



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:15 AM UTC

PDB ID : 7T7C / pdb_00007t7c
EMDB ID : EMD-25737
Title : The hexagonal organization of Munc13-1 C1-C2B-MUN-C2C domains between lipid bilayers
Authors : Grushin, K.; Sindelar, C.V.
Deposited on : 2021-12-15
Resolution : 10.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

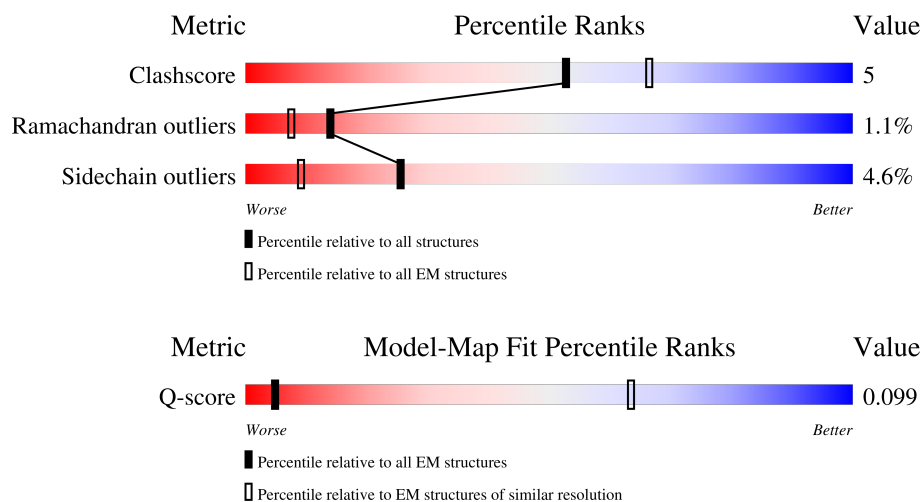
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 10.00 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	147 (9.50 - 10.50)

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	1154	14% 85% 12% ..
1	B	1154	37% 82% 14% ..
1	C	1154	14% 85% 12% ..
1	D	1154	14% 85% 12% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	1154	
1	F	1154	
1	G	1154	
1	H	1154	
1	I	1154	
1	J	1154	
1	K	1154	
1	L	1154	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 216120 atoms, of which 107712 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 Protein unc-13 homolog A Chimera.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	B	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	C	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	D	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	E	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	F	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	G	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	H	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	I	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	J	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	K	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		
1	L	1132	Total	C	H	N	O	S	0	0
			18010	5715	8976	1545	1719	55		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A822AJ50
A	-6	PRO	-	expression tag	UNP A0A822AJ50
A	-5	LEU	-	expression tag	UNP A0A822AJ50
A	-4	GLY	-	expression tag	UNP A0A822AJ50
A	-3	SER	-	expression tag	UNP A0A822AJ50
A	-2	GLU	-	expression tag	UNP A0A822AJ50

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PHE	-	expression tag	UNP A0A822AJ50
A	0	MET	-	expression tag	UNP A0A822AJ50
A	880	GLU	-	linker	UNP A0A822AJ50
A	881	PHE	-	linker	UNP A0A822AJ50
B	-7	GLY	-	expression tag	UNP A0A822AJ50
B	-6	PRO	-	expression tag	UNP A0A822AJ50
B	-5	LEU	-	expression tag	UNP A0A822AJ50
B	-4	GLY	-	expression tag	UNP A0A822AJ50
B	-3	SER	-	expression tag	UNP A0A822AJ50
B	-2	GLU	-	expression tag	UNP A0A822AJ50
B	-1	PHE	-	expression tag	UNP A0A822AJ50
B	0	MET	-	expression tag	UNP A0A822AJ50
B	880	GLU	-	linker	UNP A0A822AJ50
B	881	PHE	-	linker	UNP A0A822AJ50
C	-7	GLY	-	expression tag	UNP A0A822AJ50
C	-6	PRO	-	expression tag	UNP A0A822AJ50
C	-5	LEU	-	expression tag	UNP A0A822AJ50
C	-4	GLY	-	expression tag	UNP A0A822AJ50
C	-3	SER	-	expression tag	UNP A0A822AJ50
C	-2	GLU	-	expression tag	UNP A0A822AJ50
C	-1	PHE	-	expression tag	UNP A0A822AJ50
C	0	MET	-	expression tag	UNP A0A822AJ50
C	880	GLU	-	linker	UNP A0A822AJ50
C	881	PHE	-	linker	UNP A0A822AJ50
D	-7	GLY	-	expression tag	UNP A0A822AJ50
D	-6	PRO	-	expression tag	UNP A0A822AJ50
D	-5	LEU	-	expression tag	UNP A0A822AJ50
D	-4	GLY	-	expression tag	UNP A0A822AJ50
D	-3	SER	-	expression tag	UNP A0A822AJ50
D	-2	GLU	-	expression tag	UNP A0A822AJ50
D	-1	PHE	-	expression tag	UNP A0A822AJ50
D	0	MET	-	expression tag	UNP A0A822AJ50
D	880	GLU	-	linker	UNP A0A822AJ50
D	881	PHE	-	linker	UNP A0A822AJ50
E	-7	GLY	-	expression tag	UNP A0A822AJ50
E	-6	PRO	-	expression tag	UNP A0A822AJ50
E	-5	LEU	-	expression tag	UNP A0A822AJ50
E	-4	GLY	-	expression tag	UNP A0A822AJ50
E	-3	SER	-	expression tag	UNP A0A822AJ50
E	-2	GLU	-	expression tag	UNP A0A822AJ50
E	-1	PHE	-	expression tag	UNP A0A822AJ50
E	0	MET	-	expression tag	UNP A0A822AJ50

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	880	GLU	-	linker	UNP A0A822AJ50
E	881	PHE	-	linker	UNP A0A822AJ50
F	-7	GLY	-	expression tag	UNP A0A822AJ50
F	-6	PRO	-	expression tag	UNP A0A822AJ50
F	-5	LEU	-	expression tag	UNP A0A822AJ50
F	-4	GLY	-	expression tag	UNP A0A822AJ50
F	-3	SER	-	expression tag	UNP A0A822AJ50
F	-2	GLU	-	expression tag	UNP A0A822AJ50
F	-1	PHE	-	expression tag	UNP A0A822AJ50
F	0	MET	-	expression tag	UNP A0A822AJ50
F	880	GLU	-	linker	UNP A0A822AJ50
F	881	PHE	-	linker	UNP A0A822AJ50
G	-7	GLY	-	expression tag	UNP A0A822AJ50
G	-6	PRO	-	expression tag	UNP A0A822AJ50
G	-5	LEU	-	expression tag	UNP A0A822AJ50
G	-4	GLY	-	expression tag	UNP A0A822AJ50
G	-3	SER	-	expression tag	UNP A0A822AJ50
G	-2	GLU	-	expression tag	UNP A0A822AJ50
G	-1	PHE	-	expression tag	UNP A0A822AJ50
G	0	MET	-	expression tag	UNP A0A822AJ50
G	880	GLU	-	linker	UNP A0A822AJ50
G	881	PHE	-	linker	UNP A0A822AJ50
H	-7	GLY	-	expression tag	UNP A0A822AJ50
H	-6	PRO	-	expression tag	UNP A0A822AJ50
H	-5	LEU	-	expression tag	UNP A0A822AJ50
H	-4	GLY	-	expression tag	UNP A0A822AJ50
H	-3	SER	-	expression tag	UNP A0A822AJ50
H	-2	GLU	-	expression tag	UNP A0A822AJ50
H	-1	PHE	-	expression tag	UNP A0A822AJ50
H	0	MET	-	expression tag	UNP A0A822AJ50
H	880	GLU	-	linker	UNP A0A822AJ50
H	881	PHE	-	linker	UNP A0A822AJ50
I	-7	GLY	-	expression tag	UNP A0A822AJ50
I	-6	PRO	-	expression tag	UNP A0A822AJ50
I	-5	LEU	-	expression tag	UNP A0A822AJ50
I	-4	GLY	-	expression tag	UNP A0A822AJ50
I	-3	SER	-	expression tag	UNP A0A822AJ50
I	-2	GLU	-	expression tag	UNP A0A822AJ50
I	-1	PHE	-	expression tag	UNP A0A822AJ50
I	0	MET	-	expression tag	UNP A0A822AJ50
I	880	GLU	-	linker	UNP A0A822AJ50
I	881	PHE	-	linker	UNP A0A822AJ50

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-7	GLY	-	expression tag	UNP A0A822AJ50
J	-6	PRO	-	expression tag	UNP A0A822AJ50
J	-5	LEU	-	expression tag	UNP A0A822AJ50
J	-4	GLY	-	expression tag	UNP A0A822AJ50
J	-3	SER	-	expression tag	UNP A0A822AJ50
J	-2	GLU	-	expression tag	UNP A0A822AJ50
J	-1	PHE	-	expression tag	UNP A0A822AJ50
J	0	MET	-	expression tag	UNP A0A822AJ50
J	880	GLU	-	linker	UNP A0A822AJ50
J	881	PHE	-	linker	UNP A0A822AJ50
K	-7	GLY	-	expression tag	UNP A0A822AJ50
K	-6	PRO	-	expression tag	UNP A0A822AJ50
K	-5	LEU	-	expression tag	UNP A0A822AJ50
K	-4	GLY	-	expression tag	UNP A0A822AJ50
K	-3	SER	-	expression tag	UNP A0A822AJ50
K	-2	GLU	-	expression tag	UNP A0A822AJ50
K	-1	PHE	-	expression tag	UNP A0A822AJ50
K	0	MET	-	expression tag	UNP A0A822AJ50
K	880	GLU	-	linker	UNP A0A822AJ50
K	881	PHE	-	linker	UNP A0A822AJ50
L	-7	GLY	-	expression tag	UNP A0A822AJ50
L	-6	PRO	-	expression tag	UNP A0A822AJ50
L	-5	LEU	-	expression tag	UNP A0A822AJ50
L	-4	GLY	-	expression tag	UNP A0A822AJ50
L	-3	SER	-	expression tag	UNP A0A822AJ50
L	-2	GLU	-	expression tag	UNP A0A822AJ50
L	-1	PHE	-	expression tag	UNP A0A822AJ50
L	0	MET	-	expression tag	UNP A0A822AJ50
L	880	GLU	-	linker	UNP A0A822AJ50
L	881	PHE	-	linker	UNP A0A822AJ50

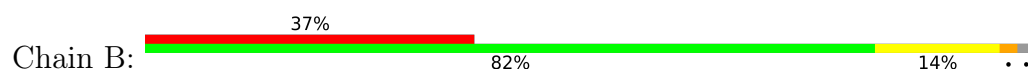
3 Residue-property plots

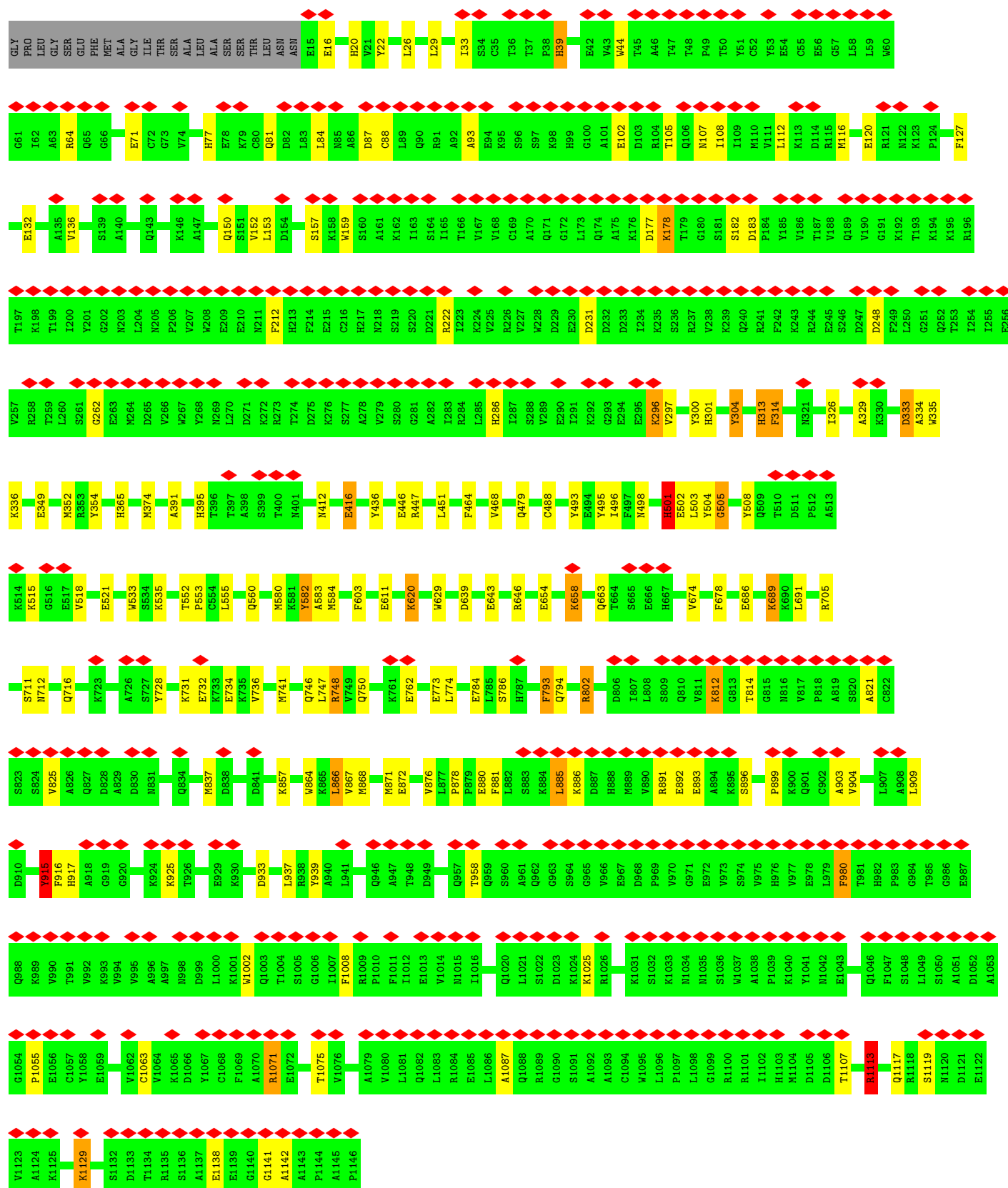
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Protein unc-13 homolog A Chimera

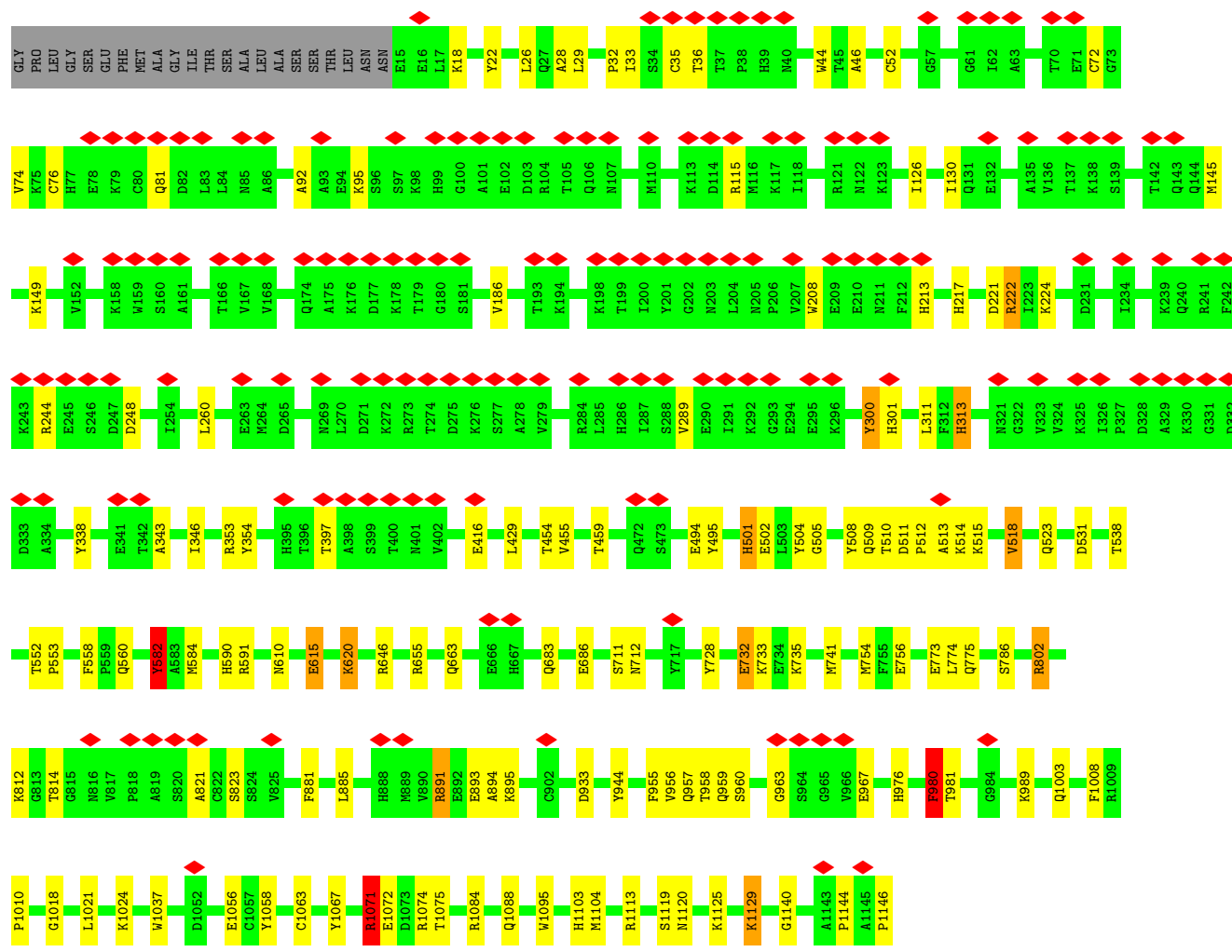


- Molecule 1: Protein unc-13 homolog A Chimera

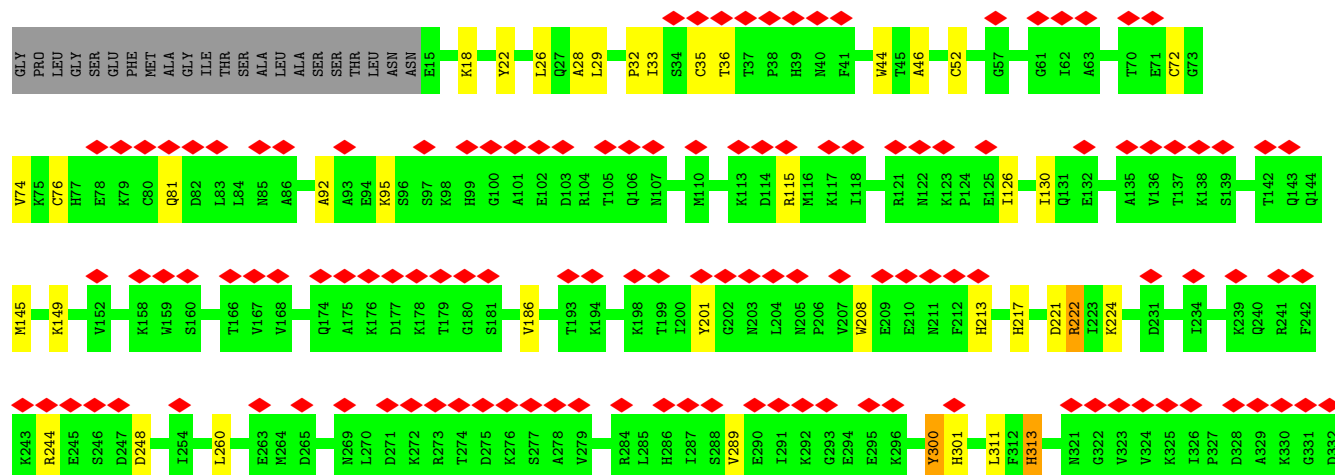


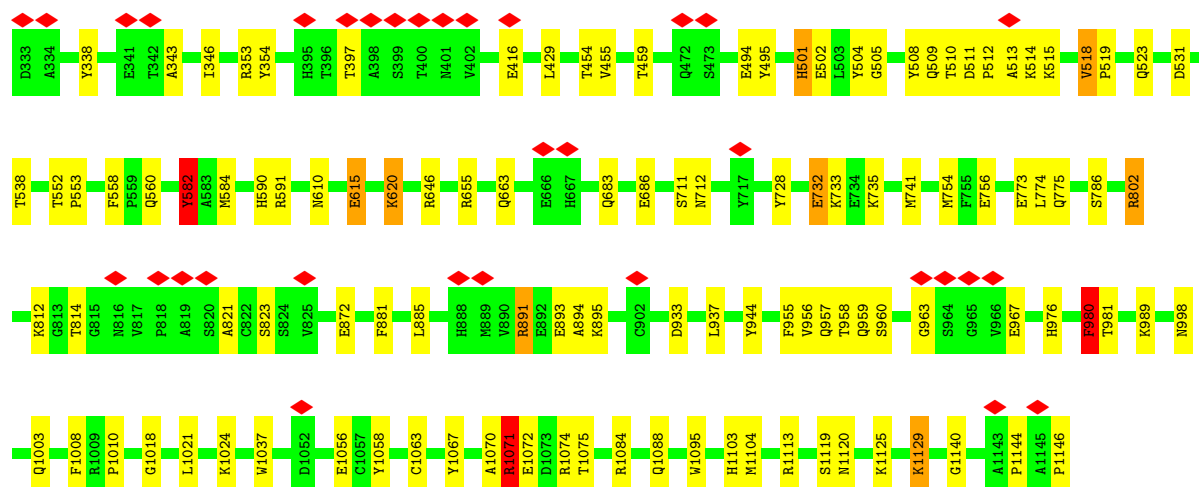


• Molecule 1: Protein unc-13 homolog A Chimera

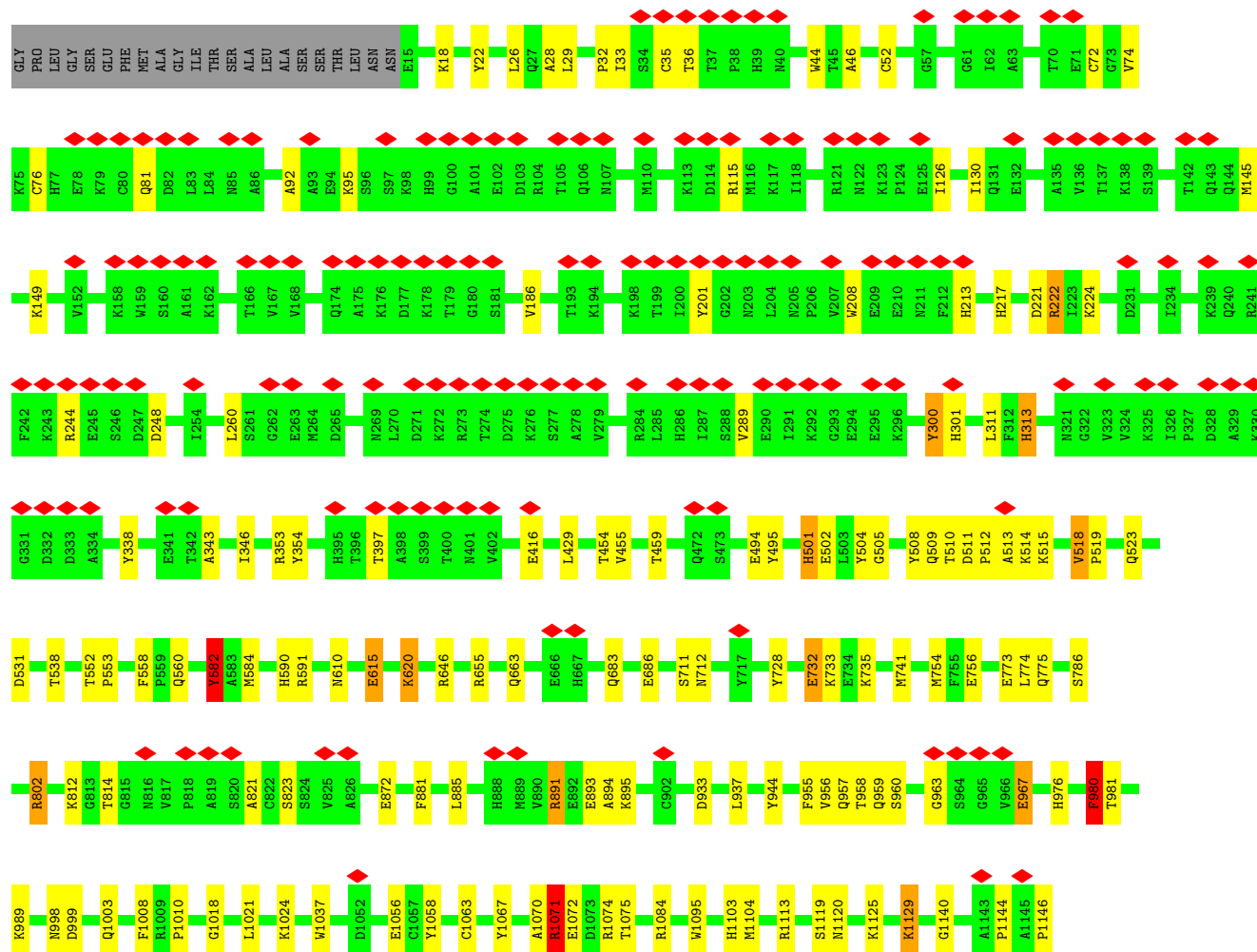
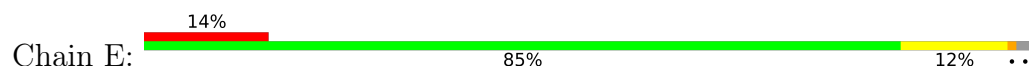


Chain D: 14% 85% 12%

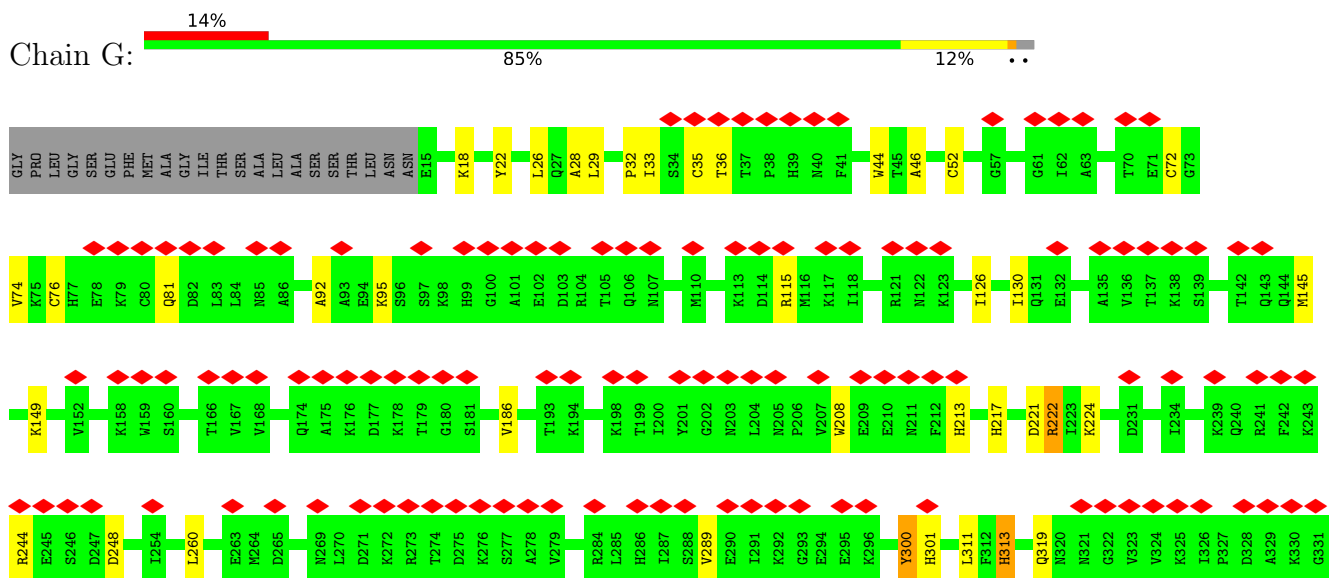
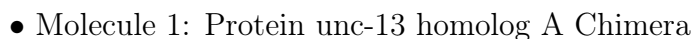


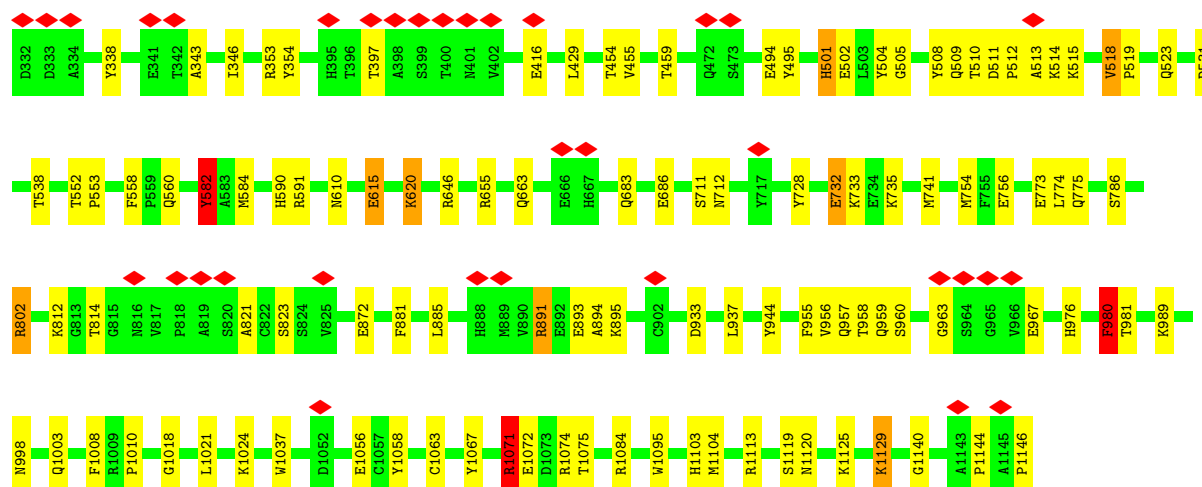


• Molecule 1: Protein unc-13 homolog A Chimera

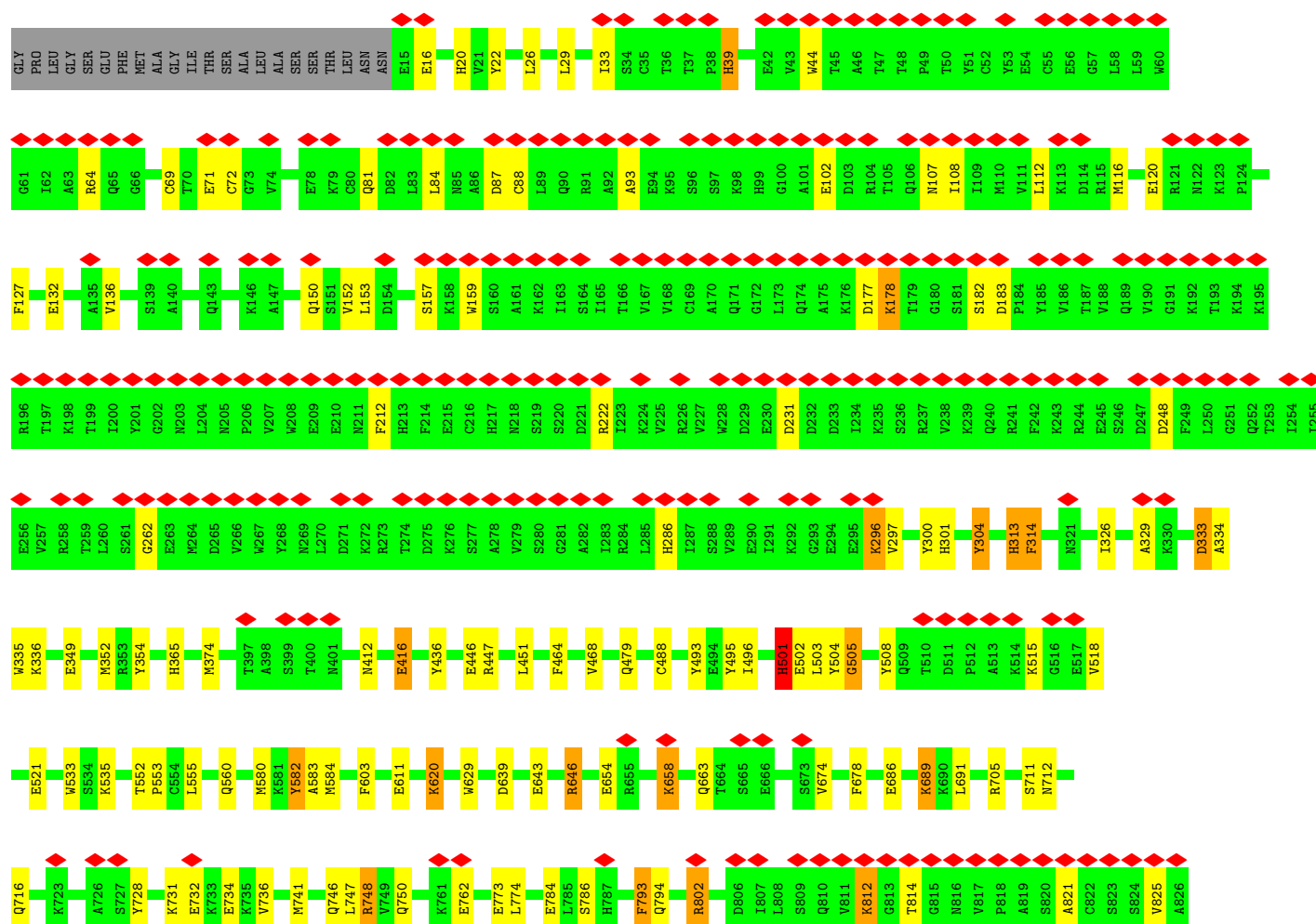
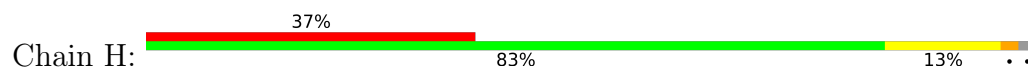


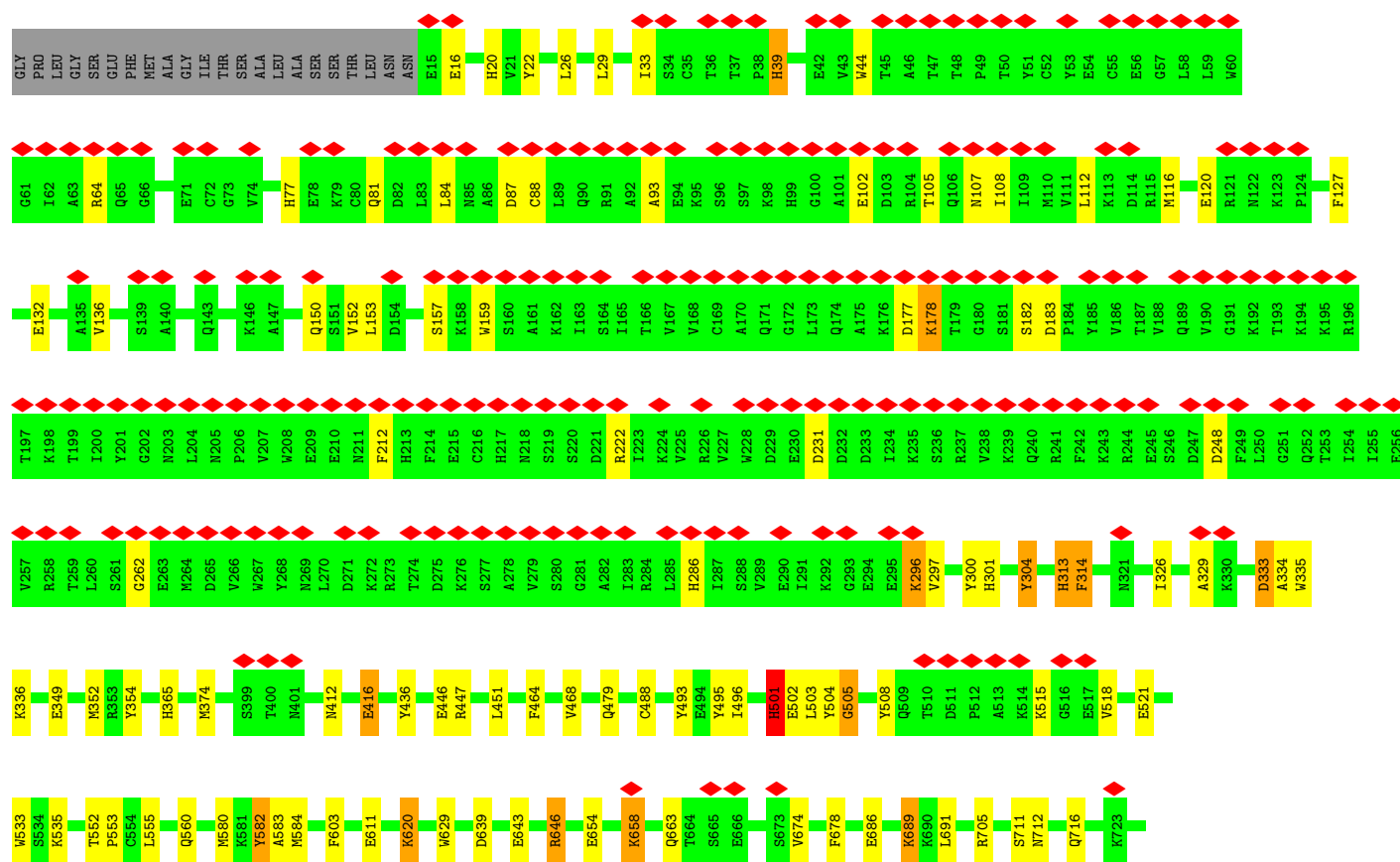
• Molecule 1: Protein unc-13 homolog A Chimera

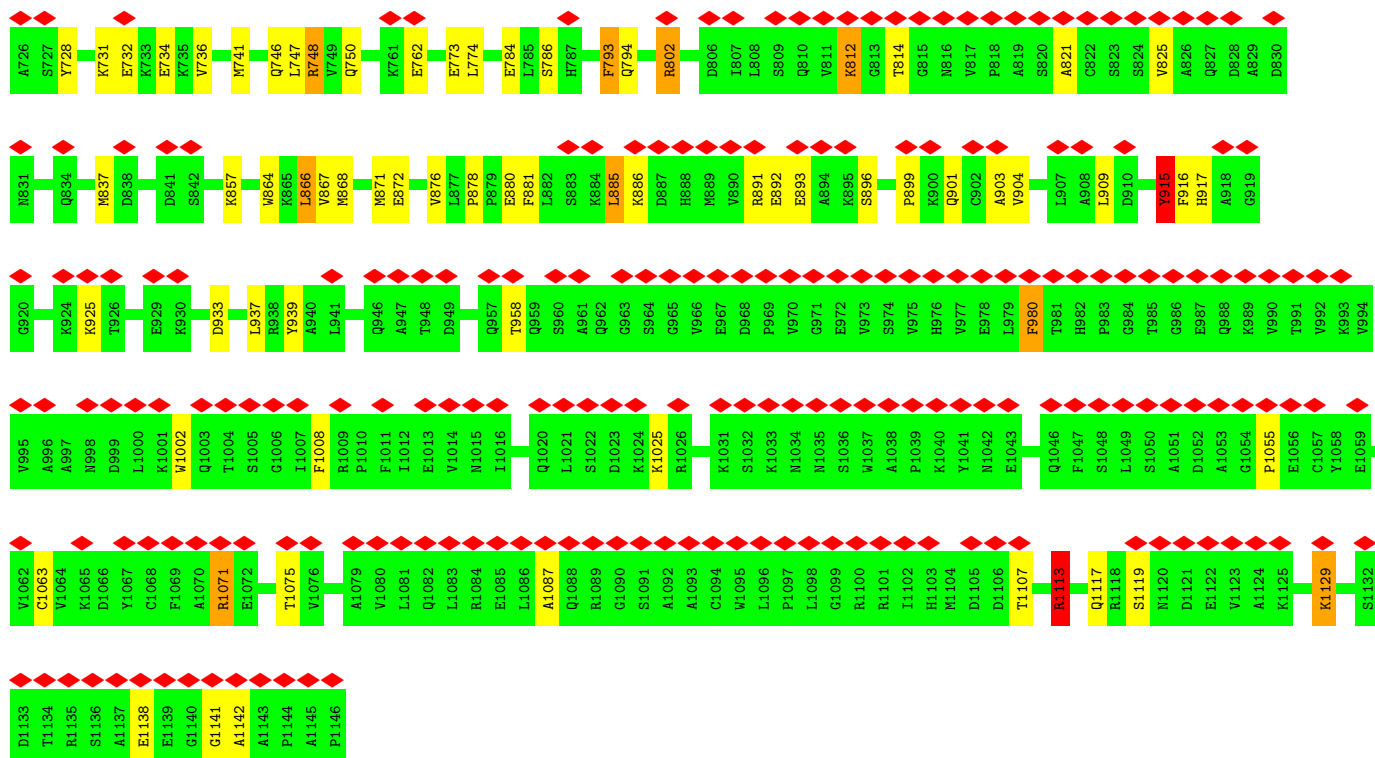




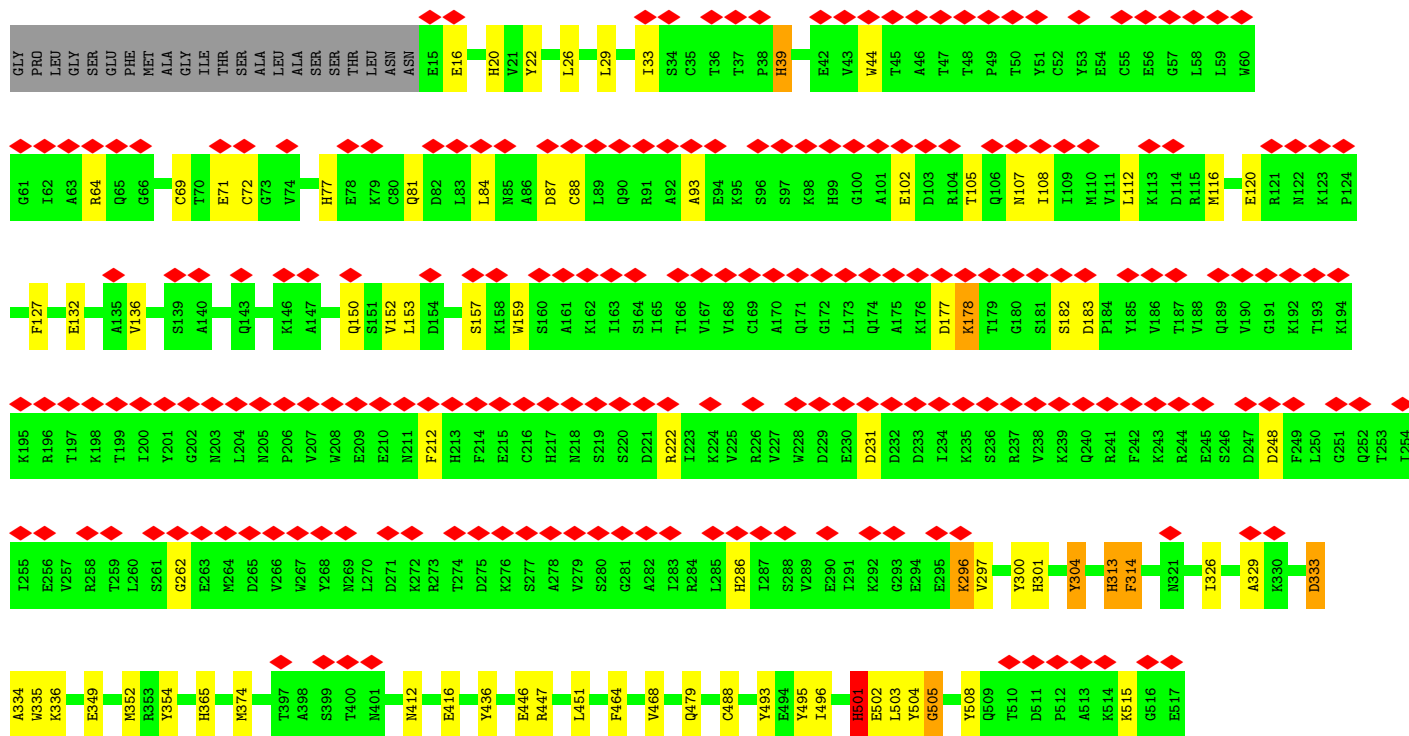
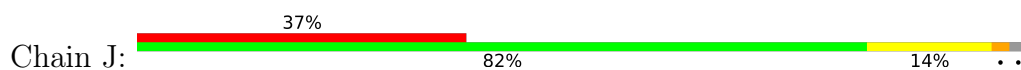
• Molecule 1: Protein unc-13 homolog A Chimera

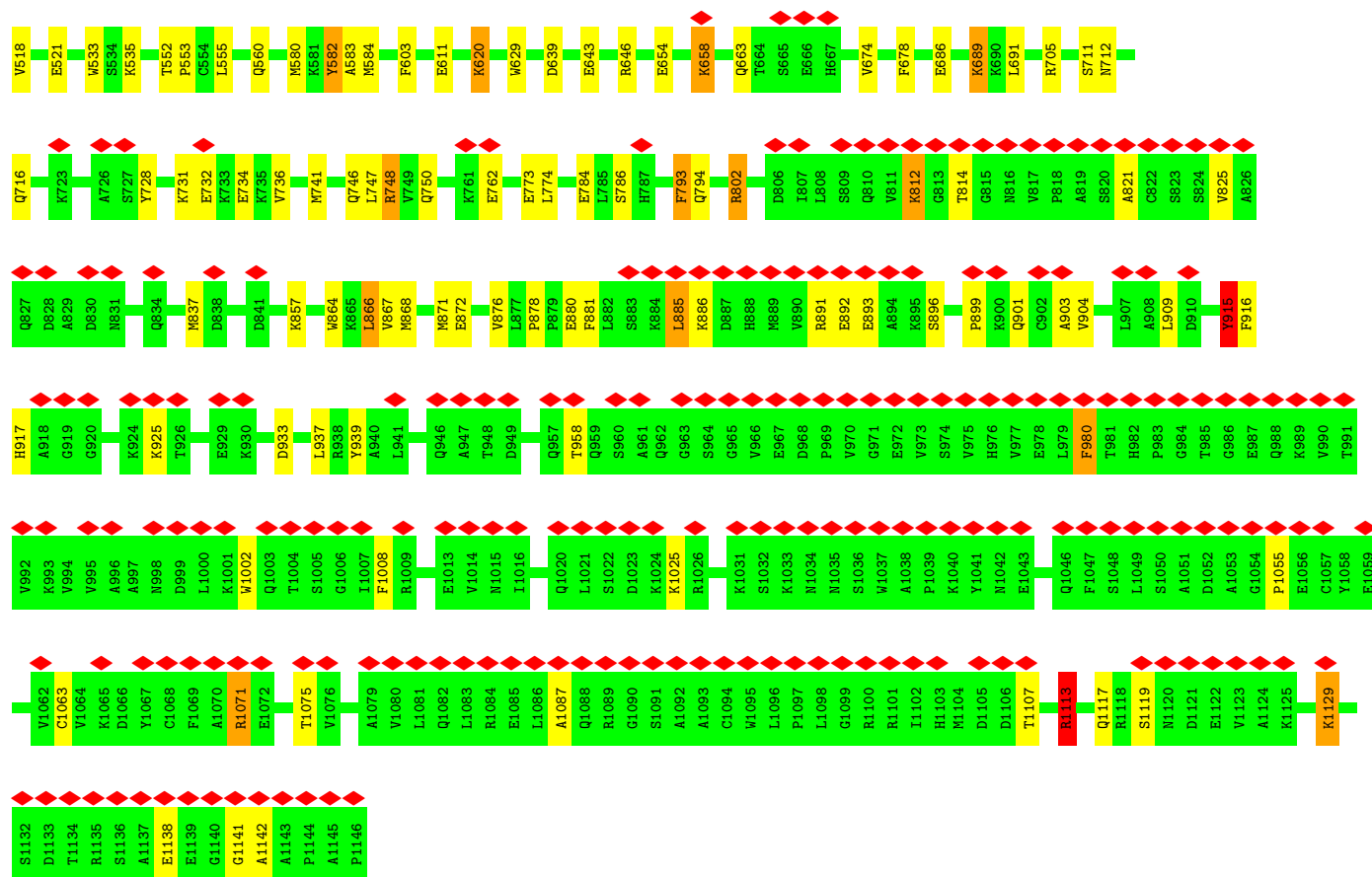




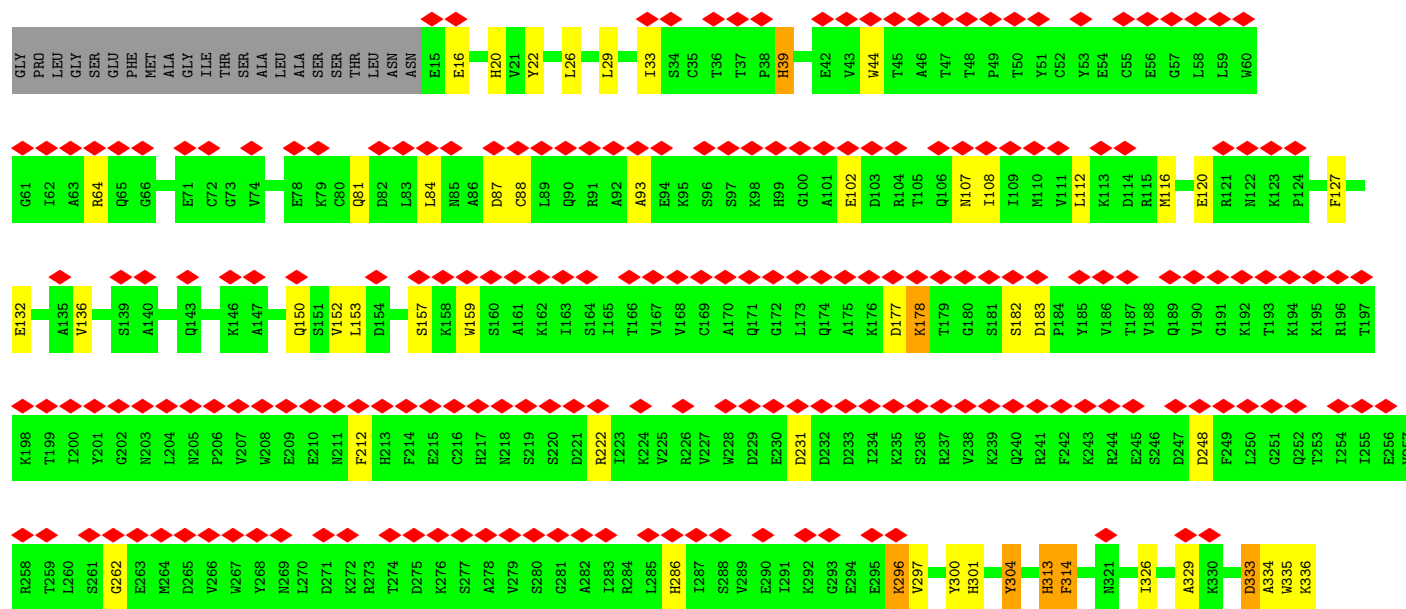
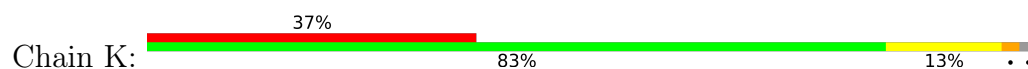


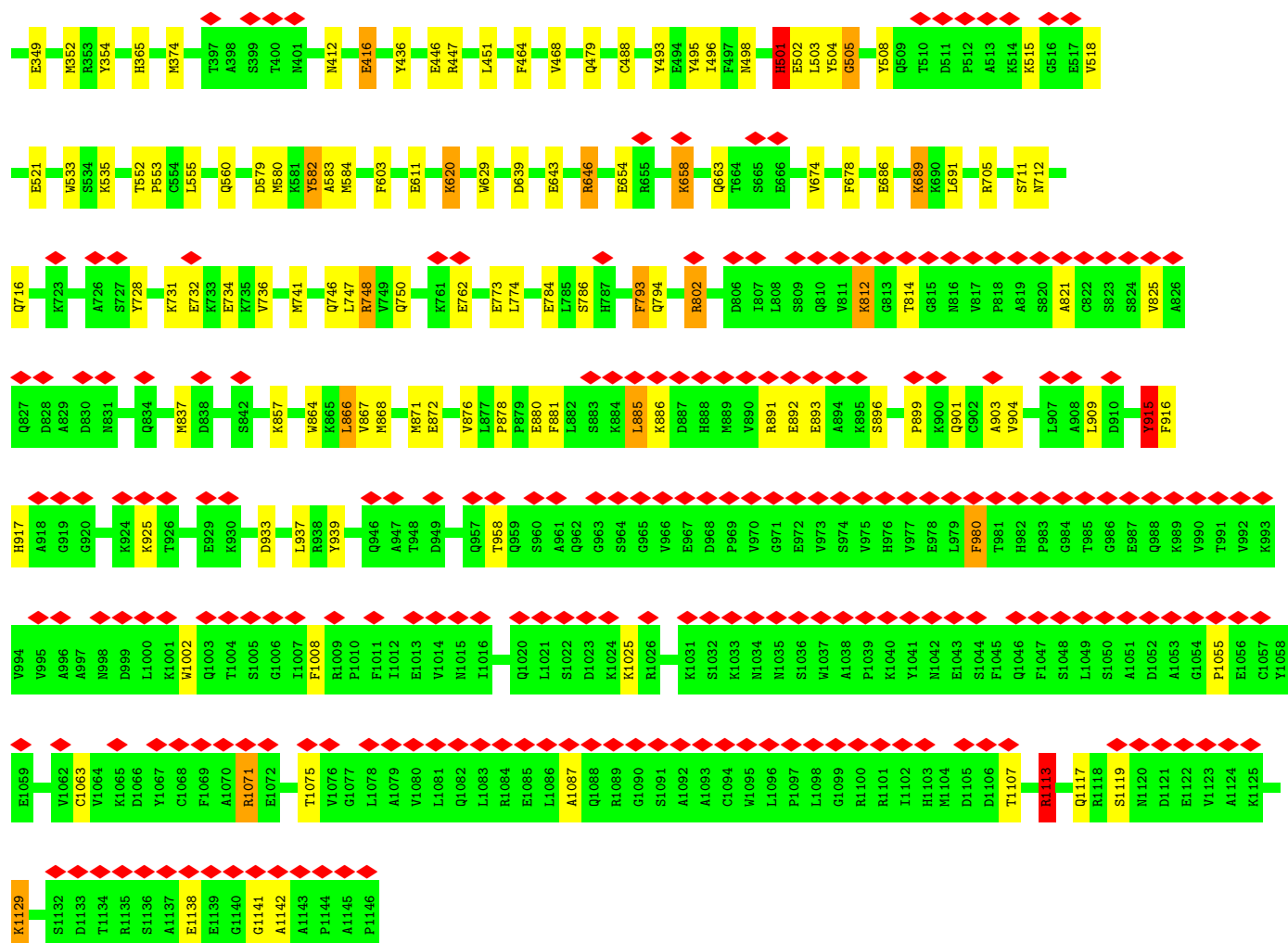
• Molecule 1: Protein unc-13 homolog A Chimera



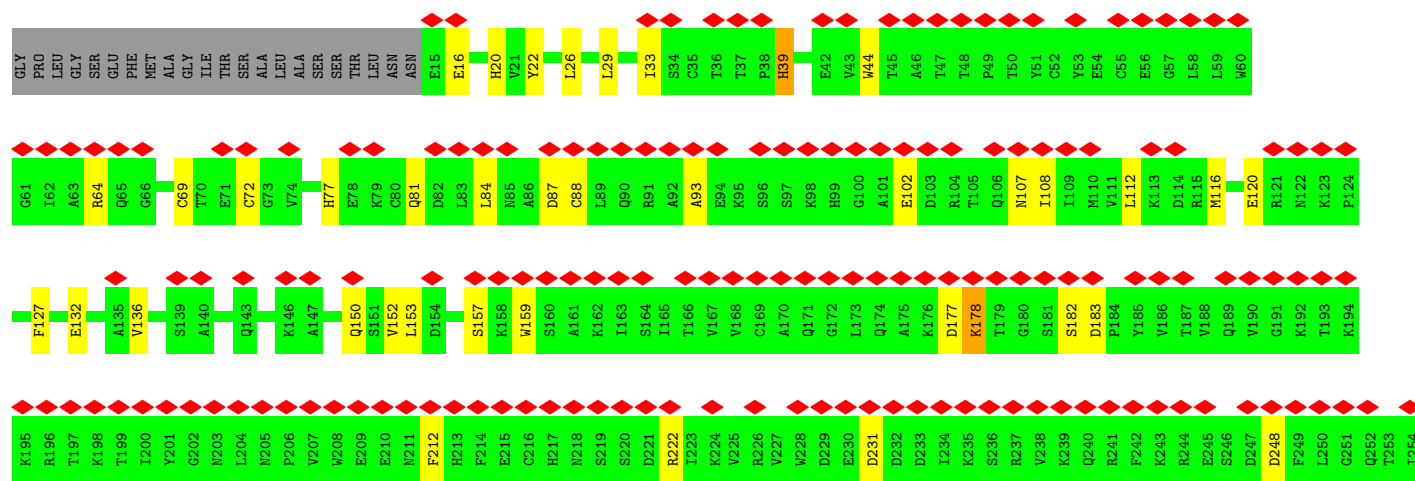
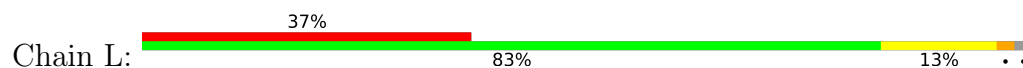


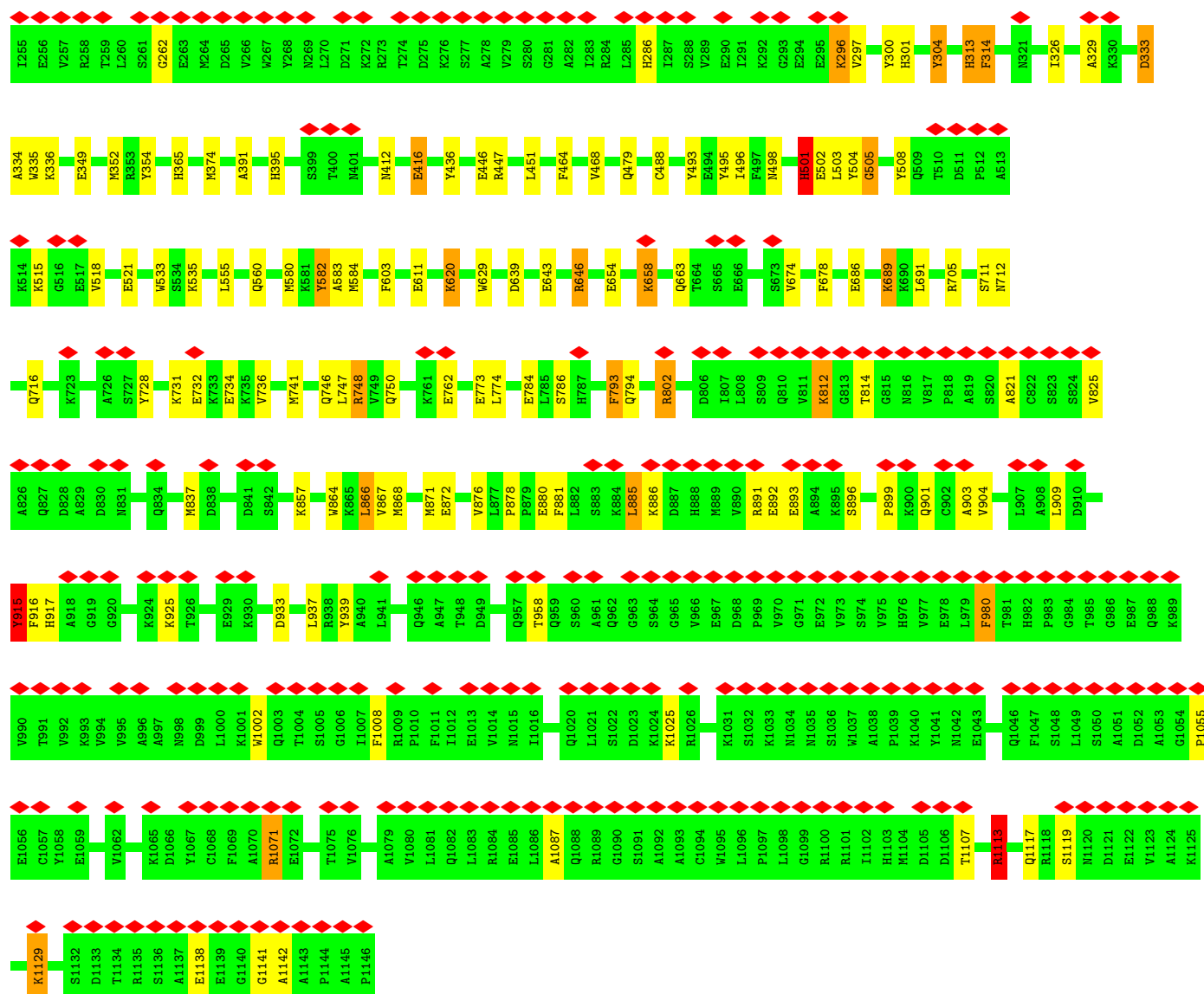
• Molecule 1: Protein unc-13 homolog A Chimera





• Molecule 1: Protein unc-13 homolog A Chimera





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of subtomograms used	12149	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed during 3D reconstruction in RELION 3.1	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	110	Depositor
Minimum defocus (nm)	3500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.853	Depositor
Minimum map value	-0.528	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	411.59998, 411.59998, 411.59998	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.1, 2.1, 2.1	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	0.78	0/9220	1.33	18/12466 (0.1%)
1	B	0.79	0/9220	1.41	16/12466 (0.1%)
1	C	0.78	0/9220	1.33	17/12466 (0.1%)
1	D	0.78	0/9220	1.33	17/12466 (0.1%)
1	E	0.78	0/9220	1.33	17/12466 (0.1%)
1	F	0.78	0/9220	1.33	17/12466 (0.1%)
1	G	0.78	0/9220	1.33	18/12466 (0.1%)
1	H	0.79	0/9220	1.41	16/12466 (0.1%)
1	I	0.79	0/9220	1.41	17/12466 (0.1%)
1	J	0.79	0/9220	1.41	16/12466 (0.1%)
1	K	0.79	0/9220	1.41	16/12466 (0.1%)
1	L	0.79	0/9220	1.41	17/12466 (0.1%)
All	All	0.78	0/110640	1.37	202/149592 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	14
1	C	0	9
1	D	0	10
1	E	0	10
1	F	0	9
1	G	0	9
1	H	0	14
1	I	0	14
1	J	0	14
1	K	0	14
1	L	0	14
All	All	0	140

There are no bond length outliers.

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	980	PHE	CA-CB-CG	10.31	124.11	113.80
1	H	980	PHE	CA-CB-CG	10.29	124.09	113.80
1	K	980	PHE	CA-CB-CG	10.28	124.08	113.80
1	J	980	PHE	CA-CB-CG	10.26	124.06	113.80
1	B	980	PHE	CA-CB-CG	10.25	124.05	113.80
1	L	980	PHE	CA-CB-CG	10.25	124.05	113.80
1	L	501	HIS	CA-CB-CG	-10.11	103.69	113.80
1	J	501	HIS	CA-CB-CG	-10.10	103.70	113.80
1	B	501	HIS	CA-CB-CG	-10.09	103.71	113.80
1	H	501	HIS	CA-CB-CG	-10.08	103.72	113.80
1	I	501	HIS	CA-CB-CG	-10.05	103.75	113.80
1	K	501	HIS	CA-CB-CG	-10.05	103.75	113.80
1	F	980	PHE	CA-CB-CG	9.41	123.21	113.80
1	E	980	PHE	CA-CB-CG	9.40	123.20	113.80
1	C	980	PHE	CA-CB-CG	9.39	123.19	113.80
1	A	980	PHE	CA-CB-CG	9.38	123.18	113.80
1	D	980	PHE	CA-CB-CG	9.37	123.17	113.80
1	G	980	PHE	CA-CB-CG	9.37	123.17	113.80
1	C	523	GLN	CA-C-N	8.00	134.43	121.87
1	C	523	GLN	C-N-CA	8.00	134.43	121.87
1	D	523	GLN	CA-C-N	8.00	134.43	121.87
1	D	523	GLN	C-N-CA	8.00	134.43	121.87
1	G	523	GLN	CA-C-N	8.00	134.42	121.87
1	G	523	GLN	C-N-CA	8.00	134.42	121.87
1	E	523	GLN	CA-C-N	8.00	134.42	121.87
1	E	523	GLN	C-N-CA	8.00	134.42	121.87
1	A	523	GLN	CA-C-N	7.99	134.41	121.87
1	A	523	GLN	C-N-CA	7.99	134.41	121.87
1	F	523	GLN	CA-C-N	7.97	134.38	121.87
1	F	523	GLN	C-N-CA	7.97	134.38	121.87
1	A	313	HIS	CA-CB-CG	7.75	121.55	113.80
1	C	313	HIS	CA-CB-CG	7.73	121.53	113.80
1	D	313	HIS	CA-CB-CG	7.73	121.53	113.80
1	G	313	HIS	CA-CB-CG	7.71	121.51	113.80
1	E	313	HIS	CA-CB-CG	7.71	121.51	113.80
1	F	313	HIS	CA-CB-CG	7.69	121.49	113.80
1	J	678	PHE	CA-CB-CG	-7.62	106.18	113.80
1	I	678	PHE	CA-CB-CG	-7.62	106.18	113.80
1	L	678	PHE	CA-CB-CG	-7.62	106.19	113.80
1	H	678	PHE	CA-CB-CG	-7.58	106.22	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	678	PHE	CA-CB-CG	-7.55	106.25	113.80
1	K	678	PHE	CA-CB-CG	-7.54	106.26	113.80
1	E	501	HIS	CA-CB-CG	-7.26	106.54	113.80
1	G	501	HIS	CA-CB-CG	-7.26	106.54	113.80
1	D	501	HIS	CA-CB-CG	-7.23	106.57	113.80
1	C	501	HIS	CA-CB-CG	-7.21	106.59	113.80
1	A	501	HIS	CA-CB-CG	-7.20	106.60	113.80
1	F	501	HIS	CA-CB-CG	-7.18	106.62	113.80
1	B	663	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	H	663	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	I	663	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	J	663	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	L	663	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	K	663	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	E	775	GLN	OE1-CD-NE2	-6.28	116.32	122.60
1	A	775	GLN	OE1-CD-NE2	-6.26	116.33	122.60
1	G	775	GLN	OE1-CD-NE2	-6.25	116.34	122.60
1	F	775	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	D	775	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	C	775	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	I	793	PHE	CA-CB-CG	-6.18	107.62	113.80
1	H	793	PHE	CA-CB-CG	-6.15	107.65	113.80
1	L	793	PHE	CA-CB-CG	-6.15	107.65	113.80
1	K	793	PHE	CA-CB-CG	-6.13	107.67	113.80
1	J	793	PHE	CA-CB-CG	-6.13	107.67	113.80
1	B	793	PHE	CA-CB-CG	-6.11	107.69	113.80
1	L	365	HIS	CB-CG-CD2	-5.81	123.64	131.20
1	J	365	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	H	365	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	I	365	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	B	365	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	K	365	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	K	301	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	J	301	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	L	301	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	B	301	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	B	39	HIS	CA-CB-CG	5.68	119.48	113.80
1	I	301	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	H	39	HIS	CA-CB-CG	5.68	119.48	113.80
1	H	301	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	K	39	HIS	CA-CB-CG	5.66	119.46	113.80
1	I	39	HIS	CA-CB-CG	5.63	119.43	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	39	HIS	CA-CB-CG	5.62	119.42	113.80
1	J	39	HIS	CA-CB-CG	5.61	119.41	113.80
1	G	967	GLU	CB-CA-C	5.59	119.45	109.38
1	F	967	GLU	CB-CA-C	5.59	119.44	109.38
1	D	967	GLU	CB-CA-C	5.57	119.41	109.38
1	A	967	GLU	CB-CA-C	5.57	119.41	109.38
1	C	967	GLU	CB-CA-C	5.57	119.41	109.38
1	E	967	GLU	CB-CA-C	5.56	119.39	109.38
1	D	590	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	E	590	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	F	590	HIS	CB-CG-CD2	-5.54	123.99	131.20
1	C	313	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	C	590	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	590	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	G	590	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	D	313	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	G	313	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	B	20	HIS	CA-CB-CG	5.46	119.26	113.80
1	K	20	HIS	CA-CB-CG	5.46	119.25	113.80
1	F	313	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	E	313	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	H	20	HIS	CA-CB-CG	5.44	119.24	113.80
1	E	976	HIS	CA-CB-CG	-5.43	108.37	113.80
1	A	313	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	D	976	HIS	CA-CB-CG	-5.42	108.38	113.80
1	J	20	HIS	CA-CB-CG	5.42	119.22	113.80
1	F	976	HIS	CA-CB-CG	-5.42	108.38	113.80
1	G	976	HIS	CA-CB-CG	-5.42	108.38	113.80
1	A	976	HIS	CA-CB-CG	-5.41	108.39	113.80
1	L	20	HIS	CA-CB-CG	5.41	119.21	113.80
1	I	20	HIS	CA-CB-CG	5.40	119.20	113.80
1	I	314	PHE	CA-CB-CG	-5.39	108.41	113.80
1	C	976	HIS	CA-CB-CG	-5.39	108.41	113.80
1	E	610	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	D	893	GLU	CA-C-N	5.38	131.82	121.54
1	D	893	GLU	C-N-CA	5.38	131.82	121.54
1	E	893	GLU	CA-C-N	5.37	131.79	121.54
1	E	893	GLU	C-N-CA	5.37	131.79	121.54
1	J	314	PHE	CA-CB-CG	-5.37	108.44	113.80
1	K	314	PHE	CA-CB-CG	-5.36	108.44	113.80
1	A	893	GLU	CA-C-N	5.36	131.77	121.54
1	A	893	GLU	C-N-CA	5.36	131.77	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	893	GLU	CA-C-N	5.36	131.77	121.54
1	C	893	GLU	C-N-CA	5.36	131.77	121.54
1	F	610	ASN	OD1-CG-ND2	-5.36	117.25	122.60
1	F	893	GLU	CA-C-N	5.36	131.77	121.54
1	F	893	GLU	C-N-CA	5.36	131.77	121.54
1	G	610	ASN	OD1-CG-ND2	-5.36	117.25	122.60
1	K	748	ARG	CD-NE-CZ	5.35	131.90	124.40
1	L	748	ARG	CD-NE-CZ	5.35	131.90	124.40
1	A	610	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	G	893	GLU	CA-C-N	5.35	131.76	121.54
1	G	893	GLU	C-N-CA	5.35	131.76	121.54
1	H	748	ARG	CD-NE-CZ	5.35	131.89	124.40
1	I	748	ARG	CD-NE-CZ	5.35	131.89	124.40
1	B	314	PHE	CA-CB-CG	-5.34	108.45	113.80
1	L	314	PHE	CA-CB-CG	-5.34	108.46	113.80
1	J	748	ARG	CD-NE-CZ	5.32	131.84	124.40
1	H	314	PHE	CA-CB-CG	-5.31	108.49	113.80
1	I	326	ILE	CB-CA-C	5.31	116.62	110.89
1	C	610	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	B	748	ARG	CD-NE-CZ	5.29	131.81	124.40
1	D	610	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	H	326	ILE	CB-CA-C	5.29	116.60	110.89
1	B	1142	ALA	N-CA-C	5.27	116.73	110.19
1	L	326	ILE	CB-CA-C	5.27	116.58	110.89
1	J	326	ILE	CB-CA-C	5.27	116.58	110.89
1	J	1142	ALA	N-CA-C	5.26	116.72	110.19
1	K	326	ILE	CB-CA-C	5.26	116.57	110.89
1	L	1142	ALA	N-CA-C	5.26	116.71	110.19
1	K	1142	ALA	N-CA-C	5.25	116.70	110.19
1	B	326	ILE	CB-CA-C	5.25	116.56	110.89
1	H	1142	ALA	N-CA-C	5.24	116.69	110.19
1	I	1142	ALA	N-CA-C	5.24	116.69	110.19
1	B	1141	GLY	N-CA-C	5.23	119.84	110.95
1	K	1141	GLY	N-CA-C	5.22	119.82	110.95
1	I	1141	GLY	N-CA-C	5.22	119.82	110.95
1	H	1141	GLY	N-CA-C	5.21	119.80	110.95
1	E	213	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	213	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	J	1141	GLY	N-CA-C	5.20	119.79	110.95
1	I	716	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	C	213	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	L	1141	GLY	N-CA-C	5.18	119.76	110.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	213	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	J	716	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	D	213	HIS	CB-CG-CD2	-5.17	124.47	131.20
1	B	716	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	F	213	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	K	716	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	L	716	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	H	716	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	C	733	LYS	CA-C-N	5.10	127.83	120.38
1	C	733	LYS	C-N-CA	5.10	127.83	120.38
1	E	733	LYS	CA-C-N	5.09	127.82	120.38
1	E	733	LYS	C-N-CA	5.09	127.82	120.38
1	D	733	LYS	CA-C-N	5.07	127.79	120.38
1	D	733	LYS	C-N-CA	5.07	127.79	120.38
1	F	301	HIS	CB-CG-CD2	-5.07	124.60	131.20
1	G	733	LYS	CA-C-N	5.07	127.78	120.38
1	G	733	LYS	C-N-CA	5.07	127.78	120.38
1	E	301	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	D	301	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	733	LYS	CA-C-N	5.05	127.75	120.38
1	A	733	LYS	C-N-CA	5.05	127.75	120.38
1	A	301	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	F	733	LYS	CA-C-N	5.04	127.74	120.38
1	F	733	LYS	C-N-CA	5.04	127.74	120.38
1	G	319	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	G	301	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	C	301	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	I	646	ARG	CA-CB-CG	-5.03	104.05	114.10
1	I	77	HIS	CB-CG-CD2	-5.01	124.68	131.20
1	A	319	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	L	77	HIS	CB-CG-CD2	-5.01	124.68	131.20
1	J	77	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	L	646	ARG	CA-CB-CG	-5.01	104.08	114.10
1	B	77	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	H	646	ARG	CA-CB-CG	-5.01	104.09	114.10
1	K	646	ARG	CA-CB-CG	-5.00	104.09	114.10

There are no chirality outliers.

All (140) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1071	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	244	ARG	Sidechain
1	A	300	TYR	Sidechain
1	A	495	TYR	Sidechain
1	A	582	TYR	Sidechain
1	A	591	ARG	Sidechain
1	A	728	TYR	Sidechain
1	A	802	ARG	Sidechain
1	A	944	TYR	Sidechain
1	B	1071	ARG	Sidechain
1	B	1113	ARG	Sidechain
1	B	127	PHE	Sidechain
1	B	212	PHE	Sidechain
1	B	304	TYR	Sidechain
1	B	313	HIS	Sidechain
1	B	447	ARG	Sidechain
1	B	493	TYR	Sidechain
1	B	495	TYR	Sidechain
1	B	501	HIS	Sidechain
1	B	793	PHE	Sidechain
1	B	802	ARG	Sidechain
1	B	915	TYR	Sidechain
1	B	939	TYR	Sidechain
1	C	1071	ARG	Sidechain
1	C	244	ARG	Sidechain
1	C	300	TYR	Sidechain
1	C	495	TYR	Sidechain
1	C	582	TYR	Sidechain
1	C	591	ARG	Sidechain
1	C	728	TYR	Sidechain
1	C	802	ARG	Sidechain
1	C	944	TYR	Sidechain
1	D	1071	ARG	Sidechain
1	D	201	TYR	Sidechain
1	D	244	ARG	Sidechain
1	D	300	TYR	Sidechain
1	D	495	TYR	Sidechain
1	D	582	TYR	Sidechain
1	D	591	ARG	Sidechain
1	D	728	TYR	Sidechain
1	D	802	ARG	Sidechain
1	D	944	TYR	Sidechain
1	E	1071	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	201	TYR	Sidechain
1	E	244	ARG	Sidechain
1	E	300	TYR	Sidechain
1	E	495	TYR	Sidechain
1	E	582	TYR	Sidechain
1	E	591	ARG	Sidechain
1	E	728	TYR	Sidechain
1	E	802	ARG	Sidechain
1	E	944	TYR	Sidechain
1	F	1071	ARG	Sidechain
1	F	244	ARG	Sidechain
1	F	300	TYR	Sidechain
1	F	495	TYR	Sidechain
1	F	582	TYR	Sidechain
1	F	591	ARG	Sidechain
1	F	728	TYR	Sidechain
1	F	802	ARG	Sidechain
1	F	944	TYR	Sidechain
1	G	1071	ARG	Sidechain
1	G	244	ARG	Sidechain
1	G	300	TYR	Sidechain
1	G	495	TYR	Sidechain
1	G	582	TYR	Sidechain
1	G	591	ARG	Sidechain
1	G	728	TYR	Sidechain
1	G	802	ARG	Sidechain
1	G	944	TYR	Sidechain
1	H	1071	ARG	Sidechain
1	H	1113	ARG	Sidechain
1	H	127	PHE	Sidechain
1	H	212	PHE	Sidechain
1	H	304	TYR	Sidechain
1	H	313	HIS	Sidechain
1	H	447	ARG	Sidechain
1	H	493	TYR	Sidechain
1	H	495	TYR	Sidechain
1	H	501	HIS	Sidechain
1	H	793	PHE	Sidechain
1	H	802	ARG	Sidechain
1	H	915	TYR	Sidechain
1	H	939	TYR	Sidechain
1	I	1071	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	I	1113	ARG	Sidechain
1	I	127	PHE	Sidechain
1	I	212	PHE	Sidechain
1	I	304	TYR	Sidechain
1	I	313	HIS	Sidechain
1	I	447	ARG	Sidechain
1	I	493	TYR	Sidechain
1	I	495	TYR	Sidechain
1	I	501	HIS	Sidechain
1	I	793	PHE	Sidechain
1	I	802	ARG	Sidechain
1	I	915	TYR	Sidechain
1	I	939	TYR	Sidechain
1	J	1071	ARG	Sidechain
1	J	1113	ARG	Sidechain
1	J	127	PHE	Sidechain
1	J	212	PHE	Sidechain
1	J	304	TYR	Sidechain
1	J	313	HIS	Sidechain
1	J	447	ARG	Sidechain
1	J	493	TYR	Sidechain
1	J	495	TYR	Sidechain
1	J	501	HIS	Sidechain
1	J	793	PHE	Sidechain
1	J	802	ARG	Sidechain
1	J	915	TYR	Sidechain
1	J	939	TYR	Sidechain
1	K	1071	ARG	Sidechain
1	K	1113	ARG	Sidechain
1	K	127	PHE	Sidechain
1	K	212	PHE	Sidechain
1	K	304	TYR	Sidechain
1	K	313	HIS	Sidechain
1	K	447	ARG	Sidechain
1	K	493	TYR	Sidechain
1	K	495	TYR	Sidechain
1	K	501	HIS	Sidechain
1	K	793	PHE	Sidechain
1	K	802	ARG	Sidechain
1	K	915	TYR	Sidechain
1	K	939	TYR	Sidechain
1	L	1071	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	L	1113	ARG	Sidechain
1	L	127	PHE	Sidechain
1	L	212	PHE	Sidechain
1	L	304	TYR	Sidechain
1	L	313	HIS	Sidechain
1	L	447	ARG	Sidechain
1	L	493	TYR	Sidechain
1	L	495	TYR	Sidechain
1	L	501	HIS	Sidechain
1	L	793	PHE	Sidechain
1	L	802	ARG	Sidechain
1	L	915	TYR	Sidechain
1	L	939	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9034	8976	8957	190	0
1	B	9034	8976	8973	72	0
1	C	9034	8976	8957	190	0
1	D	9034	8976	8960	201	0
1	E	9034	8976	8959	204	0
1	F	9034	8976	8958	204	0
1	G	9034	8976	8958	196	0
1	H	9034	8976	8973	71	0
1	I	9034	8976	8973	70	0
1	J	9034	8976	8973	73	0
1	K	9034	8976	8973	76	0
1	L	9034	8976	8973	71	0
All	All	108408	107712	107587	1152	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 (1152) 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:A:655:ARG:CD	1:G:1003:GLN:HE22	1.09	1.64
1:A:1003:GLN:HE22	1:C:655:ARG:CD	1.08	1.63
1:E:1003:GLN:HE22	1:F:655:ARG:CD	1.07	1.61
1:C:1003:GLN:CD	1:D:655:ARG:HD3	1.26	1.60
1:C:1003:GLN:HE22	1:D:655:ARG:CD	1.10	1.57
1:F:1003:GLN:CD	1:G:655:ARG:HD3	1.28	1.55
1:F:1003:GLN:HE22	1:G:655:ARG:CD	1.11	1.53
1:D:1003:GLN:HE22	1:E:655:ARG:CD	1.16	1.51
1:E:1003:GLN:CD	1:F:655:ARG:HD3	1.33	1.51
1:A:1003:GLN:CD	1:C:655:ARG:HD3	1.29	1.49
1:D:1003:GLN:CD	1:E:655:ARG:HD3	1.35	1.48
1:A:655:ARG:HD3	1:G:1003:GLN:CD	1.31	1.48
1:D:1003:GLN:NE2	1:E:655:ARG:HD3	1.14	1.40
1:F:1003:GLN:NE2	1:G:655:ARG:HD3	1.09	1.40
1:A:1003:GLN:NE2	1:C:655:ARG:HD3	1.07	1.39
1:C:1003:GLN:NE2	1:D:655:ARG:HD3	1.08	1.36
1:E:967:GLU:CD	1:F:594:LYS:NZ	1.81	1.35
1:A:655:ARG:HD3	1:G:1003:GLN:NE2	1.08	1.35
1:E:1003:GLN:NE2	1:F:655:ARG:HD3	1.07	1.34
1:E:967:GLU:OE2	1:F:594:LYS:NZ	1.56	1.32
1:A:510:THR:C	1:G:957:GLN:HG2	1.08	1.27
1:C:957:GLN:HG2	1:D:510:THR:C	1.08	1.26
1:C:1003:GLN:NE2	1:D:655:ARG:CD	1.76	1.26
1:A:957:GLN:HG2	1:C:510:THR:C	1.04	1.25
1:E:1003:GLN:NE2	1:F:655:ARG:CD	1.75	1.25
1:F:1003:GLN:NE2	1:G:655:ARG:CD	1.77	1.25
1:A:655:ARG:CD	1:G:1003:GLN:NE2	1.77	1.25
1:D:957:GLN:OE1	1:E:512:PRO:HD3	1.36	1.24
1:E:967:GLU:CD	1:F:594:LYS:HZ2	1.42	1.21
1:F:957:GLN:HG2	1:G:510:THR:C	1.06	1.21
1:C:1003:GLN:HE22	1:D:655:ARG:NE	1.37	1.20
1:F:1003:GLN:HE22	1:G:655:ARG:NE	1.40	1.19
1:A:512:PRO:HD3	1:G:957:GLN:OE1	1.43	1.19
1:A:957:GLN:OE1	1:C:512:PRO:HD3	1.42	1.19
1:E:957:GLN:OE1	1:F:512:PRO:HD3	1.41	1.19
1:D:960:SER:H	1:E:514:LYS:NZ	1.39	1.18
1:E:1095:TRP:CH2	1:F:683:GLN:O	1.96	1.18
1:C:1003:GLN:OE1	1:D:655:ARG:HD3	1.43	1.18
1:A:1003:GLN:HE22	1:C:655:ARG:NE	1.42	1.18
1:A:1003:GLN:NE2	1:C:655:ARG:CD	1.75	1.17
1:D:1003:GLN:NE2	1:E:655:ARG:CD	1.83	1.17
1:F:957:GLN:OE1	1:G:512:PRO:HD3	1.43	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:NZ	1:G:960:SER:H	1.42	1.16
1:A:655:ARG:NE	1:G:1003:GLN:HE22	1.42	1.16
1:A:1095:TRP:CH2	1:C:683:GLN:O	1.98	1.16
1:A:960:SER:H	1:C:514:LYS:NZ	1.45	1.15
1:D:957:GLN:CB	1:E:512:PRO:CD	2.16	1.15
1:E:957:GLN:HG2	1:F:510:THR:C	1.00	1.14
1:F:960:SER:H	1:G:514:LYS:NZ	1.45	1.14
1:F:1003:GLN:OE1	1:G:655:ARG:HD3	1.44	1.14
1:D:998:ASN:OD1	1:E:683:GLN:NE2	1.58	1.14
1:E:960:SER:H	1:F:514:LYS:NZ	1.45	1.14
1:F:957:GLN:CB	1:G:510:THR:O	1.91	1.14
1:F:1095:TRP:CH2	1:G:683:GLN:O	2.01	1.14
1:C:957:GLN:OE1	1:D:512:PRO:HD3	1.46	1.14
1:C:957:GLN:CB	1:D:510:THR:O	1.89	1.13
1:D:1003:GLN:OE1	1:E:655:ARG:HD3	1.46	1.13
1:C:960:SER:H	1:D:514:LYS:NZ	1.45	1.13
1:C:1095:TRP:CH2	1:D:683:GLN:O	2.02	1.13
1:A:512:PRO:CD	1:G:957:GLN:CB	2.23	1.12
1:D:960:SER:N	1:E:514:LYS:NZ	1.96	1.12
1:D:1003:GLN:HE22	1:E:655:ARG:NE	1.45	1.12
1:A:512:PRO:HD2	1:G:957:GLN:HB2	1.22	1.12
1:D:957:GLN:HB2	1:E:512:PRO:HD2	1.14	1.12
1:A:510:THR:O	1:G:957:GLN:CG	0.82	1.11
1:A:683:GLN:O	1:G:1095:TRP:CH2	2.03	1.11
1:E:1003:GLN:HE22	1:F:655:ARG:NE	1.47	1.11
1:F:957:GLN:CB	1:G:512:PRO:CD	2.26	1.11
1:A:655:ARG:HD3	1:G:1003:GLN:OE1	1.48	1.11
1:A:1003:GLN:OE1	1:C:655:ARG:HD3	1.48	1.10
1:D:958:THR:HG22	1:E:513:ALA:CB	1.80	1.10
1:E:957:GLN:HB2	1:F:512:PRO:HD2	1.31	1.10
1:E:967:GLU:OE1	1:F:594:LYS:NZ	1.76	1.10
1:F:957:GLN:HB2	1:G:512:PRO:HD2	1.25	1.09
1:C:957:GLN:CG	1:D:510:THR:O	0.79	1.09
1:E:957:GLN:CB	1:F:510:THR:O	1.90	1.09
1:A:514:LYS:NZ	1:G:960:SER:N	2.01	1.09
1:C:957:GLN:HB2	1:D:512:PRO:HD2	1.26	1.09
1:A:957:GLN:CB	1:C:510:THR:O	1.91	1.08
1:A:998:ASN:OD1	1:C:683:GLN:NE2	1.60	1.08
1:E:1003:GLN:OE1	1:F:655:ARG:HD3	1.53	1.08
1:A:957:GLN:HB2	1:C:512:PRO:HD2	1.28	1.08
1:C:958:THR:CG2	1:D:511:ASP:OD1	1.97	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:957:GLN:CG	1:G:510:THR:O	0.78	1.08
1:A:510:THR:O	1:G:957:GLN:CB	1.94	1.07
1:E:957:GLN:CB	1:F:512:PRO:CD	2.32	1.07
1:C:957:GLN:CB	1:D:512:PRO:CD	2.26	1.07
1:A:957:GLN:CB	1:C:512:PRO:CD	2.29	1.06
1:A:957:GLN:CG	1:C:510:THR:O	0.77	1.06
1:C:1003:GLN:OE1	1:D:655:ARG:CD	2.02	1.06
1:F:998:ASN:OD1	1:G:683:GLN:NE2	1.56	1.06
1:F:1003:GLN:OE1	1:G:655:ARG:CD	2.04	1.06
1:D:957:GLN:CD	1:E:512:PRO:HD3	1.81	1.05
1:D:1095:TRP:CH2	1:E:683:GLN:O	2.08	1.05
1:C:960:SER:N	1:D:514:LYS:NZ	2.04	1.05
1:F:960:SER:N	1:G:514:LYS:NZ	2.04	1.05
1:C:957:GLN:HG3	1:D:510:THR:O	1.23	1.04
1:A:958:THR:CG2	1:C:511:ASP:OD1	1.99	1.04
1:A:957:GLN:HG3	1:C:510:THR:O	1.23	1.04
1:A:1003:GLN:OE1	1:C:655:ARG:CD	2.06	1.04
1:E:998:ASN:OD1	1:F:683:GLN:NE2	1.65	1.03
1:A:510:THR:O	1:G:957:GLN:HG3	1.24	1.03
1:A:960:SER:N	1:C:514:LYS:NZ	2.05	1.03
1:E:960:SER:N	1:F:514:LYS:NZ	2.06	1.03
1:F:958:THR:HG22	1:G:513:ALA:CB	1.89	1.03
1:E:957:GLN:CG	1:F:510:THR:O	0.73	1.03
1:A:512:PRO:HD2	1:G:957:GLN:CB	1.87	1.02
1:A:513:ALA:CB	1:G:958:THR:HG22	1.88	1.02
1:A:655:ARG:CD	1:G:1003:GLN:OE1	2.08	1.02
1:E:958:THR:HG23	1:F:511:ASP:OD1	1.55	1.02
1:D:958:THR:HG22	1:E:513:ALA:HB2	1.42	1.02
1:C:958:THR:HG23	1:D:511:ASP:OD1	1.57	1.01
1:D:958:THR:CG2	1:E:511:ASP:OD1	2.05	1.01
1:E:958:THR:CG2	1:F:511:ASP:OD1	1.98	1.01
1:E:957:GLN:HG3	1:F:510:THR:O	1.21	1.01
1:A:509:GLN:HA	1:G:1084:ARG:CZ	1.90	1.01
1:A:511:ASP:OD1	1:G:958:THR:CG2	2.01	1.01
1:A:958:THR:HG23	1:C:511:ASP:OD1	1.57	1.01
1:F:958:THR:CG2	1:G:511:ASP:OD1	1.98	1.01
1:C:1084:ARG:CZ	1:D:509:GLN:HA	1.89	1.01
1:E:957:GLN:CD	1:F:510:THR:O	2.03	1.00
1:D:957:GLN:CB	1:E:512:PRO:HD2	1.81	1.00
1:F:957:GLN:CB	1:G:512:PRO:HD2	1.90	1.00
1:F:957:GLN:HG3	1:G:510:THR:O	1.22	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:958:THR:HG23	1:G:511:ASP:OD1	1.56	1.00
1:A:958:THR:HG22	1:C:513:ALA:CB	1.90	1.00
1:D:958:THR:HG23	1:E:511:ASP:OD1	1.60	1.00
1:E:958:THR:HG22	1:F:513:ALA:CB	1.91	1.00
1:C:958:THR:HG22	1:D:513:ALA:CB	1.92	1.00
1:D:1003:GLN:OE1	1:E:655:ARG:CD	2.08	1.00
1:D:1084:ARG:CZ	1:E:509:GLN:HA	1.89	0.99
1:A:511:ASP:OD1	1:G:958:THR:HG23	1.59	0.98
1:A:683:GLN:NE2	1:G:998:ASN:OD1	1.58	0.98
1:A:957:GLN:CB	1:C:512:PRO:HD2	1.92	0.98
1:A:957:GLN:CD	1:C:510:THR:O	2.07	0.98
1:E:1003:GLN:OE1	1:F:655:ARG:CD	2.10	0.98
1:D:957:GLN:HB2	1:E:512:PRO:CD	1.86	0.97
1:A:1084:ARG:CZ	1:C:509:GLN:HA	1.95	0.97
1:A:1003:GLN:CD	1:C:655:ARG:CD	2.21	0.97
1:A:512:PRO:HD3	1:G:957:GLN:CD	1.89	0.96
1:E:957:GLN:CB	1:F:512:PRO:HD2	1.95	0.96
1:F:1084:ARG:CZ	1:G:509:GLN:HA	1.91	0.96
1:A:512:PRO:CD	1:G:957:GLN:HB2	1.93	0.95
1:F:957:GLN:HB2	1:G:512:PRO:CD	1.95	0.95
1:A:957:GLN:CD	1:C:512:PRO:HD3	1.92	0.95
1:C:957:GLN:CB	1:D:512:PRO:HD2	1.90	0.94
1:D:960:SER:H	1:E:514:LYS:CE	1.81	0.94
1:F:957:GLN:CD	1:G:510:THR:O	2.10	0.94
1:D:960:SER:H	1:E:514:LYS:HZ3	1.06	0.93
1:F:957:GLN:CD	1:G:512:PRO:HD3	1.92	0.93
1:C:957:GLN:HB2	1:D:512:PRO:CD	1.95	0.93
1:C:957:GLN:CD	1:D:512:PRO:HD3	1.94	0.93
1:A:1095:TRP:HH2	1:C:683:GLN:O	1.47	0.93
1:A:683:GLN:O	1:G:1095:TRP:HH2	1.50	0.92
1:C:957:GLN:CD	1:D:510:THR:O	2.12	0.92
1:D:960:SER:N	1:E:514:LYS:HZ3	1.60	0.91
1:E:957:GLN:CD	1:F:512:PRO:HD3	1.94	0.91
1:E:967:GLU:CD	1:F:594:LYS:HZ3	1.59	0.91
1:C:1095:TRP:HH2	1:D:683:GLN:O	1.50	0.91
1:D:958:THR:HG22	1:E:513:ALA:HB3	1.53	0.91
1:E:1084:ARG:CZ	1:F:509:GLN:HA	1.98	0.90
1:E:1095:TRP:HH2	1:F:683:GLN:O	1.46	0.89
1:A:510:THR:O	1:G:957:GLN:CD	2.13	0.89
1:E:1037:TRP:CH2	1:F:655:ARG:HD2	2.07	0.89
1:F:958:THR:HG22	1:G:513:ALA:HB2	1.54	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ALA:HB2	1:G:958:THR:HG22	1.51	0.88
1:C:958:THR:HG22	1:D:513:ALA:HB2	1.55	0.88
1:E:958:THR:HG22	1:F:513:ALA:HB2	1.57	0.87
1:F:1003:GLN:CD	1:G:655:ARG:CD	2.21	0.87
1:D:960:SER:OG	1:E:514:LYS:HE2	1.75	0.87
1:G:29:LEU:HD21	1:G:346:ILE:HA	1.57	0.87
1:D:1095:TRP:HH2	1:E:683:GLN:O	1.56	0.87
1:A:514:LYS:HE2	1:G:960:SER:OG	1.75	0.86
1:D:29:LEU:HD21	1:D:346:ILE:HA	1.57	0.86
1:A:957:GLN:HB2	1:C:512:PRO:CD	1.98	0.86
1:E:958:THR:HG22	1:F:513:ALA:HB3	1.57	0.86
1:C:29:LEU:HD21	1:C:346:ILE:HA	1.57	0.86
1:A:960:SER:OG	1:C:514:LYS:HE2	1.76	0.86
1:A:29:LEU:HD21	1:A:346:ILE:HA	1.57	0.86
1:A:958:THR:HG22	1:C:513:ALA:HB2	1.55	0.86
1:A:958:THR:HG22	1:C:513:ALA:HB3	1.58	0.85
1:E:29:LEU:HD21	1:E:346:ILE:HA	1.57	0.85
1:F:29:LEU:HD21	1:F:346:ILE:HA	1.57	0.85
1:A:513:ALA:HB3	1:G:958:THR:HG22	1.59	0.85
1:A:1037:TRP:CH2	1:C:655:ARG:HD2	2.12	0.85
1:C:1003:GLN:CD	1:D:655:ARG:CD	2.19	0.85
1:A:1067:TYR:HH	1:I:582:TYR:HE1	1.25	0.85
1:C:960:SER:OG	1:D:514:LYS:HE2	1.77	0.85
1:A:514:LYS:CE	1:G:960:SER:H	1.89	0.84
1:E:960:SER:OG	1:F:514:LYS:HE2	1.76	0.84
1:F:1095:TRP:HH2	1:G:683:GLN:O	1.50	0.84
1:E:957:GLN:HB2	1:F:512:PRO:CD	2.01	0.84
1:F:960:SER:OG	1:G:514:LYS:HE2	1.77	0.84
1:G:1067:TYR:HH	1:H:582:TYR:HE1	1.26	0.84
1:D:957:GLN:OE1	1:E:512:PRO:CD	2.26	0.83
1:F:958:THR:HG22	1:G:513:ALA:HB3	1.58	0.83
1:F:960:SER:H	1:G:514:LYS:CE	1.91	0.83
1:A:960:SER:H	1:C:514:LYS:CE	1.92	0.83
1:C:960:SER:H	1:D:514:LYS:CE	1.92	0.82
1:C:957:GLN:HB3	1:D:512:PRO:CD	1.83	0.82
1:E:960:SER:H	1:F:514:LYS:CE	1.92	0.82
1:E:1003:GLN:CD	1:F:655:ARG:CD	2.24	0.81
1:F:1037:TRP:CH2	1:G:655:ARG:HD2	2.16	0.81
1:E:957:GLN:HG2	1:F:510:THR:CA	2.10	0.81
1:B:582:TYR:HE1	1:F:1067:TYR:HH	1.26	0.80
1:D:957:GLN:CB	1:E:512:PRO:HD3	2.10	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1003:GLN:HE22	1:F:655:ARG:CG	1.95	0.80
1:C:958:THR:HG22	1:D:513:ALA:HB3	1.61	0.80
1:D:960:SER:OG	1:E:514:LYS:HG2	1.81	0.79
1:D:1037:TRP:CH2	1:E:655:ARG:HD2	2.17	0.79
1:F:957:GLN:HG2	1:G:510:THR:CA	2.13	0.78
1:A:655:ARG:HD2	1:G:1037:TRP:CH2	2.18	0.78
1:C:1037:TRP:CH2	1:D:655:ARG:HD2	2.19	0.77
1:E:891:ARG:HD3	1:L:479:GLN:HG2	1.65	0.77
1:A:891:ARG:HD3	1:I:479:GLN:HG2	1.66	0.77
1:A:512:PRO:HD3	1:G:957:GLN:CB	2.14	0.77
1:A:957:GLN:HG2	1:C:510:THR:CA	2.13	0.76
1:A:957:GLN:HB3	1:C:512:PRO:CD	1.86	0.76
1:C:957:GLN:CB	1:D:512:PRO:HD3	2.15	0.76
1:C:957:GLN:HG2	1:D:510:THR:CA	2.14	0.76
1:E:1003:GLN:NE2	1:F:655:ARG:CG	2.49	0.75
1:E:1095:TRP:CZ2	1:F:683:GLN:O	2.39	0.75
1:A:514:LYS:HG2	1:G:960:SER:OG	1.88	0.74
1:C:1003:GLN:NE2	1:D:655:ARG:NE	2.16	0.74
1:D:1084:ARG:HH11	1:E:504:TYR:HE1	1.36	0.74
1:D:1067:TYR:HH	1:K:582:TYR:HE1	1.30	0.73
1:B:479:GLN:HG2	1:F:891:ARG:HD3	1.69	0.73
1:E:1067:TYR:OH	1:L:582:TYR:CE1	2.42	0.73
1:G:891:ARG:HD3	1:H:479:GLN:HG2	1.70	0.73
1:A:1003:GLN:NE2	1:C:655:ARG:CG	2.52	0.73
1:C:891:ARG:HD3	1:J:479:GLN:HG2	1.70	0.73
1:F:957:GLN:CB	1:G:512:PRO:HD3	2.17	0.72
1:A:655:ARG:CD	1:G:1003:GLN:CD	2.24	0.72
1:A:957:GLN:OE1	1:C:512:PRO:CD	2.33	0.72
1:D:1003:GLN:NE2	1:E:655:ARG:NE	2.24	0.72
1:A:512:PRO:CD	1:G:957:GLN:OE1	2.33	0.72
1:C:960:SER:OG	1:D:514:LYS:HG2	1.90	0.72
1:D:960:SER:HB3	1:E:514:LYS:HD3	1.72	0.72
1:F:960:SER:OG	1:G:514:LYS:HG2	1.90	0.72
1:D:891:ARG:HD3	1:K:479:GLN:HG2	1.71	0.71
1:D:957:GLN:HB3	1:E:512:PRO:CD	1.76	0.71
1:C:1003:GLN:NE2	1:D:655:ARG:CZ	2.53	0.71
1:E:1037:TRP:CZ3	1:F:655:ARG:CD	2.73	0.71
1:A:957:GLN:CB	1:C:512:PRO:HD3	2.20	0.71
1:A:1003:GLN:HE22	1:C:655:ARG:CG	2.00	0.71
1:A:514:LYS:CE	1:G:960:SER:OG	2.39	0.70
1:F:1084:ARG:HH11	1:G:504:TYR:HE1	1.37	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1084:ARG:HH11	1:D:504:TYR:HE1	1.38	0.70
1:D:959:GLN:C	1:E:514:LYS:HZ1	1.79	0.70
1:D:960:SER:OG	1:E:514:LYS:CE	2.39	0.70
1:F:1003:GLN:NE2	1:G:655:ARG:NE	2.18	0.70
1:D:960:SER:OG	1:E:514:LYS:CD	2.39	0.70
1:A:510:THR:CA	1:G:957:GLN:HG2	2.17	0.70
1:D:1067:TYR:OH	1:K:582:TYR:CE1	2.44	0.70
1:A:514:LYS:CD	1:G:960:SER:OG	2.39	0.70
1:E:1067:TYR:HH	1:L:582:TYR:HE1	1.31	0.69
1:A:960:SER:OG	1:C:514:LYS:HG2	1.92	0.69
1:A:1095:TRP:CZ2	1:C:683:GLN:O	2.44	0.69
1:C:960:SER:OG	1:D:514:LYS:CD	2.40	0.69
1:A:512:PRO:CD	1:G:957:GLN:HB3	1.80	0.69
1:E:957:GLN:OE1	1:F:512:PRO:CD	2.32	0.69
1:F:1003:GLN:NE2	1:G:655:ARG:CG	2.56	0.69
1:E:958:THR:HA	1:F:514:LYS:HD2	1.75	0.69
1:A:504:TYR:HE1	1:G:1084:ARG:HH11	1.39	0.68
1:C:311:LEU:HD21	1:C:343:ALA:HB1	1.75	0.68
1:C:960:SER:OG	1:D:514:LYS:CE	2.41	0.68
1:F:957:GLN:HB3	1:G:512:PRO:CD	1.84	0.68
1:A:1067:TYR:OH	1:I:582:TYR:CE1	2.44	0.68
1:F:1003:GLN:NE2	1:G:655:ARG:CZ	2.56	0.68
1:E:957:GLN:CB	1:F:512:PRO:HD3	2.24	0.68
1:F:960:SER:OG	1:G:514:LYS:CD	2.42	0.68
1:A:1084:ARG:HH11	1:C:504:TYR:HE1	1.40	0.68
1:E:1037:TRP:CZ3	1:F:655:ARG:HD2	2.29	0.68
1:A:514:LYS:HD3	1:G:960:SER:HB3	1.76	0.68
1:F:960:SER:OG	1:G:514:LYS:CE	2.42	0.68
1:A:960:SER:OG	1:C:514:LYS:CE	2.42	0.68
1:A:311:LEU:HD21	1:A:343:ALA:HB1	1.76	0.68
1:E:1084:ARG:HH11	1:F:504:TYR:HE1	1.40	0.68
1:F:957:GLN:CG	1:G:510:THR:C	1.86	0.68
1:C:1067:TYR:HH	1:J:582:TYR:HE1	1.32	0.67
1:E:960:SER:OG	1:F:514:LYS:HG2	1.95	0.67
1:E:960:SER:OG	1:F:514:LYS:CE	2.43	0.67
1:A:655:ARG:CZ	1:G:1003:GLN:NE2	2.58	0.67
1:E:957:GLN:CG	1:F:510:THR:C	1.82	0.67
1:A:655:ARG:CG	1:G:1003:GLN:NE2	2.57	0.67
1:B:582:TYR:CE1	1:F:1067:TYR:OH	2.42	0.67
1:D:960:SER:CB	1:E:514:LYS:HD3	2.24	0.67
1:F:311:LEU:HD21	1:F:343:ALA:HB1	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:LEU:HD21	1:D:343:ALA:HB1	1.75	0.67
1:D:958:THR:HA	1:E:514:LYS:HD2	1.76	0.67
1:F:957:GLN:OE1	1:G:512:PRO:CD	2.34	0.67
1:G:311:LEU:HD21	1:G:343:ALA:HB1	1.75	0.66
1:F:958:THR:HA	1:G:514:LYS:HD2	1.77	0.66
1:F:1095:TRP:CZ2	1:G:683:GLN:O	2.48	0.66
1:C:957:GLN:CA	1:D:510:THR:O	2.40	0.66
1:E:1003:GLN:NE2	1:F:655:ARG:NE	2.23	0.66
1:E:311:LEU:HD21	1:E:343:ALA:HB1	1.76	0.66
1:D:1003:GLN:CD	1:E:655:ARG:CD	2.28	0.66
1:C:960:SER:HB3	1:D:514:LYS:HD3	1.78	0.66
1:G:1067:TYR:OH	1:H:582:TYR:CE1	2.45	0.66
1:A:958:THR:HA	1:C:514:LYS:HD2	1.77	0.66
1:D:960:SER:N	1:E:514:LYS:HZ1	1.80	0.66
1:A:960:SER:OG	1:C:514:LYS:CD	2.44	0.65
1:D:1003:GLN:NE2	1:E:655:ARG:CZ	2.59	0.65
1:E:957:GLN:HB3	1:F:512:PRO:CD	1.89	0.65
1:A:509:GLN:CA	1:G:1084:ARG:CZ	2.70	0.65
1:F:1003:GLN:HE22	1:G:655:ARG:CG	2.04	0.65
1:A:1037:TRP:CZ3	1:C:655:ARG:CD	2.80	0.65
1:C:1095:TRP:CZ2	1:D:683:GLN:O	2.50	0.65
1:F:960:SER:HB3	1:G:514:LYS:HD3	1.79	0.65
1:A:960:SER:HB3	1:C:514:LYS:HD3	1.79	0.65
1:C:1003:GLN:NE2	1:D:655:ARG:CG	2.57	0.65
1:A:514:LYS:HD3	1:G:960:SER:CB	2.27	0.64
1:A:514:LYS:HD2	1:G:958:THR:HA	1.79	0.64
1:C:957:GLN:OE1	1:D:512:PRO:CD	2.36	0.64
1:D:960:SER:OG	1:E:514:LYS:CG	2.45	0.64
1:A:683:GLN:O	1:G:1095:TRP:CZ2	2.51	0.63
1:E:260:LEU:HB3	1:E:289:VAL:HG21	1.80	0.63
1:F:260:LEU:HB3	1:F:289:VAL:HG21	1.80	0.63
1:E:29:LEU:HD22	1:E:130:ILE:HD11	1.80	0.63
1:D:29:LEU:HD22	1:D:130:ILE:HD11	1.80	0.63
1:F:29:LEU:HD22	1:F:130:ILE:HD11	1.80	0.63
1:C:260:LEU:HB3	1:C:289:VAL:HG21	1.80	0.63
1:C:958:THR:HA	1:D:514:LYS:HD2	1.80	0.63
1:D:958:THR:CG2	1:E:513:ALA:HB2	2.25	0.63
1:E:960:SER:OG	1:F:514:LYS:CD	2.47	0.63
1:A:1003:GLN:NE2	1:C:655:ARG:CZ	2.60	0.63
1:C:960:SER:CB	1:D:514:LYS:HD3	2.28	0.62
1:A:514:LYS:NZ	1:G:959:GLN:C	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:GLN:NE2	1:C:655:ARG:NE	2.20	0.62
1:G:29:LEU:HD22	1:G:130:ILE:HD11	1.80	0.62
1:A:260:LEU:HB3	1:A:289:VAL:HG21	1.80	0.62
1:A:655:ARG:NE	1:G:1003:GLN:NE2	2.21	0.62
1:D:260:LEU:HB3	1:D:289:VAL:HG21	1.80	0.62
1:E:960:SER:HB3	1:F:514:LYS:HD3	1.81	0.62
1:A:510:THR:O	1:G:957:GLN:CA	2.43	0.62
1:D:1084:ARG:CZ	1:E:509:GLN:CA	2.67	0.62
1:A:957:GLN:CA	1:C:510:THR:O	2.45	0.62
1:C:29:LEU:HD22	1:C:130:ILE:HD11	1.80	0.62
1:A:29:LEU:HD22	1:A:130:ILE:HD11	1.80	0.61
1:E:1037:TRP:CH2	1:F:655:ARG:CD	2.83	0.61
1:G:260:LEU:HB3	1:G:289:VAL:HG21	1.80	0.61
1:C:1067:TYR:OH	1:J:582:TYR:CE1	2.47	0.61
1:E:1003:GLN:OE1	1:F:655:ARG:CG	2.49	0.61
1:E:958:THR:HG22	1:F:511:ASP:OD1	1.98	0.61
1:H:533:TRP:CZ2	1:H:583:ALA:HB2	2.36	0.61
1:B:533:TRP:CZ2	1:B:583:ALA:HB2	2.36	0.61
1:F:960:SER:CB	1:G:514:LYS:HD3	2.30	0.60
1:C:958:THR:HG22	1:D:511:ASP:OD1	1.97	0.60
1:E:967:GLU:OE2	1:F:594:LYS:CE	2.46	0.60
1:F:1037:TRP:CZ3	1:G:655:ARG:CD	2.84	0.60
1:A:1003:GLN:OE1	1:C:655:ARG:CG	2.49	0.60
1:F:957:GLN:CA	1:G:510:THR:O	2.42	0.60
1:I:533:TRP:CZ2	1:I:583:ALA:HB2	2.36	0.60
1:L:533:TRP:CZ2	1:L:583:ALA:HB2	2.36	0.60
1:A:960:SER:CB	1:C:514:LYS:HD3	2.32	0.60
1:K:533:TRP:CZ2	1:K:583:ALA:HB2	2.36	0.60
1:A:1037:TRP:CZ3	1:C:655:ARG:HD2	2.36	0.60
1:D:1003:GLN:NE2	1:E:655:ARG:CG	2.62	0.59
1:J:533:TRP:CZ2	1:J:583:ALA:HB2	2.36	0.59
1:D:1037:TRP:CZ3	1:E:655:ARG:CD	2.83	0.59
1:K:812:LYS:O	1:K:814:THR:HG23	2.03	0.59
1:L:812:LYS:O	1:L:814:THR:HG23	2.03	0.59
1:A:582:TYR:C	1:A:582:TYR:CD2	2.81	0.59
1:C:582:TYR:C	1:C:582:TYR:CD2	2.81	0.59
1:H:178:LYS:HE3	1:H:178:LYS:H	1.68	0.59
1:B:178:LYS:HE3	1:B:178:LYS:H	1.68	0.59
1:C:1003:GLN:NE2	1:D:655:ARG:NH1	2.51	0.59
1:F:1003:GLN:OE1	1:G:655:ARG:CG	2.50	0.59
1:J:178:LYS:HE3	1:J:178:LYS:H	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:812:LYS:O	1:B:814:THR:HG23	2.03	0.59
1:E:1003:GLN:NE2	1:F:655:ARG:CZ	2.66	0.59
1:K:178:LYS:HE3	1:K:178:LYS:H	1.68	0.59
1:A:514:LYS:CG	1:G:960:SER:OG	2.50	0.59
1:H:812:LYS:O	1:H:814:THR:HG23	2.03	0.59
1:J:812:LYS:O	1:J:814:THR:HG23	2.03	0.59
1:G:582:TYR:C	1:G:582:TYR:CD2	2.81	0.59
1:F:958:THR:HG22	1:G:511:ASP:OD1	1.99	0.58
1:I:812:LYS:O	1:I:814:THR:HG23	2.03	0.58
1:E:582:TYR:CD2	1:E:582:TYR:C	2.81	0.58
1:D:582:TYR:C	1:D:582:TYR:CD2	2.81	0.58
1:F:582:TYR:C	1:F:582:TYR:CD2	2.81	0.58
1:A:655:ARG:CG	1:G:1003:GLN:HE22	2.06	0.58
1:E:891:ARG:CD	1:L:479:GLN:HG2	2.33	0.58
1:C:1003:GLN:OE1	1:D:655:ARG:CG	2.51	0.58
1:L:885:LEU:HD13	1:L:1113:ARG:HA	1.86	0.58
1:J:885:LEU:HD13	1:J:1113:ARG:HA	1.86	0.58
1:K:885:LEU:HD13	1:K:1113:ARG:HA	1.86	0.58
1:I:885:LEU:HD13	1:I:1113:ARG:HA	1.86	0.57
1:A:510:THR:C	1:G:957:GLN:CG	1.90	0.57
1:B:711:SER:HA	1:B:774:LEU:HD22	1.87	0.57
1:C:1037:TRP:CZ3	1:D:655:ARG:CD	2.87	0.57
1:D:1103:HIS:CG	1:D:1146:PRO:HA	2.40	0.57
1:E:1067:TYR:OH	1:L:582:TYR:HE1	1.84	0.57
1:L:178:LYS:HE3	1:L:178:LYS:H	1.68	0.57
1:F:960:SER:OG	1:G:514:LYS:CG	2.52	0.57
1:C:960:SER:OG	1:D:514:LYS:CG	2.51	0.57
1:A:655:ARG:CD	1:G:1037:TRP:CZ3	2.85	0.57
1:C:1103:HIS:CG	1:C:1146:PRO:HA	2.40	0.57
1:D:1095:TRP:CZ2	1:E:683:GLN:O	2.56	0.57
1:E:960:SER:CB	1:F:514:LYS:HD3	2.34	0.57
1:F:1084:ARG:NH1	1:G:504:TYR:HE1	2.03	0.57
1:A:891:ARG:CD	1:I:479:GLN:HG2	2.34	0.57
1:E:1103:HIS:CG	1:E:1146:PRO:HA	2.40	0.57
1:I:711:SER:HA	1:I:774:LEU:HD22	1.87	0.57
1:B:885:LEU:HD13	1:B:1113:ARG:HA	1.86	0.57
1:H:885:LEU:HD13	1:H:1113:ARG:HA	1.86	0.57
1:H:711:SER:HA	1:H:774:LEU:HD22	1.87	0.57
1:I:178:LYS:HE3	1:I:178:LYS:H	1.68	0.57
1:A:958:THR:HG22	1:C:511:ASP:OD1	1.99	0.56
1:A:1103:HIS:CG	1:A:1146:PRO:HA	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:711:SER:HA	1:L:774:LEU:HD22	1.87	0.56
1:E:1084:ARG:NH1	1:F:504:TYR:HE1	2.04	0.56
1:F:1103:HIS:CG	1:F:1146:PRO:HA	2.40	0.56
1:A:655:ARG:NH1	1:G:1003:GLN:NE2	2.53	0.56
1:G:1103:HIS:CG	1:G:1146:PRO:HA	2.40	0.56
1:F:1037:TRP:CZ3	1:G:655:ARG:HD2	2.41	0.56
1:J:711:SER:HA	1:J:774:LEU:HD22	1.87	0.56
1:E:959:GLN:C	1:F:514:LYS:NZ	2.42	0.56
1:A:655:ARG:HD2	1:G:1037:TRP:CZ3	2.41	0.56
1:F:1003:GLN:NE2	1:G:655:ARG:NH1	2.54	0.56
1:K:711:SER:HA	1:K:774:LEU:HD22	1.87	0.56
1:C:1021:LEU:HD23	1:C:1024:LYS:HE2	1.88	0.56
1:D:1037:TRP:CZ3	1:E:655:ARG:HD2	2.41	0.56
1:E:957:GLN:CA	1:F:510:THR:O	2.47	0.56
1:J:674:VAL:HG11	1:J:746:GLN:HG3	1.88	0.55
1:D:956:VAL:O	1:E:511:ASP:HB2	2.05	0.55
1:A:655:ARG:CG	1:G:1003:GLN:OE1	2.55	0.55
1:H:674:VAL:HG11	1:H:746:GLN:HG3	1.88	0.55
1:C:1084:ARG:NH1	1:D:504:TYR:HE1	2.04	0.55
1:D:1003:GLN:NE2	1:E:655:ARG:NH1	2.54	0.55
1:G:1021:LEU:HD23	1:G:1024:LYS:HE2	1.88	0.55
1:B:674:VAL:HG11	1:B:746:GLN:HG3	1.88	0.55
1:A:511:ASP:OD1	1:G:958:THR:HG22	2.02	0.55
1:A:1037:TRP:CH2	1:C:655:ARG:CD	2.87	0.55
1:A:1084:ARG:NH1	1:C:504:TYR:HE1	2.04	0.55
1:C:1003:GLN:HE22	1:D:655:ARG:CG	2.06	0.55
1:D:957:GLN:CG	1:E:512:PRO:HD3	2.34	0.55
1:D:1021:LEU:HD23	1:D:1024:LYS:HE2	1.88	0.55
1:E:1003:GLN:CD	1:F:655:ARG:CG	2.79	0.55
1:F:1021:LEU:HD23	1:F:1024:LYS:HE2	1.88	0.55
1:A:1021:LEU:HD23	1:A:1024:LYS:HE2	1.88	0.54
1:F:1037:TRP:CH2	1:G:655:ARG:CD	2.89	0.54
1:K:674:VAL:HG11	1:K:746:GLN:HG3	1.88	0.54
1:L:674:VAL:HG11	1:L:746:GLN:HG3	1.88	0.54
1:A:504:TYR:HE1	1:G:1084:ARG:NH1	2.05	0.54
1:I:674:VAL:HG11	1:I:746:GLN:HG3	1.88	0.54
1:D:958:THR:CG2	1:E:513:ALA:CB	2.71	0.54
1:A:960:SER:OG	1:C:514:LYS:CG	2.55	0.54
1:C:891:ARG:CD	1:J:479:GLN:HG2	2.38	0.54
1:A:1003:GLN:CD	1:C:655:ARG:CG	2.80	0.53
1:D:735:LYS:H	1:D:735:LYS:HD2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:891:ARG:CD	1:K:479:GLN:HG2	2.38	0.53
1:D:960:SER:N	1:E:514:LYS:CE	2.55	0.53
1:D:1037:TRP:CH2	1:E:655:ARG:CD	2.89	0.53
1:D:1067:TYR:OH	1:K:582:TYR:HE1	1.87	0.53
1:B:479:GLN:HG2	1:F:891:ARG:CD	2.38	0.53
1:E:1021:LEU:HD23	1:E:1024:LYS:HE2	1.88	0.53
1:B:674:VAL:HG13	1:B:747:LEU:HD23	1.91	0.53
1:C:615:GLU:CD	1:C:615:GLU:H	2.17	0.53
1:D:1056:GLU:HG2	1:E:510:THR:HA	1.90	0.53
1:D:1084:ARG:NH1	1:E:504:TYR:HE1	2.04	0.53
1:G:735:LYS:H	1:G:735:LYS:HD2	1.74	0.53
1:A:735:LYS:H	1:A:735:LYS:HD2	1.74	0.53
1:E:615:GLU:H	1:E:615:GLU:CD	2.17	0.53
1:L:674:VAL:HG13	1:L:747:LEU:HD23	1.91	0.53
1:L:69:CYS:CB	1:L:72:CYS:HG	2.22	0.53
1:H:876:VAL:C	1:H:878:PRO:HD3	2.34	0.53
1:F:735:LYS:H	1:F:735:LYS:HD2	1.74	0.52
1:C:1003:GLN:CD	1:D:655:ARG:CG	2.83	0.52
1:D:1003:GLN:OE1	1:E:655:ARG:CG	2.55	0.52
1:B:876:VAL:C	1:B:878:PRO:HD3	2.34	0.52
1:H:674:VAL:HG13	1:H:747:LEU:HD23	1.91	0.52
1:L:876:VAL:C	1:L:878:PRO:HD3	2.34	0.52
1:A:615:GLU:CD	1:A:615:GLU:H	2.17	0.52
1:I:876:VAL:C	1:I:878:PRO:HD3	2.34	0.52
1:J:876:VAL:C	1:J:878:PRO:HD3	2.34	0.52
1:C:735:LYS:H	1:C:735:LYS:HD2	1.74	0.52
1:F:501:HIS:CG	1:F:518:VAL:HB	2.45	0.52
1:G:891:ARG:CD	1:H:479:GLN:HG2	2.39	0.52
1:J:674:VAL:HG13	1:J:747:LEU:HD23	1.91	0.52
1:K:876:VAL:C	1:K:878:PRO:HD3	2.34	0.52
1:E:501:HIS:CG	1:E:518:VAL:HB	2.45	0.52
1:G:615:GLU:H	1:G:615:GLU:CD	2.17	0.52
1:H:1055:PRO:HG2	1:H:1087:ALA:HB2	1.92	0.52
1:E:735:LYS:H	1:E:735:LYS:HD2	1.74	0.52
1:F:615:GLU:CD	1:F:615:GLU:H	2.17	0.52
1:L:329:ALA:HB1	1:L:334:ALA:HA	1.92	0.52
1:K:1055:PRO:HG2	1:K:1087:ALA:HB2	1.92	0.52
1:D:1003:GLN:HE22	1:E:655:ARG:CZ	2.13	0.51
1:F:1003:GLN:CD	1:G:655:ARG:CG	2.82	0.51
1:G:501:HIS:CG	1:G:518:VAL:HB	2.45	0.51
1:H:958:THR:HG21	1:H:1107:THR:HG21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1055:PRO:HG2	1:L:1087:ALA:HB2	1.92	0.51
1:A:1003:GLN:NE2	1:C:655:ARG:NH1	2.59	0.51
1:B:958:THR:HG21	1:B:1107:THR:HG21	1.93	0.51
1:I:674:VAL:HG13	1:I:747:LEU:HD23	1.91	0.51
1:I:1055:PRO:HG2	1:I:1087:ALA:HB2	1.92	0.51
1:C:1037:TRP:CZ3	1:D:655:ARG:HD2	2.44	0.51
1:D:501:HIS:CG	1:D:518:VAL:HB	2.45	0.51
1:D:615:GLU:CD	1:D:615:GLU:H	2.17	0.51
1:I:958:THR:HG21	1:I:1107:THR:HG21	1.93	0.51
1:K:674:VAL:HG13	1:K:747:LEU:HD23	1.91	0.51
1:K:958:THR:HG21	1:K:1107:THR:HG21	1.92	0.51
1:J:349:GLU:HA	1:J:352:MET:HE3	1.93	0.51
1:J:958:THR:HG21	1:J:1107:THR:HG21	1.93	0.51
1:B:1055:PRO:HG2	1:B:1087:ALA:HB2	1.92	0.51
1:C:501:HIS:CG	1:C:518:VAL:HB	2.45	0.51
1:E:960:SER:OG	1:F:514:LYS:CG	2.58	0.51
1:K:329:ALA:HB1	1:K:334:ALA:HA	1.92	0.51
1:A:501:HIS:CG	1:A:518:VAL:HB	2.45	0.51
1:A:513:ALA:HB2	1:G:958:THR:CG2	2.34	0.51
1:I:349:GLU:HA	1:I:352:MET:HE3	1.93	0.51
1:J:814:THR:HG21	1:J:821:ALA:O	2.11	0.51
1:B:620:LYS:HE3	1:B:620:LYS:HA	1.93	0.51
1:I:329:ALA:HB1	1:I:334:ALA:HA	1.92	0.51
1:L:958:THR:HG21	1:L:1107:THR:HG21	1.92	0.51
1:J:1055:PRO:HG2	1:J:1087:ALA:HB2	1.92	0.51
1:L:620:LYS:HE3	1:L:620:LYS:HA	1.93	0.51
1:J:329:ALA:HB1	1:J:334:ALA:HA	1.92	0.51
1:L:93:ALA:HB2	1:L:108:ILE:HD12	1.92	0.51
1:B:674:VAL:CG1	1:B:750:GLN:HE22	2.24	0.51
1:D:958:THR:CG2	1:E:513:ALA:HB3	2.34	0.51
1:K:674:VAL:CG1	1:K:750:GLN:HE22	2.24	0.51
1:A:655:ARG:CD	1:G:1037:TRP:CH2	2.92	0.50
1:B:329:ALA:HB1	1:B:334:ALA:HA	1.92	0.50
1:H:329:ALA:HB1	1:H:334:ALA:HA	1.92	0.50
1:H:814:THR:HG21	1:H:821:ALA:O	2.11	0.50
1:B:93:ALA:HB2	1:B:108:ILE:HD12	1.92	0.50
1:H:496:ILE:HA	1:H:503:LEU:CD1	2.42	0.50
1:J:93:ALA:HB2	1:J:108:ILE:HD12	1.92	0.50
1:J:496:ILE:HA	1:J:503:LEU:CD1	2.42	0.50
1:L:178:LYS:HE2	1:L:231:ASP:OD1	2.12	0.50
1:C:812:LYS:O	1:C:814:THR:HG23	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1003:GLN:OE1	1:F:655:ARG:HG2	2.11	0.50
1:H:178:LYS:HE2	1:H:231:ASP:OD1	2.12	0.50
1:K:620:LYS:HE3	1:K:620:LYS:HA	1.93	0.50
1:D:812:LYS:O	1:D:814:THR:HG23	2.12	0.50
1:G:812:LYS:O	1:G:814:THR:HG23	2.12	0.50
1:H:93:ALA:HB2	1:H:108:ILE:HD12	1.92	0.50
1:J:674:VAL:CG1	1:J:750:GLN:HE22	2.24	0.50
1:K:814:THR:HG21	1:K:821:ALA:O	2.11	0.50
1:L:674:VAL:CG1	1:L:750:GLN:HE22	2.24	0.50
1:A:1067:TYR:OH	1:I:582:TYR:HE1	1.87	0.50
1:H:674:VAL:CG1	1:H:750:GLN:HE22	2.24	0.50
1:K:93:ALA:HB2	1:K:108:ILE:HD12	1.92	0.50
1:K:178:LYS:HE2	1:K:231:ASP:OD1	2.12	0.50
1:A:812:LYS:O	1:A:814:THR:HG23	2.12	0.50
1:B:814:THR:HG21	1:B:821:ALA:O	2.11	0.50
1:I:178:LYS:HE2	1:I:231:ASP:OD1	2.12	0.50
1:I:496:ILE:HA	1:I:503:LEU:CD1	2.42	0.50
1:I:674:VAL:CG1	1:I:750:GLN:HE22	2.24	0.50
1:L:349:GLU:HA	1:L:352:MET:HE3	1.93	0.50
1:B:178:LYS:HE2	1:B:231:ASP:OD1	2.12	0.50
1:H:620:LYS:HE3	1:H:620:LYS:HA	1.93	0.50
1:L:496:ILE:HA	1:L:503:LEU:CD1	2.42	0.50
1:L:814:THR:HG21	1:L:821:ALA:O	2.11	0.50
1:D:959:GLN:C	1:E:514:LYS:HZ3	2.04	0.50
1:E:812:LYS:O	1:E:814:THR:HG23	2.12	0.50
1:F:812:LYS:O	1:F:814:THR:HG23	2.12	0.50
1:I:814:THR:HG21	1:I:821:ALA:O	2.11	0.50
1:J:178:LYS:HE2	1:J:231:ASP:OD1	2.12	0.50
1:J:620:LYS:HA	1:J:620:LYS:HE3	1.93	0.50
1:K:349:GLU:HA	1:K:352:MET:HE3	1.93	0.50
1:B:349:GLU:HA	1:B:352:MET:HE3	1.93	0.49
1:I:93:ALA:HB2	1:I:108:ILE:HD12	1.92	0.49
1:K:496:ILE:HA	1:K:503:LEU:CD1	2.42	0.49
1:B:496:ILE:HA	1:B:503:LEU:CD1	2.42	0.49
1:B:582:TYR:HE1	1:F:1067:TYR:OH	1.86	0.49
1:K:504:TYR:CE1	1:K:535:LYS:HG2	2.48	0.49
1:A:512:PRO:HD3	1:G:957:GLN:CG	2.42	0.49
1:I:620:LYS:HE3	1:I:620:LYS:HA	1.93	0.49
1:L:504:TYR:CE1	1:L:535:LYS:HG2	2.48	0.49
1:B:504:TYR:CE1	1:B:535:LYS:HG2	2.48	0.49
1:J:504:TYR:CE1	1:J:535:LYS:HG2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:GLU:HA	1:H:352:MET:HE3	1.93	0.49
1:H:300:TYR:CG	1:H:354:TYR:HB3	2.48	0.49
1:I:300:TYR:CG	1:I:354:TYR:HB3	2.48	0.49
1:H:504:TYR:CE1	1:H:535:LYS:HG2	2.47	0.49
1:I:504:TYR:CE1	1:I:535:LYS:HG2	2.47	0.49
1:I:658:LYS:HE3	1:I:658:LYS:HA	1.95	0.49
1:A:511:ASP:HB2	1:G:956:VAL:O	2.13	0.48
1:C:958:THR:CG2	1:D:513:ALA:HB2	2.37	0.48
1:H:658:LYS:HE3	1:H:658:LYS:HA	1.95	0.48
1:B:300:TYR:CG	1:B:354:TYR:HB3	2.48	0.48
1:L:300:TYR:CG	1:L:354:TYR:HB3	2.48	0.48
1:F:1129:LYS:HE3	1:F:1129:LYS:HA	1.95	0.48
1:J:300:TYR:CG	1:J:354:TYR:HB3	2.48	0.48
1:C:1037:TRP:CH2	1:D:655:ARG:CD	2.92	0.48
1:K:300:TYR:CG	1:K:354:TYR:HB3	2.48	0.48
1:D:1063:CYS:SG	1:D:1075:THR:HG23	2.54	0.48
1:G:1063:CYS:SG	1:G:1075:THR:HG23	2.54	0.48
1:G:1129:LYS:HE3	1:G:1129:LYS:HA	1.95	0.48
1:A:1003:GLN:OE1	1:C:655:ARG:HG2	2.13	0.48
1:G:32:PRO:HG2	1:G:35:CYS:SG	2.54	0.48
1:L:177:ASP:HB2	1:L:182:SER:HA	1.96	0.48
1:A:1063:CYS:SG	1:A:1075:THR:HG23	2.54	0.48
1:A:1129:LYS:HE3	1:A:1129:LYS:HA	1.95	0.48
1:C:1063:CYS:SG	1:C:1075:THR:HG23	2.54	0.48
1:E:1129:LYS:HE3	1:E:1129:LYS:HA	1.95	0.48
1:F:959:GLN:C	1:G:514:LYS:NZ	2.38	0.48
1:C:1067:TYR:OH	1:J:582:TYR:HE1	1.91	0.48
1:J:658:LYS:HA	1:J:658:LYS:HE3	1.95	0.48
1:K:436:TYR:CE1	1:K:488:CYS:HB3	2.49	0.48
1:B:436:TYR:CE1	1:B:488:CYS:HB3	2.49	0.47
1:F:32:PRO:HG2	1:F:35:CYS:SG	2.54	0.47
1:F:1063:CYS:SG	1:F:1075:THR:HG23	2.54	0.47
1:L:658:LYS:HE3	1:L:658:LYS:HA	1.95	0.47
1:A:32:PRO:HG2	1:A:35:CYS:SG	2.54	0.47
1:A:510:THR:HA	1:G:1056:GLU:HG2	1.96	0.47
1:B:658:LYS:HE3	1:B:658:LYS:HA	1.95	0.47
1:E:1063:CYS:SG	1:E:1075:THR:HG23	2.54	0.47
1:J:436:TYR:CE1	1:J:488:CYS:HB3	2.49	0.47
1:K:658:LYS:HE3	1:K:658:LYS:HA	1.95	0.47
1:A:655:ARG:CG	1:G:1003:GLN:CD	2.85	0.47
1:C:957:GLN:CG	1:D:510:THR:C	1.88	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:GLN:C	1:D:514:LYS:NZ	2.38	0.47
1:D:32:PRO:HG2	1:D:35:CYS:SG	2.54	0.47
1:H:436:TYR:CE1	1:H:488:CYS:HB3	2.49	0.47
1:D:1067:TYR:HH	1:K:582:TYR:HD1	1.53	0.47
1:F:958:THR:CG2	1:G:513:ALA:HB2	2.36	0.47
1:H:872:GLU:HA	1:H:937:LEU:HD13	1.97	0.47
1:A:958:THR:CG2	1:C:513:ALA:HB2	2.38	0.47
1:B:689:LYS:HE3	1:B:689:LYS:HA	1.97	0.47
1:F:960:SER:N	1:G:514:LYS:CE	2.66	0.47
1:H:177:ASP:HB2	1:H:182:SER:HA	1.96	0.47
1:I:689:LYS:HE3	1:I:689:LYS:HA	1.97	0.47
1:I:872:GLU:HA	1:I:937:LEU:HD13	1.97	0.47
1:K:177:ASP:HB2	1:K:182:SER:HA	1.96	0.47
1:A:814:THR:HG21	1:A:821:ALA:O	2.15	0.47
1:A:957:GLN:CG	1:C:510:THR:C	1.85	0.47
1:B:872:GLU:HA	1:B:937:LEU:HD13	1.97	0.47
1:C:814:THR:HG21	1:C:821:ALA:O	2.15	0.47
1:D:1129:LYS:HA	1:D:1129:LYS:HE3	1.95	0.47
1:E:814:THR:HG21	1:E:821:ALA:O	2.15	0.47
1:E:958:THR:CG2	1:F:513:ALA:HB2	2.39	0.47
1:G:29:LEU:HD23	1:G:126:ILE:CG2	2.45	0.47
1:H:689:LYS:HA	1:H:689:LYS:HE3	1.97	0.47
1:L:436:TYR:CE1	1:L:488:CYS:HB3	2.49	0.47
1:L:872:GLU:HA	1:L:937:LEU:HD13	1.97	0.47
1:A:1056:GLU:HG2	1:C:510:THR:HA	1.97	0.47
1:C:1129:LYS:HE3	1:C:1129:LYS:HA	1.95	0.47
1:D:814:THR:HG21	1:D:821:ALA:O	2.15	0.47
1:C:32:PRO:HG2	1:C:35:CYS:SG	2.54	0.47
1:E:32:PRO:HG2	1:E:35:CYS:SG	2.54	0.47
1:I:177:ASP:HB2	1:I:182:SER:HA	1.96	0.47
1:I:436:TYR:CE1	1:I:488:CYS:HB3	2.49	0.47
1:A:29:LEU:HD23	1:A:126:ILE:CG2	2.45	0.46
1:A:514:LYS:CE	1:G:960:SER:N	2.63	0.46
1:F:29:LEU:HD23	1:F:126:ILE:CG2	2.45	0.46
1:J:689:LYS:HE3	1:J:689:LYS:HA	1.97	0.46
1:K:580:MET:HG3	1:K:629:TRP:CE3	2.50	0.46
1:L:689:LYS:HE3	1:L:689:LYS:HA	1.97	0.46
1:F:957:GLN:CG	1:G:512:PRO:HD3	2.46	0.46
1:D:29:LEU:HD23	1:D:126:ILE:CG2	2.45	0.46
1:D:1067:TYR:CZ	1:K:582:TYR:CD1	3.03	0.46
1:E:29:LEU:HD23	1:E:126:ILE:CG2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:580:MET:HG3	1:J:629:TRP:CE3	2.51	0.46
1:L:580:MET:HG3	1:L:629:TRP:CE3	2.50	0.46
1:B:177:ASP:HB2	1:B:182:SER:HA	1.96	0.46
1:F:814:THR:HG21	1:F:821:ALA:O	2.15	0.46
1:K:872:GLU:HA	1:K:937:LEU:HD13	1.97	0.46
1:A:33:ILE:HA	1:A:36:THR:HG23	1.97	0.46
1:A:300:TYR:CG	1:A:354:TYR:HB3	2.51	0.46
1:G:33:ILE:HA	1:G:36:THR:HG23	1.98	0.46
1:G:814:THR:HG21	1:G:821:ALA:O	2.15	0.46
1:C:29:LEU:HD23	1:C:126:ILE:CG2	2.45	0.46
1:C:300:TYR:CG	1:C:354:TYR:HB3	2.51	0.46
1:D:300:TYR:CG	1:D:354:TYR:HB3	2.51	0.46
1:J:177:ASP:HB2	1:J:182:SER:HA	1.96	0.46
1:F:956:VAL:O	1:G:511:ASP:HB2	2.16	0.46
1:H:580:MET:HG3	1:H:629:TRP:CE3	2.50	0.46
1:I:580:MET:HG3	1:I:629:TRP:CE3	2.51	0.46
1:F:1003:GLN:OE1	1:G:655:ARG:HG2	2.16	0.46
1:J:872:GLU:HA	1:J:937:LEU:HD13	1.97	0.46
1:B:580:MET:HG3	1:B:629:TRP:CE3	2.50	0.46
1:E:300:TYR:CG	1:E:354:TYR:HB3	2.51	0.46
1:F:881:PHE:CE2	1:F:1113:ARG:HG3	2.51	0.46
1:I:837:MET:HE1	1:I:915:TYR:CE2	2.51	0.46
1:D:1003:GLN:CD	1:E:655:ARG:CG	2.89	0.46
1:F:22:TYR:CE2	1:F:26:LEU:HD11	2.51	0.46
1:F:33:ILE:HA	1:F:36:THR:HG23	1.97	0.46
1:G:881:PHE:CE2	1:G:1113:ARG:HG3	2.51	0.46
1:I:814:THR:HG21	1:I:821:ALA:C	2.41	0.46
1:K:689:LYS:HE3	1:K:689:LYS:HA	1.97	0.46
1:E:72:CYS:HA	1:E:92:ALA:CB	2.46	0.45
1:F:72:CYS:HA	1:F:92:ALA:CB	2.46	0.45
1:G:300:TYR:CG	1:G:354:TYR:HB3	2.51	0.45
1:K:837:MET:HE1	1:K:915:TYR:CE2	2.52	0.45
1:E:1056:GLU:HG2	1:F:510:THR:HA	1.97	0.45
1:H:814:THR:HG21	1:H:821:ALA:C	2.41	0.45
1:J:837:MET:HE1	1:J:915:TYR:CE2	2.51	0.45
1:C:960:SER:N	1:D:514:LYS:CE	2.66	0.45
1:D:22:TYR:CE2	1:D:26:LEU:HD11	2.51	0.45
1:D:957:GLN:O	1:E:511:ASP:O	2.33	0.45
1:G:1018:GLY:HA3	1:G:1058:TYR:CD1	2.52	0.45
1:H:837:MET:HE1	1:H:915:TYR:CE2	2.52	0.45
1:A:1018:GLY:HA3	1:A:1058:TYR:CD1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:TYR:CE2	1:C:26:LEU:HD11	2.51	0.45
1:D:1088:GLN:HG2	1:E:538:THR:HG23	1.97	0.45
1:E:1018:GLY:HA3	1:E:1058:TYR:CD1	2.52	0.45
1:J:69:CYS:CB	1:J:72:CYS:HG	2.29	0.45
1:J:814:THR:HG21	1:J:821:ALA:C	2.41	0.45
1:L:837:MET:HE1	1:L:915:TYR:CE2	2.51	0.45
1:B:582:TYR:CD1	1:F:1067:TYR:CZ	3.04	0.45
1:D:33:ILE:HA	1:D:36:THR:HG23	1.97	0.45
1:E:33:ILE:HA	1:E:36:THR:HG23	1.98	0.45
1:E:958:THR:CA	1:F:514:LYS:HD2	2.46	0.45
1:G:1067:TYR:OH	1:H:582:TYR:HE1	1.88	0.45
1:B:837:MET:HE1	1:B:915:TYR:CE2	2.51	0.45
1:C:956:VAL:O	1:D:511:ASP:HB2	2.17	0.45
1:D:1018:GLY:HA3	1:D:1058:TYR:CD1	2.52	0.45
1:E:22:TYR:CE2	1:E:26:LEU:HD11	2.52	0.45
1:A:22:TYR:CE2	1:A:26:LEU:HD11	2.52	0.45
1:E:881:PHE:CE2	1:E:1113:ARG:HG3	2.51	0.45
1:F:300:TYR:CG	1:F:354:TYR:HB3	2.51	0.45
1:I:451:LEU:HG	1:I:555:LEU:HD21	1.99	0.45
1:K:22:TYR:CZ	1:K:26:LEU:HD11	2.52	0.45
1:B:451:LEU:HG	1:B:555:LEU:HD21	1.99	0.45
1:F:1018:GLY:HA3	1:F:1058:TYR:CD1	2.52	0.45
1:G:22:TYR:CE2	1:G:26:LEU:HD11	2.52	0.45
1:H:69:CYS:CB	1:H:72:CYS:HG	2.29	0.45
1:A:881:PHE:CE2	1:A:1113:ARG:HG3	2.51	0.45
1:B:814:THR:HG21	1:B:821:ALA:C	2.41	0.45
1:C:1018:GLY:HA3	1:C:1058:TYR:CD1	2.52	0.45
1:D:72:CYS:HA	1:D:92:ALA:CB	2.46	0.45
1:F:72:CYS:HA	1:F:92:ALA:HA	1.99	0.45
1:G:72:CYS:HA	1:G:92:ALA:CB	2.47	0.45
1:I:825:VAL:HG13	1:I:904:VAL:H	1.82	0.45
1:A:959:GLN:C	1:C:514:LYS:NZ	2.40	0.45
1:B:22:TYR:CZ	1:B:26:LEU:HD11	2.52	0.45
1:C:72:CYS:HA	1:C:92:ALA:CB	2.46	0.45
1:E:221:ASP:HA	1:E:222:ARG:HH21	1.82	0.45
1:L:814:THR:HG21	1:L:821:ALA:C	2.41	0.45
1:A:72:CYS:HA	1:A:92:ALA:CB	2.46	0.44
1:C:33:ILE:HA	1:C:36:THR:HG23	1.97	0.44
1:D:505:GLY:HA3	1:D:515:LYS:HA	1.99	0.44
1:E:72:CYS:HA	1:E:92:ALA:HA	1.99	0.44
1:H:22:TYR:CZ	1:H:136:VAL:HG21	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:451:LEU:HG	1:H:555:LEU:HD21	1.99	0.44
1:J:22:TYR:CZ	1:J:136:VAL:HG21	2.53	0.44
1:C:72:CYS:HA	1:C:92:ALA:HA	1.99	0.44
1:D:221:ASP:HA	1:D:222:ARG:HH21	1.82	0.44
1:D:881:PHE:CE2	1:D:1113:ARG:HG3	2.51	0.44
1:I:794:GLN:CD	1:I:866:LEU:HD13	2.43	0.44
1:J:451:LEU:HG	1:J:555:LEU:HD21	1.99	0.44
1:J:1002:TRP:CD1	1:J:1008:PHE:CE2	3.06	0.44
1:K:794:GLN:CD	1:K:866:LEU:HD13	2.43	0.44
1:B:868:MET:HE1	1:B:909:LEU:CD2	2.48	0.44
1:C:72:CYS:SG	1:C:74:VAL:HG12	2.58	0.44
1:E:1003:GLN:NE2	1:F:655:ARG:NH1	2.65	0.44
1:F:72:CYS:SG	1:F:74:VAL:HG12	2.58	0.44
1:H:1002:TRP:CD1	1:H:1008:PHE:CE2	3.06	0.44
1:K:22:TYR:CZ	1:K:136:VAL:HG21	2.52	0.44
1:K:814:THR:HG21	1:K:821:ALA:C	2.41	0.44
1:K:868:MET:HE1	1:K:909:LEU:CD2	2.48	0.44
1:L:868:MET:HE1	1:L:909:LEU:CD2	2.48	0.44
1:E:72:CYS:SG	1:E:74:VAL:HG12	2.58	0.44
1:G:505:GLY:HA3	1:G:515:LYS:HA	1.99	0.44
1:I:22:TYR:CZ	1:I:136:VAL:HG21	2.53	0.44
1:K:451:LEU:HG	1:K:555:LEU:HD21	1.99	0.44
1:L:22:TYR:CZ	1:L:26:LEU:HD11	2.52	0.44
1:L:451:LEU:HG	1:L:555:LEU:HD21	1.99	0.44
1:D:72:CYS:SG	1:D:74:VAL:HG12	2.58	0.44
1:F:221:ASP:HA	1:F:222:ARG:HH21	1.82	0.44
1:H:868:MET:HE1	1:H:909:LEU:CD2	2.48	0.44
1:J:22:TYR:CZ	1:J:26:LEU:HD11	2.52	0.44
1:J:335:TRP:CZ2	1:J:336:LYS:HE3	2.53	0.44
1:K:335:TRP:CZ2	1:K:336:LYS:HE3	2.53	0.44
1:K:864:TRP:HA	1:K:916:PHE:CZ	2.53	0.44
1:B:1002:TRP:CD1	1:B:1008:PHE:CE2	3.06	0.44
1:C:145:MET:SD	1:C:149:LYS:HE3	2.58	0.44
1:D:145:MET:SD	1:D:149:LYS:HE3	2.58	0.44
1:G:72:CYS:HA	1:G:92:ALA:HA	1.99	0.44
1:H:794:GLN:CD	1:H:866:LEU:HD13	2.43	0.44
1:I:22:TYR:CZ	1:I:26:LEU:HD11	2.52	0.44
1:I:335:TRP:CZ2	1:I:336:LYS:HE3	2.53	0.44
1:J:794:GLN:CD	1:J:866:LEU:HD13	2.43	0.44
1:K:1002:TRP:CD1	1:K:1008:PHE:CE2	3.06	0.44
1:A:221:ASP:HA	1:A:222:ARG:HH21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ASP:HA	1:C:222:ARG:HH21	1.82	0.44
1:C:957:GLN:CG	1:D:512:PRO:HD3	2.46	0.44
1:G:221:ASP:HA	1:G:222:ARG:HH21	1.82	0.44
1:H:335:TRP:CZ2	1:H:336:LYS:HE3	2.53	0.44
1:J:825:VAL:HG13	1:J:904:VAL:H	1.82	0.44
1:L:116:MET:HE3	1:L:153:LEU:HD21	2.00	0.44
1:L:335:TRP:CZ2	1:L:336:LYS:HE3	2.53	0.44
1:L:868:MET:HE2	1:L:871:MET:SD	2.58	0.44
1:A:505:GLY:HA3	1:A:515:LYS:HA	1.99	0.44
1:B:825:VAL:HG13	1:B:904:VAL:H	1.82	0.44
1:C:881:PHE:CE2	1:C:1113:ARG:HG3	2.51	0.44
1:D:958:THR:CA	1:E:514:LYS:HD2	2.43	0.44
1:E:145:MET:SD	1:E:149:LYS:HE3	2.58	0.44
1:F:505:GLY:HA3	1:F:515:LYS:HA	1.99	0.44
1:G:881:PHE:CZ	1:G:1113:ARG:HG3	2.53	0.44
1:H:825:VAL:HG13	1:H:904:VAL:H	1.82	0.44
1:H:864:TRP:HA	1:H:916:PHE:CZ	2.53	0.44
1:J:868:MET:HE2	1:J:871:MET:SD	2.58	0.44
1:K:868:MET:HE2	1:K:871:MET:SD	2.58	0.44
1:L:794:GLN:CD	1:L:866:LEU:HD13	2.43	0.44
1:L:864:TRP:HA	1:L:916:PHE:CZ	2.53	0.44
1:A:881:PHE:CZ	1:A:1113:ARG:HG3	2.53	0.44
1:B:335:TRP:CZ2	1:B:336:LYS:HE3	2.53	0.44
1:D:552:THR:HB	1:D:553:PRO:HD3	2.00	0.44
1:F:741:MET:HE1	1:F:786:SER:HB3	2.00	0.44
1:F:1056:GLU:HG2	1:G:510:THR:HA	1.98	0.44
1:G:429:LEU:HD22	1:G:454:THR:HG23	2.00	0.44
1:H:22:TYR:CZ	1:H:26:LEU:HD11	2.52	0.44
1:B:22:TYR:CZ	1:B:136:VAL:HG21	2.53	0.43
1:C:552:THR:HB	1:C:553:PRO:HD3	2.00	0.43
1:E:552:THR:HB	1:E:553:PRO:HD3	2.00	0.43
1:G:72:CYS:SG	1:G:74:VAL:HG12	2.58	0.43
1:I:116:MET:HE3	1:I:153:LEU:HD21	2.00	0.43
1:J:864:TRP:HA	1:J:916:PHE:CZ	2.53	0.43
1:L:22:TYR:CZ	1:L:136:VAL:HG21	2.53	0.43
1:L:825:VAL:HG13	1:L:904:VAL:H	1.82	0.43
1:L:1002:TRP:CD1	1:L:1008:PHE:CE2	3.06	0.43
1:A:145:MET:SD	1:A:149:LYS:HE3	2.58	0.43
1:A:956:VAL:O	1:C:511:ASP:HB2	2.18	0.43
1:B:748:ARG:CZ	1:B:748:ARG:HB3	2.49	0.43
1:B:794:GLN:CD	1:B:866:LEU:HD13	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:SER:HA	1:C:774:LEU:HD22	2.00	0.43
1:C:1056:GLU:HG2	1:D:510:THR:HA	2.00	0.43
1:D:72:CYS:HA	1:D:92:ALA:HA	1.99	0.43
1:D:960:SER:CB	1:E:514:LYS:CD	2.90	0.43
1:F:881:PHE:CZ	1:F:1113:ARG:HG3	2.53	0.43
1:J:868:MET:HE1	1:J:909:LEU:CD2	2.48	0.43
1:A:429:LEU:HD22	1:A:454:THR:HG23	2.00	0.43
1:A:711:SER:HA	1:A:774:LEU:HD22	2.00	0.43
1:B:116:MET:HE3	1:B:153:LEU:HD21	2.00	0.43
1:B:864:TRP:HA	1:B:916:PHE:CZ	2.53	0.43
1:G:1067:TYR:CZ	1:H:582:TYR:CD1	3.06	0.43
1:G:1071:ARG:CZ	1:G:1071:ARG:HB3	2.48	0.43
1:A:72:CYS:SG	1:A:74:VAL:HG12	2.58	0.43
1:A:552:THR:HB	1:A:553:PRO:HD3	2.00	0.43
1:A:957:GLN:CG	1:C:512:PRO:HD3	2.48	0.43
1:B:868:MET:HE2	1:B:871:MET:SD	2.58	0.43
1:B:917:HIS:CD2	1:B:925:LYS:HE3	2.54	0.43
1:D:881:PHE:CZ	1:D:1113:ARG:HG3	2.53	0.43
1:F:429:LEU:HD22	1:F:454:THR:HG23	2.01	0.43
1:F:1071:ARG:CZ	1:F:1071:ARG:HB3	2.49	0.43
1:H:748:ARG:CZ	1:H:748:ARG:HB3	2.49	0.43
1:I:917:HIS:CD2	1:I:925:LYS:HE3	2.54	0.43
1:J:116:MET:HE3	1:J:153:LEU:HD21	2.00	0.43
1:C:881:PHE:CZ	1:C:1113:ARG:HG3	2.53	0.43
1:E:505:GLY:HA3	1:E:515:LYS:HA	1.99	0.43
1:I:1002:TRP:CD1	1:I:1008:PHE:CE2	3.06	0.43
1:A:72:CYS:HA	1:A:92:ALA:HA	1.99	0.43
1:F:145:MET:SD	1:F:149:LYS:HE3	2.58	0.43
1:F:552:THR:HB	1:F:553:PRO:HD3	2.00	0.43
1:I:868:MET:HE1	1:I:909:LEU:CD2	2.48	0.43
1:A:508:TYR:CZ	1:A:538:THR:HG22	2.54	0.43
1:A:1071:ARG:HB3	1:A:1071:ARG:CZ	2.48	0.43
1:C:429:LEU:HD22	1:C:454:THR:HG23	2.00	0.43
1:C:1071:ARG:CZ	1:C:1071:ARG:HB3	2.49	0.43
1:E:429:LEU:HD22	1:E:454:THR:HG23	2.00	0.43
1:I:864:TRP:HA	1:I:916:PHE:CZ	2.53	0.43
1:K:116:MET:HE3	1:K:153:LEU:HD21	2.00	0.43
1:L:876:VAL:HG21	1:L:937:LEU:HD11	2.00	0.43
1:A:455:VAL:O	1:A:459:THR:HG23	2.19	0.43
1:C:741:MET:HE1	1:C:786:SER:HB3	2.01	0.43
1:C:1003:GLN:OE1	1:D:655:ARG:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:LEU:HD22	1:D:454:THR:HG23	2.00	0.43
1:D:1071:ARG:HB3	1:D:1071:ARG:CZ	2.49	0.43
1:E:881:PHE:CZ	1:E:1113:ARG:HG3	2.53	0.43
1:G:145:MET:SD	1:G:149:LYS:HE3	2.58	0.43
1:H:868:MET:HE2	1:H:871:MET:SD	2.58	0.43
1:H:917:HIS:CD2	1:H:925:LYS:HE3	2.54	0.43
1:I:748:ARG:HB3	1:I:748:ARG:CZ	2.48	0.43
1:J:893:GLU:HG3	1:J:1117:GLN:HA	2.01	0.43
1:A:741:MET:HE1	1:A:786:SER:HB3	2.00	0.43
1:G:455:VAL:O	1:G:459:THR:HG23	2.19	0.43
1:G:508:TYR:CZ	1:G:538:THR:HG22	2.54	0.43
1:G:552:THR:HB	1:G:553:PRO:HD3	2.01	0.43
1:G:711:SER:HA	1:G:774:LEU:HD22	2.00	0.43
1:J:917:HIS:CD2	1:J:925:LYS:HE3	2.54	0.43
1:K:825:VAL:HG13	1:K:904:VAL:H	1.82	0.43
1:K:893:GLU:HG3	1:K:1117:GLN:HA	2.01	0.43
1:K:893:GLU:CG	1:K:1117:GLN:HA	2.49	0.43
1:B:893:GLU:HG3	1:B:1117:GLN:HA	2.01	0.43
1:C:508:TYR:CZ	1:C:538:THR:HG22	2.54	0.43
1:D:711:SER:HA	1:D:774:LEU:HD22	2.00	0.43
1:G:741:MET:HE1	1:G:786:SER:HB3	2.00	0.43
1:H:116:MET:HE3	1:H:153:LEU:HD21	2.00	0.43
1:L:748:ARG:CZ	1:L:748:ARG:HB3	2.49	0.43
1:E:741:MET:HE1	1:E:786:SER:HB3	2.01	0.42
1:L:893:GLU:HG3	1:L:1117:GLN:HA	2.01	0.42
1:L:893:GLU:CG	1:L:1117:GLN:HA	2.49	0.42
1:A:72:CYS:HA	1:A:92:ALA:HB2	2.01	0.42
1:C:505:GLY:HA3	1:C:515:LYS:HA	1.99	0.42
1:D:1067:TYR:OH	1:K:579:ASP:OD1	2.36	0.42
1:D:1067:TYR:OH	1:K:582:TYR:CD1	2.59	0.42
1:E:1071:ARG:HB3	1:E:1071:ARG:CZ	2.48	0.42
1:I:866:LEU:HD12	1:I:866:LEU:C	2.44	0.42
1:J:639:ASP:HA	1:J:705:ARG:HH21	1.84	0.42
1:J:866:LEU:C	1:J:866:LEU:HD12	2.44	0.42
1:J:876:VAL:HG21	1:J:937:LEU:HD11	2.00	0.42
1:A:956:VAL:C	1:C:511:ASP:HB2	2.38	0.42
1:E:508:TYR:CZ	1:E:538:THR:HG22	2.54	0.42
1:F:455:VAL:O	1:F:459:THR:HG23	2.19	0.42
1:F:508:TYR:CZ	1:F:538:THR:HG22	2.54	0.42
1:H:639:ASP:HA	1:H:705:ARG:HH21	1.85	0.42
1:H:1129:LYS:HE3	1:H:1129:LYS:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:893:GLU:HG3	1:I:1117:GLN:HA	2.01	0.42
1:K:639:ASP:HA	1:K:705:ARG:HH21	1.85	0.42
1:K:867:VAL:HG12	1:K:871:MET:SD	2.60	0.42
1:K:1129:LYS:HE3	1:K:1129:LYS:HA	2.01	0.42
1:L:867:VAL:HG12	1:L:871:MET:SD	2.60	0.42
1:L:917:HIS:CD2	1:L:925:LYS:HE3	2.54	0.42
1:B:876:VAL:HG21	1:B:937:LEU:HD11	2.00	0.42
1:C:1120:ASN:HA	1:C:1125:LYS:HE3	2.02	0.42
1:H:893:GLU:HG3	1:H:1117:GLN:HA	2.01	0.42
1:I:876:VAL:HG21	1:I:937:LEU:HD11	2.00	0.42
1:K:866:LEU:HD12	1:K:866:LEU:C	2.44	0.42
1:A:513:ALA:CB	1:G:958:THR:CG2	2.80	0.42
1:A:655:ARG:HG2	1:G:1003:GLN:OE1	2.20	0.42
1:D:960:SER:H	1:E:514:LYS:CD	2.31	0.42
1:D:1120:ASN:HA	1:D:1125:LYS:HE3	2.02	0.42
1:J:748:ARG:CZ	1:J:748:ARG:HB3	2.49	0.42
1:J:881:PHE:CE1	1:J:892:GLU:HB3	2.55	0.42
1:K:505:GLY:CA	1:K:515:LYS:HA	2.50	0.42
1:L:881:PHE:CE1	1:L:892:GLU:HB3	2.55	0.42
1:A:1120:ASN:HA	1:A:1125:LYS:HE3	2.02	0.42
1:B:881:PHE:CE1	1:B:892:GLU:HB3	2.55	0.42
1:C:72:CYS:HA	1:C:92:ALA:HB2	2.01	0.42
1:E:711:SER:HA	1:E:774:LEU:HD22	2.00	0.42
1:E:999:ASP:OD1	1:F:648:PHE:CD2	2.72	0.42
1:F:44:TRP:CH2	1:F:46:ALA:HA	2.55	0.42
1:H:893:GLU:CG	1:H:1117:GLN:HA	2.49	0.42
1:I:333:ASP:HA	1:I:335:TRP:CD1	2.55	0.42
1:I:868:MET:HE2	1:I:871:MET:SD	2.58	0.42
1:J:304:TYR:CD1	1:J:304:TYR:C	2.98	0.42
1:J:505:GLY:CA	1:J:515:LYS:HA	2.50	0.42
1:K:748:ARG:CZ	1:K:748:ARG:HB3	2.49	0.42
1:L:505:GLY:CA	1:L:515:LYS:HA	2.50	0.42
1:B:304:TYR:CD1	1:B:304:TYR:C	2.98	0.42
1:B:867:VAL:HG12	1:B:871:MET:SD	2.60	0.42
1:B:1129:LYS:HE3	1:B:1129:LYS:HA	2.01	0.42
1:C:455:VAL:O	1:C:459:THR:HG23	2.19	0.42
1:C:620:LYS:HE3	1:C:620:LYS:HA	2.02	0.42
1:D:620:LYS:HE3	1:D:620:LYS:HA	2.02	0.42
1:F:711:SER:HA	1:F:774:LEU:HD22	2.00	0.42
1:I:639:ASP:HA	1:I:705:ARG:HH21	1.84	0.42
1:I:741:MET:HE1	1:I:786:SER:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:867:VAL:HG12	1:J:871:MET:SD	2.60	0.42
1:K:917:HIS:CD2	1:K:925:LYS:HE3	2.54	0.42
1:B:866:LEU:HD12	1:B:866:LEU:C	2.45	0.42
1:B:893:GLU:CG	1:B:1117:GLN:HA	2.49	0.42
1:E:1120:ASN:HA	1:E:1125:LYS:HE3	2.02	0.42
1:G:955:PHE:CZ	1:G:1104:MET:SD	3.13	0.42
1:G:1008:PHE:CD2	1:G:1010:PRO:HD3	2.55	0.42
1:H:304:TYR:CD1	1:H:304:TYR:C	2.97	0.42
1:H:866:LEU:C	1:H:866:LEU:HD12	2.45	0.42
1:I:893:GLU:CG	1:I:1117:GLN:HA	2.49	0.42
1:J:741:MET:HE1	1:J:786:SER:HB3	2.01	0.42
1:K:876:VAL:HG21	1:K:937:LEU:HD11	2.00	0.42
1:C:955:PHE:CZ	1:C:1104:MET:SD	3.13	0.42
1:D:508:TYR:CZ	1:D:538:THR:HG22	2.54	0.42
1:D:955:PHE:CZ	1:D:1104:MET:SD	3.13	0.42
1:E:44:TRP:CH2	1:E:46:ALA:HA	2.55	0.42
1:L:639:ASP:HA	1:L:705:ARG:HH21	1.85	0.42
1:A:955:PHE:CZ	1:A:1104:MET:SD	3.13	0.42
1:D:1067:TYR:CE1	1:K:582:TYR:CD1	3.08	0.42
1:F:732:GLU:CD	1:F:732:GLU:H	2.28	0.42
1:F:958:THR:CG2	1:G:513:ALA:HB3	2.40	0.42
1:F:1008:PHE:CD2	1:F:1010:PRO:HD3	2.55	0.42
1:H:881:PHE:CE1	1:H:892:GLU:HB3	2.55	0.42
1:I:304:TYR:CD1	1:I:304:TYR:C	2.97	0.42
1:K:132:GLU:HB3	1:K:314:PHE:CZ	2.55	0.42
1:K:333:ASP:HA	1:K:335:TRP:CD1	2.55	0.42
1:L:132:GLU:HB3	1:L:314:PHE:CZ	2.55	0.42
1:L:333:ASP:HA	1:L:335:TRP:CD1	2.55	0.42
1:L:866:LEU:C	1:L:866:LEU:HD12	2.44	0.42
1:A:958:THR:CA	1:C:514:LYS:HD2	2.47	0.41
1:B:333:ASP:HA	1:B:335:TRP:CD1	2.55	0.41
1:D:455:VAL:O	1:D:459:THR:HG23	2.19	0.41
1:E:455:VAL:O	1:E:459:THR:HG23	2.19	0.41
1:E:732:GLU:H	1:E:732:GLU:CD	2.28	0.41
1:E:1008:PHE:CD2	1:E:1010:PRO:HD3	2.55	0.41
1:G:732:GLU:H	1:G:732:GLU:CD	2.28	0.41
1:H:464:PHE:CZ	1:H:468:VAL:HG11	2.55	0.41
1:H:867:VAL:HG12	1:H:871:MET:SD	2.60	0.41
1:I:867:VAL:HG12	1:I:871:MET:SD	2.60	0.41
1:I:881:PHE:CE1	1:I:892:GLU:HB3	2.55	0.41
1:J:728:TYR:CD1	1:J:736:VAL:HG11	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:893:GLU:CG	1:J:1117:GLN:HA	2.49	0.41
1:K:728:TYR:CD1	1:K:736:VAL:HG11	2.55	0.41
1:L:304:TYR:CD1	1:L:304:TYR:C	2.98	0.41
1:L:646:ARG:CZ	1:L:712:ASN:HB3	2.50	0.41
1:A:1008:PHE:CD2	1:A:1010:PRO:HD3	2.55	0.41
1:B:639:ASP:HA	1:B:705:ARG:HH21	1.85	0.41
1:D:741:MET:HE1	1:D:786:SER:HB3	2.00	0.41
1:G:72:CYS:HA	1:G:92:ALA:HB2	2.02	0.41
1:H:674:VAL:HG11	1:H:746:GLN:CG	2.50	0.41
1:H:876:VAL:HG21	1:H:937:LEU:HD11	2.00	0.41
1:I:505:GLY:CA	1:I:515:LYS:HA	2.50	0.41
1:J:132:GLU:HB3	1:J:314:PHE:CZ	2.55	0.41
1:J:1129:LYS:HE3	1:J:1129:LYS:HA	2.01	0.41
1:K:646:ARG:CZ	1:K:712:ASN:HB3	2.50	0.41
1:L:1129:LYS:HE3	1:L:1129:LYS:HA	2.01	0.41
1:B:416:GLU:CD	1:B:416:GLU:H	2.29	0.41
1:B:646:ARG:CZ	1:B:712:ASN:HB3	2.50	0.41
1:D:646:ARG:CZ	1:D:712:ASN:HB3	2.51	0.41
1:D:1084:ARG:NE	1:E:509:GLN:HA	2.29	0.41
1:F:955:PHE:CZ	1:F:1104:MET:SD	3.13	0.41
1:F:1120:ASN:HA	1:F:1125:LYS:HE3	2.02	0.41
1:G:44:TRP:CH2	1:G:46:ALA:HA	2.55	0.41
1:H:741:MET:HE1	1:H:786:SER:HB3	2.02	0.41
1:K:881:PHE:CE1	1:K:892:GLU:HB3	2.55	0.41
1:A:732:GLU:CD	1:A:732:GLU:H	2.28	0.41
1:D:52:CYS:SG	1:D:76:CYS:HA	2.61	0.41
1:E:646:ARG:CZ	1:E:712:ASN:HB3	2.51	0.41
1:H:1063:CYS:SG	1:H:1075:THR:HG23	2.61	0.41
1:I:132:GLU:HB3	1:I:314:PHE:CZ	2.55	0.41
1:I:464:PHE:CZ	1:I:468:VAL:HG11	2.55	0.41
1:I:646:ARG:CZ	1:I:712:ASN:HB3	2.50	0.41
1:J:333:ASP:HA	1:J:335:TRP:CD1	2.55	0.41
1:J:646:ARG:CZ	1:J:712:ASN:HB3	2.50	0.41
1:A:620:LYS:HE3	1:A:620:LYS:HA	2.02	0.41
1:B:132:GLU:HB3	1:B:314:PHE:CZ	2.55	0.41
1:C:52:CYS:SG	1:C:76:CYS:HA	2.61	0.41
1:C:956:VAL:C	1:D:511:ASP:HB2	2.38	0.41
1:E:620:LYS:HA	1:E:620:LYS:HE3	2.02	0.41
1:E:955:PHE:CZ	1:E:1104:MET:SD	3.13	0.41
1:G:52:CYS:SG	1:G:76:CYS:HA	2.61	0.41
1:G:1120:ASN:HA	1:G:1125:LYS:HE3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1129:LYS:HA	1:I:1129:LYS:HE3	2.01	0.41
1:A:44:TRP:CH2	1:A:46:ALA:HA	2.55	0.41
1:B:93:ALA:HB1	1:B:105:THR:HA	2.03	0.41
1:B:741:MET:HE1	1:B:786:SER:HB3	2.02	0.41
1:D:1008:PHE:CD2	1:D:1010:PRO:HD3	2.55	0.41
1:E:52:CYS:SG	1:E:76:CYS:HA	2.61	0.41
1:E:1070:ALA:HB1	1:L:498:ASN:HD21	1.86	0.41
1:F:56:GLU:CD	1:F:224:LYS:HZ2	2.28	0.41
1:F:1088:GLN:HG2	1:G:538:THR:HG23	2.02	0.41
1:I:917:HIS:CG	1:I:925:LYS:HE3	2.56	0.41
1:K:304:TYR:CD1	1:K:304:TYR:C	2.97	0.41
1:B:505:GLY:CA	1:B:515:LYS:HA	2.50	0.41
1:D:958:THR:HG22	1:E:511:ASP:OD1	2.09	0.41
1:E:1003:GLN:NE2	1:F:655:ARG:HG3	2.35	0.41
1:H:132:GLU:HB3	1:H:314:PHE:CZ	2.55	0.41
1:H:646:ARG:CZ	1:H:712:ASN:HB3	2.50	0.41
1:J:464:PHE:CZ	1:J:468:VAL:HG11	2.55	0.41
1:C:44:TRP:CH2	1:C:46:ALA:HA	2.55	0.41
1:C:1008:PHE:CD2	1:C:1010:PRO:HD3	2.55	0.41
1:C:1088:GLN:HG2	1:D:538:THR:HG23	2.02	0.41
1:D:72:CYS:HA	1:D:92:ALA:HB2	2.02	0.41
1:G:28:ALA:HA	1:G:353:ARG:CD	2.51	0.41
1:H:333:ASP:HA	1:H:335:TRP:CD1	2.55	0.41
1:J:917:HIS:CG	1:J:925:LYS:HE3	2.56	0.41
1:K:674:VAL:HG11	1:K:746:GLN:CG	2.50	0.41
1:K:812:LYS:HA	1:K:901:GLN:NE2	2.36	0.41
1:K:1063:CYS:SG	1:K:1075:THR:HG23	2.61	0.41
1:A:28:ALA:HA	1:A:353:ARG:CD	2.51	0.41
1:B:464:PHE:CZ	1:B:468:VAL:HG11	2.55	0.41
1:B:1063:CYS:SG	1:B:1075:THR:HG23	2.61	0.41
1:C:732:GLU:CD	1:C:732:GLU:H	2.28	0.41
1:D:732:GLU:CD	1:D:732:GLU:H	2.28	0.41
1:D:980:PHE:CE2	1:D:989:LYS:HB2	2.56	0.41
1:D:1070:ALA:HB1	1:K:498:ASN:HD21	1.86	0.41
1:E:186:VAL:HG23	1:E:208:TRP:CZ2	2.56	0.41
1:F:72:CYS:HA	1:F:92:ALA:HB2	2.01	0.41
1:F:646:ARG:CZ	1:F:712:ASN:HB3	2.51	0.41
1:F:956:VAL:C	1:G:511:ASP:HB2	2.37	0.41
1:G:518:VAL:HG13	1:G:519:PRO:HD2	2.03	0.41
1:H:505:GLY:CA	1:H:515:LYS:HA	2.50	0.41
1:H:728:TYR:CD1	1:H:736:VAL:HG11	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:917:HIS:CG	1:H:925:LYS:HE3	2.56	0.41
1:I:39:HIS:HA	1:I:88:CYS:SG	2.61	0.41
1:I:93:ALA:HB1	1:I:105:THR:HA	2.03	0.41
1:I:603:PHE:CE1	1:I:691:LEU:HD23	2.56	0.41
1:I:728:TYR:CD1	1:I:736:VAL:HG11	2.55	0.41
1:J:603:PHE:CE1	1:J:691:LEU:HD23	2.56	0.41
1:K:39:HIS:HA	1:K:88:CYS:SG	2.61	0.41
1:K:464:PHE:CZ	1:K:468:VAL:HG11	2.55	0.41
1:L:39:HIS:HA	1:L:88:CYS:SG	2.61	0.41
1:L:728:TYR:CD1	1:L:736:VAL:HG11	2.55	0.41
1:C:186:VAL:HG23	1:C:208:TRP:CZ2	2.56	0.41
1:C:646:ARG:CZ	1:C:712:ASN:HB3	2.51	0.41
1:D:186:VAL:HG23	1:D:208:TRP:CZ2	2.56	0.41
1:E:72:CYS:HA	1:E:92:ALA:HB2	2.01	0.41
1:F:505:GLY:CA	1:F:515:LYS:HA	2.51	0.41
1:F:980:PHE:CE2	1:F:989:LYS:HB2	2.56	0.41
1:G:620:LYS:HA	1:G:620:LYS:HE3	2.02	0.41
1:G:980:PHE:CE2	1:G:989:LYS:HB2	2.56	0.41
1:H:416:GLU:CD	1:H:416:GLU:H	2.28	0.41
1:I:1063:CYS:SG	1:I:1075:THR:HG23	2.61	0.41
1:J:812:LYS:HA	1:J:901:GLN:NE2	2.36	0.41
1:K:741:MET:HE1	1:K:786:SER:HB3	2.02	0.41
1:L:416:GLU:CD	1:L:416:GLU:H	2.29	0.41
1:L:603:PHE:CE1	1:L:691:LEU:HD23	2.56	0.41
1:B:39:HIS:HA	1:B:88:CYS:SG	2.61	0.40
1:B:498:ASN:HD21	1:F:1070:ALA:HB1	1.86	0.40
1:B:728:TYR:CD1	1:B:736:VAL:HG11	2.55	0.40
1:C:958:THR:CA	1:D:514:LYS:HD2	2.48	0.40
1:C:980:PHE:CE2	1:C:989:LYS:HB2	2.56	0.40
1:D:44:TRP:CH2	1:D:46:ALA:HA	2.55	0.40
1:E:956:VAL:O	1:F:511:ASP:HB2	2.21	0.40
1:F:186:VAL:HG23	1:F:208:TRP:CZ2	2.56	0.40
1:J:674:VAL:HG11	1:J:746:GLN:CG	2.50	0.40
1:K:603:PHE:CE1	1:K:691:LEU:HD23	2.56	0.40
1:L:674:VAL:HG11	1:L:746:GLN:CG	2.50	0.40
1:L:812:LYS:HA	1:L:901:GLN:NE2	2.36	0.40
1:A:514:LYS:CD	1:G:960:SER:CB	2.94	0.40
1:A:646:ARG:CZ	1:A:712:ASN:HB3	2.51	0.40
1:C:28:ALA:HA	1:C:353:ARG:CD	2.51	0.40
1:E:28:ALA:HA	1:E:353:ARG:CD	2.51	0.40
1:E:999:ASP:OD1	1:F:648:PHE:HD2	2.05	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:518:VAL:HG13	1:F:519:PRO:HD2	2.03	0.40
1:F:620:LYS:HE3	1:F:620:LYS:HA	2.02	0.40
1:F:872:GLU:HA	1:F:937:LEU:HD13	2.04	0.40
1:H:552:THR:HB	1:H:553:PRO:HD3	2.03	0.40
1:K:416:GLU:CD	1:K:416:GLU:H	2.29	0.40
1:A:872:GLU:HA	1:A:937:LEU:HD13	2.04	0.40
1:E:518:VAL:HG13	1:E:519:PRO:HD2	2.03	0.40
1:E:872:GLU:HA	1:E:937:LEU:HD13	2.04	0.40
1:E:1070:ALA:CB	1:L:498:ASN:HD21	2.35	0.40
1:G:186:VAL:HG23	1:G:208:TRP:CZ2	2.56	0.40
1:G:646:ARG:CZ	1:G:712:ASN:HB3	2.51	0.40
1:G:872:GLU:HA	1:G:937:LEU:HD13	2.04	0.40
1:H:39:HIS:HA	1:H:88:CYS:SG	2.61	0.40
1:I:552:THR:HB	1:I:553:PRO:HD3	2.04	0.40
1:I:812:LYS:HA	1:I:901:GLN:NE2	2.36	0.40
1:J:39:HIS:HA	1:J:88:CYS:SG	2.61	0.40
1:J:552:THR:HB	1:J:553:PRO:HD3	2.03	0.40
1:K:917:HIS:CG	1:K:925:LYS:HE3	2.56	0.40
1:L:391:ALA:HA	1:L:395:HIS:CD2	2.56	0.40
1:L:464:PHE:CZ	1:L:468:VAL:HG11	2.55	0.40
1:L:741:MET:HE1	1:L:786:SER:HB3	2.02	0.40
1:A:52:CYS:SG	1:A:76:CYS:HA	2.61	0.40
1:B:552:THR:HB	1:B:553:PRO:HD3	2.04	0.40
1:B:917:HIS:CG	1:B:925:LYS:HE3	2.56	0.40
1:C:1067:TYR:CZ	1:J:582:TYR:CD1	3.09	0.40
1:D:28:ALA:HA	1:D:353:ARG:CD	2.51	0.40
1:D:505:GLY:CA	1:D:515:LYS:HA	2.51	0.40
1:D:518:VAL:HG13	1:D:519:PRO:HD2	2.03	0.40
1:D:872:GLU:HA	1:D:937:LEU:HD13	2.03	0.40
1:E:960:SER:N	1:F:514:LYS:CE	2.68	0.40
1:F:28:ALA:HA	1:F:353:ARG:CD	2.51	0.40
1:F:1008:PHE:CG	1:F:1010:PRO:HD3	2.57	0.40
1:G:505:GLY:CA	1:G:515:LYS:HA	2.51	0.40
1:J:93:ALA:HB1	1:J:105:THR:HA	2.03	0.40
1:J:496:ILE:HG22	1:J:503:LEU:HD13	2.04	0.40
1:J:1063:CYS:SG	1:J:1075:THR:HG23	2.61	0.40
1:K:552:THR:HB	1:K:553:PRO:HD3	2.04	0.40
1:A:186:VAL:HG23	1:A:208:TRP:CZ2	2.56	0.40
1:B:391:ALA:HA	1:B:395:HIS:CD2	2.57	0.40
1:B:603:PHE:CE1	1:B:691:LEU:HD23	2.56	0.40
1:E:505:GLY:CA	1:E:515:LYS:HA	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:980:PHE:CE2	1:E:989:LYS:HB2	2.56	0.40
1:H:603:PHE:CE1	1:H:691:LEU:HD23	2.56	0.40
1:I:416:GLU:CD	1:I:416:GLU:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1130/1154 (98%)	1059 (94%)	61 (5%)	10 (1%)	14	51
1	B	1130/1154 (98%)	1030 (91%)	85 (8%)	15 (1%)	9	42
1	C	1130/1154 (98%)	1059 (94%)	61 (5%)	10 (1%)	14	51
1	D	1130/1154 (98%)	1060 (94%)	60 (5%)	10 (1%)	14	51
1	E	1130/1154 (98%)	1060 (94%)	60 (5%)	10 (1%)	14	51
1	F	1130/1154 (98%)	1060 (94%)	60 (5%)	10 (1%)	14	51
1	G	1130/1154 (98%)	1059 (94%)	61 (5%)	10 (1%)	14	51
1	H	1130/1154 (98%)	1030 (91%)	85 (8%)	15 (1%)	9	42
1	I	1130/1154 (98%)	1030 (91%)	85 (8%)	15 (1%)	9	42
1	J	1130/1154 (98%)	1030 (91%)	85 (8%)	15 (1%)	9	42
1	K	1130/1154 (98%)	1030 (91%)	85 (8%)	15 (1%)	9	42
1	L	1130/1154 (98%)	1030 (91%)	85 (8%)	15 (1%)	9	42
All	All	13560/13848 (98%)	12537 (92%)	873 (6%)	150 (1%)	14	46

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	894	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	899	PRO
1	C	894	ALA
1	D	894	ALA
1	E	894	ALA
1	F	894	ALA
1	G	894	ALA
1	H	899	PRO
1	I	899	PRO
1	J	899	PRO
1	K	899	PRO
1	L	899	PRO
1	A	397	THR
1	A	895	LYS
1	B	84	LEU
1	B	333	ASP
1	B	505	GLY
1	B	891	ARG
1	C	397	THR
1	C	895	LYS
1	D	397	THR
1	D	895	LYS
1	E	397	THR
1	E	895	LYS
1	F	397	THR
1	F	895	LYS
1	G	397	THR
1	G	895	LYS
1	H	84	LEU
1	H	333	ASP
1	H	505	GLY
1	H	891	ARG
1	I	84	LEU
1	I	333	ASP
1	I	505	GLY
1	I	891	ARG
1	J	84	LEU
1	J	333	ASP
1	J	505	GLY
1	J	891	ARG
1	K	84	LEU
1	K	333	ASP
1	K	505	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	891	ARG
1	L	84	LEU
1	L	333	ASP
1	L	505	GLY
1	L	891	ARG
1	A	1071	ARG
1	B	157	SER
1	B	262	GLY
1	B	296	LYS
1	C	1071	ARG
1	D	1071	ARG
1	E	1071	ARG
1	F	1071	ARG
1	G	1071	ARG
1	H	157	SER
1	H	262	GLY
1	H	296	LYS
1	I	157	SER
1	I	262	GLY
1	I	296	LYS
1	J	157	SER
1	J	262	GLY
1	J	296	LYS
1	K	157	SER
1	K	262	GLY
1	K	296	LYS
1	L	157	SER
1	L	262	GLY
1	L	296	LYS
1	A	885	LEU
1	A	1119	SER
1	A	1140	GLY
1	B	731	LYS
1	B	880	GLU
1	C	885	LEU
1	C	981	THR
1	C	1119	SER
1	C	1140	GLY
1	D	885	LEU
1	D	1119	SER
1	D	1140	GLY
1	E	885	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1119	SER
1	E	1140	GLY
1	F	885	LEU
1	F	1119	SER
1	F	1140	GLY
1	G	885	LEU
1	G	981	THR
1	G	1119	SER
1	G	1140	GLY
1	H	731	LYS
1	H	880	GLU
1	I	731	LYS
1	I	880	GLU
1	J	731	LYS
1	J	880	GLU
1	K	731	LYS
1	K	880	GLU
1	L	731	LYS
1	L	880	GLU
1	A	981	THR
1	A	1144	PRO
1	B	1071	ARG
1	C	1144	PRO
1	D	981	THR
1	D	1144	PRO
1	E	981	THR
1	E	1144	PRO
1	F	981	THR
1	F	1144	PRO
1	G	1144	PRO
1	H	1071	ARG
1	I	1071	ARG
1	J	1071	ARG
1	K	903	ALA
1	K	1071	ARG
1	L	1071	ARG
1	B	183	ASP
1	B	896	SER
1	B	903	ALA
1	B	1025	LYS
1	H	183	ASP
1	H	896	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	903	ALA
1	H	1025	LYS
1	I	183	ASP
1	I	896	SER
1	I	903	ALA
1	I	1025	LYS
1	J	183	ASP
1	J	896	SER
1	J	903	ALA
1	J	1025	LYS
1	K	183	ASP
1	K	896	SER
1	K	1025	LYS
1	L	183	ASP
1	L	896	SER
1	L	903	ALA
1	L	1025	LYS
1	A	963	GLY
1	C	963	GLY
1	D	963	GLY
1	E	963	GLY
1	F	963	GLY
1	G	963	GLY

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	1006/1022 (98%)	971 (96%)	35 (4%)	32	53
1	B	1006/1022 (98%)	947 (94%)	59 (6%)	18	39
1	C	1006/1022 (98%)	971 (96%)	35 (4%)	32	53
1	D	1006/1022 (98%)	971 (96%)	35 (4%)	32	53
1	E	1006/1022 (98%)	971 (96%)	35 (4%)	32	53
1	F	1006/1022 (98%)	971 (96%)	35 (4%)	32	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	1006/1022 (98%)	971 (96%)	35 (4%)	32	53
1	H	1006/1022 (98%)	947 (94%)	59 (6%)	18	39
1	I	1006/1022 (98%)	948 (94%)	58 (6%)	18	40
1	J	1006/1022 (98%)	947 (94%)	59 (6%)	18	39
1	K	1006/1022 (98%)	948 (94%)	58 (6%)	18	40
1	L	1006/1022 (98%)	948 (94%)	58 (6%)	18	40
All	All	12072/12264 (98%)	11511 (95%)	561 (5%)	25	45

All (561) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	81	GLN
1	A	95	LYS
1	A	115	ARG
1	A	217	HIS
1	A	222	ARG
1	A	224	LYS
1	A	248	ASP
1	A	313	HIS
1	A	338	TYR
1	A	416	GLU
1	A	494	GLU
1	A	502	GLU
1	A	518	VAL
1	A	531	ASP
1	A	558	PHE
1	A	560	GLN
1	A	582	TYR
1	A	584	MET
1	A	615	GLU
1	A	620	LYS
1	A	663	GLN
1	A	686	GLU
1	A	732	GLU
1	A	754	MET
1	A	756	GLU
1	A	773	GLU
1	A	802	ARG
1	A	823	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	891	ARG
1	A	933	ASP
1	A	980	PHE
1	A	1072	GLU
1	A	1074	ARG
1	A	1129	LYS
1	B	16	GLU
1	B	29	LEU
1	B	33	ILE
1	B	44	TRP
1	B	64	ARG
1	B	71	GLU
1	B	81	GLN
1	B	87	ASP
1	B	102	GLU
1	B	107	ASN
1	B	112	LEU
1	B	120	GLU
1	B	150	GLN
1	B	152	VAL
1	B	159	TRP
1	B	178	LYS
1	B	222	ARG
1	B	248	ASP
1	B	286	HIS
1	B	296	LYS
1	B	297	VAL
1	B	313	HIS
1	B	374	MET
1	B	412	ASN
1	B	416	GLU
1	B	446	GLU
1	B	501	HIS
1	B	502	GLU
1	B	508	TYR
1	B	518	VAL
1	B	521	GLU
1	B	560	GLN
1	B	582	TYR
1	B	584	MET
1	B	611	GLU
1	B	620	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	643	GLU
1	B	654	GLU
1	B	658	LYS
1	B	686	GLU
1	B	689	LYS
1	B	732	GLU
1	B	734	GLU
1	B	762	GLU
1	B	773	GLU
1	B	784	GLU
1	B	802	ARG
1	B	812	LYS
1	B	857	LYS
1	B	866	LEU
1	B	885	LEU
1	B	886	LYS
1	B	915	TYR
1	B	933	ASP
1	B	980	PHE
1	B	1113	ARG
1	B	1119	SER
1	B	1129	LYS
1	B	1138	GLU
1	C	18	LYS
1	C	81	GLN
1	C	95	LYS
1	C	115	ARG
1	C	217	HIS
1	C	222	ARG
1	C	224	LYS
1	C	248	ASP
1	C	313	HIS
1	C	338	TYR
1	C	416	GLU
1	C	494	GLU
1	C	502	GLU
1	C	518	VAL
1	C	531	ASP
1	C	558	PHE
1	C	560	GLN
1	C	582	TYR
1	C	584	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	615	GLU
1	C	620	LYS
1	C	663	GLN
1	C	686	GLU
1	C	732	GLU
1	C	754	MET
1	C	756	GLU
1	C	773	GLU
1	C	802	ARG
1	C	823	SER
1	C	891	ARG
1	C	933	ASP
1	C	980	PHE
1	C	1072	GLU
1	C	1074	ARG
1	C	1129	LYS
1	D	18	LYS
1	D	81	GLN
1	D	95	LYS
1	D	115	ARG
1	D	217	HIS
1	D	222	ARG
1	D	224	LYS
1	D	248	ASP
1	D	313	HIS
1	D	338	TYR
1	D	416	GLU
1	D	494	GLU
1	D	502	GLU
1	D	518	VAL
1	D	531	ASP
1	D	558	PHE
1	D	560	GLN
1	D	582	TYR
1	D	584	MET
1	D	615	GLU
1	D	620	LYS
1	D	663	GLN
1	D	686	GLU
1	D	732	GLU
1	D	754	MET
1	D	756	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	773	GLU
1	D	802	ARG
1	D	823	SER
1	D	891	ARG
1	D	933	ASP
1	D	980	PHE
1	D	1072	GLU
1	D	1074	ARG
1	D	1129	LYS
1	E	18	LYS
1	E	81	GLN
1	E	95	LYS
1	E	115	ARG
1	E	217	HIS
1	E	222	ARG
1	E	224	LYS
1	E	248	ASP
1	E	313	HIS
1	E	338	TYR
1	E	416	GLU
1	E	494	GLU
1	E	502	GLU
1	E	518	VAL
1	E	531	ASP
1	E	558	PHE
1	E	560	GLN
1	E	582	TYR
1	E	584	MET
1	E	615	GLU
1	E	620	LYS
1	E	663	GLN
1	E	686	GLU
1	E	732	GLU
1	E	754	MET
1	E	756	GLU
1	E	773	GLU
1	E	802	ARG
1	E	823	SER
1	E	891	ARG
1	E	933	ASP
1	E	980	PHE
1	E	1072	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1074	ARG
1	E	1129	LYS
1	F	18	LYS
1	F	81	GLN
1	F	95	LYS
1	F	115	ARG
1	F	217	HIS
1	F	222	ARG
1	F	224	LYS
1	F	248	ASP
1	F	313	HIS
1	F	338	TYR
1	F	416	GLU
1	F	494	GLU
1	F	502	GLU
1	F	518	VAL
1	F	531	ASP
1	F	558	PHE
1	F	560	GLN
1	F	582	TYR
1	F	584	MET
1	F	615	GLU
1	F	620	LYS
1	F	663	GLN
1	F	686	GLU
1	F	732	GLU
1	F	754	MET
1	F	756	GLU
1	F	773	GLU
1	F	802	ARG
1	F	823	SER
1	F	891	ARG
1	F	933	ASP
1	F	980	PHE
1	F	1072	GLU
1	F	1074	ARG
1	F	1129	LYS
1	G	18	LYS
1	G	81	GLN
1	G	95	LYS
1	G	115	ARG
1	G	217	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	222	ARG
1	G	224	LYS
1	G	248	ASP
1	G	313	HIS
1	G	338	TYR
1	G	416	GLU
1	G	494	GLU
1	G	502	GLU
1	G	518	VAL
1	G	531	ASP
1	G	558	PHE
1	G	560	GLN
1	G	582	TYR
1	G	584	MET
1	G	615	GLU
1	G	620	LYS
1	G	663	GLN
1	G	686	GLU
1	G	732	GLU
1	G	754	MET
1	G	756	GLU
1	G	773	GLU
1	G	802	ARG
1	G	823	SER
1	G	891	ARG
1	G	933	ASP
1	G	980	PHE
1	G	1072	GLU
1	G	1074	ARG
1	G	1129	LYS
1	H	16	GLU
1	H	29	LEU
1	H	33	ILE
1	H	44	TRP
1	H	64	ARG
1	H	71	GLU
1	H	81	GLN
1	H	87	ASP
1	H	102	GLU
1	H	107	ASN
1	H	112	LEU
1	H	120	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	150	GLN
1	H	152	VAL
1	H	159	TRP
1	H	178	LYS
1	H	222	ARG
1	H	248	ASP
1	H	286	HIS
1	H	296	LYS
1	H	297	VAL
1	H	313	HIS
1	H	374	MET
1	H	412	ASN
1	H	416	GLU
1	H	446	GLU
1	H	501	HIS
1	H	502	GLU
1	H	508	TYR
1	H	518	VAL
1	H	521	GLU
1	H	560	GLN
1	H	582	TYR
1	H	584	MET
1	H	611	GLU
1	H	620	LYS
1	H	643	GLU
1	H	654	GLU
1	H	658	LYS
1	H	686	GLU
1	H	689	LYS
1	H	732	GLU
1	H	734	GLU
1	H	762	GLU
1	H	773	GLU
1	H	784	GLU
1	H	802	ARG
1	H	812	LYS
1	H	857	LYS
1	H	866	LEU
1	H	885	LEU
1	H	886	LYS
1	H	915	TYR
1	H	933	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	980	PHE
1	H	1113	ARG
1	H	1119	SER
1	H	1129	LYS
1	H	1138	GLU
1	I	16	GLU
1	I	29	LEU
1	I	33	ILE
1	I	44	TRP
1	I	64	ARG
1	I	81	GLN
1	I	87	ASP
1	I	102	GLU
1	I	107	ASN
1	I	112	LEU
1	I	120	GLU
1	I	150	GLN
1	I	152	VAL
1	I	159	TRP
1	I	178	LYS
1	I	222	ARG
1	I	248	ASP
1	I	286	HIS
1	I	296	LYS
1	I	297	VAL
1	I	313	HIS
1	I	374	MET
1	I	412	ASN
1	I	416	GLU
1	I	446	GLU
1	I	501	HIS
1	I	502	GLU
1	I	508	TYR
1	I	518	VAL
1	I	521	GLU
1	I	560	GLN
1	I	582	TYR
1	I	584	MET
1	I	611	GLU
1	I	620	LYS
1	I	643	GLU
1	I	654	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	658	LYS
1	I	686	GLU
1	I	689	LYS
1	I	732	GLU
1	I	734	GLU
1	I	762	GLU
1	I	773	GLU
1	I	784	GLU
1	I	802	ARG
1	I	812	LYS
1	I	857	LYS
1	I	866	LEU
1	I	885	LEU
1	I	886	LYS
1	I	915	TYR
1	I	933	ASP
1	I	980	PHE
1	I	1113	ARG
1	I	1119	SER
1	I	1129	LYS
1	I	1138	GLU
1	J	16	GLU
1	J	29	LEU
1	J	33	ILE
1	J	44	TRP
1	J	64	ARG
1	J	71	GLU
1	J	81	GLN
1	J	87	ASP
1	J	102	GLU
1	J	107	ASN
1	J	112	LEU
1	J	120	GLU
1	J	150	GLN
1	J	152	VAL
1	J	159	TRP
1	J	178	LYS
1	J	222	ARG
1	J	248	ASP
1	J	286	HIS
1	J	296	LYS
1	J	297	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	313	HIS
1	J	374	MET
1	J	412	ASN
1	J	416	GLU
1	J	446	GLU
1	J	501	HIS
1	J	502	GLU
1	J	508	TYR
1	J	518	VAL
1	J	521	GLU
1	J	560	GLN
1	J	582	TYR
1	J	584	MET
1	J	611	GLU
1	J	620	LYS
1	J	643	GLU
1	J	654	GLU
1	J	658	LYS
1	J	686	GLU
1	J	689	LYS
1	J	732	GLU
1	J	734	GLU
1	J	762	GLU
1	J	773	GLU
1	J	784	GLU
1	J	802	ARG
1	J	812	LYS
1	J	857	LYS
1	J	866	LEU
1	J	885	LEU
1	J	886	LYS
1	J	915	TYR
1	J	933	ASP
1	J	980	PHE
1	J	1113	ARG
1	J	1119	SER
1	J	1129	LYS
1	J	1138	GLU
1	K	16	GLU
1	K	29	LEU
1	K	33	ILE
1	K	44	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	64	ARG
1	K	81	GLN
1	K	87	ASP
1	K	102	GLU
1	K	107	ASN
1	K	112	LEU
1	K	120	GLU
1	K	150	GLN
1	K	152	VAL
1	K	159	TRP
1	K	178	LYS
1	K	222	ARG
1	K	248	ASP
1	K	286	HIS
1	K	296	LYS
1	K	297	VAL
1	K	313	HIS
1	K	374	MET
1	K	412	ASN
1	K	416	GLU
1	K	446	GLU
1	K	501	HIS
1	K	502	GLU
1	K	508	TYR
1	K	518	VAL
1	K	521	GLU
1	K	560	GLN
1	K	582	TYR
1	K	584	MET
1	K	611	GLU
1	K	620	LYS
1	K	643	GLU
1	K	654	GLU
1	K	658	LYS
1	K	686	GLU
1	K	689	LYS
1	K	732	GLU
1	K	734	GLU
1	K	762	GLU
1	K	773	GLU
1	K	784	GLU
1	K	802	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	812	LYS
1	K	857	LYS
1	K	866	LEU
1	K	885	LEU
1	K	886	LYS
1	K	915	TYR
1	K	933	ASP
1	K	980	PHE
1	K	1113	ARG
1	K	1119	SER
1	K	1129	LYS
1	K	1138	GLU
1	L	16	GLU
1	L	29	LEU
1	L	33	ILE
1	L	44	TRP
1	L	64	ARG
1	L	81	GLN
1	L	87	ASP
1	L	102	GLU
1	L	107	ASN
1	L	112	LEU
1	L	120	GLU
1	L	150	GLN
1	L	152	VAL
1	L	159	TRP
1	L	178	LYS
1	L	222	ARG
1	L	248	ASP
1	L	286	HIS
1	L	296	LYS
1	L	297	VAL
1	L	313	HIS
1	L	374	MET
1	L	412	ASN
1	L	416	GLU
1	L	446	GLU
1	L	501	HIS
1	L	502	GLU
1	L	508	TYR
1	L	518	VAL
1	L	521	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	560	GLN
1	L	582	TYR
1	L	584	MET
1	L	611	GLU
1	L	620	LYS
1	L	643	GLU
1	L	654	GLU
1	L	658	LYS
1	L	686	GLU
1	L	689	LYS
1	L	732	GLU
1	L	734	GLU
1	L	762	GLU
1	L	773	GLU
1	L	784	GLU
1	L	802	ARG
1	L	812	LYS
1	L	857	LYS
1	L	866	LEU
1	L	885	LEU
1	L	886	LYS
1	L	915	TYR
1	L	933	ASP
1	L	980	PHE
1	L	1113	ARG
1	L	1119	SER
1	L	1129	LYS
1	L	1138	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	81	GLN
1	A	141	HIS
1	A	143	GLN
1	A	395	HIS
1	A	449	GLN
1	A	587	HIS
1	A	843	ASN
1	A	1003	GLN
1	A	1015	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1035	ASN
1	A	1042	ASN
1	B	65	GLN
1	B	77	HIS
1	B	90	GLN
1	B	107	ASN
1	B	143	GLN
1	B	144	GLN
1	B	171	GLN
1	B	213	HIS
1	B	269	ASN
1	B	388	ASN
1	B	395	HIS
1	B	427	ASN
1	B	641	ASN
1	B	680	GLN
1	B	682	ASN
1	B	683	GLN
1	B	750	GLN
1	B	803	GLN
1	B	810	GLN
1	B	816	ASN
1	B	1034	ASN
1	B	1035	ASN
1	B	1042	ASN
1	C	65	GLN
1	C	81	GLN
1	C	141	HIS
1	C	143	GLN
1	C	144	GLN
1	C	395	HIS
1	C	449	GLN
1	C	490	ASN
1	C	587	HIS
1	C	843	ASN
1	C	1003	GLN
1	C	1015	ASN
1	C	1035	ASN
1	C	1042	ASN
1	D	65	GLN
1	D	81	GLN
1	D	141	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	143	GLN
1	D	252	GLN
1	D	395	HIS
1	D	449	GLN
1	D	587	HIS
1	D	843	ASN
1	D	998	ASN
1	D	1003	GLN
1	D	1015	ASN
1	D	1035	ASN
1	D	1042	ASN
1	E	65	GLN
1	E	81	GLN
1	E	141	HIS
1	E	143	GLN
1	E	252	GLN
1	E	395	HIS
1	E	449	GLN
1	E	587	HIS
1	E	680	GLN
1	E	843	ASN
1	E	1003	GLN
1	E	1015	ASN
1	E	1035	ASN
1	E	1042	ASN
1	F	65	GLN
1	F	81	GLN
1	F	141	HIS
1	F	143	GLN
1	F	174	GLN
1	F	395	HIS
1	F	449	GLN
1	F	587	HIS
1	F	843	ASN
1	F	1003	GLN
1	F	1015	ASN
1	F	1035	ASN
1	F	1042	ASN
1	G	65	GLN
1	G	81	GLN
1	G	141	HIS
1	G	143	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	395	HIS
1	G	449	GLN
1	G	587	HIS
1	G	843	ASN
1	G	1003	GLN
1	G	1015	ASN
1	G	1035	ASN
1	G	1042	ASN
1	H	65	GLN
1	H	77	HIS
1	H	90	GLN
1	H	107	ASN
1	H	143	GLN
1	H	144	GLN
1	H	171	GLN
1	H	213	HIS
1	H	395	HIS
1	H	427	ASN
1	H	641	ASN
1	H	680	GLN
1	H	682	ASN
1	H	683	GLN
1	H	750	GLN
1	H	810	GLN
1	H	816	ASN
1	H	1034	ASN
1	H	1035	ASN
1	H	1042	ASN
1	I	65	GLN
1	I	77	HIS
1	I	107	ASN
1	I	143	GLN
1	I	144	GLN
1	I	150	GLN
1	I	171	GLN
1	I	213	HIS
1	I	269	ASN
1	I	303	GLN
1	I	395	HIS
1	I	427	ASN
1	I	641	ASN
1	I	680	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	682	ASN
1	I	683	GLN
1	I	750	GLN
1	I	810	GLN
1	I	816	ASN
1	I	1034	ASN
1	I	1035	ASN
1	I	1042	ASN
1	J	65	GLN
1	J	77	HIS
1	J	90	GLN
1	J	107	ASN
1	J	143	GLN
1	J	144	GLN
1	J	171	GLN
1	J	213	HIS
1	J	395	HIS
1	J	427	ASN
1	J	641	ASN
1	J	680	GLN
1	J	682	ASN
1	J	683	GLN
1	J	750	GLN
1	J	810	GLN
1	J	816	ASN
1	J	1034	ASN
1	J	1035	ASN
1	J	1042	ASN
1	K	65	GLN
1	K	77	HIS
1	K	90	GLN
1	K	107	ASN
1	K	143	GLN
1	K	144	GLN
1	K	150	GLN
1	K	171	GLN
1	K	213	HIS
1	K	269	ASN
1	K	395	HIS
1	K	427	ASN
1	K	641	ASN
1	K	680	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	682	ASN
1	K	683	GLN
1	K	750	GLN
1	K	816	ASN
1	K	1034	ASN
1	K	1035	ASN
1	K	1042	ASN
1	L	65	GLN
1	L	77	HIS
1	L	90	GLN
1	L	107	ASN
1	L	143	GLN
1	L	144	GLN
1	L	171	GLN
1	L	213	HIS
1	L	269	ASN
1	L	395	HIS
1	L	427	ASN
1	L	641	ASN
1	L	680	GLN
1	L	682	ASN
1	L	683	GLN
1	L	750	GLN
1	L	803	GLN
1	L	816	ASN
1	L	1034	ASN
1	L	1035	ASN
1	L	1042	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 ⓘ

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.

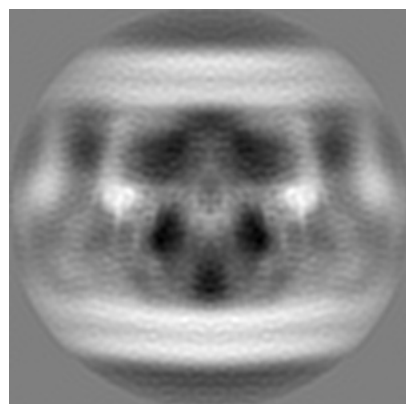
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25737. These allow visual inspection of the internal detail of the map and identification of artifacts.

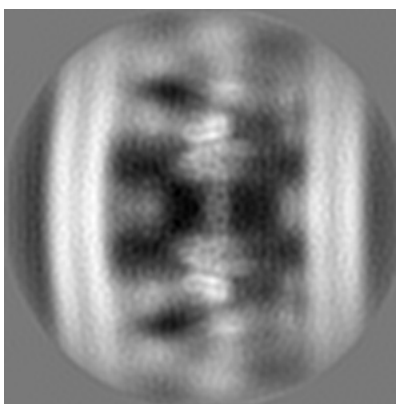
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

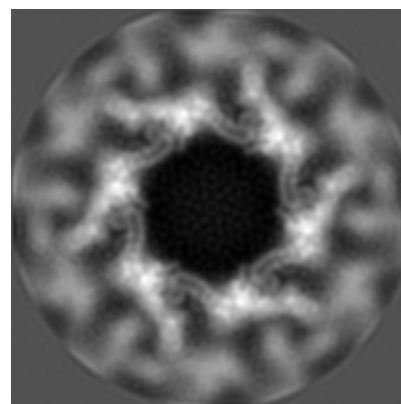
6.1.1 Primary map



X

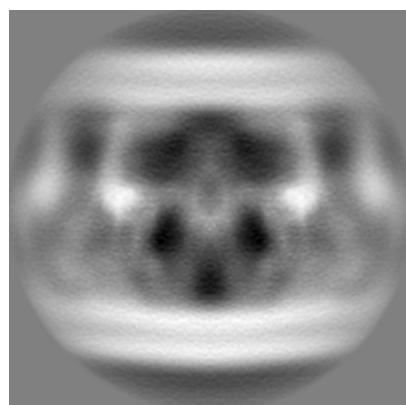


Y

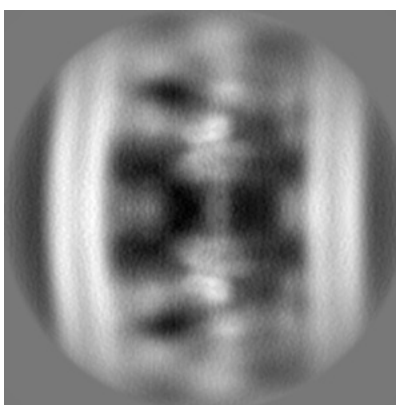


Z

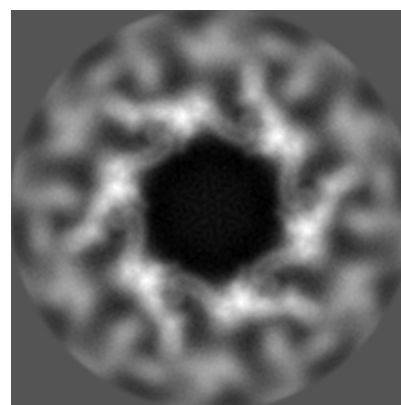
6.1.2 Raw map



X



Y

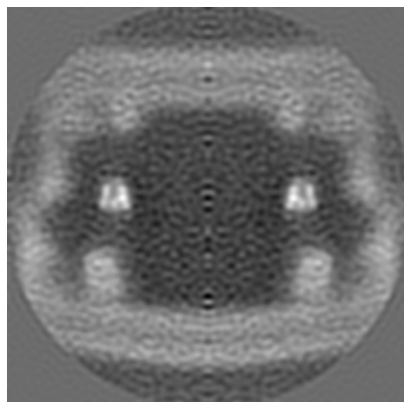


Z

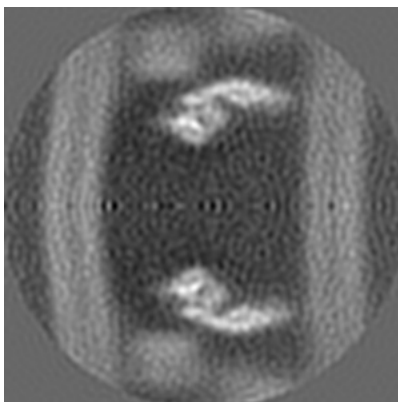
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

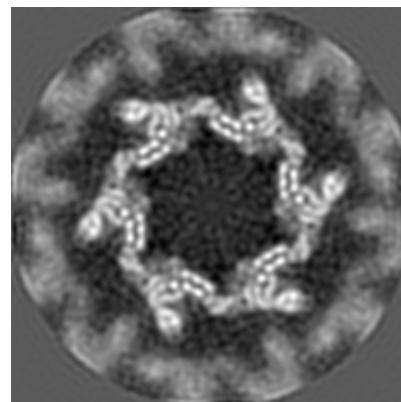
6.2.1 Primary map



X Index: 98

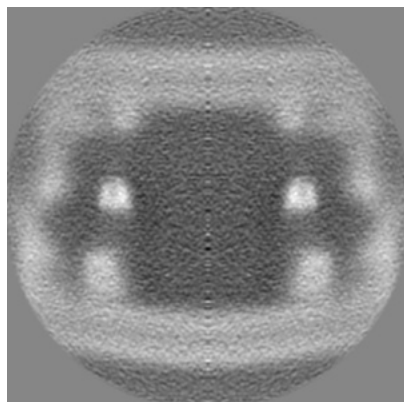


Y Index: 98

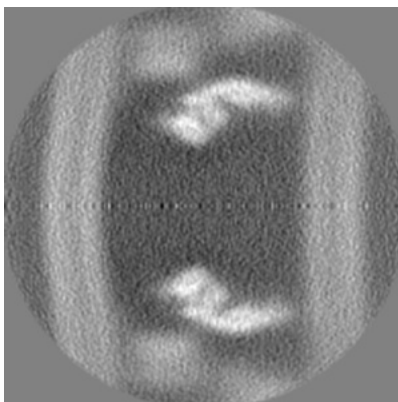


Z Index: 98

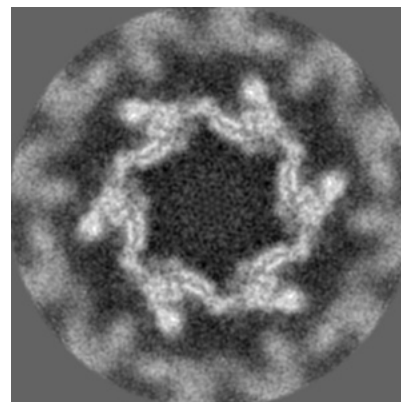
6.2.2 Raw map



X Index: 98



Y Index: 98

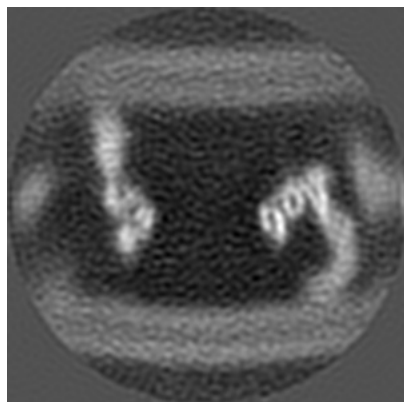


Z Index: 98

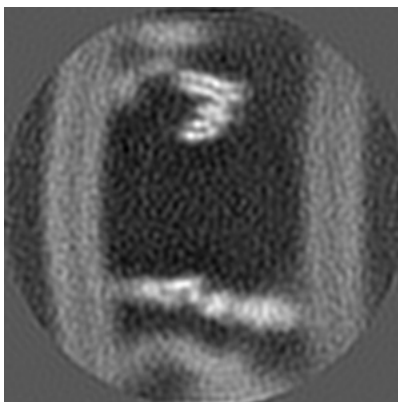
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

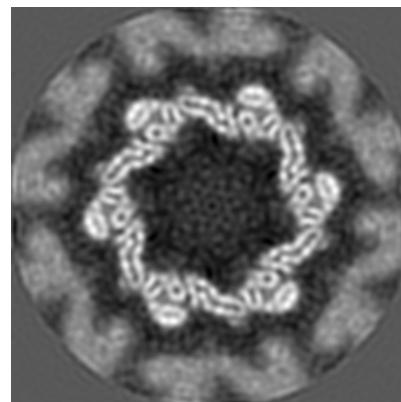
6.3.1 Primary map



X Index: 117

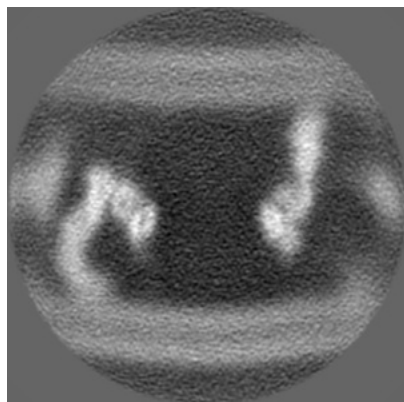


Y Index: 106

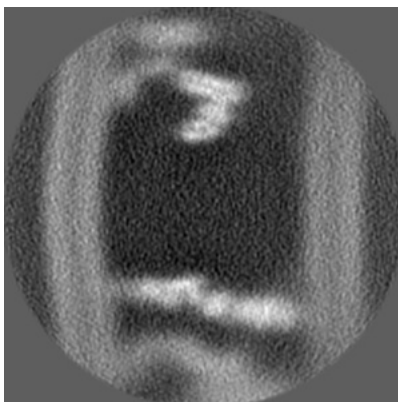


Z Index: 103

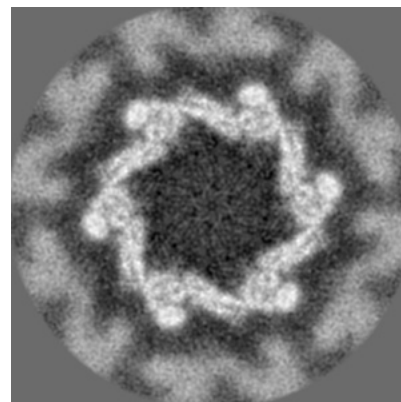
6.3.2 Raw map



X Index: 78



Y Index: 106

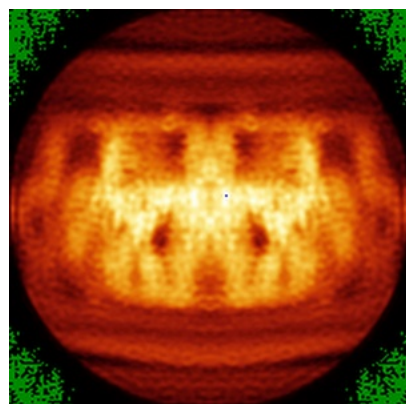


Z Index: 102

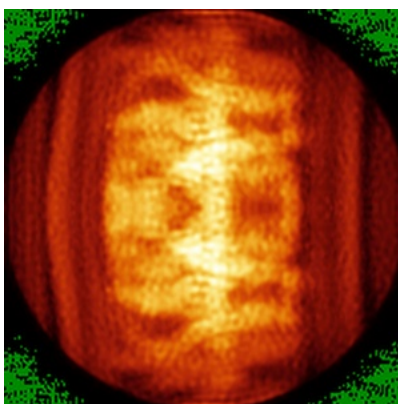
The images above show the largest variance slices of the map in three orthogonal directions.

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

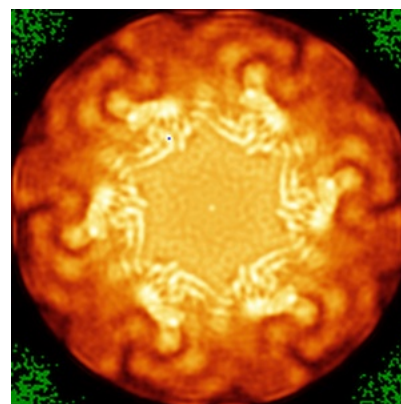
6.4.1 Primary map



X

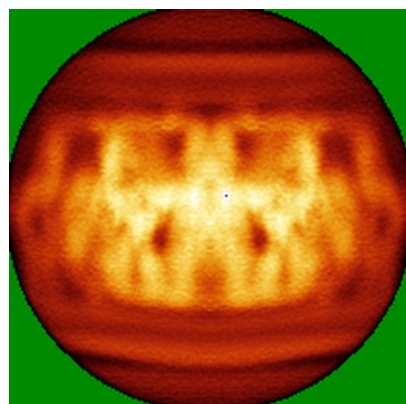


Y

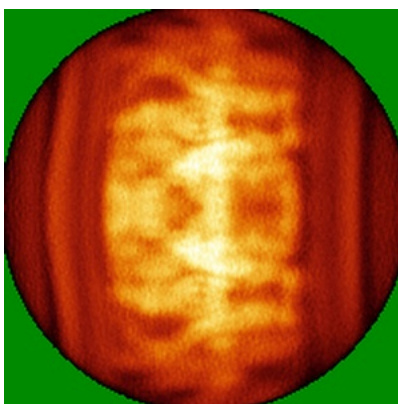


Z

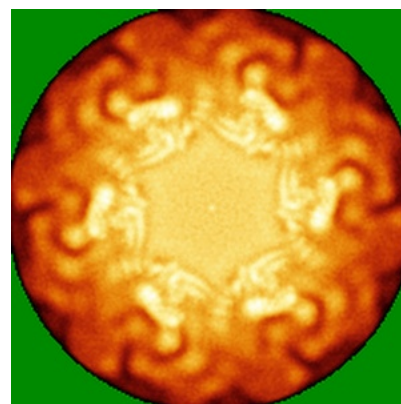
6.4.2 Raw map



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.

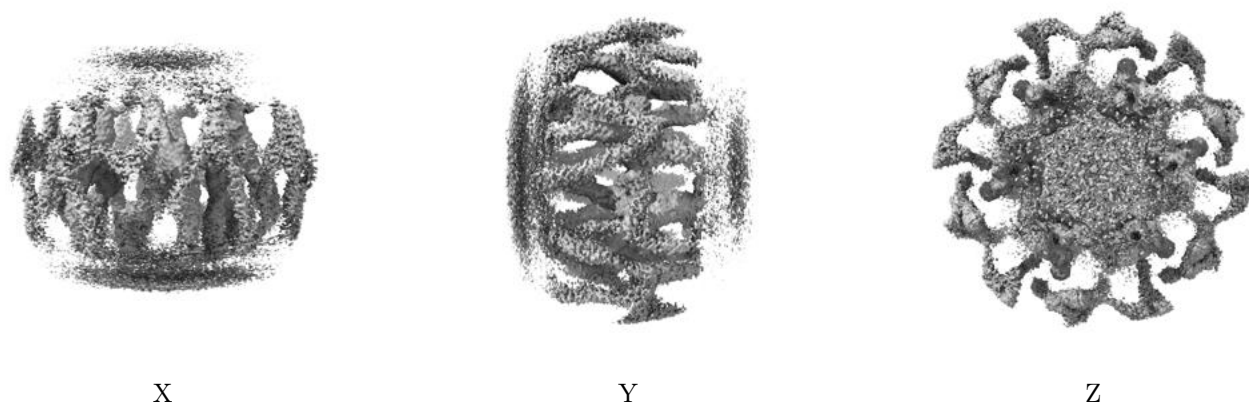
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

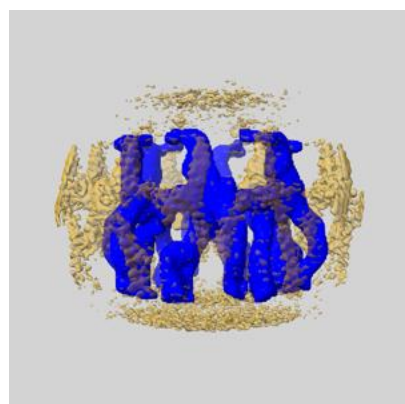
6.6 Mask visualisation [i](#)

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

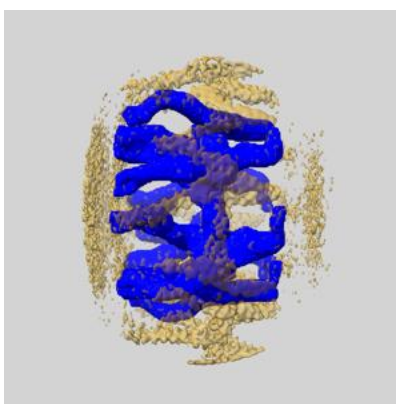
A mask typically either:

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

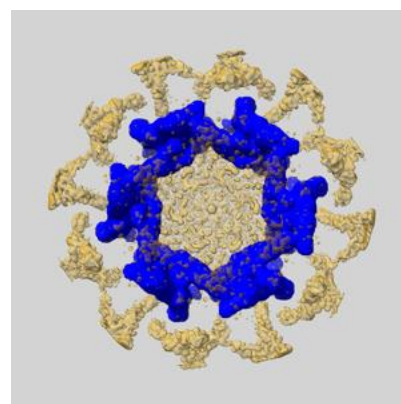
6.6.1 emd_25737_msk_1.map [i](#)



X



Y

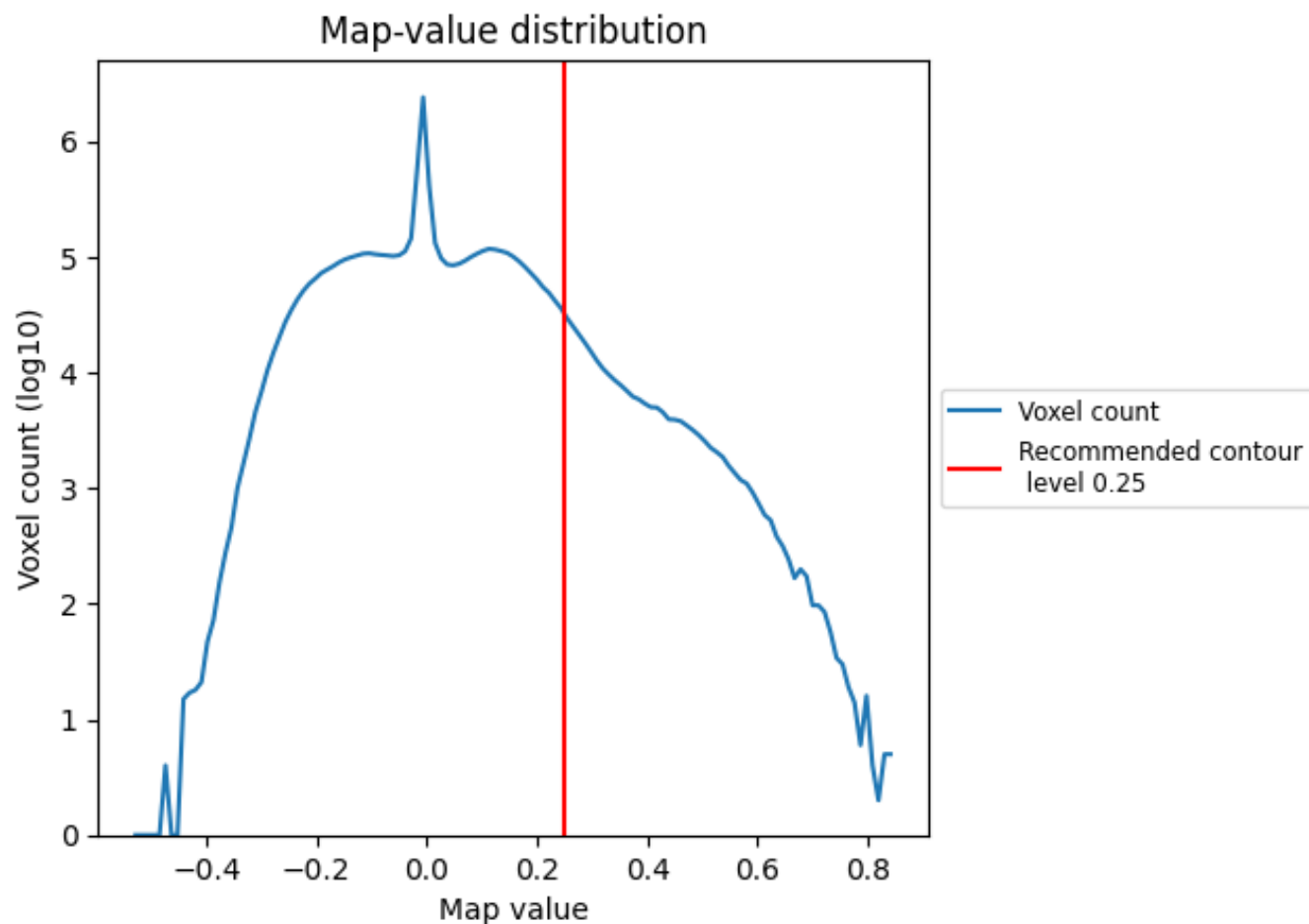


Z

7 Map analysis [i](#)

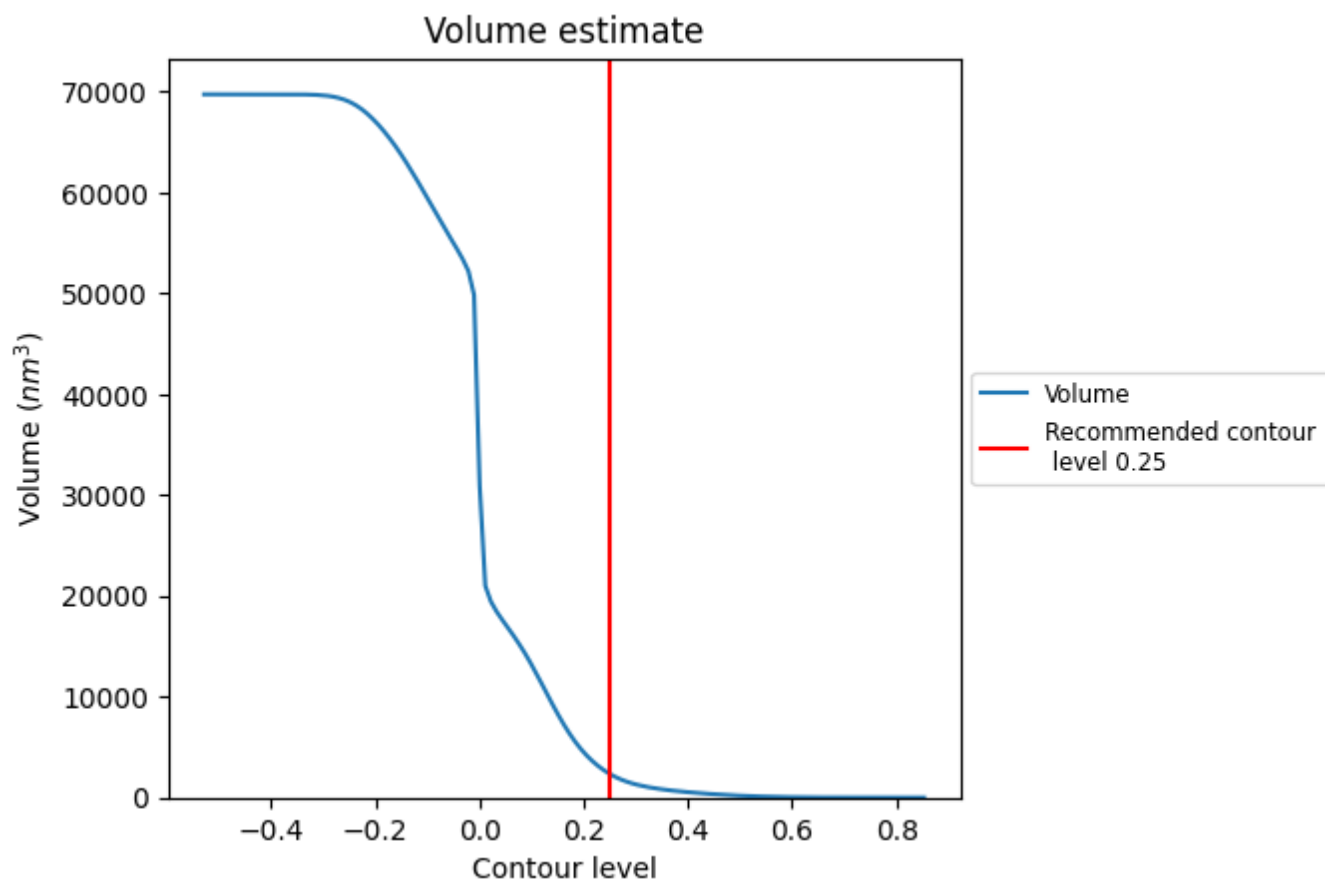
This section contains the results of statistical analysis of the map.

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.

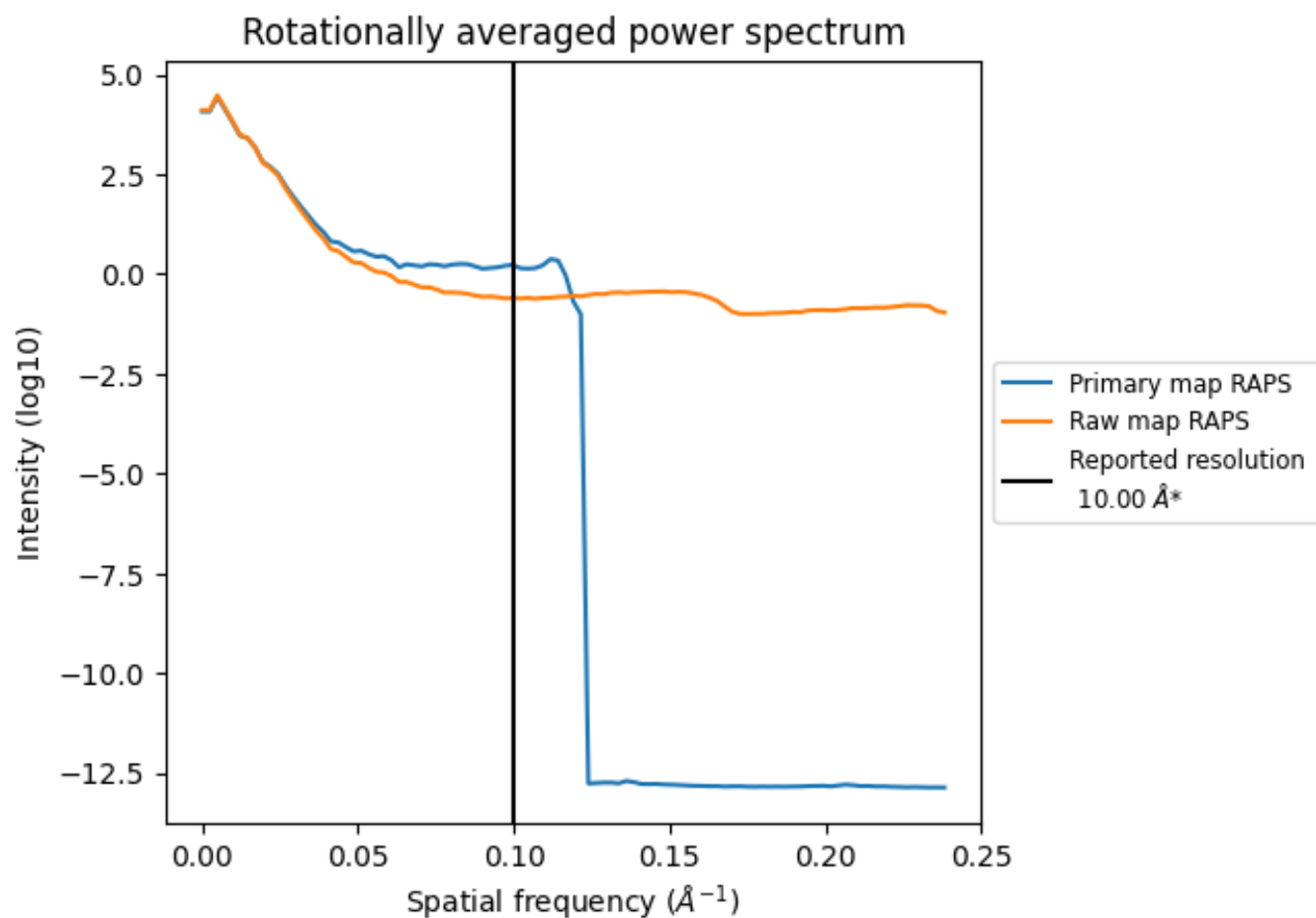
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2345 nm³; this corresponds to an approximate mass of 2118 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 ⓘ

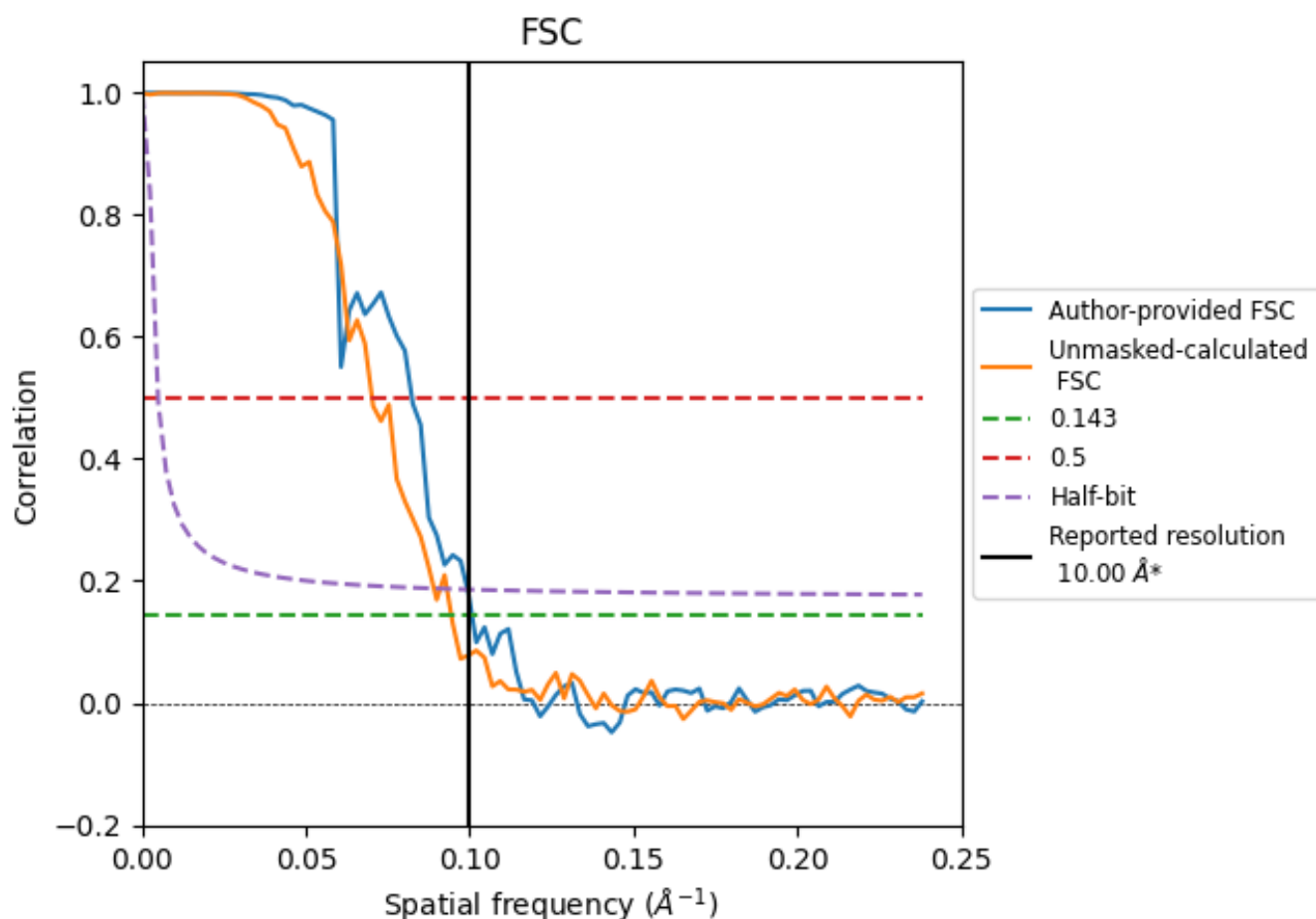


*Reported resolution corresponds to spatial frequency of 0.100 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.100 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

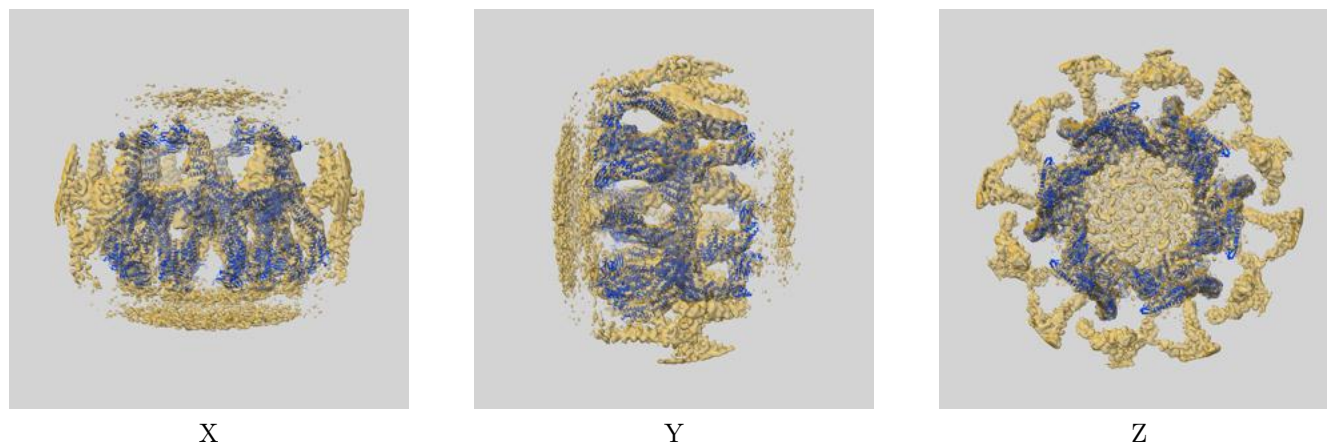
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.93	12.15	10.07
Unmasked-calculated*	10.59	14.27	11.24

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

9 Map-model fit [i](#)

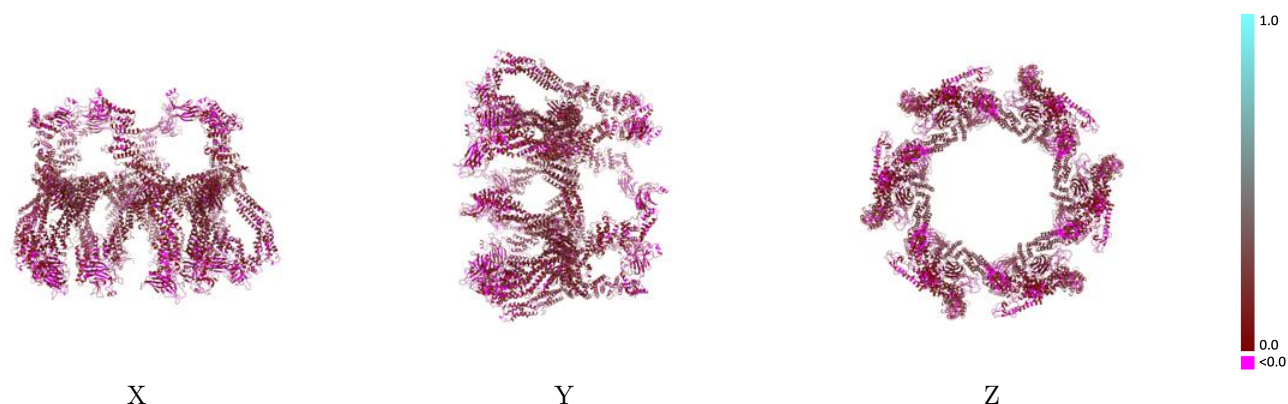
This section contains information regarding the fit between EMDB map EMD-25737 and PDB model 7T7C. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



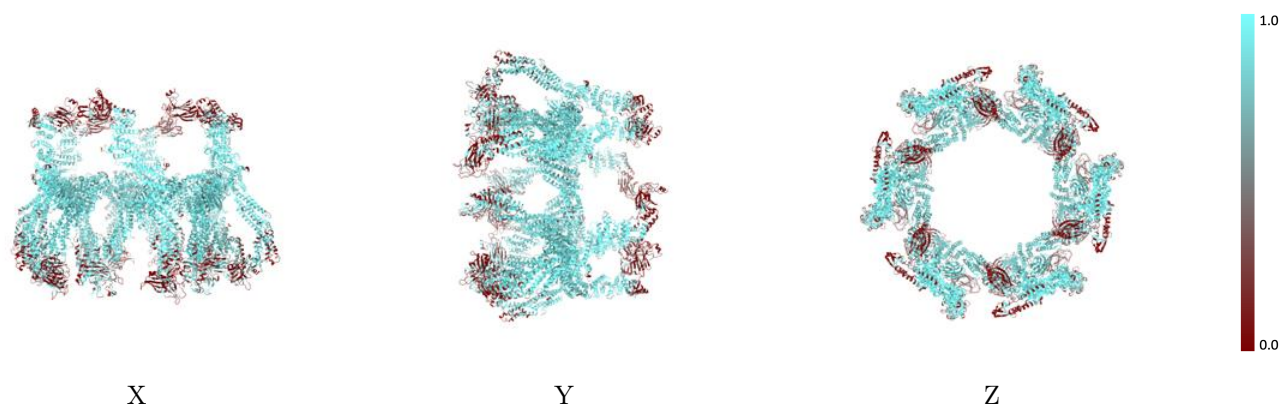
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



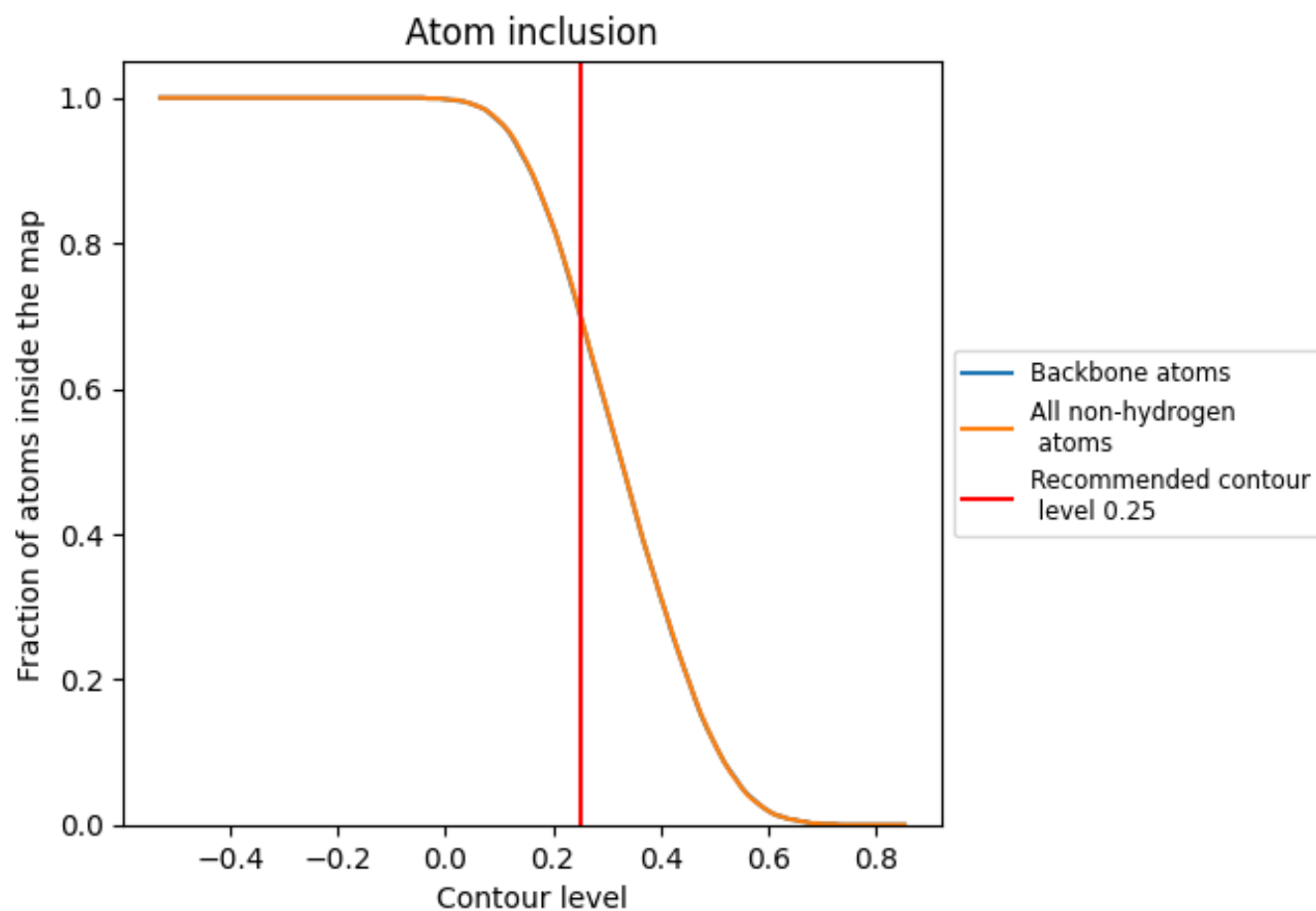
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.0990
A	0.7940	0.1160
B	0.6110	0.0830
C	0.7970	0.1160
D	0.7940	0.1160
E	0.7930	0.1160
F	0.7960	0.1160
G	0.7940	0.1160
H	0.6100	0.0820
I	0.6100	0.0820
J	0.6110	0.0830
K	0.6100	0.0820
L	0.6110	0.0820

