



Full wwPDB EM Validation Report ⓘ

Apr 27, 2026 – 10:45 PM JST

PDB ID : 9WSZ / pdb_00009wsz
EMDB ID : EMD-66211
Title : CryoEM structure of baseplate iris structure in the contracted AlgoCIS
Authors : Xu, J.; Ericson, C.F.; Toenshoff, E.R.; Pilhofer, M.
Deposited on : 2025-09-15
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

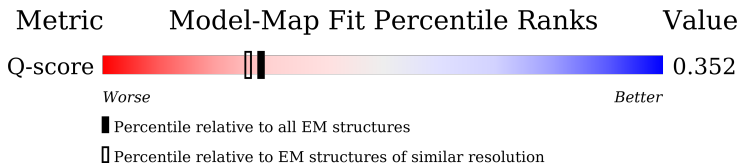
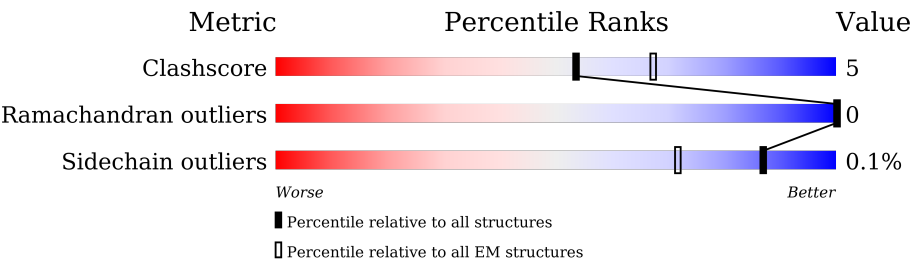
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	922	<div><div>32%</div><div><div></div><div>83%</div><div>10%</div><div>6%</div></div></div>
1	B	922	<div><div>32%</div><div><div></div><div>83%</div><div>10%</div><div>6%</div></div></div>
1	C	922	<div><div>32%</div><div><div></div><div>84%</div><div>10%</div><div>6%</div></div></div>
1	D	922	<div><div>32%</div><div><div></div><div>84%</div><div>10%</div><div>6%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	922	
1	F	922	
2	G	1050	
2	H	1050	
2	I	1050	
2	J	1050	
2	K	1050	
2	L	1050	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 92154 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Baseplate protein Alg12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	866	Total	C	N	O	S	0	0
			7059	4523	1149	1364	23		
1	B	866	Total	C	N	O	S	0	0
			7059	4523	1149	1364	23		
1	C	866	Total	C	N	O	S	0	0
			7059	4523	1149	1364	23		
1	D	866	Total	C	N	O	S	0	0
			7059	4523	1149	1364	23		
1	E	866	Total	C	N	O	S	0	0
			7059	4523	1149	1364	23		
1	F	866	Total	C	N	O	S	0	0
			7059	4523	1149	1364	23		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	THR	-	insertion	UNP A3HTB3
A	728	PHE	-	insertion	UNP A3HTB3
B	727	THR	-	insertion	UNP A3HTB3
B	728	PHE	-	insertion	UNP A3HTB3
C	727	THR	-	insertion	UNP A3HTB3
C	728	PHE	-	insertion	UNP A3HTB3
D	727	THR	-	insertion	UNP A3HTB3
D	728	PHE	-	insertion	UNP A3HTB3
E	727	THR	-	insertion	UNP A3HTB3
E	728	PHE	-	insertion	UNP A3HTB3
F	727	THR	-	insertion	UNP A3HTB3
F	728	PHE	-	insertion	UNP A3HTB3

- Molecule 2 is a protein called Baseplate protein J-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	1035	Total	C	N	O	S	0	0
			8300	5321	1351	1610	18		
2	H	1035	Total	C	N	O	S	0	0
			8300	5321	1351	1610	18		
2	I	1035	Total	C	N	O	S	0	0
			8300	5321	1351	1610	18		
2	J	1035	Total	C	N	O	S	0	0
			8300	5321	1351	1610	18		
2	K	1035	Total	C	N	O	S	0	0
			8300	5321	1351	1610	18		
2	L	1035	Total	C	N	O	S	0	0
			8300	5321	1351	1610	18		

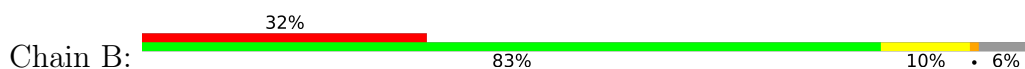
3 Residue-property plots

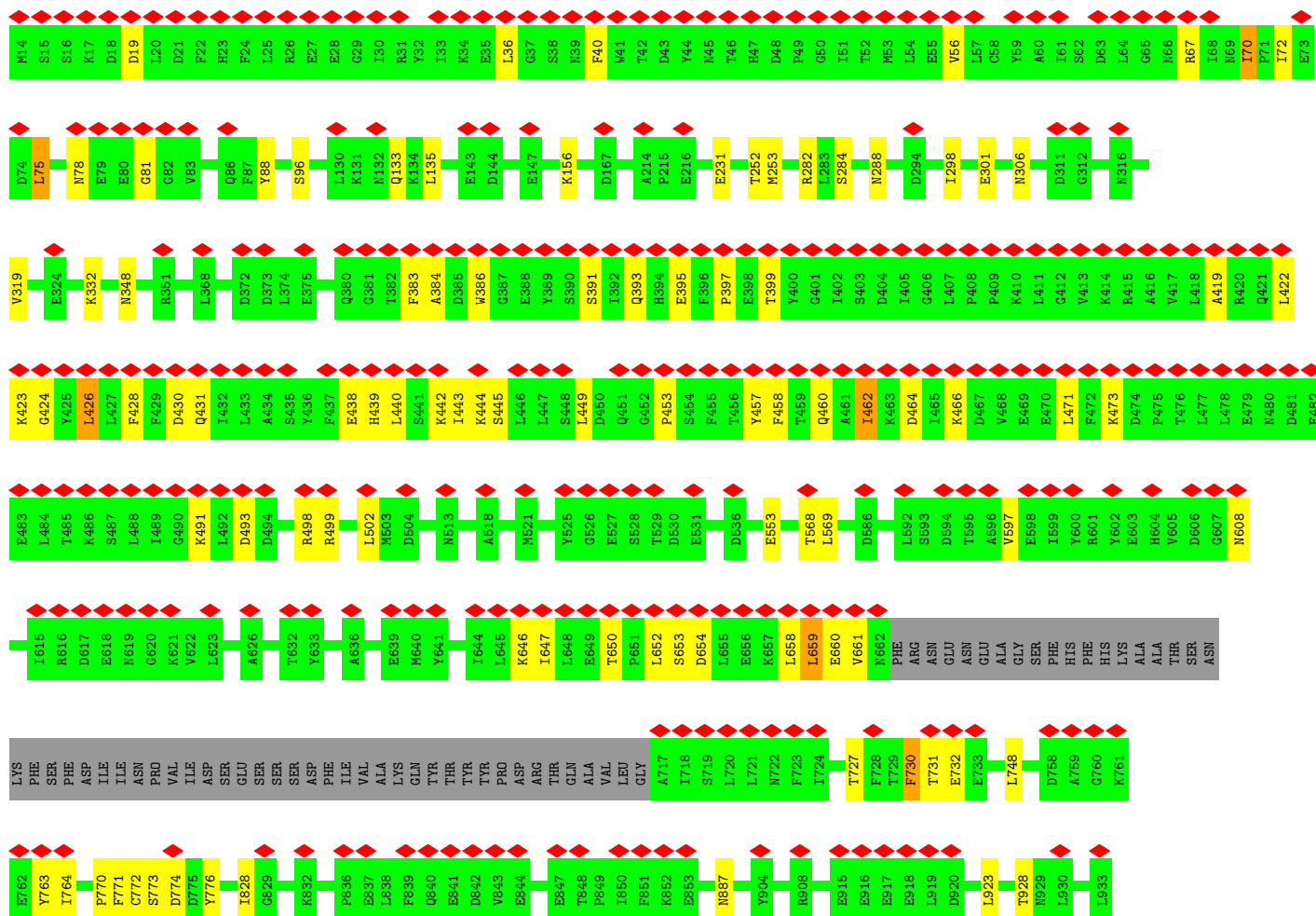
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Baseplate protein Alg12

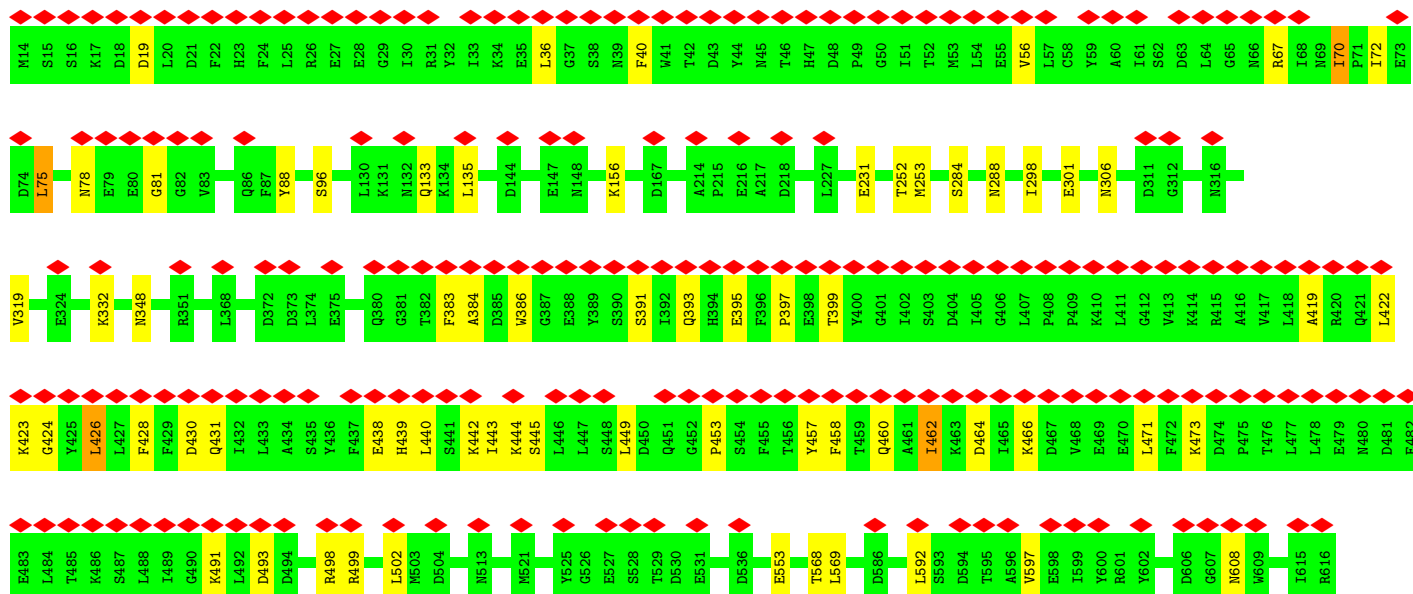
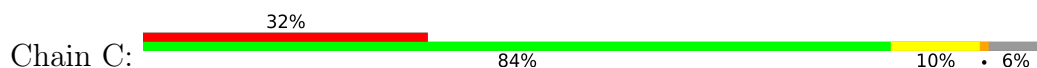


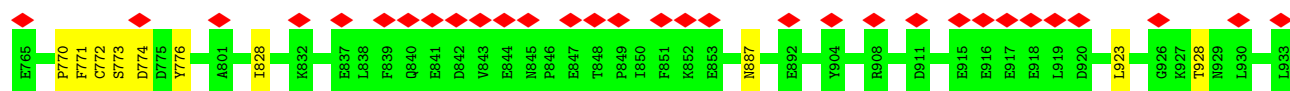
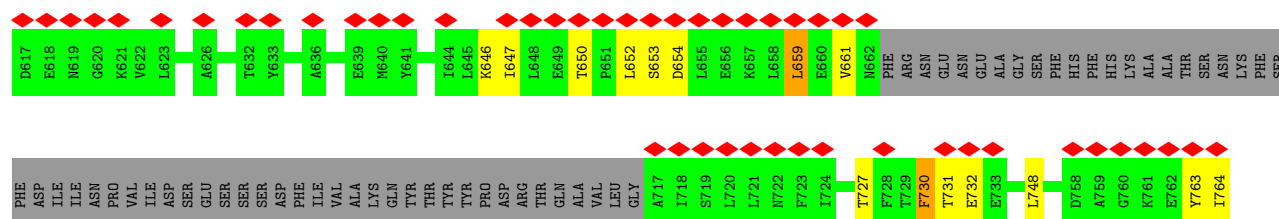
• Molecule 1: Baseplate protein Alg12



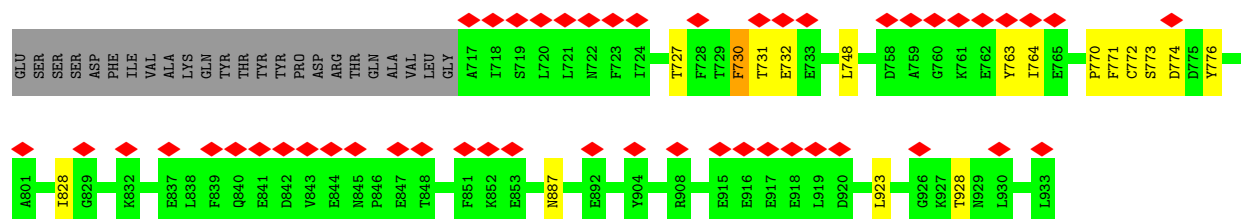
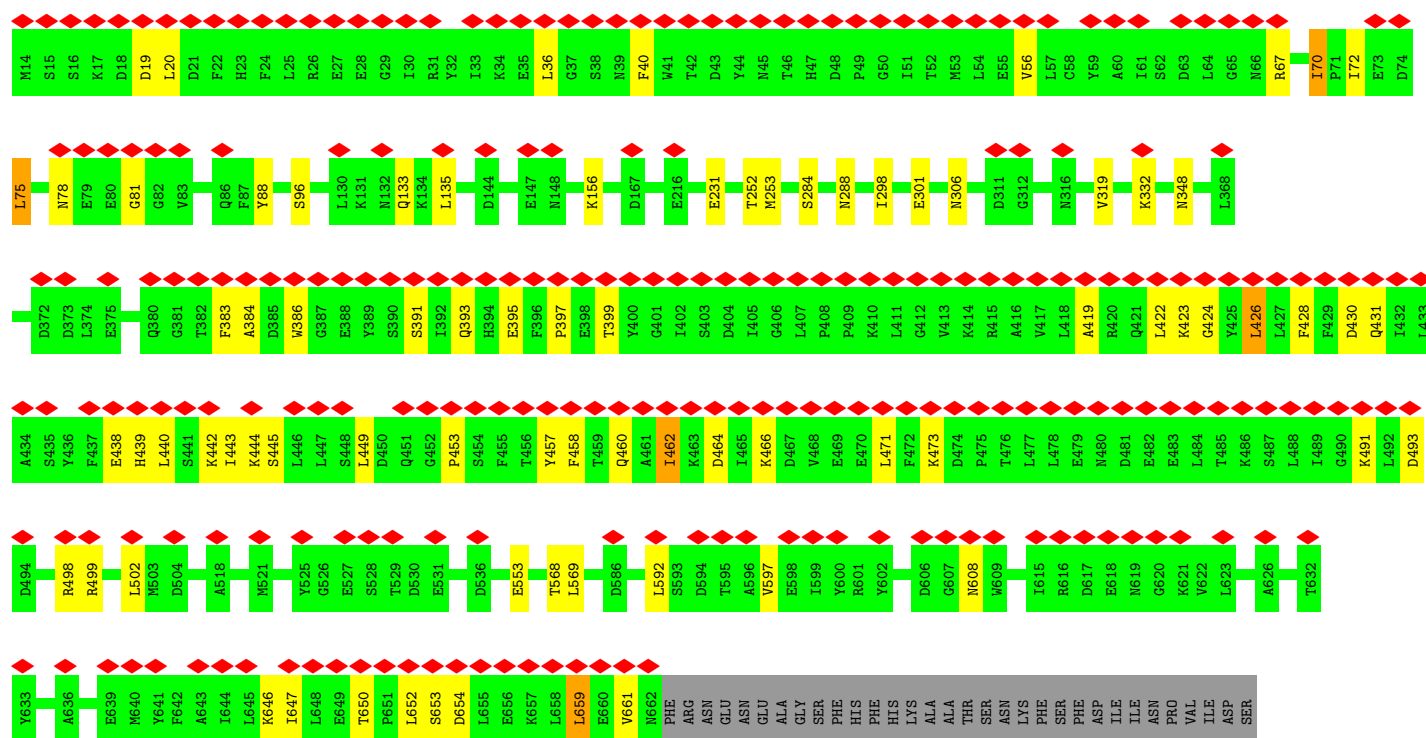
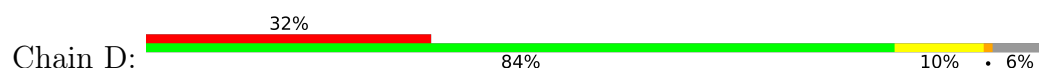


• Molecule 1: Baseplate protein Alg12

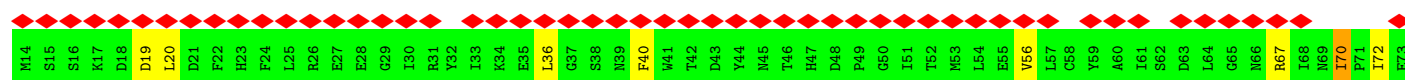
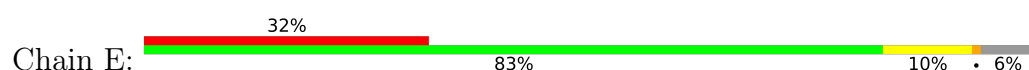


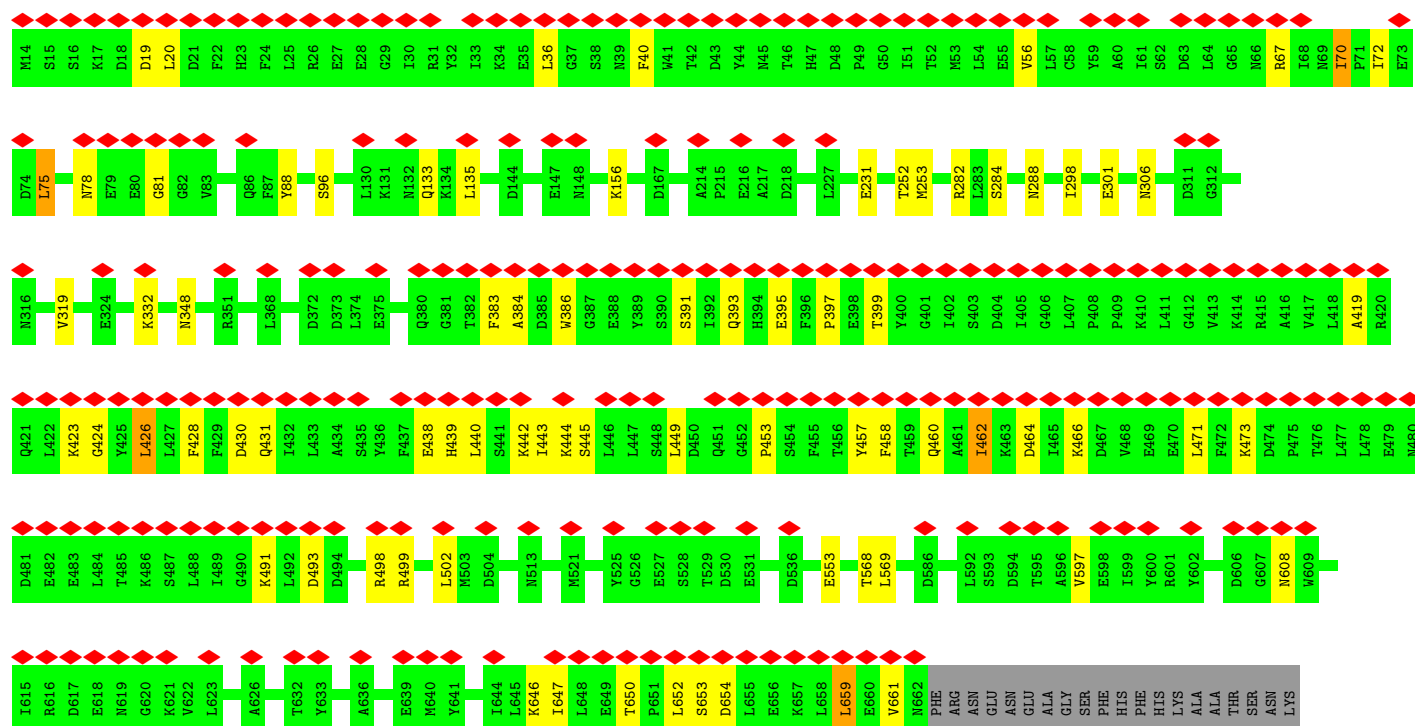


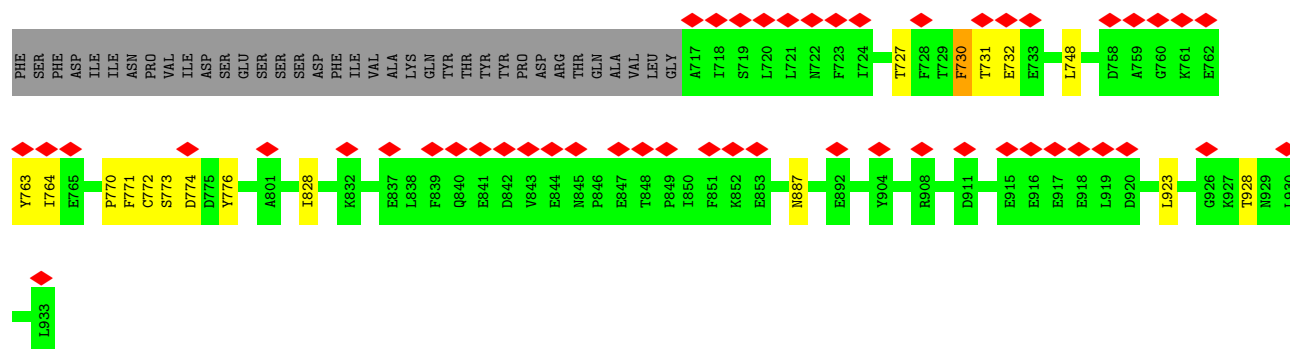
• Molecule 1: Baseplate protein Alg12



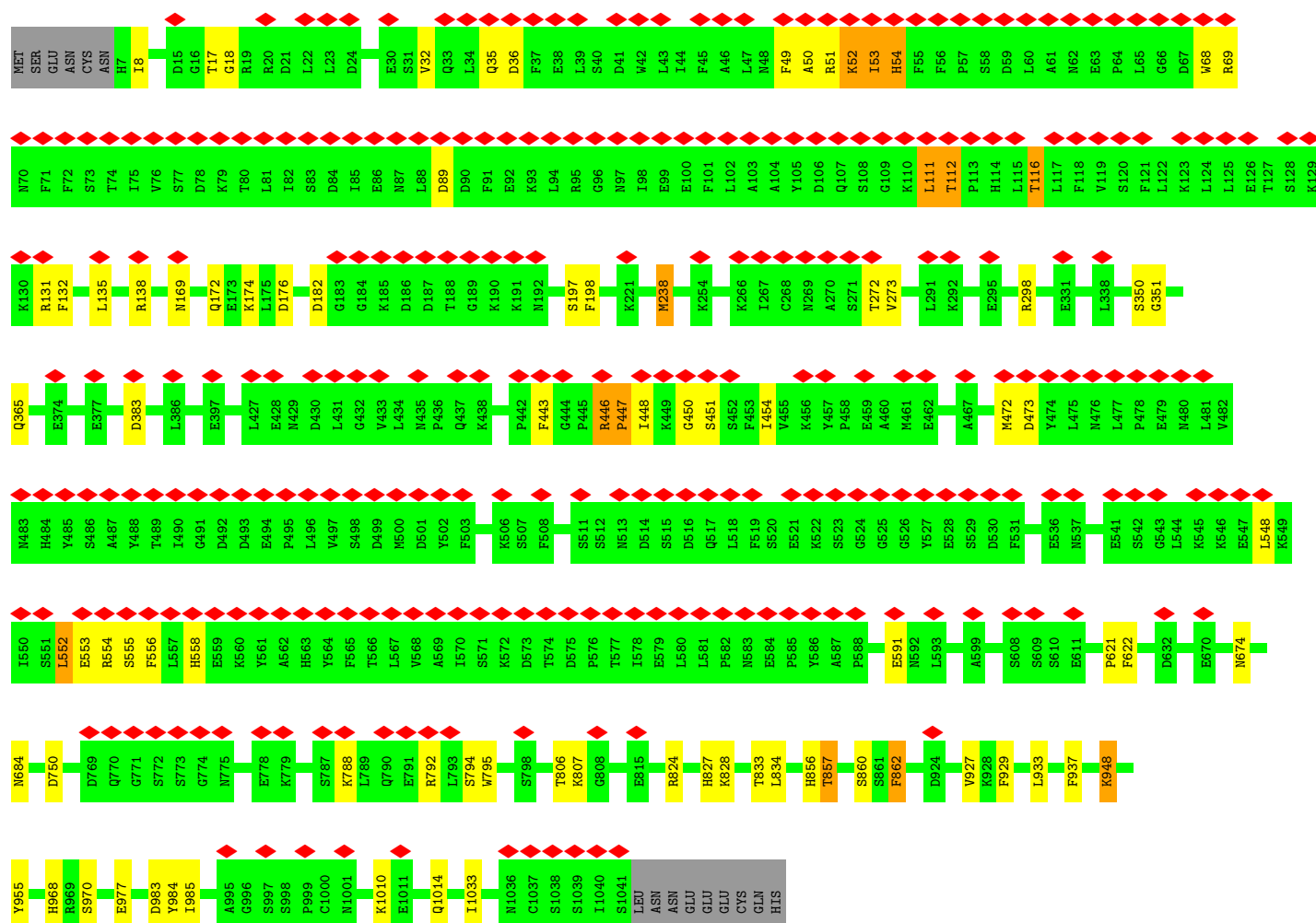
• Molecule 1: Baseplate protein Alg12



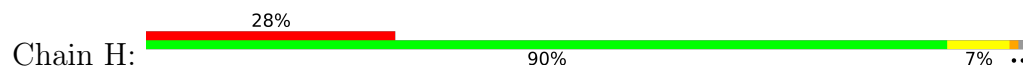


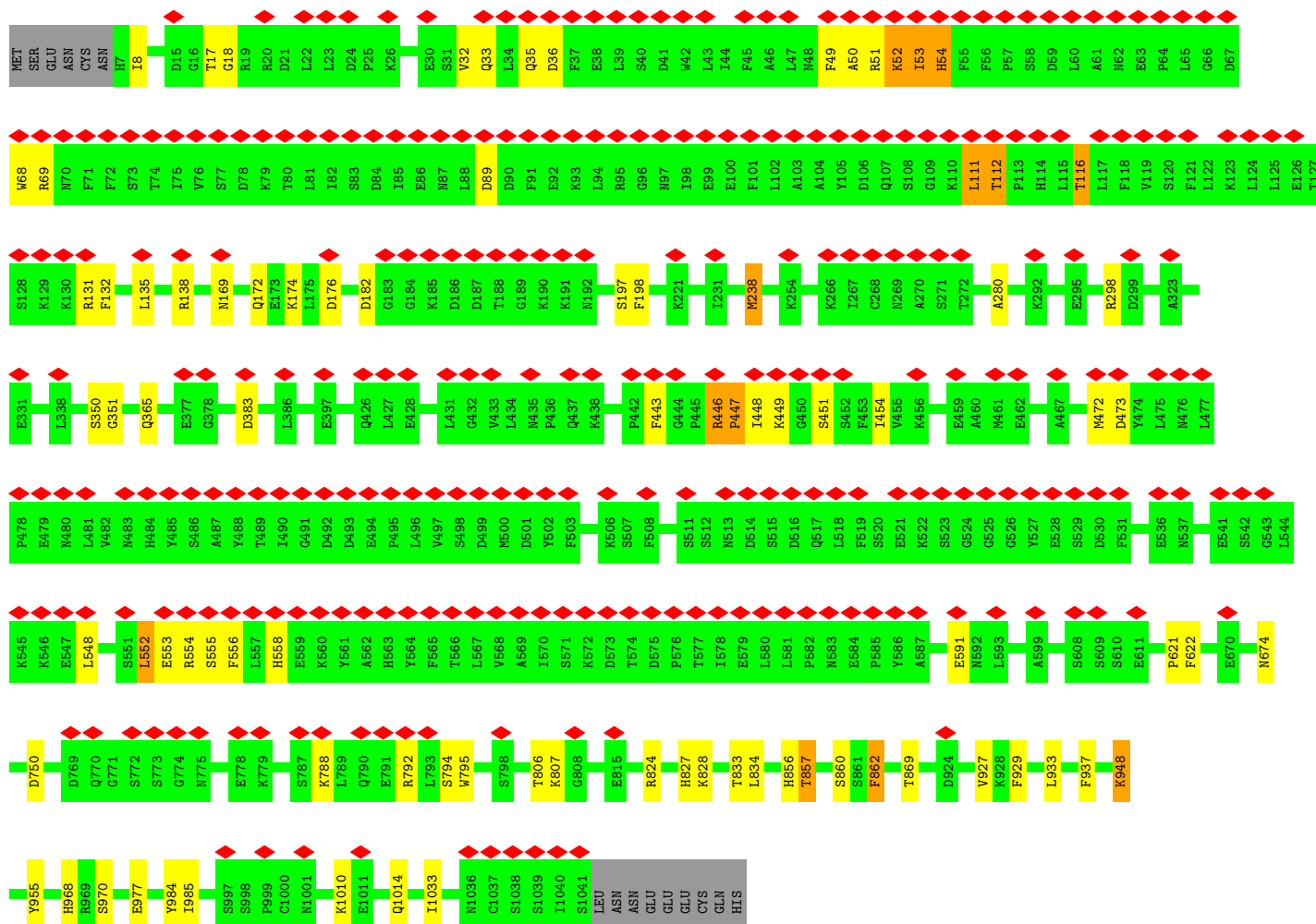


• Molecule 2: Baseplate protein J-like domain-containing protein

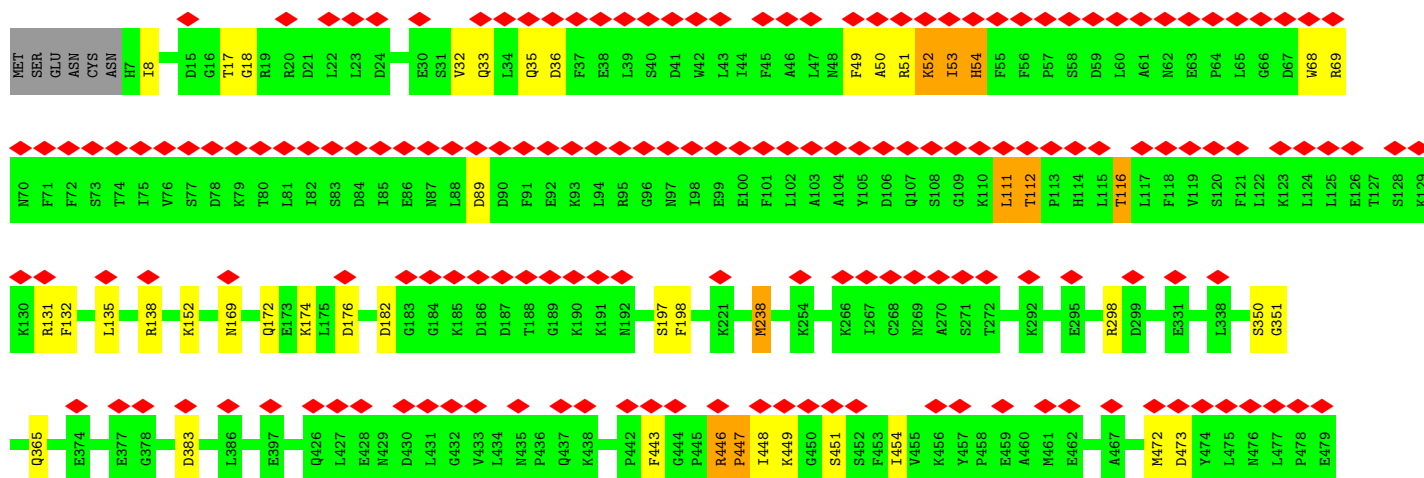
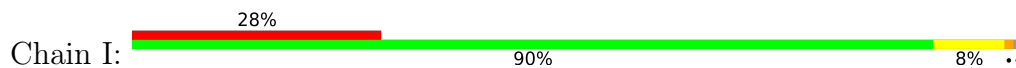


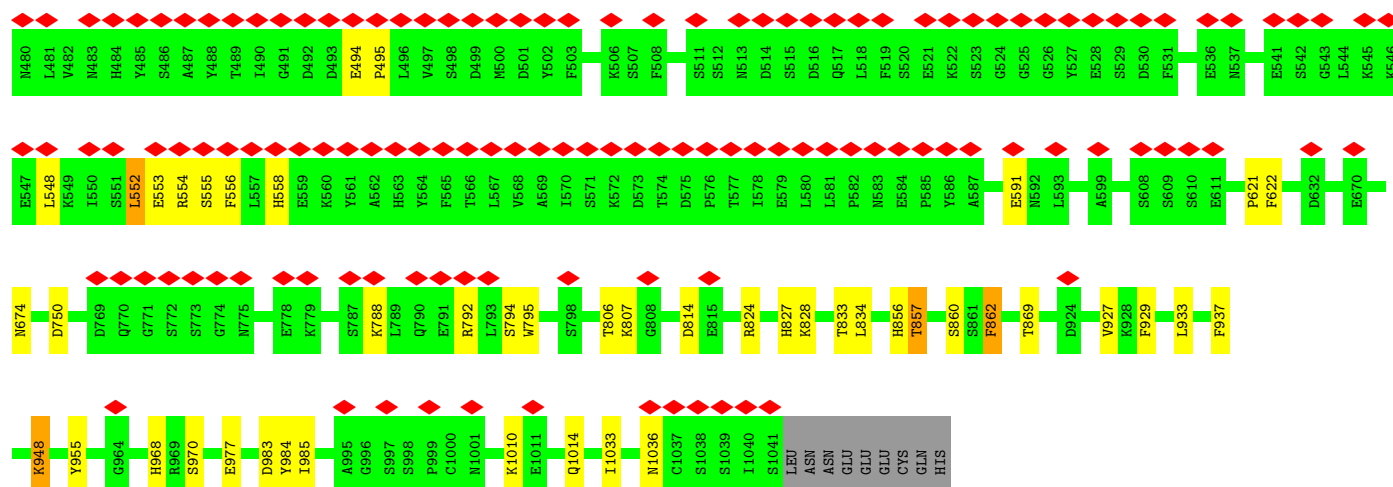
• Molecule 2: Baseplate protein J-like domain-containing protein



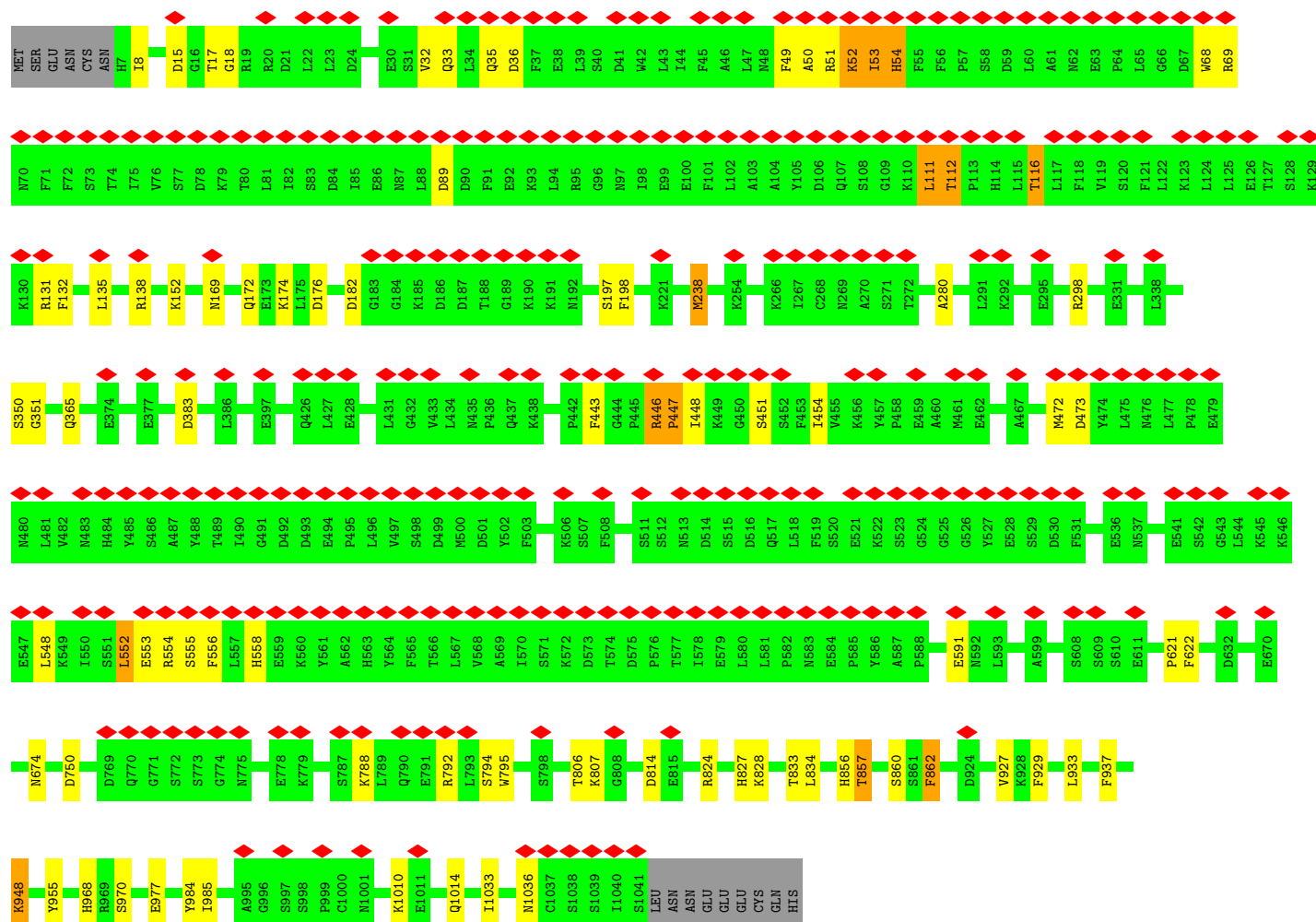
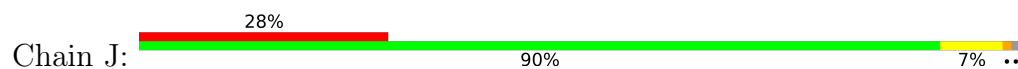


• Molecule 2: Baseplate protein J-like domain-containing protein

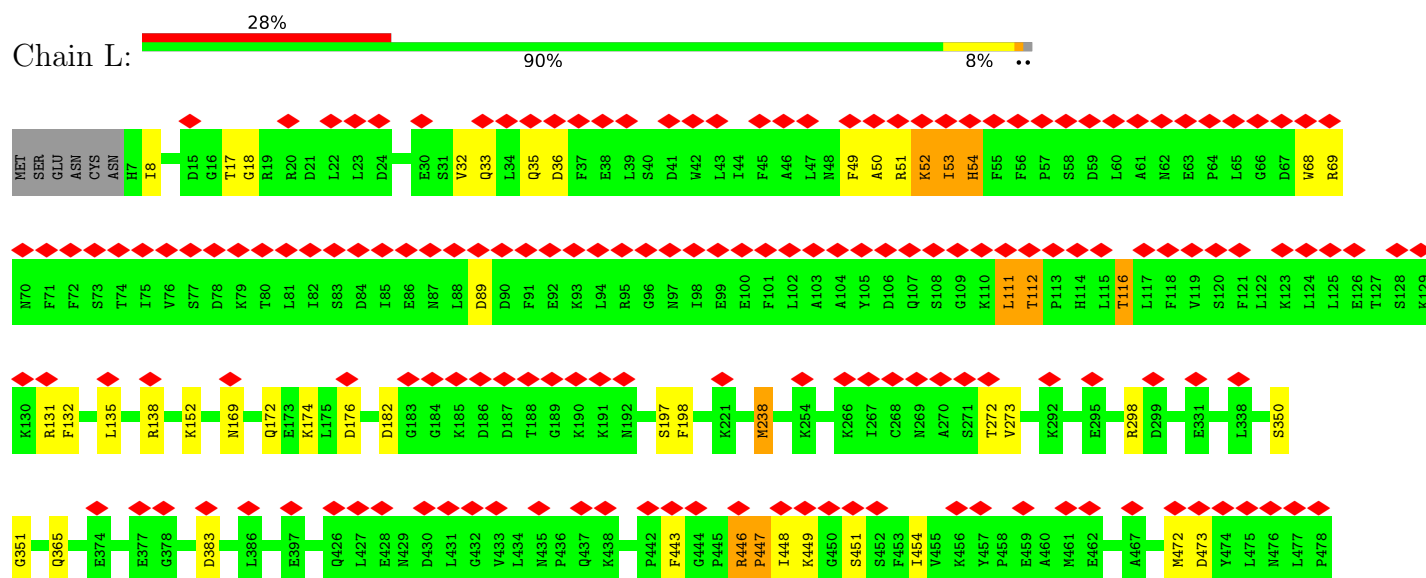


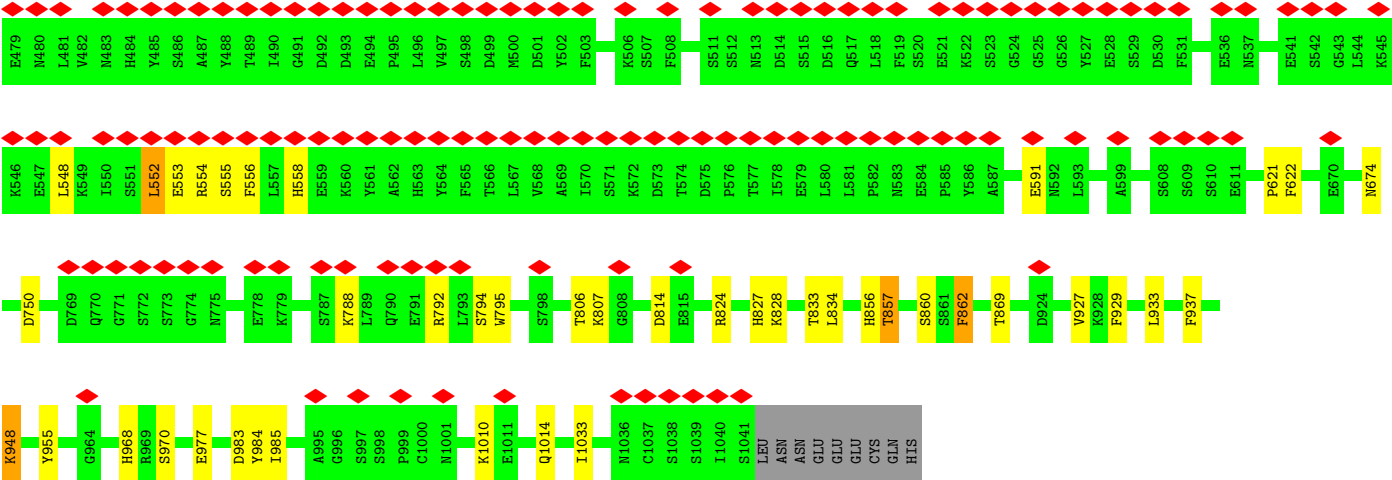


• Molecule 2: Baseplate protein J-like domain-containing protein



• Molecule 2: Baseplate protein J-like domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30251	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	616.0, 616.0, 616.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.81	9/7205 (0.1%)	1.00	19/9739 (0.2%)
1	B	0.81	9/7205 (0.1%)	1.00	19/9739 (0.2%)
1	C	0.81	8/7205 (0.1%)	1.00	19/9739 (0.2%)
1	D	0.81	9/7205 (0.1%)	1.00	19/9739 (0.2%)
1	E	0.81	8/7205 (0.1%)	1.00	19/9739 (0.2%)
1	F	0.81	9/7205 (0.1%)	1.00	19/9739 (0.2%)
2	G	0.79	21/8497 (0.2%)	1.01	22/11522 (0.2%)
2	H	0.80	20/8497 (0.2%)	1.01	22/11522 (0.2%)
2	I	0.80	21/8497 (0.2%)	1.01	22/11522 (0.2%)
2	J	0.80	20/8497 (0.2%)	1.01	22/11522 (0.2%)
2	K	0.80	20/8497 (0.2%)	1.01	21/11522 (0.2%)
2	L	0.80	21/8497 (0.2%)	1.01	22/11522 (0.2%)
All	All	0.80	175/94212 (0.2%)	1.01	245/127566 (0.2%)

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	238	MET	SD-CE	-11.46	1.50	1.79
2	K	238	MET	SD-CE	-11.46	1.50	1.79
2	L	238	MET	SD-CE	-11.46	1.50	1.79
2	J	238	MET	SD-CE	-11.44	1.50	1.79
2	G	238	MET	SD-CE	-11.43	1.50	1.79
2	H	238	MET	SD-CE	-11.43	1.50	1.79
1	E	462	ILE	CG1-CD1	-10.60	1.10	1.51
1	A	462	ILE	CG1-CD1	-10.59	1.10	1.51
1	C	462	ILE	CG1-CD1	-10.59	1.10	1.51
1	D	462	ILE	CG1-CD1	-10.59	1.10	1.51
1	F	462	ILE	CG1-CD1	-10.58	1.10	1.51
1	B	462	ILE	CG1-CD1	-10.58	1.10	1.51
2	K	473	ASP	N-CA	7.95	1.56	1.45
2	J	473	ASP	N-CA	7.95	1.56	1.45
2	L	473	ASP	N-CA	7.94	1.56	1.45
2	G	473	ASP	N-CA	7.88	1.56	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	473	ASP	N-CA	7.85	1.56	1.45
2	I	473	ASP	N-CA	7.83	1.56	1.45
2	J	857	THR	CB-CG2	-7.64	1.27	1.52
2	L	857	THR	CB-CG2	-7.63	1.27	1.52
2	G	857	THR	CB-CG2	-7.62	1.27	1.52
2	I	857	THR	CB-CG2	-7.61	1.27	1.52
2	K	857	THR	CB-CG2	-7.61	1.27	1.52
2	H	857	THR	CB-CG2	-7.60	1.27	1.52
2	H	112	THR	C-O	-7.04	1.15	1.24
2	K	112	THR	C-O	-7.04	1.15	1.24
2	G	112	THR	C-O	-7.03	1.15	1.24
2	J	112	THR	C-O	-7.03	1.15	1.24
2	I	112	THR	C-O	-7.00	1.15	1.24
2	L	112	THR	C-O	-7.00	1.15	1.24
2	H	473	ASP	CA-C	6.84	1.61	1.52
2	G	473	ASP	CA-C	6.83	1.61	1.52
2	I	473	ASP	CA-C	6.82	1.61	1.52
2	L	473	ASP	CA-C	6.82	1.61	1.52
2	J	473	ASP	CA-C	6.81	1.61	1.52
2	K	591	GLU	C-N	6.81	1.43	1.33
2	I	591	GLU	C-N	6.80	1.43	1.33
2	L	591	GLU	C-N	6.80	1.43	1.33
2	G	591	GLU	C-N	6.79	1.43	1.33
2	J	591	GLU	C-N	6.79	1.43	1.33
2	H	591	GLU	C-N	6.78	1.43	1.33
2	K	473	ASP	CA-C	6.78	1.61	1.52
2	H	447	PRO	CG-CD	-6.74	1.27	1.50
2	I	447	PRO	CG-CD	-6.74	1.27	1.50
2	L	447	PRO	CG-CD	-6.74	1.27	1.50
2	G	447	PRO	CG-CD	-6.73	1.27	1.50
2	J	447	PRO	CG-CD	-6.71	1.27	1.50
2	K	447	PRO	CG-CD	-6.71	1.27	1.50
1	A	383	PHE	C-N	6.38	1.43	1.33
1	D	383	PHE	C-N	6.38	1.43	1.33
1	B	383	PHE	C-N	6.36	1.43	1.33
1	E	383	PHE	C-N	6.36	1.43	1.33
1	C	383	PHE	C-N	6.35	1.43	1.33
1	F	383	PHE	C-N	6.35	1.43	1.33
2	H	552	LEU	CG-CD1	-6.23	1.32	1.52
2	I	552	LEU	CG-CD1	-6.21	1.32	1.52
2	L	552	LEU	CG-CD1	-6.21	1.32	1.52
2	G	552	LEU	CG-CD1	-6.20	1.32	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	552	LEU	CG-CD1	-6.20	1.32	1.52
2	K	552	LEU	CG-CD1	-6.19	1.32	1.52
2	H	53	ILE	N-CA	-6.12	1.39	1.46
2	K	53	ILE	N-CA	-6.12	1.39	1.46
2	G	53	ILE	N-CA	-6.11	1.39	1.46
2	J	53	ILE	N-CA	-6.11	1.39	1.46
2	L	53	ILE	N-CA	-6.08	1.39	1.46
2	G	53	ILE	C-N	-6.08	1.25	1.33
2	J	53	ILE	C-N	-6.08	1.25	1.33
2	H	53	ILE	C-N	-6.07	1.25	1.33
2	K	53	ILE	C-N	-6.07	1.25	1.33
2	I	53	ILE	N-CA	-6.06	1.39	1.46
2	I	53	ILE	C-N	-6.05	1.25	1.33
2	L	53	ILE	C-N	-6.05	1.25	1.33
2	J	238	MET	CG-SD	-6.04	1.65	1.80
2	I	238	MET	CG-SD	-6.02	1.65	1.80
2	L	238	MET	CG-SD	-6.02	1.65	1.80
1	C	75	LEU	CB-CG	-6.02	1.41	1.53
1	A	70	ILE	CG1-CD1	-6.01	1.28	1.51
2	G	238	MET	CG-SD	-6.01	1.65	1.80
1	C	70	ILE	CG1-CD1	-6.01	1.28	1.51
1	B	70	ILE	CG1-CD1	-6.01	1.28	1.51
1	E	70	ILE	CG1-CD1	-6.01	1.28	1.51
1	F	70	ILE	CG1-CD1	-6.01	1.28	1.51
1	B	75	LEU	CB-CG	-6.01	1.41	1.53
1	D	70	ILE	CG1-CD1	-6.01	1.28	1.51
2	K	238	MET	CG-SD	-6.00	1.65	1.80
2	H	238	MET	CG-SD	-6.00	1.65	1.80
1	A	75	LEU	CB-CG	-5.99	1.41	1.53
1	E	75	LEU	CB-CG	-5.98	1.41	1.53
1	F	75	LEU	CB-CG	-5.98	1.41	1.53
1	D	75	LEU	CB-CG	-5.96	1.41	1.53
2	L	54	HIS	N-CA	-5.78	1.39	1.46
1	C	70	ILE	CB-CG1	-5.77	1.42	1.53
1	F	70	ILE	CB-CG1	-5.77	1.42	1.53
1	A	70	ILE	CB-CG1	-5.76	1.42	1.53
1	B	70	ILE	CB-CG1	-5.75	1.42	1.53
2	I	54	HIS	N-CA	-5.75	1.39	1.46
1	D	70	ILE	CB-CG1	-5.75	1.42	1.53
1	E	70	ILE	CB-CG1	-5.74	1.42	1.53
2	I	116	THR	CB-CG2	-5.74	1.33	1.52
2	L	116	THR	CB-CG2	-5.72	1.33	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	116	THR	CB-CG2	-5.72	1.33	1.52
2	G	54	HIS	N-CA	-5.71	1.39	1.46
2	J	54	HIS	N-CA	-5.71	1.39	1.46
2	G	116	THR	CB-CG2	-5.71	1.33	1.52
2	J	116	THR	CB-CG2	-5.71	1.33	1.52
2	H	116	THR	CB-CG2	-5.71	1.33	1.52
2	H	54	HIS	N-CA	-5.71	1.39	1.46
2	K	54	HIS	N-CA	-5.69	1.39	1.46
1	E	81	GLY	N-CA	5.65	1.50	1.45
1	A	81	GLY	N-CA	5.61	1.50	1.45
1	C	81	GLY	N-CA	5.60	1.50	1.45
1	F	81	GLY	N-CA	5.59	1.50	1.45
1	D	81	GLY	N-CA	5.57	1.50	1.45
1	B	81	GLY	N-CA	5.54	1.50	1.45
2	H	552	LEU	C-O	-5.52	1.17	1.23
2	K	552	LEU	C-O	-5.52	1.17	1.23
2	L	111	LEU	C-N	5.49	1.39	1.33
2	G	552	LEU	C-O	-5.49	1.17	1.23
2	J	552	LEU	C-O	-5.49	1.17	1.23
2	I	552	LEU	C-O	-5.46	1.17	1.23
2	L	552	LEU	C-O	-5.46	1.17	1.23
2	K	111	LEU	C-N	5.44	1.39	1.33
2	G	111	LEU	C-N	5.43	1.39	1.33
2	J	111	LEU	C-N	5.43	1.39	1.33
2	H	111	LEU	C-N	5.42	1.39	1.33
2	K	446	ARG	CZ-NH1	-5.40	1.25	1.32
2	I	111	LEU	C-N	5.39	1.39	1.33
2	I	446	ARG	CZ-NH1	-5.36	1.25	1.32
2	G	446	ARG	CZ-NH1	-5.33	1.25	1.32
2	J	446	ARG	CZ-NH1	-5.33	1.25	1.32
2	L	446	ARG	CZ-NH1	-5.33	1.25	1.32
2	J	591	GLU	CA-C	5.30	1.58	1.52
1	D	770	PRO	N-CA	5.30	1.52	1.46
2	H	591	GLU	CA-C	5.29	1.58	1.52
2	K	591	GLU	CA-C	5.29	1.58	1.52
2	H	446	ARG	CZ-NH1	-5.29	1.25	1.32
2	I	591	GLU	CA-C	5.28	1.58	1.52
2	I	112	THR	N-CA	5.28	1.51	1.46
1	B	770	PRO	N-CA	5.27	1.52	1.46
2	G	591	GLU	CA-C	5.26	1.58	1.52
2	I	52	LYS	CA-C	-5.26	1.46	1.53
2	H	112	THR	N-CA	5.23	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	112	THR	N-CA	5.23	1.51	1.46
2	L	591	GLU	CA-C	5.22	1.58	1.52
2	H	52	LYS	CA-C	-5.22	1.46	1.53
2	K	52	LYS	CA-C	-5.22	1.46	1.53
2	G	112	THR	N-CA	5.21	1.50	1.46
1	C	426	LEU	CG-CD1	-5.21	1.35	1.52
1	C	770	PRO	N-CA	5.21	1.52	1.46
2	J	52	LYS	CA-C	-5.21	1.46	1.53
2	G	52	LYS	CA-C	-5.21	1.46	1.53
1	E	770	PRO	N-CA	5.19	1.52	1.46
1	A	770	PRO	N-CA	5.19	1.52	1.46
2	K	112	THR	N-CA	5.19	1.50	1.46
2	L	52	LYS	CA-C	-5.19	1.46	1.53
1	A	426	LEU	CG-CD1	-5.18	1.35	1.52
1	D	426	LEU	CG-CD1	-5.18	1.35	1.52
2	L	112	THR	N-CA	5.18	1.50	1.46
1	B	426	LEU	CG-CD1	-5.18	1.35	1.52
1	F	426	LEU	CG-CD1	-5.17	1.35	1.52
1	E	426	LEU	CG-CD1	-5.16	1.35	1.52
1	F	770	PRO	N-CA	5.13	1.52	1.46
2	L	591	GLU	N-CA	5.11	1.52	1.46
1	B	81	GLY	CA-C	5.10	1.59	1.52
2	G	591	GLU	N-CA	5.08	1.51	1.46
2	H	591	GLU	N-CA	5.07	1.51	1.46
2	K	591	GLU	N-CA	5.07	1.51	1.46
2	I	53	ILE	CA-C	-5.05	1.46	1.52
2	L	53	ILE	CA-C	-5.05	1.46	1.52
2	J	591	GLU	N-CA	5.04	1.51	1.46
1	A	81	GLY	CA-C	5.03	1.59	1.52
2	I	591	GLU	N-CA	5.03	1.51	1.46
1	D	81	GLY	CA-C	5.03	1.59	1.52
2	G	53	ILE	CA-C	-5.03	1.46	1.52
1	F	81	GLY	CA-C	5.01	1.59	1.52

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	473	ASP	N-CA-C	8.97	123.54	109.81
2	H	473	ASP	N-CA-C	8.96	123.51	109.81
2	G	473	ASP	N-CA-C	8.95	123.50	109.81
2	K	473	ASP	N-CA-C	8.95	123.51	109.81
2	L	473	ASP	N-CA-C	8.93	123.47	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	473	ASP	N-CA-C	8.93	123.47	109.81
2	K	856	HIS	CA-C-N	-8.72	110.70	122.99
2	K	856	HIS	C-N-CA	-8.72	110.70	122.99
2	L	856	HIS	CA-C-N	-8.71	110.70	122.99
2	L	856	HIS	C-N-CA	-8.71	110.70	122.99
2	G	856	HIS	CA-C-N	-8.71	110.71	122.99
2	G	856	HIS	C-N-CA	-8.71	110.71	122.99
2	I	856	HIS	CA-C-N	-8.70	110.72	122.99
2	I	856	HIS	C-N-CA	-8.70	110.72	122.99
2	J	856	HIS	CA-C-N	-8.70	110.72	122.99
2	J	856	HIS	C-N-CA	-8.70	110.72	122.99
2	H	856	HIS	CA-C-N	-8.69	110.74	122.99
2	H	856	HIS	C-N-CA	-8.69	110.74	122.99
2	H	446	ARG	NE-CZ-NH1	8.54	130.04	121.50
2	L	446	ARG	NE-CZ-NH1	8.50	130.00	121.50
2	G	446	ARG	NE-CZ-NH1	8.48	129.98	121.50
2	K	446	ARG	NE-CZ-NH1	8.48	129.98	121.50
2	I	446	ARG	NE-CZ-NH1	8.47	129.97	121.50
2	J	446	ARG	NE-CZ-NH1	8.46	129.96	121.50
2	H	446	ARG	NH1-CZ-NH2	-8.31	108.50	119.30
2	L	446	ARG	NH1-CZ-NH2	-8.26	108.56	119.30
2	G	446	ARG	NH1-CZ-NH2	-8.25	108.57	119.30
2	I	446	ARG	NH1-CZ-NH2	-8.24	108.59	119.30
2	J	446	ARG	NH1-CZ-NH2	-8.24	108.59	119.30
2	K	446	ARG	NH1-CZ-NH2	-8.24	108.59	119.30
1	C	81	GLY	N-CA-C	7.92	119.48	111.95
1	E	81	GLY	N-CA-C	7.92	119.48	111.95
1	F	81	GLY	N-CA-C	7.91	119.46	111.95
1	A	81	GLY	N-CA-C	7.90	119.45	111.95
1	B	81	GLY	N-CA-C	7.88	119.43	111.95
1	D	81	GLY	N-CA-C	7.88	119.43	111.95
2	L	53	ILE	CG1-CB-CG2	-7.59	87.94	110.70
2	I	53	ILE	CG1-CB-CG2	-7.58	87.96	110.70
2	G	53	ILE	CG1-CB-CG2	-7.58	87.98	110.70
2	H	53	ILE	CG1-CB-CG2	-7.57	87.98	110.70
2	J	53	ILE	CG1-CB-CG2	-7.57	87.98	110.70
2	K	53	ILE	CG1-CB-CG2	-7.57	87.98	110.70
1	D	653	SER	CA-C-N	7.28	130.35	120.38
1	D	653	SER	C-N-CA	7.28	130.35	120.38
1	F	653	SER	CA-C-N	7.27	130.34	120.38
1	F	653	SER	C-N-CA	7.27	130.34	120.38
1	A	653	SER	CA-C-N	7.25	130.32	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	653	SER	C-N-CA	7.25	130.32	120.38
1	C	653	SER	CA-C-N	7.24	130.29	120.38
1	C	653	SER	C-N-CA	7.24	130.29	120.38
1	B	653	SER	CA-C-N	7.23	130.29	120.38
1	B	653	SER	C-N-CA	7.23	130.29	120.38
1	E	653	SER	CA-C-N	7.21	130.26	120.38
1	E	653	SER	C-N-CA	7.21	130.26	120.38
2	J	857	THR	N-CA-C	7.18	120.60	108.90
2	G	857	THR	N-CA-C	7.17	120.59	108.90
2	H	857	THR	N-CA-C	7.17	120.60	108.90
2	I	857	THR	N-CA-C	7.17	120.59	108.90
2	L	857	THR	N-CA-C	7.16	120.56	108.90
2	K	857	THR	N-CA-C	7.15	120.55	108.90
2	I	795	TRP	N-CA-C	-6.77	102.49	113.19
2	H	795	TRP	N-CA-C	-6.77	102.50	113.19
2	K	795	TRP	N-CA-C	-6.77	102.50	113.19
2	L	795	TRP	N-CA-C	-6.77	102.50	113.19
2	G	795	TRP	N-CA-C	-6.76	102.50	113.19
2	J	795	TRP	N-CA-C	-6.73	102.56	113.19
2	H	827	HIS	CB-CA-C	-6.70	100.37	110.88
2	K	827	HIS	CB-CA-C	-6.70	100.37	110.88
2	I	827	HIS	CB-CA-C	-6.69	100.37	110.88
2	G	827	HIS	CB-CA-C	-6.69	100.38	110.88
2	J	827	HIS	CB-CA-C	-6.67	100.40	110.88
2	L	827	HIS	CB-CA-C	-6.66	100.37	110.90
2	J	591	GLU	N-CA-C	6.40	117.94	108.60
2	K	591	GLU	N-CA-C	6.38	117.92	108.60
2	I	591	GLU	N-CA-C	6.38	117.91	108.60
2	G	591	GLU	N-CA-C	6.38	117.91	108.60
2	L	591	GLU	N-CA-C	6.37	117.90	108.60
2	H	591	GLU	N-CA-C	6.36	117.89	108.60
2	I	472	MET	O-C-N	-6.26	116.01	123.27
2	K	472	MET	O-C-N	-6.26	116.01	123.27
2	L	473	ASP	O-C-N	-6.26	113.99	122.94
2	I	52	LYS	CA-C-N	-6.25	112.33	122.33
2	I	52	LYS	C-N-CA	-6.25	112.33	122.33
2	J	473	ASP	O-C-N	-6.25	114.00	122.94
2	H	52	LYS	CA-C-N	-6.25	112.33	122.33
2	H	52	LYS	C-N-CA	-6.25	112.33	122.33
2	K	52	LYS	CA-C-N	-6.25	112.33	122.33
2	K	52	LYS	C-N-CA	-6.25	112.33	122.33
2	L	862	PHE	CG-CD2-CE2	6.25	131.32	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	473	ASP	O-C-N	-6.24	114.01	122.94
2	I	862	PHE	CG-CD2-CE2	6.24	131.30	120.70
2	G	862	PHE	CG-CD2-CE2	6.24	131.30	120.70
2	G	473	ASP	O-C-N	-6.24	114.02	122.94
2	K	862	PHE	CG-CD2-CE2	6.23	131.30	120.70
2	G	52	LYS	CA-C-N	-6.22	112.37	122.33
2	G	52	LYS	C-N-CA	-6.22	112.37	122.33
2	J	52	LYS	CA-C-N	-6.22	112.37	122.33
2	J	52	LYS	C-N-CA	-6.22	112.37	122.33
2	J	862	PHE	CG-CD2-CE2	6.22	131.28	120.70
2	H	473	ASP	O-C-N	-6.22	114.05	122.94
2	G	472	MET	O-C-N	-6.21	116.06	123.27
2	I	473	ASP	O-C-N	-6.21	114.06	122.94
2	L	52	LYS	CA-C-N	-6.21	112.39	122.33
2	L	52	LYS	C-N-CA	-6.21	112.39	122.33
2	H	862	PHE	CG-CD2-CE2	6.21	131.25	120.70
2	H	472	MET	O-C-N	-6.20	116.08	123.27
2	L	472	MET	O-C-N	-6.20	116.08	123.27
2	J	472	MET	O-C-N	-6.17	116.11	123.27
2	I	794	SER	CA-C-N	5.97	130.97	121.18
2	I	794	SER	C-N-CA	5.97	130.97	121.18
2	G	794	SER	CA-C-N	5.97	130.97	121.18
2	G	794	SER	C-N-CA	5.97	130.97	121.18
2	J	794	SER	CA-C-N	5.97	130.97	121.18
2	J	794	SER	C-N-CA	5.97	130.97	121.18
2	H	794	SER	CA-C-N	5.96	130.96	121.18
2	H	794	SER	C-N-CA	5.96	130.96	121.18
1	B	763	TYR	CA-C-N	5.96	128.88	120.42
1	B	763	TYR	C-N-CA	5.96	128.88	120.42
2	L	794	SER	CA-C-N	5.95	130.94	121.18
2	L	794	SER	C-N-CA	5.95	130.94	121.18
1	C	763	TYR	CA-C-N	5.95	128.87	120.42
1	C	763	TYR	C-N-CA	5.95	128.87	120.42
1	F	763	TYR	CA-C-N	5.95	128.87	120.42
1	F	763	TYR	C-N-CA	5.95	128.87	120.42
1	A	763	TYR	CA-C-N	5.94	128.85	120.42
1	A	763	TYR	C-N-CA	5.94	128.85	120.42
2	K	794	SER	CA-C-N	5.94	130.92	121.18
2	K	794	SER	C-N-CA	5.94	130.92	121.18
1	E	763	TYR	CA-C-N	5.92	128.83	120.42
1	E	763	TYR	C-N-CA	5.92	128.83	120.42
1	D	763	TYR	CA-C-N	5.92	128.82	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	763	TYR	C-N-CA	5.92	128.82	120.42
1	C	466	LYS	CA-C-N	-5.88	113.20	122.79
1	C	466	LYS	C-N-CA	-5.88	113.20	122.79
1	B	466	LYS	CA-C-N	-5.88	113.21	122.79
1	B	466	LYS	C-N-CA	-5.88	113.21	122.79
1	A	466	LYS	CA-C-N	-5.88	113.21	122.79
1	A	466	LYS	C-N-CA	-5.88	113.21	122.79
1	D	466	LYS	CA-C-N	-5.87	113.22	122.79
1	D	466	LYS	C-N-CA	-5.87	113.22	122.79
1	F	466	LYS	CA-C-N	-5.87	113.22	122.79
1	F	466	LYS	C-N-CA	-5.87	113.22	122.79
1	E	466	LYS	CA-C-N	-5.87	113.23	122.79
1	E	466	LYS	C-N-CA	-5.87	113.23	122.79
1	E	608	ASN	N-CA-C	-5.86	107.12	114.56
1	C	608	ASN	N-CA-C	-5.84	107.14	114.56
1	D	608	ASN	N-CA-C	-5.83	107.15	114.56
1	A	608	ASN	N-CA-C	-5.83	107.16	114.56
1	F	608	ASN	N-CA-C	-5.83	107.16	114.56
1	B	608	ASN	N-CA-C	-5.81	107.18	114.56
1	D	828	ILE	N-CA-C	5.73	115.81	108.82
1	A	828	ILE	N-CA-C	5.70	115.77	108.82
1	F	828	ILE	N-CA-C	5.69	115.76	108.82
1	C	828	ILE	N-CA-C	5.68	115.75	108.82
1	E	828	ILE	N-CA-C	5.68	115.75	108.82
1	B	828	ILE	N-CA-C	5.67	115.74	108.82
1	D	732	GLU	N-CA-C	5.38	119.10	112.54
1	B	732	GLU	N-CA-C	5.36	119.08	112.54
1	E	732	GLU	N-CA-C	5.36	119.08	112.54
1	F	732	GLU	N-CA-C	5.36	119.07	112.54
1	F	156	LYS	N-CA-C	5.35	119.79	112.68
1	F	81	GLY	O-C-N	-5.34	117.31	122.87
1	A	732	GLU	N-CA-C	5.34	119.06	112.54
1	D	156	LYS	N-CA-C	5.34	119.78	112.68
1	C	732	GLU	N-CA-C	5.33	119.04	112.54
1	C	748	LEU	N-CA-C	-5.32	108.55	114.62
1	A	156	LYS	N-CA-C	5.32	119.76	112.68
1	E	156	LYS	N-CA-C	5.32	119.75	112.68
1	D	81	GLY	O-C-N	-5.31	117.35	122.87
1	D	748	LEU	N-CA-C	-5.31	108.57	114.62
1	C	156	LYS	N-CA-C	5.30	119.73	112.68
1	B	156	LYS	N-CA-C	5.29	119.72	112.68
1	E	748	LEU	N-CA-C	-5.29	108.59	114.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	GLY	O-C-N	-5.29	117.37	122.87
1	C	81	GLY	O-C-N	-5.29	117.37	122.87
1	A	748	LEU	N-CA-C	-5.28	108.60	114.62
1	E	81	GLY	O-C-N	-5.28	117.38	122.87
1	A	348	ASN	CA-C-N	5.27	124.94	119.56
1	A	348	ASN	C-N-CA	5.27	124.94	119.56
1	B	748	LEU	N-CA-C	-5.26	108.62	114.62
1	B	348	ASN	CA-C-N	5.26	124.93	119.56
1	B	348	ASN	C-N-CA	5.26	124.93	119.56
1	F	348	ASN	CA-C-N	5.26	124.92	119.56
1	F	348	ASN	C-N-CA	5.26	124.92	119.56
1	F	770	PRO	N-CA-C	5.26	120.55	111.77
1	C	348	ASN	CA-C-N	5.25	124.92	119.56
1	C	348	ASN	C-N-CA	5.25	124.92	119.56
1	B	81	GLY	O-C-N	-5.25	117.41	122.87
1	D	348	ASN	CA-C-N	5.25	124.91	119.56
1	D	348	ASN	C-N-CA	5.25	124.91	119.56
1	E	348	ASN	CA-C-N	5.25	124.91	119.56
1	E	348	ASN	C-N-CA	5.25	124.91	119.56
1	F	748	LEU	N-CA-C	-5.24	108.64	114.62
1	E	770	PRO	N-CA-C	5.24	120.52	111.77
1	B	770	PRO	N-CA-C	5.24	120.52	111.77
1	C	770	PRO	N-CA-C	5.23	120.51	111.77
1	A	770	PRO	N-CA-C	5.23	120.51	111.77
1	D	770	PRO	N-CA-C	5.23	120.51	111.77
2	I	182	ASP	N-CA-C	5.22	115.94	108.74
1	B	652	LEU	N-CA-C	-5.21	103.51	110.55
1	F	731	THR	N-CA-C	5.21	118.43	111.24
1	C	652	LEU	N-CA-C	-5.21	103.52	110.55
2	H	182	ASP	N-CA-C	5.21	115.92	108.74
1	E	652	LEU	N-CA-C	-5.21	103.52	110.55
2	J	182	ASP	N-CA-C	5.21	115.92	108.74
1	E	731	THR	N-CA-C	5.20	118.42	111.24
1	A	652	LEU	N-CA-C	-5.20	103.53	110.55
1	F	652	LEU	N-CA-C	-5.20	103.53	110.55
1	A	731	THR	N-CA-C	5.19	118.40	111.24
1	C	731	THR	N-CA-C	5.19	118.40	111.24
1	D	731	THR	N-CA-C	5.19	118.40	111.24
2	G	182	ASP	N-CA-C	5.19	115.90	108.74
2	L	182	ASP	N-CA-C	5.17	115.88	108.74
1	D	652	LEU	N-CA-C	-5.17	103.57	110.55
2	K	182	ASP	N-CA-C	5.16	115.86	108.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	731	THR	N-CA-C	5.16	118.36	111.24
1	B	730	PHE	N-CA-CB	-5.15	102.00	109.82
1	C	730	PHE	N-CA-CB	-5.14	102.00	109.82
1	F	730	PHE	N-CA-CB	-5.14	102.00	109.82
1	A	730	PHE	N-CA-CB	-5.13	102.02	109.82
1	D	730	PHE	N-CA-CB	-5.13	102.02	109.82
2	L	948	LYS	CB-CG-CD	5.11	123.06	111.30
2	K	948	LYS	CB-CG-CD	5.11	123.04	111.30
1	E	730	PHE	N-CA-CB	-5.10	102.07	109.82
2	G	948	LYS	CB-CG-CD	5.09	123.02	111.30
2	J	948	LYS	CB-CG-CD	5.09	123.02	111.30
2	H	948	LYS	CB-CG-CD	5.09	123.01	111.30
2	I	948	LYS	CB-CG-CD	5.08	122.98	111.30
2	K	1014	GLN	CA-C-N	5.06	125.34	119.47
2	K	1014	GLN	C-N-CA	5.06	125.34	119.47
2	I	116	THR	CA-CB-CG2	5.04	119.07	110.50
2	J	1014	GLN	CA-C-N	5.03	125.31	119.47
2	J	1014	GLN	C-N-CA	5.03	125.31	119.47
2	I	1014	GLN	CA-C-N	5.03	125.31	119.47
2	I	1014	GLN	C-N-CA	5.03	125.31	119.47
2	G	1014	GLN	CA-C-N	5.03	125.30	119.47
2	G	1014	GLN	C-N-CA	5.03	125.30	119.47
2	H	116	THR	CA-CB-CG2	5.02	119.03	110.50
2	G	116	THR	CA-CB-CG2	5.02	119.03	110.50
2	H	1014	GLN	CA-C-N	5.01	125.29	119.47
2	H	1014	GLN	C-N-CA	5.01	125.29	119.47
2	L	1014	GLN	CA-C-N	5.01	125.28	119.47
2	L	1014	GLN	C-N-CA	5.01	125.28	119.47
2	L	116	THR	CA-CB-CG2	5.01	119.01	110.50
2	J	116	THR	CA-CB-CG2	5.01	119.01	110.50

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	7059	0	6979	100	0
1	B	7059	0	6979	101	0
1	C	7059	0	6979	96	0
1	D	7059	0	6979	100	0
1	E	7059	0	6979	102	0
1	F	7059	0	6979	103	0
2	G	8300	0	8185	112	0
2	H	8300	0	8185	111	0
2	I	8300	0	8185	114	0
2	J	8300	0	8185	109	0
2	K	8300	0	8185	111	0
2	L	8300	0	8185	113	0
All	All	92154	0	90984	955	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (955) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:HIS:HD2	2:H:132:PHE:CZ	1.47	1.32
1:A:439:HIS:HD2	2:G:132:PHE:CZ	1.47	1.31
1:C:439:HIS:HD2	2:I:132:PHE:CZ	1.47	1.31
1:F:439:HIS:HD2	2:L:132:PHE:CZ	1.47	1.30
1:E:439:HIS:HD2	2:K:132:PHE:CZ	1.47	1.30
1:D:439:HIS:HD2	2:J:132:PHE:CZ	1.47	1.29
2:H:857:THR:HG21	2:H:862:PHE:CD2	1.74	1.23
2:J:857:THR:HG21	2:J:862:PHE:CD2	1.74	1.23
2:K:857:THR:HG21	2:K:862:PHE:CD2	1.74	1.22
2:G:857:THR:HG21	2:G:862:PHE:CD2	1.74	1.22
2:I:857:THR:HG21	2:I:862:PHE:CD2	1.74	1.21
2:L:857:THR:HG21	2:L:862:PHE:CD2	1.74	1.20
1:A:36:LEU:HB3	2:G:111:LEU:CD1	1.75	1.17
1:B:36:LEU:HB3	2:H:111:LEU:CD1	1.75	1.17
1:C:36:LEU:HB3	2:I:111:LEU:CD1	1.75	1.17
1:F:36:LEU:HB3	2:L:111:LEU:CD1	1.75	1.16
2:J:857:THR:HG21	2:J:862:PHE:HD2	0.99	1.16
1:D:36:LEU:HB3	2:J:111:LEU:CD1	1.75	1.15
1:E:36:LEU:HB3	2:K:111:LEU:CD1	1.75	1.15
2:I:857:THR:HG21	2:I:862:PHE:HD2	0.99	1.14
2:K:857:THR:HG21	2:K:862:PHE:HD2	0.99	1.13
1:B:439:HIS:CD2	2:H:132:PHE:CZ	2.38	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:HIS:CD2	2:G:132:PHE:CZ	2.38	1.11
1:C:439:HIS:CD2	2:I:132:PHE:CZ	2.38	1.11
2:H:857:THR:HG21	2:H:862:PHE:HD2	0.99	1.10
1:E:439:HIS:CD2	2:K:132:PHE:CZ	2.38	1.10
1:D:439:HIS:CD2	2:J:132:PHE:CZ	2.38	1.10
2:L:857:THR:HG21	2:L:862:PHE:HD2	0.99	1.09
1:F:439:HIS:CD2	2:L:132:PHE:CZ	2.38	1.09
2:G:857:THR:HG21	2:G:862:PHE:HD2	0.99	1.08
1:A:36:LEU:CB	2:G:111:LEU:HD12	1.85	1.07
1:E:36:LEU:CB	2:K:111:LEU:HD12	1.85	1.07
1:D:36:LEU:CB	2:J:111:LEU:HD12	1.85	1.06
1:B:36:LEU:CB	2:H:111:LEU:HD12	1.85	1.06
1:C:36:LEU:CB	2:I:111:LEU:HD12	1.85	1.05
1:F:36:LEU:CB	2:L:111:LEU:HD12	1.85	1.05
2:J:857:THR:HG22	2:J:862:PHE:HA	1.40	1.04
2:K:857:THR:HG22	2:K:862:PHE:HA	1.40	1.04
2:G:857:THR:HG22	2:G:862:PHE:HA	1.39	1.03
2:I:857:THR:HG22	2:I:862:PHE:HA	1.40	1.03
2:L:857:THR:HG22	2:L:862:PHE:HA	1.40	1.03
2:H:857:THR:HG22	2:H:862:PHE:HA	1.40	1.02
1:D:70:ILE:HD11	1:D:75:LEU:HD21	1.39	1.02
1:F:70:ILE:HD11	1:F:75:LEU:HD21	1.39	1.01
1:B:70:ILE:HD11	1:B:75:LEU:HD21	1.39	1.01
1:C:70:ILE:HD11	1:C:75:LEU:HD21	1.39	1.00
1:E:70:ILE:HD11	1:E:75:LEU:HD21	1.39	1.00
1:A:70:ILE:HD11	1:A:75:LEU:HD21	1.39	1.00
1:B:439:HIS:HD2	2:H:132:PHE:HZ	1.15	0.95
2:H:238:MET:SD	2:H:621:PRO:HB3	2.07	0.95
2:K:238:MET:SD	2:K:621:PRO:HB3	2.07	0.95
1:C:439:HIS:HD2	2:I:132:PHE:HZ	1.14	0.95
2:L:446:ARG:HH11	2:L:558:HIS:CE1	1.85	0.95
2:G:446:ARG:HH11	2:G:558:HIS:CE1	1.85	0.95
2:G:238:MET:SD	2:G:621:PRO:HB3	2.07	0.95
2:H:446:ARG:HH11	2:H:558:HIS:CE1	1.85	0.95
2:K:446:ARG:HH11	2:K:558:HIS:CE1	1.85	0.95
2:J:238:MET:SD	2:J:621:PRO:HB3	2.07	0.94
2:I:446:ARG:HH11	2:I:558:HIS:CE1	1.85	0.94
2:I:238:MET:SD	2:I:621:PRO:HB3	2.07	0.94
2:L:238:MET:SD	2:L:621:PRO:HB3	2.07	0.94
1:A:439:HIS:HD2	2:G:132:PHE:HZ	1.14	0.94
2:J:446:ARG:HH11	2:J:558:HIS:CE1	1.85	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LEU:HB3	2:J:111:LEU:HD12	0.94	0.94
1:D:439:HIS:HD2	2:J:132:PHE:HZ	1.14	0.94
1:F:36:LEU:HB3	2:L:111:LEU:HD12	0.94	0.93
1:C:36:LEU:HB3	2:I:111:LEU:HD12	0.94	0.92
1:F:439:HIS:HD2	2:L:132:PHE:HZ	1.14	0.91
1:E:439:HIS:HD2	2:K:132:PHE:HZ	1.14	0.91
1:E:36:LEU:HB3	2:K:111:LEU:HD12	0.94	0.90
1:B:36:LEU:HB3	2:H:111:LEU:HD12	0.94	0.89
1:A:36:LEU:HB3	2:G:111:LEU:HD12	0.94	0.88
2:G:857:THR:CG2	2:G:862:PHE:HA	2.07	0.85
2:H:857:THR:CG2	2:H:862:PHE:HA	2.07	0.85
2:J:857:THR:CG2	2:J:862:PHE:HA	2.07	0.84
2:I:857:THR:CG2	2:I:862:PHE:HA	2.07	0.83
1:A:428:PHE:CE2	2:G:49:PHE:HD2	1.96	0.83
2:K:857:THR:CG2	2:K:862:PHE:HA	2.07	0.83
1:F:428:PHE:CE2	2:L:49:PHE:HD2	1.96	0.83
2:L:857:THR:CG2	2:L:862:PHE:HA	2.07	0.83
1:B:428:PHE:CE2	2:H:49:PHE:HD2	1.96	0.82
1:C:428:PHE:CE2	2:I:49:PHE:HD2	1.96	0.82
1:D:298:ILE:HD11	2:K:968:HIS:CG	2.14	0.82
1:E:428:PHE:CE2	2:K:49:PHE:HD2	1.96	0.82
1:D:428:PHE:CE2	2:J:49:PHE:HD2	1.96	0.82
1:A:298:ILE:HD11	2:H:968:HIS:CG	2.14	0.82
2:G:968:HIS:CG	1:F:298:ILE:HD11	2.16	0.80
1:B:298:ILE:HD11	2:I:968:HIS:CG	2.17	0.79
1:D:298:ILE:HD11	2:K:968:HIS:ND1	1.96	0.79
1:A:298:ILE:HD11	2:H:968:HIS:ND1	1.96	0.79
1:B:70:ILE:HD11	1:B:75:LEU:CD2	2.13	0.79
1:F:70:ILE:HD11	1:F:75:LEU:CD2	2.13	0.79
1:C:70:ILE:HD11	1:C:75:LEU:CD2	2.13	0.78
1:E:70:ILE:HD11	1:E:75:LEU:CD2	2.13	0.78
1:B:298:ILE:HD11	2:I:968:HIS:ND1	1.98	0.78
1:A:70:ILE:HD11	1:A:75:LEU:CD2	2.13	0.78
1:C:298:ILE:HD11	2:J:968:HIS:CG	2.18	0.78
2:G:968:HIS:ND1	1:F:298:ILE:HD11	1.98	0.78
1:E:298:ILE:HD11	2:L:968:HIS:CG	2.19	0.77
1:F:491:LYS:HG2	2:L:89:ASP:HA	1.67	0.77
1:D:439:HIS:CD2	2:J:132:PHE:HZ	1.94	0.77
1:E:491:LYS:HG2	2:K:89:ASP:HA	1.67	0.77
1:E:298:ILE:HD11	2:L:968:HIS:ND1	2.00	0.77
1:D:491:LYS:HG2	2:J:89:ASP:HA	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LYS:HG2	2:G:89:ASP:HA	1.67	0.76
1:D:70:ILE:HD11	1:D:75:LEU:CD2	2.13	0.76
1:C:491:LYS:HG2	2:I:89:ASP:HA	1.67	0.76
1:C:298:ILE:HD11	2:J:968:HIS:ND1	2.01	0.76
1:A:439:HIS:CD2	2:G:132:PHE:HZ	1.94	0.76
1:B:491:LYS:HG2	2:H:89:ASP:HA	1.67	0.76
1:C:439:HIS:CD2	2:I:132:PHE:HZ	1.94	0.74
1:F:439:HIS:CD2	2:L:132:PHE:HZ	1.94	0.73
1:C:439:HIS:CD2	2:I:132:PHE:CE2	2.77	0.73
1:B:439:HIS:CD2	2:H:132:PHE:CE2	2.77	0.73
1:E:439:HIS:CD2	2:K:132:PHE:CE2	2.77	0.73
1:F:439:HIS:CD2	2:L:132:PHE:CE2	2.77	0.73
1:A:72:ILE:HD11	2:G:138:ARG:HD2	1.71	0.73
1:D:439:HIS:CD2	2:J:132:PHE:CE2	2.77	0.73
1:A:473:LYS:HG2	2:G:54:HIS:CD2	2.24	0.72
1:D:473:LYS:HE3	2:J:53:ILE:O	1.89	0.72
1:E:473:LYS:HE3	2:K:53:ILE:O	1.89	0.72
1:E:473:LYS:HG2	2:K:54:HIS:CD2	2.24	0.72
1:D:473:LYS:HG2	2:J:54:HIS:CD2	2.24	0.72
2:K:948:LYS:HG2	2:K:955:TYR:CD1	2.25	0.72
1:A:439:HIS:CD2	2:G:132:PHE:CE2	2.77	0.72
1:F:473:LYS:HG2	2:L:54:HIS:CD2	2.24	0.72
2:L:948:LYS:HG2	2:L:955:TYR:CD1	2.25	0.72
1:B:439:HIS:CD2	2:H:132:PHE:HZ	1.94	0.72
2:J:948:LYS:HG2	2:J:955:TYR:CD1	2.25	0.72
1:F:473:LYS:HE3	2:L:53:ILE:O	1.89	0.72
1:D:72:ILE:HD11	2:J:138:ARG:HD2	1.71	0.72
1:B:473:LYS:HG2	2:H:54:HIS:CD2	2.24	0.72
1:C:72:ILE:HD11	2:I:138:ARG:HD2	1.71	0.71
2:G:948:LYS:HG2	2:G:955:TYR:CD1	2.25	0.71
1:E:72:ILE:HD11	2:K:138:ARG:HD2	1.71	0.71
1:B:473:LYS:HE3	2:H:53:ILE:O	1.89	0.71
1:C:473:LYS:HG2	2:I:54:HIS:CD2	2.24	0.71
1:C:473:LYS:HE3	2:I:53:ILE:O	1.89	0.71
2:I:857:THR:CG2	2:I:862:PHE:CD2	2.67	0.71
1:E:439:HIS:CD2	2:K:132:PHE:HZ	1.94	0.71
1:C:393:GLN:NE2	1:C:430:ASP:OD2	2.24	0.71
1:D:288:ASN:HD21	2:K:977:GLU:CB	2.04	0.71
1:D:393:GLN:NE2	1:D:430:ASP:OD2	2.24	0.71
2:G:977:GLU:CB	1:F:288:ASN:HD21	2.02	0.71
2:I:948:LYS:HG2	2:I:955:TYR:CD1	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:ILE:HD11	2:L:138:ARG:HD2	1.71	0.71
1:B:72:ILE:HD11	2:H:138:ARG:HD2	1.71	0.71
1:A:473:LYS:HE3	2:G:53:ILE:O	1.89	0.70
2:H:948:LYS:HG2	2:H:955:TYR:CD1	2.24	0.70
1:E:393:GLN:NE2	1:E:430:ASP:OD2	2.24	0.70
1:B:393:GLN:NE2	1:B:430:ASP:OD2	2.24	0.70
2:J:857:THR:CG2	2:J:862:PHE:CD2	2.67	0.70
1:A:393:GLN:NE2	1:A:430:ASP:OD2	2.24	0.70
2:H:857:THR:CG2	2:H:862:PHE:CD2	2.67	0.70
1:F:393:GLN:NE2	1:F:430:ASP:OD2	2.24	0.70
2:G:448:ILE:HD13	2:G:555:SER:HB2	1.74	0.69
2:L:448:ILE:HD13	2:L:555:SER:HB2	1.74	0.69
1:B:428:PHE:CD2	2:H:49:PHE:HD2	2.10	0.69
1:A:428:PHE:CD2	2:G:49:PHE:HD2	2.10	0.69
2:J:448:ILE:HD13	2:J:555:SER:HB2	1.74	0.69
1:E:288:ASN:HD21	2:L:977:GLU:CB	2.05	0.69
2:H:448:ILE:HD13	2:H:555:SER:HB2	1.74	0.69
2:I:448:ILE:HD13	2:I:555:SER:HB2	1.74	0.69
1:B:288:ASN:HD21	2:I:977:GLU:CB	2.04	0.69
1:C:288:ASN:HD21	2:J:977:GLU:CB	2.04	0.69
1:C:428:PHE:CD2	2:I:49:PHE:HD2	2.10	0.69
2:K:448:ILE:HD13	2:K:555:SER:HB2	1.75	0.69
1:F:428:PHE:CD2	2:L:49:PHE:HD2	2.10	0.69
1:A:288:ASN:HD21	2:H:977:GLU:CB	2.05	0.68
1:B:96:SER:OG	2:H:828:LYS:HB3	1.94	0.68
1:C:96:SER:OG	2:I:828:LYS:HB3	1.94	0.68
1:D:428:PHE:CD2	2:J:49:PHE:HD2	2.10	0.68
1:A:457:TYR:OH	2:G:36:ASP:N	2.26	0.67
1:E:428:PHE:CD2	2:K:49:PHE:HD2	2.10	0.67
1:A:96:SER:OG	2:G:828:LYS:HB3	1.94	0.67
1:D:96:SER:OG	2:J:828:LYS:HB3	1.94	0.67
1:E:96:SER:OG	2:K:828:LYS:HB3	1.94	0.67
2:K:857:THR:CG2	2:K:862:PHE:CD2	2.67	0.67
1:F:96:SER:OG	2:L:828:LYS:HB3	1.94	0.67
1:C:457:TYR:OH	2:I:36:ASP:N	2.26	0.67
1:A:288:ASN:ND2	2:H:977:GLU:OE1	2.29	0.66
2:G:857:THR:CG2	2:G:862:PHE:CD2	2.67	0.66
1:B:457:TYR:OH	2:H:36:ASP:N	2.26	0.66
2:J:112:THR:O	2:J:116:THR:OG1	2.14	0.66
1:F:457:TYR:OH	2:L:36:ASP:N	2.26	0.65
1:A:428:PHE:CD2	2:G:49:PHE:CD2	2.85	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ASN:ND2	2:K:977:GLU:OE1	2.29	0.65
1:F:428:PHE:CD2	2:L:49:PHE:CD2	2.85	0.65
1:B:428:PHE:CD2	2:H:49:PHE:CD2	2.85	0.65
2:G:112:THR:O	2:G:116:THR:OG1	2.14	0.65
2:L:857:THR:CG2	2:L:862:PHE:CD2	2.67	0.65
2:G:977:GLU:HB3	1:F:288:ASN:HD21	1.61	0.64
1:E:457:TYR:OH	2:K:36:ASP:N	2.26	0.64
1:E:428:PHE:CD2	2:K:49:PHE:CD2	2.85	0.64
1:A:40:PHE:CD1	2:G:111:LEU:O	2.51	0.64
1:C:428:PHE:CD2	2:I:49:PHE:CD2	2.85	0.64
1:D:428:PHE:CD2	2:J:49:PHE:CD2	2.85	0.64
1:D:457:TYR:OH	2:J:36:ASP:N	2.26	0.64
1:E:78:ASN:OD1	1:E:444:LYS:NZ	2.31	0.64
1:E:288:ASN:HD21	2:L:977:GLU:HB3	1.63	0.64
1:E:70:ILE:HG13	1:E:75:LEU:HG	1.80	0.64
1:F:78:ASN:OD1	1:F:444:LYS:NZ	2.31	0.64
1:B:288:ASN:HD21	2:I:977:GLU:HB3	1.63	0.64
2:I:112:THR:O	2:I:116:THR:OG1	2.14	0.64
1:D:70:ILE:HG13	1:D:75:LEU:HG	1.80	0.64
1:D:40:PHE:CD1	2:J:111:LEU:O	2.51	0.63
1:B:288:ASN:ND2	2:I:977:GLU:OE1	2.32	0.63
1:B:40:PHE:CD1	2:H:111:LEU:O	2.51	0.63
1:D:78:ASN:OD1	1:D:444:LYS:NZ	2.31	0.63
1:C:40:PHE:CD1	2:I:111:LEU:O	2.51	0.63
1:F:40:PHE:CD1	2:L:111:LEU:O	2.51	0.63
1:F:70:ILE:HG13	1:F:75:LEU:HG	1.80	0.63
1:B:70:ILE:HG13	1:B:75:LEU:HG	1.80	0.63
2:G:977:GLU:OE1	1:F:288:ASN:ND2	2.31	0.63
1:A:78:ASN:OD1	1:A:444:LYS:NZ	2.31	0.63
1:E:40:PHE:CD1	2:K:111:LEU:O	2.51	0.63
1:A:36:LEU:HD22	2:G:111:LEU:HD11	1.81	0.62
1:B:78:ASN:OD1	1:B:444:LYS:NZ	2.31	0.62
1:C:78:ASN:OD1	1:C:444:LYS:NZ	2.31	0.62
1:C:36:LEU:HD22	2:I:111:LEU:HD11	1.82	0.62
1:B:36:LEU:HD22	2:H:111:LEU:HD11	1.82	0.62
1:D:288:ASN:HD21	2:K:977:GLU:HB3	1.63	0.62
2:L:112:THR:O	2:L:116:THR:OG1	2.14	0.62
1:D:36:LEU:HD22	2:J:111:LEU:HD11	1.81	0.62
1:E:36:LEU:HD22	2:K:111:LEU:HD11	1.81	0.62
1:A:70:ILE:HG13	1:A:75:LEU:HG	1.80	0.62
2:H:112:THR:O	2:H:116:THR:OG1	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:927:VAL:C	2:I:1033:ILE:HG22	2.25	0.62
1:F:36:LEU:HD22	2:L:111:LEU:HD11	1.82	0.62
2:G:927:VAL:C	2:G:1033:ILE:HG22	2.25	0.62
1:C:70:ILE:HG13	1:C:75:LEU:HG	1.80	0.62
2:L:927:VAL:C	2:L:1033:ILE:HG22	2.25	0.62
1:A:288:ASN:HD21	2:H:977:GLU:HB3	1.64	0.62
2:K:927:VAL:C	2:K:1033:ILE:HG22	2.25	0.61
2:L:238:MET:CE	2:L:621:PRO:HB3	2.30	0.61
1:B:923:LEU:HD23	1:B:928:THR:HB	1.83	0.61
2:H:238:MET:CE	2:H:621:PRO:HB3	2.30	0.61
1:C:288:ASN:ND2	2:J:977:GLU:OE1	2.33	0.61
2:H:788:LYS:NZ	2:H:792:ARG:HD3	2.16	0.61
1:E:384:ALA:HB3	1:E:386:TRP:CE2	2.35	0.61
1:C:288:ASN:HD21	2:J:977:GLU:HB3	1.63	0.61
1:A:923:LEU:HD23	1:A:928:THR:HB	1.83	0.61
2:G:970:SER:OG	1:F:298:ILE:HG13	2.00	0.61
2:I:238:MET:CE	2:I:621:PRO:HB3	2.31	0.61
1:A:384:ALA:HB3	1:A:386:TRP:CE2	2.36	0.61
1:A:438:GLU:HB2	1:A:460:GLN:HG3	1.83	0.61
1:B:384:ALA:HB3	1:B:386:TRP:CE2	2.35	0.61
1:B:438:GLU:HB2	1:B:460:GLN:HG3	1.83	0.61
2:H:927:VAL:C	2:H:1033:ILE:HG22	2.25	0.61
1:C:923:LEU:HD23	1:C:928:THR:HB	1.82	0.61
2:I:788:LYS:NZ	2:I:792:ARG:HD3	2.16	0.61
1:D:384:ALA:HB3	1:D:386:TRP:CE2	2.35	0.61
2:J:927:VAL:C	2:J:1033:ILE:HG22	2.25	0.61
1:F:384:ALA:HB3	1:F:386:TRP:CE2	2.35	0.61
1:C:654:ASP:OD1	1:C:654:ASP:N	2.34	0.61
1:D:298:ILE:HG13	2:K:970:SER:OG	2.01	0.61
2:J:788:LYS:NZ	2:J:792:ARG:HD3	2.16	0.61
1:F:438:GLU:HB2	1:F:460:GLN:HG3	1.83	0.61
1:A:473:LYS:HE3	2:G:53:ILE:C	2.26	0.61
1:C:384:ALA:HB3	1:C:386:TRP:CE2	2.35	0.61
2:G:238:MET:CE	2:G:621:PRO:HB3	2.31	0.60
2:I:984:TYR:HE2	2:I:1033:ILE:HD13	1.66	0.60
2:J:238:MET:CE	2:J:621:PRO:HB3	2.31	0.60
2:J:984:TYR:HE2	2:J:1033:ILE:HD13	1.66	0.60
1:C:438:GLU:HB2	1:C:460:GLN:HG3	1.83	0.60
2:J:446:ARG:HH11	2:J:558:HIS:HE1	1.46	0.60
1:A:298:ILE:HG13	2:H:970:SER:OG	2.01	0.60
2:G:788:LYS:NZ	2:G:792:ARG:HD3	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:923:LEU:HD23	1:D:928:THR:HB	1.83	0.60
2:K:238:MET:CE	2:K:621:PRO:HB3	2.30	0.60
2:K:788:LYS:NZ	2:K:792:ARG:HD3	2.16	0.60
1:B:298:ILE:HG13	2:I:970:SER:OG	2.01	0.60
1:E:298:ILE:HG13	2:L:970:SER:OG	2.02	0.60
1:F:654:ASP:OD1	1:F:654:ASP:N	2.34	0.60
2:I:446:ARG:HH11	2:I:558:HIS:HE1	1.46	0.60
2:K:112:THR:O	2:K:116:THR:OG1	2.14	0.60
1:F:923:LEU:HD23	1:F:928:THR:HB	1.83	0.60
1:B:654:ASP:N	1:B:654:ASP:OD1	2.34	0.60
2:L:788:LYS:NZ	2:L:792:ARG:HD3	2.16	0.60
1:B:473:LYS:HE3	2:H:53:ILE:C	2.26	0.60
1:C:597:VAL:HG11	1:C:730:PHE:CE1	2.37	0.60
1:D:438:GLU:HB2	1:D:460:GLN:HG3	1.83	0.60
1:E:438:GLU:HB2	1:E:460:GLN:HG3	1.83	0.60
1:D:473:LYS:HE3	2:J:53:ILE:C	2.26	0.59
1:E:654:ASP:OD1	1:E:654:ASP:N	2.34	0.59
1:E:923:LEU:HD23	1:E:928:THR:HB	1.83	0.59
2:L:984:TYR:HE2	2:L:1033:ILE:HD13	1.66	0.59
1:D:597:VAL:HG11	1:D:730:PHE:CE1	2.37	0.59
1:E:288:ASN:ND2	2:L:977:GLU:OE1	2.34	0.59
2:K:948:LYS:HG2	2:K:955:TYR:CE1	2.38	0.59
1:F:473:LYS:HE3	2:L:53:ILE:C	2.26	0.59
1:C:298:ILE:HG13	2:J:970:SER:OG	2.02	0.59
1:E:473:LYS:HE3	2:K:53:ILE:C	2.26	0.59
1:E:597:VAL:HG11	1:E:730:PHE:CE1	2.37	0.59
2:H:984:TYR:HE2	2:H:1033:ILE:HD13	1.66	0.59
1:C:473:LYS:HE3	2:I:53:ILE:C	2.26	0.59
2:J:948:LYS:HG2	2:J:955:TYR:CE1	2.38	0.59
2:K:984:TYR:HE2	2:K:1033:ILE:HD13	1.66	0.59
2:L:948:LYS:HG2	2:L:955:TYR:CE1	2.38	0.59
2:G:174:LYS:NZ	2:G:176:ASP:OD1	2.36	0.59
2:K:174:LYS:NZ	2:K:176:ASP:OD1	2.36	0.59
1:F:393:GLN:HG2	1:F:426:LEU:HD13	1.85	0.59
1:F:597:VAL:HG11	1:F:730:PHE:CE1	2.38	0.59
1:E:72:ILE:HD11	2:K:138:ARG:CD	2.33	0.59
1:A:393:GLN:HG2	1:A:426:LEU:HD13	1.85	0.59
2:G:984:TYR:HE2	2:G:1033:ILE:HD13	1.66	0.59
1:E:393:GLN:HG2	1:E:426:LEU:HD13	1.85	0.59
1:F:72:ILE:HD11	2:L:138:ARG:CD	2.32	0.59
2:J:174:LYS:NZ	2:J:176:ASP:OD1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:HD11	2:J:138:ARG:CD	2.33	0.58
2:K:446:ARG:HH11	2:K:558:HIS:HE1	1.46	0.58
2:G:948:LYS:HG2	2:G:955:TYR:CE1	2.38	0.58
2:I:948:LYS:HG2	2:I:955:TYR:CE1	2.38	0.58
2:L:174:LYS:NZ	2:L:176:ASP:OD1	2.36	0.58
1:A:72:ILE:HD11	2:G:138:ARG:CD	2.33	0.58
1:B:393:GLN:HG2	1:B:426:LEU:HD13	1.85	0.58
1:B:597:VAL:HG11	1:B:730:PHE:CE1	2.38	0.58
1:C:72:ILE:HD11	2:I:138:ARG:CD	2.32	0.58
1:C:473:LYS:HG2	2:I:54:HIS:NE2	2.19	0.58
2:L:51:ARG:NH2	2:L:69:ARG:HG3	2.19	0.58
1:A:431:GLN:HA	1:A:462:ILE:HD11	1.86	0.58
2:H:948:LYS:HG2	2:H:955:TYR:CE1	2.37	0.58
1:E:431:GLN:HA	1:E:462:ILE:HD11	1.86	0.58
1:A:70:ILE:HG21	1:A:386:TRP:CZ3	2.39	0.58
1:A:473:LYS:HG2	2:G:54:HIS:NE2	2.19	0.58
1:A:597:VAL:HG11	1:A:730:PHE:CE1	2.37	0.58
1:B:70:ILE:HG21	1:B:386:TRP:CZ3	2.39	0.58
2:I:174:LYS:NZ	2:I:176:ASP:OD1	2.36	0.58
1:D:393:GLN:HG2	1:D:426:LEU:HD13	1.85	0.58
2:K:51:ARG:NH2	2:K:69:ARG:HG3	2.19	0.58
1:F:70:ILE:HG21	1:F:386:TRP:CZ3	2.39	0.58
1:F:431:GLN:HA	1:F:462:ILE:HD11	1.86	0.58
1:D:473:LYS:HA	2:J:54:HIS:CE1	2.39	0.57
1:C:393:GLN:HG2	1:C:426:LEU:HD13	1.85	0.57
2:K:948:LYS:HG2	2:K:955:TYR:HD1	1.68	0.57
1:B:72:ILE:HD11	2:H:138:ARG:CD	2.32	0.57
1:D:473:LYS:HG2	2:J:54:HIS:NE2	2.19	0.57
1:F:473:LYS:HG2	2:L:54:HIS:NE2	2.19	0.57
2:L:948:LYS:HG2	2:L:955:TYR:HD1	1.68	0.57
2:G:51:ARG:NH2	2:G:69:ARG:HG3	2.19	0.57
1:B:473:LYS:HA	2:H:54:HIS:CE1	2.39	0.57
1:A:473:LYS:HA	2:G:54:HIS:CE1	2.39	0.57
1:B:431:GLN:HA	1:B:462:ILE:HD11	1.86	0.57
1:D:654:ASP:N	1:D:654:ASP:OD1	2.34	0.57
1:E:473:LYS:HA	2:K:54:HIS:CE1	2.39	0.57
1:B:473:LYS:HG2	2:H:54:HIS:NE2	2.19	0.57
2:H:174:LYS:NZ	2:H:176:ASP:OD1	2.36	0.57
1:C:70:ILE:HG21	1:C:386:TRP:CZ3	2.39	0.57
1:D:70:ILE:HG21	1:D:386:TRP:CZ3	2.39	0.57
1:D:431:GLN:HA	1:D:462:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:473:LYS:HA	2:L:54:HIS:CE1	2.39	0.57
2:H:51:ARG:NH2	2:H:69:ARG:HG3	2.19	0.57
1:C:473:LYS:HA	2:I:54:HIS:CE1	2.39	0.57
2:J:51:ARG:NH2	2:J:69:ARG:HG3	2.19	0.57
1:A:654:ASP:OD1	1:A:654:ASP:N	2.34	0.57
1:C:442:LYS:HB2	1:C:458:PHE:CZ	2.40	0.57
1:C:431:GLN:HA	1:C:462:ILE:HD11	1.86	0.56
2:J:447:PRO:HG2	2:J:556:PHE:CD1	2.41	0.56
1:E:473:LYS:HG2	2:K:54:HIS:NE2	2.19	0.56
1:A:442:LYS:HB2	1:A:458:PHE:CZ	2.40	0.56
1:C:439:HIS:CE1	2:I:35:GLN:NE2	2.73	0.56
2:I:51:ARG:NH2	2:I:69:ARG:HG3	2.19	0.56
1:D:439:HIS:CE1	2:J:35:GLN:NE2	2.73	0.56
1:E:70:ILE:HG21	1:E:386:TRP:CZ3	2.39	0.56
1:E:439:HIS:CE1	2:K:35:GLN:NE2	2.73	0.56
1:F:439:HIS:CE1	2:L:35:GLN:NE2	2.73	0.56
1:A:439:HIS:CE1	2:G:35:GLN:NE2	2.73	0.56
2:K:447:PRO:HG2	2:K:556:PHE:CD1	2.41	0.56
1:F:442:LYS:HB2	1:F:458:PHE:CZ	2.40	0.56
2:L:447:PRO:HG2	2:L:556:PHE:CD1	2.41	0.56
1:B:442:LYS:HB2	1:B:458:PHE:CZ	2.40	0.56
2:I:447:PRO:HG2	2:I:556:PHE:CD1	2.41	0.56
1:D:442:LYS:HB2	1:D:458:PHE:CZ	2.40	0.56
1:B:391:SER:N	1:B:464:ASP:OD2	2.38	0.56
1:B:439:HIS:CE1	2:H:35:GLN:NE2	2.73	0.56
1:A:391:SER:N	1:A:464:ASP:OD2	2.38	0.56
2:J:860:SER:O	2:J:860:SER:OG	2.22	0.56
1:B:430:ASP:HB3	1:B:462:ILE:HD13	1.88	0.56
2:J:52:LYS:O	2:J:53:ILE:HD13	2.06	0.56
1:F:430:ASP:HB3	1:F:462:ILE:HD13	1.88	0.56
2:L:52:LYS:O	2:L:53:ILE:HD13	2.06	0.56
1:E:442:LYS:HB2	1:E:458:PHE:CZ	2.40	0.55
2:H:53:ILE:HG22	2:H:54:HIS:O	2.06	0.55
2:H:447:PRO:HG2	2:H:556:PHE:CD1	2.41	0.55
2:J:948:LYS:HG2	2:J:955:TYR:HD1	1.68	0.55
2:L:446:ARG:HH11	2:L:558:HIS:HE1	1.46	0.55
2:G:52:LYS:O	2:G:53:ILE:HD13	2.06	0.55
2:G:53:ILE:HG22	2:G:54:HIS:O	2.07	0.55
2:G:948:LYS:HG2	2:G:955:TYR:HD1	1.68	0.55
2:I:238:MET:HE1	2:I:621:PRO:HB3	1.89	0.55
2:K:52:LYS:O	2:K:53:ILE:HD13	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:447:PRO:HG2	2:G:556:PHE:CD1	2.41	0.55
1:F:391:SER:N	1:F:464:ASP:OD2	2.38	0.55
1:C:430:ASP:HB3	1:C:462:ILE:HD13	1.89	0.55
2:I:860:SER:O	2:I:860:SER:OG	2.22	0.55
1:E:430:ASP:HB3	1:E:462:ILE:HD13	1.88	0.55
2:I:52:LYS:O	2:I:53:ILE:HD13	2.06	0.55
2:J:238:MET:HE1	2:J:621:PRO:HB3	1.89	0.55
1:C:391:SER:N	1:C:464:ASP:OD2	2.38	0.54
2:K:860:SER:O	2:K:860:SER:OG	2.22	0.54
2:H:52:LYS:O	2:H:53:ILE:HD13	2.07	0.54
2:I:53:ILE:HG22	2:I:54:HIS:O	2.07	0.54
2:J:50:ALA:HB1	2:J:68:TRP:HB2	1.89	0.54
2:L:53:ILE:HG22	2:L:54:HIS:O	2.07	0.54
2:L:238:MET:HE1	2:L:621:PRO:HB3	1.89	0.54
1:B:70:ILE:HD12	1:B:386:TRP:CH2	2.43	0.54
2:J:53:ILE:HG22	2:J:54:HIS:O	2.07	0.54
1:E:70:ILE:HD12	1:E:386:TRP:CH2	2.43	0.54
1:F:70:ILE:HD12	1:F:386:TRP:CH2	2.43	0.54
1:E:391:SER:N	1:E:464:ASP:OD2	2.38	0.54
2:I:50:ALA:HB1	2:I:68:TRP:HB2	1.89	0.54
1:A:430:ASP:HB3	1:A:462:ILE:HD13	1.89	0.54
1:A:70:ILE:HD12	1:A:386:TRP:CH2	2.43	0.54
1:C:70:ILE:HD12	1:C:386:TRP:CH2	2.43	0.54
1:D:70:ILE:HD12	1:D:386:TRP:CH2	2.43	0.54
1:E:568:THR:OG1	1:E:569:LEU:N	2.41	0.54
2:K:50:ALA:HB1	2:K:68:TRP:HB2	1.89	0.53
2:K:53:ILE:HG22	2:K:54:HIS:O	2.07	0.53
2:K:238:MET:HE1	2:K:621:PRO:HB3	1.89	0.53
2:G:50:ALA:HB1	2:G:68:TRP:HB2	1.89	0.53
1:B:568:THR:OG1	1:B:569:LEU:N	2.41	0.53
2:H:50:ALA:HB1	2:H:68:TRP:HB2	1.89	0.53
2:H:238:MET:HE1	2:H:621:PRO:HB3	1.89	0.53
1:D:391:SER:N	1:D:464:ASP:OD2	2.38	0.53
2:G:238:MET:HE1	2:G:621:PRO:HB3	1.89	0.53
1:F:133:GLN:OE1	1:F:772:CYS:HA	2.09	0.53
1:A:568:THR:OG1	1:A:569:LEU:N	2.42	0.53
1:C:133:GLN:OE1	1:C:772:CYS:HA	2.09	0.53
1:D:430:ASP:HB3	1:D:462:ILE:HD13	1.89	0.53
1:E:133:GLN:OE1	1:E:772:CYS:HA	2.09	0.53
1:B:133:GLN:OE1	1:B:772:CYS:HA	2.09	0.53
1:D:133:GLN:OE1	1:D:772:CYS:HA	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:SER:O	1:A:776:TYR:N	2.42	0.53
2:G:446:ARG:HH11	2:G:558:HIS:HE1	1.46	0.53
1:D:568:THR:OG1	1:D:569:LEU:N	2.42	0.52
2:H:860:SER:O	2:H:860:SER:OG	2.22	0.52
2:H:948:LYS:HG2	2:H:955:TYR:HD1	1.68	0.52
1:D:773:SER:O	1:D:776:TYR:N	2.42	0.52
1:F:773:SER:O	1:F:776:TYR:N	2.42	0.52
2:I:948:LYS:HG2	2:I:955:TYR:HD1	1.68	0.52
2:L:50:ALA:HB1	2:L:68:TRP:HB2	1.89	0.52
1:B:773:SER:O	1:B:776:TYR:N	2.42	0.52
1:C:773:SER:O	1:C:776:TYR:N	2.42	0.52
2:I:927:VAL:O	2:I:1033:ILE:HG22	2.10	0.52
2:L:383:ASP:OD1	2:L:383:ASP:N	2.42	0.52
1:A:284:SER:OG	2:H:985:ILE:O	2.28	0.52
1:D:19:ASP:OD2	2:J:131:ARG:NE	2.40	0.52
2:K:927:VAL:O	2:K:1033:ILE:HG22	2.10	0.52
2:G:927:VAL:O	2:G:1033:ILE:HG22	2.10	0.52
2:G:985:ILE:O	1:F:284:SER:OG	2.28	0.52
2:H:927:VAL:O	2:H:1033:ILE:HG22	2.10	0.52
2:L:860:SER:O	2:L:860:SER:OG	2.22	0.52
2:L:927:VAL:O	2:L:1033:ILE:HG22	2.10	0.52
1:A:133:GLN:OE1	1:A:772:CYS:HA	2.09	0.52
2:H:383:ASP:OD1	2:H:383:ASP:N	2.42	0.52
2:H:833:THR:OG1	2:H:834:LEU:N	2.43	0.52
2:I:833:THR:OG1	2:I:834:LEU:N	2.43	0.52
2:H:984:TYR:CE2	2:H:1033:ILE:HD13	2.45	0.52
1:E:773:SER:O	1:E:776:TYR:N	2.42	0.51
2:J:927:VAL:O	2:J:1033:ILE:HG22	2.10	0.51
2:K:984:TYR:CE2	2:K:1033:ILE:HD13	2.45	0.51
2:G:984:TYR:CE2	2:G:1033:ILE:HD13	2.45	0.51
2:I:984:TYR:CE2	2:I:1033:ILE:HD13	2.45	0.51
2:G:833:THR:OG1	2:G:834:LEU:N	2.43	0.51
2:J:833:THR:OG1	2:J:834:LEU:N	2.43	0.51
2:K:833:THR:OG1	2:K:834:LEU:N	2.43	0.51
2:J:152:LYS:NZ	2:J:814:ASP:OD1	2.37	0.51
1:B:19:ASP:OD2	2:H:131:ARG:NE	2.41	0.51
2:L:984:TYR:CE2	2:L:1033:ILE:HD13	2.45	0.51
1:A:773:SER:O	1:A:774:ASP:C	2.54	0.51
1:B:428:PHE:CE2	2:H:49:PHE:CD2	2.89	0.51
1:C:568:THR:OG1	1:C:569:LEU:N	2.41	0.51
1:C:19:ASP:OD2	2:I:131:ARG:NE	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:152:LYS:NZ	2:L:814:ASP:OD1	2.37	0.51
1:A:19:ASP:OD1	2:G:131:ARG:NH2	2.44	0.50
1:B:19:ASP:OD1	2:H:131:ARG:NH2	2.44	0.50
1:D:438:GLU:HG3	1:D:458:PHE:CD2	2.47	0.50
2:K:383:ASP:OD1	2:K:383:ASP:N	2.42	0.50
1:F:19:ASP:OD1	2:L:131:ARG:NH2	2.44	0.50
2:J:984:TYR:CE2	2:J:1033:ILE:HD13	2.45	0.50
1:E:438:GLU:HG3	1:E:458:PHE:CD2	2.47	0.50
1:F:438:GLU:HG3	1:F:458:PHE:CD2	2.47	0.50
1:A:438:GLU:HG3	1:A:458:PHE:CD2	2.47	0.50
2:H:674:ASN:HB2	2:H:750:ASP:HB3	1.94	0.50
1:D:284:SER:OG	2:K:985:ILE:O	2.27	0.50
1:E:19:ASP:OD1	2:K:131:ARG:NH2	2.44	0.50
1:E:773:SER:O	1:E:774:ASP:C	2.54	0.50
1:C:19:ASP:OD1	2:I:131:ARG:NH2	2.44	0.50
1:D:19:ASP:OD1	2:J:131:ARG:NH2	2.44	0.50
1:F:428:PHE:CE2	2:L:49:PHE:CD2	2.89	0.50
1:C:773:SER:O	1:C:774:ASP:C	2.54	0.50
1:B:284:SER:OG	2:I:985:ILE:O	2.30	0.50
2:H:446:ARG:HH11	2:H:558:HIS:HE1	1.46	0.50
2:I:674:ASN:HB2	2:I:750:ASP:HB3	1.94	0.50
2:J:674:ASN:HB2	2:J:750:ASP:HB3	1.93	0.50
1:C:438:GLU:HG3	1:C:458:PHE:CD2	2.47	0.50
2:K:152:LYS:NZ	2:K:814:ASP:OD1	2.37	0.50
1:E:428:PHE:CE2	2:K:49:PHE:CD2	2.89	0.49
1:D:773:SER:O	1:D:774:ASP:C	2.54	0.49
1:F:56:VAL:HG13	1:F:395:GLU:HB2	1.95	0.49
1:D:502:LEU:HD23	2:J:32:VAL:HG11	1.94	0.49
1:A:40:PHE:HD1	2:G:111:LEU:O	1.95	0.49
2:G:674:ASN:HB2	2:G:750:ASP:HB3	1.93	0.49
2:G:860:SER:O	2:G:860:SER:OG	2.22	0.49
1:B:438:GLU:HG3	1:B:458:PHE:CD2	2.47	0.49
2:I:443:PHE:HB3	2:I:451:SER:HB2	1.95	0.49
2:J:15:ASP:OD1	2:J:15:ASP:N	2.43	0.49
1:E:56:VAL:HG13	1:E:395:GLU:HB2	1.95	0.49
2:K:674:ASN:HB2	2:K:750:ASP:HB3	1.93	0.49
1:A:56:VAL:HG13	1:A:395:GLU:HB2	1.95	0.49
1:C:502:LEU:HD23	2:I:32:VAL:HG11	1.94	0.49
2:I:49:PHE:O	2:I:53:ILE:HG12	2.13	0.49
2:I:383:ASP:OD1	2:I:383:ASP:N	2.42	0.49
2:J:49:PHE:O	2:J:53:ILE:HG12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:TYR:HB2	1:E:493:ASP:OD2	2.13	0.49
1:A:502:LEU:HD23	2:G:32:VAL:HG11	1.94	0.49
2:G:977:GLU:OE2	1:F:284:SER:HB3	2.13	0.49
1:B:773:SER:O	1:B:774:ASP:C	2.54	0.49
2:H:49:PHE:O	2:H:53:ILE:HG12	2.13	0.49
1:D:301:GLU:OE2	2:K:1010:LYS:NZ	2.46	0.49
1:E:502:LEU:HD23	2:K:32:VAL:HG11	1.94	0.49
2:K:49:PHE:O	2:K:53:ILE:HG12	2.13	0.49
1:F:457:TYR:HB2	1:F:493:ASP:OD2	2.13	0.49
2:G:49:PHE:O	2:G:53:ILE:HG12	2.13	0.48
2:G:1010:LYS:NZ	1:F:301:GLU:OE2	2.46	0.48
1:B:40:PHE:HD1	2:H:111:LEU:O	1.95	0.48
1:C:284:SER:OG	2:J:985:ILE:O	2.31	0.48
2:J:446:ARG:HD2	2:J:558:HIS:CG	2.48	0.48
1:F:40:PHE:HD1	2:L:111:LEU:O	1.95	0.48
2:L:49:PHE:O	2:L:53:ILE:HG12	2.13	0.48
2:L:443:PHE:HB3	2:L:451:SER:HB2	1.95	0.48
2:G:383:ASP:OD1	2:G:383:ASP:N	2.42	0.48
2:H:443:PHE:HB3	2:H:451:SER:HB2	1.95	0.48
2:K:446:ARG:HD2	2:K:558:HIS:CG	2.48	0.48
1:F:502:LEU:HD23	2:L:32:VAL:HG11	1.94	0.48
2:L:446:ARG:HD2	2:L:558:HIS:CG	2.48	0.48
2:L:674:ASN:HB2	2:L:750:ASP:HB3	1.94	0.48
2:G:446:ARG:HD2	2:G:558:HIS:CG	2.48	0.48
2:H:446:ARG:HD2	2:H:558:HIS:CG	2.48	0.48
1:C:445:SER:O	1:C:453:PRO:HD3	2.14	0.48
2:I:446:ARG:HD2	2:I:558:HIS:CG	2.48	0.48
2:J:443:PHE:HB3	2:J:451:SER:HB2	1.95	0.48
1:A:397:PRO:HB2	1:A:399:THR:HG22	1.96	0.48
1:B:502:LEU:HD23	2:H:32:VAL:HG11	1.94	0.48
1:C:284:SER:HB3	2:J:977:GLU:OE2	2.13	0.48
1:D:457:TYR:HB2	1:D:493:ASP:OD2	2.13	0.48
1:E:284:SER:OG	2:L:985:ILE:O	2.32	0.48
1:E:397:PRO:HB2	1:E:399:THR:HG22	1.96	0.48
1:D:56:VAL:HG13	1:D:395:GLU:HB2	1.95	0.48
1:D:298:ILE:CD1	2:K:968:HIS:CG	2.94	0.48
1:E:445:SER:O	1:E:453:PRO:HD3	2.13	0.48
1:F:568:THR:OG1	1:F:569:LEU:N	2.41	0.48
1:A:457:TYR:HB2	1:A:493:ASP:OD2	2.13	0.48
1:B:445:SER:O	1:B:453:PRO:HD3	2.14	0.48
1:B:457:TYR:HB2	1:B:493:ASP:OD2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:SER:HB3	2:L:977:GLU:OE2	2.14	0.48
2:H:857:THR:O	2:H:869:THR:OG1	2.27	0.48
1:E:40:PHE:HD1	2:K:111:LEU:O	1.95	0.48
2:L:553:GLU:O	2:L:554:ARG:HG3	2.14	0.48
1:A:301:GLU:OE2	2:H:1010:LYS:NZ	2.47	0.47
1:B:56:VAL:HG13	1:B:395:GLU:HB2	1.95	0.47
1:D:397:PRO:HB2	1:D:399:THR:HG22	1.96	0.47
1:D:445:SER:O	1:D:453:PRO:HD3	2.14	0.47
1:E:319:VAL:HG21	2:L:984:TYR:CE1	2.49	0.47
2:K:172:GLN:HE21	2:L:937:PHE:HD1	1.61	0.47
2:K:443:PHE:HB3	2:K:451:SER:HB2	1.95	0.47
1:A:764:ILE:O	1:A:887:ASN:ND2	2.48	0.47
2:G:443:PHE:HB3	2:G:451:SER:HB2	1.95	0.47
1:B:397:PRO:HB2	1:B:399:THR:HG22	1.96	0.47
2:H:553:GLU:O	2:H:554:ARG:HG3	2.14	0.47
1:C:56:VAL:HG13	1:C:395:GLU:HB2	1.95	0.47
1:C:301:GLU:OE2	2:J:1010:LYS:NZ	2.47	0.47
1:F:397:PRO:HB2	1:F:399:THR:HG22	1.96	0.47
2:I:172:GLN:NE2	2:J:937:PHE:HD1	2.12	0.47
2:K:172:GLN:NE2	2:L:937:PHE:HD1	2.12	0.47
1:F:764:ILE:O	1:F:887:ASN:ND2	2.48	0.47
1:C:135:LEU:HD21	1:C:771:PHE:CE2	2.50	0.47
2:I:53:ILE:HD12	2:I:53:ILE:HG23	1.65	0.47
2:I:172:GLN:HE21	2:J:937:PHE:HD1	1.61	0.47
1:B:135:LEU:HD21	1:B:771:PHE:CE2	2.50	0.47
1:F:773:SER:O	1:F:774:ASP:C	2.54	0.47
2:G:553:GLU:O	2:G:554:ARG:HG3	2.14	0.47
2:G:937:PHE:HD1	2:L:172:GLN:HE21	1.62	0.47
2:H:53:ILE:HD12	2:H:53:ILE:HG23	1.65	0.47
1:C:397:PRO:HB2	1:C:399:THR:HG22	1.96	0.47
2:K:553:GLU:O	2:K:554:ARG:HG3	2.14	0.47
1:A:298:ILE:HD11	2:H:968:HIS:CE1	2.48	0.47
1:B:72:ILE:HD11	2:H:138:ARG:HG3	1.97	0.47
1:B:764:ILE:O	1:B:887:ASN:ND2	2.48	0.47
2:H:172:GLN:NE2	2:I:937:PHE:HD1	2.13	0.47
1:C:428:PHE:CE2	2:I:49:PHE:CD2	2.89	0.47
2:I:553:GLU:O	2:I:554:ARG:HG3	2.14	0.47
2:I:824:ARG:O	2:I:824:ARG:HD3	2.15	0.47
1:D:428:PHE:CE2	2:J:49:PHE:CD2	2.89	0.47
2:J:824:ARG:HD3	2:J:824:ARG:O	2.15	0.47
1:E:72:ILE:HD11	2:K:138:ARG:CG	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:15:ASP:OD1	2:K:15:ASP:N	2.43	0.47
1:F:72:ILE:HD11	2:L:138:ARG:CG	2.45	0.47
1:A:72:ILE:HD11	2:G:138:ARG:CG	2.45	0.47
1:A:72:ILE:HD11	2:G:138:ARG:HG3	1.97	0.47
1:A:135:LEU:HD21	1:A:771:PHE:CE2	2.50	0.47
2:G:824:ARG:O	2:G:824:ARG:HD3	2.15	0.47
2:G:968:HIS:CG	1:F:298:ILE:CD1	2.96	0.47
1:C:231:GLU:OE2	1:C:332:LYS:NZ	2.48	0.47
1:C:457:TYR:HB2	1:C:493:ASP:OD2	2.13	0.47
2:K:857:THR:O	2:K:869:THR:OG1	2.27	0.47
1:F:72:ILE:HD11	2:L:138:ARG:HG3	1.97	0.47
1:B:284:SER:HB3	2:I:977:GLU:OE2	2.14	0.47
2:H:824:ARG:O	2:H:824:ARG:HD3	2.15	0.47
1:C:72:ILE:HD11	2:I:138:ARG:HG3	1.97	0.47
1:D:231:GLU:OE2	1:D:332:LYS:NZ	2.48	0.47
1:F:445:SER:O	1:F:453:PRO:HD3	2.14	0.47
1:B:231:GLU:OE2	1:B:332:LYS:NZ	2.48	0.47
1:D:135:LEU:HD21	1:D:771:PHE:CE2	2.50	0.47
1:E:764:ILE:O	1:E:887:ASN:ND2	2.48	0.47
1:B:72:ILE:HD11	2:H:138:ARG:CG	2.45	0.46
1:D:72:ILE:HD11	2:J:138:ARG:CG	2.45	0.46
1:D:453:PRO:O	1:D:499:ARG:HD3	2.16	0.46
2:J:383:ASP:OD1	2:J:383:ASP:N	2.42	0.46
1:A:231:GLU:OE2	1:A:332:LYS:NZ	2.48	0.46
1:A:445:SER:O	1:A:453:PRO:HD3	2.14	0.46
1:B:453:PRO:O	1:B:499:ARG:HD3	2.16	0.46
1:C:764:ILE:O	1:C:887:ASN:ND2	2.48	0.46
1:E:72:ILE:HD11	2:K:138:ARG:HG3	1.97	0.46
2:H:172:GLN:HE21	2:I:937:PHE:HD1	1.62	0.46
2:J:553:GLU:O	2:J:554:ARG:HG3	2.14	0.46
1:F:231:GLU:OE2	1:F:332:LYS:NZ	2.48	0.46
1:A:453:PRO:O	1:A:499:ARG:HD3	2.16	0.46
1:C:72:ILE:HD11	2:I:138:ARG:CG	2.45	0.46
1:D:72:ILE:HD11	2:J:138:ARG:HG3	1.97	0.46
1:D:439:HIS:HA	1:D:458:PHE:CZ	2.51	0.46
1:D:764:ILE:O	1:D:887:ASN:ND2	2.48	0.46
1:E:135:LEU:HD21	1:E:771:PHE:CE2	2.50	0.46
2:G:172:GLN:HE21	2:H:937:PHE:HD1	1.64	0.46
1:C:40:PHE:HD1	2:I:111:LEU:O	1.95	0.46
2:J:238:MET:HE1	2:J:621:PRO:CB	2.46	0.46
2:K:824:ARG:O	2:K:824:ARG:HD3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:LEU:HD21	1:F:771:PHE:CE2	2.50	0.46
1:B:439:HIS:HA	1:B:458:PHE:CZ	2.51	0.46
2:I:350:SER:OG	2:I:351:GLY:N	2.49	0.46
1:B:306:ASN:OD1	1:B:306:ASN:N	2.49	0.46
2:H:238:MET:HE1	2:H:621:PRO:CB	2.45	0.46
1:E:439:HIS:HA	1:E:458:PHE:CZ	2.51	0.46
2:L:824:ARG:HD3	2:L:824:ARG:O	2.15	0.46
2:G:238:MET:HE1	2:G:621:PRO:CB	2.46	0.46
1:C:453:PRO:O	1:C:499:ARG:HD3	2.16	0.46
1:E:231:GLU:OE2	1:E:332:LYS:NZ	2.48	0.46
2:K:929:PHE:HB3	2:K:933:LEU:HD22	1.98	0.46
1:A:306:ASN:OD1	1:A:306:ASN:N	2.49	0.45
1:A:419:ALA:O	1:A:423:LYS:N	2.48	0.45
2:G:350:SER:OG	2:G:351:GLY:N	2.49	0.45
2:G:937:PHE:HD1	2:L:172:GLN:NE2	2.14	0.45
1:D:88:TYR:CE1	1:D:449:LEU:HD13	2.51	0.45
1:D:419:ALA:O	1:D:423:LYS:N	2.48	0.45
1:E:423:LYS:HB3	1:E:471:LEU:HD11	1.98	0.45
1:F:453:PRO:O	1:F:499:ARG:HD3	2.16	0.45
1:B:70:ILE:HD12	1:B:386:TRP:CZ2	2.52	0.45
1:C:439:HIS:HA	1:C:458:PHE:CZ	2.51	0.45
1:D:70:ILE:HD12	1:D:386:TRP:CZ2	2.52	0.45
1:D:423:LYS:HB3	1:D:471:LEU:HD11	1.98	0.45
2:J:172:GLN:HE21	2:K:937:PHE:HD1	1.63	0.45
1:E:70:ILE:HD12	1:E:386:TRP:CZ2	2.52	0.45
1:A:439:HIS:HA	1:A:458:PHE:CZ	2.51	0.45
1:D:284:SER:HB3	2:K:977:GLU:OE2	2.16	0.45
1:D:288:ASN:HD21	2:K:977:GLU:HB2	1.81	0.45
1:E:453:PRO:O	1:E:499:ARG:HD3	2.16	0.45
2:K:197:SER:C	2:K:198:PHE:HD1	2.25	0.45
1:F:70:ILE:HD12	1:F:386:TRP:CZ2	2.51	0.45
2:L:238:MET:HE1	2:L:621:PRO:CB	2.46	0.45
1:A:423:LYS:HB3	1:A:471:LEU:HD11	1.98	0.45
2:H:806:THR:OG1	2:H:807:LYS:N	2.50	0.45
1:C:306:ASN:OD1	1:C:306:ASN:N	2.49	0.45
2:J:197:SER:C	2:J:198:PHE:HD1	2.25	0.45
1:E:88:TYR:CE1	1:E:449:LEU:HD13	2.51	0.45
1:E:422:LEU:HA	1:E:422:LEU:HD12	1.72	0.45
2:L:197:SER:C	2:L:198:PHE:HD1	2.25	0.45
2:H:454:ILE:HA	2:H:548:LEU:O	2.17	0.45
2:I:238:MET:HE1	2:I:621:PRO:CB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:350:SER:OG	2:J:351:GLY:N	2.49	0.45
2:J:929:PHE:HB3	2:J:933:LEU:HD22	1.98	0.45
1:B:319:VAL:HG21	2:I:984:TYR:CE1	2.50	0.45
1:C:88:TYR:CE1	1:C:449:LEU:HD13	2.51	0.45
2:K:454:ILE:HA	2:K:548:LEU:O	2.17	0.45
2:L:806:THR:OG1	2:L:807:LYS:N	2.50	0.45
2:J:447:PRO:CB	2:J:552:LEU:HD11	2.47	0.45
2:K:238:MET:HE1	2:K:621:PRO:CB	2.45	0.45
1:F:439:HIS:HA	1:F:458:PHE:CZ	2.51	0.45
1:A:70:ILE:HD12	1:A:386:TRP:CZ2	2.52	0.45
1:C:319:VAL:HG21	2:J:984:TYR:CE1	2.52	0.45
1:D:298:ILE:HD11	2:K:968:HIS:CE1	2.49	0.45
2:K:350:SER:OG	2:K:351:GLY:N	2.49	0.45
2:K:806:THR:OG1	2:K:807:LYS:N	2.50	0.45
1:A:284:SER:HB3	2:H:977:GLU:OE2	2.17	0.45
2:G:454:ILE:HA	2:G:548:LEU:O	2.17	0.45
1:B:88:TYR:CE1	1:B:449:LEU:HD13	2.51	0.45
1:B:422:LEU:HA	1:B:422:LEU:HD12	1.72	0.45
2:H:350:SER:OG	2:H:351:GLY:N	2.49	0.45
1:C:288:ASN:HD21	2:J:977:GLU:HB2	1.81	0.45
2:J:454:ILE:HA	2:J:548:LEU:O	2.17	0.45
1:F:88:TYR:CE1	1:F:449:LEU:HD13	2.51	0.45
1:A:88:TYR:CE1	1:A:449:LEU:HD13	2.51	0.45
2:G:984:TYR:CE1	1:F:319:VAL:HG21	2.51	0.45
1:B:298:ILE:HD11	2:I:968:HIS:CE1	2.51	0.45
1:C:423:LYS:HB3	1:C:471:LEU:HD11	1.98	0.45
2:I:806:THR:OG1	2:I:807:LYS:N	2.50	0.45
1:D:40:PHE:HD1	2:J:111:LEU:O	1.95	0.45
2:J:53:ILE:HD12	2:J:53:ILE:HG23	1.65	0.45
2:K:53:ILE:HD12	2:K:53:ILE:HG23	1.65	0.45
2:G:806:THR:OG1	2:G:807:LYS:N	2.50	0.44
1:C:419:ALA:O	1:C:423:LYS:N	2.48	0.44
2:L:929:PHE:HB3	2:L:933:LEU:HD22	1.98	0.44
1:B:419:ALA:O	1:B:423:LYS:N	2.48	0.44
2:I:929:PHE:HB3	2:I:933:LEU:HD22	1.98	0.44
1:E:419:ALA:O	1:E:423:LYS:N	2.48	0.44
1:F:306:ASN:N	1:F:306:ASN:OD1	2.49	0.44
2:L:833:THR:OG1	2:L:834:LEU:N	2.43	0.44
2:G:929:PHE:HB3	2:G:933:LEU:HD22	1.98	0.44
2:G:977:GLU:HB2	1:F:288:ASN:HD21	1.79	0.44
1:E:443:ILE:HD11	2:K:135:LEU:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:LYS:HB3	1:F:471:LEU:HD11	1.98	0.44
1:C:70:ILE:HD12	1:C:386:TRP:CZ2	2.52	0.44
2:I:197:SER:C	2:I:198:PHE:HD1	2.25	0.44
2:I:454:ILE:HA	2:I:548:LEU:O	2.17	0.44
1:E:301:GLU:OE2	2:L:1010:LYS:NZ	2.51	0.44
2:L:298:ARG:NH2	2:L:365:GLN:O	2.51	0.44
2:L:447:PRO:CB	2:L:552:LEU:HD11	2.47	0.44
2:H:197:SER:C	2:H:198:PHE:HD1	2.25	0.44
2:K:447:PRO:CB	2:K:552:LEU:HD11	2.47	0.44
1:F:19:ASP:OD2	2:L:131:ARG:NE	2.41	0.44
2:L:454:ILE:HA	2:L:548:LEU:O	2.17	0.44
1:D:306:ASN:OD1	1:D:306:ASN:N	2.49	0.44
1:D:592:LEU:HA	1:D:592:LEU:HD12	1.81	0.44
2:G:447:PRO:CB	2:G:552:LEU:HD11	2.47	0.44
1:B:288:ASN:HD21	2:I:977:GLU:HB2	1.81	0.44
2:I:298:ARG:NH2	2:I:365:GLN:O	2.50	0.44
2:G:298:ARG:NH2	2:G:365:GLN:O	2.51	0.44
2:H:929:PHE:HB3	2:H:933:LEU:HD22	1.98	0.44
2:J:169:ASN:OD1	2:J:169:ASN:N	2.49	0.44
2:L:857:THR:O	2:L:869:THR:OG1	2.27	0.44
1:B:301:GLU:OE2	2:I:1010:LYS:NZ	2.50	0.44
1:B:423:LYS:HB3	1:B:471:LEU:HD11	1.98	0.44
1:C:422:LEU:HD12	1:C:422:LEU:HA	1.72	0.44
1:C:443:ILE:HD11	2:I:135:LEU:HD13	1.99	0.44
2:I:152:LYS:NZ	2:I:814:ASP:OD1	2.37	0.44
2:J:8:ILE:HD11	2:J:862:PHE:CD1	2.53	0.44
2:J:806:THR:OG1	2:J:807:LYS:N	2.50	0.44
1:E:306:ASN:OD1	1:E:306:ASN:N	2.49	0.44
1:A:443:ILE:HD11	2:G:135:LEU:HD13	1.99	0.43
2:G:8:ILE:HD11	2:G:862:PHE:CD1	2.53	0.43
2:H:8:ILE:HD11	2:H:862:PHE:CD1	2.53	0.43
2:H:298:ARG:NH2	2:H:365:GLN:O	2.51	0.43
2:H:447:PRO:CB	2:H:552:LEU:HD11	2.47	0.43
2:I:447:PRO:CB	2:I:552:LEU:HD11	2.47	0.43
2:J:298:ARG:NH2	2:J:365:GLN:O	2.51	0.43
2:G:197:SER:C	2:G:198:PHE:HD1	2.25	0.43
1:B:443:ILE:HD11	2:H:135:LEU:HD13	1.99	0.43
1:C:70:ILE:HG13	1:C:75:LEU:CG	2.48	0.43
1:D:646:LYS:O	1:D:650:THR:HG23	2.19	0.43
1:E:440:LEU:HD22	2:K:132:PHE:HE1	1.83	0.43
1:E:646:LYS:O	1:E:650:THR:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:443:ILE:HD11	2:L:135:LEU:HD13	1.99	0.43
1:A:36:LEU:O	2:G:111:LEU:HB2	2.19	0.43
1:B:36:LEU:O	2:H:111:LEU:HB2	2.19	0.43
1:B:923:LEU:HD23	1:B:923:LEU:HA	1.88	0.43
2:I:8:ILE:HD11	2:I:862:PHE:CD1	2.53	0.43
2:I:857:THR:O	2:I:869:THR:OG1	2.27	0.43
1:E:288:ASN:HD21	2:L:977:GLU:HB2	1.82	0.43
2:K:446:ARG:HD2	2:K:558:HIS:ND1	2.33	0.43
2:L:350:SER:OG	2:L:351:GLY:N	2.49	0.43
1:A:440:LEU:HD22	2:G:132:PHE:HE1	1.84	0.43
2:G:172:GLN:NE2	2:H:937:PHE:HD1	2.16	0.43
1:C:36:LEU:O	2:I:111:LEU:HB2	2.18	0.43
1:C:646:LYS:O	1:C:650:THR:HG23	2.19	0.43
1:D:443:ILE:HD11	2:J:135:LEU:HD13	1.99	0.43
2:J:172:GLN:NE2	2:K:937:PHE:HD1	2.15	0.43
1:F:440:LEU:HD22	2:L:132:PHE:HE1	1.84	0.43
2:L:446:ARG:HD2	2:L:558:HIS:ND1	2.33	0.43
1:A:647:ILE:HG21	1:A:727:THR:HG21	2.01	0.43
1:C:252:THR:OG1	1:C:253:MET:N	2.51	0.43
1:E:319:VAL:HG21	2:L:984:TYR:CZ	2.53	0.43
1:F:646:LYS:O	1:F:650:THR:HG23	2.19	0.43
1:D:647:ILE:HG21	1:D:727:THR:HG21	2.01	0.43
2:K:8:ILE:HD11	2:K:862:PHE:CD1	2.53	0.43
2:L:8:ILE:HD11	2:L:862:PHE:CD1	2.53	0.43
2:G:984:TYR:CZ	1:F:319:VAL:HG21	2.54	0.43
1:B:462:ILE:HD13	1:B:462:ILE:HG21	1.87	0.43
2:I:169:ASN:OD1	2:I:169:ASN:N	2.49	0.43
1:D:252:THR:OG1	1:D:253:MET:N	2.51	0.43
1:E:647:ILE:HG21	1:E:727:THR:HG21	2.01	0.43
1:F:252:THR:OG1	1:F:253:MET:N	2.51	0.43
2:G:968:HIS:CE1	1:F:298:ILE:HD11	2.52	0.43
1:B:440:LEU:HD22	2:H:132:PHE:HE1	1.84	0.43
2:I:446:ARG:HD2	2:I:558:HIS:ND1	2.33	0.43
1:D:36:LEU:O	2:J:111:LEU:HB2	2.19	0.43
1:E:19:ASP:OD2	2:K:131:ARG:NE	2.41	0.43
1:B:319:VAL:HG21	2:I:984:TYR:CZ	2.54	0.43
1:B:646:LYS:O	1:B:650:THR:HG23	2.19	0.43
2:J:446:ARG:HD2	2:J:558:HIS:ND1	2.33	0.43
1:F:597:VAL:HG11	1:F:730:PHE:HE1	1.84	0.43
1:A:252:THR:OG1	1:A:253:MET:N	2.51	0.43
2:G:684:ASN:OD1	2:G:684:ASN:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:LEU:HD22	2:I:132:PHE:HE1	1.84	0.43
2:K:169:ASN:OD1	2:K:169:ASN:N	2.49	0.43
1:A:646:LYS:O	1:A:650:THR:HG23	2.19	0.42
1:D:70:ILE:HG13	1:D:75:LEU:CG	2.48	0.42
1:D:597:VAL:HG11	1:D:730:PHE:HE1	1.84	0.42
1:E:36:LEU:O	2:K:111:LEU:HB2	2.19	0.42
1:E:252:THR:OG1	1:E:253:MET:N	2.51	0.42
1:E:592:LEU:HA	1:E:592:LEU:HD12	1.81	0.42
2:K:298:ARG:NH2	2:K:365:GLN:O	2.51	0.42
1:F:36:LEU:O	2:L:111:LEU:HB2	2.18	0.42
1:A:438:GLU:HG3	1:A:458:PHE:CE2	2.54	0.42
1:D:440:LEU:HD22	2:J:132:PHE:HE1	1.84	0.42
1:F:419:ALA:O	1:F:423:LYS:N	2.48	0.42
2:G:53:ILE:HD12	2:G:53:ILE:HG23	1.65	0.42
2:G:446:ARG:HD2	2:G:558:HIS:ND1	2.33	0.42
2:G:1033:ILE:HD13	2:G:1033:ILE:HG21	1.81	0.42
2:I:238:MET:HE3	2:I:622:PHE:CZ	2.54	0.42
1:D:319:VAL:HG21	2:K:984:TYR:CE1	2.55	0.42
1:D:438:GLU:HG3	1:D:458:PHE:CE2	2.54	0.42
1:B:438:GLU:HG3	1:B:458:PHE:CE2	2.54	0.42
1:B:647:ILE:HG21	1:B:727:THR:HG21	2.01	0.42
1:E:438:GLU:HG3	1:E:458:PHE:CE2	2.54	0.42
1:E:439:HIS:CE1	2:K:35:GLN:HE22	2.38	0.42
2:H:446:ARG:HD2	2:H:558:HIS:ND1	2.33	0.42
1:E:462:ILE:HD13	1:E:462:ILE:HG21	1.87	0.42
1:A:319:VAL:HG21	2:H:984:TYR:CE1	2.54	0.42
1:B:439:HIS:CE1	2:H:35:GLN:HE22	2.38	0.42
2:H:238:MET:HE3	2:H:622:PHE:CZ	2.54	0.42
1:C:647:ILE:HG21	1:C:727:THR:HG21	2.01	0.42
1:D:659:LEU:HB2	1:D:661:VAL:HG13	2.02	0.42
1:F:659:LEU:HB2	1:F:661:VAL:HG13	2.02	0.42
1:A:19:ASP:OD2	2:G:131:ARG:NE	2.41	0.42
1:A:298:ILE:CD1	2:H:968:HIS:CG	2.94	0.42
1:D:422:LEU:HD12	1:D:422:LEU:HA	1.72	0.42
2:I:197:SER:O	2:I:198:PHE:CD1	2.73	0.42
1:E:298:ILE:CD1	2:L:968:HIS:CG	2.98	0.42
1:E:659:LEU:HB2	1:E:661:VAL:HG13	2.02	0.42
2:K:238:MET:HE3	2:K:622:PHE:CZ	2.54	0.42
1:F:647:ILE:HG21	1:F:727:THR:HG21	2.01	0.42
1:C:438:GLU:HG3	1:C:458:PHE:CE2	2.54	0.42
1:E:923:LEU:HD23	1:E:923:LEU:HA	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:243:ASN:OD1	2:K:243:ASN:N	2.53	0.42
1:A:658:LEU:C	1:A:660:GLU:N	2.78	0.41
2:G:238:MET:HE3	2:G:622:PHE:CZ	2.54	0.41
2:J:238:MET:HE3	2:J:622:PHE:CZ	2.54	0.41
2:L:238:MET:HE3	2:L:622:PHE:CZ	2.54	0.41
1:A:439:HIS:CE1	2:G:35:GLN:HE22	2.38	0.41
1:B:252:THR:OG1	1:B:253:MET:N	2.51	0.41
2:H:197:SER:O	2:H:198:PHE:CD1	2.73	0.41
1:E:298:ILE:HD11	2:L:968:HIS:CE1	2.53	0.41
2:K:238:MET:HE3	2:K:238:MET:HB2	1.86	0.41
1:F:438:GLU:HG3	1:F:458:PHE:CE2	2.54	0.41
2:L:53:ILE:HD12	2:L:53:ILE:HG23	1.65	0.41
1:A:422:LEU:HD12	1:A:422:LEU:HA	1.72	0.41
1:A:659:LEU:H	1:A:659:LEU:HG	1.73	0.41
2:H:17:THR:OG1	2:H:18:GLY:N	2.53	0.41
1:C:659:LEU:HB2	1:C:661:VAL:HG13	2.02	0.41
1:F:440:LEU:CD2	2:L:132:PHE:HE1	2.34	0.41
1:B:424:GLY:HA2	1:B:471:LEU:HD22	2.02	0.41
1:C:597:VAL:HG11	1:C:730:PHE:HE1	1.84	0.41
2:I:17:THR:OG1	2:I:18:GLY:N	2.53	0.41
1:A:659:LEU:HB2	1:A:661:VAL:HG13	2.02	0.41
1:B:298:ILE:CD1	2:I:968:HIS:CG	2.96	0.41
2:I:89:ASP:OD1	2:I:89:ASP:N	2.54	0.41
1:F:36:LEU:CA	2:L:111:LEU:HD12	2.49	0.41
2:L:197:SER:O	2:L:198:PHE:CD1	2.73	0.41
2:H:169:ASN:OD1	2:H:169:ASN:N	2.50	0.41
2:J:17:THR:OG1	2:J:18:GLY:N	2.53	0.41
2:J:197:SER:O	2:J:198:PHE:CD1	2.73	0.41
2:K:197:SER:O	2:K:198:PHE:CD1	2.73	0.41
2:K:450:GLY:N	2:K:552:LEU:O	2.51	0.41
1:F:67:ARG:O	1:F:70:ILE:HG12	2.21	0.41
1:A:424:GLY:HA2	1:A:471:LEU:HD22	2.02	0.41
1:A:504:ASP:OD1	1:A:537:LYS:NZ	2.48	0.41
1:C:67:ARG:O	1:C:70:ILE:HG12	2.21	0.41
1:C:592:LEU:HA	1:C:592:LEU:HD12	1.81	0.41
2:G:17:THR:OG1	2:G:18:GLY:N	2.53	0.41
1:B:659:LEU:HB2	1:B:661:VAL:HG13	2.02	0.41
2:H:89:ASP:OD1	2:H:89:ASP:N	2.54	0.41
2:I:494:GLU:HA	2:I:495:PRO:HD3	1.95	0.41
1:D:440:LEU:CD2	2:J:132:PHE:HE1	2.33	0.41
1:A:440:LEU:CD2	2:G:132:PHE:HE1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:GLU:N	1:A:553:GLU:OE1	2.54	0.41
2:G:446:ARG:NH1	2:G:558:HIS:ND1	2.69	0.41
2:G:983:ASP:OD2	1:F:282:ARG:NH2	2.54	0.41
1:B:440:LEU:CD2	2:H:132:PHE:HE1	2.34	0.41
1:C:298:ILE:HD11	2:J:968:HIS:CE1	2.54	0.41
2:I:449:LYS:HB2	2:I:554:ARG:HA	2.03	0.41
2:I:1036:ASN:N	2:I:1036:ASN:HD22	2.19	0.41
1:D:67:ARG:O	1:D:70:ILE:HG12	2.21	0.41
1:D:424:GLY:HA2	1:D:471:LEU:HD22	2.02	0.41
1:E:70:ILE:HG13	1:E:75:LEU:CG	2.48	0.41
1:E:553:GLU:N	1:E:553:GLU:OE1	2.54	0.41
2:K:17:THR:OG1	2:K:18:GLY:N	2.53	0.41
1:F:439:HIS:CE1	2:L:35:GLN:HE22	2.38	0.41
1:F:553:GLU:N	1:F:553:GLU:OE1	2.54	0.41
1:F:647:ILE:HG23	1:F:647:ILE:HD12	1.76	0.41
1:F:659:LEU:H	1:F:659:LEU:HG	1.73	0.41
2:L:169:ASN:OD1	2:L:169:ASN:N	2.49	0.41
1:A:288:ASN:HD21	2:H:977:GLU:HB2	1.82	0.41
2:G:197:SER:O	2:G:198:PHE:CD1	2.73	0.41
1:B:67:ARG:O	1:B:70:ILE:HG12	2.21	0.41
1:B:282:ARG:NH2	2:I:983:ASP:OD2	2.54	0.41
1:B:658:LEU:C	1:B:660:GLU:N	2.78	0.41
2:H:449:LYS:HB2	2:H:554:ARG:HA	2.03	0.41
1:C:439:HIS:CE1	2:I:35:GLN:HE22	2.38	0.41
1:C:498:ARG:NH2	2:I:33:GLN:O	2.55	0.41
2:J:197:SER:O	2:J:198:PHE:HD1	2.04	0.41
1:A:319:VAL:HG21	2:H:984:TYR:CZ	2.57	0.40
1:A:428:PHE:CE2	2:G:49:PHE:CD2	2.89	0.40
1:B:498:ARG:NH2	2:H:33:GLN:O	2.54	0.40
1:B:553:GLU:N	1:B:553:GLU:OE1	2.54	0.40
2:H:446:ARG:NH1	2:H:558:HIS:ND1	2.69	0.40
2:I:197:SER:O	2:I:198:PHE:HD1	2.04	0.40
2:J:1036:ASN:N	2:J:1036:ASN:HD22	2.19	0.40
2:K:449:LYS:HB2	2:K:554:ARG:HA	2.03	0.40
2:L:17:THR:OG1	2:L:18:GLY:N	2.53	0.40
2:L:788:LYS:HZ2	2:L:792:ARG:HD3	1.85	0.40
2:G:238:MET:CE	2:G:622:PHE:CE2	3.05	0.40
2:G:450:GLY:N	2:G:552:LEU:O	2.51	0.40
1:C:553:GLU:N	1:C:553:GLU:OE1	2.54	0.40
1:E:19:ASP:OD1	1:E:20:LEU:HG	2.21	0.40
1:E:282:ARG:NH2	2:L:983:ASP:OD2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ASP:OD1	1:F:20:LEU:HG	2.22	0.40
2:L:446:ARG:NH1	2:L:558:HIS:ND1	2.69	0.40
2:L:449:LYS:HB2	2:L:554:ARG:HA	2.03	0.40
1:A:402:ILE:HG21	1:A:422:LEU:HG	2.04	0.40
2:I:238:MET:HE3	2:I:238:MET:HB2	1.86	0.40
1:E:658:LEU:C	1:E:660:GLU:N	2.78	0.40
1:F:424:GLY:HA2	1:F:471:LEU:HD22	2.02	0.40
2:L:272:THR:OG1	2:L:273:VAL:N	2.55	0.40
1:A:70:ILE:HG13	1:A:75:LEU:CG	2.48	0.40
1:A:462:ILE:HD13	1:A:462:ILE:HG21	1.87	0.40
2:H:238:MET:SD	2:H:280:ALA:HA	2.62	0.40
2:I:238:MET:CE	2:I:622:PHE:CE2	3.05	0.40
1:D:462:ILE:HD13	1:D:462:ILE:HG21	1.87	0.40
1:D:498:ARG:NH2	2:J:33:GLN:O	2.55	0.40
1:D:553:GLU:OE1	1:D:553:GLU:N	2.54	0.40
2:J:929:PHE:CB	2:J:933:LEU:HD22	2.52	0.40
1:E:424:GLY:HA2	1:E:471:LEU:HD22	2.02	0.40
1:F:384:ALA:HB3	1:F:386:TRP:NE1	2.37	0.40
1:F:498:ARG:NH2	2:L:33:GLN:O	2.55	0.40
2:G:169:ASN:OD1	2:G:169:ASN:N	2.49	0.40
2:G:272:THR:OG1	2:G:273:VAL:N	2.55	0.40
2:G:929:PHE:CB	2:G:933:LEU:HD22	2.52	0.40
1:B:443:ILE:CD1	2:H:135:LEU:HD13	2.52	0.40
1:C:424:GLY:HA2	1:C:471:LEU:HD22	2.02	0.40
1:D:19:ASP:OD1	1:D:20:LEU:HG	2.21	0.40
1:D:439:HIS:CE1	2:J:35:GLN:HE22	2.38	0.40
2:J:238:MET:SD	2:J:280:ALA:HA	2.62	0.40
1:E:67:ARG:O	1:E:70:ILE:HG12	2.21	0.40
1:E:498:ARG:NH2	2:K:33:GLN:O	2.55	0.40
2:K:929:PHE:CB	2:K:933:LEU:HD22	2.52	0.40
1:F:462:ILE:HD13	1:F:462:ILE:HG21	1.87	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	862/922 (94%)	834 (97%)	28 (3%)	0	100	100
1	B	862/922 (94%)	834 (97%)	28 (3%)	0	100	100
1	C	862/922 (94%)	834 (97%)	28 (3%)	0	100	100
1	D	862/922 (94%)	833 (97%)	29 (3%)	0	100	100
1	E	862/922 (94%)	834 (97%)	28 (3%)	0	100	100
1	F	862/922 (94%)	833 (97%)	29 (3%)	0	100	100
2	G	1033/1050 (98%)	1003 (97%)	30 (3%)	0	100	100
2	H	1033/1050 (98%)	1003 (97%)	30 (3%)	0	100	100
2	I	1033/1050 (98%)	1003 (97%)	30 (3%)	0	100	100
2	J	1033/1050 (98%)	1003 (97%)	30 (3%)	0	100	100
2	K	1033/1050 (98%)	1003 (97%)	30 (3%)	0	100	100
2	L	1033/1050 (98%)	1003 (97%)	30 (3%)	0	100	100
All	All	11370/11832 (96%)	11020 (97%)	350 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	782/831 (94%)	781 (100%)	1 (0%)	88	88
1	B	782/831 (94%)	781 (100%)	1 (0%)	88	88
1	C	782/831 (94%)	781 (100%)	1 (0%)	88	88
1	D	782/831 (94%)	781 (100%)	1 (0%)	88	88
1	E	782/831 (94%)	781 (100%)	1 (0%)	88	88
1	F	782/831 (94%)	781 (100%)	1 (0%)	88	88
2	G	940/955 (98%)	940 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	940/955 (98%)	940 (100%)	0	100	100
2	I	940/955 (98%)	940 (100%)	0	100	100
2	J	940/955 (98%)	940 (100%)	0	100	100
2	K	940/955 (98%)	940 (100%)	0	100	100
2	L	940/955 (98%)	940 (100%)	0	100	100
All	All	10332/10716 (96%)	10326 (100%)	6 (0%)	87	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	659	LEU
1	B	659	LEU
1	C	659	LEU
1	D	659	LEU
1	E	659	LEU
1	F	659	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	288	ASN
1	A	439	HIS
2	G	7	HIS
2	G	35	GLN
2	G	54	HIS
2	G	172	GLN
2	G	192	ASN
2	G	558	HIS
2	G	625	GLN
2	G	626	GLN
2	G	891	GLN
2	G	908	HIS
2	G	974	HIS
2	G	1036	ASN
1	B	86	GLN
1	B	288	ASN
1	B	317	GLN
1	B	337	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	439	HIS
2	H	7	HIS
2	H	35	GLN
2	H	54	HIS
2	H	172	GLN
2	H	192	ASN
2	H	558	HIS
2	H	625	GLN
2	H	626	GLN
2	H	891	GLN
2	H	908	HIS
2	H	974	HIS
2	H	1036	ASN
1	C	86	GLN
1	C	288	ASN
1	C	337	ASN
1	C	439	HIS
2	I	7	HIS
2	I	35	GLN
2	I	54	HIS
2	I	172	GLN
2	I	192	ASN
2	I	558	HIS
2	I	625	GLN
2	I	891	GLN
2	I	908	HIS
2	I	974	HIS
2	I	1035	GLN
2	I	1036	ASN
1	D	86	GLN
1	D	288	ASN
1	D	317	GLN
1	D	439	HIS
2	J	7	HIS
2	J	35	GLN
2	J	54	HIS
2	J	172	GLN
2	J	192	ASN
2	J	558	HIS
2	J	625	GLN
2	J	908	HIS
2	J	974	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	1035	GLN
2	J	1036	ASN
1	E	86	GLN
1	E	288	ASN
1	E	317	GLN
1	E	439	HIS
2	K	7	HIS
2	K	35	GLN
2	K	54	HIS
2	K	172	GLN
2	K	192	ASN
2	K	437	GLN
2	K	558	HIS
2	K	625	GLN
2	K	908	HIS
2	K	974	HIS
2	K	1036	ASN
1	F	86	GLN
1	F	288	ASN
1	F	317	GLN
1	F	337	ASN
1	F	439	HIS
2	L	7	HIS
2	L	35	GLN
2	L	54	HIS
2	L	172	GLN
2	L	192	ASN
2	L	558	HIS
2	L	625	GLN
2	L	626	GLN
2	L	908	HIS
2	L	974	HIS
2	L	1036	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

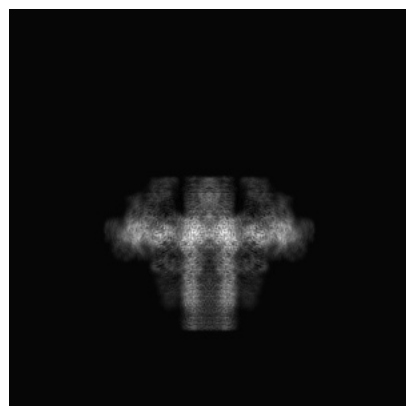
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66211. These allow visual inspection of the internal detail of the map and identification of artifacts.

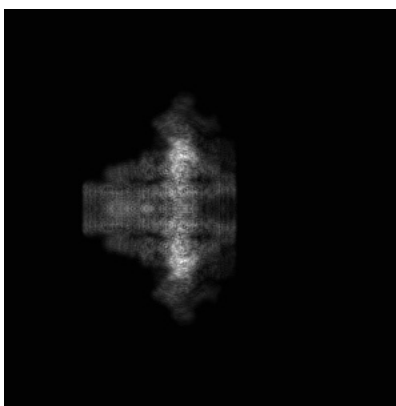
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

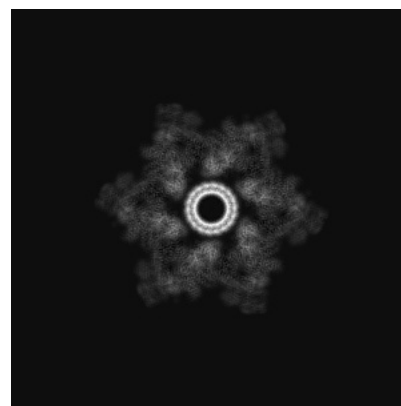
6.1.1 Primary map



X

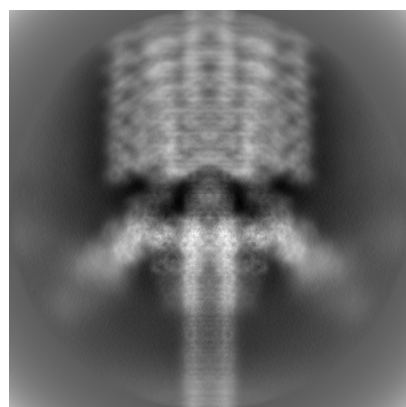


Y

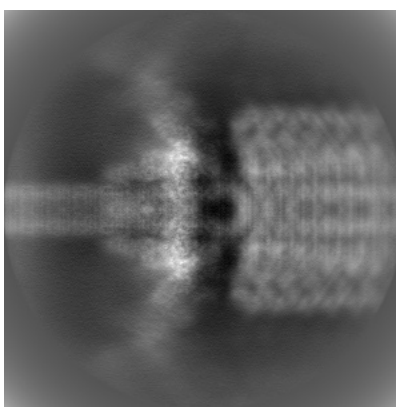


Z

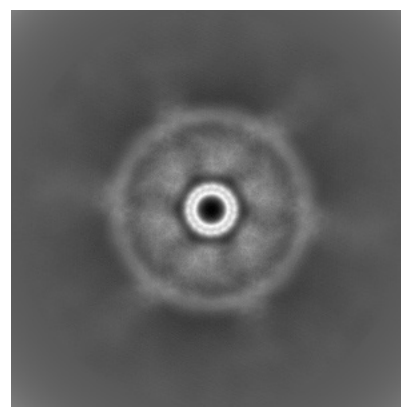
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

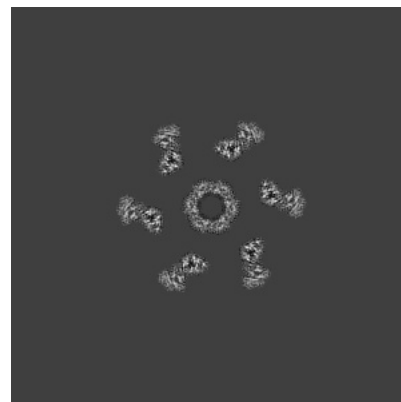
6.2.1 Primary map



X Index: 280

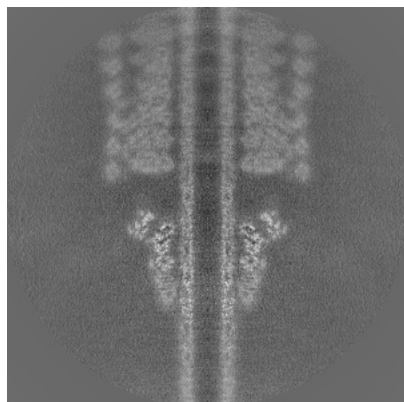


Y Index: 280

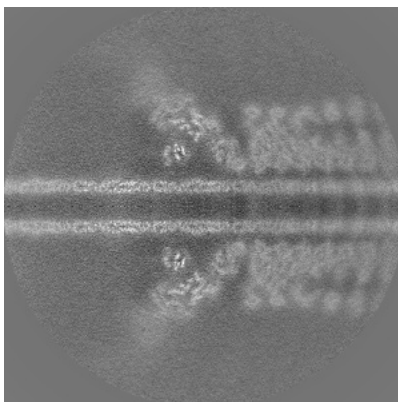


Z Index: 280

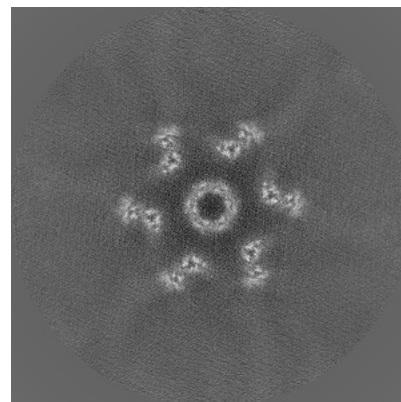
6.2.2 Raw map



X Index: 280



Y Index: 280



Z Index: 280

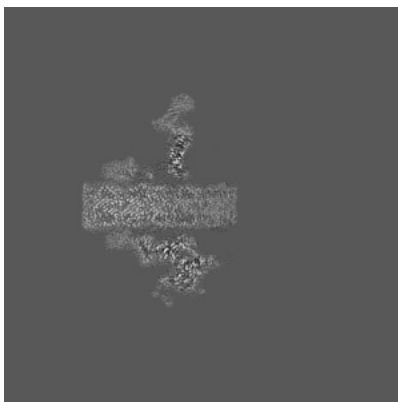
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 303

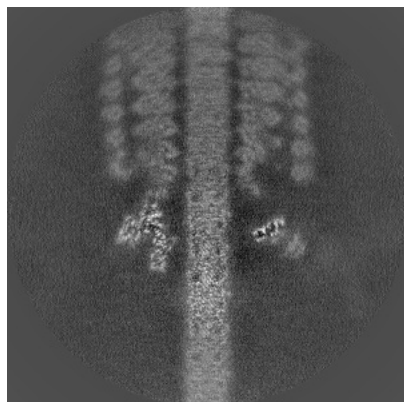


Y Index: 258

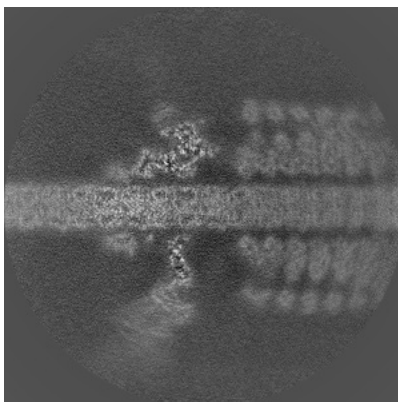


Z Index: 246

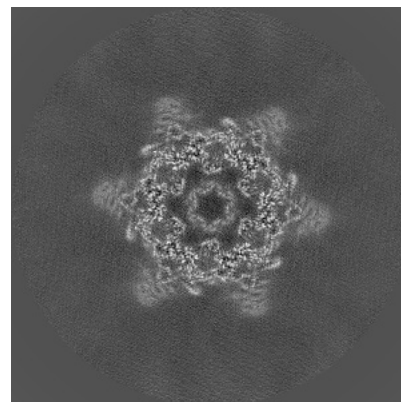
6.3.2 Raw map



X Index: 257



Y Index: 302

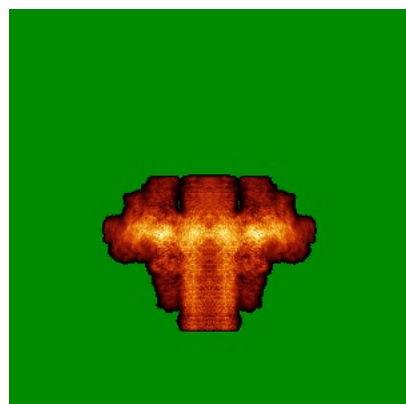


Z Index: 244

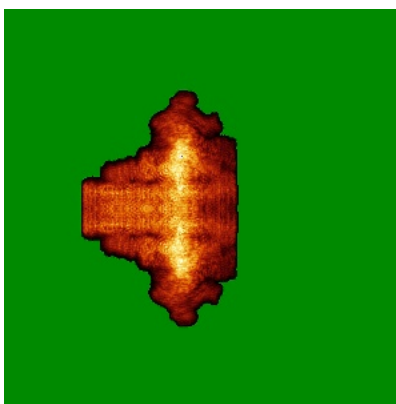
The images above show the largest variance slices of the map in three orthogonal directions.

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

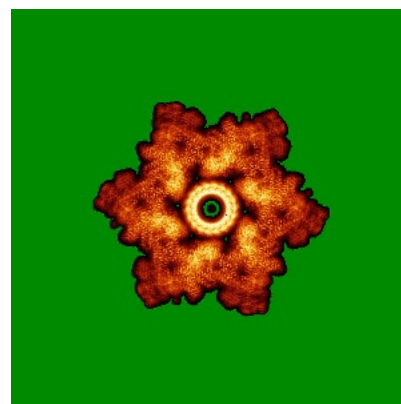
6.4.1 Primary map



X

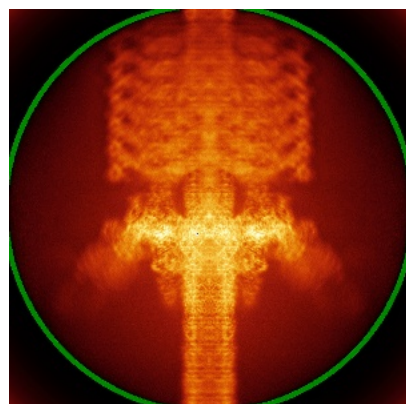


Y

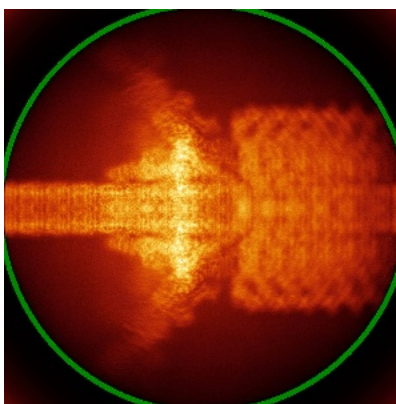


Z

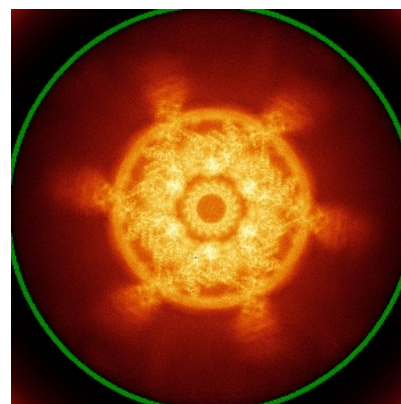
6.4.2 Raw map



X



Y

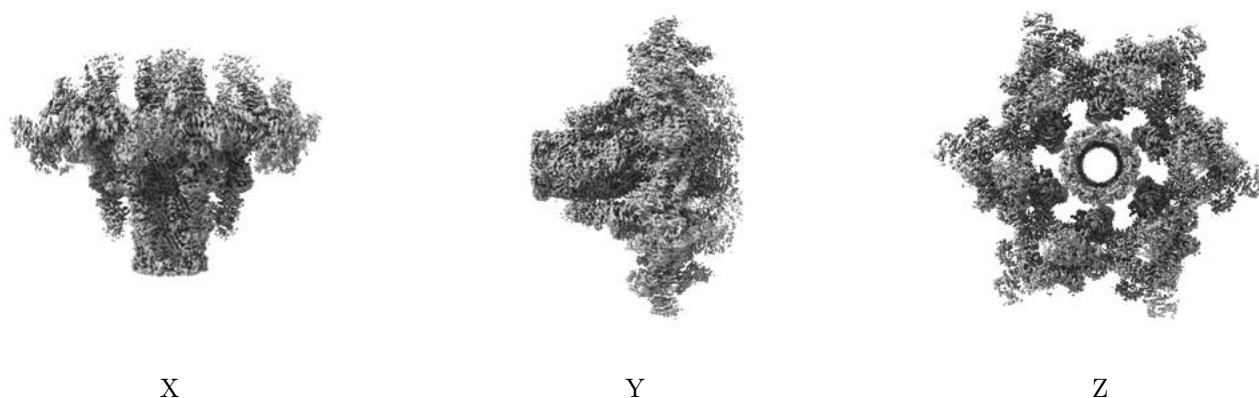


Z

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.

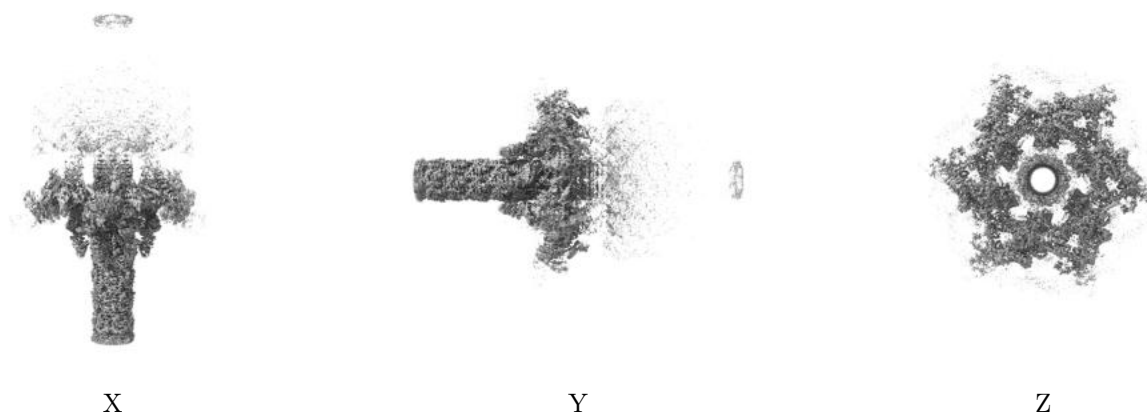
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

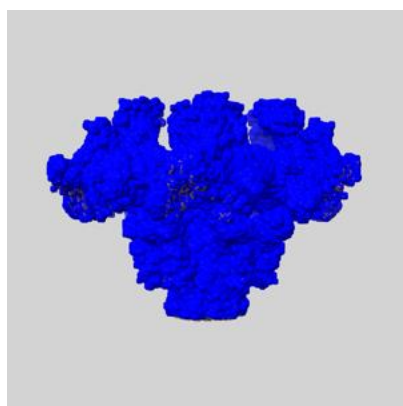
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

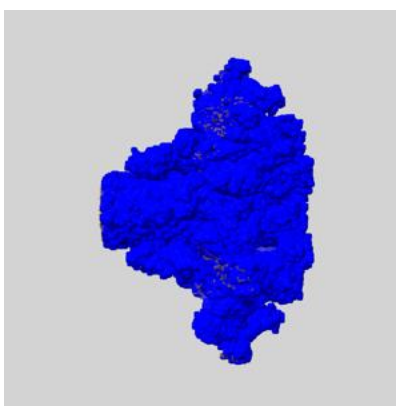
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

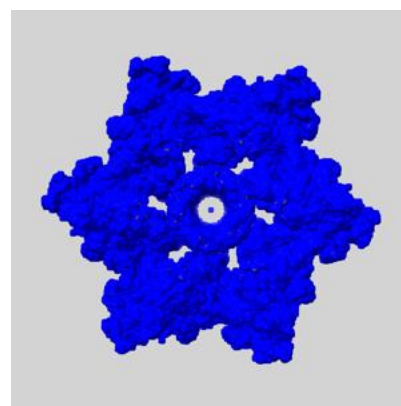
6.6.1 emd_66211_msk_1.map [i](#)



X



Y

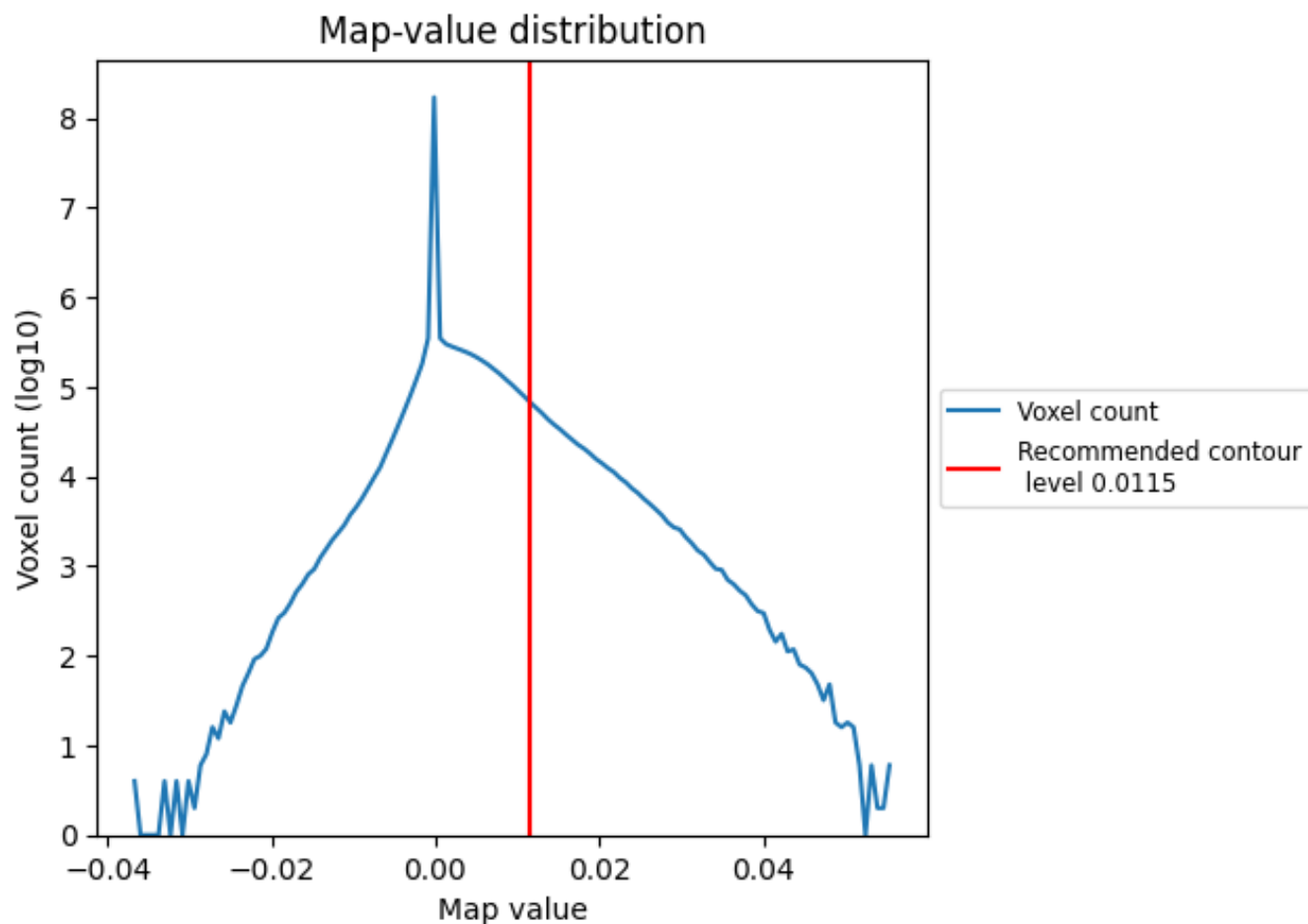


Z

7 Map analysis [i](#)

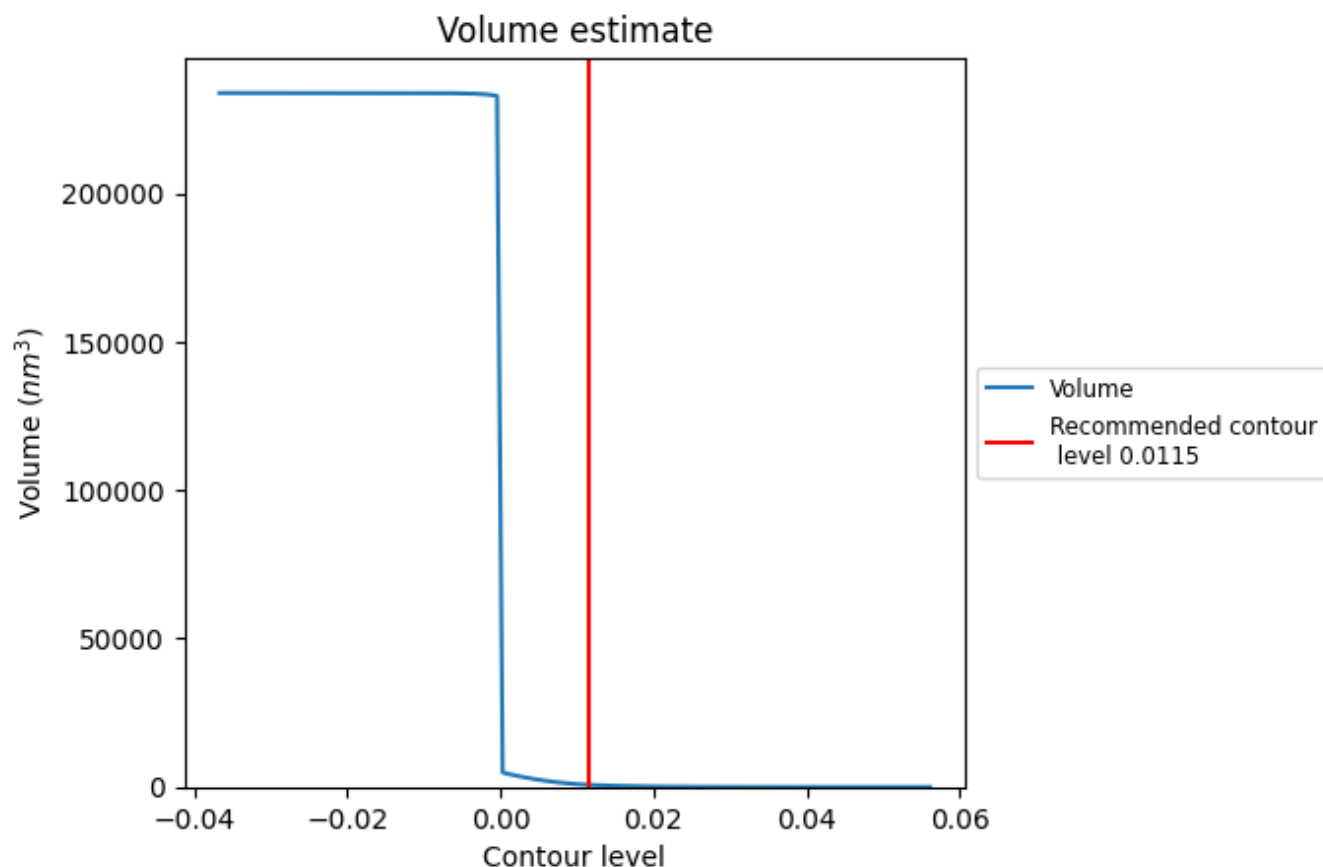
This section contains the results of statistical analysis of the map.

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.

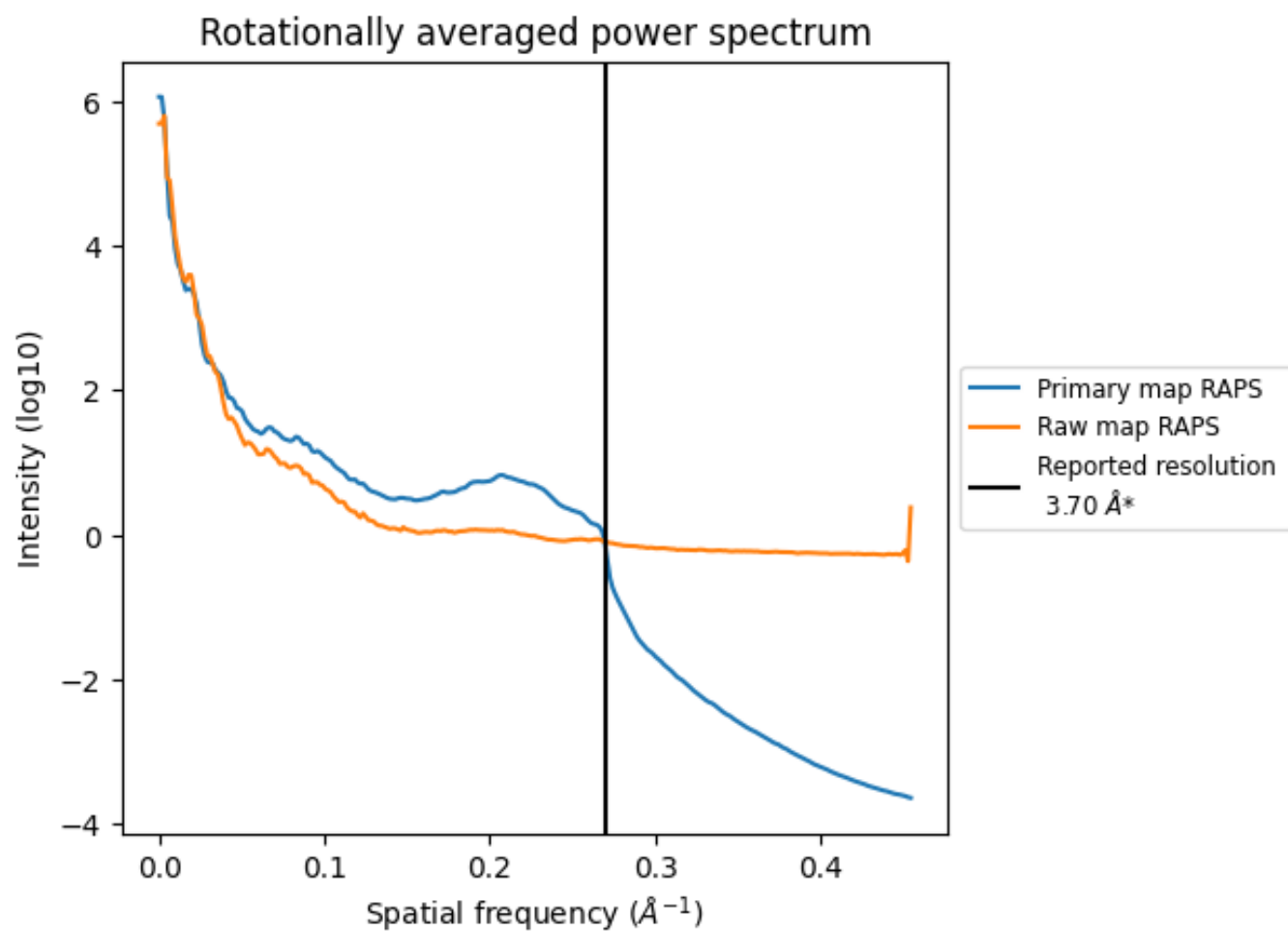
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 723 nm³; this corresponds to an approximate mass of 653 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 ⓘ

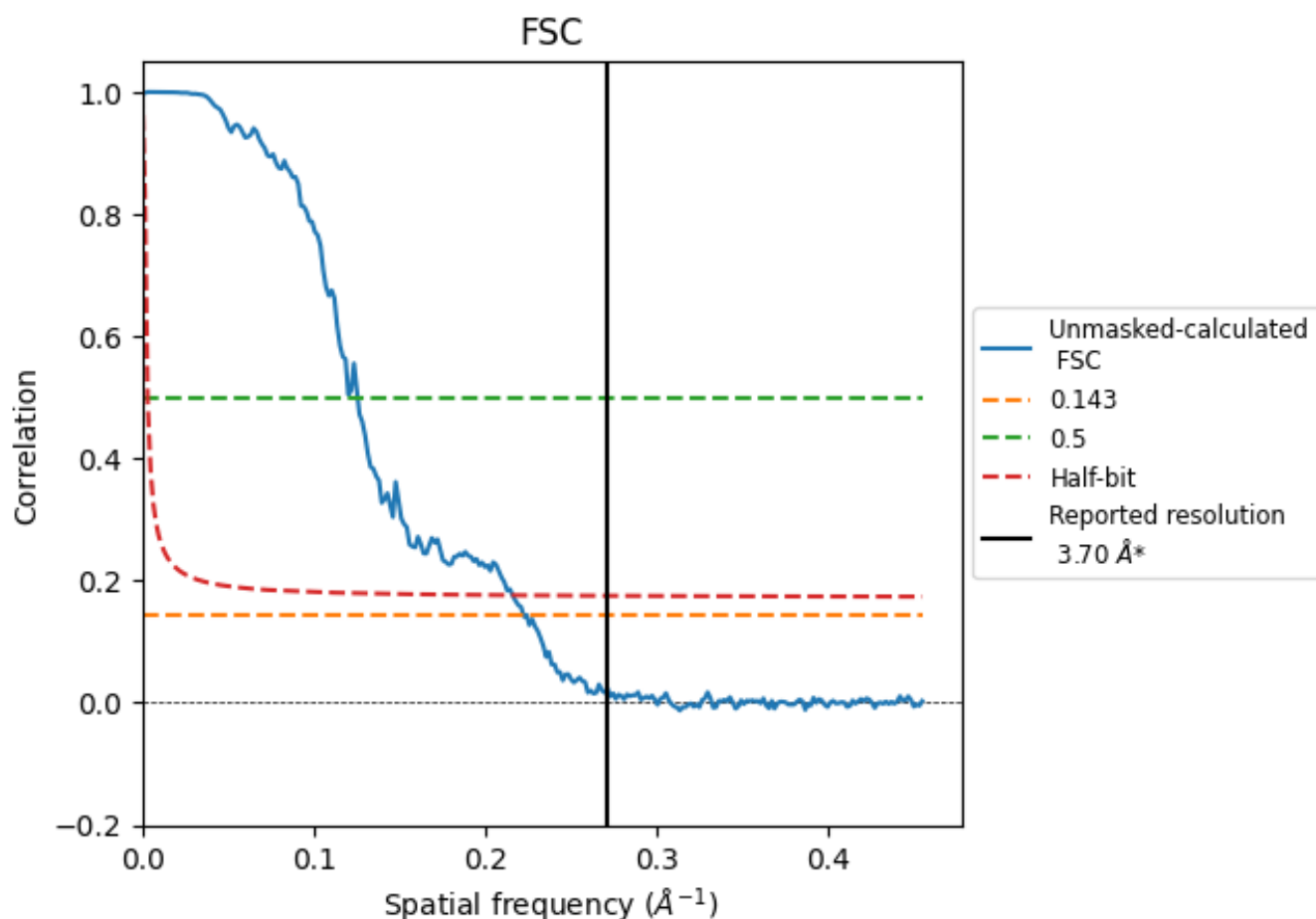


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

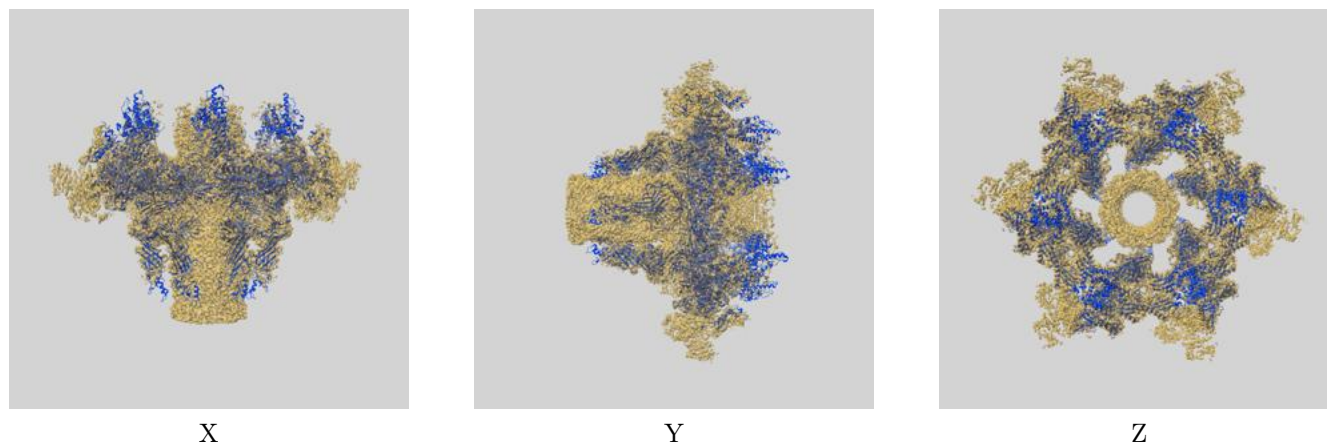
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	7.97	4.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

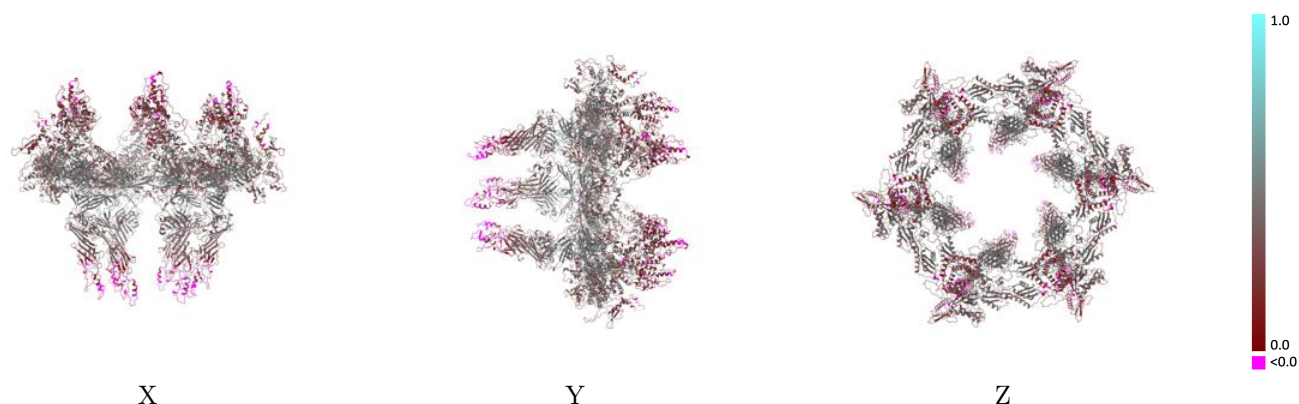
This section contains information regarding the fit between EMDB map EMD-66211 and PDB model 9WSZ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



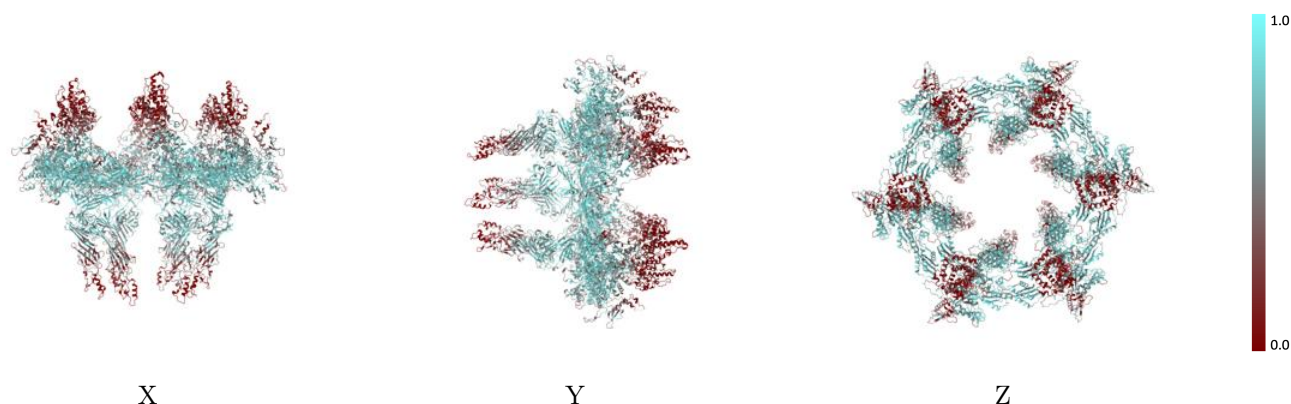
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



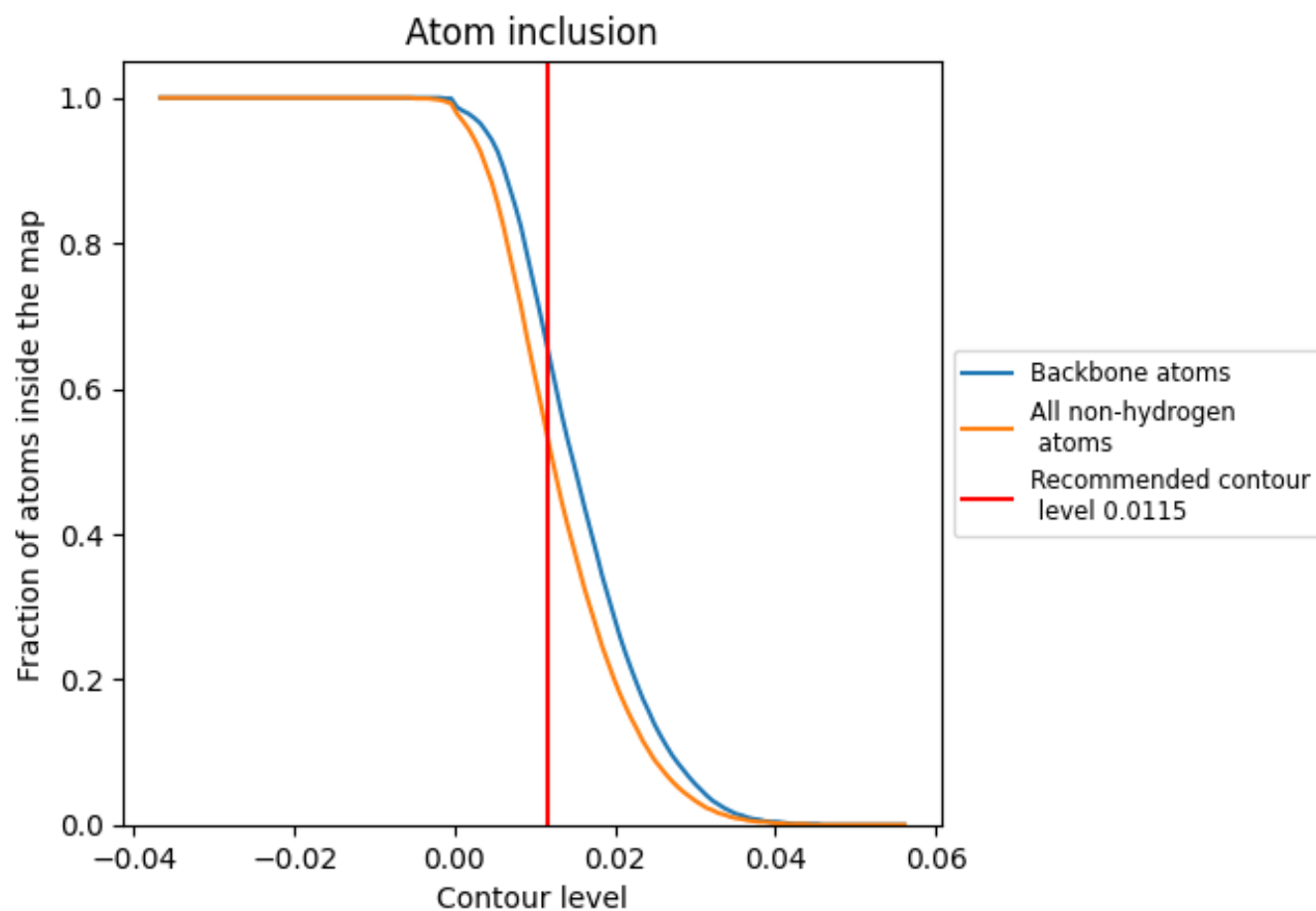
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0115).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 54% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5380	<div><div></div></div> 0.3520
A	<div><div></div></div> 0.5130	<div><div></div></div> 0.3390
B	<div><div></div></div> 0.5090	<div><div></div></div> 0.3390
C	<div><div></div></div> 0.5100	<div><div></div></div> 0.3380
D	<div><div></div></div> 0.5130	<div><div></div></div> 0.3380
E	<div><div></div></div> 0.5090	<div><div></div></div> 0.3380
F	<div><div></div></div> 0.5100	<div><div></div></div> 0.3370
G	<div><div></div></div> 0.5630	<div><div></div></div> 0.3650
H	<div><div></div></div> 0.5610	<div><div></div></div> 0.3640
I	<div><div></div></div> 0.5600	<div><div></div></div> 0.3630
J	<div><div></div></div> 0.5640	<div><div></div></div> 0.3640
K	<div><div></div></div> 0.5610	<div><div></div></div> 0.3640
L	<div><div></div></div> 0.5600	<div><div></div></div> 0.3630

1.0

0.0

<0.0