



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:13 AM UTC

PDB ID : 7AEB / pdb_00007aeb
EMDB ID : EMD-11743
Title : Cryo-EM structure of an extracellular contractile injection system in marine bacterium *Algoriphagus machipongonensis*, the baseplate complex in extended state applied 6-fold symmetry.
Authors : Xu, J.; Ericson, C.; Feldmueller, M.; Lien, Y.W.; Pilhofer, M.
Deposited on : 2020-09-17
Resolution : 2.70 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

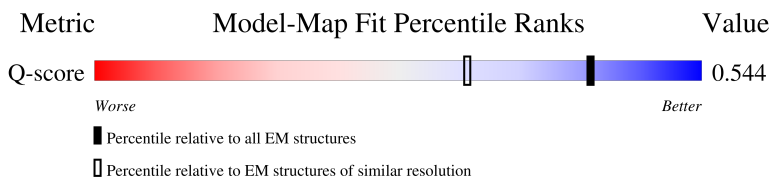
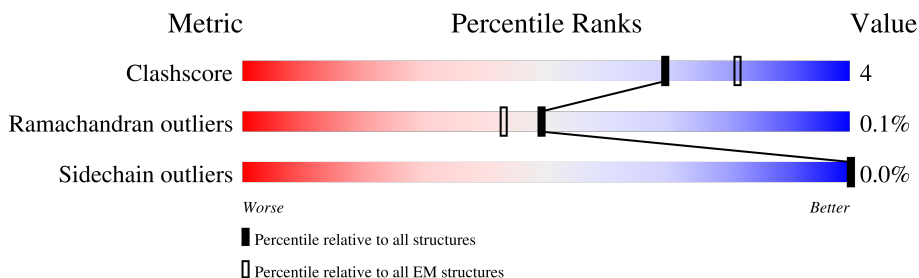
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	
1	B	933	
1	C	933	
1	D	933	



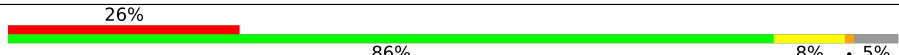
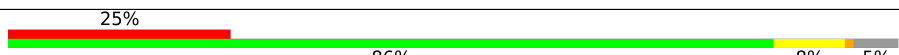
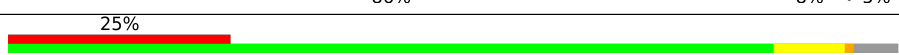
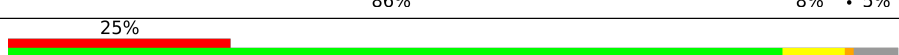

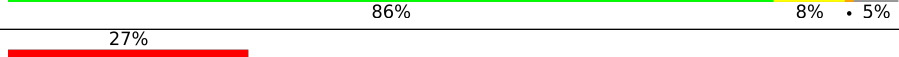


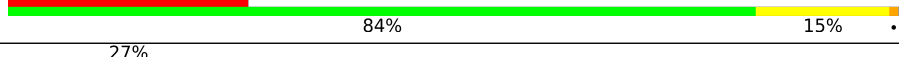

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Mol	Chain	Length	Quality of chain
1	E	933	
1	F	933	
2	G	1050	
2	H	1050	
2	I	1050	
2	J	1050	
2	K	1050	
2	L	1050	
3	M	228	
3	N	228	
3	O	228	
3	P	228	
3	Q	228	
3	R	228	
4	S	137	
4	T	137	
4	U	137	
4	V	137	
4	W	137	
4	X	137	
5	Y	147	
5	Z	147	
5	a	147	
5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

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Mol	Chain	Length	Quality of chain
5	d	147	 88% 10% •
6	e	692	 25% 86% 8% • 5%
6	f	692	 26% 86% 8% • 5%
6	g	692	 25% 86% 8% • 5%
6	h	692	 25% 86% 8% • 5%
6	i	692	 25% 87% 7% • 5%
6	j	692	 26% 86% 8% • 5%
7	k	142	 27% 85% 15% •
7	l	142	 26% 84% 15% •
7	m	142	 27% 84% 15% ••
7	n	142	 27% 85% 15% •
7	o	142	 26% 86% 13% •
7	p	142	 27% 85% 14% •

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 135156 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
			Total	C	N	O	S		
1	A	549	4447	2845	730	858	14	0	0
1	B	549	4447	2845	730	858	14	0	0
1	C	549	4447	2845	730	858	14	0	0
1	D	549	4447	2845	730	858	14	0	0
1	E	549	4447	2845	730	858	14	0	0
1	F	549	4447	2845	730	858	14	0	0

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

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

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

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

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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.

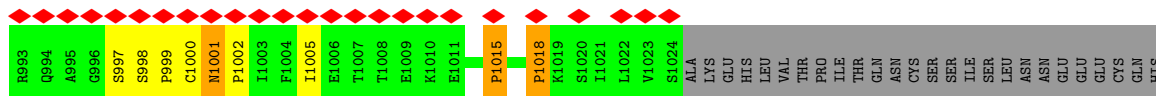
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	Z	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	a	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	b	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	c	145	Total	C	N	O	S	0	0
			1192	773	190	226	3		
5	d	145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

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

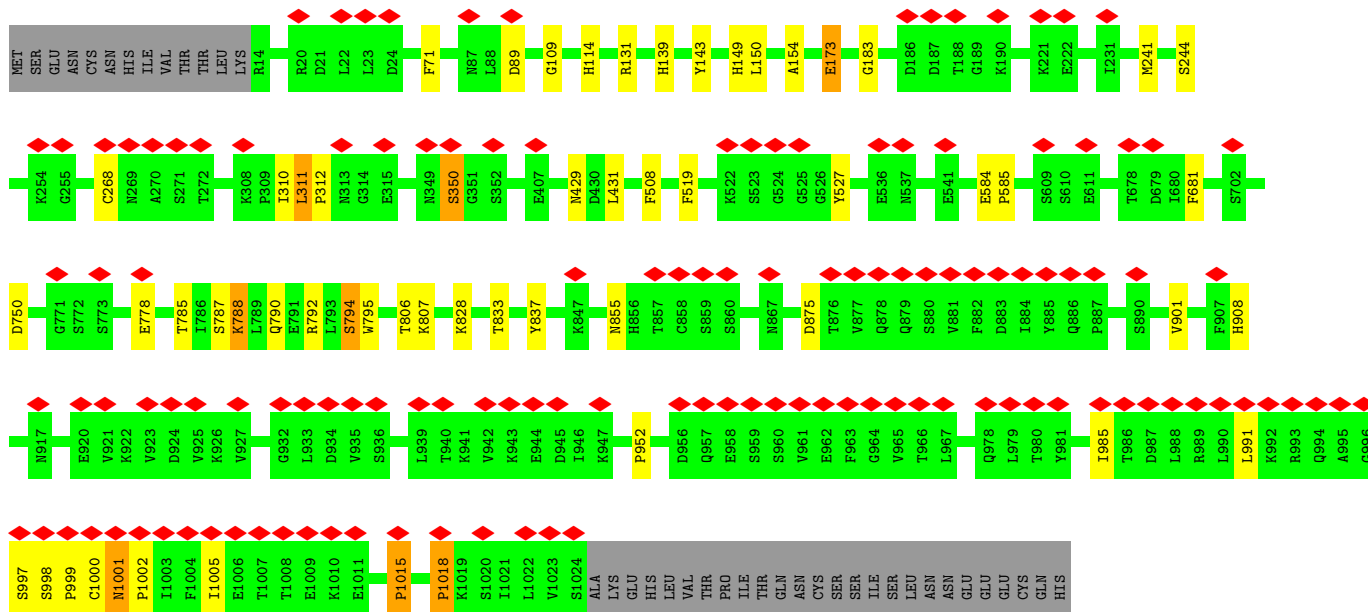
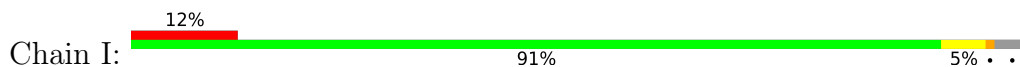
Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	f	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	g	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	h	655	Total	C	N	O	S	0	0
			5057	3204	832	1009	12		
6	i	655	Total	C	N	O	S	0	0
			5057	3204	832	1009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

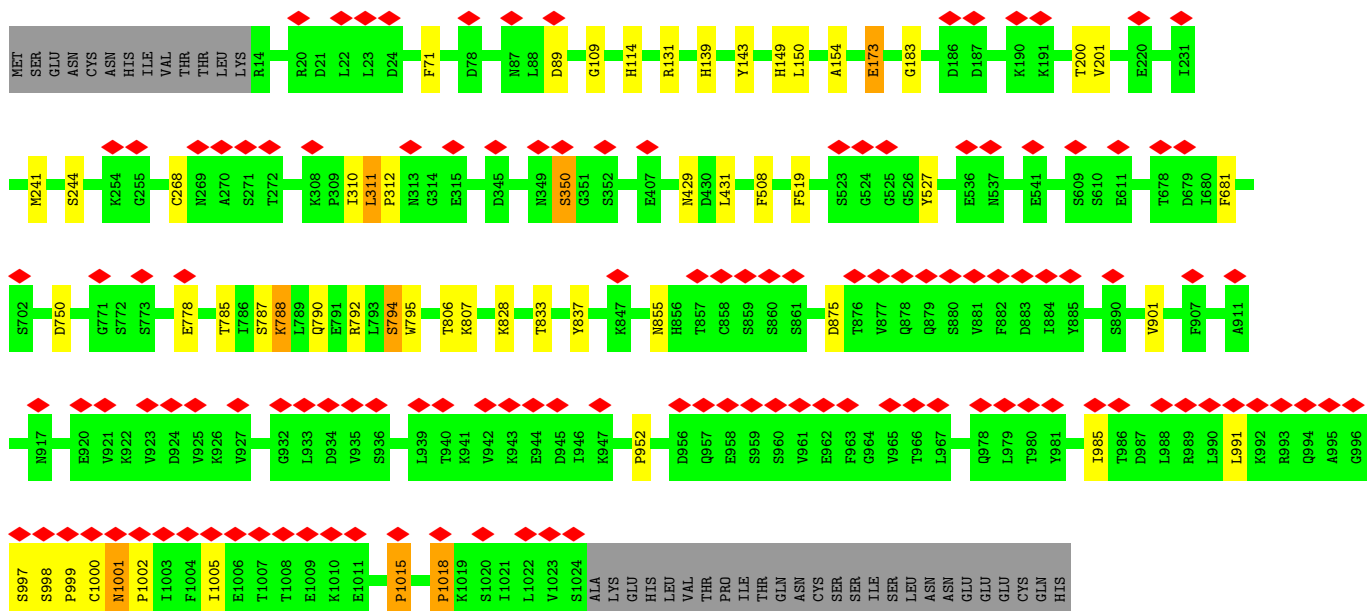
Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	l	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	m	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	n	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	o	141	Total	C	N	O	S	0	0
			1145	731	190	221	3		
7	p	141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



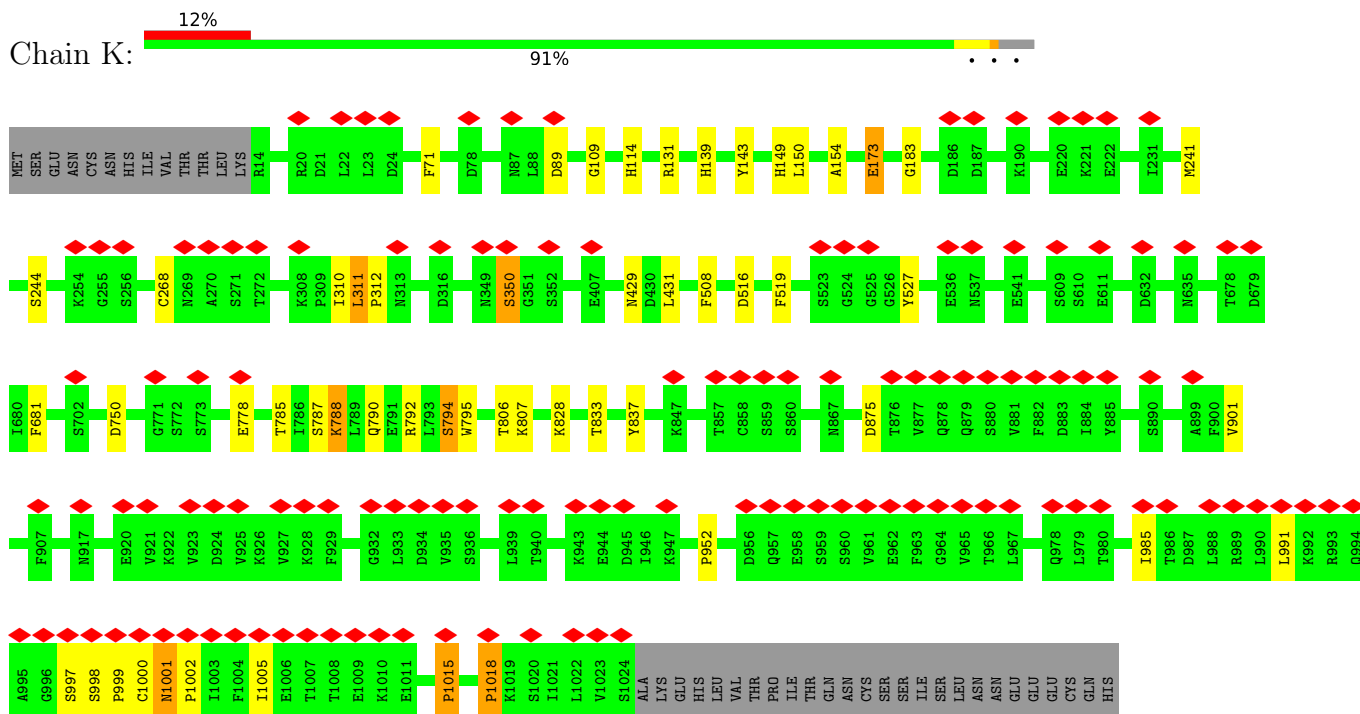
• Molecule 2: Baseplate_J domain-containing protein



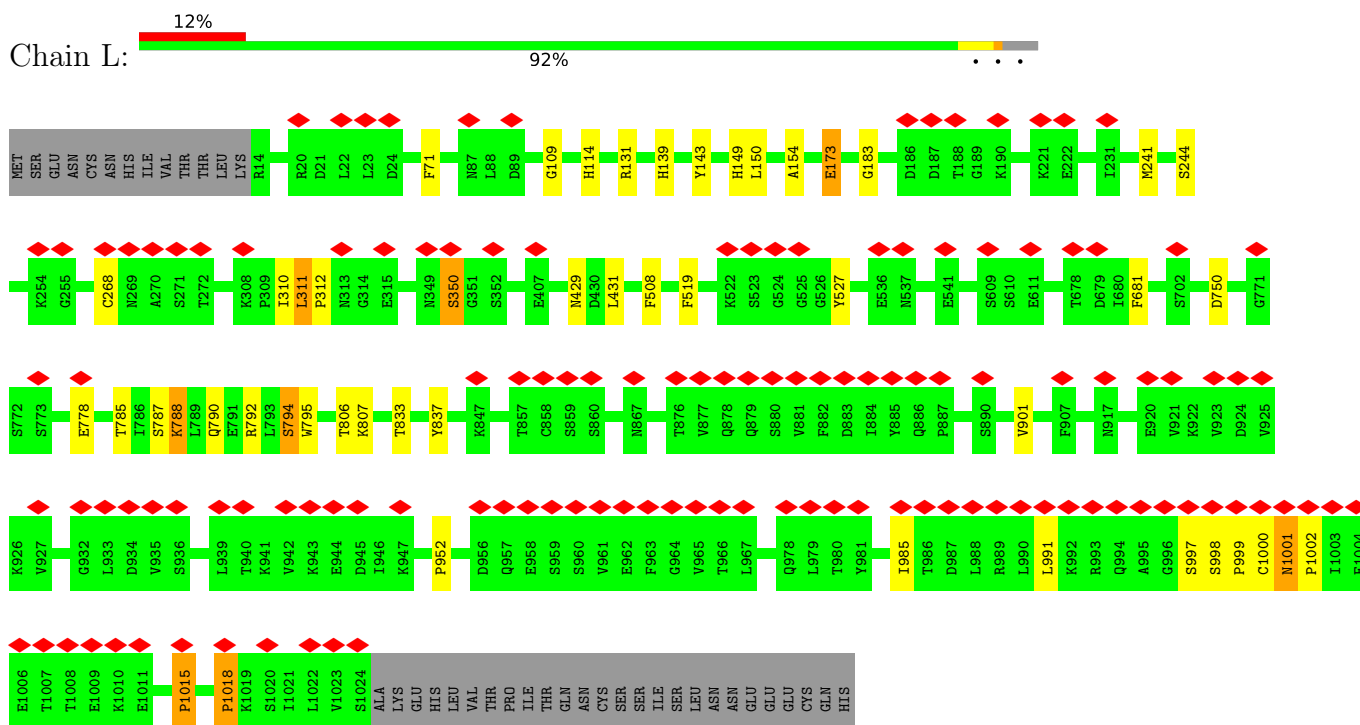
• Molecule 2: Baseplate_J domain-containing protein



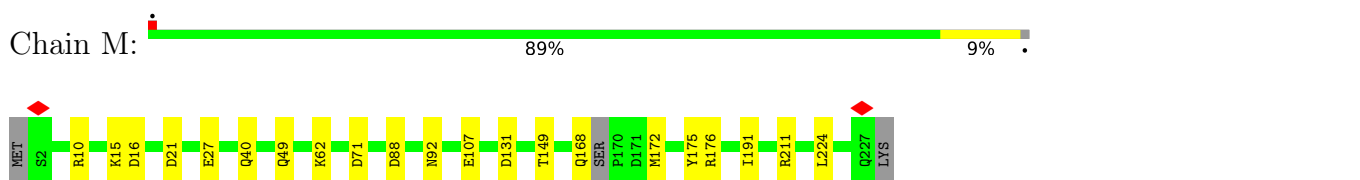
• Molecule 2: Baseplate_J domain-containing protein



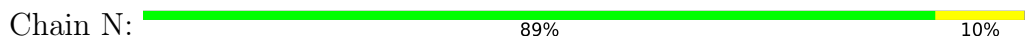
• Molecule 2: Baseplate_J domain-containing protein



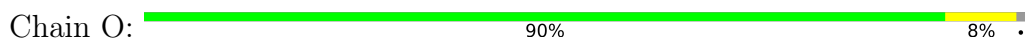
• Molecule 3: LysM domain-containing protein



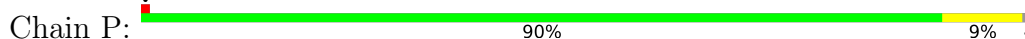
• Molecule 3: LysM domain-containing protein



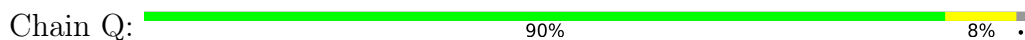
• Molecule 3: LysM domain-containing protein



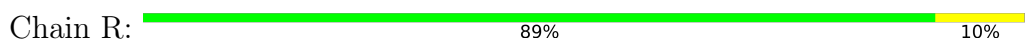
• Molecule 3: LysM domain-containing protein



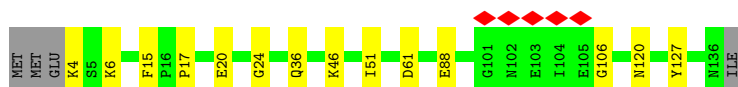
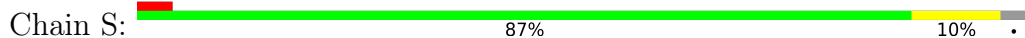
• Molecule 3: LysM domain-containing protein



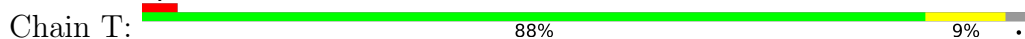
• Molecule 3: LysM domain-containing protein



• Molecule 4: Putative tail lysozyme

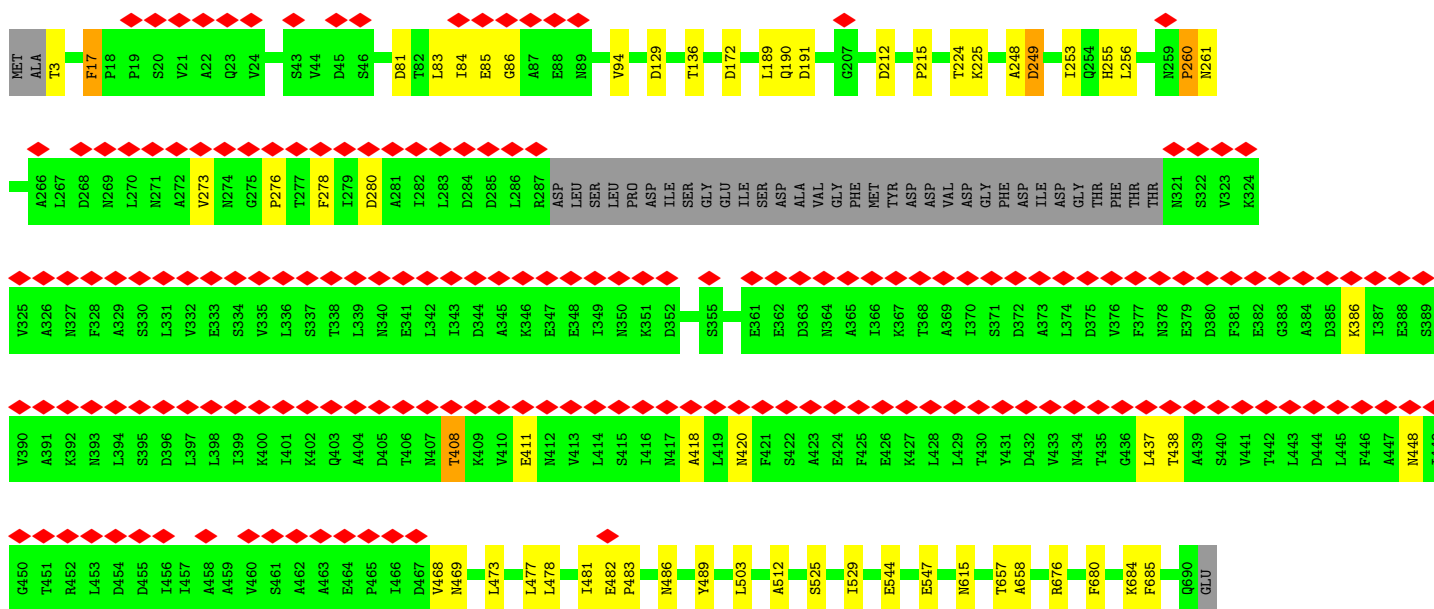
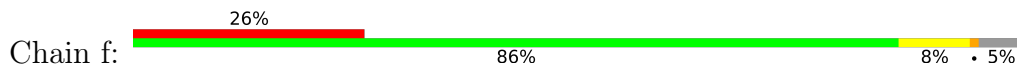


• Molecule 4: Putative tail lysozyme



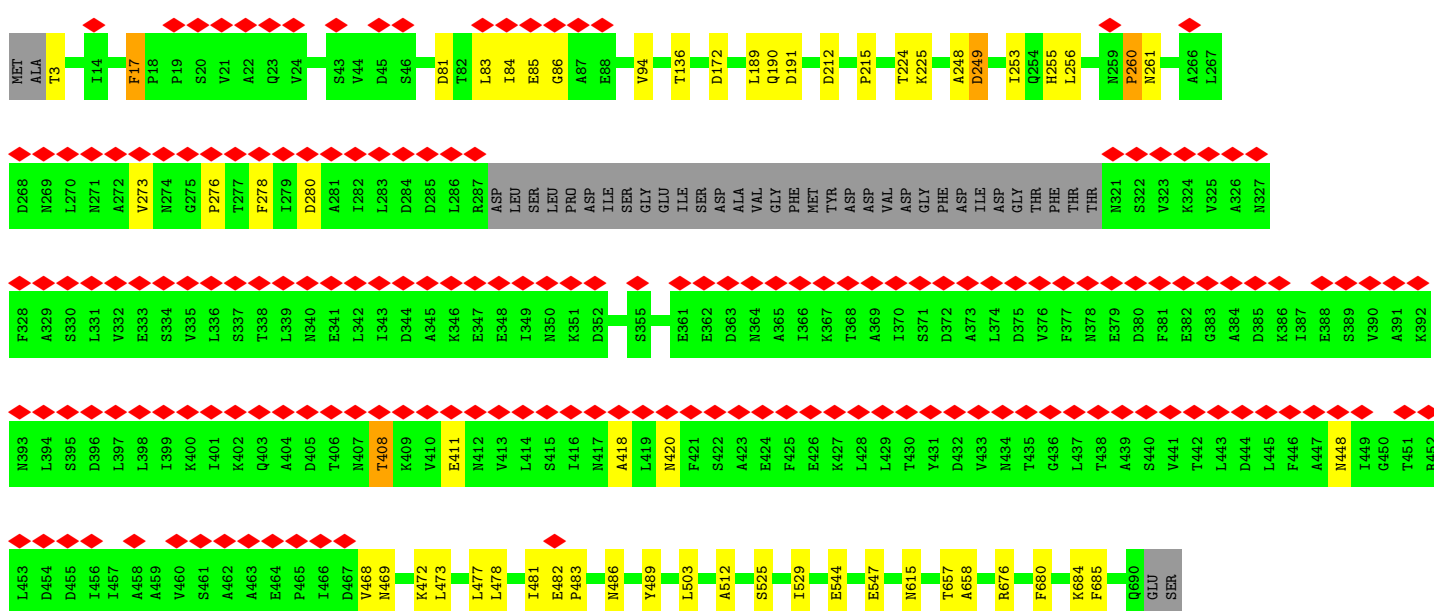
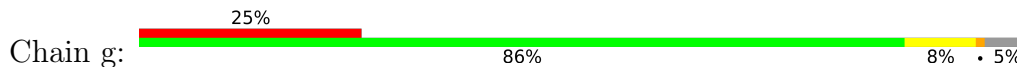
SER

Molecule 6: Putative phage tail sheath protein FI

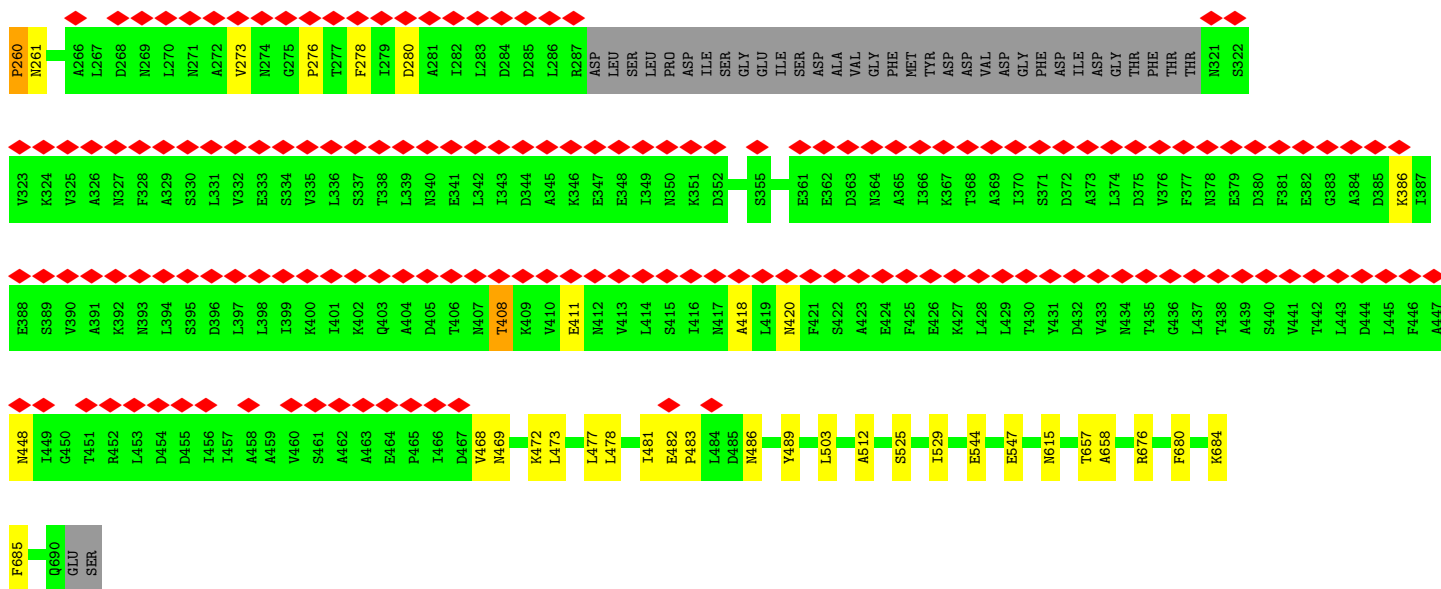


SER

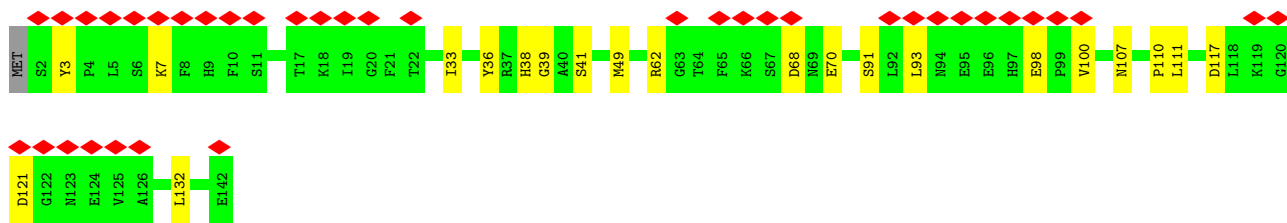
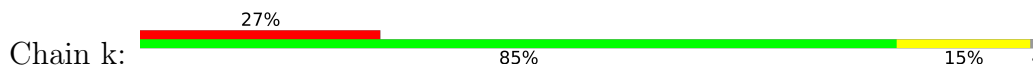
Molecule 6: Putative phage tail sheath protein FI



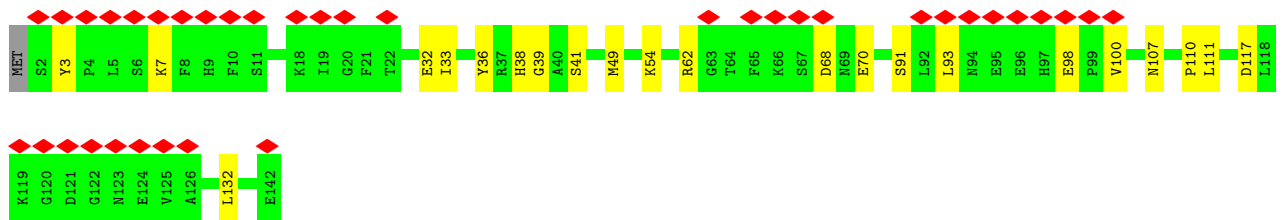
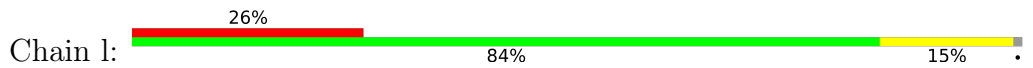
Molecule 6: Putative phage tail sheath protein FI



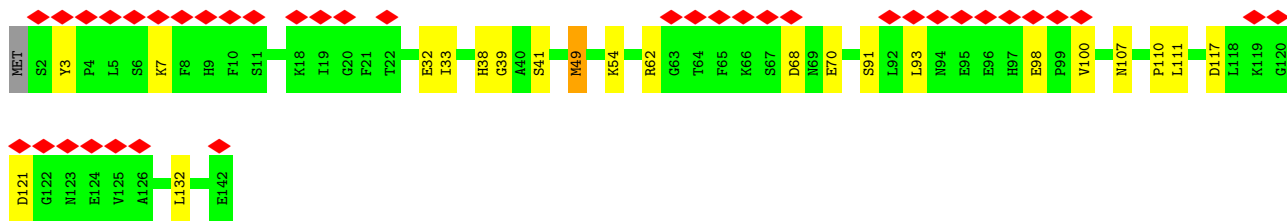
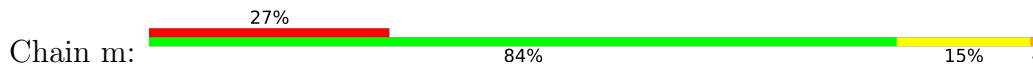
• Molecule 7: Phage tail protein



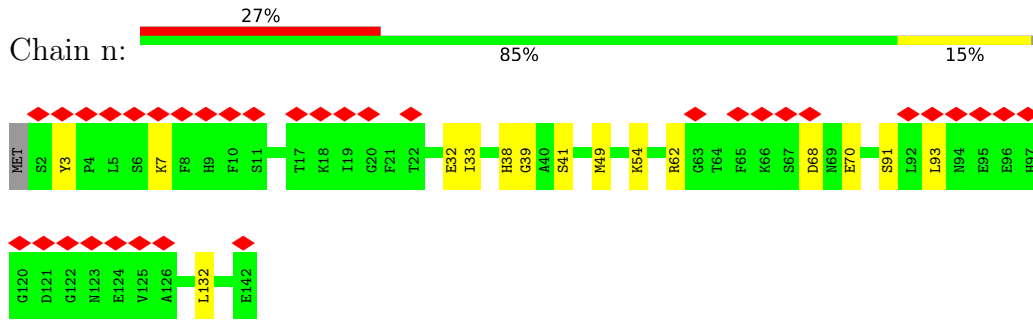
• Molecule 7: Phage tail protein



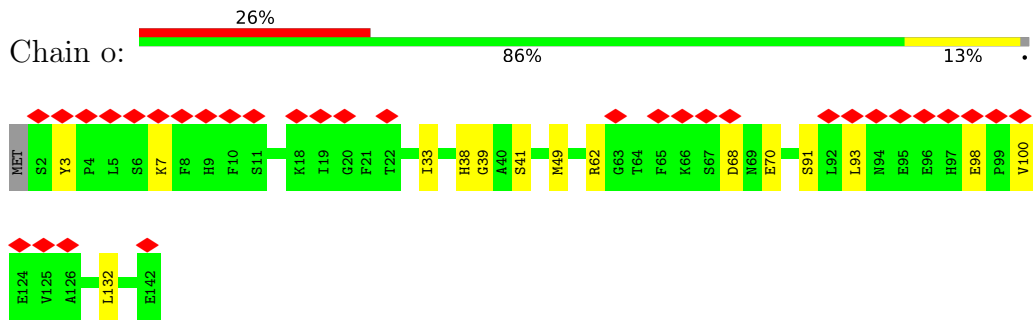
• Molecule 7: Phage tail protein



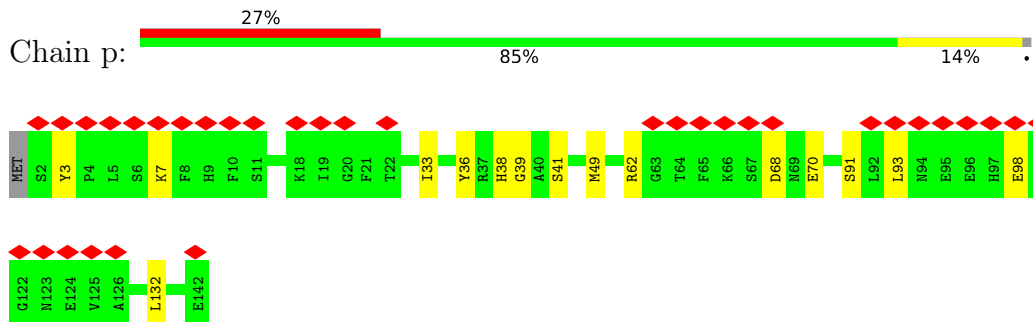
• Molecule 7: Phage tail protein



• Molecule 7: Phage tail protein



• Molecule 7: Phage tail protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
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	0.181	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.77	0/4531	1.05	20/6117 (0.3%)
1	B	0.77	0/4531	1.06	20/6117 (0.3%)
1	C	0.77	0/4531	1.06	19/6117 (0.3%)
1	D	0.77	0/4531	1.06	19/6117 (0.3%)
1	E	0.77	0/4531	1.06	19/6117 (0.3%)
1	F	0.77	0/4531	1.06	19/6117 (0.3%)
2	G	0.66	3/7935 (0.0%)	1.05	17/10781 (0.2%)
2	H	0.66	3/7935 (0.0%)	1.05	18/10781 (0.2%)
2	I	0.66	3/7935 (0.0%)	1.05	18/10781 (0.2%)
2	J	0.66	3/7935 (0.0%)	1.05	18/10781 (0.2%)
2	K	0.66	3/7935 (0.0%)	1.05	17/10781 (0.2%)
2	L	0.66	3/7935 (0.0%)	1.05	17/10781 (0.2%)
3	M	0.35	0/1889	0.55	0/2544
3	N	0.35	0/1889	0.55	0/2544
3	O	0.35	0/1889	0.55	0/2544
3	P	0.35	0/1889	0.55	0/2544
3	Q	0.35	0/1889	0.55	0/2544
3	R	0.35	0/1889	0.55	0/2544
4	S	0.64	0/1096	1.03	4/1483 (0.3%)
4	T	0.64	0/1096	1.03	2/1483 (0.1%)
4	U	0.64	0/1096	1.03	4/1483 (0.3%)
4	V	0.64	0/1096	1.03	2/1483 (0.1%)
4	W	0.64	0/1096	1.03	2/1483 (0.1%)
4	X	0.64	0/1096	1.03	4/1483 (0.3%)
5	Y	0.69	0/1226	1.06	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	1/1226 (0.1%)	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	22/7021 (0.3%)
6	f	0.74	1/5155 (0.0%)	1.09	23/7021 (0.3%)
6	g	0.74	1/5155 (0.0%)	1.09	22/7021 (0.3%)
6	h	0.74	1/5155 (0.0%)	1.09	25/7021 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	i	0.74	1/5155 (0.0%)	1.09	22/7021 (0.3%)
6	j	0.74	1/5155 (0.0%)	1.09	23/7021 (0.3%)
7	k	0.90	0/1172	1.28	16/1584 (1.0%)
7	l	0.90	0/1172	1.28	16/1584 (1.0%)
7	m	0.90	0/1172	1.27	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	16/1584 (1.0%)
All	All	0.70	25/138024 (0.0%)	1.04	487/187164 (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	1
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
All	All	0	6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	794	SER	C-O	-6.56	1.15	1.24
2	H	794	SER	C-O	-6.51	1.15	1.24
2	J	794	SER	C-O	-6.48	1.15	1.24
2	L	794	SER	C-O	-6.43	1.16	1.24
2	I	794	SER	C-O	-6.43	1.16	1.24
2	G	794	SER	C-O	-6.41	1.16	1.24
2	L	173	GLU	CA-CB	-6.36	1.43	1.53
2	H	173	GLU	CA-CB	-6.35	1.43	1.53
2	J	173	GLU	CA-CB	-6.33	1.43	1.53
2	G	173	GLU	CA-CB	-6.30	1.43	1.53
2	I	173	GLU	CA-CB	-6.29	1.43	1.53
2	K	173	GLU	CA-CB	-6.25	1.43	1.53
6	j	249	ASP	C-O	-5.97	1.16	1.24
6	i	249	ASP	C-O	-5.93	1.16	1.24
6	g	249	ASP	C-O	-5.93	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	249	ASP	C-O	-5.93	1.16	1.24
6	e	249	ASP	C-O	-5.87	1.16	1.24
6	h	249	ASP	C-O	-5.81	1.16	1.24
2	L	750	ASP	CG-OD1	-5.17	1.15	1.25
2	J	750	ASP	CG-OD1	-5.10	1.15	1.25
2	I	750	ASP	CG-OD1	-5.07	1.15	1.25
2	G	750	ASP	CG-OD1	-5.05	1.15	1.25
2	K	750	ASP	CG-OD1	-5.04	1.15	1.25
2	H	750	ASP	CG-OD1	-5.01	1.15	1.25
5	c	37	ASP	CG-OD2	-5.01	1.15	1.25

All (487) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1018	PRO	N-CA-CB	10.97	114.77	103.25
2	L	1018	PRO	N-CA-CB	10.91	114.71	103.25
2	H	1018	PRO	N-CA-CB	10.88	114.67	103.25
2	K	1018	PRO	N-CA-CB	10.87	114.66	103.25
2	G	1018	PRO	N-CA-CB	10.83	114.62	103.25
2	I	1018	PRO	N-CA-CB	10.83	114.62	103.25
2	G	998	SER	N-CA-C	-9.32	96.10	109.62
2	I	998	SER	N-CA-C	-9.31	96.12	109.62
2	L	998	SER	N-CA-C	-9.31	96.12	109.62
2	K	998	SER	N-CA-C	-9.30	96.13	109.62
2	H	998	SER	N-CA-C	-9.29	96.16	109.62
2	J	998	SER	N-CA-C	-9.28	96.17	109.62
2	H	310	ILE	N-CA-C	8.58	118.60	110.53
2	L	310	ILE	N-CA-C	8.54	118.56	110.53
2	G	310	ILE	N-CA-C	8.51	118.53	110.53
2	I	310	ILE	N-CA-C	8.48	118.51	110.53
2	J	310	ILE	N-CA-C	8.46	118.54	110.42
2	K	310	ILE	N-CA-C	8.41	118.49	110.42
2	I	1002	PRO	N-CA-CB	7.96	110.40	103.31
2	L	1002	PRO	N-CA-CB	7.93	110.36	103.31
2	J	1002	PRO	N-CA-CB	7.92	110.36	103.31
2	H	1002	PRO	N-CA-CB	7.92	110.36	103.31
2	G	1002	PRO	N-CA-CB	7.90	110.34	103.31
2	K	1002	PRO	N-CA-CB	7.89	110.33	103.31
6	j	420	ASN	N-CA-C	7.75	122.46	112.92
6	g	420	ASN	N-CA-C	7.73	122.43	112.92
2	I	999	PRO	N-CA-CB	7.72	109.81	103.32
6	i	420	ASN	N-CA-C	7.72	122.42	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	420	ASN	N-CA-C	7.72	122.42	112.92
6	e	420	ASN	N-CA-C	7.71	122.40	112.92
6	f	420	ASN	N-CA-C	7.71	122.40	112.92
2	L	999	PRO	N-CA-CB	7.67	109.77	103.32
2	H	999	PRO	N-CA-CB	7.61	109.71	103.32
2	G	999	PRO	N-CA-CB	7.58	109.68	103.32
2	J	999	PRO	N-CA-CB	7.58	109.69	103.32
2	K	999	PRO	N-CA-CB	7.57	109.67	103.32
1	C	384	ALA	N-CA-C	7.41	119.15	110.41
1	D	384	ALA	N-CA-C	7.36	119.09	110.41
1	A	384	ALA	N-CA-C	7.35	119.08	110.41
1	F	384	ALA	N-CA-C	7.33	119.06	110.41
1	E	384	ALA	N-CA-C	7.33	119.06	110.41
1	B	384	ALA	N-CA-C	7.33	119.06	110.41
7	l	41	SER	CA-C-N	7.32	127.02	119.56
7	l	41	SER	C-N-CA	7.32	127.02	119.56
7	k	41	SER	CA-C-N	7.31	127.02	119.56
7	k	41	SER	C-N-CA	7.31	127.02	119.56
7	n	41	SER	CA-C-N	7.30	127.01	119.56
7	n	41	SER	C-N-CA	7.30	127.01	119.56
7	p	41	SER	CA-C-N	7.24	126.95	119.56
7	p	41	SER	C-N-CA	7.24	126.95	119.56
7	m	41	SER	CA-C-N	7.23	126.93	119.56
7	m	41	SER	C-N-CA	7.23	126.93	119.56
7	o	41	SER	CA-C-N	7.22	126.92	119.56
7	o	41	SER	C-N-CA	7.22	126.92	119.56
6	h	525	SER	CA-C-N	7.15	126.82	119.82
6	h	525	SER	C-N-CA	7.15	126.82	119.82
6	j	525	SER	CA-C-N	7.14	126.82	119.82
6	j	525	SER	C-N-CA	7.14	126.82	119.82
6	e	525	SER	CA-C-N	7.13	126.81	119.82
6	e	525	SER	C-N-CA	7.13	126.81	119.82
6	i	525	SER	CA-C-N	7.13	126.81	119.82
6	i	525	SER	C-N-CA	7.13	126.81	119.82
6	i	448	ASN	CA-C-N	7.12	130.21	120.46
6	i	448	ASN	C-N-CA	7.12	130.21	120.46
6	g	448	ASN	CA-C-N	7.10	130.19	120.46
6	g	448	ASN	C-N-CA	7.10	130.19	120.46
6	j	448	ASN	CA-C-N	7.09	130.17	120.46
6	j	448	ASN	C-N-CA	7.09	130.17	120.46
6	f	448	ASN	CA-C-N	7.08	130.17	120.46
6	f	448	ASN	C-N-CA	7.08	130.17	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	448	ASN	CA-C-N	7.08	130.16	120.46
6	h	448	ASN	C-N-CA	7.08	130.16	120.46
6	e	448	ASN	CA-C-N	7.06	130.14	120.46
6	e	448	ASN	C-N-CA	7.06	130.14	120.46
6	g	525	SER	CA-C-N	7.06	126.74	119.82
6	g	525	SER	C-N-CA	7.06	126.74	119.82
6	f	525	SER	CA-C-N	7.03	126.71	119.82
6	f	525	SER	C-N-CA	7.03	126.71	119.82
6	i	469	ASN	N-CA-C	7.02	122.84	112.94
6	g	469	ASN	N-CA-C	7.00	122.81	112.94
6	j	469	ASN	N-CA-C	6.95	122.74	112.94
6	e	469	ASN	N-CA-C	6.93	122.72	112.94
1	A	324	GLU	N-CA-C	6.91	121.33	112.34
6	h	81	ASP	CA-CB-CG	6.91	119.51	112.60
6	f	469	ASN	N-CA-C	6.91	122.68	112.94
6	h	469	ASN	N-CA-C	6.90	122.67	112.94
1	B	324	GLU	N-CA-C	6.90	121.31	112.34
7	m	107	ASN	N-CA-C	6.90	121.05	111.74
7	l	107	ASN	N-CA-C	6.90	121.05	111.74
1	D	324	GLU	N-CA-C	6.89	121.30	112.34
7	o	107	ASN	N-CA-C	6.89	121.05	111.74
7	p	107	ASN	N-CA-C	6.88	121.02	111.74
7	k	107	ASN	N-CA-C	6.87	121.02	111.74
7	n	107	ASN	N-CA-C	6.87	121.02	111.74
7	l	3	TYR	CA-C-N	6.86	126.82	120.03
7	l	3	TYR	C-N-CA	6.86	126.82	120.03
1	F	324	GLU	N-CA-C	6.86	121.25	112.34
6	f	81	ASP	CA-CB-CG	6.85	119.45	112.60
6	i	81	ASP	CA-CB-CG	6.84	119.44	112.60
1	E	324	GLU	N-CA-C	6.84	121.23	112.34
1	C	324	GLU	N-CA-C	6.83	121.22	112.34
6	j	81	ASP	CA-CB-CG	6.83	119.43	112.60
6	e	81	ASP	CA-CB-CG	6.80	119.40	112.60
6	f	17	PHE	CA-C-N	6.79	127.38	120.38
6	f	17	PHE	C-N-CA	6.79	127.38	120.38
6	j	17	PHE	CA-C-N	6.79	127.38	120.38
6	j	17	PHE	C-N-CA	6.79	127.38	120.38
6	g	81	ASP	CA-CB-CG	6.79	119.39	112.60
7	n	3	TYR	CA-C-N	6.79	126.75	120.03
7	n	3	TYR	C-N-CA	6.79	126.75	120.03
1	C	466	LYS	CA-C-N	-6.78	111.89	122.67
1	C	466	LYS	C-N-CA	-6.78	111.89	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	952	PRO	N-CA-CB	6.78	110.26	103.48
7	k	3	TYR	CA-C-N	6.78	126.74	120.03
7	k	3	TYR	C-N-CA	6.78	126.74	120.03
6	e	17	PHE	CA-C-N	6.77	127.35	120.38
6	e	17	PHE	C-N-CA	6.77	127.35	120.38
7	o	3	TYR	CA-C-N	6.76	126.73	120.03
7	o	3	TYR	C-N-CA	6.76	126.73	120.03
1	A	466	LYS	CA-C-N	-6.76	111.92	122.67
1	A	466	LYS	C-N-CA	-6.76	111.92	122.67
2	H	952	PRO	N-CA-CB	6.75	110.23	103.48
1	F	466	LYS	CA-C-N	-6.74	111.95	122.67
1	F	466	LYS	C-N-CA	-6.74	111.95	122.67
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
7	p	3	TYR	CA-C-N	6.73	126.70	120.03
7	p	3	TYR	C-N-CA	6.73	126.70	120.03
2	J	952	PRO	N-CA-CB	6.73	110.21	103.48
1	D	466	LYS	CA-C-N	-6.72	111.98	122.67
1	D	466	LYS	C-N-CA	-6.72	111.98	122.67
6	h	17	PHE	CA-C-N	6.71	127.29	120.38
6	h	17	PHE	C-N-CA	6.71	127.29	120.38
2	G	952	PRO	N-CA-CB	6.70	110.18	103.48
7	m	3	TYR	CA-C-N	6.70	126.66	120.03
7	m	3	TYR	C-N-CA	6.70	126.66	120.03
6	i	17	PHE	CA-C-N	6.67	127.25	120.38
6	i	17	PHE	C-N-CA	6.67	127.25	120.38
1	B	466	LYS	CA-C-N	-6.67	112.06	122.67
1	B	466	LYS	C-N-CA	-6.67	112.06	122.67
2	K	952	PRO	N-CA-CB	6.66	110.14	103.48
2	I	952	PRO	N-CA-CB	6.66	110.14	103.48
1	E	466	LYS	CA-C-N	-6.65	112.10	122.67
1	E	466	LYS	C-N-CA	-6.65	112.10	122.67
2	K	1015	PRO	N-CA-CB	6.60	110.18	103.25
2	J	1015	PRO	N-CA-CB	6.56	110.14	103.25
2	L	1015	PRO	N-CA-CB	6.54	110.12	103.25
2	G	1015	PRO	N-CA-CB	6.53	110.10	103.25
2	I	1015	PRO	N-CA-CB	6.51	110.09	103.25
2	H	1015	PRO	N-CA-CB	6.46	110.03	103.25
1	B	343	LEU	CA-C-N	6.28	126.04	119.76
1	B	343	LEU	C-N-CA	6.28	126.04	119.76
1	F	343	LEU	CA-C-N	6.25	126.01	119.76
1	F	343	LEU	C-N-CA	6.25	126.01	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	l	49	MET	CA-C-N	6.21	126.16	119.76
7	l	49	MET	C-N-CA	6.21	126.16	119.76
1	E	343	LEU	CA-C-N	6.20	125.96	119.76
1	E	343	LEU	C-N-CA	6.20	125.96	119.76
1	D	343	LEU	CA-C-N	6.18	125.94	119.76
1	D	343	LEU	C-N-CA	6.18	125.94	119.76
7	k	49	MET	CA-C-N	6.18	126.12	119.76
7	k	49	MET	C-N-CA	6.18	126.12	119.76
7	n	49	MET	CA-C-N	6.17	126.12	119.76
7	n	49	MET	C-N-CA	6.17	126.12	119.76
1	A	343	LEU	CA-C-N	6.17	125.93	119.76
1	A	343	LEU	C-N-CA	6.17	125.93	119.76
1	C	343	LEU	CA-C-N	6.16	125.92	119.76
1	C	343	LEU	C-N-CA	6.16	125.92	119.76
7	m	49	MET	CA-C-N	6.15	126.09	119.76
7	m	49	MET	C-N-CA	6.15	126.09	119.76
7	o	49	MET	CA-C-N	6.14	126.08	119.76
7	o	49	MET	C-N-CA	6.14	126.08	119.76
7	p	49	MET	CA-C-N	6.11	126.05	119.76
7	p	49	MET	C-N-CA	6.11	126.05	119.76
2	H	311	LEU	N-CA-C	6.03	118.00	108.23
2	G	311	LEU	N-CA-C	6.01	117.97	108.23
2	L	311	LEU	N-CA-C	6.01	117.96	108.23
2	I	311	LEU	N-CA-C	5.99	117.94	108.23
1	C	474	ASP	CA-C-N	5.98	125.66	119.56
1	C	474	ASP	C-N-CA	5.98	125.66	119.56
2	K	311	LEU	N-CA-C	5.98	117.92	108.23
2	J	311	LEU	N-CA-C	5.96	117.89	108.23
2	H	901	VAL	N-CA-C	5.96	116.74	110.72
2	K	901	VAL	N-CA-C	5.95	116.73	110.72
1	D	474	ASP	CA-C-N	5.94	125.62	119.56
1	D	474	ASP	C-N-CA	5.94	125.62	119.56
1	A	474	ASP	CA-C-N	5.94	125.61	119.56
1	A	474	ASP	C-N-CA	5.94	125.61	119.56
1	E	474	ASP	CA-C-N	5.93	125.61	119.56
1	E	474	ASP	C-N-CA	5.93	125.61	119.56
1	F	474	ASP	CA-C-N	5.93	125.61	119.56
1	F	474	ASP	C-N-CA	5.93	125.61	119.56
1	B	474	ASP	CA-C-N	5.92	125.59	119.56
1	B	474	ASP	C-N-CA	5.92	125.59	119.56
2	G	901	VAL	N-CA-C	5.91	116.69	110.72
2	J	901	VAL	N-CA-C	5.89	116.67	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	901	VAL	N-CA-C	5.88	116.66	110.72
2	I	901	VAL	N-CA-C	5.88	116.66	110.72
6	g	418	ALA	N-CA-C	-5.87	106.66	113.88
6	h	418	ALA	N-CA-C	-5.86	106.68	113.88
6	e	418	ALA	N-CA-C	-5.85	106.68	113.88
6	i	418	ALA	N-CA-C	-5.85	106.69	113.88
6	j	418	ALA	N-CA-C	-5.85	106.69	113.88
6	f	418	ALA	N-CA-C	-5.84	106.69	113.88
1	B	159	TYR	N-CA-C	5.78	119.14	109.95
7	p	110	PRO	CA-C-N	5.76	128.47	120.29
7	p	110	PRO	C-N-CA	5.76	128.47	120.29
6	j	408	THR	N-CA-C	5.76	117.28	108.52
7	k	110	PRO	CA-C-N	5.75	128.45	120.29
7	k	110	PRO	C-N-CA	5.75	128.45	120.29
7	o	110	PRO	CA-C-N	5.75	128.45	120.29
7	o	110	PRO	C-N-CA	5.75	128.45	120.29
1	E	159	TYR	N-CA-C	5.74	119.08	109.95
1	C	159	TYR	N-CA-C	5.74	119.07	109.95
6	g	408	THR	N-CA-C	5.73	117.24	108.52
1	D	159	TYR	N-CA-C	5.73	119.06	109.95
7	n	110	PRO	CA-C-N	5.72	128.42	120.29
7	n	110	PRO	C-N-CA	5.72	128.42	120.29
6	e	408	THR	N-CA-C	5.72	117.21	108.52
6	f	408	THR	N-CA-C	5.71	117.20	108.52
1	A	159	TYR	N-CA-C	5.71	119.03	109.95
6	h	408	THR	N-CA-C	5.71	117.19	108.52
7	p	98	GLU	CA-C-N	5.69	125.62	119.76
7	p	98	GLU	C-N-CA	5.69	125.62	119.76
7	m	110	PRO	CA-C-N	5.69	128.37	120.29
7	m	110	PRO	C-N-CA	5.69	128.37	120.29
7	l	110	PRO	CA-C-N	5.68	128.36	120.29
7	l	110	PRO	C-N-CA	5.68	128.36	120.29
6	i	408	THR	N-CA-C	5.68	117.16	108.52
1	F	159	TYR	N-CA-C	5.66	118.95	109.95
6	f	676	ARG	CA-C-N	5.63	125.83	120.31
6	f	676	ARG	C-N-CA	5.63	125.83	120.31
7	o	98	GLU	CA-C-N	5.62	125.55	119.76
7	o	98	GLU	C-N-CA	5.62	125.55	119.76
7	p	100	VAL	N-CA-C	-5.62	107.18	111.62
7	o	100	VAL	N-CA-C	-5.62	107.18	111.62
7	m	98	GLU	CA-C-N	5.60	125.53	119.76
7	m	98	GLU	C-N-CA	5.60	125.53	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	n	100	VAL	N-CA-C	-5.60	107.20	111.62
6	h	136	THR	CA-C-N	5.59	126.14	120.38
6	h	136	THR	C-N-CA	5.59	126.14	120.38
6	e	676	ARG	CA-C-N	5.59	125.79	120.31
6	e	676	ARG	C-N-CA	5.59	125.79	120.31
6	e	136	THR	CA-C-N	5.59	126.14	120.38
6	e	136	THR	C-N-CA	5.59	126.14	120.38
6	g	136	THR	CA-C-N	5.58	126.13	120.38
6	g	136	THR	C-N-CA	5.58	126.13	120.38
7	k	98	GLU	CA-C-N	5.58	125.51	119.76
7	k	98	GLU	C-N-CA	5.58	125.51	119.76
7	l	100	VAL	N-CA-C	-5.58	107.21	111.62
7	n	98	GLU	CA-C-N	5.57	125.50	119.76
7	n	98	GLU	C-N-CA	5.57	125.50	119.76
6	i	420	ASN	CA-C-N	-5.57	112.81	120.28
6	i	420	ASN	C-N-CA	-5.57	112.81	120.28
6	g	676	ARG	CA-C-N	5.57	125.77	120.31
6	g	676	ARG	C-N-CA	5.57	125.77	120.31
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
7	l	98	GLU	CA-C-N	5.57	125.50	119.76
7	l	98	GLU	C-N-CA	5.57	125.50	119.76
2	G	183	GLY	N-CA-C	5.56	126.36	113.18
2	H	183	GLY	N-CA-C	5.56	126.36	113.18
2	K	183	GLY	N-CA-C	5.55	126.34	113.18
2	J	183	GLY	N-CA-C	5.55	126.34	113.18
6	i	676	ARG	CA-C-N	5.55	125.75	120.31
6	i	676	ARG	C-N-CA	5.55	125.75	120.31
6	f	136	THR	CA-C-N	5.54	126.09	120.38
6	f	136	THR	C-N-CA	5.54	126.09	120.38
7	k	100	VAL	N-CA-C	-5.54	107.25	111.62
6	i	136	THR	CA-C-N	5.54	126.08	120.38
6	i	136	THR	C-N-CA	5.54	126.08	120.38
2	I	183	GLY	N-CA-C	5.54	126.30	113.18
6	e	420	ASN	CA-C-N	-5.54	112.86	120.28
6	e	420	ASN	C-N-CA	-5.54	112.86	120.28
6	j	136	THR	CA-C-N	5.54	126.08	120.38
6	j	136	THR	C-N-CA	5.54	126.08	120.38
7	m	100	VAL	N-CA-C	-5.53	107.25	111.62
2	L	183	GLY	N-CA-C	5.53	126.29	113.18
2	L	794	SER	CA-C-O	-5.52	114.69	120.32
6	h	676	ARG	CA-C-N	5.52	125.72	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	676	ARG	C-N-CA	5.52	125.72	120.31
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
1	F	408	PRO	CA-C-N	5.52	125.87	119.47
1	F	408	PRO	C-N-CA	5.52	125.87	119.47
2	J	788	LYS	N-CA-C	5.51	117.45	109.07
2	H	794	SER	CA-C-O	-5.50	114.71	120.32
1	E	408	PRO	CA-C-N	5.50	125.85	119.47
1	E	408	PRO	C-N-CA	5.50	125.85	119.47
6	g	420	ASN	CA-C-N	-5.49	112.92	120.28
6	g	420	ASN	C-N-CA	-5.49	112.92	120.28
1	B	452	GLY	CA-C-N	5.49	125.69	120.31
1	B	452	GLY	C-N-CA	5.49	125.69	120.31
1	F	452	GLY	CA-C-N	5.48	125.68	120.31
1	F	452	GLY	C-N-CA	5.48	125.68	120.31
6	f	420	ASN	CA-C-N	-5.48	112.94	120.28
6	f	420	ASN	C-N-CA	-5.48	112.94	120.28
2	H	788	LYS	N-CA-C	5.47	117.39	109.07
2	G	794	SER	CA-C-O	-5.47	114.74	120.32
2	G	788	LYS	N-CA-C	5.46	117.38	109.07
2	K	788	LYS	N-CA-C	5.46	117.38	109.07
1	B	408	PRO	CA-C-N	5.46	125.81	119.47
1	B	408	PRO	C-N-CA	5.46	125.81	119.47
2	L	788	LYS	N-CA-C	5.46	117.36	109.07
6	h	420	ASN	CA-C-N	-5.45	112.97	120.28
6	h	420	ASN	C-N-CA	-5.45	112.97	120.28
2	I	788	LYS	N-CA-C	5.44	117.34	109.07
1	B	235	ALA	CA-C-N	5.44	125.74	119.92
1	B	235	ALA	C-N-CA	5.44	125.74	119.92
1	F	235	ALA	CA-C-N	5.43	125.73	119.92
1	F	235	ALA	C-N-CA	5.43	125.73	119.92
1	D	235	ALA	CA-C-N	5.43	125.73	119.92
1	D	235	ALA	C-N-CA	5.43	125.73	119.92
2	I	794	SER	CA-C-O	-5.43	114.78	120.32
2	K	794	SER	CA-C-O	-5.43	114.78	120.32
1	C	452	GLY	CA-C-N	5.42	125.62	120.31
1	C	452	GLY	C-N-CA	5.42	125.62	120.31
1	D	404	ASP	N-CA-C	5.42	117.94	111.71
1	D	408	PRO	CA-C-N	5.42	125.75	119.47
1	D	408	PRO	C-N-CA	5.42	125.75	119.47
1	A	408	PRO	CA-C-N	5.41	125.75	119.47
1	A	408	PRO	C-N-CA	5.41	125.75	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	794	SER	CA-C-O	-5.41	114.80	120.32
7	p	93	LEU	N-CA-C	5.40	118.53	109.95
1	A	452	GLY	CA-C-N	5.39	125.59	120.31
1	A	452	GLY	C-N-CA	5.39	125.59	120.31
7	o	93	LEU	N-CA-C	5.39	118.52	109.95
7	n	93	LEU	N-CA-C	5.39	118.52	109.95
7	l	93	LEU	N-CA-C	5.39	118.52	109.95
7	k	93	LEU	N-CA-C	5.38	118.50	109.95
1	A	235	ALA	CA-C-N	5.38	125.68	119.92
1	A	235	ALA	C-N-CA	5.38	125.68	119.92
7	m	93	LEU	N-CA-C	5.38	118.50	109.95
7	p	132	LEU	N-CA-C	5.37	118.24	109.59
1	B	404	ASP	N-CA-C	5.37	117.88	111.71
7	o	132	LEU	N-CA-C	5.37	118.23	109.59
1	C	235	ALA	CA-C-N	5.36	125.66	119.92
1	C	235	ALA	C-N-CA	5.36	125.66	119.92
2	K	681	PHE	CB-CA-C	-5.36	104.28	112.11
2	J	681	PHE	CB-CA-C	-5.35	104.30	112.11
1	C	408	PRO	CA-C-N	5.35	125.68	119.47
1	C	408	PRO	C-N-CA	5.35	125.68	119.47
1	C	404	ASP	N-CA-C	5.35	117.86	111.71
1	E	235	ALA	CA-C-N	5.35	125.64	119.92
1	E	235	ALA	C-N-CA	5.35	125.64	119.92
1	E	404	ASP	N-CA-C	5.35	117.86	111.71
1	A	404	ASP	N-CA-C	5.34	117.85	111.71
1	D	452	GLY	CA-C-N	5.34	125.54	120.31
1	D	452	GLY	C-N-CA	5.34	125.54	120.31
2	I	681	PHE	CB-CA-C	-5.33	104.32	112.11
2	H	681	PHE	CB-CA-C	-5.33	104.32	112.11
2	L	681	PHE	CB-CA-C	-5.33	104.32	112.11
2	G	681	PHE	CB-CA-C	-5.33	104.33	112.11
1	F	404	ASP	N-CA-C	5.32	117.83	111.71
7	n	132	LEU	N-CA-C	5.32	118.16	109.59
5	c	90	LYS	CA-C-N	5.32	125.26	119.78
5	c	90	LYS	C-N-CA	5.32	125.26	119.78
7	l	132	LEU	N-CA-C	5.32	118.15	109.59
7	k	132	LEU	N-CA-C	5.32	118.15	109.59
1	E	452	GLY	CA-C-N	5.31	125.51	120.31
1	E	452	GLY	C-N-CA	5.31	125.51	120.31
2	G	154	ALA	CA-C-N	5.30	128.40	120.87
2	G	154	ALA	C-N-CA	5.30	128.40	120.87
7	m	132	LEU	N-CA-C	5.30	118.13	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	88	GLU	CA-C-N	5.30	124.97	119.56
4	X	88	GLU	C-N-CA	5.30	124.97	119.56
4	S	88	GLU	CA-C-N	5.30	124.96	119.56
4	S	88	GLU	C-N-CA	5.30	124.96	119.56
4	V	88	GLU	CA-C-N	5.29	124.96	119.56
4	V	88	GLU	C-N-CA	5.29	124.96	119.56
7	o	91	SER	N-CA-C	5.29	118.05	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	I	154	ALA	CA-C-N	5.27	128.36	120.87
2	I	154	ALA	C-N-CA	5.27	128.36	120.87
7	p	91	SER	N-CA-C	5.26	118.01	108.69
4	T	88	GLU	CA-C-N	5.26	124.93	119.56
4	T	88	GLU	C-N-CA	5.26	124.93	119.56
7	k	91	SER	N-CA-C	5.26	118.00	108.69
7	n	91	SER	N-CA-C	5.26	118.00	108.69
5	d	94	LEU	CA-CB-CG	5.25	134.69	116.30
2	J	508	PHE	CA-CB-CG	-5.25	108.55	113.80
2	J	154	ALA	CA-C-N	5.25	128.33	120.87
2	J	154	ALA	C-N-CA	5.25	128.33	120.87
5	Z	90	LYS	CA-C-N	5.25	125.19	119.78
5	Z	90	LYS	C-N-CA	5.25	125.19	119.78
5	b	90	LYS	CA-C-N	5.25	125.19	119.78
5	b	90	LYS	C-N-CA	5.25	125.19	119.78
5	a	94	LEU	CA-CB-CG	5.25	134.68	116.30
2	K	154	ALA	CA-C-N	5.25	128.32	120.87
2	K	154	ALA	C-N-CA	5.25	128.32	120.87
5	Y	90	LYS	CA-C-N	5.24	125.18	119.78
5	Y	90	LYS	C-N-CA	5.24	125.18	119.78
5	Y	94	LEU	CA-CB-CG	5.24	134.64	116.30
1	E	375	GLU	CA-C-N	5.24	125.44	120.31
1	E	375	GLU	C-N-CA	5.24	125.44	120.31
7	m	91	SER	N-CA-C	5.23	117.95	108.69
5	a	90	LYS	CA-C-N	5.23	125.17	119.78
5	a	90	LYS	C-N-CA	5.23	125.17	119.78
5	d	90	LYS	CA-C-N	5.23	125.17	119.78
5	d	90	LYS	C-N-CA	5.23	125.17	119.78
6	i	94	VAL	CA-C-N	5.23	125.44	120.31
6	i	94	VAL	C-N-CA	5.23	125.44	120.31
5	c	94	LEU	CA-CB-CG	5.23	134.59	116.30
7	l	91	SER	N-CA-C	5.23	117.94	108.69
1	D	375	GLU	CA-C-N	5.22	125.43	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	375	GLU	C-N-CA	5.22	125.43	120.31
2	G	508	PHE	CA-CB-CG	-5.22	108.58	113.80
5	Z	94	LEU	CA-CB-CG	5.22	134.58	116.30
5	b	94	LEU	CA-CB-CG	5.22	134.57	116.30
6	h	94	VAL	CA-C-N	5.22	125.43	120.31
6	h	94	VAL	C-N-CA	5.22	125.43	120.31
2	L	154	ALA	CA-C-N	5.21	128.27	120.87
2	L	154	ALA	C-N-CA	5.21	128.27	120.87
4	W	88	GLU	CA-C-N	5.21	124.88	119.56
4	W	88	GLU	C-N-CA	5.21	124.88	119.56
6	f	94	VAL	CA-C-N	5.21	125.42	120.31
6	f	94	VAL	C-N-CA	5.21	125.42	120.31
6	e	94	VAL	CA-C-N	5.20	125.41	120.31
6	e	94	VAL	C-N-CA	5.20	125.41	120.31
2	I	508	PHE	CA-CB-CG	-5.19	108.61	113.80
6	g	94	VAL	CA-C-N	5.19	125.39	120.31
6	g	94	VAL	C-N-CA	5.19	125.39	120.31
6	f	503	LEU	CA-C-N	5.18	123.44	119.66
6	f	503	LEU	C-N-CA	5.18	123.44	119.66
6	j	94	VAL	CA-C-N	5.17	125.37	120.31
6	j	94	VAL	C-N-CA	5.17	125.37	120.31
2	H	154	ALA	CA-C-N	5.16	128.20	120.87
2	H	154	ALA	C-N-CA	5.16	128.20	120.87
1	A	375	GLU	CA-C-N	5.16	125.36	120.31
1	A	375	GLU	C-N-CA	5.16	125.36	120.31
2	L	508	PHE	CA-CB-CG	-5.15	108.65	113.80
2	H	508	PHE	CA-CB-CG	-5.15	108.65	113.80
6	e	503	LEU	CA-C-N	5.14	123.41	119.66
6	e	503	LEU	C-N-CA	5.14	123.41	119.66
1	B	375	GLU	CA-C-N	5.13	125.34	120.31
1	B	375	GLU	C-N-CA	5.13	125.34	120.31
1	C	209	ALA	N-CA-C	5.13	116.63	108.79
6	i	503	LEU	CA-C-N	5.12	123.40	119.66
6	i	503	LEU	C-N-CA	5.12	123.40	119.66
1	F	375	GLU	CA-C-N	5.12	125.32	120.31
1	F	375	GLU	C-N-CA	5.12	125.32	120.31
6	j	503	LEU	CA-C-N	5.11	123.39	119.66
6	j	503	LEU	C-N-CA	5.11	123.39	119.66
1	C	375	GLU	CA-C-N	5.09	125.30	120.31
1	C	375	GLU	C-N-CA	5.09	125.30	120.31
2	K	508	PHE	CA-CB-CG	-5.09	108.71	113.80
6	h	503	LEU	CA-C-N	5.09	123.38	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	503	LEU	C-N-CA	5.09	123.38	119.66
2	I	350	SER	CB-CA-C	-5.08	102.84	110.92
6	g	260	PRO	CB-CG-CD	5.07	122.34	106.10
6	h	260	PRO	CB-CG-CD	5.07	122.31	106.10
2	H	350	SER	CB-CA-C	-5.06	102.88	110.92
1	A	209	ALA	N-CA-C	5.06	116.53	108.79
6	i	260	PRO	CB-CG-CD	5.05	122.27	106.10
1	B	209	ALA	N-CA-C	5.05	116.52	108.79
4	U	51	ILE	CA-C-N	-5.05	114.72	122.60
4	U	51	ILE	C-N-CA	-5.05	114.72	122.60
6	e	260	PRO	CB-CG-CD	5.05	122.27	106.10
6	f	260	PRO	CB-CG-CD	5.05	122.27	106.10
2	J	350	SER	CB-CA-C	-5.05	102.89	110.92
1	D	209	ALA	N-CA-C	5.04	116.50	108.79
1	F	209	ALA	N-CA-C	5.04	116.50	108.79
6	j	260	PRO	CB-CG-CD	5.04	122.23	106.10
2	L	350	SER	CB-CA-C	-5.04	102.91	110.92
6	g	503	LEU	CA-C-N	5.04	123.34	119.66
6	g	503	LEU	C-N-CA	5.04	123.34	119.66
6	h	163	PHE	CA-C-N	5.04	124.70	119.56
6	h	163	PHE	C-N-CA	5.04	124.70	119.56
2	I	855	ASN	N-CA-C	5.03	116.77	111.28
2	K	350	SER	CB-CA-C	-5.02	102.93	110.92
2	G	350	SER	CB-CA-C	-5.02	102.93	110.92
2	J	855	ASN	N-CA-C	5.02	116.75	111.28
1	B	397	PRO	N-CA-C	5.02	118.94	111.41
6	f	386	LYS	N-CA-C	5.02	117.42	107.98
1	A	397	PRO	N-CA-C	5.02	118.94	111.41
1	E	397	PRO	N-CA-C	5.02	118.94	111.41
2	H	855	ASN	N-CA-C	5.02	116.75	111.28
6	h	386	LYS	N-CA-C	5.02	117.41	107.98
7	p	36	TYR	N-CA-C	5.02	117.33	108.75
7	k	36	TYR	N-CA-C	5.01	117.31	108.75
7	l	36	TYR	N-CA-C	5.01	117.31	108.75
4	X	51	ILE	CA-C-N	-5.00	114.71	122.67
4	X	51	ILE	C-N-CA	-5.00	114.71	122.67
4	S	51	ILE	CA-C-N	-5.00	114.80	122.60
4	S	51	ILE	C-N-CA	-5.00	114.80	122.60
6	j	386	LYS	N-CA-C	5.00	117.39	107.98

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	778	GLU	Sidechain
2	H	778	GLU	Sidechain
2	I	778	GLU	Sidechain
2	J	778	GLU	Sidechain
2	K	778	GLU	Sidechain
2	L	778	GLU	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4447	0	4459	43	0
1	B	4447	0	4459	39	0
1	C	4447	0	4459	41	0
1	D	4447	0	4459	40	0
1	E	4447	0	4459	38	0
1	F	4447	0	4459	40	0
2	G	7762	0	7321	46	0
2	H	7762	0	7321	44	0
2	I	7762	0	7321	47	0
2	J	7762	0	7321	46	0
2	K	7762	0	7321	46	0
2	L	7762	0	7321	41	0
3	M	1849	0	1819	21	0
3	N	1849	0	1819	23	0
3	O	1849	0	1819	21	0
3	P	1849	0	1819	21	0
3	Q	1849	0	1819	20	0
3	R	1849	0	1819	23	0
4	S	1074	0	1076	16	0
4	T	1074	0	1076	15	0
4	U	1074	0	1076	15	0
4	V	1074	0	1076	15	0
4	W	1074	0	1076	15	0
4	X	1074	0	1076	15	0
5	Y	1192	0	1147	11	0
5	Z	1192	0	1147	14	0
5	a	1192	0	1147	13	0
5	b	1192	0	1147	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	c	1192	0	1147	13	0
5	d	1192	0	1147	13	0
6	e	5057	0	4910	61	0
6	f	5057	0	4910	61	0
6	g	5057	0	4910	60	0
6	h	5057	0	4910	58	0
6	i	5057	0	4910	61	0
6	j	5057	0	4910	61	0
7	k	1145	0	1118	12	0
7	l	1145	0	1118	11	0
7	m	1145	0	1118	13	0
7	n	1145	0	1118	12	0
7	o	1145	0	1118	12	0
7	p	1145	0	1118	11	0
All	All	135156	0	131100	954	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 4.

All (954) 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)
6:h:260:PRO:HG3	6:h:468:VAL:O	1.44	1.18
6:j:260:PRO:HG3	6:j:468:VAL:O	1.44	1.17
6:e:260:PRO:HG3	6:e:468:VAL:O	1.44	1.17
6:g:260:PRO:HG3	6:g:468:VAL:O	1.44	1.15
6:f:260:PRO:HG3	6:f:468:VAL:O	1.44	1.15
6:i:260:PRO:HG3	6:i:468:VAL:O	1.44	1.15
1:F:318:TRP:CD2	2:K:985:ILE:O	2.01	1.13
1:D:318:TRP:CD2	2:I:985:ILE:O	2.02	1.12
1:A:318:TRP:CD2	2:L:985:ILE:O	2.02	1.12
1:E:318:TRP:CD2	2:J:985:ILE:O	2.02	1.12
1:B:318:TRP:CD2	2:G:985:ILE:O	2.01	1.12
1:C:318:TRP:CD2	2:H:985:ILE:O	2.02	1.11
6:g:249:ASP:O	6:g:477:LEU:HD22	1.61	1.01
6:i:249:ASP:O	6:i:477:LEU:HD22	1.61	1.01
6:f:249:ASP:O	6:f:477:LEU:HD22	1.61	1.00
6:h:249:ASP:O	6:h:477:LEU:HD22	1.61	1.00
6:j:249:ASP:O	6:j:477:LEU:HD22	1.61	1.00
6:e:249:ASP:O	6:e:477:LEU:HD22	1.61	1.00
6:e:83:LEU:HD21	6:e:86:GLY:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:83:LEU:HD21	6:i:86:GLY:H	1.33	0.92
2:J:173:GLU:HG3	2:J:795:TRP:CE3	2.05	0.92
2:K:173:GLU:HG3	2:K:795:TRP:CE3	2.05	0.92
2:I:173:GLU:HG3	2:I:795:TRP:CE3	2.05	0.91
6:h:83:LEU:HD21	6:h:86:GLY:H	1.33	0.91
6:j:83:LEU:HD21	6:j:86:GLY:H	1.33	0.91
2:L:173:GLU:HG3	2:L:795:TRP:CE3	2.05	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:H	1.33	0.91
6:e:83:LEU:HD21	6:e:86:GLY:N	1.86	0.91
6:g:83:LEU:HD21	6:g:86:GLY:H	1.33	0.90
6:i:83:LEU:HD21	6:i:86:GLY:N	1.86	0.90
2:G:173:GLU:HG3	2:G:795:TRP:CE3	2.05	0.90
2:H:173:GLU:HG3	2:H:795:TRP:CE3	2.05	0.90
6:f:83:LEU:HD21	6:f:86:GLY:N	1.86	0.90
6:g:83:LEU:HD21	6:g:86:GLY:N	1.86	0.90
6:j:83:LEU:HD21	6:j:86:GLY:N	1.86	0.89
6:h:260:PRO:HG3	6:h:468:VAL:C	1.99	0.88
6:j:260:PRO:HG3	6:j:468:VAL:C	1.99	0.88
6:g:260:PRO:HG3	6:g:468:VAL:C	1.99	0.87
6:i:260:PRO:HG3	6:i:468:VAL:C	1.99	0.87
1:B:318:TRP:CG	2:G:985:ILE:O	2.28	0.87
6:e:260:PRO:HG3	6:e:468:VAL:C	1.99	0.86
1:D:318:TRP:CG	2:I:985:ILE:O	2.29	0.86
6:f:260:PRO:HG3	6:f:468:VAL:C	1.99	0.86
1:C:318:TRP:CE3	2:H:985:ILE:O	2.29	0.86
6:i:408:THR:HG23	6:i:411:GLU:HG2	1.58	0.85
1:D:318:TRP:CE3	2:I:985:ILE:O	2.29	0.85
1:F:318:TRP:CE3	2:K:985:ILE:O	2.28	0.85
1:C:318:TRP:CG	2:H:985:ILE:O	2.29	0.85
1:E:318:TRP:CE3	2:J:985:ILE:O	2.30	0.85
1:F:318:TRP:CG	2:K:985:ILE:O	2.29	0.85
1:E:318:TRP:CG	2:J:985:ILE:O	2.28	0.84
6:j:408:THR:HG23	6:j:411:GLU:HG2	1.58	0.84
1:A:318:TRP:CE3	2:L:985:ILE:O	2.29	0.84
1:B:318:TRP:CE3	2:G:985:ILE:O	2.30	0.84
1:A:318:TRP:CG	2:L:985:ILE:O	2.29	0.84
6:h:408:THR:HG23	6:h:411:GLU:HG2	1.59	0.84
6:g:408:THR:HG23	6:g:411:GLU:HG2	1.58	0.83
6:f:408:THR:HG23	6:f:411:GLU:HG2	1.58	0.83
1:C:89:LYS:NZ	6:g:85:GLU:OE1	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LYS:NZ	6:h:85:GLU:OE1	2.12	0.82
1:E:89:LYS:NZ	6:i:85:GLU:OE1	2.11	0.82
6:e:408:THR:HG23	6:e:411:GLU:HG2	1.58	0.82
1:B:89:LYS:NZ	6:f:85:GLU:OE1	2.11	0.82
6:g:83:LEU:CD2	6:g:86:GLY:H	1.94	0.81
6:h:83:LEU:CD2	6:h:86:GLY:H	1.95	0.80
6:f:83:LEU:CD2	6:f:86:GLY:H	1.94	0.80
3:N:175:TYR:CE1	4:V:6:LYS:HE2	2.17	0.80
1:A:89:LYS:NZ	6:e:85:GLU:OE1	2.12	0.80
1:D:340:LYS:HG3	1:D:345:ILE:HD11	1.64	0.80
1:C:340:LYS:HG3	1:C:345:ILE:HD11	1.64	0.80
3:M:175:TYR:CE1	4:T:6:LYS:HE2	2.16	0.80
3:P:175:TYR:CE1	4:W:6:LYS:HE2	2.16	0.80
3:Q:175:TYR:CE1	4:X:6:LYS:HE2	2.17	0.80
6:i:83:LEU:HD21	6:i:86:GLY:CA	2.12	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:B:340:LYS:HG3	1:B:345:ILE:HD11	1.64	0.79
3:O:175:TYR:CE1	4:U:6:LYS:HE2	2.17	0.79
3:R:175:TYR:CE1	4:S:6:LYS:HE2	2.17	0.79
1:E:340:LYS:HG3	1:E:345:ILE:HD11	1.64	0.79
1:A:340:LYS:HG3	1:A:345:ILE:HD11	1.64	0.79
1:F:89:LYS:NZ	6:j:85:GLU:OE1	2.12	0.79
6:e:83:LEU:HD21	6:e:86:GLY:CA	2.12	0.79
6:e:83:LEU:CD2	6:e:86:GLY:H	1.94	0.79
6:h:83:LEU:HD21	6:h:86:GLY:CA	2.12	0.79
1:F:340:LYS:HG3	1:F:345:ILE:HD11	1.64	0.79
1:C:133:GLN:N	1:C:133:GLN:OE1	2.16	0.79
6:f:83:LEU:HD21	6:f:86:GLY:CA	2.12	0.78
1:E:133:GLN:N	1:E:133:GLN:OE1	2.16	0.78
6:g:83:LEU:HD21	6:g:86:GLY:CA	2.12	0.78
1:A:133:GLN:OE1	1:A:133:GLN:N	2.16	0.78
1:D:39:ASN:HB2	2:J:109:GLY:O	1.84	0.78
6:j:83:LEU:CD2	6:j:86:GLY:H	1.95	0.78
1:C:39:ASN:HB2	2:I:109:GLY:O	1.83	0.77
1:B:39:ASN:HB2	2:H:109:GLY:O	1.84	0.77
1:F:39:ASN:HB2	2:L:109:GLY:O	1.84	0.77
1:E:39:ASN:HB2	2:K:109:GLY:O	1.84	0.76
6:e:408:THR:CG2	6:e:411:GLU:HG2	2.16	0.76
4:S:36:GLN:HE22	6:e:685:PHE:HB2	1.50	0.76
4:T:36:GLN:HE22	6:f:685:PHE:HB2	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:408:THR:CG2	6:j:411:GLU:HG2	2.16	0.76
1:A:39:ASN:HB2	2:G:109:GLY:O	1.84	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:342:ILE:HG13	1:F:343:LEU:HD12	1.67	0.76
4:X:36:GLN:HE22	6:j:685:PHE:HB2	1.50	0.76
4:W:36:GLN:HE22	6:i:685:PHE:HB2	1.50	0.76
1:E:342:ILE:HG13	1:E:343:LEU:HD12	1.67	0.75
6:i:408:THR:CG2	6:i:411:GLU:HG2	2.15	0.75
6:h:408:THR:CG2	6:h:411:GLU:HG2	2.16	0.75
1:B:133:GLN:N	1:B:133:GLN:OE1	2.16	0.75
1:D:133:GLN:OE1	1:D:133:GLN:N	2.16	0.75
4:V:36:GLN:HE22	6:h:685:PHE:HB2	1.50	0.75
1:C:342:ILE:HG13	1:C:343:LEU:HD12	1.67	0.75
7:n:33:ILE:HD11	7:o:111:LEU:HD12	1.69	0.75
1:A:342:ILE:HG13	1:A:343:LEU:HD12	1.67	0.74
1:B:342:ILE:HG13	1:B:343:LEU:HD12	1.67	0.74
4:U:36:GLN:HE22	6:g:685:PHE:HB2	1.50	0.74
6:f:512:ALA:HB1	6:f:529:ILE:HD12	1.69	0.74
1:F:133:GLN:OE1	1:F:133:GLN:N	2.16	0.74
6:j:512:ALA:HB1	6:j:529:ILE:HD12	1.69	0.74
7:m:33:ILE:HD11	7:n:111:LEU:HD12	1.70	0.74
6:e:512:ALA:HB1	6:e:529:ILE:HD12	1.69	0.74
6:i:512:ALA:HB1	6:i:529:ILE:HD12	1.69	0.74
6:f:473:LEU:HD22	6:f:481:ILE:HG22	1.70	0.74
6:g:473:LEU:HD22	6:g:481:ILE:HG22	1.70	0.74
1:D:342:ILE:HG13	1:D:343:LEU:HD12	1.67	0.73
6:h:473:LEU:HD22	6:h:481:ILE:HG22	1.70	0.73
7:l:33:ILE:HD11	7:m:111:LEU:HD12	1.69	0.73
7:o:33:ILE:HD11	7:p:111:LEU:HD12	1.69	0.73
7:k:33:ILE:HD11	7:l:111:LEU:HD12	1.69	0.73
6:e:473:LEU:HD22	6:e:481:ILE:HG22	1.70	0.72
6:h:512:ALA:HB1	6:h:529:ILE:HD12	1.69	0.72
6:g:512:ALA:HB1	6:g:529:ILE:HD12	1.69	0.72
2:H:794:SER:O	2:H:795:TRP:CG	2.43	0.72
2:I:794:SER:O	2:I:795:TRP:CG	2.43	0.72
2:G:794:SER:O	2:G:795:TRP:CG	2.43	0.72
6:i:473:LEU:HD22	6:i:481:ILE:HG22	1.70	0.72
2:J:794:SER:O	2:J:795:TRP:CG	2.43	0.71
7:k:111:LEU:HD12	7:p:33:ILE:HD11	1.70	0.71
6:j:473:LEU:HD22	6:j:481:ILE:HG22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:790:GLN:HA	2:J:790:GLN:OE1	1.91	0.70
2:K:794:SER:O	2:K:795:TRP:CG	2.43	0.70
1:E:99:THR:HG23	1:E:189:ASN:OD1	1.92	0.70
1:F:99:THR:HG23	1:F:189:ASN:OD1	1.92	0.70
2:K:790:GLN:OE1	2:K:790:GLN:HA	1.91	0.70
2:L:794:SER:O	2:L:795:TRP:CG	2.43	0.70
1:A:99:THR:HG23	1:A:189:ASN:OD1	1.92	0.70
3:N:172:MET:HE2	4:V:120:ASN:O	1.91	0.70
5:b:32:SER:HB2	5:c:123:ASP:OD1	1.92	0.70
1:B:99:THR:HG23	1:B:189:ASN:OD1	1.92	0.70
2:G:790:GLN:HA	2:G:790:GLN:OE1	1.91	0.70
3:P:172:MET:HE2	4:W:120:ASN:O	1.91	0.70
2:I:790:GLN:OE1	2:I:790:GLN:HA	1.91	0.70
3:R:172:MET:HE2	4:S:120:ASN:O	1.92	0.70
6:h:255:HIS:O	6:h:256:LEU:HD23	1.92	0.70
1:D:99:THR:HG23	1:D:189:ASN:OD1	1.92	0.70
2:H:790:GLN:HA	2:H:790:GLN:OE1	1.91	0.70
6:g:83:LEU:C	6:g:83:LEU:HD23	2.17	0.70
5:c:32:SER:HB2	5:d:123:ASP:OD1	1.92	0.69
6:e:255:HIS:O	6:e:256:LEU:HD23	1.92	0.69
6:f:83:LEU:C	6:f:83:LEU:HD23	2.17	0.69
6:j:255:HIS:O	6:j:256:LEU:HD23	1.92	0.69
2:L:790:GLN:HA	2:L:790:GLN:OE1	1.91	0.69
6:j:478:LEU:HD22	6:j:481:ILE:HD11	1.74	0.69
6:i:83:LEU:HD23	6:i:83:LEU:C	2.17	0.69
3:M:172:MET:HE2	4:T:120:ASN:O	1.92	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	2.18	0.69
5:Z:32:SER:HB2	5:a:123:ASP:OD1	1.92	0.69
6:e:478:LEU:HD22	6:e:481:ILE:HD11	1.74	0.69
3:Q:172:MET:HE2	4:X:120:ASN:O	1.93	0.69
5:a:32:SER:HB2	5:b:123:ASP:OD1	1.93	0.69
6:f:255:HIS:O	6:f:256:LEU:HD23	1.92	0.69
1:C:99:THR:HG23	1:C:189:ASN:OD1	1.92	0.69
6:g:255:HIS:O	6:g:256:LEU:HD23	1.92	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
2:H:794:SER:O	2:H:795:TRP:CD2	2.46	0.69
2:G:173:GLU:HG3	2:G:795:TRP:CD2	2.28	0.68
2:K:173:GLU:HB3	2:K:795:TRP:CZ2	2.28	0.68
2:K:794:SER:O	2:K:795:TRP:CD2	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:478:LEU:HD22	6:i:481:ILE:HD11	1.74	0.68
2:G:794:SER:O	2:G:795:TRP:CD2	2.46	0.68
2:H:173:GLU:HB3	2:H:795:TRP:CH2	2.29	0.68
2:J:173:GLU:HB3	2:J:795:TRP:CZ2	2.28	0.68
2:G:173:GLU:HB3	2:G:795:TRP:CH2	2.29	0.68
2:H:173:GLU:HG3	2:H:795:TRP:CD2	2.28	0.68
2:I:173:GLU:HB3	2:I:795:TRP:CZ2	2.28	0.68
5:Y:123:ASP:OD1	5:d:32:SER:HB2	1.93	0.68
2:G:173:GLU:HB3	2:G:795:TRP:CZ2	2.28	0.68
1:C:409:PRO:HD2	6:g:547:GLU:OE2	1.94	0.68
2:I:794:SER:O	2:I:795:TRP:CD2	2.46	0.68
2:J:794:SER:O	2:J:795:TRP:CD2	2.46	0.68
2:L:173:GLU:HG3	2:L:795:TRP:CD2	2.28	0.68
2:L:794:SER:O	2:L:795:TRP:CD2	2.46	0.68
1:B:409:PRO:HD2	6:f:547:GLU:OE2	1.94	0.68
5:Y:32:SER:HB2	5:Z:123:ASP:OD1	1.92	0.68
2:I:114:HIS:CE1	4:U:24:GLY:O	2.47	0.68
2:I:173:GLU:HB3	2:I:795:TRP:CH2	2.29	0.68
2:I:173:GLU:HG3	2:I:795:TRP:CD2	2.28	0.68
2:L:114:HIS:CE1	4:X:24:GLY:O	2.47	0.68
2:L:173:GLU:HB3	2:L:795:TRP:CZ2	2.28	0.68
6:f:478:LEU:HD22	6:f:481:ILE:HD11	1.74	0.68
3:O:172:MET:HE2	4:U:120:ASN:O	1.93	0.68
2:H:173:GLU:HB3	2:H:795:TRP:CZ2	2.28	0.67
2:L:173:GLU:HB3	2:L:795:TRP:CH2	2.29	0.67
3:N:71:ASP:OD1	3:N:149:THR:HG22	1.95	0.67
3:Q:71:ASP:OD1	3:Q:149:THR:HG22	1.95	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	1.94	0.67
3:P:71:ASP:OD1	3:P:149:THR:HG22	1.95	0.67
1:F:89:LYS:HZ1	6:j:85:GLU:CD	2.01	0.67
2:J:173:GLU:HG3	2:J:795:TRP:CD2	2.28	0.67
1:A:409:PRO:HD2	6:e:547:GLU:OE2	1.95	0.67
1:F:409:PRO:HD2	6:j:547:GLU:OE2	1.94	0.67
2:J:114:HIS:CE1	4:V:24:GLY:O	2.48	0.67
6:h:478:LEU:HD22	6:h:481:ILE:HD11	1.74	0.67
2:K:173:GLU:HG3	2:K:795:TRP:CD2	2.28	0.67
2:J:173:GLU:HB3	2:J:795:TRP:CH2	2.29	0.67
6:g:478:LEU:HD22	6:g:481:ILE:HD11	1.74	0.67
1:E:409:PRO:HD2	6:i:547:GLU:OE2	1.94	0.67
2:K:114:HIS:CE1	4:W:24:GLY:O	2.48	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:173:GLU:HB3	2:K:795:TRP:CH2	2.29	0.67
3:M:71:ASP:OD1	3:M:149:THR:HG22	1.95	0.67
5:Y:3:THR:HG22	5:Y:4:TYR:H	1.60	0.66
1:E:89:LYS:HZ1	6:i:85:GLU:CD	2.01	0.66
1:D:409:PRO:HD2	6:h:547:GLU:OE2	1.95	0.66
2:H:114:HIS:CE1	4:T:24:GLY:O	2.48	0.66
5:Z:3:THR:HG22	5:Z:4:TYR:H	1.61	0.66
1:C:10:ILE:HG13	3:M:224:LEU:HD23	1.78	0.66
1:B:10:ILE:HG13	3:R:224:LEU:HD23	1.77	0.66
5:c:3:THR:HG22	5:c:4:TYR:H	1.61	0.66
5:a:3:THR:HG22	5:a:4:TYR:H	1.61	0.65
1:D:10:ILE:HG13	3:O:224:LEU:HD23	1.78	0.65
1:F:10:ILE:HG13	3:P:224:LEU:HD23	1.78	0.65
5:b:3:THR:HG22	5:b:4:TYR:H	1.60	0.65
2:G:114:HIS:CE1	4:S:24:GLY:O	2.48	0.65
5:d:105:PRO:HD3	6:j:615:ASN:OD1	1.96	0.65
2:L:312:PRO:O	2:L:350:SER:HB2	1.97	0.65
5:d:3:THR:HG22	5:d:4:TYR:H	1.61	0.65
5:Y:105:PRO:HD3	6:e:615:ASN:OD1	1.97	0.65
1:E:10:ILE:HG13	3:N:224:LEU:HD23	1.77	0.64
5:a:105:PRO:HD3	6:g:615:ASN:OD1	1.96	0.64
5:c:105:PRO:HD3	6:i:615:ASN:OD1	1.96	0.64
1:A:10:ILE:HG13	3:Q:224:LEU:HD23	1.78	0.64
2:K:312:PRO:O	2:K:350:SER:HB2	1.97	0.64
5:Z:105:PRO:HD3	6:f:615:ASN:OD1	1.96	0.64
2:J:312:PRO:O	2:J:350:SER:HB2	1.97	0.64
2:G:312:PRO:O	2:G:350:SER:HB2	1.97	0.64
4:X:15:PHE:O	4:X:17:PRO:HD3	1.98	0.64
5:b:105:PRO:HD3	6:h:615:ASN:OD1	1.97	0.64
6:i:83:LEU:HD21	6:i:86:GLY:HA2	1.80	0.64
4:U:46:LYS:NZ	4:U:61:ASP:OD2	2.31	0.64
2:I:312:PRO:O	2:I:350:SER:HB2	1.97	0.64
4:S:15:PHE:O	4:S:17:PRO:HD3	1.98	0.64
4:V:15:PHE:O	4:V:17:PRO:HD3	1.98	0.64
4:W:15:PHE:O	4:W:17:PRO:HD3	1.98	0.64
6:h:83:LEU:HD21	6:h:86:GLY:HA2	1.80	0.64
4:T:15:PHE:O	4:T:17:PRO:HD3	1.98	0.63
4:W:46:LYS:NZ	4:W:61:ASP:OD2	2.31	0.63
4:U:15:PHE:O	4:U:17:PRO:HD3	1.98	0.63
2:H:312:PRO:O	2:H:350:SER:HB2	1.97	0.63
6:h:684:LYS:HD3	6:i:17:PHE:HZ	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:83:LEU:HD21	6:j:86:GLY:HA2	1.80	0.63
2:I:312:PRO:O	2:I:350:SER:CB	2.47	0.63
2:L:991:LEU:H	2:L:1005:ILE:H	1.47	0.63
4:V:46:LYS:NZ	4:V:61:ASP:OD2	2.31	0.63
6:i:684:LYS:HD3	6:j:17:PHE:HZ	1.64	0.63
2:H:312:PRO:O	2:H:350:SER:CB	2.47	0.63
2:K:991:LEU:H	2:K:1005:ILE:H	1.47	0.63
4:X:46:LYS:NZ	4:X:61:ASP:OD2	2.31	0.63
5:Z:36:VAL:O	5:Z:37:ASP:OD2	2.17	0.63
2:J:991:LEU:H	2:J:1005:ILE:H	1.47	0.63
6:e:17:PHE:HZ	6:j:684:LYS:HD3	1.63	0.63
6:e:684:LYS:HD3	6:f:17:PHE:HZ	1.63	0.63
6:g:83:LEU:HD21	6:g:86:GLY:HA2	1.80	0.63
2:G:991:LEU:H	2:G:1005:ILE:H	1.47	0.63
6:f:684:LYS:HD3	6:g:17:PHE:HZ	1.63	0.63
1:A:410:LYS:HE2	6:f:3:THR:O	1.99	0.62
2:G:312:PRO:O	2:G:350:SER:CB	2.47	0.62
2:J:312:PRO:O	2:J:350:SER:CB	2.47	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
2:L:312:PRO:O	2:L:350:SER:CB	2.47	0.62
2:H:991:LEU:H	2:H:1005:ILE:H	1.47	0.62
1:B:410:LYS:HE2	6:g:3:THR:O	2.00	0.62
2:I:991:LEU:H	2:I:1005:ILE:H	1.47	0.62
5:c:36:VAL:O	5:c:37:ASP:OD2	2.17	0.62
1:E:410:LYS:HE2	6:j:3:THR:O	1.99	0.62
5:Z:27:GLU:HB3	7:l:38:HIS:ND1	2.14	0.62
2:K:312:PRO:O	2:K:350:SER:CB	2.47	0.62
1:B:34:LYS:HD2	4:T:127:TYR:CE1	2.35	0.62
4:T:46:LYS:NZ	4:T:61:ASP:OD2	2.31	0.62
5:Y:36:VAL:O	5:Y:37:ASP:OD2	2.17	0.62
5:d:36:VAL:O	5:d:37:ASP:OD2	2.17	0.62
5:c:27:GLU:HB3	7:o:38:HIS:ND1	2.14	0.62
5:a:27:GLU:HB3	7:m:38:HIS:ND1	2.15	0.62
5:b:36:VAL:O	5:b:37:ASP:OD2	2.17	0.62
1:C:410:LYS:HE2	6:h:3:THR:O	2.00	0.61
1:D:410:LYS:HE2	6:i:3:THR:O	1.99	0.61
1:F:410:LYS:HE2	6:e:3:THR:O	2.00	0.61
2:I:794:SER:O	2:I:795:TRP:CD1	2.53	0.61
6:f:83:LEU:HD21	6:f:86:GLY:HA2	1.80	0.61
6:g:684:LYS:HD3	6:h:17:PHE:HZ	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:LYS:HD2	4:X:127:TYR:CE1	2.35	0.61
6:e:83:LEU:HD21	6:e:86:GLY:HA2	1.80	0.61
6:e:512:ALA:HB1	6:e:529:ILE:CD1	2.30	0.61
2:H:794:SER:O	2:H:795:TRP:CD1	2.53	0.61
5:d:27:GLU:HB3	7:p:38:HIS:ND1	2.15	0.61
1:C:89:LYS:NZ	6:g:85:GLU:CD	2.59	0.61
2:G:794:SER:O	2:G:795:TRP:CD1	2.54	0.61
6:h:248:ALA:HB1	6:h:478:LEU:HD12	1.83	0.61
1:D:89:LYS:NZ	6:h:85:GLU:CD	2.59	0.61
1:E:34:LYS:HD2	4:W:127:TYR:CE1	2.35	0.61
6:g:512:ALA:HB1	6:g:529:ILE:CD1	2.30	0.61
5:Y:27:GLU:HB3	7:k:38:HIS:ND1	2.15	0.61
6:i:248:ALA:HB1	6:i:478:LEU:HD12	1.83	0.61
6:j:478:LEU:O	6:j:481:ILE:HG12	2.01	0.61
1:A:34:LYS:HD2	4:S:127:TYR:CE1	2.36	0.61
2:L:794:SER:O	2:L:795:TRP:CD1	2.54	0.61
6:g:248:ALA:HB1	6:g:478:LEU:HD12	1.83	0.61
6:h:224:THR:HG22	6:h:225:LYS:N	2.16	0.61
6:h:512:ALA:HB1	6:h:529:ILE:CD1	2.30	0.61
6:j:512:ALA:HB1	6:j:529:ILE:CD1	2.30	0.61
2:J:794:SER:O	2:J:795:TRP:CD1	2.54	0.61
2:L:788:LYS:HD3	2:L:792:ARG:HD3	1.83	0.61
6:e:478:LEU:O	6:e:481:ILE:HG12	2.01	0.61
6:f:512:ALA:HB1	6:f:529:ILE:CD1	2.30	0.61
1:C:34:LYS:HD2	4:U:127:TYR:CE1	2.35	0.60
5:b:27:GLU:HB3	7:n:38:HIS:ND1	2.15	0.60
1:E:89:LYS:NZ	6:i:85:GLU:CD	2.58	0.60
2:K:794:SER:O	2:K:795:TRP:CD1	2.54	0.60
6:i:224:THR:HG22	6:i:225:LYS:N	2.16	0.60
1:B:89:LYS:NZ	6:f:85:GLU:CD	2.59	0.60
6:i:478:LEU:O	6:i:481:ILE:HG12	2.01	0.60
1:B:316:ASN:HD22	1:B:318:TRP:HE1	1.50	0.60
2:J:788:LYS:HD3	2:J:792:ARG:HD3	1.84	0.60
6:j:248:ALA:HB1	6:j:478:LEU:HD12	1.83	0.60
2:K:788:LYS:HD3	2:K:792:ARG:HD3	1.83	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
1:F:89:LYS:NZ	6:j:85:GLU:CD	2.59	0.60
2:G:788:LYS:HD3	2:G:792:ARG:HD3	1.83	0.60
4:T:36:GLN:HE22	6:f:685:PHE:CB	2.14	0.60
1:A:89:LYS:NZ	6:e:85:GLU:CD	2.59	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ASN:HD22	1:C:318:TRP:HE1	1.50	0.60
1:D:34:LYS:HD2	4:V:127:TYR:CE1	2.36	0.60
6:h:478:LEU:O	6:h:481:ILE:HG12	2.01	0.60
6:i:512:ALA:HB1	6:i:529:ILE:CD1	2.30	0.60
6:f:248:ALA:HB1	6:f:478:LEU:HD12	1.83	0.60
1:A:316:ASN:HD22	1:A:318:TRP:HE1	1.50	0.60
1:F:316:ASN:HD22	1:F:318:TRP:HE1	1.50	0.60
2:H:788:LYS:HD3	2:H:792:ARG:HD3	1.83	0.60
6:f:224:THR:HG22	6:f:225:LYS:N	2.16	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
1:E:316:ASN:HD22	1:E:318:TRP:HE1	1.50	0.59
2:I:788:LYS:HD3	2:I:792:ARG:HD3	1.84	0.59
6:g:224:THR:HG22	6:g:225:LYS:N	2.16	0.59
6:i:253:ILE:HD11	6:i:478:LEU:HD23	1.84	0.59
2:H:241:MET:HG2	2:H:244:SER:HB3	1.85	0.59
1:D:316:ASN:HD22	1:D:318:TRP:HE1	1.50	0.59
6:j:224:THR:HG22	6:j:225:LYS:N	2.16	0.59
6:j:253:ILE:HD11	6:j:478:LEU:HD23	1.85	0.59
2:H:268:CYS:SG	2:H:997:SER:O	2.55	0.59
6:e:253:ILE:HD11	6:e:478:LEU:HD23	1.85	0.59
4:S:36:GLN:HE22	6:e:685:PHE:CB	2.15	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
2:I:241:MET:HG2	2:I:244:SER:HB3	1.85	0.59
2:K:241:MET:HG2	2:K:244:SER:HB3	1.85	0.59
2:G:241:MET:HG2	2:G:244:SER:HB3	1.85	0.59
6:g:478:LEU:C	6:g:478:LEU:HD13	2.28	0.59
6:i:478:LEU:HD13	6:i:478:LEU:C	2.28	0.59
5:a:48:GLU:O	5:b:58:LYS:NZ	2.36	0.58
6:j:478:LEU:C	6:j:478:LEU:HD13	2.28	0.58
1:D:409:PRO:HG3	6:h:544:GLU:OE1	2.03	0.58
4:V:36:GLN:HE22	6:h:685:PHE:CB	2.15	0.58
6:f:253:ILE:HD11	6:f:478:LEU:HD23	1.85	0.58
6:g:253:ILE:HD11	6:g:478:LEU:HD23	1.85	0.58
6:h:478:LEU:HD13	6:h:478:LEU:C	2.28	0.58
2:I:71:PHE:CZ	4:U:20:GLU:O	2.57	0.58
2:L:241:MET:HG2	2:L:244:SER:HB3	1.85	0.58
6:h:482:GLU:HB3	6:h:483:PRO:HD3	1.85	0.58
1:A:409:PRO:HG3	6:e:544:GLU:OE1	2.03	0.58
4:U:36:GLN:HE22	6:g:685:PHE:CB	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:36:GLN:HE22	6:i:685:PHE:CB	2.14	0.58
6:g:482:GLU:HB3	6:g:483:PRO:HD3	1.86	0.58
2:L:71:PHE:CZ	4:X:20:GLU:O	2.57	0.58
6:e:478:LEU:C	6:e:478:LEU:HD13	2.28	0.58
5:Z:48:GLU:O	5:a:58:LYS:NZ	2.37	0.58
2:K:268:CYS:SG	2:K:997:SER:O	2.55	0.58
5:Y:58:LYS:NZ	5:d:48:GLU:O	2.36	0.58
6:i:482:GLU:HB3	6:i:483:PRO:HD3	1.85	0.58
6:j:482:GLU:HB3	6:j:483:PRO:HD3	1.85	0.58
2:J:241:MET:HG2	2:J:244:SER:HB3	1.85	0.57
5:c:48:GLU:O	5:d:58:LYS:NZ	2.37	0.57
1:C:409:PRO:HG3	6:g:544:GLU:OE1	2.04	0.57
1:B:345:ILE:C	1:B:346:ASN:HD22	2.13	0.57
1:F:409:PRO:HG3	6:j:544:GLU:OE1	2.04	0.57
1:B:409:PRO:HG3	6:f:544:GLU:OE1	2.04	0.57
2:J:71:PHE:CZ	4:V:20:GLU:O	2.58	0.57
4:X:36:GLN:HE22	6:j:685:PHE:CB	2.16	0.57
1:E:345:ILE:C	1:E:346:ASN:HD22	2.13	0.57
2:H:71:PHE:CZ	4:T:20:GLU:O	2.58	0.57
2:I:268:CYS:SG	2:I:997:SER:O	2.55	0.57
5:a:118:LYS:HB3	5:a:137:GLU:HB3	1.87	0.56
2:K:71:PHE:CZ	4:W:20:GLU:O	2.58	0.56
6:e:482:GLU:HB3	6:e:483:PRO:HD3	1.85	0.56
1:A:345:ILE:C	1:A:346:ASN:HD22	2.13	0.56
5:d:118:LYS:HB3	5:d:137:GLU:HB3	1.87	0.56
6:g:684:LYS:CD	6:h:17:PHE:HZ	2.18	0.56
5:b:48:GLU:O	5:c:58:LYS:NZ	2.39	0.56
5:c:118:LYS:HB3	5:c:137:GLU:HB3	1.87	0.56
1:F:345:ILE:C	1:F:346:ASN:HD22	2.13	0.56
2:L:114:HIS:HE1	4:X:24:GLY:O	1.89	0.56
5:Y:48:GLU:O	5:Z:58:LYS:NZ	2.39	0.56
6:f:83:LEU:HD23	6:f:84:ILE:N	2.21	0.56
1:C:345:ILE:C	1:C:346:ASN:HD22	2.13	0.56
1:E:409:PRO:HG3	6:i:544:GLU:OE1	2.04	0.56
5:Z:118:LYS:HB3	5:Z:137:GLU:HB3	1.88	0.56
6:e:83:LEU:HD23	6:e:84:ILE:N	2.21	0.56
6:f:482:GLU:HB3	6:f:483:PRO:HD3	1.85	0.56
6:f:684:LYS:CD	6:g:17:PHE:HZ	2.18	0.56
6:h:83:LEU:HD23	6:h:84:ILE:N	2.21	0.56
6:i:83:LEU:HD23	6:i:84:ILE:N	2.21	0.56
2:I:114:HIS:HE1	4:U:24:GLY:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:268:CYS:SG	2:L:997:SER:O	2.55	0.56
1:D:345:ILE:C	1:D:346:ASN:HD22	2.13	0.56
6:e:17:PHE:HZ	6:j:684:LYS:CD	2.18	0.56
6:e:684:LYS:CD	6:f:17:PHE:HZ	2.18	0.56
6:h:684:LYS:CD	6:i:17:PHE:HZ	2.18	0.56
2:G:71:PHE:CZ	4:S:20:GLU:O	2.58	0.55
6:j:83:LEU:HD23	6:j:84:ILE:N	2.21	0.55
2:J:268:CYS:SG	2:J:997:SER:O	2.55	0.55
2:G:114:HIS:HE1	4:S:24:GLY:O	1.90	0.55
5:b:118:LYS:HB3	5:b:137:GLU:HB3	1.87	0.55
6:j:172:ASP:OD1	6:j:172:ASP:N	2.40	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
6:g:83:LEU:HD23	6:g:84:ILE:N	2.21	0.55
5:Y:118:LYS:HB3	5:Y:137:GLU:HB3	1.87	0.55
6:e:478:LEU:CD1	6:e:489:TYR:HE1	2.20	0.55
6:f:478:LEU:CD1	6:f:489:TYR:HE1	2.20	0.55
6:i:684:LYS:CD	6:j:17:PHE:HZ	2.19	0.55
6:j:478:LEU:HD11	6:j:489:TYR:CE1	2.42	0.55
6:g:478:LEU:CD1	6:g:489:TYR:HE1	2.20	0.55
6:f:478:LEU:HD11	6:f:489:TYR:CE1	2.42	0.54
2:J:114:HIS:HE1	4:V:24:GLY:O	1.90	0.54
6:g:478:LEU:HD11	6:g:489:TYR:CE1	2.42	0.54
6:h:478:LEU:CD1	6:h:489:TYR:HE1	2.20	0.54
6:j:478:LEU:CD1	6:j:489:TYR:HE1	2.20	0.54
6:h:172:ASP:OD1	6:h:172:ASP:N	2.40	0.54
2:G:173:GLU:CB	2:G:795:TRP:CH2	2.91	0.54
2:H:173:GLU:CB	2:H:795:TRP:CH2	2.91	0.54
2:I:173:GLU:CB	2:I:795:TRP:CH2	2.91	0.53
2:K:114:HIS:HE1	4:W:24:GLY:O	1.90	0.53
6:e:478:LEU:HD11	6:e:489:TYR:CE1	2.42	0.53
6:e:172:ASP:OD1	6:e:172:ASP:N	2.40	0.53
2:L:173:GLU:CB	2:L:795:TRP:CH2	2.91	0.53
6:i:478:LEU:CD1	6:i:489:TYR:HE1	2.20	0.53
2:G:268:CYS:SG	2:G:997:SER:O	2.55	0.53
2:I:785:THR:HG22	2:I:785:THR:O	2.09	0.53
2:K:173:GLU:CB	2:K:795:TRP:CH2	2.91	0.53
2:K:785:THR:HG22	2:K:785:THR:O	2.09	0.53
2:G:785:THR:O	2:G:785:THR:HG22	2.09	0.53
3:M:62:LYS:CD	3:R:49:GLN:HG3	2.39	0.53
3:N:49:GLN:HG3	3:P:62:LYS:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:173:GLU:CB	2:J:795:TRP:CH2	2.91	0.52
6:i:191:ASP:OD1	6:i:191:ASP:N	2.42	0.52
2:H:785:THR:O	2:H:785:THR:HG22	2.09	0.52
3:N:62:LYS:CD	3:O:49:GLN:HG3	2.39	0.52
6:g:478:LEU:O	6:g:478:LEU:HD13	2.10	0.52
2:J:785:THR:O	2:J:785:THR:HG22	2.09	0.52
4:T:36:GLN:NE2	6:f:685:PHE:HB2	2.22	0.52
6:j:478:LEU:O	6:j:478:LEU:HD13	2.10	0.52
3:Q:49:GLN:HG3	3:R:62:LYS:CD	2.39	0.52
6:h:478:LEU:O	6:h:478:LEU:HD13	2.10	0.52
6:i:478:LEU:O	6:i:478:LEU:HD13	2.10	0.52
6:f:478:LEU:O	6:f:478:LEU:HD13	2.10	0.52
3:M:62:LYS:HD3	3:R:49:GLN:HG3	1.92	0.52
6:f:478:LEU:CD1	6:f:489:TYR:CE1	2.93	0.52
2:I:429:ASN:HB3	2:I:431:LEU:H	1.76	0.51
2:L:785:THR:HG22	2:L:785:THR:O	2.09	0.51
3:N:49:GLN:HG3	3:P:62:LYS:HD3	1.92	0.51
6:e:478:LEU:O	6:e:478:LEU:HD13	2.10	0.51
6:f:482:GLU:O	6:f:486:ASN:OD1	2.29	0.51
6:g:478:LEU:CD1	6:g:489:TYR:CE1	2.94	0.51
2:H:429:ASN:HB3	2:H:431:LEU:H	1.76	0.51
6:h:482:GLU:O	6:h:486:ASN:OD1	2.29	0.51
1:D:87:PHE:CD2	2:J:143:TYR:CD1	2.98	0.51
6:e:482:GLU:O	6:e:486:ASN:OD1	2.29	0.51
6:g:191:ASP:N	6:g:191:ASP:OD1	2.42	0.51
6:h:478:LEU:CD1	6:h:489:TYR:CE1	2.93	0.51
6:i:482:GLU:O	6:i:486:ASN:OD1	2.29	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
1:E:87:PHE:CD2	2:K:143:TYR:CD1	2.99	0.51
3:Q:49:GLN:HG3	3:R:62:LYS:HD3	1.92	0.51
6:g:482:GLU:O	6:g:486:ASN:OD1	2.29	0.51
1:B:87:PHE:CD2	2:H:143:TYR:CD1	2.99	0.51
2:J:429:ASN:HB3	2:J:431:LEU:H	1.75	0.51
6:e:260:PRO:C	6:e:261:ASN:HD22	2.19	0.51
6:f:172:ASP:OD1	6:f:172:ASP:N	2.40	0.51
6:g:260:PRO:C	6:g:261:ASN:HD22	2.19	0.51
6:f:260:PRO:C	6:f:261:ASN:HD22	2.19	0.51
2:G:429:ASN:HB3	2:G:431:LEU:H	1.76	0.51
1:C:87:PHE:CD2	2:I:143:TYR:CD1	2.99	0.50
1:F:87:PHE:CD2	2:L:143:TYR:CD1	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1000:CYS:O	2:G:1001:ASN:CB	2.59	0.50
2:J:1000:CYS:O	2:J:1001:ASN:CB	2.59	0.50
1:A:87:PHE:CD2	2:G:143:TYR:CD1	2.98	0.50
3:P:49:GLN:HG3	3:Q:62:LYS:HD3	1.94	0.50
6:e:212:ASP:OD1	6:e:215:PRO:HD2	2.11	0.50
6:e:478:LEU:CD1	6:e:489:TYR:CE1	2.94	0.50
6:f:191:ASP:OD1	6:f:191:ASP:N	2.41	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
6:j:478:LEU:CD1	6:j:489:TYR:CE1	2.94	0.50
3:M:49:GLN:HG3	3:O:62:LYS:CD	2.41	0.50
4:U:36:GLN:NE2	6:g:685:PHE:HB2	2.24	0.50
6:f:212:ASP:OD1	6:f:215:PRO:HD2	2.11	0.50
1:F:10:ILE:CG1	3:P:224:LEU:HD23	2.42	0.50
2:K:1000:CYS:O	2:K:1001:ASN:CB	2.59	0.50
2:L:1000:CYS:O	2:L:1001:ASN:CB	2.59	0.50
3:P:49:GLN:HG3	3:Q:62:LYS:CD	2.41	0.50
2:H:114:HIS:HE1	4:T:24:GLY:O	1.90	0.50
3:N:62:LYS:HD3	3:O:49:GLN:HG3	1.92	0.50
6:h:260:PRO:C	6:h:261:ASN:HD22	2.19	0.50
6:j:191:ASP:OD1	6:j:191:ASP:N	2.42	0.50
3:Q:176:ARG:HD2	3:Q:191:ILE:HD11	1.94	0.50
4:S:36:GLN:NE2	6:e:685:PHE:HB2	2.23	0.50
4:V:36:GLN:NE2	6:h:685:PHE:HB2	2.23	0.49
3:M:176:ARG:HD2	3:M:191:ILE:HD11	1.94	0.49
6:h:191:ASP:OD1	6:h:191:ASP:N	2.42	0.49
6:j:212:ASP:OD1	6:j:215:PRO:HD2	2.11	0.49
2:K:429:ASN:HB3	2:K:431:LEU:H	1.76	0.49
6:i:212:ASP:OD1	6:i:215:PRO:HD2	2.11	0.49
1:E:10:ILE:CG1	3:N:224:LEU:HD23	2.41	0.49
1:D:253:MET:HG3	2:J:149:HIS:HB2	1.94	0.49
1:E:253:MET:HG3	2:K:149:HIS:HB2	1.93	0.49
2:H:1000:CYS:O	2:H:1001:ASN:CB	2.60	0.49
2:I:1000:CYS:O	2:I:1001:ASN:CB	2.60	0.49
3:N:176:ARG:HD2	3:N:191:ILE:HD11	1.94	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
1:A:253:MET:HG3	2:G:149:HIS:HB2	1.94	0.49
3:M:49:GLN:HG3	3:O:62:LYS:HD3	1.93	0.49
6:h:212:ASP:OD1	6:h:215:PRO:HD2	2.11	0.49
1:A:10:ILE:CG1	3:Q:224:LEU:HD23	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:MET:HG3	2:L:149:HIS:HB2	1.94	0.49
2:L:429:ASN:HB3	2:L:431:LEU:H	1.76	0.49
3:O:176:ARG:HD2	3:O:191:ILE:HD11	1.94	0.49
1:C:253:MET:HG3	2:I:149:HIS:HB2	1.94	0.49
1:B:253:MET:HG3	2:H:149:HIS:HB2	1.94	0.49
3:P:176:ARG:HD2	3:P:191:ILE:HD11	1.94	0.48
3:R:176:ARG:HD2	3:R:191:ILE:HD11	1.94	0.48
6:j:276:PRO:HA	6:j:280:ASP:HB2	1.96	0.48
2:H:875:ASP:N	2:H:875:ASP:OD1	2.47	0.48
2:J:875:ASP:OD1	2:J:875:ASP:N	2.47	0.48
6:g:276:PRO:HA	6:g:280:ASP:HB2	1.96	0.48
6:e:276:PRO:HA	6:e:280:ASP:HB2	1.96	0.48
6:f:276:PRO:HA	6:f:280:ASP:HB2	1.96	0.48
6:g:224:THR:CG2	6:g:225:LYS:N	2.77	0.48
4:V:106:GLY:O	6:h:680:PHE:N	2.41	0.48
4:W:36:GLN:NE2	6:i:685:PHE:HB2	2.22	0.48
6:f:224:THR:CG2	6:f:225:LYS:N	2.77	0.48
1:B:10:ILE:CG1	3:R:224:LEU:HD23	2.42	0.48
6:i:172:ASP:N	6:i:172:ASP:OD1	2.40	0.48
2:L:312:PRO:O	2:L:350:SER:HB3	2.14	0.48
5:Z:36:VAL:HG22	5:Z:37:ASP:N	2.29	0.48
6:i:276:PRO:HA	6:i:280:ASP:HB2	1.96	0.48
4:X:36:GLN:NE2	6:j:685:PHE:HB2	2.24	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:I:312:PRO:O	2:I:350:SER:HB3	2.14	0.47
6:h:224:THR:CG2	6:h:225:LYS:N	2.77	0.47
3:Q:40:GLN:HG2	3:R:131:ASP:OD2	2.14	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:d:36:VAL:HG22	5:d:37:ASP:N	2.29	0.47
6:j:224:THR:CG2	6:j:225:LYS:N	2.77	0.47
3:N:131:ASP:OD2	3:O:40:GLN:HG2	2.14	0.47
5:c:36:VAL:HG22	5:c:37:ASP:N	2.29	0.47
6:e:224:THR:CG2	6:e:225:LYS:N	2.77	0.47
1:C:10:ILE:CG1	3:M:224:LEU:HD23	2.42	0.47
3:M:131:ASP:OD2	3:R:40:GLN:HG2	2.14	0.47
6:e:189:LEU:O	6:e:190:GLN:HB2	2.15	0.47
7:l:7:LYS:HE3	7:m:117:ASP:O	2.15	0.47
1:D:397:PRO:HB2	1:D:399:THR:HG22	1.97	0.47
2:J:795:TRP:HE3	2:J:795:TRP:O	1.98	0.47

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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	0.47
1:E:397:PRO:HB2	1:E:399:THR:HG22	1.97	0.47
7:l:62:ARG:HH22	7:l:70:GLU:HB2	1.80	0.47
2:J:312:PRO:O	2:J:350:SER:HB3	2.14	0.47
3:N:40:GLN:HG2	3:P:131:ASP:OD2	2.14	0.47
6:f:189:LEU:O	6:f:190:GLN:HB2	2.15	0.47
7:m:62:ARG:HH22	7:m:70:GLU:HB2	1.80	0.47
1:B:409:PRO:HG2	6:f:547:GLU:OE1	2.15	0.46
1:D:10:ILE:CG1	3:O:224:LEU:HD23	2.43	0.46
2:G:312:PRO:O	2:G:350:SER:HB3	2.14	0.46
3:P:16:ASP:OD1	3:P:16:ASP:N	2.48	0.46
6:g:189:LEU:O	6:g:190:GLN:HB2	2.15	0.46
2:I:173:GLU:HG3	2:I:795:TRP:CZ3	2.50	0.46
2:J:833:THR:O	2:J:837:TYR:HD2	1.98	0.46
3:O:16:ASP:OD1	3:O:16:ASP:N	2.48	0.46
7:o:7:LYS:HE3	7:p:117:ASP:O	2.15	0.46
1:B:397:PRO:HB2	1:B:399:THR:HG22	1.97	0.46
1:F:409:PRO:HG2	6:j:547:GLU:OE1	2.15	0.46
3:R:16:ASP:OD1	3:R:16:ASP:N	2.49	0.46
5:b:36:VAL:HG22	5:b:37:ASP:N	2.29	0.46
7:k:117:ASP:O	7:p:7:LYS:HE3	2.15	0.46
7:o:33:ILE:CD1	7:p:111:LEU:HD12	2.44	0.46
1:C:397:PRO:HB2	1:C:399:THR:HG22	1.97	0.46
2:L:833:THR:O	2:L:837:TYR:HD2	1.98	0.46
3:M:40:GLN:HG2	3:O:131:ASP:OD2	2.15	0.46
7:k:62:ARG:HH22	7:k:70:GLU:HB2	1.80	0.46
7:m:33:ILE:CD1	7:n:111:LEU:HD12	2.44	0.46
1:B:410:LYS:O	1:B:410:LYS:HG3	2.16	0.46
2:G:833:THR:O	2:G:837:TYR:HD2	1.98	0.46
2:K:875:ASP:OD1	2:K:875:ASP:N	2.47	0.46
2:I:833:THR:O	2:I:837:TYR:HD2	1.98	0.46
6:j:189:LEU:O	6:j:190:GLN:HB2	2.15	0.46
7:n:62:ARG:HH22	7:n:70:GLU:HB2	1.80	0.46
1:A:397:PRO:HB2	1:A:399:THR:HG22	1.97	0.46
1:C:409:PRO:HG2	6:g:547:GLU:OE1	2.15	0.46
7:k:7:LYS:HE3	7:l:117:ASP:O	2.16	0.46
1:C:68:ILE:HG21	2:I:131:ARG:HG2	1.98	0.46
2:H:312:PRO:O	2:H:350:SER:HB3	2.14	0.46
2:H:795:TRP:O	2:H:795:TRP:HE3	1.98	0.46
2:L:795:TRP:HE3	2:L:795:TRP:O	1.98	0.46
7:n:33:ILE:CD1	7:o:111:LEU:HD12	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ILE:HG21	2:J:131:ARG:HG2	1.98	0.46
6:h:189:LEU:O	6:h:190:GLN:HB2	2.15	0.46
6:i:45:ASP:OD1	6:i:45:ASP:N	2.47	0.46
6:j:478:LEU:HD13	6:j:489:TYR:HE1	1.81	0.46
7:m:7:LYS:HE3	7:n:117:ASP:O	2.15	0.46
7:p:62:ARG:HH22	7:p:70:GLU:HB2	1.80	0.46
6:h:212:ASP:HB3	6:h:215:PRO:HG2	1.98	0.46
7:o:62:ARG:HH22	7:o:70:GLU:HB2	1.80	0.46
1:A:68:ILE:HG21	2:G:131:ARG:HG2	1.98	0.45
1:D:59:TYR:CE2	3:O:211:ARG:HG2	2.51	0.45
1:E:409:PRO:HG2	6:i:547:GLU:OE1	2.15	0.45
2:G:795:TRP:HE3	2:G:795:TRP:O	1.98	0.45
2:I:795:TRP:HE3	2:I:795:TRP:O	1.98	0.45
2:K:795:TRP:HE3	2:K:795:TRP:O	1.98	0.45
2:K:833:THR:O	2:K:837:TYR:HD2	1.98	0.45
1:A:409:PRO:HG2	6:e:547:GLU:OE1	2.17	0.45
1:B:68:ILE:HG21	2:H:131:ARG:HG2	1.99	0.45
1:C:410:LYS:HG3	1:C:410:LYS:O	2.16	0.45
1:F:397:PRO:HB2	1:F:399:THR:HG22	1.97	0.45
2:H:833:THR:O	2:H:837:TYR:HD2	1.98	0.45
3:P:40:GLN:HG2	3:Q:131:ASP:OD2	2.15	0.45
6:g:212:ASP:HB3	6:g:215:PRO:HG2	1.98	0.45
1:A:410:LYS:O	1:A:410:LYS:HG3	2.16	0.45
1:F:68:ILE:HG21	2:L:131:ARG:HG2	1.98	0.45
1:C:59:TYR:CE2	3:M:211:ARG:HG2	2.51	0.45
2:J:173:GLU:HG3	2:J:795:TRP:CZ3	2.50	0.45
6:f:129:ASP:OD1	6:f:129:ASP:N	2.49	0.45
1:A:59:TYR:CE2	3:Q:211:ARG:HG2	2.51	0.45
3:M:16:ASP:OD1	3:M:16:ASP:N	2.48	0.45
3:N:16:ASP:OD1	3:N:16:ASP:N	2.49	0.45
6:h:273:VAL:HG13	6:h:278:PHE:CE2	2.52	0.45
4:W:106:GLY:O	6:i:680:PHE:N	2.41	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
7:n:62:ARG:NH2	7:n:70:GLU:HB2	2.32	0.45
7:o:68:ASP:OD1	7:o:70:GLU:HG2	2.17	0.45
2:K:312:PRO:O	2:K:350:SER:HB3	2.14	0.45
6:i:212:ASP:HB3	6:i:215:PRO:HG2	1.98	0.45
7:o:62:ARG:NH2	7:o:70:GLU:HB2	2.32	0.45
6:i:273:VAL:HG13	6:i:278:PHE:CE2	2.52	0.45
7:p:62:ARG:NH2	7:p:70:GLU:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:TYR:CE2	3:N:211:ARG:HG2	2.51	0.45
2:G:794:SER:O	2:G:795:TRP:CE2	2.70	0.45
2:I:794:SER:O	2:I:795:TRP:CE2	2.70	0.45
6:e:478:LEU:HD13	6:e:489:TYR:HE1	1.81	0.45
1:E:68:ILE:HG21	2:K:131:ARG:HG2	1.99	0.45
1:E:410:LYS:HG3	1:E:410:LYS:O	2.16	0.45
2:J:794:SER:O	2:J:795:TRP:CE2	2.70	0.45
2:L:794:SER:O	2:L:795:TRP:CE2	2.70	0.45
3:Q:16:ASP:OD1	3:Q:16:ASP:N	2.48	0.45
6:g:273:VAL:HG13	6:g:278:PHE:CE2	2.52	0.45
7:k:68:ASP:OD1	7:k:70:GLU:HG2	2.17	0.45
1:D:93:ILE:O	2:J:828:LYS:NZ	2.50	0.44
1:D:410:LYS:O	1:D:410:LYS:HG3	2.16	0.44
1:F:59:TYR:CE2	3:P:211:ARG:HG2	2.52	0.44
6:f:478:LEU:HD13	6:f:489:TYR:HE1	1.81	0.44
6:g:478:LEU:HD13	6:g:489:TYR:HE1	1.81	0.44
6:j:273:VAL:HG13	6:j:278:PHE:CE2	2.52	0.44
7:n:7:LYS:HE3	7:o:117:ASP:O	2.16	0.44
1:B:59:TYR:CE2	3:R:211:ARG:HG2	2.51	0.44
1:D:409:PRO:HG2	6:h:547:GLU:OE1	2.16	0.44
2:K:516:ASP:OD1	2:K:516:ASP:N	2.46	0.44
2:K:794:SER:O	2:K:795:TRP:CE2	2.70	0.44
3:Q:88:ASP:OD2	3:Q:92:ASN:ND2	2.51	0.44
6:e:212:ASP:HB3	6:e:215:PRO:HG2	1.98	0.44
6:f:212:ASP:HB3	6:f:215:PRO:HG2	1.98	0.44
6:f:273:VAL:HG13	6:f:278:PHE:CE2	2.52	0.44
7:l:62:ARG:NH2	7:l:70:GLU:HB2	2.32	0.44
7:l:68:ASP:OD1	7:l:70:GLU:HG2	2.17	0.44
7:k:62:ARG:NH2	7:k:70:GLU:HB2	2.32	0.44
7:m:62:ARG:NH2	7:m:70:GLU:HB2	2.32	0.44
7:p:68:ASP:OD1	7:p:70:GLU:HG2	2.17	0.44
1:C:99:THR:HG23	1:C:189:ASN:CG	2.43	0.44
6:e:273:VAL:HG13	6:e:278:PHE:CE2	2.52	0.44
1:B:99:THR:HG23	1:B:189:ASN:CG	2.43	0.44
1:F:409:PRO:HD2	6:j:547:GLU:CD	2.43	0.44
1:F:410:LYS:O	1:F:410:LYS:HG3	2.16	0.44
2:H:794:SER:C	2:H:795:TRP:CG	2.96	0.44
2:I:173:GLU:CB	2:I:795:TRP:CZ3	3.01	0.44
2:K:173:GLU:HG3	2:K:795:TRP:CZ3	2.50	0.44
2:L:173:GLU:HG3	2:L:795:TRP:CZ3	2.50	0.44
3:P:88:ASP:OD2	3:P:92:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:175:TYR:HE1	4:W:6:LYS:HE2	1.77	0.44
4:S:106:GLY:O	6:e:680:PHE:N	2.41	0.44
6:e:83:LEU:CD2	6:e:83:LEU:C	2.90	0.44
1:B:99:THR:O	1:B:99:THR:HG22	2.18	0.44
3:R:88:ASP:OD2	3:R:92:ASN:ND2	2.51	0.44
1:E:409:PRO:HD2	6:i:547:GLU:CD	2.43	0.44
2:J:173:GLU:CB	2:J:795:TRP:CZ3	3.01	0.44
2:K:173:GLU:CB	2:K:795:TRP:CZ3	3.01	0.44
2:L:173:GLU:CB	2:L:795:TRP:CZ3	3.01	0.44
3:O:88:ASP:OD2	3:O:92:ASN:ND2	2.51	0.44
5:Y:11:HIS:HA	7:k:39:GLY:O	2.18	0.44
6:j:83:LEU:CD2	6:j:83:LEU:C	2.90	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:E:254:ASP:OD1	2:K:150:LEU:CD2	2.66	0.44
2:G:794:SER:C	2:G:795:TRP:CG	2.96	0.44
2:I:89:ASP:OD1	2:I:89:ASP:N	2.50	0.44
3:M:88:ASP:OD2	3:M:92:ASN:ND2	2.51	0.44
3:M:175:TYR:CZ	4:T:6:LYS:HG2	2.53	0.44
3:N:175:TYR:CZ	4:V:6:LYS:HG2	2.53	0.44
3:R:175:TYR:CZ	4:S:6:LYS:HG2	2.53	0.44
2:H:173:GLU:CB	2:H:795:TRP:CZ3	3.01	0.44
2:I:806:THR:O	2:I:807:LYS:HB2	2.18	0.44
6:i:478:LEU:HD13	6:i:489:TYR:HE1	1.81	0.44
1:A:99:THR:HG23	1:A:189:ASN:CG	2.43	0.43
1:A:410:LYS:CE	6:f:3:THR:O	2.66	0.43
1:B:410:LYS:CE	6:g:3:THR:O	2.66	0.43
2:G:875:ASP:OD1	2:G:875:ASP:N	2.47	0.43
2:L:794:SER:C	2:L:795:TRP:CG	2.96	0.43
3:P:175:TYR:CZ	4:W:6:LYS:HG2	2.53	0.43
7:n:68:ASP:OD1	7:n:70:GLU:HG2	2.17	0.43
1:C:99:THR:HG22	1:C:99:THR:O	2.18	0.43
1:D:99:THR:HG23	1:D:189:ASN:CG	2.43	0.43
1:B:254:ASP:OD1	2:H:150:LEU:CD2	2.66	0.43
1:E:99:THR:O	1:E:99:THR:HG22	2.18	0.43
2:G:806:THR:O	2:G:807:LYS:HB2	2.19	0.43
2:H:794:SER:O	2:H:795:TRP:CE2	2.70	0.43
2:J:806:THR:O	2:J:807:LYS:HB2	2.18	0.43
3:N:88:ASP:OD2	3:N:92:ASN:ND2	2.51	0.43
1:A:99:THR:O	1:A:99:THR:HG22	2.18	0.43
1:F:99:THR:O	1:F:99:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:173:GLU:CB	2:G:795:TRP:CZ3	3.01	0.43
2:I:794:SER:C	2:I:795:TRP:CG	2.96	0.43
2:K:806:THR:O	2:K:807:LYS:HB2	2.19	0.43
3:O:175:TYR:CZ	4:U:6:LYS:HG2	2.54	0.43
1:A:254:ASP:OD1	2:G:150:LEU:CD2	2.67	0.43
1:F:254:ASP:OD1	2:L:150:LEU:CD2	2.67	0.43
7:k:121:ASP:OD1	7:k:121:ASP:N	2.49	0.43
2:G:173:GLU:HG3	2:G:795:TRP:CZ3	2.50	0.43
2:L:806:THR:O	2:L:807:LYS:HB2	2.19	0.43
7:l:32:GLU:OE2	7:l:54:LYS:NZ	2.49	0.43
2:J:794:SER:C	2:J:795:TRP:CG	2.96	0.43
5:b:11:HIS:HA	7:n:39:GLY:O	2.18	0.43
1:A:409:PRO:HD2	6:e:547:GLU:CD	2.44	0.43
3:P:168:GLN:NE2	3:Q:107:GLU:HG3	2.34	0.43
1:B:409:PRO:HD2	6:f:547:GLU:CD	2.43	0.43
1:C:409:PRO:HD2	6:g:547:GLU:CD	2.43	0.43
1:E:98:PRO:CB	1:E:103:ASP:HB3	2.49	0.43
1:F:99:THR:HG23	1:F:189:ASN:CG	2.43	0.43
2:H:806:THR:O	2:H:807:LYS:HB2	2.19	0.43
6:j:411:GLU:HA	6:j:411:GLU:OE1	2.19	0.43
1:E:99:THR:HG23	1:E:189:ASN:CG	2.43	0.43
3:N:168:GLN:NE2	3:P:107:GLU:HG3	2.34	0.43
1:D:316:ASN:ND2	1:D:318:TRP:HE1	2.16	0.42
2:I:875:ASP:OD1	2:I:875:ASP:N	2.47	0.42
2:K:794:SER:C	2:K:795:TRP:CG	2.96	0.42
6:h:411:GLU:OE1	6:h:411:GLU:HA	2.19	0.42
6:i:411:GLU:OE1	6:i:411:GLU:HA	2.19	0.42
1:C:254:ASP:OD1	2:I:150:LEU:CD2	2.67	0.42
1:D:409:PRO:HD2	6:h:547:GLU:CD	2.44	0.42
1:F:98:PRO:CB	1:F:103:ASP:HB3	2.49	0.42
1:E:316:ASN:ND2	1:E:318:TRP:HE1	2.16	0.42
1:E:509:ARG:HH12	2:K:139:HIS:CD2	2.37	0.42
3:Q:175:TYR:CZ	4:X:6:LYS:HG2	2.54	0.42
1:F:10:ILE:HA	1:F:11:PRO:HD3	1.87	0.42
2:K:89:ASP:OD1	2:K:89:ASP:N	2.50	0.42
4:X:106:GLY:O	6:j:680:PHE:N	2.41	0.42
6:e:411:GLU:HA	6:e:411:GLU:OE1	2.19	0.42
1:A:98:PRO:CB	1:A:103:ASP:HB3	2.49	0.42
1:B:98:PRO:CB	1:B:103:ASP:HB3	2.49	0.42
1:B:219:GLU:HB2	1:B:347:LEU:HD21	2.02	0.42
1:D:254:ASP:OD1	2:J:150:LEU:CD2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:LYS:CE	6:e:3:THR:O	2.66	0.42
1:F:509:ARG:HH12	2:L:139:HIS:CD2	2.37	0.42
6:g:411:GLU:HA	6:g:411:GLU:OE1	2.19	0.42
1:D:99:THR:HG22	1:D:99:THR:O	2.18	0.42
1:B:509:ARG:HH12	2:H:139:HIS:CD2	2.37	0.42
1:C:219:GLU:HB2	1:C:347:LEU:HD21	2.02	0.42
1:D:219:GLU:HB2	1:D:347:LEU:HD21	2.02	0.42
1:D:346:ASN:HD22	1:D:346:ASN:N	2.18	0.42
3:M:107:GLU:HG3	3:R:168:GLN:NE2	2.34	0.42
3:M:168:GLN:NE2	3:O:107:GLU:HG3	2.34	0.42
3:Q:168:GLN:NE2	3:R:107:GLU:HG3	2.35	0.42
3:R:2:SER:O	3:R:2:SER:OG	2.37	0.42
5:d:11:HIS:HA	7:p:39:GLY:O	2.20	0.42
1:C:316:ASN:ND2	1:C:318:TRP:HE1	2.16	0.42
4:T:4:LYS:HG2	4:T:4:LYS:O	2.20	0.42
1:A:408:PRO:HA	1:A:409:PRO:HD3	1.95	0.42
1:D:98:PRO:CB	1:D:103:ASP:HB3	2.49	0.42
1:E:219:GLU:HB2	1:E:347:LEU:HD21	2.02	0.42
2:G:787:SER:C	2:G:788:LYS:HG3	2.45	0.42
2:K:519:PHE:HB3	2:K:527:TYR:CD2	2.55	0.42
2:K:787:SER:C	2:K:788:LYS:HG3	2.45	0.42
4:U:4:LYS:O	4:U:4:LYS:HG2	2.20	0.42
6:g:172:ASP:OD1	6:g:172:ASP:N	2.40	0.42
1:E:10:ILE:HA	1:E:11:PRO:HD3	1.87	0.42
2:H:519:PHE:HB3	2:H:527:TYR:CD2	2.55	0.42
2:L:787:SER:C	2:L:788:LYS:HG3	2.45	0.42
3:N:2:SER:O	3:N:2:SER:OG	2.36	0.42
5:a:11:HIS:HA	7:m:39:GLY:O	2.20	0.42
1:A:132:ASN:O	1:A:133:GLN:C	2.62	0.41
1:A:219:GLU:HB2	1:A:347:LEU:HD21	2.02	0.41
1:A:509:ARG:HH12	2:G:139:HIS:CD2	2.38	0.41
1:B:346:ASN:HD22	1:B:346:ASN:N	2.18	0.41
1:C:98:PRO:CB	1:C:103:ASP:HB3	2.49	0.41
4:W:4:LYS:O	4:W:4:LYS:HG2	2.20	0.41
6:h:83:LEU:CD2	6:h:83:LEU:C	2.91	0.41
1:B:93:ILE:O	2:H:828:LYS:NZ	2.51	0.41
1:C:93:ILE:O	2:I:828:LYS:NZ	2.50	0.41
1:E:93:ILE:O	2:K:828:LYS:NZ	2.51	0.41
3:M:172:MET:CE	4:T:120:ASN:O	2.65	0.41
3:N:107:GLU:HG3	3:O:168:GLN:NE2	2.35	0.41
6:f:255:HIS:HD2	6:f:256:LEU:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:657:THR:OG1	6:f:658:ALA:N	2.54	0.41
1:A:159:TYR:CZ	2:G:908:HIS:NE2	2.87	0.41
1:F:132:ASN:O	1:F:133:GLN:C	2.62	0.41
2:G:311:LEU:O	2:G:350:SER:O	2.39	0.41
2:L:519:PHE:HB3	2:L:527:TYR:CD2	2.55	0.41
3:N:175:TYR:HE1	4:V:6:LYS:HE2	1.77	0.41
4:X:4:LYS:O	4:X:4:LYS:HG2	2.20	0.41
5:c:3:THR:HG22	5:c:4:TYR:N	2.32	0.41
2:H:311:LEU:O	2:H:350:SER:O	2.39	0.41
2:H:787:SER:C	2:H:788:LYS:HG3	2.45	0.41
2:I:584:GLU:HA	2:I:585:PRO:HD3	1.95	0.41
3:P:15:LYS:HE3	3:P:21:ASP:HB3	2.03	0.41
3:Q:175:TYR:HE1	4:X:6:LYS:HE2	1.78	0.41
6:j:205:ASN:OD1	6:j:207:GLY:N	2.46	0.41
6:j:472:LYS:HB2	6:j:472:LYS:HE3	1.66	0.41
1:C:348:ASN:N	1:C:348:ASN:HD22	2.19	0.41
1:C:467:ASP:O	1:C:468:VAL:C	2.63	0.41
1:D:410:LYS:CE	6:i:3:THR:O	2.66	0.41
1:E:346:ASN:HD22	1:E:346:ASN:N	2.18	0.41
2:H:173:GLU:HG3	2:H:795:TRP:CZ3	2.50	0.41
4:S:4:LYS:O	4:S:4:LYS:HG2	2.20	0.41
5:Z:11:HIS:HA	7:l:39:GLY:O	2.21	0.41
6:f:411:GLU:OE1	6:f:411:GLU:HA	2.19	0.41
6:g:255:HIS:HD2	6:g:256:LEU:N	2.19	0.41
2:I:311:LEU:O	2:I:350:SER:O	2.39	0.41
3:O:15:LYS:HE3	3:O:21:ASP:HB3	2.03	0.41
4:T:106:GLY:O	6:f:680:PHE:N	2.41	0.41
7:k:33:ILE:CD1	7:l:111:LEU:HD12	2.43	0.41
1:A:93:ILE:O	2:G:828:LYS:NZ	2.50	0.41
1:B:467:ASP:O	1:B:468:VAL:C	2.63	0.41
1:C:159:TYR:CZ	2:I:908:HIS:NE2	2.88	0.41
2:I:787:SER:C	2:I:788:LYS:HG3	2.45	0.41
2:J:519:PHE:HB3	2:J:527:TYR:CD2	2.55	0.41
3:N:15:LYS:HE3	3:N:21:ASP:HB3	2.03	0.41
4:V:4:LYS:O	4:V:4:LYS:HG2	2.20	0.41
1:A:348:ASN:HA	1:A:349:PRO:HD2	1.93	0.41
1:C:252:THR:OG1	1:C:253:MET:N	2.54	0.41
1:D:348:ASN:N	1:D:348:ASN:HD22	2.19	0.41
1:D:509:ARG:HH12	2:J:139:HIS:CD2	2.38	0.41
1:E:348:ASN:N	1:E:348:ASN:HD22	2.19	0.41
1:F:316:ASN:ND2	1:F:318:TRP:HE1	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:89:ASP:OD1	2:J:89:ASP:N	2.50	0.41
2:J:311:LEU:O	2:J:350:SER:O	2.39	0.41
2:J:787:SER:C	2:J:788:LYS:HG3	2.45	0.41
2:L:311:LEU:O	2:L:350:SER:O	2.39	0.41
3:Q:15:LYS:HE3	3:Q:21:ASP:HB3	2.03	0.41
5:a:3:THR:HG22	5:a:4:TYR:N	2.32	0.41
6:j:657:THR:OG1	6:j:658:ALA:N	2.54	0.41
7:n:32:GLU:OE2	7:n:54:LYS:NZ	2.49	0.41
1:A:467:ASP:O	1:A:468:VAL:C	2.63	0.41
1:C:132:ASN:O	1:C:133:GLN:C	2.62	0.41
1:F:219:GLU:HB2	1:F:347:LEU:HD21	2.02	0.41
2:I:519:PHE:HB3	2:I:527:TYR:CD2	2.55	0.41
2:I:787:SER:O	2:I:788:LYS:CG	2.69	0.41
2:J:787:SER:O	2:J:788:LYS:CG	2.69	0.41
3:M:15:LYS:HE3	3:M:21:ASP:HB3	2.03	0.41
3:P:98:LYS:HE2	3:P:98:LYS:HB3	1.80	0.41
3:R:175:TYR:HE1	4:S:6:LYS:HE2	1.78	0.41
4:U:106:GLY:O	6:g:680:PHE:N	2.41	0.41
5:b:3:THR:HG22	5:b: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: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:h:437:LEU:O	6:h:438:THR:C	2.63	0.41
7:k:70:GLU:OE1	7:k:70:GLU:HA	2.21	0.41
7:m:32:GLU:OE2	7:m:54:LYS:NZ	2.49	0.41
1:A:347:LEU:C	1:A:348:ASN:HD22	2.29	0.41
2:G:308:LYS:HA	2:G:309:PRO:HD3	1.88	0.41
5:Z:32:SER:HB2	5:a:123:ASP:CG	2.46	0.41
5:c:32:SER:HB2	5:d:123:ASP:CG	2.46	0.41
6:g:472:LYS:HE3	6:g:472:LYS:HB2	1.66	0.41
6:h:657:THR:OG1	6:h:658:ALA:N	2.54	0.41
1:A:10:ILE:HA	1:A:11:PRO:HD3	1.87	0.40
1:B:348:ASN:N	1:B:348:ASN:HD22	2.19	0.40
1:C:346:ASN:HD22	1:C:346:ASN:N	2.18	0.40
1:C:509:ARG:HH12	2:I:139:HIS:CD2	2.38	0.40
2:G:519:PHE:HB3	2:G:527:TYR:CD2	2.55	0.40
2:K:311:LEU:O	2:K:350:SER:O	2.39	0.40
3:R:172:MET:CE	4:S:120:ASN:O	2.65	0.40
6:f:437:LEU:O	6:f:438:THR:C	2.63	0.40
1:F:347:LEU:C	1:F:348:ASN:HD22	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:464:ASP:OD1	1:F:464:ASP:N	2.50	0.40
2:G:200:THR:OG1	2:G:201:VAL:N	2.55	0.40
3:M:10:ARG:NH1	3:M:27:GLU:OE1	2.55	0.40
3:N:62:LYS:HD2	3:O:49:GLN:HG3	2.03	0.40
3:R:10:ARG:NH1	3:R:27:GLU:OE1	2.55	0.40
1:B:347:LEU:C	1:B:348:ASN:HD22	2.29	0.40
3:R:15:LYS:HE3	3:R:21:ASP:HB3	2.03	0.40
5:Z:3:THR:HG22	5:Z:4:TYR:N	2.32	0.40
5:d:36:VAL:C	5:d:37:ASP:OD2	2.65	0.40
6:e:437:LEU:O	6:e:438:THR:C	2.63	0.40
6:g:83:LEU:CD2	6:g:83:LEU:C	2.90	0.40
1:A:346:ASN:HD22	1:A:346:ASN:N	2.18	0.40
1:D:132:ASN:O	1:D:133:GLN:C	2.62	0.40
1:D:343:LEU:HA	1:D:344:PRO:HD2	1.86	0.40
1:F:348:ASN:HD22	1:F:348:ASN:N	2.19	0.40
2:J:200:THR:OG1	2:J:201:VAL:N	2.55	0.40
2:K:787:SER:O	2:K:788:LYS:CG	2.69	0.40
3:N:10:ARG:NH1	3:N:27:GLU:OE1	2.54	0.40
3:O:172:MET:CE	4:U:120:ASN:O	2.66	0.40
5:Z:6:PRO:O	7:m:49:MET:HE1	2.22	0.40
6:e:205:ASN:OD1	6:e:207:GLY:N	2.46	0.40
6:g:657:THR:OG1	6:g:658:ALA:N	2.54	0.40
6:i:253:ILE:HD11	6:i:478:LEU:CD2	2.51	0.40
6:i:255:HIS:C	6:i:256:LEU:HD23	2.47	0.40
7:p:70:GLU:HA	7:p:70:GLU:OE1	2.21	0.40
1:A:252:THR:OG1	1:A:253:MET:N	2.54	0.40
1:B:132:ASN:O	1:B:133:GLN:C	2.62	0.40
1:C:10:ILE:HA	1:C:11:PRO:HD3	1.87	0.40
1:D:148:ASN:OD1	1:D:148:ASN:N	2.54	0.40
2:H:787:SER:O	2:H:788:LYS:CG	2.69	0.40
6:i:420:ASN:O	6:i:421:PHE:C	2.64	0.40
6:j:255:HIS:C	6:j:256:LEU:HD23	2.47	0.40
7:o:70:GLU:OE1	7:o:70:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	969 (96%)	37 (4%)	3 (0%)	36	60
2	H	1009/1050 (96%)	969 (96%)	37 (4%)	3 (0%)	36	60
2	I	1009/1050 (96%)	969 (96%)	37 (4%)	3 (0%)	36	60
2	J	1009/1050 (96%)	969 (96%)	37 (4%)	3 (0%)	36	60
2	K	1009/1050 (96%)	969 (96%)	37 (4%)	3 (0%)	36	60
2	L	1009/1050 (96%)	969 (96%)	37 (4%)	3 (0%)	36	60
3	M	221/228 (97%)	220 (100%)	1 (0%)	0	100	100
3	N	221/228 (97%)	219 (99%)	2 (1%)	0	100	100
3	O	221/228 (97%)	219 (99%)	2 (1%)	0	100	100
3	P	221/228 (97%)	219 (99%)	2 (1%)	0	100	100
3	Q	221/228 (97%)	219 (99%)	2 (1%)	0	100	100
3	R	221/228 (97%)	219 (99%)	2 (1%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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
All	All	17046/19974 (85%)	16591 (97%)	437 (3%)	18 (0%)	49	73

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

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

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	497/842 (59%)	496 (100%)	1 (0%)	87	95
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%)	814 (100%)	0	100	100
2	H	814/955 (85%)	814 (100%)	0	100	100
2	I	814/955 (85%)	814 (100%)	0	100	100
2	J	814/955 (85%)	814 (100%)	0	100	100
2	K	814/955 (85%)	814 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	U	121/125 (97%)	121 (100%)	0	100	100
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
All	All	14646/17892 (82%)	14645 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN

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Mol	Chain	Res	Type
1	A	316	ASN
1	A	346	ASN
1	A	348	ASN
1	A	431	GLN
1	B	288	ASN
1	B	316	ASN
1	B	346	ASN
1	B	348	ASN
1	B	431	GLN
1	C	288	ASN
1	C	316	ASN
1	C	346	ASN
1	C	348	ASN
1	C	431	GLN
1	D	288	ASN
1	D	316	ASN
1	D	346	ASN
1	D	348	ASN
1	D	431	GLN
1	E	316	ASN
1	E	346	ASN
1	E	348	ASN
1	E	431	GLN
1	F	288	ASN
1	F	316	ASN
1	F	346	ASN
1	F	348	ASN
1	F	431	GLN
2	G	114	HIS
2	G	139	HIS
2	G	149	HIS
2	G	172	GLN
2	G	856	HIS
2	G	878	GLN
2	G	886	GLN
2	H	114	HIS
2	H	139	HIS
2	H	149	HIS
2	H	172	GLN
2	H	759	HIS
2	H	856	HIS
2	H	886	GLN

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Mol	Chain	Res	Type
2	I	114	HIS
2	I	149	HIS
2	I	172	GLN
2	I	759	HIS
2	I	856	HIS
2	I	878	GLN
2	I	886	GLN
2	J	114	HIS
2	J	139	HIS
2	J	149	HIS
2	J	172	GLN
2	J	759	HIS
2	J	856	HIS
2	J	886	GLN
2	K	114	HIS
2	K	139	HIS
2	K	149	HIS
2	K	172	GLN
2	K	856	HIS
2	K	878	GLN
2	K	886	GLN
2	L	114	HIS
2	L	139	HIS
2	L	149	HIS
2	L	172	GLN
2	L	856	HIS
2	L	878	GLN
2	L	886	GLN
3	M	46	ASN
3	M	92	ASN
3	N	46	ASN
3	N	92	ASN
3	O	46	ASN
3	O	92	ASN
3	P	46	ASN
3	P	168	GLN
3	Q	46	ASN
3	Q	92	ASN
3	R	46	ASN
3	R	92	ASN
3	R	168	GLN
4	S	36	GLN

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Mol	Chain	Res	Type
4	S	87	HIS
4	S	102	ASN
4	T	36	GLN
4	T	59	ASN
4	T	87	HIS
4	U	36	GLN
4	U	87	HIS
4	V	36	GLN
4	V	87	HIS
4	V	102	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	36	GLN
6	g	245	GLN
6	g	420	ASN
6	g	631	GLN
6	h	36	GLN
6	h	245	GLN
6	h	631	GLN
6	i	245	GLN
6	i	631	GLN
6	j	245	GLN
6	j	631	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

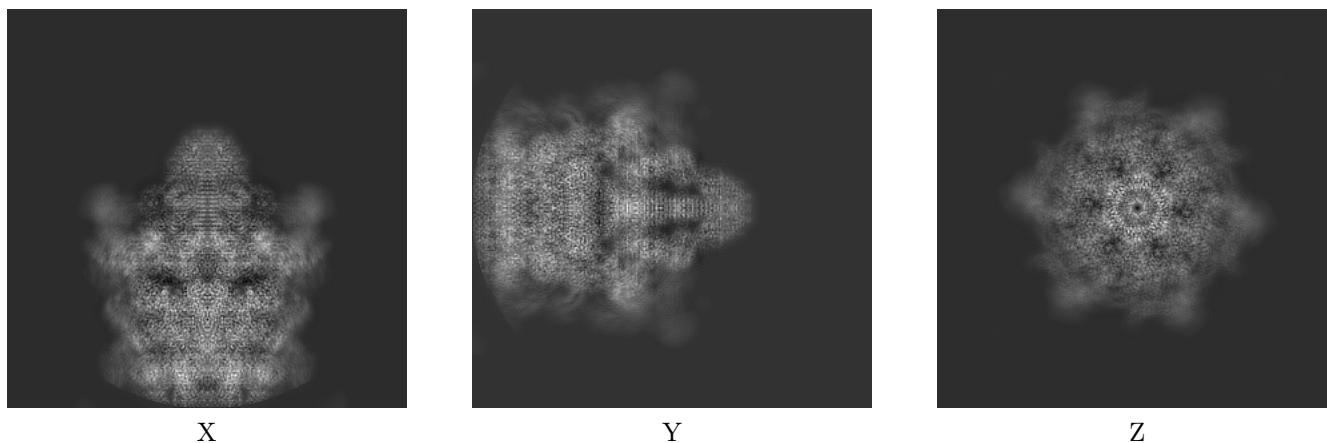
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11743. 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](#)

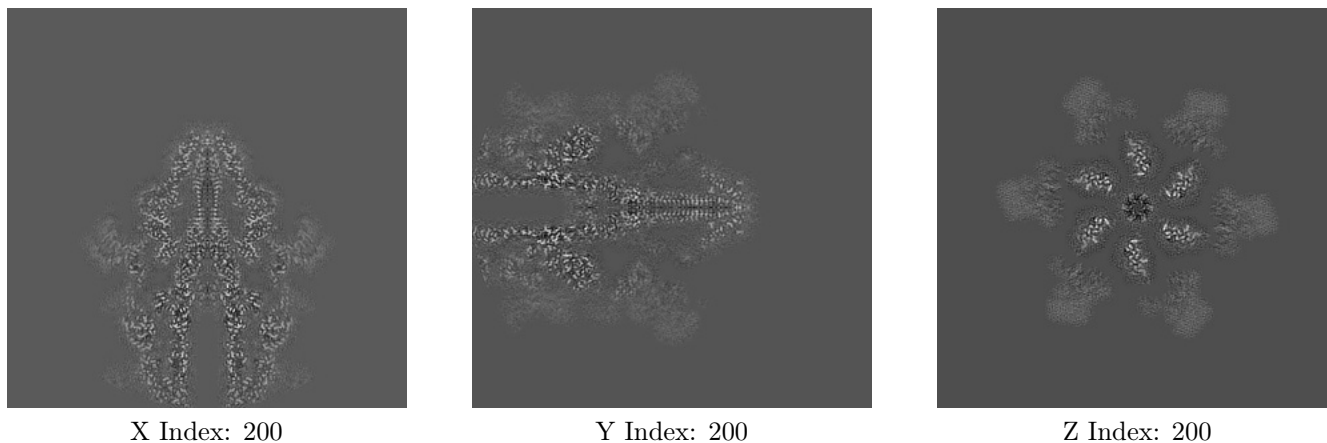
6.1.1 Primary map



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

6.2 Central slices [i](#)

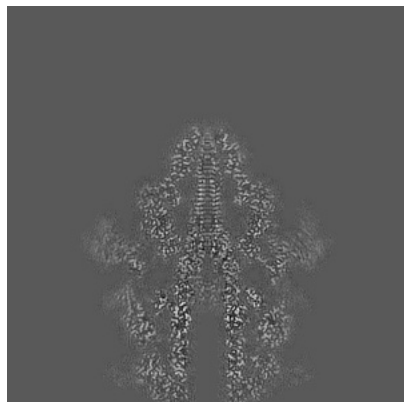
6.2.1 Primary map



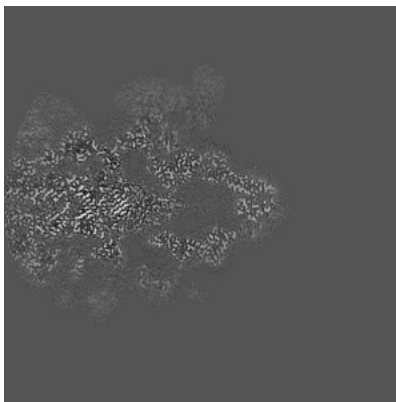
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

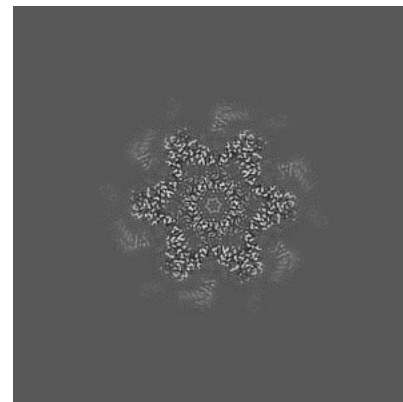
6.3.1 Primary map



X Index: 198



Y Index: 180

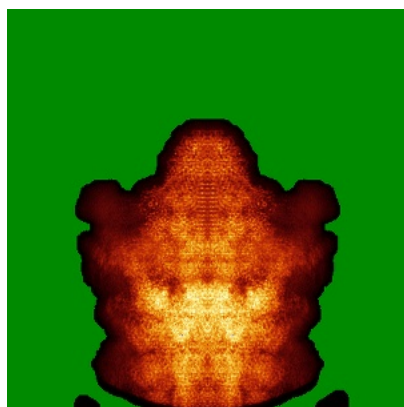


Z Index: 110

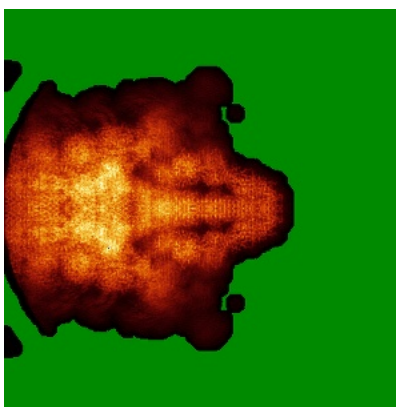
The images above show the largest variance slices of the map in three orthogonal directions.

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

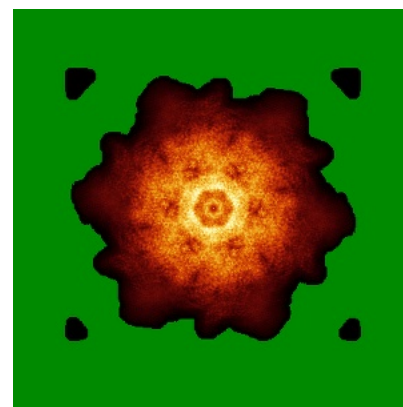
6.4.1 Primary map



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

This section was not generated.

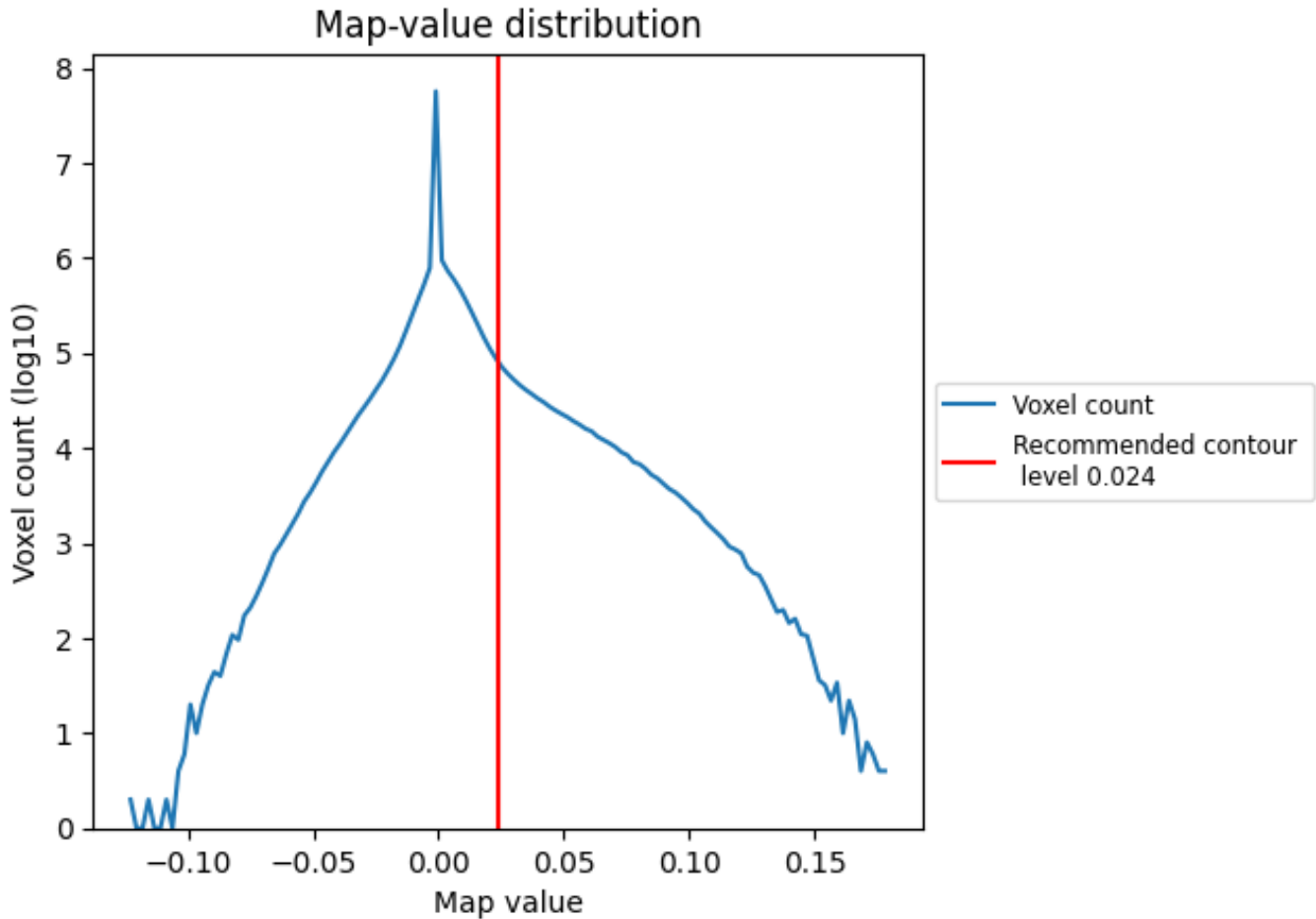
6.6 Mask visualisation

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

7 Map analysis [i](#)

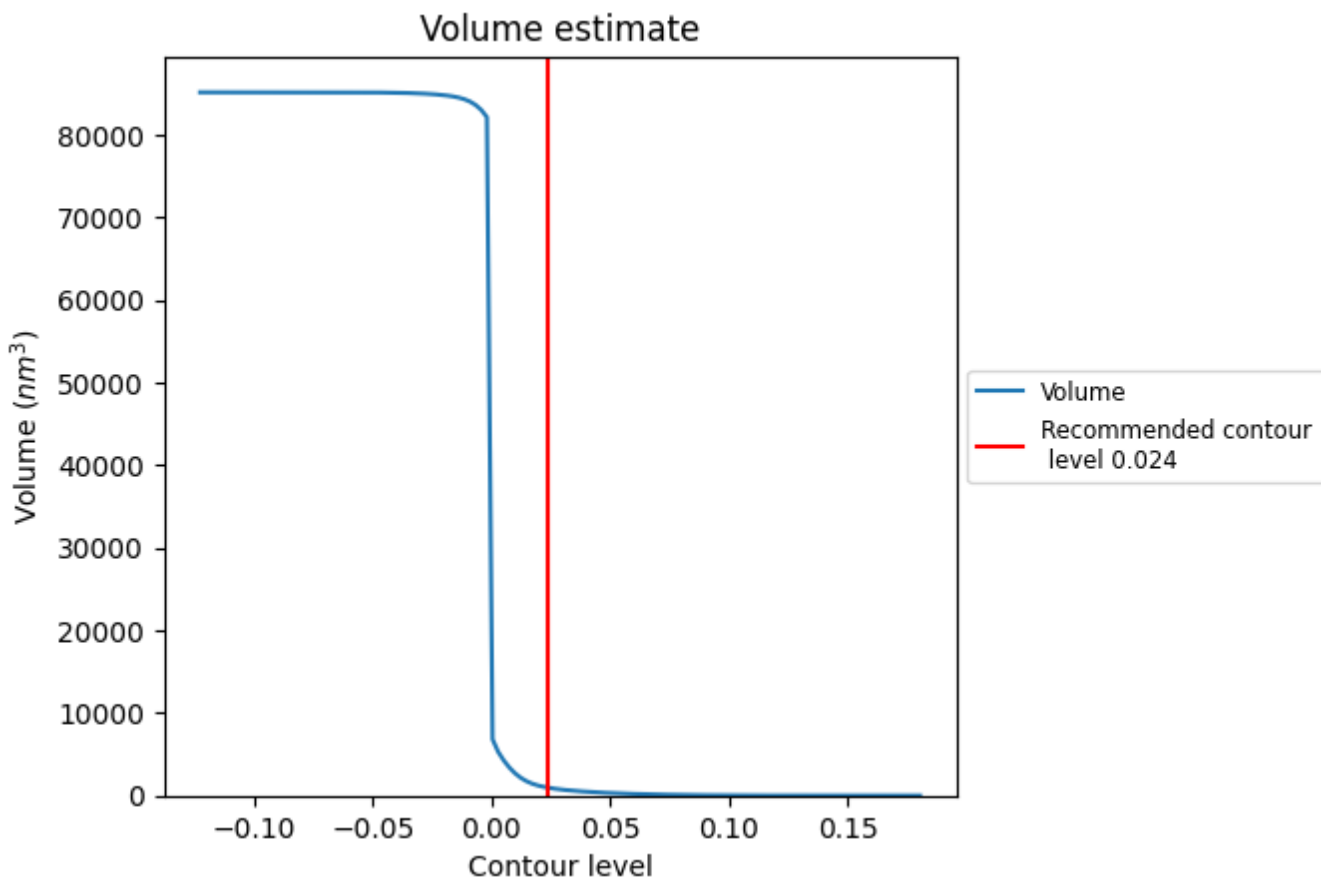
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

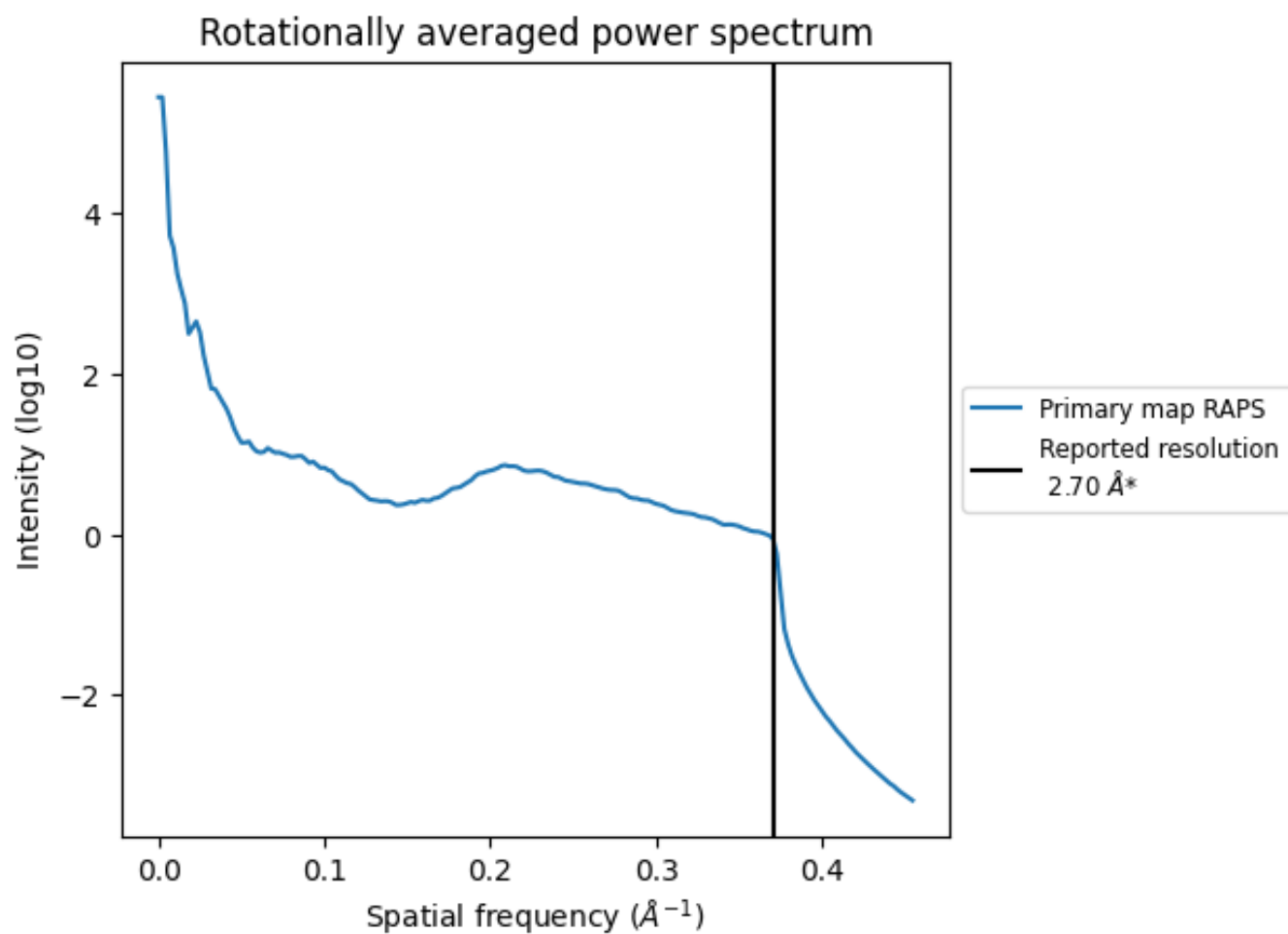
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 941 nm³; this corresponds to an approximate mass of 850 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.370\AA^{-1}

8 Fourier-Shell correlation

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

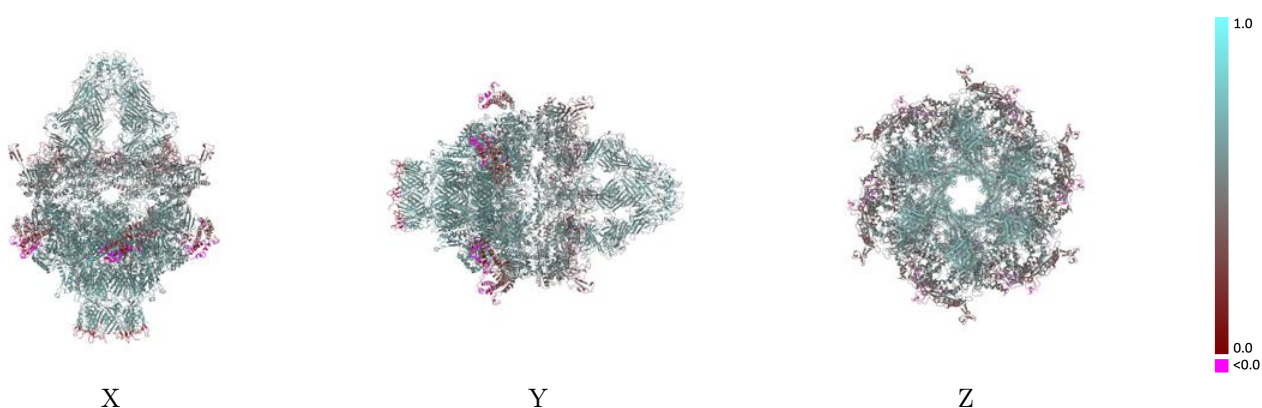
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11743 and PDB model 7AEB. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

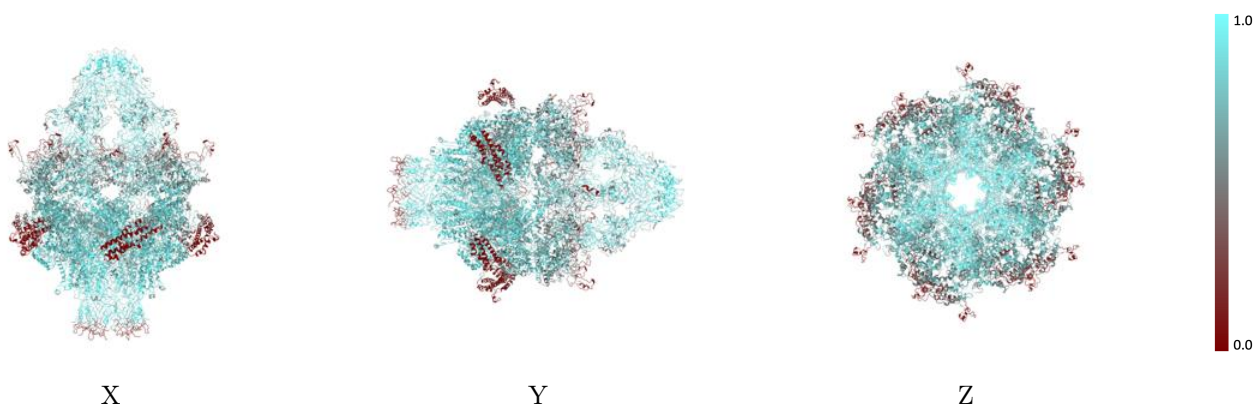
This section was not generated.

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



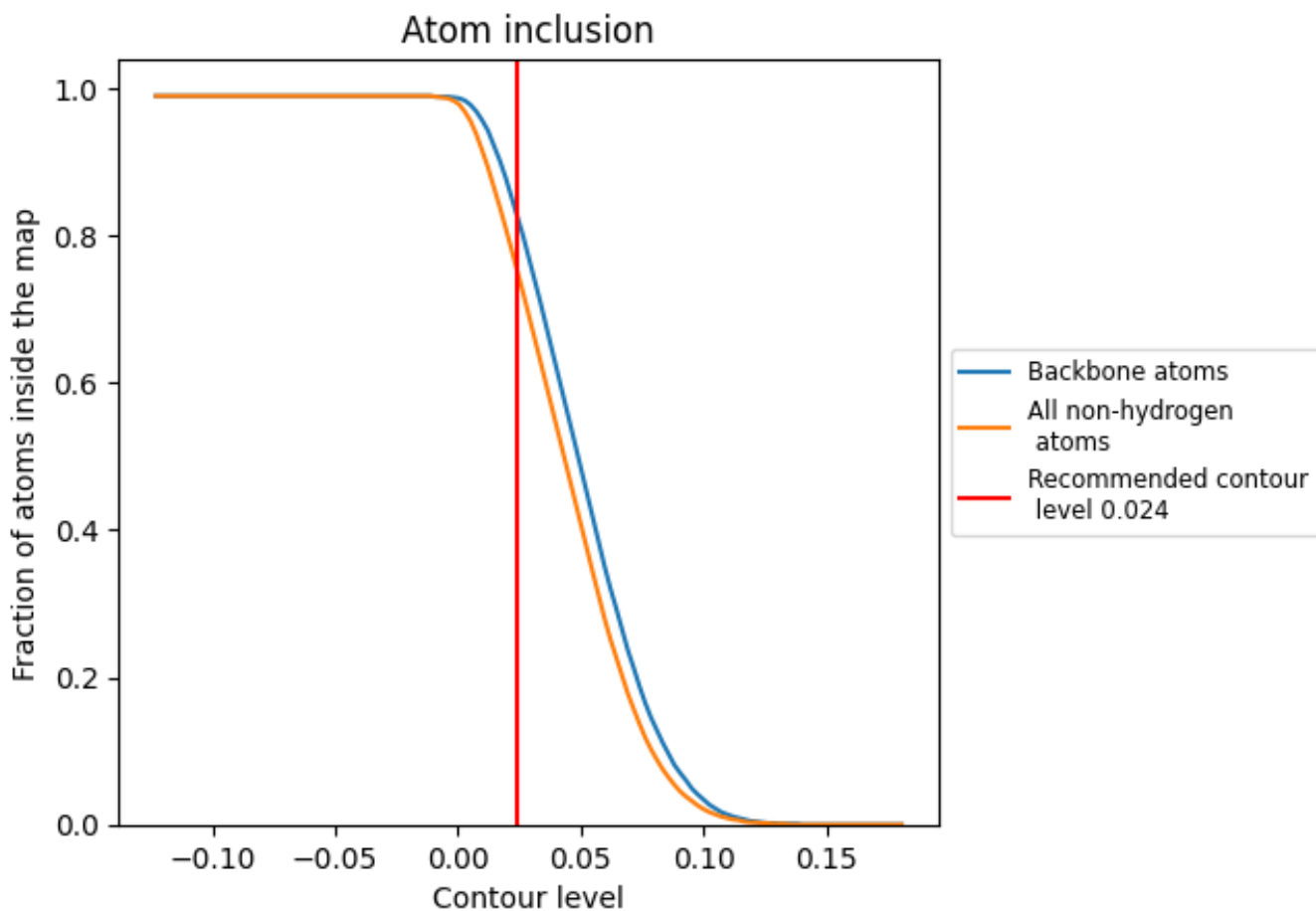
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.024).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7540	 0.5440
A	 0.6980	 0.5270
B	 0.6980	 0.5250
C	 0.6990	 0.5250
D	 0.6980	 0.5250
E	 0.6970	 0.5230
F	 0.6990	 0.5240
G	 0.7750	 0.5470
H	 0.7760	 0.5470
I	 0.7730	 0.5460
J	 0.7750	 0.5470
K	 0.7760	 0.5470
L	 0.7730	 0.5460
M	 0.9290	 0.6560
N	 0.9270	 0.6510
O	 0.9240	 0.6510
P	 0.9300	 0.6560
Q	 0.9250	 0.6520
R	 0.9270	 0.6510
S	 0.8750	 0.6060
T	 0.8700	 0.6030
U	 0.8750	 0.6030
V	 0.8750	 0.6050
W	 0.8700	 0.6020
X	 0.8750	 0.6040
Y	 0.9160	 0.6350
Z	 0.9110	 0.6340
a	 0.9130	 0.6340
b	 0.9150	 0.6340
c	 0.9110	 0.6340
d	 0.9130	 0.6350
e	 0.6620	 0.4970
f	 0.6610	 0.4970
g	 0.6670	 0.4950
h	 0.6620	 0.4970



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Chain	Atom inclusion	Q-score
i	 0.6620	 0.4960
j	 0.6650	 0.4950
k	 0.6670	 0.4860
l	 0.6670	 0.4850
m	 0.6680	 0.4860
n	 0.6670	 0.4860
o	 0.6670	 0.4860
p	 0.6680	 0.4870