



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:25 PM UTC

PDB ID : 7X30 / pdb_00007x30
EMDB ID : EMD-32974
Title : Capsid structure of Staphylococcus jumbo bacteriophage S6
Authors : Koibuchi, W.; Uchiyama, J.; Matsuzaki, S.; Murata, K.; Iwasaki, K.; Miyazaki, N.
Deposited on : 2022-02-27
Resolution : 3.60 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

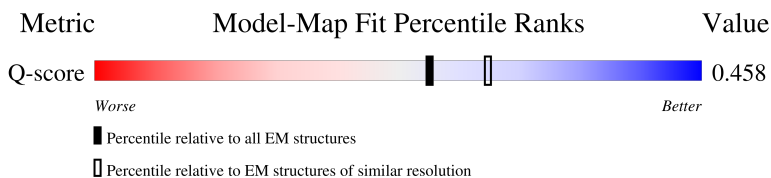
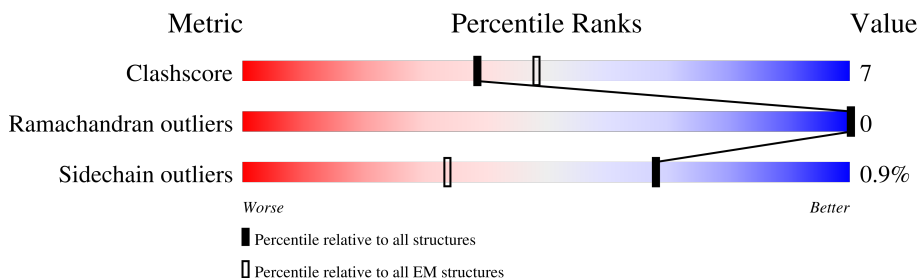
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	534	
1	a	534	
1	b	534	
1	c	534	

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Mol	Chain	Length	Quality of chain
1	d	534	
1	e	534	
1	f	534	
1	g	534	
1	h	534	
1	i	534	
1	j	534	
1	k	534	
1	l	534	
1	m	534	
1	n	534	
1	o	534	
1	p	534	
1	q	534	
1	r	534	
1	s	534	
1	t	534	
1	u	534	
1	v	534	
1	w	534	
1	x	534	
1	y	534	
1	z	534	
2	P	476	
2	Q	476	

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Mol	Chain	Length	Quality of chain
2	R	476	6% 50% 13% 37%
2	S	476	6% 50% 12% 37%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105389 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 Major structural protein ORF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	434	Total	C	N	O	S	0	0
			3394	2151	566	668	9		
1	a	444	Total	C	N	O	S	0	0
			3479	2207	581	682	9		
1	b	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	c	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	d	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	e	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	f	454	Total	C	N	O	S	0	0
			3549	2247	594	699	9		
1	g	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	h	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	i	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	j	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	k	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	l	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	m	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	n	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	o	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	p	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	q	454	Total	C	N	O	S	0	0
			3549	2247	594	699	9		
1	r	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	s	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	t	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	u	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	v	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	w	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	x	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	y	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		
1	z	454	Total	C	N	O	S	0	0
			3550	2247	595	699	9		

- Molecule 2 is a protein called Hoc-like protein ORF90.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	301	Total	C	N	O	0	0
			2442	1572	395	475		
2	Q	301	Total	C	N	O	0	0
			2442	1572	395	475		
2	R	301	Total	C	N	O	0	0
			2442	1572	395	475		
2	S	301	Total	C	N	O	0	0
			2442	1572	395	475		

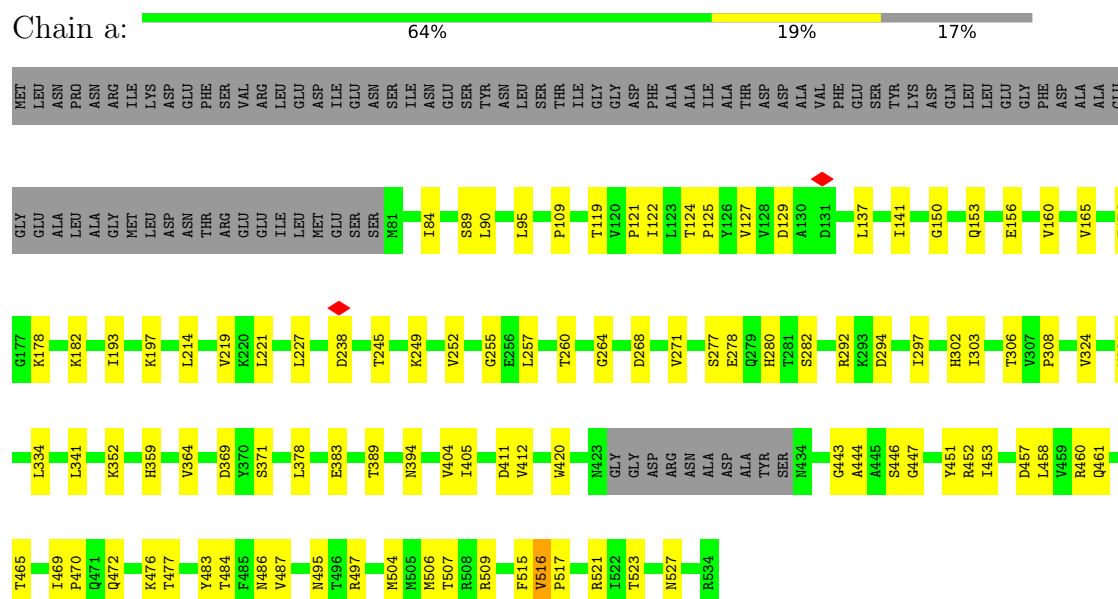
3 Residue-property plots [i](#)

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.

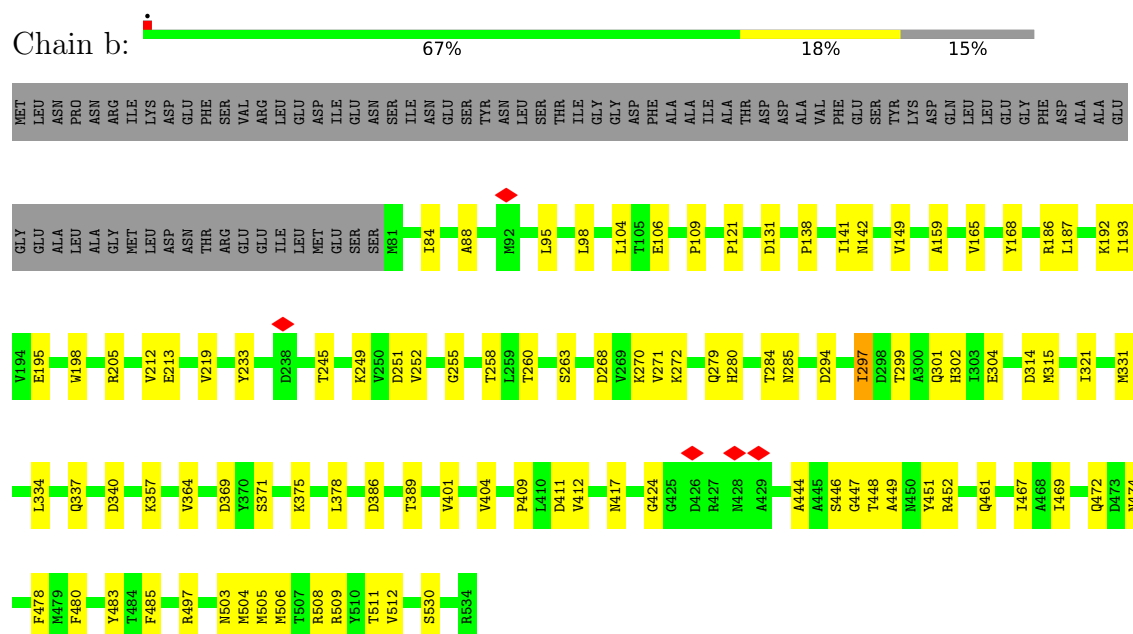
• Molecule 1: Major structural protein ORF12



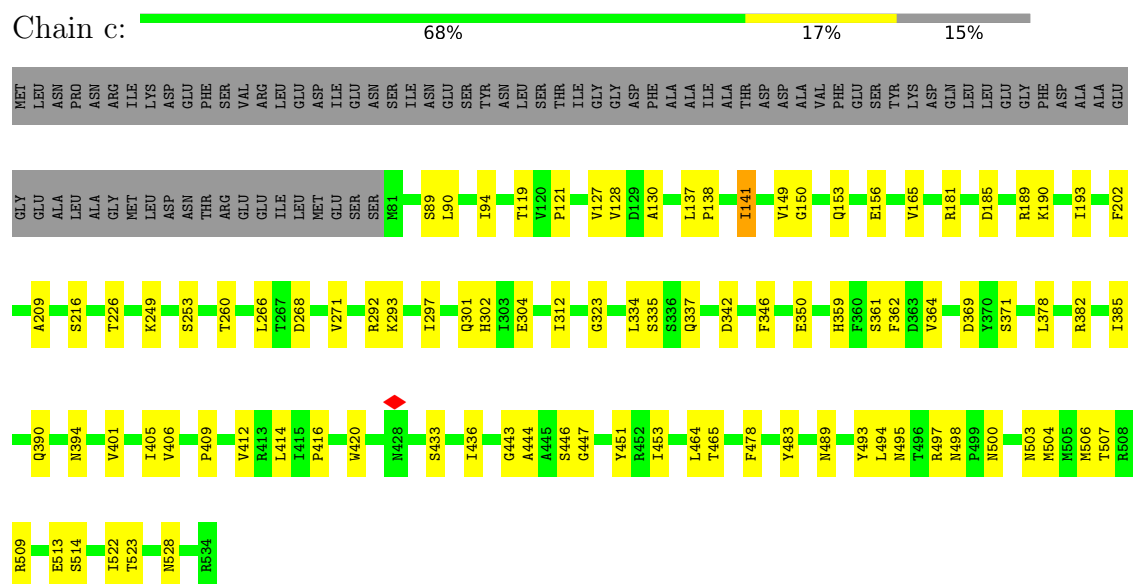
• Molecule 1: Major structural protein ORF12



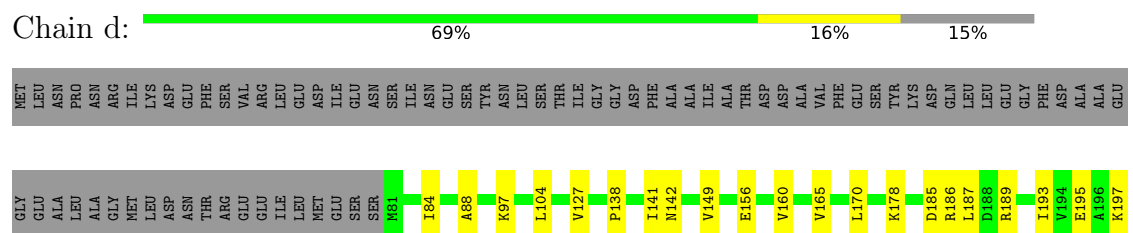
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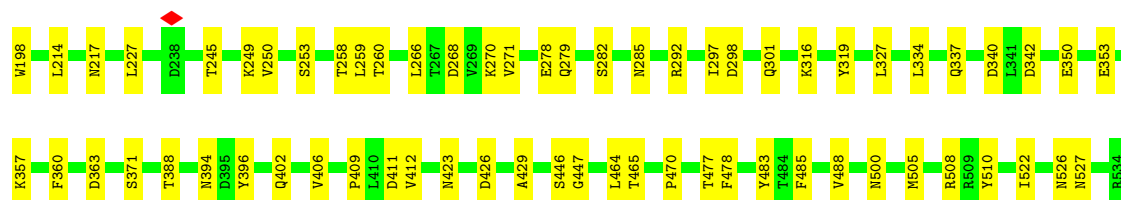


- Molecule 1: Major structural protein ORF12



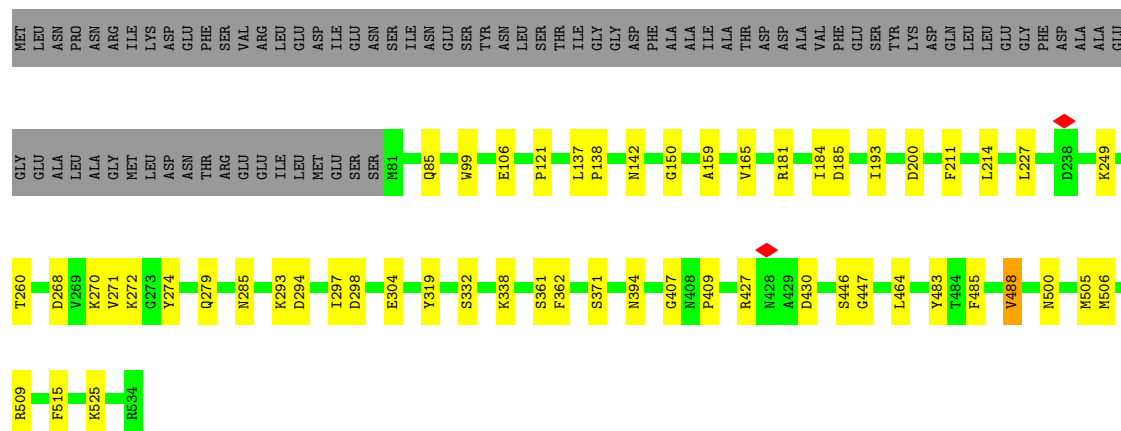
- Molecule 1: Major structural protein ORF12





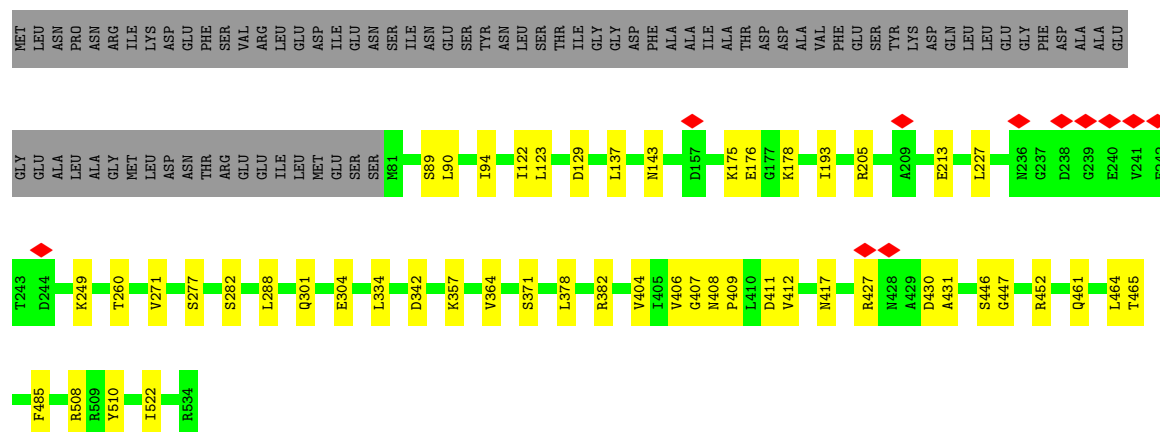
• Molecule 1: Major structural protein ORF12

Chain e: 75% 10% 15%



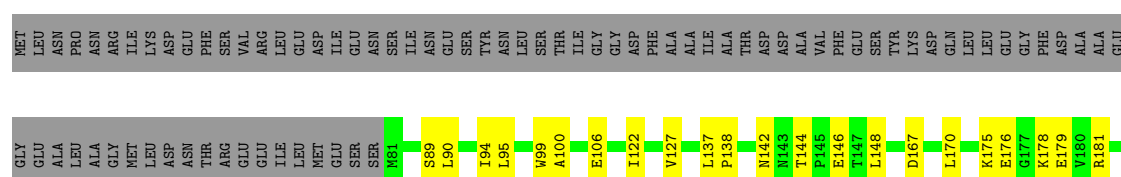
• Molecule 1: Major structural protein ORF12

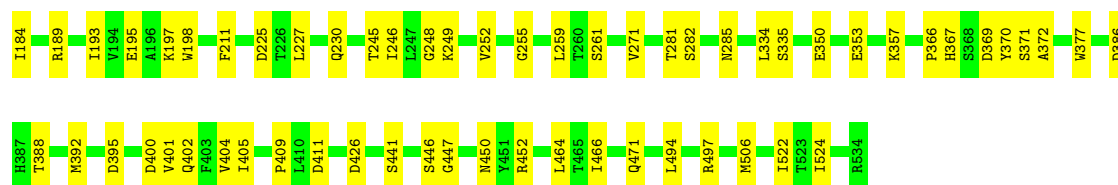
Chain f: 75% 10% 15%



• Molecule 1: Major structural protein ORF12

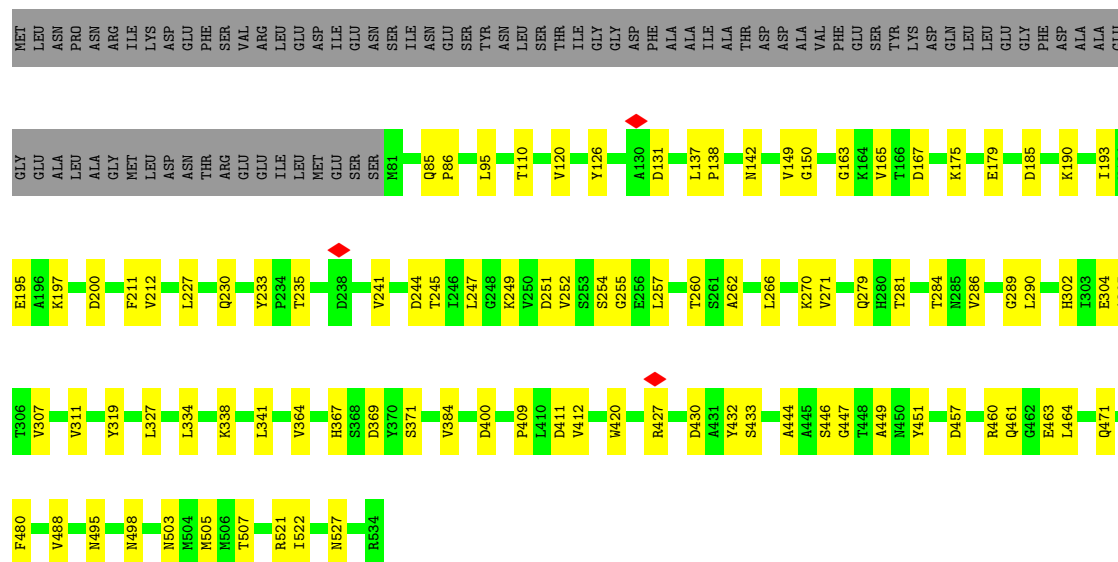
Chain g: 70% 15% 15%





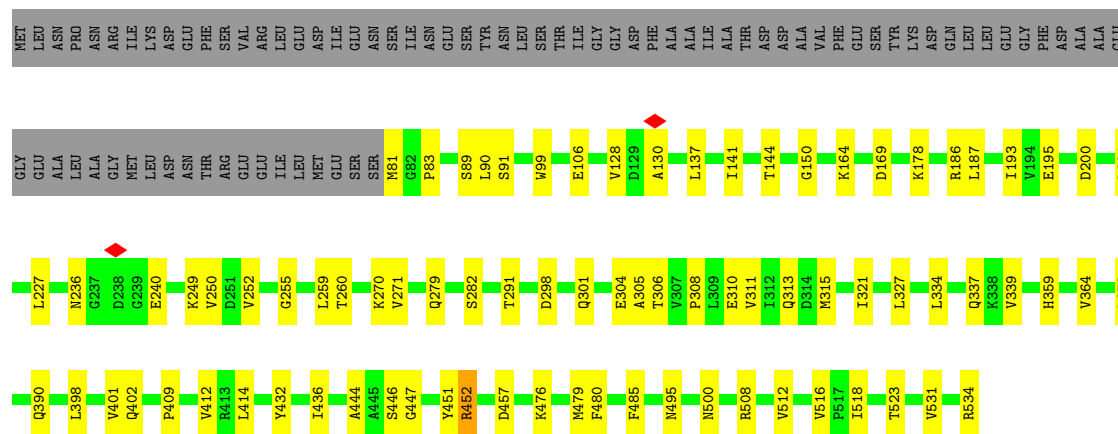
• Molecule 1: Major structural protein ORF12

Chain h: 67% 18% 15%



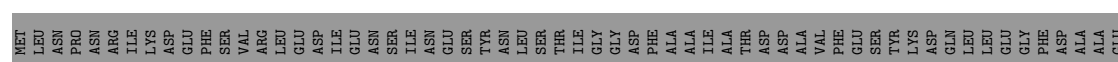
• Molecule 1: Major structural protein ORF12

Chain i: 70% 15% 15%



• Molecule 1: Major structural protein ORF12

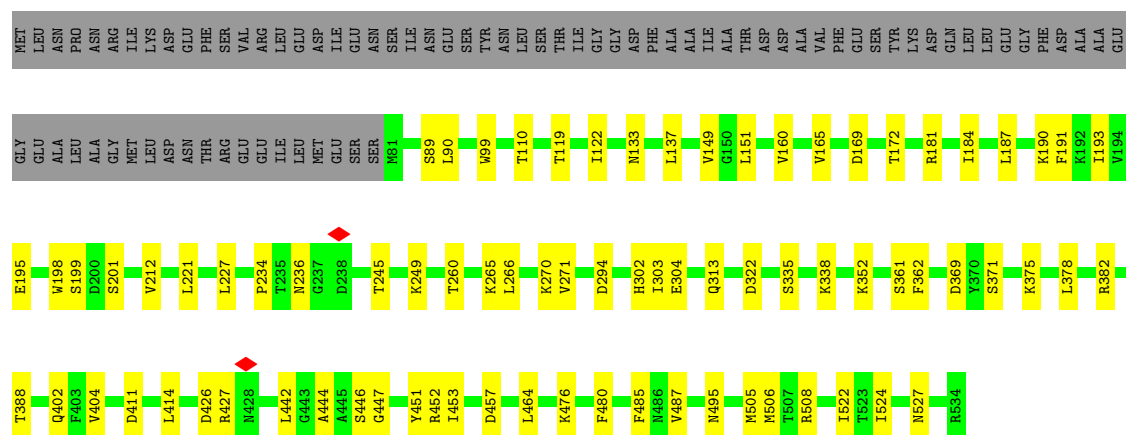
Chain j: 70% 15% 15%





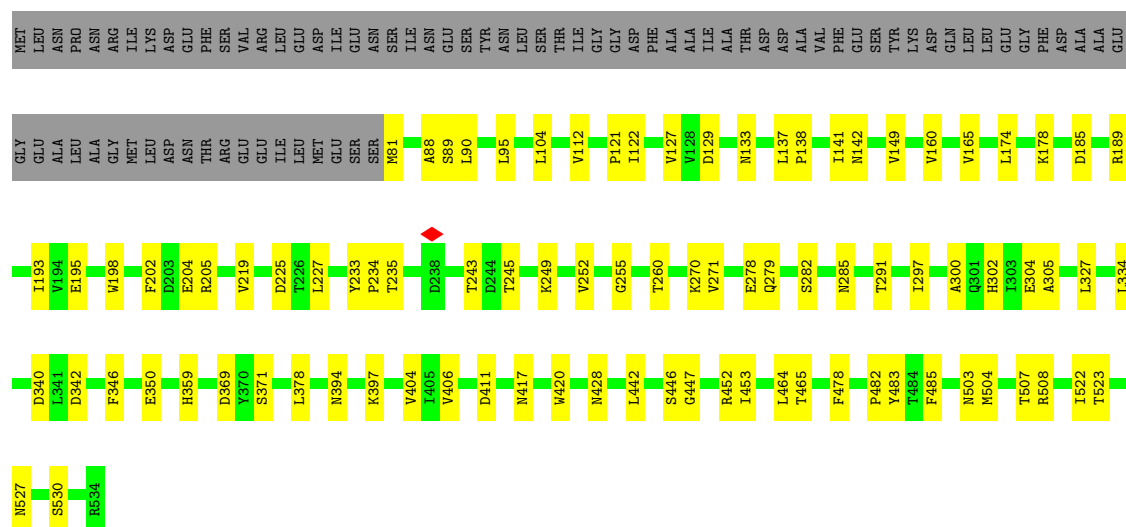
• Molecule 1: Major structural protein ORF12

Chain k: 70% 15% 15%



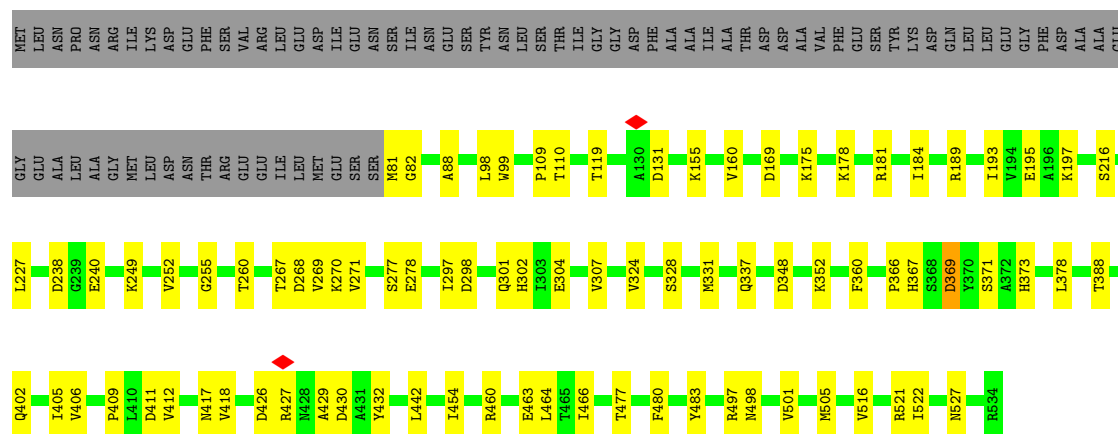
• Molecule 1: Major structural protein ORF12

Chain l: 68% 17% 15%



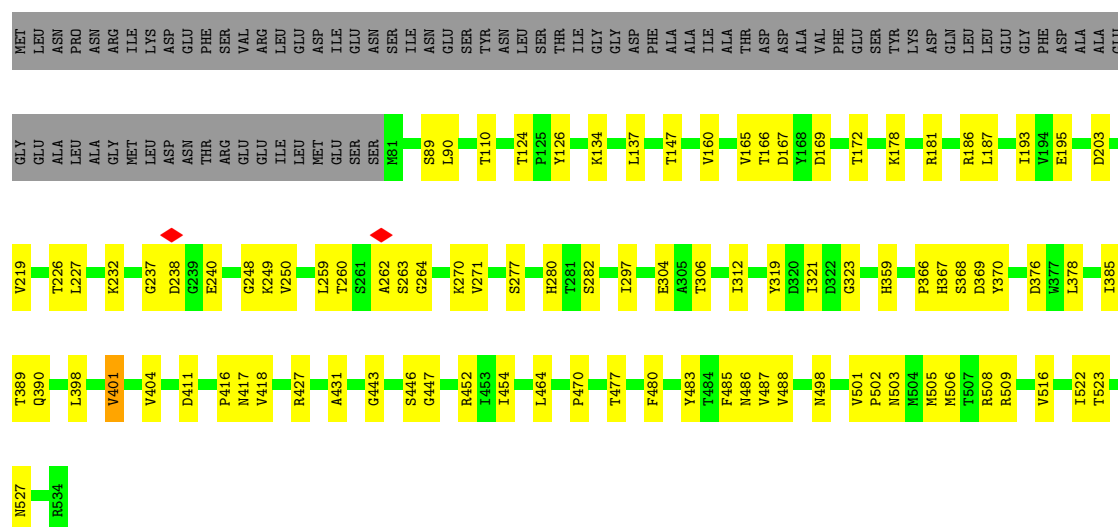
• Molecule 1: Major structural protein ORF12

Chain m: 69% 16% 15%



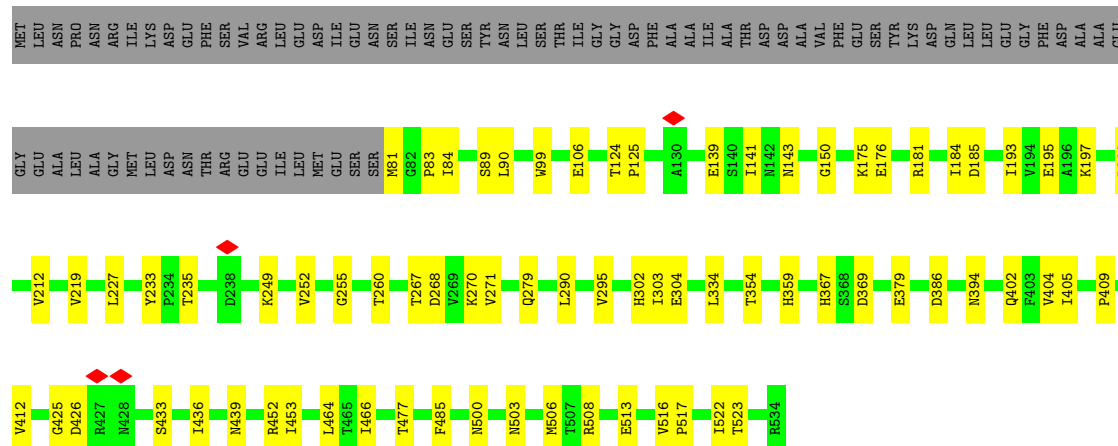
• Molecule 1: Major structural protein ORF12

Chain q: 67% 17% 15%

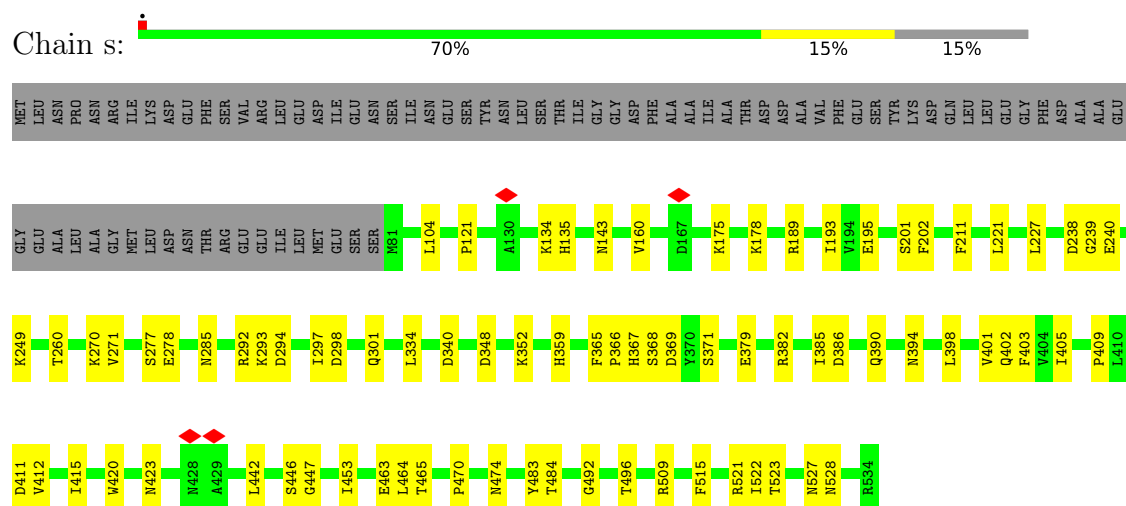


• Molecule 1: Major structural protein ORF12

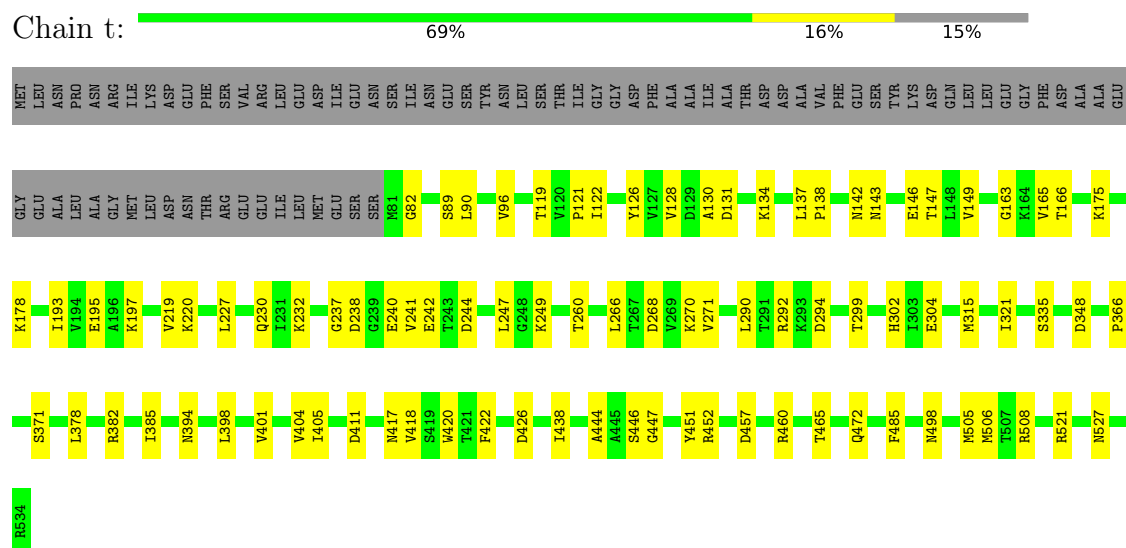
Chain r: 71% 14% 15%



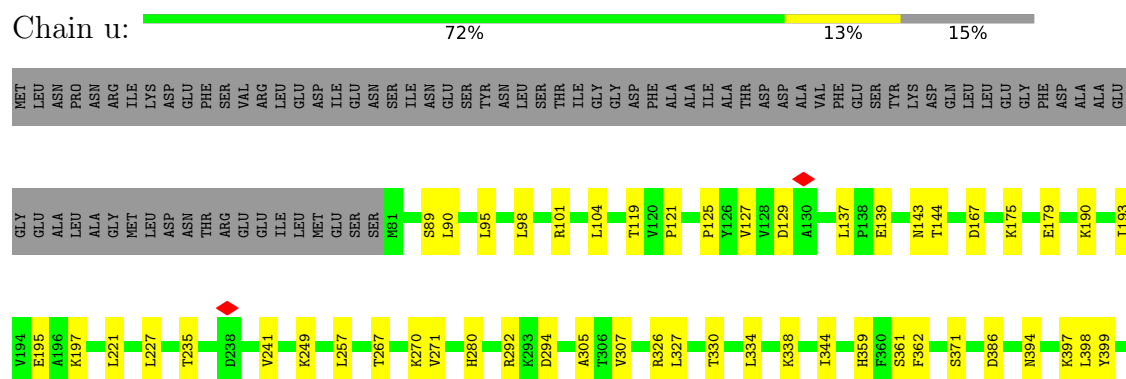
- Molecule 1: Major structural protein ORF12

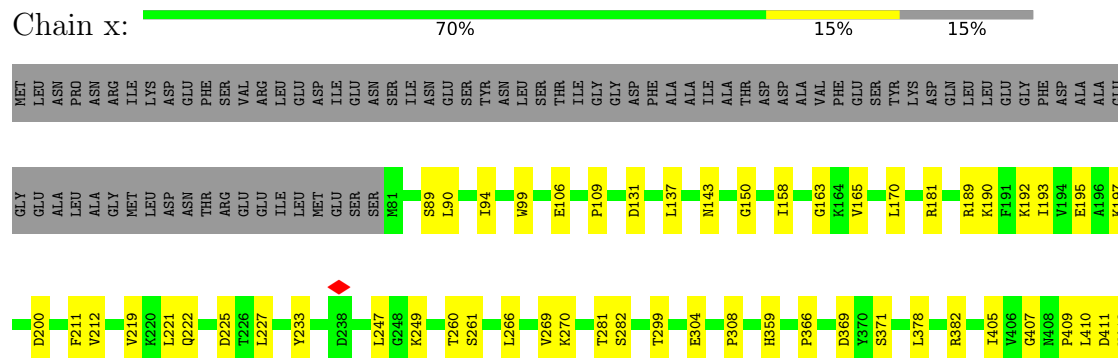
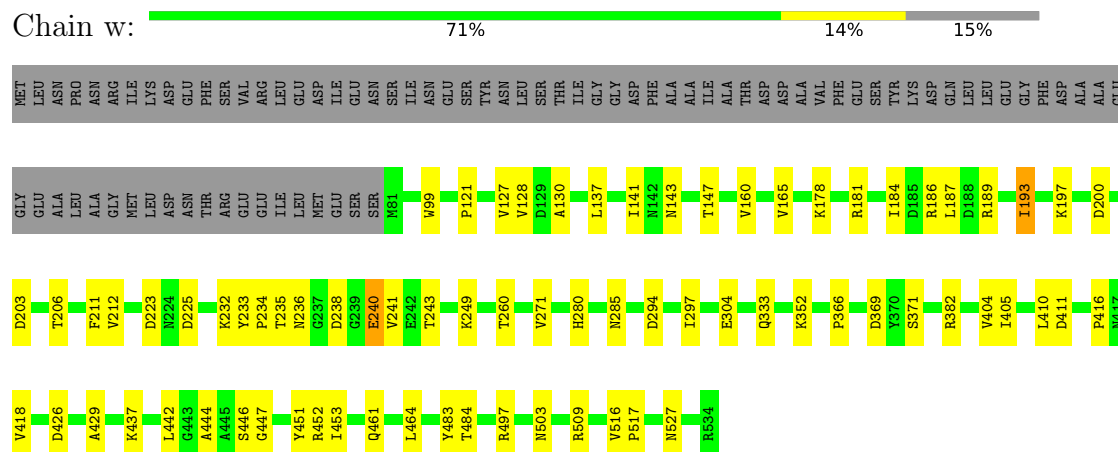
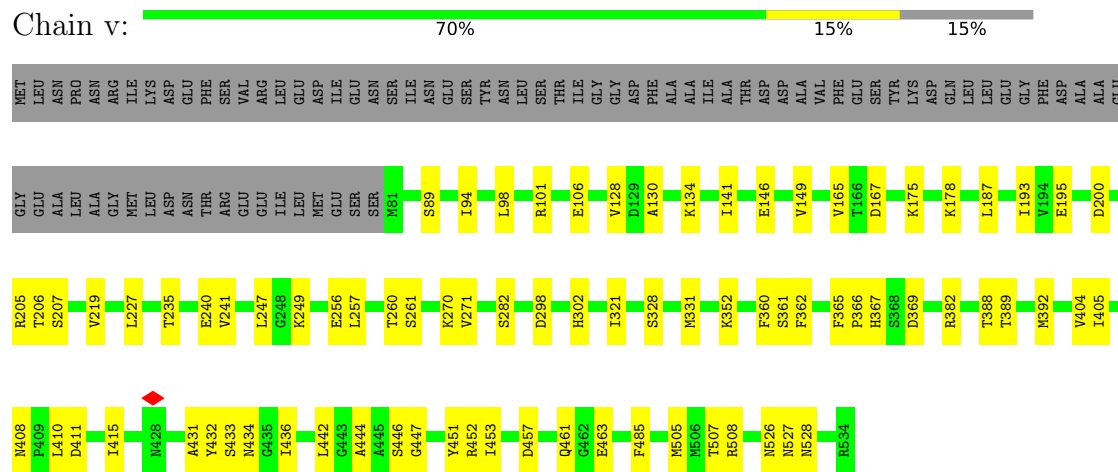
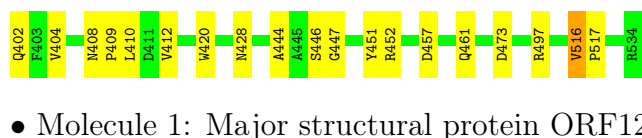


- Molecule 1: Major structural protein ORF12



- Molecule 1: Major structural protein ORF12

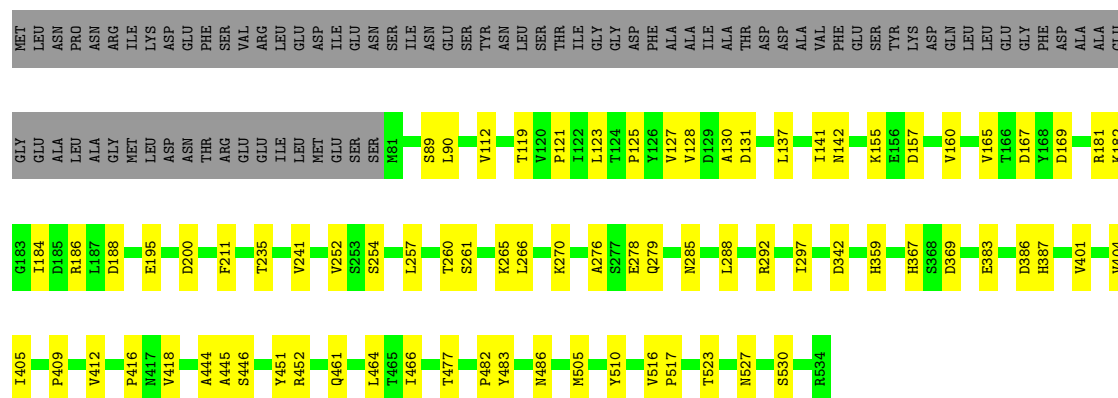






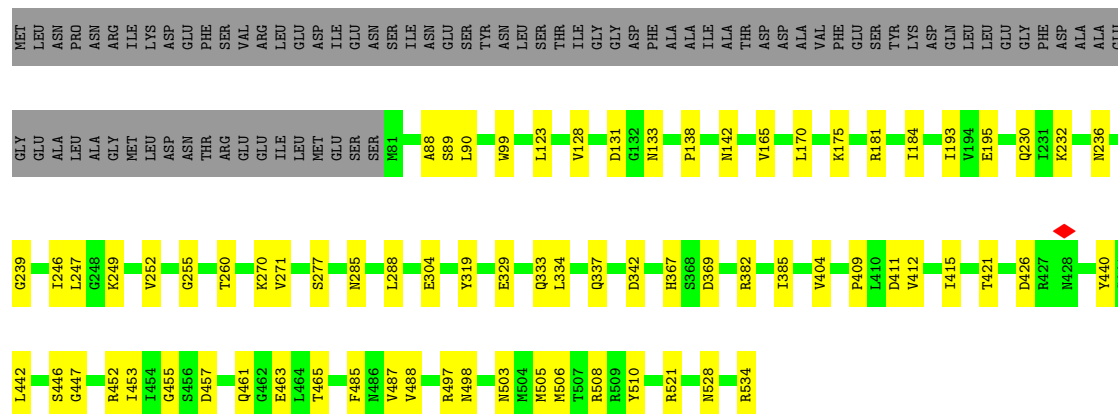
• Molecule 1: Major structural protein ORF12

Chain y: 70% 15% 15%



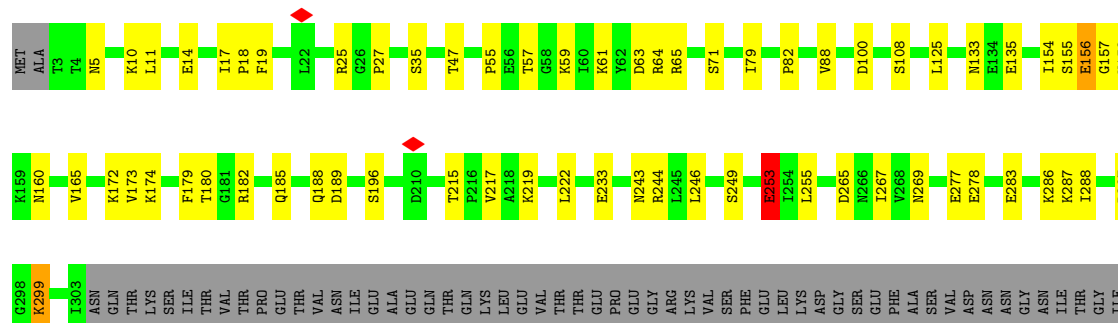
• Molecule 1: Major structural protein ORF12

Chain z: 71% 14% 15%

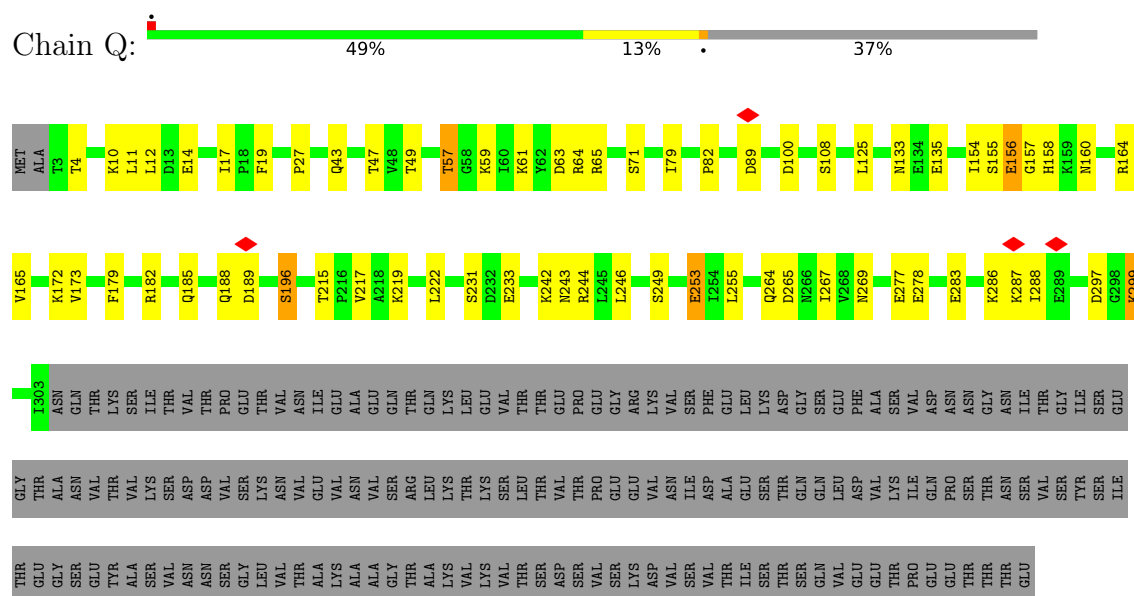


• Molecule 2: Hoc-like protein ORF90

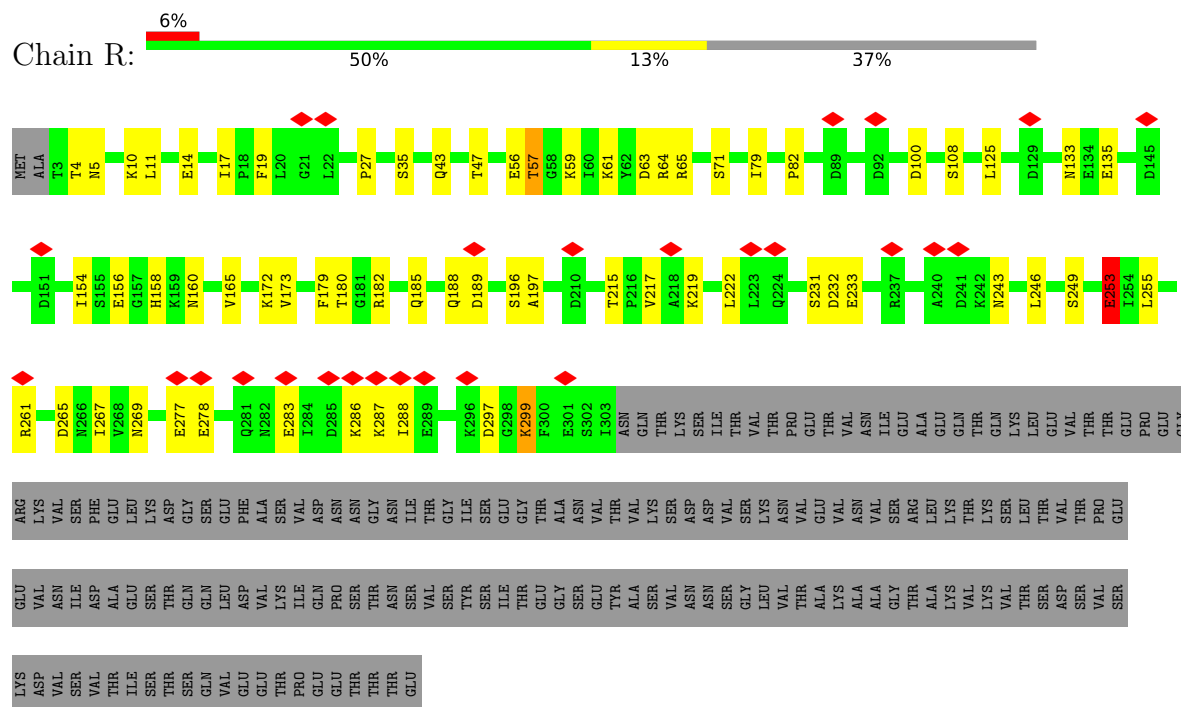
Chain P: 49% 13% 37%



- Molecule 2: Hoc-like protein ORF90

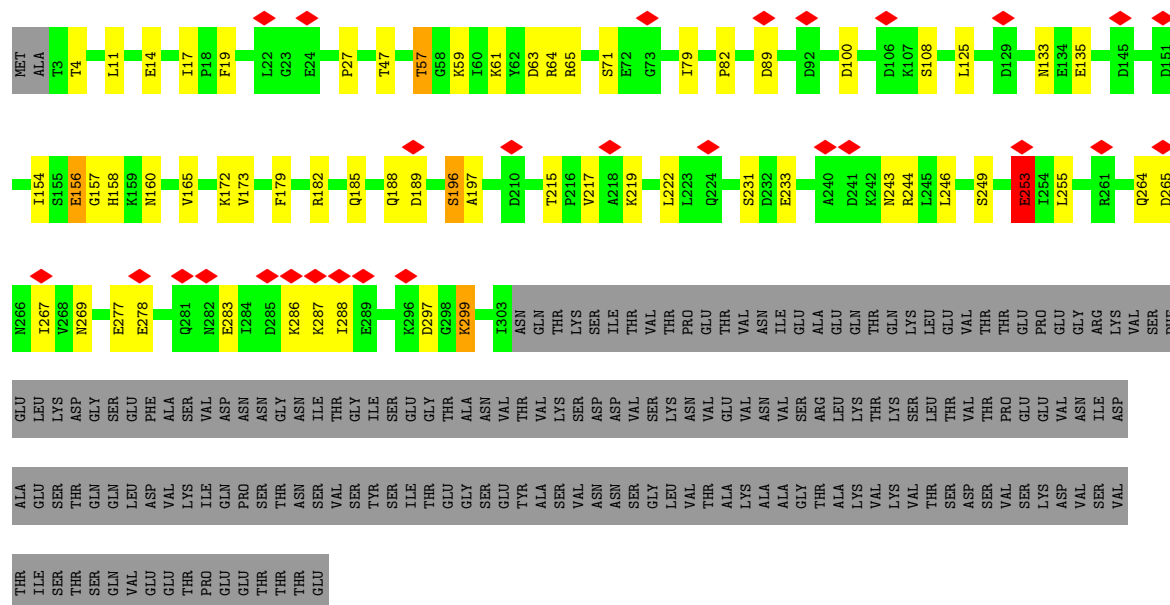


- Molecule 2: Hoc-like protein ORF90



- Molecule 2: Hoc-like protein ORF90





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	27164	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	1394.0, 1394.0, 1394.0	wwPDB
Map dimensions	820, 820, 820	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7, 1.7, 1.7	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	0/3459	0.51	0/4701
1	a	0.25	0/3547	0.49	1/4821 (0.0%)
1	b	0.25	0/3620	0.51	0/4921
1	c	0.28	1/3620 (0.0%)	0.51	0/4921
1	d	0.25	0/3620	0.51	0/4921
1	e	0.26	0/3620	0.52	2/4921 (0.0%)
1	f	0.24	0/3619	0.50	0/4919
1	g	0.26	0/3620	0.54	0/4921
1	h	0.25	0/3620	0.54	3/4921 (0.1%)
1	i	0.25	0/3620	0.51	2/4921 (0.0%)
1	j	0.25	0/3620	0.50	0/4921
1	k	0.25	0/3620	0.52	0/4921
1	l	0.24	0/3620	0.48	0/4921
1	m	0.28	1/3620 (0.0%)	0.54	0/4921
1	n	0.27	0/3620	0.54	0/4921
1	o	0.26	0/3620	0.54	2/4921 (0.0%)
1	p	0.26	0/3620	0.52	0/4921
1	q	0.26	0/3619	0.55	2/4919 (0.0%)
1	r	0.27	0/3620	0.51	0/4921
1	s	0.26	0/3620	0.54	0/4921
1	t	0.31	2/3620 (0.1%)	0.58	0/4921
1	u	0.25	0/3620	0.51	0/4921
1	v	0.26	0/3620	0.54	0/4921
1	w	0.28	0/3620	0.54	0/4921
1	x	0.28	1/3620 (0.0%)	0.53	1/4921 (0.0%)
1	y	0.29	2/3620 (0.1%)	0.49	0/4921
1	z	0.24	0/3620	0.51	0/4921
2	P	0.24	0/2484	0.50	1/3353 (0.0%)
2	Q	0.24	0/2484	0.50	1/3353 (0.0%)
2	R	0.24	0/2484	0.50	1/3353 (0.0%)
2	S	0.24	0/2484	0.50	1/3353 (0.0%)
All	All	0.26	7/107440 (0.0%)	0.52	17/145955 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	y	270	LYS	C-N	-7.59	1.23	1.33
1	x	261	SER	C-N	-6.78	1.23	1.33
1	y	265	LYS	C-N	6.58	1.42	1.33
1	m	126	TYR	C-N	-6.36	1.25	1.33
1	c	226	THR	C-N	-6.36	1.24	1.33
1	t	126	TYR	C-N	-5.68	1.26	1.33
1	t	131	ASP	C-N	-5.37	1.25	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	h	384	VAL	N-CA-C	-7.79	105.17	112.96
1	h	311	VAL	N-CA-C	-6.99	106.68	113.53
1	o	384	VAL	N-CA-C	-6.96	106.00	112.96
1	o	364	VAL	N-CA-C	-6.10	106.56	111.81
1	x	366	PRO	O-C-N	-6.01	115.40	122.86
1	h	281	THR	N-CA-C	-5.57	107.48	114.56
1	e	525	LYS	CA-C-N	5.35	130.01	122.46
1	e	525	LYS	C-N-CA	5.35	130.01	122.46
1	i	452	ARG	CA-C-N	5.33	128.47	120.69
1	i	452	ARG	C-N-CA	5.33	128.47	120.69
2	S	253	GLU	CB-CG-CD	5.27	121.56	112.60
2	Q	253	GLU	CB-CG-CD	5.25	121.53	112.60
2	R	253	GLU	CB-CG-CD	5.21	121.46	112.60
2	P	253	GLU	CB-CG-CD	5.20	121.44	112.60
1	q	203	ASP	CA-C-N	5.13	131.34	121.54
1	q	203	ASP	C-N-CA	5.13	131.34	121.54
1	a	84	ILE	N-CA-C	-5.04	108.59	113.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3394	0	3371	39	0
1	a	3479	0	3453	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	3550	0	3511	76	0
1	c	3550	0	3511	69	0
1	d	3550	0	3511	55	0
1	e	3550	0	3511	42	0
1	f	3549	0	3510	35	0
1	g	3550	0	3511	63	0
1	h	3550	0	3511	72	0
1	i	3550	0	3511	55	0
1	j	3550	0	3511	52	0
1	k	3550	0	3511	57	0
1	l	3550	0	3511	64	0
1	m	3550	0	3511	83	0
1	n	3550	0	3511	56	0
1	o	3550	0	3511	67	0
1	p	3550	0	3511	76	0
1	q	3549	0	3510	73	0
1	r	3550	0	3511	69	0
1	s	3550	0	3511	74	0
1	t	3550	0	3511	60	0
1	u	3550	0	3511	62	0
1	v	3550	0	3511	74	0
1	w	3550	0	3511	59	0
1	x	3550	0	3511	76	0
1	y	3550	0	3511	52	0
1	z	3550	0	3511	49	0
2	P	2442	0	2486	62	0
2	Q	2442	0	2486	86	0
2	R	2442	0	2486	64	0
2	S	2442	0	2486	74	0
All	All	105389	0	104541	1533	0

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

All (1533) 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:r:143:ASN:OD1	2:Q:19:PHE:CE1	1.68	1.44
1:x:143:ASN:OD1	2:S:19:PHE:CE1	1.71	1.41
1:u:143:ASN:OD1	2:R:19:PHE:CE1	1.72	1.40
1:p:238:ASP:OD1	2:P:244:ARG:CZ	1.75	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:143:ASN:CG	2:R:19:PHE:CE1	2.09	1.30
1:p:238:ASP:OD1	2:P:244:ARG:NE	1.63	1.26
1:s:240:GLU:OE1	2:S:246:LEU:HD13	1.40	1.20
1:o:143:ASN:OD1	2:P:19:PHE:CD1	2.05	1.10
1:r:143:ASN:CG	2:Q:19:PHE:CD1	2.29	1.09
1:s:240:GLU:CD	2:S:246:LEU:HD13	1.77	1.09
1:r:143:ASN:CG	2:Q:19:PHE:CE1	2.31	1.07
1:s:238:ASP:OD2	2:S:244:ARG:NE	1.88	1.06
1:u:143:ASN:ND2	2:R:19:PHE:CZ	2.22	1.05
1:m:463:GLU:OE1	2:Q:158:HIS:CE1	2.11	1.04
1:x:143:ASN:CG	2:S:19:PHE:CE1	2.36	1.03
1:w:232:LYS:HE2	2:S:47:THR:CG2	1.89	1.02
1:r:143:ASN:OD1	2:Q:19:PHE:CD1	2.14	1.00
1:q:232:LYS:HZ3	2:Q:47:THR:HG21	1.21	1.00
1:u:143:ASN:ND2	2:R:19:PHE:CE1	2.30	1.00
1:o:131:ASP:OD2	2:P:25:ARG:NH1	1.94	0.99
1:s:238:ASP:OD2	2:S:244:ARG:CZ	2.09	0.99
1:o:143:ASN:ND2	2:P:19:PHE:CD2	2.30	0.98
1:s:463:GLU:CD	2:S:158:HIS:CE1	2.44	0.96
1:w:232:LYS:CE	2:S:47:THR:HG21	1.95	0.94
1:v:367:HIS:CE1	2:R:64:ARG:HE	1.84	0.94
1:s:463:GLU:OE1	2:S:158:HIS:CE1	2.21	0.94
1:u:143:ASN:CG	2:R:19:PHE:CD1	2.46	0.93
1:u:143:ASN:OD1	2:R:19:PHE:HE1	1.29	0.92
1:s:240:GLU:CD	2:S:246:LEU:CD1	2.43	0.91
1:v:365:PHE:HE2	2:R:57:THR:HG23	1.35	0.91
1:t:232:LYS:HE2	2:R:47:THR:HG21	1.54	0.90
1:m:238:ASP:CG	2:Q:244:ARG:CZ	2.45	0.90
1:q:232:LYS:NZ	2:Q:47:THR:HG21	1.85	0.90
1:x:460:ARG:NH2	2:R:231:SER:O	2.05	0.90
1:x:143:ASN:ND2	2:S:19:PHE:CE2	2.40	0.89
1:m:365:PHE:HE2	2:Q:57:THR:HG23	1.35	0.88
1:q:232:LYS:NZ	2:Q:47:THR:CG2	2.36	0.88
1:u:359:HIS:HD2	2:S:264:GLN:HE21	1.20	0.88
1:r:143:ASN:OD1	2:Q:19:PHE:HE1	1.51	0.87
1:o:143:ASN:ND2	2:P:19:PHE:CG	2.41	0.87
1:s:463:GLU:OE2	2:S:158:HIS:CE1	2.28	0.87
1:v:240:GLU:CD	2:R:246:LEU:CD1	2.48	0.86
1:n:232:LYS:HE2	2:P:47:THR:HG21	1.58	0.86
1:w:232:LYS:CE	2:S:47:THR:CG2	2.52	0.86
1:t:240:GLU:OE1	1:t:242:GLU:HG2	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:143:ASN:ND2	2:P:19:PHE:CE2	2.46	0.83
1:p:238:ASP:CG	2:P:244:ARG:CZ	2.51	0.83
1:x:143:ASN:CG	2:S:19:PHE:CD1	2.56	0.82
1:p:238:ASP:OD1	2:P:244:ARG:NH2	2.12	0.82
1:q:147:THR:HG21	2:P:253:GLU:HB2	1.63	0.81
1:o:143:ASN:CG	2:P:19:PHE:CD1	2.58	0.80
1:n:143:ASN:ND2	2:Q:231:SER:O	2.16	0.79
1:x:143:ASN:ND2	2:S:19:PHE:CZ	2.48	0.79
1:u:359:HIS:CD2	2:S:264:GLN:HE21	2.01	0.79
1:s:463:GLU:OE1	2:S:158:HIS:HE1	1.66	0.78
1:v:240:GLU:CD	2:R:246:LEU:HD13	2.06	0.78
1:q:232:LYS:HZ3	2:Q:47:THR:CG2	1.93	0.78
1:p:238:ASP:CG	2:P:244:ARG:NE	2.40	0.78
1:x:143:ASN:ND2	2:S:19:PHE:CD2	2.51	0.78
1:n:205:ARG:NE	2:Q:188:GLN:NE2	2.33	0.77
1:w:232:LYS:HE2	2:S:47:THR:HG21	1.59	0.77
1:x:143:ASN:OD1	2:S:19:PHE:CZ	2.35	0.77
1:w:232:LYS:HE2	2:S:47:THR:HG22	1.66	0.77
1:m:365:PHE:CE2	2:Q:57:THR:HG23	2.19	0.76
1:n:232:LYS:HE2	2:P:47:THR:CG2	2.16	0.76
1:o:143:ASN:OD1	2:P:19:PHE:CG	2.40	0.75
1:d:227:LEU:HB2	1:d:249:LYS:HB2	1.68	0.75
1:v:240:GLU:HG2	2:R:246:LEU:HD11	1.67	0.74
1:p:521:ARG:NH1	2:P:157:GLY:C	2.44	0.74
1:x:143:ASN:OD1	2:S:19:PHE:HE1	1.62	0.74
1:w:147:THR:HG21	2:R:253:GLU:HB2	1.69	0.74
1:r:143:ASN:ND2	2:Q:19:PHE:CE1	2.56	0.73
1:v:365:PHE:CE2	2:R:57:THR:HG23	2.21	0.73
1:p:348:ASP:OD1	2:P:157:GLY:N	2.15	0.73
1:m:348:ASP:CG	2:Q:157:GLY:H	1.95	0.73
1:n:205:ARG:HD2	2:Q:188:GLN:HE22	1.53	0.73
1:u:195:GLU:HB2	1:u:270:LYS:HB2	1.71	0.72
1:u:143:ASN:ND2	2:R:19:PHE:CE2	2.53	0.72
1:l:195:GLU:HB3	1:l:270:LYS:HB2	1.72	0.71
1:s:175:LYS:HB3	1:s:178:LYS:HZ3	1.56	0.71
1:w:371:SER:HB2	1:x:371:SER:HB2	1.71	0.71
1:r:143:ASN:ND2	2:Q:19:PHE:CZ	2.58	0.71
1:v:240:GLU:CD	2:R:246:LEU:HD11	2.14	0.71
1:v:240:GLU:OE2	2:R:197:ALA:HB2	1.92	0.69
1:r:143:ASN:ND2	2:Q:19:PHE:CD1	2.60	0.69
1:v:227:LEU:HB2	1:v:249:LYS:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:227:LEU:HB2	1:h:249:LYS:HB3	1.73	0.69
1:m:348:ASP:OD2	2:Q:156:GLU:CB	2.41	0.69
1:h:488:VAL:HB	1:h:505:MET:HB3	1.75	0.69
1:m:238:ASP:OD2	2:Q:244:ARG:CD	2.39	0.69
1:r:227:LEU:HB2	1:r:249:LYS:HB3	1.75	0.69
1:n:227:LEU:HB3	1:n:249:LYS:HB3	1.75	0.68
1:p:378:LEU:HB2	1:p:417:ASN:HD21	1.58	0.68
1:t:227:LEU:HB2	1:t:249:LYS:HB3	1.76	0.68
1:x:249:LYS:HE3	1:x:260:THR:HB	1.74	0.68
1:u:104:LEU:HD22	1:u:344:ILE:HD11	1.75	0.68
1:l:129:ASP:HB3	1:l:133:ASN:H	1.58	0.68
1:w:232:LYS:HE3	2:S:47:THR:HG21	1.76	0.68
1:m:238:ASP:OD1	2:Q:244:ARG:CZ	2.42	0.68
1:v:240:GLU:CG	2:R:246:LEU:HD11	2.24	0.67
1:z:409:PRO:HA	1:z:412:VAL:HG12	1.76	0.67
1:x:143:ASN:OD1	2:S:19:PHE:CD1	2.42	0.67
1:o:143:ASN:CG	2:P:19:PHE:CG	2.73	0.67
1:p:238:ASP:OD2	2:P:244:ARG:CD	2.43	0.67
1:q:232:LYS:HZ2	2:Q:47:THR:HG22	1.59	0.67
1:r:195:GLU:HB3	1:r:270:LYS:HB2	1.76	0.67
1:j:227:LEU:HB2	1:j:249:LYS:HB2	1.77	0.66
1:c:405:ILE:HB	1:c:453:ILE:HG23	1.77	0.66
1:u:139:GLU:OE2	2:R:43:GLN:HB3	1.96	0.65
1:q:498:ASN:HD22	1:x:181:ARG:HH22	1.43	0.65
1:u:404:VAL:HG12	1:u:452:ARG:HB3	1.78	0.65
1:x:143:ASN:CG	2:S:19:PHE:CZ	2.74	0.65
1:y:165:VAL:HG22	1:y:260:THR:HG22	1.77	0.65
1:d:197:LYS:HB3	1:d:268:ASP:HB2	1.79	0.65
1:r:143:ASN:ND2	2:Q:19:PHE:CE2	2.64	0.65
1:n:378:LEU:HB2	1:n:417:ASN:HD21	1.61	0.65
1:a:227:LEU:HB2	1:a:249:LYS:HB2	1.77	0.65
1:s:238:ASP:OD2	2:S:244:ARG:CD	2.44	0.65
1:u:409:PRO:HA	1:u:412:VAL:HG12	1.78	0.65
1:m:348:ASP:OD1	2:Q:157:GLY:N	2.21	0.64
1:x:195:GLU:HB3	1:x:270:LYS:HB2	1.79	0.64
1:h:195:GLU:HB3	1:h:270:LYS:HB3	1.79	0.64
1:v:240:GLU:CD	2:R:197:ALA:HB2	2.22	0.64
1:w:234:PRO:HB3	1:w:240:GLU:HG3	1.80	0.64
1:A:164:LYS:HG2	1:A:261:SER:HA	1.78	0.64
1:x:249:LYS:HG2	1:x:260:THR:HA	1.80	0.64
1:c:494:LEU:HB2	1:m:500:ASN:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:163:GLY:HA2	1:h:266:LEU:HB2	1.80	0.64
1:l:193:ILE:HG22	1:l:271:VAL:HG12	1.80	0.64
1:A:404:VAL:HG12	1:A:452:ARG:HB3	1.78	0.64
1:e:332:SER:HA	1:e:506:MET:HE1	1.78	0.64
1:q:232:LYS:HZ2	2:Q:47:THR:CG2	2.11	0.63
1:s:409:PRO:HA	1:s:412:VAL:HG12	1.80	0.63
1:j:404:VAL:HG12	1:j:452:ARG:HB3	1.81	0.63
1:s:104:LEU:HD12	1:s:340:ASP:HB3	1.81	0.63
1:x:143:ASN:ND2	2:S:19:PHE:CE1	2.66	0.63
1:y:285:ASN:HD22	1:z:497:ARG:HE	1.47	0.63
1:g:285:ASN:HD21	1:h:495:ASN:HD21	1.44	0.63
1:u:143:ASN:CG	2:R:19:PHE:CZ	2.69	0.63
1:r:143:ASN:ND2	2:Q:19:PHE:CG	2.66	0.63
1:a:405:ILE:HB	1:a:453:ILE:HG22	1.81	0.63
1:p:521:ARG:HH11	2:P:157:GLY:C	2.06	0.63
1:i:236:ASN:HB3	1:i:240:GLU:H	1.64	0.62
1:i:409:PRO:HA	1:i:412:VAL:HG12	1.81	0.62
1:k:227:LEU:HB3	1:k:249:LYS:HB3	1.81	0.62
1:y:252:VAL:HG22	1:y:254:SER:H	1.64	0.62
1:q:368:SER:HB3	2:P:63:ASP:HB2	1.79	0.62
1:p:460:ARG:NH1	2:P:155:SER:OG	2.23	0.62
1:q:404:VAL:HG12	1:q:452:ARG:HB3	1.80	0.62
1:x:143:ASN:ND2	2:S:19:PHE:CG	2.68	0.62
1:a:197:LYS:HB3	1:a:268:ASP:HB2	1.82	0.62
1:f:409:PRO:HA	1:f:412:VAL:HG12	1.82	0.62
1:q:237:GLY:HA2	1:q:240:GLU:OE1	1.98	0.62
1:s:369:ASP:OD2	2:S:63:ASP:HB3	2.00	0.62
1:q:137:LEU:HD22	1:r:99:TRP:HH2	1.64	0.62
1:a:359:HIS:HE2	1:a:523:THR:HG1	1.47	0.62
1:i:227:LEU:HB3	1:i:249:LYS:HB2	1.82	0.61
1:h:409:PRO:HA	1:h:412:VAL:HG12	1.82	0.61
1:t:378:LEU:HB2	1:t:417:ASN:HD21	1.66	0.61
1:m:252:VAL:HG22	1:m:255:GLY:H	1.65	0.61
1:m:337:GLN:NE2	1:r:141:ILE:O	2.34	0.61
1:t:404:VAL:HG12	1:t:452:ARG:HB3	1.82	0.61
1:e:371:SER:HB2	1:f:371:SER:HB2	1.81	0.61
1:i:444:ALA:HB3	1:i:451:TYR:HB2	1.83	0.61
1:y:367:HIS:ND1	1:y:369:ASP:OD1	2.33	0.61
1:b:263:SER:HB3	1:q:166:THR:HG22	1.83	0.61
1:m:460:ARG:NH1	2:Q:155:SER:OG	2.34	0.60
1:v:431:ALA:HB1	1:v:434:ASN:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:227:LEU:HB2	1:e:249:LYS:HB3	1.83	0.60
1:g:95:LEU:HB2	1:l:122:ILE:HG22	1.83	0.60
1:m:240:GLU:OE2	2:Q:196:SER:N	2.35	0.60
1:r:143:ASN:ND2	2:Q:19:PHE:CD2	2.69	0.60
1:A:236:ASN:H	1:A:241:VAL:HB	1.66	0.60
1:w:143:ASN:ND2	2:R:231:SER:O	2.33	0.60
1:s:367:HIS:HE1	2:S:64:ARG:NE	2.00	0.60
1:i:310:GLU:HB2	1:p:278:GLU:HG3	1.84	0.60
1:e:193:ILE:HG12	1:e:271:VAL:HG12	1.83	0.60
1:v:367:HIS:CE1	2:R:64:ARG:NE	2.66	0.60
1:m:365:PHE:HD2	2:Q:59:LYS:HD2	1.66	0.60
1:n:205:ARG:HD2	2:Q:188:GLN:NE2	2.16	0.60
1:o:143:ASN:ND2	2:P:19:PHE:CD1	2.68	0.60
1:k:227:LEU:HD23	1:k:249:LYS:HD2	1.84	0.60
1:l:359:HIS:HE2	1:l:523:THR:HG1	1.47	0.60
2:Q:297:ASP:HB2	2:Q:299:LYS:HZ3	1.66	0.59
1:g:441:SER:HB2	1:h:427:ARG:HH12	1.68	0.59
1:m:238:ASP:CG	2:Q:244:ARG:NE	2.60	0.59
1:v:249:LYS:HD3	1:v:260:THR:HA	1.84	0.59
1:z:128:VAL:HG21	1:z:285:ASN:HD22	1.65	0.59
1:k:122:ILE:HG22	1:l:95:LEU:HB2	1.84	0.59
1:p:227:LEU:HD13	1:p:249:LYS:HZ3	1.66	0.59
1:q:232:LYS:NZ	2:Q:47:THR:HG22	2.13	0.59
1:s:143:ASN:HA	1:t:460:ARG:HH12	1.67	0.59
1:q:366:PRO:O	2:P:65:ARG:NH1	2.34	0.59
1:k:402:GLN:HE22	1:k:452:ARG:HB2	1.67	0.59
1:q:193:ILE:HG22	1:q:271:VAL:HG12	1.84	0.59
1:n:193:ILE:HG13	1:n:271:VAL:HG12	1.85	0.59
1:o:359:HIS:NE2	1:o:523:THR:OG1	2.36	0.59
1:v:128:VAL:HG23	1:v:134:LYS:HG2	1.84	0.59
1:v:240:GLU:OE1	2:R:246:LEU:CD1	2.50	0.59
1:h:252:VAL:HG22	1:h:255:GLY:H	1.68	0.59
1:o:409:PRO:HA	1:o:412:VAL:HG12	1.85	0.59
1:o:411:ASP:HB3	1:o:524:ILE:HD12	1.85	0.59
1:x:378:LEU:HB2	1:x:417:ASN:HD21	1.67	0.59
1:o:193:ILE:HG22	1:o:271:VAL:HG12	1.85	0.59
1:q:186:ARG:NH1	1:q:187:LEU:O	2.36	0.59
1:o:404:VAL:HG12	1:o:452:ARG:HB3	1.84	0.59
1:k:149:VAL:HG21	1:l:334:LEU:HD21	1.84	0.58
1:r:212:VAL:HG21	1:r:233:TYR:HB2	1.85	0.58
1:g:122:ILE:HG22	1:h:95:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:382:ARG:NH1	1:s:415:ILE:O	2.35	0.58
1:u:143:ASN:ND2	2:R:19:PHE:CD1	2.67	0.58
1:A:235:THR:HG23	1:A:241:VAL:H	1.68	0.58
1:c:249:LYS:HG2	1:c:260:THR:HA	1.84	0.58
1:k:487:VAL:HG12	1:k:506:MET:HB3	1.86	0.58
1:x:525:LYS:HG3	2:R:261:ARG:HD2	1.86	0.58
1:l:297:ILE:HD13	1:l:483:TYR:HB2	1.86	0.58
1:r:139:GLU:OE1	2:Q:43:GLN:HB3	2.04	0.58
1:v:367:HIS:HE1	2:R:64:ARG:HE	1.48	0.58
1:t:137:LEU:HD11	1:u:334:LEU:HD13	1.86	0.58
1:t:457:ASP:OD1	1:t:457:ASP:N	2.37	0.58
1:e:137:LEU:HD11	1:f:334:LEU:HD13	1.86	0.57
1:e:488:VAL:HG23	1:e:505:MET:HB3	1.85	0.57
1:g:404:VAL:HG12	1:g:452:ARG:HB3	1.87	0.57
1:k:404:VAL:HG12	1:k:452:ARG:HB3	1.84	0.57
1:m:238:ASP:OD2	2:Q:244:ARG:HD3	2.03	0.57
1:v:360:PHE:HD2	1:v:388:THR:HG22	1.68	0.57
1:v:526:ASN:ND2	2:R:56:GLU:O	2.37	0.57
1:c:149:VAL:HG21	1:d:334:LEU:HD11	1.85	0.57
1:i:221:LEU:HD12	1:i:227:LEU:HD13	1.85	0.57
1:m:238:ASP:OD2	2:Q:244:ARG:CZ	2.53	0.57
1:z:404:VAL:HG12	1:z:452:ARG:HB3	1.86	0.57
1:c:371:SER:HB3	1:d:371:SER:HB2	1.85	0.57
1:n:205:ARG:CD	2:Q:188:GLN:NE2	2.67	0.57
1:r:402:GLN:HE22	1:r:452:ARG:HB2	1.69	0.57
1:y:278:GLU:HG2	1:y:279:GLN:HE21	1.69	0.57
2:Q:63:ASP:OD2	2:Q:63:ASP:N	2.38	0.57
1:d:285:ASN:HB3	1:e:304:GLU:HG3	1.85	0.57
1:v:167:ASP:HB3	1:v:257:LEU:HD22	1.87	0.57
1:o:472:GLN:HE22	1:p:98:LEU:HD21	1.70	0.57
1:r:405:ILE:HB	1:r:453:ILE:HG23	1.84	0.57
1:m:238:ASP:OD1	2:Q:244:ARG:NE	2.38	0.57
1:q:378:LEU:HB2	1:q:417:ASN:HD21	1.69	0.57
2:R:182:ARG:NH2	2:R:265:ASP:O	2.38	0.57
1:e:165:VAL:HB	1:e:260:THR:HB	1.85	0.57
1:o:143:ASN:ND2	2:P:19:PHE:CZ	2.73	0.57
1:z:446:SER:OG	1:z:447:GLY:N	2.38	0.57
1:i:485:PHE:HD1	1:i:508:ARG:HB3	1.70	0.57
1:n:205:ARG:NH2	1:n:213:GLU:OE2	2.38	0.57
1:p:360:PHE:HD2	1:p:388:THR:HG22	1.69	0.57
1:v:240:GLU:CG	2:R:246:LEU:CD1	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:123:LEU:HD11	1:y:288:LEU:HD23	1.85	0.57
1:k:165:VAL:HB	1:k:260:THR:HB	1.85	0.56
1:k:304:GLU:HB3	1:k:505:MET:HG3	1.86	0.56
1:q:167:ASP:H	1:q:259:LEU:HD13	1.69	0.56
1:y:160:VAL:HG21	1:y:266:LEU:HD13	1.86	0.56
1:r:81:MET:HG3	1:r:83:PRO:HD2	1.87	0.56
1:c:150:GLY:O	1:d:301:GLN:NE2	2.38	0.56
1:l:104:LEU:HD23	1:l:340:ASP:HB3	1.85	0.56
1:n:446:SER:OG	1:n:447:GLY:N	2.39	0.56
1:s:240:GLU:CD	2:S:197:ALA:HB2	2.30	0.56
1:y:235:THR:HB	1:y:241:VAL:HB	1.87	0.56
1:y:404:VAL:HG12	1:y:452:ARG:HB3	1.86	0.56
1:z:457:ASP:OD1	1:z:457:ASP:N	2.38	0.56
2:S:63:ASP:N	2:S:63:ASP:OD2	2.38	0.56
2:S:182:ARG:NH2	2:S:265:ASP:O	2.38	0.56
1:i:306:THR:OG1	1:i:495:ASN:ND2	2.38	0.56
1:q:367:HIS:ND1	1:q:369:ASP:OD1	2.38	0.56
2:R:63:ASP:OD2	2:R:63:ASP:N	2.38	0.56
1:a:371:SER:HB2	1:b:371:SER:HB2	1.87	0.56
1:m:238:ASP:OD2	2:Q:244:ARG:NE	2.39	0.56
1:i:364:VAL:HG13	1:i:378:LEU:HD21	1.87	0.56
1:p:110:THR:HG22	1:p:480:PHE:HB3	1.87	0.56
1:t:444:ALA:HB3	1:t:451:TYR:HB2	1.88	0.56
2:P:182:ARG:NH2	2:P:265:ASP:O	2.38	0.56
1:a:446:SER:OG	1:a:447:GLY:N	2.39	0.56
1:v:240:GLU:OE1	2:R:246:LEU:HD11	2.04	0.56
1:h:149:VAL:HG23	1:h:284:THR:HG21	1.88	0.56
1:m:367:HIS:NE2	2:Q:64:ARG:NE	2.54	0.56
1:v:235:THR:HB	1:v:241:VAL:HB	1.88	0.56
2:Q:182:ARG:NH2	2:Q:265:ASP:O	2.38	0.56
1:b:104:LEU:HD12	1:b:340:ASP:HB3	1.88	0.56
1:b:284:THR:HG23	1:c:301:GLN:HE21	1.70	0.56
1:h:400:ASP:HB3	1:h:471:GLN:HG2	1.88	0.56
1:j:405:ILE:HG12	1:j:466:ILE:HG12	1.88	0.56
1:a:150:GLY:O	1:b:301:GLN:NE2	2.39	0.56
1:b:121:PRO:HG2	1:c:94:ILE:HA	1.88	0.56
1:m:193:ILE:HG12	1:m:271:VAL:HG12	1.87	0.56
2:P:297:ASP:HB2	2:P:299:LYS:HZ3	1.71	0.56
2:S:297:ASP:HB2	2:S:299:LYS:HZ3	1.70	0.56
1:A:227:LEU:HB3	1:A:249:LYS:HB2	1.88	0.55
1:b:467:ILE:HD12	1:b:478:PHE:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:240:GLU:OE1	2:S:197:ALA:HB2	2.06	0.55
1:s:352:LYS:HG2	2:S:156:GLU:HG2	1.89	0.55
1:f:342:ASP:OD2	1:f:510:TYR:OH	2.24	0.55
1:m:365:PHE:HE2	2:Q:57:THR:CG2	2.12	0.55
1:v:444:ALA:HB3	1:v:451:TYR:HB2	1.88	0.55
1:w:444:ALA:HB3	1:w:451:TYR:HB2	1.87	0.55
1:b:404:VAL:HG12	1:b:452:ARG:HB3	1.88	0.55
1:i:193:ILE:HG22	1:i:271:VAL:HG12	1.89	0.55
1:k:198:TRP:HB2	1:k:201:SER:HB2	1.87	0.55
1:p:367:HIS:NE2	2:P:64:ARG:NE	2.55	0.55
1:t:165:VAL:HG22	1:t:260:THR:HG22	1.88	0.55
1:y:387:HIS:NE2	1:z:528:ASN:O	2.39	0.55
2:P:63:ASP:OD2	2:P:63:ASP:N	2.38	0.55
1:b:483:TYR:HB3	1:b:509:ARG:HB2	1.88	0.55
1:q:485:PHE:HD1	1:q:508:ARG:HB2	1.72	0.55
1:r:106:GLU:O	1:r:452:ARG:NH2	2.39	0.55
1:s:465:THR:OG1	1:s:521:ARG:NH1	2.40	0.55
1:v:240:GLU:HG2	2:R:246:LEU:CD1	2.33	0.55
1:k:199:SER:HB2	1:k:265:LYS:HD3	1.88	0.55
1:l:127:VAL:HB	1:l:137:LEU:HD13	1.88	0.55
1:w:143:ASN:HD22	1:x:460:ARG:HH22	1.54	0.55
1:g:138:PRO:O	1:g:142:ASN:ND2	2.40	0.55
1:n:199:SER:HB3	1:n:265:LYS:HD3	1.87	0.55
1:w:147:THR:CG2	2:R:253:GLU:HB2	2.36	0.55
1:z:252:VAL:HG22	1:z:255:GLY:H	1.71	0.55
1:a:306:THR:OG1	1:a:495:ASN:ND2	2.40	0.55
1:m:465:THR:OG1	1:m:521:ARG:NH1	2.39	0.55
1:v:219:VAL:HG21	1:v:247:LEU:HD21	1.88	0.55
1:w:280:HIS:NE2	1:x:505:MET:SD	2.70	0.55
1:x:212:VAL:HG21	1:x:233:TYR:HB2	1.89	0.55
1:j:360:PHE:HD2	1:j:388:THR:HG22	1.71	0.55
1:s:367:HIS:HE1	2:S:64:ARG:HG2	1.72	0.55
1:t:348:ASP:OD1	1:t:521:ARG:NH2	2.40	0.55
1:A:199:SER:HB3	1:A:265:LYS:HB2	1.88	0.55
1:A:375:LYS:O	1:A:417:ASN:ND2	2.40	0.55
1:b:279:GLN:HE21	1:m:498:ASN:HD21	1.55	0.55
1:d:193:ILE:HG22	1:d:271:VAL:HG12	1.88	0.55
1:k:193:ILE:HG22	1:k:271:VAL:HG12	1.89	0.55
1:n:89:SER:OG	1:n:90:LEU:N	2.40	0.55
1:n:411:ASP:OD1	1:n:527:ASN:ND2	2.40	0.55
1:t:446:SER:OG	1:t:447:GLY:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:410:LEU:HB3	1:u:461:GLN:HG3	1.88	0.55
1:v:365:PHE:HD2	2:R:59:LYS:HD2	1.72	0.55
1:d:84:ILE:HG13	1:r:290:LEU:HB3	1.88	0.54
1:g:193:ILE:HG22	1:g:271:VAL:HG12	1.89	0.54
1:h:193:ILE:HG22	1:h:271:VAL:HG12	1.88	0.54
1:i:315:MET:HB3	1:i:321:ILE:HG13	1.87	0.54
1:m:154:ILE:HD12	1:m:170:LEU:HD22	1.89	0.54
1:w:366:PRO:O	2:R:65:ARG:NH1	2.41	0.54
1:z:485:PHE:HD1	1:z:508:ARG:HB3	1.72	0.54
1:q:160:VAL:HG13	1:q:165:VAL:HG13	1.89	0.54
1:q:240:GLU:HG3	2:Q:49:THR:HB	1.89	0.54
1:q:370:TYR:OH	1:q:376:ASP:OD2	2.25	0.54
1:t:219:VAL:HG21	1:t:247:LEU:HD23	1.90	0.54
1:y:169:ASP:OD1	1:y:182:LYS:NZ	2.40	0.54
1:f:378:LEU:HB2	1:f:417:ASN:HD21	1.73	0.54
1:m:348:ASP:OD2	2:Q:156:GLU:N	2.40	0.54
1:a:411:ASP:OD1	1:a:461:GLN:NE2	2.40	0.54
1:c:193:ILE:HG22	1:c:271:VAL:HG12	1.90	0.54
1:h:200:ASP:OD1	1:h:200:ASP:N	2.40	0.54
1:k:169:ASP:N	1:k:169:ASP:OD1	2.40	0.54
1:l:446:SER:OG	1:l:447:GLY:N	2.41	0.54
1:s:442:LEU:HD11	1:t:422:PHE:HB3	1.90	0.54
1:t:472:GLN:HE22	1:u:98:LEU:HD21	1.72	0.54
1:t:485:PHE:HD1	1:t:508:ARG:HB3	1.73	0.54
1:d:249:LYS:HD3	1:d:260:THR:HA	1.88	0.54
1:g:144:THR:OG1	1:h:460:ARG:NH1	2.40	0.54
1:i:359:HIS:HE2	1:i:523:THR:HG1	1.56	0.54
1:l:304:GLU:OE1	1:l:503:ASN:ND2	2.37	0.54
1:r:404:VAL:HG12	1:r:452:ARG:HB3	1.89	0.54
1:r:409:PRO:HA	1:r:412:VAL:HG12	1.88	0.54
1:c:443:GLY:O	1:d:423:ASN:ND2	2.41	0.54
1:j:252:VAL:HG22	1:j:255:GLY:H	1.71	0.54
1:o:304:GLU:OE1	1:o:503:ASN:ND2	2.40	0.54
1:e:150:GLY:O	1:f:301:GLN:NE2	2.41	0.54
1:l:342:ASP:O	1:l:346:PHE:N	2.40	0.54
1:o:460:ARG:HH22	2:Q:231:SER:HA	1.71	0.54
1:z:138:PRO:O	1:z:142:ASN:ND2	2.41	0.54
1:a:389:THR:HG21	1:a:451:TYR:HE1	1.73	0.54
1:b:364:VAL:HG13	1:b:378:LEU:HD11	1.89	0.54
1:c:409:PRO:HA	1:c:412:VAL:HG12	1.88	0.54
1:h:150:GLY:O	1:i:301:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:249:LYS:HG3	1:h:260:THR:HA	1.88	0.54
1:l:302:HIS:ND1	1:l:507:THR:OG1	2.40	0.54
1:m:463:GLU:OE2	2:Q:158:HIS:HA	2.06	0.54
1:p:189:ARG:NH2	1:r:81:MET:O	2.40	0.54
1:q:446:SER:OG	1:q:447:GLY:N	2.39	0.54
1:s:371:SER:HB2	1:t:371:SER:HB3	1.89	0.54
1:w:411:ASP:OD1	1:w:527:ASN:ND2	2.41	0.54
1:b:193:ILE:HB	1:b:219:VAL:HG23	1.90	0.54
1:c:489:ASN:ND2	1:c:504:MET:SD	2.81	0.54
1:i:311:VAL:HG23	1:r:81:MET:HB2	1.89	0.54
1:p:369:ASP:OD1	1:p:369:ASP:N	2.35	0.54
1:z:131:ASP:OD2	1:z:133:ASN:ND2	2.41	0.54
1:i:304:GLU:OE1	1:i:495:ASN:ND2	2.41	0.54
1:s:446:SER:OG	1:s:447:GLY:N	2.38	0.54
1:t:175:LYS:HD3	1:t:178:LYS:HE3	1.89	0.54
1:v:130:ALA:HA	1:w:497:ARG:HD2	1.90	0.54
1:y:461:GLN:HE22	1:y:527:ASN:HB3	1.73	0.54
1:a:443:GLY:N	1:b:424:GLY:O	2.38	0.53
1:e:184:ILE:O	1:e:279:GLN:NE2	2.40	0.53
1:g:371:SER:HG	1:l:371:SER:HG	1.56	0.53
1:i:81:MET:HG3	1:i:83:PRO:HD2	1.90	0.53
1:j:249:LYS:HG2	1:j:260:THR:HA	1.89	0.53
1:l:404:VAL:HG12	1:l:452:ARG:HB3	1.89	0.53
1:r:175:LYS:NZ	1:r:176:GLU:O	2.41	0.53
1:r:295:VAL:HG22	1:r:513:GLU:HG3	1.89	0.53
1:s:195:GLU:HB2	1:s:270:LYS:HB2	1.89	0.53
1:u:227:LEU:HB3	1:u:249:LYS:HB2	1.90	0.53
1:c:89:SER:OG	1:c:90:LEU:N	2.39	0.53
1:c:361:SER:OG	1:c:362:PHE:N	2.41	0.53
1:p:307:VAL:HG21	1:p:324:VAL:HG12	1.90	0.53
1:b:411:ASP:OD1	1:b:461:GLN:NE2	2.42	0.53
1:c:312:ILE:HD12	1:c:323:GLY:HA3	1.91	0.53
1:g:99:TRP:HZ3	1:l:141:ILE:HD11	1.74	0.53
1:h:254:SER:HB3	1:j:82:GLY:HA3	1.90	0.53
1:y:444:ALA:HB3	1:y:451:TYR:HB2	1.89	0.53
1:i:169:ASP:OD2	1:i:169:ASP:N	2.41	0.53
1:k:411:ASP:OD1	1:k:527:ASN:ND2	2.42	0.53
1:s:367:HIS:CE1	2:S:64:ARG:HE	2.27	0.53
1:v:411:ASP:OD1	1:v:527:ASN:ND2	2.41	0.53
1:A:445:ALA:HA	1:A:450:ASN:HA	1.90	0.53
1:a:249:LYS:HG2	1:a:260:THR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:431:ALA:HB1	1:m:434:ASN:HB2	1.91	0.53
1:o:297:ILE:HD13	1:o:483:TYR:HB2	1.91	0.53
1:w:446:SER:OG	1:w:447:GLY:N	2.42	0.53
1:x:143:ASN:ND2	2:S:19:PHE:CD1	2.75	0.53
2:R:297:ASP:HB2	2:R:299:LYS:HZ3	1.74	0.53
1:a:89:SER:OG	1:a:90:LEU:N	2.41	0.53
1:b:297:ILE:HG12	1:b:511:THR:HG21	1.91	0.53
1:n:346:PHE:HZ	1:n:514:SER:HB3	1.74	0.53
1:r:367:HIS:ND1	1:r:369:ASP:OD2	2.42	0.53
1:s:367:HIS:CE1	2:S:64:ARG:NE	2.76	0.53
1:e:121:PRO:HG2	1:f:94:ILE:HA	1.91	0.53
1:o:252:VAL:HG22	1:o:255:GLY:H	1.73	0.53
1:t:149:VAL:HG21	1:u:334:LEU:HD11	1.90	0.53
1:g:137:LEU:HD11	1:h:334:LEU:HD13	1.91	0.53
1:u:457:ASP:OD1	1:u:457:ASP:N	2.41	0.53
1:w:193:ILE:HA	1:w:271:VAL:HA	1.90	0.53
1:w:232:LYS:CE	2:S:47:THR:HG22	2.30	0.53
2:R:100:ASP:N	2:R:100:ASP:OD1	2.41	0.53
1:e:446:SER:OG	1:e:447:GLY:N	2.42	0.52
1:f:123:LEU:HD11	1:f:288:LEU:HD12	1.92	0.52
1:f:464:LEU:HB2	1:f:522:ILE:HB	1.92	0.52
1:g:405:ILE:HG12	1:g:466:ILE:HG23	1.90	0.52
1:i:106:GLU:O	1:i:452:ARG:NH2	2.42	0.52
1:g:335:SER:HB3	1:g:506:MET:HE1	1.90	0.52
1:h:138:PRO:O	1:h:142:ASN:ND2	2.41	0.52
1:n:498:ASN:HD22	1:n:501:VAL:HG22	1.73	0.52
1:o:426:ASP:OD1	1:o:426:ASP:N	2.41	0.52
1:v:446:SER:OG	1:v:447:GLY:N	2.41	0.52
2:Q:100:ASP:OD1	2:Q:100:ASP:N	2.41	0.52
1:c:165:VAL:H	1:c:260:THR:HG22	1.74	0.52
1:d:198:TRP:HE1	1:d:245:THR:HG21	1.75	0.52
1:g:357:LYS:NZ	1:g:395:ASP:OD2	2.42	0.52
1:g:452:ARG:HG2	1:h:427:ARG:HH21	1.74	0.52
1:j:277:SER:O	1:k:302:HIS:NE2	2.41	0.52
1:k:457:ASP:OD1	1:k:457:ASP:N	2.41	0.52
1:l:252:VAL:HG22	1:l:255:GLY:H	1.74	0.52
1:n:141:ILE:O	1:o:337:GLN:NE2	2.42	0.52
1:o:463:GLU:OE1	1:o:521:ARG:NH1	2.41	0.52
1:x:446:SER:OG	1:x:447:GLY:N	2.42	0.52
1:b:480:PHE:HD1	1:b:512:VAL:HB	1.74	0.52
1:d:411:ASP:OD1	1:d:527:ASN:ND2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:366:PRO:O	2:S:65:ARG:NH1	2.43	0.52
1:u:193:ILE:HG22	1:u:271:VAL:HG12	1.91	0.52
1:x:304:GLU:HB3	1:x:505:MET:HG3	1.91	0.52
2:S:100:ASP:OD1	2:S:100:ASP:N	2.41	0.52
1:A:290:LEU:HD23	1:b:84:ILE:HG23	1.92	0.52
1:g:464:LEU:HD22	1:g:524:ILE:HD11	1.90	0.52
1:n:402:GLN:HE22	1:n:452:ARG:HB2	1.74	0.52
1:v:195:GLU:OE2	1:v:205:ARG:NH2	2.42	0.52
1:z:89:SER:OG	1:z:90:LEU:N	2.43	0.52
1:a:129:ASP:O	1:b:497:ARG:NH2	2.42	0.52
1:b:304:GLU:OE2	1:b:503:ASN:ND2	2.38	0.52
1:d:446:SER:OG	1:d:447:GLY:N	2.43	0.52
1:f:249:LYS:HD3	1:f:260:THR:HA	1.91	0.52
1:p:406:VAL:HG12	1:p:454:ILE:HB	1.92	0.52
1:x:359:HIS:NE2	1:x:523:THR:OG1	2.40	0.52
1:d:292:ARG:NH1	1:h:86:PRO:O	2.43	0.52
1:e:298:ASP:OD1	1:e:298:ASP:N	2.41	0.52
1:k:485:PHE:HD1	1:k:508:ARG:HB3	1.75	0.52
1:p:497:ARG:HG3	1:p:498:ASN:HB2	1.91	0.52
1:r:252:VAL:HG22	1:r:255:GLY:H	1.75	0.52
1:r:426:ASP:N	1:r:426:ASP:OD2	2.43	0.52
1:s:348:ASP:OD1	2:S:157:GLY:N	2.40	0.52
1:x:411:ASP:HB3	1:x:524:ILE:HD12	1.92	0.52
2:P:100:ASP:N	2:P:100:ASP:OD1	2.41	0.52
2:Q:154:ILE:HD13	2:Q:160:ASN:HB3	1.92	0.52
1:f:446:SER:OG	1:f:447:GLY:N	2.43	0.52
1:h:190:LYS:HG3	1:i:298:ASP:HB2	1.92	0.52
1:j:195:GLU:OE2	1:j:205:ARG:NH1	2.43	0.52
1:v:404:VAL:HG12	1:v:452:ARG:HB3	1.92	0.52
1:v:442:LEU:HD23	1:v:453:ILE:HD11	1.91	0.52
1:c:216:SER:HB3	1:d:353:GLU:HB3	1.92	0.52
1:d:138:PRO:O	1:d:142:ASN:ND2	2.42	0.52
1:e:227:LEU:HD12	1:e:249:LYS:HD2	1.91	0.52
1:f:175:LYS:NZ	1:f:176:GLU:O	2.42	0.52
1:j:359:HIS:NE2	1:j:523:THR:OG1	2.39	0.52
1:l:485:PHE:HD1	1:l:508:ARG:HB3	1.75	0.52
1:A:406:VAL:HG12	1:A:454:ILE:HB	1.93	0.51
1:f:411:ASP:OD1	1:f:461:GLN:NE2	2.43	0.51
1:r:359:HIS:NE2	1:r:523:THR:OG1	2.42	0.51
1:u:89:SER:OG	1:u:90:LEU:N	2.42	0.51
1:n:128:VAL:HG21	1:o:497:ARG:HH22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:409:PRO:HA	1:x:412:VAL:HB	1.90	0.51
1:x:411:ASP:OD1	1:x:461:GLN:NE2	2.42	0.51
1:A:160:VAL:HG23	1:A:165:VAL:HG12	1.92	0.51
1:a:153:GLN:NE2	1:a:156:GLU:OE1	2.44	0.51
1:j:446:SER:OG	1:j:447:GLY:N	2.44	0.51
1:k:313:GLN:NE2	1:y:486:ASN:OD1	2.37	0.51
1:v:106:GLU:O	1:v:452:ARG:NH2	2.44	0.51
1:v:382:ARG:NH2	1:v:415:ILE:O	2.43	0.51
2:P:154:ILE:HD13	2:P:160:ASN:HB3	1.92	0.51
1:b:449:ALA:HA	1:c:436:ILE:HD13	1.93	0.51
1:g:127:VAL:HG13	1:g:137:LEU:HD13	1.91	0.51
1:h:411:ASP:OD1	1:h:461:GLN:NE2	2.43	0.51
1:j:141:ILE:HD11	1:k:99:TRP:HZ3	1.75	0.51
1:m:446:SER:OG	1:m:447:GLY:N	2.43	0.51
1:p:409:PRO:HA	1:p:412:VAL:HB	1.91	0.51
1:t:411:ASP:OD1	1:t:527:ASN:ND2	2.43	0.51
1:w:197:LYS:HB2	1:w:211:PHE:HA	1.91	0.51
1:y:125:PRO:HG2	1:y:137:LEU:HB3	1.93	0.51
1:a:280:HIS:NE2	1:b:304:GLU:OE1	2.43	0.51
1:i:313:GLN:OE1	1:q:486:ASN:ND2	2.43	0.51
1:j:201:SER:OG	1:j:202:PHE:N	2.43	0.51
1:s:402:GLN:NE2	1:s:403:PHE:O	2.43	0.51
1:k:371:SER:HB3	1:l:371:SER:HB2	1.93	0.51
1:t:138:PRO:O	1:t:142:ASN:ND2	2.44	0.51
1:w:128:VAL:HG23	1:w:130:ALA:H	1.76	0.51
1:w:232:LYS:HE3	2:S:47:THR:CG2	2.34	0.51
1:x:106:GLU:O	1:x:452:ARG:NH2	2.42	0.51
1:a:95:LEU:HB2	1:f:122:ILE:HA	1.93	0.51
1:q:195:GLU:HB3	1:q:270:LYS:HB2	1.92	0.51
1:s:334:LEU:HD13	1:x:137:LEU:HD11	1.92	0.51
1:a:245:THR:HG23	1:a:264:GLY:H	1.75	0.51
1:g:497:ARG:NH1	1:l:285:ASN:OD1	2.44	0.51
1:i:446:SER:OG	1:i:447:GLY:N	2.44	0.51
1:n:405:ILE:HD12	1:n:453:ILE:HG12	1.92	0.51
1:o:200:ASP:OD1	1:o:200:ASP:N	2.42	0.51
1:t:398:LEU:HG	1:t:401:VAL:HG22	1.92	0.51
1:w:404:VAL:HG12	1:w:452:ARG:HB3	1.93	0.51
1:x:89:SER:OG	1:x:90:LEU:N	2.44	0.51
2:R:154:ILE:HD13	2:R:160:ASN:HB3	1.92	0.51
1:c:268:ASP:N	1:c:268:ASP:OD1	2.43	0.51
1:k:89:SER:OG	1:k:90:LEU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:367:HIS:HD2	2:P:64:ARG:HH21	1.59	0.51
1:w:236:ASN:O	1:w:240:GLU:HA	2.11	0.51
2:S:154:ILE:HD13	2:S:160:ASN:HB3	1.92	0.51
1:A:165:VAL:H	1:A:260:THR:HG1	1.59	0.50
1:a:121:PRO:HA	1:a:292:ARG:HA	1.92	0.50
1:b:472:GLN:NE2	1:b:474:ASN:OD1	2.43	0.50
1:t:426:ASP:OD1	1:t:426:ASP:N	2.44	0.50
1:u:119:THR:HG22	1:u:294:ASP:HA	1.93	0.50
1:j:313:GLN:HE22	1:x:486:ASN:HD21	1.57	0.50
1:k:369:ASP:OD1	1:k:369:ASP:N	2.44	0.50
1:n:473:ASP:OD2	1:n:473:ASP:N	2.42	0.50
1:t:304:GLU:HB3	1:t:505:MET:HG2	1.92	0.50
1:b:302:HIS:ND1	1:b:505:MET:SD	2.84	0.50
1:d:360:PHE:HD2	1:d:388:THR:HG22	1.75	0.50
1:g:426:ASP:N	1:g:426:ASP:OD1	2.44	0.50
1:r:249:LYS:HG3	1:r:260:THR:HA	1.92	0.50
1:w:249:LYS:HE2	1:w:260:THR:HA	1.92	0.50
1:a:497:ARG:NH2	1:f:129:ASP:O	2.45	0.50
1:c:137:LEU:HD11	1:d:334:LEU:HD13	1.93	0.50
1:d:185:ASP:HA	1:d:279:GLN:HG3	1.92	0.50
1:d:189:ARG:NH1	1:d:253:SER:OG	2.45	0.50
1:p:304:GLU:HA	1:p:505:MET:HA	1.94	0.50
1:q:502:PRO:HB3	1:s:492:GLY:HA3	1.92	0.50
2:R:255:LEU:HD11	2:R:269:ASN:HB3	1.94	0.50
1:A:321:ILE:HG22	1:A:323:GLY:H	1.77	0.50
1:a:369:ASP:OD1	1:a:369:ASP:N	2.45	0.50
1:b:138:PRO:O	1:b:142:ASN:ND2	2.44	0.50
1:h:446:SER:OG	1:h:447:GLY:N	2.43	0.50
1:m:528:ASN:HD22	2:Q:4:THR:HA	1.77	0.50
1:s:227:LEU:HB2	1:s:249:LYS:HG3	1.92	0.50
1:s:367:HIS:CE1	2:S:64:ARG:HG2	2.46	0.50
1:t:143:ASN:OD1	2:S:231:SER:O	2.28	0.50
1:a:252:VAL:HG22	1:a:255:GLY:H	1.76	0.50
1:a:476:LYS:HE2	1:a:515:PHE:HE2	1.77	0.50
1:h:235:THR:HB	1:h:241:VAL:HB	1.93	0.50
1:l:227:LEU:HD13	1:l:249:LYS:HZ1	1.76	0.50
1:q:178:LYS:O	1:q:282:SER:OG	2.29	0.50
1:y:137:LEU:HD11	1:z:334:LEU:HD13	1.94	0.50
1:h:230:GLN:NE2	1:h:245:THR:O	2.45	0.50
1:k:446:SER:OG	1:k:447:GLY:N	2.44	0.50
1:m:404:VAL:HG12	1:m:452:ARG:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:305:ALA:HB1	1:u:327:LEU:HD13	1.93	0.50
1:v:193:ILE:HG22	1:v:271:VAL:HG12	1.93	0.50
1:w:410:LEU:HD23	1:w:461:GLN:HG3	1.93	0.50
1:z:195:GLU:HB2	1:z:270:LYS:HB2	1.94	0.50
1:c:446:SER:OG	1:c:447:GLY:N	2.44	0.50
1:d:195:GLU:HB2	1:d:270:LYS:HB3	1.94	0.50
1:g:402:GLN:NE2	1:g:450:ASN:O	2.45	0.50
1:g:411:ASP:HB3	1:g:524:ILE:HD12	1.94	0.50
1:h:120:VAL:HG12	1:i:91:SER:HB3	1.93	0.50
1:n:495:ASN:OD1	1:n:503:ASN:ND2	2.45	0.50
1:w:189:ARG:NH1	1:w:225:ASP:OD2	2.45	0.50
1:x:221:LEU:HD12	1:x:227:LEU:HD21	1.94	0.50
1:y:405:ILE:HG12	1:y:466:ILE:HG12	1.94	0.50
2:S:255:LEU:HD11	2:S:269:ASN:HB3	1.94	0.50
1:b:186:ARG:NH1	1:b:187:LEU:O	2.42	0.50
1:b:268:ASP:OD1	1:b:268:ASP:N	2.44	0.50
1:w:442:LEU:HD23	1:w:453:ILE:HD11	1.94	0.50
1:y:186:ARG:NE	1:y:278:GLU:OE1	2.42	0.50
1:A:240:GLU:HG2	1:A:241:VAL:HG23	1.94	0.49
1:A:249:LYS:HD3	1:A:260:THR:HA	1.94	0.49
1:a:383:GLU:OE1	1:b:375:LYS:NZ	2.44	0.49
1:c:128:VAL:HG23	1:c:130:ALA:H	1.77	0.49
1:m:137:LEU:HD11	1:n:334:LEU:HD13	1.93	0.49
1:m:312:ILE:HG23	1:m:323:GLY:H	1.77	0.49
1:v:141:ILE:HD11	1:w:99:TRP:HZ3	1.76	0.49
1:x:410:LEU:HD12	1:x:461:GLN:HG3	1.94	0.49
2:R:180:THR:OG1	2:S:89:ASP:OD2	2.25	0.49
1:a:324:VAL:HG23	1:a:504:MET:HE1	1.94	0.49
1:b:205:ARG:NH1	1:b:213:GLU:OE2	2.45	0.49
1:e:361:SER:OG	1:e:362:PHE:N	2.45	0.49
1:j:193:ILE:HG22	1:j:271:VAL:HG12	1.94	0.49
1:q:169:ASP:O	1:q:172:THR:OG1	2.28	0.49
1:u:294:ASP:OD1	1:u:294:ASP:N	2.42	0.49
1:a:193:ILE:HG22	1:a:271:VAL:HG12	1.93	0.49
1:b:285:ASN:OD1	1:c:497:ARG:NH1	2.46	0.49
1:m:426:ASP:HB2	1:m:429:ALA:HB3	1.94	0.49
1:n:160:VAL:HG13	1:n:165:VAL:HG13	1.94	0.49
1:o:294:ASP:OD1	1:o:294:ASP:N	2.42	0.49
1:x:405:ILE:HB	1:x:453:ILE:HG23	1.93	0.49
1:x:498:ASN:ND2	1:y:279:GLN:OE1	2.46	0.49
1:y:89:SER:OG	1:y:90:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:160:VAL:HG23	1:a:165:VAL:HG13	1.93	0.49
1:c:119:THR:HG23	1:d:88:ALA:HB1	1.94	0.49
1:j:409:PRO:HA	1:j:412:VAL:HB	1.93	0.49
1:o:141:ILE:O	1:p:337:GLN:NE2	2.41	0.49
1:s:386:ASP:OD2	1:t:420:TRP:NE1	2.41	0.49
1:t:128:VAL:HG12	1:t:134:LYS:HG2	1.94	0.49
2:Q:255:LEU:HD11	2:Q:269:ASN:HB3	1.94	0.49
1:b:249:LYS:NZ	1:b:251:ASP:OD1	2.44	0.49
1:f:193:ILE:HG22	1:f:271:VAL:HG12	1.94	0.49
1:h:167:ASP:HB3	1:h:257:LEU:HD23	1.95	0.49
1:t:193:ILE:HG22	1:t:271:VAL:HG12	1.95	0.49
1:A:473:ASP:N	1:A:473:ASP:OD1	2.45	0.49
1:b:446:SER:OG	1:b:447:GLY:N	2.46	0.49
1:j:335:SER:HG	1:j:508:ARG:HE	1.58	0.49
1:l:464:LEU:HB2	1:l:522:ILE:HB	1.94	0.49
1:o:141:ILE:HD11	1:p:99:TRP:HZ3	1.78	0.49
1:s:201:SER:OG	1:s:202:PHE:N	2.45	0.49
1:t:240:GLU:OE1	1:t:242:GLU:CG	2.56	0.49
2:Q:133:ASN:N	2:Q:173:VAL:O	2.45	0.49
1:a:119:THR:HG23	1:b:88:ALA:HB1	1.94	0.49
1:b:106:GLU:O	1:b:452:ARG:NH2	2.45	0.49
1:f:485:PHE:HD1	1:f:508:ARG:HB2	1.77	0.49
1:i:150:GLY:O	1:j:301:GLN:NE2	2.45	0.49
1:p:181:ARG:HB3	1:p:184:ILE:HD13	1.94	0.49
1:p:328:SER:HA	1:p:331:MET:HE2	1.95	0.49
1:s:301:GLN:NE2	1:x:150:GLY:O	2.46	0.49
1:v:240:GLU:OE1	2:R:197:ALA:HB2	2.12	0.49
1:w:206:THR:HG22	2:R:185:GLN:HB2	1.94	0.49
1:x:463:GLU:HB3	1:x:521:ARG:HD2	1.95	0.49
1:y:141:ILE:HD11	1:z:99:TRP:HZ3	1.78	0.49
1:d:178:LYS:O	1:d:282:SER:OG	2.31	0.49
1:i:339:VAL:HG11	1:i:508:ARG:HH11	1.78	0.49
1:m:240:GLU:HG2	2:Q:246:LEU:CD1	2.43	0.49
1:m:348:ASP:OD2	2:Q:156:GLU:HB3	2.11	0.49
1:r:184:ILE:O	1:r:279:GLN:NE2	2.46	0.49
1:w:143:ASN:ND2	2:R:232:ASP:HA	2.27	0.49
1:A:193:ILE:HG22	1:A:271:VAL:HG12	1.94	0.49
1:a:487:VAL:HG12	1:a:506:MET:HG3	1.93	0.49
1:c:297:ILE:O	1:c:509:ARG:NH2	2.46	0.49
1:d:350:GLU:HG2	1:d:478:PHE:HE1	1.77	0.49
1:g:175:LYS:NZ	1:g:176:GLU:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:165:VAL:HG22	1:h:260:THR:HB	1.95	0.49
1:i:279:GLN:HB3	1:z:498:ASN:HD21	1.78	0.49
1:o:371:SER:OG	1:p:371:SER:O	2.31	0.49
1:a:137:LEU:HD11	1:b:334:LEU:HD13	1.95	0.49
1:a:472:GLN:HE22	1:b:98:LEU:HD11	1.78	0.49
1:b:141:ILE:HD12	1:c:337:GLN:HG2	1.94	0.49
1:d:149:VAL:HB	1:e:338:LYS:HE3	1.94	0.49
1:d:186:ARG:NE	1:d:278:GLU:OE2	2.45	0.49
1:i:195:GLU:HB2	1:i:270:LYS:HB2	1.94	0.49
1:j:212:VAL:HG21	1:j:233:TYR:HB2	1.95	0.49
1:l:249:LYS:HG3	1:l:260:THR:HA	1.95	0.49
1:r:200:ASP:N	1:r:200:ASP:OD1	2.45	0.48
1:s:195:GLU:HB3	1:s:211:PHE:HB3	1.95	0.48
1:A:252:VAL:HG22	1:A:255:GLY:H	1.78	0.48
1:e:297:ILE:HG21	1:e:483:TYR:HB2	1.94	0.48
1:g:167:ASP:H	1:g:259:LEU:HD23	1.78	0.48
1:h:110:THR:HG22	1:h:480:PHE:HB3	1.95	0.48
1:h:142:ASN:OD1	1:i:337:GLN:NE2	2.38	0.48
1:m:131:ASP:N	1:m:131:ASP:OD1	2.46	0.48
1:m:373:HIS:HE2	1:r:379:GLU:HB3	1.76	0.48
1:o:89:SER:OG	1:o:90:LEU:N	2.46	0.48
1:p:238:ASP:CG	2:P:244:ARG:CD	2.86	0.48
1:t:315:MET:HB3	1:t:321:ILE:HB	1.95	0.48
1:u:197:LYS:O	1:u:267:THR:OG1	2.31	0.48
2:P:255:LEU:HD11	2:P:269:ASN:HB3	1.94	0.48
1:g:89:SER:OG	1:g:90:LEU:N	2.47	0.48
1:j:189:ARG:NH2	1:l:81:MET:O	2.46	0.48
1:q:89:SER:OG	1:q:90:LEU:N	2.45	0.48
1:s:239:GLY:O	2:S:196:SER:HA	2.13	0.48
1:u:326:ARG:O	1:u:330:THR:OG1	2.29	0.48
1:a:119:THR:HG22	1:a:294:ASP:HA	1.94	0.48
1:a:277:SER:O	1:b:302:HIS:NE2	2.40	0.48
1:b:149:VAL:HG21	1:c:334:LEU:HD11	1.94	0.48
1:e:106:GLU:HB2	1:f:427:ARG:HD2	1.95	0.48
1:h:185:ASP:HB3	1:h:279:GLN:HB2	1.94	0.48
1:j:106:GLU:HB2	1:k:427:ARG:HD2	1.95	0.48
1:u:221:LEU:HD22	1:u:227:LEU:HD13	1.96	0.48
1:w:186:ARG:NH1	1:w:187:LEU:O	2.44	0.48
1:b:389:THR:HG21	1:b:451:TYR:HE2	1.78	0.48
1:g:446:SER:OG	1:g:447:GLY:N	2.46	0.48
1:h:175:LYS:NZ	1:h:179:GLU:OE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:175:LYS:HE3	1:o:178:LYS:HD2	1.96	0.48
1:o:473:ASP:OD2	1:o:473:ASP:N	2.42	0.48
1:r:405:ILE:HG12	1:r:466:ILE:HG12	1.95	0.48
1:s:463:GLU:CD	2:S:158:HIS:NE2	2.69	0.48
1:p:175:LYS:HD2	1:p:178:LYS:HG2	1.95	0.48
1:q:464:LEU:HB2	1:q:522:ILE:HB	1.95	0.48
1:v:463:GLU:OE2	2:R:158:HIS:HA	2.14	0.48
1:g:189:ARG:NH1	1:g:225:ASP:OD1	2.47	0.48
1:j:426:ASP:OD1	1:j:426:ASP:N	2.45	0.48
1:x:444:ALA:HB3	1:x:451:TYR:HB2	1.95	0.48
1:a:178:LYS:O	1:a:282:SER:OG	2.30	0.48
1:b:212:VAL:HG21	1:b:233:TYR:HB2	1.95	0.48
1:f:89:SER:OG	1:f:90:LEU:N	2.45	0.48
1:f:364:VAL:HG13	1:f:378:LEU:HD21	1.96	0.48
1:i:306:THR:HG22	1:i:308:PRO:HD3	1.95	0.48
1:k:151:LEU:HD11	1:l:300:ALA:HA	1.96	0.48
1:l:530:SER:O	1:l:530:SER:OG	2.32	0.48
1:m:89:SER:OG	1:m:90:LEU:N	2.46	0.48
1:r:303:ILE:HB	1:r:506:MET:HB3	1.96	0.48
1:s:411:ASP:OD1	1:s:527:ASN:ND2	2.46	0.48
1:u:444:ALA:HB3	1:u:451:TYR:HB2	1.96	0.48
1:z:411:ASP:OD1	1:z:461:GLN:NE2	2.43	0.48
1:A:235:THR:HG22	1:A:237:GLY:H	1.79	0.48
1:j:489:ASN:OD1	1:j:489:ASN:N	2.46	0.48
1:u:386:ASP:OD2	1:u:446:SER:OG	2.30	0.48
1:w:141:ILE:HD11	1:x:99:TRP:HZ3	1.78	0.48
1:x:131:ASP:OD1	1:x:131:ASP:N	2.46	0.48
1:x:500:ASN:OD1	1:y:181:ARG:NH1	2.39	0.48
1:p:521:ARG:NH1	2:P:157:GLY:O	2.40	0.48
1:q:487:VAL:HB	1:q:506:MET:HG3	1.96	0.48
1:r:219:VAL:HG12	1:r:227:LEU:HD12	1.96	0.48
1:t:249:LYS:HG3	1:t:260:THR:HA	1.96	0.48
1:u:359:HIS:HD2	2:S:264:GLN:NE2	2.01	0.48
1:v:485:PHE:HB2	1:v:508:ARG:HG3	1.94	0.48
1:y:195:GLU:HG2	1:y:211:PHE:HB3	1.96	0.48
1:a:193:ILE:HA	1:a:271:VAL:HA	1.96	0.47
1:a:457:ASP:OD1	1:a:457:ASP:N	2.46	0.47
1:c:165:VAL:HG22	1:c:260:THR:HG22	1.95	0.47
1:c:202:PHE:HA	1:c:209:ALA:HA	1.95	0.47
1:d:214:LEU:HB3	1:d:217:ASN:HB2	1.95	0.47
1:d:394:ASN:HD21	1:e:409:PRO:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:235:THR:HG1	1:l:243:THR:HG1	1.58	0.47
1:o:195:GLU:HB3	1:o:270:LYS:HB2	1.96	0.47
1:t:465:THR:OG1	1:t:521:ARG:NH1	2.46	0.47
1:k:198:TRP:HE1	1:k:245:THR:HG21	1.79	0.47
1:m:154:ILE:HA	1:m:174:LEU:HD11	1.95	0.47
2:P:133:ASN:N	2:P:173:VAL:O	2.45	0.47
2:P:180:THR:OG1	2:Q:89:ASP:OD2	2.25	0.47
1:c:385:ILE:HD13	1:c:405:ILE:HD13	1.96	0.47
1:g:181:ARG:NH1	1:r:500:ASN:OD1	2.46	0.47
1:t:121:PRO:HB2	1:t:290:LEU:HD11	1.96	0.47
1:v:206:THR:OG1	1:v:207:SER:N	2.47	0.47
1:v:433:SER:HA	1:v:436:ILE:HD13	1.97	0.47
1:y:386:ASP:OD2	1:y:446:SER:OG	2.32	0.47
1:c:190:LYS:HG3	1:d:298:ASP:HB2	1.96	0.47
1:h:212:VAL:HG21	1:h:233:TYR:HB2	1.96	0.47
1:l:193:ILE:HG12	1:l:219:VAL:HB	1.96	0.47
1:m:449:ALA:HA	1:n:436:ILE:HD13	1.96	0.47
1:q:263:SER:OG	1:q:264:GLY:N	2.47	0.47
1:z:123:LEU:HD11	1:z:288:LEU:HD23	1.95	0.47
1:c:498:ASN:OD1	1:c:500:ASN:ND2	2.43	0.47
1:d:363:ASP:OD1	1:d:526:ASN:ND2	2.47	0.47
1:g:248:GLY:O	1:g:261:SER:OG	2.32	0.47
1:n:366:PRO:O	2:Q:65:ARG:NH1	2.46	0.47
1:u:167:ASP:HB3	1:u:257:LEU:HD13	1.96	0.47
1:v:366:PRO:O	2:R:59:LYS:NZ	2.47	0.47
1:w:200:ASP:N	1:w:200:ASP:OD1	2.46	0.47
1:z:426:ASP:N	1:z:426:ASP:OD1	2.46	0.47
1:a:341:LEU:HD21	1:a:458:LEU:HD22	1.96	0.47
1:n:138:PRO:O	1:n:142:ASN:ND2	2.48	0.47
1:n:371:SER:HB2	1:o:371:SER:HB2	1.96	0.47
1:q:304:GLU:OE2	1:q:503:ASN:ND2	2.47	0.47
1:w:121:PRO:HG2	1:x:94:ILE:HA	1.94	0.47
1:w:160:VAL:HG13	1:w:165:VAL:HG13	1.97	0.47
1:b:193:ILE:HG12	1:b:271:VAL:HG12	1.96	0.47
1:b:195:GLU:HB2	1:b:270:LYS:HB2	1.95	0.47
1:b:503:ASN:OD1	1:b:503:ASN:N	2.47	0.47
1:c:369:ASP:OD1	1:c:369:ASP:N	2.48	0.47
1:e:294:ASP:OD2	1:e:294:ASP:N	2.43	0.47
1:g:146:GLU:HB2	1:h:341:LEU:HD23	1.97	0.47
1:l:89:SER:OG	1:l:90:LEU:N	2.46	0.47
1:m:152:VAL:HG21	1:m:179:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:365:PHE:HB3	2:Q:59:LYS:NZ	2.30	0.47
1:p:463:GLU:HG3	2:P:158:HIS:CE1	2.50	0.47
1:q:411:ASP:OD1	1:q:527:ASN:ND2	2.47	0.47
1:s:390:GLN:NE2	1:s:394:ASN:OD1	2.47	0.47
1:t:146:GLU:OE2	1:u:338:LYS:NZ	2.38	0.47
1:u:121:PRO:HB3	1:u:292:ARG:HG2	1.97	0.47
1:x:181:ARG:HG3	1:x:281:THR:HG23	1.96	0.47
2:P:283:GLU:HA	2:P:286:LYS:HG2	1.97	0.47
2:Q:283:GLU:HA	2:Q:286:LYS:HG2	1.97	0.47
2:R:283:GLU:HA	2:R:286:LYS:HG2	1.97	0.47
2:S:283:GLU:HA	2:S:286:LYS:HG2	1.97	0.47
1:a:303:ILE:HG13	1:a:506:MET:HB3	1.97	0.47
1:c:153:GLN:NE2	1:c:156:GLU:OE1	2.47	0.47
1:g:471:GLN:HB3	1:h:432:TYR:CG	2.49	0.47
1:m:420:TRP:NE1	1:r:386:ASP:OD2	2.44	0.47
1:n:205:ARG:CZ	2:Q:188:GLN:NE2	2.78	0.47
1:o:143:ASN:ND2	2:P:19:PHE:CE1	2.83	0.47
1:s:121:PRO:HA	1:s:292:ARG:HA	1.97	0.47
1:y:155:LYS:NZ	1:y:157:ASP:O	2.48	0.47
1:q:248:GLY:HA3	1:q:262:ALA:HB3	1.96	0.47
1:r:304:GLU:OE1	1:r:503:ASN:ND2	2.42	0.47
1:s:298:ASP:HB2	1:x:190:LYS:HG3	1.97	0.47
1:u:399:TYR:HE2	1:v:101:ARG:H	1.62	0.47
1:b:315:MET:HB3	1:b:321:ILE:HB	1.97	0.47
1:c:185:ASP:OD1	1:c:185:ASP:N	2.48	0.47
1:d:402:GLN:NE2	1:e:430:ASP:OD1	2.48	0.47
1:h:302:HIS:HB3	1:h:507:THR:HB	1.97	0.47
1:h:304:GLU:OE1	1:h:503:ASN:ND2	2.47	0.47
1:o:400:ASP:HB3	1:o:471:GLN:HG2	1.97	0.47
1:u:175:LYS:N	1:u:179:GLU:OE2	2.45	0.47
1:z:463:GLU:HG2	1:z:521:ARG:HD3	1.97	0.47
2:R:133:ASN:N	2:R:173:VAL:O	2.45	0.47
1:A:409:PRO:HA	1:A:412:VAL:HB	1.96	0.46
1:b:168:TYR:HB3	1:b:258:THR:HB	1.97	0.46
1:h:230:GLN:NE2	1:h:244:ASP:OD2	2.45	0.46
1:j:457:ASP:N	1:j:457:ASP:OD1	2.41	0.46
1:l:227:LEU:HB2	1:l:249:LYS:HB3	1.97	0.46
1:p:240:GLU:OE2	2:P:246:LEU:HD11	2.14	0.46
1:p:297:ILE:HG21	1:p:483:TYR:HB2	1.96	0.46
1:q:193:ILE:HG12	1:q:219:VAL:HB	1.97	0.46
1:a:306:THR:HG22	1:a:308:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:331:MET:HE2	1:a:506:MET:HE3	1.96	0.46
1:h:364:VAL:HG21	1:h:527:ASN:HB2	1.97	0.46
1:i:144:THR:HA	1:j:341:LEU:HD12	1.97	0.46
1:i:500:ASN:OD1	1:p:181:ARG:NH1	2.47	0.46
1:k:160:VAL:HG21	1:k:266:LEU:HD22	1.97	0.46
1:l:112:VAL:HA	1:l:482:PRO:HD2	1.97	0.46
1:y:342:ASP:OD1	1:y:510:TYR:OH	2.32	0.46
1:y:359:HIS:NE2	1:y:523:THR:OG1	2.42	0.46
1:b:294:ASP:OD2	1:b:294:ASP:N	2.40	0.46
1:c:293:LYS:NZ	1:c:513:GLU:OE2	2.47	0.46
1:f:227:LEU:HD23	1:f:249:LYS:HG2	1.97	0.46
1:j:305:ALA:HB1	1:j:327:LEU:HD13	1.96	0.46
1:l:428:ASN:N	1:l:428:ASN:OD1	2.47	0.46
1:r:506:MET:HE2	1:r:506:MET:HB2	1.78	0.46
1:v:389:THR:HG21	1:v:451:TYR:HE1	1.81	0.46
1:w:99:TRP:NE1	1:w:333:GLN:OE1	2.48	0.46
1:z:165:VAL:HG22	1:z:260:THR:HB	1.96	0.46
1:z:382:ARG:HA	1:z:385:ILE:HB	1.98	0.46
1:z:534:ARG:HE	1:z:534:ARG:HB3	1.57	0.46
1:c:359:HIS:NE2	1:c:523:THR:OG1	2.49	0.46
1:c:390:GLN:NE2	1:c:394:ASN:OD1	2.44	0.46
1:d:250:VAL:HG13	1:d:259:LEU:HD13	1.96	0.46
1:h:457:ASP:OD1	1:h:457:ASP:N	2.43	0.46
1:m:427:ARG:NH1	1:m:428:ASN:OD1	2.42	0.46
1:z:488:VAL:HG23	1:z:505:MET:HB3	1.97	0.46
1:b:371:SER:OG	1:c:371:SER:OG	2.31	0.46
1:d:186:ARG:NH1	1:d:187:LEU:O	2.46	0.46
1:i:89:SER:OG	1:i:90:LEU:N	2.46	0.46
1:i:137:LEU:HD11	1:j:334:LEU:HD13	1.97	0.46
1:p:216:SER:O	1:p:216:SER:OG	2.33	0.46
1:q:319:TYR:HB2	1:q:321:ILE:HG12	1.97	0.46
1:v:165:VAL:H	1:v:260:THR:HB	1.80	0.46
1:a:176:GLU:OE2	1:a:182:LYS:N	2.44	0.46
1:d:406:VAL:HG23	1:d:465:THR:HB	1.97	0.46
1:e:427:ARG:NH1	1:e:430:ASP:OD2	2.48	0.46
1:o:447:GLY:HA3	1:p:418:VAL:HG11	1.96	0.46
2:S:14:GLU:HB3	2:S:27:PRO:HD3	1.98	0.46
2:S:133:ASN:N	2:S:173:VAL:O	2.45	0.46
1:A:108:LEU:HD23	1:A:480:PHE:HB2	1.96	0.46
1:A:364:VAL:HG11	1:A:530:SER:HA	1.98	0.46
1:g:175:LYS:HE3	1:g:175:LYS:HB3	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:402:GLN:HE22	1:i:452:ARG:HB2	1.81	0.46
1:l:406:VAL:O	1:l:465:THR:OG1	2.33	0.46
1:m:121:PRO:HA	1:m:292:ARG:HA	1.98	0.46
1:o:219:VAL:HG12	1:o:227:LEU:HB3	1.98	0.46
1:s:359:HIS:NE2	1:s:523:THR:OG1	2.38	0.46
2:P:185:GLN:OE1	2:P:188:GLN:NE2	2.49	0.46
1:n:200:ASP:OD1	1:n:200:ASP:N	2.47	0.46
1:r:193:ILE:HG22	1:r:271:VAL:HG12	1.98	0.46
1:v:457:ASP:OD1	1:v:457:ASP:N	2.39	0.46
1:w:426:ASP:HB2	1:w:429:ALA:HB3	1.98	0.46
1:y:167:ASP:HB3	1:y:257:LEU:HD22	1.98	0.46
2:R:185:GLN:OE1	2:R:188:GLN:NE2	2.49	0.46
1:o:402:GLN:HB2	1:p:432:TYR:CD2	2.51	0.46
1:x:464:LEU:HB2	1:x:522:ILE:HB	1.98	0.46
1:A:153:GLN:H	1:A:153:GLN:HG2	1.46	0.46
1:d:141:ILE:HD11	1:e:99:TRP:HZ3	1.80	0.46
1:h:367:HIS:ND1	1:h:369:ASP:OD1	2.49	0.46
1:m:463:GLU:OE1	2:Q:158:HIS:NE2	2.43	0.46
1:p:249:LYS:HD3	1:p:260:THR:HG23	1.98	0.46
1:p:298:ASP:OD2	1:p:298:ASP:N	2.48	0.46
1:y:131:ASP:N	1:y:131:ASP:OD1	2.48	0.46
1:y:477:THR:OG1	1:y:516:VAL:O	2.30	0.46
1:b:409:PRO:HA	1:b:412:VAL:HB	1.97	0.45
1:g:409:PRO:HG2	1:l:394:ASN:HD21	1.81	0.45
1:i:141:ILE:O	1:j:337:GLN:NE2	2.49	0.45
1:u:361:SER:OG	1:u:362:PHE:N	2.48	0.45
1:A:198:TRP:HA	1:A:266:LEU:HA	1.98	0.45
1:c:378:LEU:HD13	1:c:414:LEU:HD22	1.98	0.45
1:d:500:ASN:OD1	1:q:181:ARG:NH1	2.48	0.45
1:g:100:ALA:HA	1:l:397:LYS:HG2	1.98	0.45
1:g:350:GLU:HA	1:g:353:GLU:HG2	1.98	0.45
1:l:411:ASP:OD1	1:l:527:ASN:ND2	2.49	0.45
1:m:411:ASP:OD1	1:m:527:ASN:ND2	2.46	0.45
1:n:169:ASP:OD1	1:n:169:ASP:N	2.42	0.45
1:p:405:ILE:HG12	1:p:466:ILE:HG12	1.97	0.45
1:w:203:ASP:OD2	1:w:206:THR:OG1	2.24	0.45
1:z:230:GLN:HA	1:z:246:ILE:HA	1.97	0.45
1:c:127:VAL:HG13	1:c:137:LEU:HD13	1.97	0.45
1:c:493:TYR:HE2	1:m:309:LEU:HD13	1.81	0.45
1:c:506:MET:HE3	1:c:506:MET:HB3	1.90	0.45
1:h:449:ALA:HA	1:i:436:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:195:GLU:HB2	1:k:270:LYS:HB3	1.97	0.45
1:r:181:ARG:HB3	1:r:184:ILE:HD12	1.98	0.45
1:a:444:ALA:HB3	1:a:451:TYR:HB2	1.98	0.45
1:g:371:SER:HB3	1:h:371:SER:HB2	1.98	0.45
1:j:175:LYS:N	1:j:179:GLU:OE1	2.45	0.45
1:k:221:LEU:HD12	1:k:227:LEU:HD13	1.98	0.45
1:b:530:SER:O	1:b:530:SER:OG	2.31	0.45
1:c:335:SER:HB3	1:c:506:MET:HE1	1.98	0.45
1:d:464:LEU:HB2	1:d:522:ILE:HB	1.97	0.45
1:h:197:LYS:HB2	1:h:211:PHE:HA	1.99	0.45
1:h:338:LYS:HD2	1:h:338:LYS:HA	1.83	0.45
1:i:378:LEU:HD13	1:i:414:LEU:HD22	1.99	0.45
1:i:480:PHE:HD1	1:i:512:VAL:HB	1.82	0.45
1:j:146:GLU:HG2	1:k:338:LYS:HE2	1.98	0.45
1:j:149:VAL:HB	1:k:338:LYS:HE3	1.97	0.45
1:m:240:GLU:HG2	2:Q:246:LEU:HD13	1.98	0.45
1:q:238:ASP:OD1	1:q:238:ASP:N	2.46	0.45
1:s:379:GLU:OE2	1:s:382:ARG:NE	2.48	0.45
1:t:195:GLU:HB2	1:t:270:LYS:HB3	1.98	0.45
2:Q:185:GLN:OE1	2:Q:188:GLN:NE2	2.49	0.45
2:S:185:GLN:OE1	2:S:188:GLN:NE2	2.49	0.45
1:g:466:ILE:HD11	1:g:522:ILE:HD11	1.99	0.45
1:h:463:GLU:HG2	1:h:521:ARG:HD3	1.98	0.45
1:j:195:GLU:HB2	1:j:270:LYS:HB2	1.98	0.45
1:j:383:GLU:HG3	1:k:375:LYS:HG3	1.99	0.45
1:m:279:GLN:NE2	1:m:281:THR:OG1	2.45	0.45
1:x:485:PHE:HD1	1:x:508:ARG:HB2	1.81	0.45
1:a:141:ILE:O	1:b:337:GLN:NE2	2.50	0.45
1:g:227:LEU:HB2	1:g:249:LYS:HG2	1.98	0.45
1:j:304:GLU:OE1	1:j:503:ASN:ND2	2.50	0.45
1:s:528:ASN:HD22	2:S:4:THR:HA	1.81	0.45
1:v:528:ASN:HD22	2:R:4:THR:HA	1.81	0.45
1:z:249:LYS:HE2	1:z:260:THR:HG23	1.98	0.45
2:P:14:GLU:HB3	2:P:27:PRO:HD3	1.98	0.45
1:g:106:GLU:O	1:g:452:ARG:NH2	2.50	0.45
1:g:400:ASP:HB3	1:g:471:GLN:HE21	1.80	0.45
1:m:238:ASP:OD1	2:Q:244:ARG:NH2	2.50	0.45
1:o:106:GLU:HG2	1:p:427:ARG:HB3	1.99	0.45
1:o:143:ASN:CG	2:P:19:PHE:CE1	2.95	0.45
1:p:411:ASP:OD1	1:p:527:ASN:ND2	2.38	0.45
1:s:160:VAL:HG11	1:s:260:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:190:LYS:HG2	1:v:298:ASP:HB3	1.99	0.45
1:v:193:ILE:HG12	1:v:219:VAL:HB	1.99	0.45
1:w:285:ASN:ND2	1:x:304:GLU:OE2	2.50	0.45
1:y:181:ARG:HB3	1:y:184:ILE:HD13	1.98	0.45
1:a:302:HIS:HD1	1:a:507:THR:HG1	1.63	0.45
1:b:357:LYS:HE3	1:b:357:LYS:HB2	1.78	0.45
1:e:285:ASN:HB3	1:f:304:GLU:HG2	1.98	0.45
1:j:411:ASP:OD1	1:j:527:ASN:ND2	2.49	0.45
1:k:137:LEU:HD21	1:l:334:LEU:HD12	1.98	0.45
1:k:304:GLU:OE1	1:k:495:ASN:ND2	2.49	0.45
1:n:134:LYS:HB2	1:n:134:LYS:HE3	1.84	0.45
1:n:485:PHE:HD1	1:n:508:ARG:HB2	1.82	0.45
2:Q:79:ILE:HG23	2:Q:125:LEU:HB2	1.99	0.45
2:R:14:GLU:HB3	2:R:27:PRO:HD3	1.98	0.45
1:c:464:LEU:HB2	1:c:522:ILE:HB	1.98	0.45
1:e:407:GLY:HA3	1:e:464:LEU:HD23	1.99	0.45
1:i:128:VAL:HG23	1:i:130:ALA:H	1.82	0.45
1:k:169:ASP:O	1:k:172:THR:OG1	2.35	0.45
1:n:197:LYS:HE3	1:n:268:ASP:HB2	1.99	0.45
1:o:299:THR:HA	1:o:509:ARG:HE	1.80	0.45
1:p:464:LEU:HB3	1:p:522:ILE:HB	1.99	0.45
1:b:109:PRO:HG3	1:b:469:ILE:HG23	1.99	0.44
1:e:485:PHE:HE1	1:e:506:MET:HE3	1.82	0.44
1:h:369:ASP:OD1	1:h:369:ASP:N	2.49	0.44
1:h:505:MET:HE2	1:h:505:MET:HB2	1.77	0.44
1:k:110:THR:HG22	1:k:480:PHE:HB3	2.00	0.44
1:l:198:TRP:HE1	1:l:245:THR:HG21	1.82	0.44
1:t:394:ASN:ND2	1:u:408:ASN:OD1	2.49	0.44
1:u:402:GLN:HB2	1:v:432:TYR:HA	1.99	0.44
2:P:79:ILE:HG23	2:P:125:LEU:HB2	1.99	0.44
1:b:192:LYS:HB3	1:b:272:LYS:HB3	2.00	0.44
1:f:178:LYS:O	1:f:282:SER:OG	2.36	0.44
1:k:119:THR:HG23	1:l:88:ALA:HB1	1.98	0.44
1:l:185:ASP:HA	1:l:279:GLN:HG3	1.98	0.44
1:m:247:LEU:HD23	1:m:247:LEU:HA	1.86	0.44
1:n:127:VAL:O	1:n:135:HIS:N	2.50	0.44
1:q:165:VAL:HG22	1:q:260:THR:HG22	1.99	0.44
1:q:219:VAL:HG12	1:q:227:LEU:HB3	1.99	0.44
1:s:294:ASP:OD1	1:x:222:GLN:NE2	2.50	0.44
1:s:398:LEU:HD21	1:s:470:PRO:HG3	1.98	0.44
1:w:484:THR:HG22	1:w:509:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:200:ASP:OD1	1:y:200:ASP:N	2.50	0.44
1:c:121:PRO:HA	1:c:292:ARG:HG2	1.99	0.44
1:e:293:LYS:HD3	1:e:515:PHE:HD1	1.82	0.44
1:k:378:LEU:HD13	1:k:414:LEU:HD22	1.99	0.44
1:n:304:GLU:OE2	1:n:496:THR:N	2.50	0.44
1:r:404:VAL:HG11	1:r:452:ARG:HH21	1.83	0.44
1:s:464:LEU:HB2	1:s:522:ILE:HB	2.00	0.44
1:t:163:GLY:HA2	1:t:266:LEU:HB2	1.99	0.44
1:u:101:ARG:HA	1:u:101:ARG:HD3	1.84	0.44
1:u:235:THR:HB	1:u:241:VAL:HB	1.99	0.44
1:z:329:GLU:O	1:z:333:GLN:NE2	2.50	0.44
2:S:79:ILE:HG23	2:S:125:LEU:HB2	1.99	0.44
1:d:409:PRO:HA	1:d:412:VAL:HB	1.99	0.44
1:g:230:GLN:HB2	1:g:246:ILE:HD12	1.98	0.44
1:p:277:SER:O	1:p:277:SER:OG	2.31	0.44
1:z:382:ARG:NH2	1:z:415:ILE:O	2.46	0.44
1:c:346:PHE:HZ	1:c:514:SER:HB3	1.81	0.44
1:d:297:ILE:HG21	1:d:483:TYR:HB2	1.99	0.44
1:e:200:ASP:OD1	1:e:200:ASP:N	2.50	0.44
1:g:334:LEU:HD11	1:l:149:VAL:HG21	1.98	0.44
1:k:382:ARG:HB3	1:l:420:TRP:CE2	2.53	0.44
1:k:444:ALA:HB3	1:k:451:TYR:HB2	1.99	0.44
1:q:137:LEU:HD22	1:r:99:TRP:CH2	2.49	0.44
1:t:382:ARG:HB3	1:u:420:TRP:CE2	2.52	0.44
1:z:487:VAL:HG23	1:z:506:MET:HB3	1.98	0.44
1:b:401:VAL:O	1:c:433:SER:OG	2.34	0.44
1:m:298:ASP:OD2	1:m:298:ASP:N	2.50	0.44
1:m:460:ARG:HD2	2:Q:158:HIS:CD2	2.52	0.44
1:o:148:LEU:HD21	2:P:18:PRO:HB3	1.98	0.44
1:r:477:THR:OG1	1:r:516:VAL:O	2.28	0.44
1:x:163:GLY:HA2	1:x:266:LEU:HB2	1.99	0.44
1:e:181:ARG:HB2	1:e:184:ILE:HG22	1.99	0.44
1:g:369:ASP:OD1	1:g:369:ASP:N	2.47	0.44
1:o:120:VAL:HG23	1:o:293:LYS:HB3	2.00	0.44
1:p:268:ASP:OD1	1:p:268:ASP:N	2.48	0.44
1:q:359:HIS:NE2	1:q:523:THR:OG1	2.40	0.44
1:t:335:SER:HB2	1:t:508:ARG:HD2	2.00	0.44
1:u:125:PRO:HB2	1:u:137:LEU:HD23	1.99	0.44
1:u:446:SER:OG	1:u:447:GLY:N	2.51	0.44
1:w:304:GLU:HG3	1:w:503:ASN:HD22	1.81	0.44
1:w:405:ILE:HG22	1:w:464:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:189:ARG:NH1	1:x:225:ASP:OD1	2.51	0.44
2:P:11:LEU:HD13	2:P:17:ILE:HD12	2.00	0.44
2:Q:14:GLU:HB3	2:Q:27:PRO:HD3	1.98	0.44
1:f:277:SER:O	1:f:277:SER:OG	2.33	0.44
1:i:305:ALA:HB1	1:i:327:LEU:HD13	2.00	0.44
1:i:398:LEU:HD13	1:i:401:VAL:HG21	1.99	0.44
1:k:352:LYS:HA	1:k:352:LYS:HD2	1.79	0.44
1:l:278:GLU:HG3	1:l:279:GLN:HG2	2.00	0.44
1:m:484:THR:HG22	1:m:509:ARG:HB2	2.00	0.44
1:q:277:SER:O	1:r:302:HIS:NE2	2.43	0.44
1:q:280:HIS:NE2	1:r:304:GLU:OE2	2.50	0.44
1:s:193:ILE:HG12	1:s:271:VAL:HG12	2.00	0.44
1:s:297:ILE:HD13	1:s:483:TYR:HB2	1.99	0.44
1:v:361:SER:OG	1:v:362:PHE:N	2.51	0.44
1:y:142:ASN:OD1	1:z:337:GLN:NE2	2.51	0.44
1:A:350:GLU:HG3	1:A:478:PHE:HE2	1.82	0.44
1:b:371:SER:HG	1:c:371:SER:HG	1.62	0.44
1:d:485:PHE:HD1	1:d:508:ARG:HB2	1.83	0.44
1:k:181:ARG:HB3	1:k:184:ILE:HD13	2.00	0.44
1:l:160:VAL:HG13	1:l:165:VAL:HG13	1.99	0.44
1:l:178:LYS:O	1:l:282:SER:OG	2.33	0.44
1:m:240:GLU:OE2	2:Q:196:SER:O	2.35	0.44
1:o:266:LEU:HD23	1:o:266:LEU:HA	1.91	0.44
1:w:352:LYS:HE2	1:w:352:LYS:HB3	1.81	0.44
1:x:505:MET:HE3	1:x:505:MET:HB2	1.75	0.44
1:b:252:VAL:HG22	1:b:255:GLY:H	1.83	0.43
1:b:331:MET:HE2	1:b:506:MET:HE3	1.99	0.43
1:h:175:LYS:N	1:h:179:GLU:OE1	2.51	0.43
1:h:471:GLN:HB3	1:i:432:TYR:CG	2.53	0.43
1:m:365:PHE:CD2	2:Q:59:LYS:HD2	2.50	0.43
1:m:525:LYS:NZ	2:Q:164:ARG:O	2.49	0.43
1:p:193:ILE:HG12	1:p:271:VAL:HG12	2.00	0.43
1:t:230:GLN:NE2	1:t:244:ASP:OD1	2.51	0.43
1:t:394:ASN:HD21	1:u:409:PRO:HG2	1.83	0.43
1:u:127:VAL:HG12	1:u:129:ASP:H	1.82	0.43
1:v:146:GLU:OE2	1:v:149:VAL:N	2.43	0.43
1:A:530:SER:OG	1:A:531:VAL:N	2.50	0.43
1:a:364:VAL:HG21	1:a:527:ASN:HB2	2.00	0.43
1:f:227:LEU:HB3	1:f:249:LYS:HB3	1.99	0.43
1:j:121:PRO:HA	1:j:292:ARG:HA	2.01	0.43
1:k:212:VAL:HG11	1:k:234:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:307:VAL:HB	1:m:312:ILE:HD11	2.01	0.43
1:o:364:VAL:HG13	1:o:378:LEU:HD11	1.99	0.43
1:p:430:ASP:N	1:p:430:ASP:OD1	2.51	0.43
1:s:405:ILE:HD12	1:s:453:ILE:HG22	2.00	0.43
1:v:200:ASP:OD1	1:v:200:ASP:N	2.50	0.43
1:x:426:ASP:N	1:x:426:ASP:OD1	2.50	0.43
1:z:342:ASP:OD2	1:z:510:TYR:OH	2.28	0.43
1:g:181:ARG:HG3	1:g:281:THR:HG23	2.01	0.43
1:h:185:ASP:HA	1:h:279:GLN:HE21	1.83	0.43
1:h:286:VAL:HG23	1:i:327:LEU:HD22	2.00	0.43
1:h:290:LEU:HB3	1:r:84:ILE:HG23	2.01	0.43
1:k:361:SER:OG	1:k:362:PHE:N	2.51	0.43
1:m:486:ASN:N	1:m:486:ASN:OD1	2.49	0.43
1:n:444:ALA:HB3	1:n:451:TYR:HB2	2.01	0.43
1:o:349:HIS:HA	1:o:352:LYS:HE2	2.00	0.43
1:r:185:ASP:HA	1:r:279:GLN:HE21	1.84	0.43
1:t:122:ILE:HG22	1:u:95:LEU:HB3	2.00	0.43
1:y:292:ARG:NH1	1:z:319:TYR:OH	2.46	0.43
1:z:442:LEU:HB3	1:z:453:ILE:HB	1.99	0.43
1:a:127:VAL:HG13	1:a:137:LEU:HD13	2.01	0.43
1:g:94:ILE:HG23	1:l:121:PRO:HG2	2.01	0.43
1:g:366:PRO:HA	1:g:377:TRP:CE2	2.53	0.43
1:h:430:ASP:OD1	1:h:430:ASP:N	2.49	0.43
1:p:477:THR:OG1	1:p:516:VAL:O	2.31	0.43
1:q:488:VAL:HG23	1:q:505:MET:HB3	2.01	0.43
1:t:506:MET:HE3	1:t:506:MET:HB2	1.92	0.43
1:y:416:PRO:HB2	1:y:418:VAL:HG23	2.00	0.43
1:z:304:GLU:OE1	1:z:503:ASN:ND2	2.50	0.43
1:A:199:SER:OG	1:A:200:ASP:N	2.52	0.43
1:A:509:ARG:NH1	1:b:314:ASP:OD1	2.51	0.43
1:c:292:ARG:NH1	1:d:319:TYR:OH	2.51	0.43
1:e:185:ASP:OD2	1:e:279:GLN:NE2	2.51	0.43
1:h:464:LEU:HB2	1:h:522:ILE:HB	2.01	0.43
1:k:464:LEU:HG	1:k:524:ILE:HD11	2.01	0.43
1:k:476:LYS:H	1:l:95:LEU:HD22	1.82	0.43
1:m:192:LYS:HB3	1:m:220:LYS:HG2	2.01	0.43
1:o:379:GLU:HB3	1:p:373:HIS:HE1	1.83	0.43
1:w:382:ARG:HB3	1:x:420:TRP:CE2	2.54	0.43
2:P:286:LYS:HG3	2:P:288:ILE:HG12	2.01	0.43
1:A:121:PRO:HB2	1:A:290:LEU:HD11	2.00	0.43
1:c:382:ARG:NH2	1:c:416:PRO:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:504:MET:HE3	1:c:504:MET:HB3	1.91	0.43
1:e:500:ASN:HA	1:g:494:LEU:HB2	2.00	0.43
1:g:388:THR:HG22	1:g:392:MET:HE3	2.00	0.43
1:h:444:ALA:HB3	1:h:451:TYR:HB2	2.00	0.43
1:k:426:ASP:N	1:k:426:ASP:OD1	2.52	0.43
1:m:409:PRO:HG2	1:r:394:ASN:HD21	1.83	0.43
1:o:119:THR:HG23	1:p:88:ALA:HB1	1.99	0.43
1:q:312:ILE:HG22	1:q:323:GLY:HA3	2.01	0.43
1:s:278:GLU:HB2	1:t:299:THR:HG21	2.00	0.43
1:v:302:HIS:ND1	1:v:507:THR:OG1	2.42	0.43
1:v:405:ILE:HD13	1:v:453:ILE:HG22	2.00	0.43
1:x:219:VAL:HG21	1:x:247:LEU:HD12	2.00	0.43
1:x:464:LEU:HD23	1:x:464:LEU:HA	1.91	0.43
2:P:135:GLU:HG3	2:P:172:LYS:HG2	2.00	0.43
2:R:11:LEU:HD13	2:R:17:ILE:HD12	2.00	0.43
2:R:79:ILE:HG23	2:R:125:LEU:HB2	1.99	0.43
2:S:11:LEU:HD13	2:S:17:ILE:HD12	2.00	0.43
2:S:135:GLU:HG3	2:S:172:LYS:HG2	2.00	0.43
1:a:394:ASN:HD21	1:b:409:PRO:HG2	1.83	0.43
1:b:504:MET:HE3	1:b:504:MET:HB2	1.81	0.43
1:c:297:ILE:HD13	1:c:483:TYR:HB2	2.01	0.43
1:i:476:LYS:HD3	1:i:479:MET:HE2	2.01	0.43
1:n:312:ILE:HD12	1:n:323:GLY:HA3	2.00	0.43
1:o:411:ASP:OD1	1:o:527:ASN:ND2	2.51	0.43
1:r:143:ASN:CG	2:Q:19:PHE:CG	2.92	0.43
1:x:304:GLU:OE1	1:x:495:ASN:ND2	2.51	0.43
1:x:407:GLY:HA3	1:x:464:LEU:HD23	2.00	0.43
1:y:127:VAL:HG13	1:y:137:LEU:HD13	2.01	0.43
1:z:247:LEU:HD23	1:z:247:LEU:HA	1.89	0.43
1:z:367:HIS:ND1	1:z:369:ASP:OD1	2.51	0.43
1:a:122:ILE:HG22	1:b:95:LEU:HD12	2.00	0.43
1:a:460:ARG:HH21	1:f:143:ASN:HB2	1.82	0.43
1:a:486:ASN:OD1	1:a:486:ASN:N	2.50	0.43
1:a:516:VAL:HA	1:a:517:PRO:HD3	1.91	0.43
1:b:165:VAL:HG22	1:b:260:THR:H	1.83	0.43
1:c:189:ARG:NH1	1:c:253:SER:OG	2.52	0.43
1:g:197:LYS:HB2	1:g:211:PHE:HA	2.01	0.43
1:j:500:ASN:OD1	1:w:181:ARG:NH1	2.46	0.43
1:m:282:SER:O	1:n:301:GLN:NE2	2.51	0.43
1:n:465:THR:OG1	1:n:521:ARG:NH1	2.51	0.43
1:p:521:ARG:HE	1:p:521:ARG:HB2	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:306:THR:HG23	1:q:501:VAL:HG21	2.00	0.43
1:v:175:LYS:HB3	1:v:178:LYS:HZ1	1.83	0.43
1:w:181:ARG:HB3	1:w:184:ILE:HD12	2.00	0.43
1:w:235:THR:HG1	1:w:243:THR:HG1	1.61	0.43
2:P:10:LYS:HE3	2:P:10:LYS:HB2	1.87	0.43
1:h:247:LEU:HD23	1:h:262:ALA:HB2	2.01	0.43
1:k:303:ILE:HD11	1:k:335:SER:HB2	2.01	0.43
1:l:371:SER:O	1:l:371:SER:OG	2.37	0.43
1:n:121:PRO:HG2	1:o:94:ILE:HA	2.00	0.43
1:o:405:ILE:HD12	1:o:453:ILE:HD12	2.00	0.43
1:r:197:LYS:O	1:r:267:THR:OG1	2.34	0.43
1:u:371:SER:O	1:u:371:SER:OG	2.31	0.43
1:y:383:GLU:HA	1:y:386:ASP:HB2	2.00	0.43
1:b:297:ILE:HG21	1:b:483:TYR:HB2	2.01	0.43
1:n:404:VAL:HG12	1:n:452:ARG:HB3	2.00	0.43
1:q:398:LEU:HG	1:q:401:VAL:HG22	2.01	0.43
1:w:130:ALA:O	1:w:178:LYS:NZ	2.52	0.43
2:R:135:GLU:HG3	2:R:172:LYS:HG2	2.00	0.43
1:h:126:TYR:HE1	1:h:289:GLY:HA3	1.84	0.42
1:p:98:LEU:HD23	1:p:98:LEU:HA	1.91	0.42
1:p:169:ASP:OD1	1:p:169:ASP:N	2.41	0.42
1:p:252:VAL:HG22	1:p:255:GLY:H	1.84	0.42
1:q:297:ILE:O	1:q:509:ARG:NH2	2.51	0.42
1:r:433:SER:HA	1:r:436:ILE:HD13	2.01	0.42
1:s:277:SER:O	1:t:302:HIS:NE2	2.43	0.42
1:s:496:THR:HG21	1:x:282:SER:HA	2.01	0.42
1:t:197:LYS:HB3	1:t:268:ASP:HB2	1.99	0.42
1:v:369:ASP:OD2	2:R:63:ASP:HB3	2.19	0.42
1:w:294:ASP:OD2	1:w:294:ASP:N	2.44	0.42
1:x:109:PRO:HD3	1:x:469:ILE:HD12	2.01	0.42
2:P:61:LYS:HB3	2:P:82:PRO:HB2	2.01	0.42
2:Q:286:LYS:HG3	2:Q:288:ILE:HG12	2.01	0.42
1:i:200:ASP:N	1:i:200:ASP:OD1	2.52	0.42
1:i:457:ASP:OD1	1:i:457:ASP:N	2.39	0.42
1:l:202:PHE:HD2	1:l:204:GLU:HG2	1.84	0.42
1:m:301:GLN:NE2	1:r:150:GLY:O	2.52	0.42
1:q:110:THR:HG22	1:q:480:PHE:HB3	2.01	0.42
1:t:385:ILE:HD12	1:t:405:ILE:HD13	2.01	0.42
1:u:98:LEU:HD23	1:u:98:LEU:HA	1.85	0.42
2:Q:10:LYS:HE3	2:Q:10:LYS:HB2	1.87	0.42
1:d:160:VAL:HG13	1:d:165:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:461:GLN:HE22	1:h:527:ASN:HB3	1.84	0.42
1:i:186:ARG:NH1	1:i:187:LEU:O	2.51	0.42
1:i:252:VAL:HG22	1:i:255:GLY:H	1.84	0.42
1:m:303:ILE:HD11	1:m:335:SER:HB2	2.00	0.42
1:p:197:LYS:O	1:p:267:THR:OG1	2.38	0.42
1:q:147:THR:HG21	2:P:253:GLU:CB	2.39	0.42
1:r:359:HIS:ND1	2:P:265:ASP:OD1	2.52	0.42
1:s:474:ASN:HB3	1:t:96:VAL:HG22	2.01	0.42
1:v:388:THR:O	1:v:392:MET:N	2.51	0.42
1:y:137:LEU:HG	1:z:99:TRP:HH2	1.83	0.42
1:a:412:VAL:HG13	1:a:453:ILE:HD12	2.02	0.42
1:b:444:ALA:HB3	1:b:451:TYR:HB2	2.02	0.42
1:d:470:PRO:HD3	1:d:477:THR:HG22	2.01	0.42
1:m:121:PRO:HG2	1:n:94:ILE:HA	2.01	0.42
1:n:205:ARG:CD	2:Q:188:GLN:HE22	2.22	0.42
1:q:137:LEU:HD21	1:r:334:LEU:HD13	2.01	0.42
1:q:193:ILE:HA	1:q:271:VAL:HA	2.01	0.42
1:s:484:THR:HG22	1:s:509:ARG:HB2	2.01	0.42
1:x:192:LYS:HB3	1:x:192:LYS:HE2	1.91	0.42
1:y:188:ASP:HB3	1:y:276:ALA:HB2	2.02	0.42
2:Q:11:LEU:HD13	2:Q:17:ILE:HD12	2.00	0.42
2:R:243:ASN:OD1	2:R:243:ASN:N	2.52	0.42
1:b:280:HIS:NE2	1:c:304:GLU:OE2	2.39	0.42
1:c:444:ALA:HB3	1:c:451:TYR:HB2	2.01	0.42
1:d:488:VAL:HB	1:d:505:MET:HB3	2.01	0.42
1:f:406:VAL:O	1:f:465:THR:OG1	2.34	0.42
1:g:506:MET:HE3	1:g:506:MET:HB3	1.86	0.42
1:i:398:LEU:HD11	1:i:518:ILE:HD13	2.01	0.42
1:j:200:ASP:OD1	1:j:200:ASP:N	2.52	0.42
1:o:205:ARG:HH12	1:p:352:LYS:NZ	2.18	0.42
1:z:193:ILE:HG22	1:z:271:VAL:HG12	2.01	0.42
2:Q:243:ASN:OD1	2:Q:243:ASN:N	2.52	0.42
1:A:335:SER:HB3	1:A:506:MET:HE1	2.02	0.42
1:b:369:ASP:OD1	1:b:369:ASP:N	2.51	0.42
1:c:138:PRO:HG2	1:d:97:LYS:HB3	2.01	0.42
1:c:181:ARG:NH2	1:h:498:ASN:OD1	2.52	0.42
1:i:531:VAL:O	1:i:534:ARG:NE	2.45	0.42
1:j:310:GLU:HG3	1:x:299:THR:HG21	2.01	0.42
1:l:378:LEU:HB2	1:l:417:ASN:HD21	1.83	0.42
1:p:109:PRO:HB3	1:q:427:ARG:HH22	1.83	0.42
1:p:426:ASP:OD2	1:p:429:ALA:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:130:ALA:HA	1:u:497:ARG:HH12	1.83	0.42
1:x:170:LEU:HD23	1:x:170:LEU:HA	1.84	0.42
1:x:498:ASN:HD21	1:y:279:GLN:HB3	1.84	0.42
1:a:297:ILE:HG21	1:a:483:TYR:HB2	2.02	0.42
1:d:170:LEU:HD11	1:d:258:THR:HB	2.02	0.42
1:d:327:LEU:HD23	1:d:327:LEU:HA	1.94	0.42
1:h:305:ALA:HB1	1:h:327:LEU:HD13	2.02	0.42
1:m:250:VAL:HG13	1:m:259:LEU:HD13	2.02	0.42
1:n:338:LYS:HA	1:n:338:LYS:HD2	1.88	0.42
1:o:303:ILE:HG22	1:o:331:MET:HG2	2.01	0.42
1:o:359:HIS:ND1	2:Q:264:GLN:NE2	2.53	0.42
1:p:301:GLN:HE21	1:p:302:HIS:H	1.68	0.42
1:p:367:HIS:HD2	2:P:64:ARG:NH2	2.17	0.42
1:p:498:ASN:HB3	1:p:501:VAL:HG22	2.01	0.42
1:r:464:LEU:HB2	1:r:522:ILE:HB	2.01	0.42
1:u:143:ASN:ND2	2:R:19:PHE:CD2	2.88	0.42
1:u:394:ASN:ND2	1:v:408:ASN:OD1	2.50	0.42
1:v:410:LEU:HD23	1:v:461:GLN:HG3	2.02	0.42
1:w:127:VAL:HG13	1:w:137:LEU:HD13	2.01	0.42
2:Q:135:GLU:HG3	2:Q:172:LYS:HG2	2.00	0.42
1:a:221:LEU:HD23	1:a:221:LEU:HA	1.92	0.42
1:c:528:ASN:OD1	1:c:528:ASN:N	2.52	0.42
1:f:407:GLY:HA3	1:f:464:LEU:HD23	2.02	0.42
1:i:164:LYS:HA	1:i:260:THR:HG23	2.02	0.42
1:m:485:PHE:HD1	1:m:508:ARG:HB2	1.85	0.42
1:p:81:MET:HB3	1:p:82:GLY:H	1.65	0.42
1:r:200:ASP:HB2	1:r:235:THR:HG23	2.02	0.42
1:t:147:THR:HG21	2:S:253:GLU:HB2	2.01	0.42
1:t:220:LYS:HB3	1:t:220:LYS:HE2	1.86	0.42
1:w:297:ILE:HG21	1:w:483:TYR:HB2	2.02	0.42
1:y:112:VAL:HA	1:y:482:PRO:HD2	2.02	0.42
1:A:404:VAL:HG23	1:A:467:ILE:HB	2.01	0.42
1:a:193:ILE:HG12	1:a:219:VAL:HB	2.00	0.42
1:c:406:VAL:O	1:c:465:THR:OG1	2.36	0.42
1:f:205:ARG:HH12	1:f:213:GLU:HG3	1.85	0.42
1:j:170:LEU:HD23	1:j:170:LEU:HA	1.90	0.42
1:l:350:GLU:HG3	1:l:478:PHE:HE1	1.84	0.42
1:n:165:VAL:H	1:n:260:THR:HG23	1.84	0.42
1:o:444:ALA:HB3	1:o:451:TYR:HB2	2.02	0.42
1:q:249:LYS:HA	1:q:260:THR:HA	2.00	0.42
1:s:385:ILE:HD13	1:s:405:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:119:THR:N	1:v:89:SER:O	2.50	0.42
1:y:445:ALA:N	1:z:421:THR:O	2.53	0.42
2:S:286:LYS:HG3	2:S:288:ILE:HG12	2.01	0.42
1:a:477:THR:OG1	1:a:516:VAL:O	2.32	0.42
1:b:485:PHE:HB2	1:b:508:ARG:HG3	2.00	0.42
1:e:85:GLN:O	1:h:319:TYR:OH	2.34	0.42
1:e:159:ALA:HA	1:e:268:ASP:HB3	2.02	0.42
1:e:249:LYS:HG3	1:e:260:THR:HA	2.01	0.42
1:e:464:LEU:HD23	1:e:464:LEU:HA	1.92	0.42
1:m:179:GLU:HA	1:m:282:SER:HB2	2.01	0.42
1:s:134:LYS:O	1:s:135:HIS:ND1	2.53	0.42
1:v:352:LYS:HD2	1:v:352:LYS:HA	1.93	0.42
1:w:416:PRO:HB2	1:w:418:VAL:HG23	2.01	0.42
2:P:179:PHE:HD1	2:P:222:LEU:HD22	1.85	0.42
2:Q:242:LYS:HD2	2:Q:242:LYS:HA	1.91	0.42
2:R:10:LYS:HE3	2:R:10:LYS:HB2	1.86	0.42
1:b:386:ASP:OD2	1:c:420:TRP:NE1	2.53	0.41
1:h:433:SER:O	1:h:433:SER:OG	2.37	0.41
1:j:225:ASP:OD2	1:j:253:SER:OG	2.37	0.41
1:l:464:LEU:HD23	1:l:464:LEU:HA	1.93	0.41
1:n:286:VAL:HG23	1:o:327:LEU:HD22	2.02	0.41
1:o:322:ASP:HB3	1:o:325:ALA:HB3	2.01	0.41
1:p:366:PRO:O	2:P:59:LYS:NZ	2.53	0.41
1:q:464:LEU:HD23	1:q:464:LEU:HA	1.95	0.41
1:s:368:SER:HA	1:x:369:ASP:OD2	2.20	0.41
1:t:121:PRO:HA	1:t:292:ARG:HA	2.02	0.41
1:v:321:ILE:HD13	1:v:321:ILE:HA	1.89	0.41
1:y:128:VAL:HG23	1:y:130:ALA:H	1.85	0.41
1:z:440:TYR:O	1:z:455:GLY:N	2.48	0.41
1:A:506:MET:HE3	1:A:506:MET:HB3	1.79	0.41
1:b:378:LEU:HB3	1:b:417:ASN:HD21	1.85	0.41
1:d:357:LYS:NZ	1:d:396:TYR:OH	2.52	0.41
1:e:485:PHE:CE1	1:e:506:MET:HE3	2.54	0.41
1:n:221:LEU:HD22	1:n:227:LEU:HD13	2.03	0.41
1:n:249:LYS:HB2	1:n:249:LYS:HE3	1.77	0.41
1:q:126:TYR:HB3	1:q:134:LYS:HB2	2.01	0.41
1:u:428:ASN:OD1	1:u:428:ASN:N	2.53	0.41
1:y:409:PRO:HA	1:y:412:VAL:HB	2.02	0.41
1:z:170:LEU:HD23	1:z:170:LEU:HA	1.93	0.41
2:Q:179:PHE:HD1	2:Q:222:LEU:HD22	1.85	0.41
1:a:469:ILE:HA	1:a:470:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:495:ASN:HB2	1:c:503:ASN:HD21	1.85	0.41
1:d:426:ASP:OD1	1:d:429:ALA:N	2.51	0.41
1:l:305:ALA:HB1	1:l:327:LEU:HD13	2.02	0.41
1:m:122:ILE:N	1:m:291:THR:O	2.48	0.41
1:r:464:LEU:HD23	1:r:464:LEU:HA	1.92	0.41
1:s:367:HIS:HE1	2:S:64:ARG:CG	2.32	0.41
1:s:398:LEU:HG	1:s:401:VAL:HG13	2.02	0.41
1:v:195:GLU:HB3	1:v:270:LYS:HB2	2.02	0.41
1:y:119:THR:HG23	1:z:88:ALA:HB1	2.02	0.41
1:y:464:LEU:HD23	1:y:464:LEU:HA	1.91	0.41
2:R:286:LYS:HG3	2:R:288:ILE:HG12	2.01	0.41
1:e:297:ILE:O	1:e:509:ARG:NH2	2.53	0.41
1:g:146:GLU:OE2	1:g:148:LEU:N	2.50	0.41
1:j:530:SER:O	1:j:530:SER:OG	2.34	0.41
1:m:365:PHE:CD1	1:m:531:VAL:HG12	2.56	0.41
1:n:428:ASN:OD1	1:n:428:ASN:N	2.50	0.41
1:p:155:LYS:HD3	1:p:155:LYS:HA	1.84	0.41
1:p:193:ILE:HD13	1:p:269:VAL:HG21	2.02	0.41
1:q:134:LYS:HE2	1:q:134:LYS:HB3	1.86	0.41
1:v:463:GLU:OE1	2:R:158:HIS:CG	2.73	0.41
1:d:156:GLU:HG3	1:d:270:LYS:HG3	2.01	0.41
1:m:230:GLN:NE2	1:m:244:ASP:OD1	2.45	0.41
1:o:506:MET:HE3	1:o:506:MET:HB3	1.78	0.41
1:p:238:ASP:OD2	2:P:244:ARG:HD2	2.16	0.41
1:u:280:HIS:NE2	1:v:505:MET:SD	2.76	0.41
1:v:193:ILE:HA	1:v:271:VAL:HA	2.01	0.41
1:w:212:VAL:HG21	1:w:233:TYR:HB2	2.02	0.41
1:z:232:LYS:HE2	1:z:232:LYS:HB3	1.92	0.41
1:a:109:PRO:HD3	1:a:469:ILE:HG12	2.02	0.41
1:a:420:TRP:CE2	1:f:382:ARG:HB3	2.55	0.41
1:a:484:THR:HG22	1:a:509:ARG:HB2	2.03	0.41
1:f:357:LYS:HE2	1:f:357:LYS:HB3	1.85	0.41
1:j:226:THR:HA	1:j:250:VAL:HA	2.02	0.41
1:k:322:ASP:OD1	1:k:322:ASP:N	2.53	0.41
1:l:233:TYR:HA	1:l:234:PRO:HD3	1.96	0.41
1:m:235:THR:HB	1:m:241:VAL:HB	2.02	0.41
1:o:181:ARG:HE	1:o:184:ILE:HG21	1.84	0.41
1:q:398:LEU:HD21	1:q:470:PRO:HB3	2.02	0.41
1:v:98:LEU:HA	1:v:98:LEU:HD23	1.81	0.41
1:x:158:ILE:HB	1:x:269:VAL:HG12	2.01	0.41
1:x:197:LYS:HB2	1:x:211:PHE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:382:ARG:H	1:z:382:ARG:HG3	1.70	0.41
2:P:243:ASN:OD1	2:P:243:ASN:N	2.52	0.41
2:S:61:LYS:HB3	2:S:82:PRO:HB2	2.01	0.41
1:A:331:MET:HE2	1:A:504:MET:HE3	2.03	0.41
1:c:266:LEU:HD23	1:c:266:LEU:HA	1.92	0.41
1:d:342:ASP:OD2	1:d:510:TYR:OH	2.39	0.41
1:j:182:LYS:HE3	1:j:182:LYS:HB2	1.88	0.41
1:j:495:ASN:OD1	1:j:496:THR:N	2.52	0.41
1:k:165:VAL:O	1:k:260:THR:N	2.53	0.41
1:l:504:MET:HE2	1:l:504:MET:HB3	1.98	0.41
1:n:359:HIS:NE2	1:n:523:THR:OG1	2.43	0.41
1:p:442:LEU:HD12	1:p:442:LEU:HA	1.91	0.41
1:v:187:LEU:HD13	1:v:256:GLU:HG2	2.02	0.41
1:y:505:MET:HE2	1:y:505:MET:HB3	1.91	0.41
1:c:350:GLU:HG2	1:c:478:PHE:HE1	1.85	0.41
1:g:178:LYS:O	1:g:282:SER:OG	2.34	0.41
1:g:195:GLU:HB3	1:g:211:PHE:HB3	2.03	0.41
1:h:137:LEU:HD11	1:i:334:LEU:HD13	2.02	0.41
1:i:250:VAL:HG12	1:i:259:LEU:HB2	2.03	0.41
1:j:167:ASP:HB3	1:j:257:LEU:HD13	2.03	0.41
1:j:198:TRP:HE1	1:j:245:THR:HG21	1.86	0.41
1:k:187:LEU:HD21	1:k:191:PHE:HB2	2.03	0.41
1:l:369:ASP:OD1	1:l:369:ASP:N	2.47	0.41
1:q:390:GLN:OE1	1:r:439:ASN:ND2	2.54	0.41
1:s:293:LYS:HE3	1:s:515:PHE:HA	2.02	0.41
1:s:365:PHE:CE2	2:S:57:THR:HG23	2.55	0.41
1:t:89:SER:OG	1:t:90:LEU:N	2.53	0.41
1:u:327:LEU:HD23	1:u:327:LEU:HA	1.94	0.41
1:v:261:SER:HB3	1:y:261:SER:HB3	2.03	0.41
1:w:516:VAL:HA	1:w:517:PRO:HD3	1.89	0.41
1:x:200:ASP:OD1	1:x:200:ASP:N	2.51	0.41
1:y:121:PRO:HA	1:y:292:ARG:HG2	2.03	0.41
1:y:297:ILE:HD13	1:y:483:TYR:HB2	2.03	0.41
1:y:516:VAL:HA	1:y:517:PRO:HD3	1.89	0.41
1:y:530:SER:O	1:y:530:SER:OG	2.33	0.41
1:A:235:THR:HG21	1:A:239:GLY:N	2.36	0.41
1:A:446:SER:O	1:A:446:SER:OG	2.37	0.41
1:a:278:GLU:HG2	1:b:299:THR:HG21	2.03	0.41
1:a:364:VAL:HG13	1:a:378:LEU:HD21	2.02	0.41
1:a:465:THR:OG1	1:a:521:ARG:NH1	2.54	0.41
1:b:131:ASP:OD1	1:b:131:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:386:ASP:OD1	1:b:451:TYR:OH	2.34	0.41
1:c:364:VAL:HG13	1:c:378:LEU:HD21	2.03	0.41
1:d:316:LYS:HA	1:d:316:LYS:HD3	1.87	0.41
1:e:138:PRO:O	1:e:142:ASN:ND2	2.54	0.41
1:e:211:PHE:HE1	1:e:270:LYS:HB2	1.86	0.41
1:e:272:LYS:NZ	1:e:274:TYR:OH	2.53	0.41
1:e:319:TYR:OH	1:h:85:GLN:O	2.35	0.41
1:f:404:VAL:HG12	1:f:452:ARG:HB3	2.02	0.41
1:g:181:ARG:HB3	1:g:184:ILE:HD12	2.03	0.41
1:g:452:ARG:HE	1:h:427:ARG:HE	1.69	0.41
1:j:378:LEU:HB3	1:j:417:ASN:HD21	1.86	0.41
1:k:294:ASP:OD2	1:k:294:ASP:N	2.49	0.41
1:k:442:LEU:HD23	1:k:453:ILE:HD11	2.02	0.41
1:l:205:ARG:HE	1:l:205:ARG:HB2	1.68	0.41
1:m:221:LEU:HD12	1:m:221:LEU:HA	1.95	0.41
1:m:348:ASP:OD2	2:Q:156:GLU:HB2	2.18	0.41
1:n:137:LEU:HD11	1:o:334:LEU:HD13	2.01	0.41
1:n:401:VAL:O	1:o:433:SER:OG	2.33	0.41
1:o:185:ASP:OD1	1:o:185:ASP:N	2.52	0.41
1:q:443:GLY:N	1:r:425:GLY:H	2.19	0.41
1:q:454:ILE:HD13	1:q:454:ILE:HA	1.96	0.41
1:r:268:ASP:OD2	1:r:268:ASP:N	2.53	0.41
1:r:485:PHE:HD1	1:r:508:ARG:HB2	1.85	0.41
1:r:516:VAL:HA	1:r:517:PRO:HD3	1.91	0.41
1:s:240:GLU:OE1	2:S:246:LEU:HA	2.21	0.41
1:s:240:GLU:CG	2:S:246:LEU:CD1	2.98	0.41
1:s:366:PRO:O	2:S:59:LYS:NZ	2.54	0.41
1:s:420:TRP:CE2	1:x:382:ARG:HB3	2.56	0.41
1:w:223:ASP:OD1	1:w:223:ASP:N	2.53	0.41
1:x:308:PRO:HG3	1:x:501:VAL:HG11	2.03	0.41
1:z:249:LYS:HD2	1:z:260:THR:HA	2.03	0.41
2:R:61:LYS:HB3	2:R:82:PRO:HB2	2.02	0.41
2:S:243:ASN:OD1	2:S:243:ASN:N	2.52	0.41
1:A:99:TRP:CD1	1:A:101:ARG:HG2	2.56	0.41
1:A:290:LEU:HB3	1:b:84:ILE:HA	2.02	0.41
1:b:386:ASP:OD1	1:b:448:THR:OG1	2.39	0.41
1:c:141:ILE:O	1:d:337:GLN:NE2	2.54	0.41
1:c:464:LEU:HD23	1:c:464:LEU:HA	1.91	0.41
1:g:252:VAL:HG22	1:g:255:GLY:H	1.85	0.41
1:h:251:ASP:OD1	1:h:251:ASP:N	2.53	0.41
1:k:190:LYS:HE3	1:k:190:LYS:HB3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:174:LEU:HD23	1:l:174:LEU:HA	1.96	0.41
1:l:219:VAL:HG12	1:l:227:LEU:HB3	2.03	0.41
1:o:279:GLN:HB3	1:t:498:ASN:HD21	1.86	0.41
1:p:119:THR:N	1:q:89:SER:O	2.52	0.41
1:p:402:GLN:NE2	1:q:431:ALA:O	2.54	0.41
1:u:473:ASP:OD1	1:u:473:ASP:N	2.50	0.41
1:x:193:ILE:HB	1:x:219:VAL:HB	2.02	0.41
1:z:277:SER:O	1:z:277:SER:OG	2.38	0.41
2:R:5:ASN:HA	2:R:35:SER:HB3	2.03	0.41
1:a:238:ASP:OD2	1:a:238:ASP:N	2.45	0.40
1:d:104:LEU:HD12	1:d:340:ASP:HB3	2.02	0.40
1:g:198:TRP:HE1	1:g:245:THR:HG21	1.85	0.40
1:h:131:ASP:OD1	1:h:131:ASP:N	2.53	0.40
1:j:89:SER:OG	1:j:90:LEU:N	2.55	0.40
1:j:119:THR:HG22	1:j:294:ASP:HA	2.03	0.40
1:j:400:ASP:OD1	1:j:400:ASP:N	2.54	0.40
1:k:388:THR:HG21	1:k:522:ILE:HD11	2.04	0.40
1:m:297:ILE:HD13	1:m:483:TYR:HB2	2.02	0.40
1:m:332:SER:HA	1:m:506:MET:HE1	2.03	0.40
1:n:410:LEU:HD12	1:n:461:GLN:HG3	2.03	0.40
1:q:477:THR:HG22	1:q:516:VAL:HG13	2.03	0.40
1:t:237:GLY:H	1:t:240:GLU:HB3	1.85	0.40
1:u:516:VAL:HA	1:u:517:PRO:HD3	1.84	0.40
1:x:165:VAL:CG2	1:x:260:THR:HG22	2.51	0.40
1:x:266:LEU:HD23	1:x:266:LEU:HA	1.94	0.40
2:P:5:ASN:HA	2:P:35:SER:HB3	2.03	0.40
2:Q:61:LYS:HB3	2:Q:82:PRO:HB2	2.01	0.40
1:g:170:LEU:HA	1:g:170:LEU:HD23	1.87	0.40
1:g:370:TYR:CZ	1:g:372:ALA:HB3	2.55	0.40
1:h:137:LEU:HG	1:i:99:TRP:HH2	1.86	0.40
1:i:178:LYS:O	1:i:282:SER:OG	2.36	0.40
1:k:236:ASN:OD1	1:k:236:ASN:N	2.54	0.40
1:m:282:SER:O	1:m:282:SER:OG	2.34	0.40
1:p:195:GLU:HB2	1:p:270:LYS:HB3	2.03	0.40
1:p:348:ASP:OD2	2:P:156:GLU:CB	2.69	0.40
1:q:240:GLU:O	2:Q:12:LEU:HD11	2.21	0.40
1:q:385:ILE:O	1:q:389:THR:OG1	2.27	0.40
1:q:416:PRO:HB2	1:q:418:VAL:HG23	2.04	0.40
1:v:328:SER:HA	1:v:331:MET:HE2	2.02	0.40
1:z:175:LYS:HE2	1:z:175:LYS:HB2	1.94	0.40
1:z:181:ARG:HB3	1:z:184:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:236:ASN:HB3	1:z:239:GLY:H	1.86	0.40
2:P:55:PRO:HD3	2:P:88:VAL:HG11	2.03	0.40
2:R:179:PHE:HD1	2:R:222:LEU:HD22	1.85	0.40
1:A:249:LYS:HZ1	1:A:261:SER:H	1.69	0.40
1:a:124:THR:HA	1:a:125:PRO:HD3	1.97	0.40
1:a:334:LEU:HD13	1:f:137:LEU:HD11	2.03	0.40
1:a:352:LYS:HE3	1:a:352:LYS:HB3	1.90	0.40
1:c:342:ASP:O	1:c:346:PHE:N	2.46	0.40
1:d:198:TRP:CD1	1:d:266:LEU:H	2.39	0.40
1:l:138:PRO:O	1:l:142:ASN:ND2	2.54	0.40
1:l:442:LEU:HB3	1:l:453:ILE:HD11	2.03	0.40
1:o:521:ARG:HD3	1:o:521:ARG:HA	1.92	0.40
1:q:226:THR:HA	1:q:250:VAL:HA	2.03	0.40
1:r:89:SER:OG	1:r:90:LEU:N	2.54	0.40
1:r:124:THR:HA	1:r:125:PRO:HD3	1.87	0.40
1:s:189:ARG:HG3	1:s:221:LEU:HD23	2.03	0.40
1:s:240:GLU:OE2	2:S:197:ALA:HB2	2.22	0.40
1:s:285:ASN:ND2	1:t:304:GLU:OE2	2.54	0.40
1:t:82:GLY:O	1:x:189:ARG:NH2	2.53	0.40
1:t:119:THR:HG22	1:t:294:ASP:HA	2.03	0.40
1:v:94:ILE:HD13	1:v:321:ILE:HD11	2.03	0.40
2:P:174:LYS:HE2	2:P:174:LYS:HB3	1.92	0.40
1:A:373:HIS:HD2	1:A:375:LYS:HB2	1.87	0.40
1:b:159:ALA:HA	1:b:268:ASP:HB3	2.03	0.40
1:b:198:TRP:HE1	1:b:245:THR:HG21	1.87	0.40
1:c:302:HIS:ND1	1:c:507:THR:OG1	2.38	0.40
1:e:394:ASN:ND2	1:f:408:ASN:OD1	2.54	0.40
1:f:430:ASP:OD2	1:f:431:ALA:N	2.55	0.40
1:g:146:GLU:HG2	1:h:338:LYS:HE2	2.02	0.40
1:g:175:LYS:N	1:g:179:GLU:OE2	2.51	0.40
1:g:367:HIS:ND1	1:g:369:ASP:OD1	2.55	0.40
1:g:371:SER:OG	1:l:371:SER:OG	2.27	0.40
1:m:246:ILE:HG22	1:m:263:SER:HB3	2.03	0.40
1:p:464:LEU:HD12	1:p:464:LEU:HA	1.91	0.40
1:q:297:ILE:HG21	1:q:483:TYR:HB2	2.03	0.40
1:s:423:ASN:OD1	1:s:423:ASN:N	2.53	0.40
1:t:418:VAL:HG11	1:t:438:ILE:HD11	2.03	0.40
2:S:179:PHE:HD1	2:S:222:LEU:HD22	1.85	0.40
1:a:404:VAL:HG12	1:a:452:ARG:HB3	2.03	0.40
1:g:386:ASP:OD2	1:h:420:TRP:NE1	2.49	0.40
1:i:390:GLN:HB3	1:j:410:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:133:ASN:OD1	1:k:133:ASN:N	2.54	0.40
1:l:189:ARG:NH1	1:l:225:ASP:OD1	2.55	0.40
1:m:348:ASP:OD2	2:Q:156:GLU:CA	2.70	0.40
1:m:480:PHE:HD1	1:m:512:VAL:HG12	1.87	0.40
1:n:249:LYS:HG3	1:n:260:THR:HA	2.02	0.40
1:o:236:ASN:HB3	1:o:240:GLU:H	1.87	0.40
1:o:446:SER:OG	1:o:447:GLY:N	2.53	0.40
1:p:131:ASP:N	1:p:131:ASP:OD1	2.52	0.40
1:u:394:ASN:O	1:u:397:LYS:NZ	2.51	0.40
1:v:178:LYS:O	1:v:282:SER:OG	2.31	0.40
1:w:369:ASP:OD1	1:w:369:ASP:N	2.40	0.40
1:w:437:LYS:HB2	1:w:437:LYS:HE3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/534 (80%)	394 (92%)	36 (8%)	0	100	100
1	a	440/534 (82%)	404 (92%)	36 (8%)	0	100	100
1	b	452/534 (85%)	409 (90%)	43 (10%)	0	100	100
1	c	452/534 (85%)	422 (93%)	30 (7%)	0	100	100
1	d	452/534 (85%)	420 (93%)	32 (7%)	0	100	100
1	e	452/534 (85%)	421 (93%)	31 (7%)	0	100	100
1	f	452/534 (85%)	421 (93%)	31 (7%)	0	100	100
1	g	452/534 (85%)	418 (92%)	34 (8%)	0	100	100
1	h	452/534 (85%)	413 (91%)	39 (9%)	0	100	100
1	i	452/534 (85%)	417 (92%)	35 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	452/534 (85%)	414 (92%)	38 (8%)	0	100	100
1	k	452/534 (85%)	417 (92%)	35 (8%)	0	100	100
1	l	452/534 (85%)	423 (94%)	29 (6%)	0	100	100
1	m	452/534 (85%)	415 (92%)	37 (8%)	0	100	100
1	n	452/534 (85%)	415 (92%)	37 (8%)	0	100	100
1	o	452/534 (85%)	413 (91%)	39 (9%)	0	100	100
1	p	452/534 (85%)	410 (91%)	42 (9%)	0	100	100
1	q	452/534 (85%)	402 (89%)	50 (11%)	0	100	100
1	r	452/534 (85%)	420 (93%)	32 (7%)	0	100	100
1	s	452/534 (85%)	416 (92%)	36 (8%)	0	100	100
1	t	452/534 (85%)	412 (91%)	40 (9%)	0	100	100
1	u	452/534 (85%)	414 (92%)	38 (8%)	0	100	100
1	v	452/534 (85%)	409 (90%)	43 (10%)	0	100	100
1	w	452/534 (85%)	407 (90%)	45 (10%)	0	100	100
1	x	452/534 (85%)	420 (93%)	32 (7%)	0	100	100
1	y	452/534 (85%)	419 (93%)	33 (7%)	0	100	100
1	z	452/534 (85%)	416 (92%)	36 (8%)	0	100	100
2	P	299/476 (63%)	277 (93%)	22 (7%)	0	100	100
2	Q	299/476 (63%)	277 (93%)	22 (7%)	0	100	100
2	R	299/476 (63%)	277 (93%)	22 (7%)	0	100	100
2	S	299/476 (63%)	277 (93%)	22 (7%)	0	100	100
All	All	13366/16322 (82%)	12289 (92%)	1077 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/461 (82%)	376 (99%)	3 (1%)	73	77
1	a	388/461 (84%)	385 (99%)	3 (1%)	73	77
1	b	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	c	394/461 (86%)	392 (100%)	2 (0%)	81	80
1	d	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	e	394/461 (86%)	392 (100%)	2 (0%)	81	80
1	f	393/461 (85%)	393 (100%)	0	100	100
1	g	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	h	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	i	394/461 (86%)	392 (100%)	2 (0%)	81	80
1	j	394/461 (86%)	392 (100%)	2 (0%)	81	80
1	k	394/461 (86%)	394 (100%)	0	100	100
1	l	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	m	394/461 (86%)	394 (100%)	0	100	100
1	n	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	o	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	p	394/461 (86%)	392 (100%)	2 (0%)	81	80
1	q	393/461 (85%)	391 (100%)	2 (0%)	81	80
1	r	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	s	394/461 (86%)	394 (100%)	0	100	100
1	t	394/461 (86%)	391 (99%)	3 (1%)	73	77
1	u	394/461 (86%)	390 (99%)	4 (1%)	68	75
1	v	394/461 (86%)	394 (100%)	0	100	100
1	w	394/461 (86%)	390 (99%)	4 (1%)	68	75
1	x	394/461 (86%)	394 (100%)	0	100	100
1	y	394/461 (86%)	393 (100%)	1 (0%)	86	83
1	z	394/461 (86%)	393 (100%)	1 (0%)	86	83
2	P	277/434 (64%)	259 (94%)	18 (6%)	15	43
2	Q	277/434 (64%)	259 (94%)	18 (6%)	15	43
2	R	277/434 (64%)	259 (94%)	18 (6%)	15	43
2	S	277/434 (64%)	259 (94%)	18 (6%)	15	43
All	All	11723/14183 (83%)	11612 (99%)	111 (1%)	68	76

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	VAL
1	A	153	GLN
1	A	401	VAL
1	a	214	LEU
1	a	257	LEU
1	a	516	VAL
1	b	297	ILE
1	c	141	ILE
1	c	401	VAL
1	d	127	VAL
1	e	214	LEU
1	e	488	VAL
1	g	401	VAL
1	h	307	VAL
1	i	291	THR
1	i	516	VAL
1	j	127	VAL
1	j	307	VAL
1	l	291	THR
1	n	241	VAL
1	o	401	VAL
1	p	160	VAL
1	p	369	ASP
1	q	124	THR
1	q	401	VAL
1	r	354	THR
1	t	166	THR
1	t	238	ASP
1	t	241	VAL
1	u	144	THR
1	u	307	VAL
1	u	398	LEU
1	u	516	VAL
1	w	193	ILE
1	w	238	ASP
1	w	240	GLU
1	w	241	VAL
1	y	401	VAL
1	z	465	THR
2	P	57	THR
2	P	71	SER
2	P	108	SER

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Mol	Chain	Res	Type
2	P	156	GLU
2	P	165	VAL
2	P	189	ASP
2	P	196	SER
2	P	215	THR
2	P	217	VAL
2	P	219	LYS
2	P	233	GLU
2	P	249	SER
2	P	253	GLU
2	P	267	ILE
2	P	277	GLU
2	P	278	GLU
2	P	287	LYS
2	P	299	LYS
2	Q	57	THR
2	Q	71	SER
2	Q	108	SER
2	Q	156	GLU
2	Q	165	VAL
2	Q	189	ASP
2	Q	196	SER
2	Q	215	THR
2	Q	217	VAL
2	Q	219	LYS
2	Q	233	GLU
2	Q	249	SER
2	Q	253	GLU
2	Q	267	ILE
2	Q	277	GLU
2	Q	278	GLU
2	Q	287	LYS
2	Q	299	LYS
2	R	57	THR
2	R	71	SER
2	R	108	SER
2	R	156	GLU
2	R	165	VAL
2	R	189	ASP
2	R	196	SER
2	R	215	THR
2	R	217	VAL

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Mol	Chain	Res	Type
2	R	219	LYS
2	R	233	GLU
2	R	249	SER
2	R	253	GLU
2	R	267	ILE
2	R	277	GLU
2	R	278	GLU
2	R	287	LYS
2	R	299	LYS
2	S	57	THR
2	S	71	SER
2	S	108	SER
2	S	156	GLU
2	S	165	VAL
2	S	189	ASP
2	S	196	SER
2	S	215	THR
2	S	217	VAL
2	S	219	LYS
2	S	233	GLU
2	S	249	SER
2	S	253	GLU
2	S	267	ILE
2	S	277	GLU
2	S	278	GLU
2	S	287	LYS
2	S	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (217) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	236	ASN
1	A	333	GLN
1	A	373	HIS
1	A	394	ASN
1	A	472	GLN
1	A	489	ASN
1	A	526	ASN
1	A	527	ASN
1	a	133	ASN
1	a	142	ASN

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Mol	Chain	Res	Type
1	a	153	GLN
1	a	222	GLN
1	a	236	ASN
1	a	333	GLN
1	a	439	ASN
1	a	472	GLN
1	b	135	HIS
1	b	279	GLN
1	b	301	GLN
1	b	373	HIS
1	b	434	ASN
1	b	472	GLN
1	b	474	ASN
1	b	500	ASN
1	c	224	ASN
1	c	301	GLN
1	c	423	ASN
1	c	450	ASN
1	c	489	ASN
1	c	503	ASN
1	c	527	ASN
1	d	117	ASN
1	d	222	GLN
1	d	349	HIS
1	d	359	HIS
1	d	402	GLN
1	d	423	ASN
1	d	434	ASN
1	d	439	ASN
1	e	153	GLN
1	e	313	GLN
1	e	471	GLN
1	e	500	ASN
1	f	230	GLN
1	f	236	ASN
1	f	301	GLN
1	f	313	GLN
1	f	373	HIS
1	f	486	ASN
1	g	280	HIS
1	g	285	ASN
1	g	337	GLN

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Mol	Chain	Res	Type
1	g	408	ASN
1	g	434	ASN
1	g	471	GLN
1	g	500	ASN
1	g	528	ASN
1	h	153	GLN
1	h	279	GLN
1	h	302	HIS
1	h	408	ASN
1	h	423	ASN
1	h	439	ASN
1	h	526	ASN
1	i	135	HIS
1	i	285	ASN
1	i	301	GLN
1	i	367	HIS
1	i	402	GLN
1	i	495	ASN
1	i	526	ASN
1	j	117	ASN
1	j	402	GLN
1	j	428	ASN
1	j	486	ASN
1	j	528	ASN
1	k	85	GLN
1	k	117	ASN
1	k	153	GLN
1	k	224	ASN
1	k	402	GLN
1	k	439	ASN
1	k	486	ASN
1	l	142	ASN
1	l	390	GLN
1	l	495	ASN
1	l	500	ASN
1	m	117	ASN
1	m	390	GLN
1	m	417	ASN
1	m	489	ASN
1	m	503	ASN
1	n	85	GLN
1	n	143	ASN

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Mol	Chain	Res	Type
1	n	224	ASN
1	n	280	HIS
1	n	285	ASN
1	n	373	HIS
1	n	390	GLN
1	n	402	GLN
1	n	417	ASN
1	n	439	ASN
1	n	471	GLN
1	n	498	ASN
1	o	390	GLN
1	o	472	GLN
1	o	526	ASN
1	o	528	ASN
1	p	117	ASN
1	p	236	ASN
1	p	279	GLN
1	p	280	HIS
1	p	373	HIS
1	p	390	GLN
1	p	402	GLN
1	p	417	ASN
1	p	423	ASN
1	p	439	ASN
1	p	489	ASN
1	q	133	ASN
1	q	143	ASN
1	q	279	GLN
1	q	285	ASN
1	q	313	GLN
1	q	337	GLN
1	q	417	ASN
1	q	486	ASN
1	q	498	ASN
1	q	526	ASN
1	r	135	HIS
1	r	222	GLN
1	r	224	ASN
1	r	279	GLN
1	r	285	ASN
1	r	394	ASN
1	r	402	GLN

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Mol	Chain	Res	Type
1	r	428	ASN
1	s	230	GLN
1	s	301	GLN
1	s	367	HIS
1	s	373	HIS
1	s	387	HIS
1	s	402	GLN
1	s	471	GLN
1	s	486	ASN
1	s	503	ASN
1	t	143	ASN
1	t	230	GLN
1	t	236	ASN
1	t	301	GLN
1	t	359	HIS
1	t	394	ASN
1	t	417	ASN
1	t	472	GLN
1	t	526	ASN
1	u	135	HIS
1	u	143	ASN
1	u	301	GLN
1	u	423	ASN
1	u	526	ASN
1	v	301	GLN
1	v	367	HIS
1	v	373	HIS
1	v	390	GLN
1	v	423	ASN
1	v	472	GLN
1	v	500	ASN
1	v	526	ASN
1	w	117	ASN
1	w	143	ASN
1	w	222	GLN
1	w	230	GLN
1	w	359	HIS
1	w	402	GLN
1	w	434	ASN
1	w	439	ASN
1	w	474	ASN
1	w	498	ASN

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Mol	Chain	Res	Type
1	x	135	HIS
1	x	142	ASN
1	x	222	GLN
1	x	224	ASN
1	x	301	GLN
1	x	313	GLN
1	x	349	HIS
1	x	367	HIS
1	x	417	ASN
1	x	471	GLN
1	x	486	ASN
1	y	117	ASN
1	y	349	HIS
1	y	373	HIS
1	y	474	ASN
1	y	500	ASN
1	y	503	ASN
1	y	526	ASN
1	z	114	ASN
1	z	133	ASN
1	z	143	ASN
1	z	285	ASN
1	z	333	GLN
1	z	349	HIS
1	z	423	ASN
2	P	52	GLN
2	P	188	GLN
2	P	229	ASN
2	P	264	GLN
2	Q	52	GLN
2	Q	188	GLN
2	R	52	GLN
2	R	188	GLN
2	R	264	GLN
2	S	52	GLN
2	S	158	HIS
2	S	188	GLN
2	S	264	GLN

5.3.3 RNA ⓘ

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.

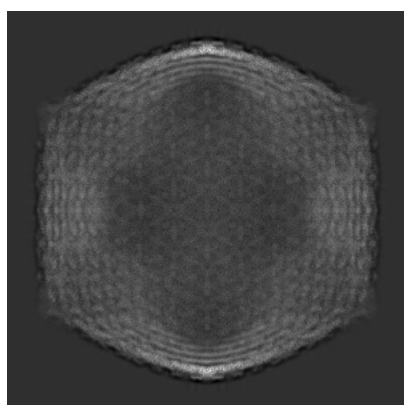
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32974. These allow visual inspection of the internal detail of the map and identification of artifacts.

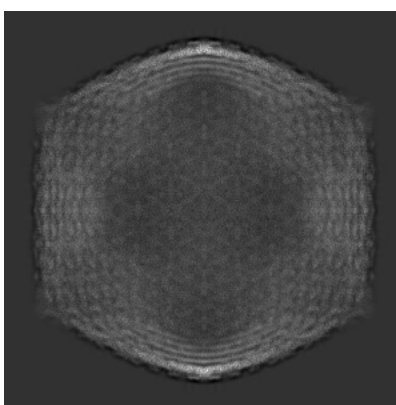
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

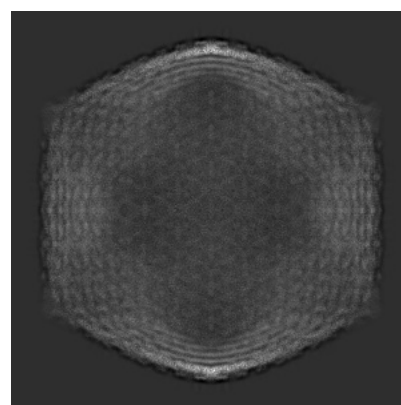
6.1.1 Primary map



X



Y



Z

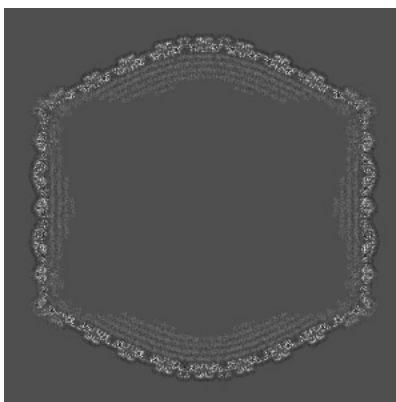
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

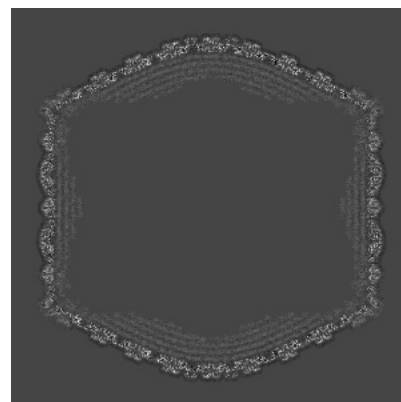
6.2.1 Primary map



X Index: 410



Y Index: 410



Z Index: 410

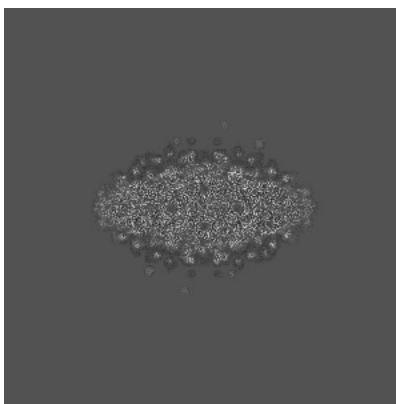
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

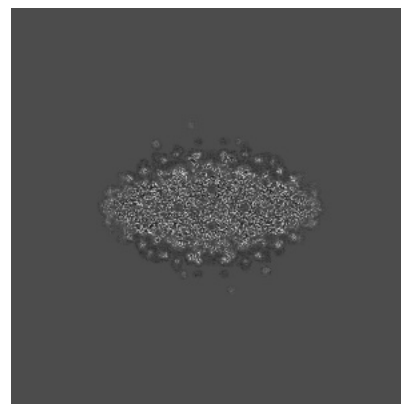
6.3.1 Primary map



X Index: 344



Y Index: 86

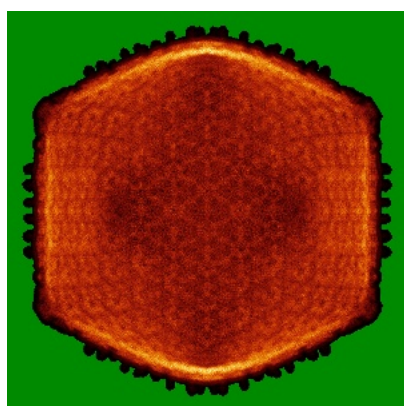


Z Index: 734

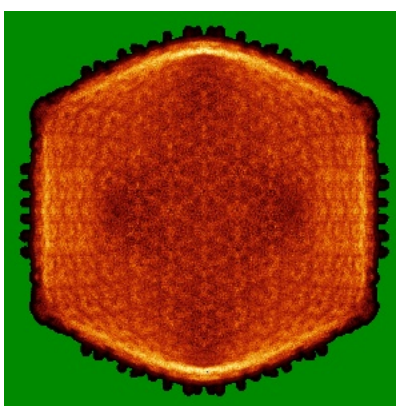
The images above show the largest variance slices of the map in three orthogonal directions.

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

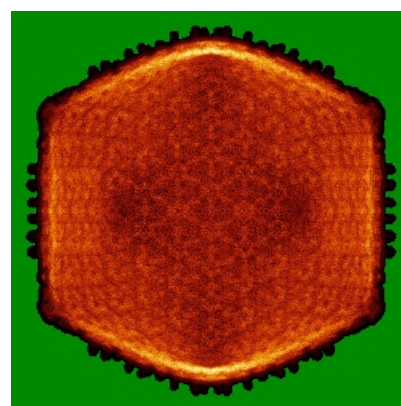
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

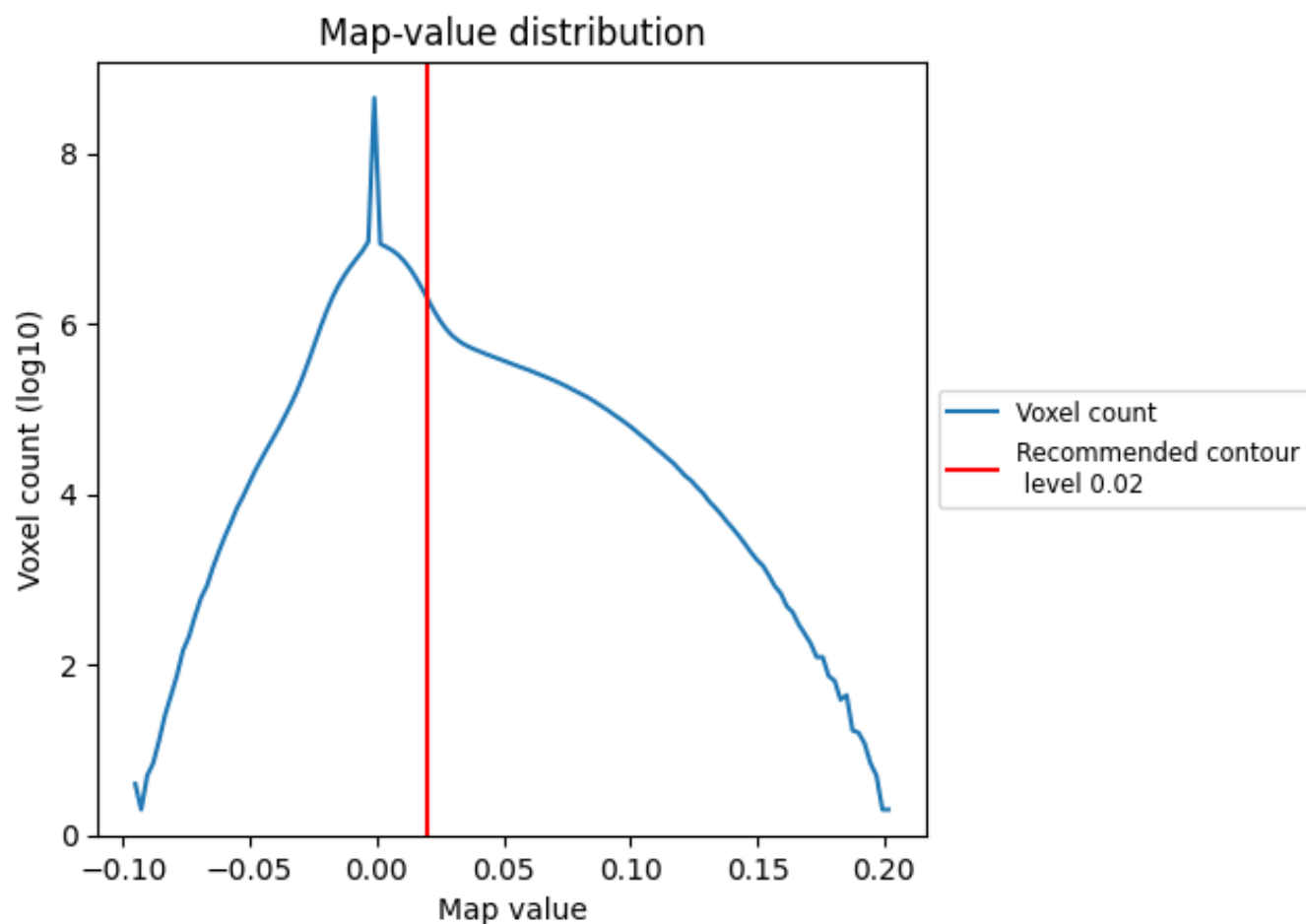
6.6 Mask visualisation

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

7 Map analysis [i](#)

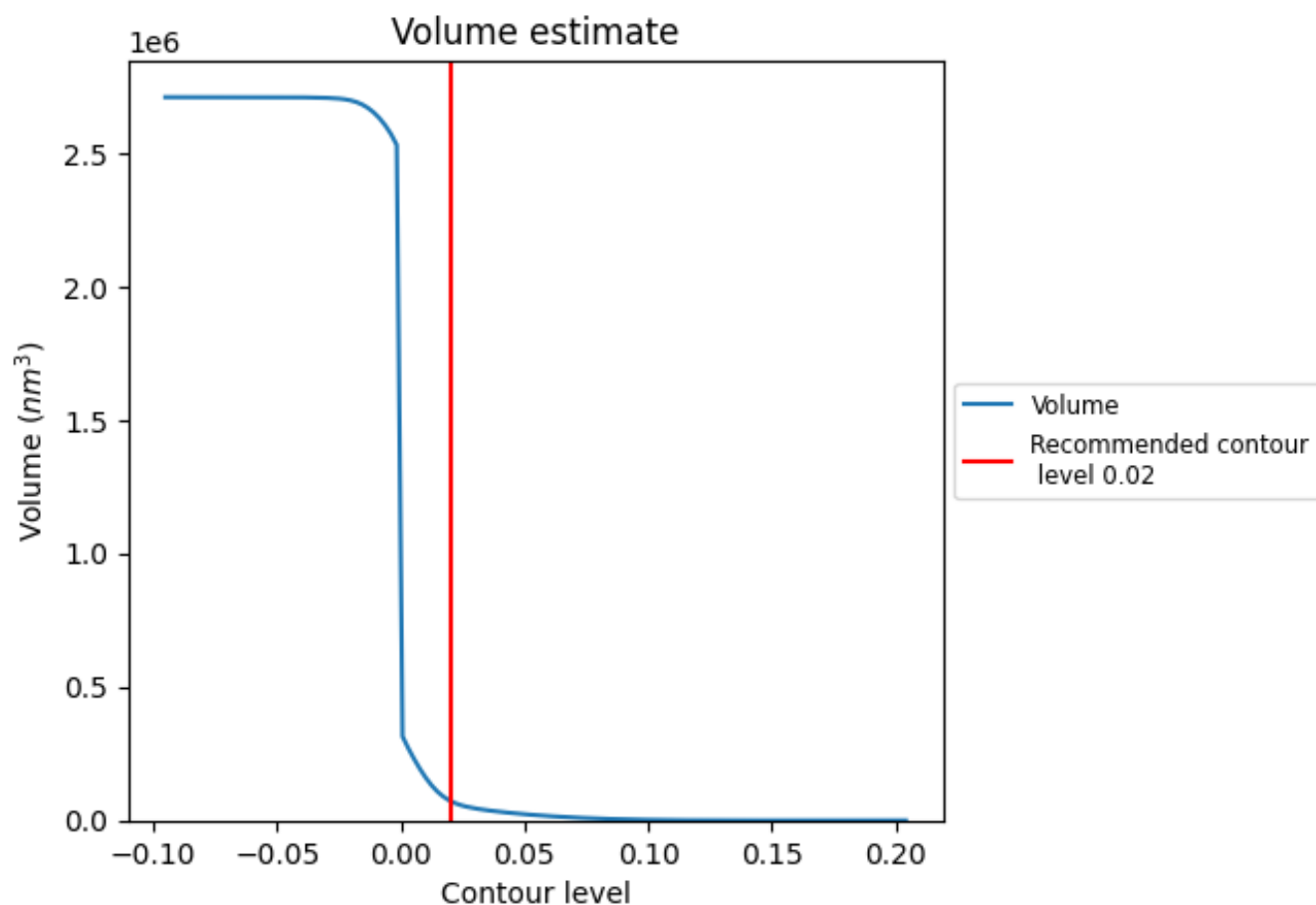
This section contains the results of statistical analysis of the map.

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.

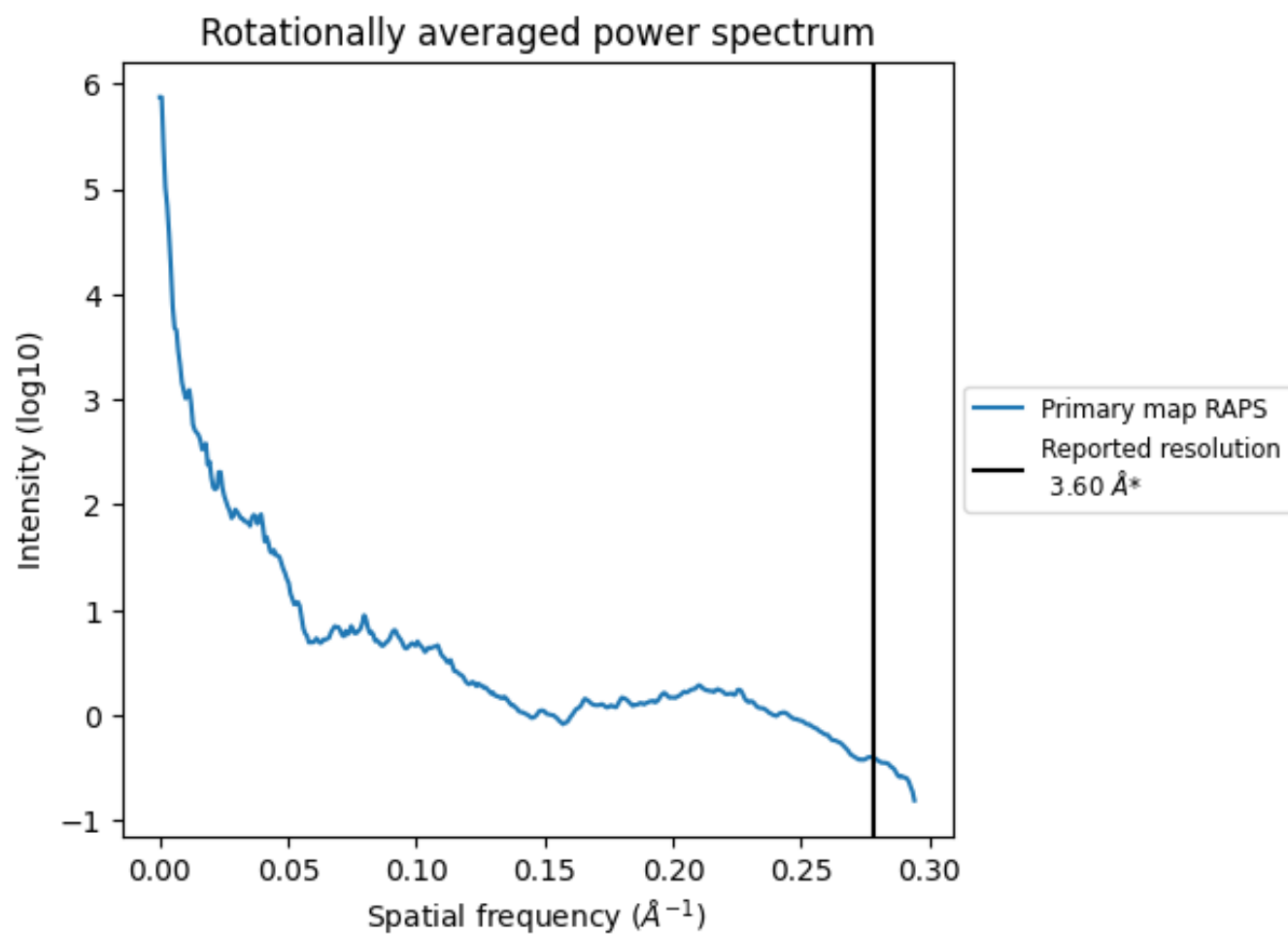
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73369 nm³; this corresponds to an approximate mass of 66276 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 ⓘ

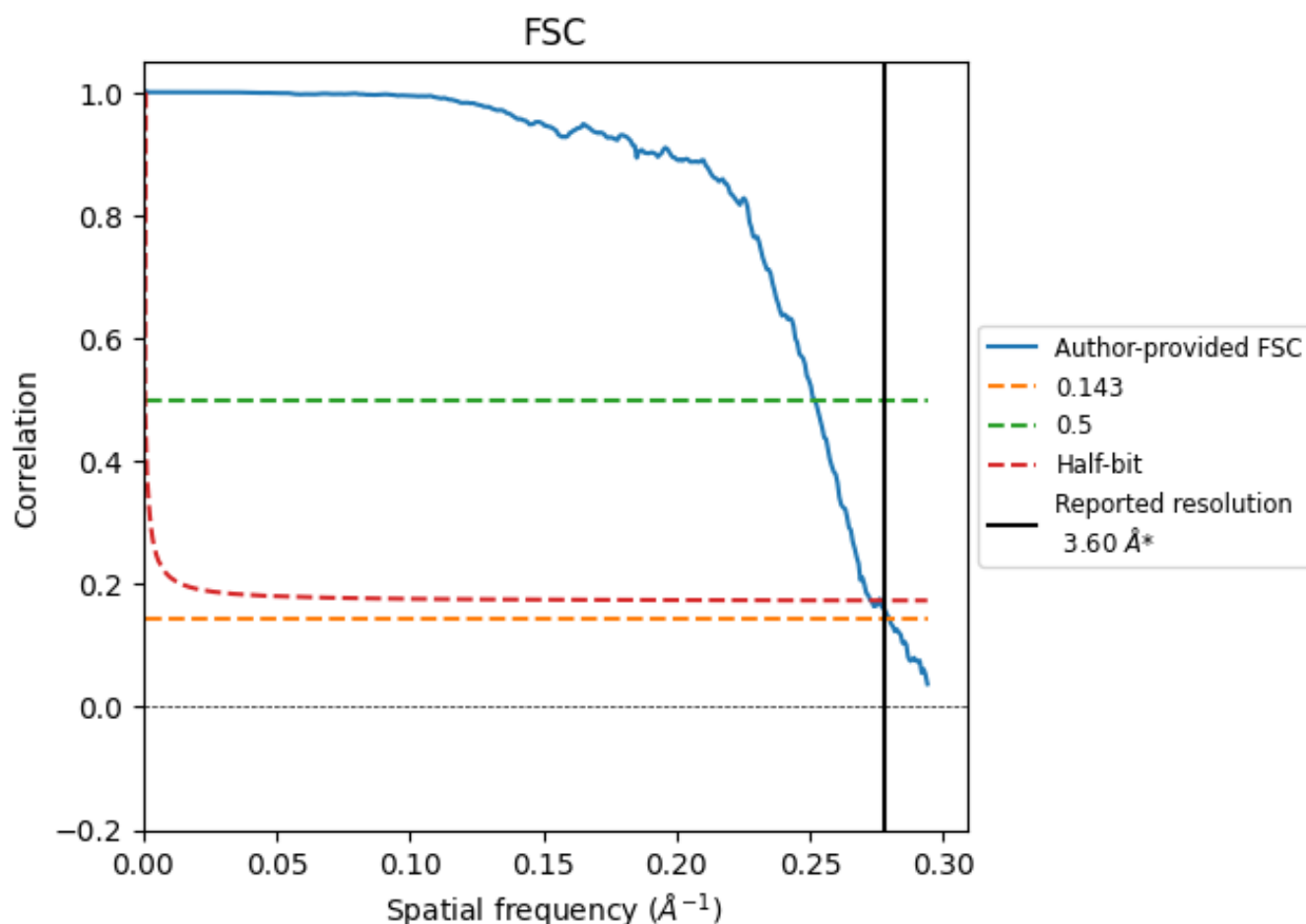


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	3.97	3.66
Unmasked-calculated*	-	-	-

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

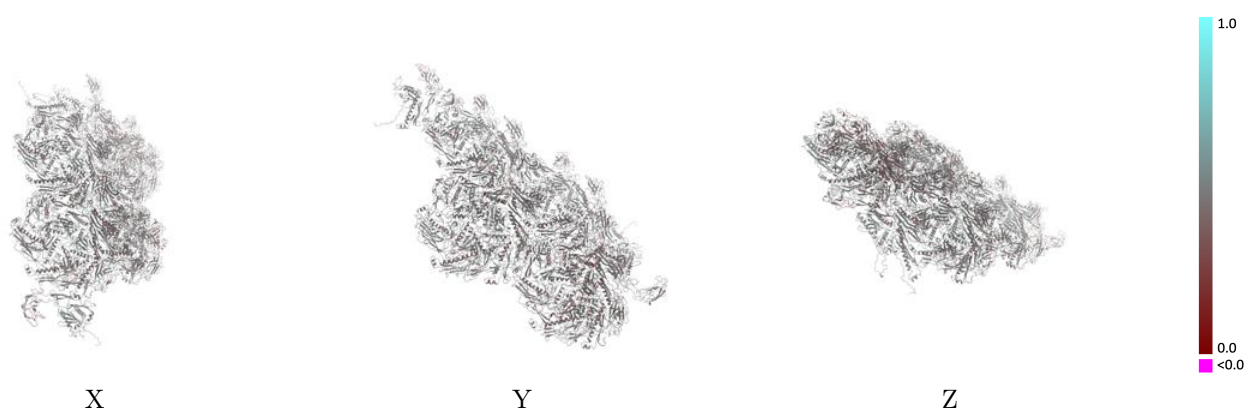
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32974 and PDB model 7X30. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

This section was not generated.

9.2 Q-score mapped to coordinate model ⓘ

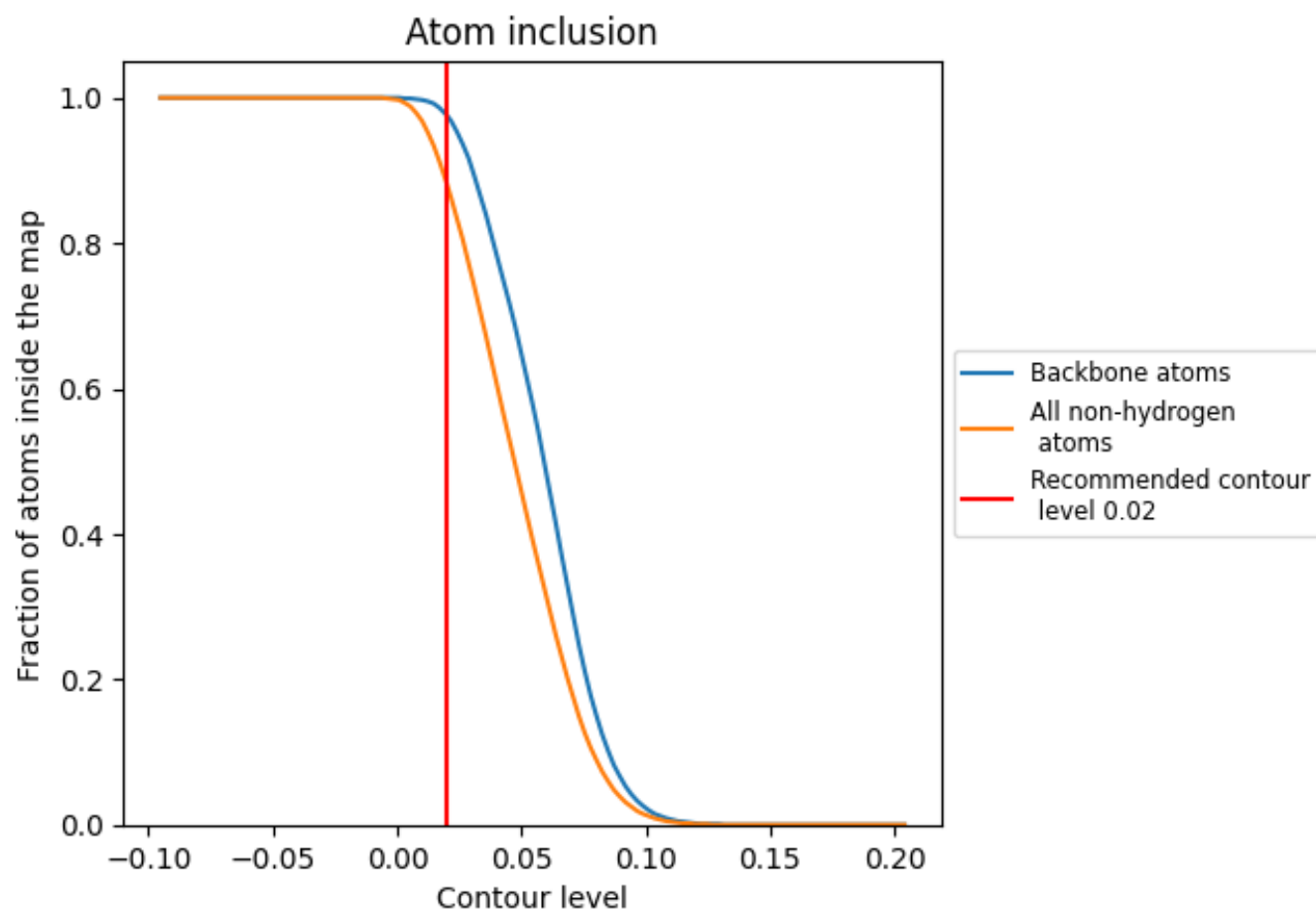


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.4580
A	 0.8320	 0.4430
P	 0.8520	 0.4280
Q	 0.8460	 0.4260
R	 0.7070	 0.3870
S	 0.6910	 0.3680
a	 0.8950	 0.4640
b	 0.8910	 0.4630
c	 0.8900	 0.4650
d	 0.8920	 0.4680
e	 0.8940	 0.4630
f	 0.8590	 0.4570
g	 0.9040	 0.4660
h	 0.9020	 0.4650
i	 0.8990	 0.4660
j	 0.9010	 0.4680
k	 0.9060	 0.4680
l	 0.9000	 0.4650
m	 0.8930	 0.4630
n	 0.8930	 0.4670
o	 0.8920	 0.4630
p	 0.8980	 0.4600
q	 0.8880	 0.4660
r	 0.8850	 0.4620
s	 0.8960	 0.4630
t	 0.8930	 0.4620
u	 0.8950	 0.4580
v	 0.9020	 0.4640
w	 0.8980	 0.4630
x	 0.8980	 0.4660
y	 0.9100	 0.4640
z	 0.9030	 0.4670

