



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:30 AM UTC

PDB ID : 7AEF / pdb_00007aef
EMDB ID : EMD-11745
Title : Cryo-EM structure of an extracellular contractile injection system in marine bacterium *Algoriphagus machipongonensis*, the baseplate complex in extended state applied 3-fold symmetry.
Authors : Xu, J.; Ericson, C.; Feldmueller, M.; Lien, Y.W.; Pilhofer, M.
Deposited on : 2020-09-17
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

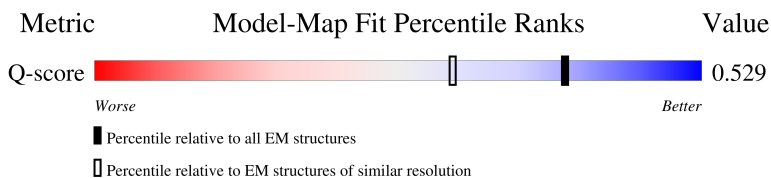
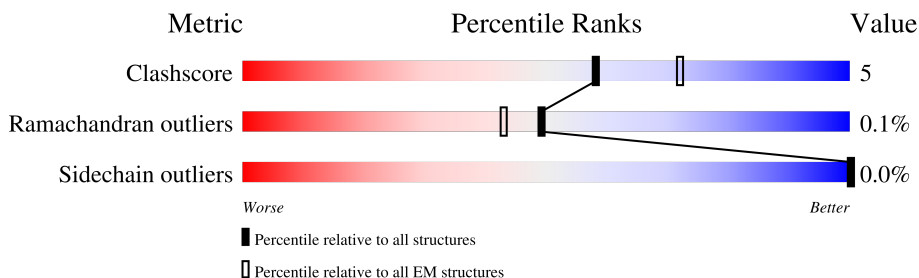
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	933	10% 54% 5% 41%
1	B	933	11% 54% 5% 41%
1	C	933	10% 55% . 41%
1	D	933	12% 52% 6% 41%

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Mol	Chain	Length	Quality of chain
1	E	933	
1	F	933	
2	G	1050	
2	H	1050	
2	I	1050	
2	J	1050	
2	K	1050	
2	L	1050	
3	M	228	
3	N	228	
3	O	228	
3	P	228	
3	Q	228	
3	R	228	
4	S	137	
4	T	137	
4	U	137	
4	V	137	
4	W	137	
4	X	137	
5	Y	147	
5	Z	147	
5	a	147	
5	b	147	
5	c	147	

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Mol	Chain	Length	Quality of chain
5	d	147	
6	e	692	
6	f	692	
6	g	692	
6	h	692	
6	i	692	
6	j	692	
7	k	142	
7	l	142	
7	m	142	
7	n	142	
7	o	142	
7	p	142	
8	t	52	
8	u	52	
8	v	52	
9	q	581	
9	r	581	
9	s	581	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 149535 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 baseplate protein (Algo12).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	549	Total	C	N	O	S	0	0
			4447	2845	730	858	14		
1	B	549	Total	C	N	O	S	0	0
			4447	2845	730	858	14		
1	C	549	Total	C	N	O	S	0	0
			4447	2845	730	858	14		
1	D	549	Total	C	N	O	S	0	0
			4447	2845	730	858	14		
1	E	549	Total	C	N	O	S	0	0
			4447	2845	730	858	14		
1	F	549	Total	C	N	O	S	0	0
			4447	2845	730	858	14		

- Molecule 2 is a protein called Baseplate_J domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	1011	Total	C	N	O	S	0	0
			7762	4951	1284	1512	15		
2	H	1011	Total	C	N	O	S	0	0
			7762	4951	1284	1512	15		
2	I	1011	Total	C	N	O	S	0	0
			7762	4951	1284	1512	15		
2	J	1011	Total	C	N	O	S	0	0
			7762	4951	1284	1512	15		
2	K	1011	Total	C	N	O	S	0	0
			7762	4951	1284	1512	15		
2	L	1011	Total	C	N	O	S	0	0
			7762	4951	1284	1512	15		

- Molecule 3 is a protein called LysM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		
3	O	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		
3	P	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		
3	Q	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		
3	R	225	Total	C	N	O	S	0	0
			1849	1185	304	355	5		

- Molecule 4 is a protein called Putative tail lysozyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	T	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	U	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	V	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	W	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		
4	X	133	Total	C	N	O	S	0	0
			1074	690	174	207	3		

- Molecule 5 is a protein called Phospholipid/glycerol acyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	Z	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	a	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	b	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	c	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	d	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		

- Molecule 6 is a protein called Putative phage tail sheath protein FI.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	f	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	g	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	h	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	i	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	j	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		

- Molecule 7 is a protein called Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	l	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	m	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	n	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	o	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	p	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		

- Molecule 8 is a protein called inner protein (Algo6).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	t	40	Total	C	N	O	S	0	0
			324	202	55	66	1		
8	u	40	Total	C	N	O	S	0	0
			324	202	55	66	1		
8	v	40	Total	C	N	O	S	0	0
			324	202	55	66	1		

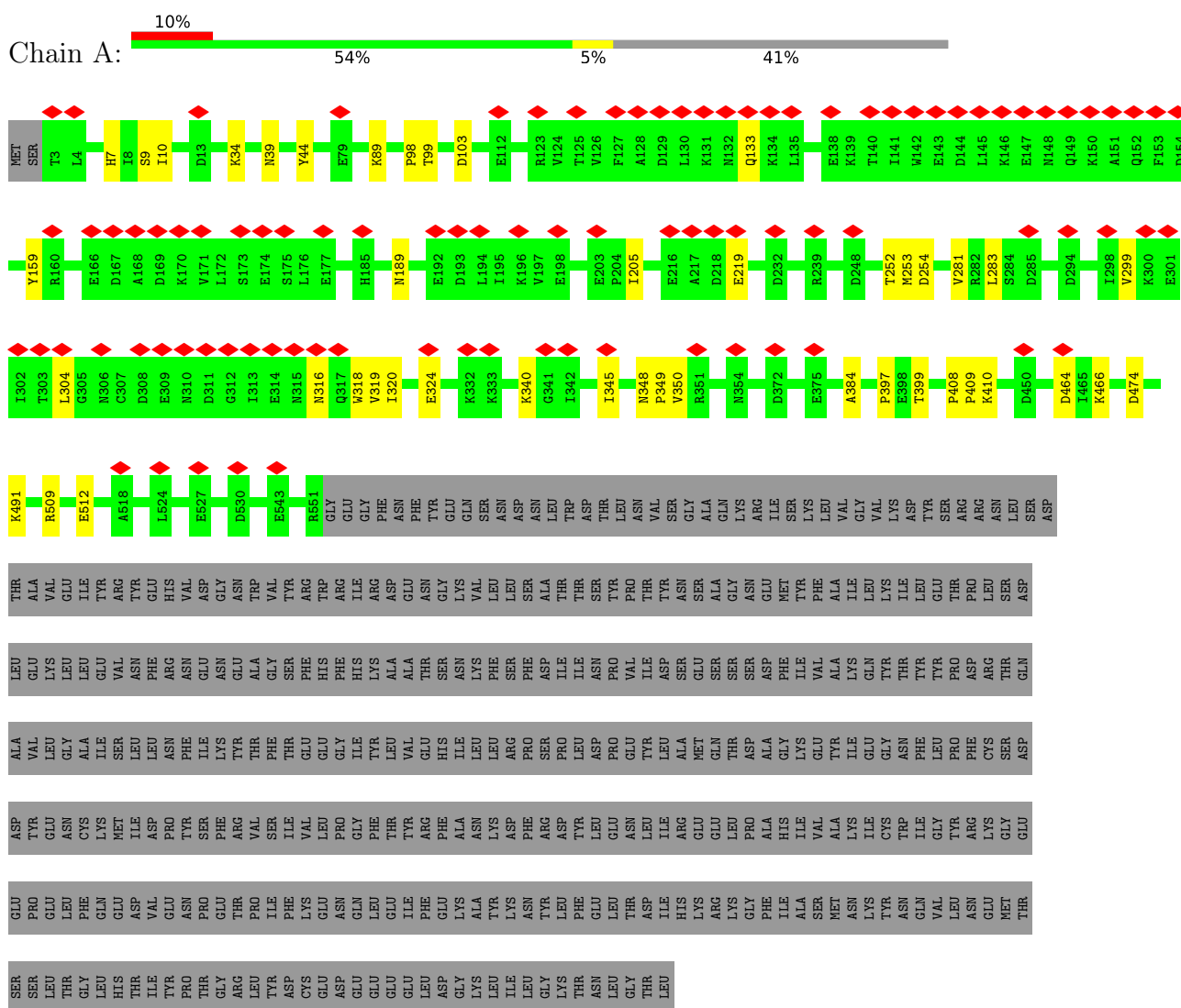
- Molecule 9 is a protein called Phosphoserine phosphatase SerB.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	q	580	Total 4469	C 2771	N 765	O 920	S 13	0	0
9	r	580	Total 4469	C 2771	N 765	O 920	S 13	0	0
9	s	580	Total 4469	C 2771	N 765	O 920	S 13	0	0

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.

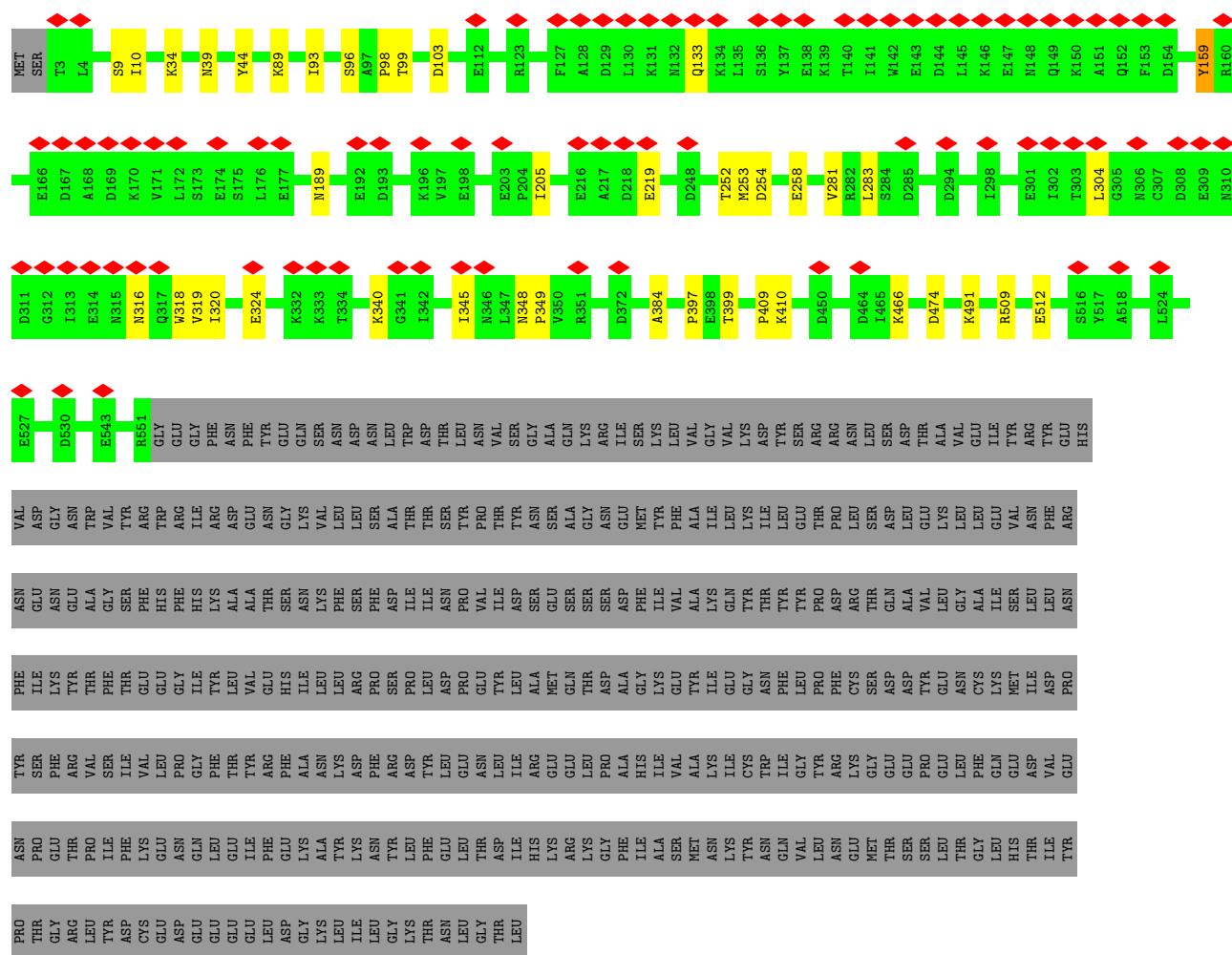
- Molecule 1: baseplate protein (Algo12)



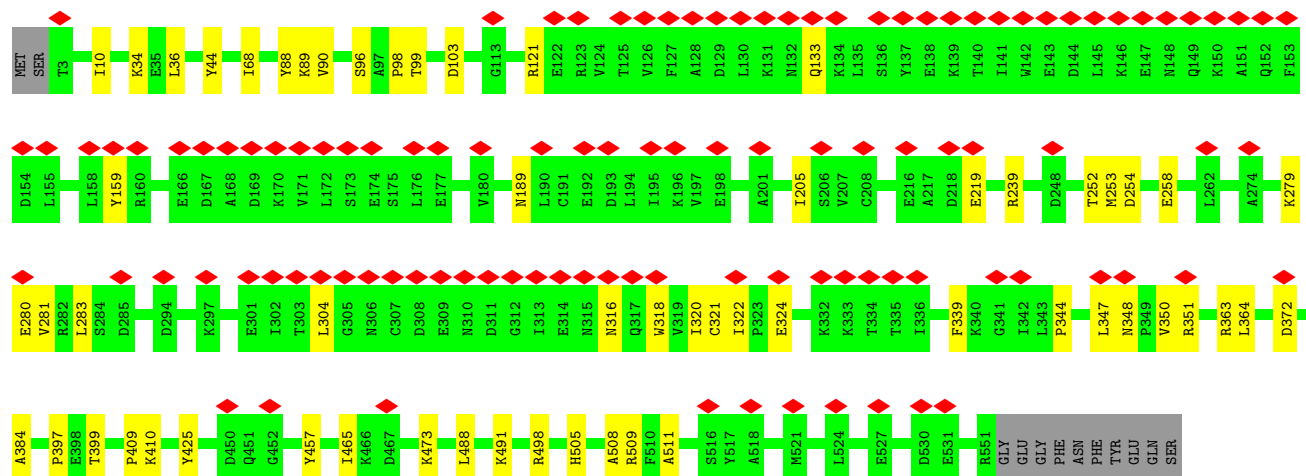
- Molecule 1: baseplate protein (Algo12)





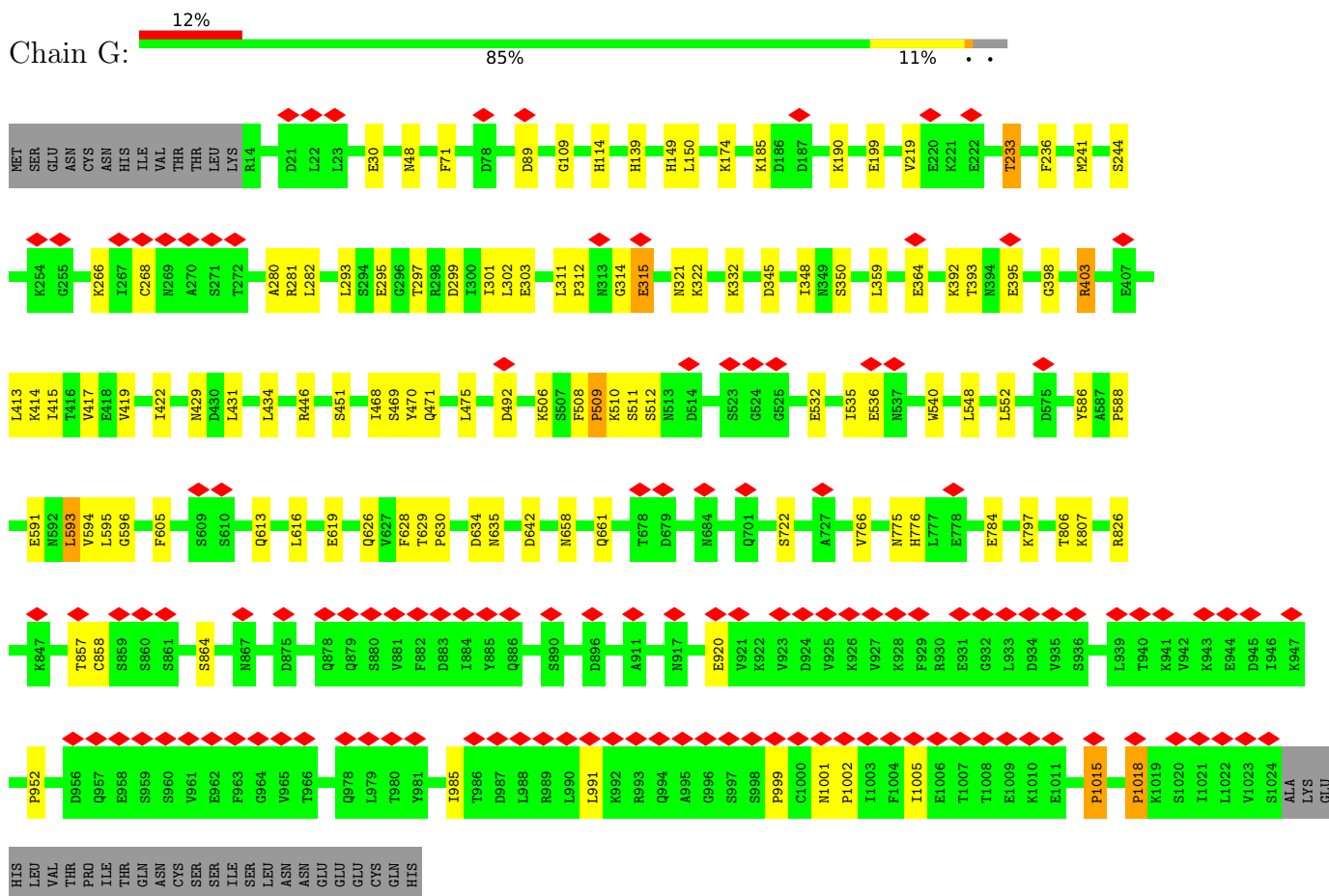


• Molecule 1: baseplate protein (Algo12)

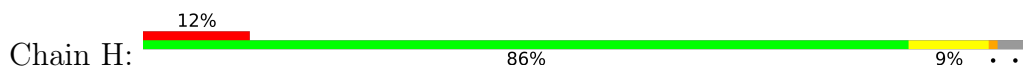


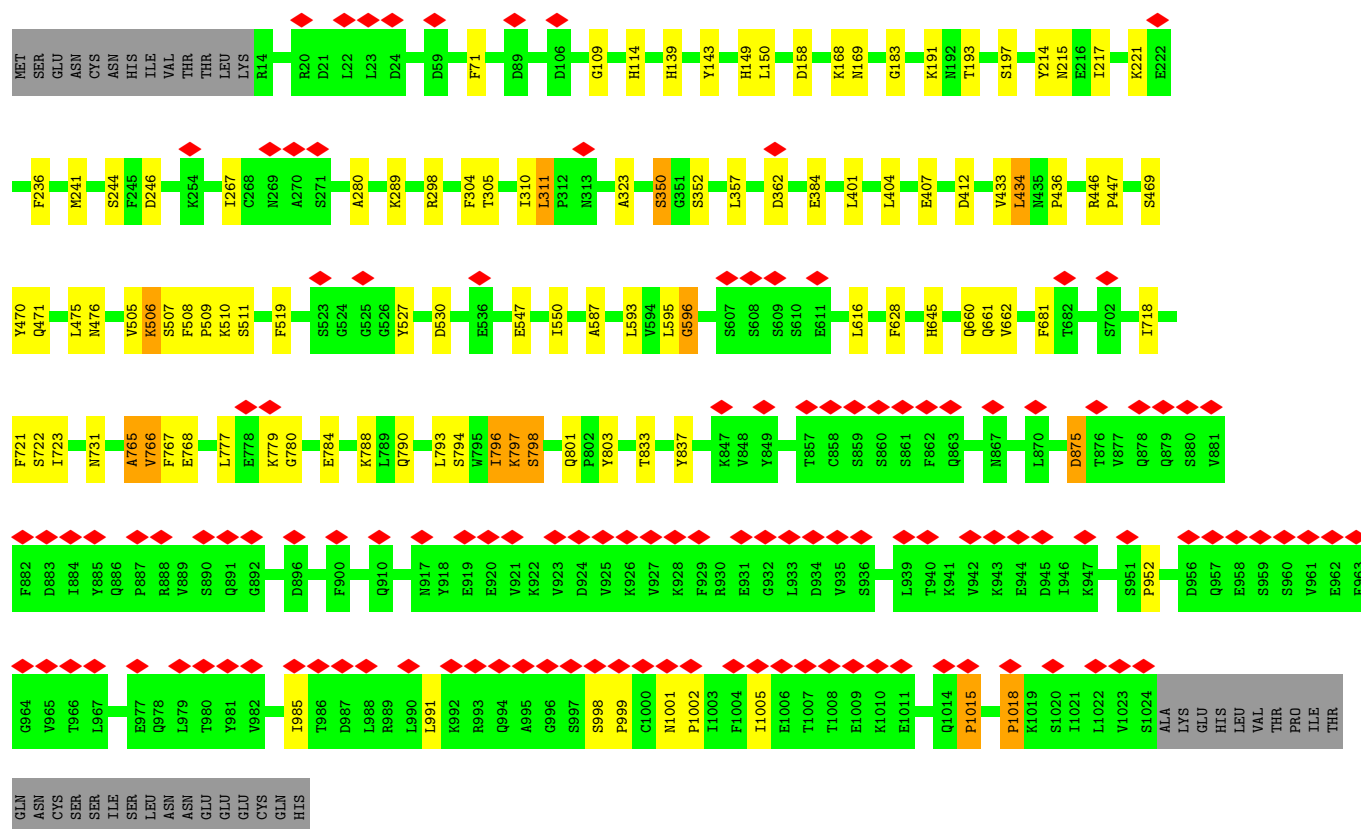
LYS	ALA	ASN	LEU	LYS
LEU	TYP	LYS	LEU	PHE
ILE	LYS	ASP	ARG	SER
LEU	ASN	PHE	PRO	ASP
GLY	TYP	ARG	SER	ASP
LYS	LEU	ASP	PRO	ILE
THR	PHE	TYP	LEU	ILE
ASN	GLU	LEU	ASP	LEU
LEU	LEU	GLU	PRO	TYP
GLY	THR	ASN	GLU	VAL
THR	ASP	LEU	TYP	ILE
LEU	ILE	ILE	LEU	ASP
	HIS	ARG	ALA	SER
	LYS	GLU	MET	GLU
	ARG	GLU	GLN	SER
	LYS	LEU	THR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

- Molecule 2: Baseplate_J domain-containing protein

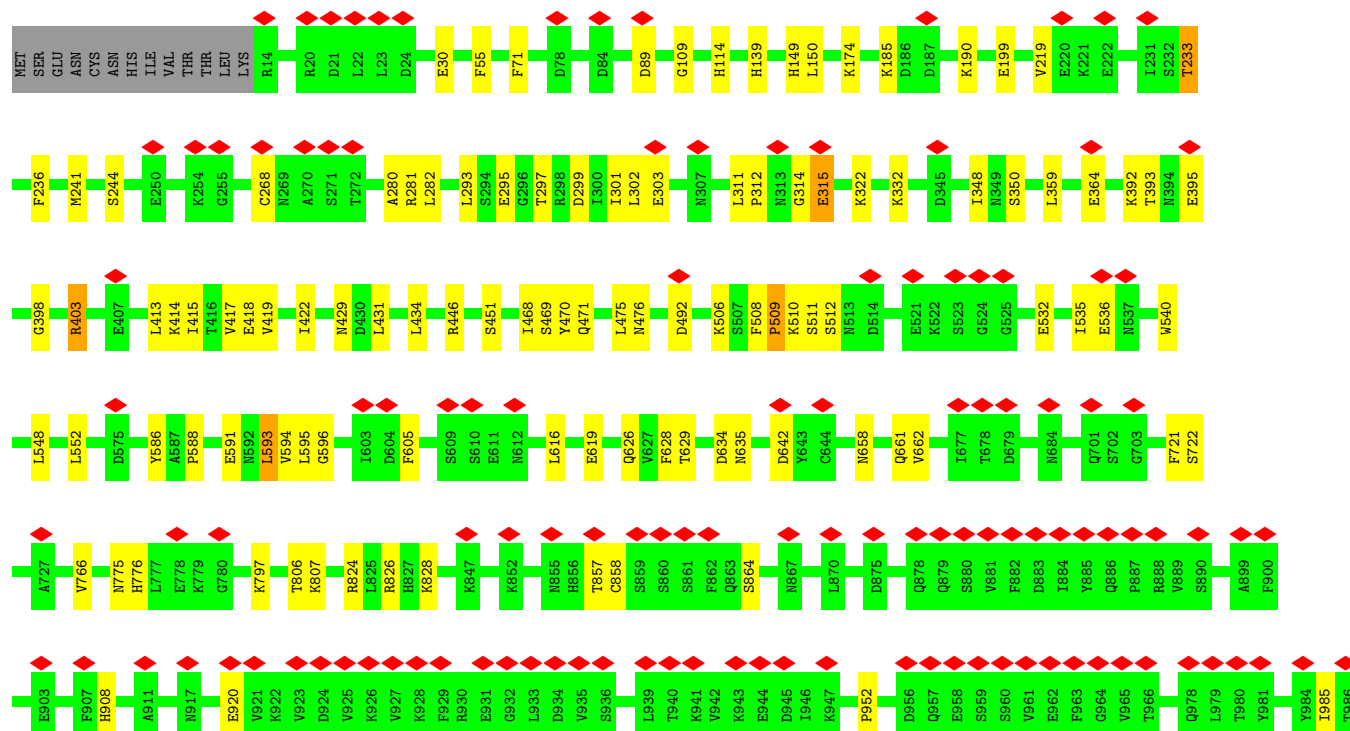
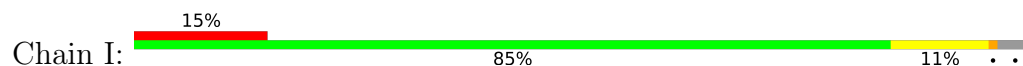


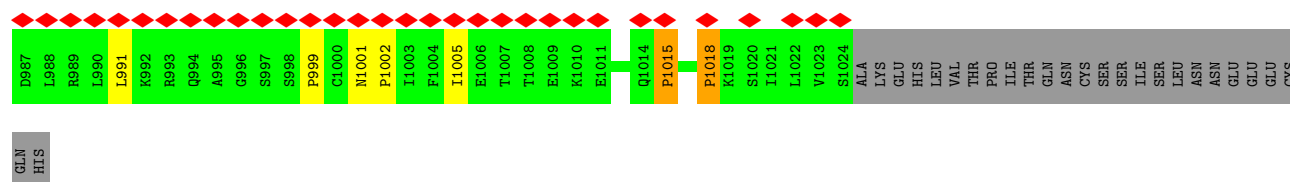
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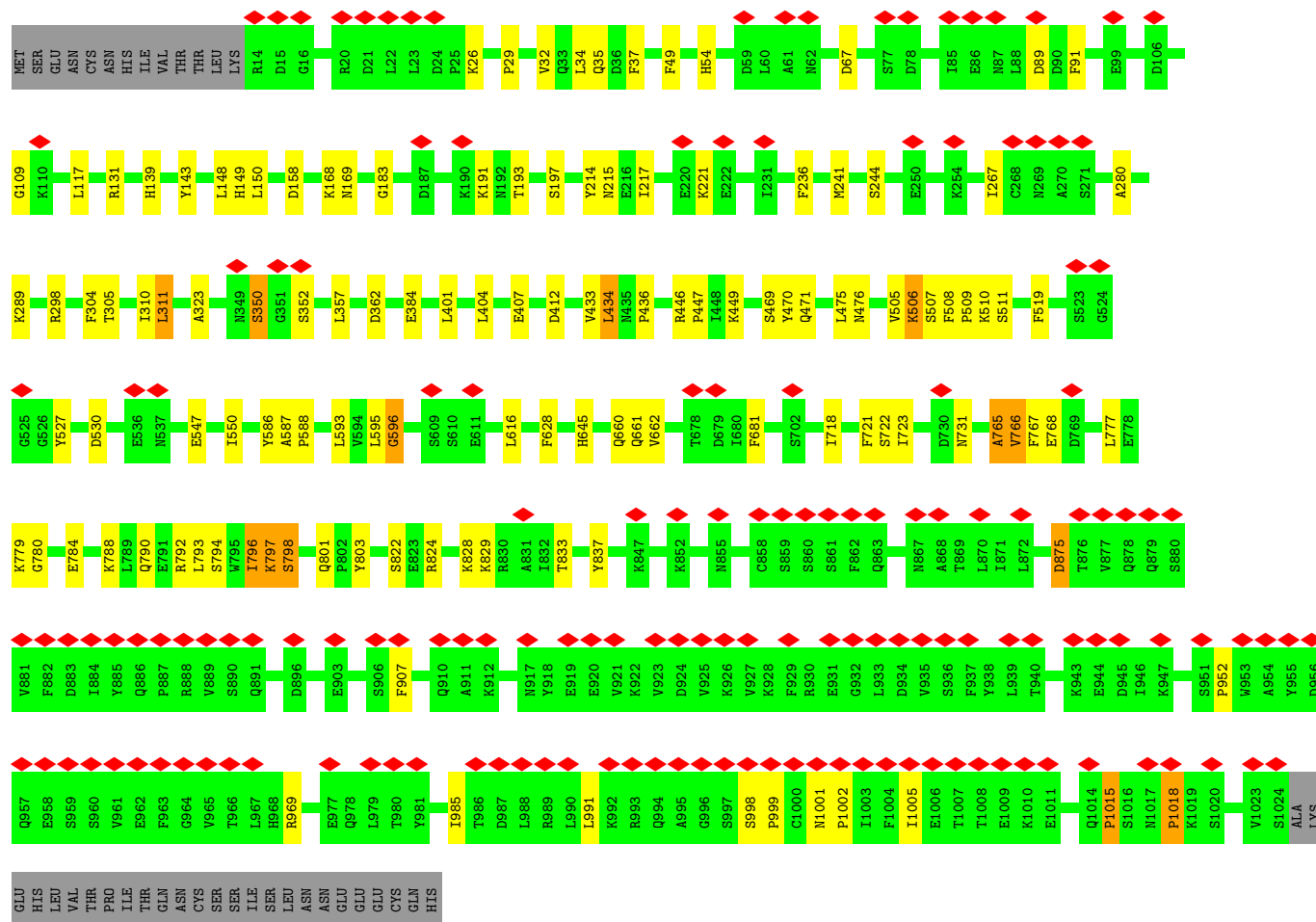
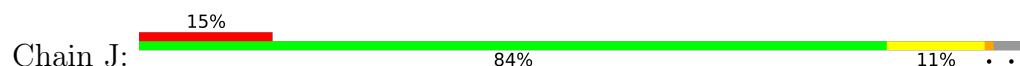


• Molecule 2: Baseplate_J domain-containing protein

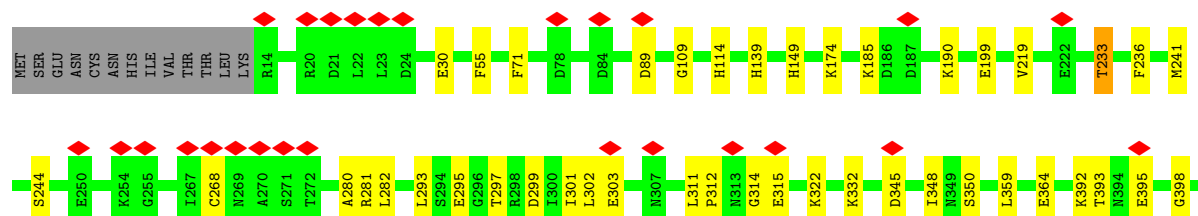
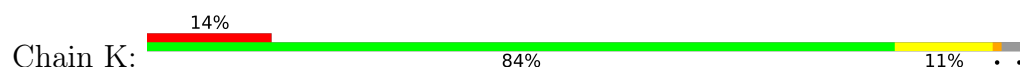


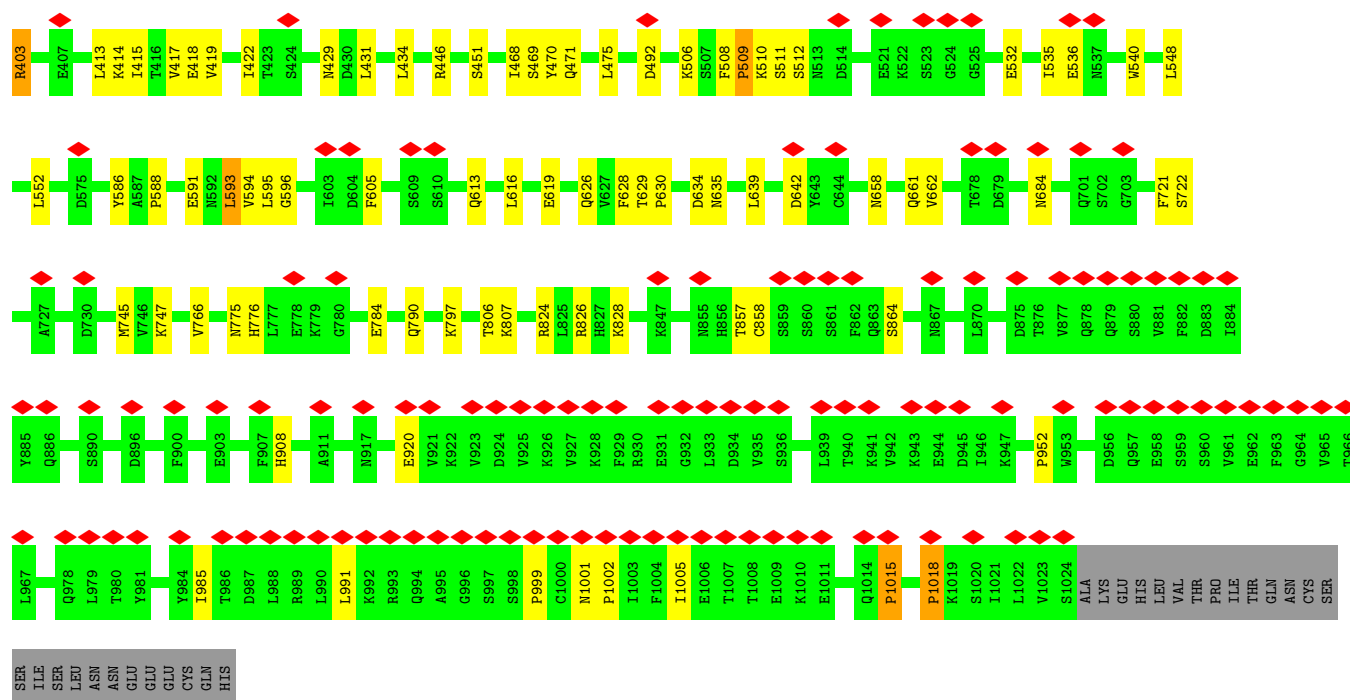


• Molecule 2: Baseplate_J domain-containing protein

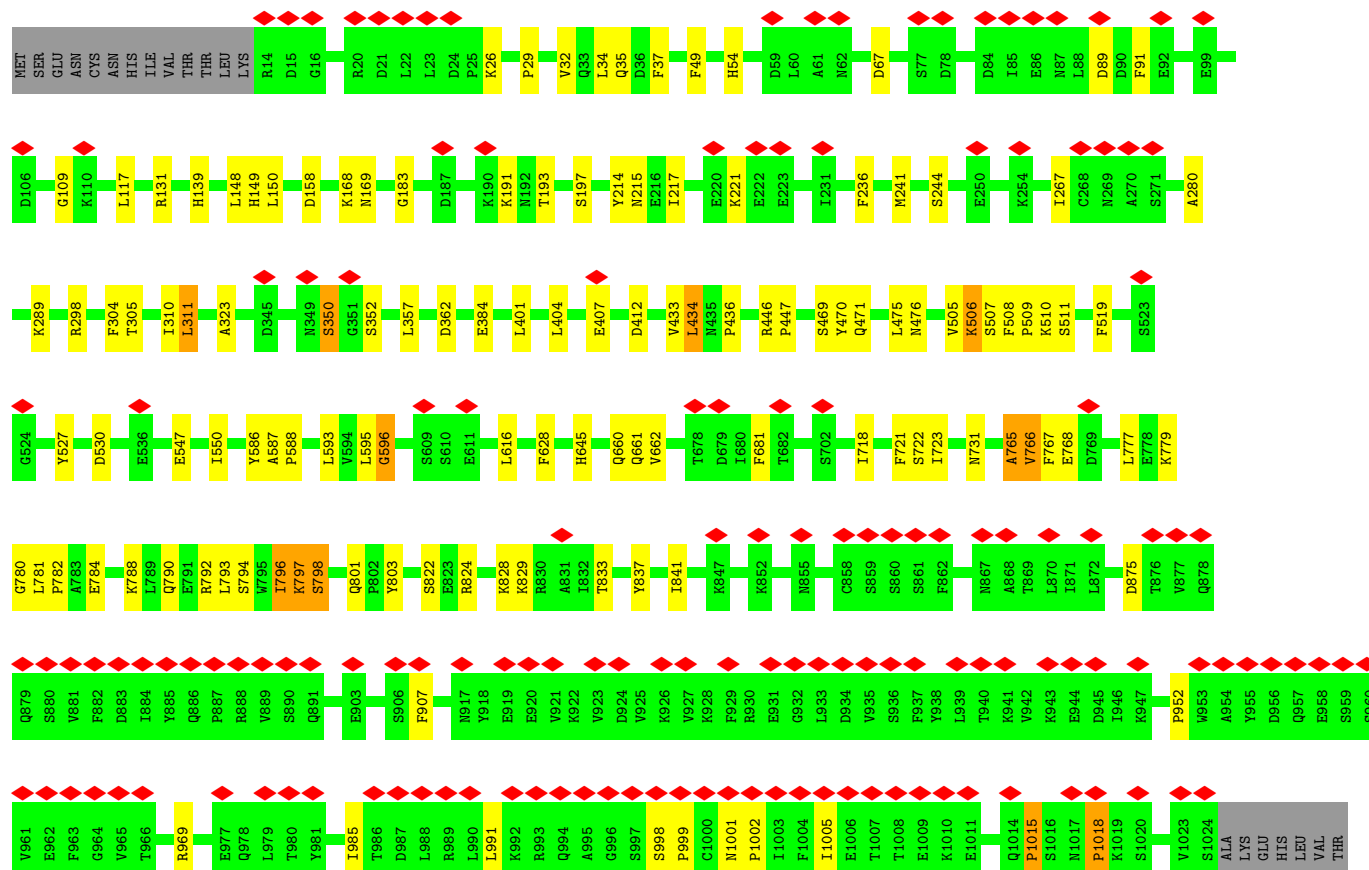
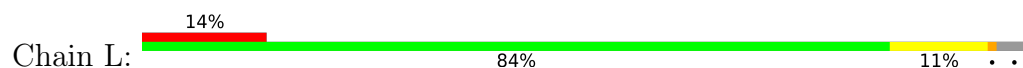


• Molecule 2: Baseplate_J domain-containing protein





• Molecule 2: Baseplate_J domain-containing protein



PRO
ILE
THR
GLN
ASN
CYS
SER
SER
ILE
SER
LEU
ASN
ASN
GLU
GLU
GLU
CYS
GLN
HIS

- Molecule 3: LysM domain-containing protein

Chain M:  89% 10%



- Molecule 3: LysM domain-containing protein

Chain N:  90% 8%



- Molecule 3: LysM domain-containing protein

Chain O:  89% 10%



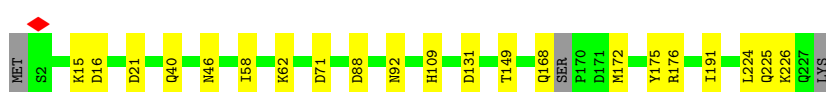
- Molecule 3: LysM domain-containing protein

Chain P:  90% 9%



- Molecule 3: LysM domain-containing protein

Chain Q:  89% 9%



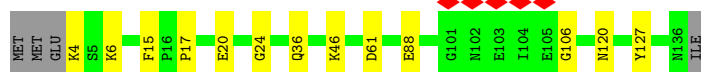
- Molecule 3: LysM domain-containing protein

Chain R:  89% 10%



- Molecule 4: Putative tail lysozyme

Chain S:  88% 9%



- Molecule 4: Putative tail lysozyme

Chain T:  87% 10%



- Molecule 4: Putative tail lysozyme

Chain U:  87% 10%



- Molecule 4: Putative tail lysozyme

Chain V:  88% 9%



- Molecule 4: Putative tail lysozyme

Chain W:  86% 11%



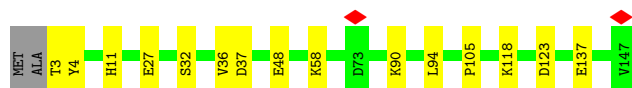
- Molecule 4: Putative tail lysozyme

Chain X:  88% 9%



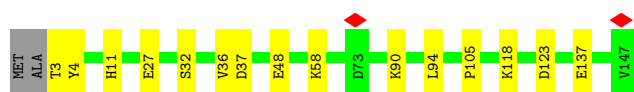
- Molecule 5: Phospholipid/glycerol acyltransferase

Chain Y:  88% 10%



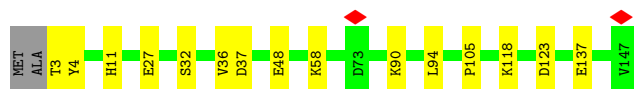
- Molecule 5: Phospholipid/glycerol acyltransferase

Chain Z:  88% 10%



- Molecule 5: Phospholipid/glycerol acyltransferase

Chain a:  88% 10%



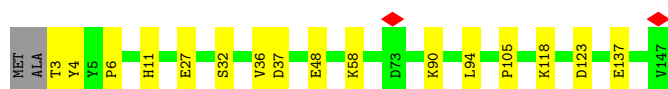
- Molecule 5: Phospholipid/glycerol acyltransferase

Chain b:  88% 11%



- Molecule 5: Phospholipid/glycerol acyltransferase

Chain c:  88% 11%



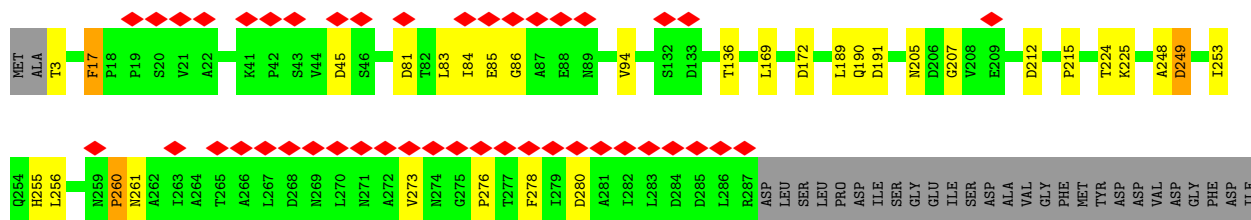
- Molecule 5: Phospholipid/glycerol acyltransferase

Chain d:  89% 10%

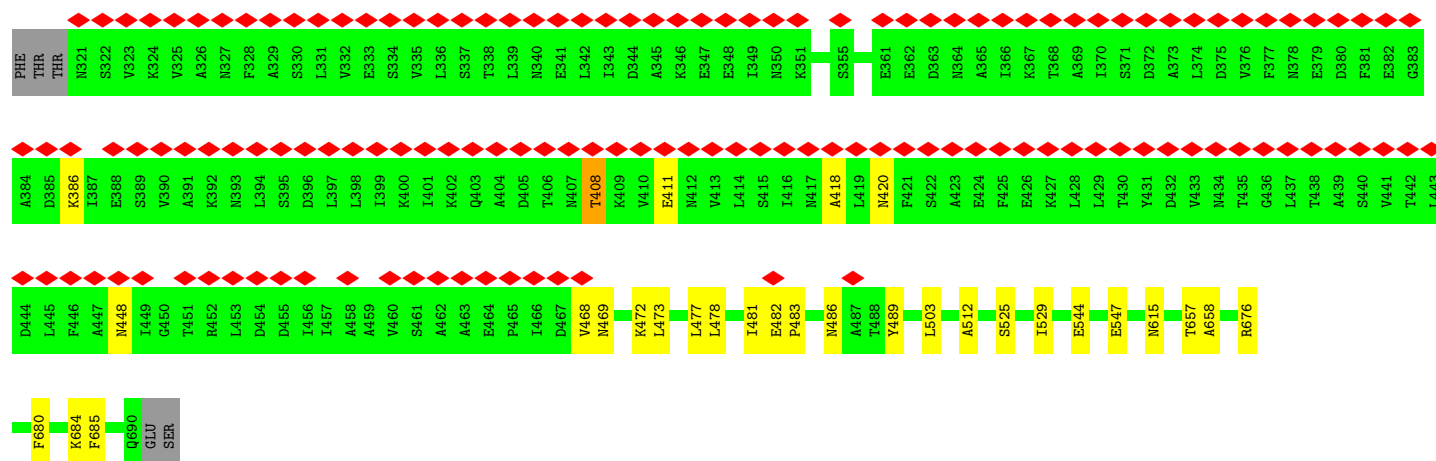


- Molecule 6: Putative phage tail sheath protein FI

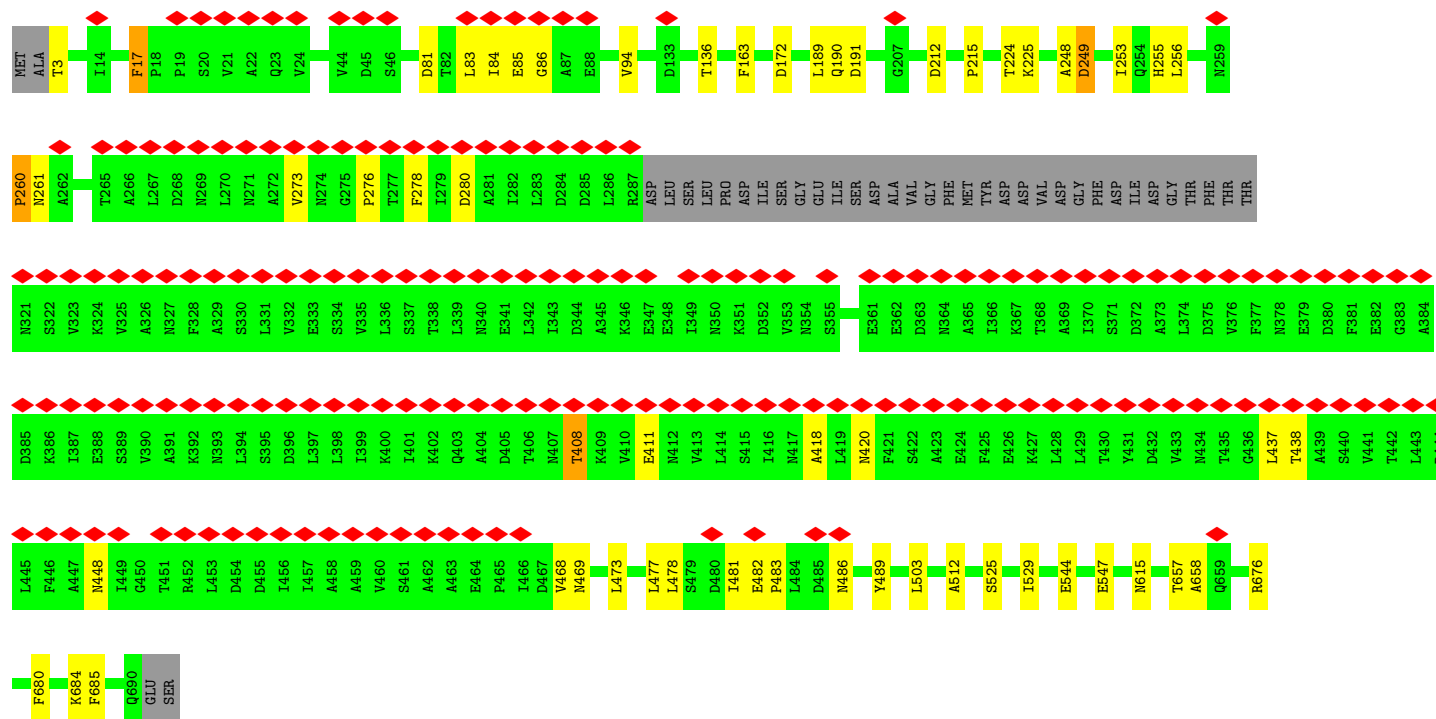
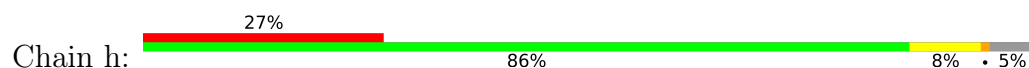
Chain e:  27% 86% 8% 5%



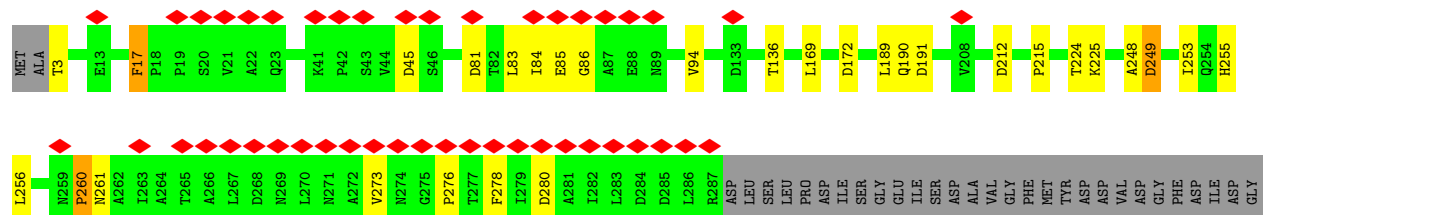
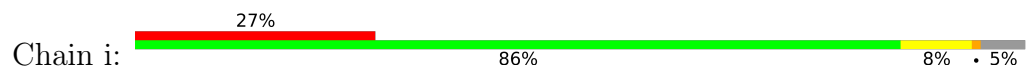


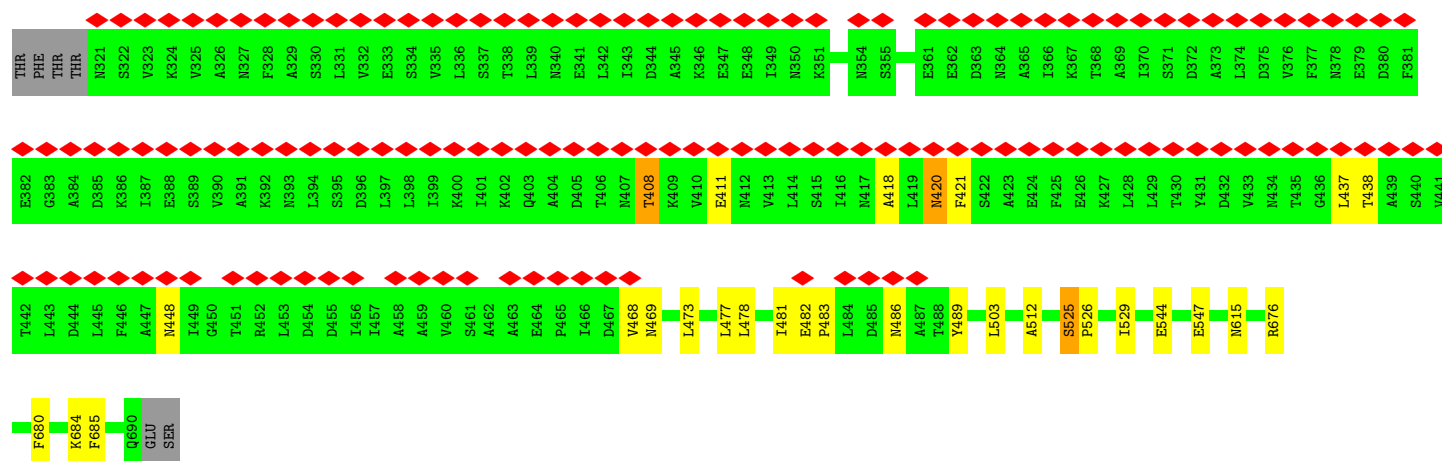


• Molecule 6: Putative phage tail sheath protein FI

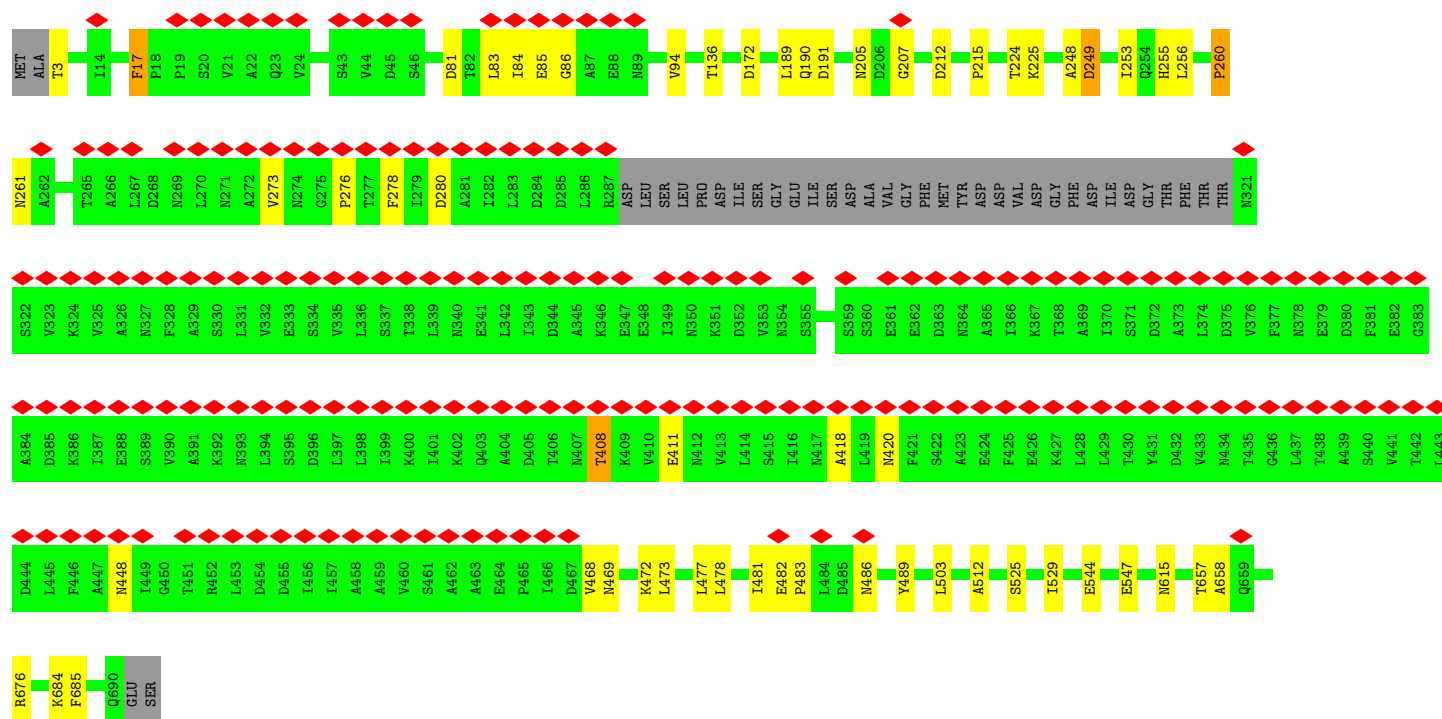
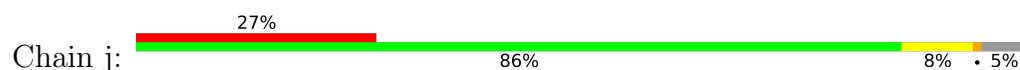


• Molecule 6: Putative phage tail sheath protein FI

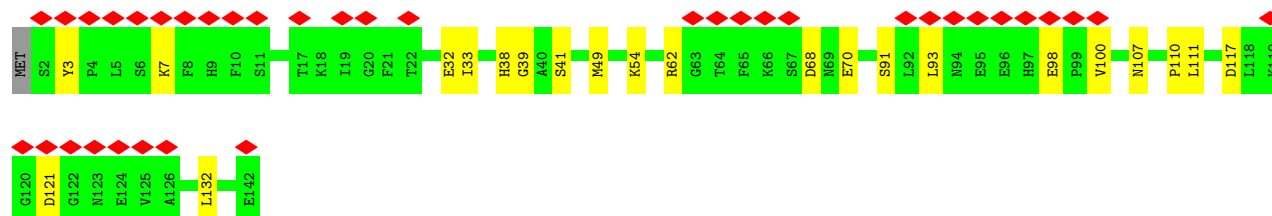
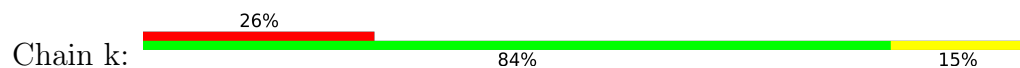




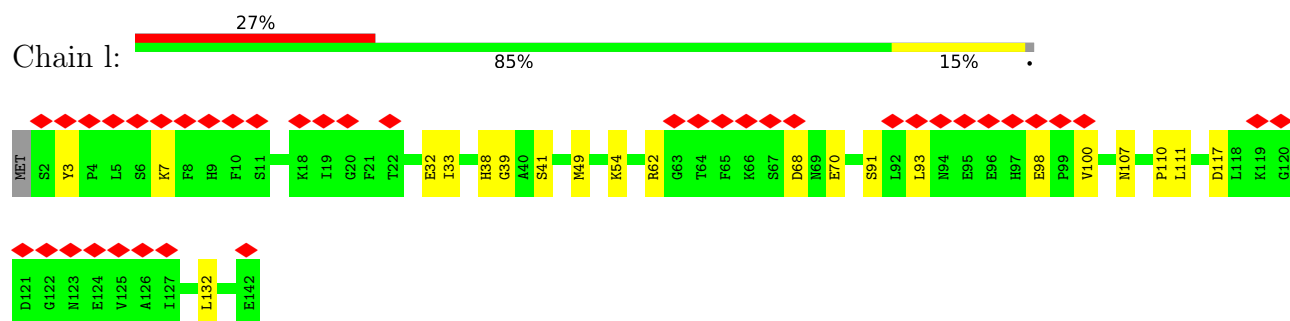
• Molecule 6: Putative phage tail sheath protein FI



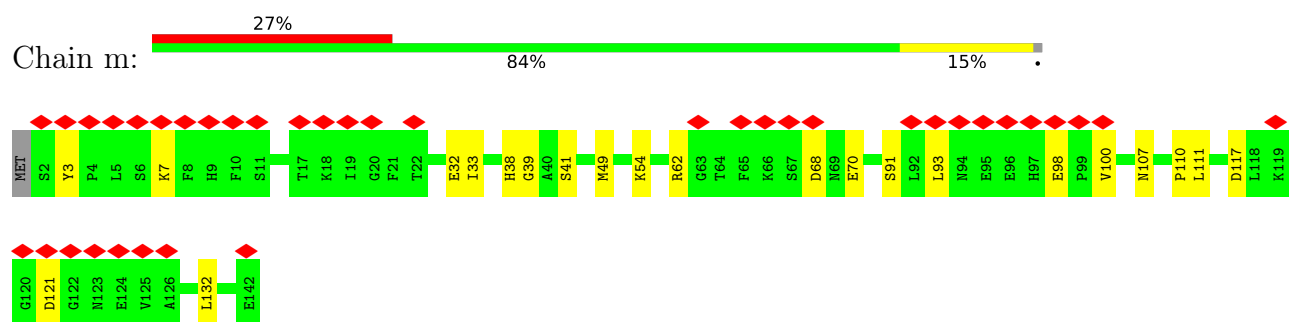
• Molecule 7: Phage tail protein



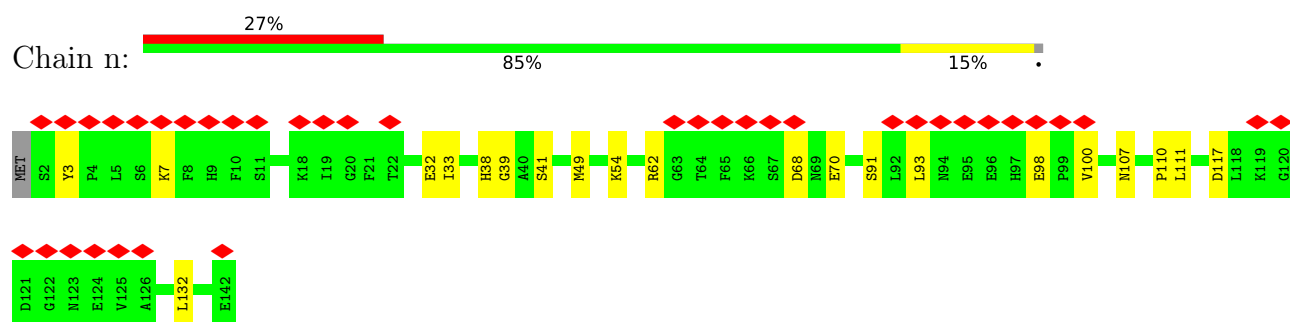
- Molecule 7: Phage tail protein



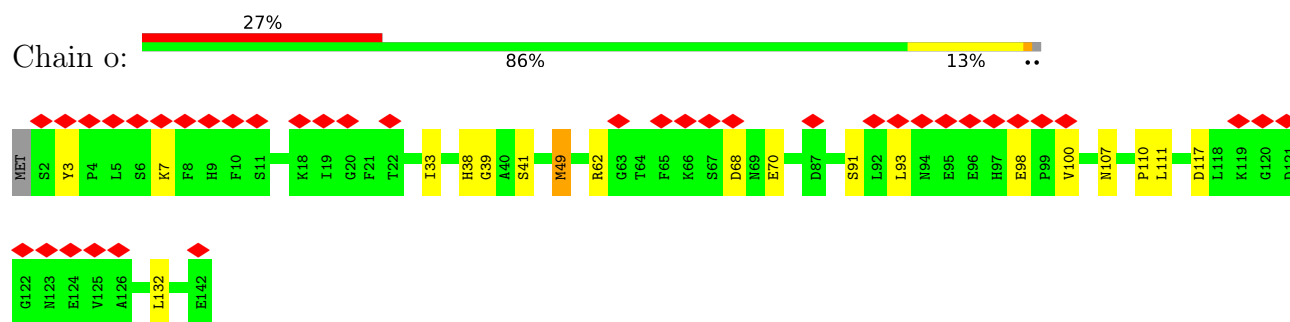
- Molecule 7: Phage tail protein



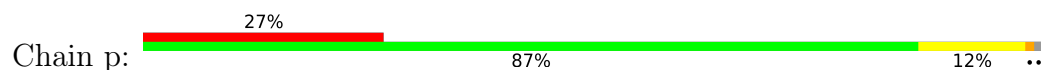
- Molecule 7: Phage tail protein

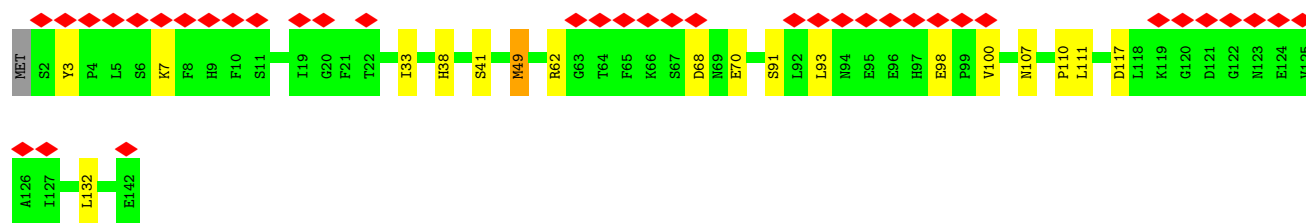


- Molecule 7: Phage tail protein

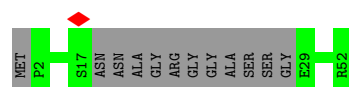
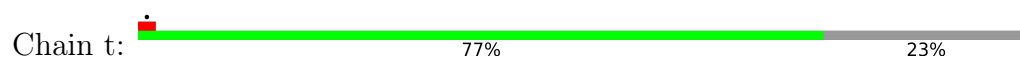


- Molecule 7: Phage tail protein

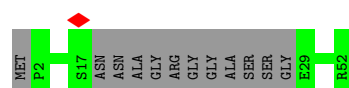
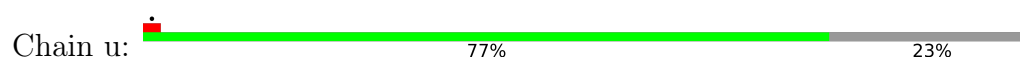




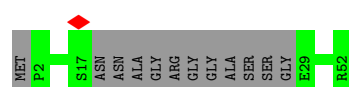
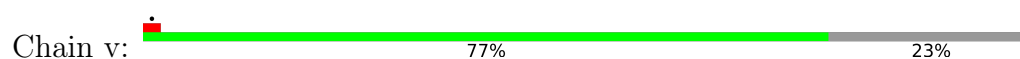
- Molecule 8: inner protein (Algo6)



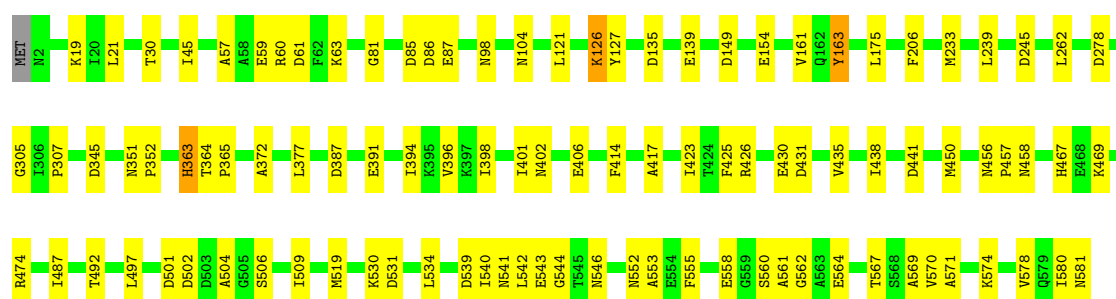
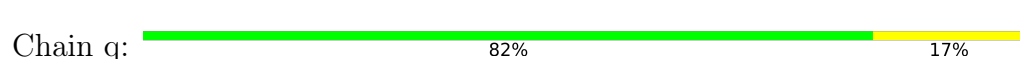
- Molecule 8: inner protein (Algo6)



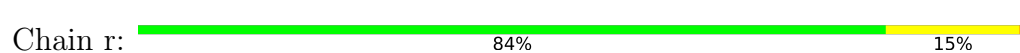
- Molecule 8: inner protein (Algo6)

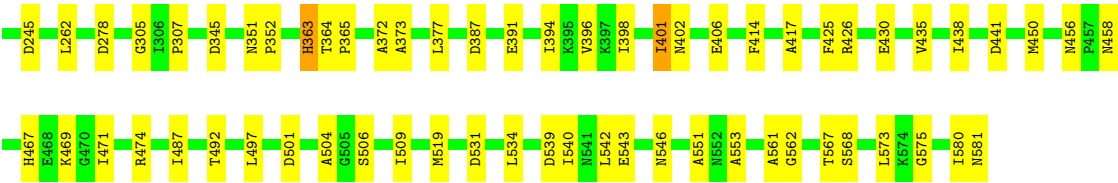


- Molecule 9: Phosphoserine phosphatase SerB

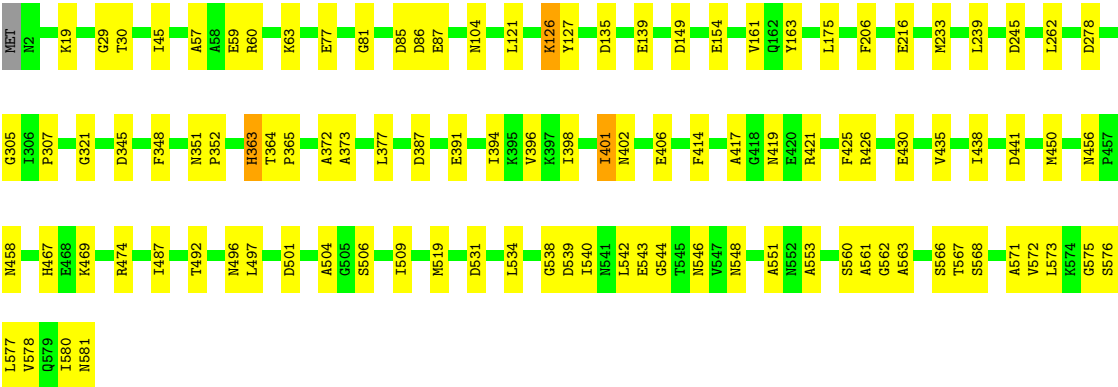
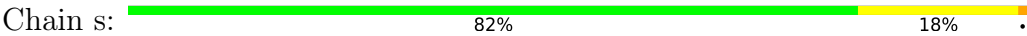


- Molecule 9: Phosphoserine phosphatase SerB





• Molecule 9: Phosphoserine phosphatase SerB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	82969	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.219	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.69	0/4531	1.00	7/6117 (0.1%)
1	B	0.69	0/4531	1.01	7/6117 (0.1%)
1	C	0.69	0/4531	1.00	7/6117 (0.1%)
1	D	0.69	0/4531	1.01	7/6117 (0.1%)
1	E	0.69	0/4531	1.00	7/6117 (0.1%)
1	F	0.69	0/4531	1.01	7/6117 (0.1%)
2	G	0.73	7/7935 (0.1%)	1.08	28/10781 (0.3%)
2	H	0.94	16/7935 (0.2%)	1.18	56/10781 (0.5%)
2	I	0.73	7/7935 (0.1%)	1.08	27/10781 (0.3%)
2	J	0.94	17/7935 (0.2%)	1.18	56/10781 (0.5%)
2	K	0.73	7/7935 (0.1%)	1.08	27/10781 (0.3%)
2	L	0.94	17/7935 (0.2%)	1.18	56/10781 (0.5%)
3	M	0.41	0/1889	0.64	2/2544 (0.1%)
3	N	0.45	0/1889	0.60	0/2544
3	O	0.41	0/1889	0.64	2/2544 (0.1%)
3	P	0.45	0/1889	0.60	0/2544
3	Q	0.41	0/1889	0.64	2/2544 (0.1%)
3	R	0.45	0/1889	0.60	0/2544
4	S	0.64	0/1096	1.03	2/1483 (0.1%)
4	T	0.66	0/1096	1.03	4/1483 (0.3%)
4	U	0.64	0/1096	1.03	2/1483 (0.1%)
4	V	0.66	0/1096	1.03	4/1483 (0.3%)
4	W	0.64	0/1096	1.03	4/1483 (0.3%)
4	X	0.66	0/1096	1.03	4/1483 (0.3%)
5	Y	0.69	0/1226	1.05	3/1664 (0.2%)
5	Z	0.69	0/1226	1.05	3/1664 (0.2%)
5	a	0.69	0/1226	1.05	3/1664 (0.2%)
5	b	0.69	0/1226	1.05	3/1664 (0.2%)
5	c	0.69	0/1226	1.05	3/1664 (0.2%)
5	d	0.69	0/1226	1.05	3/1664 (0.2%)
6	e	0.74	1/5155 (0.0%)	1.09	24/7021 (0.3%)
6	f	0.74	1/5155 (0.0%)	1.09	22/7021 (0.3%)
6	g	0.74	1/5155 (0.0%)	1.09	25/7021 (0.4%)
6	h	0.74	1/5155 (0.0%)	1.09	24/7021 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	i	0.74	1/5155 (0.0%)	1.09	24/7021 (0.3%)
6	j	0.74	1/5155 (0.0%)	1.09	22/7021 (0.3%)
7	k	0.90	0/1172	1.28	15/1584 (0.9%)
7	l	0.90	0/1172	1.28	15/1584 (0.9%)
7	m	0.90	0/1172	1.28	15/1584 (0.9%)
7	n	0.90	0/1172	1.28	15/1584 (0.9%)
7	o	0.90	0/1172	1.28	15/1584 (0.9%)
7	p	0.90	0/1172	1.28	15/1584 (0.9%)
8	t	0.35	0/324	0.48	0/432
8	u	0.35	0/324	0.48	0/432
8	v	0.35	0/324	0.48	0/432
9	q	0.94	1/4536 (0.0%)	1.28	46/6145 (0.7%)
9	r	0.94	2/4536 (0.0%)	1.28	48/6145 (0.8%)
9	s	0.94	1/4536 (0.0%)	1.28	47/6145 (0.8%)
All	All	0.77	81/152604 (0.1%)	1.08	708/206895 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	5
2	H	0	2
2	I	0	4
2	J	0	2
2	K	0	4
2	L	0	2
All	All	0	19

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	509	PRO	C-N	26.38	1.70	1.33
2	I	509	PRO	C-N	26.38	1.70	1.33
2	G	509	PRO	C-N	26.36	1.70	1.33
2	L	506	LYS	C-N	20.74	1.67	1.33
2	H	506	LYS	C-N	20.67	1.67	1.33
2	J	506	LYS	C-N	20.66	1.67	1.33
2	H	433	VAL	C-N	20.24	1.61	1.33
2	J	433	VAL	C-N	20.23	1.61	1.33
2	L	433	VAL	C-N	20.22	1.61	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	357	LEU	C-N	20.20	1.59	1.33
2	H	357	LEU	C-N	20.20	1.59	1.33
2	L	357	LEU	C-N	20.16	1.59	1.33
2	L	304	PHE	C-N	19.75	1.59	1.33
2	H	304	PHE	C-N	19.72	1.59	1.33
2	J	304	PHE	C-N	19.69	1.59	1.33
2	L	446	ARG	C-N	19.69	1.57	1.33
2	H	446	ARG	C-N	19.68	1.57	1.33
2	J	446	ARG	C-N	19.64	1.57	1.33
2	J	731	ASN	C-N	18.31	1.61	1.33
2	H	731	ASN	C-N	18.30	1.61	1.33
2	L	731	ASN	C-N	18.29	1.61	1.33
2	J	765	ALA	C-N	13.01	1.47	1.33
2	I	233	THR	CB-CG2	-13.00	1.09	1.52
2	G	233	THR	CB-CG2	-12.99	1.09	1.52
2	K	233	THR	CB-CG2	-12.99	1.09	1.52
2	H	765	ALA	C-N	12.98	1.47	1.33
2	L	765	ALA	C-N	12.91	1.47	1.33
2	L	547	GLU	C-N	12.76	1.51	1.33
2	H	547	GLU	C-N	12.74	1.51	1.33
2	J	547	GLU	C-N	12.73	1.51	1.33
2	J	214	TYR	C-N	12.54	1.51	1.33
2	L	214	TYR	C-N	12.52	1.51	1.33
2	H	214	TYR	C-N	12.51	1.51	1.33
2	K	506	LYS	C-N	12.28	1.51	1.33
2	G	506	LYS	C-N	12.27	1.51	1.33
2	I	506	LYS	C-N	10.66	1.51	1.33
2	K	403	ARG	CZ-NH1	-10.12	1.18	1.32
2	I	403	ARG	CZ-NH1	-10.09	1.18	1.32
2	G	403	ARG	CZ-NH1	-10.08	1.18	1.32
2	H	587	ALA	C-N	9.79	1.56	1.33
2	J	587	ALA	C-N	9.79	1.56	1.33
2	L	587	ALA	C-N	9.72	1.56	1.33
2	K	766	VAL	C-N	-8.75	1.21	1.33
2	I	766	VAL	C-N	-8.72	1.22	1.33
2	G	766	VAL	C-N	-8.71	1.22	1.33
2	H	447	PRO	N-CA	8.08	1.56	1.46
2	L	447	PRO	N-CA	8.04	1.56	1.46
2	J	447	PRO	N-CA	8.04	1.56	1.46
2	J	446	ARG	CA-C	7.88	1.64	1.52
2	H	446	ARG	CA-C	7.88	1.64	1.52
2	L	446	ARG	CA-C	7.86	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	446	ARG	C-N	6.55	1.42	1.33
2	J	596	GLY	C-N	-6.52	1.24	1.33
2	K	446	ARG	C-N	6.51	1.42	1.33
2	H	596	GLY	C-N	-6.49	1.24	1.33
2	G	446	ARG	C-N	6.46	1.42	1.33
2	L	596	GLY	C-N	-6.36	1.24	1.33
9	q	394	ILE	C-O	-6.05	1.18	1.24
9	s	394	ILE	C-O	-5.99	1.18	1.24
9	r	394	ILE	C-O	-5.95	1.18	1.24
6	j	249	ASP	C-O	-5.92	1.16	1.24
6	f	249	ASP	C-O	-5.91	1.16	1.24
6	i	249	ASP	C-O	-5.87	1.16	1.24
6	g	249	ASP	C-O	-5.86	1.16	1.24
6	h	249	ASP	C-O	-5.86	1.16	1.24
6	e	249	ASP	C-O	-5.84	1.16	1.24
2	J	311	LEU	C-O	-5.48	1.17	1.24
2	L	311	LEU	C-O	-5.48	1.17	1.24
2	H	311	LEU	C-O	-5.46	1.17	1.24
2	K	593	LEU	CG-CD1	-5.35	1.34	1.52
2	I	593	LEU	CG-CD1	-5.33	1.34	1.52
2	G	593	LEU	CG-CD1	-5.31	1.35	1.52
2	J	587	ALA	C-O	-5.30	1.20	1.25
2	L	587	ALA	C-O	-5.27	1.20	1.25
2	H	587	ALA	C-O	-5.25	1.20	1.25
2	H	433	VAL	CA-C	5.07	1.59	1.52
2	L	433	VAL	CA-C	5.06	1.59	1.52
2	J	433	VAL	CA-C	5.04	1.59	1.52
2	L	792	ARG	C-O	-5.02	1.18	1.24
9	r	80	VAL	C-O	-5.01	1.18	1.23
2	J	792	ARG	C-O	-5.01	1.18	1.24

All (708) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	446	ARG	CA-C-N	19.97	141.31	120.14
2	J	446	ARG	C-N-CA	19.97	141.31	120.14
2	H	446	ARG	CA-C-N	19.92	141.25	120.14
2	H	446	ARG	C-N-CA	19.92	141.25	120.14
2	L	446	ARG	CA-C-N	19.91	141.24	120.14
2	L	446	ARG	C-N-CA	19.91	141.24	120.14
2	L	587	ALA	CA-C-N	14.53	138.00	119.84
2	L	587	ALA	C-N-CA	14.53	138.00	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	506	LYS	O-C-N	-14.53	106.15	123.29
2	H	587	ALA	CA-C-N	14.52	137.98	119.84
2	H	587	ALA	C-N-CA	14.52	137.98	119.84
2	G	506	LYS	O-C-N	-14.51	106.16	123.29
2	J	587	ALA	CA-C-N	14.51	137.97	119.84
2	J	587	ALA	C-N-CA	14.51	137.97	119.84
2	I	506	LYS	O-C-N	-14.48	106.21	123.29
2	J	446	ARG	O-C-N	-13.04	112.10	121.23
2	H	446	ARG	O-C-N	-12.99	112.14	121.23
2	L	446	ARG	O-C-N	-12.96	112.16	121.23
2	L	434	LEU	O-C-N	12.01	137.36	123.31
2	H	434	LEU	O-C-N	11.95	137.29	123.31
2	J	434	LEU	O-C-N	11.90	137.23	123.31
2	L	1018	PRO	N-CA-CB	11.08	114.89	103.25
2	J	1018	PRO	N-CA-CB	11.05	114.85	103.25
2	H	1018	PRO	N-CA-CB	11.01	114.81	103.25
2	G	1018	PRO	N-CA-CB	10.71	114.49	103.25
2	I	1018	PRO	N-CA-CB	10.68	114.46	103.25
2	K	1018	PRO	N-CA-CB	10.65	114.43	103.25
2	H	433	VAL	CA-C-N	9.97	138.09	122.74
2	H	433	VAL	C-N-CA	9.97	138.09	122.74
2	L	433	VAL	CA-C-N	9.97	138.09	122.74
2	L	433	VAL	C-N-CA	9.97	138.09	122.74
2	J	433	VAL	CA-C-N	9.96	138.07	122.74
2	J	433	VAL	C-N-CA	9.96	138.07	122.74
2	H	998	SER	N-CA-C	-9.24	98.17	109.72
2	J	998	SER	N-CA-C	-9.24	98.17	109.72
2	L	998	SER	N-CA-C	-9.24	98.17	109.72
9	r	364	THR	CA-C-N	8.99	126.22	119.66
9	r	364	THR	C-N-CA	8.99	126.22	119.66
9	q	364	THR	CA-C-N	8.91	126.16	119.66
9	q	364	THR	C-N-CA	8.91	126.16	119.66
9	s	364	THR	CA-C-N	8.87	126.14	119.66
9	s	364	THR	C-N-CA	8.87	126.14	119.66
2	L	509	PRO	N-CA-C	-8.59	94.78	112.47
2	H	509	PRO	N-CA-C	-8.57	94.81	112.47
2	J	509	PRO	N-CA-C	-8.57	94.81	112.47
2	L	510	LYS	N-CA-C	8.56	122.85	110.10
2	H	510	LYS	N-CA-C	8.55	122.85	110.10
2	J	510	LYS	N-CA-C	8.53	122.82	110.10
9	r	398	ILE	CA-C-N	8.51	128.24	119.56
9	r	398	ILE	C-N-CA	8.51	128.24	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	s	398	ILE	CA-C-N	8.47	128.20	119.56
9	s	398	ILE	C-N-CA	8.47	128.20	119.56
9	q	398	ILE	CA-C-N	8.45	128.18	119.56
9	q	398	ILE	C-N-CA	8.45	128.18	119.56
9	s	30	THR	N-CA-C	-8.38	103.92	114.56
9	q	30	THR	N-CA-C	-8.34	103.97	114.56
9	r	30	THR	N-CA-C	-8.33	103.98	114.56
2	G	506	LYS	CA-C-N	8.28	133.43	122.42
2	G	506	LYS	C-N-CA	8.28	133.43	122.42
2	K	506	LYS	CA-C-N	8.27	133.42	122.42
2	K	506	LYS	C-N-CA	8.27	133.42	122.42
2	I	506	LYS	CA-C-N	8.09	133.36	122.84
2	I	506	LYS	C-N-CA	8.09	133.36	122.84
2	L	797	LYS	CA-C-N	-8.07	105.54	121.91
2	L	797	LYS	C-N-CA	-8.07	105.54	121.91
2	J	797	LYS	CA-C-N	-8.06	105.54	121.91
2	J	797	LYS	C-N-CA	-8.06	105.54	121.91
2	H	797	LYS	CA-C-N	-8.06	105.54	121.91
2	H	797	LYS	C-N-CA	-8.06	105.54	121.91
2	G	1002	PRO	N-CA-CB	8.04	110.47	103.31
2	K	1002	PRO	N-CA-CB	8.00	110.43	103.31
2	J	197	SER	N-CA-C	7.98	121.50	111.69
2	L	197	SER	N-CA-C	7.98	121.50	111.69
2	I	1002	PRO	N-CA-CB	7.98	110.41	103.31
2	H	197	SER	N-CA-C	7.95	121.46	111.69
2	J	1002	PRO	N-CA-CB	7.88	110.33	103.31
2	H	1002	PRO	N-CA-CB	7.88	110.32	103.31
2	L	1002	PRO	N-CA-CB	7.88	110.32	103.31
6	i	420	ASN	N-CA-C	7.75	122.45	112.92
2	G	509	PRO	CA-C-N	7.74	136.32	121.54
2	G	509	PRO	C-N-CA	7.74	136.32	121.54
2	K	999	PRO	N-CA-CB	7.74	110.08	103.35
2	K	509	PRO	CA-C-N	7.71	136.27	121.54
2	K	509	PRO	C-N-CA	7.71	136.27	121.54
6	g	420	ASN	N-CA-C	7.71	122.41	112.92
2	I	509	PRO	CA-C-N	7.71	136.27	121.54
2	I	509	PRO	C-N-CA	7.71	136.27	121.54
6	e	420	ASN	N-CA-C	7.71	122.40	112.92
6	h	420	ASN	N-CA-C	7.70	122.40	112.92
6	j	420	ASN	N-CA-C	7.69	122.38	112.92
2	G	999	PRO	N-CA-CB	7.68	110.03	103.35
2	L	350	SER	N-CA-C	7.67	119.65	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	420	ASN	N-CA-C	7.67	122.35	112.92
2	H	350	SER	N-CA-C	7.66	119.63	111.28
2	I	999	PRO	N-CA-CB	7.63	109.99	103.35
2	J	350	SER	N-CA-C	7.62	119.58	111.28
9	q	492	THR	CA-C-N	7.62	127.33	119.56
9	q	492	THR	C-N-CA	7.62	127.33	119.56
9	s	492	THR	CA-C-N	7.61	127.32	119.56
9	s	492	THR	C-N-CA	7.61	127.32	119.56
9	r	492	THR	CA-C-N	7.59	127.31	119.56
9	r	492	THR	C-N-CA	7.59	127.31	119.56
2	L	446	ARG	CA-C-O	-7.51	113.78	121.06
2	H	446	ARG	CA-C-O	-7.50	113.79	121.06
2	H	587	ALA	O-C-N	-7.49	111.16	121.12
2	J	446	ARG	CA-C-O	-7.49	113.80	121.06
2	J	587	ALA	O-C-N	-7.47	111.18	121.12
2	J	508	PHE	CA-C-N	-7.43	110.55	119.84
2	J	508	PHE	C-N-CA	-7.43	110.55	119.84
2	L	587	ALA	O-C-N	-7.43	111.24	121.12
7	n	41	SER	CA-C-N	7.41	127.12	119.56
7	n	41	SER	C-N-CA	7.41	127.12	119.56
2	H	508	PHE	CA-C-N	-7.41	110.58	119.84
2	H	508	PHE	C-N-CA	-7.41	110.58	119.84
2	L	508	PHE	CA-C-N	-7.38	110.61	119.84
2	L	508	PHE	C-N-CA	-7.38	110.61	119.84
7	l	41	SER	CA-C-N	7.34	127.04	119.56
7	l	41	SER	C-N-CA	7.34	127.04	119.56
2	L	434	LEU	CA-C-N	-7.30	103.98	121.80
2	L	434	LEU	C-N-CA	-7.30	103.98	121.80
7	o	41	SER	CA-C-N	7.30	127.00	119.56
7	o	41	SER	C-N-CA	7.30	127.00	119.56
7	m	41	SER	CA-C-N	7.28	126.98	119.56
7	m	41	SER	C-N-CA	7.28	126.98	119.56
7	p	41	SER	CA-C-N	7.27	126.97	119.56
7	p	41	SER	C-N-CA	7.27	126.97	119.56
2	H	434	LEU	CA-C-N	-7.27	104.07	121.80
2	H	434	LEU	C-N-CA	-7.27	104.07	121.80
2	J	434	LEU	CA-C-N	-7.25	104.10	121.80
2	J	434	LEU	C-N-CA	-7.25	104.10	121.80
2	J	505	VAL	N-CA-C	7.24	119.15	108.65
7	k	41	SER	CA-C-N	7.24	126.94	119.56
7	k	41	SER	C-N-CA	7.24	126.94	119.56
2	H	505	VAL	N-CA-C	7.22	119.12	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	505	VAL	N-CA-C	7.22	119.12	108.65
6	e	525	SER	CA-C-N	7.16	126.83	119.82
6	e	525	SER	C-N-CA	7.16	126.83	119.82
9	q	45	ILE	CA-C-N	7.15	127.15	119.78
9	q	45	ILE	C-N-CA	7.15	127.15	119.78
2	H	999	PRO	N-CA-CB	7.14	109.57	103.35
6	j	448	ASN	CA-C-N	7.14	130.25	120.46
6	j	448	ASN	C-N-CA	7.14	130.25	120.46
9	s	45	ILE	CA-C-N	7.14	127.14	119.78
9	s	45	ILE	C-N-CA	7.14	127.14	119.78
2	J	999	PRO	N-CA-CB	7.14	109.56	103.35
2	L	999	PRO	N-CA-CB	7.13	109.55	103.35
6	g	448	ASN	CA-C-N	7.13	130.23	120.46
6	g	448	ASN	C-N-CA	7.13	130.23	120.46
6	h	448	ASN	CA-C-N	7.13	130.23	120.46
6	h	448	ASN	C-N-CA	7.13	130.23	120.46
9	r	45	ILE	CA-C-N	7.12	127.11	119.78
9	r	45	ILE	C-N-CA	7.12	127.11	119.78
6	f	448	ASN	CA-C-N	7.11	130.21	120.46
6	f	448	ASN	C-N-CA	7.11	130.21	120.46
6	h	525	SER	CA-C-N	7.11	126.79	119.82
6	h	525	SER	C-N-CA	7.11	126.79	119.82
6	i	525	SER	CA-C-N	7.11	126.79	119.82
6	i	525	SER	C-N-CA	7.11	126.79	119.82
2	G	952	PRO	N-CA-CB	7.11	110.59	103.48
6	f	525	SER	CA-C-N	7.11	126.78	119.82
6	f	525	SER	C-N-CA	7.11	126.78	119.82
6	e	448	ASN	CA-C-N	7.10	130.19	120.46
6	e	448	ASN	C-N-CA	7.10	130.19	120.46
6	i	448	ASN	CA-C-N	7.10	130.19	120.46
6	i	448	ASN	C-N-CA	7.10	130.19	120.46
6	g	525	SER	CA-C-N	7.08	126.76	119.82
6	g	525	SER	C-N-CA	7.08	126.76	119.82
2	I	952	PRO	N-CA-CB	7.08	110.56	103.48
6	j	525	SER	CA-C-N	7.08	126.75	119.82
6	j	525	SER	C-N-CA	7.08	126.75	119.82
2	K	952	PRO	N-CA-CB	7.06	110.54	103.48
1	C	466	LYS	CA-C-N	-7.04	111.48	122.67
1	C	466	LYS	C-N-CA	-7.04	111.48	122.67
9	s	387	ASP	CA-C-N	7.03	126.73	119.56
9	s	387	ASP	C-N-CA	7.03	126.73	119.56
1	A	466	LYS	CA-C-N	-7.01	111.52	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	LYS	C-N-CA	-7.01	111.52	122.67
6	j	469	ASN	N-CA-C	7.00	122.81	112.94
9	q	245	ASP	CA-C-N	7.00	127.15	119.87
9	q	245	ASP	C-N-CA	7.00	127.15	119.87
1	E	466	LYS	CA-C-N	-7.00	111.54	122.67
1	E	466	LYS	C-N-CA	-7.00	111.54	122.67
9	r	387	ASP	CA-C-N	7.00	126.69	119.56
9	r	387	ASP	C-N-CA	7.00	126.69	119.56
9	q	387	ASP	CA-C-N	6.98	126.68	119.56
9	q	387	ASP	C-N-CA	6.98	126.68	119.56
9	s	245	ASP	CA-C-N	6.97	127.12	119.87
9	s	245	ASP	C-N-CA	6.97	127.12	119.87
2	L	798	SER	N-CA-C	6.97	119.15	108.42
6	i	469	ASN	N-CA-C	6.96	122.76	112.94
9	r	245	ASP	CA-C-N	6.96	127.11	119.87
9	r	245	ASP	C-N-CA	6.96	127.11	119.87
6	e	469	ASN	N-CA-C	6.96	122.75	112.94
2	J	798	SER	N-CA-C	6.95	119.12	108.42
6	g	469	ASN	N-CA-C	6.95	122.74	112.94
2	H	798	SER	N-CA-C	6.94	119.11	108.42
6	h	469	ASN	N-CA-C	6.93	122.72	112.94
2	H	183	GLY	N-CA-C	6.92	127.84	115.80
2	L	183	GLY	N-CA-C	6.91	127.81	115.80
7	o	107	ASN	N-CA-C	6.90	121.06	111.74
7	m	3	TYR	CA-C-N	6.89	126.85	120.03
7	m	3	TYR	C-N-CA	6.89	126.85	120.03
6	f	469	ASN	N-CA-C	6.88	122.65	112.94
2	J	183	GLY	N-CA-C	6.88	127.77	115.80
7	l	107	ASN	N-CA-C	6.88	121.03	111.74
7	m	107	ASN	N-CA-C	6.87	121.01	111.74
7	k	107	ASN	N-CA-C	6.86	121.01	111.74
7	p	107	ASN	N-CA-C	6.86	121.00	111.74
6	i	81	ASP	CA-CB-CG	6.85	119.45	112.60
6	f	81	ASP	CA-CB-CG	6.84	119.44	112.60
6	e	81	ASP	CA-CB-CG	6.84	119.44	112.60
6	g	81	ASP	CA-CB-CG	6.84	119.44	112.60
7	n	107	ASN	N-CA-C	6.83	120.96	111.74
6	h	81	ASP	CA-CB-CG	6.83	119.43	112.60
2	I	1015	PRO	N-CA-CB	6.82	110.41	103.25
6	j	81	ASP	CA-CB-CG	6.82	119.42	112.60
2	K	1015	PRO	N-CA-CB	6.81	110.40	103.25
9	r	435	VAL	N-CA-C	6.81	117.65	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	l	3	TYR	CA-C-N	6.80	126.76	120.03
7	l	3	TYR	C-N-CA	6.80	126.76	120.03
2	L	952	PRO	N-CA-CB	6.80	110.28	103.48
7	p	3	TYR	CA-C-N	6.79	126.75	120.03
7	p	3	TYR	C-N-CA	6.79	126.75	120.03
2	H	952	PRO	N-CA-CB	6.78	110.26	103.48
2	J	952	PRO	N-CA-CB	6.78	110.26	103.48
7	k	3	TYR	CA-C-N	6.77	126.74	120.03
7	k	3	TYR	C-N-CA	6.77	126.74	120.03
7	o	3	TYR	CA-C-N	6.77	126.73	120.03
7	o	3	TYR	C-N-CA	6.77	126.73	120.03
9	q	435	VAL	N-CA-C	6.77	117.58	108.11
9	s	435	VAL	N-CA-C	6.76	117.57	108.11
2	G	1015	PRO	N-CA-CB	6.75	110.34	103.25
7	n	3	TYR	CA-C-N	6.75	126.71	120.03
7	n	3	TYR	C-N-CA	6.75	126.71	120.03
6	i	17	PHE	CA-C-N	6.74	127.33	120.38
6	i	17	PHE	C-N-CA	6.74	127.33	120.38
6	g	17	PHE	CA-C-N	6.74	127.32	120.38
6	g	17	PHE	C-N-CA	6.74	127.32	120.38
6	h	17	PHE	CA-C-N	6.74	127.32	120.38
6	h	17	PHE	C-N-CA	6.74	127.32	120.38
2	J	718	ILE	O-C-N	6.72	130.00	123.14
2	H	718	ILE	O-C-N	6.71	129.99	123.14
6	j	17	PHE	CA-C-N	6.71	127.29	120.38
6	j	17	PHE	C-N-CA	6.71	127.29	120.38
9	r	175	LEU	CA-CB-CG	6.71	139.77	116.30
6	e	17	PHE	CA-C-N	6.71	127.29	120.38
6	e	17	PHE	C-N-CA	6.71	127.29	120.38
9	s	175	LEU	CA-CB-CG	6.70	139.76	116.30
9	q	175	LEU	CA-CB-CG	6.69	139.73	116.30
9	r	456	ASN	CA-C-N	6.68	126.66	119.78
9	r	456	ASN	C-N-CA	6.68	126.66	119.78
2	L	718	ILE	O-C-N	6.68	129.95	123.14
6	f	17	PHE	CA-C-N	6.67	127.25	120.38
6	f	17	PHE	C-N-CA	6.67	127.25	120.38
9	q	365	PRO	CA-C-N	6.67	126.71	119.90
9	q	365	PRO	C-N-CA	6.67	126.71	119.90
9	s	456	ASN	CA-C-N	6.66	126.64	119.78
9	s	456	ASN	C-N-CA	6.66	126.64	119.78
2	L	433	VAL	O-C-N	-6.65	114.30	122.61
9	q	456	ASN	CA-C-N	6.64	126.62	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	q	456	ASN	C-N-CA	6.64	126.62	119.78
9	s	365	PRO	CA-C-N	6.64	126.67	119.90
9	s	365	PRO	C-N-CA	6.64	126.67	119.90
2	H	1015	PRO	N-CA-CB	6.64	110.22	103.25
2	J	1015	PRO	N-CA-CB	6.64	110.22	103.25
2	L	1015	PRO	N-CA-CB	6.63	110.22	103.25
2	H	433	VAL	O-C-N	-6.63	114.32	122.61
9	r	365	PRO	CA-C-N	6.62	126.66	119.90
9	r	365	PRO	C-N-CA	6.62	126.66	119.90
2	J	433	VAL	O-C-N	-6.62	114.33	122.61
1	C	384	ALA	N-CA-C	6.59	118.19	110.41
1	A	384	ALA	N-CA-C	6.59	118.18	110.41
1	F	384	ALA	N-CA-C	6.58	118.18	110.41
2	J	168	LYS	N-CA-C	6.58	118.45	111.28
2	L	168	LYS	N-CA-C	6.58	118.45	111.28
1	E	384	ALA	N-CA-C	6.55	118.14	110.41
2	G	403	ARG	NE-CZ-NH2	6.55	125.09	119.20
2	I	403	ARG	NE-CZ-NH2	6.55	125.09	119.20
1	B	384	ALA	N-CA-C	6.54	118.13	110.41
1	D	384	ALA	N-CA-C	6.54	118.13	110.41
2	H	168	LYS	N-CA-C	6.53	118.40	111.28
2	K	403	ARG	NE-CZ-NH2	6.51	125.06	119.20
9	q	305	GLY	N-CA-C	6.47	120.34	111.54
9	r	305	GLY	N-CA-C	6.46	120.33	111.54
2	I	658	ASN	CA-C-N	-6.45	112.43	122.37
2	I	658	ASN	C-N-CA	-6.45	112.43	122.37
2	G	658	ASN	CA-C-N	-6.45	112.43	122.37
2	G	658	ASN	C-N-CA	-6.45	112.43	122.37
2	J	801	GLN	CA-C-N	6.45	125.88	118.85
2	J	801	GLN	C-N-CA	6.45	125.88	118.85
9	s	305	GLY	N-CA-C	6.44	120.30	111.54
2	K	658	ASN	CA-C-N	-6.43	112.46	122.37
2	K	658	ASN	C-N-CA	-6.43	112.46	122.37
2	L	801	GLN	CA-C-N	6.41	125.84	118.85
2	L	801	GLN	C-N-CA	6.41	125.84	118.85
2	H	784	GLU	N-CA-C	6.39	120.37	111.74
2	L	784	GLU	N-CA-C	6.39	120.37	111.74
2	J	784	GLU	N-CA-C	6.39	120.36	111.74
1	B	465	ILE	CA-C-N	6.38	129.70	120.38
1	B	465	ILE	C-N-CA	6.38	129.70	120.38
1	F	465	ILE	CA-C-N	6.38	129.70	120.38
1	F	465	ILE	C-N-CA	6.38	129.70	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	GLN	CA-C-N	6.37	125.80	118.85
2	H	801	GLN	C-N-CA	6.37	125.80	118.85
2	K	30	GLU	CB-CA-C	-6.37	99.85	110.68
1	D	465	ILE	CA-C-N	6.36	129.66	120.38
1	D	465	ILE	C-N-CA	6.36	129.66	120.38
2	G	30	GLU	CB-CA-C	-6.35	99.88	110.68
2	I	30	GLU	CB-CA-C	-6.32	99.93	110.68
2	L	511	SER	N-CA-C	6.29	119.04	110.55
2	H	777	LEU	N-CA-C	6.29	118.21	111.36
2	K	857	THR	CA-C-N	6.28	133.37	122.81
2	K	857	THR	C-N-CA	6.28	133.37	122.81
1	C	324	GLU	N-CA-C	6.28	120.50	112.34
2	G	857	THR	CA-C-N	6.28	133.35	122.81
2	G	857	THR	C-N-CA	6.28	133.35	122.81
9	s	345	ASP	CA-CB-CG	6.27	118.87	112.60
1	E	324	GLU	N-CA-C	6.27	120.49	112.34
9	r	414	PHE	CA-C-N	6.25	125.93	119.56
9	r	414	PHE	C-N-CA	6.25	125.93	119.56
2	J	777	LEU	N-CA-C	6.25	118.17	111.36
2	I	857	THR	CA-C-N	6.24	133.30	122.81
2	I	857	THR	C-N-CA	6.24	133.30	122.81
1	A	324	GLU	N-CA-C	6.24	120.45	112.34
2	J	511	SER	N-CA-C	6.24	118.97	110.55
1	F	324	GLU	N-CA-C	6.23	120.44	112.34
2	H	511	SER	N-CA-C	6.23	118.96	110.55
2	H	214	TYR	O-C-N	6.22	131.10	123.44
9	s	414	PHE	CA-C-N	6.22	125.90	119.56
9	s	414	PHE	C-N-CA	6.22	125.90	119.56
2	G	332	LYS	CA-CB-CG	-6.21	101.67	114.10
2	L	777	LEU	N-CA-C	6.21	118.13	111.36
9	q	345	ASP	CA-CB-CG	6.21	118.81	112.60
2	K	332	LYS	CA-CB-CG	-6.21	101.68	114.10
2	L	214	TYR	O-C-N	6.21	131.07	123.44
9	r	345	ASP	CA-CB-CG	6.21	118.81	112.60
1	D	324	GLU	N-CA-C	6.20	120.40	112.34
1	B	324	GLU	N-CA-C	6.20	120.40	112.34
9	q	414	PHE	CA-C-N	6.18	125.86	119.56
9	q	414	PHE	C-N-CA	6.18	125.86	119.56
2	I	332	LYS	CA-CB-CG	-6.18	101.75	114.10
2	J	214	TYR	O-C-N	6.18	131.04	123.44
2	L	506	LYS	O-C-N	-6.17	115.95	123.30
9	r	163	TYR	N-CA-C	6.16	118.49	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	s	163	TYR	N-CA-C	6.16	118.48	108.26
3	O	58	ILE	N-CA-C	6.15	117.01	108.89
9	q	163	TYR	N-CA-C	6.15	118.47	108.26
7	l	49	MET	CA-C-N	6.14	126.08	119.76
7	l	49	MET	C-N-CA	6.14	126.08	119.76
3	M	58	ILE	N-CA-C	6.13	116.98	108.89
2	H	506	LYS	O-C-N	-6.12	116.02	123.30
3	Q	58	ILE	N-CA-C	6.11	116.96	108.89
7	m	49	MET	CA-C-N	6.11	126.06	119.76
7	m	49	MET	C-N-CA	6.11	126.06	119.76
7	p	49	MET	CA-C-N	6.11	126.06	119.76
7	p	49	MET	C-N-CA	6.11	126.06	119.76
2	J	506	LYS	O-C-N	-6.11	116.03	123.30
7	n	49	MET	CA-C-N	6.10	126.04	119.76
7	n	49	MET	C-N-CA	6.10	126.04	119.76
7	o	49	MET	CA-C-N	6.09	126.03	119.76
7	o	49	MET	C-N-CA	6.09	126.03	119.76
7	k	49	MET	CA-C-N	6.08	126.02	119.76
7	k	49	MET	C-N-CA	6.08	126.02	119.76
9	q	161	VAL	N-CA-C	6.04	116.57	108.11
2	K	403	ARG	NH1-CZ-NH2	-6.03	111.47	119.30
9	r	161	VAL	N-CA-C	6.02	116.54	108.11
9	r	406	GLU	N-CA-C	6.01	117.91	111.36
9	q	406	GLU	N-CA-C	6.01	117.91	111.36
9	r	149	ASP	CA-CB-CG	6.00	118.60	112.60
2	G	403	ARG	NH1-CZ-NH2	-6.00	111.51	119.30
9	s	406	GLU	N-CA-C	5.99	117.89	111.36
9	s	161	VAL	N-CA-C	5.98	116.48	108.11
9	q	149	ASP	CA-CB-CG	5.98	118.58	112.60
2	I	403	ARG	NH1-CZ-NH2	-5.97	111.53	119.30
9	s	149	ASP	CA-CB-CG	5.96	118.56	112.60
2	K	268	CYS	CA-CB-SG	-5.92	100.79	114.40
2	G	268	CYS	CA-CB-SG	-5.91	100.82	114.40
2	I	268	CYS	CA-CB-SG	-5.90	100.83	114.40
6	e	418	ALA	N-CA-C	-5.86	106.67	113.88
6	f	418	ALA	N-CA-C	-5.85	106.69	113.88
6	h	418	ALA	N-CA-C	-5.84	106.69	113.88
6	i	418	ALA	N-CA-C	-5.84	106.69	113.88
6	j	418	ALA	N-CA-C	-5.84	106.69	113.88
9	s	396	VAL	N-CA-C	5.84	116.53	108.12
9	q	396	VAL	N-CA-C	5.83	116.52	108.12
6	g	418	ALA	N-CA-C	-5.82	106.72	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	396	VAL	N-CA-C	5.80	116.47	108.12
9	q	506	SER	N-CA-C	5.78	117.97	109.24
9	s	506	SER	N-CA-C	5.77	117.95	109.24
3	Q	226	LYS	N-CA-C	5.76	118.99	110.46
3	M	226	LYS	N-CA-C	5.76	118.98	110.46
9	r	506	SER	N-CA-C	5.76	117.93	109.24
3	O	226	LYS	N-CA-C	5.72	118.93	110.46
7	o	110	PRO	CA-C-N	5.72	128.41	120.29
7	o	110	PRO	C-N-CA	5.72	128.41	120.29
7	l	110	PRO	CA-C-N	5.72	128.41	120.29
7	l	110	PRO	C-N-CA	5.72	128.41	120.29
7	p	110	PRO	CA-C-N	5.72	128.41	120.29
7	p	110	PRO	C-N-CA	5.72	128.41	120.29
6	i	408	THR	N-CA-C	5.71	117.20	108.52
7	m	110	PRO	CA-C-N	5.71	128.40	120.29
7	m	110	PRO	C-N-CA	5.71	128.40	120.29
2	L	794	SER	N-CA-C	5.71	117.50	111.28
6	e	408	THR	N-CA-C	5.71	117.19	108.52
2	J	794	SER	N-CA-C	5.70	117.50	111.28
6	g	408	THR	N-CA-C	5.70	117.19	108.52
6	f	408	THR	N-CA-C	5.70	117.18	108.52
6	j	408	THR	N-CA-C	5.70	117.18	108.52
7	k	110	PRO	CA-C-N	5.69	128.38	120.29
7	k	110	PRO	C-N-CA	5.69	128.38	120.29
6	h	408	THR	N-CA-C	5.69	117.17	108.52
7	n	110	PRO	CA-C-N	5.69	128.37	120.29
7	n	110	PRO	C-N-CA	5.69	128.37	120.29
9	r	262	LEU	N-CA-C	5.69	118.25	111.71
9	q	262	LEU	N-CA-C	5.68	118.24	111.71
2	H	794	SER	N-CA-C	5.67	117.46	111.28
2	J	508	PHE	CA-CB-CG	-5.66	108.14	113.80
7	m	100	VAL	N-CA-C	-5.66	107.15	111.62
2	H	508	PHE	CA-CB-CG	-5.65	108.15	113.80
9	s	262	LEU	N-CA-C	5.64	118.20	111.71
7	l	100	VAL	N-CA-C	-5.64	107.17	111.62
2	G	508	PHE	CA-CB-CG	-5.63	108.17	113.80
7	l	98	GLU	CA-C-N	5.63	125.56	119.76
7	l	98	GLU	C-N-CA	5.63	125.56	119.76
2	K	508	PHE	CA-CB-CG	-5.62	108.18	113.80
7	o	98	GLU	CA-C-N	5.62	125.54	119.76
7	o	98	GLU	C-N-CA	5.62	125.54	119.76
2	L	508	PHE	CA-CB-CG	-5.61	108.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	i	676	ARG	CA-C-N	5.61	125.80	120.31
6	i	676	ARG	C-N-CA	5.61	125.80	120.31
7	p	100	VAL	N-CA-C	-5.60	107.19	111.62
7	k	100	VAL	N-CA-C	-5.60	107.20	111.62
9	r	121	LEU	N-CA-C	5.59	120.38	113.50
6	g	676	ARG	CA-C-N	5.59	125.79	120.31
6	g	676	ARG	C-N-CA	5.59	125.79	120.31
2	I	508	PHE	CA-CB-CG	-5.58	108.22	113.80
7	p	98	GLU	CA-C-N	5.58	125.51	119.76
7	p	98	GLU	C-N-CA	5.58	125.51	119.76
6	f	676	ARG	CA-C-N	5.57	125.77	120.31
6	f	676	ARG	C-N-CA	5.57	125.77	120.31
7	m	98	GLU	CA-C-N	5.57	125.50	119.76
7	m	98	GLU	C-N-CA	5.57	125.50	119.76
6	j	676	ARG	CA-C-N	5.57	125.77	120.31
6	j	676	ARG	C-N-CA	5.57	125.77	120.31
6	i	136	THR	CA-C-N	5.57	126.11	120.38
6	i	136	THR	C-N-CA	5.57	126.11	120.38
7	k	98	GLU	CA-C-N	5.57	125.50	119.76
7	k	98	GLU	C-N-CA	5.57	125.50	119.76
9	r	426	ARG	CA-C-N	5.57	125.47	119.85
9	r	426	ARG	C-N-CA	5.57	125.47	119.85
6	e	676	ARG	CA-C-N	5.56	125.76	120.31
6	e	676	ARG	C-N-CA	5.56	125.76	120.31
7	n	100	VAL	N-CA-C	-5.56	107.22	111.62
1	D	372	ASP	N-CA-C	5.56	117.42	111.36
6	h	676	ARG	CA-C-N	5.55	125.75	120.31
6	h	676	ARG	C-N-CA	5.55	125.75	120.31
6	e	136	THR	CA-C-N	5.55	126.09	120.38
6	e	136	THR	C-N-CA	5.55	126.09	120.38
9	q	121	LEU	N-CA-C	5.54	120.32	113.50
1	B	372	ASP	N-CA-C	5.54	117.40	111.36
1	F	372	ASP	N-CA-C	5.54	117.40	111.36
7	n	98	GLU	CA-C-N	5.54	125.47	119.76
7	n	98	GLU	C-N-CA	5.54	125.47	119.76
7	o	100	VAL	N-CA-C	-5.54	107.24	111.62
6	h	136	THR	CA-C-N	5.54	126.08	120.38
6	h	136	THR	C-N-CA	5.54	126.08	120.38
9	q	426	ARG	CA-C-N	5.54	125.44	119.85
9	q	426	ARG	C-N-CA	5.54	125.44	119.85
6	f	420	ASN	CA-C-N	-5.53	112.87	120.28
6	f	420	ASN	C-N-CA	-5.53	112.87	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	q	401	ILE	N-CA-C	-5.53	106.80	111.56
9	s	121	LEU	N-CA-C	5.53	120.30	113.50
6	g	420	ASN	CA-C-N	-5.53	112.87	120.28
6	g	420	ASN	C-N-CA	-5.53	112.87	120.28
6	j	136	THR	CA-C-N	5.53	126.07	120.38
6	j	136	THR	C-N-CA	5.53	126.07	120.38
9	s	401	ILE	N-CA-C	-5.53	106.81	111.56
6	j	420	ASN	CA-C-N	-5.52	112.88	120.28
6	j	420	ASN	C-N-CA	-5.52	112.88	120.28
6	g	136	THR	CA-C-N	5.52	126.07	120.38
6	g	136	THR	C-N-CA	5.52	126.07	120.38
9	s	426	ARG	CA-C-N	5.52	125.43	119.85
9	s	426	ARG	C-N-CA	5.52	125.43	119.85
6	f	136	THR	CA-C-N	5.52	126.06	120.38
6	f	136	THR	C-N-CA	5.52	126.06	120.38
6	i	420	ASN	CA-C-N	-5.51	112.89	120.28
6	i	420	ASN	C-N-CA	-5.51	112.89	120.28
1	C	159	TYR	N-CA-C	5.51	118.71	109.95
1	D	350	VAL	N-CA-C	5.51	116.28	110.72
6	h	420	ASN	CA-C-N	-5.51	112.90	120.28
6	h	420	ASN	C-N-CA	-5.51	112.90	120.28
9	r	401	ILE	N-CA-C	-5.51	106.83	111.56
1	B	350	VAL	N-CA-C	5.48	116.25	110.72
1	F	350	VAL	N-CA-C	5.47	116.24	110.72
2	L	191	LYS	N-CA-C	5.46	118.57	110.48
1	A	159	TYR	N-CA-C	5.46	118.64	109.95
1	E	159	TYR	N-CA-C	5.46	118.63	109.95
6	e	420	ASN	CA-C-N	-5.46	112.96	120.28
6	e	420	ASN	C-N-CA	-5.46	112.96	120.28
2	H	191	LYS	N-CA-C	5.45	118.55	110.48
2	J	765	ALA	O-C-N	-5.45	115.53	122.78
2	L	357	LEU	CA-C-N	5.44	130.45	121.86
2	L	357	LEU	C-N-CA	5.44	130.45	121.86
2	J	357	LEU	CA-C-N	5.44	130.45	121.86
2	J	357	LEU	C-N-CA	5.44	130.45	121.86
2	H	765	ALA	O-C-N	-5.43	115.55	122.78
2	L	765	ALA	O-C-N	-5.43	115.55	122.78
9	r	504	ALA	N-CA-C	-5.43	107.30	114.04
2	H	357	LEU	CA-C-N	5.42	130.43	121.86
2	H	357	LEU	C-N-CA	5.42	130.43	121.86
2	J	191	LYS	N-CA-C	5.42	118.51	110.48
1	F	159	TYR	N-CA-C	5.42	118.57	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	267	ILE	N-CA-C	5.42	115.62	110.53
9	q	504	ALA	N-CA-C	-5.42	107.32	114.04
1	B	159	TYR	N-CA-C	5.42	118.56	109.95
9	s	504	ALA	N-CA-C	-5.40	107.34	114.04
2	K	511	SER	N-CA-C	5.40	117.69	110.35
7	k	93	LEU	N-CA-C	5.39	118.52	109.95
1	D	159	TYR	N-CA-C	5.39	118.52	109.95
2	L	796	ILE	CB-CA-C	-5.39	104.41	111.25
2	J	796	ILE	CB-CA-C	-5.38	104.42	111.25
7	n	93	LEU	N-CA-C	5.38	118.50	109.95
2	I	511	SER	N-CA-C	5.37	117.65	110.35
7	o	93	LEU	N-CA-C	5.37	118.48	109.95
7	m	93	LEU	N-CA-C	5.36	118.47	109.95
7	p	93	LEU	N-CA-C	5.36	118.47	109.95
2	H	267	ILE	N-CA-C	5.35	115.56	110.53
2	H	796	ILE	CB-CA-C	-5.35	104.45	111.25
7	l	93	LEU	N-CA-C	5.35	118.46	109.95
2	G	511	SER	N-CA-C	5.35	117.62	110.35
7	p	132	LEU	N-CA-C	5.35	118.20	109.59
7	n	132	LEU	N-CA-C	5.34	118.19	109.59
7	k	132	LEU	N-CA-C	5.33	118.18	109.59
7	m	132	LEU	N-CA-C	5.33	118.17	109.59
9	r	501	ASP	N-CA-C	5.33	117.34	108.02
7	o	132	LEU	N-CA-C	5.33	118.16	109.59
9	s	441	ASP	CA-C-N	5.32	126.50	119.84
9	s	441	ASP	C-N-CA	5.32	126.50	119.84
9	r	487	ILE	N-CA-C	5.32	115.55	108.11
4	V	88	GLU	CA-C-N	5.32	124.98	119.56
4	V	88	GLU	C-N-CA	5.32	124.98	119.56
9	r	441	ASP	CA-C-N	5.31	126.48	119.84
9	r	441	ASP	C-N-CA	5.31	126.48	119.84
7	l	132	LEU	N-CA-C	5.31	118.14	109.59
9	q	487	ILE	N-CA-C	5.31	115.54	108.11
2	J	267	ILE	N-CA-C	5.30	115.52	110.53
2	H	766	VAL	N-CA-C	5.30	114.84	108.06
5	Y	90	LYS	CA-C-N	5.30	125.24	119.78
5	Y	90	LYS	C-N-CA	5.30	125.24	119.78
5	c	90	LYS	CA-C-N	5.30	125.24	119.78
5	c	90	LYS	C-N-CA	5.30	125.24	119.78
9	q	501	ASP	N-CA-C	5.30	117.29	108.02
2	J	766	VAL	N-CA-C	5.30	114.84	108.06
5	b	90	LYS	CA-C-N	5.29	125.23	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	90	LYS	C-N-CA	5.29	125.23	119.78
9	s	458	ASN	CA-C-N	5.29	124.95	119.56
9	s	458	ASN	C-N-CA	5.29	124.95	119.56
4	T	88	GLU	CA-C-N	5.29	124.95	119.56
4	T	88	GLU	C-N-CA	5.29	124.95	119.56
9	q	458	ASN	CA-C-N	5.29	124.95	119.56
9	q	458	ASN	C-N-CA	5.29	124.95	119.56
5	Z	90	LYS	CA-C-N	5.28	125.22	119.78
5	Z	90	LYS	C-N-CA	5.28	125.22	119.78
9	s	487	ILE	N-CA-C	5.28	115.51	108.11
7	m	91	SER	N-CA-C	5.28	118.04	108.69
4	U	88	GLU	CA-C-N	5.28	124.95	119.56
4	U	88	GLU	C-N-CA	5.28	124.95	119.56
2	L	766	VAL	N-CA-C	5.28	114.81	108.06
7	l	91	SER	N-CA-C	5.28	118.03	108.69
9	q	441	ASP	CA-C-N	5.28	126.44	119.84
9	q	441	ASP	C-N-CA	5.28	126.44	119.84
9	s	501	ASP	N-CA-C	5.27	117.25	108.02
4	X	88	GLU	CA-C-N	5.27	124.94	119.56
4	X	88	GLU	C-N-CA	5.27	124.94	119.56
5	d	90	LYS	CA-C-N	5.27	125.21	119.78
5	d	90	LYS	C-N-CA	5.27	125.21	119.78
7	n	91	SER	N-CA-C	5.27	118.02	108.69
2	J	803	TYR	CA-C-N	5.27	125.21	119.78
2	J	803	TYR	C-N-CA	5.27	125.21	119.78
9	r	458	ASN	CA-C-N	5.27	124.94	119.56
9	r	458	ASN	C-N-CA	5.27	124.94	119.56
5	a	90	LYS	CA-C-N	5.27	125.21	119.78
5	a	90	LYS	C-N-CA	5.27	125.21	119.78
7	p	91	SER	N-CA-C	5.27	118.01	108.69
9	r	497	LEU	N-CA-C	5.27	117.39	109.23
7	k	91	SER	N-CA-C	5.26	118.00	108.69
9	q	135	ASP	N-CA-C	-5.26	105.61	112.23
2	J	780	GLY	N-CA-C	5.25	120.55	112.51
5	c	94	LEU	CA-CB-CG	5.25	134.68	116.30
2	L	681	PHE	CB-CA-C	-5.25	104.45	112.11
7	o	91	SER	N-CA-C	5.25	117.98	108.69
4	S	88	GLU	CA-C-N	5.25	124.91	119.56
4	S	88	GLU	C-N-CA	5.25	124.91	119.56
2	K	797	LYS	CA-C-N	5.24	131.12	121.85
2	K	797	LYS	C-N-CA	5.24	131.12	121.85
2	L	780	GLY	N-CA-C	5.23	120.52	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	803	TYR	CA-C-N	5.23	125.17	119.78
2	H	803	TYR	C-N-CA	5.23	125.17	119.78
2	J	779	LYS	N-CA-C	-5.23	100.37	108.90
5	Y	94	LEU	CA-CB-CG	5.23	134.62	116.30
4	W	88	GLU	CA-C-N	5.23	124.89	119.56
4	W	88	GLU	C-N-CA	5.23	124.89	119.56
5	Z	94	LEU	CA-CB-CG	5.23	134.61	116.30
9	r	135	ASP	N-CA-C	-5.23	105.64	112.23
9	s	135	ASP	N-CA-C	-5.23	105.64	112.23
5	d	94	LEU	CA-CB-CG	5.23	134.60	116.30
9	q	497	LEU	N-CA-C	5.23	117.33	109.23
2	G	797	LYS	CA-C-N	5.23	131.10	121.85
2	G	797	LYS	C-N-CA	5.23	131.10	121.85
5	b	94	LEU	CA-CB-CG	5.22	134.59	116.30
2	H	681	PHE	CB-CA-C	-5.22	104.48	112.11
2	H	780	GLY	N-CA-C	5.22	120.50	112.51
2	I	797	LYS	CA-C-N	5.22	131.09	121.85
2	I	797	LYS	C-N-CA	5.22	131.09	121.85
9	s	497	LEU	N-CA-C	5.22	117.32	109.23
5	a	94	LEU	CA-CB-CG	5.22	134.57	116.30
2	H	779	LYS	N-CA-C	-5.22	100.40	108.90
2	L	803	TYR	CA-C-N	5.22	125.15	119.78
2	L	803	TYR	C-N-CA	5.22	125.15	119.78
6	j	94	VAL	CA-C-N	5.22	125.42	120.31
6	j	94	VAL	C-N-CA	5.22	125.42	120.31
6	e	94	VAL	CA-C-N	5.21	125.42	120.31
6	e	94	VAL	C-N-CA	5.21	125.42	120.31
2	J	681	PHE	CB-CA-C	-5.20	104.52	112.11
2	L	779	LYS	N-CA-C	-5.19	100.44	108.90
2	L	357	LEU	CA-C-O	-5.18	115.29	121.56
6	g	94	VAL	CA-C-N	5.17	125.38	120.31
6	g	94	VAL	C-N-CA	5.17	125.38	120.31
6	h	94	VAL	CA-C-N	5.17	125.37	120.31
6	h	94	VAL	C-N-CA	5.17	125.37	120.31
2	H	357	LEU	CA-C-O	-5.16	115.31	121.56
2	J	357	LEU	CA-C-O	-5.16	115.31	121.56
9	s	363	HIS	CA-C-N	5.16	127.56	120.39
9	s	363	HIS	C-N-CA	5.16	127.56	120.39
2	K	536	GLU	CB-CA-C	-5.16	102.55	110.81
2	I	536	GLU	CB-CA-C	-5.13	102.61	110.81
6	f	94	VAL	CA-C-N	5.13	125.33	120.31
6	f	94	VAL	C-N-CA	5.13	125.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	i	94	VAL	CA-C-N	5.13	125.34	120.31
6	i	94	VAL	C-N-CA	5.13	125.34	120.31
9	r	363	HIS	CA-C-N	5.13	127.52	120.39
9	r	363	HIS	C-N-CA	5.13	127.52	120.39
2	G	536	GLU	CB-CA-C	-5.12	102.61	110.81
9	q	363	HIS	CA-C-N	5.12	127.51	120.39
9	q	363	HIS	C-N-CA	5.12	127.51	120.39
1	A	474	ASP	CA-C-N	5.12	124.78	119.56
1	A	474	ASP	C-N-CA	5.12	124.78	119.56
1	C	474	ASP	CA-C-N	5.11	124.77	119.56
1	C	474	ASP	C-N-CA	5.11	124.77	119.56
2	I	920	GLU	CA-C-N	5.11	129.46	121.85
2	I	920	GLU	C-N-CA	5.11	129.46	121.85
2	J	788	LYS	N-CA-C	5.11	116.95	109.24
9	r	126	LYS	N-CA-C	5.11	116.83	108.76
2	G	920	GLU	CA-C-N	5.10	129.46	121.85
2	G	920	GLU	C-N-CA	5.10	129.46	121.85
6	j	503	LEU	CA-C-N	5.10	123.39	119.66
6	j	503	LEU	C-N-CA	5.10	123.39	119.66
2	K	920	GLU	CA-C-N	5.10	129.45	121.85
2	K	920	GLU	C-N-CA	5.10	129.45	121.85
2	J	352	SER	N-CA-C	5.10	117.26	110.53
6	h	503	LEU	CA-C-N	5.09	123.38	119.66
6	h	503	LEU	C-N-CA	5.09	123.38	119.66
6	i	503	LEU	CA-C-N	5.09	123.38	119.66
6	i	503	LEU	C-N-CA	5.09	123.38	119.66
1	E	474	ASP	CA-C-N	5.08	124.74	119.56
1	E	474	ASP	C-N-CA	5.08	124.74	119.56
6	g	503	LEU	CA-C-N	5.08	123.36	119.66
6	g	503	LEU	C-N-CA	5.08	123.36	119.66
2	H	352	SER	N-CA-C	5.07	117.22	110.53
6	f	503	LEU	CA-C-N	5.07	123.36	119.66
6	f	503	LEU	C-N-CA	5.07	123.36	119.66
9	q	126	LYS	N-CA-C	5.07	116.76	108.76
2	L	788	LYS	N-CA-C	5.06	116.89	109.24
2	H	788	LYS	N-CA-C	5.06	116.88	109.24
6	e	260	PRO	CB-CG-CD	5.06	122.28	106.10
6	f	260	PRO	CB-CG-CD	5.06	122.28	106.10
6	g	260	PRO	CB-CG-CD	5.05	122.26	106.10
2	L	352	SER	N-CA-C	5.05	117.19	110.53
6	e	503	LEU	CA-C-N	5.05	123.35	119.66
6	e	503	LEU	C-N-CA	5.05	123.35	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	i	169	LEU	CA-C-N	5.05	125.33	119.47
6	i	169	LEU	C-N-CA	5.05	125.33	119.47
6	j	260	PRO	CB-CG-CD	5.05	122.25	106.10
6	h	260	PRO	CB-CG-CD	5.04	122.22	106.10
4	T	51	ILE	CA-C-N	-5.04	114.75	122.60
4	T	51	ILE	C-N-CA	-5.04	114.75	122.60
4	V	51	ILE	CA-C-N	-5.04	114.74	122.60
4	V	51	ILE	C-N-CA	-5.04	114.74	122.60
6	e	169	LEU	CA-C-N	5.04	125.31	119.47
6	e	169	LEU	C-N-CA	5.04	125.31	119.47
9	s	126	LYS	N-CA-C	5.04	116.72	108.76
4	X	51	ILE	CA-C-N	-5.03	114.75	122.60
4	X	51	ILE	C-N-CA	-5.03	114.75	122.60
6	i	260	PRO	CB-CG-CD	5.03	122.21	106.10
6	g	169	LEU	CA-C-N	5.03	125.30	119.47
6	g	169	LEU	C-N-CA	5.03	125.30	119.47
9	r	193	LYS	CA-C-N	5.02	125.02	119.90
9	r	193	LYS	C-N-CA	5.02	125.02	119.90
9	s	348	PHE	CA-CB-CG	5.02	118.82	113.80
2	G	784	GLU	N-CA-C	5.02	120.77	113.40
6	h	163	PHE	CA-C-N	5.02	124.68	119.56
6	h	163	PHE	C-N-CA	5.02	124.68	119.56
4	W	51	ILE	CA-C-N	-5.00	114.79	122.60
4	W	51	ILE	C-N-CA	-5.00	114.79	122.60
2	I	315	GLU	CB-CG-CD	5.00	121.10	112.60
2	K	784	GLU	N-CA-C	5.00	120.76	113.40
2	G	315	GLU	CB-CG-CD	5.00	121.10	112.60
6	g	386	LYS	N-CA-C	5.00	117.38	107.98

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	364	GLU	Sidechain
2	G	48	ASN	Sidechain
2	G	492	ASP	Sidechain
2	G	635	ASN	Sidechain
2	G	642	ASP	Sidechain
2	H	596	GLY	Mainchain
2	H	875	ASP	Sidechain
2	I	364	GLU	Sidechain
2	I	492	ASP	Sidechain

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Mol	Chain	Res	Type	Group
2	I	635	ASN	Sidechain
2	I	642	ASP	Sidechain
2	J	596	GLY	Mainchain
2	J	875	ASP	Sidechain
2	K	364	GLU	Sidechain
2	K	492	ASP	Sidechain
2	K	635	ASN	Sidechain
2	K	642	ASP	Sidechain
2	L	596	GLY	Mainchain
2	L	875	ASP	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4447	0	4459	56	0
1	B	4447	0	4459	45	0
1	C	4447	0	4459	53	0
1	D	4447	0	4459	96	0
1	E	4447	0	4459	57	0
1	F	4447	0	4459	100	0
2	G	7762	0	7320	70	0
2	H	7762	0	7321	58	0
2	I	7762	0	7320	77	0
2	J	7762	0	7321	111	0
2	K	7762	0	7320	79	0
2	L	7762	0	7321	105	0
3	M	1849	0	1819	19	0
3	N	1849	0	1819	17	0
3	O	1849	0	1819	20	0
3	P	1849	0	1819	20	0
3	Q	1849	0	1819	20	0
3	R	1849	0	1819	20	0
4	S	1074	0	1076	17	0
4	T	1074	0	1076	15	0
4	U	1074	0	1076	18	0
4	V	1074	0	1076	16	0
4	W	1074	0	1076	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	X	1074	0	1076	13	0
5	Y	1192	0	1147	11	0
5	Z	1192	0	1147	12	0
5	a	1192	0	1147	12	0
5	b	1192	0	1147	13	0
5	c	1192	0	1147	13	0
5	d	1192	0	1147	11	0
6	e	5057	0	4910	62	0
6	f	5057	0	4910	63	0
6	g	5057	0	4910	61	0
6	h	5057	0	4910	60	0
6	i	5057	0	4910	62	0
6	j	5057	0	4910	59	0
7	k	1145	0	1118	12	0
7	l	1145	0	1118	10	0
7	m	1145	0	1118	12	0
7	n	1145	0	1118	13	0
7	o	1145	0	1118	12	0
7	p	1145	0	1118	11	0
8	t	324	0	337	0	0
8	u	324	0	337	0	0
8	v	324	0	337	0	0
9	q	4469	0	4361	107	0
9	r	4469	0	4361	91	0
9	s	4469	0	4361	113	0
All	All	149535	0	145191	1387	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 5.

All (1387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:506:LYS:C	2:L:507:SER:N	1.67	1.50
2:G:509:PRO:C	2:G:510:LYS:N	1.70	1.49
2:H:506:LYS:C	2:H:507:SER:N	1.67	1.48
2:J:506:LYS:C	2:J:507:SER:N	1.67	1.47
2:I:509:PRO:C	2:I:510:LYS:N	1.70	1.47
2:K:509:PRO:C	2:K:510:LYS:N	1.70	1.45
9:q:553:ALA:O	9:s:561:ALA:HB3	1.17	1.27
2:H:169:ASN:ND2	9:q:430:GLU:OE2	1.66	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:561:ALA:HB3	9:s:553:ALA:O	1.19	1.25
6:h:260:PRO:HG3	6:h:468:VAL:O	1.44	1.18
6:e:260:PRO:HG3	6:e:468:VAL:O	1.44	1.17
6:j:260:PRO:HG3	6:j:468:VAL:O	1.44	1.17
1:F:318:TRP:CD2	2:I:985:ILE:O	1.96	1.16
6:f:260:PRO:HG3	6:f:468:VAL:O	1.44	1.16
6:i:260:PRO:HG3	6:i:468:VAL:O	1.44	1.16
6:g:260:PRO:HG3	6:g:468:VAL:O	1.44	1.15
1:D:318:TRP:CD2	2:K:985:ILE:O	2.00	1.15
1:D:488:LEU:HD22	2:L:49:PHE:HD1	1.04	1.14
1:F:488:LEU:HD22	2:J:49:PHE:HD1	1.04	1.13
1:D:253:MET:HG3	2:L:149:HIS:HB2	1.28	1.11
1:D:488:LEU:HD22	2:L:49:PHE:CD1	1.84	1.11
9:q:561:ALA:HB3	9:r:553:ALA:O	1.52	1.10
1:D:254:ASP:OD1	2:L:150:LEU:CD2	1.99	1.09
1:F:488:LEU:HD22	2:J:49:PHE:CD1	1.86	1.09
9:q:534:LEU:HD12	9:s:542:LEU:CD2	1.80	1.09
1:F:254:ASP:OD1	2:J:150:LEU:CD2	2.01	1.08
1:F:253:MET:HG3	2:J:149:HIS:HB2	1.27	1.08
1:D:509:ARG:HH12	2:L:139:HIS:CD2	1.76	1.04
9:q:553:ALA:O	9:s:561:ALA:CB	2.05	1.03
1:F:254:ASP:OD1	2:J:150:LEU:HD22	1.57	1.03
1:C:318:TRP:CD2	2:J:985:ILE:O	2.12	1.03
9:q:540:ILE:HD11	9:s:543:GLU:O	1.59	1.02
9:q:450:MET:HE2	9:s:417:ALA:O	1.58	1.02
9:r:543:GLU:O	9:s:540:ILE:HD11	1.60	1.02
6:g:249:ASP:O	6:g:477:LEU:HD22	1.61	1.01
1:F:509:ARG:HH12	2:J:139:HIS:CD2	1.78	1.01
6:i:249:ASP:O	6:i:477:LEU:HD22	1.61	1.01
1:A:318:TRP:CD2	2:L:985:ILE:O	2.13	1.00
1:D:254:ASP:OD1	2:L:150:LEU:HD22	1.56	1.00
1:F:318:TRP:CG	2:I:985:ILE:O	2.15	1.00
6:f:249:ASP:O	6:f:477:LEU:HD22	1.61	1.00
6:j:249:ASP:O	6:j:477:LEU:HD22	1.61	1.00
6:h:249:ASP:O	6:h:477:LEU:HD22	1.61	1.00
6:e:249:ASP:O	6:e:477:LEU:HD22	1.61	1.00
9:r:561:ALA:CB	9:s:553:ALA:O	2.09	0.99
9:r:567:THR:OG1	9:s:562:GLY:HA2	1.61	0.98
1:E:318:TRP:CD2	2:H:985:ILE:O	2.16	0.98
9:q:534:LEU:HD12	9:s:542:LEU:HD21	1.44	0.97
1:D:318:TRP:CG	2:K:985:ILE:O	2.16	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:NZ	6:e:85:GLU:OE1	1.98	0.96
1:B:318:TRP:CD2	2:G:985:ILE:O	2.18	0.96
9:r:543:GLU:O	9:s:540:ILE:CD1	2.13	0.95
9:q:531:ASP:OD1	9:s:539:ASP:O	1.84	0.95
1:E:89:LYS:NZ	6:g:85:GLU:OE1	1.98	0.95
1:D:473:LYS:HG2	2:L:54:HIS:CD2	2.02	0.94
9:r:567:THR:OG1	9:s:562:GLY:CA	2.16	0.94
9:q:509:ILE:HG22	9:r:519:MET:HE1	1.49	0.94
1:B:89:LYS:NZ	6:f:85:GLU:OE1	1.99	0.93
6:e:83:LEU:HD21	6:e:86:GLY:H	1.33	0.93
6:i:83:LEU:HD21	6:i:86:GLY:H	1.33	0.93
2:G:806:THR:HG22	2:G:807:LYS:HG3	1.51	0.92
6:h:83:LEU:HD21	6:h:86:GLY:H	1.33	0.92
6:j:83:LEU:HD21	6:j:86:GLY:H	1.33	0.92
2:K:806:THR:HG22	2:K:807:LYS:HG3	1.51	0.91
9:q:539:ASP:OD1	9:s:546:ASN:HB2	1.69	0.91
1:D:89:LYS:NZ	6:j:85:GLU:OE1	2.03	0.91
1:F:473:LYS:HG2	2:J:54:HIS:CD2	2.04	0.91
2:I:806:THR:HG22	2:I:807:LYS:HG3	1.52	0.91
6:f:83:LEU:HD21	6:f:86:GLY:H	1.33	0.91
6:g:83:LEU:HD21	6:g:86:GLY:H	1.33	0.91
6:h:83:LEU:HD21	6:h:86:GLY:N	1.86	0.91
6:f:83:LEU:HD21	6:f:86:GLY:N	1.86	0.91
6:i:83:LEU:HD21	6:i:86:GLY:N	1.86	0.91
9:r:417:ALA:O	9:s:450:MET:HE2	1.71	0.91
6:e:83:LEU:HD21	6:e:86:GLY:N	1.86	0.91
1:F:509:ARG:HH12	2:J:139:HIS:HD2	0.98	0.90
2:J:169:ASN:ND2	9:r:430:GLU:OE2	2.04	0.90
1:F:89:LYS:NZ	6:h:85:GLU:OE1	2.03	0.90
1:D:473:LYS:NZ	2:L:67:ASP:HB3	1.86	0.90
1:C:89:LYS:NZ	6:i:85:GLU:OE1	2.03	0.90
1:E:318:TRP:CG	2:H:985:ILE:O	2.24	0.90
6:g:83:LEU:HD21	6:g:86:GLY:N	1.86	0.90
1:D:509:ARG:HH12	2:L:139:HIS:HD2	0.97	0.89
1:F:258:GLU:HA	2:J:824:ARG:NH2	1.86	0.89
6:j:83:LEU:HD21	6:j:86:GLY:N	1.86	0.89
9:s:59:GLU:O	9:s:60:ARG:HB2	1.73	0.88
1:D:121:ARG:HB2	2:L:907:PHE:HE2	1.39	0.88
2:L:169:ASN:ND2	9:s:430:GLU:OE2	2.06	0.88
1:F:473:LYS:NZ	2:J:67:ASP:HB3	1.88	0.88
1:D:254:ASP:OD1	2:L:150:LEU:HD21	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:260:PRO:HG3	6:j:468:VAL:C	1.99	0.88
6:h:260:PRO:HG3	6:h:468:VAL:C	1.99	0.88
6:g:260:PRO:HG3	6:g:468:VAL:C	1.99	0.87
1:B:318:TRP:CG	2:G:985:ILE:O	2.26	0.87
1:F:96:SER:HB2	2:J:828:LYS:HB3	1.57	0.87
1:D:511:ALA:HB2	2:L:822:SER:OG	1.74	0.87
2:J:221:LYS:NZ	2:J:407:GLU:OE1	2.08	0.87
6:e:260:PRO:HG3	6:e:468:VAL:C	1.99	0.87
6:i:260:PRO:HG3	6:i:468:VAL:C	1.99	0.87
9:r:59:GLU:O	9:r:60:ARG:HB2	1.73	0.86
2:L:221:LYS:NZ	2:L:407:GLU:OE1	2.08	0.86
9:q:59:GLU:O	9:q:60:ARG:HB2	1.73	0.86
6:f:260:PRO:HG3	6:f:468:VAL:C	1.99	0.86
1:A:318:TRP:CG	2:L:985:ILE:O	2.28	0.86
2:H:221:LYS:NZ	2:H:407:GLU:OE1	2.08	0.85
1:F:254:ASP:OD1	2:J:150:LEU:HD21	1.75	0.85
6:i:408:THR:HG23	6:i:411:GLU:HG2	1.58	0.85
9:q:540:ILE:CD1	9:s:543:GLU:O	2.24	0.85
1:D:258:GLU:HA	2:L:824:ARG:NH2	1.92	0.85
9:r:542:LEU:CD2	9:s:534:LEU:HD12	2.07	0.85
1:C:318:TRP:CG	2:J:985:ILE:O	2.29	0.85
1:F:10:ILE:HG13	3:N:224:LEU:HD23	1.59	0.84
6:j:408:THR:HG23	6:j:411:GLU:HG2	1.59	0.84
6:h:408:THR:HG23	6:h:411:GLU:HG2	1.59	0.84
1:B:10:ILE:HG13	3:R:224:LEU:HD23	1.59	0.84
1:F:121:ARG:HB2	2:J:907:PHE:HE2	1.42	0.84
6:g:408:THR:HG23	6:g:411:GLU:HG2	1.59	0.83
6:f:408:THR:HG23	6:f:411:GLU:HG2	1.58	0.83
1:D:10:ILE:HG13	3:P:224:LEU:HD23	1.59	0.83
1:D:509:ARG:NH1	2:L:139:HIS:HD2	1.77	0.83
1:F:511:ALA:HB2	2:J:822:SER:OG	1.80	0.82
1:E:34:LYS:HD2	4:U:127:TYR:CE1	2.13	0.82
1:D:488:LEU:CD2	2:L:49:PHE:CD1	2.63	0.82
6:e:408:THR:HG23	6:e:411:GLU:HG2	1.59	0.82
1:A:34:LYS:HD2	4:S:127:TYR:CE1	2.15	0.82
9:r:509:ILE:HG22	9:s:519:MET:HE1	1.60	0.82
1:F:34:LYS:HD2	4:V:127:TYR:CE1	2.15	0.81
9:q:402:ASN:HB3	9:s:127:TYR:HE1	1.44	0.81
1:D:488:LEU:CD2	2:L:49:PHE:HD1	1.91	0.81
1:C:318:TRP:CE2	2:J:985:ILE:O	2.33	0.81
1:D:254:ASP:CG	2:L:150:LEU:HD22	2.06	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:83:LEU:CD2	6:h:86:GLY:H	1.94	0.81
6:g:83:LEU:CD2	6:g:86:GLY:H	1.95	0.80
6:f:83:LEU:CD2	6:f:86:GLY:H	1.95	0.80
9:q:233:MET:HE2	9:r:391:GLU:OE1	1.82	0.80
9:r:567:THR:OG1	9:s:562:GLY:N	2.15	0.80
1:D:457:TYR:HE2	2:L:35:GLN:NE2	1.80	0.80
6:i:83:LEU:CD2	6:i:86:GLY:H	1.94	0.80
6:j:83:LEU:HD21	6:j:86:GLY:CA	2.12	0.80
1:A:318:TRP:CE2	2:L:985:ILE:O	2.34	0.80
1:D:96:SER:HB2	2:L:828:LYS:HB3	1.62	0.80
6:i:83:LEU:HD21	6:i:86:GLY:CA	2.12	0.80
1:C:34:LYS:HD2	4:W:127:TYR:CE1	2.17	0.79
4:X:36:GLN:HE22	6:j:685:PHE:HB2	1.46	0.79
1:D:239:ARG:NH2	1:D:363:ARG:HD3	1.97	0.79
6:h:83:LEU:HD21	6:h:86:GLY:CA	2.12	0.79
1:F:254:ASP:CG	2:J:150:LEU:HD22	2.06	0.79
6:e:83:LEU:HD21	6:e:86:GLY:CA	2.12	0.79
1:F:239:ARG:NH2	1:F:363:ARG:HD3	1.97	0.79
6:e:83:LEU:CD2	6:e:86:GLY:H	1.94	0.79
9:q:417:ALA:O	9:r:450:MET:HE2	1.83	0.79
1:B:239:ARG:NH2	1:B:363:ARG:HD3	1.97	0.79
1:F:457:TYR:CZ	2:J:37:PHE:CE1	2.71	0.79
6:f:83:LEU:HD21	6:f:86:GLY:CA	2.12	0.78
1:F:36:LEU:O	2:J:109:GLY:HA2	1.84	0.78
6:g:83:LEU:HD21	6:g:86:GLY:CA	2.12	0.78
6:j:83:LEU:CD2	6:j:86:GLY:H	1.94	0.78
1:F:488:LEU:CD2	2:J:49:PHE:CD1	2.65	0.78
1:F:488:LEU:CD2	2:J:49:PHE:HD1	1.91	0.78
1:D:36:LEU:O	2:L:109:GLY:HA2	1.84	0.77
1:B:34:LYS:HD2	4:T:127:TYR:CE1	2.19	0.77
1:E:283:LEU:HD23	1:E:304:LEU:HG	1.67	0.76
9:q:402:ASN:HB3	9:s:127:TYR:CE1	2.19	0.76
6:e:408:THR:CG2	6:e:411:GLU:HG2	2.16	0.76
6:j:408:THR:CG2	6:j:411:GLU:HG2	2.16	0.76
9:r:546:ASN:HB2	9:s:539:ASP:OD1	1.85	0.76
6:f:408:THR:CG2	6:f:411:GLU:HG2	2.16	0.76
6:g:408:THR:CG2	6:g:411:GLU:HG2	2.16	0.76
1:F:473:LYS:HZ1	2:J:67:ASP:HB3	1.49	0.76
1:D:34:LYS:HD2	4:X:127:TYR:CE1	2.20	0.76
4:S:36:GLN:HE22	6:e:685:PHE:HB2	1.51	0.76
1:F:509:ARG:NH1	2:J:139:HIS:HD2	1.79	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:408:THR:CG2	6:i:411:GLU:HG2	2.16	0.75
6:h:408:THR:CG2	6:h:411:GLU:HG2	2.16	0.75
9:q:163:TYR:CD1	9:r:401:ILE:HG12	2.21	0.75
9:q:544:GLY:O	9:s:551:ALA:HA	1.86	0.75
9:s:87:GLU:OE1	9:s:307:PRO:CG	2.35	0.75
9:r:87:GLU:OE1	9:r:307:PRO:CG	2.35	0.75
9:q:87:GLU:OE1	9:q:307:PRO:CG	2.35	0.75
1:D:457:TYR:CZ	2:L:37:PHE:CE1	2.75	0.75
6:f:512:ALA:HB1	6:f:529:ILE:HD12	1.69	0.74
1:A:512:GLU:OE2	2:G:826:ARG:HD2	1.86	0.74
6:j:512:ALA:HB1	6:j:529:ILE:HD12	1.69	0.74
9:q:567:THR:O	9:s:575:GLY:HA2	1.87	0.74
1:F:508:ALA:CB	2:J:26:LYS:O	2.35	0.74
1:A:283:LEU:HD23	1:A:304:LEU:HG	1.67	0.74
1:C:283:LEU:HD23	1:C:304:LEU:HG	1.67	0.74
6:i:512:ALA:HB1	6:i:529:ILE:HD12	1.69	0.74
1:F:219:GLU:HB3	1:F:347:LEU:HD21	1.69	0.74
3:R:175:TYR:CE1	4:S:6:LYS:HE2	2.23	0.74
6:e:512:ALA:HB1	6:e:529:ILE:HD12	1.69	0.74
6:f:473:LEU:HD22	6:f:481:ILE:HG22	1.69	0.74
6:g:473:LEU:HD22	6:g:481:ILE:HG22	1.70	0.74
1:B:219:GLU:HB3	1:B:347:LEU:HD21	1.69	0.73
1:F:457:TYR:HE2	2:J:35:GLN:NE2	1.86	0.73
3:N:175:TYR:CE1	4:U:6:LYS:HE2	2.24	0.73
6:h:473:LEU:HD22	6:h:481:ILE:HG22	1.70	0.73
9:q:567:THR:OG1	9:r:562:GLY:HA2	1.88	0.73
1:A:409:PRO:HD2	6:e:547:GLU:OE2	1.88	0.73
4:T:36:GLN:HE22	6:f:685:PHE:HB2	1.51	0.73
1:D:508:ALA:CB	2:L:26:LYS:O	2.36	0.73
1:E:133:GLN:N	1:E:133:GLN:OE1	2.21	0.73
2:K:315:GLU:HB2	2:K:348:ILE:HB	1.71	0.73
9:r:542:LEU:HD21	9:s:534:LEU:HD12	1.69	0.73
1:C:133:GLN:N	1:C:133:GLN:OE1	2.21	0.73
3:O:46:ASN:ND2	9:r:104:ASN:O	2.22	0.73
9:r:567:THR:CB	9:s:562:GLY:HA2	2.19	0.73
1:B:39:ASN:HB2	2:H:109:GLY:O	1.89	0.73
1:D:253:MET:HG3	2:L:149:HIS:CB	2.15	0.73
1:A:133:GLN:OE1	1:A:133:GLN:N	2.21	0.72
7:n:33:ILE:HD11	7:o:111:LEU:HD12	1.71	0.72
9:q:87:GLU:OE1	9:q:307:PRO:HG3	1.89	0.72
1:E:409:PRO:HD2	6:g:547:GLU:OE2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:315:GLU:HB2	2:I:348:ILE:HB	1.71	0.72
3:M:175:TYR:CE1	4:T:6:LYS:HE2	2.24	0.72
6:e:473:LEU:HD22	6:e:481:ILE:HG22	1.70	0.72
7:l:33:ILE:HD11	7:m:111:LEU:HD12	1.70	0.72
9:r:87:GLU:OE1	9:r:307:PRO:HG3	1.88	0.72
1:C:10:ILE:HG13	3:O:224:LEU:HD23	1.72	0.72
6:g:512:ALA:HB1	6:g:529:ILE:HD12	1.69	0.72
6:h:512:ALA:HB1	6:h:529:ILE:HD12	1.69	0.72
1:D:219:GLU:HB3	1:D:347:LEU:HD21	1.69	0.72
3:P:175:TYR:CE1	4:W:6:LYS:HE2	2.23	0.72
7:m:33:ILE:HD11	7:n:111:LEU:HD12	1.71	0.72
2:G:174:LYS:HD2	2:G:199:GLU:OE2	1.89	0.72
2:I:174:LYS:HD2	2:I:199:GLU:OE2	1.89	0.72
1:A:89:LYS:HZ1	6:e:85:GLU:CD	1.96	0.72
2:G:315:GLU:HB2	2:G:348:ILE:HB	1.71	0.72
4:V:36:GLN:HE22	6:h:685:PHE:HB2	1.53	0.72
7:o:33:ILE:HD11	7:p:111:LEU:HD12	1.71	0.72
6:i:473:LEU:HD22	6:i:481:ILE:HG22	1.70	0.72
4:U:36:GLN:HE22	6:g:685:PHE:HB2	1.54	0.71
9:s:87:GLU:OE1	9:s:307:PRO:HG3	1.89	0.71
6:j:473:LEU:HD22	6:j:481:ILE:HG22	1.70	0.71
2:K:174:LYS:HD2	2:K:199:GLU:OE2	1.89	0.71
2:K:626:GLN:NE2	2:K:629:THR:HG22	2.06	0.71
7:k:33:ILE:HD11	7:l:111:LEU:HD12	1.71	0.71
1:A:10:ILE:HG13	3:Q:224:LEU:HD23	1.71	0.70
2:G:661:GLN:HA	2:G:722:SER:HA	1.73	0.70
2:I:626:GLN:NE2	2:I:629:THR:HG22	2.06	0.70
2:K:661:GLN:HA	2:K:722:SER:HA	1.73	0.70
7:k:111:LEU:HD12	7:p:33:ILE:HD11	1.71	0.70
1:D:409:PRO:HD2	6:j:547:GLU:OE2	1.91	0.70
1:D:473:LYS:HZ1	2:L:67:ASP:HB3	1.54	0.70
2:J:661:GLN:HA	2:J:722:SER:HA	1.73	0.70
1:B:409:PRO:HD2	6:f:547:GLU:OE2	1.91	0.70
9:q:539:ASP:O	9:r:531:ASP:OD1	2.09	0.70
6:h:255:HIS:O	6:h:256:LEU:HD23	1.92	0.70
5:d:27:GLU:HB3	7:p:38:HIS:ND1	2.06	0.70
1:B:133:GLN:N	1:B:133:GLN:OE1	2.22	0.70
2:L:661:GLN:HA	2:L:722:SER:HA	1.73	0.70
5:Y:123:ASP:OD1	5:d:32:SER:HB2	1.92	0.70
9:q:561:ALA:CB	9:r:553:ALA:O	2.35	0.70
1:A:89:LYS:NZ	6:e:85:GLU:CD	2.50	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:661:GLN:HA	2:I:722:SER:HA	1.73	0.69
6:f:83:LEU:C	6:f:83:LEU:HD23	2.17	0.69
6:g:83:LEU:C	6:g:83:LEU:HD23	2.17	0.69
6:j:478:LEU:HD22	6:j:481:ILE:HD11	1.74	0.69
6:e:255:HIS:O	6:e:256:LEU:HD23	1.92	0.69
1:F:133:GLN:OE1	1:F:133:GLN:N	2.22	0.69
2:G:616:LEU:HB2	2:G:628:PHE:HB3	1.74	0.69
2:G:626:GLN:NE2	2:G:629:THR:HG22	2.06	0.69
3:O:175:TYR:CE1	4:V:6:LYS:HE2	2.27	0.69
6:j:255:HIS:O	6:j:256:LEU:HD23	1.92	0.69
2:H:169:ASN:ND2	9:q:430:GLU:CD	2.51	0.69
6:e:83:LEU:C	6:e:83:LEU:HD23	2.17	0.69
6:h:83:LEU:C	6:h:83:LEU:HD23	2.17	0.69
6:i:83:LEU:HD23	6:i:83:LEU:C	2.17	0.69
9:q:363:HIS:CE1	9:r:373:ALA:H	2.10	0.69
9:r:543:GLU:O	9:s:540:ILE:HD12	1.92	0.69
1:E:10:ILE:HG13	3:M:224:LEU:HD23	1.72	0.69
2:I:616:LEU:HB2	2:I:628:PHE:HB3	1.74	0.69
6:f:255:HIS:O	6:f:256:LEU:HD23	1.92	0.69
1:E:89:LYS:NZ	6:g:85:GLU:CD	2.50	0.69
6:e:478:LEU:HD22	6:e:481:ILE:HD11	1.74	0.69
6:g:255:HIS:O	6:g:256:LEU:HD23	1.92	0.69
1:D:491:LYS:CG	2:L:91:PHE:HE2	2.06	0.69
2:H:661:GLN:HA	2:H:722:SER:HA	1.73	0.69
5:c:27:GLU:HB3	7:o:38:HIS:ND1	2.06	0.69
5:c:32:SER:HB2	5:d:123:ASP:OD1	1.93	0.69
6:i:255:HIS:O	6:i:256:LEU:HD23	1.92	0.69
6:j:83:LEU:C	6:j:83:LEU:HD23	2.17	0.69
9:q:57:ALA:HA	9:s:206:PHE:CE2	2.27	0.69
1:D:133:GLN:OE1	1:D:133:GLN:N	2.22	0.69
5:a:32:SER:HB2	5:b:123:ASP:OD1	1.93	0.69
1:F:253:MET:HG3	2:J:149:HIS:CB	2.15	0.69
2:H:310:ILE:HG22	2:H:311:LEU:HG	1.75	0.69
6:i:478:LEU:HD22	6:i:481:ILE:HD11	1.74	0.68
1:F:90:VAL:CG1	2:J:148:LEU:HA	2.23	0.68
1:F:409:PRO:HD2	6:h:547:GLU:OE2	1.94	0.68
2:K:616:LEU:HB2	2:K:628:PHE:HB3	1.74	0.68
4:W:36:GLN:HE22	6:i:685:PHE:HB2	1.56	0.68
5:Z:32:SER:HB2	5:a:123:ASP:OD1	1.93	0.68
1:F:89:LYS:HZ1	6:h:85:GLU:CD	1.99	0.68
2:J:310:ILE:HG22	2:J:311:LEU:HG	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:175:TYR:CE1	4:X:6:LYS:HE2	2.29	0.68
1:F:491:LYS:CG	2:J:91:PHE:HE2	2.06	0.68
5:b:32:SER:HB2	5:c:123:ASP:OD1	1.94	0.68
1:A:39:ASN:HB2	2:G:109:GLY:O	1.94	0.68
1:B:89:LYS:NZ	6:f:85:GLU:CD	2.51	0.68
1:C:409:PRO:HD2	6:i:547:GLU:OE2	1.94	0.68
6:f:478:LEU:HD22	6:f:481:ILE:HD11	1.74	0.68
2:H:193:THR:HG23	2:H:768:GLU:HB3	1.76	0.68
1:D:90:VAL:CG1	2:L:148:LEU:HA	2.24	0.67
2:J:471:GLN:HE22	2:J:530:ASP:CG	2.02	0.67
3:R:71:ASP:OD1	3:R:149:THR:HG22	1.95	0.67
3:O:71:ASP:OD1	3:O:149:THR:HG22	1.95	0.67
1:E:159:TYR:CZ	2:I:908:HIS:NE2	2.61	0.67
3:P:71:ASP:OD1	3:P:149:THR:HG22	1.95	0.67
3:Q:71:ASP:OD1	3:Q:149:THR:HG22	1.95	0.67
3:N:71:ASP:OD1	3:N:149:THR:HG22	1.95	0.67
9:q:519:MET:HE1	9:s:509:ILE:HG22	1.76	0.67
6:h:478:LEU:HD22	6:h:481:ILE:HD11	1.74	0.67
2:J:193:THR:HG23	2:J:768:GLU:HB3	1.76	0.67
5:Y:105:PRO:HD3	6:e:615:ASN:OD1	1.95	0.67
6:g:478:LEU:HD22	6:g:481:ILE:HD11	1.74	0.67
3:N:172:MET:HE2	4:U:120:ASN:O	1.94	0.67
9:r:233:MET:HE2	9:s:391:GLU:OE1	1.93	0.67
2:L:310:ILE:HG22	2:L:311:LEU:HG	1.75	0.67
2:H:471:GLN:HE22	2:H:530:ASP:CG	2.02	0.66
2:I:297:THR:O	2:I:419:VAL:HA	1.95	0.66
3:M:71:ASP:OD1	3:M:149:THR:HG22	1.95	0.66
2:L:193:THR:HG23	2:L:768:GLU:HB3	1.76	0.66
3:R:172:MET:HE2	4:S:120:ASN:O	1.96	0.66
5:Y:3:THR:HG22	5:Y:4:TYR:H	1.61	0.66
2:G:297:THR:O	2:G:419:VAL:HA	1.95	0.66
5:Z:3:THR:HG22	5:Z:4:TYR:H	1.61	0.66
1:D:473:LYS:HA	2:L:54:HIS:CE1	2.30	0.66
2:L:471:GLN:HE22	2:L:530:ASP:CG	2.02	0.66
9:q:530:LYS:O	9:s:538:GLY:HA3	1.96	0.66
1:F:457:TYR:CE1	2:J:37:PHE:HE1	2.14	0.66
2:K:297:THR:O	2:K:419:VAL:HA	1.95	0.66
5:d:105:PRO:HD3	6:j:615:ASN:OD1	1.95	0.66
5:c:3:THR:HG22	5:c:4:TYR:H	1.61	0.66
9:q:543:GLU:O	9:r:540:ILE:CD1	2.44	0.66
3:M:172:MET:HE2	4:T:120:ASN:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:TYR:CZ	2:K:908:HIS:NE2	2.63	0.65
1:E:89:LYS:HZ1	6:g:85:GLU:CD	2.03	0.65
1:F:473:LYS:HA	2:J:54:HIS:CE1	2.30	0.65
1:B:89:LYS:HZ1	6:f:85:GLU:CD	2.02	0.65
1:E:93:ILE:O	2:I:828:LYS:NZ	2.30	0.65
5:a:3:THR:HG22	5:a:4:TYR:H	1.61	0.65
1:B:10:ILE:CG1	3:R:224:LEU:HD23	2.26	0.65
3:P:172:MET:HE2	4:W:120:ASN:O	1.96	0.65
5:b:3:THR:HG22	5:b:4:TYR:H	1.61	0.65
1:D:425:TYR:OH	2:L:117:LEU:HD12	1.97	0.65
9:r:127:TYR:CE1	9:s:402:ASN:HB3	2.32	0.65
5:d:3:THR:HG22	5:d:4:TYR:H	1.61	0.65
9:q:206:PHE:CE1	9:r:101:ILE:HD13	2.32	0.65
9:q:543:GLU:O	9:r:540:ILE:HD11	1.97	0.65
5:a:105:PRO:HD3	6:g:615:ASN:OD1	1.97	0.64
9:q:552:ASN:O	9:s:560:SER:OG	2.14	0.64
9:q:562:GLY:CA	9:s:567:THR:OG1	2.45	0.64
1:D:10:ILE:CG1	3:P:224:LEU:HD23	2.26	0.64
1:F:10:ILE:CG1	3:N:224:LEU:HD23	2.25	0.64
5:Y:32:SER:HB2	5:Z:123:ASP:OD1	1.96	0.64
9:q:539:ASP:CG	9:s:546:ASN:HB2	2.21	0.64
9:q:569:ALA:O	9:s:576:SER:OG	2.09	0.64
2:L:217:ILE:H	2:L:645:HIS:CD2	2.15	0.64
5:c:105:PRO:HD3	6:i:615:ASN:OD1	1.97	0.64
1:D:89:LYS:NZ	6:j:85:GLU:CD	2.56	0.64
9:q:450:MET:CE	9:s:417:ALA:O	2.42	0.64
9:r:539:ASP:O	9:s:531:ASP:OD1	2.15	0.64
5:b:105:PRO:HD3	6:h:615:ASN:OD1	1.97	0.64
1:B:280:GLU:HG2	1:B:321:CYS:SG	2.38	0.64
1:C:512:GLU:OE2	2:K:826:ARG:HD2	1.97	0.64
2:K:626:GLN:HE21	2:K:629:THR:HG22	1.63	0.64
4:V:15:PHE:O	4:V:17:PRO:HD3	1.98	0.64
4:X:15:PHE:O	4:X:17:PRO:HD3	1.98	0.64
6:i:83:LEU:HD21	6:i:86:GLY:HA2	1.80	0.64
1:F:258:GLU:HA	2:J:824:ARG:HH22	1.59	0.64
1:F:280:GLU:HG2	1:F:321:CYS:SG	2.38	0.64
2:G:626:GLN:HE21	2:G:629:THR:HG22	1.63	0.64
3:O:172:MET:HE2	4:V:120:ASN:O	1.98	0.64
6:h:83:LEU:HD21	6:h:86:GLY:HA2	1.80	0.64
1:D:280:GLU:HG2	1:D:321:CYS:SG	2.38	0.64
1:D:457:TYR:CE1	2:L:37:PHE:HE1	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:GLU:OE2	2:I:826:ARG:HD2	1.97	0.64
2:J:217:ILE:H	2:J:645:HIS:CD2	2.15	0.64
2:J:434:LEU:O	2:J:436:PRO:HD3	1.98	0.64
4:S:15:PHE:O	4:S:17:PRO:HD3	1.98	0.64
4:T:15:PHE:O	4:T:17:PRO:HD3	1.98	0.64
4:U:46:LYS:NZ	4:U:61:ASP:OD2	2.31	0.64
2:H:217:ILE:H	2:H:645:HIS:CD2	2.15	0.63
4:U:15:PHE:O	4:U:17:PRO:HD3	1.98	0.63
1:C:93:ILE:O	2:K:828:LYS:NZ	2.30	0.63
4:V:46:LYS:NZ	4:V:61:ASP:OD2	2.31	0.63
4:W:15:PHE:O	4:W:17:PRO:HD3	1.98	0.63
9:q:431:ASP:OD2	9:s:421:ARG:NH2	2.32	0.63
1:A:318:TRP:CD1	2:L:985:ILE:O	2.50	0.63
2:L:215:ASN:HB2	2:L:236:PHE:CE2	2.34	0.63
4:W:46:LYS:NZ	4:W:61:ASP:OD2	2.31	0.63
6:j:83:LEU:HD21	6:j:86:GLY:HA2	1.80	0.63
2:H:434:LEU:O	2:H:436:PRO:HD3	1.98	0.63
9:q:509:ILE:CG2	9:r:519:MET:HE1	2.26	0.63
2:I:626:GLN:HE21	2:I:629:THR:HG22	1.63	0.63
4:X:46:LYS:NZ	4:X:61:ASP:OD2	2.31	0.63
9:q:546:ASN:HB2	9:r:539:ASP:OD1	1.99	0.63
1:A:99:THR:HG23	1:A:189:ASN:OD1	1.99	0.63
1:C:99:THR:HG23	1:C:189:ASN:OD1	1.99	0.63
2:J:215:ASN:HB2	2:J:236:PHE:CE2	2.34	0.63
5:Y:48:GLU:O	5:Z:58:LYS:NZ	2.32	0.63
5:Z:36:VAL:O	5:Z:37:ASP:OD2	2.17	0.63
5:Z:105:PRO:HD3	6:f:615:ASN:OD1	1.98	0.63
2:H:215:ASN:HB2	2:H:236:PHE:CE2	2.34	0.63
6:g:83:LEU:HD21	6:g:86:GLY:HA2	1.80	0.63
1:B:339:PHE:HE2	1:B:344:PRO:HG3	1.64	0.63
1:C:89:LYS:NZ	6:i:85:GLU:CD	2.57	0.63
1:D:339:PHE:CE2	1:D:344:PRO:HG3	2.34	0.62
4:S:46:LYS:NZ	4:S:61:ASP:OD2	2.31	0.62
5:a:36:VAL:O	5:a:37:ASP:OD2	2.17	0.62
1:F:339:PHE:HE2	1:F:344:PRO:HG3	1.64	0.62
9:q:425:PHE:CD2	9:r:469:LYS:HD2	2.34	0.62
1:D:99:THR:HG23	1:D:189:ASN:OD1	1.99	0.62
1:D:258:GLU:HA	2:L:824:ARG:HH22	1.64	0.62
1:D:473:LYS:HZ2	2:L:67:ASP:HB3	1.63	0.62
2:L:434:LEU:O	2:L:436:PRO:HD3	1.98	0.62
5:c:36:VAL:O	5:c:37:ASP:OD2	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:q:562:GLY:HA2	9:s:567:THR:OG1	1.98	0.62
1:F:99:THR:HG23	1:F:189:ASN:OD1	1.99	0.62
2:J:991:LEU:H	2:J:1005:ILE:H	1.48	0.62
2:L:991:LEU:H	2:L:1005:ILE:H	1.48	0.62
3:P:162:THR:HG21	9:r:29:GLY:O	1.99	0.62
4:T:46:LYS:NZ	4:T:61:ASP:OD2	2.31	0.62
1:B:99:THR:HG23	1:B:189:ASN:OD1	1.99	0.62
1:B:339:PHE:CE2	1:B:344:PRO:HG3	2.34	0.62
1:D:339:PHE:HE2	1:D:344:PRO:HG3	1.64	0.62
9:q:562:GLY:N	9:s:567:THR:OG1	2.32	0.62
1:C:318:TRP:CD1	2:J:985:ILE:O	2.52	0.62
1:F:339:PHE:CE2	1:F:344:PRO:HG3	2.34	0.62
2:H:991:LEU:H	2:H:1005:ILE:H	1.48	0.62
2:K:114:HIS:CE1	4:W:24:GLY:O	2.53	0.62
5:d:36:VAL:O	5:d:37:ASP:OD2	2.17	0.62
1:A:10:ILE:CG1	3:Q:224:LEU:HD23	2.29	0.62
6:i:684:LYS:HD3	6:j:17:PHE:HZ	1.65	0.62
5:Y:36:VAL:O	5:Y:37:ASP:OD2	2.17	0.62
1:C:10:ILE:CG1	3:O:224:LEU:HD23	2.30	0.62
5:b:36:VAL:O	5:b:37:ASP:OD2	2.17	0.61
6:f:83:LEU:HD21	6:f:86:GLY:HA2	1.80	0.61
6:e:684:LYS:HD3	6:f:17:PHE:HZ	1.64	0.61
6:h:684:LYS:HD3	6:i:17:PHE:HZ	1.65	0.61
1:A:512:GLU:OE1	2:G:826:ARG:NH1	2.33	0.61
6:e:512:ALA:HB1	6:e:529:ILE:CD1	2.30	0.61
1:D:68:ILE:HG21	2:L:131:ARG:HG2	1.83	0.61
1:F:89:LYS:NZ	6:h:85:GLU:CD	2.57	0.61
1:F:96:SER:CB	2:J:828:LYS:HB3	2.30	0.61
6:e:83:LEU:HD21	6:e:86:GLY:HA2	1.80	0.61
6:h:248:ALA:HB1	6:h:478:LEU:HD12	1.83	0.61
6:j:478:LEU:O	6:j:481:ILE:HG12	2.01	0.61
6:h:512:ALA:HB1	6:h:529:ILE:CD1	2.30	0.61
9:r:575:GLY:HA2	9:s:567:THR:O	2.01	0.61
1:E:99:THR:HG23	1:E:189:ASN:OD1	1.99	0.61
6:e:478:LEU:O	6:e:481:ILE:HG12	2.01	0.61
6:g:512:ALA:HB1	6:g:529:ILE:CD1	2.30	0.61
9:q:474:ARG:HH22	9:r:467:HIS:HD2	1.47	0.61
9:q:567:THR:OG1	9:r:562:GLY:CA	2.48	0.61
6:f:512:ALA:HB1	6:f:529:ILE:CD1	2.30	0.61
6:g:248:ALA:HB1	6:g:478:LEU:HD12	1.83	0.61
6:i:248:ALA:HB1	6:i:478:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ILE:HG21	2:J:131:ARG:HG2	1.83	0.61
6:h:224:THR:HG22	6:h:225:LYS:N	2.16	0.61
6:i:224:THR:HG22	6:i:225:LYS:N	2.16	0.61
6:j:512:ALA:HB1	6:j:529:ILE:CD1	2.30	0.61
6:e:17:PHE:HZ	6:j:684:LYS:HD3	1.66	0.60
3:R:162:THR:HG21	9:s:29:GLY:O	2.01	0.60
6:i:478:LEU:O	6:i:481:ILE:HG12	2.01	0.60
1:F:457:TYR:CZ	2:J:37:PHE:CD1	2.90	0.60
3:Q:172:MET:HE2	4:X:120:ASN:O	2.02	0.60
6:e:224:THR:HG22	6:e:225:LYS:N	2.16	0.60
6:f:478:LEU:O	6:f:481:ILE:HG12	2.01	0.60
6:j:248:ALA:HB1	6:j:478:LEU:HD12	1.83	0.60
6:f:248:ALA:HB1	6:f:478:LEU:HD12	1.83	0.60
2:K:241:MET:HG2	2:K:244:SER:HB3	1.83	0.60
6:h:478:LEU:O	6:h:481:ILE:HG12	2.01	0.60
2:G:241:MET:HG2	2:G:244:SER:HB3	1.83	0.60
6:f:224:THR:HG22	6:f:225:LYS:N	2.16	0.60
6:i:512:ALA:HB1	6:i:529:ILE:CD1	2.30	0.60
2:H:241:MET:HG2	2:H:244:SER:HB3	1.84	0.60
6:e:248:ALA:HB1	6:e:478:LEU:HD12	1.83	0.60
6:g:478:LEU:O	6:g:481:ILE:HG12	2.01	0.60
9:r:573:LEU:HD11	9:s:571:ALA:HB1	1.83	0.60
6:g:224:THR:HG22	6:g:225:LYS:N	2.16	0.59
6:j:224:THR:HG22	6:j:225:LYS:N	2.16	0.59
9:q:534:LEU:HD12	9:s:542:LEU:HD22	1.79	0.59
1:D:457:TYR:HH	2:L:37:PHE:HD1	1.49	0.59
6:f:684:LYS:HD3	6:g:17:PHE:HZ	1.66	0.59
1:E:10:ILE:CG1	3:M:224:LEU:HD23	2.32	0.59
6:g:684:LYS:HD3	6:h:17:PHE:HZ	1.65	0.59
6:j:253:ILE:HD11	6:j:478:LEU:HD23	1.85	0.59
9:r:417:ALA:O	9:s:450:MET:CE	2.48	0.59
9:r:509:ILE:CG2	9:s:519:MET:HE1	2.32	0.59
1:A:253:MET:HG3	2:G:149:HIS:HB2	1.83	0.59
2:I:233:THR:HG21	2:I:403:ARG:HH11	1.67	0.59
3:Q:46:ASN:ND2	9:s:104:ASN:O	2.36	0.59
6:e:253:ILE:HD11	6:e:478:LEU:HD23	1.85	0.59
6:f:478:LEU:HD13	6:f:478:LEU:C	2.28	0.59
6:h:253:ILE:HD11	6:h:478:LEU:HD23	1.85	0.59
6:i:253:ILE:HD11	6:i:478:LEU:HD23	1.85	0.59
5:b:48:GLU:O	5:c:58:LYS:NZ	2.36	0.59
2:K:233:THR:HG21	2:K:403:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ILE:CD1	1:B:281:VAL:HG21	2.33	0.59
4:X:36:GLN:HE22	6:j:685:PHE:CB	2.15	0.59
6:f:253:ILE:HD11	6:f:478:LEU:HD23	1.85	0.59
6:h:478:LEU:HD13	6:h:478:LEU:C	2.28	0.59
6:i:478:LEU:HD13	6:i:478:LEU:C	2.28	0.59
9:q:391:GLU:OE1	9:s:233:MET:HE2	2.03	0.59
2:I:114:HIS:CE1	4:U:24:GLY:O	2.56	0.58
2:I:241:MET:HG2	2:I:244:SER:HB3	1.83	0.58
6:g:253:ILE:HD11	6:g:478:LEU:HD23	1.85	0.58
6:g:478:LEU:C	6:g:478:LEU:HD13	2.28	0.58
6:g:482:GLU:HB3	6:g:483:PRO:HD3	1.85	0.58
6:j:478:LEU:C	6:j:478:LEU:HD13	2.28	0.58
9:q:363:HIS:HE1	9:r:372:ALA:HA	1.68	0.58
1:F:318:TRP:CE3	2:I:985:ILE:O	2.54	0.58
1:F:425:TYR:OH	2:J:117:LEU:HD12	2.02	0.58
6:h:482:GLU:HB3	6:h:483:PRO:HD3	1.85	0.58
1:B:316:ASN:HD22	1:B:318:TRP:HE1	1.52	0.58
1:D:205:ILE:CD1	1:D:281:VAL:HG21	2.33	0.58
1:D:316:ASN:HD22	1:D:318:TRP:HE1	1.52	0.58
2:J:241:MET:HG2	2:J:244:SER:HB3	1.84	0.58
5:b:27:GLU:HB3	7:n:38:HIS:ND1	2.18	0.58
1:A:316:ASN:HD22	1:A:318:TRP:HE1	1.52	0.58
1:F:205:ILE:CD1	1:F:281:VAL:HG21	2.33	0.58
2:G:233:THR:HG21	2:G:403:ARG:HH11	1.67	0.58
5:Y:27:GLU:HB3	7:k:38:HIS:ND1	2.18	0.58
1:F:36:LEU:O	2:J:109:GLY:CA	2.52	0.58
1:F:457:TYR:CE1	2:J:37:PHE:CE1	2.91	0.58
6:e:478:LEU:C	6:e:478:LEU:HD13	2.28	0.58
1:E:316:ASN:HD22	1:E:318:TRP:HE1	1.52	0.58
1:F:318:TRP:CE2	2:I:985:ILE:O	2.54	0.58
2:I:303:GLU:O	2:I:413:LEU:HA	2.04	0.58
2:K:303:GLU:O	2:K:413:LEU:HA	2.04	0.58
2:L:241:MET:HG2	2:L:244:SER:HB3	1.84	0.58
6:j:482:GLU:HB3	6:j:483:PRO:HD3	1.85	0.58
1:C:316:ASN:HD22	1:C:318:TRP:HE1	1.52	0.58
1:F:316:ASN:HD22	1:F:318:TRP:HE1	1.52	0.58
9:r:363:HIS:HE1	9:s:372:ALA:HA	1.68	0.58
1:B:253:MET:HG3	2:H:149:HIS:HB2	1.86	0.57
6:i:482:GLU:HB3	6:i:483:PRO:HD3	1.85	0.57
9:q:534:LEU:HB2	9:s:542:LEU:HD23	1.85	0.57
1:D:399:THR:HG1	4:X:15:PHE:HZ	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:425:PHE:CD2	9:s:469:LYS:HD2	2.39	0.57
1:D:457:TYR:CZ	2:L:37:PHE:CD1	2.92	0.57
2:K:991:LEU:H	2:K:1005:ILE:H	1.53	0.57
1:C:512:GLU:OE1	2:K:826:ARG:NH1	2.38	0.57
1:E:512:GLU:OE1	2:I:826:ARG:NH1	2.37	0.57
2:L:311:LEU:HD21	2:L:404:LEU:HD22	1.86	0.57
1:D:121:ARG:HB2	2:L:907:PHE:CE2	2.31	0.57
2:G:71:PHE:CZ	4:S:20:GLU:O	2.58	0.57
2:G:303:GLU:O	2:G:413:LEU:HA	2.04	0.57
2:H:71:PHE:CZ	4:T:20:GLU:O	2.57	0.57
2:J:311:LEU:HD21	2:J:404:LEU:HD22	1.87	0.57
1:D:457:TYR:CE1	2:L:37:PHE:CE1	2.93	0.57
1:D:457:TYR:CE2	2:L:35:GLN:NE2	2.67	0.57
2:G:991:LEU:H	2:G:1005:ILE:H	1.53	0.57
2:H:311:LEU:HD21	2:H:404:LEU:HD22	1.86	0.57
2:K:55:PHE:CE2	4:W:21:THR:OG1	2.57	0.57
6:e:482:GLU:HB3	6:e:483:PRO:HD3	1.85	0.57
9:r:127:TYR:HE1	9:s:402:ASN:HB3	1.68	0.57
2:I:991:LEU:H	2:I:1005:ILE:H	1.53	0.56
2:J:298:ARG:NH2	2:J:362:ASP:O	2.38	0.56
2:L:298:ARG:NH2	2:L:362:ASP:O	2.38	0.56
5:a:118:LYS:HB3	5:a:137:GLU:HB3	1.87	0.56
9:r:239:LEU:HD21	9:r:278:ASP:OD1	2.05	0.56
1:A:219:GLU:OE1	1:A:345:ILE:HG21	2.04	0.56
1:E:283:LEU:CD2	1:E:304:LEU:HG	2.36	0.56
1:E:318:TRP:CE3	2:H:985:ILE:O	2.57	0.56
2:H:236:PHE:HD1	2:H:280:ALA:CB	2.19	0.56
4:S:36:GLN:HE22	6:e:685:PHE:CB	2.18	0.56
5:d:118:LYS:HB3	5:d:137:GLU:HB3	1.88	0.56
6:e:684:LYS:CD	6:f:17:PHE:HZ	2.18	0.56
9:q:127:TYR:CE1	9:r:402:ASN:HB3	2.41	0.56
9:q:239:LEU:HD21	9:q:278:ASP:OD1	2.05	0.56
9:q:553:ALA:C	9:s:561:ALA:HB3	2.17	0.56
1:C:219:GLU:OE1	1:C:345:ILE:HG21	2.04	0.56
6:e:83:LEU:HD23	6:e:84:ILE:N	2.21	0.56
2:K:470:TYR:CD1	2:K:593:LEU:HD11	2.41	0.56
3:P:227:GLN:HG2	9:r:77:GLU:OE1	2.06	0.56
5:c:118:LYS:HB3	5:c:137:GLU:HB3	1.87	0.56
6:f:83:LEU:HD23	6:f:84:ILE:N	2.21	0.56
6:f:482:GLU:HB3	6:f:483:PRO:HD3	1.85	0.56
6:h:83:LEU:HD23	6:h:84:ILE:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LEU:O	2:L:109:GLY:CA	2.54	0.56
1:E:34:LYS:HD2	4:U:127:TYR:CD1	2.41	0.56
1:E:219:GLU:OE1	1:E:345:ILE:HG21	2.04	0.56
1:E:491:LYS:HG2	2:I:89:ASP:HA	1.87	0.56
2:I:470:TYR:CD1	2:I:593:LEU:HD11	2.41	0.56
2:J:236:PHE:HD1	2:J:280:ALA:CB	2.19	0.56
5:Z:118:LYS:HB3	5:Z:137:GLU:HB3	1.87	0.56
1:B:318:TRP:CE3	2:G:985:ILE:O	2.57	0.56
1:F:44:TYR:CE1	4:V:127:TYR:HB2	2.41	0.56
2:L:236:PHE:HD1	2:L:280:ALA:CB	2.19	0.56
6:i:83:LEU:HD23	6:i:84:ILE:N	2.21	0.56
9:q:567:THR:OG1	9:r:562:GLY:N	2.38	0.56
1:C:283:LEU:CD2	1:C:304:LEU:HG	2.36	0.56
2:H:298:ARG:NH2	2:H:362:ASP:O	2.38	0.55
6:i:684:LYS:CD	6:j:17:PHE:HZ	2.18	0.55
6:j:83:LEU:HD23	6:j:84:ILE:N	2.21	0.55
9:q:567:THR:CB	9:r:562:GLY:HA2	2.36	0.55
4:T:36:GLN:HE22	6:f:685:PHE:CB	2.19	0.55
5:Z:11:His:HA	7:l:39:GLY:O	2.06	0.55
5:b:118:LYS:HB3	5:b:137:GLU:HB3	1.87	0.55
9:s:239:LEU:HD21	9:s:278:ASP:OD1	2.05	0.55
5:a:48:GLU:O	5:b:58:LYS:NZ	2.40	0.55
1:B:205:ILE:HD13	1:B:281:VAL:HG21	1.89	0.55
1:D:205:ILE:HD13	1:D:281:VAL:HG21	1.89	0.55
1:D:281:VAL:N	1:D:320:ILE:O	2.32	0.55
2:G:470:TYR:CD1	2:G:593:LEU:HD11	2.41	0.55
6:j:172:ASP:OD1	6:j:172:ASP:N	2.40	0.55
1:E:205:ILE:CD1	1:E:281:VAL:HG21	2.37	0.55
1:E:96:SER:HB2	2:I:828:LYS:HB3	1.88	0.55
2:L:217:ILE:N	2:L:645:HIS:CD2	2.75	0.55
6:g:83:LEU:HD23	6:g:84:ILE:N	2.21	0.55
6:h:478:LEU:HD11	6:h:489:TYR:CE1	2.42	0.55
6:i:478:LEU:HD11	6:i:489:TYR:CE1	2.42	0.55
1:D:318:TRP:CE2	2:K:985:ILE:O	2.59	0.55
5:Y:118:LYS:HB3	5:Y:137:GLU:HB3	1.88	0.55
6:e:478:LEU:CD1	6:e:489:TYR:HE1	2.20	0.55
6:g:478:LEU:CD1	6:g:489:TYR:HE1	2.20	0.55
6:h:684:LYS:CD	6:i:17:PHE:HZ	2.19	0.55
6:j:478:LEU:HD11	6:j:489:TYR:CE1	2.42	0.55
9:r:163:TYR:CD1	9:s:401:ILE:HG12	2.42	0.55
4:U:36:GLN:HE22	6:g:685:PHE:CB	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:478:LEU:CD1	6:f:489:TYR:HE1	2.20	0.54
9:q:571:ALA:HB3	9:s:578:VAL:HG22	1.88	0.54
1:D:96:SER:CB	2:L:828:LYS:HB3	2.34	0.54
1:D:509:ARG:NH1	2:L:139:HIS:CD2	2.60	0.54
1:E:44:TYR:CE1	4:U:127:TYR:HB2	2.41	0.54
4:V:36:GLN:HE22	6:h:685:PHE:CB	2.20	0.54
6:g:684:LYS:CD	6:h:17:PHE:HZ	2.20	0.54
1:A:205:ILE:CD1	1:A:281:VAL:HG21	2.37	0.54
1:C:205:ILE:CD1	1:C:281:VAL:HG21	2.37	0.54
1:D:498:ARG:NH2	2:L:34:LEU:O	2.37	0.54
2:H:217:ILE:N	2:H:645:HIS:CD2	2.75	0.54
6:g:478:LEU:HD11	6:g:489:TYR:CE1	2.42	0.54
9:r:474:ARG:HH22	9:s:467:HIS:HD2	1.55	0.54
6:f:478:LEU:HD11	6:f:489:TYR:CE1	2.42	0.54
6:f:684:LYS:CD	6:g:17:PHE:HZ	2.20	0.54
6:h:478:LEU:CD1	6:h:489:TYR:HE1	2.20	0.54
9:q:417:ALA:O	9:r:450:MET:CE	2.53	0.54
2:J:469:SER:O	2:J:595:LEU:HD12	2.08	0.54
2:L:797:LYS:O	2:L:798:SER:HB2	2.08	0.54
5:a:11:HIS:HA	7:m:39:GLY:O	2.06	0.54
6:h:172:ASP:OD1	6:h:172:ASP:N	2.40	0.54
1:A:283:LEU:CD2	1:A:304:LEU:HG	2.36	0.54
2:J:217:ILE:N	2:J:645:HIS:CD2	2.75	0.54
6:j:478:LEU:CD1	6:j:489:TYR:HE1	2.20	0.54
1:A:44:TYR:CE1	4:S:127:TYR:HB2	2.43	0.54
2:I:475:LEU:HD11	2:I:591:GLU:HG2	1.90	0.54
2:J:797:LYS:O	2:J:798:SER:HB2	2.08	0.54
6:e:17:PHE:HZ	6:j:684:LYS:CD	2.20	0.54
9:q:467:HIS:HD2	9:s:474:ARG:HH22	1.54	0.54
1:F:457:TYR:CE2	2:J:35:GLN:NE2	2.72	0.54
2:H:469:SER:O	2:H:595:LEU:HD12	2.08	0.54
5:Z:48:GLU:O	5:a:58:LYS:NZ	2.41	0.54
6:e:172:ASP:OD1	6:e:172:ASP:N	2.40	0.54
5:Y:58:LYS:NZ	5:d:48:GLU:O	2.41	0.54
5:c:48:GLU:O	5:d:58:LYS:NZ	2.41	0.54
9:r:546:ASN:HB2	9:s:539:ASP:CG	2.32	0.54
1:F:36:LEU:C	2:J:109:GLY:HA2	2.32	0.53
2:G:114:HIS:CE1	4:S:24:GLY:O	2.61	0.53
2:H:114:HIS:CE1	4:T:24:GLY:O	2.61	0.53
1:F:205:ILE:HD13	1:F:281:VAL:HG21	1.89	0.53
1:E:258:GLU:HA	2:I:824:ARG:NH2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:392:LYS:O	2:K:398:GLY:HA3	2.08	0.53
6:i:478:LEU:CD1	6:i:489:TYR:HE1	2.20	0.53
9:q:457:PRO:HD2	9:s:419:ASN:OD1	2.09	0.53
9:r:567:THR:CG2	9:s:562:GLY:HA2	2.38	0.53
1:A:254:ASP:OD1	2:G:150:LEU:CD2	2.57	0.53
2:H:797:LYS:O	2:H:798:SER:HB2	2.08	0.53
2:L:469:SER:O	2:L:595:LEU:HD12	2.08	0.53
6:e:478:LEU:HD11	6:e:489:TYR:CE1	2.42	0.53
1:C:34:LYS:HD2	4:W:127:TYR:CD1	2.43	0.53
1:F:281:VAL:N	1:F:320:ILE:O	2.32	0.53
2:L:790:GLN:HA	2:L:790:GLN:OE1	2.09	0.53
2:G:392:LYS:O	2:G:398:GLY:HA3	2.09	0.53
2:H:790:GLN:HA	2:H:790:GLN:OE1	2.09	0.53
2:I:55:PHE:CE2	4:U:21:THR:OG1	2.61	0.53
1:C:491:LYS:HG2	2:K:89:ASP:HA	1.90	0.53
2:J:790:GLN:HA	2:J:790:GLN:OE1	2.09	0.53
2:I:392:LYS:O	2:I:398:GLY:HA3	2.08	0.53
2:L:660:GLN:O	2:L:723:ILE:N	2.33	0.53
1:A:34:LYS:HD2	4:S:127:TYR:CD1	2.43	0.52
1:D:44:TYR:CE1	4:X:127:TYR:HB2	2.44	0.52
3:R:227:GLN:HG2	9:s:77:GLU:OE1	2.10	0.52
3:N:49:GLN:HG3	3:O:62:LYS:CD	2.39	0.52
6:g:478:LEU:O	6:g:478:LEU:HD13	2.10	0.52
6:h:478:LEU:O	6:h:478:LEU:HD13	2.10	0.52
6:j:478:LEU:O	6:j:478:LEU:HD13	2.10	0.52
1:C:44:TYR:CE1	4:W:127:TYR:HB2	2.45	0.52
6:i:191:ASP:OD1	6:i:191:ASP:N	2.42	0.52
1:D:318:TRP:CE3	2:K:985:ILE:O	2.57	0.52
2:I:451:SER:OG	2:I:552:LEU:HD12	2.10	0.52
6:i:478:LEU:O	6:i:478:LEU:HD13	2.10	0.52
2:G:451:SER:OG	2:G:552:LEU:HD12	2.10	0.52
2:K:71:PHE:CZ	4:W:20:GLU:O	2.62	0.52
6:f:478:LEU:O	6:f:478:LEU:HD13	2.10	0.52
9:q:81:GLY:HA3	9:q:85:ASP:O	2.10	0.52
9:q:562:GLY:HA2	9:s:567:THR:HG21	1.91	0.52
2:G:475:LEU:HD11	2:G:591:GLU:HG2	1.90	0.52
2:G:512:SER:HB2	2:G:532:GLU:OE2	2.10	0.52
2:K:282:LEU:HD12	2:K:393:THR:HG21	1.92	0.52
2:K:451:SER:OG	2:K:552:LEU:HD12	2.10	0.52
2:K:605:PHE:O	2:K:634:ASP:N	2.40	0.52
3:P:49:GLN:HG3	3:Q:62:LYS:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:q:542:LEU:CD2	9:r:534:LEU:HD12	2.40	0.52
9:r:551:ALA:HA	9:s:544:GLY:O	2.09	0.52
1:A:509:ARG:HH12	2:G:139:HIS:CD2	2.28	0.52
2:G:282:LEU:HD12	2:G:393:THR:HG21	1.92	0.52
2:I:282:LEU:HD12	2:I:393:THR:HG21	1.92	0.52
9:q:474:ARG:HH22	9:r:467:HIS:CD2	2.28	0.52
9:r:59:GLU:O	9:r:60:ARG:CB	2.51	0.52
9:r:81:GLY:HA3	9:r:85:ASP:O	2.10	0.52
1:A:9:SER:OG	3:Q:225:GLN:CG	2.57	0.51
1:C:340:LYS:HD2	1:C:345:ILE:HD11	1.91	0.51
2:L:311:LEU:O	2:L:350:SER:O	2.28	0.51
4:X:36:GLN:NE2	6:j:685:PHE:HB2	2.22	0.51
6:g:478:LEU:CD1	6:g:489:TYR:CE1	2.94	0.51
9:r:568:SER:OG	9:s:560:SER:O	2.28	0.51
1:D:410:LYS:HE2	6:e:3:THR:O	2.11	0.51
1:D:505:HIS:HB2	2:L:32:VAL:CG2	2.41	0.51
1:E:340:LYS:HD2	1:E:345:ILE:HD11	1.91	0.51
1:F:34:LYS:HD2	4:V:127:TYR:CD1	2.45	0.51
1:F:121:ARG:HB2	2:J:907:PHE:CE2	2.33	0.51
1:F:409:PRO:HG3	6:h:544:GLU:OE1	2.11	0.51
2:H:311:LEU:O	2:H:350:SER:O	2.28	0.51
6:f:478:LEU:CD1	6:f:489:TYR:CE1	2.94	0.51
6:f:482:GLU:O	6:f:486:ASN:OD1	2.29	0.51
6:e:478:LEU:O	6:e:478:LEU:HD13	2.10	0.51
6:i:482:GLU:O	6:i:486:ASN:OD1	2.29	0.51
1:C:9:SER:OG	3:O:225:GLN:CG	2.59	0.51
1:F:505:HIS:HB2	2:J:32:VAL:CG2	2.41	0.51
2:G:605:PHE:O	2:G:634:ASP:N	2.40	0.51
3:M:62:LYS:HD3	3:R:49:GLN:HG3	1.93	0.51
6:e:482:GLU:O	6:e:486:ASN:OD1	2.29	0.51
6:f:172:ASP:OD1	6:f:172:ASP:N	2.40	0.51
6:h:478:LEU:CD1	6:h:489:TYR:CE1	2.94	0.51
6:h:482:GLU:O	6:h:486:ASN:OD1	2.29	0.51
9:q:571:ALA:HB1	9:s:573:LEU:HD11	1.92	0.51
9:s:81:GLY:HA3	9:s:85:ASP:O	2.10	0.51
1:A:9:SER:OG	3:Q:225:GLN:HG2	2.09	0.51
1:B:44:TYR:CE1	4:T:127:TYR:HB2	2.45	0.51
2:G:311:LEU:HD23	2:G:312:PRO:HD2	1.93	0.51
2:I:512:SER:HB2	2:I:532:GLU:OE2	2.10	0.51
6:j:260:PRO:C	6:j:261:ASN:HD22	2.19	0.51
6:j:482:GLU:O	6:j:486:ASN:OD1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG13	3:Q:224:LEU:CD2	2.40	0.51
1:A:340:LYS:HD2	1:A:345:ILE:HD11	1.91	0.51
1:E:253:MET:HG3	2:I:149:HIS:HB2	1.92	0.51
6:g:482:GLU:O	6:g:486:ASN:OD1	2.29	0.51
2:K:475:LEU:HD11	2:K:591:GLU:HG2	1.90	0.51
2:K:512:SER:HB2	2:K:532:GLU:OE2	2.10	0.51
3:N:227:GLN:HE21	9:q:21:LEU:HD13	1.75	0.51
6:e:260:PRO:C	6:e:261:ASN:HD22	2.19	0.51
6:f:260:PRO:C	6:f:261:ASN:HD22	2.19	0.51
2:J:793:LEU:HB2	2:J:796:ILE:HD12	1.93	0.51
6:g:260:PRO:C	6:g:261:ASN:HD22	2.19	0.51
1:D:488:LEU:HD22	2:L:49:PHE:CE1	2.42	0.51
2:H:660:GLN:O	2:H:723:ILE:N	2.33	0.51
3:N:49:GLN:HG3	3:O:62:LYS:HD3	1.92	0.51
2:H:793:LEU:HB2	2:H:796:ILE:HD12	1.93	0.51
2:I:311:LEU:HD23	2:I:312:PRO:HD2	1.93	0.51
9:q:560:SER:O	9:s:568:SER:OG	2.29	0.51
1:D:36:LEU:C	2:L:109:GLY:HA2	2.36	0.50
2:J:311:LEU:O	2:J:350:SER:O	2.28	0.50
2:J:662:VAL:HB	2:J:721:PHE:CZ	2.46	0.50
6:e:478:LEU:CD1	6:e:489:TYR:CE1	2.94	0.50
9:q:502:ASP:OD1	9:s:496:ASN:ND2	2.44	0.50
4:W:36:GLN:HE22	6:i:685:PHE:CB	2.22	0.50
6:i:260:PRO:C	6:i:261:ASN:HD22	2.19	0.50
6:i:478:LEU:CD1	6:i:489:TYR:CE1	2.94	0.50
9:q:534:LEU:HB2	9:s:542:LEU:CD2	2.40	0.50
1:A:410:LYS:HE2	6:f:3:THR:O	2.12	0.50
1:E:410:LYS:HE2	6:h:3:THR:O	2.12	0.50
6:e:212:ASP:OD1	6:e:215:PRO:HD2	2.11	0.50
6:j:478:LEU:CD1	6:j:489:TYR:CE1	2.94	0.50
9:s:126:LYS:NZ	9:s:139:GLU:OE2	2.44	0.50
2:H:662:VAL:HB	2:H:721:PHE:CZ	2.46	0.50
2:L:793:LEU:HB2	2:L:796:ILE:HD12	1.93	0.50
3:P:49:GLN:HG3	3:Q:62:LYS:CD	2.40	0.50
6:f:191:ASP:OD1	6:f:191:ASP:N	2.42	0.50
6:f:212:ASP:OD1	6:f:215:PRO:HD2	2.11	0.50
9:q:578:VAL:HG23	9:s:581:ASN:HD21	1.76	0.50
2:I:429:ASN:HB3	2:I:431:LEU:H	1.76	0.50
1:C:9:SER:OG	3:O:225:GLN:HG2	2.11	0.50
2:L:471:GLN:O	2:L:593:LEU:HA	2.12	0.50
6:h:260:PRO:C	6:h:261:ASN:HD22	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:VAL:N	1:B:320:ILE:O	2.32	0.50
2:J:311:LEU:HD11	2:J:404:LEU:HD13	1.94	0.50
1:F:473:LYS:HZ2	2:J:67:ASP:HB3	1.74	0.50
2:L:311:LEU:HD11	2:L:404:LEU:HD13	1.94	0.50
3:M:62:LYS:CD	3:R:49:GLN:HG3	2.42	0.50
3:Q:176:ARG:HD2	3:Q:191:ILE:HD11	1.94	0.50
6:j:191:ASP:OD1	6:j:191:ASP:N	2.42	0.50
1:E:409:PRO:HG3	6:g:544:GLU:OE1	2.12	0.49
2:G:219:VAL:HB	2:G:233:THR:HG23	1.93	0.49
2:L:662:VAL:HB	2:L:721:PHE:CZ	2.46	0.49
3:Q:109:HIS:HB3	9:r:15:ARG:HH21	1.77	0.49
4:W:106:GLY:O	6:i:680:PHE:N	2.36	0.49
6:j:212:ASP:OD1	6:j:215:PRO:HD2	2.11	0.49
9:q:425:PHE:HD2	9:r:469:LYS:HD2	1.73	0.49
9:r:567:THR:HG21	9:s:562:GLY:HA2	1.93	0.49
1:D:488:LEU:CD2	2:L:49:PHE:CE1	2.94	0.49
2:I:219:VAL:HB	2:I:233:THR:HG23	1.93	0.49
2:J:471:GLN:O	2:J:593:LEU:HA	2.12	0.49
2:K:311:LEU:HD23	2:K:312:PRO:HD2	1.93	0.49
3:M:176:ARG:HD2	3:M:191:ILE:HD11	1.94	0.49
1:A:409:PRO:HG2	6:e:547:GLU:OE1	2.12	0.49
2:K:219:VAL:HB	2:K:233:THR:HG23	1.93	0.49
3:O:176:ARG:HD2	3:O:191:ILE:HD11	1.94	0.49
6:i:212:ASP:OD1	6:i:215:PRO:HD2	2.11	0.49
1:B:254:ASP:OD1	2:H:150:LEU:CD2	2.60	0.49
1:B:409:PRO:HG3	6:f:544:GLU:OE1	2.12	0.49
1:B:410:LYS:HE2	6:g:3:THR:O	2.13	0.49
2:H:471:GLN:O	2:H:593:LEU:HA	2.12	0.49
6:h:191:ASP:OD1	6:h:191:ASP:N	2.42	0.49
7:k:117:ASP:O	7:p:7:LYS:HE3	2.12	0.49
1:C:39:ASN:HB2	2:K:109:GLY:O	2.12	0.49
1:F:410:LYS:HE2	6:i:3:THR:O	2.12	0.49
2:L:616:LEU:HB2	2:L:628:PHE:HB3	1.95	0.49
3:N:176:ARG:HD2	3:N:191:ILE:HD11	1.94	0.49
4:U:106:GLY:O	6:g:680:PHE:N	2.40	0.49
4:V:106:GLY:O	6:h:680:PHE:N	2.38	0.49
1:C:409:PRO:HG3	6:i:544:GLU:OE1	2.13	0.49
1:F:508:ALA:HB3	2:J:26:LYS:O	2.13	0.49
2:I:71:PHE:CZ	4:U:20:GLU:O	2.66	0.49
9:r:363:HIS:CE1	9:s:373:ALA:H	2.30	0.49
1:C:96:SER:HB2	2:K:828:LYS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:457:TYR:HH	2:J:37:PHE:HD1	1.59	0.49
2:H:236:PHE:HD1	2:H:280:ALA:HB2	1.78	0.49
2:H:475:LEU:O	2:H:476:ASN:HB3	2.13	0.49
2:J:616:LEU:HB2	2:J:628:PHE:HB3	1.95	0.49
2:K:314:GLY:H	2:K:350:SER:HB3	1.78	0.49
2:K:429:ASN:HB3	2:K:431:LEU:H	1.76	0.49
6:e:191:ASP:OD1	6:e:191:ASP:N	2.42	0.49
6:g:212:ASP:OD1	6:g:215:PRO:HD2	2.11	0.49
6:h:212:ASP:OD1	6:h:215:PRO:HD2	2.11	0.49
1:E:9:SER:OG	3:M:225:GLN:CG	2.61	0.49
2:L:236:PHE:HD1	2:L:280:ALA:HB2	1.78	0.49
4:S:36:GLN:NE2	6:e:685:PHE:HB2	2.25	0.49
9:q:372:ALA:HA	9:s:363:HIS:HE1	1.78	0.49
1:B:348:ASN:HD22	1:B:351:ARG:HD2	1.78	0.49
2:H:311:LEU:HD11	2:H:404:LEU:HD13	1.94	0.49
9:q:564:GLU:HG3	9:s:572:VAL:HB	1.94	0.49
1:E:509:ARG:HH12	2:I:139:HIS:CD2	2.30	0.49
1:F:498:ARG:NH2	2:J:34:LEU:O	2.44	0.49
2:G:293:LEU:HD21	2:G:417:VAL:HG11	1.95	0.49
2:G:429:ASN:HB3	2:G:431:LEU:H	1.76	0.49
2:H:616:LEU:HB2	2:H:628:PHE:HB3	1.95	0.49
7:k:7:LYS:HE3	7:l:117:ASP:O	2.13	0.49
1:D:348:ASN:HD22	1:D:351:ARG:HD2	1.77	0.48
1:E:9:SER:OG	3:M:225:GLN:HG2	2.13	0.48
7:m:7:LYS:HE3	7:n:117:ASP:O	2.12	0.48
2:K:293:LEU:HD21	2:K:417:VAL:HG11	1.95	0.48
2:L:475:LEU:O	2:L:476:ASN:HB3	2.13	0.48
3:R:176:ARG:HD2	3:R:191:ILE:HD11	1.94	0.48
9:q:61:ASP:OD1	9:s:321:GLY:HA2	2.13	0.48
3:P:176:ARG:HD2	3:P:191:ILE:HD11	1.94	0.48
6:i:172:ASP:N	6:i:172:ASP:OD1	2.40	0.48
6:j:276:PRO:HA	6:j:280:ASP:HB2	1.96	0.48
2:I:236:PHE:CD1	2:I:280:ALA:CB	2.97	0.48
2:J:236:PHE:HD1	2:J:280:ALA:HB2	1.78	0.48
2:K:236:PHE:CD1	2:K:280:ALA:CB	2.97	0.48
6:i:276:PRO:HA	6:i:280:ASP:HB2	1.96	0.48
9:s:19:LYS:NZ	9:s:86:ASP:OD2	2.47	0.48
1:A:254:ASP:OD1	2:G:150:LEU:HD21	2.14	0.48
1:B:509:ARG:HH12	2:H:139:HIS:CD2	2.31	0.48
1:F:348:ASN:HD22	1:F:351:ARG:HD2	1.78	0.48
2:I:314:GLY:H	2:I:350:SER:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:36:VAL:HG22	5:Z:37:ASP:N	2.29	0.48
6:f:224:THR:CG2	6:f:225:LYS:N	2.77	0.48
9:q:542:LEU:HD21	9:r:534:LEU:HD12	1.96	0.48
2:I:293:LEU:HD21	2:I:417:VAL:HG11	1.95	0.48
2:J:875:ASP:OD1	2:J:875:ASP:N	2.47	0.48
6:g:224:THR:CG2	6:g:225:LYS:N	2.77	0.48
6:g:276:PRO:HA	6:g:280:ASP:HB2	1.96	0.48
1:D:409:PRO:HG3	6:j:544:GLU:OE1	2.14	0.48
1:F:258:GLU:OE2	2:J:829:LYS:HG2	2.13	0.48
2:I:322:LYS:O	2:I:392:LYS:HD2	2.14	0.48
6:f:276:PRO:HA	6:f:280:ASP:HB2	1.96	0.48
7:l:7:LYS:HE3	7:m:117:ASP:O	2.14	0.48
9:q:570:VAL:HA	9:s:577:LEU:O	2.13	0.48
1:E:39:ASN:HB2	2:I:109:GLY:O	2.14	0.48
2:G:236:PHE:CD1	2:G:280:ALA:CB	2.97	0.48
2:G:314:GLY:H	2:G:350:SER:HB3	1.78	0.48
2:K:315:GLU:N	2:K:348:ILE:O	2.47	0.48
5:b:6:PRO:O	7:o:49:MET:HE1	2.14	0.48
6:e:276:PRO:HA	6:e:280:ASP:HB2	1.96	0.48
7:n:7:LYS:HE3	7:o:117:ASP:O	2.13	0.48
9:q:363:HIS:HE1	9:r:372:ALA:CA	2.27	0.48
1:E:10:ILE:HG13	3:M:224:LEU:CD2	2.42	0.48
3:M:40:GLN:HG2	3:N:131:ASP:OD2	2.14	0.48
6:h:276:PRO:HA	6:h:280:ASP:HB2	1.96	0.48
6:i:224:THR:CG2	6:i:225:LYS:N	2.77	0.48
2:J:475:LEU:O	2:J:476:ASN:HB3	2.13	0.47
3:Q:40:GLN:HG2	3:R:131:ASP:OD2	2.14	0.47
5:Y:11:HIS:HA	7:k:39:GLY:O	2.14	0.47
6:j:224:THR:CG2	6:j:225:LYS:N	2.77	0.47
2:G:322:LYS:O	2:G:392:LYS:HD2	2.14	0.47
1:E:409:PRO:HG2	6:g:547:GLU:OE1	2.14	0.47
2:K:233:THR:CG2	2:K:403:ARG:HH11	2.28	0.47
5:Y:36:VAL:HG22	5:Y:37:ASP:N	2.29	0.47
5:a:36:VAL:HG22	5:a:37:ASP:N	2.29	0.47
5:c:36:VAL:HG22	5:c:37:ASP:N	2.29	0.47
6:g:191:ASP:N	6:g:191:ASP:OD1	2.41	0.47
6:h:224:THR:CG2	6:h:225:LYS:N	2.77	0.47
9:q:351:ASN:OD1	9:q:352:PRO:HD2	2.14	0.47
9:r:351:ASN:OD1	9:r:352:PRO:HD2	2.14	0.47
3:O:40:GLN:HG2	3:P:131:ASP:OD2	2.14	0.47
6:e:224:THR:CG2	6:e:225:LYS:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:o:7:LYS:HE3	7:p:117:ASP:O	2.14	0.47
9:q:363:HIS:CE1	9:r:372:ALA:HA	2.49	0.47
9:r:19:LYS:NZ	9:r:86:ASP:OD2	2.47	0.47
9:s:351:ASN:OD1	9:s:352:PRO:HD2	2.14	0.47
2:J:311:LEU:HD21	2:J:404:LEU:CD2	2.44	0.47
1:C:509:ARG:HH12	2:K:139:HIS:CD2	2.31	0.47
1:D:279:LYS:O	1:D:322:ILE:N	2.46	0.47
5:d:36:VAL:HG22	5:d:37:ASP:N	2.29	0.47
6:e:189:LEU:O	6:e:190:GLN:HB2	2.15	0.47
1:B:34:LYS:HD2	4:T:127:TYR:CD1	2.48	0.47
1:C:10:ILE:HG13	3:O:224:LEU:CD2	2.41	0.47
1:C:410:LYS:HE2	6:j:3:THR:O	2.14	0.47
1:E:205:ILE:HD13	1:E:281:VAL:HG21	1.97	0.47
1:F:397:PRO:HB2	1:F:399:THR:HG22	1.97	0.47
2:H:311:LEU:HD21	2:H:404:LEU:CD2	2.44	0.47
2:H:506:LYS:O	2:H:550:ILE:HA	2.15	0.47
2:J:236:PHE:CD1	2:J:280:ALA:CB	2.98	0.47
1:C:258:GLU:HA	2:K:824:ARG:NH2	2.29	0.47
2:L:289:LYS:HG2	2:L:384:GLU:OE2	2.15	0.47
9:q:552:ASN:C	9:s:560:SER:OG	2.57	0.47
1:C:205:ILE:HD13	1:C:281:VAL:HG21	1.97	0.47
1:E:219:GLU:OE2	1:E:345:ILE:HD12	2.15	0.47
2:I:233:THR:CG2	2:I:403:ARG:HH11	2.28	0.47
2:I:429:ASN:ND2	2:I:434:LEU:HD21	2.30	0.47
2:K:322:LYS:O	2:K:392:LYS:HD2	2.14	0.47
2:L:506:LYS:O	2:L:550:ILE:HA	2.15	0.47
6:f:189:LEU:O	6:f:190:GLN:HB2	2.15	0.47
7:l:62:ARG:HH22	7:l:70:GLU:HB2	1.80	0.47
1:A:219:GLU:OE2	1:A:345:ILE:HD12	2.15	0.47
1:C:397:PRO:HB2	1:C:399:THR:HG22	1.97	0.47
1:F:68:ILE:CG2	2:J:131:ARG:HG2	2.45	0.47
2:K:468:ILE:HA	2:K:596:GLY:O	2.15	0.47
4:U:36:GLN:NE2	6:g:685:PHE:HB2	2.27	0.47
1:A:205:ILE:HD13	1:A:281:VAL:HG21	1.97	0.46
1:B:397:PRO:HB2	1:B:399:THR:HG22	1.96	0.46
2:G:233:THR:CG2	2:G:403:ARG:HH11	2.28	0.46
2:K:429:ASN:ND2	2:K:434:LEU:HD21	2.30	0.46
3:P:16:ASP:OD1	3:P:16:ASP:N	2.49	0.46
5:a:27:GLU:HB3	7:m:38:HIS:ND1	2.30	0.46
5:b:36:VAL:HG22	5:b:37:ASP:N	2.29	0.46
6:g:189:LEU:O	6:g:190:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:189:LEU:O	6:i:190:GLN:HB2	2.15	0.46
7:m:62:ARG:HH22	7:m:70:GLU:HB2	1.80	0.46
9:q:438:ILE:HG23	9:r:377:LEU:O	2.15	0.46
9:q:543:GLU:O	9:r:540:ILE:HD12	2.13	0.46
2:J:506:LYS:O	2:J:550:ILE:HA	2.15	0.46
1:E:34:LYS:CD	4:U:127:TYR:CD1	2.98	0.46
3:R:16:ASP:OD1	3:R:16:ASP:N	2.49	0.46
9:q:423:ILE:HG12	9:r:471:ILE:HG12	1.97	0.46
1:A:409:PRO:HG3	6:e:544:GLU:OE1	2.15	0.46
1:A:491:LYS:HG2	2:G:89:ASP:HA	1.98	0.46
1:C:253:MET:HG3	2:K:149:HIS:HB2	1.97	0.46
1:E:397:PRO:HB2	1:E:399:THR:HG22	1.97	0.46
2:J:289:LYS:HG2	2:J:384:GLU:OE2	2.15	0.46
3:N:16:ASP:OD1	3:N:16:ASP:N	2.49	0.46
5:Z:27:GLU:HB3	7:l:38:HIS:ND1	2.31	0.46
7:k:62:ARG:HH22	7:k:70:GLU:HB2	1.80	0.46
1:D:409:PRO:HG2	6:j:547:GLU:OE1	2.16	0.46
1:E:509:ARG:HH12	2:I:139:HIS:HD2	1.62	0.46
1:F:488:LEU:CD2	2:J:49:PHE:CE1	2.99	0.46
2:G:315:GLU:N	2:G:348:ILE:O	2.47	0.46
2:I:605:PHE:O	2:I:634:ASP:N	2.40	0.46
6:j:189:LEU:O	6:j:190:GLN:HB2	2.15	0.46
1:A:509:ARG:HH12	2:G:139:HIS:HD2	1.62	0.46
1:B:409:PRO:HG2	6:f:547:GLU:OE1	2.16	0.46
2:I:315:GLU:N	2:I:348:ILE:O	2.47	0.46
2:G:429:ASN:ND2	2:G:434:LEU:HD21	2.30	0.46
2:G:468:ILE:HA	2:G:596:GLY:O	2.15	0.46
2:I:468:ILE:HA	2:I:596:GLY:O	2.15	0.46
5:b:11:HIS:HA	7:n:39:GLY:O	2.15	0.46
1:C:219:GLU:OE2	1:C:345:ILE:HD12	2.15	0.46
1:E:512:GLU:CD	2:I:826:ARG:NH1	2.74	0.46
2:H:289:LYS:HG2	2:H:384:GLU:OE2	2.15	0.46
6:h:189:LEU:O	6:h:190:GLN:HB2	2.15	0.46
6:j:478:LEU:HD13	6:j:489:TYR:HE1	1.81	0.46
1:A:397:PRO:HB2	1:A:399:THR:HG22	1.97	0.46
7:n:62:ARG:HH22	7:n:70:GLU:HB2	1.81	0.46
9:r:438:ILE:HG23	9:s:377:LEU:O	2.15	0.46
2:L:311:LEU:HD21	2:L:404:LEU:CD2	2.44	0.46
3:N:40:GLN:HG2	3:O:131:ASP:OD2	2.16	0.46
6:g:212:ASP:HB3	6:g:215:PRO:HG2	1.98	0.46
7:p:62:ARG:HH22	7:p:70:GLU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:221:LYS:NZ	2:J:407:GLU:CD	2.74	0.45
6:h:212:ASP:HB3	6:h:215:PRO:HG2	1.98	0.45
9:r:580:ILE:O	9:r:581:ASN:C	2.60	0.45
3:O:16:ASP:OD1	3:O:16:ASP:N	2.48	0.45
6:i:45:ASP:OD1	6:i:45:ASP:N	2.47	0.45
7:o:62:ARG:HH22	7:o:70:GLU:HB2	1.80	0.45
1:D:397:PRO:HB2	1:D:399:THR:HG22	1.96	0.45
2:L:471:GLN:O	2:L:593:LEU:HD12	2.16	0.45
4:T:106:GLY:O	6:f:680:PHE:N	2.42	0.45
1:B:279:LYS:O	1:B:322:ILE:N	2.46	0.45
1:D:34:LYS:HD2	4:X:127:TYR:CD1	2.50	0.45
2:H:221:LYS:NZ	2:H:407:GLU:CD	2.74	0.45
2:H:471:GLN:O	2:H:593:LEU:HD12	2.17	0.45
6:f:129:ASP:OD1	6:f:129:ASP:N	2.49	0.45
1:A:409:PRO:HD2	6:e:547:GLU:CD	2.40	0.45
1:B:87:PHE:CD2	2:H:143:TYR:CD1	3.05	0.45
1:E:89:LYS:HZ2	6:g:85:GLU:CD	2.23	0.45
6:h:273:VAL:HG13	6:h:278:PHE:CE2	2.52	0.45
6:h:478:LEU:HD13	6:h:489:TYR:HE1	1.81	0.45
7:m:68:ASP:OD1	7:m:70:GLU:HG2	2.17	0.45
9:q:580:ILE:O	9:q:581:ASN:C	2.60	0.45
9:r:59:GLU:OE1	9:r:63:LYS:NZ	2.50	0.45
2:L:236:PHE:CD1	2:L:280:ALA:CB	2.98	0.45
7:o:33:ILE:CD1	7:p:111:LEU:HD12	2.45	0.45
7:o:68:ASP:OD1	7:o:70:GLU:HG2	2.17	0.45
1:D:68:ILE:CG2	2:L:131:ARG:HG2	2.46	0.45
1:D:219:GLU:CB	1:D:347:LEU:HD21	2.45	0.45
2:G:185:LYS:HA	2:G:190:LYS:O	2.16	0.45
3:M:16:ASP:OD1	3:M:16:ASP:N	2.48	0.45
6:i:212:ASP:HB3	6:i:215:PRO:HG2	1.98	0.45
7:n:62:ARG:NH2	7:n:70:GLU:HB2	2.32	0.45
1:D:68:ILE:HG21	2:L:131:ARG:CG	2.46	0.45
2:I:185:LYS:HA	2:I:190:LYS:O	2.16	0.45
3:N:126:TYR:CD1	3:N:126:TYR:N	2.85	0.45
6:g:478:LEU:HD13	6:g:489:TYR:HE1	1.81	0.45
6:i:273:VAL:HG13	6:i:278:PHE:CE2	2.52	0.45
7:o:62:ARG:NH2	7:o:70:GLU:HB2	2.32	0.45
7:p:62:ARG:NH2	7:p:70:GLU:HB2	2.32	0.45
1:A:34:LYS:CD	4:S:127:TYR:CD1	3.00	0.45
1:E:409:PRO:HD2	6:g:547:GLU:CD	2.41	0.45
2:L:221:LYS:NZ	2:L:407:GLU:CD	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:16:ASP:OD1	3:Q:16:ASP:N	2.48	0.45
6:j:273:VAL:HG13	6:j:278:PHE:CE2	2.52	0.45
7:k:68:ASP:OD1	7:k:70:GLU:HG2	2.17	0.45
9:q:19:LYS:NZ	9:q:86:ASP:OD2	2.47	0.45
1:C:512:GLU:CD	2:K:826:ARG:NH1	2.75	0.45
2:J:471:GLN:O	2:J:593:LEU:HD12	2.17	0.45
2:K:71:PHE:HZ	4:W:20:GLU:O	1.99	0.45
2:K:185:LYS:HA	2:K:190:LYS:O	2.16	0.45
2:K:345:ASP:OD1	2:K:345:ASP:N	2.49	0.45
6:e:478:LEU:HD13	6:e:489:TYR:HE1	1.81	0.45
6:i:478:LEU:HD13	6:i:489:TYR:HE1	1.81	0.45
1:D:508:ALA:HB3	2:L:26:LYS:O	2.16	0.44
2:H:236:PHE:CD1	2:H:280:ALA:CB	2.98	0.44
2:I:470:TYR:HA	2:I:594:VAL:O	2.17	0.44
2:K:395:GLU:HB2	2:K:398:GLY:H	1.82	0.44
6:f:212:ASP:HB3	6:f:215:PRO:HG2	1.98	0.44
2:H:71:PHE:HZ	4:T:20:GLU:O	2.00	0.44
3:Q:88:ASP:OD2	3:Q:92:ASN:ND2	2.51	0.44
6:e:273:VAL:HG13	6:e:278:PHE:CE2	2.52	0.44
6:g:273:VAL:HG13	6:g:278:PHE:CE2	2.52	0.44
7:l:68:ASP:OD1	7:l:70:GLU:HG2	2.17	0.44
7:m:62:ARG:NH2	7:m:70:GLU:HB2	2.32	0.44
9:q:450:MET:HE1	9:s:421:ARG:HH22	1.82	0.44
9:q:574:LYS:HA	9:s:581:ASN:OD1	2.18	0.44
1:F:509:ARG:NH1	2:J:139:HIS:CD2	2.63	0.44
2:I:174:LYS:HD2	2:I:199:GLU:CD	2.43	0.44
3:P:126:TYR:CD1	3:P:126:TYR:N	2.85	0.44
6:e:212:ASP:HB3	6:e:215:PRO:HG2	1.98	0.44
7:l:62:ARG:NH2	7:l:70:GLU:HB2	2.32	0.44
9:q:553:ALA:O	9:s:561:ALA:CA	2.63	0.44
1:A:281:VAL:O	1:A:319:VAL:HA	2.18	0.44
1:F:279:LYS:O	1:F:322:ILE:N	2.46	0.44
1:F:409:PRO:HG2	6:h:547:GLU:OE1	2.18	0.44
2:I:469:SER:O	2:I:595:LEU:HA	2.17	0.44
2:K:470:TYR:HA	2:K:594:VAL:O	2.18	0.44
3:P:40:GLN:HG2	3:Q:131:ASP:OD2	2.17	0.44
6:e:83:LEU:CD2	6:e:83:LEU:C	2.90	0.44
6:f:273:VAL:HG13	6:f:278:PHE:CE2	2.52	0.44
7:k:62:ARG:NH2	7:k:70:GLU:HB2	2.32	0.44
7:p:68:ASP:OD1	7:p:70:GLU:HG2	2.17	0.44
1:B:89:LYS:HZ2	6:f:85:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:VAL:O	1:C:319:VAL:HA	2.17	0.44
1:C:509:ARG:HH12	2:K:139:HIS:HD2	1.65	0.44
2:G:469:SER:O	2:G:595:LEU:HA	2.17	0.44
2:K:299:ASP:O	2:K:417:VAL:HA	2.18	0.44
3:P:88:ASP:OD2	3:P:92:ASN:ND2	2.51	0.44
3:R:126:TYR:CD1	3:R:126:TYR:N	2.85	0.44
6:f:478:LEU:HD13	6:f:489:TYR:HE1	1.81	0.44
9:q:59:GLU:OE1	9:q:63:LYS:NZ	2.50	0.44
2:K:469:SER:O	2:K:595:LEU:HA	2.17	0.44
3:N:88:ASP:OD2	3:N:92:ASN:ND2	2.51	0.44
3:R:88:ASP:OD2	3:R:92:ASN:ND2	2.51	0.44
1:C:34:LYS:CD	4:W:127:TYR:CD1	3.01	0.44
1:F:457:TYR:CE2	2:J:37:PHE:CE1	3.06	0.44
2:H:323:ALA:HB1	2:H:401:LEU:HD12	2.00	0.44
4:T:36:GLN:NE2	6:f:685:PHE:HB2	2.26	0.44
4:V:36:GLN:NE2	6:h:685:PHE:HB2	2.27	0.44
6:j:83:LEU:CD2	6:j:83:LEU:C	2.91	0.44
7:n:68:ASP:OD1	7:n:70:GLU:HG2	2.17	0.44
9:q:539:ASP:OD1	9:s:546:ASN:ND2	2.46	0.44
9:s:59:GLU:OE1	9:s:63:LYS:NZ	2.50	0.44
2:I:586:TYR:CE2	2:I:588:PRO:HA	2.53	0.44
2:K:586:TYR:CE2	2:K:588:PRO:HA	2.53	0.44
3:M:88:ASP:OD2	3:M:92:ASN:ND2	2.51	0.44
6:j:212:ASP:HB3	6:j:215:PRO:HG2	1.98	0.44
7:m:121:ASP:OD1	7:m:121:ASP:N	2.49	0.44
1:B:364:LEU:HD23	1:B:364:LEU:HA	1.77	0.44
1:D:10:ILE:HG13	3:P:224:LEU:CD2	2.41	0.44
1:F:364:LEU:HD23	1:F:364:LEU:HA	1.77	0.44
2:G:299:ASP:O	2:G:417:VAL:HA	2.18	0.44
2:I:395:GLU:HB2	2:I:398:GLY:H	1.82	0.44
3:M:46:ASN:ND2	9:q:104:ASN:O	2.51	0.44
3:M:131:ASP:OD2	3:R:40:GLN:HG2	2.18	0.44
1:A:299:VAL:O	2:L:969:ARG:CB	2.66	0.43
1:C:409:PRO:HG2	6:i:547:GLU:OE1	2.19	0.43
2:G:471:GLN:O	2:G:593:LEU:HA	2.19	0.43
2:K:471:GLN:O	2:K:593:LEU:HD12	2.18	0.43
7:n:33:ILE:CD1	7:o:111:LEU:HD12	2.45	0.43
1:E:159:TYR:OH	2:I:908:HIS:CD2	2.72	0.43
2:G:71:PHE:HZ	4:S:20:GLU:O	2.01	0.43
2:G:395:GLU:HB2	2:G:398:GLY:H	1.82	0.43
2:J:660:GLN:O	2:J:723:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:LEU:HG	1:D:304:LEU:HG	2.00	0.43
3:O:88:ASP:OD2	3:O:92:ASN:ND2	2.51	0.43
9:q:126:LYS:NZ	9:q:139:GLU:OE2	2.44	0.43
9:r:126:LYS:NZ	9:r:139:GLU:OE2	2.44	0.43
1:F:68:ILE:HG21	2:J:131:ARG:CG	2.47	0.43
1:F:505:HIS:CE1	2:J:29:PRO:HA	2.54	0.43
2:G:471:GLN:O	2:G:593:LEU:HD12	2.18	0.43
2:G:586:TYR:CE2	2:G:588:PRO:HA	2.53	0.43
2:J:323:ALA:HB1	2:J:401:LEU:HD12	2.00	0.43
1:A:7:HIS:CE1	4:X:132:GLU:HB3	2.54	0.43
1:A:410:LYS:HD3	6:f:3:THR:O	2.18	0.43
1:E:281:VAL:O	1:E:319:VAL:HA	2.18	0.43
2:G:295:GLU:HG3	2:G:422:ILE:HG12	2.01	0.43
2:I:471:GLN:O	2:I:593:LEU:HA	2.18	0.43
2:I:471:GLN:O	2:I:593:LEU:HD12	2.18	0.43
7:l:32:GLU:OE2	7:l:54:LYS:NZ	2.49	0.43
9:r:567:THR:HG1	9:s:562:GLY:H	1.62	0.43
1:F:34:LYS:CD	4:V:127:TYR:CD1	3.01	0.43
1:F:283:LEU:HG	1:F:304:LEU:HG	2.00	0.43
2:I:299:ASP:O	2:I:417:VAL:HA	2.18	0.43
3:Q:109:HIS:HB3	9:r:15:ARG:NH2	2.33	0.43
9:q:534:LEU:CD1	9:s:542:LEU:CD2	2.73	0.43
2:G:174:LYS:HD2	2:G:199:GLU:CD	2.43	0.43
2:G:295:GLU:OE2	2:G:422:ILE:HG23	2.19	0.43
2:I:295:GLU:OE2	2:I:422:ILE:HG23	2.19	0.43
2:J:833:THR:O	2:J:837:TYR:HD2	2.02	0.43
2:L:833:THR:O	2:L:837:TYR:HD2	2.02	0.43
5:c:6:PRO:O	7:p:49:MET:HE1	2.18	0.43
6:i:411:GLU:OE1	6:i:411:GLU:HA	2.19	0.43
9:r:542:LEU:HD23	9:s:534:LEU:HB2	2.01	0.43
2:G:470:TYR:HA	2:G:594:VAL:O	2.18	0.43
2:K:684:ASN:OD1	2:K:684:ASN:N	2.51	0.43
2:L:323:ALA:HB1	2:L:401:LEU:HD12	2.00	0.43
6:h:411:GLU:OE1	6:h:411:GLU:HA	2.19	0.43
6:j:411:GLU:HA	6:j:411:GLU:OE1	2.19	0.43
7:k:121:ASP:OD1	7:k:121:ASP:N	2.49	0.43
9:r:206:PHE:CE2	9:s:57:ALA:HA	2.53	0.43
1:C:281:VAL:HB	1:C:320:ILE:HB	2.01	0.43
1:E:281:VAL:HB	1:E:320:ILE:HB	2.01	0.43
2:G:345:ASP:OD1	2:G:345:ASP:N	2.49	0.43
2:I:509:PRO:HG2	2:I:548:LEU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:765:ALA:C	2:J:766:VAL:HG23	2.44	0.43
2:L:305:THR:HB	2:L:412:ASP:HB2	2.01	0.43
3:Q:168:GLN:NE2	3:R:107:GLU:HG3	2.34	0.43
9:q:558:GLU:HA	9:s:566:SER:O	2.19	0.43
9:q:552:ASN:C	9:s:560:SER:HG	2.25	0.42
9:s:154:GLU:OE1	9:s:154:GLU:N	2.52	0.42
1:B:254:ASP:OD1	2:H:150:LEU:HD21	2.18	0.42
1:D:409:PRO:HD2	6:j:547:GLU:CD	2.44	0.42
1:F:258:GLU:HA	2:J:824:ARG:HH21	1.73	0.42
2:G:321:ASN:O	2:G:392:LYS:NZ	2.42	0.42
1:B:509:ARG:HH12	2:H:139:HIS:HD2	1.65	0.42
1:F:491:LYS:HB3	2:J:91:PHE:CE2	2.54	0.42
2:H:875:ASP:N	2:H:875:ASP:OD1	2.47	0.42
2:J:310:ILE:O	2:J:311:LEU:HD23	2.20	0.42
2:K:471:GLN:O	2:K:593:LEU:HA	2.18	0.42
2:K:662:VAL:N	2:K:721:PHE:O	2.35	0.42
3:O:168:GLN:NE2	3:P:107:GLU:HG3	2.34	0.42
6:e:411:GLU:HA	6:e:411:GLU:OE1	2.19	0.42
9:q:377:LEU:O	9:s:438:ILE:HG23	2.19	0.42
1:A:281:VAL:HB	1:A:320:ILE:HB	2.01	0.42
1:D:283:LEU:HD23	1:D:283:LEU:HA	1.88	0.42
2:H:158:ASP:OD1	2:H:767:PHE:HB2	2.20	0.42
2:H:310:ILE:O	2:H:311:LEU:HD23	2.19	0.42
2:K:295:GLU:OE2	2:K:422:ILE:HG23	2.19	0.42
6:g:411:GLU:HA	6:g:411:GLU:OE1	2.19	0.42
1:A:44:TYR:HE1	4:S:127:TYR:HB2	1.83	0.42
1:B:283:LEU:HG	1:B:304:LEU:HG	2.00	0.42
1:B:410:LYS:O	1:B:410:LYS:HG3	2.20	0.42
2:G:775:ASN:OD1	2:G:776:HIS:N	2.53	0.42
6:g:172:ASP:OD1	6:g:172:ASP:N	2.40	0.42
1:F:34:LYS:HD2	4:V:127:TYR:HE1	1.78	0.42
3:R:2:SER:O	3:R:2:SER:OG	2.37	0.42
1:D:505:HIS:CE1	2:L:29:PRO:HA	2.53	0.42
2:I:314:GLY:N	2:I:350:SER:HB3	2.35	0.42
2:J:470:TYR:HB2	2:J:593:LEU:HD11	2.02	0.42
2:K:301:ILE:O	2:K:415:ILE:HA	2.20	0.42
2:L:765:ALA:C	2:L:766:VAL:HG23	2.44	0.42
2:L:841:ILE:HD13	2:L:841:ILE:HA	1.93	0.42
4:T:4:LYS:HG2	4:T:4:LYS:O	2.20	0.42
4:V:125:MET:HE3	4:V:125:MET:HB3	1.93	0.42
9:r:154:GLU:OE1	9:r:154:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:ASP:OD1	2:I:150:LEU:CD2	2.68	0.42
2:H:470:TYR:HB2	2:H:593:LEU:HD11	2.02	0.42
2:H:765:ALA:C	2:H:766:VAL:HG23	2.44	0.42
2:H:833:THR:O	2:H:837:TYR:HD2	2.02	0.42
2:J:305:THR:HB	2:J:412:ASP:HB2	2.01	0.42
2:K:174:LYS:HD2	2:K:199:GLU:CD	2.43	0.42
2:K:509:PRO:HG2	2:K:548:LEU:HA	2.01	0.42
2:L:310:ILE:O	2:L:311:LEU:HD23	2.20	0.42
4:U:4:LYS:O	4:U:4:LYS:HG2	2.20	0.42
9:q:127:TYR:HE1	9:r:402:ASN:HB3	1.82	0.42
1:C:299:VAL:O	2:J:969:ARG:CB	2.67	0.42
1:E:252:THR:OG1	1:E:253:MET:N	2.53	0.42
2:I:775:ASN:OD1	2:I:776:HIS:N	2.53	0.42
2:K:314:GLY:N	2:K:350:SER:HB3	2.35	0.42
2:K:535:ILE:HD11	2:K:540:TRP:CZ3	2.55	0.42
2:L:470:TYR:HB2	2:L:593:LEU:HD11	2.02	0.42
3:M:168:GLN:NE2	3:N:107:GLU:HG3	2.34	0.42
6:i:525:SER:HA	6:i:526:PRO:HD3	1.94	0.42
1:B:409:PRO:HD2	6:f:547:GLU:CD	2.43	0.42
1:C:159:TYR:OH	2:K:908:HIS:CD2	2.73	0.42
2:K:858:CYS:SG	2:K:864:SER:HB3	2.60	0.42
6:h:83:LEU:CD2	6:h:83:LEU:C	2.90	0.42
6:i:437:LEU:O	6:i:438:THR:C	2.63	0.42
7:m:33:ILE:CD1	7:n:111:LEU:HD12	2.46	0.42
9:q:530:LYS:O	9:s:538:GLY:CA	2.66	0.42
9:q:570:VAL:HG22	9:s:577:LEU:HB3	2.02	0.42
9:s:580:ILE:O	9:s:581:ASN:C	2.60	0.42
1:E:410:LYS:HG3	1:E:410:LYS:O	2.20	0.41
1:F:44:TYR:HE1	4:V:127:TYR:HB2	1.83	0.41
1:F:316:ASN:ND2	1:F:318:TRP:HE1	2.17	0.41
2:J:158:ASP:OD1	2:J:767:PHE:HB2	2.20	0.41
2:K:281:ARG:NH2	2:K:619:GLU:OE1	2.53	0.41
4:W:36:GLN:NE2	6:i:685:PHE:HB2	2.30	0.41
5:c:3:THR:HG22	5:c:4:TYR:N	2.32	0.41
1:A:410:LYS:O	1:A:410:LYS:HG3	2.20	0.41
1:D:258:GLU:OE2	2:L:829:LYS:HG2	2.19	0.41
2:G:858:CYS:SG	2:G:864:SER:HB3	2.60	0.41
2:H:305:THR:HB	2:H:412:ASP:HB2	2.01	0.41
2:K:295:GLU:HG3	2:K:422:ILE:HG12	2.01	0.41
4:W:4:LYS:O	4:W:4:LYS:HG2	2.20	0.41
9:q:540:ILE:HD12	9:s:543:GLU:O	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:OD1	2:G:150:LEU:HD22	2.19	0.41
1:E:258:GLU:HA	2:I:824:ARG:HH22	1.85	0.41
1:F:505:HIS:CB	2:J:32:VAL:HG21	2.50	0.41
2:G:535:ILE:HD11	2:G:540:TRP:CZ3	2.55	0.41
2:I:295:GLU:HG3	2:I:422:ILE:HG12	2.01	0.41
3:P:15:LYS:HE3	3:P:21:ASP:HB3	2.03	0.41
4:X:4:LYS:O	4:X:4:LYS:HG2	2.20	0.41
9:q:98:ASN:OD1	9:s:216:GLU:HG3	2.21	0.41
9:q:469:LYS:HD2	9:s:425:PHE:CD2	2.55	0.41
1:A:283:LEU:HD12	1:A:318:TRP:CD2	2.56	0.41
1:C:98:PRO:CB	1:C:103:ASP:HB3	2.50	0.41
1:D:505:HIS:HB2	2:L:32:VAL:HG21	2.03	0.41
1:D:505:HIS:CB	2:L:32:VAL:HG21	2.50	0.41
1:F:36:LEU:O	2:J:109:GLY:C	2.64	0.41
2:K:302:LEU:HA	2:K:414:LYS:O	2.21	0.41
4:S:106:GLY:O	6:e:680:PHE:N	2.44	0.41
4:V:4:LYS:O	4:V:4:LYS:HG2	2.20	0.41
6:f:255:HIS:HD2	6:f:256:LEU:N	2.19	0.41
6:f:411:GLU:OE1	6:f:411:GLU:HA	2.19	0.41
6:f:657:THR:OG1	6:f:658:ALA:N	2.54	0.41
6:j:205:ASN:OD1	6:j:207:GLY:N	2.46	0.41
9:q:154:GLU:OE1	9:q:154:GLU:N	2.52	0.41
9:r:363:HIS:HE1	9:s:372:ALA:CA	2.33	0.41
1:A:348:ASN:OD1	1:A:349:PRO:HD2	2.21	0.41
1:A:464:ASP:OD1	1:A:464:ASP:N	2.50	0.41
1:C:316:ASN:ND2	1:C:318:TRP:HE1	2.17	0.41
1:D:368:LEU:HD23	1:D:368:LEU:HA	1.85	0.41
2:G:509:PRO:HG2	2:G:548:LEU:HA	2.01	0.41
2:H:519:PHE:HB3	2:H:527:TYR:CD2	2.55	0.41
2:I:281:ARG:NH2	2:I:619:GLU:OE1	2.53	0.41
2:L:158:ASP:OD1	2:L:767:PHE:HB2	2.20	0.41
2:G:314:GLY:N	2:G:350:SER:HB3	2.35	0.41
3:N:15:LYS:HE3	3:N:21:ASP:HB3	2.03	0.41
4:S:4:LYS:O	4:S:4:LYS:HG2	2.20	0.41
9:q:59:GLU:O	9:q:60:ARG:CB	2.51	0.41
9:q:562:GLY:HA2	9:s:567:THR:CG2	2.50	0.41
1:C:283:LEU:HD12	1:C:318:TRP:CD2	2.56	0.41
1:D:98:PRO:CB	1:D:103:ASP:HB3	2.51	0.41
1:F:491:LYS:HB3	2:J:91:PHE:HE2	1.86	0.41
2:I:301:ILE:O	2:I:415:ILE:HA	2.20	0.41
2:I:662:VAL:N	2:I:721:PHE:O	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:775:ASN:OD1	2:K:776:HIS:N	2.53	0.41
3:O:15:LYS:HE3	3:O:21:ASP:HB3	2.03	0.41
3:P:98:LYS:HE2	3:P:98:LYS:HB3	1.80	0.41
5:a:3:THR:HG22	5:a:4:TYR:N	2.32	0.41
5:c:11:HIS:HA	7:o:39:GLY:O	2.21	0.41
6:e:255:HIS:HD2	6:e:256:LEU:N	2.19	0.41
6:g:255:HIS:HD2	6:g:256:LEU:N	2.19	0.41
6:j:472:LYS:HB2	6:j:472:LYS:HE3	1.66	0.41
1:C:252:THR:OG1	1:C:253:MET:N	2.53	0.41
1:F:252:THR:OG1	1:F:253:MET:N	2.53	0.41
1:F:409:PRO:HD2	6:h:547:GLU:CD	2.45	0.41
2:I:476:ASN:HB3	2:J:449:LYS:O	2.21	0.41
3:Q:15:LYS:HE3	3:Q:21:ASP:HB3	2.03	0.41
6:e:657:THR:OG1	6:e:658:ALA:N	2.54	0.41
6:f:83:LEU:CD2	6:f:83:LEU:C	2.90	0.41
6:g:472:LYS:HE3	6:g:472:LYS:HB2	1.66	0.41
7:m:32:GLU:OE2	7:m:54:LYS:NZ	2.49	0.41
9:r:363:HIS:CE1	9:s:372:ALA:HA	2.53	0.41
1:A:98:PRO:CB	1:A:103:ASP:HB3	2.51	0.41
1:A:252:THR:OG1	1:A:253:MET:N	2.53	0.41
1:B:98:PRO:CB	1:B:103:ASP:HB3	2.51	0.41
1:C:410:LYS:HG3	1:C:410:LYS:O	2.20	0.41
1:D:10:ILE:HA	1:D:11:PRO:HD3	1.89	0.41
1:D:239:ARG:HH21	1:D:363:ARG:HD3	1.83	0.41
1:E:44:TYR:HE1	4:U:127:TYR:HB2	1.81	0.41
1:E:283:LEU:HD12	1:E:318:TRP:CD2	2.56	0.41
1:E:316:ASN:ND2	1:E:318:TRP:HE1	2.17	0.41
1:E:348:ASN:OD1	1:E:349:PRO:HD2	2.21	0.41
1:F:410:LYS:O	1:F:410:LYS:HG3	2.20	0.41
2:G:281:ARG:NH2	2:G:619:GLU:OE1	2.53	0.41
2:G:302:LEU:HA	2:G:414:LYS:O	2.20	0.41
2:J:519:PHE:HB3	2:J:527:TYR:CD2	2.55	0.41
2:K:639:LEU:HD23	2:K:639:LEU:HA	1.92	0.41
2:K:790:GLN:HA	2:K:790:GLN:OE1	2.21	0.41
2:L:89:ASP:OD1	2:L:89:ASP:N	2.52	0.41
3:P:172:MET:CE	4:W:120:ASN:O	2.69	0.41
6:h:657:THR:OG1	6:h:658:ALA:N	2.54	0.41
6:j:657:THR:OG1	6:j:658:ALA:N	2.54	0.41
7:k:32:GLU:OE2	7:k:54:LYS:NZ	2.49	0.41
7:n:32:GLU:OE2	7:n:54:LYS:NZ	2.49	0.41
9:q:555:PHE:O	9:s:563:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:PRO:HA	1:A:409:PRO:HD3	1.96	0.41
1:D:90:VAL:HG12	2:L:148:LEU:HA	2.01	0.41
1:D:258:GLU:HA	2:L:824:ARG:HH21	1.79	0.41
1:D:464:ASP:OD1	1:D:464:ASP:N	2.50	0.41
1:F:90:VAL:HG12	2:J:148:LEU:HA	2.02	0.41
2:G:301:ILE:O	2:G:415:ILE:HA	2.20	0.41
2:I:858:CYS:SG	2:I:864:SER:HB3	2.60	0.41
3:N:168:GLN:NE2	3:O:107:GLU:HG3	2.35	0.41
5:b:3:THR:HG22	5:b:4:TYR:N	2.32	0.41
7:k:70:GLU:OE1	7:k:70:GLU:HA	2.21	0.41
9:q:57:ALA:HA	9:s:206:PHE:HE2	1.78	0.41
1:A:348:ASN:HD21	1:A:350:VAL:HB	1.87	0.40
1:B:252:THR:OG1	1:B:253:MET:N	2.53	0.40
1:F:491:LYS:CB	2:J:91:PHE:HE2	2.34	0.40
2:I:71:PHE:HZ	4:U:20:GLU:O	2.03	0.40
2:I:302:LEU:HA	2:I:414:LYS:O	2.21	0.40
2:J:169:ASN:ND2	9:r:430:GLU:CD	2.78	0.40
2:J:797:LYS:O	2:J:798:SER:CB	2.63	0.40
3:M:15:LYS:HE3	3:M:21:ASP:HB3	2.03	0.40
6:h:437:LEU:O	6:h:438:THR:C	2.63	0.40
1:F:98:PRO:CB	1:F:103:ASP:HB3	2.51	0.40
2:G:613:GLN:HA	2:G:630:PRO:HB3	2.04	0.40
2:K:613:GLN:HA	2:K:630:PRO:HB3	2.04	0.40
2:L:781:LEU:HA	2:L:782:PRO:HD3	1.87	0.40
3:M:10:ARG:NH1	3:M:27:GLU:OE1	2.55	0.40
5:Z:3:THR:HG22	5:Z:4:TYR:N	2.32	0.40
6:f:437:LEU:O	6:f:438:THR:C	2.63	0.40
9:q:541:ASN:OD1	9:s:548:ASN:HB2	2.21	0.40
9:r:56:ASP:C	9:r:56:ASP:OD1	2.65	0.40
1:B:281:VAL:O	1:B:319:VAL:HA	2.22	0.40
1:E:98:PRO:CB	1:E:103:ASP:HB3	2.51	0.40
2:I:535:ILE:HD11	2:I:540:TRP:CZ3	2.55	0.40
2:K:299:ASP:HB2	2:K:418:GLU:HB3	2.03	0.40
2:L:519:PHE:HB3	2:L:527:TYR:CD2	2.55	0.40
3:R:10:ARG:NH1	3:R:27:GLU:OE1	2.55	0.40
6:g:83:LEU:CD2	6:g:83:LEU:C	2.90	0.40
6:g:657:THR:OG1	6:g:658:ALA:N	2.54	0.40
1:C:89:LYS:HZ1	6:i:85:GLU:CD	2.05	0.40
1:C:409:PRO:HD2	6:i:547:GLU:CD	2.47	0.40
1:D:410:LYS:O	1:D:410:LYS:HG3	2.20	0.40
2:I:299:ASP:HB2	2:I:418:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:89:ASP:OD1	2:J:89:ASP:N	2.52	0.40
2:J:586:TYR:CZ	2:J:588:PRO:HA	2.57	0.40
2:L:586:TYR:CZ	2:L:588:PRO:HA	2.57	0.40
3:R:15:LYS:HE3	3:R:21:ASP:HB3	2.03	0.40
5:d:36:VAL:C	5:d:37:ASP:OD2	2.65	0.40
6:e:45:ASP:OD1	6:e:45:ASP:N	2.47	0.40
6:e:437:LEU:O	6:e:438:THR:C	2.63	0.40
6:i:253:ILE:HD11	6:i:478:LEU:CD2	2.51	0.40
6:i:420:ASN:O	6:i:421:PHE:C	2.64	0.40
7:n:70:GLU:OE1	7:n:70:GLU:HA	2.21	0.40
7:p:70:GLU:HA	7:p:70:GLU:OE1	2.21	0.40
9:r:80:VAL:HG12	9:r:89:ILE:HG13	2.03	0.40
1:B:10:ILE:HG13	3:R:224:LEU:CD2	2.41	0.40
1:D:281:VAL:O	1:D:319:VAL:HA	2.22	0.40
1:E:410:LYS:HD3	6:h:3:THR:O	2.22	0.40
1:F:88:TYR:O	2:J:143:TYR:HE1	2.04	0.40
1:F:219:GLU:CB	1:F:347:LEU:HD21	2.45	0.40
1:F:318:TRP:CD1	2:I:985:ILE:O	2.71	0.40
2:G:266:LYS:HE2	2:G:266:LYS:HB3	1.89	0.40
2:H:246:ASP:OD1	2:H:246:ASP:N	2.54	0.40
2:K:745:MET:HG2	2:K:747:LYS:H	1.86	0.40
3:O:10:ARG:NH1	3:O:27:GLU:OE1	2.55	0.40
6:e:205:ASN:OD1	6:e:207:GLY:N	2.46	0.40
6:i:255:HIS:C	6:i:256:LEU:HD23	2.47	0.40
6:j:255:HIS:C	6:j:256:LEU:HD23	2.47	0.40
9:s:59:GLU:O	9:s:60:ARG:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	B	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	C	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	D	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	E	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
1	F	547/933 (59%)	533 (97%)	14 (3%)	0	100	100
2	G	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	36	66
2	H	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	36	66
2	I	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	36	66
2	J	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	36	66
2	K	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	36	66
2	L	1009/1050 (96%)	971 (96%)	35 (4%)	3 (0%)	36	66
3	M	221/228 (97%)	218 (99%)	3 (1%)	0	100	100
3	N	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
3	O	221/228 (97%)	218 (99%)	3 (1%)	0	100	100
3	P	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
3	Q	221/228 (97%)	219 (99%)	2 (1%)	0	100	100
3	R	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
4	S	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	T	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	U	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	V	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	W	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
4	X	131/137 (96%)	130 (99%)	1 (1%)	0	100	100
5	Y	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	Z	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	a	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	b	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	c	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
5	d	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
6	e	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	f	651/692 (94%)	635 (98%)	16 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	g	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	h	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	i	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
6	j	651/692 (94%)	635 (98%)	16 (2%)	0	100	100
7	k	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	l	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	m	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	n	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	o	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
7	p	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
8	t	36/52 (69%)	36 (100%)	0	0	100	100
8	u	36/52 (69%)	36 (100%)	0	0	100	100
8	v	36/52 (69%)	36 (100%)	0	0	100	100
9	q	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
9	r	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
9	s	578/581 (100%)	565 (98%)	13 (2%)	0	100	100
All	All	18888/21873 (86%)	18397 (97%)	473 (2%)	18 (0%)	49	77

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	1001	ASN
2	G	1015	PRO
2	G	1018	PRO
2	H	1001	ASN
2	H	1015	PRO
2	H	1018	PRO
2	I	1001	ASN
2	I	1015	PRO
2	I	1018	PRO
2	J	1001	ASN
2	J	1015	PRO
2	J	1018	PRO
2	K	1001	ASN
2	K	1015	PRO
2	K	1018	PRO

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Mol	Chain	Res	Type
2	L	1001	ASN
2	L	1015	PRO
2	L	1018	PRO

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	497/842 (59%)	497 (100%)	0	100	100
1	B	497/842 (59%)	497 (100%)	0	100	100
1	C	497/842 (59%)	497 (100%)	0	100	100
1	D	497/842 (59%)	497 (100%)	0	100	100
1	E	497/842 (59%)	497 (100%)	0	100	100
1	F	497/842 (59%)	497 (100%)	0	100	100
2	G	814/955 (85%)	813 (100%)	1 (0%)	88	97
2	H	814/955 (85%)	814 (100%)	0	100	100
2	I	814/955 (85%)	813 (100%)	1 (0%)	88	97
2	J	814/955 (85%)	814 (100%)	0	100	100
2	K	814/955 (85%)	813 (100%)	1 (0%)	88	97
2	L	814/955 (85%)	814 (100%)	0	100	100
3	M	201/204 (98%)	201 (100%)	0	100	100
3	N	201/204 (98%)	201 (100%)	0	100	100
3	O	201/204 (98%)	201 (100%)	0	100	100
3	P	201/204 (98%)	201 (100%)	0	100	100
3	Q	201/204 (98%)	201 (100%)	0	100	100
3	R	201/204 (98%)	201 (100%)	0	100	100
4	S	121/125 (97%)	121 (100%)	0	100	100
4	T	121/125 (97%)	121 (100%)	0	100	100
4	U	121/125 (97%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	V	121/125 (97%)	121 (100%)	0	100	100
4	W	121/125 (97%)	121 (100%)	0	100	100
4	X	121/125 (97%)	121 (100%)	0	100	100
5	Y	134/135 (99%)	134 (100%)	0	100	100
5	Z	134/135 (99%)	134 (100%)	0	100	100
5	a	134/135 (99%)	134 (100%)	0	100	100
5	b	134/135 (99%)	134 (100%)	0	100	100
5	c	134/135 (99%)	134 (100%)	0	100	100
5	d	134/135 (99%)	134 (100%)	0	100	100
6	e	547/593 (92%)	547 (100%)	0	100	100
6	f	547/593 (92%)	547 (100%)	0	100	100
6	g	547/593 (92%)	547 (100%)	0	100	100
6	h	547/593 (92%)	547 (100%)	0	100	100
6	i	547/593 (92%)	547 (100%)	0	100	100
6	j	547/593 (92%)	547 (100%)	0	100	100
7	k	127/128 (99%)	127 (100%)	0	100	100
7	l	127/128 (99%)	127 (100%)	0	100	100
7	m	127/128 (99%)	127 (100%)	0	100	100
7	n	127/128 (99%)	127 (100%)	0	100	100
7	o	127/128 (99%)	127 (100%)	0	100	100
7	p	127/128 (99%)	127 (100%)	0	100	100
8	t	39/45 (87%)	39 (100%)	0	100	100
8	u	39/45 (87%)	39 (100%)	0	100	100
8	v	39/45 (87%)	39 (100%)	0	100	100
9	q	499/500 (100%)	499 (100%)	0	100	100
9	r	499/500 (100%)	499 (100%)	0	100	100
9	s	499/500 (100%)	499 (100%)	0	100	100
All	All	16260/19527 (83%)	16257 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	359	LEU

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Mol	Chain	Res	Type
2	I	359	LEU
2	K	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	A	431	GLN
1	B	316	ASN
1	B	348	ASN
1	B	431	GLN
1	C	316	ASN
1	C	431	GLN
1	D	316	ASN
1	D	348	ASN
1	D	431	GLN
1	E	316	ASN
1	E	431	GLN
1	F	316	ASN
1	F	348	ASN
1	F	431	GLN
2	G	139	HIS
2	G	149	HIS
2	G	437	GLN
2	G	471	GLN
2	G	563	HIS
2	G	626	GLN
2	G	856	HIS
2	G	879	GLN
2	H	139	HIS
2	H	149	HIS
2	H	172	GLN
2	H	513	ASN
2	H	759	HIS
2	H	800	GLN
2	H	856	HIS
2	H	886	GLN
2	I	139	HIS
2	I	149	HIS
2	I	437	GLN
2	I	471	GLN
2	I	626	GLN

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Mol	Chain	Res	Type
2	I	856	HIS
2	I	879	GLN
2	J	54	HIS
2	J	139	HIS
2	J	172	GLN
2	J	471	GLN
2	J	513	ASN
2	J	759	HIS
2	J	800	GLN
2	J	856	HIS
2	J	886	GLN
2	K	114	HIS
2	K	139	HIS
2	K	149	HIS
2	K	437	GLN
2	K	471	GLN
2	K	563	HIS
2	K	626	GLN
2	K	856	HIS
2	K	886	GLN
2	L	54	HIS
2	L	139	HIS
2	L	172	GLN
2	L	513	ASN
2	L	759	HIS
2	L	800	GLN
2	L	856	HIS
2	L	878	GLN
2	L	886	GLN
3	M	92	ASN
3	N	46	ASN
3	N	92	ASN
3	N	227	GLN
3	Q	92	ASN
3	R	92	ASN
4	S	36	GLN
4	S	87	HIS
4	S	102	ASN
4	T	36	GLN
4	T	59	ASN
4	T	87	HIS
4	U	36	GLN

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Mol	Chain	Res	Type
4	U	87	HIS
4	V	36	GLN
4	V	87	HIS
4	V	102	ASN
4	V	124	ASN
4	W	36	GLN
4	W	87	HIS
4	W	102	ASN
4	X	36	GLN
4	X	87	HIS
4	X	102	ASN
6	e	245	GLN
6	e	631	GLN
6	f	245	GLN
6	f	631	GLN
6	g	245	GLN
6	g	420	ASN
6	g	631	GLN
6	h	36	GLN
6	h	631	GLN
6	i	245	GLN
6	i	420	ASN
6	i	631	GLN
6	j	245	GLN
6	j	631	GLN
8	t	9	HIS
8	u	9	HIS
8	u	37	GLN
8	v	9	HIS
9	q	105	GLN
9	q	282	GLN
9	q	292	GLN
9	q	314	ASN
9	q	363	HIS
9	q	467	HIS
9	r	69	HIS
9	r	98	ASN
9	r	105	GLN
9	r	236	GLN
9	r	282	GLN
9	r	292	GLN
9	r	314	ASN

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Mol	Chain	Res	Type
9	r	363	HIS
9	r	456	ASN
9	r	467	HIS
9	r	533	ASN
9	r	546	ASN
9	s	69	HIS
9	s	282	GLN
9	s	292	GLN
9	s	314	ASN
9	s	363	HIS
9	s	467	HIS
9	s	513	ASN
9	s	533	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	3
2	J	3
2	L	3
2	G	1
2	I	1
2	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	509:PRO	C	510:LYS	N	1.70
1	I	509:PRO	C	510:LYS	N	1.70
1	K	509:PRO	C	510:LYS	N	1.70
1	H	506:LYS	C	507:SER	N	1.67
1	J	506:LYS	C	507:SER	N	1.67
1	L	506:LYS	C	507:SER	N	1.67
1	H	433:VAL	C	434:LEU	N	1.61
1	H	731:ASN	C	732:THR	N	1.61
1	J	433:VAL	C	434:LEU	N	1.61
1	J	731:ASN	C	732:THR	N	1.61
1	L	433:VAL	C	434:LEU	N	1.61
1	L	731:ASN	C	732:THR	N	1.61

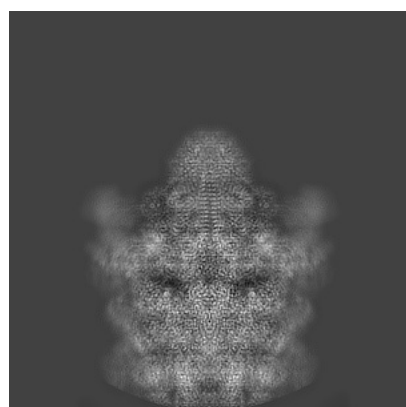
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11745. These allow visual inspection of the internal detail of the map and identification of artifacts.

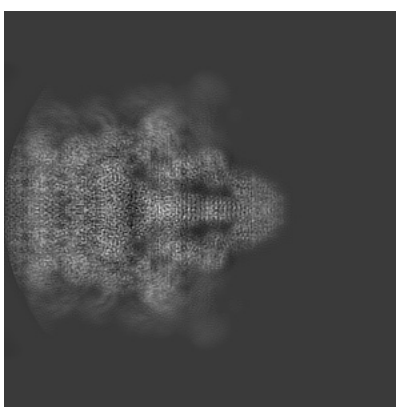
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

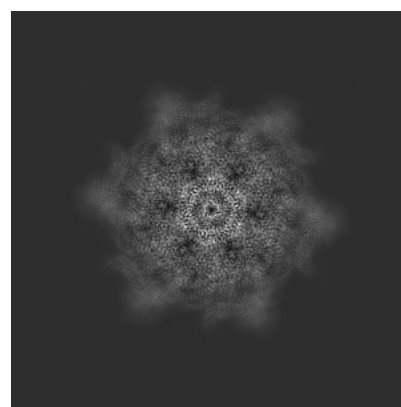
6.1.1 Primary map



X



Y

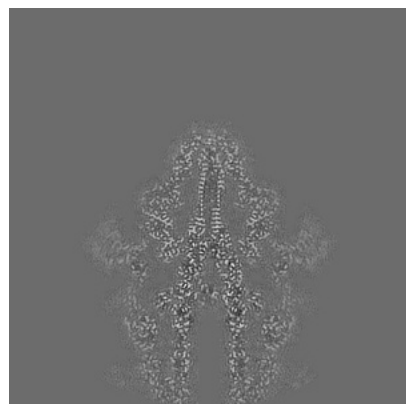


Z

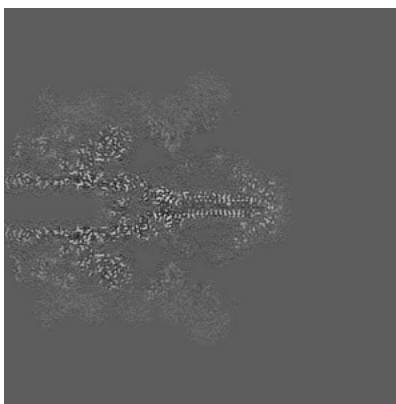
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

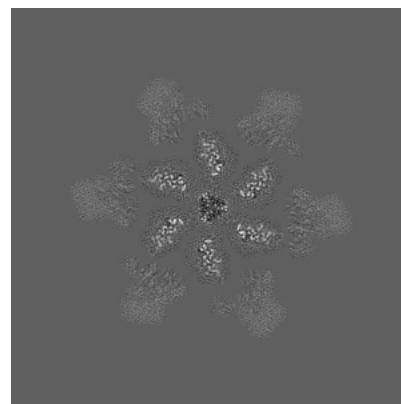
6.2.1 Primary map



X Index: 200



Y Index: 200

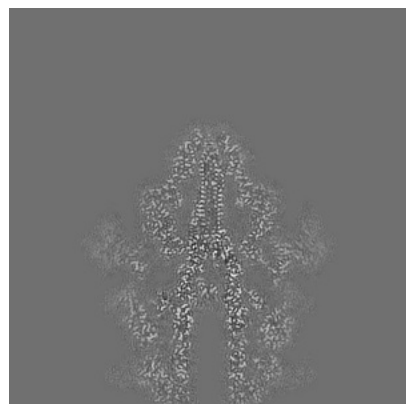


Z Index: 200

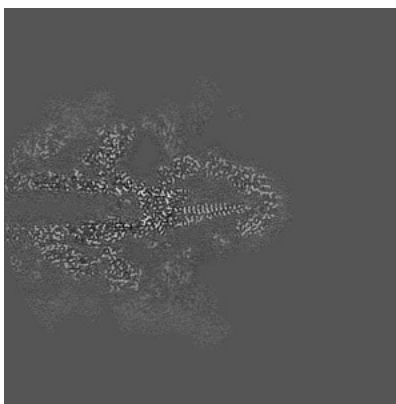
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

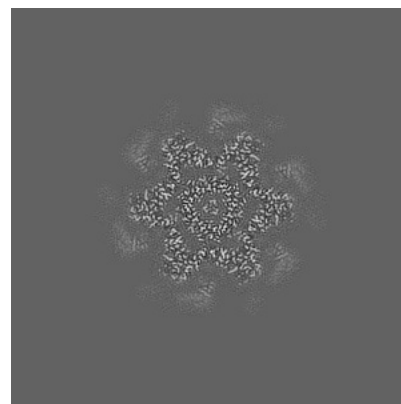
6.3.1 Primary map



X Index: 198



Y Index: 210

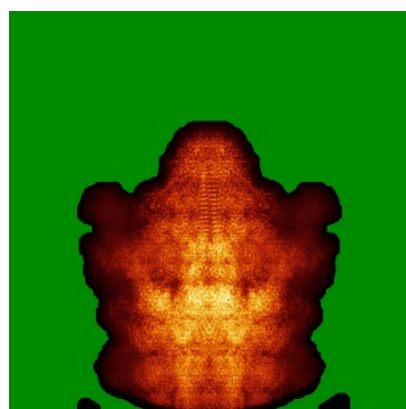


Z Index: 110

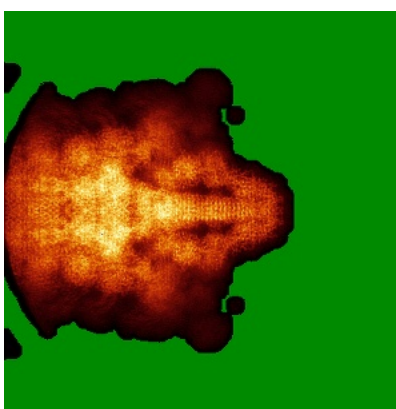
The images above show the largest variance slices of the map in three orthogonal directions.

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

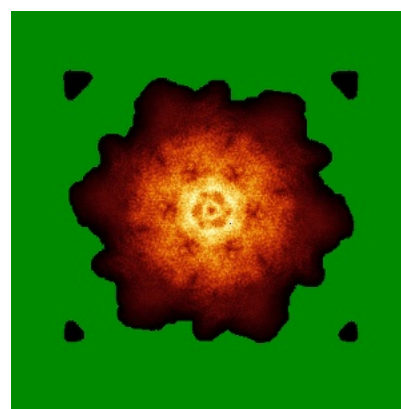
6.4.1 Primary map



X



Y

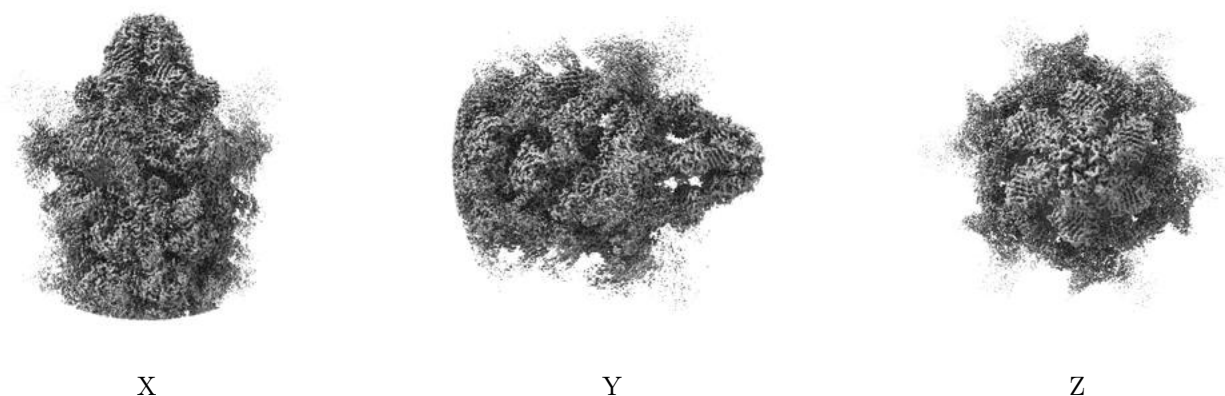


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

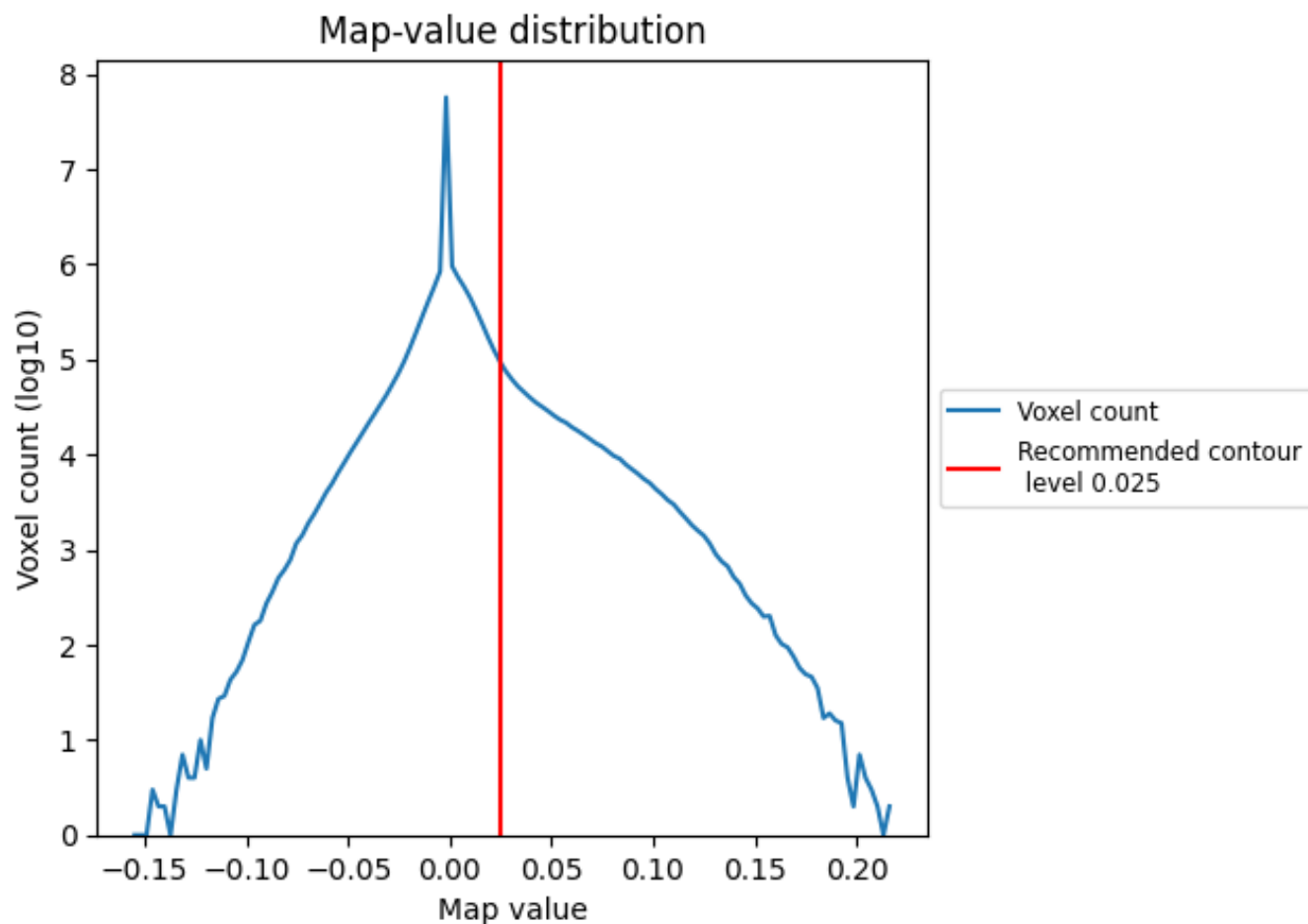
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

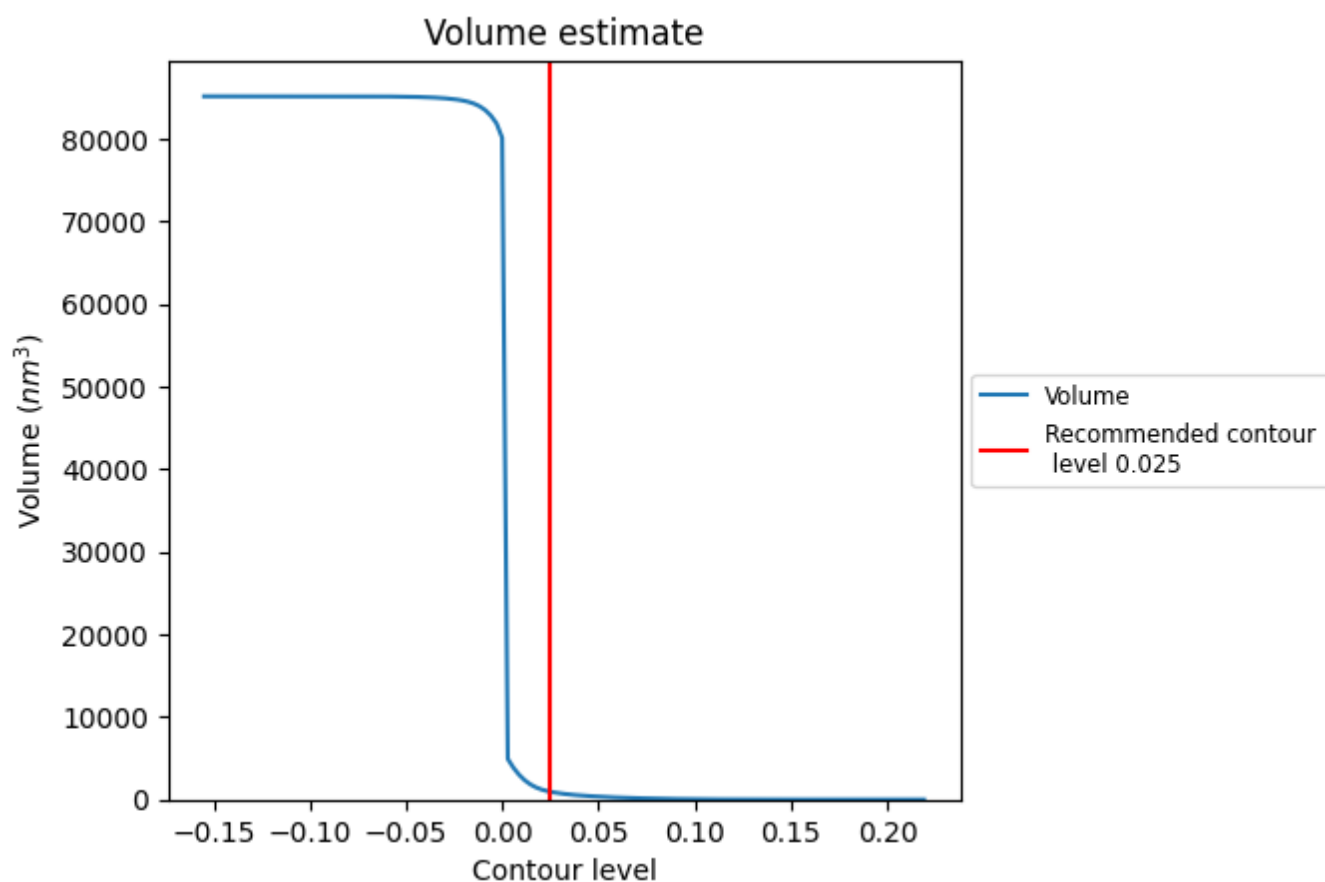
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

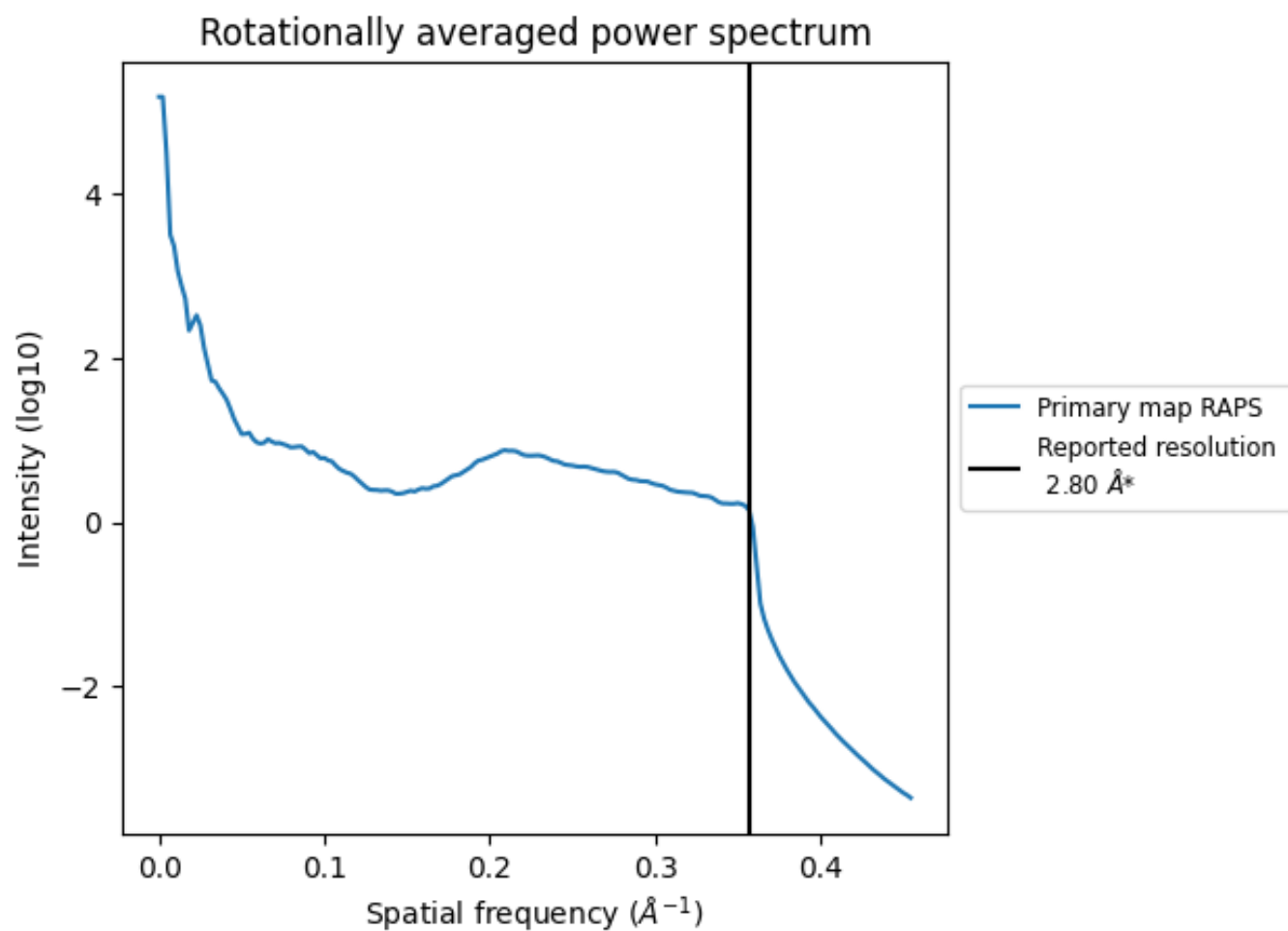
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 948 nm³; this corresponds to an approximate mass of 856 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

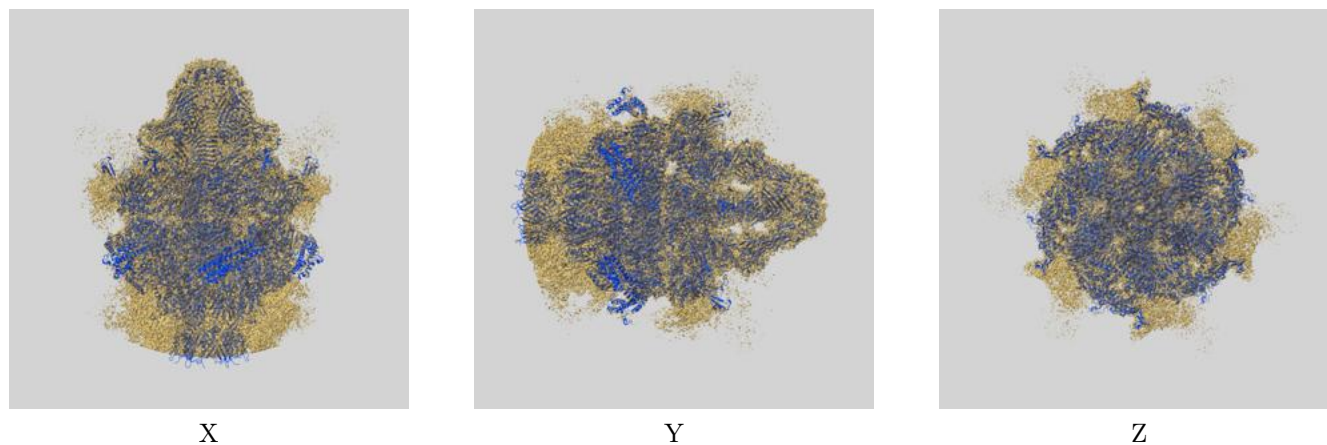
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

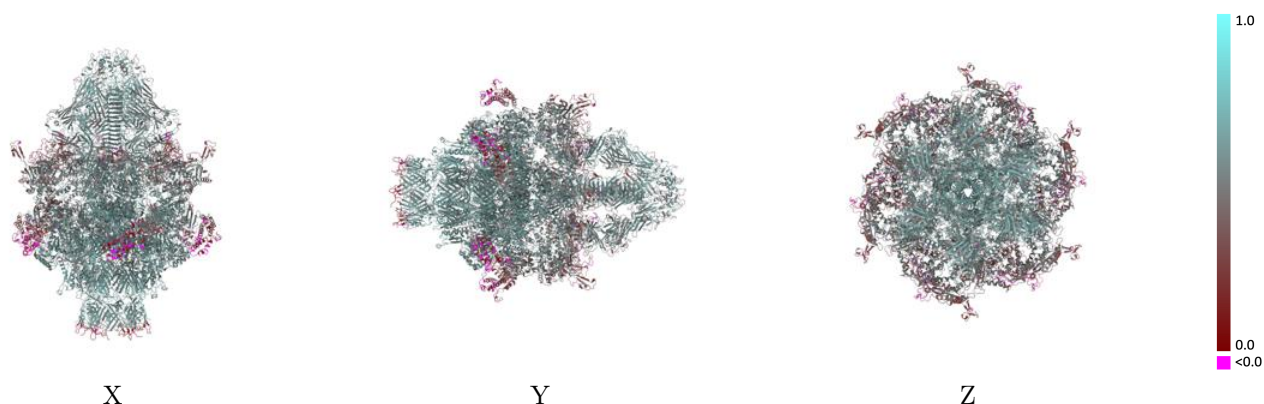
This section contains information regarding the fit between EMDB map EMD-11745 and PDB model 7AEF. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



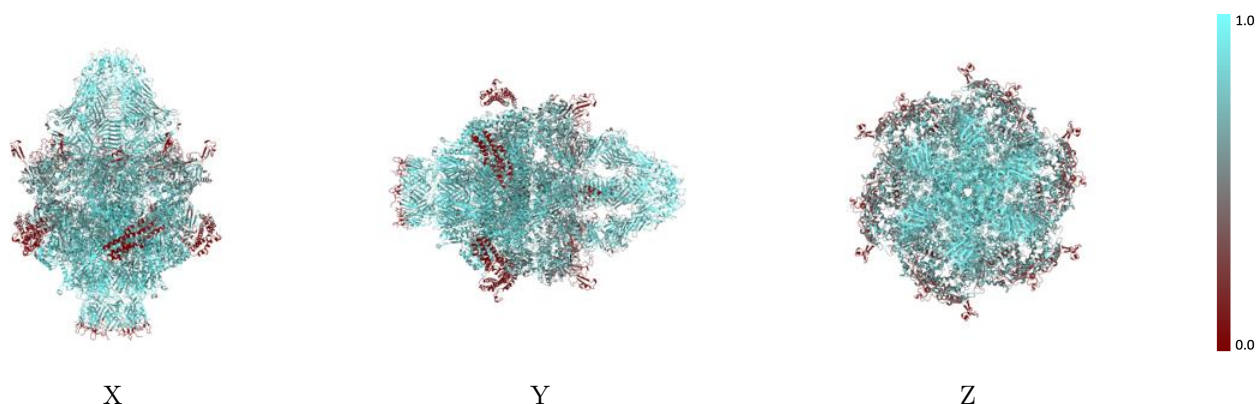
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



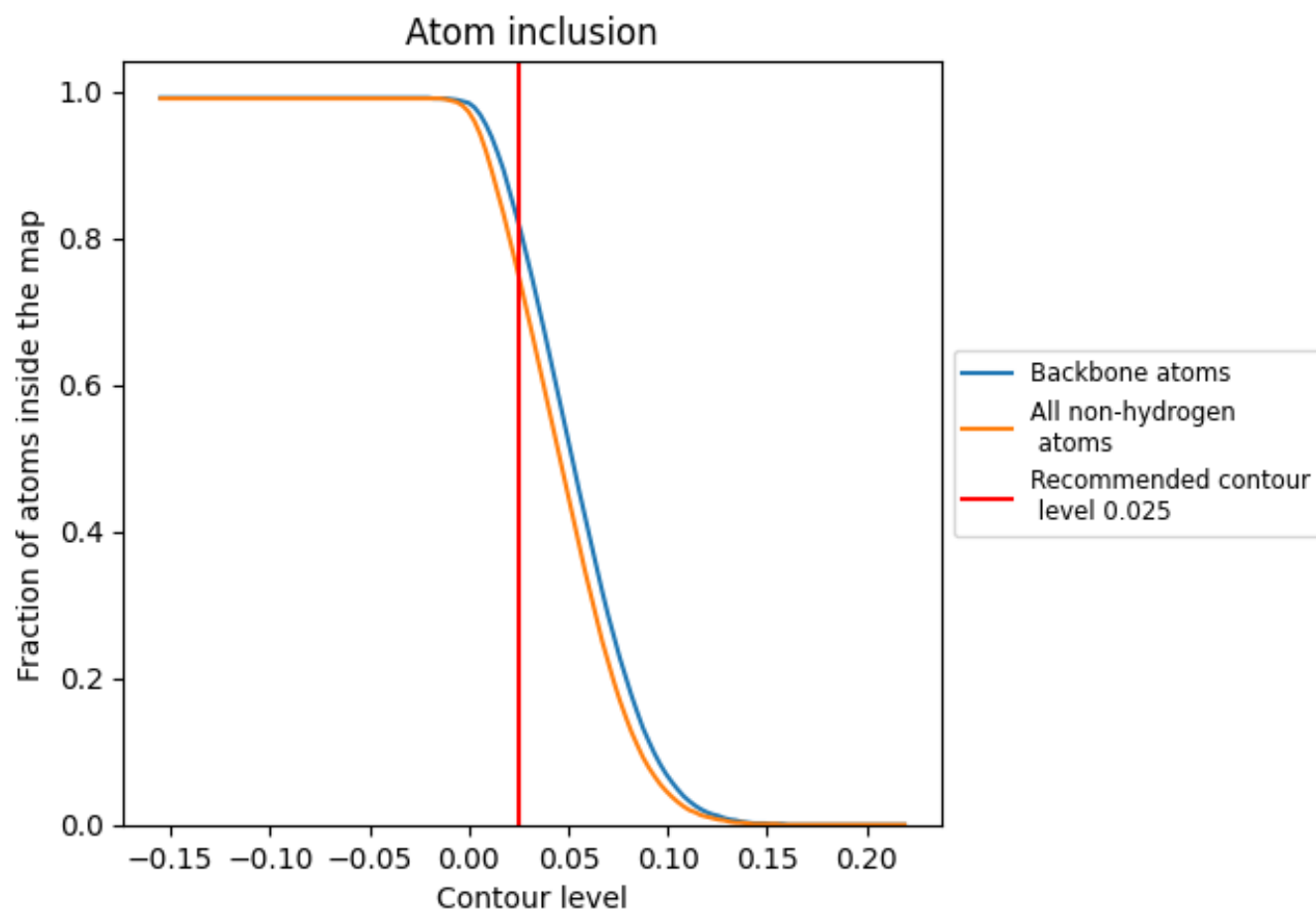
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7500	 0.5290
A	 0.6790	 0.5040
B	 0.6610	 0.5020
C	 0.6770	 0.5040
D	 0.6670	 0.5010
E	 0.6840	 0.5050
F	 0.6670	 0.5000
G	 0.7750	 0.5410
H	 0.7820	 0.5400
I	 0.7500	 0.5140
J	 0.7230	 0.4740
K	 0.7520	 0.5180
L	 0.7210	 0.4740
M	 0.9230	 0.6340
N	 0.9170	 0.6300
O	 0.9230	 0.6320
P	 0.9160	 0.6340
Q	 0.9180	 0.6330
R	 0.9140	 0.6300
S	 0.8740	 0.5930
T	 0.8520	 0.5840
U	 0.8720	 0.5890
V	 0.8540	 0.5850
W	 0.8750	 0.5910
X	 0.8510	 0.5850
Y	 0.8970	 0.6160
Z	 0.9010	 0.6190
a	 0.8900	 0.6150
b	 0.8960	 0.6190
c	 0.8950	 0.6160
d	 0.9000	 0.6210
e	 0.6400	 0.4800
f	 0.6480	 0.4780
g	 0.6440	 0.4810
h	 0.6450	 0.4790



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Chain	Atom inclusion	Q-score
i	 0.6380	 0.4800
j	 0.6430	 0.4780
k	 0.6480	 0.4770
l	 0.6460	 0.4760
m	 0.6430	 0.4710
n	 0.6520	 0.4690
o	 0.6460	 0.4710
p	 0.6460	 0.4780
q	 0.9240	 0.6240
r	 0.9230	 0.6200
s	 0.9230	 0.6240
t	 0.8110	 0.6230
u	 0.8140	 0.6180
v	 0.8070	 0.6160