



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:43 AM UTC

PDB ID : 8KEE / pdb_00008kee
EMDB ID : EMD-37153
Title : Cyanophage A-1(L) sheath-tube
Authors : Yu, R.C.; Li, Q.; Zhou, C.Z.
Deposited on : 2023-08-11
Resolution : 3.26 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

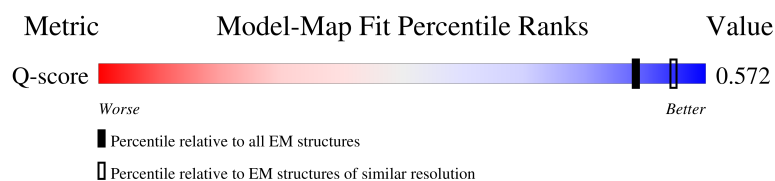
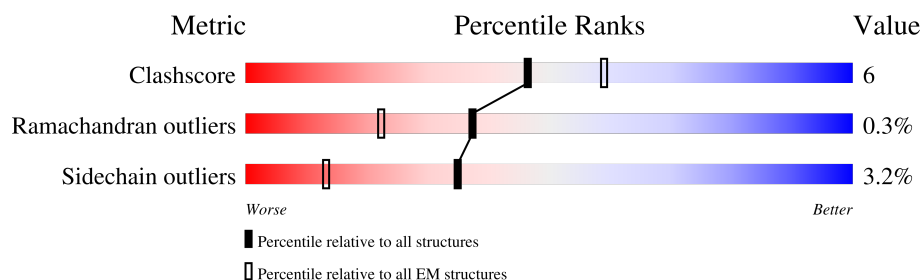
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.26 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	14557 (2.76 - 3.76)

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	506	
1	B	506	
1	C	506	
1	D	506	

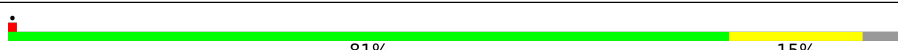
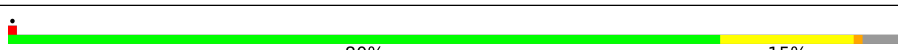
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Mol	Chain	Length	Quality of chain
1	E	506	
1	F	506	
1	G	506	
1	H	506	
1	I	506	
1	J	506	
1	K	506	
1	L	506	
1	M	506	
1	N	506	
1	O	506	
1	P	506	
1	Q	506	
1	R	506	
2	S	167	
2	T	167	
2	U	167	
2	V	167	
2	W	167	
2	X	167	
2	Y	167	
2	Z	167	
2	a	167	
2	b	167	
2	c	167	

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Mol	Chain	Length	Quality of chain
2	d	167	
2	e	167	
2	f	167	
2	g	167	
2	h	167	
2	i	167	
2	j	167	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 91095 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 sheath.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		
1	B	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		
1	C	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	D	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		
1	E	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	F	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		
1	G	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	H	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		
1	I	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	J	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	K	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	L	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	M	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		
1	N	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	O	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		
1	P	505	Total	C	N	O	S	0	0
			3802	2417	621	755	9		
1	Q	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	504	Total	C	N	O	S	0	0
			3794	2412	620	754	8		

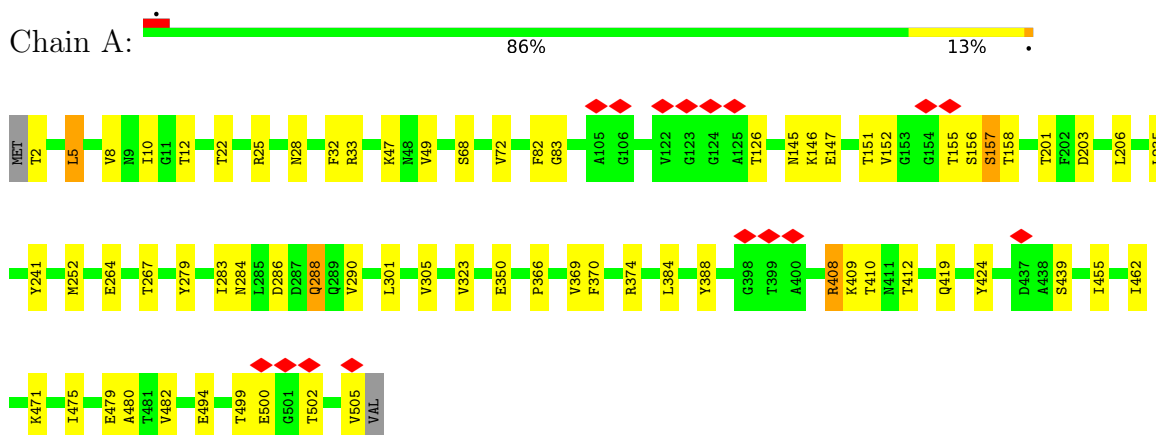
- Molecule 2 is a protein called tube.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	163	Total	C	N	O	S	0	0
			1274	814	213	242	5		
2	T	162	Total	C	N	O	S	0	0
			1267	809	212	241	5		
2	U	163	Total	C	N	O	S	0	0
			1275	814	213	242	6		
2	V	163	Total	C	N	O	S	0	0
			1275	814	213	242	6		
2	W	161	Total	C	N	O	S	0	0
			1258	804	210	239	5		
2	X	163	Total	C	N	O	S	0	0
			1275	814	213	242	6		
2	Y	162	Total	C	N	O	S	0	0
			1267	809	212	241	5		
2	Z	163	Total	C	N	O	S	0	0
			1275	814	213	242	6		
2	a	161	Total	C	N	O	S	0	0
			1258	804	210	239	5		
2	b	161	Total	C	N	O	S	0	0
			1258	804	210	239	5		
2	c	160	Total	C	N	O	S	0	0
			1253	801	209	238	5		
2	d	160	Total	C	N	O	S	0	0
			1253	801	209	238	5		
2	e	161	Total	C	N	O	S	0	0
			1258	804	210	239	5		
2	f	159	Total	C	N	O	S	0	0
			1246	796	208	237	5		
2	g	163	Total	C	N	O	S	0	0
			1275	814	213	242	6		
2	h	160	Total	C	N	O	S	0	0
			1253	801	209	238	5		
2	i	161	Total	C	N	O	S	0	0
			1258	804	210	239	5		
2	j	160	Total	C	N	O	S	0	0
			1253	801	209	238	5		

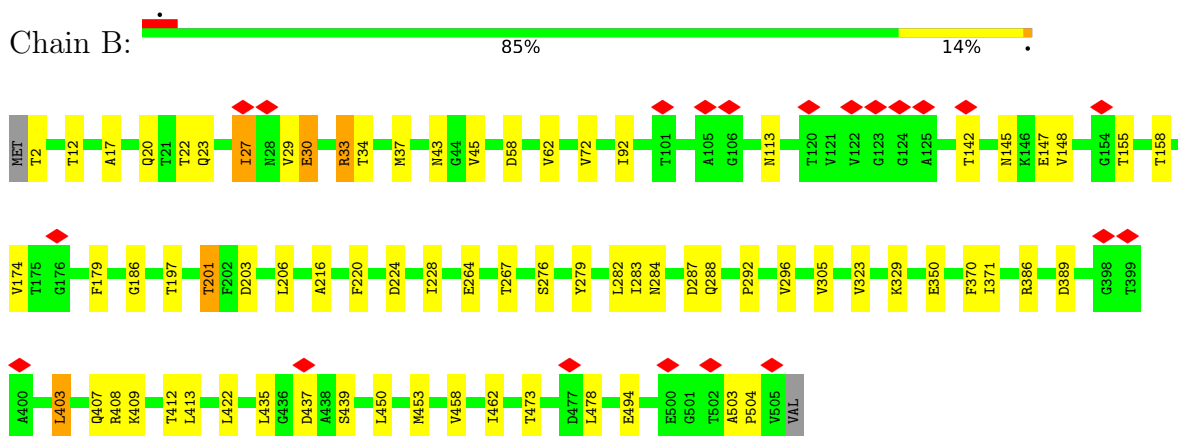
3 Residue-property plots

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

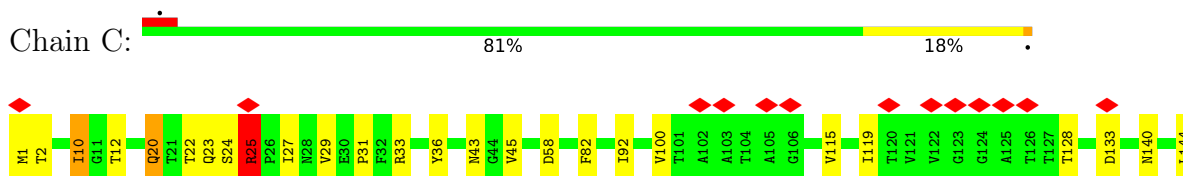
- Molecule 1: sheath

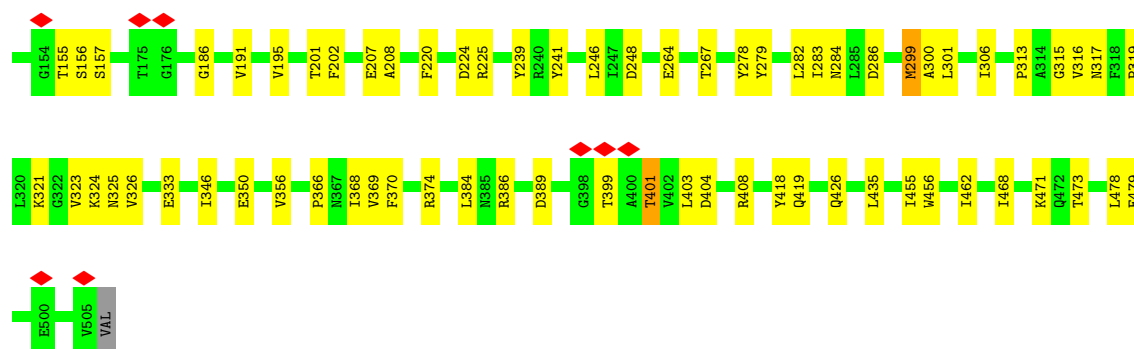


- Molecule 1: sheath



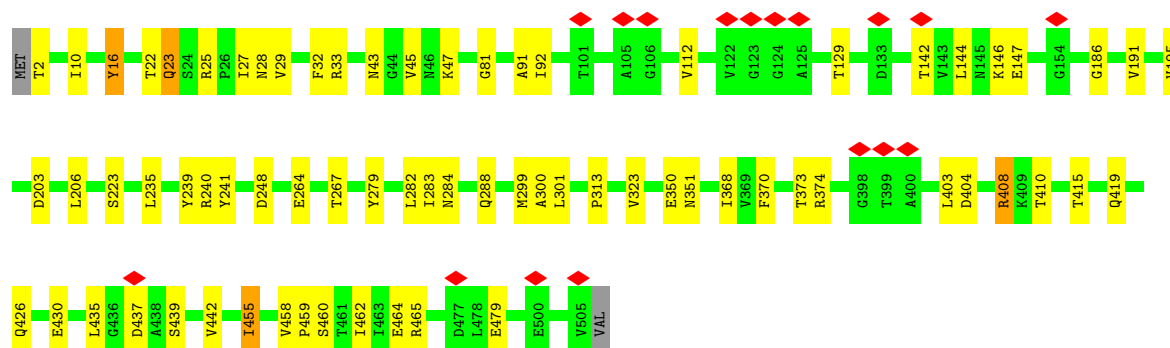
- Molecule 1: sheath





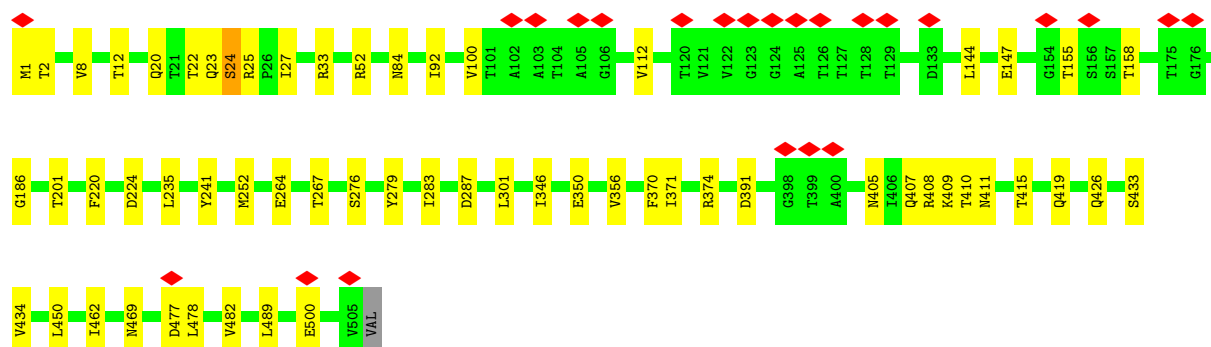
- Molecule 1: sheath

Chain D: 85% 13% .



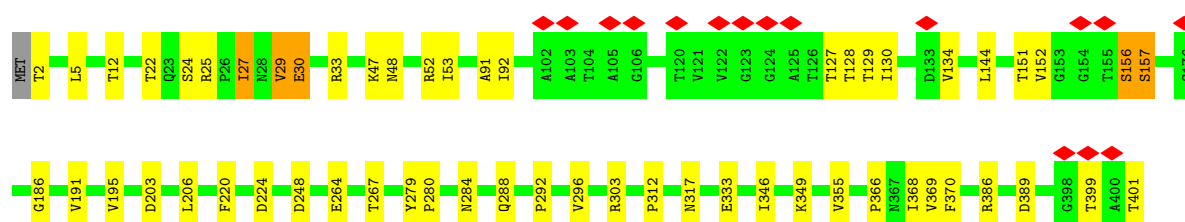
- Molecule 1: sheath

Chain E: 5% 88% 12% .



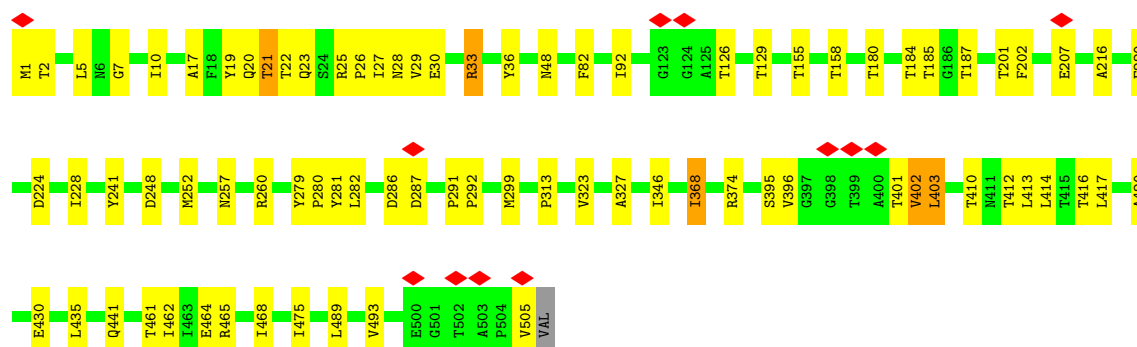
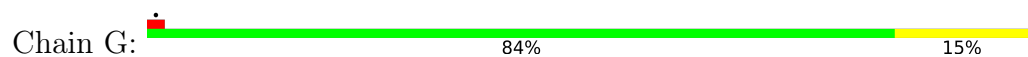
- Molecule 1: sheath

Chain F: 85% 13% .

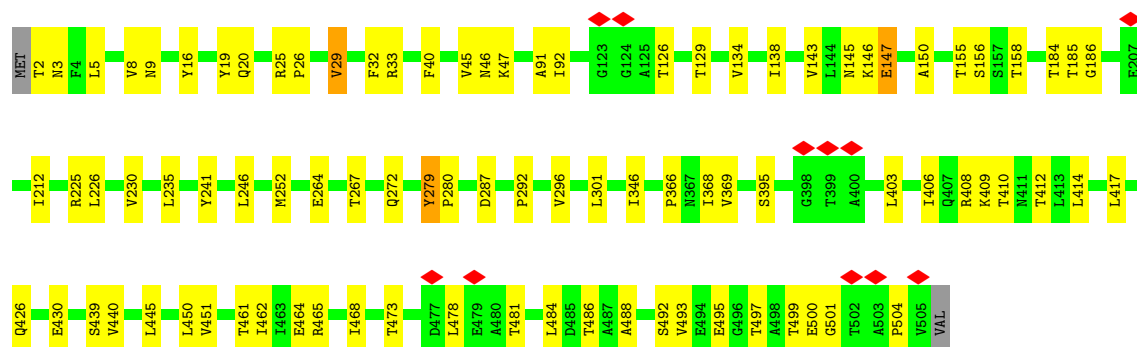
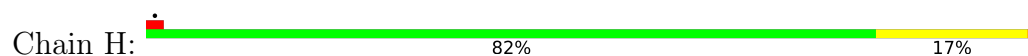




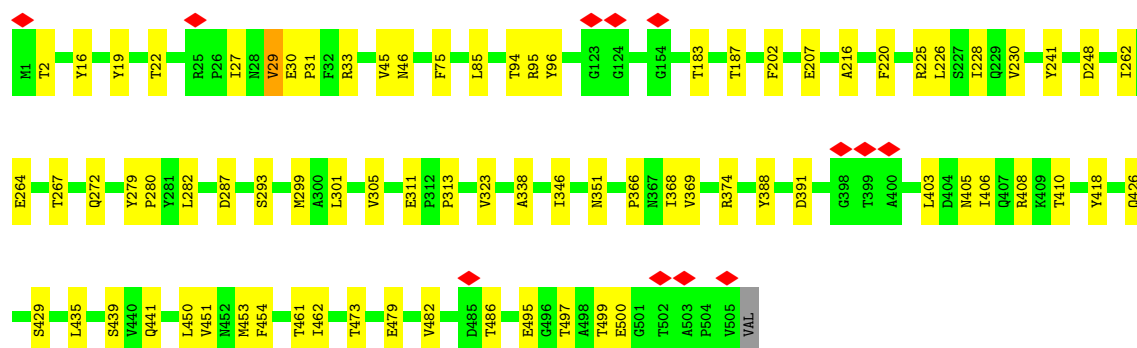
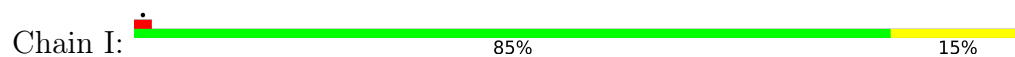
- Molecule 1: sheath



- Molecule 1: sheath

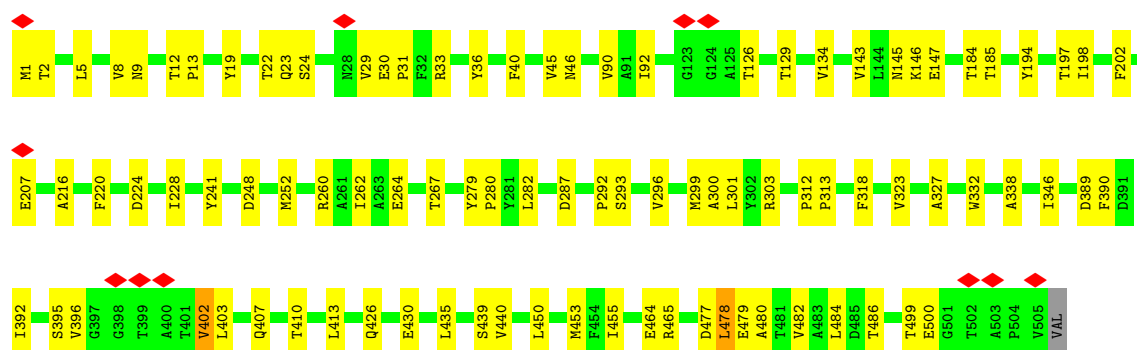


- Molecule 1: sheath



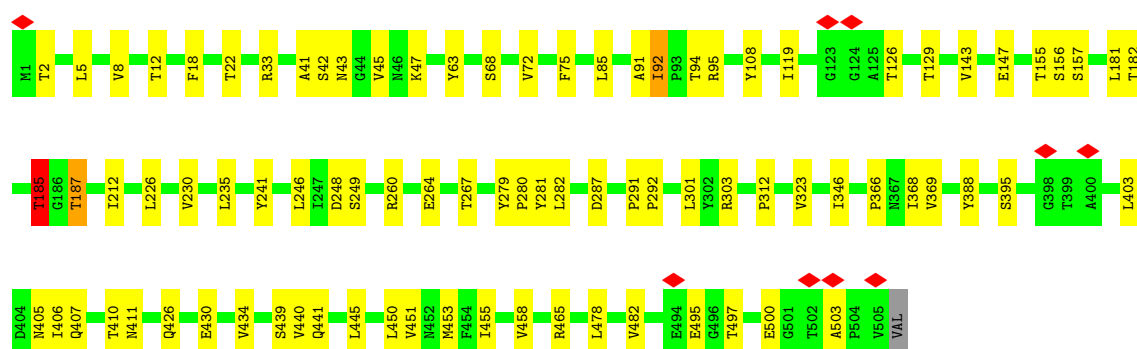
- Molecule 1: sheath

Chain J:  81% 18%



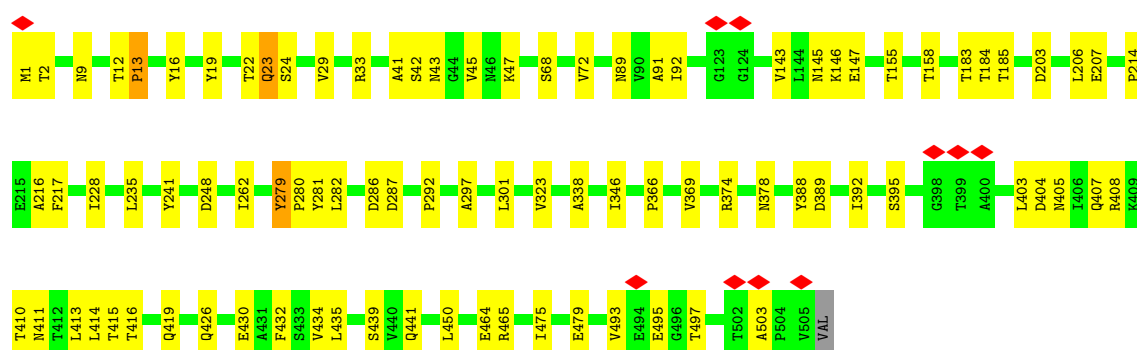
• Molecule 1: sheath

Chain K:  83% 17%



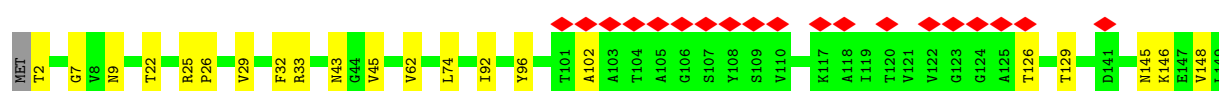
• Molecule 1: sheath

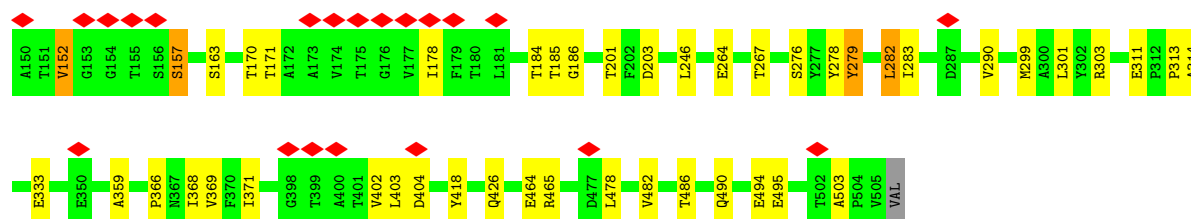
Chain L:  82% 17%



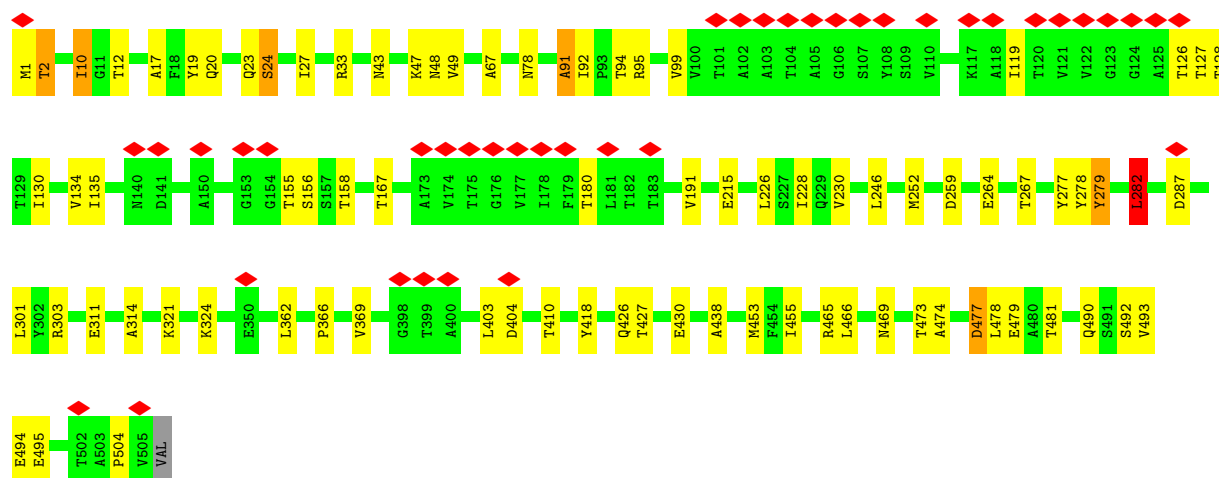
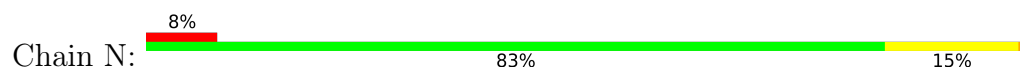
• Molecule 1: sheath

Chain M:  8% 86% 12%

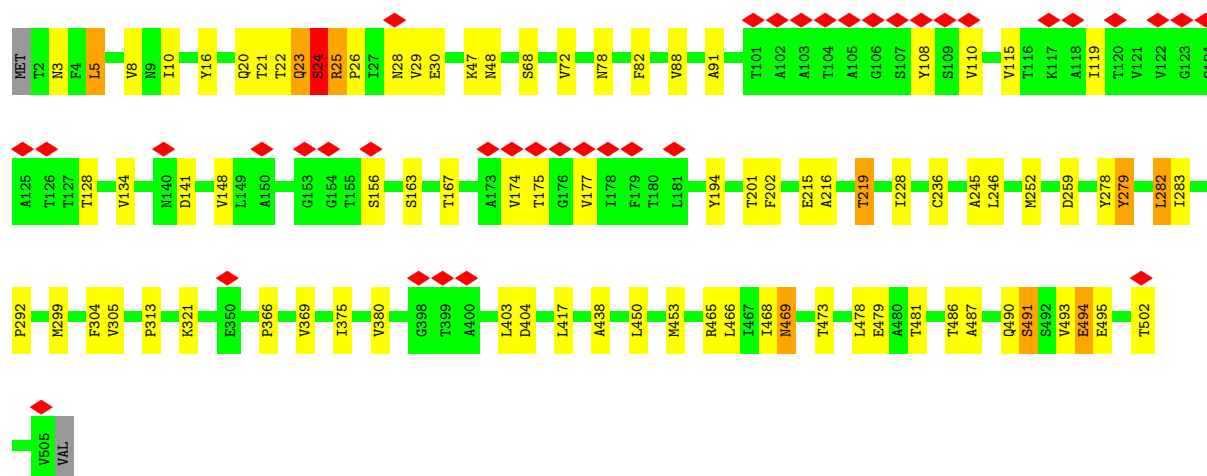
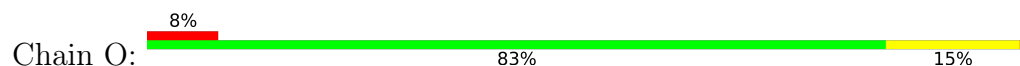




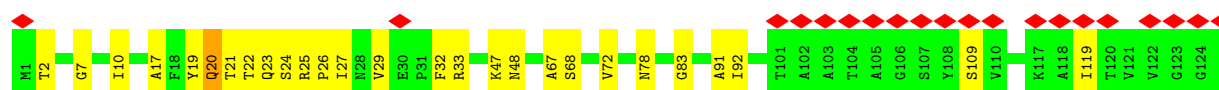
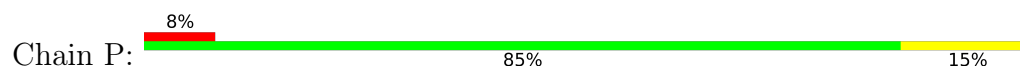
• Molecule 1: sheath

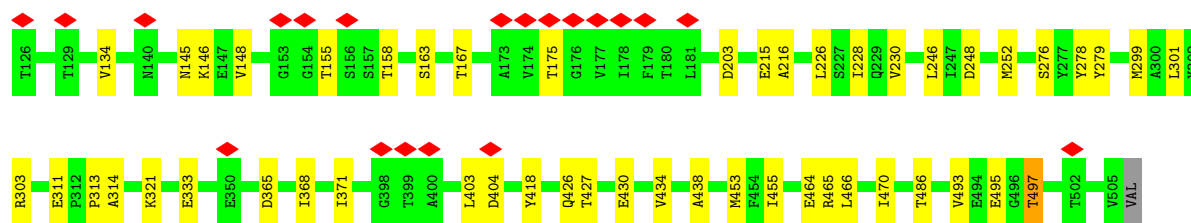


• Molecule 1: sheath

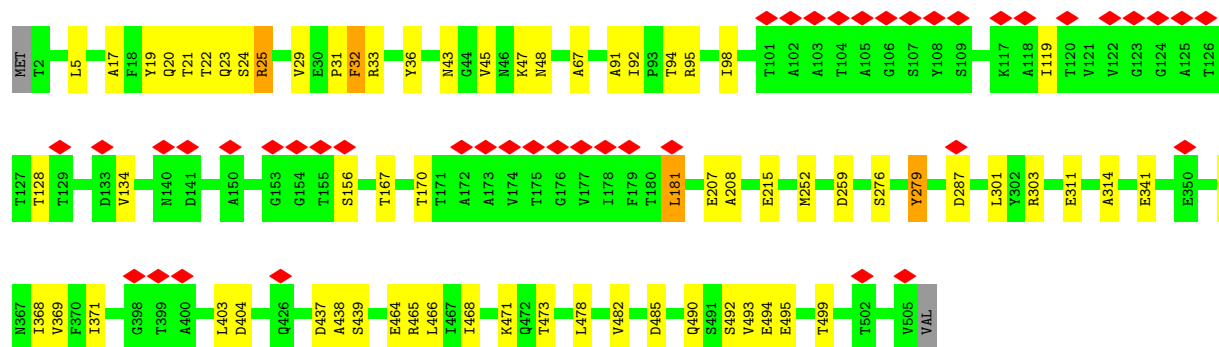
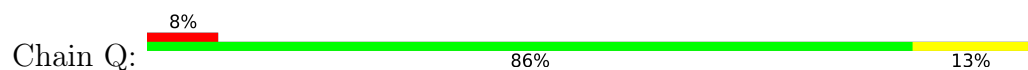


• Molecule 1: sheath

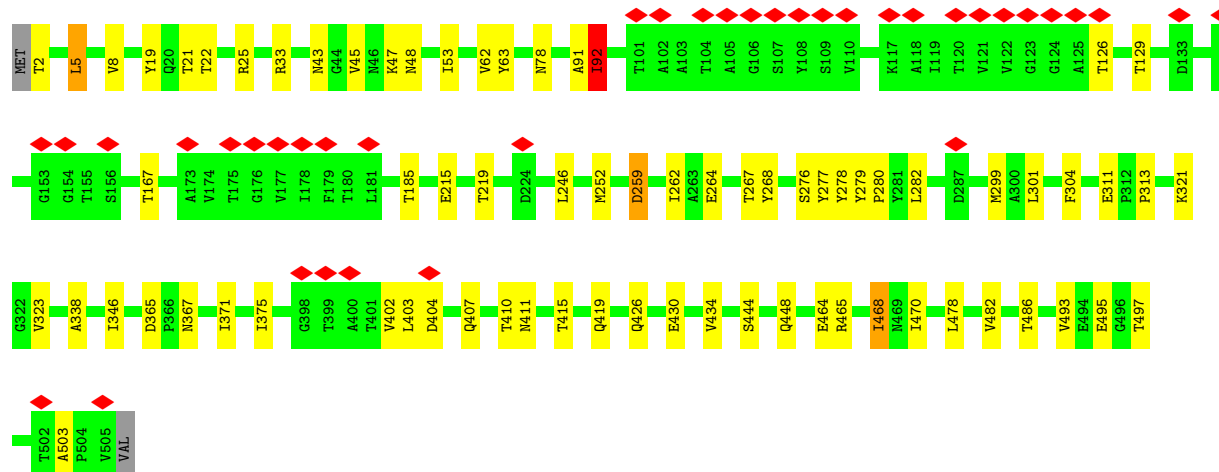
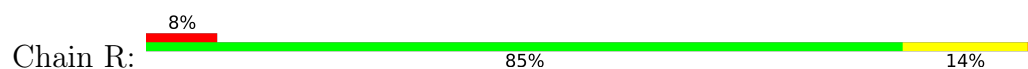




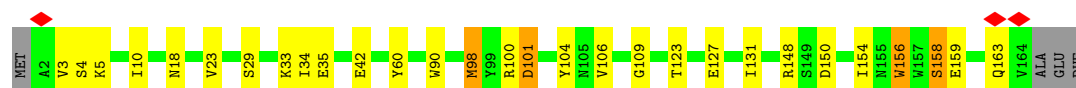
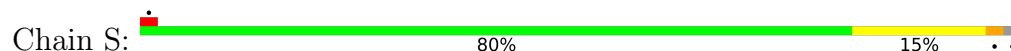
- Molecule 1: sheath



- Molecule 1: sheath

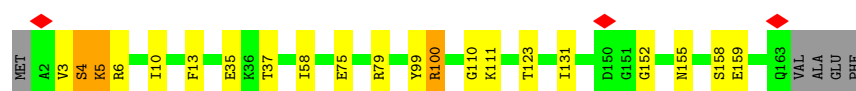


- Molecule 2: tube



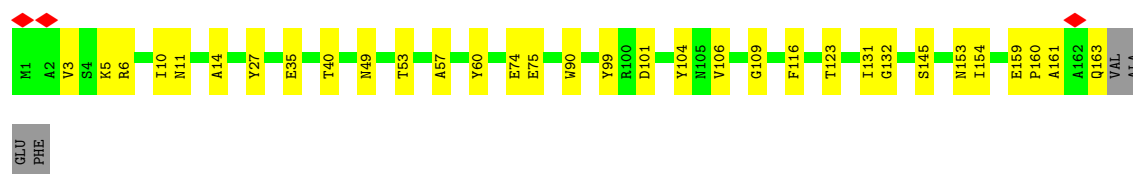
- Molecule 2: tube

Chain T:  84% 11% ..



• Molecule 2: tube

Chain U:  78% 19% .



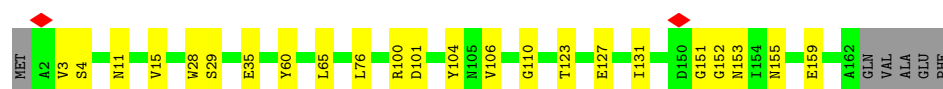
• Molecule 2: tube

Chain V:  86% 11% ..



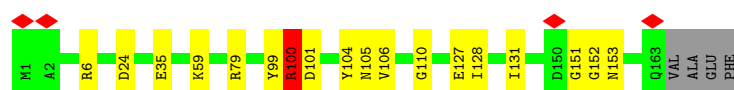
• Molecule 2: tube

Chain W:  83% 14% .



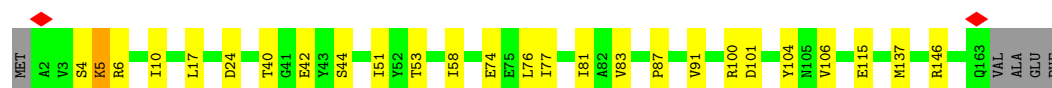
• Molecule 2: tube

Chain X:  87% 10% ..



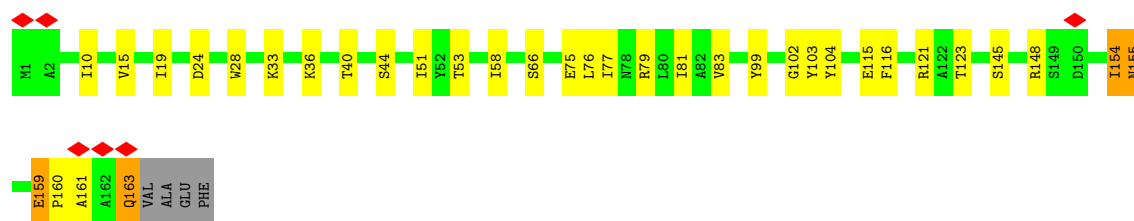
• Molecule 2: tube

Chain Y:  81% 15% ..

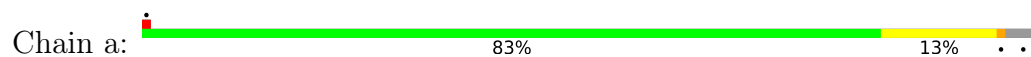


• Molecule 2: tube

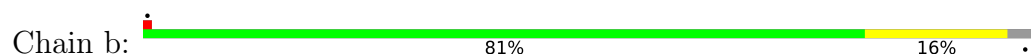
Chain Z:  77% 19% ..



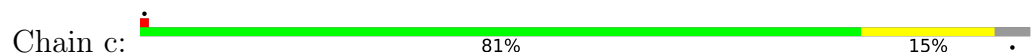
- Molecule 2: tube



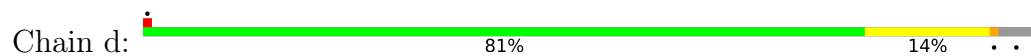
- Molecule 2: tube



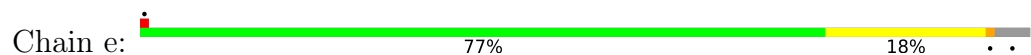
- Molecule 2: tube



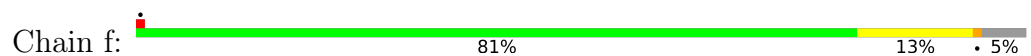
- Molecule 2: tube

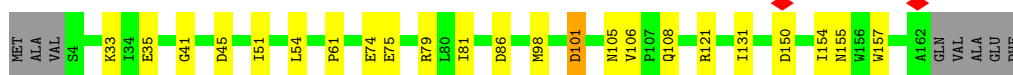


- Molecule 2: tube

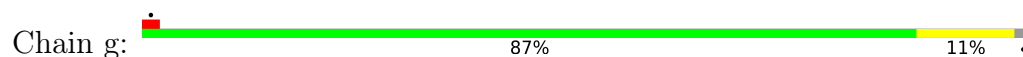


- Molecule 2: tube

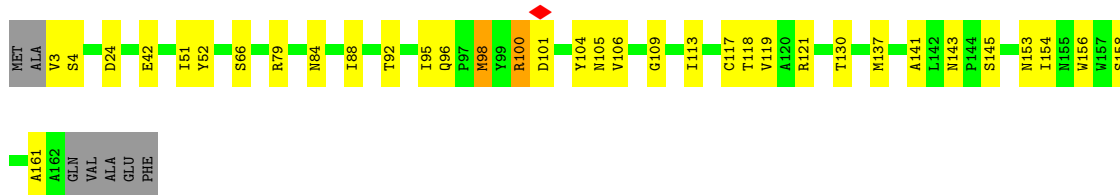
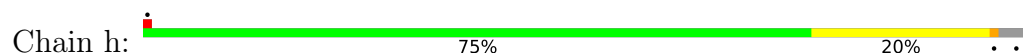




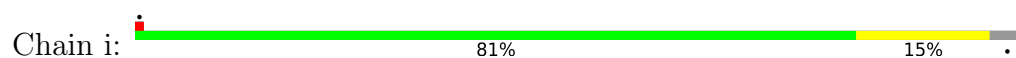
- Molecule 2: tube



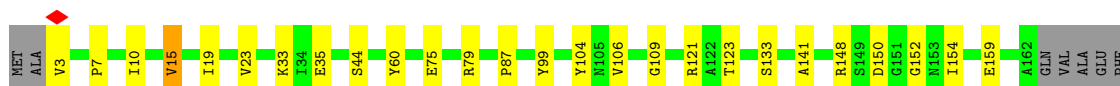
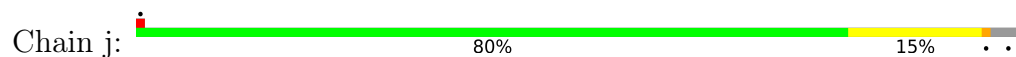
- Molecule 2: tube



- Molecule 2: tube



- Molecule 2: tube



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0065	Depositor
Map size ($\text{\AA}$)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	1/3867 (0.0%)	0.50	4/5302 (0.1%)
1	B	0.18	0/3867	0.45	3/5302 (0.1%)
1	C	0.22	0/3875	0.50	6/5312 (0.1%)
1	D	0.19	0/3867	0.49	7/5302 (0.1%)
1	E	0.15	0/3875	0.41	1/5312 (0.0%)
1	F	0.21	1/3867 (0.0%)	0.43	4/5302 (0.1%)
1	G	0.23	0/3875	0.47	4/5312 (0.1%)
1	H	0.21	0/3867	0.44	3/5302 (0.1%)
1	I	0.15	0/3875	0.37	1/5312 (0.0%)
1	J	0.19	0/3875	0.47	6/5312 (0.1%)
1	K	0.19	0/3875	0.45	7/5312 (0.1%)
1	L	0.17	0/3875	0.44	5/5312 (0.1%)
1	M	0.16	0/3867	0.42	5/5302 (0.1%)
1	N	0.21	0/3875	0.46	5/5312 (0.1%)
1	O	0.20	0/3867	0.47	3/5302 (0.1%)
1	P	0.19	0/3875	0.42	2/5312 (0.0%)
1	Q	0.21	0/3867	0.46	2/5302 (0.0%)
1	R	0.18	0/3867	0.44	8/5302 (0.2%)
2	S	0.23	1/1306 (0.1%)	0.44	0/1780
2	T	0.20	0/1299	0.49	2/1770 (0.1%)
2	U	0.18	0/1307	0.54	4/1780 (0.2%)
2	V	0.28	1/1307 (0.1%)	0.46	0/1780
2	W	0.29	1/1290 (0.1%)	0.52	1/1758 (0.1%)
2	X	0.18	0/1307	0.45	1/1780 (0.1%)
2	Y	0.26	1/1299 (0.1%)	0.53	4/1770 (0.2%)
2	Z	0.24	1/1307 (0.1%)	0.62	7/1780 (0.4%)
2	a	0.14	0/1290	0.40	0/1758
2	b	0.26	0/1290	0.55	5/1758 (0.3%)
2	c	0.16	0/1285	0.40	0/1751
2	d	0.23	0/1285	0.56	5/1751 (0.3%)
2	e	0.22	0/1290	0.51	0/1758
2	f	0.18	0/1278	0.47	2/1741 (0.1%)
2	g	0.15	0/1307	0.41	1/1780 (0.1%)
2	h	0.23	0/1285	0.54	4/1751 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	i	0.16	0/1290	0.55	4/1758 (0.2%)
2	j	0.16	0/1285	0.49	3/1751 (0.2%)
All	All	0.20	7/92985 (0.0%)	0.46	119/127281 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	101	ASP	C-O	-6.06	1.17	1.23
2	Z	159	GLU	C-N	5.78	1.38	1.33
1	A	290	VAL	C-N	5.75	1.38	1.33
2	V	101	ASP	C-O	-5.59	1.17	1.24
1	F	30	GLU	CA-C	5.14	1.57	1.52
2	Y	101	ASP	C-O	-5.02	1.17	1.24
2	S	101	ASP	C-O	-5.02	1.17	1.24

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	101	ASP	N-CA-C	-9.71	100.82	108.78
1	J	480	ALA	N-CA-C	-9.65	101.52	113.38
2	T	99	TYR	CA-C-N	8.49	133.56	121.42
2	T	99	TYR	C-N-CA	8.49	133.56	121.42
2	Z	99	TYR	CA-C-N	8.40	133.45	121.02
2	Z	99	TYR	C-N-CA	8.40	133.45	121.02
2	i	103	TYR	CA-C-N	8.35	132.72	120.87
2	i	103	TYR	C-N-CA	8.35	132.72	120.87
1	D	22	THR	CA-C-N	8.13	133.51	121.72
1	D	22	THR	C-N-CA	8.13	133.51	121.72
2	j	99	TYR	CA-C-N	8.10	134.13	121.26
2	j	99	TYR	C-N-CA	8.10	134.13	121.26
1	L	22	THR	CA-C-N	7.87	134.07	123.05
1	L	22	THR	C-N-CA	7.87	134.07	123.05
1	Q	170	THR	CB-CA-C	7.81	122.69	109.50
1	A	22	THR	CA-C-N	7.67	132.81	122.84
1	A	22	THR	C-N-CA	7.67	132.81	122.84
1	O	26	PRO	CA-C-N	7.62	132.03	122.43
1	O	26	PRO	C-N-CA	7.62	132.03	122.43
2	U	99	TYR	CA-C-N	7.58	131.50	120.82
2	U	99	TYR	C-N-CA	7.58	131.50	120.82
2	Z	154	ILE	CA-C-N	7.54	132.80	122.77
2	Z	154	ILE	C-N-CA	7.54	132.80	122.77
1	K	18	PHE	CA-C-N	7.22	133.16	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	18	PHE	C-N-CA	7.22	133.16	123.05
1	B	33	ARG	N-CA-C	-7.13	101.72	111.56
2	d	103	TYR	N-CA-C	-7.02	102.76	112.30
1	G	420	ALA	N-CA-C	-7.00	103.70	111.82
2	Z	159	GLU	CA-C-N	-6.90	113.79	120.83
2	Z	159	GLU	C-N-CA	-6.90	113.79	120.83
1	G	19	TYR	N-CA-C	6.76	121.29	113.38
2	i	99	TYR	CA-C-N	6.59	132.88	122.74
2	i	99	TYR	C-N-CA	6.59	132.88	122.74
1	N	10	ILE	N-CA-C	-6.41	98.81	108.17
1	D	32	PHE	N-CA-C	6.40	120.37	111.74
2	f	157	TRP	N-CA-C	6.39	118.19	109.11
2	Y	100	ARG	N-CA-C	6.31	119.38	110.23
1	J	13	PRO	CA-C-N	6.19	132.50	121.48
1	J	13	PRO	C-N-CA	6.19	132.50	121.48
1	C	25	ARG	CA-C-N	-6.15	113.61	119.76
1	C	25	ARG	C-N-CA	-6.15	113.61	119.76
1	R	185	THR	CA-C-N	6.12	125.80	119.92
1	R	185	THR	C-N-CA	6.12	125.80	119.92
1	Q	170	THR	N-CA-C	-6.12	100.31	110.17
2	h	96	GLN	CA-C-N	-6.11	113.39	119.99
2	h	96	GLN	C-N-CA	-6.11	113.39	119.99
1	N	282	LEU	N-CA-C	6.05	118.78	110.24
1	F	29	VAL	N-CA-C	5.96	115.83	107.37
1	H	156	SER	N-CA-C	-5.95	106.02	113.28
2	b	159	GLU	CA-C-N	-5.95	113.41	119.83
2	b	159	GLU	C-N-CA	-5.95	113.41	119.83
1	L	279	TYR	N-CA-C	5.91	122.86	109.81
1	N	2	THR	OG1-CB-CG2	5.81	120.92	109.30
1	C	2	THR	OG1-CB-CG2	5.76	120.81	109.30
1	B	2	THR	OG1-CB-CG2	5.74	120.79	109.30
1	G	33	ARG	N-CA-C	-5.72	104.05	111.71
1	H	279	TYR	N-CA-C	5.70	122.40	109.81
1	D	2	THR	OG1-CB-CG2	5.69	120.68	109.30
1	L	2	THR	OG1-CB-CG2	5.69	120.67	109.30
1	A	22	THR	OG1-CB-CG2	5.68	120.65	109.30
1	M	22	THR	OG1-CB-CG2	5.67	120.63	109.30
1	F	2	THR	OG1-CB-CG2	5.66	120.61	109.30
1	K	2	THR	OG1-CB-CG2	5.65	120.60	109.30
2	Y	5	LYS	CA-C-O	-5.65	111.98	119.10
1	R	2	THR	OG1-CB-CG2	5.64	120.58	109.30
1	D	22	THR	OG1-CB-CG2	5.62	120.53	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2	THR	OG1-CB-CG2	5.62	120.53	109.30
1	M	157	SER	N-CA-C	-5.61	106.48	113.38
1	M	279	TYR	N-CA-C	5.59	122.16	109.81
1	D	458	VAL	CA-C-N	-5.58	114.22	120.14
1	D	458	VAL	C-N-CA	-5.58	114.22	120.14
1	P	2	THR	OG1-CB-CG2	5.57	120.44	109.30
1	J	2	THR	OG1-CB-CG2	5.55	120.41	109.30
1	K	22	THR	OG1-CB-CG2	5.55	120.40	109.30
1	G	2	THR	OG1-CB-CG2	5.53	120.37	109.30
2	W	101	ASP	N-CA-C	-5.53	102.47	111.04
1	C	315	GLY	N-CA-C	5.49	119.12	112.48
1	C	10	ILE	N-CA-C	-5.48	100.17	108.17
1	L	22	THR	OG1-CB-CG2	5.46	120.22	109.30
1	R	92	ILE	CA-C-N	-5.46	114.31	119.76
1	R	92	ILE	C-N-CA	-5.46	114.31	119.76
1	R	21	THR	CB-CA-C	-5.45	109.22	117.07
1	I	2	THR	OG1-CB-CG2	5.45	120.19	109.30
1	J	12	THR	OG1-CB-CG2	5.43	120.16	109.30
1	B	12	THR	OG1-CB-CG2	5.43	120.16	109.30
1	F	502	THR	OG1-CB-CG2	5.43	120.15	109.30
2	U	6	ARG	CA-C-N	-5.41	115.00	120.85
2	U	6	ARG	C-N-CA	-5.41	115.00	120.85
1	J	13	PRO	N-CA-C	5.37	123.53	112.47
1	K	92	ILE	CA-C-N	-5.36	114.40	119.76
1	K	92	ILE	C-N-CA	-5.36	114.40	119.76
1	M	2	THR	OG1-CB-CG2	5.36	120.02	109.30
1	R	25	ARG	CA-C-N	-5.35	114.41	119.76
1	R	25	ARG	C-N-CA	-5.35	114.41	119.76
2	Z	160	PRO	N-CA-C	-5.32	109.15	114.68
1	C	20	GLN	N-CA-C	5.25	121.99	110.80
1	N	91	ALA	CA-C-N	-5.25	118.81	122.59
1	N	91	ALA	C-N-CA	-5.25	118.81	122.59
1	K	185	THR	N-CA-C	5.24	121.96	110.80
2	f	101	ASP	N-CA-C	-5.21	104.68	112.54
2	Y	5	LYS	CA-C-N	5.20	134.49	121.80
2	Y	5	LYS	C-N-CA	5.20	134.49	121.80
1	O	279	TYR	N-CA-C	5.20	121.30	109.81
2	b	86	ASP	CA-C-N	-5.20	114.73	119.82
2	b	86	ASP	C-N-CA	-5.20	114.73	119.82
2	X	100	ARG	N-CA-C	5.18	117.74	110.23
2	h	153	ASN	N-CA-C	5.17	116.60	111.07
1	M	2	THR	CA-CB-CG2	5.12	119.21	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	15	VAL	N-CA-C	5.12	115.34	108.17
2	d	159	GLU	CA-C-N	-5.09	114.33	119.83
2	d	159	GLU	C-N-CA	-5.09	114.33	119.83
2	d	101	ASP	CB-CA-C	-5.06	109.78	117.07
1	H	20	GLN	N-CA-C	5.06	117.57	110.23
2	h	100	ARG	N-CA-C	5.05	117.47	109.24
1	A	10	ILE	N-CA-C	-5.05	100.98	108.45
1	P	2	THR	CA-CB-CG2	5.03	119.05	110.50
2	g	150	ASP	N-CA-C	5.03	121.50	110.80
1	F	502	THR	CA-CB-CG2	5.02	119.04	110.50
2	b	161	ALA	N-CA-C	-5.02	104.99	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3794	0	3754	40	0
1	B	3794	0	3754	62	0
1	C	3802	0	3766	61	0
1	D	3794	0	3754	45	0
1	E	3802	0	3766	42	0
1	F	3794	0	3754	37	0
1	G	3802	0	3766	56	0
1	H	3794	0	3754	63	0
1	I	3802	0	3766	60	0
1	J	3802	0	3766	57	0
1	K	3802	0	3766	58	0
1	L	3802	0	3766	66	0
1	M	3794	0	3754	37	0
1	N	3802	0	3766	56	0
1	O	3794	0	3754	52	0
1	P	3802	0	3766	42	0
1	Q	3794	0	3754	41	0
1	R	3794	0	3754	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	1274	0	1242	21	0
2	T	1267	0	1233	16	0
2	U	1275	0	1245	22	0
2	V	1275	0	1245	20	0
2	W	1258	0	1225	11	0
2	X	1275	0	1245	13	0
2	Y	1267	0	1233	18	0
2	Z	1275	0	1245	24	0
2	a	1258	0	1225	21	0
2	b	1258	0	1225	12	0
2	c	1253	0	1220	22	0
2	d	1253	0	1220	17	0
2	e	1258	0	1225	19	0
2	f	1246	0	1211	33	0
2	g	1275	0	1245	19	0
2	h	1253	0	1220	23	0
2	i	1258	0	1225	21	0
2	j	1253	0	1220	17	0
All	All	91095	0	89829	1098	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 6.

All (1098) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:35:GLU:HG3	2:f:61:PRO:CG	1.47	1.43
1:B:27:ILE:CG1	1:B:33:ARG:HH21	1.35	1.39
1:B:27:ILE:HG13	1:B:33:ARG:NH2	1.40	1.36
1:G:26:PRO:HG3	1:H:497:THR:CG2	1.56	1.34
1:K:248:ASP:OD2	1:K:291:PRO:HB3	1.16	1.32
1:I:29:VAL:HG23	1:I:207:GLU:OE2	1.34	1.26
2:f:35:GLU:CG	2:f:61:PRO:CG	2.14	1.26
1:O:25:ARG:CB	1:O:25:ARG:HH11	1.52	1.23
1:N:155:THR:HG22	1:N:158:THR:OG1	1.16	1.22
2:f:35:GLU:CD	2:f:61:PRO:HG2	1.66	1.21
1:B:27:ILE:CG1	1:B:33:ARG:NH2	1.99	1.21
1:R:264:GLU:O	1:R:267:THR:HG22	1.43	1.18
1:G:248:ASP:OD1	1:G:292:PRO:HD2	1.44	1.17
2:f:35:GLU:CG	2:f:61:PRO:HG2	1.71	1.16
2:f:35:GLU:CG	2:f:61:PRO:HD2	1.74	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:407:GLN:O	1:K:410:THR:HG22	1.46	1.15
2:h:145:SER:HB2	2:i:52:TYR:CE1	1.81	1.14
2:e:35:GLU:OE2	2:j:121:ARG:HG3	1.47	1.14
1:G:26:PRO:CG	1:H:497:THR:HG21	1.77	1.14
2:f:35:GLU:CG	2:f:61:PRO:CD	2.26	1.12
1:I:29:VAL:CG2	1:I:207:GLU:OE2	2.03	1.07
1:K:248:ASP:OD2	1:K:291:PRO:CB	2.02	1.07
2:f:35:GLU:HG2	2:f:61:PRO:CD	1.83	1.05
1:O:25:ARG:HH11	1:O:25:ARG:CG	1.68	1.04
1:L:217:PHE:CB	1:L:248:ASP:OD1	2.06	1.03
2:f:35:GLU:HG3	2:f:61:PRO:HG3	1.38	1.03
1:N:155:THR:CG2	1:N:158:THR:OG1	2.07	1.02
2:g:33:LYS:HE3	2:g:35:GLU:OE1	1.59	1.00
1:R:407:GLN:O	1:R:410:THR:HG22	1.61	1.00
1:O:25:ARG:CB	1:O:25:ARG:NH1	2.24	0.99
2:f:35:GLU:HG2	2:f:61:PRO:HD2	1.01	0.99
1:G:26:PRO:CG	1:H:497:THR:CG2	2.37	0.98
2:f:35:GLU:OE2	2:f:61:PRO:HG2	1.62	0.98
1:O:25:ARG:HH11	1:O:25:ARG:HB3	1.24	0.98
1:B:27:ILE:CD1	1:B:33:ARG:NH2	2.26	0.97
1:L:407:GLN:O	1:L:410:THR:HG22	1.65	0.95
1:E:410:THR:HG21	1:E:434:VAL:HG11	1.49	0.92
2:h:145:SER:HB2	2:i:52:TYR:HE1	1.14	0.92
1:L:410:THR:HG21	1:L:434:VAL:HG11	1.50	0.91
1:K:410:THR:HG21	1:K:434:VAL:HG11	1.52	0.91
1:E:407:GLN:O	1:E:410:THR:HG22	1.72	0.90
1:N:17:ALA:HA	1:O:468:ILE:O	1.73	0.89
1:G:25:ARG:NH2	1:G:82:PHE:CZ	2.42	0.88
1:L:217:PHE:HB3	1:L:248:ASP:OD1	1.73	0.88
2:f:35:GLU:HG3	2:f:61:PRO:HG2	1.31	0.87
1:A:388:TYR:HH	1:A:410:THR:HG1	1.09	0.87
1:A:147:GLU:OE2	1:G:257:ASN:ND2	2.07	0.87
1:R:264:GLU:O	1:R:267:THR:CG2	2.23	0.86
1:C:128:THR:HG22	1:C:156:SER:CB	2.05	0.86
1:J:194:TYR:O	1:J:197:THR:HG22	1.76	0.86
1:B:30:GLU:HB2	1:B:33:ARG:HD3	1.56	0.85
1:I:388:TYR:HH	1:I:410:THR:HG1	1.06	0.84
1:A:408:ARG:NH1	2:Y:17:LEU:O	2.10	0.84
1:B:27:ILE:HD11	1:B:33:ARG:HH22	1.42	0.84
1:B:30:GLU:CB	1:B:33:ARG:HD3	2.08	0.83
2:h:145:SER:CB	2:i:52:TYR:CE1	2.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HG13	1:B:33:ARG:HH21	0.68	0.83
1:B:27:ILE:CD1	1:B:33:ARG:HH21	1.87	0.83
1:C:128:THR:HG22	1:C:156:SER:HB3	1.60	0.82
1:B:27:ILE:HD11	1:B:33:ARG:NH2	1.92	0.81
1:O:25:ARG:NH1	1:O:25:ARG:HB3	1.89	0.81
1:G:25:ARG:HG2	1:H:488:ALA:HA	1.61	0.80
1:R:410:THR:HG21	1:R:434:VAL:HG11	1.63	0.80
2:a:103:TYR:OH	2:h:52:TYR:OH	1.99	0.80
1:B:435:LEU:HD22	1:H:486:THR:HG23	1.63	0.79
2:f:35:GLU:OE2	2:f:61:PRO:CG	2.29	0.79
1:G:248:ASP:OD1	1:G:292:PRO:CD	2.30	0.79
1:K:407:GLN:O	1:K:410:THR:CG2	2.26	0.79
1:N:155:THR:HG22	1:N:158:THR:HG1	1.46	0.79
1:O:25:ARG:HH11	1:O:25:ARG:HG2	1.48	0.78
1:M:464:GLU:OE1	1:M:465:ARG:NH1	2.17	0.77
1:N:1:MET:SD	1:N:2:THR:N	2.58	0.76
1:C:155:THR:HG22	1:C:157:SER:H	1.51	0.76
1:F:479:GLU:OE1	1:F:479:GLU:N	2.19	0.75
1:L:217:PHE:CG	1:L:248:ASP:OD1	2.39	0.75
1:H:143:VAL:HG12	1:H:147:GLU:OE1	1.85	0.75
1:A:350:GLU:N	1:A:350:GLU:OE1	2.20	0.75
1:M:333:GLU:N	1:M:333:GLU:OE1	2.20	0.74
1:H:5:LEU:HD11	1:I:499:THR:O	1.87	0.74
1:I:29:VAL:HG23	1:I:207:GLU:CD	2.13	0.74
1:P:7:GLY:O	1:Q:465:ARG:NH1	2.21	0.74
1:N:303:ARG:NH1	1:N:314:ALA:O	2.21	0.74
1:G:26:PRO:HG3	1:H:497:THR:HG21	0.81	0.74
1:O:194:TYR:OH	1:O:215:GLU:OE1	2.04	0.74
1:C:202:PHE:O	1:C:241:TYR:OH	2.05	0.73
1:O:25:ARG:CG	1:O:25:ARG:NH1	2.40	0.73
1:J:143:VAL:HG12	1:J:147:GLU:OE1	1.89	0.73
1:K:143:VAL:HG12	1:K:147:GLU:OE1	1.88	0.73
1:M:303:ARG:NH1	1:M:314:ALA:O	2.21	0.73
1:N:474:ALA:HB3	1:N:477:ASP:OD1	1.89	0.73
1:H:464:GLU:OE1	1:H:465:ARG:NH1	2.21	0.73
2:f:35:GLU:HG3	2:f:61:PRO:CD	2.03	0.72
1:C:333:GLU:N	1:C:333:GLU:OE1	2.20	0.72
2:e:35:GLU:OE2	2:j:121:ARG:CG	2.33	0.72
1:H:280:PRO:HG2	1:H:346:ILE:H	1.53	0.72
1:I:29:VAL:CB	1:I:207:GLU:OE2	2.36	0.72
1:K:495:GLU:OE1	1:K:497:THR:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:148:ARG:NH2	2:j:150:ASP:OD2	2.22	0.72
1:J:426:GLN:N	1:J:430:GLU:OE1	2.23	0.72
1:L:410:THR:CG2	1:L:434:VAL:HG11	2.20	0.71
1:N:47:LYS:HB3	1:N:91:ALA:HB2	1.73	0.71
1:C:282:LEU:HB3	1:C:323:VAL:HG11	1.73	0.70
2:i:13:PHE:O	2:i:100:ARG:NH2	2.24	0.70
1:J:248:ASP:OD2	1:J:293:SER:OG	2.05	0.70
1:D:43:ASN:OD1	1:D:45:VAL:HG13	1.91	0.69
1:G:464:GLU:OE1	1:G:465:ARG:NH1	2.25	0.69
1:L:495:GLU:OE1	1:L:497:THR:N	2.25	0.69
1:G:202:PHE:O	1:G:241:TYR:OH	2.10	0.69
1:N:33:ARG:HA	1:N:301:LEU:HD22	1.75	0.69
1:K:8:VAL:HG21	1:L:503:ALA:HB1	1.75	0.69
1:E:426:GLN:OE1	1:E:426:GLN:N	2.25	0.68
1:H:495:GLU:OE1	1:H:497:THR:N	2.26	0.68
1:L:143:VAL:HG12	1:L:147:GLU:OE1	1.92	0.68
1:B:155:THR:HG1	1:B:158:THR:HG1	1.36	0.68
1:C:386:ARG:NH1	1:C:389:ASP:OD2	2.27	0.68
1:B:350:GLU:OE1	1:B:350:GLU:N	2.26	0.68
1:K:407:GLN:C	1:K:410:THR:HG22	2.18	0.68
1:R:426:GLN:N	1:R:430:GLU:OE1	2.27	0.68
1:B:30:GLU:CB	1:B:33:ARG:CD	2.72	0.68
1:B:113:ASN:HD22	1:B:147:GLU:HG2	1.58	0.68
1:C:27:ILE:HD11	1:C:82:PHE:HA	1.76	0.68
2:T:13:PHE:O	2:T:100:ARG:NH2	2.26	0.68
2:a:101:ASP:O	2:g:58:ILE:HD12	1.94	0.68
1:B:386:ARG:NH1	1:B:389:ASP:OD2	2.27	0.67
1:G:17:ALA:HA	1:H:468:ILE:O	1.94	0.67
1:R:264:GLU:C	1:R:267:THR:HG22	2.17	0.67
2:U:106:VAL:HG13	2:U:106:VAL:O	1.93	0.67
1:A:155:THR:HG22	1:A:156:SER:N	2.09	0.67
1:R:407:GLN:O	1:R:410:THR:CG2	2.41	0.67
1:M:7:GLY:O	1:N:465:ARG:NH1	2.28	0.67
1:Q:471:LYS:NZ	1:Q:485:ASP:OD2	2.22	0.67
1:C:43:ASN:OD1	1:C:45:VAL:HG13	1.95	0.66
1:Q:33:ARG:HA	1:Q:301:LEU:HD22	1.77	0.66
1:C:479:GLU:OE1	1:C:479:GLU:N	2.27	0.66
1:P:33:ARG:HA	1:P:301:LEU:HD22	1.78	0.66
2:g:3:VAL:HG11	2:g:7:PRO:HD3	1.77	0.66
1:C:128:THR:HG22	1:C:156:SER:HB2	1.77	0.66
2:i:3:VAL:HG13	2:i:3:VAL:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:3:VAL:HG11	2:j:7:PRO:HD3	1.78	0.66
1:B:30:GLU:HB2	1:B:33:ARG:CD	2.24	0.66
1:C:92:ILE:HG21	1:C:186:GLY:O	1.96	0.66
1:K:410:THR:CG2	1:K:434:VAL:HG11	2.26	0.66
1:I:479:GLU:OE2	1:I:479:GLU:N	2.25	0.65
1:N:287:ASP:OD1	1:N:324:LYS:NZ	2.22	0.65
1:M:33:ARG:HA	1:M:301:LEU:HD22	1.77	0.65
1:R:33:ARG:HA	1:R:301:LEU:HD22	1.78	0.65
1:L:407:GLN:O	1:L:410:THR:CG2	2.44	0.65
2:V:106:VAL:HG23	2:V:106:VAL:O	1.96	0.65
1:L:217:PHE:HB2	1:L:248:ASP:OD1	1.95	0.65
1:C:435:LEU:HD22	1:I:486:THR:HG23	1.79	0.65
1:O:23:GLN:O	1:O:24:SER:C	2.40	0.65
1:G:26:PRO:CG	1:H:497:THR:HG22	2.27	0.65
1:P:48:ASN:HB2	1:P:167:THR:HG22	1.78	0.65
2:h:145:SER:HB3	2:i:52:TYR:CD1	2.31	0.65
2:Y:5:LYS:O	2:j:87:PRO:HB2	1.96	0.64
1:Q:303:ARG:NH1	1:Q:314:ALA:O	2.30	0.64
1:E:52:ARG:NH1	1:E:84:ASN:OD1	2.31	0.64
1:N:119:ILE:HG13	1:N:134:VAL:HG22	1.80	0.64
2:h:145:SER:CB	2:i:52:TYR:CD1	2.80	0.64
1:H:8:VAL:HG23	1:H:9:ASN:OD1	1.98	0.64
1:P:333:GLU:OE1	1:P:333:GLU:N	2.29	0.64
1:Q:5:LEU:HD12	1:R:503:ALA:HB2	1.79	0.64
2:Y:24:ASP:OD2	2:Y:76:LEU:HD13	1.98	0.64
1:O:25:ARG:NH1	1:O:25:ARG:HG2	2.10	0.64
2:Z:123:THR:HG23	2:a:35:GLU:HG2	1.80	0.63
2:h:121:ARG:HB2	2:h:141:ALA:HB3	1.80	0.63
1:E:112:VAL:HB	1:E:144:LEU:HD11	1.81	0.63
2:X:101:ASP:O	2:Y:58:ILE:HD12	1.99	0.63
1:K:426:GLN:N	1:K:430:GLU:OE1	2.32	0.62
1:F:127:THR:HB	1:F:157:SER:HB2	1.80	0.62
1:P:47:LYS:HB3	1:P:91:ALA:HB2	1.79	0.62
1:P:252:MET:HE2	1:P:252:MET:HA	1.81	0.62
2:S:148:ARG:NH2	2:S:150:ASP:OD2	2.31	0.62
1:G:248:ASP:CG	1:G:291:PRO:HB3	2.25	0.62
1:J:33:ARG:HA	1:J:301:LEU:HD22	1.81	0.62
1:E:33:ARG:HA	1:E:301:LEU:HD22	1.81	0.62
1:L:439:SER:O	1:R:493:VAL:HG11	2.00	0.62
1:R:410:THR:CG2	1:R:434:VAL:HG11	2.31	0.61
2:e:35:GLU:OE1	2:j:123:THR:OG1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLU:OE1	1:A:479:GLU:N	2.33	0.61
2:c:83:VAL:HG11	2:c:91:VAL:HG23	1.82	0.61
1:O:115:VAL:HG11	1:O:141:ASP:OD2	2.01	0.61
1:R:444:SER:O	1:R:448:GLN:NE2	2.33	0.61
1:G:25:ARG:CG	1:H:488:ALA:HA	2.30	0.61
2:e:109:GLY:HA3	2:e:154:ILE:HD12	1.83	0.61
1:A:374:ARG:NH2	1:L:19:TYR:OH	2.31	0.61
1:H:184:THR:O	1:H:185:THR:HG23	2.01	0.61
1:C:419:GLN:NE2	2:U:3:VAL:O	2.34	0.61
1:D:374:ARG:NH2	1:I:19:TYR:OH	2.32	0.61
1:G:257:ASN:OD1	1:G:260:ARG:HG3	1.99	0.61
2:a:154:ILE:HG21	2:a:156:TRP:CE3	2.35	0.61
1:K:155:THR:HG22	1:K:156:SER:N	2.15	0.61
2:U:160:PRO:O	2:U:163:GLN:NE2	2.32	0.61
1:C:374:ARG:NH2	1:H:19:TYR:OH	2.34	0.61
1:E:276:SER:OG	1:E:371:ILE:HD12	2.01	0.61
1:D:142:THR:O	1:D:146:LYS:NZ	2.27	0.60
2:V:109:GLY:CA	2:V:154:ILE:HD12	2.31	0.60
1:L:47:LYS:HB2	1:L:91:ALA:HB2	1.83	0.60
2:X:110:GLY:HA2	2:X:152:GLY:H	1.65	0.60
2:f:108:GLN:O	2:f:108:GLN:NE2	2.34	0.60
1:N:128:THR:HG23	1:N:156:SER:HB3	1.82	0.60
1:D:350:GLU:OE1	1:D:351:ASN:ND2	2.34	0.60
1:I:439:SER:O	1:O:493:VAL:HG11	2.01	0.60
1:H:5:LEU:O	1:H:8:VAL:HG22	2.02	0.60
1:L:404:ASP:OD1	1:L:408:ARG:NE	2.34	0.60
1:C:92:ILE:HD13	1:C:186:GLY:O	2.01	0.60
1:D:203:ASP:H	1:D:206:LEU:HD12	1.65	0.60
1:I:495:GLU:OE1	1:I:497:THR:N	2.34	0.60
1:N:426:GLN:N	1:N:430:GLU:OE1	2.35	0.60
1:O:252:MET:HA	1:O:252:MET:HE2	1.82	0.60
1:I:368:ILE:HG22	1:I:368:ILE:O	2.02	0.60
1:I:287:ASP:OD1	1:I:287:ASP:O	2.19	0.59
1:D:479:GLU:N	1:D:479:GLU:OE1	2.34	0.59
1:E:350:GLU:N	1:E:350:GLU:OE2	2.36	0.59
1:F:386:ARG:NH1	1:F:389:ASP:OD2	2.35	0.59
1:B:27:ILE:HG13	1:B:33:ARG:CZ	2.25	0.59
1:H:26:PRO:CG	1:I:497:THR:HG21	2.32	0.59
1:Q:47:LYS:HB3	1:Q:91:ALA:HB2	1.85	0.59
1:A:33:ARG:HA	1:A:301:LEU:HD22	1.85	0.59
1:L:280:PRO:HG2	1:L:346:ILE:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:434:VAL:HG13	1:P:453:MET:HE1	1.84	0.59
1:F:399:THR:HG22	1:L:426:GLN:OE1	2.03	0.59
1:Q:464:GLU:OE1	1:Q:465:ARG:NE	2.32	0.59
1:G:248:ASP:OD2	1:G:281:TYR:CE1	2.56	0.59
1:L:413:LEU:O	1:L:416:THR:HG22	2.02	0.59
1:A:471:LYS:HZ1	1:A:482:VAL:HA	1.66	0.59
1:J:252:MET:HE2	1:J:327:ALA:HB3	1.85	0.59
1:B:30:GLU:HB3	1:B:33:ARG:CD	2.33	0.58
1:G:403:LEU:HG	1:G:441:GLN:HG3	1.83	0.58
2:V:109:GLY:HA3	2:V:154:ILE:HD12	1.85	0.58
1:A:203:ASP:H	1:A:206:LEU:HD12	1.67	0.58
1:B:92:ILE:HG21	1:B:186:GLY:O	2.04	0.58
1:K:303:ARG:NH1	1:K:312:PRO:O	2.37	0.58
1:C:1:MET:HE2	1:C:1:MET:N	2.18	0.58
1:C:27:ILE:CD1	1:C:82:PHE:HA	2.32	0.58
1:M:126:THR:O	1:M:129:THR:OG1	2.19	0.58
1:D:370:PHE:CD1	1:D:462:ILE:HD11	2.38	0.58
1:C:300:ALA:HB2	1:C:313:PRO:HB3	1.86	0.58
1:O:68:SER:O	1:O:72:VAL:HG23	2.04	0.57
1:R:5:LEU:O	1:R:8:VAL:HG22	2.04	0.57
1:F:368:ILE:O	1:F:368:ILE:HG22	2.05	0.57
1:P:17:ALA:HA	1:Q:468:ILE:O	2.04	0.57
1:Q:43:ASN:OD1	1:Q:45:VAL:HG13	2.04	0.57
1:O:47:LYS:HB3	1:O:91:ALA:HB2	1.86	0.57
1:Q:341:GLU:OE1	1:Q:341:GLU:N	2.36	0.57
1:B:437:ASP:OD1	1:B:439:SER:N	2.34	0.57
1:D:147:GLU:OE2	1:J:260:ARG:NH1	2.38	0.57
1:N:43:ASN:OD1	1:N:43:ASN:O	2.23	0.57
2:d:75:GLU:OE1	2:d:75:GLU:N	2.27	0.57
2:Y:104:TYR:CG	2:Y:104:TYR:O	2.57	0.57
1:E:147:GLU:OE2	1:K:260:ARG:CZ	2.52	0.57
1:K:94:THR:HA	1:K:185:THR:HG23	1.86	0.57
1:M:402:VAL:HG23	1:M:403:LEU:HD22	1.87	0.57
2:Z:104:TYR:CG	2:Z:104:TYR:O	2.58	0.57
2:f:121:ARG:HD3	2:g:35:GLU:OE2	2.04	0.57
1:L:29:VAL:HG23	1:L:29:VAL:O	2.05	0.57
1:R:407:GLN:C	1:R:410:THR:HG22	2.28	0.57
1:C:33:ARG:HA	1:C:301:LEU:HD22	1.85	0.57
1:E:1:MET:HE2	1:E:24:SER:H	1.70	0.57
1:P:276:SER:OG	1:P:371:ILE:HD12	2.04	0.57
1:L:407:GLN:C	1:L:410:THR:HG22	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:156:TRP:H	2:V:156:TRP:CD1	2.23	0.56
1:K:47:LYS:HG2	1:K:91:ALA:HB2	1.86	0.56
1:K:405:ASN:HA	2:i:23:VAL:HG11	1.86	0.56
1:F:399:THR:OG1	1:F:401:THR:HG23	2.05	0.56
1:G:252:MET:HE2	1:G:327:ALA:HB3	1.87	0.56
1:J:145:ASN:OD1	1:J:146:LYS:N	2.39	0.56
1:L:184:THR:O	1:L:185:THR:OG1	2.23	0.56
2:h:109:GLY:HA2	2:h:154:ILE:H	1.69	0.56
2:j:109:GLY:HA3	2:j:154:ILE:HD12	1.87	0.56
1:A:155:THR:HG22	1:A:157:SER:H	1.71	0.56
1:E:100:VAL:HG13	1:E:100:VAL:O	2.04	0.56
1:F:27:ILE:HG13	1:F:33:ARG:HH11	1.71	0.56
1:F:439:SER:O	1:L:493:VAL:HG11	2.05	0.56
1:O:215:GLU:O	1:O:219:THR:OG1	2.18	0.56
2:W:106:VAL:HG13	2:W:106:VAL:O	2.06	0.56
2:d:109:GLY:HA3	2:d:154:ILE:HD12	1.87	0.56
1:G:1:MET:N	1:H:500:GLU:O	2.38	0.56
1:L:479:GLU:OE2	1:L:479:GLU:N	2.28	0.56
1:M:26:PRO:HG2	1:N:495:GLU:HG2	1.87	0.56
1:C:128:THR:CG2	1:C:156:SER:HB3	2.32	0.55
1:E:155:THR:OG1	1:E:158:THR:OG1	2.20	0.55
1:G:430:GLU:OE1	2:e:161:ALA:HB1	2.06	0.55
1:A:408:ARG:NH2	2:Y:24:ASP:O	2.37	0.55
1:Q:48:ASN:HB2	1:Q:167:THR:HG22	1.88	0.55
1:R:48:ASN:HB2	1:R:167:THR:HG22	1.87	0.55
2:Y:77:ILE:O	2:Y:81:ILE:HG12	2.06	0.55
1:Q:252:MET:HA	1:Q:252:MET:HE2	1.87	0.55
1:N:252:MET:HE2	1:N:252:MET:HA	1.87	0.55
2:j:106:VAL:HG13	2:j:106:VAL:O	2.07	0.55
1:D:437:ASP:OD1	1:D:439:SER:OG	2.22	0.55
1:F:333:GLU:OE1	1:F:333:GLU:N	2.37	0.55
1:N:27:ILE:HD12	1:N:27:ILE:O	2.07	0.55
2:Y:83:VAL:HG11	2:Y:91:VAL:HG23	1.89	0.55
1:E:1:MET:N	1:F:500:GLU:O	2.33	0.55
1:M:102:ALA:HB3	1:M:178:ILE:HG22	1.88	0.55
1:Q:490:GLN:O	1:Q:494:GLU:HG2	2.07	0.55
2:V:155:ASN:OD1	2:V:155:ASN:O	2.24	0.55
1:B:45:VAL:HG21	1:B:62:VAL:HG12	1.88	0.55
1:C:115:VAL:HG11	1:C:144:LEU:HD21	1.89	0.55
1:D:284:ASN:OD1	1:D:288:GLN:N	2.39	0.55
2:S:156:TRP:H	2:S:156:TRP:CD1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:395:SER:N	1:P:311:GLU:OE1	2.37	0.55
2:a:149:SER:O	2:a:155:ASN:ND2	2.38	0.55
1:I:33:ARG:HA	1:I:301:LEU:HD22	1.88	0.54
2:a:104:TYR:O	2:a:104:TYR:CG	2.60	0.54
1:B:43:ASN:OD1	1:B:43:ASN:O	2.25	0.54
1:C:404:ASP:O	1:C:408:ARG:HG2	2.07	0.54
1:J:303:ARG:NH1	1:J:312:PRO:O	2.40	0.54
1:K:33:ARG:HA	1:K:301:LEU:HD22	1.88	0.54
1:K:108:TYR:O	1:K:119:ILE:N	2.35	0.54
1:F:203:ASP:H	1:F:206:LEU:HD12	1.71	0.54
2:i:3:VAL:O	2:i:3:VAL:CG1	2.56	0.54
1:E:407:GLN:O	1:E:410:THR:CG2	2.51	0.54
1:G:216:ALA:HB1	1:G:228:ILE:HD13	1.90	0.54
1:G:299:MET:HE1	1:G:313:PRO:C	2.33	0.54
1:I:29:VAL:HB	1:I:207:GLU:OE2	2.05	0.54
1:P:155:THR:OG1	1:P:158:THR:OG1	2.20	0.54
1:E:410:THR:CG2	1:E:434:VAL:HG11	2.29	0.54
1:I:299:MET:HE1	1:I:313:PRO:C	2.31	0.54
1:L:155:THR:HG1	1:L:158:THR:HG1	1.56	0.54
2:S:60:TYR:OH	2:S:159:GLU:OE2	2.24	0.54
2:c:75:GLU:OE1	2:c:75:GLU:N	2.32	0.54
1:H:40:PHE:CE1	1:H:92:ILE:HD11	2.43	0.54
1:Q:36:TYR:OH	1:Q:207:GLU:O	2.16	0.54
1:C:36:TYR:OH	1:C:207:GLU:O	2.21	0.54
1:P:303:ARG:NH1	1:P:314:ALA:O	2.40	0.54
1:R:402:VAL:HG23	1:R:403:LEU:HD22	1.89	0.54
1:A:82:PHE:CD1	1:A:305:VAL:HG11	2.43	0.54
1:R:252:MET:HE2	1:R:252:MET:HA	1.90	0.54
1:D:368:ILE:O	1:D:368:ILE:HG22	2.08	0.54
1:B:370:PHE:CD1	1:B:462:ILE:HD11	2.43	0.53
1:J:90:VAL:HG22	1:J:197:THR:HG21	1.90	0.53
1:O:25:ARG:NH1	1:O:25:ARG:HB2	2.21	0.53
2:Z:75:GLU:OE2	2:Z:75:GLU:N	2.29	0.53
1:A:145:ASN:OD1	1:A:146:LYS:N	2.40	0.53
1:G:396:VAL:HA	1:G:402:VAL:HG21	1.91	0.53
1:K:5:LEU:O	1:K:8:VAL:HG22	2.08	0.53
1:K:445:LEU:HD22	1:K:450:LEU:HD12	1.90	0.53
2:T:131:ILE:HD12	2:c:51:ILE:HG12	1.89	0.53
2:X:104:TYR:CG	2:X:104:TYR:O	2.62	0.53
1:O:148:VAL:HG12	1:O:163:SER:HA	1.89	0.53
2:V:34:ILE:HD12	2:V:34:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:THR:HG1	1:E:158:THR:HG1	1.52	0.53
1:J:5:LEU:O	1:J:8:VAL:HG22	2.08	0.53
1:J:194:TYR:O	1:J:197:THR:CG2	2.54	0.53
1:P:78:ASN:OD1	1:P:321:LYS:N	2.36	0.53
2:b:77:ILE:O	2:b:81:ILE:HG12	2.09	0.53
2:i:150:ASP:OD1	2:i:151:GLY:N	2.41	0.53
1:C:100:VAL:HG13	1:C:100:VAL:O	2.08	0.53
1:C:264:GLU:O	1:C:267:THR:OG1	2.22	0.53
2:h:104:TYR:CD2	2:h:104:TYR:O	2.62	0.53
1:J:389:ASP:HA	1:J:392:ILE:HD12	1.90	0.53
1:K:248:ASP:OD1	1:K:249:SER:N	2.42	0.53
1:Q:119:ILE:HG13	1:Q:134:VAL:HG22	1.91	0.53
2:U:109:GLY:HA2	2:U:154:ILE:H	1.72	0.53
1:F:471:LYS:HE2	1:F:481:THR:HG22	1.90	0.53
1:N:27:ILE:HD12	1:N:27:ILE:C	2.34	0.53
1:H:126:THR:O	1:H:129:THR:OG1	2.22	0.52
1:L:287:ASP:OD1	1:L:287:ASP:O	2.27	0.52
2:Z:24:ASP:OD2	2:Z:76:LEU:HD13	2.09	0.52
1:J:216:ALA:HB1	1:J:228:ILE:HD13	1.92	0.52
1:J:280:PRO:HG2	1:J:346:ILE:H	1.74	0.52
1:P:148:VAL:HG12	1:P:163:SER:HA	1.91	0.52
1:A:155:THR:CG2	1:A:156:SER:N	2.72	0.52
1:D:240:ARG:HA	1:I:16:TYR:HB3	1.91	0.52
1:I:311:GLU:N	1:I:311:GLU:OE1	2.42	0.52
1:J:396:VAL:HA	1:J:402:VAL:HG21	1.90	0.52
1:P:27:ILE:HG12	1:P:83:GLY:H	1.75	0.52
2:c:121:ARG:NH2	2:c:139:GLU:OE2	2.42	0.52
1:B:473:THR:HG21	1:B:478:LEU:HA	1.92	0.52
2:Y:106:VAL:HG12	2:Y:106:VAL:O	2.10	0.52
1:C:418:TYR:OH	1:C:426:GLN:O	2.27	0.52
1:D:264:GLU:O	1:D:267:THR:OG1	2.24	0.52
1:K:440:VAL:HA	1:Q:493:VAL:HG21	1.92	0.52
1:O:3:ASN:HD21	1:O:20:GLN:HA	1.75	0.52
1:P:48:ASN:CB	1:P:167:THR:HG22	2.39	0.52
1:H:33:ARG:HA	1:H:301:LEU:HD22	1.92	0.52
1:K:248:ASP:OD2	1:K:291:PRO:CA	2.58	0.52
1:L:68:SER:O	1:L:72:VAL:HG23	2.10	0.52
1:P:404:ASP:C	1:P:404:ASP:OD1	2.53	0.52
1:R:259:ASP:OD1	1:R:259:ASP:N	2.42	0.52
1:G:184:THR:O	1:G:185:THR:OG1	2.27	0.52
1:H:26:PRO:HG2	1:I:497:THR:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:426:GLN:N	1:H:430:GLU:OE1	2.39	0.52
1:I:497:THR:OG1	1:I:500:GLU:OE1	2.27	0.52
1:E:1:MET:N	1:F:497:THR:O	2.42	0.52
1:E:433:SER:OG	2:c:150:ASP:OD1	2.28	0.52
1:L:248:ASP:OD1	1:L:248:ASP:O	2.28	0.52
2:j:109:GLY:CA	2:j:154:ILE:HD12	2.39	0.52
1:D:28:ASN:OD1	1:D:28:ASN:C	2.53	0.51
1:I:418:TYR:OH	1:I:426:GLN:O	2.27	0.51
2:S:34:ILE:HD12	2:S:34:ILE:N	2.25	0.51
2:g:74:GLU:HB2	2:h:156:TRP:HA	1.91	0.51
1:A:155:THR:HG22	1:A:156:SER:H	1.74	0.51
1:Q:404:ASP:OD1	1:Q:404:ASP:C	2.53	0.51
1:A:68:SER:O	1:A:72:VAL:HG23	2.11	0.51
1:D:239:TYR:HH	1:J:332:TRP:HH2	1.57	0.51
1:J:455:ILE:HB	1:P:470:ILE:HG22	1.91	0.51
1:K:406:ILE:HG22	1:K:453:MET:HE1	1.91	0.51
1:B:17:ALA:HA	1:C:468:ILE:O	2.10	0.51
1:B:92:ILE:HD13	1:B:186:GLY:O	2.11	0.51
1:D:403:LEU:HD22	1:D:403:LEU:H	1.76	0.51
1:Q:276:SER:OG	1:Q:371:ILE:HD12	2.11	0.51
2:f:150:ASP:N	2:f:150:ASP:OD1	2.44	0.51
1:H:450:LEU:HD21	1:N:465:ARG:NH1	2.25	0.51
1:K:248:ASP:CG	1:K:292:PRO:HD2	2.36	0.51
2:U:160:PRO:O	2:U:161:ALA:C	2.53	0.51
2:g:104:TYR:CG	2:g:104:TYR:O	2.63	0.51
1:F:264:GLU:O	1:F:267:THR:OG1	2.26	0.51
1:I:30:GLU:HB2	1:I:31:PRO:HD2	1.92	0.51
1:O:128:THR:HG23	1:O:156:SER:HB3	1.92	0.51
2:Z:103:TYR:OH	2:g:47:GLN:OE1	2.29	0.51
2:b:155:ASN:OD1	2:b:158:SER:OG	2.27	0.51
1:F:280:PRO:HG2	1:F:346:ILE:H	1.76	0.51
1:J:1:MET:N	1:K:497:THR:O	2.44	0.51
1:J:389:ASP:OD1	1:J:390:PHE:N	2.43	0.51
1:J:439:SER:O	1:P:493:VAL:HG11	2.10	0.51
1:O:23:GLN:O	1:O:24:SER:O	2.27	0.51
1:R:365:ASP:OD1	1:R:367:ASN:N	2.41	0.51
2:T:123:THR:HG23	2:U:35:GLU:HG2	1.92	0.51
2:V:154:ILE:HG21	2:V:156:TRP:CE3	2.46	0.51
1:B:203:ASP:H	1:B:206:LEU:HD12	1.75	0.51
1:J:194:TYR:C	1:J:197:THR:HG22	2.35	0.51
2:e:75:GLU:OE1	2:e:75:GLU:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PHE:CE1	1:A:305:VAL:HG11	2.46	0.51
1:F:464:GLU:OE1	1:F:465:ARG:NH1	2.43	0.51
2:Y:5:LYS:O	2:Y:5:LYS:HG3	2.10	0.51
1:D:408:ARG:NH1	2:b:17:LEU:O	2.44	0.51
1:G:435:LEU:HD22	1:M:486:THR:HG23	1.91	0.51
1:R:464:GLU:OE1	1:R:465:ARG:NH1	2.40	0.51
1:K:143:VAL:HG12	1:K:147:GLU:CD	2.36	0.50
2:a:99:TYR:HD2	2:a:108:GLN:HE22	1.58	0.50
1:A:264:GLU:O	1:A:267:THR:OG1	2.23	0.50
1:L:145:ASN:OD1	1:L:146:LYS:N	2.43	0.50
2:S:131:ILE:HD12	2:b:51:ILE:HG13	1.93	0.50
2:S:154:ILE:HG21	2:S:156:TRP:CE3	2.45	0.50
1:M:418:TYR:OH	1:M:426:GLN:O	2.30	0.50
1:R:215:GLU:O	1:R:219:THR:OG1	2.22	0.50
1:R:478:LEU:O	1:R:482:VAL:HG23	2.11	0.50
2:e:15:VAL:HB	2:e:28:TRP:HB2	1.94	0.50
2:a:33:LYS:HD2	2:a:35:GLU:OE2	2.12	0.50
2:c:19:ILE:HG21	2:c:79:ARG:HB3	1.92	0.50
1:B:174:VAL:HG21	1:B:179:PHE:HB2	1.93	0.50
1:C:399:THR:HB	1:C:401:THR:HG23	1.93	0.50
1:C:403:LEU:HD22	1:C:403:LEU:H	1.77	0.50
1:J:8:VAL:HG21	1:K:503:ALA:HB1	1.92	0.50
1:K:155:THR:HG22	1:K:157:SER:H	1.77	0.50
1:M:9:ASN:ND2	1:N:504:PRO:O	2.44	0.50
1:Q:48:ASN:CB	1:Q:167:THR:HG22	2.42	0.50
1:R:299:MET:HE1	1:R:313:PRO:C	2.37	0.50
1:R:495:GLU:OE1	1:R:497:THR:HG23	2.11	0.50
2:X:24:ASP:OD1	2:X:79:ARG:NH1	2.38	0.50
1:A:5:LEU:O	1:A:8:VAL:HG22	2.11	0.50
1:I:391:ASP:HB3	1:I:406:ILE:HD11	1.94	0.50
1:Q:128:THR:HG23	1:Q:156:SER:HB2	1.94	0.50
2:S:163:GLN:HA	2:S:163:GLN:OE1	2.12	0.50
1:D:33:ARG:HA	1:D:301:LEU:HD22	1.93	0.50
1:O:48:ASN:HB2	1:O:167:THR:HG22	1.94	0.50
2:c:19:ILE:HG23	2:c:83:VAL:HG22	1.94	0.50
1:D:10:ILE:HG21	1:D:16:TYR:CZ	2.47	0.50
2:S:101:ASP:O	2:Z:58:ILE:HD12	2.11	0.50
2:h:106:VAL:HG12	2:h:106:VAL:O	2.11	0.50
2:j:60:TYR:OH	2:j:159:GLU:OE2	2.27	0.50
1:L:216:ALA:HB1	1:L:228:ILE:HD13	1.94	0.49
2:W:131:ILE:HD12	2:Z:51:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:109:GLY:HA3	2:g:154:ILE:HD12	1.93	0.49
1:E:407:GLN:C	1:E:410:THR:HG22	2.35	0.49
1:J:292:PRO:O	1:J:296:VAL:HG23	2.12	0.49
1:M:96:TYR:HE2	1:M:170:THR:HG22	1.78	0.49
1:M:478:LEU:O	1:M:482:VAL:HG23	2.12	0.49
2:U:132:GLY:HA3	2:V:10:ILE:HD11	1.93	0.49
1:I:262:ILE:HD11	1:I:338:ALA:HB2	1.94	0.49
1:N:252:MET:HE1	1:N:279:TYR:CE1	2.46	0.49
1:R:280:PRO:HG2	1:R:346:ILE:H	1.77	0.49
2:S:106:VAL:O	2:S:106:VAL:HG13	2.12	0.49
2:W:15:VAL:HG11	2:W:65:LEU:HD22	1.94	0.49
2:f:35:GLU:CD	2:f:61:PRO:CG	2.50	0.49
1:D:373:THR:HG23	1:D:459:PRO:HG2	1.93	0.49
1:M:276:SER:OG	1:M:371:ILE:HD12	2.12	0.49
1:N:226:LEU:O	1:N:230:VAL:HG23	2.12	0.49
1:D:112:VAL:HB	1:D:144:LEU:HD11	1.95	0.49
1:D:282:LEU:HB3	1:D:323:VAL:HG11	1.95	0.49
1:H:292:PRO:O	1:H:296:VAL:HG23	2.13	0.49
1:I:216:ALA:HB1	1:I:228:ILE:HD13	1.93	0.49
1:M:490:GLN:O	1:M:494:GLU:HG2	2.12	0.49
2:U:75:GLU:OE2	2:U:75:GLU:N	2.27	0.49
1:B:292:PRO:O	1:B:296:VAL:HG23	2.13	0.49
1:J:450:LEU:HD23	1:P:465:ARG:HG3	1.94	0.49
1:B:37:MET:HE1	1:B:72:VAL:HG23	1.93	0.49
1:J:435:LEU:HD22	1:P:486:THR:HG23	1.93	0.49
2:d:83:VAL:HG11	2:d:91:VAL:HG23	1.95	0.49
1:C:368:ILE:HG22	1:C:368:ILE:O	2.13	0.49
1:F:370:PHE:CD1	1:F:462:ILE:HD11	2.47	0.49
1:G:36:TYR:OH	1:G:207:GLU:O	2.20	0.49
1:J:440:VAL:HA	1:P:493:VAL:HG21	1.94	0.49
1:F:47:LYS:HB3	1:F:91:ALA:HB2	1.95	0.49
1:H:26:PRO:HG3	1:I:497:THR:HG21	1.93	0.49
1:I:351:ASN:C	1:I:351:ASN:OD1	2.54	0.49
2:X:104:TYR:O	2:X:104:TYR:CD2	2.66	0.49
1:C:346:ILE:HG12	1:C:356:VAL:HG22	1.95	0.48
1:F:424:TYR:CD1	1:L:475:ILE:HG23	2.48	0.48
2:W:110:GLY:HA2	2:W:152:GLY:H	1.78	0.48
2:f:121:ARG:CD	2:g:35:GLU:OE2	2.61	0.48
1:A:439:SER:O	1:G:493:VAL:HG11	2.12	0.48
1:B:45:VAL:HG21	1:B:62:VAL:CG1	2.44	0.48
1:J:8:VAL:HG23	1:J:9:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:LEU:HD21	1:C:346:ILE:HG21	1.95	0.48
1:Q:437:ASP:OD1	1:Q:439:SER:OG	2.24	0.48
1:B:174:VAL:HG21	1:B:179:PHE:CB	2.44	0.48
1:C:246:LEU:HD22	1:C:278:TYR:HE2	1.78	0.48
1:O:119:ILE:HG13	1:O:134:VAL:HG22	1.96	0.48
1:Q:17:ALA:HA	1:R:468:ILE:O	2.14	0.48
2:V:36:LYS:HB2	2:V:157:TRP:HH2	1.77	0.48
2:Z:15:VAL:HB	2:Z:28:TRP:HB2	1.95	0.48
1:D:464:GLU:OE1	1:D:465:ARG:NH1	2.47	0.48
1:G:48:ASN:O	1:G:201:THR:HG23	2.14	0.48
1:R:282:LEU:HD13	1:R:323:VAL:HG11	1.95	0.48
2:Z:19:ILE:HG21	2:Z:79:ARG:HB3	1.94	0.48
2:h:24:ASP:OD1	2:h:79:ARG:NH1	2.47	0.48
1:C:366:PRO:HA	1:C:369:VAL:HG23	1.95	0.48
1:I:282:LEU:HB3	1:I:323:VAL:HG11	1.96	0.48
1:N:48:ASN:HB2	1:N:167:THR:HG22	1.96	0.48
2:c:19:ILE:CG2	2:c:83:VAL:HG22	2.44	0.48
2:f:131:ILE:O	2:f:131:ILE:HG22	2.12	0.48
1:L:33:ARG:HA	1:L:301:LEU:HD22	1.95	0.48
2:V:131:ILE:HD11	2:Y:44:SER:HB2	1.96	0.48
1:I:454:PHE:CD2	1:O:469:ASN:ND2	2.82	0.48
1:B:37:MET:HE1	1:B:72:VAL:CG2	2.44	0.48
1:D:426:GLN:N	1:D:430:GLU:OE1	2.41	0.48
1:E:346:ILE:HG12	1:E:356:VAL:HG22	1.95	0.48
1:L:47:LYS:HA	1:L:89:ASN:HB3	1.95	0.48
2:U:104:TYR:O	2:U:104:TYR:CG	2.65	0.48
1:J:464:GLU:OE1	1:J:465:ARG:NH1	2.47	0.47
1:P:119:ILE:HG13	1:P:134:VAL:HG22	1.96	0.47
1:B:403:LEU:H	1:B:403:LEU:HD22	1.78	0.47
1:E:408:ARG:NH1	2:c:16:ASN:HB3	2.29	0.47
1:J:143:VAL:HG12	1:J:147:GLU:CD	2.39	0.47
1:K:226:LEU:O	1:K:230:VAL:HG23	2.14	0.47
1:N:78:ASN:OD1	1:N:321:LYS:N	2.41	0.47
1:Q:31:PRO:O	1:Q:208:ALA:HB3	2.14	0.47
2:Z:102:GLY:O	2:g:48:SER:HB2	2.14	0.47
1:F:292:PRO:O	1:F:296:VAL:HG23	2.13	0.47
1:D:27:ILE:HD11	1:D:81:GLY:O	2.15	0.47
1:K:155:THR:CG2	1:K:156:SER:N	2.76	0.47
1:L:41:ALA:HB3	1:L:89:ASN:HD21	1.80	0.47
1:O:495:GLU:OE2	1:O:495:GLU:HA	2.14	0.47
2:Z:19:ILE:CG2	2:Z:83:VAL:HG22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:155:ASN:O	2:Z:155:ASN:ND2	2.47	0.47
2:a:101:ASP:OD2	2:g:38:TYR:OH	2.32	0.47
2:i:33:LYS:HE3	2:i:35:GLU:OE2	2.14	0.47
1:A:384:LEU:HD13	1:A:455:ILE:HD13	1.97	0.47
1:L:217:PHE:HB2	1:L:248:ASP:CG	2.39	0.47
1:R:47:LYS:HB3	1:R:91:ALA:HB2	1.97	0.47
2:S:98:MET:HE3	2:S:98:MET:HB3	1.63	0.47
2:Z:121:ARG:HG2	2:a:35:GLU:OE1	2.14	0.47
2:c:74:GLU:HG2	2:c:75:GLU:OE1	2.15	0.47
1:A:366:PRO:HA	1:A:369:VAL:HG23	1.96	0.47
1:B:33:ARG:HH12	1:B:305:VAL:HG22	1.80	0.47
1:F:284:ASN:OD1	1:F:288:GLN:N	2.43	0.47
1:L:143:VAL:HG12	1:L:147:GLU:CD	2.39	0.47
2:e:26:ARG:CZ	2:e:75:GLU:OE2	2.63	0.47
1:B:276:SER:OG	1:B:371:ILE:HD12	2.15	0.47
1:G:248:ASP:OD2	1:G:291:PRO:HB3	2.15	0.47
1:R:53:ILE:HD11	1:R:63:TYR:HE2	1.79	0.47
2:U:131:ILE:HD11	2:d:43:TYR:C	2.40	0.47
2:X:131:ILE:HD12	2:a:51:ILE:HG12	1.97	0.47
2:j:104:TYR:CG	2:j:104:TYR:O	2.67	0.47
1:A:155:THR:CG2	1:A:156:SER:H	2.27	0.47
1:F:92:ILE:HD13	1:F:186:GLY:O	2.15	0.47
1:H:368:ILE:O	1:H:368:ILE:HG22	2.14	0.47
1:O:110:VAL:HG22	1:O:174:VAL:HG12	1.96	0.47
1:Q:403:LEU:HD12	1:Q:438:ALA:HB2	1.97	0.47
2:S:104:TYR:CG	2:S:104:TYR:O	2.68	0.47
2:X:106:VAL:HG12	2:X:106:VAL:O	2.15	0.47
2:h:117:CYS:HA	2:h:143:ASN:O	2.15	0.47
1:H:2:THR:OG1	1:H:3:ASN:N	2.45	0.47
1:K:282:LEU:HB3	1:K:323:VAL:HG11	1.95	0.47
1:P:68:SER:O	1:P:72:VAL:HG23	2.15	0.47
1:P:427:THR:OG1	1:P:430:GLU:OE2	2.32	0.47
2:Y:5:LYS:O	2:Y:5:LYS:CG	2.63	0.47
2:i:17:LEU:CD2	2:i:93:VAL:HG22	2.45	0.47
2:i:159:GLU:HB3	2:i:160:PRO:HD2	1.96	0.47
1:B:216:ALA:HB1	1:B:228:ILE:HD12	1.97	0.47
1:M:299:MET:HE1	1:M:313:PRO:C	2.40	0.47
1:O:380:VAL:HG22	1:O:417:LEU:HD13	1.97	0.47
1:O:487:ALA:O	1:O:491:SER:OG	2.24	0.47
1:R:404:ASP:C	1:R:404:ASP:OD1	2.58	0.47
1:R:486:THR:HG21	2:j:152:GLY:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:42:GLU:OE2	2:X:59:LYS:NZ	2.48	0.46
2:V:104:TYR:CG	2:V:104:TYR:O	2.69	0.46
2:f:33:LYS:O	2:f:35:GLU:OE1	2.33	0.46
2:f:75:GLU:O	2:f:79:ARG:HG3	2.15	0.46
1:B:58:ASP:C	1:B:58:ASP:OD1	2.57	0.46
1:C:370:PHE:CD1	1:C:462:ILE:HD11	2.50	0.46
1:J:184:THR:O	1:J:185:THR:OG1	2.27	0.46
1:K:287:ASP:OD1	1:K:287:ASP:O	2.34	0.46
1:O:78:ASN:OD1	1:O:321:LYS:N	2.40	0.46
2:W:104:TYR:CG	2:W:104:TYR:O	2.68	0.46
2:Y:40:THR:HB	2:Y:53:THR:HG23	1.98	0.46
2:Y:42:GLU:HG2	2:Y:51:ILE:HG23	1.97	0.46
1:A:203:ASP:HB3	1:A:206:LEU:HG	1.97	0.46
1:E:478:LEU:O	1:E:482:VAL:HG23	2.15	0.46
1:H:145:ASN:OD1	1:H:146:LYS:N	2.47	0.46
1:L:282:LEU:HD13	1:L:323:VAL:HG11	1.96	0.46
1:N:126:THR:HG23	1:N:128:THR:HB	1.97	0.46
1:O:403:LEU:HD12	1:O:438:ALA:HB2	1.96	0.46
1:Q:252:MET:HE1	1:Q:279:TYR:CE1	2.51	0.46
2:T:159:GLU:HA	2:T:159:GLU:OE2	2.16	0.46
1:D:47:LYS:HB3	1:D:91:ALA:HB2	1.98	0.46
1:H:235:LEU:HD12	1:H:241:TYR:CD2	2.50	0.46
2:S:18:ASN:OD1	2:S:23:VAL:HG22	2.16	0.46
2:U:57:ALA:HB1	2:V:51:ILE:HD11	1.96	0.46
2:V:123:THR:HG23	2:W:35:GLU:HG2	1.98	0.46
1:A:288:GLN:HE21	1:A:288:GLN:HB3	1.49	0.46
1:B:494:GLU:OE2	1:B:494:GLU:C	2.59	0.46
1:D:248:ASP:OD1	1:D:248:ASP:N	2.48	0.46
1:L:395:SER:N	1:R:311:GLU:OE1	2.42	0.46
1:K:410:THR:HG23	1:K:411:ASN:N	2.30	0.46
1:L:450:LEU:HD21	1:R:465:ARG:CZ	2.45	0.46
2:W:60:TYR:OH	2:W:159:GLU:OE1	2.34	0.46
2:d:131:ILE:O	2:e:57:ALA:HB2	2.16	0.46
2:h:145:SER:HB3	2:i:52:TYR:HD1	1.78	0.46
1:D:404:ASP:O	1:D:408:ARG:HG2	2.15	0.46
2:e:84:ASN:ND2	2:e:119:VAL:O	2.43	0.46
1:A:370:PHE:CD1	1:A:462:ILE:HD11	2.50	0.46
1:E:374:ARG:NH2	1:J:19:TYR:OH	2.44	0.46
1:E:450:LEU:HD11	1:K:465:ARG:HH12	1.80	0.46
1:L:426:GLN:N	1:L:430:GLU:OE1	2.47	0.46
1:O:108:TYR:OH	1:O:177:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:25:ARG:HE	1:Q:25:ARG:HB2	1.46	0.46
2:f:81:ILE:HD12	2:g:36:LYS:HD2	1.97	0.46
1:A:28:ASN:C	1:A:28:ASN:OD1	2.58	0.46
1:A:384:LEU:CD1	1:A:455:ILE:HD13	2.46	0.46
1:C:115:VAL:CG1	1:C:144:LEU:HD21	2.46	0.46
1:L:388:TYR:OH	1:L:410:THR:HB	2.16	0.46
1:M:282:LEU:H	1:M:282:LEU:HG	1.27	0.46
2:S:123:THR:OG1	2:T:35:GLU:OE2	2.27	0.46
2:Y:115:GLU:OE2	2:Y:146:ARG:NE	2.49	0.46
2:a:97:PRO:HG2	2:a:156:TRP:CZ2	2.51	0.46
2:d:131:ILE:HG23	2:f:51:ILE:HD13	1.98	0.46
1:J:40:PHE:CE1	1:J:92:ILE:HD11	2.51	0.45
1:K:453:MET:HG2	1:K:455:ILE:HD11	1.97	0.45
1:L:262:ILE:HD11	1:L:338:ALA:HB2	1.97	0.45
1:P:418:TYR:OH	1:P:426:GLN:O	2.34	0.45
2:g:109:GLY:CA	2:g:154:ILE:HD12	2.46	0.45
1:B:439:SER:O	1:H:493:VAL:HG11	2.17	0.45
1:H:500:GLU:CD	1:H:501:GLY:N	2.74	0.45
1:J:202:PHE:O	1:J:241:TYR:OH	2.32	0.45
1:J:282:LEU:HB3	1:J:323:VAL:HG11	1.98	0.45
1:N:495:GLU:HA	1:N:495:GLU:OE2	2.15	0.45
1:Q:67:ALA:HB3	1:Q:215:GLU:HG3	1.98	0.45
2:V:106:VAL:O	2:V:106:VAL:CG2	2.62	0.45
1:A:8:VAL:CG2	1:B:503:ALA:HB1	2.46	0.45
2:d:131:ILE:HG23	2:f:51:ILE:CD1	2.46	0.45
2:g:33:LYS:CE	2:g:35:GLU:OE1	2.48	0.45
2:h:42:GLU:HG2	2:h:51:ILE:CG2	2.46	0.45
1:E:370:PHE:CD1	1:E:462:ILE:HD11	2.51	0.45
1:G:374:ARG:NH2	1:R:19:TYR:OH	2.45	0.45
1:H:252:MET:HE2	1:H:252:MET:HA	1.99	0.45
1:H:450:LEU:HD21	1:N:465:ARG:CZ	2.47	0.45
1:I:264:GLU:O	1:I:267:THR:OG1	2.29	0.45
1:Q:478:LEU:O	1:Q:482:VAL:HG23	2.17	0.45
1:A:284:ASN:HA	1:A:323:VAL:HA	1.98	0.45
1:C:473:THR:HG21	1:C:478:LEU:HA	1.98	0.45
1:E:92:ILE:HD13	1:E:186:GLY:O	2.17	0.45
1:G:26:PRO:HG2	1:H:497:THR:HG22	1.96	0.45
2:T:4:SER:HB3	2:T:5:LYS:H	1.60	0.45
2:Y:74:GLU:HG2	2:Z:154:ILE:CG2	2.46	0.45
1:G:155:THR:OG1	1:G:158:THR:OG1	2.20	0.45
1:M:246:LEU:HD22	1:M:278:TYR:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:158:SER:O	2:T:158:SER:OG	2.35	0.45
2:U:106:VAL:O	2:U:106:VAL:CG1	2.64	0.45
2:f:86:ASP:OD1	2:f:86:ASP:C	2.60	0.45
2:i:131:ILE:HG22	2:i:131:ILE:O	2.17	0.45
1:A:83:GLY:HA3	1:A:301:LEU:HD13	1.98	0.45
1:D:442:VAL:HG11	1:J:499:THR:HG21	1.98	0.45
1:F:128:THR:HG23	1:F:156:SER:HB2	1.99	0.45
1:H:272:GLN:O	1:H:368:ILE:HG21	2.17	0.45
1:I:451:VAL:HB	1:O:466:LEU:HD12	1.99	0.45
1:K:395:SER:N	1:Q:311:GLU:OE1	2.45	0.45
1:O:299:MET:HE1	1:O:313:PRO:C	2.42	0.45
1:O:490:GLN:O	1:O:494:GLU:OE2	2.34	0.45
1:P:495:GLU:OE1	1:P:497:THR:HG23	2.17	0.45
2:X:100:ARG:HB3	2:X:105:ASN:HA	1.98	0.45
1:B:450:LEU:HD21	1:G:7:GLY:O	2.16	0.45
1:F:349:LYS:HG3	1:F:355:VAL:HG21	1.99	0.45
1:G:489:LEU:HD23	1:L:23:GLN:HG3	1.99	0.45
2:b:100:ARG:HD2	2:i:48:SER:HA	1.99	0.45
1:I:408:ARG:NH2	2:g:24:ASP:O	2.49	0.45
1:K:212:ILE:HG22	1:K:246:LEU:HB2	1.99	0.45
1:L:286:ASP:O	1:L:287:ASP:HB3	2.16	0.45
1:L:374:ARG:NH2	1:L:378:ASN:OD1	2.45	0.45
1:L:464:GLU:OE1	1:L:465:ARG:NH1	2.50	0.45
1:O:304:PHE:HZ	1:O:375:ILE:HD13	1.81	0.45
2:e:42:GLU:HG2	2:e:51:ILE:HG22	1.97	0.45
2:f:35:GLU:CD	2:f:61:PRO:CD	2.86	0.45
1:B:437:ASP:OD1	1:B:439:SER:OG	2.30	0.45
1:I:33:ARG:HH21	1:I:305:VAL:HG22	1.81	0.45
2:U:131:ILE:HG23	2:d:51:ILE:HG12	1.98	0.45
2:d:19:ILE:CG2	2:d:83:VAL:HG22	2.46	0.45
1:D:415:THR:O	1:D:419:GLN:HG2	2.17	0.44
1:I:406:ILE:HG22	1:I:453:MET:HE1	1.98	0.44
1:L:410:THR:HG23	1:L:411:ASN:N	2.31	0.44
1:M:26:PRO:HG3	1:N:492:SER:HA	1.99	0.44
1:N:127:THR:HA	1:N:130:ILE:HD12	1.99	0.44
2:T:75:GLU:OE1	2:T:79:ARG:NH2	2.50	0.44
2:d:97:PRO:HG3	2:d:156:TRP:CZ2	2.52	0.44
2:e:86:ASP:C	2:e:86:ASP:OD1	2.61	0.44
1:G:25:ARG:HH22	1:G:82:PHE:HZ	1.58	0.44
1:I:94:THR:HG22	1:I:95:ARG:N	2.33	0.44
1:M:264:GLU:O	1:M:267:THR:OG1	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:226:LEU:O	1:P:230:VAL:HG23	2.17	0.44
1:R:304:PHE:HZ	1:R:375:ILE:HD13	1.82	0.44
2:W:11:ASN:OD1	2:W:11:ASN:C	2.60	0.44
2:h:104:TYR:O	2:h:104:TYR:CG	2.70	0.44
1:C:299:MET:HE3	1:C:299:MET:HB3	1.70	0.44
1:C:384:LEU:HD13	1:C:455:ILE:HD13	1.98	0.44
1:C:419:GLN:OE1	1:C:419:GLN:HA	2.16	0.44
1:N:155:THR:HG23	1:N:158:THR:N	2.33	0.44
2:Z:115:GLU:OE2	2:Z:148:ARG:HG2	2.17	0.44
2:e:109:GLY:CA	2:e:154:ILE:HD12	2.46	0.44
1:B:458:VAL:HG22	1:H:473:THR:OG1	2.17	0.44
1:I:226:LEU:O	1:I:230:VAL:HG23	2.16	0.44
1:K:366:PRO:HA	1:K:369:VAL:HG23	1.98	0.44
1:K:403:LEU:HD13	1:K:441:GLN:HG3	2.00	0.44
1:C:128:THR:CG2	1:C:156:SER:CB	2.85	0.44
1:C:456:TRP:CD2	1:I:482:VAL:HG22	2.52	0.44
1:F:191:VAL:O	1:F:195:VAL:HG23	2.17	0.44
1:G:282:LEU:HB3	1:G:323:VAL:HG11	1.99	0.44
1:H:264:GLU:O	1:H:267:THR:OG1	2.30	0.44
1:M:368:ILE:HG23	1:M:368:ILE:O	2.18	0.44
2:c:19:ILE:HG23	2:c:83:VAL:CG2	2.48	0.44
2:f:45:ASP:OD1	2:f:45:ASP:N	2.42	0.44
1:D:23:GLN:HG3	1:E:489:LEU:HD23	1.98	0.44
1:K:430:GLU:OE2	2:i:161:ALA:HB1	2.17	0.44
1:L:214:PRO:HA	1:L:248:ASP:OD2	2.18	0.44
1:O:259:ASP:OD1	1:O:259:ASP:N	2.51	0.44
1:P:299:MET:HE1	1:P:313:PRO:C	2.43	0.44
1:P:368:ILE:O	1:P:368:ILE:HG23	2.16	0.44
2:X:131:ILE:HD11	2:a:44:SER:HB2	1.98	0.44
2:a:109:GLY:HA3	2:a:154:ILE:HD12	2.00	0.44
2:d:101:ASP:HB3	2:d:102:GLY:H	1.64	0.44
1:B:147:GLU:HG3	1:B:148:VAL:HG13	1.99	0.44
1:C:225:ARG:NE	1:C:264:GLU:OE2	2.46	0.44
1:F:130:ILE:O	1:F:134:VAL:HG23	2.17	0.44
1:I:248:ASP:OD2	1:I:293:SER:OG	2.22	0.44
1:K:41:ALA:CB	1:K:63:TYR:HB3	2.47	0.44
1:L:435:LEU:HD22	1:R:486:THR:HG23	1.99	0.44
1:R:78:ASN:OD1	1:R:321:LYS:N	2.41	0.44
2:d:112:ILE:HD11	2:d:156:TRP:CE2	2.53	0.44
2:d:112:ILE:HD11	2:d:156:TRP:NE1	2.32	0.44
1:B:435:LEU:CD2	1:H:486:THR:HG23	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:THR:HG21	1:D:455:ILE:HD11	2.00	0.44
1:G:414:LEU:HD23	1:G:417:LEU:HD12	1.99	0.44
1:H:451:VAL:HB	1:N:466:LEU:HD12	1.99	0.44
1:K:280:PRO:HG2	1:K:346:ILE:H	1.82	0.44
1:O:404:ASP:OD1	1:O:404:ASP:C	2.61	0.44
1:O:502:THR:HG23	1:O:502:THR:O	2.18	0.44
2:X:6:ARG:O	2:X:99:TYR:OH	2.28	0.44
2:h:84:ASN:ND2	2:h:119:VAL:O	2.48	0.44
1:B:113:ASN:ND2	1:B:147:GLU:HG2	2.29	0.44
1:G:25:ARG:NH2	1:G:82:PHE:CE1	2.86	0.44
1:G:286:ASP:O	1:G:287:ASP:HB3	2.18	0.44
1:I:418:TYR:HH	1:I:426:GLN:C	2.26	0.44
1:M:29:VAL:O	1:M:29:VAL:HG13	2.18	0.44
1:B:20:GLN:HB3	1:C:471:LYS:HB2	2.00	0.43
1:F:48:ASN:ND2	1:F:91:ALA:HB3	2.33	0.43
1:G:287:ASP:CG	1:G:287:ASP:O	2.60	0.43
1:H:226:LEU:O	1:H:230:VAL:HG23	2.18	0.43
1:J:300:ALA:HB2	1:J:313:PRO:HB3	2.00	0.43
1:J:500:GLU:OE1	1:J:500:GLU:C	2.60	0.43
1:O:282:LEU:HD11	1:O:292:PRO:HA	1.99	0.43
1:P:453:MET:HE1	1:P:455:ILE:HD11	2.00	0.43
2:a:156:TRP:CD1	2:a:156:TRP:H	2.34	0.43
1:B:284:ASN:OD1	1:B:288:GLN:N	2.47	0.43
1:E:264:GLU:O	1:E:267:THR:OG1	2.32	0.43
1:E:415:THR:O	1:E:419:GLN:HG2	2.19	0.43
1:I:391:ASP:CB	1:I:406:ILE:HD11	2.48	0.43
1:K:451:VAL:HB	1:Q:466:LEU:HD12	1.98	0.43
1:N:490:GLN:O	1:N:494:GLU:HG2	2.18	0.43
2:a:92:THR:HG22	2:a:94:PHE:CE1	2.53	0.43
2:f:35:GLU:OE2	2:f:61:PRO:CD	2.66	0.43
1:B:264:GLU:O	1:B:267:THR:OG1	2.32	0.43
1:D:300:ALA:HB2	1:D:313:PRO:HB3	2.00	0.43
1:E:27:ILE:HD11	1:E:84:ASN:OD1	2.17	0.43
1:E:410:THR:HG23	1:E:411:ASN:N	2.33	0.43
1:E:477:ASP:OD1	1:E:477:ASP:N	2.51	0.43
1:G:5:LEU:HB2	1:H:504:PRO:HD2	2.00	0.43
1:H:287:ASP:CG	1:H:287:ASP:O	2.61	0.43
1:N:191:VAL:HG23	1:N:228:ILE:HD11	2.01	0.43
1:N:246:LEU:HD22	1:N:278:TYR:HE2	1.84	0.43
2:U:116:PHE:O	2:U:145:SER:OG	2.33	0.43
1:I:374:ARG:NH2	1:N:19:TYR:OH	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:453:MET:HG2	1:J:455:ILE:HD11	2.00	0.43
1:M:74:LEU:HD12	1:M:290:VAL:HG11	2.00	0.43
1:M:148:VAL:HG12	1:M:163:SER:HA	2.00	0.43
1:P:216:ALA:HB1	1:P:228:ILE:HD13	2.00	0.43
1:Q:366:PRO:HA	1:Q:369:VAL:HG23	2.00	0.43
1:R:267:THR:HG23	1:R:268:TYR:N	2.32	0.43
1:R:415:THR:O	1:R:419:GLN:HG2	2.18	0.43
1:C:201:THR:O	1:C:201:THR:HG22	2.19	0.43
1:J:197:THR:HG23	1:J:198:ILE:N	2.34	0.43
1:N:1:MET:HE1	1:N:24:SER:HB3	2.01	0.43
1:P:403:LEU:HD12	1:P:438:ALA:HB2	2.00	0.43
2:S:158:SER:O	2:S:158:SER:OG	2.37	0.43
2:U:123:THR:HG23	2:V:35:GLU:HG3	2.01	0.43
1:B:407:GLN:HA	1:B:453:MET:HE1	2.00	0.43
1:D:299:MET:HE1	1:D:313:PRO:C	2.43	0.43
1:F:5:LEU:N	1:F:5:LEU:HD22	2.34	0.43
1:F:303:ARG:NE	1:F:312:PRO:O	2.52	0.43
1:I:287:ASP:O	1:I:287:ASP:CG	2.62	0.43
1:I:429:SER:HA	2:g:148:ARG:NH1	2.33	0.43
1:J:430:GLU:OE2	2:h:161:ALA:HB1	2.19	0.43
1:N:99:VAL:HB	1:N:180:THR:HG22	2.00	0.43
1:N:259:ASP:OD1	1:N:259:ASP:N	2.52	0.43
2:S:33:LYS:HD2	2:S:35:GLU:OE2	2.18	0.43
2:e:3:VAL:HG12	2:e:4:SER:H	1.83	0.43
1:E:220:PHE:HB3	1:E:224:ASP:HB2	2.01	0.43
1:L:407:GLN:HA	1:L:410:THR:HG22	2.01	0.43
1:M:366:PRO:HA	1:M:369:VAL:HG23	2.00	0.43
1:N:403:LEU:HD12	1:N:438:ALA:HB2	2.01	0.43
1:N:418:TYR:OH	1:N:426:GLN:O	2.36	0.43
1:Q:287:ASP:O	1:Q:287:ASP:CG	2.62	0.43
2:d:150:ASP:OD1	2:d:151:GLY:N	2.50	0.43
1:H:45:VAL:HG23	1:H:46:ASN:N	2.33	0.43
1:H:92:ILE:HD13	1:H:186:GLY:O	2.19	0.43
1:J:403:LEU:H	1:J:403:LEU:HG	1.70	0.43
1:K:68:SER:O	1:K:72:VAL:HG23	2.19	0.43
1:L:9:ASN:N	1:L:9:ASN:OD1	2.51	0.43
1:O:366:PRO:HA	1:O:369:VAL:HG23	2.00	0.43
1:R:264:GLU:OE1	1:R:277:TYR:OH	2.34	0.43
2:S:5:LYS:HD2	2:Y:87:PRO:HB2	1.99	0.43
2:a:22:PHE:CD2	2:a:79:ARG:HD2	2.54	0.43
2:e:160:PRO:O	2:e:161:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLU:HB3	1:B:33:ARG:HD3	1.92	0.43
1:D:92:ILE:HD13	1:D:186:GLY:O	2.19	0.43
1:D:235:LEU:HD12	1:D:241:TYR:CD2	2.54	0.43
1:H:225:ARG:NE	1:H:264:GLU:OE2	2.49	0.43
1:H:440:VAL:HA	1:N:493:VAL:HG21	2.00	0.43
1:K:95:ARG:H	1:K:185:THR:HA	1.83	0.43
1:K:126:THR:O	1:K:129:THR:OG1	2.25	0.43
1:K:264:GLU:O	1:K:267:THR:OG1	2.29	0.43
1:M:26:PRO:HG2	1:N:495:GLU:CG	2.48	0.43
1:N:67:ALA:HB3	1:N:215:GLU:HG3	2.00	0.43
2:U:11:ASN:OD1	2:U:11:ASN:C	2.61	0.43
2:b:109:GLY:HA3	2:b:154:ILE:HD12	2.01	0.43
2:j:33:LYS:HE2	2:j:35:GLU:OE1	2.18	0.43
1:A:235:LEU:HD12	1:A:241:TYR:CD2	2.54	0.43
1:C:191:VAL:O	1:C:195:VAL:HG23	2.19	0.43
1:E:8:VAL:CG2	1:F:503:ALA:HB1	2.49	0.43
1:E:252:MET:HE3	1:E:252:MET:HA	2.01	0.43
1:F:500:GLU:OE2	1:F:500:GLU:HA	2.19	0.43
1:I:405:ASN:HA	2:g:23:VAL:HG11	2.01	0.43
1:P:299:MET:HE3	1:P:299:MET:HB3	1.95	0.43
1:R:43:ASN:HB3	1:R:45:VAL:HG13	2.01	0.43
1:R:262:ILE:HD11	1:R:338:ALA:HB2	2.01	0.43
1:R:495:GLU:CD	1:R:497:THR:HG23	2.44	0.43
2:T:58:ILE:N	2:U:49:ASN:O	2.52	0.43
2:T:110:GLY:HA2	2:T:152:GLY:N	2.33	0.43
2:Z:77:ILE:O	2:Z:81:ILE:HG12	2.19	0.43
2:Z:163:GLN:H	2:Z:163:GLN:HG2	1.42	0.43
1:I:96:TYR:HE1	1:I:183:THR:HG1	1.67	0.42
1:N:404:ASP:OD1	1:N:404:ASP:C	2.60	0.42
2:V:131:ILE:HG22	2:V:131:ILE:O	2.18	0.42
2:Z:19:ILE:HG23	2:Z:83:VAL:HG22	2.01	0.42
2:c:40:THR:HB	2:c:53:THR:HG23	2.01	0.42
1:A:203:ASP:H	1:A:206:LEU:CD1	2.30	0.42
1:A:424:TYR:CD2	1:G:475:ILE:HG23	2.54	0.42
1:D:33:ARG:HE	1:D:33:ARG:HB2	1.59	0.42
1:G:464:GLU:HG2	1:L:13:PRO:HB3	2.00	0.42
1:K:75:PHE:CE1	1:K:85:LEU:HB2	2.54	0.42
2:T:155:ASN:C	2:T:155:ASN:OD1	2.61	0.42
2:c:74:GLU:CB	2:d:156:TRP:HB3	2.50	0.42
2:g:36:LYS:HE2	2:g:58:ILE:HD13	2.00	0.42
1:I:45:VAL:HG23	1:I:46:ASN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:495:GLU:OE2	1:M:495:GLU:HA	2.19	0.42
1:P:145:ASN:OD1	1:P:146:LYS:N	2.53	0.42
1:P:246:LEU:HD22	1:P:278:TYR:HE2	1.84	0.42
1:R:246:LEU:HD22	1:R:278:TYR:HE1	1.84	0.42
2:S:127:GLU:HG3	2:T:10:ILE:HD12	2.01	0.42
1:H:395:SER:N	1:N:311:GLU:OE1	2.44	0.42
1:I:187:THR:O	1:I:187:THR:HG22	2.20	0.42
1:I:388:TYR:OH	1:I:410:THR:OG1	2.00	0.42
1:L:389:ASP:HA	1:L:392:ILE:HD12	2.01	0.42
1:M:404:ASP:OD1	1:M:404:ASP:N	2.51	0.42
1:N:282:LEU:H	1:N:282:LEU:HG	1.61	0.42
1:O:201:THR:O	1:O:202:PHE:C	2.61	0.42
2:U:60:TYR:OH	2:U:159:GLU:OE1	2.32	0.42
2:Y:81:ILE:HG23	2:Z:36:LYS:HZ2	1.83	0.42
1:A:409:LYS:HA	1:A:412:THR:HG22	2.02	0.42
1:C:140:ASN:N	1:C:140:ASN:OD1	2.52	0.42
1:G:248:ASP:OD2	1:G:281:TYR:HE1	2.00	0.42
1:J:126:THR:O	1:J:129:THR:OG1	2.30	0.42
1:M:45:VAL:HG21	1:M:62:VAL:HG12	2.01	0.42
1:M:145:ASN:OD1	1:M:146:LYS:N	2.51	0.42
1:N:264:GLU:O	1:N:267:THR:OG1	2.31	0.42
1:O:10:ILE:HG21	1:O:16:TYR:OH	2.19	0.42
1:O:216:ALA:HB1	1:O:228:ILE:HD13	2.01	0.42
1:R:410:THR:HG23	1:R:411:ASN:N	2.34	0.42
2:S:131:ILE:O	2:S:131:ILE:HG22	2.18	0.42
2:U:14:ALA:HB1	2:U:27:TYR:HE2	1.84	0.42
2:V:97:PRO:HG2	2:V:156:TRP:HZ2	1.84	0.42
2:W:131:ILE:HD11	2:Z:44:SER:HB2	2.01	0.42
2:h:98:MET:HE3	2:h:98:MET:HB3	1.72	0.42
1:B:220:PHE:HB3	1:B:224:ASP:HB2	2.01	0.42
1:E:391:ASP:OD2	1:E:409:LYS:NZ	2.50	0.42
1:H:47:LYS:HB2	1:H:91:ALA:HB2	2.01	0.42
1:H:212:ILE:HG22	1:H:246:LEU:HB2	2.00	0.42
1:H:439:SER:O	1:N:493:VAL:HG11	2.19	0.42
1:I:33:ARG:NH2	1:I:305:VAL:HG22	2.34	0.42
1:J:36:TYR:OH	1:J:207:GLU:O	2.20	0.42
1:K:388:TYR:OH	1:K:410:THR:HB	2.20	0.42
1:N:277:TYR:HB2	1:N:362:LEU:HD21	2.02	0.42
1:R:495:GLU:OE2	1:R:497:THR:HG23	2.20	0.42
2:Z:121:ARG:CG	2:a:35:GLU:OE1	2.68	0.42
2:j:121:ARG:HB3	2:j:141:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:LEU:HD11	1:H:499:THR:O	2.20	0.42
1:I:27:ILE:HG23	1:I:33:ARG:NH1	2.34	0.42
1:J:479:GLU:HA	1:J:482:VAL:HB	2.02	0.42
1:Q:368:ILE:O	1:Q:368:ILE:HG23	2.18	0.42
2:c:24:ASP:OD2	2:c:76:LEU:HD13	2.20	0.42
1:A:47:LYS:O	1:A:49:VAL:HG23	2.20	0.42
1:A:252:MET:HE3	1:A:252:MET:HA	2.00	0.42
1:F:248:ASP:OD1	1:F:248:ASP:N	2.52	0.42
1:F:475:ILE:HG23	1:F:475:ILE:O	2.19	0.42
1:I:461:THR:OG1	1:I:462:ILE:N	2.52	0.42
1:J:45:VAL:HG23	1:J:46:ASN:N	2.34	0.42
2:a:159:GLU:OE2	2:a:159:GLU:HA	2.20	0.42
2:b:128:ILE:HD12	2:c:31:CYS:HB3	2.02	0.42
2:h:66:SER:OG	2:h:137:MET:HE3	2.20	0.42
1:C:374:ARG:HH22	1:H:19:TYR:HH	1.65	0.42
1:F:144:LEU:N	1:F:144:LEU:HD22	2.34	0.42
1:G:126:THR:O	1:G:129:THR:OG1	2.35	0.42
1:L:403:LEU:HD13	1:L:441:GLN:HG3	2.01	0.42
2:U:40:THR:HB	2:U:53:THR:HG23	2.00	0.42
1:B:197:THR:O	1:B:201:THR:HB	2.20	0.42
1:G:187:THR:O	1:G:187:THR:HG22	2.19	0.42
1:G:395:SER:N	1:M:311:GLU:OE1	2.45	0.42
1:L:248:ASP:OD1	1:L:248:ASP:C	2.63	0.42
1:L:281:TYR:HB3	1:L:282:LEU:H	1.75	0.42
1:L:366:PRO:HA	1:L:369:VAL:HG23	2.02	0.42
1:M:43:ASN:OD1	1:M:43:ASN:N	2.53	0.42
1:M:503:ALA:HB1	1:R:8:VAL:HG21	2.02	0.42
1:P:453:MET:HE2	1:P:453:MET:HB2	1.93	0.42
1:Q:495:GLU:OE2	1:Q:495:GLU:HA	2.19	0.42
1:R:276:SER:OG	1:R:371:ILE:HD12	2.20	0.42
2:i:74:GLU:HG2	2:i:75:GLU:N	2.34	0.42
1:C:350:GLU:OE2	1:C:350:GLU:HA	2.20	0.41
1:G:461:THR:OG1	1:G:462:ILE:N	2.53	0.41
1:R:45:VAL:HG11	1:R:62:VAL:O	2.20	0.41
2:T:131:ILE:HD11	2:c:44:SER:HB2	2.01	0.41
2:f:35:GLU:OE2	2:f:61:PRO:O	2.37	0.41
2:f:41:GLY:O	2:f:54:LEU:N	2.46	0.41
1:B:142:THR:O	1:B:145:ASN:ND2	2.53	0.41
1:C:119:ILE:HG23	1:C:133:ASP:OD2	2.20	0.41
1:E:235:LEU:HD12	1:E:241:TYR:CE2	2.55	0.41
1:E:405:ASN:HA	2:c:23:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:PHE:HB3	1:G:224:ASP:HB2	2.01	0.41
1:G:280:PRO:HG2	1:G:346:ILE:H	1.85	0.41
1:G:368:ILE:HG13	1:G:368:ILE:O	2.20	0.41
1:G:505:VAL:O	1:G:505:VAL:HG13	2.20	0.41
1:I:220:PHE:O	1:I:225:ARG:NH1	2.52	0.41
1:I:435:LEU:HD22	1:O:486:THR:HG23	2.01	0.41
1:J:264:GLU:O	1:J:267:THR:OG1	2.33	0.41
1:L:203:ASP:H	1:L:206:LEU:HD12	1.85	0.41
1:L:286:ASP:O	1:L:286:ASP:CG	2.63	0.41
1:L:414:LEU:HD13	1:L:432:PHE:CD2	2.55	0.41
1:N:47:LYS:O	1:N:49:VAL:HG23	2.19	0.41
1:P:19:TYR:O	1:P:20:GLN:C	2.63	0.41
2:Z:116:PHE:HB2	2:Z:145:SER:HB2	2.02	0.41
2:b:19:ILE:CG2	2:b:83:VAL:HG22	2.49	0.41
2:c:131:ILE:HG12	2:e:44:SER:HB2	2.02	0.41
1:B:437:ASP:OD1	1:B:437:ASP:C	2.64	0.41
1:C:31:PRO:O	1:C:208:ALA:HB3	2.21	0.41
1:C:220:PHE:HB3	1:C:224:ASP:HB2	2.01	0.41
1:D:147:GLU:OE2	1:J:260:ARG:CZ	2.67	0.41
1:E:287:ASP:OD1	1:E:287:ASP:N	2.53	0.41
1:K:368:ILE:O	1:K:368:ILE:HG13	2.20	0.41
1:O:246:LEU:HD22	1:O:278:TYR:HE2	1.86	0.41
2:T:131:ILE:O	2:T:131:ILE:HG22	2.21	0.41
2:V:39:ASN:HB2	2:V:57:ALA:HB3	2.02	0.41
2:g:35:GLU:OE1	2:g:61:PRO:HG3	2.20	0.41
1:F:366:PRO:HA	1:F:369:VAL:HG23	2.01	0.41
1:H:461:THR:OG1	1:H:462:ILE:N	2.54	0.41
1:I:366:PRO:HA	1:I:369:VAL:HG23	2.01	0.41
1:J:220:PHE:HB3	1:J:224:ASP:HB2	2.01	0.41
1:K:439:SER:O	1:Q:493:VAL:HG11	2.21	0.41
1:M:359:ALA:O	1:M:371:ILE:HG22	2.20	0.41
1:Q:94:THR:HG22	1:Q:95:ARG:N	2.35	0.41
2:U:101:ASP:O	2:b:58:ILE:HD12	2.20	0.41
2:V:155:ASN:OD1	2:V:155:ASN:C	2.63	0.41
2:e:106:VAL:O	2:e:106:VAL:HG12	2.20	0.41
1:B:413:LEU:HD23	1:B:413:LEU:HA	1.88	0.41
1:D:92:ILE:HG21	1:D:186:GLY:O	2.19	0.41
1:D:435:LEU:HD22	1:J:486:THR:HG23	2.03	0.41
1:J:262:ILE:HD11	1:J:338:ALA:HB2	2.01	0.41
1:N:366:PRO:HA	1:N:369:VAL:HG23	2.01	0.41
2:X:127:GLU:HG2	2:X:128:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:35:GLU:OE2	2:f:61:PRO:C	2.63	0.41
1:F:220:PHE:HB3	1:F:224:ASP:HB2	2.02	0.41
1:I:75:PHE:CE1	1:I:85:LEU:HB2	2.55	0.41
1:J:299:MET:HE3	1:J:318:PHE:HB2	2.03	0.41
1:L:281:TYR:HA	1:L:292:PRO:HD3	2.02	0.41
1:M:184:THR:O	1:M:185:THR:OG1	2.32	0.41
1:P:26:PRO:HG2	1:Q:492:SER:HA	2.01	0.41
1:Q:98:ILE:HD11	1:Q:181:LEU:HG	2.03	0.41
2:W:28:TRP:CZ2	2:W:76:LEU:HD21	2.56	0.41
2:b:131:ILE:HG23	2:j:44:SER:HB2	2.02	0.41
2:b:148:ARG:HG3	2:b:149:SER:N	2.35	0.41
2:c:42:GLU:HG2	2:c:51:ILE:CG2	2.51	0.41
1:D:43:ASN:OD1	1:D:43:ASN:C	2.64	0.41
1:D:408:ARG:CZ	2:b:16:ASN:HB3	2.50	0.41
1:P:109:SER:OG	1:P:175:THR:OG1	2.21	0.41
2:h:130:THR:HG22	2:i:100:ARG:NH2	2.35	0.41
1:B:282:LEU:HD13	1:B:323:VAL:HG11	2.02	0.41
1:C:284:ASN:HA	1:C:323:VAL:HA	2.02	0.41
1:E:408:ARG:HG2	2:c:18:ASN:OD1	2.20	0.41
1:E:500:GLU:OE2	1:E:500:GLU:HA	2.20	0.41
1:G:286:ASP:O	1:G:286:ASP:CG	2.64	0.41
1:H:414:LEU:HD23	1:H:417:LEU:HD12	2.03	0.41
1:H:445:LEU:HD22	1:H:450:LEU:HD12	2.03	0.41
1:L:29:VAL:HB	1:L:207:GLU:OE2	2.21	0.41
1:L:405:ASN:HA	2:j:23:VAL:HG11	2.01	0.41
1:N:410:THR:HG21	1:N:455:ILE:HD11	2.02	0.41
2:e:45:ASP:OD1	2:e:45:ASP:N	2.53	0.41
2:f:74:GLU:HG2	2:f:75:GLU:N	2.35	0.41
1:A:5:LEU:O	1:B:504:PRO:HD2	2.20	0.41
1:B:27:ILE:HD12	1:B:27:ILE:HA	1.81	0.41
1:C:1:MET:HE2	1:C:1:MET:H3	1.83	0.41
1:C:100:VAL:O	1:C:100:VAL:CG1	2.69	0.41
1:C:144:LEU:HD22	1:C:144:LEU:N	2.36	0.41
1:F:52:ARG:O	1:F:53:ILE:HD13	2.21	0.41
1:H:366:PRO:HA	1:H:369:VAL:HG23	2.01	0.41
1:I:202:PHE:O	1:I:241:TYR:OH	2.35	0.41
1:I:403:LEU:HD13	1:I:441:GLN:HG3	2.03	0.41
1:I:450:LEU:HD23	1:O:465:ARG:HG3	2.03	0.41
1:J:30:GLU:HG2	1:J:33:ARG:HD2	2.03	0.41
1:K:248:ASP:OD1	1:K:281:TYR:HE1	2.04	0.41
1:K:458:VAL:HG22	1:Q:473:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:MET:HE2	1:L:24:SER:H	1.85	0.41
1:L:235:LEU:HD12	1:L:241:TYR:CD2	2.56	0.41
1:P:67:ALA:HB3	1:P:215:GLU:HG3	2.02	0.41
1:R:126:THR:O	1:R:129:THR:OG1	2.26	0.41
2:f:35:GLU:OE1	2:f:35:GLU:N	2.54	0.41
2:h:3:VAL:HG12	2:h:4:SER:N	2.35	0.41
2:i:160:PRO:O	2:i:161:ALA:C	2.63	0.41
1:C:248:ASP:N	1:C:248:ASP:OD1	2.52	0.41
1:K:478:LEU:O	1:K:482:VAL:HG23	2.20	0.41
1:N:427:THR:N	1:N:430:GLU:OE1	2.54	0.41
1:O:48:ASN:CB	1:O:167:THR:HG22	2.51	0.41
2:T:131:ILE:O	2:T:131:ILE:CG2	2.69	0.41
2:a:30:LYS:NZ	2:a:30:LYS:HB3	2.36	0.41
2:c:79:ARG:O	2:c:83:VAL:HG23	2.21	0.41
1:B:287:ASP:OD1	1:B:287:ASP:N	2.54	0.40
1:C:25:ARG:HE	1:C:25:ARG:HB3	1.35	0.40
1:C:239:TYR:HD2	1:H:16:TYR:HB3	1.87	0.40
1:E:201:THR:O	1:E:201:THR:HG22	2.20	0.40
1:J:30:GLU:O	1:J:31:PRO:C	2.64	0.40
1:N:94:THR:HG22	1:N:95:ARG:N	2.36	0.40
1:Q:19:TYR:HA	1:R:470:ILE:O	2.22	0.40
2:Z:159:GLU:C	2:Z:161:ALA:H	2.29	0.40
2:e:3:VAL:HG12	2:e:4:SER:N	2.37	0.40
1:A:479:GLU:CD	1:A:480:ALA:N	2.80	0.40
1:C:58:ASP:OD1	1:C:58:ASP:C	2.64	0.40
1:D:191:VAL:O	1:D:195:VAL:HG23	2.21	0.40
1:G:23:GLN:HB3	1:H:488:ALA:HB1	2.02	0.40
1:H:155:THR:OG1	1:H:158:THR:OG1	2.10	0.40
1:L:297:ALA:O	1:L:301:LEU:HG	2.20	0.40
1:O:3:ASN:HD22	1:O:3:ASN:HA	1.62	0.40
1:O:5:LEU:O	1:O:8:VAL:HG22	2.22	0.40
1:Q:259:ASP:OD1	1:Q:259:ASP:N	2.53	0.40
2:S:109:GLY:HA3	2:S:154:ILE:HD12	2.03	0.40
2:S:123:THR:HG23	2:T:35:GLU:HG2	2.03	0.40
2:U:74:GLU:CB	2:V:156:TRP:HB3	2.51	0.40
1:D:27:ILE:N	1:D:27:ILE:HD12	2.37	0.40
1:I:280:PRO:HG2	1:I:346:ILE:H	1.86	0.40
1:J:1:MET:N	1:K:500:GLU:O	2.52	0.40
1:K:235:LEU:HD12	1:K:241:TYR:CD2	2.56	0.40
1:N:453:MET:HE3	1:N:453:MET:HB2	1.96	0.40
1:O:236:CYS:SG	1:O:245:ALA:HB2	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:40:THR:HB	2:Z:53:THR:HG23	2.04	0.40
2:a:126:ASN:OD1	2:a:126:ASN:N	2.54	0.40
2:d:116:PHE:HB2	2:d:145:SER:HB2	2.04	0.40
2:d:126:ASN:OD1	2:d:126:ASN:N	2.54	0.40
2:j:19:ILE:HG21	2:j:79:ARG:HB3	2.03	0.40
1:D:25:ARG:O	1:D:27:ILE:HD12	2.21	0.40
1:L:415:THR:O	1:L:419:GLN:HG2	2.21	0.40
1:M:92:ILE:HD13	1:M:186:GLY:O	2.21	0.40
1:O:82:PHE:CD1	1:O:305:VAL:HG11	2.57	0.40
1:R:92:ILE:H	1:R:92:ILE:HG12	1.42	0.40
2:W:123:THR:HG23	2:X:35:GLU:HG2	2.04	0.40
2:h:158:SER:O	2:h:158:SER:OG	2.37	0.40
1:H:138:ILE:HG21	1:H:150:ALA:HB2	2.03	0.40
1:J:478:LEU:HD22	1:J:478:LEU:HA	1.84	0.40
1:P:365:ASP:HB3	1:P:368:ILE:HG22	2.03	0.40
2:c:115:GLU:OE1	2:c:148:ARG:HG2	2.21	0.40
2:i:93:VAL:HB	2:i:114:LEU:HB2	2.03	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	502/506 (99%)	488 (97%)	13 (3%)	1 (0%)	43	70
1	B	502/506 (99%)	488 (97%)	13 (3%)	1 (0%)	43	70
1	C	503/506 (99%)	487 (97%)	12 (2%)	4 (1%)	16	44
1	D	502/506 (99%)	487 (97%)	14 (3%)	1 (0%)	43	70
1	E	503/506 (99%)	486 (97%)	16 (3%)	1 (0%)	43	70
1	F	502/506 (99%)	486 (97%)	15 (3%)	1 (0%)	43	70
1	G	503/506 (99%)	487 (97%)	13 (3%)	3 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	502/506 (99%)	483 (96%)	17 (3%)	2 (0%)	30	59
1	I	503/506 (99%)	488 (97%)	14 (3%)	1 (0%)	43	70
1	J	503/506 (99%)	485 (96%)	17 (3%)	1 (0%)	43	70
1	K	503/506 (99%)	490 (97%)	10 (2%)	3 (1%)	21	51
1	L	503/506 (99%)	488 (97%)	13 (3%)	2 (0%)	30	59
1	M	502/506 (99%)	486 (97%)	14 (3%)	2 (0%)	30	59
1	N	503/506 (99%)	487 (97%)	14 (3%)	2 (0%)	30	59
1	O	502/506 (99%)	482 (96%)	18 (4%)	2 (0%)	30	59
1	P	503/506 (99%)	484 (96%)	16 (3%)	3 (1%)	21	51
1	Q	502/506 (99%)	486 (97%)	13 (3%)	3 (1%)	21	51
1	R	502/506 (99%)	484 (96%)	17 (3%)	1 (0%)	43	70
2	S	161/167 (96%)	148 (92%)	13 (8%)	0	100	100
2	T	160/167 (96%)	152 (95%)	8 (5%)	0	100	100
2	U	161/167 (96%)	150 (93%)	11 (7%)	0	100	100
2	V	161/167 (96%)	148 (92%)	13 (8%)	0	100	100
2	W	159/167 (95%)	150 (94%)	8 (5%)	1 (1%)	21	51
2	X	161/167 (96%)	151 (94%)	9 (6%)	1 (1%)	21	51
2	Y	160/167 (96%)	148 (92%)	11 (7%)	1 (1%)	21	51
2	Z	161/167 (96%)	152 (94%)	9 (6%)	0	100	100
2	a	159/167 (95%)	146 (92%)	13 (8%)	0	100	100
2	b	159/167 (95%)	153 (96%)	6 (4%)	0	100	100
2	c	158/167 (95%)	151 (96%)	7 (4%)	0	100	100
2	d	158/167 (95%)	150 (95%)	8 (5%)	0	100	100
2	e	159/167 (95%)	144 (91%)	15 (9%)	0	100	100
2	f	157/167 (94%)	144 (92%)	13 (8%)	0	100	100
2	g	161/167 (96%)	150 (93%)	11 (7%)	0	100	100
2	h	158/167 (95%)	150 (95%)	8 (5%)	0	100	100
2	i	159/167 (95%)	148 (93%)	11 (7%)	0	100	100
2	j	158/167 (95%)	147 (93%)	11 (7%)	0	100	100
All	All	11915/12114 (98%)	11434 (96%)	444 (4%)	37 (0%)	37	66

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	6	ARG
1	C	20	GLN
1	M	279	TYR
1	N	20	GLN
1	O	24	SER
1	P	32	PHE
2	W	151	GLY
2	X	151	GLY
1	A	279	TYR
1	B	279	TYR
1	D	279	TYR
1	E	279	TYR
1	G	21	THR
1	K	187	THR
1	L	13	PRO
1	L	279	TYR
1	N	279	TYR
1	O	279	TYR
1	P	279	TYR
1	Q	20	GLN
1	C	279	TYR
1	F	279	TYR
1	G	279	TYR
1	H	279	TYR
1	K	279	TYR
1	P	20	GLN
1	Q	279	TYR
1	I	279	TYR
1	K	185	THR
1	R	279	TYR
1	G	20	GLN
1	J	279	TYR
1	Q	32	PHE
1	H	29	VAL
1	C	319	PRO
1	M	152	VAL
1	C	306	ILE

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	417/419 (100%)	395 (95%)	22 (5%)	20	48
1	B	417/419 (100%)	403 (97%)	14 (3%)	32	57
1	C	418/419 (100%)	401 (96%)	17 (4%)	27	53
1	D	417/419 (100%)	408 (98%)	9 (2%)	45	65
1	E	418/419 (100%)	410 (98%)	8 (2%)	50	67
1	F	417/419 (100%)	399 (96%)	18 (4%)	26	52
1	G	418/419 (100%)	399 (96%)	19 (4%)	24	52
1	H	417/419 (100%)	402 (96%)	15 (4%)	31	56
1	I	418/419 (100%)	414 (99%)	4 (1%)	68	75
1	J	418/419 (100%)	405 (97%)	13 (3%)	35	59
1	K	418/419 (100%)	410 (98%)	8 (2%)	50	67
1	L	418/419 (100%)	410 (98%)	8 (2%)	50	67
1	M	417/419 (100%)	408 (98%)	9 (2%)	45	65
1	N	418/419 (100%)	405 (97%)	13 (3%)	35	59
1	O	417/419 (100%)	394 (94%)	23 (6%)	19	46
1	P	418/419 (100%)	405 (97%)	13 (3%)	35	59
1	Q	417/419 (100%)	407 (98%)	10 (2%)	43	64
1	R	417/419 (100%)	412 (99%)	5 (1%)	63	74
2	S	138/141 (98%)	129 (94%)	9 (6%)	15	42
2	T	137/141 (97%)	130 (95%)	7 (5%)	21	49
2	U	138/141 (98%)	134 (97%)	4 (3%)	37	60
2	V	138/141 (98%)	135 (98%)	3 (2%)	45	65
2	W	136/141 (96%)	129 (95%)	7 (5%)	21	49
2	X	138/141 (98%)	136 (99%)	2 (1%)	59	72
2	Y	137/141 (97%)	134 (98%)	3 (2%)	45	65
2	Z	138/141 (98%)	133 (96%)	5 (4%)	31	56
2	a	136/141 (96%)	133 (98%)	3 (2%)	45	65
2	b	136/141 (96%)	130 (96%)	6 (4%)	25	52
2	c	136/141 (96%)	134 (98%)	2 (2%)	57	71
2	d	136/141 (96%)	131 (96%)	5 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	e	136/141 (96%)	122 (90%)	14 (10%)	7	25
2	f	135/141 (96%)	129 (96%)	6 (4%)	25	52
2	g	138/141 (98%)	138 (100%)	0	100	100
2	h	136/141 (96%)	127 (93%)	9 (7%)	15	42
2	i	136/141 (96%)	132 (97%)	4 (3%)	37	60
2	j	136/141 (96%)	132 (97%)	4 (3%)	37	60
All	All	9976/10080 (99%)	9655 (97%)	321 (3%)	35	58

All (321) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	5	LEU
1	A	12	THR
1	A	25	ARG
1	A	32	PHE
1	A	126	THR
1	A	151	THR
1	A	152	VAL
1	A	157	SER
1	A	158	THR
1	A	201	THR
1	A	283	ILE
1	A	286	ASP
1	A	288	GLN
1	A	408	ARG
1	A	419	GLN
1	A	475	ILE
1	A	494	GLU
1	A	499	THR
1	A	500	GLU
1	A	502	THR
1	A	505	VAL
1	B	22	THR
1	B	23	GLN
1	B	27	ILE
1	B	29	VAL
1	B	30	GLU
1	B	34	THR
1	B	201	THR

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Mol	Chain	Res	Type
1	B	283	ILE
1	B	329	LYS
1	B	403	LEU
1	B	408	ARG
1	B	409	LYS
1	B	412	THR
1	B	422	LEU
1	C	10	ILE
1	C	12	THR
1	C	22	THR
1	C	23	GLN
1	C	24	SER
1	C	25	ARG
1	C	29	VAL
1	C	283	ILE
1	C	286	ASP
1	C	299	MET
1	C	316	VAL
1	C	317	ASN
1	C	321	LYS
1	C	324	LYS
1	C	325	ASN
1	C	326	VAL
1	C	401	THR
1	D	16	TYR
1	D	23	GLN
1	D	29	VAL
1	D	129	THR
1	D	223	SER
1	D	283	ILE
1	D	408	ARG
1	D	455	ILE
1	D	460	SER
1	E	12	THR
1	E	20	GLN
1	E	22	THR
1	E	23	GLN
1	E	24	SER
1	E	25	ARG
1	E	283	ILE
1	E	469	ASN
1	F	12	THR

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Mol	Chain	Res	Type
1	F	22	THR
1	F	24	SER
1	F	25	ARG
1	F	27	ILE
1	F	29	VAL
1	F	30	GLU
1	F	129	THR
1	F	151	THR
1	F	152	VAL
1	F	156	SER
1	F	157	SER
1	F	317	ASN
1	F	403	LEU
1	F	404	ASP
1	F	409	LYS
1	F	426	GLN
1	F	475	ILE
1	G	10	ILE
1	G	21	THR
1	G	22	THR
1	G	27	ILE
1	G	28	ASN
1	G	29	VAL
1	G	30	GLU
1	G	33	ARG
1	G	92	ILE
1	G	180	THR
1	G	368	ILE
1	G	401	THR
1	G	402	VAL
1	G	403	LEU
1	G	410	THR
1	G	412	THR
1	G	413	LEU
1	G	416	THR
1	G	468	ILE
1	H	25	ARG
1	H	29	VAL
1	H	32	PHE
1	H	134	VAL
1	H	147	GLU
1	H	403	LEU

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Mol	Chain	Res	Type
1	H	406	ILE
1	H	408	ARG
1	H	409	LYS
1	H	410	THR
1	H	412	THR
1	H	478	LEU
1	H	481	THR
1	H	484	LEU
1	H	492	SER
1	I	22	THR
1	I	29	VAL
1	I	272	GLN
1	I	473	THR
1	J	22	THR
1	J	23	GLN
1	J	24	SER
1	J	29	VAL
1	J	134	VAL
1	J	287	ASP
1	J	402	VAL
1	J	407	GLN
1	J	410	THR
1	J	413	LEU
1	J	477	ASP
1	J	478	LEU
1	J	484	LEU
1	K	12	THR
1	K	42	SER
1	K	43	ASN
1	K	45	VAL
1	K	92	ILE
1	K	181	LEU
1	K	182	THR
1	K	187	THR
1	L	12	THR
1	L	16	TYR
1	L	23	GLN
1	L	42	SER
1	L	43	ASN
1	L	45	VAL
1	L	92	ILE
1	L	183	THR

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Mol	Chain	Res	Type
1	M	25	ARG
1	M	32	PHE
1	M	152	VAL
1	M	157	SER
1	M	171	THR
1	M	201	THR
1	M	203	ASP
1	M	282	LEU
1	M	283	ILE
1	N	10	ILE
1	N	12	THR
1	N	23	GLN
1	N	24	SER
1	N	92	ILE
1	N	135	ILE
1	N	282	LEU
1	N	469	ASN
1	N	473	THR
1	N	477	ASP
1	N	478	LEU
1	N	479	GLU
1	N	481	THR
1	O	5	LEU
1	O	21	THR
1	O	22	THR
1	O	23	GLN
1	O	24	SER
1	O	25	ARG
1	O	28	ASN
1	O	29	VAL
1	O	30	GLU
1	O	88	VAL
1	O	175	THR
1	O	219	THR
1	O	282	LEU
1	O	283	ILE
1	O	450	LEU
1	O	453	MET
1	O	469	ASN
1	O	473	THR
1	O	478	LEU
1	O	479	GLU

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Mol	Chain	Res	Type
1	O	481	THR
1	O	491	SER
1	O	494	GLU
1	P	10	ILE
1	P	21	THR
1	P	22	THR
1	P	23	GLN
1	P	24	SER
1	P	25	ARG
1	P	29	VAL
1	P	92	ILE
1	P	203	ASP
1	P	248	ASP
1	P	464	GLU
1	P	466	LEU
1	P	497	THR
1	Q	21	THR
1	Q	22	THR
1	Q	23	GLN
1	Q	24	SER
1	Q	25	ARG
1	Q	29	VAL
1	Q	32	PHE
1	Q	92	ILE
1	Q	181	LEU
1	Q	499	THR
1	R	5	LEU
1	R	22	THR
1	R	92	ILE
1	R	259	ASP
1	R	468	ILE
2	S	3	VAL
2	S	4	SER
2	S	10	ILE
2	S	29	SER
2	S	90	TRP
2	S	98	MET
2	S	100	ARG
2	S	156	TRP
2	S	158	SER
2	T	3	VAL
2	T	4	SER

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Mol	Chain	Res	Type
2	T	5	LYS
2	T	6	ARG
2	T	37	THR
2	T	100	ARG
2	T	111	LYS
2	U	5	LYS
2	U	10	ILE
2	U	90	TRP
2	U	153	ASN
2	V	37	THR
2	V	100	ARG
2	V	156	TRP
2	W	3	VAL
2	W	4	SER
2	W	29	SER
2	W	100	ARG
2	W	127	GLU
2	W	153	ASN
2	W	155	ASN
2	X	100	ARG
2	X	153	ASN
2	Y	4	SER
2	Y	10	ILE
2	Y	137	MET
2	Z	10	ILE
2	Z	33	LYS
2	Z	66	SER
2	Z	155	ASN
2	Z	163	GLN
2	a	108	GLN
2	a	156	TRP
2	a	157	TRP
2	b	3	VAL
2	b	4	SER
2	b	10	ILE
2	b	66	SER
2	b	88	ILE
2	b	92	THR
2	c	10	ILE
2	c	100	ARG
2	d	10	ILE
2	d	59	LYS

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Mol	Chain	Res	Type
2	d	131	ILE
2	d	157	TRP
2	d	158	SER
2	e	15	VAL
2	e	17	LEU
2	e	18	ASN
2	e	19	ILE
2	e	51	ILE
2	e	53	THR
2	e	91	VAL
2	e	92	THR
2	e	95	ILE
2	e	98	MET
2	e	100	ARG
2	e	101	ASP
2	e	103	TYR
2	e	133	SER
2	f	98	MET
2	f	101	ASP
2	f	105	ASN
2	f	106	VAL
2	f	154	ILE
2	f	155	ASN
2	h	88	ILE
2	h	92	THR
2	h	95	ILE
2	h	98	MET
2	h	100	ARG
2	h	101	ASP
2	h	105	ASN
2	h	113	ILE
2	h	118	THR
2	i	108	GLN
2	i	154	ILE
2	i	155	ASN
2	i	158	SER
2	j	10	ILE
2	j	15	VAL
2	j	75	GLU
2	j	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	23	GLN
1	A	97	GLN
1	A	168	ASN
1	A	272	GLN
1	A	274	HIS
1	A	447	GLN
1	B	20	GLN
1	B	23	GLN
1	B	97	GLN
1	B	419	GLN
1	B	447	GLN
1	B	490	GLN
1	C	46	ASN
1	C	274	HIS
1	C	411	ASN
1	C	447	GLN
1	D	46	ASN
1	D	97	GLN
1	D	274	HIS
1	D	419	GLN
1	D	447	GLN
1	D	490	GLN
1	E	9	ASN
1	E	272	GLN
1	F	9	ASN
1	F	84	ASN
1	F	490	GLN
1	G	20	GLN
1	G	394	ASN
1	G	469	ASN
1	I	6	ASN
1	I	20	GLN
1	I	28	ASN
1	J	20	GLN
1	J	28	ASN
1	J	168	ASN
1	J	411	ASN
1	K	20	GLN
1	K	469	ASN
1	L	84	ASN
1	L	452	ASN
1	N	3	ASN

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Mol	Chain	Res	Type
1	N	9	ASN
1	N	43	ASN
1	N	70	ASN
1	N	382	ASN
1	N	394	ASN
1	O	3	ASN
1	O	23	GLN
1	O	382	ASN
1	P	6	ASN
1	P	80	GLN
1	P	448	GLN
1	Q	20	GLN
1	Q	23	GLN
1	Q	70	ASN
1	Q	419	GLN
1	R	20	GLN
1	R	23	GLN
1	R	46	ASN
1	R	70	ASN
1	R	274	HIS
2	S	96	GLN
2	T	39	ASN
2	T	105	ASN
2	U	153	ASN
2	U	155	ASN
2	U	163	GLN
2	V	16	ASN
2	V	47	GLN
2	V	96	GLN
2	X	16	ASN
2	c	21	ASN
2	d	16	ASN
2	d	18	ASN
2	d	105	ASN
2	e	18	ASN
2	f	96	GLN
2	f	108	GLN
2	g	96	GLN
2	h	96	GLN
2	h	143	ASN
2	i	78	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

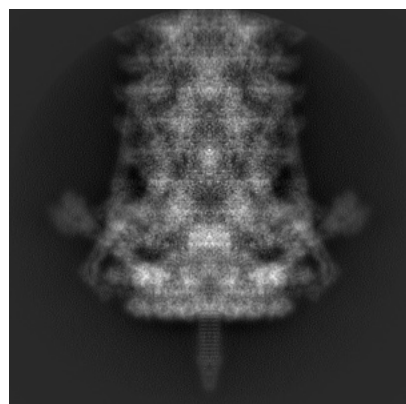
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37153. These allow visual inspection of the internal detail of the map and identification of artifacts.

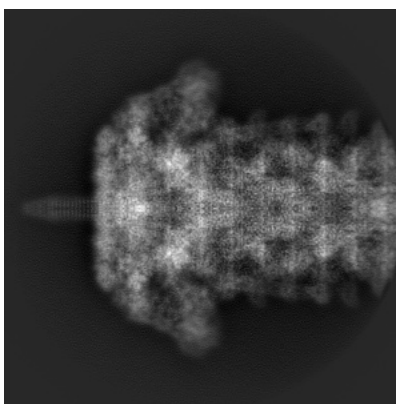
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

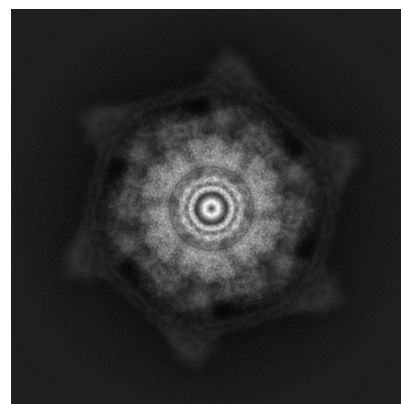
6.1.1 Primary map



X

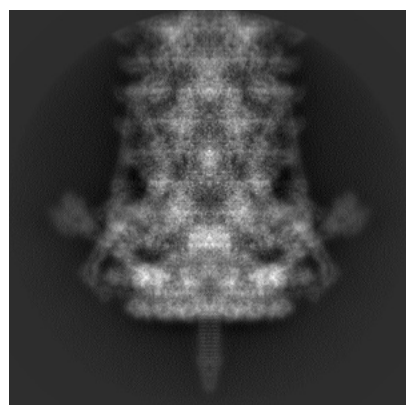


Y

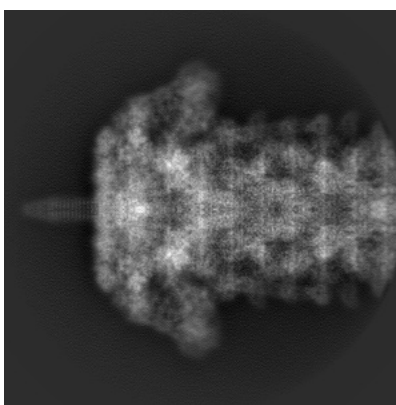


Z

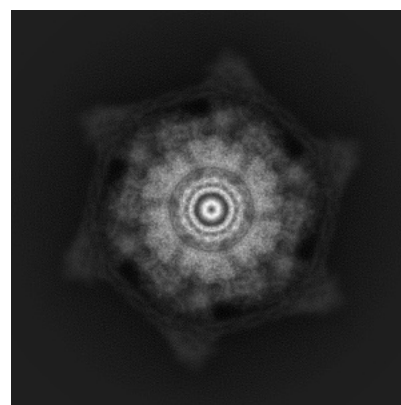
6.1.2 Raw map



X



Y

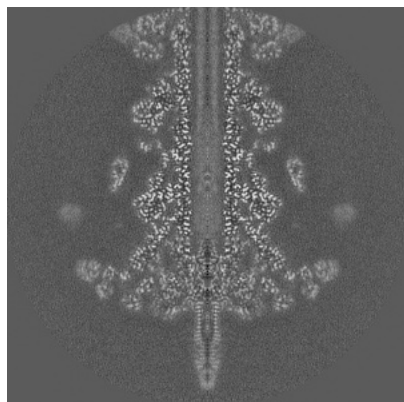


Z

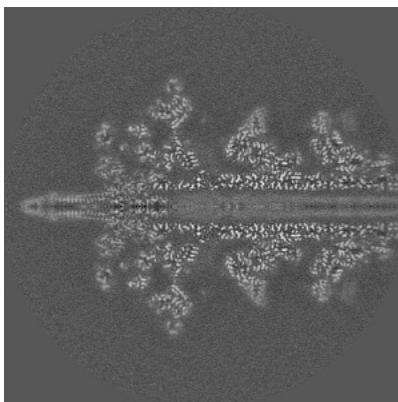
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

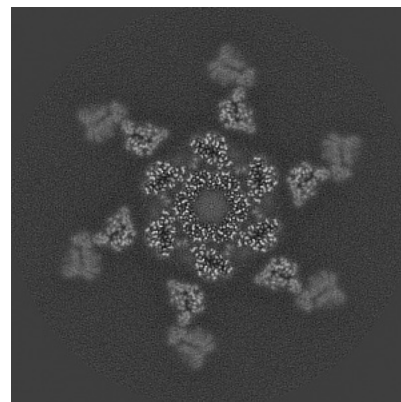
6.2.1 Primary map



X Index: 224

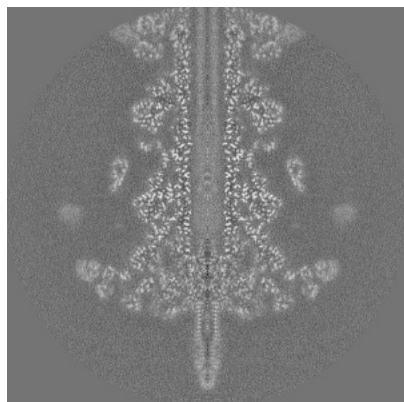


Y Index: 224

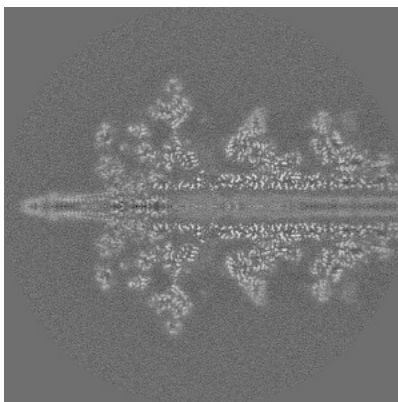


Z Index: 224

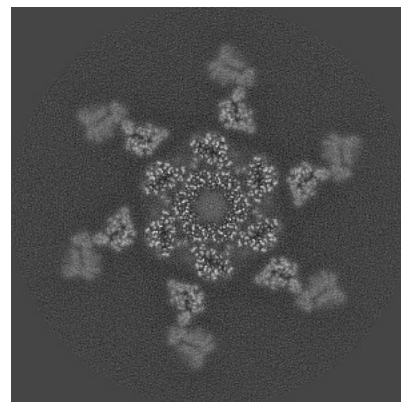
6.2.2 Raw map



X Index: 224



Y Index: 224

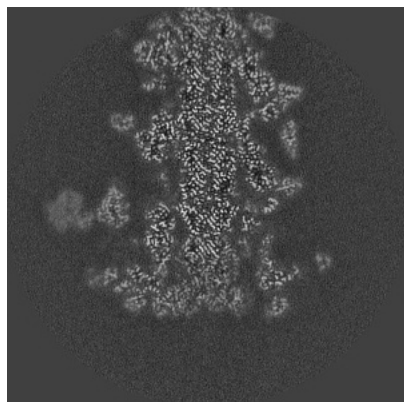


Z Index: 224

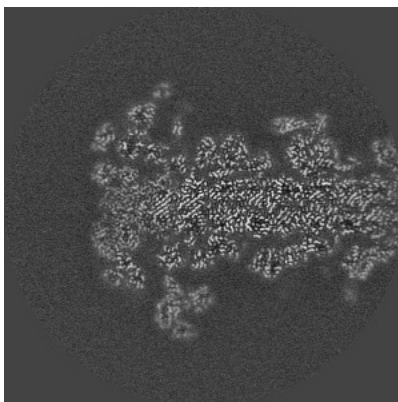
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

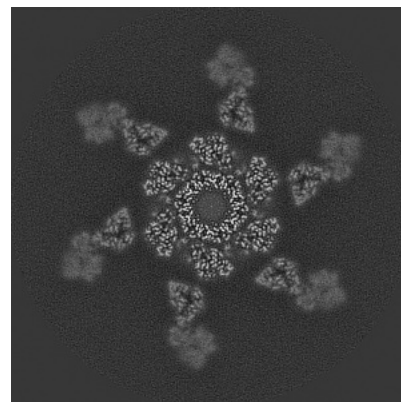
6.3.1 Primary map



X Index: 204

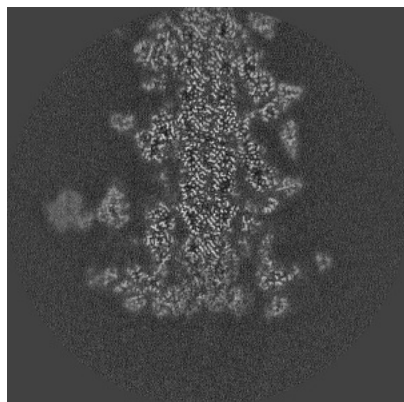


Y Index: 204

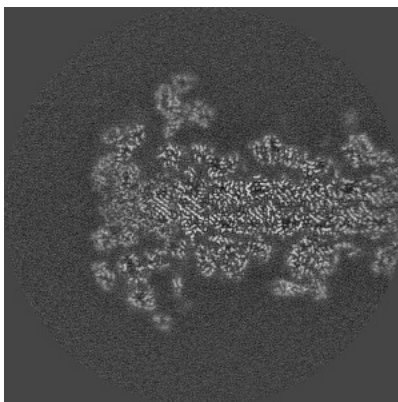


Z Index: 221

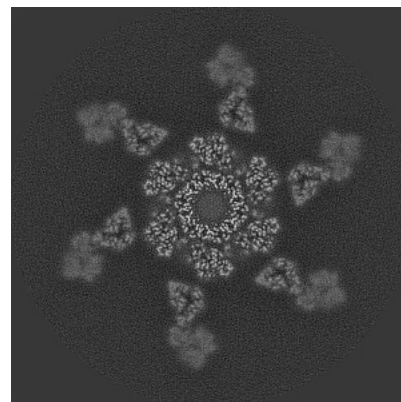
6.3.2 Raw map



X Index: 204



Y Index: 244

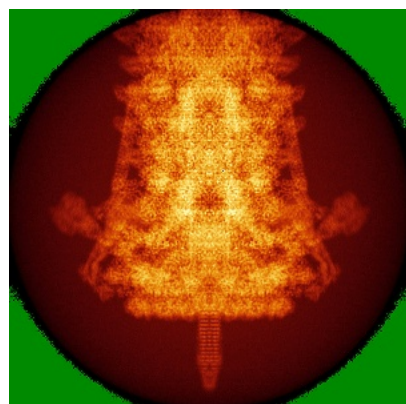


Z Index: 221

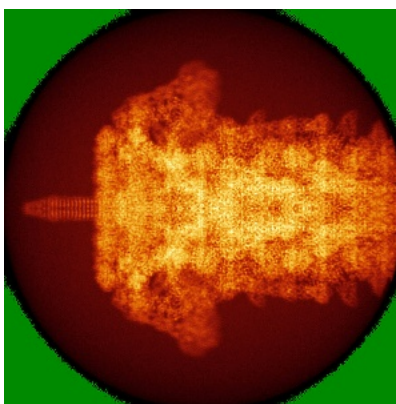
The images above show the largest variance slices of the map in three orthogonal directions.

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

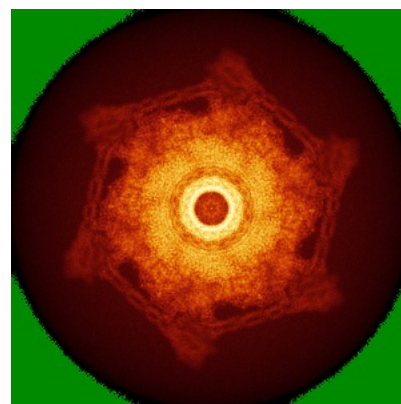
6.4.1 Primary map



X

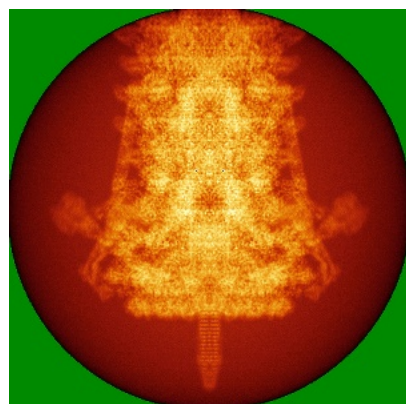


Y

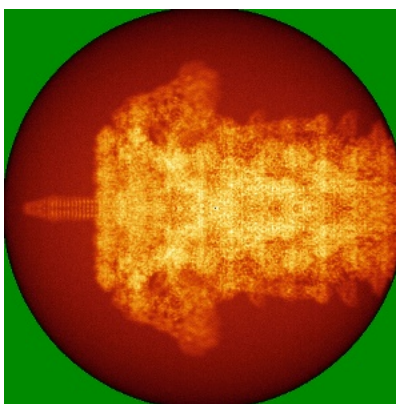


Z

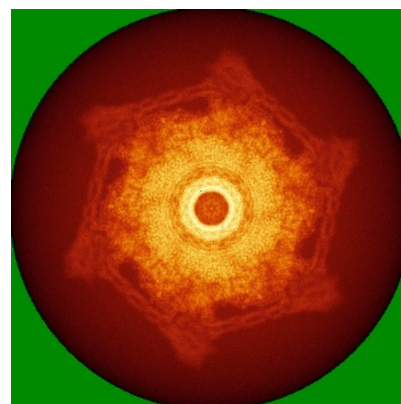
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

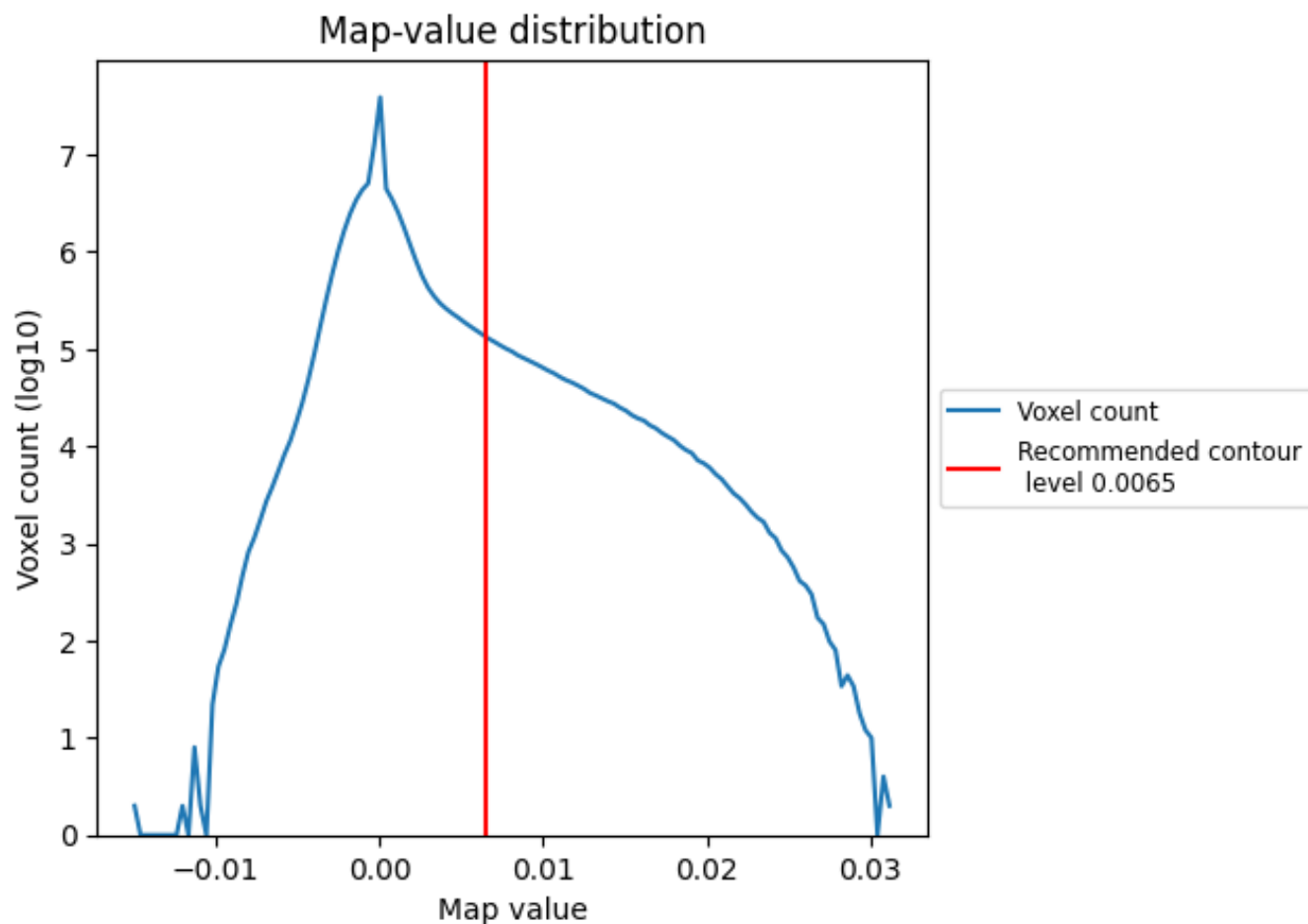
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

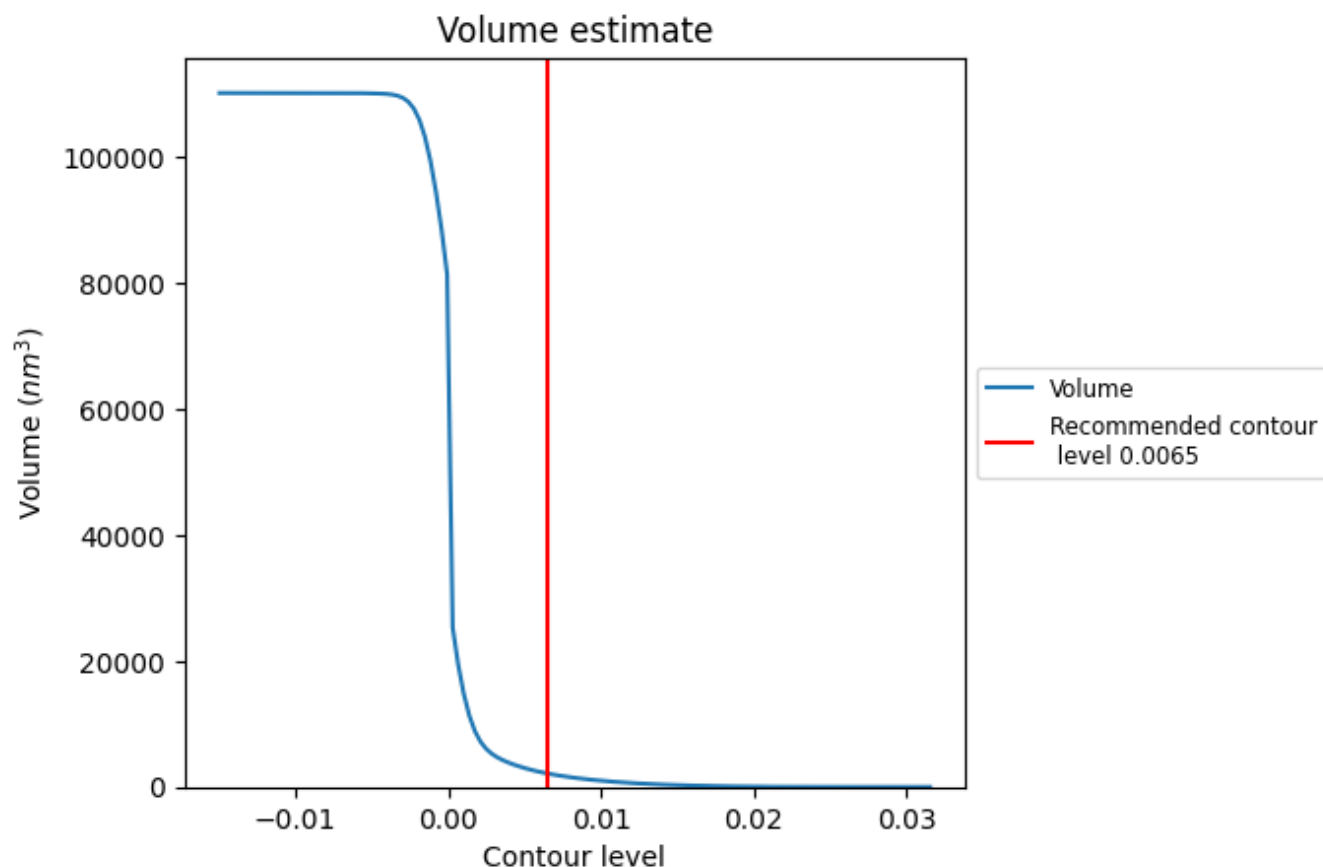
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

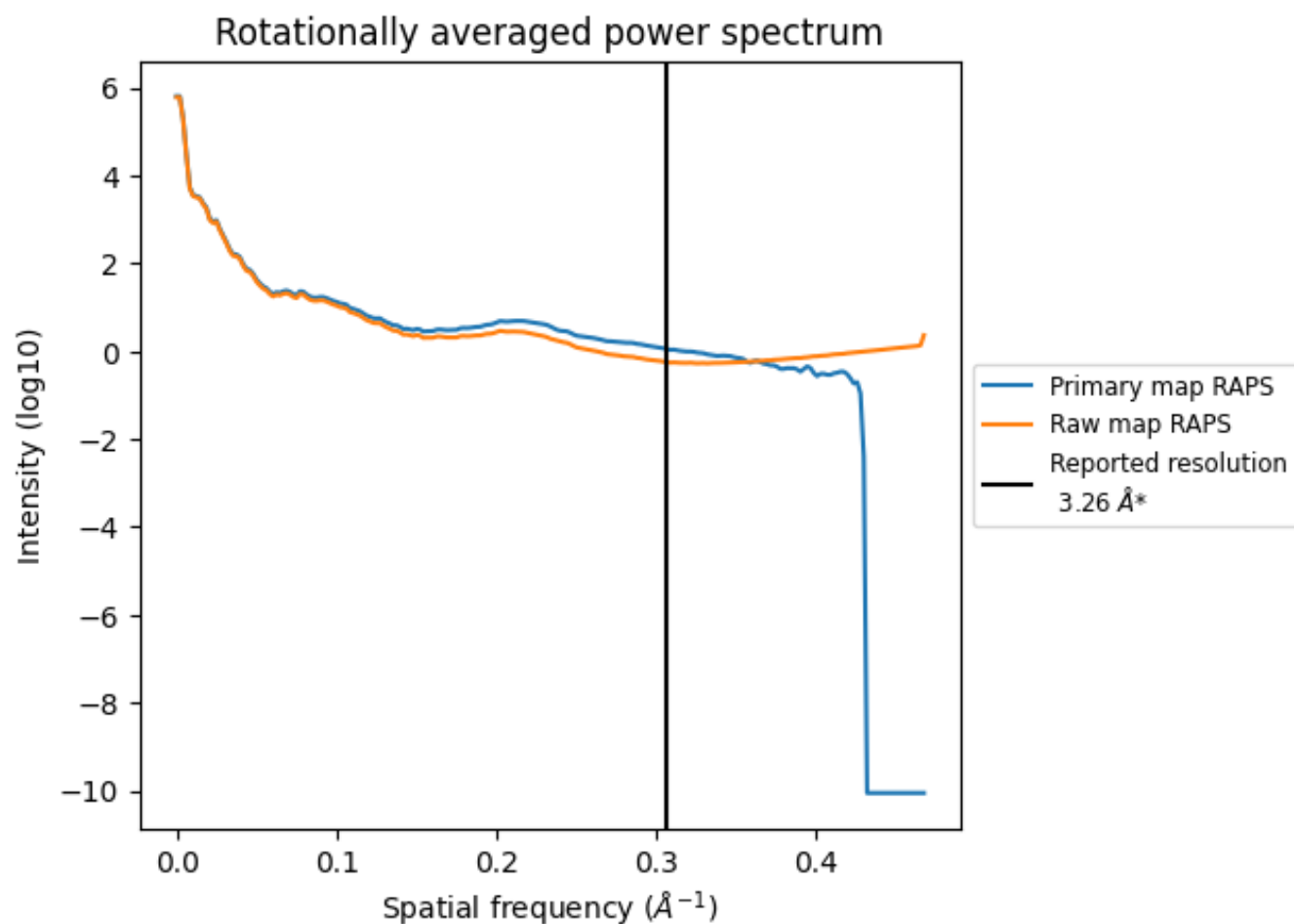
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2135 nm³; this corresponds to an approximate mass of 1929 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

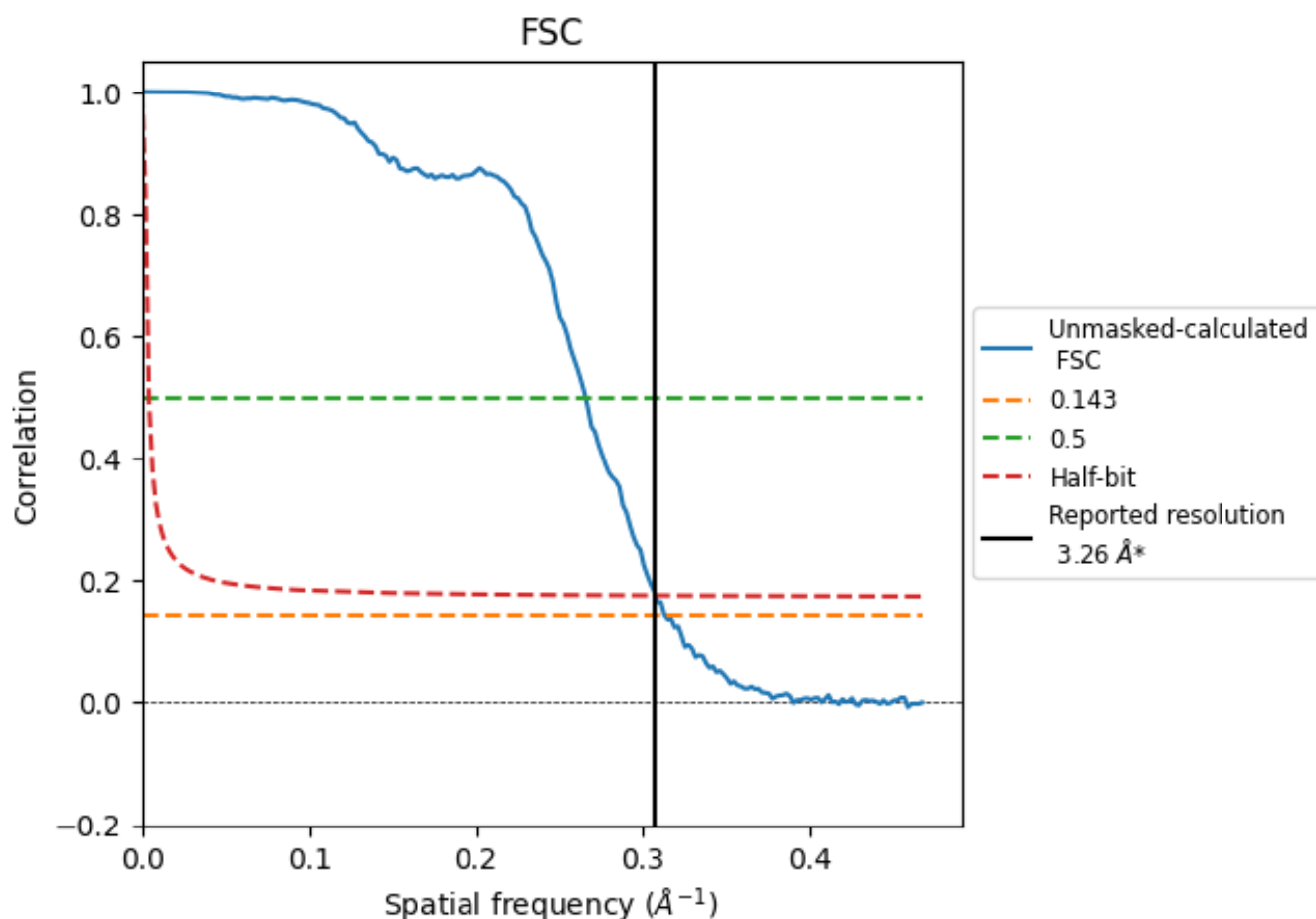


*Reported resolution corresponds to spatial frequency of 0.307 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.307 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

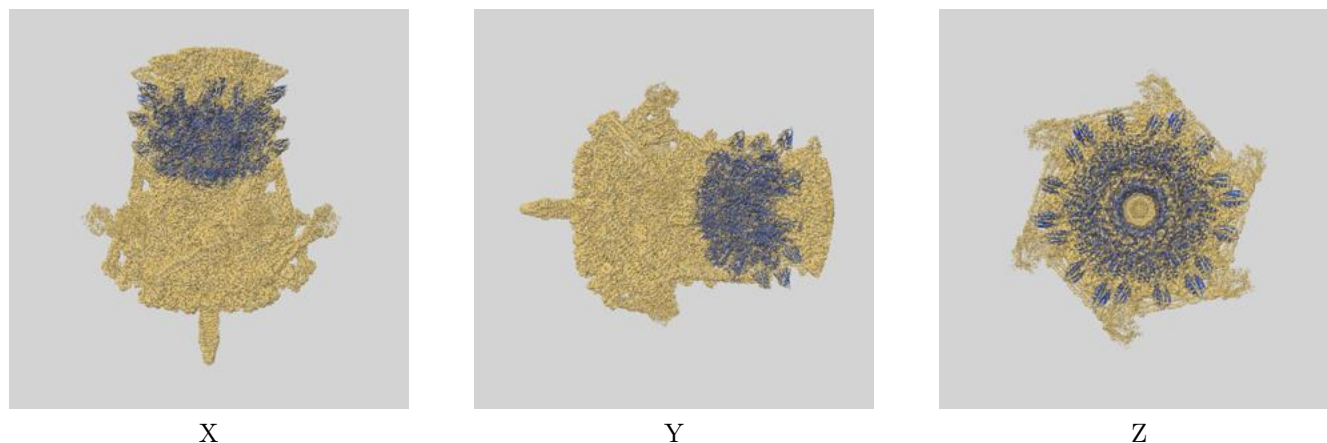
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.77	3.25

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

9 Map-model fit [i](#)

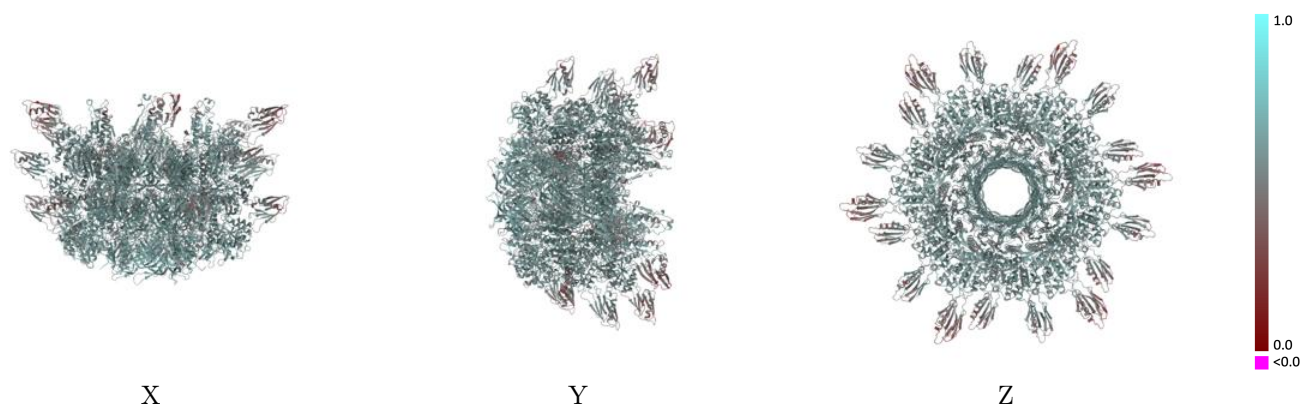
This section contains information regarding the fit between EMDB map EMD-37153 and PDB model 8KEE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

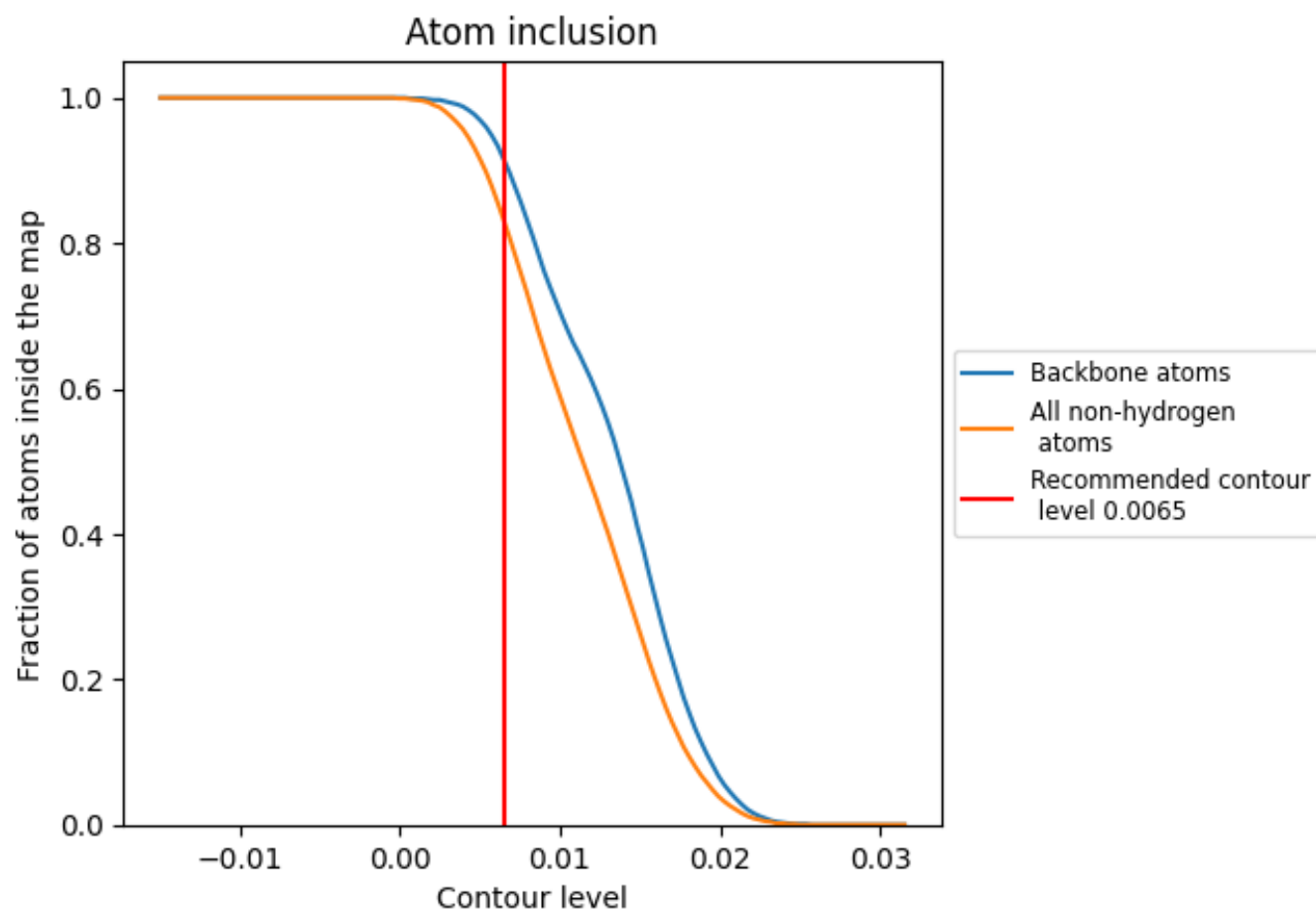


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8310	 0.5720
A	 0.8430	 0.5690
B	 0.8240	 0.5680
C	 0.8230	 0.5600
D	 0.8380	 0.5730
E	 0.8230	 0.5640
F	 0.8360	 0.5700
G	 0.8260	 0.5630
H	 0.8350	 0.5700
I	 0.8220	 0.5590
J	 0.8330	 0.5680
K	 0.8350	 0.5730
L	 0.8400	 0.5730
M	 0.7730	 0.5440
N	 0.7700	 0.5430
O	 0.7750	 0.5420
P	 0.7690	 0.5420
Q	 0.7710	 0.5460
R	 0.7770	 0.5470
S	 0.8930	 0.6230
T	 0.8810	 0.5960
U	 0.8880	 0.6090
V	 0.8860	 0.6010
W	 0.9020	 0.6260
X	 0.9010	 0.6280
Y	 0.8920	 0.6130
Z	 0.8890	 0.6080
a	 0.8950	 0.6070
b	 0.8980	 0.6070
c	 0.9040	 0.6150
d	 0.9050	 0.6160
e	 0.8700	 0.5990
f	 0.8840	 0.5980
g	 0.8790	 0.6010
h	 0.8700	 0.5970



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Chain	Atom inclusion	Q-score
i	 0.8710	 0.6030
j	 0.8870	 0.6110