HD2	1.96	0.47
2:b:5:VAL:C	2:b:50:LEU:HD12	2.39	0.47
2:b:45:ILE:HG22	2:b:50:LEU:HD23	1.94	0.47
2:d:185:ILE:HD12	2:e:153:MET:HE1	1.96	0.47
1:A:94:ILE:HB	1:A:99:SER:HB3	1.96	0.47
1:A:241:GLN:HE22	1:A:365:GLN:CD	2.22	0.47
1:F:43:SER:HB3	1:F:45:GLU:OE2	2.14	0.47
1:J:285:ASP:HA	1:K:325:ILE:HG22	1.95	0.47
1:L:365:GLN:NE2	1:L:367:ASP:OD2	2.47	0.47
1:P:79:VAL:HG22	1:R:151:LEU:HD22	1.95	0.47
2:n:244:ALA:HB2	2:o:245:ASP:N	2.28	0.47
2:k:15:LYS:HG3	2:k:78:PRO:HD3	1.96	0.47
2:a:2:THR:N	2:a:55:TYR:O	2.47	0.47
1:A:72:VAL:O	1:A:88:PRO:HA	2.14	0.47
1:A:152:PRO:HG2	1:B:123:VAL:HG13	1.97	0.47
1:B:95:ASP:OD2	1:B:96:ASN:ND2	2.47	0.47
1:B:166:ILE:HA	1:B:374:ARG:O	2.14	0.47
1:C:25:VAL:HG23	1:C:25:VAL:O	2.14	0.47
1:D:232:SER:N	1:D:235:ASP:OD2	2.47	0.47
1:G:57:TYR:CZ	1:H:52:ARG:HD2	2.49	0.47
1:I:37:VAL:HG13	1:I:41:SER:HB2	1.96	0.47
1:J:352:LEU:HB3	1:K:256:ILE:HG13	1.95	0.47
1:K:95:ASP:OD2	1:K:96:ASN:ND2	2.47	0.47
1:M:22:GLN:HG2	1:N:3:ARG:NH2	2.29	0.47
1:M:181:GLU:HG2	1:M:376:PHE:HE1	1.79	0.47
1:N:259:ASN:OD1	1:N:259:ASN:N	2.48	0.47
1:O:25:VAL:HG23	1:O:25:VAL:O	2.14	0.47
2:i:186:THR:HG22	2:g:158:GLY:HA3	1.97	0.47
2:b:40:GLU:OE2	2:b:70:TYR:OH	2.23	0.47
1:A:57:TYR:CZ	1:B:52:ARG:HD2	2.50	0.47
1:D:368:GLN:OE1	1:D:368:GLN:N	2.48	0.47
1:F:25:VAL:O	1:F:25:VAL:HG23	2.14	0.47
1:F:169:ILE:HG23	1:F:173:ALA:HB3	1.95	0.47
1:G:181:GLU:HG2	1:G:376:PHE:HE1	1.79	0.47
1:G:334:LEU:HD11	1:I:276:GLN:HG3	1.95	0.47
1:P:181:GLU:HG2	1:P:376:PHE:HE1	1.78	0.47
2:q:207:ASN:HD22	2:q:207:ASN:HA	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:204:THR:O	2:a:221:LYS:NZ	2.47	0.47
2:d:57:GLU:HG2	2:d:59:GLU:H	1.78	0.47
1:A:352:LEU:HB3	1:B:256:ILE:HG13	1.96	0.47
1:A:368:GLN:OE1	1:A:368:GLN:N	2.47	0.47
1:B:56:TRP:CZ2	1:B:146:VAL:HG12	2.49	0.47
1:D:57:TYR:CZ	1:E:52:ARG:HD2	2.50	0.47
1:D:222:ARG:NH2	1:D:237:GLY:O	2.47	0.47
1:D:249:LEU:HD12	1:D:250:PRO:HD2	1.96	0.47
1:J:22:GLN:HG2	1:K:3:ARG:NH2	2.29	0.47
1:J:148:VAL:HG11	1:K:83:ILE:HD12	1.95	0.47
1:J:354:VAL:HA	1:K:255:GLY:HA2	1.96	0.47
2:i:194:ILE:HG12	2:g:191:VAL:HA	1.97	0.47
2:j:252:GLN:HB3	2:k:253:LEU:HD21	1.97	0.47
2:k:186:THR:HG23	2:l:159:LYS:HD2	1.96	0.47
2:l:247:SER:OG	2:l:248:TYR:N	2.47	0.47
2:r:247:SER:O	2:r:251:THR:HG23	2.14	0.47
2:d:267:LYS:HD3	2:e:269:ASP:HA	1.96	0.47
2:f:178:ASP:OD1	2:f:178:ASP:N	2.48	0.47
2:g:211:LEU:H	2:h:216:ASN:CB	2.19	0.47
1:C:365:GLN:NE2	1:C:367:ASP:OD2	2.48	0.47
1:F:101:VAL:HG22	1:F:116:VAL:HG22	1.96	0.47
1:J:334:LEU:HD11	1:L:276:GLN:HG3	1.96	0.47
1:L:101:VAL:HG22	1:L:116:VAL:HG22	1.96	0.47
1:P:228:GLY:C	1:R:184:ASN:HB3	2.39	0.47
2:m:138:PRO:HA	2:m:153:MET:HE2	1.96	0.47
2:q:274:ASN:O	2:q:278:ASN:ND2	2.47	0.47
2:b:6:GLY:CA	2:c:31:PRO:HB2	2.44	0.47
2:d:191:VAL:HG23	2:d:192:SER:H	1.80	0.47
2:e:212:VAL:N	2:e:213:PRO:HD2	2.29	0.47
1:A:285:ASP:HA	1:B:325:ILE:HG22	1.96	0.47
1:C:209:ASP:OD1	1:C:213:THR:N	2.47	0.47
1:G:56:TRP:CZ2	1:G:146:VAL:HG12	2.50	0.47
1:M:249:LEU:HD12	1:M:250:PRO:HD2	1.96	0.47
1:M:368:GLN:OE1	1:M:368:GLN:N	2.47	0.47
1:N:273:THR:HB	1:O:337:ASN:HB3	1.97	0.47
1:N:353:THR:O	1:O:256:ILE:N	2.41	0.47
1:P:167:SER:HB3	1:P:376:PHE:HE2	1.80	0.47
2:n:268:ALA:HA	2:o:270:LEU:HD13	1.96	0.47
2:q:1:MET:H2	2:q:57:GLU:H	1.62	0.47
2:c:178:ASP:OD1	2:c:178:ASP:N	2.48	0.47
2:h:161:TYR:CE2	2:h:182:GLU:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLN:HG2	1:B:3:ARG:NH2	2.30	0.47
1:C:101:VAL:HG22	1:C:116:VAL:HG22	1.96	0.47
1:D:56:TRP:CZ2	1:D:146:VAL:HG12	2.50	0.47
1:D:158:ALA:HB2	1:E:158:ALA:HA	1.97	0.47
1:H:4:LYS:HB2	1:H:4:LYS:HE3	1.59	0.47
1:H:169:ILE:HG13	1:H:374:ARG:HH21	1.79	0.47
2:n:135:ALA:HB1	2:n:136:PRO:HD2	1.96	0.47
2:j:198:SER:O	2:j:200:THR:N	2.48	0.47
2:l:178:ASP:OD1	2:l:178:ASP:N	2.48	0.47
2:q:134:GLY:HA3	2:r:134:GLY:HA3	1.96	0.47
2:g:193:VAL:O	2:h:188:PRO:HD2	2.14	0.47
1:B:180:LEU:HD21	1:B:189:VAL:HG11	1.98	0.46
1:M:1:MET:H2	1:M:31:LEU:HA	1.80	0.46
1:M:54:TYR:OH	1:N:52:ARG:NH2	2.45	0.46
1:R:191:ARG:NH2	1:R:207:ASN:OD1	2.48	0.46
2:a:212:VAL:HG13	2:b:213:PRO:HA	1.96	0.46
1:H:56:TRP:CZ2	1:H:146:VAL:HG12	2.51	0.46
1:P:39:ASP:OD1	1:P:50:LYS:CE	2.63	0.46
1:Q:4:LYS:HE3	1:Q:4:LYS:HB2	1.61	0.46
2:j:61:GLN:HB2	2:j:63:VAL:HG23	1.96	0.46
2:p:25:ILE:HD12	2:c:99:ASP:HB2	1.97	0.46
2:q:186:THR:HG23	2:r:159:LYS:HD2	1.97	0.46
1:A:334:LEU:HD11	1:C:276:GLN:HG3	1.98	0.46
1:B:194:TYR:CD1	1:B:379:VAL:HG21	2.49	0.46
1:C:191:ARG:NH2	1:C:207:ASN:OD1	2.49	0.46
1:C:209:ASP:H	1:C:213:THR:HG1	1.59	0.46
1:G:310:SER:H	1:H:304:ALA:HB3	1.80	0.46
1:L:145:ASP:HB3	1:L:148:VAL:HG13	1.97	0.46
1:N:166:ILE:HA	1:N:374:ARG:O	2.15	0.46
1:Q:169:ILE:HG13	1:Q:374:ARG:HH21	1.80	0.46
2:i:7:ARG:HG3	2:d:31:PRO:HB2	1.96	0.46
2:m:194:ILE:H	2:m:194:ILE:HG13	1.30	0.46
2:o:64:THR:HG1	2:o:107:VAL:H	1.60	0.46
2:p:198:SER:O	2:p:200:THR:N	2.48	0.46
2:b:212:VAL:HG11	2:c:197:GLY:HA3	1.97	0.46
2:d:191:VAL:HA	2:f:194:ILE:HG12	1.96	0.46
1:N:366:HIS:ND1	1:O:242:ILE:HG21	2.31	0.46
1:O:296:ALA:HB2	1:O:305:PHE:O	2.16	0.46
1:Q:332:ALA:O	1:R:276:GLN:NE2	2.41	0.46
2:m:112:ASP:O	2:m:117:ARG:NE	2.48	0.46
2:m:199:ASP:HB3	2:o:210:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:10:PHE:HE2	2:r:20:LEU:HD12	1.80	0.46
2:r:15:LYS:NZ	2:r:44:ASN:OD1	2.31	0.46
2:a:35:TYR:CD1	2:f:9:GLY:HA3	2.50	0.46
2:a:81:PRO:O	2:a:82:ALA:C	2.57	0.46
2:a:172:ILE:H	2:a:172:ILE:HD12	1.80	0.46
2:g:174:PRO:HA	2:g:180:TRP:CG	2.51	0.46
1:D:46:PRO:HA	1:D:51:THR:HG21	1.97	0.46
1:E:367:ASP:OD1	1:E:367:ASP:N	2.49	0.46
1:J:343:ILE:HD12	1:L:267:ASP:HA	1.96	0.46
1:B:294:PHE:HE2	1:C:317:GLY:H	1.63	0.46
1:N:332:ALA:O	1:O:276:GLN:NE2	2.44	0.46
1:O:43:SER:HB3	1:O:45:GLU:OE2	2.14	0.46
1:Q:56:TRP:CZ2	1:Q:146:VAL:HG12	2.50	0.46
2:j:165:SER:HB2	2:j:179:SER:HB2	1.98	0.46
2:l:159:LYS:HB2	2:l:161:TYR:CE1	2.51	0.46
2:m:261:ASP:OD1	2:m:262:ALA:N	2.47	0.46
2:b:14:GLY:O	2:b:45:ILE:HG12	2.15	0.46
2:c:247:SER:OG	2:c:248:TYR:N	2.48	0.46
2:d:212:VAL:HG11	2:e:196:THR:HG23	1.97	0.46
1:A:39:ASP:OD1	1:A:40:ASN:N	2.49	0.46
1:C:296:ALA:HB2	1:C:305:PHE:O	2.16	0.46
1:D:54:TYR:OH	1:E:52:ARG:NH2	2.45	0.46
1:M:129:ARG:HH21	2:n:275:THR:HG23	1.79	0.46
1:M:267:ASP:HB3	1:N:343:ILE:HD13	1.98	0.46
2:k:202:TYR:N	2:k:218:VAL:HG21	2.30	0.46
2:o:178:ASP:OD1	2:o:178:ASP:N	2.48	0.46
2:o:247:SER:O	2:o:251:THR:HG23	2.14	0.46
2:q:59:GLU:HB2	2:q:91:PRO:HA	1.98	0.46
2:r:245:ASP:N	2:r:245:ASP:OD1	2.48	0.46
2:b:134:GLY:HA3	2:c:134:GLY:HA3	1.98	0.46
1:B:221:GLY:O	1:C:225:ARG:NE	2.42	0.46
1:E:56:TRP:CZ2	1:E:146:VAL:HG12	2.50	0.46
1:I:191:ARG:NH2	1:I:207:ASN:OD1	2.49	0.46
1:K:151:LEU:HD12	1:K:152:PRO:HD2	1.98	0.46
1:K:259:ASN:OD1	1:K:259:ASN:N	2.49	0.46
1:M:167:SER:HB3	1:M:376:PHE:HE2	1.81	0.46
1:N:56:TRP:CZ2	1:N:146:VAL:HG12	2.51	0.46
1:P:307:THR:HB	1:Q:302:ASN:HA	1.98	0.46
1:Q:259:ASN:N	1:Q:259:ASN:OD1	2.49	0.46
2:n:132:VAL:O	2:n:132:VAL:HG13	2.16	0.46
2:k:14:GLY:O	2:k:45:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:212:VAL:N	2:q:213:PRO:HD2	2.29	0.46
2:r:178:ASP:N	2:r:178:ASP:OD1	2.48	0.46
2:d:199:ASP:HB3	2:f:210:LEU:HD12	1.98	0.46
1:E:273:THR:HB	1:F:337:ASN:HB3	1.98	0.46
1:K:221:GLY:O	1:L:225:ARG:NE	2.43	0.46
1:M:361:GLY:N	1:N:249:LEU:O	2.49	0.46
1:P:310:SER:H	1:Q:304:ALA:HB3	1.79	0.46
1:R:209:ASP:H	1:R:213:THR:HG1	1.62	0.46
2:i:178:ASP:OD1	2:i:178:ASP:N	2.49	0.46
2:p:9:GLY:HA3	2:q:35:TYR:CD1	2.51	0.46
2:p:185:ILE:HD12	2:q:153:MET:HE1	1.98	0.46
2:q:97:GLU:H	2:q:97:GLU:CD	2.21	0.46
2:a:198:SER:O	2:a:200:THR:N	2.48	0.46
1:D:259:ASN:HD22	1:F:350:THR:HG23	1.81	0.46
1:K:184:ASN:ND2	1:L:229:SER:H	2.14	0.46
1:R:209:ASP:OD1	1:R:213:THR:N	2.48	0.46
2:r:159:LYS:HB2	2:r:161:TYR:CE1	2.51	0.46
2:d:199:ASP:HA	2:d:213:PRO:O	2.15	0.46
1:H:70:LEU:HD21	1:H:137:VAL:HG21	1.97	0.45
1:H:362:GLN:HE21	1:I:248:ALA:HA	1.80	0.45
1:J:267:ASP:HB3	1:K:343:ILE:HD13	1.98	0.45
1:P:368:GLN:OE1	1:P:368:GLN:N	2.48	0.45
1:Q:294:PHE:HE2	1:R:317:GLY:H	1.64	0.45
1:R:37:VAL:HG13	1:R:41:SER:HB2	1.97	0.45
2:i:270:LEU:HA	2:h:268:ALA:HB2	1.98	0.45
2:j:187:LEU:HD23	2:j:187:LEU:H	1.82	0.45
2:b:186:THR:HG23	2:c:159:LYS:HD2	1.98	0.45
1:A:56:TRP:CZ2	1:A:146:VAL:HG12	2.51	0.45
1:C:145:ASP:HB3	1:C:148:VAL:HG13	1.97	0.45
1:D:182:LEU:HB2	1:D:375:VAL:HG13	1.97	0.45
1:E:111:ALA:O	1:E:115:ARG:NH2	2.41	0.45
1:E:259:ASN:OD1	1:E:259:ASN:N	2.48	0.45
1:F:296:ALA:HB2	1:F:305:PHE:O	2.16	0.45
1:M:180:LEU:HD11	1:M:189:VAL:HG11	1.97	0.45
1:M:187:GLN:HB2	1:M:216:VAL:HB	1.98	0.45
1:P:272:HIS:HD2	1:Q:272:HIS:CD2	2.34	0.45
2:k:182:GLU:OE1	2:k:182:GLU:O	2.34	0.45
2:d:212:VAL:HG22	2:e:215:GLN:HB3	1.98	0.45
1:B:190:SER:HA	1:B:213:THR:HG22	1.97	0.45
1:J:56:TRP:CZ2	1:J:146:VAL:HG12	2.51	0.45
1:P:158:ALA:HB2	1:Q:158:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:237:THR:O	2:k:241:THR:HG22	2.16	0.45
2:k:243:LYS:HG3	2:l:246:LEU:HB3	1.98	0.45
2:p:174:PRO:HA	2:p:180:TRP:CG	2.51	0.45
2:a:199:ASP:OD1	2:a:215:GLN:N	2.38	0.45
2:d:112:ASP:O	2:d:117:ARG:NE	2.50	0.45
2:e:199:ASP:CG	2:e:215:GLN:HE21	2.24	0.45
1:F:209:ASP:H	1:F:213:THR:HG1	1.61	0.45
1:G:22:GLN:HG2	1:H:3:ARG:NH2	2.31	0.45
2:n:70:TYR:HD1	2:n:80:PHE:HA	1.82	0.45
2:i:267:LYS:HD2	2:g:267:LYS:HB3	1.98	0.45
2:j:35:TYR:CD1	2:o:9:GLY:HA3	2.51	0.45
2:e:104:THR:HG21	2:f:118:ILE:HD11	1.97	0.45
1:E:180:LEU:HB3	1:E:377:VAL:HG13	1.99	0.45
1:M:296:ALA:HB3	1:M:306:ASP:HA	1.98	0.45
1:O:111:ALA:O	1:O:115:ARG:NH2	2.46	0.45
1:P:309:GLY:HA2	1:Q:303:ASN:H	1.81	0.45
2:n:158:GLY:HA3	2:m:191:VAL:CB	2.42	0.45
2:n:202:TYR:HD2	2:n:218:VAL:HG21	1.81	0.45
2:i:9:GLY:HA3	2:d:35:TYR:CD1	2.51	0.45
2:i:138:PRO:HB2	2:h:181:TYR:HB2	1.97	0.45
2:j:57:GLU:HG2	2:j:59:GLU:H	1.82	0.45
2:m:35:TYR:CD1	2:r:9:GLY:HA3	2.51	0.45
2:p:193:VAL:HG12	2:p:194:ILE:HG23	1.99	0.45
2:a:199:ASP:H	2:a:213:PRO:HB2	1.81	0.45
2:a:199:ASP:N	2:a:213:PRO:HB2	2.31	0.45
2:d:272:TYR:OH	2:e:274:ASN:OD1	2.31	0.45
2:h:120:LYS:HG3	2:h:121:ILE:N	2.31	0.45
1:B:259:ASN:OD1	1:B:259:ASN:N	2.49	0.45
1:E:332:ALA:O	1:F:276:GLN:NE2	2.42	0.45
1:G:167:SER:HB3	1:G:376:PHE:HE2	1.82	0.45
1:G:180:LEU:HD11	1:G:189:VAL:HG11	1.99	0.45
1:G:184:ASN:HD21	1:H:229:SER:H	1.64	0.45
1:G:310:SER:O	1:H:296:ALA:HA	2.17	0.45
1:M:56:TRP:CZ2	1:M:146:VAL:HG12	2.51	0.45
2:j:79:VAL:HG12	2:j:81:PRO:HD2	1.98	0.45
2:j:211:LEU:H	2:k:216:ASN:CB	2.26	0.45
2:k:244:ALA:HB2	2:l:245:ASP:N	2.31	0.45
2:m:214:THR:HG21	2:m:217:ALA:HB3	1.98	0.45
2:p:21:ARG:HD3	2:p:64:THR:HB	1.97	0.45
2:e:156:TYR:HB3	2:e:161:TYR:CE1	2.51	0.45
2:h:160:ASN:HB3	2:h:183:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:O	1:B:356:SER:N	2.44	0.45
1:D:374:ARG:HD2	1:E:233:VAL:HG21	1.99	0.45
1:E:166:ILE:HA	1:E:374:ARG:O	2.16	0.45
1:H:259:ASN:OD1	1:H:259:ASN:N	2.49	0.45
1:K:180:LEU:HD21	1:K:189:VAL:HG11	1.99	0.45
1:K:332:ALA:O	1:L:276:GLN:NE2	2.42	0.45
1:N:26:ASP:OD1	1:N:26:ASP:N	2.50	0.45
2:j:165:SER:OG	2:j:167:SER:O	2.30	0.45
2:o:120:LYS:HE3	2:o:120:LYS:HB2	1.80	0.45
2:b:55:TYR:CG	2:b:56:PRO:HD2	2.52	0.45
2:b:244:ALA:N	2:c:246:LEU:HB2	2.29	0.45
2:e:14:GLY:O	2:e:45:ILE:HG12	2.17	0.45
2:m:80:PHE:N	2:m:81:PRO:HD2	2.31	0.45
2:r:218:VAL:O	2:r:222:ILE:HD13	2.16	0.45
2:g:261:ASP:OD1	2:g:262:ALA:N	2.50	0.45
1:C:293:PRO:HD2	1:C:294:PHE:CE2	2.52	0.45
1:F:240:ASN:HD22	1:F:365:GLN:NE2	2.15	0.45
1:L:184:ASN:OD1	1:L:184:ASN:N	2.50	0.45
1:L:209:ASP:OD1	1:L:213:THR:N	2.49	0.45
1:P:200:LEU:HD12	1:P:200:LEU:HA	1.85	0.45
2:n:102:ALA:HB3	2:o:117:ARG:NH2	2.31	0.45
2:a:211:LEU:H	2:b:216:ASN:CB	2.28	0.45
2:a:239:LEU:HD12	2:b:241:THR:HB	1.98	0.45
2:b:6:GLY:C	2:c:31:PRO:HB2	2.41	0.45
2:g:185:ILE:HD12	2:h:153:MET:HE1	1.99	0.45
1:A:65:GLN:H	1:A:70:LEU:HA	1.82	0.45
1:D:224:LEU:HD12	1:D:224:LEU:HA	1.60	0.45
1:E:62:VAL:HG22	1:E:72:VAL:HG22	1.99	0.45
1:F:180:LEU:HB3	1:F:377:VAL:HG13	1.97	0.45
1:G:224:LEU:HD22	1:G:224:LEU:HA	1.66	0.45
1:H:267:ASP:OD1	1:H:268:GLY:N	2.48	0.45
1:J:255:GLY:O	1:K:356:SER:N	2.47	0.45
2:n:194:ILE:H	2:n:194:ILE:HG13	1.39	0.45
2:g:280:LYS:HD3	2:g:280:LYS:HA	1.79	0.45
1:A:13:TYR:HB3	1:A:15:GLU:OE2	2.17	0.44
1:C:184:ASN:OD1	1:C:184:ASN:N	2.50	0.44
1:D:1:MET:H2	1:D:31:LEU:HA	1.82	0.44
1:E:4:LYS:HE3	1:E:4:LYS:HB2	1.61	0.44
1:G:259:ASN:N	1:G:259:ASN:HD22	2.15	0.44
1:H:62:VAL:HG22	1:H:72:VAL:HG22	2.00	0.44
1:M:157:ASP:OD1	1:M:157:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:347:SER:HB2	1:O:260:THR:HG23	1.99	0.44
1:P:157:ASP:OD1	1:P:157:ASP:N	2.50	0.44
2:i:274:ASN:OD1	2:h:272:TYR:OH	2.29	0.44
2:j:272:TYR:OH	2:k:274:ASN:OD1	2.33	0.44
2:k:7:ARG:HB2	2:l:31:PRO:HB2	1.99	0.44
2:k:191:VAL:O	2:k:193:VAL:HG13	2.17	0.44
2:l:248:TYR:O	2:l:252:GLN:OE1	2.35	0.44
2:m:20:LEU:HD21	2:m:58:THR:HG21	1.98	0.44
2:a:244:ALA:HB2	2:b:246:LEU:HA	1.99	0.44
2:b:206:TRP:NE1	2:c:215:GLN:HB2	2.32	0.44
2:f:159:LYS:HB2	2:f:161:TYR:CE1	2.52	0.44
1:A:361:GLY:N	1:B:249:LEU:O	2.51	0.44
1:D:74:GLN:HB3	1:D:88:PRO:HD3	2.00	0.44
1:D:222:ARG:NH2	1:D:237:GLY:H	2.15	0.44
1:E:154:SER:HA	1:F:123:VAL:HG21	1.99	0.44
1:E:181:GLU:HG2	1:E:376:PHE:CE2	2.53	0.44
1:M:259:ASN:HD22	1:O:350:THR:HG23	1.81	0.44
2:i:64:THR:HG21	2:i:87:ASP:HB3	1.98	0.44
2:b:243:LYS:HD2	2:c:245:ASP:HA	1.99	0.44
2:c:21:ARG:HG3	2:c:64:THR:HB	1.99	0.44
2:c:159:LYS:HB2	2:c:161:TYR:CE1	2.53	0.44
2:e:102:ALA:HB3	2:f:117:ARG:NH2	2.32	0.44
2:f:19:LYS:HB2	2:f:40:GLU:HG2	2.00	0.44
2:g:21:ARG:HD3	2:g:64:THR:HB	1.99	0.44
1:A:179:TYR:HE1	1:A:378:LYS:HD2	1.82	0.44
1:A:233:VAL:HG13	1:C:373:PHE:HA	2.00	0.44
1:B:4:LYS:HE3	1:B:4:LYS:HB2	1.61	0.44
1:B:151:LEU:HD12	1:B:152:PRO:HD2	1.99	0.44
1:C:222:ARG:CZ	1:C:222:ARG:HB2	2.46	0.44
1:D:1:MET:SD	1:D:1:MET:N	2.69	0.44
1:D:274:ILE:HD11	1:F:336:ILE:HG13	1.99	0.44
1:L:44:ASP:OD1	1:L:50:LYS:NZ	2.50	0.44
1:P:123:VAL:HG13	1:R:152:PRO:HG2	1.99	0.44
1:Q:367:ASP:N	1:Q:367:ASP:OD1	2.50	0.44
2:l:258:VAL:HA	2:l:261:ASP:OD2	2.18	0.44
2:m:219:TYR:O	2:m:223:VAL:HG13	2.16	0.44
2:m:264:SER:HA	2:o:263:LEU:HD11	1.99	0.44
2:o:173:LEU:HD13	2:o:173:LEU:HA	1.86	0.44
2:b:102:ALA:HB3	2:c:117:ARG:NH2	2.32	0.44
2:f:247:SER:O	2:f:251:THR:HG23	2.18	0.44
2:h:196:THR:HG22	2:h:197:GLY:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:TYR:HD1	1:F:225:ARG:HD3	1.82	0.44
1:H:353:THR:O	1:I:256:ILE:N	2.40	0.44
1:L:222:ARG:HB2	1:L:222:ARG:CZ	2.46	0.44
1:Q:224:LEU:HB2	1:R:224:LEU:HD12	2.00	0.44
2:o:222:ILE:HD13	2:o:222:ILE:HA	1.87	0.44
2:c:30:THR:CB	2:c:31:PRO:HD2	2.41	0.44
2:e:269:ASP:OD1	2:e:269:ASP:N	2.48	0.44
1:A:368:GLN:HE22	1:C:368:GLN:HB3	1.82	0.44
1:C:176:PRO:HB2	1:C:179:TYR:CD2	2.53	0.44
1:F:111:ALA:O	1:F:115:ARG:NH2	2.47	0.44
1:G:157:ASP:OD1	1:G:157:ASP:N	2.49	0.44
1:H:166:ILE:O	1:I:164:THR:OG1	2.27	0.44
1:H:367:ASP:OD1	1:H:367:ASP:N	2.50	0.44
1:M:46:PRO:HA	1:M:51:THR:HG21	1.98	0.44
1:M:74:GLN:HB3	1:M:88:PRO:HD3	1.99	0.44
1:M:304:ALA:HA	1:N:316:ILE:HD11	1.99	0.44
1:R:240:ASN:HD22	1:R:365:GLN:NE2	2.14	0.44
2:n:199:ASP:HA	2:n:215:GLN:HG3	1.99	0.44
2:j:199:ASP:HA	2:j:213:PRO:O	2.18	0.44
2:m:24:LEU:HD22	2:m:58:THR:HG22	1.99	0.44
2:b:139:ARG:HE	2:b:148:TYR:HE1	1.66	0.44
2:e:10:PHE:HE2	2:f:20:LEU:HD12	1.82	0.44
2:e:59:GLU:HB2	2:e:91:PRO:HA	2.00	0.44
2:g:138:PRO:HA	2:g:153:MET:HE2	1.99	0.44
1:A:1:MET:HE2	1:C:22:GLN:HG3	2.00	0.44
1:G:368:GLN:HE22	1:I:368:GLN:HB3	1.82	0.44
1:L:179:TYR:HB3	1:L:376:PHE:HB3	1.98	0.44
1:N:294:PHE:HE2	1:O:317:GLY:H	1.64	0.44
1:P:259:ASN:HD22	1:R:350:THR:HG23	1.83	0.44
2:k:72:VAL:HB	2:k:76:SER:HA	2.00	0.44
2:a:264:SER:HA	2:c:263:LEU:HD11	1.99	0.44
2:c:30:THR:O	2:c:31:PRO:C	2.59	0.44
2:f:15:LYS:NZ	2:f:44:ASN:OD1	2.33	0.44
1:B:367:ASP:OD1	1:B:367:ASP:N	2.51	0.44
1:M:274:ILE:HD11	1:O:336:ILE:HG13	2.00	0.44
1:N:154:SER:HA	1:O:123:VAL:HG21	1.99	0.44
1:P:22:GLN:HG2	1:Q:3:ARG:NH2	2.33	0.44
2:n:212:VAL:HG12	2:o:212:VAL:HG11	1.98	0.44
2:j:174:PRO:HA	2:j:180:TRP:CD1	2.52	0.44
2:m:2:THR:N	2:m:55:TYR:O	2.51	0.44
2:q:102:ALA:HB3	2:r:117:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:238:ASN:O	2:b:241:THR:HG22	2.17	0.44
2:e:26:ASP:HB2	2:e:35:TYR:HE2	1.82	0.44
1:A:157:ASP:OD1	1:A:157:ASP:N	2.50	0.44
1:B:184:ASN:OD1	1:B:184:ASN:N	2.51	0.44
1:D:157:ASP:N	1:D:157:ASP:OD1	2.49	0.44
1:D:180:LEU:HD11	1:D:189:VAL:HG11	2.00	0.44
1:D:310:SER:H	1:E:304:ALA:HB3	1.83	0.44
1:E:77:ILE:HG12	1:E:86:PHE:HE1	1.83	0.44
1:J:157:ASP:OD1	1:J:157:ASP:N	2.49	0.44
1:J:350:THR:HA	1:L:261:HIS:HB3	2.00	0.44
1:M:266:ASN:OD1	1:M:266:ASN:N	2.50	0.44
2:n:212:VAL:H	2:n:213:PRO:HD2	1.82	0.44
2:j:212:VAL:HG11	2:k:196:THR:HB	2.00	0.44
2:k:13:THR:HG22	2:k:72:VAL:HG21	2.00	0.44
2:e:14:GLY:HA2	2:e:72:VAL:HG13	1.99	0.44
2:e:244:ALA:N	2:f:246:LEU:HB2	2.32	0.44
2:g:174:PRO:HA	2:g:180:TRP:CD1	2.53	0.44
2:g:199:ASP:HA	2:g:213:PRO:O	2.17	0.44
2:g:253:LEU:HD23	2:g:253:LEU:HA	1.82	0.44
1:D:310:SER:O	1:E:296:ALA:HA	2.18	0.44
1:K:194:TYR:CD1	1:K:379:VAL:HG21	2.53	0.44
1:L:296:ALA:HB2	1:L:305:PHE:O	2.17	0.44
1:M:158:ALA:HB2	1:N:158:ALA:HA	2.00	0.44
1:M:205:TYR:CD2	1:M:217:PRO:HD3	2.53	0.44
1:M:224:LEU:HA	1:M:224:LEU:HD12	1.56	0.44
1:Q:212:THR:HG23	1:Q:213:THR:HG23	2.00	0.44
2:n:222:ILE:H	2:n:222:ILE:HG13	1.54	0.44
2:n:243:LYS:HB3	2:n:243:LYS:HE3	1.49	0.44
2:m:199:ASP:HB2	2:o:210:LEU:O	2.17	0.44
2:b:199:ASP:CG	2:b:215:GLN:HE21	2.25	0.44
2:d:198:SER:O	2:d:200:THR:N	2.49	0.44
2:f:246:LEU:HD12	2:f:246:LEU:O	2.17	0.44
1:G:240:ASN:ND2	1:G:366:HIS:O	2.51	0.43
1:J:24:PHE:HE1	1:K:35:LEU:HD12	1.83	0.43
1:J:98:ASN:HD21	2:k:279:SER:HA	1.82	0.43
1:J:224:LEU:HD22	1:J:224:LEU:HA	1.64	0.43
1:P:148:VAL:HG11	1:Q:83:ILE:HD12	1.99	0.43
2:n:246:LEU:HB2	2:m:243:LYS:C	2.43	0.43
2:j:118:ILE:HG21	2:l:118:ILE:HD13	2.00	0.43
2:m:139:ARG:HG3	2:m:152:GLU:HG2	2.00	0.43
2:p:199:ASP:HA	2:p:213:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:243:LYS:HG3	2:r:246:LEU:HB3	2.00	0.43
2:e:13:THR:HG22	2:e:72:VAL:HG21	2.00	0.43
1:D:368:GLN:HE22	1:F:368:GLN:HB3	1.83	0.43
1:E:228:GLY:H	1:E:231:LEU:HB2	1.83	0.43
1:E:277:THR:CG2	1:E:278:PRO:CD	2.96	0.43
1:H:168:LEU:HD11	1:H:373:PHE:CD1	2.53	0.43
1:I:182:LEU:HB2	1:I:375:VAL:HG13	2.00	0.43
1:I:249:LEU:HD12	1:I:250:PRO:HD2	2.00	0.43
1:K:367:ASP:OD1	1:K:367:ASP:N	2.51	0.43
1:L:293:PRO:HD2	1:L:294:PHE:CE2	2.52	0.43
1:O:240:ASN:HD22	1:O:365:GLN:NE2	2.16	0.43
1:R:249:LEU:HD12	1:R:250:PRO:HD2	1.99	0.43
2:i:20:LEU:HD12	2:h:10:PHE:HE2	1.82	0.43
2:i:117:ARG:NH2	2:h:102:ALA:HB3	2.33	0.43
2:l:16:LEU:HD22	2:l:50:LEU:HD22	2.00	0.43
2:b:99:ASP:HB2	2:c:32:ASN:HB2	2.00	0.43
2:g:161:TYR:CE1	2:g:182:GLU:HB2	2.53	0.43
2:g:258:VAL:HA	2:g:261:ASP:OD2	2.18	0.43
1:D:256:ILE:HG21	1:F:352:LEU:HD13	2.00	0.43
1:D:266:ASN:OD1	1:D:266:ASN:N	2.50	0.43
1:G:123:VAL:HG13	1:I:152:PRO:HG2	2.00	0.43
1:G:179:TYR:HE1	1:G:378:LYS:HD2	1.82	0.43
1:J:361:GLY:N	1:K:249:LEU:O	2.52	0.43
1:K:294:PHE:HE2	1:L:317:GLY:H	1.65	0.43
1:L:176:PRO:HB2	1:L:179:TYR:CD2	2.53	0.43
1:M:1:MET:HE1	1:M:33:HIS:O	2.18	0.43
2:j:191:VAL:HG23	2:j:192:SER:H	1.83	0.43
2:j:199:ASP:O	2:j:213:PRO:HG2	2.19	0.43
2:j:277:LEU:HG	2:l:280:LYS:HE2	1.99	0.43
2:p:174:PRO:HA	2:p:180:TRP:CD1	2.53	0.43
2:r:137:TYR:O	2:r:153:MET:N	2.41	0.43
2:a:57:GLU:HG3	2:a:92:ASN:HA	2.00	0.43
2:g:265:SER:OG	2:g:266:GLY:N	2.52	0.43
1:D:361:GLY:N	1:E:249:LEU:O	2.52	0.43
1:J:65:GLN:H	1:J:70:LEU:HA	1.84	0.43
1:K:353:THR:O	1:L:256:ILE:N	2.44	0.43
1:N:151:LEU:HD12	1:N:152:PRO:HD2	2.01	0.43
1:Q:194:TYR:CD1	1:Q:379:VAL:HG21	2.53	0.43
1:R:70:LEU:HD11	1:R:93:ALA:HB2	2.00	0.43
2:i:134:GLY:HA3	2:h:134:GLY:HA3	2.00	0.43
2:i:263:LEU:HD11	2:g:264:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:159:LYS:HB2	2:j:161:TYR:CE2	2.53	0.43
2:j:265:SER:OG	2:j:266:GLY:N	2.52	0.43
2:k:244:ALA:N	2:l:246:LEU:HB2	2.31	0.43
2:m:70:TYR:HB2	2:m:78:PRO:HB3	2.00	0.43
2:o:182:GLU:OE1	2:o:182:GLU:C	2.61	0.43
2:r:21:ARG:HG3	2:r:64:THR:HB	2.00	0.43
2:c:16:LEU:HD22	2:c:50:LEU:HD22	2.00	0.43
2:d:72:VAL:HB	2:d:76:SER:HA	1.99	0.43
1:D:35:LEU:HD12	1:D:35:LEU:HA	1.92	0.43
1:G:16:ASP:O	1:G:20:ILE:HG13	2.18	0.43
1:M:350:THR:HA	1:O:261:HIS:HB3	2.00	0.43
1:N:181:GLU:HG2	1:N:376:PHE:CE2	2.52	0.43
1:N:367:ASP:OD1	1:N:367:ASP:N	2.49	0.43
2:j:212:VAL:HB	2:j:213:PRO:HD3	2.00	0.43
2:m:70:TYR:CD2	2:m:80:PHE:HA	2.53	0.43
2:o:239:LEU:O	2:o:243:LYS:N	2.50	0.43
2:p:252:GLN:HB3	2:q:253:LEU:HD21	1.99	0.43
1:J:167:SER:HB3	1:J:376:PHE:HE2	1.83	0.43
1:M:184:ASN:OD1	1:N:228:GLY:HA2	2.18	0.43
1:P:240:ASN:ND2	1:P:366:HIS:O	2.51	0.43
2:i:229:ILE:HD11	2:g:229:ILE:HG12	1.99	0.43
2:i:246:LEU:HD22	2:h:244:ALA:H	1.82	0.43
2:k:280:LYS:HD3	2:k:280:LYS:HA	1.75	0.43
2:m:188:PRO:O	2:m:189:GLU:C	2.62	0.43
2:q:211:LEU:H	2:q:211:LEU:HG	1.61	0.43
2:d:215:GLN:HB2	2:f:213:PRO:HD3	2.01	0.43
2:d:244:ALA:HB2	2:e:246:LEU:HA	2.00	0.43
2:d:276:GLN:HG2	2:e:277:LEU:HD22	2.00	0.43
1:D:48:ASN:O	1:D:52:ARG:HG3	2.19	0.43
1:D:184:ASN:OD1	1:E:228:GLY:HA2	2.18	0.43
1:G:1:MET:HE2	1:I:22:GLN:HG3	2.01	0.43
1:I:167:SER:OG	1:I:169:ILE:HG12	2.19	0.43
1:J:368:GLN:HE22	1:L:368:GLN:HB3	1.83	0.43
1:K:26:ASP:OD1	1:K:26:ASP:N	2.50	0.43
1:M:222:ARG:NH2	1:M:237:GLY:H	2.16	0.43
1:N:62:VAL:HG22	1:N:72:VAL:HG22	2.00	0.43
1:P:256:ILE:HG21	1:R:352:LEU:HD13	2.01	0.43
1:R:182:LEU:HB2	1:R:375:VAL:HG13	2.01	0.43
2:j:258:VAL:HA	2:j:261:ASP:OD2	2.19	0.43
2:k:14:GLY:HA2	2:k:72:VAL:HG13	2.00	0.43
2:k:102:ALA:HB3	2:l:117:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:83:LEU:H	2:p:83:LEU:HG	1.69	0.43
2:p:258:VAL:HA	2:p:261:ASP:OD2	2.19	0.43
2:a:199:ASP:HA	2:a:213:PRO:O	2.19	0.43
1:F:167:SER:HB3	1:F:376:PHE:HE2	1.83	0.43
1:J:1:MET:HE2	1:L:22:GLN:HG3	1.99	0.43
1:J:191:ARG:CZ	1:J:211:SER:HA	2.49	0.43
1:M:222:ARG:NH2	1:M:237:GLY:O	2.51	0.43
1:M:267:ASP:N	1:M:267:ASP:OD1	2.52	0.43
2:i:248:TYR:O	2:i:252:GLN:HG2	2.19	0.43
2:m:205:GLY:O	2:m:206:TRP:CD1	2.72	0.43
2:o:246:LEU:HD12	2:o:246:LEU:O	2.19	0.43
2:p:199:ASP:OD2	2:p:216:ASN:ND2	2.52	0.43
2:q:244:ALA:HB2	2:r:245:ASP:N	2.31	0.43
2:q:280:LYS:HA	2:q:280:LYS:HD3	1.79	0.43
2:a:220:ASP:O	2:a:223:VAL:HG12	2.19	0.43
2:d:280:LYS:HA	2:d:280:LYS:HD3	1.83	0.43
2:f:222:ILE:HD13	2:f:222:ILE:HA	1.86	0.43
1:D:165:ILE:HG21	1:D:179:TYR:CE2	2.54	0.43
1:G:165:ILE:HD13	1:G:165:ILE:HA	1.84	0.43
1:G:359:GLY:O	1:H:251:SER:OG	2.28	0.43
1:I:176:PRO:HB2	1:I:179:TYR:CD2	2.54	0.43
1:J:184:ASN:OD1	1:K:228:GLY:HA2	2.18	0.43
1:M:205:TYR:CE2	1:O:168:LEU:HD22	2.54	0.43
2:n:267:LYS:HE3	2:o:269:ASP:OD1	2.19	0.43
2:i:245:ASP:HA	2:h:243:LYS:HD2	2.01	0.43
2:g:81:PRO:O	2:g:82:ALA:C	2.61	0.43
2:g:199:ASP:O	2:g:213:PRO:HG2	2.19	0.43
1:A:309:GLY:HA2	1:B:303:ASN:HB3	2.01	0.43
1:B:184:ASN:ND2	1:C:229:SER:H	2.16	0.43
1:D:15:GLU:H	1:D:15:GLU:CD	2.20	0.43
1:D:43:SER:HB3	1:D:48:ASN:OD1	2.19	0.43
1:D:64:VAL:HA	1:D:70:LEU:HD23	2.01	0.43
1:D:179:TYR:CE2	1:E:160:PRO:HG2	2.54	0.43
1:D:225:ARG:HA	1:F:223:PHE:HA	2.00	0.43
1:D:334:LEU:HD11	1:F:276:GLN:HG3	2.01	0.43
1:G:241:GLN:HE22	1:G:365:GLN:CD	2.27	0.43
1:I:70:LEU:HD11	1:I:93:ALA:HB2	2.00	0.43
1:J:233:VAL:HG13	1:L:373:PHE:HA	2.01	0.43
1:O:190:SER:HB3	1:O:193:THR:HG22	2.01	0.43
1:Q:154:SER:HA	1:R:123:VAL:HG21	2.00	0.43
2:k:161:TYR:HA	2:k:182:GLU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:191:VAL:HG23	2:p:192:SER:H	1.84	0.43
2:d:174:PRO:HA	2:d:180:TRP:CD1	2.54	0.43
1:A:359:GLY:O	1:B:251:SER:OG	2.26	0.42
1:B:96:ASN:N	1:B:132:ALA:O	2.52	0.42
1:E:267:ASP:OD1	1:E:268:GLY:N	2.51	0.42
1:H:332:ALA:O	1:I:276:GLN:NE2	2.37	0.42
1:J:169:ILE:HG13	1:J:374:ARG:HH11	1.84	0.42
1:K:228:GLY:H	1:K:231:LEU:HB2	1.84	0.42
1:M:224:LEU:HD11	1:O:373:PHE:CD2	2.54	0.42
1:P:16:ASP:O	1:P:20:ILE:HG13	2.19	0.42
1:P:267:ASP:OD1	1:P:267:ASP:N	2.52	0.42
2:i:11:LEU:HD12	2:i:11:LEU:HA	1.91	0.42
2:k:139:ARG:HE	2:k:148:TYR:HE1	1.67	0.42
2:b:26:ASP:HB3	2:b:33:THR:HB	2.00	0.42
2:d:199:ASP:O	2:d:213:PRO:HG2	2.19	0.42
2:g:159:LYS:HB2	2:g:161:TYR:CE2	2.53	0.42
2:g:263:LEU:HD21	2:h:263:LEU:HD22	2.01	0.42
2:h:274:ASN:O	2:h:278:ASN:ND2	2.52	0.42
1:A:24:PHE:HE1	1:B:35:LEU:HD12	1.84	0.42
1:A:224:LEU:HD22	1:A:224:LEU:HA	1.64	0.42
1:F:176:PRO:HB2	1:F:179:TYR:CD2	2.53	0.42
1:P:274:ILE:HD11	1:R:336:ILE:HG13	2.00	0.42
2:j:34:THR:O	2:o:9:GLY:N	2.38	0.42
2:l:64:THR:HG1	2:l:107:VAL:H	1.62	0.42
2:q:181:TYR:HB2	2:r:138:PRO:HB2	2.01	0.42
2:q:211:LEU:HD12	2:r:215:GLN:HE22	1.84	0.42
2:a:187:LEU:HD23	2:a:187:LEU:H	1.84	0.42
2:b:57:GLU:HG2	2:b:92:ASN:OD1	2.19	0.42
2:f:210:LEU:HD12	2:f:210:LEU:HA	1.87	0.42
2:h:189:GLU:H	2:h:189:GLU:CD	2.21	0.42
1:A:169:ILE:HG13	1:A:374:ARG:HH11	1.83	0.42
1:C:105:LYS:HB3	1:C:105:LYS:HE2	1.83	0.42
1:G:274:ILE:HD11	1:I:336:ILE:HG13	2.01	0.42
1:M:43:SER:HB3	1:M:48:ASN:OD1	2.19	0.42
1:M:256:ILE:HG21	1:O:352:LEU:HD13	2.02	0.42
1:N:45:GLU:HB2	1:N:48:ASN:CG	2.28	0.42
2:n:276:GLN:HB3	2:o:277:LEU:CD1	2.49	0.42
2:i:159:LYS:HB2	2:i:161:TYR:CE1	2.54	0.42
2:j:211:LEU:HG	2:k:216:ASN:HB2	2.01	0.42
2:m:258:VAL:HA	2:m:261:ASP:OD2	2.19	0.42
2:o:258:VAL:HA	2:o:261:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:40:GLU:OE2	2:q:70:TYR:OH	2.26	0.42
2:b:66:THR:OG1	2:b:87:ASP:OD1	2.30	0.42
2:d:216:ASN:OD1	2:f:209:SER:N	2.39	0.42
2:e:42:PHE:CE1	2:e:78:PRO:HG3	2.54	0.42
2:e:275:THR:O	2:e:279:SER:OG	2.23	0.42
2:g:9:GLY:HA3	2:h:35:TYR:CD1	2.54	0.42
1:D:1:MET:H3	1:D:1:MET:CE	2.33	0.42
1:G:184:ASN:OD1	1:G:184:ASN:N	2.52	0.42
1:K:184:ASN:OD1	1:K:184:ASN:N	2.51	0.42
1:N:45:GLU:N	1:N:48:ASN:OD1	2.52	0.42
1:N:180:LEU:HB3	1:N:377:VAL:HG13	2.00	0.42
2:j:204:THR:O	2:j:221:LYS:NZ	2.52	0.42
2:k:55:TYR:CG	2:k:56:PRO:HD2	2.54	0.42
2:m:265:SER:OG	2:m:266:GLY:N	2.52	0.42
2:o:181:TYR:HE1	2:o:183:LEU:HD12	1.84	0.42
2:q:236:ILE:HA	2:q:239:LEU:HG	2.00	0.42
2:r:64:THR:HG21	2:r:87:ASP:HB3	2.01	0.42
2:a:174:PRO:HA	2:a:180:TRP:CD1	2.55	0.42
2:d:178:ASP:OD1	2:d:179:SER:N	2.52	0.42
2:h:12:THR:O	2:h:47:ALA:N	2.52	0.42
1:D:267:ASP:OD1	1:D:267:ASP:N	2.53	0.42
1:F:179:TYR:HB3	1:F:376:PHE:HB3	2.00	0.42
1:J:222:ARG:NH2	1:J:237:GLY:H	2.18	0.42
1:M:48:ASN:O	1:M:52:ARG:HG3	2.19	0.42
1:P:249:LEU:HD12	1:P:250:PRO:HD2	2.01	0.42
1:P:297:ALA:HB2	1:R:312:TYR:CD2	2.54	0.42
1:P:361:GLY:N	1:Q:249:LEU:O	2.53	0.42
1:Q:96:ASN:N	1:Q:132:ALA:O	2.53	0.42
2:k:97:GLU:H	2:k:97:GLU:CD	2.22	0.42
2:r:162:ILE:HD12	2:r:183:LEU:HD13	2.01	0.42
2:a:57:GLU:HG3	2:a:92:ASN:CA	2.49	0.42
2:a:179:SER:HG	2:a:180:TRP:CD1	2.37	0.42
2:d:2:THR:N	2:d:55:TYR:O	2.52	0.42
1:E:294:PHE:HE2	1:F:317:GLY:H	1.66	0.42
1:H:44:ASP:OD1	1:H:50:LYS:NZ	2.34	0.42
1:J:152:PRO:HG2	1:K:123:VAL:HG13	2.01	0.42
1:J:266:ASN:OD1	1:J:266:ASN:N	2.50	0.42
1:N:77:ILE:HG12	1:N:86:PHE:HE1	1.84	0.42
1:N:277:THR:CG2	1:N:278:PRO:CD	2.98	0.42
1:O:240:ASN:HD22	1:O:365:GLN:HE22	1.68	0.42
1:P:350:THR:HA	1:R:261:HIS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:296:ALA:HB2	1:R:305:PHE:O	2.20	0.42
2:j:219:TYR:HE1	2:l:204:THR:HA	1.84	0.42
2:j:261:ASP:OD1	2:j:262:ALA:N	2.53	0.42
2:k:211:LEU:HB2	2:k:212:VAL:H	1.49	0.42
2:k:213:PRO:HB3	2:l:213:PRO:O	2.19	0.42
2:q:160:ASN:HB3	2:q:183:LEU:HD21	2.01	0.42
2:a:47:ALA:O	2:a:49:VAL:HG23	2.20	0.42
2:a:57:GLU:OE2	2:a:60:THR:N	2.41	0.42
2:a:258:VAL:HA	2:a:261:ASP:OD2	2.20	0.42
2:b:212:VAL:HG13	2:c:214:THR:HA	2.00	0.42
2:e:238:ASN:O	2:e:241:THR:HG22	2.20	0.42
2:f:239:LEU:O	2:f:243:LYS:HB3	2.19	0.42
1:A:4:LYS:HD2	1:A:4:LYS:HA	1.85	0.42
1:A:350:THR:HA	1:C:261:HIS:HB3	2.01	0.42
1:D:304:ALA:HA	1:E:316:ILE:HD11	2.00	0.42
1:G:374:ARG:HD2	1:H:233:VAL:HG21	2.01	0.42
1:I:209:ASP:H	1:I:213:THR:HG1	1.66	0.42
1:M:233:VAL:HG13	1:O:373:PHE:HA	2.02	0.42
1:P:98:ASN:HD21	2:q:279:SER:HA	1.84	0.42
2:n:216:ASN:HA	2:n:219:TYR:HB3	2.01	0.42
2:i:181:TYR:CZ	2:g:153:MET:HE3	2.55	0.42
2:j:243:LYS:HB2	2:l:243:LYS:NZ	2.35	0.42
2:k:112:ASP:OD1	2:k:113:THR:N	2.49	0.42
2:m:174:PRO:HA	2:m:180:TRP:CD1	2.54	0.42
2:m:197:GLY:HA2	2:o:210:LEU:HD12	2.01	0.42
2:b:212:VAL:N	2:b:213:PRO:HD2	2.35	0.42
1:F:182:LEU:HB2	1:F:375:VAL:HG13	2.02	0.42
1:J:13:TYR:HB3	1:J:15:GLU:OE2	2.19	0.42
2:i:31:PRO:HB2	2:h:7:ARG:HG3	2.02	0.42
2:i:35:TYR:CD1	2:h:9:GLY:HA3	2.55	0.42
2:l:210:LEU:HD12	2:l:210:LEU:HA	1.80	0.42
2:m:57:GLU:HG3	2:m:92:ASN:CA	2.49	0.42
2:p:79:VAL:HG12	2:p:81:PRO:HD2	2.01	0.42
2:p:261:ASP:OD1	2:p:262:ALA:N	2.52	0.42
2:p:265:SER:OG	2:p:266:GLY:N	2.52	0.42
2:c:64:THR:HG21	2:c:87:ASP:HB3	2.01	0.42
2:c:258:VAL:HA	2:c:261:ASP:OD2	2.19	0.42
2:f:11:LEU:HD12	2:f:11:LEU:HA	1.90	0.42
1:B:166:ILE:HD12	1:C:224:LEU:HD21	2.01	0.42
1:B:347:SER:HB2	1:C:260:THR:HG23	2.02	0.42
1:C:182:LEU:HB2	1:C:375:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:THR:HG22	1:E:247:ASN:H	1.84	0.42
1:H:294:PHE:HE2	1:I:317:GLY:H	1.66	0.42
1:L:249:LEU:HD12	1:L:250:PRO:HD2	2.02	0.42
1:O:70:LEU:HD11	1:O:93:ALA:HB2	2.01	0.42
1:Q:62:VAL:HG22	1:Q:72:VAL:HG22	2.01	0.42
2:n:193:VAL:HB	2:m:195:ALA:HA	2.02	0.42
2:i:239:LEU:O	2:i:243:LYS:HB3	2.20	0.42
2:k:206:TRP:NE1	2:l:215:GLN:HB2	2.34	0.42
2:e:99:ASP:OD1	2:f:25:ILE:HD13	2.20	0.42
2:e:210:LEU:H	2:f:215:GLN:NE2	2.18	0.42
1:A:191:ARG:CZ	1:A:211:SER:HA	2.49	0.42
1:E:308:GLY:HA3	1:F:296:ALA:HB2	2.02	0.42
1:F:190:SER:HB3	1:F:193:THR:HG22	2.02	0.42
1:J:159:VAL:HG23	1:J:163:SER:HB2	2.02	0.42
1:K:265:VAL:HG13	1:L:343:ILE:HD11	2.02	0.42
1:M:310:SER:O	1:N:296:ALA:HA	2.20	0.42
1:N:45:GLU:CA	1:N:48:ASN:OD1	2.68	0.42
1:Q:246:THR:HG22	1:Q:247:ASN:H	1.85	0.42
2:o:5:VAL:HG23	2:o:97:GLU:OE1	2.20	0.42
2:q:9:GLY:HA3	2:r:35:TYR:CD1	2.55	0.42
2:c:64:THR:HG1	2:c:107:VAL:H	1.62	0.42
1:A:222:ARG:NH2	1:A:237:GLY:H	2.17	0.41
1:A:289:ALA:O	1:B:321:ASN:ND2	2.53	0.41
1:B:37:VAL:HB	1:C:42:LEU:HD23	2.02	0.41
1:E:264:SER:OG	1:F:346:GLN:NE2	2.52	0.41
1:I:167:SER:HB3	1:I:376:PHE:HE2	1.84	0.41
1:J:200:LEU:HD12	1:J:200:LEU:HA	1.86	0.41
1:J:259:ASN:HB3	1:K:352:LEU:HD23	2.02	0.41
1:R:176:PRO:HB2	1:R:179:TYR:CD2	2.55	0.41
2:n:215:GLN:NE2	2:m:212:VAL:HG22	2.35	0.41
2:j:243:LYS:C	2:k:246:LEU:HB2	2.45	0.41
2:l:222:ILE:HD13	2:l:222:ILE:HA	1.88	0.41
2:q:11:LEU:HA	2:q:11:LEU:HD12	1.84	0.41
2:a:265:SER:OG	2:a:266:GLY:N	2.52	0.41
2:b:156:TYR:HB3	2:b:161:TYR:CE1	2.55	0.41
2:d:9:GLY:HA3	2:e:35:TYR:CD1	2.54	0.41
2:d:212:VAL:HB	2:d:213:PRO:HD3	2.02	0.41
1:D:350:THR:HA	1:F:261:HIS:HB3	2.02	0.41
1:E:151:LEU:HD12	1:E:152:PRO:HD2	2.01	0.41
1:E:181:GLU:O	1:E:187:GLN:NE2	2.47	0.41
1:G:350:THR:HA	1:I:261:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:309:GLY:HA2	1:K:303:ASN:N	2.33	0.41
1:J:310:SER:H	1:K:304:ALA:HB3	1.84	0.41
1:K:37:VAL:HB	1:L:42:LEU:HD23	2.02	0.41
2:n:221:LYS:HB3	2:n:221:LYS:HE3	1.80	0.41
2:i:243:LYS:NZ	2:g:243:LYS:HB2	2.35	0.41
2:m:277:LEU:HG	2:o:280:LYS:HE2	2.01	0.41
2:p:165:SER:OG	2:p:167:SER:O	2.26	0.41
2:q:238:ASN:O	2:q:241:THR:HG22	2.20	0.41
2:r:72:VAL:HG13	2:r:76:SER:HA	2.02	0.41
2:r:182:GLU:OE2	2:r:182:GLU:C	2.64	0.41
2:b:191:VAL:O	2:b:193:VAL:HG13	2.19	0.41
2:g:153:MET:HG3	2:g:162:ILE:HG13	2.01	0.41
1:G:46:PRO:HA	1:G:51:THR:HG21	2.02	0.41
1:I:39:ASP:OD2	1:I:54:TYR:OH	2.32	0.41
1:J:46:PRO:HA	1:J:51:THR:HG21	2.02	0.41
1:J:98:ASN:ND2	2:k:279:SER:HA	2.35	0.41
1:J:121:PRO:HB2	1:J:123:VAL:O	2.20	0.41
1:P:222:ARG:NH2	1:P:237:GLY:O	2.47	0.41
2:j:249:VAL:HG11	2:l:249:VAL:HG22	2.03	0.41
2:r:14:GLY:HA2	2:r:72:VAL:HG23	2.01	0.41
2:a:147:THR:HG23	2:a:170:ILE:HG13	2.02	0.41
2:a:199:ASP:OD2	2:a:216:ASN:ND2	2.46	0.41
2:b:14:GLY:HA2	2:b:72:VAL:HG13	2.01	0.41
2:b:42:PHE:CE1	2:b:78:PRO:HG3	2.55	0.41
2:b:280:LYS:HA	2:b:280:LYS:HD3	1.75	0.41
2:e:210:LEU:HB3	2:e:211:LEU:HD23	2.02	0.41
2:h:170:ILE:HD12	2:h:170:ILE:HA	1.88	0.41
1:A:310:SER:H	1:B:304:ALA:HB3	1.84	0.41
1:F:70:LEU:HD11	1:F:93:ALA:HB2	2.01	0.41
1:G:267:ASP:N	1:G:267:ASP:OD1	2.52	0.41
1:H:154:SER:HA	1:I:123:VAL:HG21	2.03	0.41
1:L:105:LYS:HB3	1:L:105:LYS:HE2	1.82	0.41
1:M:1:MET:H3	1:M:1:MET:CE	2.33	0.41
1:O:167:SER:OG	1:O:169:ILE:HG12	2.20	0.41
2:i:222:ILE:HD13	2:i:222:ILE:HA	1.89	0.41
2:m:280:LYS:HA	2:m:280:LYS:HD3	1.80	0.41
2:p:280:LYS:HD3	2:p:280:LYS:HA	1.82	0.41
2:r:258:VAL:HA	2:r:261:ASP:OD2	2.20	0.41
2:b:9:GLY:HA3	2:c:35:TYR:CD1	2.54	0.41
2:f:248:TYR:O	2:f:252:GLN:HG2	2.20	0.41
1:A:74:GLN:HB3	1:A:88:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:HB2	1:A:123:VAL:O	2.20	0.41
1:A:267:ASP:OD1	1:A:267:ASP:N	2.53	0.41
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.94	0.41
1:G:361:GLY:N	1:H:249:LEU:O	2.53	0.41
1:M:200:LEU:HD12	1:M:200:LEU:HA	1.85	0.41
1:O:209:ASP:OD1	1:O:213:THR:N	2.52	0.41
1:P:241:GLN:HE22	1:P:365:GLN:CD	2.27	0.41
2:j:47:ALA:O	2:j:49:VAL:HG23	2.20	0.41
2:l:64:THR:HG21	2:l:87:ASP:HB3	2.02	0.41
2:d:265:SER:OG	2:d:266:GLY:N	2.52	0.41
2:h:220:ASP:HA	2:h:223:VAL:HB	2.03	0.41
1:B:368:GLN:HE22	1:C:367:ASP:HA	1.86	0.41
1:D:18:ASN:HD21	1:E:5:VAL:HG23	1.86	0.41
1:E:184:ASN:OD1	1:E:184:ASN:N	2.53	0.41
1:G:309:GLY:HA2	1:H:303:ASN:HB3	2.01	0.41
1:I:209:ASP:OD1	1:I:213:THR:N	2.48	0.41
1:I:293:PRO:HD2	1:I:294:PHE:CE2	2.55	0.41
1:K:368:GLN:HE22	1:L:367:ASP:HA	1.84	0.41
1:M:64:VAL:HA	1:M:70:LEU:HD23	2.03	0.41
1:N:109:ASP:OD2	1:N:115:ARG:NH2	2.50	0.41
1:P:46:PRO:HA	1:P:51:THR:HG21	2.02	0.41
1:R:149:ASP:OD1	1:R:149:ASP:N	2.53	0.41
1:R:167:SER:OG	1:R:169:ILE:HG12	2.20	0.41
2:n:185:ILE:H	2:n:185:ILE:HG12	1.63	0.41
2:i:246:LEU:HB2	2:h:244:ALA:H	1.85	0.41
2:j:244:ALA:HB2	2:k:246:LEU:HA	2.02	0.41
2:k:215:GLN:HE21	2:k:215:GLN:HB3	1.62	0.41
2:m:161:TYR:CE1	2:m:182:GLU:HB2	2.55	0.41
2:p:195:ALA:CB	2:r:195:ALA:HA	2.50	0.41
2:q:45:ILE:HG23	2:q:50:LEU:HD23	2.01	0.41
2:q:139:ARG:HE	2:q:148:TYR:HE1	1.67	0.41
2:q:210:LEU:H	2:q:210:LEU:HG	1.50	0.41
2:a:205:GLY:O	2:a:206:TRP:CD1	2.73	0.41
2:f:5:VAL:HG23	2:f:97:GLU:OE1	2.20	0.41
1:C:70:LEU:HD11	1:C:93:ALA:HB2	2.02	0.41
1:E:347:SER:HB2	1:F:260:THR:HG23	2.01	0.41
1:F:200:LEU:HD23	1:F:200:LEU:HA	1.88	0.41
1:G:61:ARG:NH2	1:G:144:ARG:HH22	2.19	0.41
1:H:369:PRO:O	1:I:223:PHE:HB2	2.20	0.41
1:I:181:GLU:OE2	1:I:374:ARG:NE	2.54	0.41
1:I:323:THR:OG1	1:I:325:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:TYR:HE1	1:J:378:LYS:HD2	1.86	0.41
1:O:242:ILE:HD12	1:O:242:ILE:O	2.21	0.41
1:Q:369:PRO:O	1:R:223:PHE:HB2	2.20	0.41
2:n:91:PRO:HG2	2:n:93:VAL:HG22	2.02	0.41
2:n:204:THR:O	2:n:204:THR:HG22	2.21	0.41
2:k:208:GLY:HA2	2:l:216:ASN:HD21	1.86	0.41
2:q:11:LEU:H	2:q:48:ASN:ND2	2.19	0.41
2:q:182:GLU:OE1	2:q:182:GLU:O	2.39	0.41
2:r:246:LEU:O	2:r:246:LEU:HD12	2.20	0.41
2:c:143:SER:HB3	2:c:146:GLU:OE1	2.21	0.41
2:e:160:ASN:HB3	2:e:183:LEU:HD21	2.01	0.41
2:h:45:ILE:HG23	2:h:50:LEU:HD23	2.01	0.41
2:h:116:LEU:HD12	2:h:116:LEU:HA	1.90	0.41
1:A:123:VAL:HG23	1:C:152:PRO:HG2	2.03	0.41
1:D:16:ASP:O	1:D:20:ILE:HG13	2.21	0.41
1:D:167:SER:HB3	1:D:376:PHE:HE2	1.86	0.41
1:G:148:VAL:HG11	1:H:83:ILE:HD12	2.03	0.41
1:G:200:LEU:HD12	1:G:200:LEU:HA	1.84	0.41
1:G:352:LEU:HB3	1:H:256:ILE:HG13	2.02	0.41
1:L:200:LEU:HD23	1:L:200:LEU:HA	1.88	0.41
1:Q:183:LEU:O	1:Q:219:THR:N	2.47	0.41
1:R:181:GLU:OE2	1:R:374:ARG:NE	2.54	0.41
1:R:323:THR:OG1	1:R:325:ILE:HG13	2.20	0.41
2:m:26:ASP:HB3	2:m:33:THR:HB	2.03	0.41
2:m:165:SER:OG	2:m:167:SER:O	2.27	0.41
2:p:229:ILE:HG12	2:r:229:ILE:HD11	2.02	0.41
2:c:153:MET:HE2	2:c:153:MET:HB2	1.90	0.41
2:e:11:LEU:HD12	2:e:11:LEU:HA	1.83	0.41
1:A:16:ASP:O	1:A:20:ILE:HG13	2.20	0.41
1:B:246:THR:HG22	1:B:247:ASN:H	1.86	0.41
1:C:249:LEU:HD12	1:C:250:PRO:HD2	2.03	0.41
1:G:307:THR:HB	1:H:302:ASN:HA	2.03	0.41
1:H:180:LEU:HB3	1:H:377:VAL:HG13	2.02	0.41
1:H:188:ASN:OD1	1:H:208:GLY:HA2	2.21	0.41
1:J:4:LYS:HA	1:J:4:LYS:HD2	1.85	0.41
1:J:54:TYR:HD1	1:J:54:TYR:HA	1.75	0.41
1:L:181:GLU:OE2	1:L:374:ARG:NE	2.53	0.41
1:M:334:LEU:HD11	1:O:276:GLN:HG3	2.02	0.41
1:O:180:LEU:HB3	1:O:377:VAL:HG13	2.01	0.41
1:O:182:LEU:HB2	1:O:375:VAL:HG13	2.03	0.41
1:P:224:LEU:HD22	1:P:224:LEU:HA	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:374:ARG:HD2	1:Q:233:VAL:HG21	2.02	0.41
1:Q:336:ILE:HD13	1:R:336:ILE:HD11	2.03	0.41
1:Q:368:GLN:HE22	1:R:367:ASP:HA	1.85	0.41
1:R:167:SER:HB3	1:R:376:PHE:HE2	1.86	0.41
2:j:9:GLY:HA3	2:k:35:TYR:CD1	2.56	0.41
2:j:14:GLY:HA2	2:j:72:VAL:HG22	2.03	0.41
2:k:202:TYR:HE2	2:k:214:THR:HA	1.86	0.41
2:o:83:LEU:H	2:o:83:LEU:HG	1.66	0.41
2:p:11:LEU:O	2:p:48:ASN:ND2	2.54	0.41
2:p:47:ALA:O	2:p:49:VAL:HG23	2.21	0.41
2:q:13:THR:HG22	2:q:72:VAL:HG21	2.02	0.41
2:r:82:ALA:O	2:r:83:LEU:C	2.63	0.41
2:a:26:ASP:HB3	2:a:33:THR:HB	2.03	0.41
2:a:243:LYS:C	2:b:246:LEU:HB2	2.46	0.41
2:b:7:ARG:HD2	2:c:30:THR:HG1	1.81	0.41
2:b:99:ASP:OD1	2:c:25:ILE:HD13	2.21	0.41
2:d:258:VAL:HA	2:d:261:ASP:OD2	2.21	0.41
2:e:12:THR:O	2:e:47:ALA:N	2.54	0.41
2:f:258:VAL:HA	2:f:261:ASP:OD2	2.21	0.41
2:h:112:ASP:OD1	2:h:113:THR:N	2.54	0.41
2:h:236:ILE:HA	2:h:239:LEU:HG	2.03	0.41
1:D:296:ALA:HB3	1:D:306:ASP:HA	2.03	0.41
1:D:315:GLY:O	1:D:316:ILE:HG13	2.21	0.41
1:E:353:THR:O	1:F:256:ILE:N	2.42	0.41
1:J:296:ALA:HB3	1:J:306:ASP:HA	2.02	0.41
1:L:70:LEU:HD11	1:L:93:ALA:HB2	2.02	0.41
1:M:310:SER:H	1:N:304:ALA:HB3	1.86	0.41
1:M:368:GLN:HE22	1:O:368:GLN:HB3	1.84	0.41
1:P:368:GLN:HE22	1:R:368:GLN:HB3	1.84	0.41
1:Q:306:ASP:OD1	1:Q:307:THR:N	2.53	0.41
1:Q:353:THR:O	1:R:256:ILE:N	2.41	0.41
1:R:200:LEU:HD23	1:R:200:LEU:HA	1.88	0.41
1:R:242:ILE:O	1:R:242:ILE:HD12	2.21	0.41
2:n:99:ASP:OD1	2:n:99:ASP:C	2.62	0.41
2:b:14:GLY:C	2:b:45:ILE:HG12	2.46	0.41
2:c:210:LEU:HD12	2:c:210:LEU:HA	1.86	0.41
2:c:246:LEU:HD12	2:c:246:LEU:O	2.21	0.41
2:d:264:SER:HA	2:f:263:LEU:HD11	2.01	0.41
1:A:324:GLY:O	1:C:286:PRO:HD2	2.22	0.40
1:G:297:ALA:HB2	1:I:312:TYR:CD2	2.55	0.40
1:I:296:ALA:HB2	1:I:305:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:154:SER:HA	1:L:123:VAL:HG21	2.03	0.40
1:L:362:GLN:HA	1:L:362:GLN:OE1	2.21	0.40
1:O:249:LEU:HD12	1:O:250:PRO:HD2	2.03	0.40
1:O:300:ASN:OD1	1:O:300:ASN:C	2.65	0.40
1:P:161:VAL:HA	1:P:378:LYS:HG3	2.02	0.40
1:P:240:ASN:HD22	1:P:240:ASN:HA	1.67	0.40
1:Q:181:GLU:HG2	1:Q:376:PHE:CE2	2.56	0.40
2:n:276:GLN:HB3	2:o:277:LEU:HG	2.03	0.40
2:j:26:ASP:HB3	2:j:33:THR:HB	2.03	0.40
2:o:159:LYS:HB2	2:o:161:TYR:CE1	2.56	0.40
2:q:11:LEU:H	2:q:48:ASN:HD21	1.68	0.40
2:r:26:ASP:HB2	2:r:35:TYR:HE2	1.85	0.40
2:a:14:GLY:HA2	2:a:72:VAL:HG22	2.03	0.40
1:A:46:PRO:HA	1:A:51:THR:HG21	2.03	0.40
1:D:191:ARG:CZ	1:D:211:SER:HA	2.50	0.40
1:D:264:SER:O	1:E:346:GLN:HB2	2.22	0.40
1:M:315:GLY:O	1:M:316:ILE:HG13	2.21	0.40
1:P:98:ASN:OD1	1:P:98:ASN:N	2.54	0.40
1:P:262:THR:HG22	1:R:347:SER:HA	2.04	0.40
1:P:296:ALA:HB3	1:P:306:ASP:HA	2.04	0.40
1:Q:26:ASP:OD1	1:Q:26:ASP:N	2.51	0.40
1:Q:180:LEU:HB3	1:Q:377:VAL:HG13	2.03	0.40
2:n:26:ASP:HB2	2:n:35:TYR:HE2	1.84	0.40
2:i:72:VAL:HG13	2:i:76:SER:HA	2.04	0.40
2:i:137:TYR:O	2:i:153:MET:N	2.40	0.40
2:l:166:LEU:HD23	2:l:166:LEU:HA	1.97	0.40
2:l:206:TRP:N	2:l:206:TRP:CD1	2.89	0.40
2:a:191:VAL:HG23	2:a:192:SER:H	1.86	0.40
2:b:174:PRO:HA	2:b:180:TRP:CD1	2.56	0.40
2:d:159:LYS:HB2	2:d:161:TYR:CE2	2.57	0.40
1:A:98:ASN:HD21	2:b:279:SER:HA	1.85	0.40
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.84	0.40
1:A:296:ALA:HB3	1:A:306:ASP:HA	2.03	0.40
1:D:194:TYR:HD2	1:D:379:VAL:HG11	1.86	0.40
1:E:96:ASN:N	1:E:132:ALA:O	2.55	0.40
1:G:364:PHE:HE2	1:H:242:ILE:HD11	1.86	0.40
1:H:246:THR:HG22	1:H:247:ASN:H	1.85	0.40
1:I:200:LEU:HD23	1:I:200:LEU:HA	1.88	0.40
1:K:96:ASN:N	1:K:132:ALA:O	2.53	0.40
1:N:166:ILE:HD12	1:O:224:LEU:HD21	2.03	0.40
1:N:306:ASP:OD1	1:N:307:THR:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:107:ASP:N	1:Q:107:ASP:OD1	2.54	0.40
1:R:105:LYS:HB3	1:R:105:LYS:HE2	1.83	0.40
1:R:190:SER:HB3	1:R:193:THR:HG22	2.04	0.40
2:i:215:GLN:NE2	2:h:208:GLY:O	2.21	0.40
2:j:253:LEU:HD23	2:j:253:LEU:HA	1.91	0.40
2:p:199:ASP:O	2:p:213:PRO:HG2	2.22	0.40
2:a:280:LYS:HA	2:a:280:LYS:HD3	1.84	0.40
2:b:6:GLY:HA2	2:c:31:PRO:HB2	2.02	0.40
2:b:59:GLU:HB2	2:b:91:PRO:HA	2.03	0.40
2:g:47:ALA:O	2:g:49:VAL:HG23	2.22	0.40
2:h:238:ASN:O	2:h:241:THR:HG22	2.21	0.40
1:C:242:ILE:HG12	1:C:364:PHE:O	2.22	0.40
1:E:240:ASN:HB2	1:E:365:GLN:NE2	2.31	0.40
1:F:300:ASN:OD1	1:F:300:ASN:C	2.65	0.40
1:G:240:ASN:HD22	1:G:240:ASN:HA	1.69	0.40
1:H:96:ASN:N	1:H:132:ALA:O	2.54	0.40
1:I:312:TYR:CD1	1:I:312:TYR:C	2.99	0.40
1:J:39:ASP:OD1	1:J:50:LYS:NZ	2.54	0.40
1:K:331:ASN:OD1	1:K:331:ASN:N	2.55	0.40
1:M:179:TYR:CE2	1:N:160:PRO:HG2	2.57	0.40
1:N:246:THR:HG22	1:N:247:ASN:H	1.87	0.40
1:P:325:ILE:HD13	1:Q:325:ILE:HD11	2.04	0.40
1:R:111:ALA:O	1:R:115:ARG:NH2	2.49	0.40
2:n:160:ASN:O	2:n:183:LEU:HD23	2.22	0.40
2:i:258:VAL:HA	2:i:261:ASP:OD2	2.22	0.40
2:j:161:TYR:CE1	2:j:182:GLU:HB2	2.55	0.40
2:k:161:TYR:CD2	2:k:182:GLU:HB2	2.57	0.40
2:q:12:THR:O	2:q:47:ALA:N	2.54	0.40
2:q:55:TYR:CG	2:q:56:PRO:HD2	2.57	0.40
2:a:261:ASP:OD1	2:a:262:ALA:N	2.55	0.40
2:c:222:ILE:HD13	2:c:222:ILE:HA	1.87	0.40
2:c:248:TYR:CE1	2:c:249:VAL:HG23	2.57	0.40
2:h:198:SER:O	2:h:213:PRO:HG3	2.22	0.40
1:A:239:SER:N	1:C:367:ASP:O	2.46	0.40
1:D:226:LEU:H	1:D:226:LEU:HG	1.71	0.40
1:H:107:ASP:OD1	1:H:107:ASP:N	2.55	0.40
1:H:151:LEU:HD12	1:H:152:PRO:HD2	2.03	0.40
1:J:98:ASN:OD1	1:J:98:ASN:N	2.55	0.40
1:J:123:VAL:HG23	1:L:152:PRO:HG2	2.03	0.40
1:J:178:GLY:O	1:J:379:VAL:HG23	2.22	0.40
1:J:185:SER:OG	1:J:186:SER:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:274:ILE:HD11	1:L:336:ILE:HG13	2.03	0.40
1:M:314:ASN:OD1	1:O:302:ASN:ND2	2.55	0.40
1:P:61:ARG:NH2	1:P:144:ARG:HH22	2.20	0.40
1:P:270:HIS:NE2	1:R:270:HIS:HE1	2.20	0.40
1:Q:85:SER:O	2:r:274:ASN:ND2	2.41	0.40
2:i:192:SER:OG	2:g:189:GLU:OE2	2.38	0.40
2:o:206:TRP:N	2:o:206:TRP:CD1	2.88	0.40
2:p:260:LEU:HA	2:p:260:LEU:HD12	1.80	0.40
2:a:82:ALA:O	2:a:83:LEU:C	2.63	0.40
2:c:206:TRP:CD1	2:c:206:TRP:N	2.89	0.40
2:d:153:MET:HE2	2:d:153:MET:HB3	1.94	0.40
2:d:196:THR:OG1	2:e:187:LEU:HG	2.21	0.40
2:e:45:ILE:CG2	2:e:50:LEU:HD23	2.51	0.40
2:f:182:GLU:C	2:f:182:GLU:OE2	2.65	0.40
2:h:55:TYR:CG	2:h:56:PRO:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	311/311 (100%)	302 (97%)	9 (3%)	37	58
1	B	310/311 (100%)	295 (95%)	15 (5%)	23	48
1	C	310/311 (100%)	296 (96%)	14 (4%)	24	49
1	D	311/311 (100%)	304 (98%)	7 (2%)	44	63
1	E	310/311 (100%)	299 (96%)	11 (4%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	310/311 (100%)	297 (96%)	13 (4%)	26	50
1	G	311/311 (100%)	304 (98%)	7 (2%)	44	63
1	H	310/311 (100%)	297 (96%)	13 (4%)	26	50
1	I	310/311 (100%)	297 (96%)	13 (4%)	26	50
1	J	311/311 (100%)	302 (97%)	9 (3%)	37	58
1	K	310/311 (100%)	296 (96%)	14 (4%)	24	49
1	L	310/311 (100%)	296 (96%)	14 (4%)	24	49
1	M	311/311 (100%)	302 (97%)	9 (3%)	37	58
1	N	310/311 (100%)	300 (97%)	10 (3%)	34	56
1	O	310/311 (100%)	299 (96%)	11 (4%)	32	54
1	P	311/311 (100%)	303 (97%)	8 (3%)	40	60
1	Q	310/311 (100%)	296 (96%)	14 (4%)	24	49
1	R	310/311 (100%)	300 (97%)	10 (3%)	34	56
2	a	234/384 (61%)	224 (96%)	10 (4%)	26	49
2	b	235/384 (61%)	221 (94%)	14 (6%)	17	44
2	c	234/384 (61%)	225 (96%)	9 (4%)	29	52
2	d	234/384 (61%)	222 (95%)	12 (5%)	21	46
2	e	235/384 (61%)	228 (97%)	7 (3%)	36	57
2	f	234/384 (61%)	221 (94%)	13 (6%)	19	45
2	g	234/384 (61%)	226 (97%)	8 (3%)	32	55
2	h	235/384 (61%)	227 (97%)	8 (3%)	32	55
2	i	234/384 (61%)	224 (96%)	10 (4%)	26	49
2	j	234/384 (61%)	219 (94%)	15 (6%)	16	42
2	k	235/384 (61%)	216 (92%)	19 (8%)	11	35
2	l	234/384 (61%)	221 (94%)	13 (6%)	19	45
2	m	234/384 (61%)	221 (94%)	13 (6%)	19	45
2	n	235/384 (61%)	215 (92%)	20 (8%)	10	33
2	o	234/384 (61%)	217 (93%)	17 (7%)	13	39
2	p	234/384 (61%)	224 (96%)	10 (4%)	26	49
2	q	235/384 (61%)	220 (94%)	15 (6%)	16	42
2	r	234/384 (61%)	224 (96%)	10 (4%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	9804/12510 (78%)	9380 (96%)	424 (4%)	27	49

All (424) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	70	LEU
1	A	106	THR
1	A	159	VAL
1	A	185	SER
1	A	224	LEU
1	A	259	ASN
1	A	353	THR
1	A	379	VAL
1	B	5	VAL
1	B	7	ASN
1	B	19	ILE
1	B	44	ASP
1	B	70	LEU
1	B	105	LYS
1	B	146	VAL
1	B	148	VAL
1	B	168	LEU
1	B	184	ASN
1	B	321	ASN
1	B	334	LEU
1	B	341	THR
1	B	367	ASP
1	B	370	TYR
1	C	11	ILE
1	C	107	ASP
1	C	148	VAL
1	C	149	ASP
1	C	161	VAL
1	C	169	ILE
1	C	184	ASN
1	C	222	ARG
1	C	224	LEU
1	C	292	VAL
1	C	298	VAL
1	C	333	ASN
1	C	341	THR

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Mol	Chain	Res	Type
1	C	377	VAL
1	D	63	THR
1	D	246	THR
1	D	259	ASN
1	D	277	THR
1	D	312	TYR
1	D	353	THR
1	D	379	VAL
1	E	5	VAL
1	E	7	ASN
1	E	48	ASN
1	E	70	LEU
1	E	74	GLN
1	E	98	ASN
1	E	105	LYS
1	E	148	VAL
1	E	367	ASP
1	E	370	TYR
1	E	377	VAL
1	F	107	ASP
1	F	148	VAL
1	F	149	ASP
1	F	159	VAL
1	F	169	ILE
1	F	224	LEU
1	F	292	VAL
1	F	298	VAL
1	F	312	TYR
1	F	323	THR
1	F	341	THR
1	F	360	ASN
1	F	377	VAL
1	G	63	THR
1	G	172	THR
1	G	224	LEU
1	G	259	ASN
1	G	312	TYR
1	G	323	THR
1	G	379	VAL
1	H	5	VAL
1	H	7	ASN
1	H	19	ILE

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Mol	Chain	Res	Type
1	H	44	ASP
1	H	70	LEU
1	H	105	LYS
1	H	148	VAL
1	H	200	LEU
1	H	216	VAL
1	H	270	HIS
1	H	321	ASN
1	H	367	ASP
1	H	370	TYR
1	I	107	ASP
1	I	148	VAL
1	I	159	VAL
1	I	166	ILE
1	I	169	ILE
1	I	224	LEU
1	I	242	ILE
1	I	298	VAL
1	I	323	THR
1	I	333	ASN
1	I	341	THR
1	I	365	GLN
1	I	379	VAL
1	J	63	THR
1	J	70	LEU
1	J	106	THR
1	J	159	VAL
1	J	185	SER
1	J	224	LEU
1	J	259	ASN
1	J	353	THR
1	J	379	VAL
1	K	5	VAL
1	K	7	ASN
1	K	19	ILE
1	K	44	ASP
1	K	70	LEU
1	K	105	LYS
1	K	148	VAL
1	K	181	GLU
1	K	246	THR
1	K	321	ASN

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Mol	Chain	Res	Type
1	K	334	LEU
1	K	353	THR
1	K	367	ASP
1	K	370	TYR
1	L	107	ASP
1	L	148	VAL
1	L	149	ASP
1	L	159	VAL
1	L	169	ILE
1	L	184	ASN
1	L	224	LEU
1	L	292	VAL
1	L	298	VAL
1	L	333	ASN
1	L	341	THR
1	L	352	LEU
1	L	360	ASN
1	L	377	VAL
1	M	63	THR
1	M	211	SER
1	M	212	THR
1	M	246	THR
1	M	259	ASN
1	M	277	THR
1	M	312	TYR
1	M	353	THR
1	M	379	VAL
1	N	5	VAL
1	N	7	ASN
1	N	70	LEU
1	N	98	ASN
1	N	105	LYS
1	N	148	VAL
1	N	267	ASP
1	N	367	ASP
1	N	370	TYR
1	N	377	VAL
1	O	107	ASP
1	O	148	VAL
1	O	149	ASP
1	O	159	VAL
1	O	169	ILE

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Mol	Chain	Res	Type
1	O	224	LEU
1	O	298	VAL
1	O	323	THR
1	O	341	THR
1	O	360	ASN
1	O	377	VAL
1	P	1	MET
1	P	63	THR
1	P	172	THR
1	P	224	LEU
1	P	259	ASN
1	P	312	TYR
1	P	323	THR
1	P	379	VAL
1	Q	5	VAL
1	Q	7	ASN
1	Q	19	ILE
1	Q	44	ASP
1	Q	70	LEU
1	Q	105	LYS
1	Q	146	VAL
1	Q	148	VAL
1	Q	155	ILE
1	Q	303	ASN
1	Q	321	ASN
1	Q	336	ILE
1	Q	367	ASP
1	Q	370	TYR
1	R	107	ASP
1	R	148	VAL
1	R	159	VAL
1	R	166	ILE
1	R	169	ILE
1	R	224	LEU
1	R	298	VAL
1	R	323	THR
1	R	333	ASN
1	R	341	THR
2	n	23	VAL
2	n	25	ILE
2	n	30	THR
2	n	33	THR

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Mol	Chain	Res	Type
2	n	34	THR
2	n	79	VAL
2	n	137	TYR
2	n	186	THR
2	n	187	LEU
2	n	189	GLU
2	n	190	SER
2	n	194	ILE
2	n	196	THR
2	n	200	THR
2	n	210	LEU
2	n	214	THR
2	n	220	ASP
2	n	222	ILE
2	n	241	THR
2	n	243	LYS
2	i	5	VAL
2	i	30	THR
2	i	33	THR
2	i	34	THR
2	i	104	THR
2	i	131	LYS
2	i	225	VAL
2	i	254	SER
2	i	258	VAL
2	i	260	LEU
2	j	30	THR
2	j	33	THR
2	j	41	SER
2	j	57	GLU
2	j	60	THR
2	j	72	VAL
2	j	83	LEU
2	j	110	GLN
2	j	111	LEU
2	j	145	THR
2	j	167	SER
2	j	196	THR
2	j	239	LEU
2	j	247	SER
2	j	252	GLN
2	k	4	ILE

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Mol	Chain	Res	Type
2	k	7	ARG
2	k	28	SER
2	k	29	THR
2	k	30	THR
2	k	33	THR
2	k	34	THR
2	k	64	THR
2	k	79	VAL
2	k	84	LEU
2	k	132	VAL
2	k	178	ASP
2	k	202	TYR
2	k	211	LEU
2	k	212	VAL
2	k	215	GLN
2	k	223	VAL
2	k	248	TYR
2	k	254	SER
2	l	26	ASP
2	l	28	SER
2	l	30	THR
2	l	33	THR
2	l	34	THR
2	l	64	THR
2	l	83	LEU
2	l	104	THR
2	l	178	ASP
2	l	193	VAL
2	l	225	VAL
2	l	254	SER
2	l	258	VAL
2	m	30	THR
2	m	33	THR
2	m	83	LEU
2	m	110	GLN
2	m	147	THR
2	m	189	GLU
2	m	190	SER
2	m	192	SER
2	m	193	VAL
2	m	194	ILE
2	m	196	THR

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Mol	Chain	Res	Type
2	m	198	SER
2	m	239	LEU
2	o	30	THR
2	o	41	SER
2	o	64	THR
2	o	83	LEU
2	o	104	THR
2	o	131	LYS
2	o	178	ASP
2	o	186	THR
2	o	187	LEU
2	o	191	VAL
2	o	193	VAL
2	o	194	ILE
2	o	196	THR
2	o	200	THR
2	o	225	VAL
2	o	254	SER
2	o	258	VAL
2	p	30	THR
2	p	41	SER
2	p	57	GLU
2	p	72	VAL
2	p	80	PHE
2	p	83	LEU
2	p	111	LEU
2	p	147	THR
2	p	167	SER
2	p	239	LEU
2	q	30	THR
2	q	33	THR
2	q	45	ILE
2	q	64	THR
2	q	132	VAL
2	q	178	ASP
2	q	202	TYR
2	q	204	THR
2	q	207	ASN
2	q	210	LEU
2	q	211	LEU
2	q	212	VAL
2	q	248	TYR

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Mol	Chain	Res	Type
2	q	254	SER
2	q	279	SER
2	r	5	VAL
2	r	26	ASP
2	r	28	SER
2	r	29	THR
2	r	30	THR
2	r	104	THR
2	r	178	ASP
2	r	225	VAL
2	r	254	SER
2	r	258	VAL
2	a	30	THR
2	a	41	SER
2	a	58	THR
2	a	72	VAL
2	a	110	GLN
2	a	111	LEU
2	a	147	THR
2	a	167	SER
2	a	176	VAL
2	a	247	SER
2	b	29	THR
2	b	30	THR
2	b	32	ASN
2	b	64	THR
2	b	132	VAL
2	b	178	ASP
2	b	196	THR
2	b	202	TYR
2	b	209	SER
2	b	210	LEU
2	b	211	LEU
2	b	218	VAL
2	b	223	VAL
2	b	248	TYR
2	c	33	THR
2	c	64	THR
2	c	104	THR
2	c	131	LYS
2	c	193	VAL
2	c	225	VAL

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Mol	Chain	Res	Type
2	c	248	TYR
2	c	254	SER
2	c	258	VAL
2	d	41	SER
2	d	57	GLU
2	d	60	THR
2	d	71	SER
2	d	73	ASP
2	d	76	SER
2	d	83	LEU
2	d	111	LEU
2	d	147	THR
2	d	167	SER
2	d	239	LEU
2	d	246	LEU
2	e	30	THR
2	e	33	THR
2	e	64	THR
2	e	99	ASP
2	e	132	VAL
2	e	178	ASP
2	e	212	VAL
2	f	27	GLU
2	f	30	THR
2	f	33	THR
2	f	41	SER
2	f	64	THR
2	f	83	LEU
2	f	104	THR
2	f	131	LYS
2	f	178	ASP
2	f	225	VAL
2	f	248	TYR
2	f	254	SER
2	f	258	VAL
2	g	41	SER
2	g	57	GLU
2	g	72	VAL
2	g	83	LEU
2	g	111	LEU
2	g	147	THR
2	g	167	SER

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Mol	Chain	Res	Type
2	g	239	LEU
2	h	30	THR
2	h	34	THR
2	h	64	THR
2	h	132	VAL
2	h	178	ASP
2	h	211	LEU
2	h	212	VAL
2	h	248	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	362	GLN
1	B	7	ASN
1	B	321	ASN
1	B	322	GLN
1	B	362	GLN
1	B	368	GLN
1	C	40	ASN
1	C	92	ASN
1	C	241	GLN
1	C	259	ASN
1	C	270	HIS
1	C	320	GLN
1	C	328	ASN
1	C	360	ASN
1	D	240	ASN
1	D	259	ASN
1	D	362	GLN
1	E	7	ASN
1	E	48	ASN
1	E	247	ASN
1	E	259	ASN
1	E	321	ASN
1	E	328	ASN
1	E	333	ASN
1	E	362	GLN
1	E	368	GLN
1	F	40	ASN
1	F	92	ASN

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Continued from previous page...

Mol	Chain	Res	Type
1	F	259	ASN
1	F	302	ASN
1	F	320	GLN
1	F	365	GLN
1	G	188	ASN
1	G	240	ASN
1	G	241	GLN
1	G	300	ASN
1	G	362	GLN
1	H	7	ASN
1	H	48	ASN
1	H	321	ASN
1	H	328	ASN
1	H	362	GLN
1	H	368	GLN
1	I	40	ASN
1	I	92	ASN
1	I	187	GLN
1	I	241	GLN
1	I	259	ASN
1	I	270	HIS
1	I	320	GLN
1	I	328	ASN
1	J	48	ASN
1	J	188	ASN
1	J	313	ASN
1	J	362	GLN
1	K	7	ASN
1	K	92	ASN
1	K	247	ASN
1	K	303	ASN
1	K	362	GLN
1	K	368	GLN
1	L	40	ASN
1	L	241	GLN
1	L	259	ASN
1	L	270	HIS
1	L	302	ASN
1	L	320	GLN
1	L	328	ASN
1	L	360	ASN
1	M	240	ASN

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Mol	Chain	Res	Type
1	M	362	GLN
1	N	247	ASN
1	N	270	HIS
1	N	321	ASN
1	N	362	GLN
1	N	368	GLN
1	O	40	ASN
1	O	92	ASN
1	O	241	GLN
1	O	259	ASN
1	O	270	HIS
1	O	302	ASN
1	O	320	GLN
1	O	365	GLN
1	P	188	ASN
1	P	240	ASN
1	P	241	GLN
1	P	259	ASN
1	P	272	HIS
1	P	300	ASN
1	P	362	GLN
1	Q	7	ASN
1	Q	48	ASN
1	Q	321	ASN
1	Q	328	ASN
1	Q	362	GLN
1	Q	368	GLN
1	R	40	ASN
1	R	92	ASN
1	R	241	GLN
1	R	259	ASN
1	R	270	HIS
1	R	320	GLN
1	R	328	ASN
2	n	32	ASN
2	n	44	ASN
2	n	215	GLN
2	n	250	ASN
2	i	235	ASN
2	j	48	ASN
2	j	77	ASN
2	j	160	ASN

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Mol	Chain	Res	Type
2	k	32	ASN
2	k	77	ASN
2	k	109	ASN
2	k	215	GLN
2	l	235	ASN
2	m	48	ASN
2	m	160	ASN
2	o	3	ASN
2	o	77	ASN
2	o	215	GLN
2	o	235	ASN
2	p	48	ASN
2	p	77	ASN
2	q	48	ASN
2	q	207	ASN
2	r	3	ASN
2	r	235	ASN
2	r	238	ASN
2	a	48	ASN
2	a	77	ASN
2	b	48	ASN
2	b	109	ASN
2	c	207	ASN
2	c	215	GLN
2	c	235	ASN
2	c	238	ASN
2	d	48	ASN
2	d	61	GLN
2	d	77	ASN
2	e	48	ASN
2	e	109	ASN
2	f	3	ASN
2	f	77	ASN
2	f	171	ASN
2	f	235	ASN
2	g	48	ASN
2	g	77	ASN
2	g	160	ASN
2	h	48	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

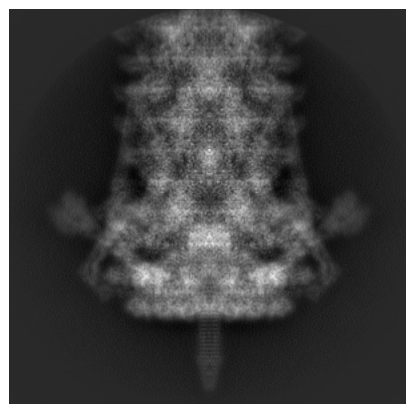
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37152. These allow visual inspection of the internal detail of the map and identification of artifacts.

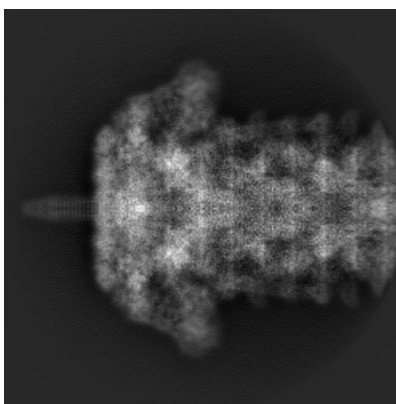
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

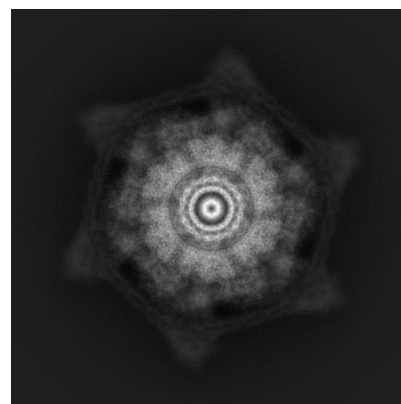
6.1.1 Primary map



X

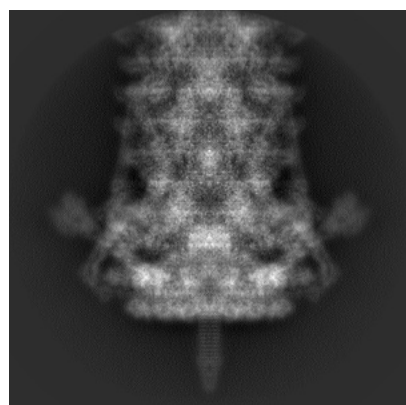


Y

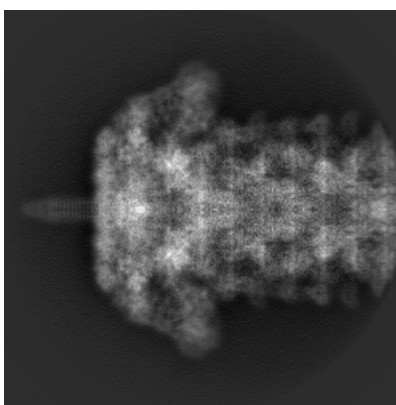


Z

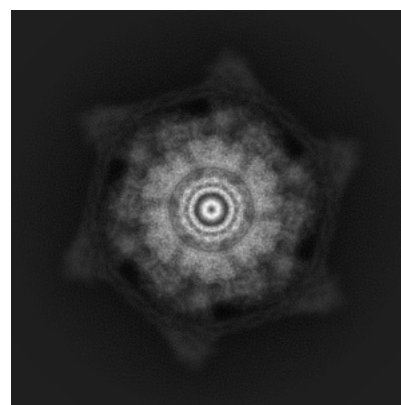
6.1.2 Raw map



X



Y

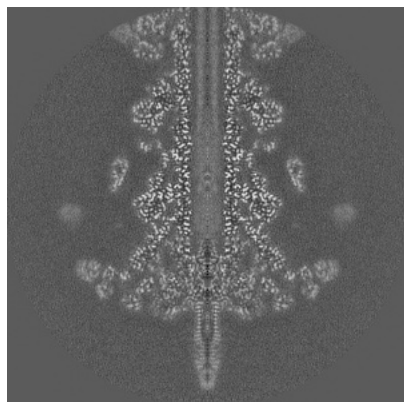


Z

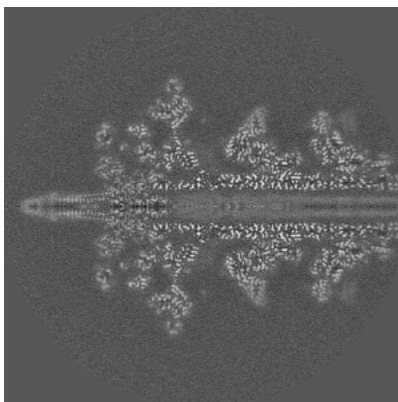
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

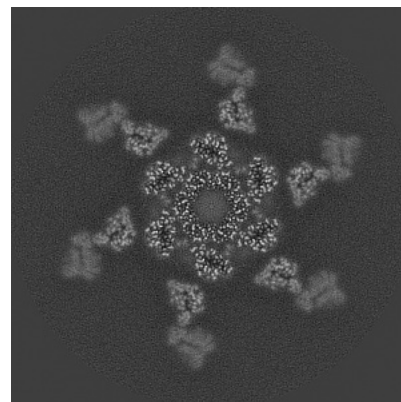
6.2.1 Primary map



X Index: 224

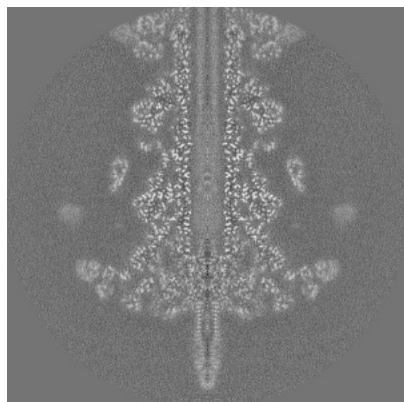


Y Index: 224

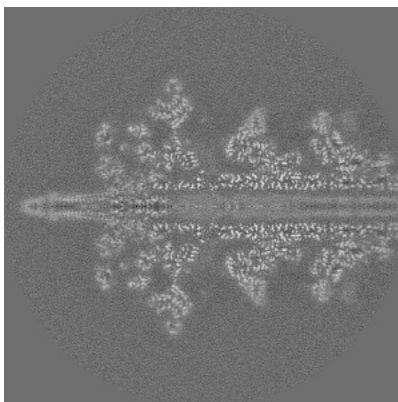


Z Index: 224

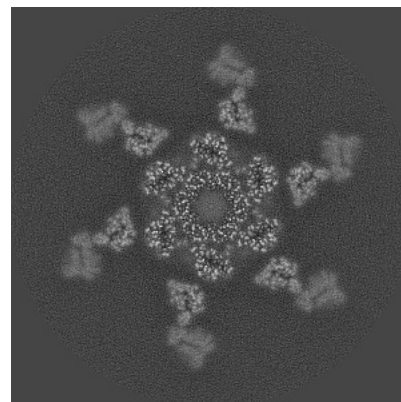
6.2.2 Raw map



X Index: 224



Y Index: 224

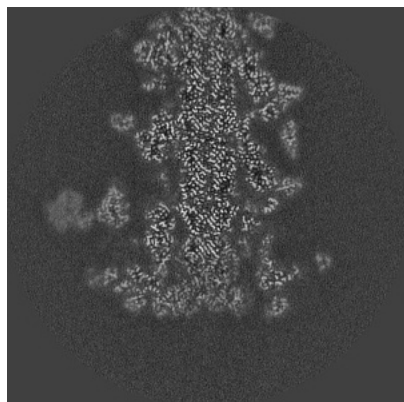


Z Index: 224

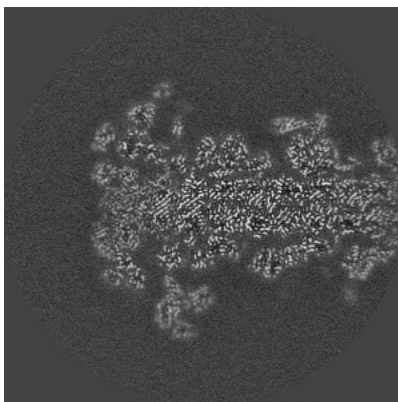
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

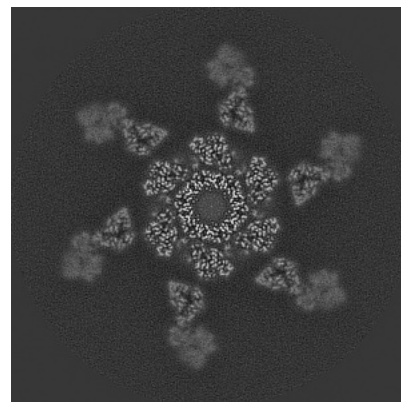
6.3.1 Primary map



X Index: 204

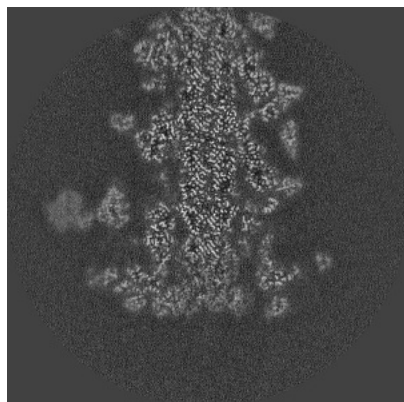


Y Index: 204

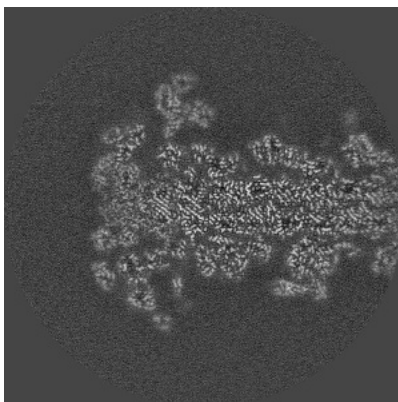


Z Index: 221

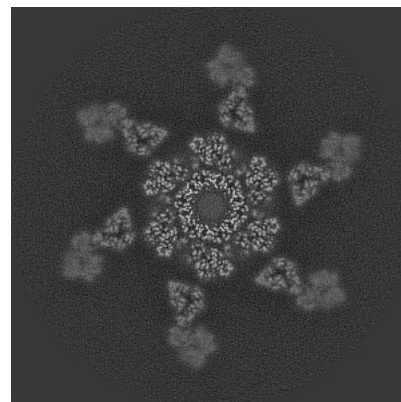
6.3.2 Raw map



X Index: 204



Y Index: 244

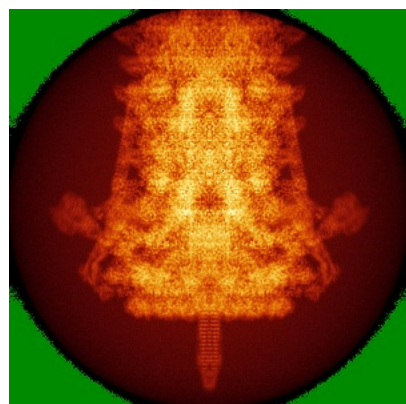


Z Index: 221

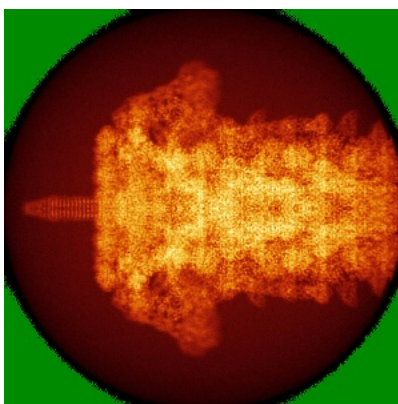
The images above show the largest variance slices of the map in three orthogonal directions.

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

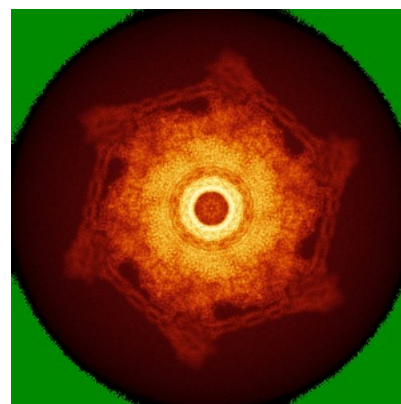
6.4.1 Primary map



X

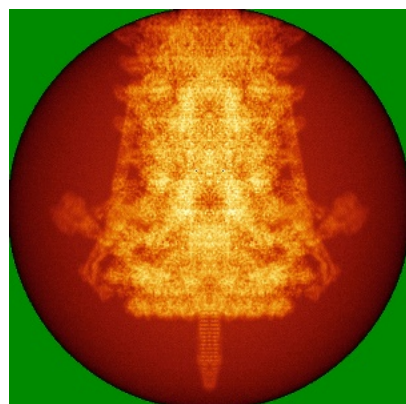


Y

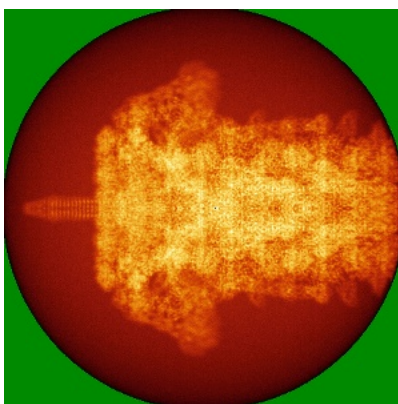


Z

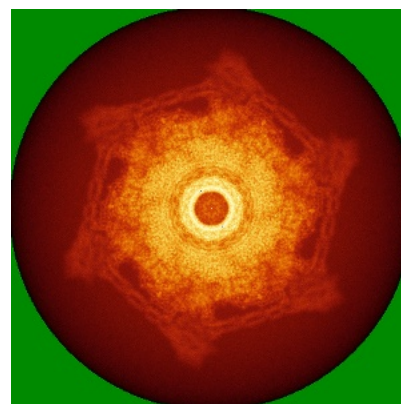
6.4.2 Raw map



X



Y

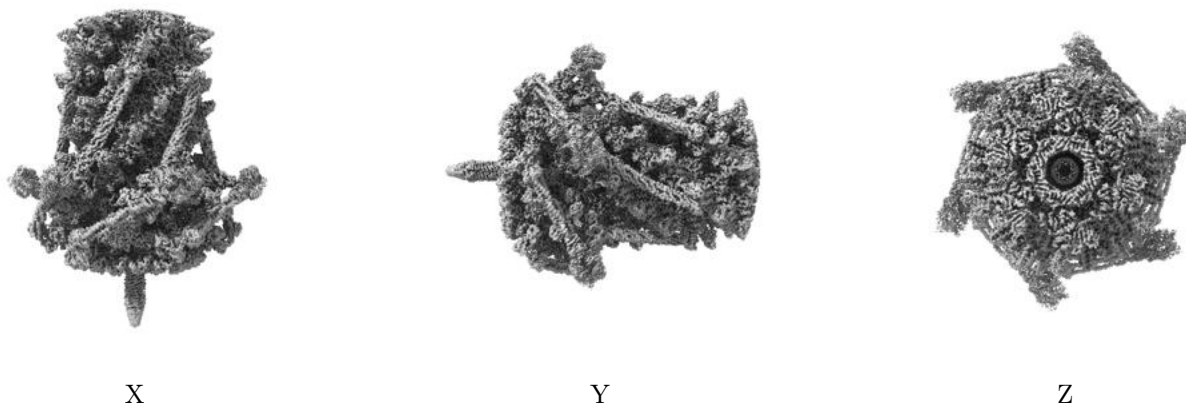


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

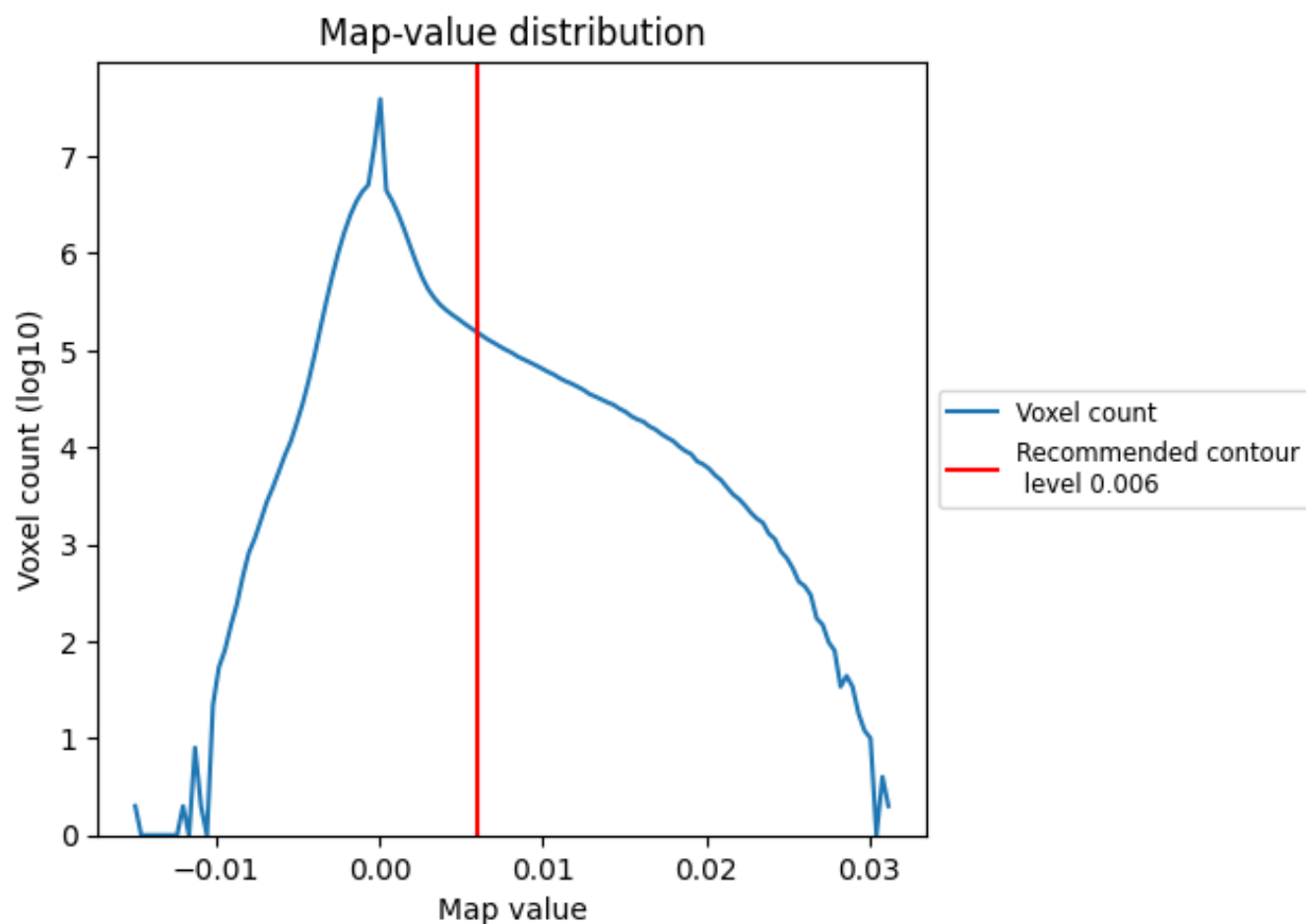
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

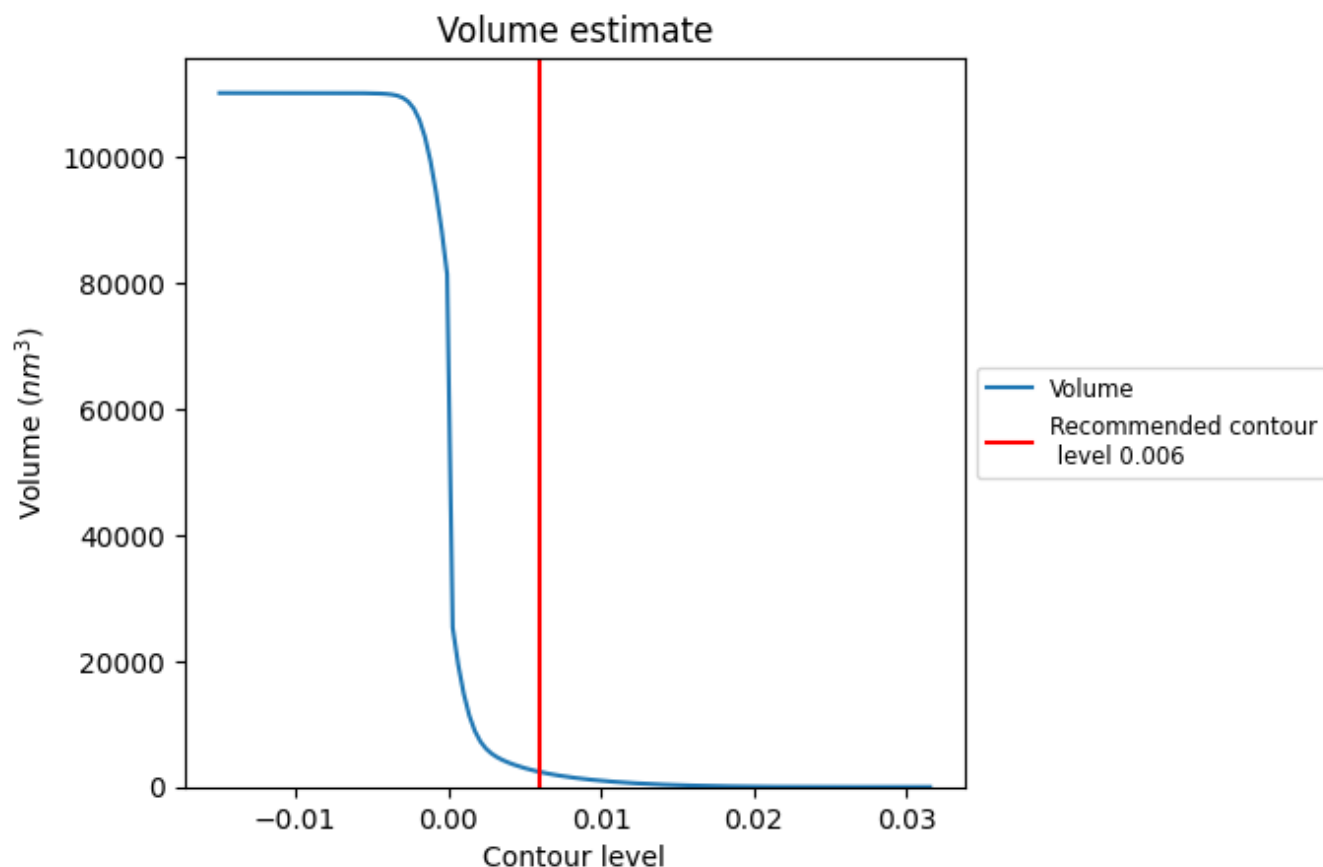
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

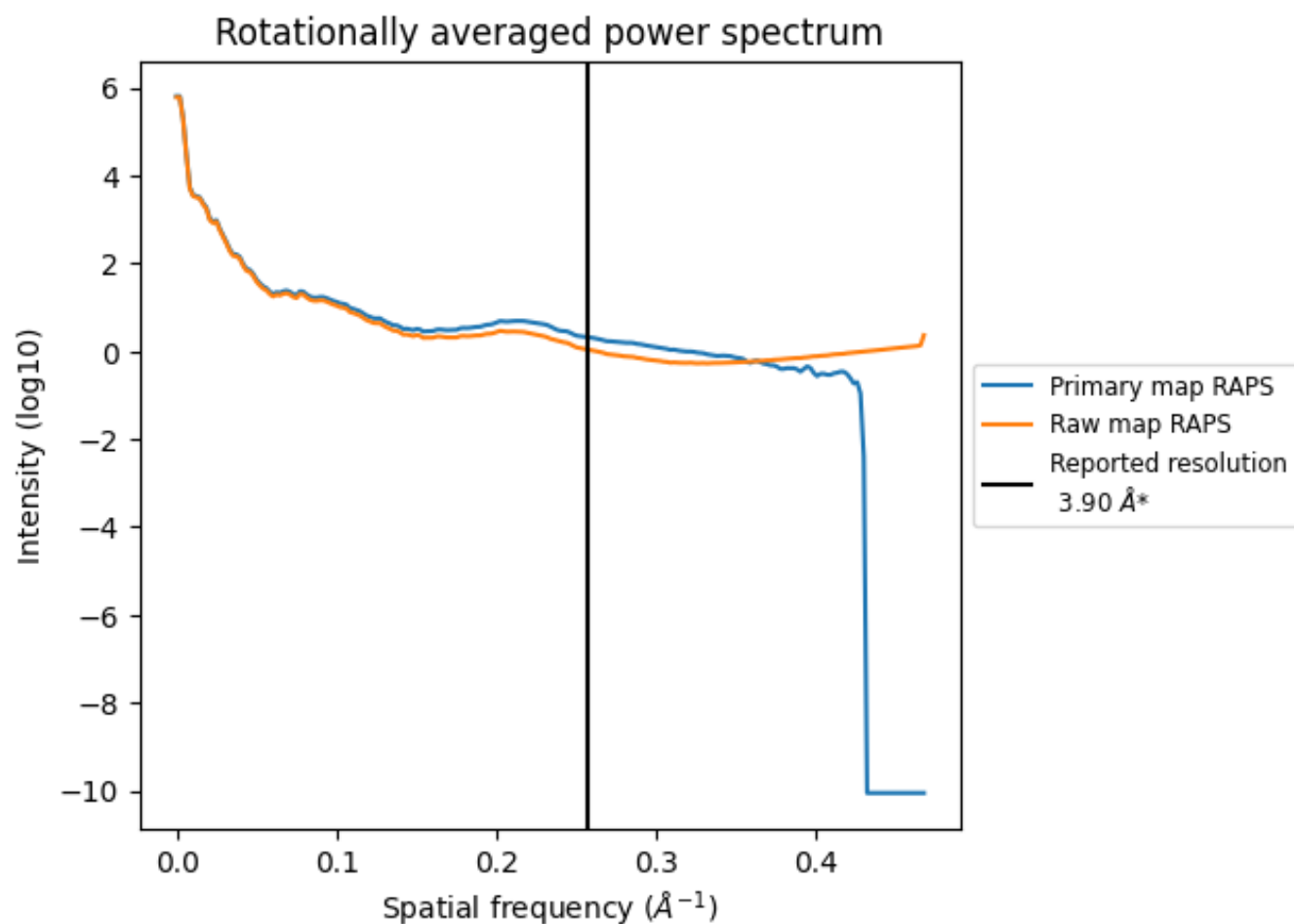
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2387 nm^3 ; this corresponds to an approximate mass of 2157 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 ⓘ

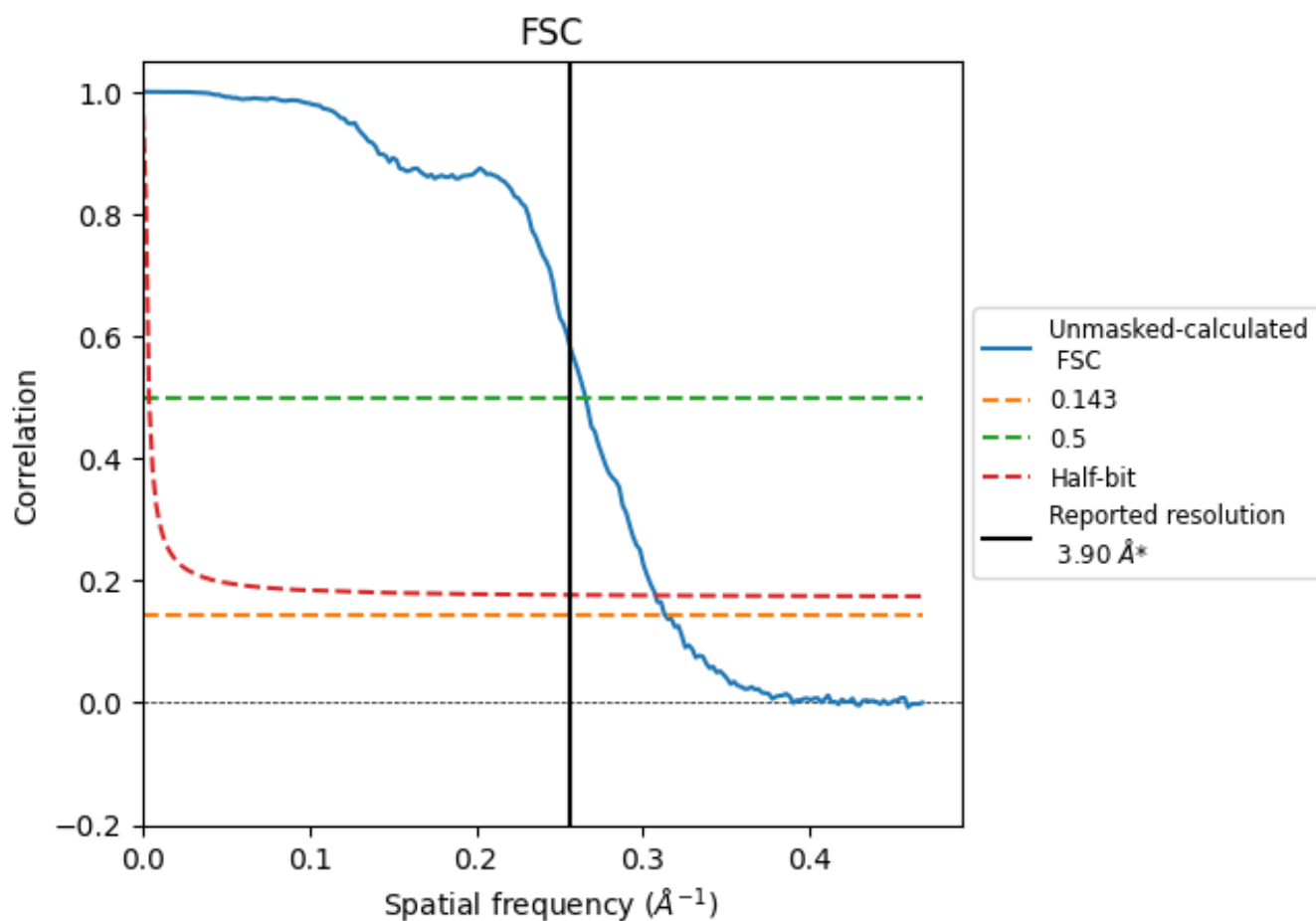


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

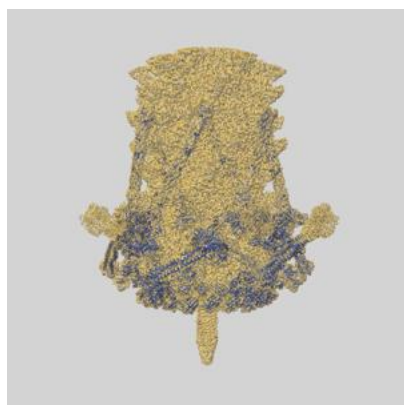
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.77	3.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 3.9 by more than 10 %

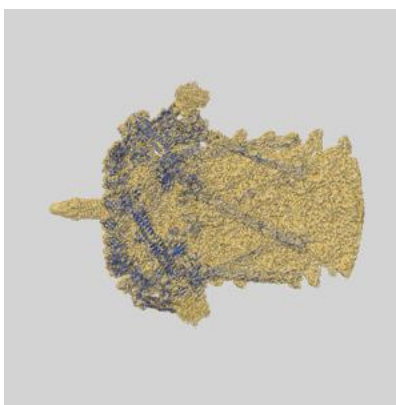
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37152 and PDB model 8KEC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

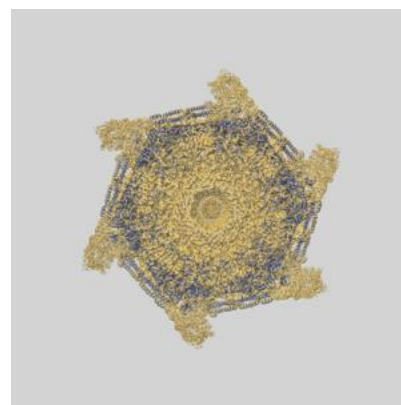
9.1 Map-model overlay [i](#)



X



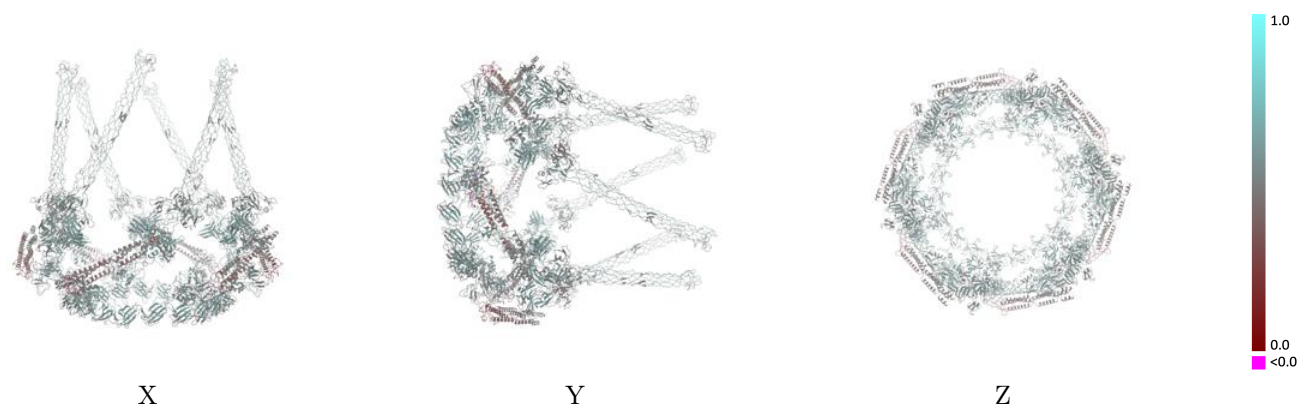
Y



Z

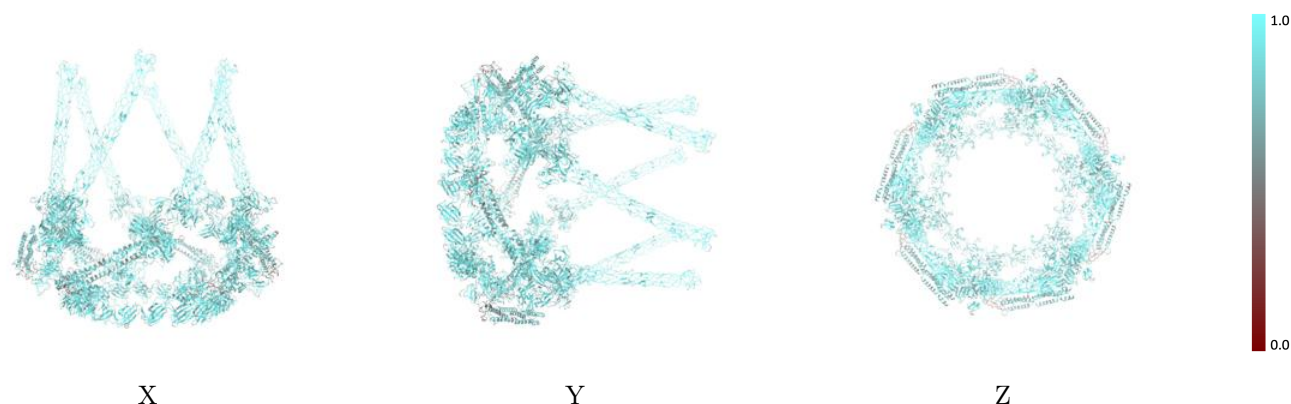
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



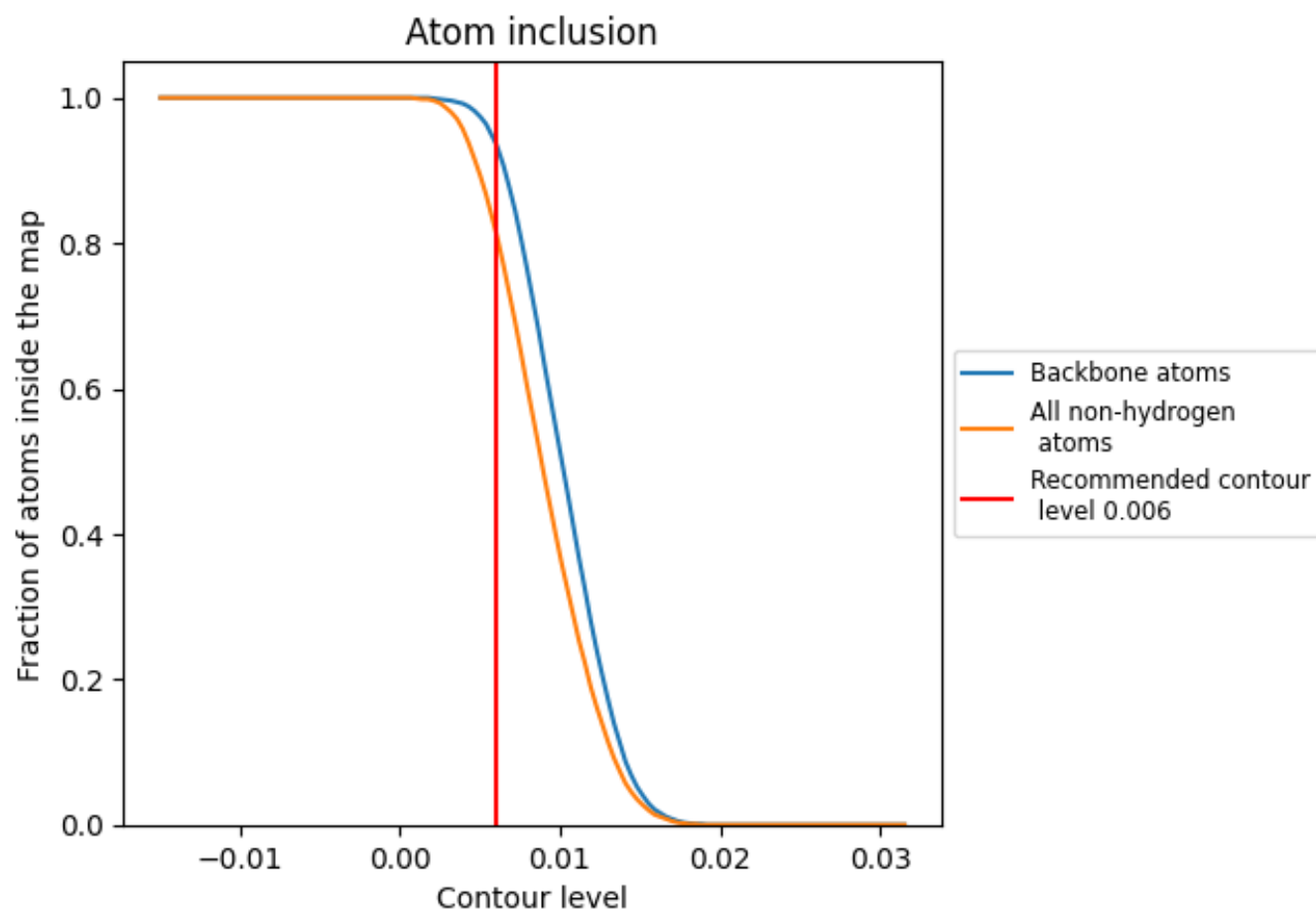
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8160	 0.5100
A	 0.8520	 0.5260
B	 0.8570	 0.5360
C	 0.8530	 0.5380
D	 0.8460	 0.5260
E	 0.8530	 0.5350
F	 0.8480	 0.5370
G	 0.8540	 0.5260
H	 0.8540	 0.5350
I	 0.8500	 0.5380
J	 0.8490	 0.5260
K	 0.8580	 0.5370
L	 0.8540	 0.5390
M	 0.8460	 0.5250
N	 0.8530	 0.5350
O	 0.8490	 0.5390
P	 0.8540	 0.5260
Q	 0.8550	 0.5370
R	 0.8500	 0.5380
a	 0.7620	 0.4730
b	 0.7540	 0.4660
c	 0.7950	 0.5070
d	 0.7670	 0.4710
e	 0.7510	 0.4660
f	 0.7930	 0.5060
g	 0.7650	 0.4740
h	 0.7450	 0.4620
i	 0.7940	 0.5030
j	 0.7680	 0.4710
k	 0.7470	 0.4630
l	 0.7900	 0.5030
m	 0.7630	 0.4720
n	 0.7240	 0.4420
o	 0.7870	 0.5000
p	 0.7620	 0.4720



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Chain	Atom inclusion	Q-score
q	 0.7490	 0.4660
r	 0.7930	 0.5060