



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:25 AM UTC

PDB ID : 5KZ5 / pdb_00005kz5
EMDB ID : EMD-8301
Title : Architecture of the Human Mitochondrial Iron-Sulfur Cluster Assembly Machinery: the Complex Formed by the Iron Donor, the Sulfur Donor, and the Scaffold
Authors : Gakh, O.; Ranatunga, W.; Smith, D.Y.; Ahlgren, E.C.; Al-Karadaghi, S.; Thompson, J.R.; Isaya, G.
Deposited on : 2016-07-22
Resolution : 14.30 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

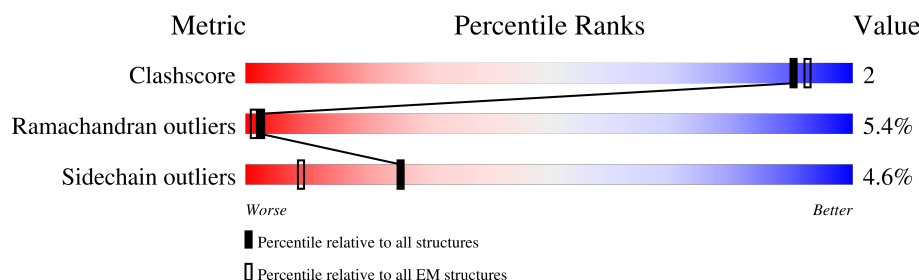
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.30 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	1	391	51% 73% 21% 6% .
1	2	391	54% 81% 15% .
1	3	391	59% 79% 17% .
1	4	391	50% 75% 22% ..
1	M	391	56% 79% 19% .
1	N	391	60% 80% 19% .
1	O	391	63% 75% 22% .
1	P	391	59% 79% 19% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	391	
1	R	391	
1	S	391	
1	T	391	
2	A	169	
2	B	169	
2	C	169	
2	D	169	
2	E	169	
2	F	169	
2	G	169	
2	H	169	
2	I	169	
2	J	169	
2	K	169	
2	L	169	
3	a	118	
3	b	118	
3	c	118	
3	d	118	
3	e	118	
3	f	118	
3	g	118	
3	h	118	
3	i	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	j	118	58% 66% 31% •
3	k	118	53% 86% 13% •
3	l	118	53% 83% 14% ••

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 62880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cysteine desulfurase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	2	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	3	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	4	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	M	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	N	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	O	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	P	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	Q	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	R	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	S	391	Total 3040	C 1905	N 540	O 576	S 19	0	0
1	T	391	Total 3040	C 1905	N 540	O 576	S 19	0	0

- Molecule 2 is a protein called Frataxin, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	169	Total 1328	C 837	N 225	O 264	S 2	0	0
2	B	169	Total 1328	C 837	N 225	O 264	S 2	0	0
2	C	169	Total 1328	C 837	N 225	O 264	S 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	E	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	F	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	G	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	H	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	I	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	J	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	K	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		
2	L	169	Total	C	N	O	S	0	0
			1328	837	225	264	2		

- Molecule 3 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	b	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	c	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	d	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	e	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	f	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	g	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	h	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	i	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	j	118	Total	C	N	O	S	0	0
			872	549	147	170	6		

Continued on next page...

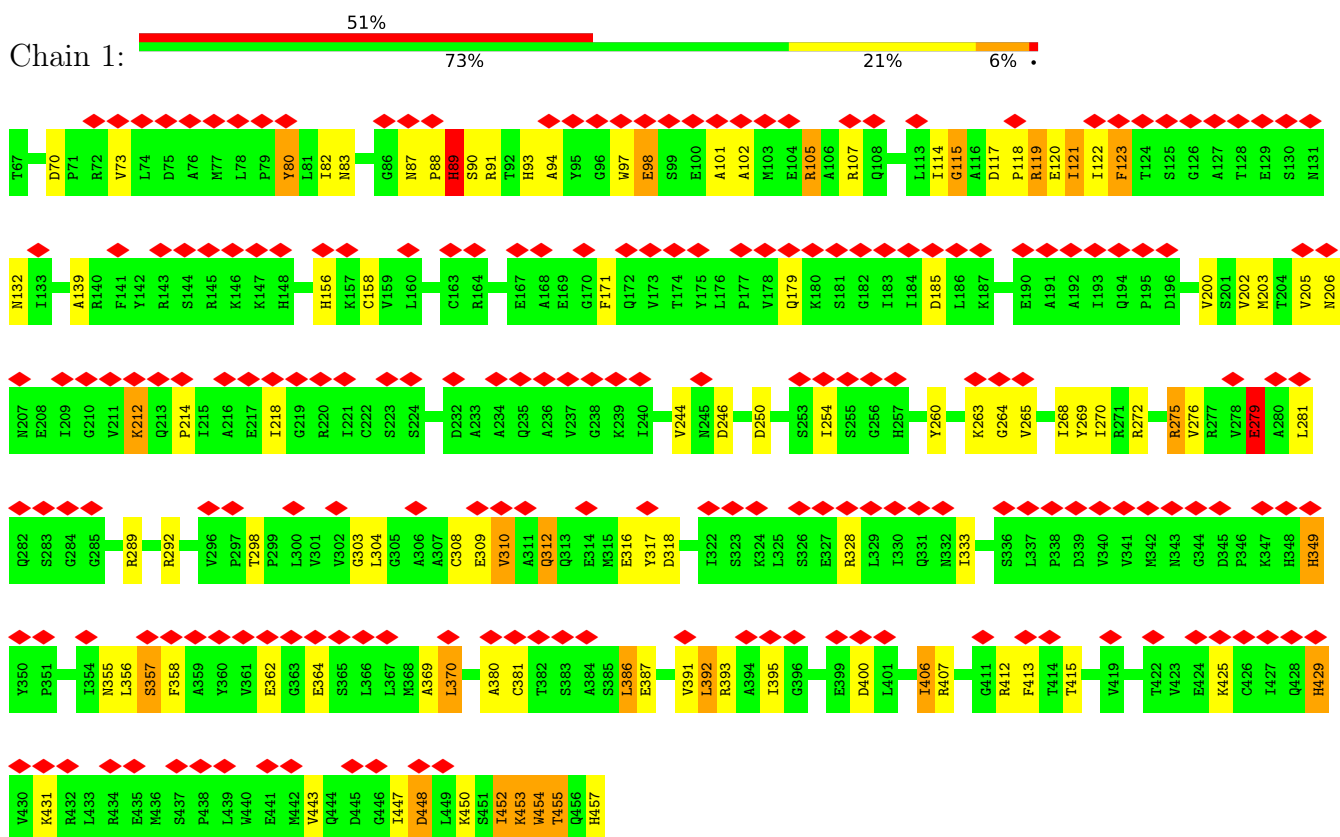
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	k	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	l	118	Total	C	N	O	S	0	0
			872	549	147	170	6		

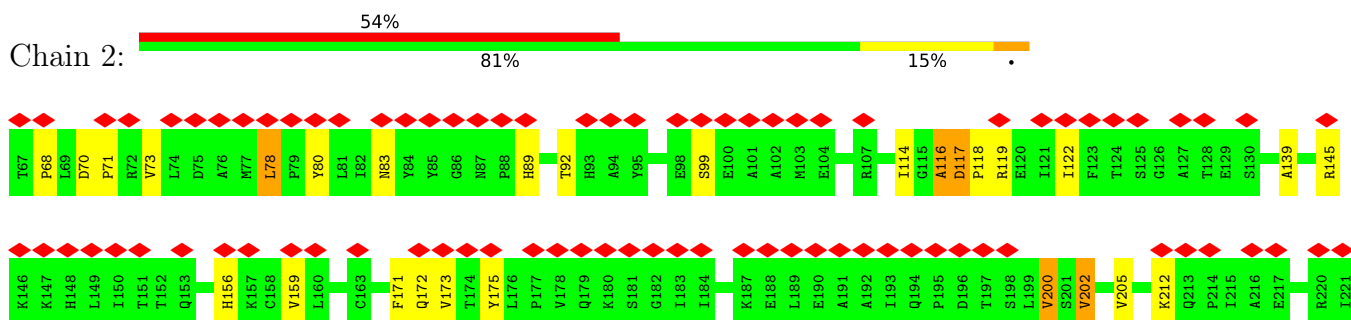
3 Residue-property plots

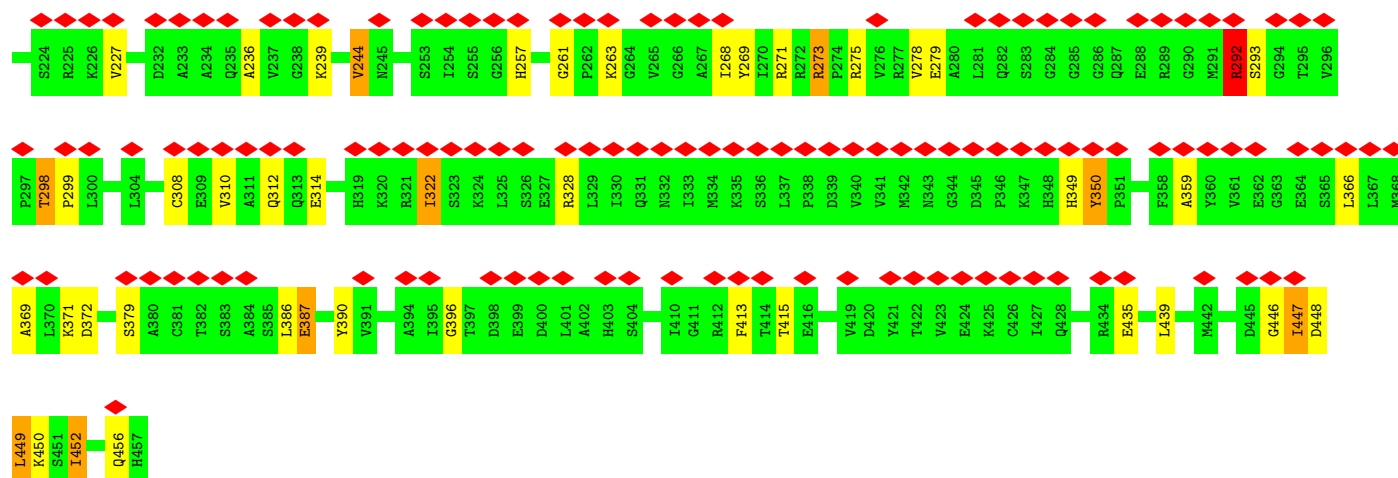
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

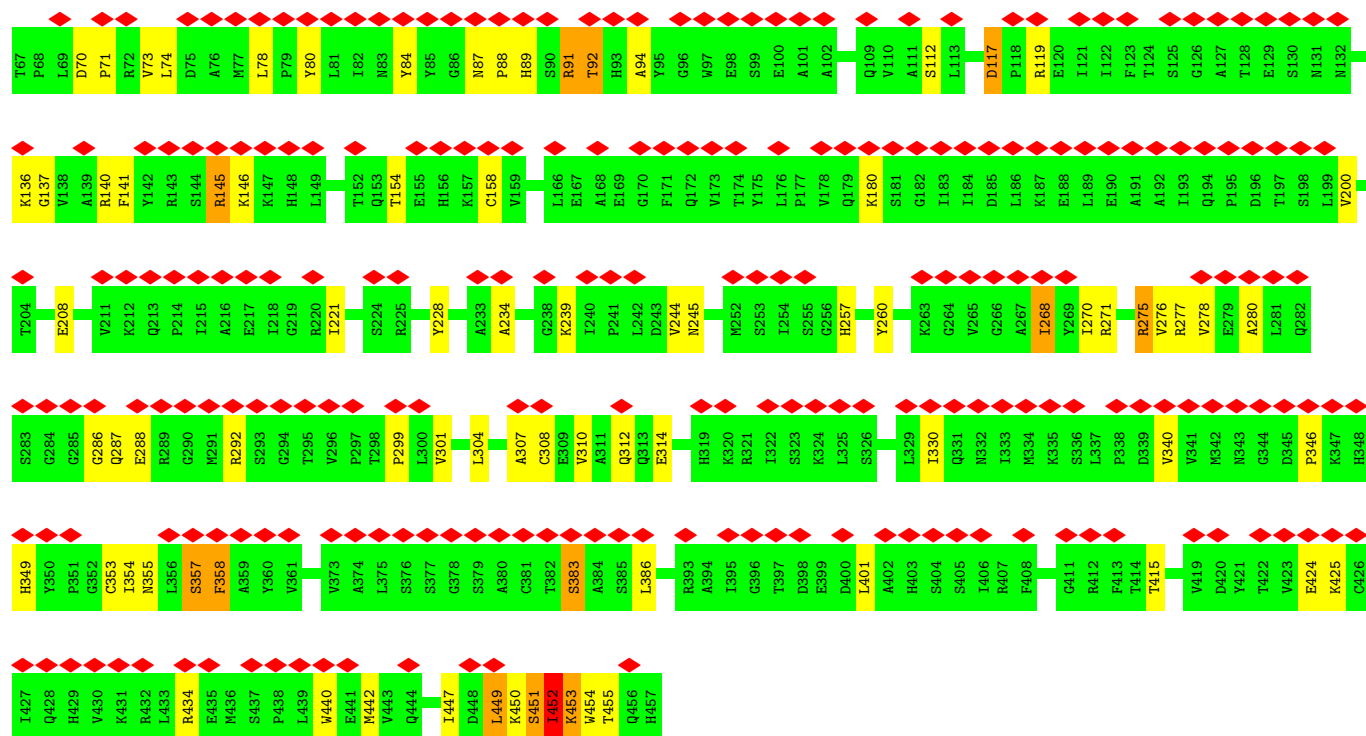
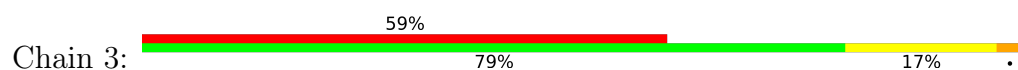


- Molecule 1: Cysteine desulfurase, mitochondrial

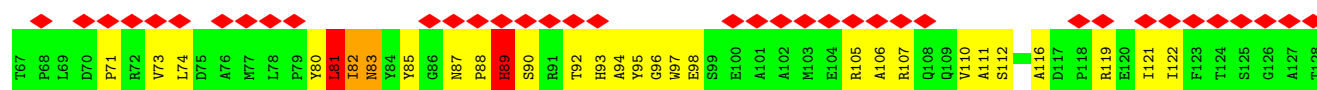
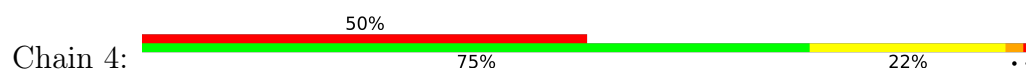


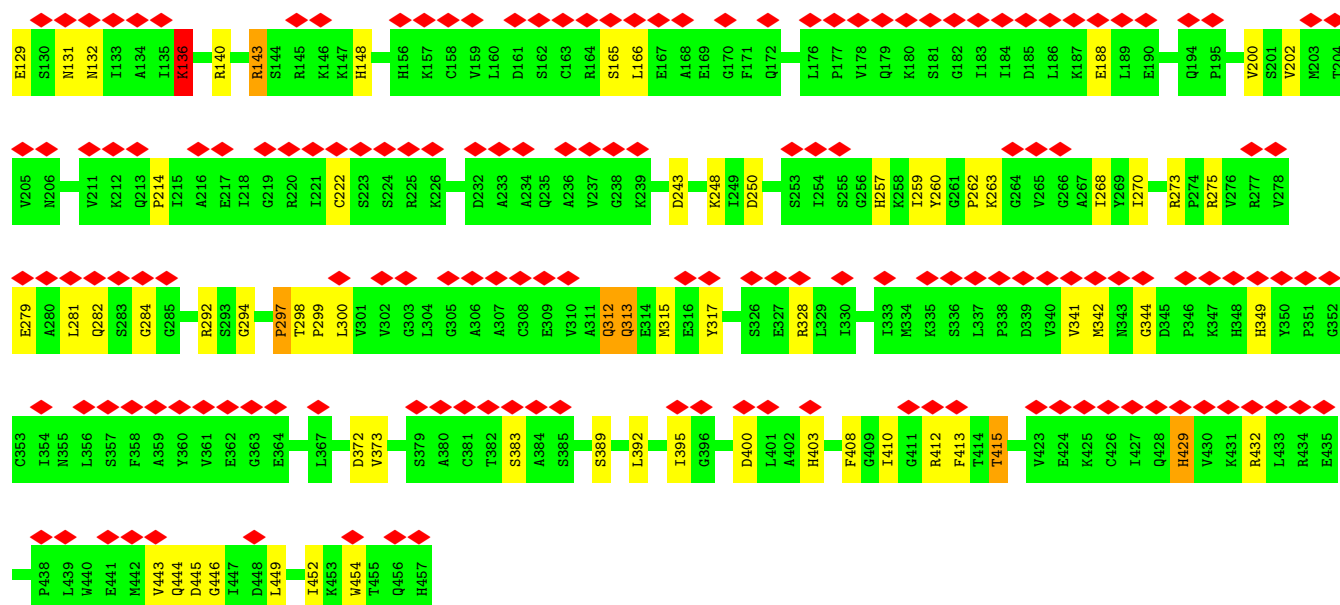


- Molecule 1: Cysteine desulfurase, mitochondrial

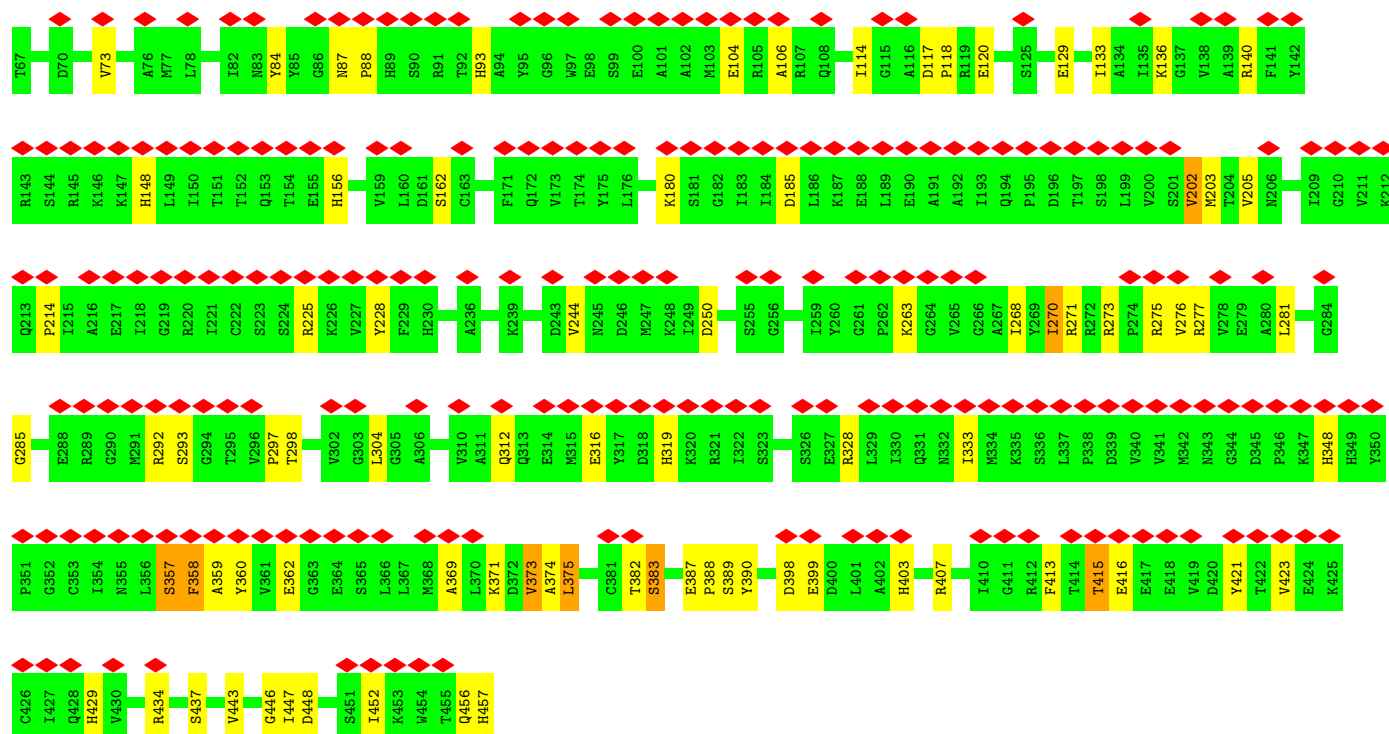
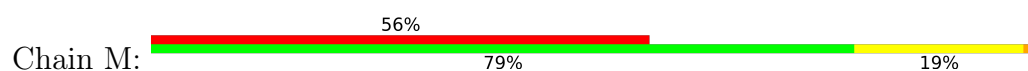


- Molecule 1: Cysteine desulfurase, mitochondrial



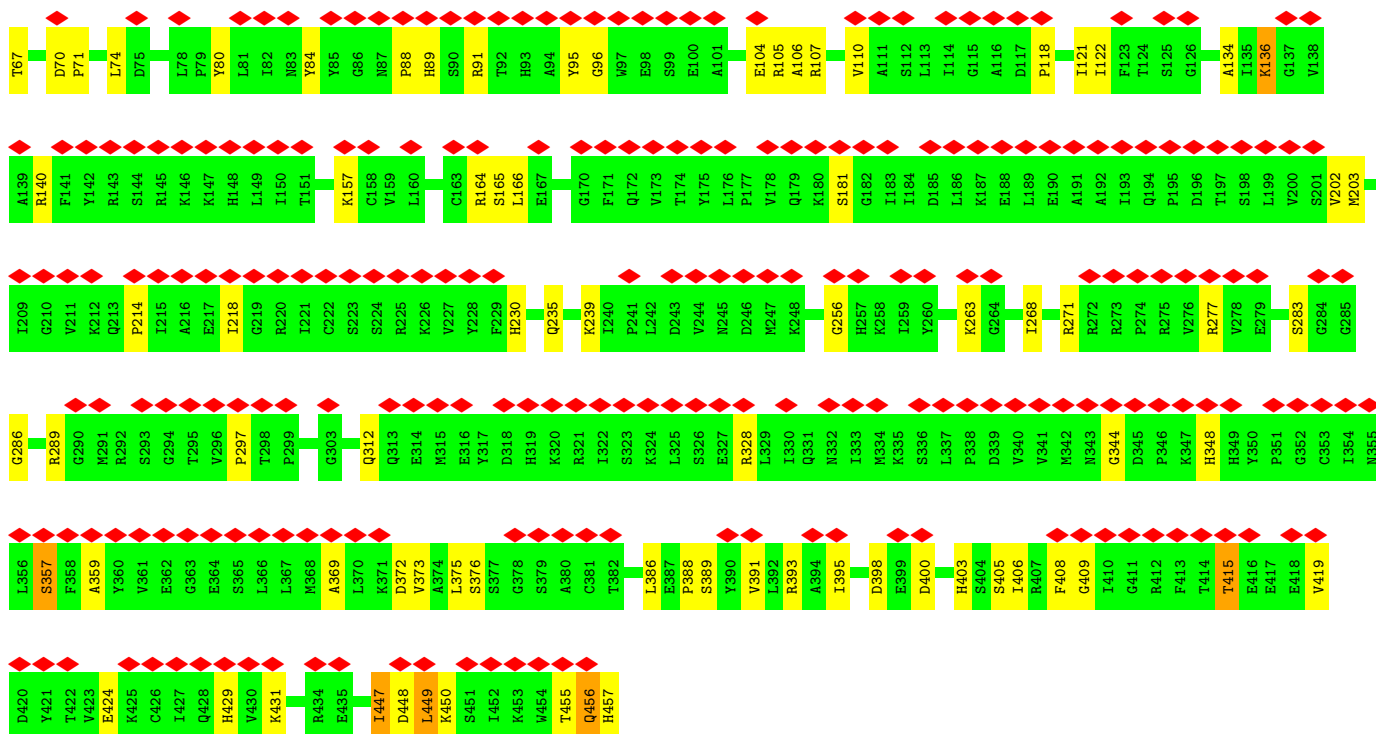


• Molecule 1: Cysteine desulfurase, mitochondrial

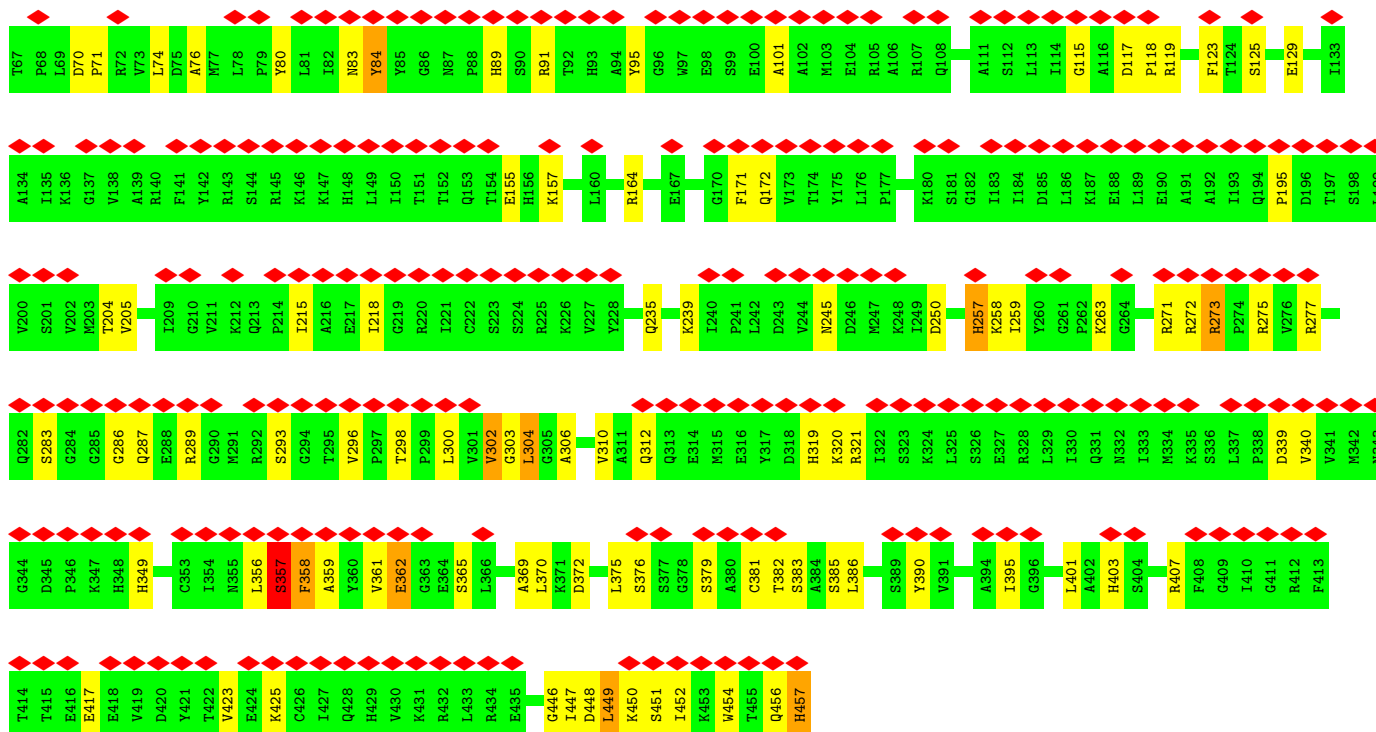
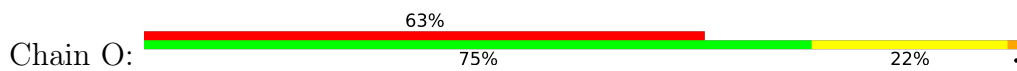


• Molecule 1: Cysteine desulfurase, mitochondrial

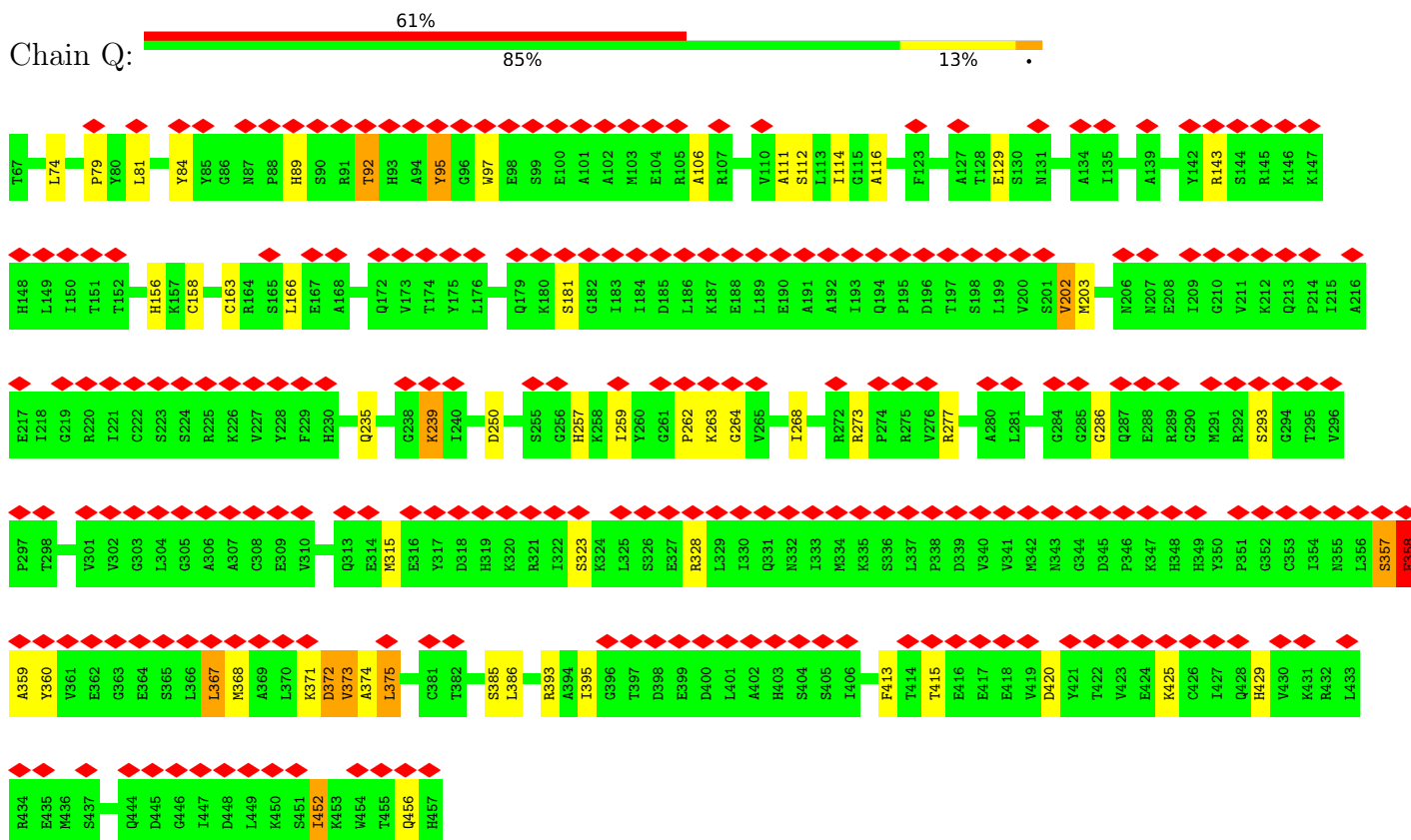




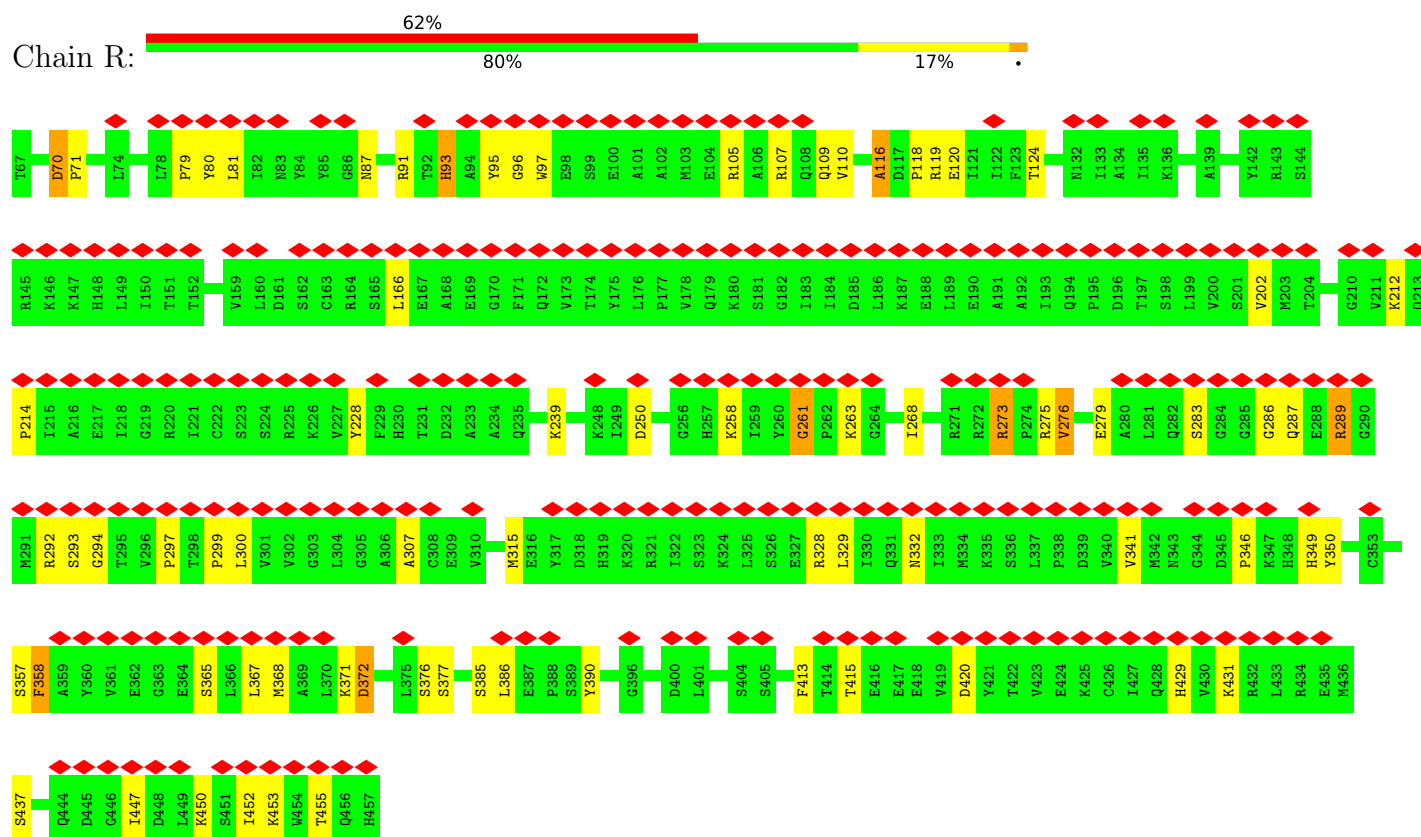
• Molecule 1: Cysteine desulfurase, mitochondrial



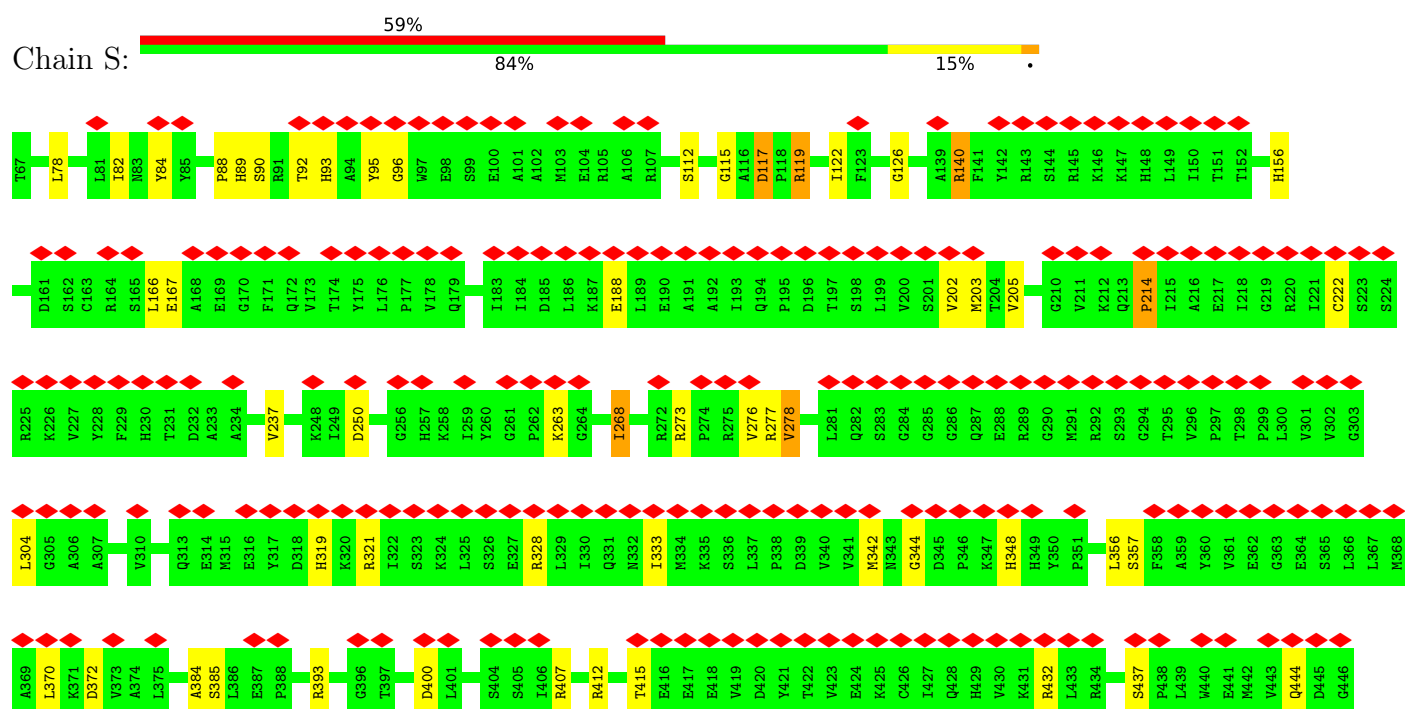
• Molecule 1: Cysteine desulfurase, mitochondrial



- Molecule 1: Cysteine desulfurase, mitochondrial

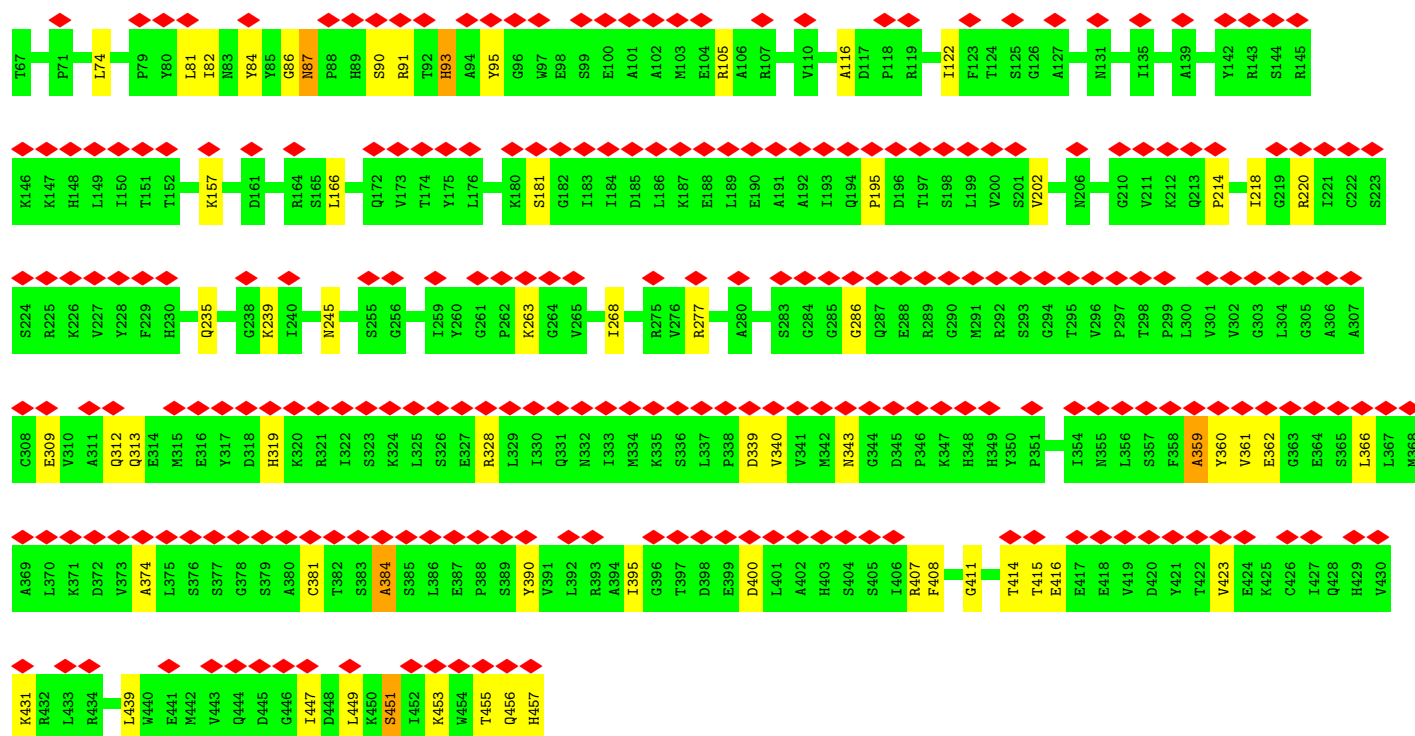
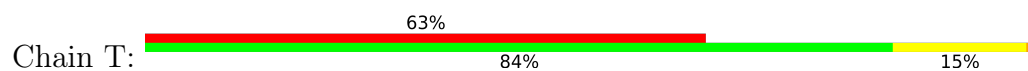


- Molecule 1: Cysteine desulfurase, mitochondrial

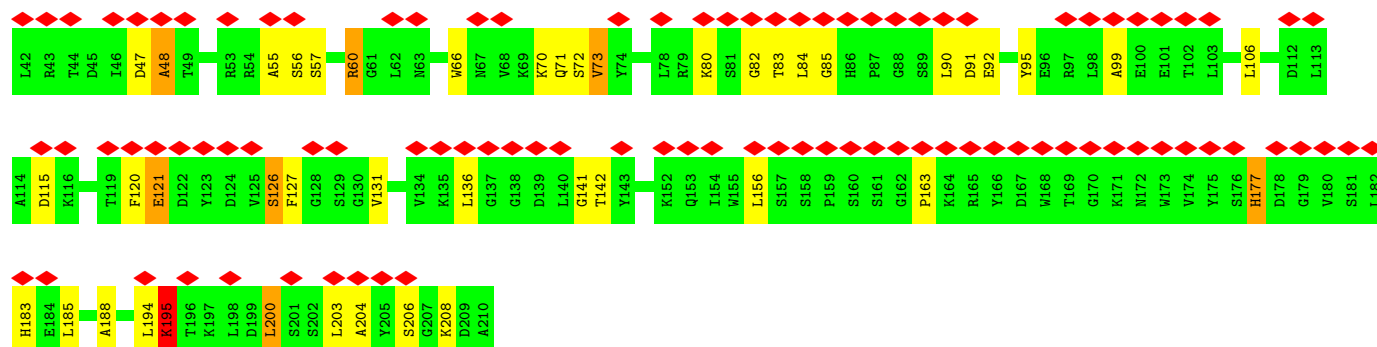
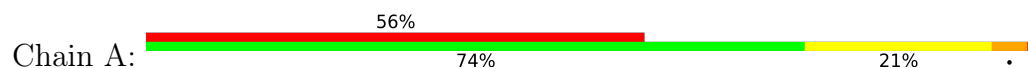




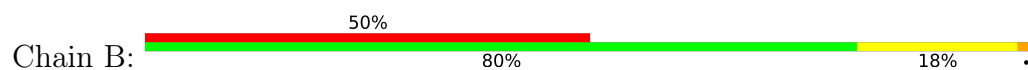
• Molecule 1: Cysteine desulfurase, mitochondrial

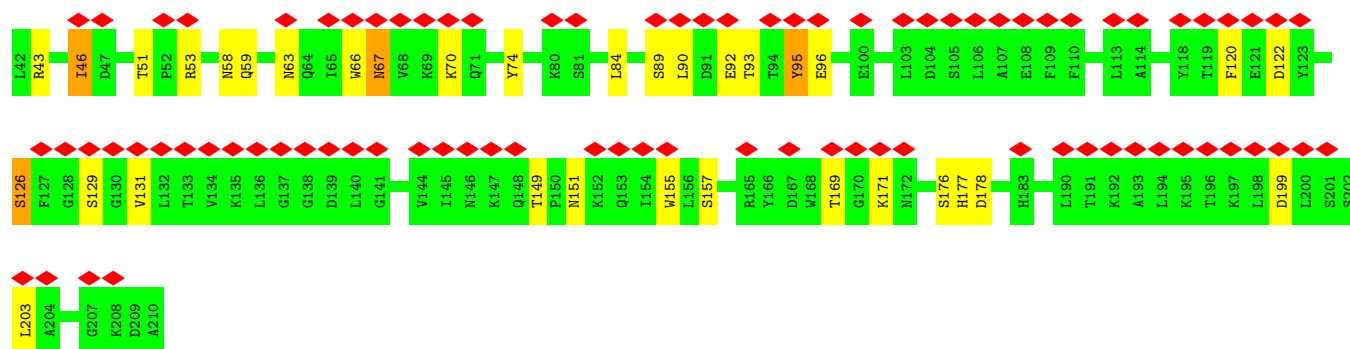


• Molecule 2: Frataxin, mitochondrial

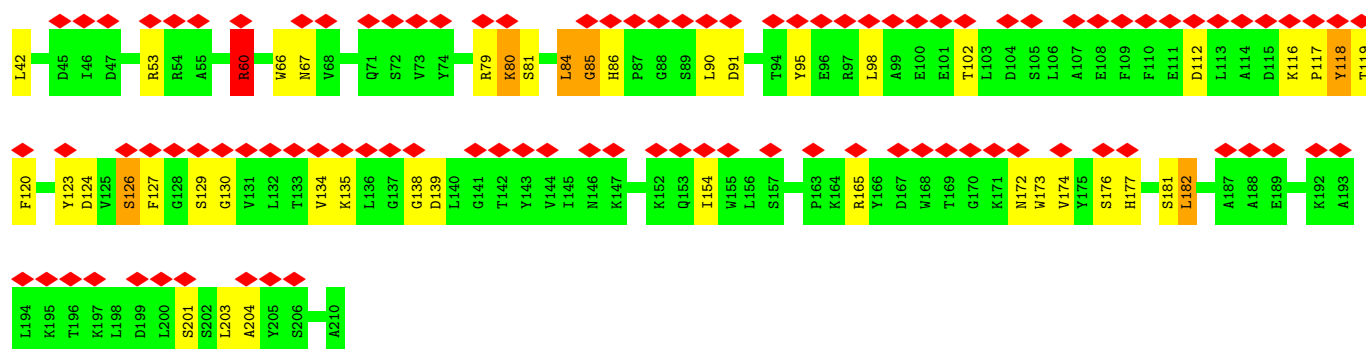
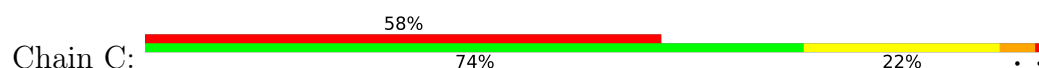


• Molecule 2: Frataxin, mitochondrial

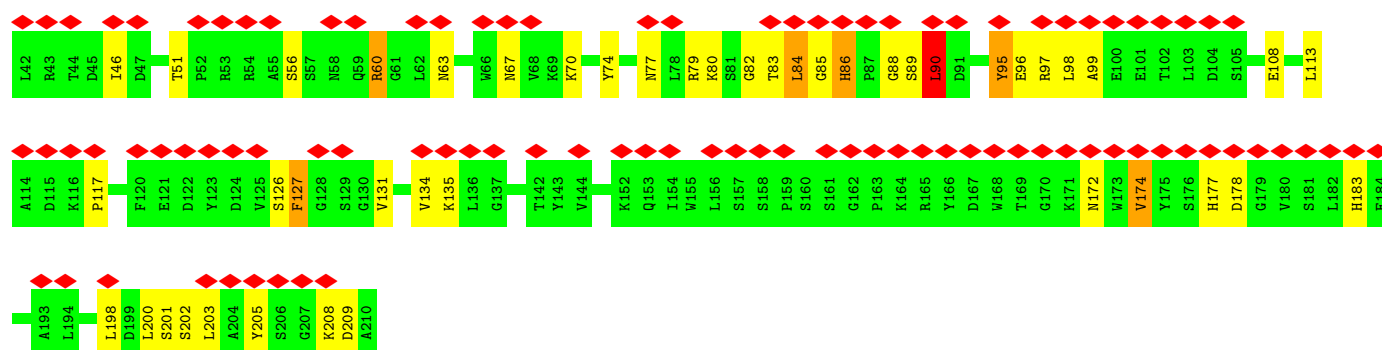
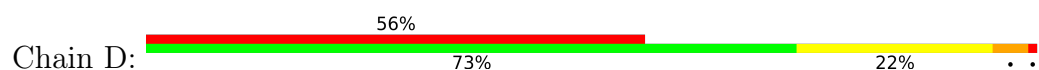




• Molecule 2: Frataxin, mitochondrial

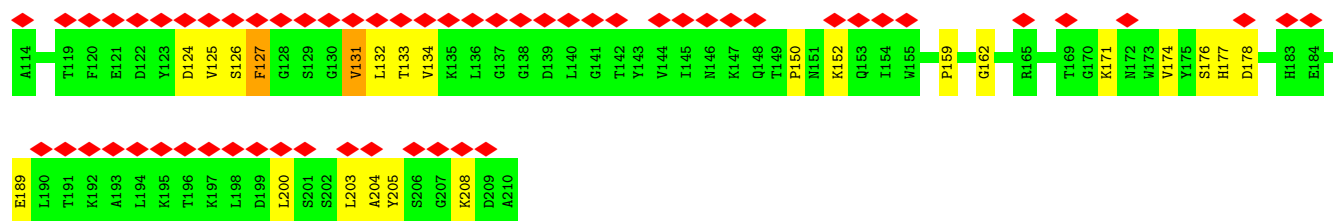


• Molecule 2: Frataxin, mitochondrial

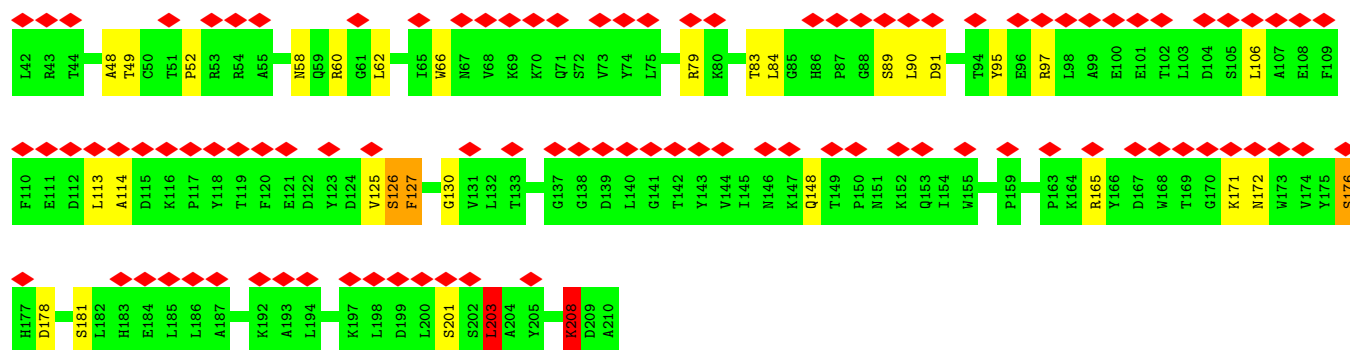
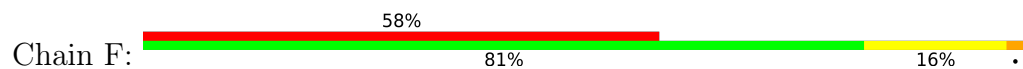


• Molecule 2: Frataxin, mitochondrial

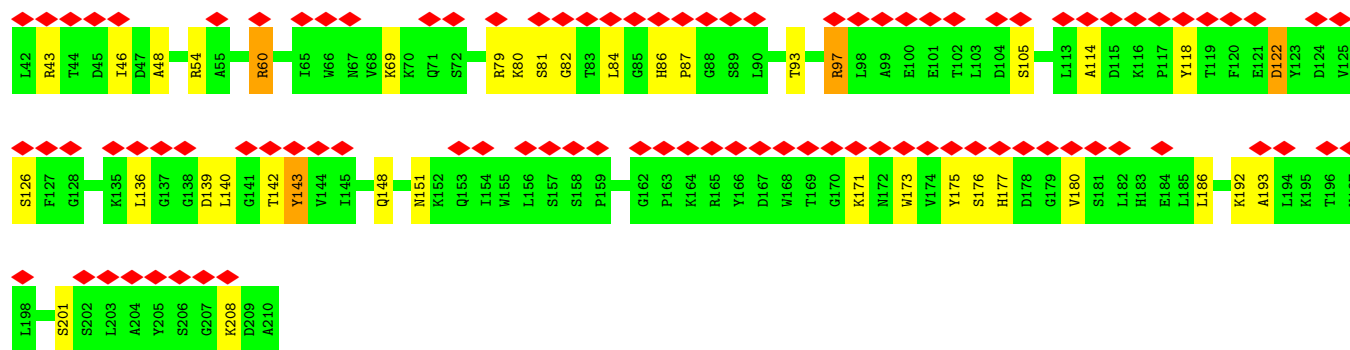
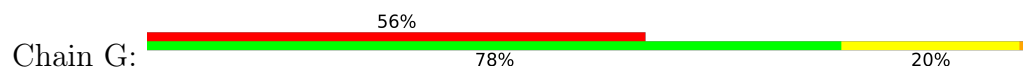




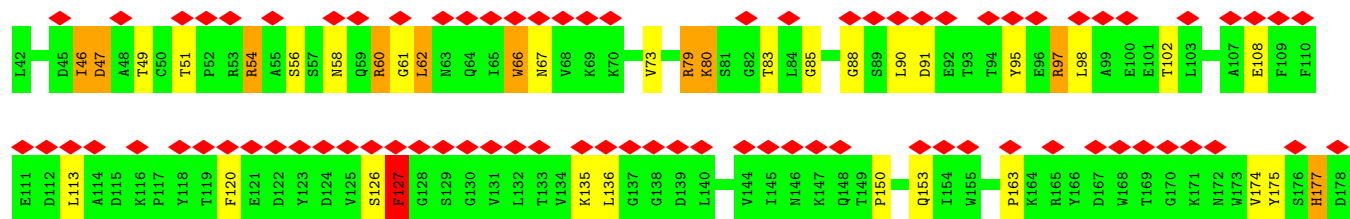
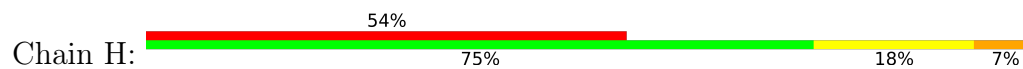
• Molecule 2: Frataxin, mitochondrial

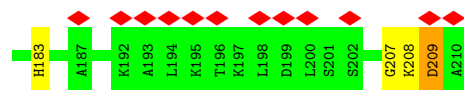


• Molecule 2: Frataxin, mitochondrial

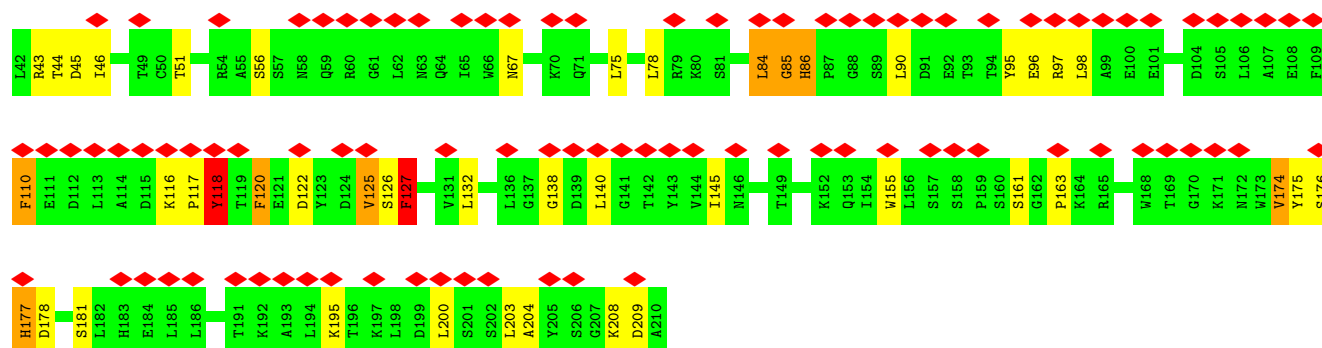


• Molecule 2: Frataxin, mitochondrial

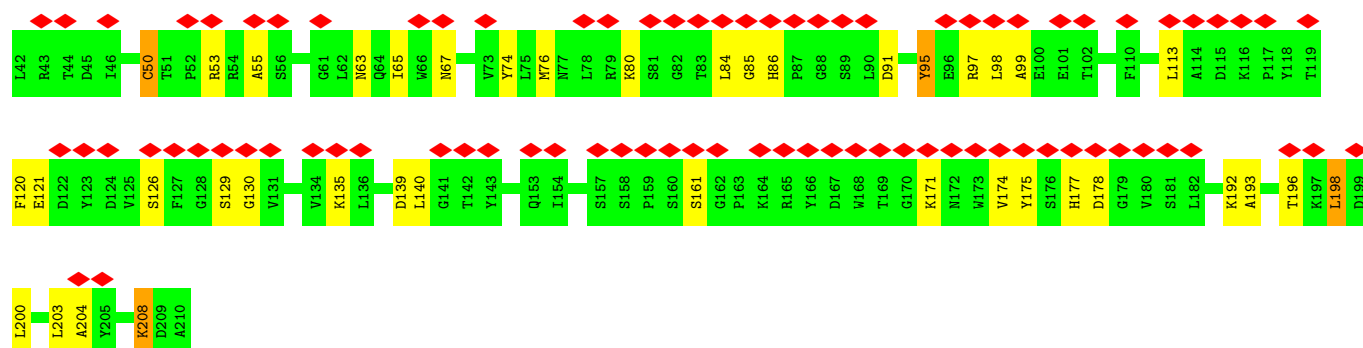
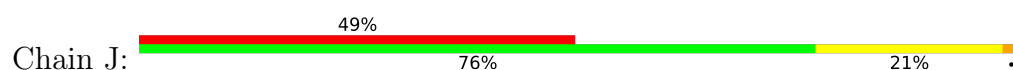




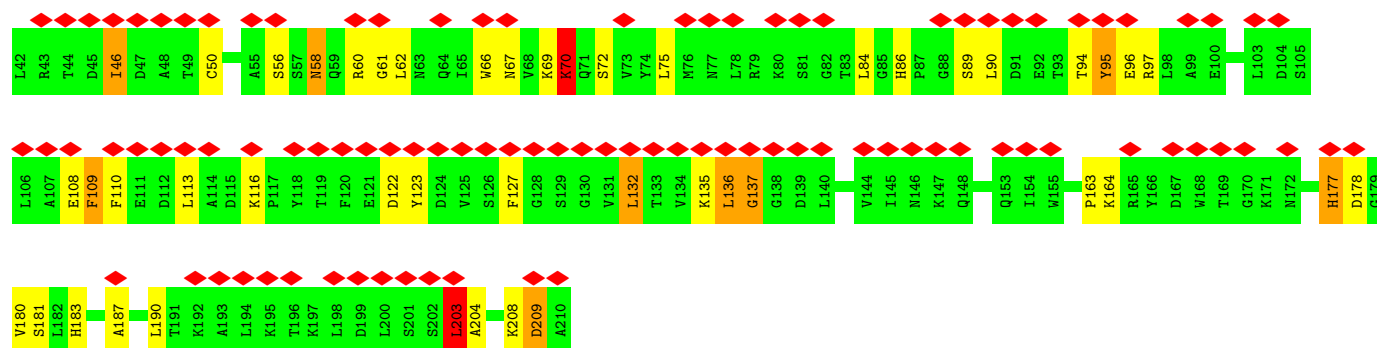
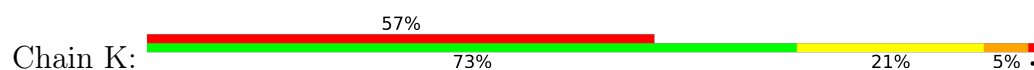
• Molecule 2: Frataxin, mitochondrial



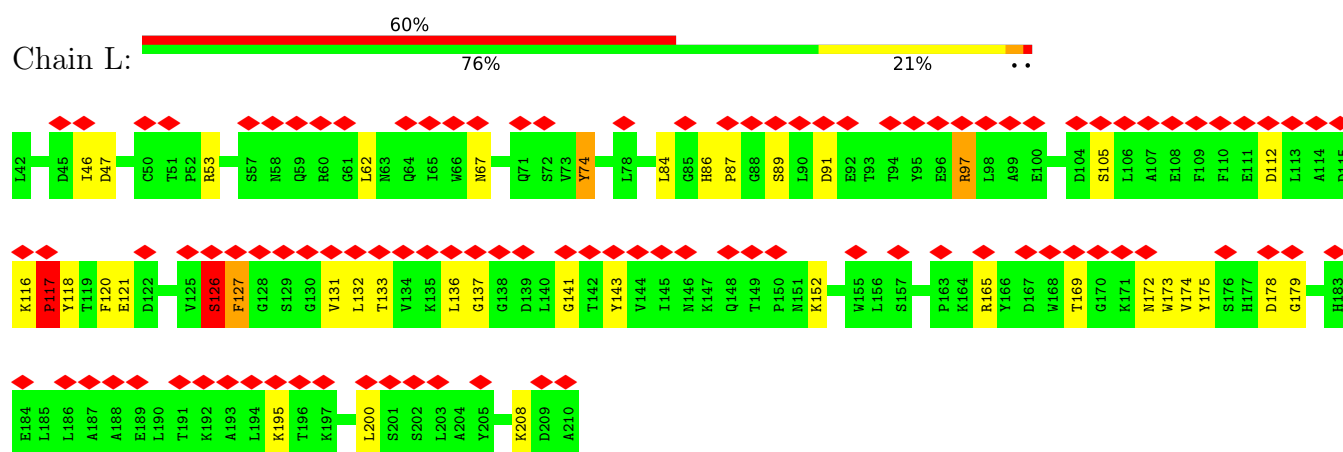
• Molecule 2: Frataxin, mitochondrial



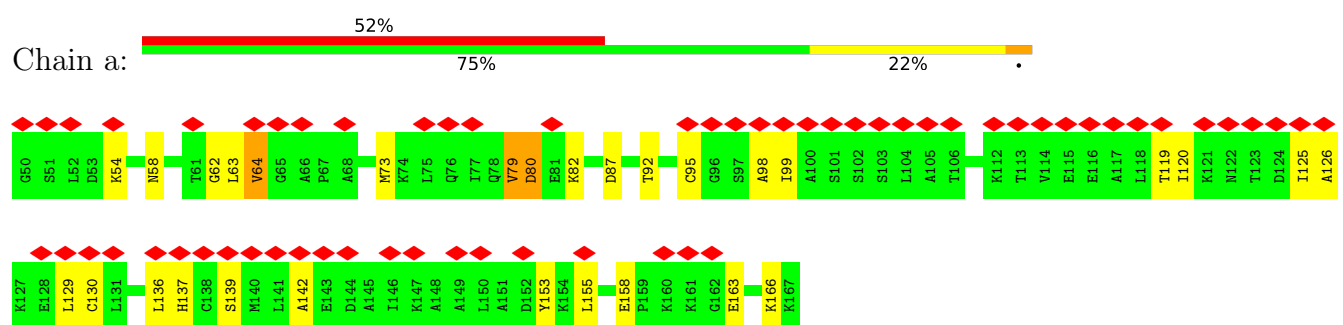
• Molecule 2: Frataxin, mitochondrial



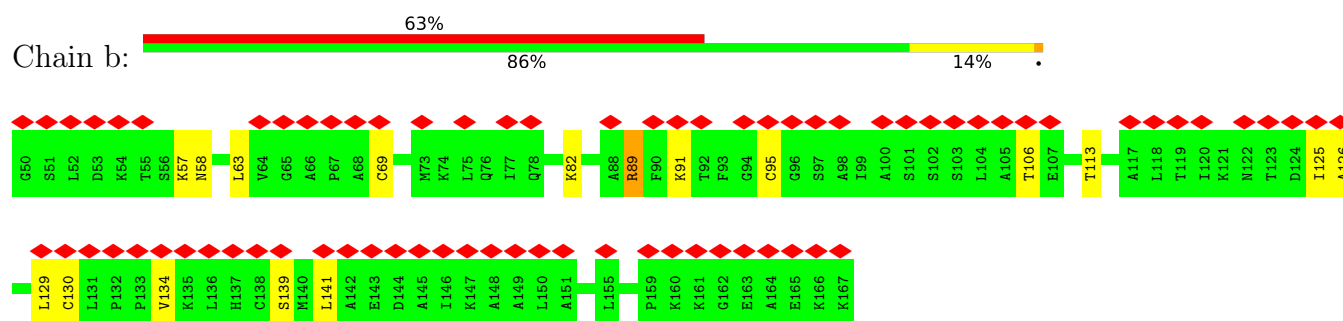
• Molecule 2: Frataxin, mitochondrial



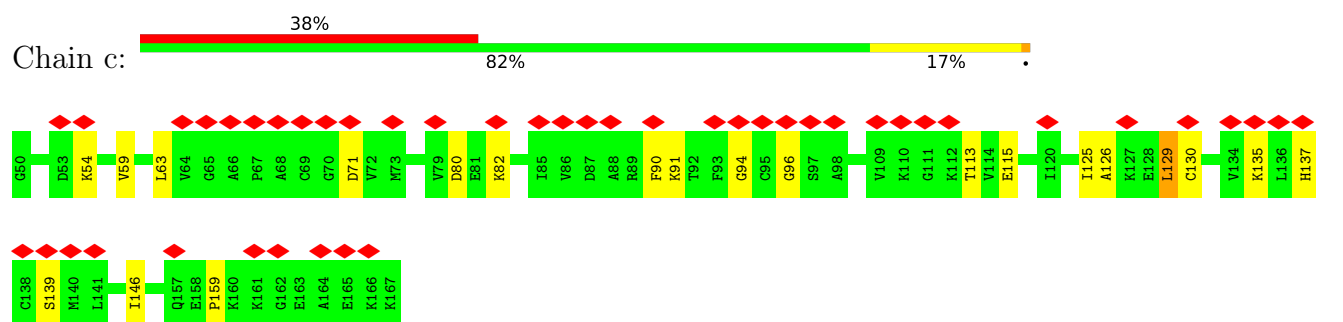
• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

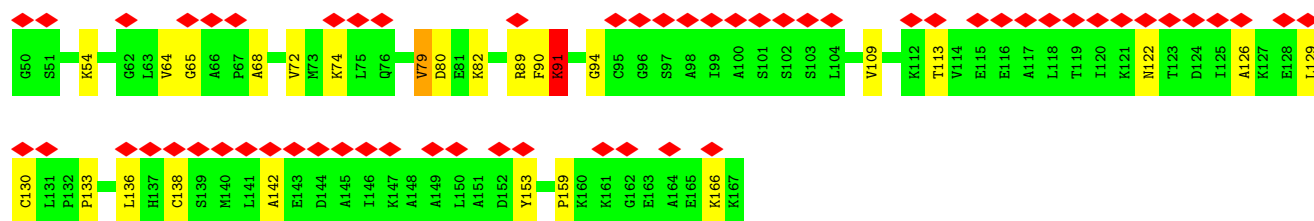


• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

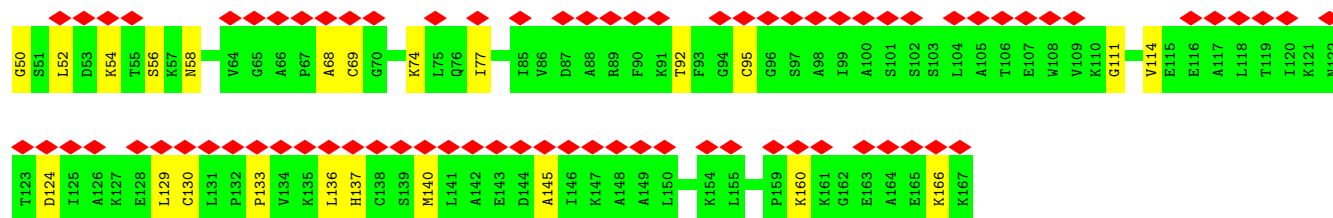
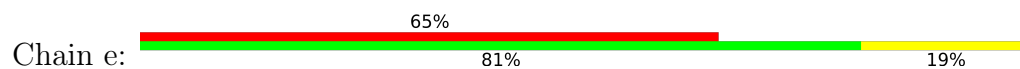


• Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

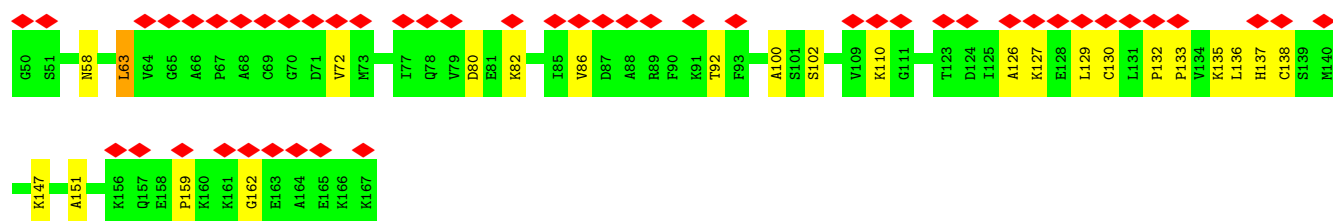
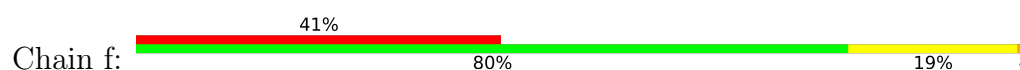




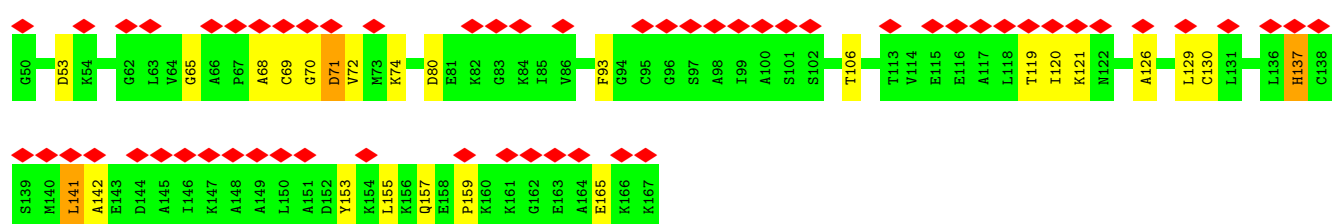
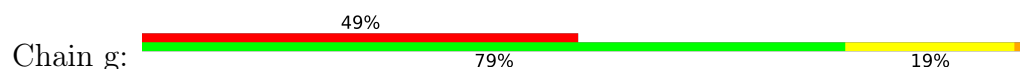
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



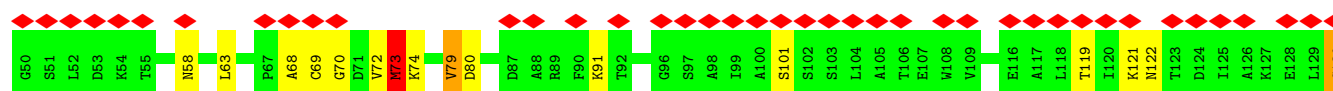
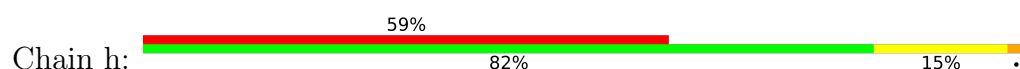
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

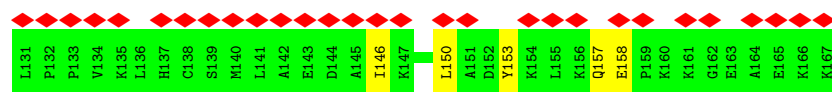


- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

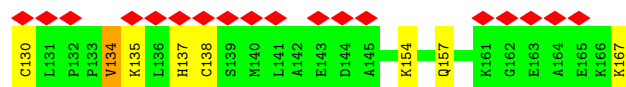
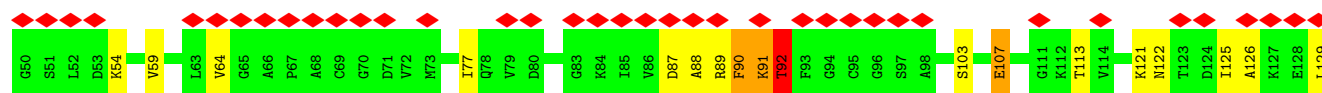
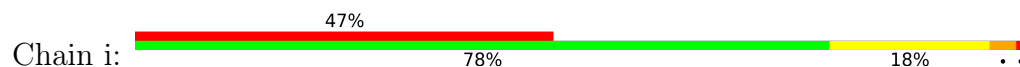


- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial

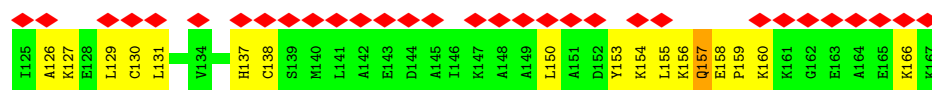
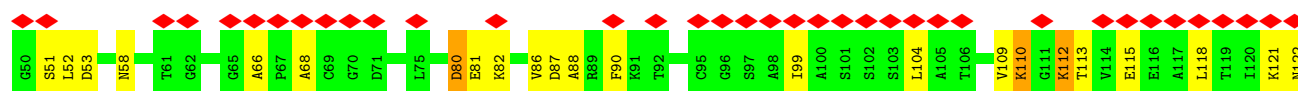




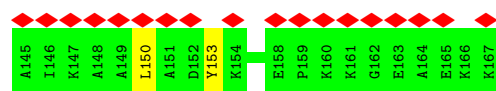
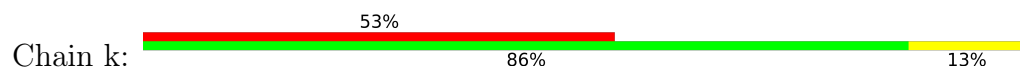
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



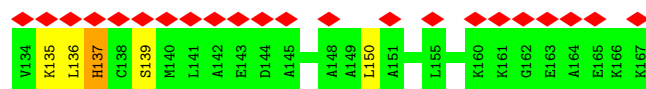
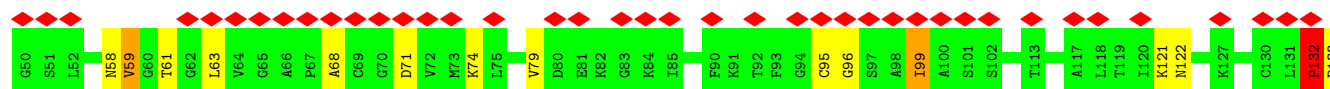
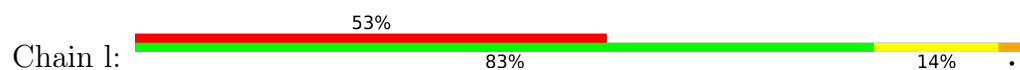
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	4124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; The ctf.auto function from EMAN2 was applied.	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	210	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	115000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	8.552	Depositor
Minimum map value	0.000	Depositor
Average map value	0.316	Depositor
Map value standard deviation	0.812	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	124.3, 181.5, 181.5	wwPDB
Map dimensions	113, 165, 165	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	1.43	4/3096 (0.1%)	1.88	82/4185 (2.0%)
1	2	1.45	3/3096 (0.1%)	1.86	58/4185 (1.4%)
1	3	1.48	8/3096 (0.3%)	1.90	72/4185 (1.7%)
1	4	1.44	4/3096 (0.1%)	1.90	87/4185 (2.1%)
1	M	1.48	5/3096 (0.2%)	1.87	77/4185 (1.8%)
1	N	1.46	8/3096 (0.3%)	1.84	81/4185 (1.9%)
1	O	1.46	8/3096 (0.3%)	1.94	80/4185 (1.9%)
1	P	1.45	5/3096 (0.2%)	1.88	74/4185 (1.8%)
1	Q	1.46	3/3096 (0.1%)	1.82	53/4185 (1.3%)
1	R	1.47	3/3096 (0.1%)	1.85	62/4185 (1.5%)
1	S	1.49	5/3096 (0.2%)	1.82	51/4185 (1.2%)
1	T	1.48	6/3096 (0.2%)	1.82	48/4185 (1.1%)
2	A	1.41	3/1356 (0.2%)	1.86	49/1838 (2.7%)
2	B	1.40	1/1356 (0.1%)	1.75	21/1838 (1.1%)
2	C	1.43	3/1356 (0.2%)	1.92	36/1838 (2.0%)
2	D	1.43	0/1356	1.87	45/1838 (2.4%)
2	E	1.42	3/1356 (0.2%)	1.85	36/1838 (2.0%)
2	F	1.44	1/1356 (0.1%)	1.83	37/1838 (2.0%)
2	G	1.44	5/1356 (0.4%)	1.82	28/1838 (1.5%)
2	H	1.44	5/1356 (0.4%)	1.88	37/1838 (2.0%)
2	I	1.42	2/1356 (0.1%)	1.86	32/1838 (1.7%)
2	J	1.41	1/1356 (0.1%)	1.78	27/1838 (1.5%)
2	K	1.41	3/1356 (0.2%)	1.81	34/1838 (1.8%)
2	L	1.37	1/1356 (0.1%)	1.80	26/1838 (1.4%)
3	a	1.37	1/881 (0.1%)	1.86	23/1181 (1.9%)
3	b	1.37	1/881 (0.1%)	1.73	13/1181 (1.1%)
3	c	1.36	0/881	1.84	21/1181 (1.8%)
3	d	1.39	1/881 (0.1%)	1.89	25/1181 (2.1%)
3	e	1.33	1/881 (0.1%)	1.83	18/1181 (1.5%)
3	f	1.33	1/881 (0.1%)	1.86	23/1181 (1.9%)
3	g	1.36	0/881	1.85	21/1181 (1.8%)
3	h	1.35	0/881	1.84	16/1181 (1.4%)
3	i	1.36	1/881 (0.1%)	1.88	22/1181 (1.9%)
3	j	1.38	0/881	1.92	28/1181 (2.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	k	1.38	1/881 (0.1%)	1.83	16/1181 (1.4%)
3	l	1.35	0/881	1.87	22/1181 (1.9%)
All	All	1.43	97/63996 (0.2%)	1.86	1481/86448 (1.7%)

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	1	0	3
1	2	0	3
1	3	0	2
1	4	0	2
1	M	0	1
1	P	0	1
1	Q	0	2
1	R	0	1
1	T	0	3
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
3	a	0	1
3	d	0	1
3	g	0	1
3	h	0	1
3	k	0	1
All	All	0	27

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	53	ARG	NE-CZ	7.00	1.40	1.33
1	T	408	PHE	C-N	6.69	1.38	1.33
1	N	297	PRO	CA-CB	6.69	1.58	1.53
3	a	62	GLY	CA-C	-6.65	1.46	1.52
1	3	275	ARG	NE-CZ	6.61	1.40	1.33
1	N	409	GLY	CA-C	-6.57	1.46	1.52
2	G	79	ARG	CD-NE	6.55	1.55	1.46
1	T	105	ARG	NE-CZ	6.40	1.40	1.33
1	R	289	ARG	NE-CZ	6.38	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	115	GLY	C-N	6.21	1.39	1.33
1	S	126	GLY	CA-C	-6.21	1.44	1.51
1	O	164	ARG	NE-CZ	6.17	1.39	1.33
1	O	403	HIS	ND1-CE1	6.12	1.38	1.32
1	M	87	ASN	CA-CB	6.10	1.56	1.52
2	C	60	ARG	NE-CZ	6.09	1.39	1.33
1	R	292	ARG	NE-CZ	5.91	1.39	1.33
2	K	86	HIS	ND1-CE1	5.83	1.38	1.32
1	2	172	GLN	CA-C	-5.81	1.46	1.52
1	P	321	ARG	CD-NE	5.80	1.54	1.46
3	k	137	HIS	ND1-CE1	5.80	1.38	1.32
1	1	349	HIS	ND1-CE1	5.79	1.38	1.32
3	b	82	LYS	CA-C	-5.78	1.45	1.52
1	S	140	ARG	NE-CZ	5.75	1.39	1.33
1	Q	328	ARG	CD-NE	5.68	1.54	1.46
1	Q	239	LYS	C-N	5.68	1.38	1.33
2	G	81	SER	C-N	5.68	1.37	1.33
2	L	53	ARG	NE-CZ	5.66	1.39	1.33
2	H	60	ARG	NE-CZ	5.57	1.39	1.33
2	B	53	ARG	NE-CZ	5.50	1.39	1.33
1	4	282	GLN	N-CA	-5.48	1.39	1.46
1	M	434	ARG	NE-CZ	5.48	1.39	1.33
2	H	54	ARG	NE-CZ	5.47	1.39	1.33
1	1	413	PHE	N-CA	-5.46	1.42	1.47
1	N	403	HIS	ND1-CE1	5.42	1.38	1.32
2	G	54	ARG	NE-CZ	5.42	1.39	1.33
1	O	273	ARG	NE-CZ	5.42	1.39	1.33
1	3	146	LYS	CA-C	-5.40	1.46	1.52
1	3	89	HIS	ND1-CE1	5.39	1.38	1.32
1	T	220	ARG	NE-CZ	5.38	1.39	1.33
1	3	141	PHE	CA-CB	5.38	1.61	1.53
2	K	209	ASP	N-CA	-5.38	1.39	1.46
1	N	328	ARG	NE-CZ	5.38	1.39	1.33
1	P	275	ARG	CD-NE	5.37	1.53	1.46
1	N	91	ARG	NE-CZ	5.37	1.39	1.33
1	S	156	HIS	ND1-CE1	5.35	1.38	1.32
1	3	257	HIS	ND1-CE1	5.34	1.37	1.32
1	N	105	ARG	NE-CZ	5.34	1.39	1.33
2	J	97	ARG	NE-CZ	5.31	1.38	1.33
3	e	137	HIS	ND1-CE1	5.30	1.37	1.32
1	M	328	ARG	NE-CZ	5.29	1.38	1.33
1	4	105	ARG	NE-CZ	5.28	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	220	ARG	NE-CZ	5.27	1.38	1.33
2	E	60	ARG	NE-CZ	5.27	1.38	1.33
3	i	89	ARG	NE-CZ	5.26	1.38	1.33
1	4	107	ARG	NE-CZ	5.26	1.38	1.33
1	S	412	ARG	NE-CZ	5.25	1.38	1.33
1	T	277	ARG	NE-CZ	5.25	1.38	1.33
1	2	435	GLU	CA-C	-5.23	1.47	1.53
2	F	97	ARG	NE-CZ	5.23	1.38	1.33
2	E	205	TYR	CA-C	-5.21	1.47	1.53
1	P	457	HIS	ND1-CE1	5.21	1.37	1.32
2	K	97	ARG	NE-CZ	5.20	1.38	1.33
2	E	53	ARG	NE-CZ	5.20	1.38	1.33
1	Q	143	ARG	NE-CZ	5.20	1.38	1.33
2	G	43	ARG	NE-CZ	5.20	1.38	1.33
2	A	183	HIS	ND1-CE1	5.19	1.37	1.32
2	A	177	HIS	ND1-CE1	5.19	1.37	1.32
2	I	177	HIS	ND1-CE1	5.18	1.37	1.32
1	O	457	HIS	ND1-CE1	5.17	1.37	1.32
1	O	321	ARG	NE-CZ	5.15	1.38	1.33
1	O	91	ARG	CD-NE	5.15	1.53	1.46
1	T	407	ARG	NE-CZ	5.15	1.38	1.33
1	R	107	ARG	NE-CZ	5.13	1.38	1.33
1	4	107	ARG	CA-C	-5.13	1.46	1.52
2	C	154	ILE	CA-C	-5.12	1.48	1.52
3	f	63	LEU	CA-C	-5.11	1.46	1.52
1	T	361	VAL	C-N	5.11	1.40	1.33
2	I	155	TRP	CA-C	-5.11	1.46	1.52
1	P	225	ARG	NE-CZ	5.10	1.38	1.33
2	G	60	ARG	NE-CZ	5.10	1.38	1.33
3	d	89	ARG	CD-NE	5.09	1.53	1.46
1	M	348	HIS	ND1-CE1	5.09	1.37	1.32
1	3	349	HIS	ND1-CE1	5.09	1.37	1.32
2	H	183	HIS	ND1-CE1	5.08	1.37	1.32
1	1	272	ARG	CD-NE	5.08	1.53	1.46
2	A	82	GLY	C-N	5.08	1.40	1.33
1	M	271	ARG	NE-CZ	5.07	1.38	1.33
1	S	93	HIS	ND1-CE1	5.06	1.37	1.32
1	2	239	LYS	C-N	5.05	1.37	1.33
1	3	271	ARG	NE-CZ	5.03	1.38	1.33
1	N	107	ARG	NE-CZ	5.03	1.38	1.33
1	O	289	ARG	NE-CZ	5.02	1.38	1.33
1	N	140	ARG	NE-CZ	5.01	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	79	ARG	NE-CZ	5.01	1.38	1.33
1	1	156	HIS	ND1-CE1	5.00	1.37	1.32
1	3	292	ARG	CD-NE	5.00	1.53	1.46
2	H	97	ARG	CA-C	-5.00	1.48	1.53

All (1481) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	175	TYR	N-CA-C	-11.58	100.16	114.75
3	i	91	LYS	CA-C-N	10.79	141.11	121.70
3	i	91	LYS	C-N-CA	10.79	141.11	121.70
2	E	72	SER	CA-C-N	10.67	140.90	121.70
2	E	72	SER	C-N-CA	10.67	140.90	121.70
1	O	381	CYS	CA-C-N	10.36	140.35	121.70
1	O	381	CYS	C-N-CA	10.36	140.35	121.70
1	S	122	ILE	N-CA-C	-9.88	93.05	107.78
1	4	82	ILE	N-CA-C	-9.85	103.15	111.91
1	3	94	ALA	CA-C-N	9.74	139.23	121.70
1	3	94	ALA	C-N-CA	9.74	139.23	121.70
1	1	454	TRP	CA-C-N	9.70	139.16	121.70
1	1	454	TRP	C-N-CA	9.70	139.16	121.70
2	I	117	PRO	CA-C-N	9.69	139.14	121.70
2	I	117	PRO	C-N-CA	9.69	139.14	121.70
1	3	452	ILE	CA-C-N	9.43	138.68	121.70
1	3	452	ILE	C-N-CA	9.43	138.68	121.70
2	C	117	PRO	CA-C-N	9.41	138.64	121.70
2	C	117	PRO	C-N-CA	9.41	138.64	121.70
1	O	450	LYS	CA-C-N	9.15	138.16	121.70
1	O	450	LYS	C-N-CA	9.15	138.16	121.70
1	T	455	THR	CA-C-N	9.12	138.12	121.70
1	T	455	THR	C-N-CA	9.12	138.12	121.70
1	R	455	THR	CA-C-N	9.10	138.08	121.70
1	R	455	THR	C-N-CA	9.10	138.08	121.70
1	1	452	ILE	CA-C-N	9.05	137.99	121.70
1	1	452	ILE	C-N-CA	9.05	137.99	121.70
2	E	85	GLY	CA-C-N	8.99	137.87	121.70
2	E	85	GLY	C-N-CA	8.99	137.87	121.70
1	4	446	GLY	N-CA-C	8.98	123.50	112.73
2	A	142	THR	N-CA-C	-8.78	99.91	110.44
2	E	84	LEU	CA-C-N	8.74	137.43	121.70
2	E	84	LEU	C-N-CA	8.74	137.43	121.70
2	H	177	HIS	CA-CB-CG	8.66	122.46	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	449	LEU	CA-C-N	8.62	137.22	121.70
1	O	449	LEU	C-N-CA	8.62	137.22	121.70
2	I	126	SER	CA-C-N	8.61	137.20	121.70
2	I	126	SER	C-N-CA	8.61	137.20	121.70
1	Q	357	SER	CA-C-N	8.57	137.12	121.70
1	Q	357	SER	C-N-CA	8.57	137.12	121.70
1	P	357	SER	CA-C-N	8.53	137.05	121.70
1	P	357	SER	C-N-CA	8.53	137.05	121.70
2	A	72	SER	CA-C-N	8.50	137.00	121.70
2	A	72	SER	C-N-CA	8.50	137.00	121.70
1	1	312	GLN	CA-C-N	8.48	132.77	120.38
1	1	312	GLN	C-N-CA	8.48	132.77	120.38
1	3	357	SER	CA-C-N	8.47	136.95	121.70
1	3	357	SER	C-N-CA	8.47	136.95	121.70
1	R	386	LEU	N-CA-C	-8.41	105.03	114.62
2	H	126	SER	CA-C-N	8.41	136.85	121.70
2	H	126	SER	C-N-CA	8.41	136.85	121.70
3	c	135	LYS	N-CA-C	-8.36	103.60	113.88
3	l	132	PRO	N-CA-C	8.34	120.88	110.70
2	L	120	PHE	CA-C-N	8.32	132.26	120.28
2	L	120	PHE	C-N-CA	8.32	132.26	120.28
1	S	250	ASP	N-CA-C	-8.28	105.18	114.62
2	A	71	GLN	CA-C-N	8.23	136.52	121.70
2	A	71	GLN	C-N-CA	8.23	136.52	121.70
2	F	66	TRP	CA-C-N	8.21	131.28	120.28
2	F	66	TRP	C-N-CA	8.21	131.28	120.28
1	1	380	ALA	N-CA-C	-8.10	98.28	109.71
1	1	122	ILE	N-CA-C	-8.06	96.82	108.11
2	K	67	ASN	CA-C-N	8.05	131.49	120.46
2	K	67	ASN	C-N-CA	8.05	131.49	120.46
1	M	456	GLN	CA-C-N	8.05	136.19	121.70
1	M	456	GLN	C-N-CA	8.05	136.19	121.70
1	P	358	PHE	N-CA-CB	8.04	124.17	110.50
1	N	297	PRO	CA-C-N	7.95	130.03	120.09
1	N	297	PRO	C-N-CA	7.95	130.03	120.09
1	2	448	ASP	CA-C-N	7.91	135.94	121.70
1	2	448	ASP	C-N-CA	7.91	135.94	121.70
2	H	83	THR	CA-C-N	7.91	135.93	121.70
2	H	83	THR	C-N-CA	7.91	135.93	121.70
2	A	71	GLN	O-C-N	-7.90	115.55	121.47
2	D	174	VAL	CA-C-N	7.88	130.84	120.28
2	D	174	VAL	C-N-CA	7.88	130.84	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	86	GLY	CA-C-N	7.86	135.85	121.70
1	T	86	GLY	C-N-CA	7.86	135.85	121.70
2	H	66	TRP	CA-C-N	7.86	130.82	120.28
2	H	66	TRP	C-N-CA	7.86	130.82	120.28
2	G	142	THR	CA-C-N	7.82	135.77	121.70
2	G	142	THR	C-N-CA	7.82	135.77	121.70
2	B	126	SER	CA-C-N	7.81	135.76	121.70
2	B	126	SER	C-N-CA	7.81	135.76	121.70
2	I	98	LEU	N-CA-C	7.77	119.75	111.28
3	c	59	VAL	CA-C-N	7.77	128.45	120.60
3	c	59	VAL	C-N-CA	7.77	128.45	120.60
1	3	268	ILE	CA-C-N	7.76	132.52	121.42
1	3	268	ILE	C-N-CA	7.76	132.52	121.42
3	e	52	LEU	N-CA-C	-7.73	102.90	113.18
3	k	134	VAL	N-CA-C	-7.72	105.24	112.96
3	i	135	LYS	N-CA-C	-7.72	104.79	112.97
1	T	87	ASN	N-CA-CB	7.72	123.62	110.50
3	g	74	LYS	N-CA-C	-7.71	95.95	109.06
2	J	76	MET	N-CA-C	-7.69	101.04	110.88
3	d	142	ALA	CA-C-N	7.64	130.37	120.44
3	d	142	ALA	C-N-CA	7.64	130.37	120.44
1	P	451	SER	CA-C-N	7.63	135.71	121.97
1	P	451	SER	C-N-CA	7.63	135.71	121.97
3	d	74	LYS	N-CA-C	-7.63	97.79	109.85
2	D	90	LEU	N-CA-C	-7.58	101.35	110.44
1	O	95	TYR	CA-C-N	7.56	128.32	120.00
1	O	95	TYR	C-N-CA	7.56	128.32	120.00
3	c	137	HIS	CA-C-N	7.54	130.39	120.28
3	c	137	HIS	C-N-CA	7.54	130.39	120.28
1	N	218	ILE	CA-C-N	7.54	129.56	120.14
1	N	218	ILE	C-N-CA	7.54	129.56	120.14
1	M	359	ALA	N-CA-C	7.51	120.57	110.35
1	1	395	ILE	N-CA-C	-7.50	96.33	107.51
1	N	391	VAL	N-CA-C	7.46	118.23	110.62
1	3	358	PHE	N-CA-CB	7.45	123.16	110.50
2	D	177	HIS	N-CA-C	-7.42	105.41	114.75
1	1	413	PHE	N-CA-C	-7.39	102.86	113.21
1	Q	358	PHE	N-CA-CB	7.39	123.07	110.50
2	D	95	TYR	CA-C-N	7.39	135.01	121.70
2	D	95	TYR	C-N-CA	7.39	135.01	121.70
1	R	357	SER	CA-C-N	7.37	134.97	121.70
1	R	357	SER	C-N-CA	7.37	134.97	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	95	TYR	N-CA-C	7.34	119.28	111.28
3	i	92	THR	N-CA-CB	7.30	123.92	111.50
2	G	126	SER	CA-C-N	7.29	134.81	121.70
2	G	126	SER	C-N-CA	7.29	134.81	121.70
1	M	390	TYR	N-CA-C	-7.27	103.51	113.18
2	F	60	ARG	CA-C-N	7.26	134.77	121.70
2	F	60	ARG	C-N-CA	7.26	134.77	121.70
3	j	115	GLU	CA-C-N	7.25	130.00	120.28
3	j	115	GLU	C-N-CA	7.25	130.00	120.28
3	g	157	GLN	CA-C-N	7.24	129.15	120.09
3	g	157	GLN	C-N-CA	7.24	129.15	120.09
3	h	58	ASN	CA-C-N	7.24	130.26	120.63
3	h	58	ASN	C-N-CA	7.24	130.26	120.63
3	d	80	ASP	CA-CB-CG	-7.18	105.42	112.60
1	O	365	SER	CA-C-N	7.18	129.90	120.28
1	O	365	SER	C-N-CA	7.18	129.90	120.28
2	C	67	ASN	CA-C-N	7.17	130.28	120.46
2	C	67	ASN	C-N-CA	7.17	130.28	120.46
2	C	126	SER	CA-C-N	7.16	134.58	121.70
2	C	126	SER	C-N-CA	7.16	134.58	121.70
1	O	258	LYS	N-CA-C	-7.12	104.07	114.39
2	I	110	PHE	CA-CB-CG	-7.11	106.69	113.80
2	A	80	LYS	CA-C-N	7.09	134.47	121.70
2	A	80	LYS	C-N-CA	7.09	134.47	121.70
1	3	117	ASP	N-CA-CB	7.07	122.96	110.37
1	O	379	SER	CA-C-N	7.06	134.41	121.70
1	O	379	SER	C-N-CA	7.06	134.41	121.70
1	3	314	GLU	CA-C-N	7.05	131.39	120.82
1	3	314	GLU	C-N-CA	7.05	131.39	120.82
1	T	395	ILE	N-CA-C	-7.04	98.31	108.17
1	4	111	ALA	CA-C-N	7.04	129.71	120.28
1	4	111	ALA	C-N-CA	7.04	129.71	120.28
3	d	80	ASP	CA-C-N	7.02	129.68	120.28
3	d	80	ASP	C-N-CA	7.02	129.68	120.28
1	4	83	ASN	N-CA-C	-7.02	98.29	109.59
1	P	387	GLU	N-CA-CB	7.01	118.46	111.10
2	D	97	ARG	N-CA-CB	7.01	122.33	110.49
2	K	66	TRP	CA-C-N	7.01	129.67	120.28
2	K	66	TRP	C-N-CA	7.01	129.67	120.28
2	E	80	LYS	CA-C-N	7.00	134.30	121.70
2	E	80	LYS	C-N-CA	7.00	134.30	121.70
1	P	390	TYR	N-CA-C	-6.99	103.87	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	109	PHE	CA-CB-CG	-6.99	106.81	113.80
2	D	77	ASN	N-CA-C	-6.98	97.03	108.41
2	D	126	SER	CA-C-N	6.97	134.25	121.70
2	D	126	SER	C-N-CA	6.97	134.25	121.70
1	S	357	SER	CA-C-N	6.97	134.25	121.70
1	S	357	SER	C-N-CA	6.97	134.25	121.70
1	2	78	LEU	CA-C-N	6.91	128.48	119.84
1	2	78	LEU	C-N-CA	6.91	128.48	119.84
1	R	328	ARG	CA-C-N	6.91	129.42	120.44
1	R	328	ARG	C-N-CA	6.91	129.42	120.44
1	R	95	TYR	CA-C-N	6.90	127.64	119.98
1	R	95	TYR	C-N-CA	6.90	127.64	119.98
3	f	137	HIS	CA-C-N	6.89	130.08	120.29
3	f	137	HIS	C-N-CA	6.89	130.08	120.29
1	S	115	GLY	N-CA-C	-6.88	105.13	112.08
3	c	125	ILE	CA-C-N	6.83	129.44	120.28
3	c	125	ILE	C-N-CA	6.83	129.44	120.28
1	M	84	TYR	N-CA-C	-6.82	103.54	112.41
1	O	362	GLU	CA-C-N	6.82	127.50	120.00
1	O	362	GLU	C-N-CA	6.82	127.50	120.00
1	P	387	GLU	N-CA-C	-6.82	102.08	108.22
1	4	98	GLU	N-CA-C	6.81	120.47	111.75
2	B	92	GLU	N-CA-C	-6.78	106.89	114.62
1	2	139	ALA	N-CA-C	6.78	118.75	111.36
1	M	437	SER	N-CA-C	-6.77	100.10	110.32
2	B	177	HIS	N-CA-C	-6.76	106.91	114.62
1	1	102	ALA	N-CA-C	6.75	118.64	111.28
3	e	54	LYS	N-CA-C	-6.75	103.75	113.21
1	S	437	SER	N-CA-C	-6.75	98.60	109.40
1	4	298	THR	CA-C-O	-6.74	111.80	118.34
1	P	450	LYS	N-CA-CB	6.73	121.86	110.49
2	C	84	LEU	CA-C-N	6.73	133.81	121.70
2	C	84	LEU	C-N-CA	6.73	133.81	121.70
1	M	319	HIS	CA-CB-CG	6.72	120.52	113.80
3	c	126	ALA	CA-C-N	6.71	129.60	120.54
3	c	126	ALA	C-N-CA	6.71	129.60	120.54
2	K	58	ASN	CA-CB-CG	6.71	119.31	112.60
1	R	415	THR	N-CA-C	-6.70	98.89	109.07
2	I	127	PHE	N-CA-CB	6.70	121.89	110.50
1	3	434	ARG	N-CA-C	6.69	119.42	111.33
3	l	95	CYS	CA-C-N	6.68	134.51	121.41
3	l	95	CYS	C-N-CA	6.68	134.51	121.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	117	ASP	CA-CB-CG	6.68	119.28	112.60
2	F	58	ASN	CA-CB-CG	6.67	119.27	112.60
2	A	85	GLY	CA-C-N	6.67	133.70	121.70
2	A	85	GLY	C-N-CA	6.67	133.70	121.70
1	1	453	LYS	CA-C-N	6.67	133.70	121.70
1	1	453	LYS	C-N-CA	6.67	133.70	121.70
1	3	208	GLU	N-CA-C	-6.66	107.03	114.62
2	D	51	THR	CA-C-N	6.65	126.59	119.28
2	D	51	THR	C-N-CA	6.65	126.59	119.28
2	G	143	TYR	N-CA-CB	6.62	121.75	110.50
1	O	451	SER	CA-C-N	6.61	133.60	121.70
1	O	451	SER	C-N-CA	6.61	133.60	121.70
1	R	349	HIS	CE1-NE2-CD2	-6.59	102.41	109.00
1	4	297	PRO	CA-C-N	6.59	128.32	120.09
1	4	297	PRO	C-N-CA	6.59	128.32	120.09
2	C	116	LYS	CA-C-N	6.57	128.06	119.84
2	C	116	LYS	C-N-CA	6.57	128.06	119.84
1	P	452	ILE	N-CA-CB	6.57	122.07	111.23
1	S	88	PRO	CA-C-N	6.56	134.08	121.54
1	S	88	PRO	C-N-CA	6.56	134.08	121.54
3	d	109	VAL	N-CA-CB	6.56	119.46	110.54
2	D	84	LEU	CA-C-N	6.54	133.48	121.70
2	D	84	LEU	C-N-CA	6.54	133.48	121.70
1	M	185	ASP	CA-C-N	6.53	129.68	120.28
1	M	185	ASP	C-N-CA	6.53	129.68	120.28
1	M	403	HIS	CA-CB-CG	-6.53	107.27	113.80
2	J	175	TYR	N-CA-C	-6.51	107.20	114.62
1	N	348	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
1	O	259	ILE	N-CA-C	-6.48	99.09	108.17
3	f	92	THR	N-CA-CB	6.48	121.44	110.49
2	B	149	THR	O-C-N	-6.47	117.32	121.85
1	Q	328	ARG	CA-C-N	6.46	128.83	120.44
1	Q	328	ARG	C-N-CA	6.46	128.83	120.44
3	c	80	ASP	CA-CB-CG	-6.45	106.15	112.60
1	Q	315	MET	N-CA-C	6.43	121.99	111.37
2	H	73	VAL	N-CA-C	-6.43	106.72	112.12
1	4	248	LYS	CA-C-N	6.43	129.28	120.35
1	4	248	LYS	C-N-CA	6.43	129.28	120.35
1	S	454	TRP	CA-C-N	6.42	133.26	121.70
1	S	454	TRP	C-N-CA	6.42	133.26	121.70
1	2	308	CYS	CA-C-N	6.42	128.79	120.44
1	2	308	CYS	C-N-CA	6.42	128.79	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	l	61	THR	CA-C-N	6.42	128.73	120.64
3	l	61	THR	C-N-CA	6.42	128.73	120.64
3	j	52	LEU	N-CA-C	-6.42	107.30	114.62
3	i	126	ALA	CA-C-N	6.41	129.19	120.54
3	i	126	ALA	C-N-CA	6.41	129.19	120.54
2	E	159	PRO	N-CA-C	-6.41	106.48	114.68
3	a	98	ALA	CA-C-N	6.40	128.63	120.56
3	a	98	ALA	C-N-CA	6.40	128.63	120.56
1	3	278	VAL	O-C-N	-6.40	117.40	122.97
1	R	372	ASP	CA-CB-CG	6.39	118.99	112.60
1	1	457	HIS	CA-CB-CG	-6.39	107.41	113.80
1	Q	386	LEU	N-CA-C	-6.37	106.72	114.75
2	I	200	LEU	N-CA-C	-6.37	105.09	112.92
1	R	437	SER	N-CA-C	-6.36	99.71	109.64
3	k	138	CYS	CA-C-N	6.36	128.80	120.28
3	k	138	CYS	C-N-CA	6.36	128.80	120.28
2	I	78	LEU	N-CA-C	-6.35	105.47	113.72
2	I	84	LEU	CA-C-N	6.35	133.12	121.70
2	I	84	LEU	C-N-CA	6.35	133.12	121.70
1	2	200	VAL	N-CA-C	-6.33	98.92	108.17
1	2	278	VAL	CA-C-N	6.33	133.09	121.70
1	2	278	VAL	C-N-CA	6.33	133.09	121.70
1	N	235	GLN	N-CA-C	-6.33	102.95	111.87
3	i	113	THR	CA-C-N	6.32	129.12	120.46
3	i	113	THR	C-N-CA	6.32	129.12	120.46
1	3	304	LEU	CA-C-N	6.32	126.82	119.94
1	3	304	LEU	C-N-CA	6.32	126.82	119.94
1	Q	250	ASP	N-CA-C	-6.31	106.11	113.88
1	2	122	ILE	N-CA-C	-6.31	98.43	107.77
1	M	369	ALA	N-CA-C	6.29	118.14	111.28
2	K	116	LYS	CA-C-N	6.29	125.79	119.24
2	K	116	LYS	C-N-CA	6.29	125.79	119.24
2	C	91	ASP	N-CA-C	-6.29	105.55	112.72
1	M	407	ARG	N-CA-C	-6.28	99.76	109.24
1	T	235	GLN	N-CA-C	-6.28	104.93	112.59
2	F	127	PHE	N-CA-CB	6.28	121.18	110.50
1	1	70	ASP	CA-C-N	6.27	126.47	119.32
1	1	70	ASP	C-N-CA	6.27	126.47	119.32
2	A	126	SER	CA-C-N	6.27	132.99	121.70
2	A	126	SER	C-N-CA	6.27	132.99	121.70
3	c	115	GLU	CA-C-N	6.27	128.68	120.28
3	c	115	GLU	C-N-CA	6.27	128.68	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	429	HIS	CE1-NE2-CD2	-6.26	102.74	109.00
1	1	392	LEU	N-CA-C	6.26	124.13	110.80
3	a	63	LEU	CA-C-N	6.26	133.23	121.97
3	a	63	LEU	C-N-CA	6.26	133.23	121.97
2	H	85	GLY	CA-C-N	6.26	132.96	121.70
2	H	85	GLY	C-N-CA	6.26	132.96	121.70
1	4	300	LEU	CA-C-N	6.25	129.02	120.46
1	4	300	LEU	C-N-CA	6.25	129.02	120.46
1	M	398	ASP	CA-CB-CG	-6.25	106.35	112.60
2	A	73	VAL	N-CA-CB	6.25	122.12	111.50
3	d	159	PRO	CA-C-N	6.24	128.97	120.54
3	d	159	PRO	C-N-CA	6.24	128.97	120.54
1	O	218	ILE	CA-C-N	6.24	127.94	120.14
1	O	218	ILE	C-N-CA	6.24	127.94	120.14
2	F	126	SER	CA-C-N	6.24	132.93	121.70
2	F	126	SER	C-N-CA	6.24	132.93	121.70
1	R	358	PHE	N-CA-CB	6.24	121.10	110.50
1	T	202	VAL	N-CA-C	-6.24	99.61	108.65
1	4	429	HIS	CE1-NE2-CD2	-6.23	102.77	109.00
1	N	357	SER	CA-C-N	6.23	132.92	121.70
1	N	357	SER	C-N-CA	6.23	132.92	121.70
1	M	88	PRO	N-CA-C	-6.23	105.88	114.98
2	L	97	ARG	N-CA-CB	6.23	121.02	110.49
1	3	87	ASN	CA-CB-CG	-6.23	106.37	112.60
3	h	157	GLN	CA-C-N	6.23	127.50	119.78
3	h	157	GLN	C-N-CA	6.23	127.50	119.78
1	P	122	ILE	N-CA-C	-6.22	98.56	107.77
1	2	390	TYR	CA-C-N	6.22	128.39	120.56
1	2	390	TYR	C-N-CA	6.22	128.39	120.56
1	P	71	PRO	CA-C-N	6.21	128.89	120.38
1	P	71	PRO	C-N-CA	6.21	128.89	120.38
2	K	90	LEU	N-CA-C	-6.21	104.96	114.16
3	h	69	CYS	N-CA-C	-6.21	104.87	112.88
1	4	106	ALA	CA-C-N	6.21	128.59	120.28
1	4	106	ALA	C-N-CA	6.21	128.59	120.28
1	Q	357	SER	O-C-N	-6.21	116.15	123.41
1	P	281	LEU	CA-C-N	6.20	133.39	121.54
1	P	281	LEU	C-N-CA	6.20	133.39	121.54
2	I	120	PHE	CA-CB-CG	6.20	120.00	113.80
1	P	319	HIS	CE1-NE2-CD2	-6.20	102.80	109.00
1	M	106	ALA	CA-C-N	6.19	128.58	120.28
1	M	106	ALA	C-N-CA	6.19	128.58	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	80	TYR	CA-C-N	6.19	128.58	120.28
1	P	80	TYR	C-N-CA	6.19	128.58	120.28
1	P	289	ARG	NE-CZ-NH2	6.19	124.77	119.20
2	H	135	LYS	N-CA-CB	6.19	118.08	110.53
2	F	91	ASP	N-CA-C	-6.18	105.38	113.17
2	J	86	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
3	k	121	LYS	CA-C-N	6.18	128.85	120.38
3	k	121	LYS	C-N-CA	6.18	128.85	120.38
1	3	92	THR	N-CA-CB	6.16	120.91	110.49
1	4	446	GLY	CA-C-N	6.15	132.78	121.70
1	4	446	GLY	C-N-CA	6.15	132.78	121.70
1	S	214	PRO	CA-C-N	6.15	128.53	120.60
1	S	214	PRO	C-N-CA	6.15	128.53	120.60
1	N	405	SER	N-CA-C	-6.15	99.18	108.96
1	P	319	HIS	CA-CB-CG	6.15	119.95	113.80
3	j	150	LEU	CA-C-N	6.14	129.01	120.29
3	j	150	LEU	C-N-CA	6.14	129.01	120.29
2	L	126	SER	CA-C-N	6.14	132.75	121.70
2	L	126	SER	C-N-CA	6.14	132.75	121.70
1	M	413	PHE	N-CA-C	-6.13	105.44	113.17
1	T	439	LEU	CA-C-N	6.13	129.00	120.29
1	T	439	LEU	C-N-CA	6.13	129.00	120.29
2	B	151	ASN	CA-CB-CG	-6.13	106.47	112.60
2	I	84	LEU	N-CA-CB	6.13	120.85	110.49
2	H	51	THR	N-CA-C	-6.13	101.09	108.14
1	2	456	GLN	CA-C-N	6.12	132.72	121.70
1	2	456	GLN	C-N-CA	6.12	132.72	121.70
1	M	357	SER	CA-C-N	6.12	132.72	121.70
1	M	357	SER	C-N-CA	6.12	132.72	121.70
1	2	387	GLU	O-C-N	-6.12	114.28	121.32
2	C	127	PHE	N-CA-CB	6.11	120.89	110.50
1	3	383	SER	N-CA-CB	6.11	120.81	110.49
1	4	165	SER	CA-C-N	6.11	128.96	120.29
1	4	165	SER	C-N-CA	6.11	128.96	120.29
1	Q	420	ASP	CA-C-N	6.11	129.59	120.31
1	Q	420	ASP	C-N-CA	6.11	129.59	120.31
2	G	114	ALA	N-CA-C	6.11	117.60	111.07
2	L	174	VAL	CA-C-N	6.11	128.46	120.28
2	L	174	VAL	C-N-CA	6.11	128.46	120.28
1	Q	395	ILE	CA-C-N	6.10	125.78	119.92
1	Q	395	ILE	C-N-CA	6.10	125.78	119.92
2	E	95	TYR	CA-C-N	6.10	132.68	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	95	TYR	C-N-CA	6.10	132.68	121.70
1	P	434	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	T	400	ASP	CA-CB-CG	-6.10	106.50	112.60
2	B	122	ASP	N-CA-C	-6.09	105.03	112.88
2	F	203	LEU	N-CA-C	-6.09	97.83	110.80
1	2	322	ILE	CB-CA-C	-6.09	103.82	112.22
3	f	138	CYS	CA-C-N	6.09	128.44	120.28
3	f	138	CYS	C-N-CA	6.09	128.44	120.28
1	O	303	GLY	CA-C-N	6.08	128.35	120.44
1	O	303	GLY	C-N-CA	6.08	128.35	120.44
1	P	156	HIS	CE1-NE2-CD2	-6.08	102.92	109.00
2	B	67	ASN	CA-C-N	6.08	128.79	120.46
2	B	67	ASN	C-N-CA	6.08	128.79	120.46
1	P	328	ARG	CA-C-N	6.07	128.33	120.44
1	P	328	ARG	C-N-CA	6.07	128.33	120.44
1	1	362	GLU	CA-C-N	6.07	126.68	120.00
1	1	362	GLU	C-N-CA	6.07	126.68	120.00
1	4	313	GLN	N-CA-C	6.07	123.73	110.80
2	B	58	ASN	CA-CB-CG	-6.07	106.53	112.60
2	K	177	HIS	ND1-CE1-NE2	6.06	114.46	108.40
1	4	413	PHE	N-CA-C	-6.06	103.23	112.99
2	H	127	PHE	N-CA-CB	6.06	120.80	110.50
1	O	89	HIS	CE1-NE2-CD2	-6.04	102.95	109.00
3	e	136	LEU	CA-C-N	6.04	128.38	120.28
3	e	136	LEU	C-N-CA	6.04	128.38	120.28
2	B	93	THR	N-CA-C	-6.04	106.23	113.97
1	M	250	ASP	N-CA-C	-6.04	106.55	114.04
1	S	278	VAL	N-CA-C	-6.04	99.79	108.42
1	N	214	PRO	CA-C-N	6.04	128.16	120.56
1	N	214	PRO	C-N-CA	6.04	128.16	120.56
3	f	92	THR	N-CA-C	-6.03	97.95	110.80
2	L	121	GLU	N-CA-C	6.03	118.64	111.71
3	a	125	ILE	CA-C-N	6.03	128.35	120.28
3	a	125	ILE	C-N-CA	6.03	128.35	120.28
1	4	298	THR	CA-C-N	6.02	127.37	119.84
1	4	298	THR	C-N-CA	6.02	127.37	119.84
1	N	386	LEU	N-CA-C	-6.02	107.76	114.62
1	4	400	ASP	CA-C-N	6.01	128.34	120.28
1	4	400	ASP	C-N-CA	6.01	128.34	120.28
1	Q	156	HIS	CE1-NE2-CD2	-6.01	102.98	109.00
1	1	202	VAL	N-CA-C	-6.01	99.93	108.65
1	N	376	SER	N-CA-C	-6.01	98.01	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	97	TRP	CA-C-N	5.99	132.99	121.54
1	1	97	TRP	C-N-CA	5.99	132.99	121.54
3	l	71	ASP	CA-C-N	5.99	129.13	120.98
3	l	71	ASP	C-N-CA	5.99	129.13	120.98
1	1	328	ARG	CA-C-N	5.98	128.22	120.44
1	1	328	ARG	C-N-CA	5.98	128.22	120.44
1	N	122	ILE	N-CA-C	-5.98	98.92	107.77
1	R	110	VAL	CA-C-N	5.98	128.29	120.28
1	R	110	VAL	C-N-CA	5.98	128.29	120.28
1	2	202	VAL	N-CA-C	-5.98	99.98	108.65
1	3	71	PRO	CA-C-N	5.97	128.57	120.38
1	3	71	PRO	C-N-CA	5.97	128.57	120.38
2	G	192	LYS	CA-C-N	5.97	128.28	120.28
2	G	192	LYS	C-N-CA	5.97	128.28	120.28
1	R	87	ASN	CA-C-N	5.97	126.31	119.92
1	R	87	ASN	C-N-CA	5.97	126.31	119.92
1	R	118	PRO	CA-C-N	5.97	130.84	122.36
1	R	118	PRO	C-N-CA	5.97	130.84	122.36
3	k	137	HIS	CA-C-N	5.96	128.76	120.29
3	k	137	HIS	C-N-CA	5.96	128.76	120.29
1	1	357	SER	CA-C-N	5.96	132.43	121.70
1	1	357	SER	C-N-CA	5.96	132.43	121.70
3	l	71	ASP	N-CA-C	5.96	118.69	110.35
1	M	429	HIS	CA-C-N	5.96	128.62	120.46
1	M	429	HIS	C-N-CA	5.96	128.62	120.46
2	H	113	LEU	CA-C-N	5.96	128.18	120.44
2	H	113	LEU	C-N-CA	5.96	128.18	120.44
1	N	344	GLY	N-CA-C	-5.95	105.54	111.85
3	d	79	VAL	N-CA-C	-5.95	100.12	108.80
3	g	159	PRO	CA-C-N	5.95	128.57	120.54
3	g	159	PRO	C-N-CA	5.95	128.57	120.54
2	D	113	LEU	CA-C-N	5.95	128.25	120.28
2	D	113	LEU	C-N-CA	5.95	128.25	120.28
1	R	390	TYR	CA-C-N	5.94	128.85	120.42
1	R	390	TYR	C-N-CA	5.94	128.85	120.42
3	f	80	ASP	CA-CB-CG	-5.94	106.66	112.60
1	O	80	TYR	CA-C-N	5.94	129.33	120.31
1	O	80	TYR	C-N-CA	5.94	129.33	120.31
1	R	452	ILE	N-CA-C	-5.94	107.34	113.10
1	O	310	VAL	CA-C-N	5.94	128.23	120.28
1	O	310	VAL	C-N-CA	5.94	128.23	120.28
2	C	135	LYS	N-CA-CB	5.93	120.17	110.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	86	HIS	ND1-CE1-NE2	5.93	114.33	108.40
2	B	95	TYR	CA-C-N	5.93	132.37	121.70
2	B	95	TYR	C-N-CA	5.93	132.37	121.70
1	N	71	PRO	CA-C-N	5.92	128.22	120.28
1	N	71	PRO	C-N-CA	5.92	128.22	120.28
2	D	79	ARG	CA-C-N	5.92	132.84	121.54
2	D	79	ARG	C-N-CA	5.92	132.84	121.54
1	4	121	ILE	N-CA-CB	5.91	117.57	110.95
2	K	95	TYR	CA-C-N	5.91	132.34	121.70
2	K	95	TYR	C-N-CA	5.91	132.34	121.70
3	g	142	ALA	CA-C-N	5.91	128.12	120.44
3	g	142	ALA	C-N-CA	5.91	128.12	120.44
1	N	372	ASP	CA-C-N	5.91	132.60	121.97
1	N	372	ASP	C-N-CA	5.91	132.60	121.97
1	M	304	LEU	CA-C-N	5.91	126.38	119.94
1	M	304	LEU	C-N-CA	5.91	126.38	119.94
2	G	122	ASP	N-CA-C	-5.91	98.22	110.80
1	4	188	GLU	CA-C-N	5.90	128.11	120.44
1	4	188	GLU	C-N-CA	5.90	128.11	120.44
1	1	380	ALA	CA-C-N	5.90	132.80	121.54
1	1	380	ALA	C-N-CA	5.90	132.80	121.54
1	4	415	THR	N-CA-C	-5.89	100.61	108.74
3	l	121	LYS	CA-C-N	5.89	128.45	120.38
3	l	121	LYS	C-N-CA	5.89	128.45	120.38
2	K	70	LYS	N-CA-CB	5.88	118.87	110.16
1	Q	429	HIS	ND1-CE1-NE2	5.88	114.28	108.40
3	e	137	HIS	ND1-CE1-NE2	5.88	114.28	108.40
2	A	194	LEU	CB-CA-C	-5.88	101.03	110.79
1	3	346	PRO	N-CA-C	-5.87	107.16	114.68
1	N	393	ARG	N-CA-C	-5.87	105.31	112.88
2	I	44	THR	CA-C-N	5.87	129.45	120.82
2	I	44	THR	C-N-CA	5.87	129.45	120.82
2	B	120	PHE	CA-CB-CG	-5.87	107.93	113.80
3	i	138	CYS	CA-C-N	5.87	128.14	120.28
3	i	138	CYS	C-N-CA	5.87	128.14	120.28
3	h	101	SER	CA-C-N	5.87	128.14	120.28
3	h	101	SER	C-N-CA	5.87	128.14	120.28
1	P	250	ASP	N-CA-C	-5.87	107.93	114.62
1	T	218	ILE	CA-C-N	5.86	127.47	120.14
1	T	218	ILE	C-N-CA	5.86	127.47	120.14
1	R	341	VAL	N-CA-C	-5.86	99.68	108.12
1	S	96	GLY	CA-C-N	5.86	128.13	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	96	GLY	C-N-CA	5.86	128.13	120.28
1	3	451	SER	N-CA-CB	5.86	120.39	110.49
1	N	406	ILE	CA-C-N	5.86	130.56	122.77
1	N	406	ILE	C-N-CA	5.86	130.56	122.77
2	A	185	LEU	CA-C-N	5.85	128.12	120.28
2	A	185	LEU	C-N-CA	5.85	128.12	120.28
1	Q	374	ALA	CA-C-N	5.85	132.71	121.54
1	Q	374	ALA	C-N-CA	5.85	132.71	121.54
1	M	136	LYS	CA-C-N	5.85	126.43	120.00
1	M	136	LYS	C-N-CA	5.85	126.43	120.00
1	2	83	ASN	CA-CB-CG	5.84	118.44	112.60
1	T	411	GLY	CA-C-N	5.84	130.42	122.07
1	T	411	GLY	C-N-CA	5.84	130.42	122.07
3	e	50	GLY	CA-C-N	5.84	132.21	121.70
3	e	50	GLY	C-N-CA	5.84	132.21	121.70
1	O	320	LYS	CA-C-N	5.84	128.03	120.44
1	O	320	LYS	C-N-CA	5.84	128.03	120.44
1	N	110	VAL	CA-C-N	5.83	128.10	120.28
1	N	110	VAL	C-N-CA	5.83	128.10	120.28
1	3	234	ALA	N-CA-C	-5.83	105.93	113.16
1	R	332	ASN	CA-C-N	5.83	127.90	120.56
1	R	332	ASN	C-N-CA	5.83	127.90	120.56
3	l	139	SER	N-CA-C	5.82	118.38	111.33
2	H	47	ASP	N-CA-C	-5.82	105.83	113.17
1	P	165	SER	CA-C-N	5.82	128.56	120.29
1	P	165	SER	C-N-CA	5.82	128.56	120.29
1	N	449	LEU	N-CA-CB	5.82	120.32	110.49
1	4	403	HIS	CE1-NE2-CD2	-5.82	103.18	109.00
1	P	70	ASP	CA-C-N	5.82	127.11	119.84
1	P	70	ASP	C-N-CA	5.82	127.11	119.84
1	Q	158	CYS	CA-C-N	5.82	128.43	120.46
1	Q	158	CYS	C-N-CA	5.82	128.43	120.46
1	O	359	ALA	N-CA-C	5.81	117.08	108.60
1	O	425	LYS	CB-CA-C	-5.81	101.14	110.79
1	P	315	MET	N-CA-C	5.81	120.96	111.37
1	P	205	VAL	N-CA-C	-5.81	99.86	108.45
1	O	283	SER	N-CA-C	-5.80	106.85	114.04
1	S	370	LEU	N-CA-C	5.80	117.60	111.28
1	R	329	LEU	CA-C-N	5.79	128.65	120.42
1	R	329	LEU	C-N-CA	5.79	128.65	120.42
1	R	124	THR	N-CA-C	-5.79	99.93	108.79
3	b	106	THR	CA-C-N	5.79	128.04	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	106	THR	C-N-CA	5.79	128.04	120.28
1	R	93	HIS	N-CA-C	-5.79	104.45	112.03
3	i	54	LYS	N-CA-C	-5.79	104.78	112.94
1	O	319	HIS	CA-CB-CG	5.78	119.58	113.80
3	f	126	ALA	CA-C-N	5.78	128.35	120.54
3	f	126	ALA	C-N-CA	5.78	128.35	120.54
1	2	312	GLN	N-CA-C	5.78	117.58	111.28
2	E	177	HIS	ND1-CE1-NE2	5.78	114.18	108.40
1	T	328	ARG	CA-C-N	5.77	128.33	120.54
1	T	328	ARG	C-N-CA	5.77	128.33	120.54
1	1	246	ASP	N-CA-C	-5.77	104.95	113.61
2	D	183	HIS	CE1-NE2-CD2	-5.77	103.23	109.00
1	M	118	PRO	CA-C-N	5.77	130.32	122.07
1	M	118	PRO	C-N-CA	5.77	130.32	122.07
3	b	126	ALA	CA-C-N	5.77	128.33	120.54
3	b	126	ALA	C-N-CA	5.77	128.33	120.54
1	M	374	ALA	CA-C-N	5.76	132.54	121.54
1	M	374	ALA	C-N-CA	5.76	132.54	121.54
1	M	297	PRO	N-CA-CB	5.76	106.44	102.35
1	4	392	LEU	N-CA-C	-5.75	104.83	112.94
3	a	82	LYS	N-CA-C	-5.75	97.79	108.02
1	4	131	ASN	CA-CB-CG	-5.74	106.86	112.60
1	2	205	VAL	N-CA-C	-5.74	99.22	107.78
1	M	156	HIS	N-CA-CB	5.74	118.47	110.26
2	C	181	SER	CA-C-N	5.74	127.96	120.28
2	C	181	SER	C-N-CA	5.74	127.96	120.28
2	A	56	SER	CA-C-N	5.73	127.96	120.28
2	A	56	SER	C-N-CA	5.73	127.96	120.28
1	Q	163	CYS	CA-C-N	5.73	127.96	120.28
1	Q	163	CYS	C-N-CA	5.73	127.96	120.28
1	P	395	ILE	N-CA-C	-5.73	99.62	107.99
1	N	388	PRO	CA-C-O	-5.73	114.61	121.48
3	d	113	THR	CA-C-N	5.73	128.31	120.46
3	d	113	THR	C-N-CA	5.73	128.31	120.46
1	T	400	ASP	CA-C-N	5.73	127.95	120.28
1	T	400	ASP	C-N-CA	5.73	127.95	120.28
2	G	136	LEU	CA-C-N	5.73	132.01	121.70
2	G	136	LEU	C-N-CA	5.73	132.01	121.70
1	2	273	ARG	N-CA-CB	5.72	120.56	110.37
1	O	304	LEU	CA-C-N	5.72	126.18	119.94
1	O	304	LEU	C-N-CA	5.72	126.18	119.94
2	H	209	ASP	N-CA-CB	5.72	120.16	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	380	ALA	N-CA-CB	5.72	116.76	110.35
1	M	281	LEU	N-CA-C	-5.72	107.30	114.56
1	3	70	ASP	CA-C-N	5.71	125.83	119.32
1	3	70	ASP	C-N-CA	5.71	125.83	119.32
1	1	391	VAL	CA-C-N	5.71	132.45	121.54
1	1	391	VAL	C-N-CA	5.71	132.45	121.54
1	R	299	PRO	CA-C-N	5.71	129.38	120.82
1	R	299	PRO	C-N-CA	5.71	129.38	120.82
1	4	95	TYR	CA-C-N	5.71	126.32	119.98
1	4	95	TYR	C-N-CA	5.71	126.32	119.98
1	Q	143	ARG	N-CA-C	5.70	117.98	111.02
1	1	369	ALA	N-CA-C	5.70	117.50	111.28
1	1	205	VAL	N-CA-C	-5.70	100.01	108.45
2	I	86	HIS	N-CA-CB	5.70	120.19	110.50
1	3	349	HIS	CE1-NE2-CD2	-5.70	103.30	109.00
2	A	92	GLU	CA-C-N	5.70	127.92	120.28
2	A	92	GLU	C-N-CA	5.70	127.92	120.28
1	N	369	ALA	N-CA-C	5.69	117.49	111.28
1	T	451	SER	N-CA-CB	5.69	120.11	110.49
2	F	208	LYS	N-CA-CB	5.69	120.11	110.49
1	3	277	ARG	CA-C-N	5.69	129.59	121.96
1	3	277	ARG	C-N-CA	5.69	129.59	121.96
2	J	192	LYS	CA-C-N	5.69	127.91	120.28
2	J	192	LYS	C-N-CA	5.69	127.91	120.28
1	4	110	VAL	CA-C-N	5.69	127.90	120.28
1	4	110	VAL	C-N-CA	5.69	127.90	120.28
1	Q	111	ALA	CA-C-N	5.69	132.40	121.54
1	Q	111	ALA	C-N-CA	5.69	132.40	121.54
1	2	70	ASP	CA-CB-CG	-5.69	106.91	112.60
1	3	200	VAL	N-CA-C	-5.69	99.31	107.78
2	G	193	ALA	CA-C-N	5.69	127.90	120.28
2	G	193	ALA	C-N-CA	5.69	127.90	120.28
1	S	319	HIS	CE1-NE2-CD2	-5.68	103.31	109.00
3	d	94	GLY	CA-C-N	5.68	128.94	120.87
3	d	94	GLY	C-N-CA	5.68	128.94	120.87
1	N	429	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
1	O	395	ILE	N-CA-C	-5.68	100.29	108.53
3	k	80	ASP	CA-CB-CG	-5.68	106.92	112.60
1	4	200	VAL	N-CA-C	-5.68	99.88	108.17
1	N	95	TYR	CA-C-N	5.68	126.24	119.94
1	N	95	TYR	C-N-CA	5.68	126.24	119.94
1	R	261	GLY	N-CA-C	-5.68	100.76	112.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	312	GLN	CA-C-N	5.67	132.38	121.54
1	4	312	GLN	C-N-CA	5.67	132.38	121.54
1	1	250	ASP	N-CA-C	-5.67	107.01	114.04
3	k	106	THR	CA-C-N	5.67	127.88	120.28
3	k	106	THR	C-N-CA	5.67	127.88	120.28
1	2	292	ARG	N-CA-CB	5.67	120.07	110.49
2	F	52	PRO	CA-C-N	5.67	127.87	120.28
2	F	52	PRO	C-N-CA	5.67	127.87	120.28
1	4	122	ILE	N-CA-C	-5.66	99.39	107.77
2	D	88	GLY	CA-C-N	5.66	132.35	121.54
2	D	88	GLY	C-N-CA	5.66	132.35	121.54
3	g	126	ALA	CA-C-N	5.65	128.17	120.54
3	g	126	ALA	C-N-CA	5.65	128.17	120.54
3	a	126	ALA	CA-C-N	5.64	128.16	120.54
3	a	126	ALA	C-N-CA	5.64	128.16	120.54
1	O	375	LEU	N-CA-C	-5.64	98.78	110.80
3	e	137	HIS	CE1-NE2-CD2	-5.64	103.36	109.00
1	P	112	SER	CA-C-N	5.64	127.84	120.28
1	P	112	SER	C-N-CA	5.64	127.84	120.28
2	E	73	VAL	N-CA-CB	5.64	121.09	111.50
2	B	90	LEU	N-CA-C	-5.63	103.79	111.56
1	4	148	HIS	CE1-NE2-CD2	-5.63	103.37	109.00
1	O	172	GLN	N-CA-C	-5.63	98.06	107.80
3	a	137	HIS	CE1-NE2-CD2	-5.63	103.37	109.00
1	Q	259	ILE	N-CA-C	-5.63	100.29	108.17
3	i	125	ILE	CA-C-N	5.63	127.82	120.28
3	i	125	ILE	C-N-CA	5.63	127.82	120.28
2	J	80	LYS	CA-C-N	5.63	131.83	121.70
2	J	80	LYS	C-N-CA	5.63	131.83	121.70
1	M	399	GLU	CA-C-N	5.63	127.75	120.44
1	M	399	GLU	C-N-CA	5.63	127.75	120.44
2	A	136	LEU	CA-C-N	5.62	125.32	119.92
2	A	136	LEU	C-N-CA	5.62	125.32	119.92
3	b	63	LEU	N-CA-C	-5.62	99.10	108.32
3	j	90	PHE	CA-CB-CG	5.62	119.42	113.80
1	4	74	LEU	CA-C-N	5.62	128.58	120.38
1	4	74	LEU	C-N-CA	5.62	128.58	120.38
1	N	456	GLN	N-CA-CB	5.62	119.99	110.49
2	D	83	THR	CA-C-N	5.62	132.27	121.54
2	D	83	THR	C-N-CA	5.62	132.27	121.54
1	1	317	TYR	CA-C-N	5.62	127.74	120.44
1	1	317	TYR	C-N-CA	5.62	127.74	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	297	PRO	CA-C-N	5.62	127.11	120.09
1	M	297	PRO	C-N-CA	5.62	127.11	120.09
2	F	89	SER	N-CA-C	-5.62	108.22	114.62
2	H	174	VAL	N-CA-C	-5.62	100.25	108.11
1	R	258	LYS	N-CA-C	-5.61	105.19	113.61
1	Q	425	LYS	CA-C-N	5.61	127.80	120.28
1	Q	425	LYS	C-N-CA	5.61	127.80	120.28
1	S	167	GLU	CA-C-N	5.61	128.84	120.31
1	S	167	GLU	C-N-CA	5.61	128.84	120.31
1	S	205	VAL	N-CA-C	-5.61	100.94	108.35
3	b	141	LEU	CB-CA-C	-5.61	101.48	110.79
1	2	173	VAL	N-CA-C	-5.60	100.26	108.11
3	l	74	LYS	N-CA-C	-5.60	100.65	109.50
3	h	146	ILE	CA-C-N	5.60	127.78	120.28
3	h	146	ILE	C-N-CA	5.60	127.78	120.28
2	L	117	PRO	N-CA-C	5.60	124.00	112.47
1	P	89	HIS	ND1-CE1-NE2	5.60	114.00	108.40
1	1	415	THR	N-CA-C	-5.59	100.80	109.14
2	J	113	LEU	CA-C-N	5.59	127.78	120.28
2	J	113	LEU	C-N-CA	5.59	127.78	120.28
1	R	91	ARG	N-CA-C	5.59	117.07	110.97
1	R	376	SER	N-CA-C	-5.59	100.21	108.99
1	R	116	ALA	N-CA-CB	5.59	119.94	110.49
1	S	415	THR	N-CA-C	-5.59	100.21	108.99
1	4	202	VAL	N-CA-C	-5.59	100.55	108.65
3	d	68	ALA	CA-C-N	5.59	127.77	120.28
3	d	68	ALA	C-N-CA	5.59	127.77	120.28
2	A	91	ASP	N-CA-CB	5.58	118.82	110.22
1	N	96	GLY	CA-C-N	5.58	127.76	120.28
1	N	96	GLY	C-N-CA	5.58	127.76	120.28
1	P	181	SER	N-CA-C	-5.58	106.13	113.17
1	S	319	HIS	CA-CB-CG	5.58	119.38	113.80
2	D	85	GLY	CA-C-N	5.58	131.75	121.70
2	D	85	GLY	C-N-CA	5.58	131.75	121.70
3	j	112	LYS	CA-C-N	5.58	132.21	121.54
3	j	112	LYS	C-N-CA	5.58	132.21	121.54
1	T	343	ASN	N-CA-C	-5.58	98.25	108.02
1	N	181	SER	N-CA-C	-5.58	106.47	113.28
2	A	95	TYR	CA-C-N	5.58	131.74	121.70
2	A	95	TYR	C-N-CA	5.58	131.74	121.70
2	A	99	ALA	N-CA-C	-5.58	105.58	112.72
2	I	90	LEU	N-CA-C	-5.57	105.69	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	119	ARG	N-CA-CB	5.57	119.90	110.49
1	3	307	ALA	CA-C-N	5.57	128.30	120.28
1	3	307	ALA	C-N-CA	5.57	128.30	120.28
1	S	304	LEU	CA-C-N	5.57	126.01	119.94
1	S	304	LEU	C-N-CA	5.57	126.01	119.94
2	D	56	SER	CA-C-N	5.57	127.68	120.44
2	D	56	SER	C-N-CA	5.57	127.68	120.44
3	i	157	GLN	CA-C-N	5.57	126.68	119.78
3	i	157	GLN	C-N-CA	5.57	126.68	119.78
3	j	121	LYS	CA-C-N	5.57	128.01	120.38
3	j	121	LYS	C-N-CA	5.57	128.01	120.38
2	L	105	SER	CA-C-N	5.57	127.74	120.28
2	L	105	SER	C-N-CA	5.57	127.74	120.28
1	1	80	TYR	N-CA-C	-5.56	98.95	110.80
1	M	205	VAL	CA-C-N	5.56	128.61	120.71
1	M	205	VAL	C-N-CA	5.56	128.61	120.71
2	J	55	ALA	CA-C-N	5.56	127.67	120.44
2	J	55	ALA	C-N-CA	5.56	127.67	120.44
2	L	117	PRO	CA-C-N	5.56	131.71	121.70
2	L	117	PRO	C-N-CA	5.56	131.71	121.70
2	K	183	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
3	e	160	LYS	N-CA-C	-5.56	105.85	113.30
2	H	120	PHE	CA-C-N	5.56	128.00	120.44
2	H	120	PHE	C-N-CA	5.56	128.00	120.44
1	P	385	SER	N-CA-C	-5.56	98.97	110.80
1	R	315	MET	N-CA-C	5.56	120.54	111.37
1	O	155	GLU	N-CA-C	-5.55	101.03	108.86
2	K	56	SER	CA-C-N	5.55	127.72	120.28
2	K	56	SER	C-N-CA	5.55	127.72	120.28
1	S	400	ASP	CA-C-N	5.55	127.72	120.28
1	S	400	ASP	C-N-CA	5.55	127.72	120.28
1	S	449	LEU	N-CA-C	-5.55	105.86	113.30
3	j	126	ALA	CA-C-N	5.55	127.65	120.44
3	j	126	ALA	C-N-CA	5.55	127.65	120.44
1	P	114	ILE	N-CA-C	-5.55	107.33	112.43
2	D	82	GLY	N-CA-C	-5.55	104.60	112.37
1	3	80	TYR	CA-C-N	5.55	127.71	120.28
1	3	80	TYR	C-N-CA	5.55	127.71	120.28
1	4	136	LYS	CA-C-N	5.55	126.14	119.98
1	4	136	LYS	C-N-CA	5.55	126.14	119.98
1	O	370	LEU	CA-C-N	5.55	127.71	120.28
1	O	370	LEU	C-N-CA	5.55	127.71	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	60	ARG	N-CA-CB	5.55	119.86	110.49
1	S	117	ASP	N-CA-C	-5.54	97.55	109.81
2	K	109	PHE	CA-CB-CG	-5.54	108.25	113.80
1	O	456	GLN	CA-C-N	5.54	131.68	121.70
1	O	456	GLN	C-N-CA	5.54	131.68	121.70
1	P	439	LEU	CA-C-N	5.54	127.71	120.28
1	P	439	LEU	C-N-CA	5.54	127.71	120.28
1	R	300	LEU	CA-C-N	5.54	128.29	120.42
1	R	300	LEU	C-N-CA	5.54	128.29	120.42
2	G	48	ALA	CA-C-N	5.54	128.71	120.95
2	G	48	ALA	C-N-CA	5.54	128.71	120.95
1	4	97	TRP	CA-C-N	5.54	128.47	120.38
1	4	97	TRP	C-N-CA	5.54	128.47	120.38
1	4	443	VAL	N-CA-CB	5.54	118.89	110.58
1	2	99	SER	CA-C-N	5.54	127.70	120.28
1	2	99	SER	C-N-CA	5.54	127.70	120.28
1	4	119	ARG	NE-CZ-NH1	-5.54	115.96	121.50
2	H	49	THR	N-CA-C	-5.54	100.29	108.99
2	K	110	PHE	CA-CB-CG	-5.54	108.26	113.80
1	4	298	THR	N-CA-C	5.53	121.02	113.16
1	4	94	ALA	CA-C-N	5.53	127.69	120.28
1	4	94	ALA	C-N-CA	5.53	127.69	120.28
1	O	452	ILE	N-CA-CB	5.53	120.90	111.50
1	N	455	THR	CA-C-N	5.53	132.10	121.54
1	N	455	THR	C-N-CA	5.53	132.10	121.54
2	D	67	ASN	CA-C-N	5.53	128.03	120.46
2	D	67	ASN	C-N-CA	5.53	128.03	120.46
3	j	137	HIS	CE1-NE2-CD2	-5.53	103.47	109.00
3	e	145	ALA	CA-C-N	5.53	127.52	120.56
3	e	145	ALA	C-N-CA	5.53	127.52	120.56
3	f	102	SER	CA-C-N	5.53	127.68	120.28
3	f	102	SER	C-N-CA	5.53	127.68	120.28
1	R	429	HIS	CE1-NE2-CD2	-5.52	103.48	109.00
2	J	67	ASN	CA-C-N	5.52	128.03	120.46
2	J	67	ASN	C-N-CA	5.52	128.03	120.46
1	3	158	CYS	CA-C-N	5.52	128.26	120.42
1	3	158	CYS	C-N-CA	5.52	128.26	120.42
2	A	200	LEU	N-CA-C	-5.52	104.39	113.50
2	C	95	TYR	CA-C-N	5.52	131.63	121.70
2	C	95	TYR	C-N-CA	5.52	131.63	121.70
2	J	126	SER	CA-C-N	5.52	131.63	121.70
2	J	126	SER	C-N-CA	5.52	131.63	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	341	VAL	N-CA-C	-5.51	100.12	108.17
2	G	148	GLN	CA-C-N	5.51	129.06	120.68
2	G	148	GLN	C-N-CA	5.51	129.06	120.68
3	l	136	LEU	N-CA-C	-5.51	106.55	113.28
3	e	140	MET	CB-CA-C	-5.51	100.43	110.63
3	j	66	ALA	CA-C-N	5.51	125.46	119.78
3	j	66	ALA	C-N-CA	5.51	125.46	119.78
1	R	250	ASP	N-CA-C	-5.51	107.56	114.56
1	O	381	CYS	CB-CA-C	5.51	121.39	110.42
1	S	344	GLY	N-CA-C	-5.51	105.30	111.63
3	d	91	LYS	N-CA-C	-5.51	99.06	110.80
2	K	113	LEU	CA-C-N	5.51	127.66	120.28
2	K	113	LEU	C-N-CA	5.51	127.66	120.28
1	T	93	HIS	N-CA-C	-5.51	100.06	108.76
1	Q	415	THR	N-CA-C	-5.50	100.94	109.14
1	M	359	ALA	CA-C-N	5.50	129.99	122.34
1	M	359	ALA	C-N-CA	5.50	129.99	122.34
1	O	417	GLU	CA-C-N	5.50	127.65	120.28
1	O	417	GLU	C-N-CA	5.50	127.65	120.28
1	2	328	ARG	CA-C-N	5.50	127.58	120.44
1	2	328	ARG	C-N-CA	5.50	127.58	120.44
3	a	136	LEU	N-CA-C	-5.50	104.83	112.30
3	b	134	VAL	N-CA-C	-5.50	106.99	113.42
3	e	111	GLY	N-CA-C	-5.49	107.74	115.32
2	C	102	THR	CA-C-N	5.49	127.64	120.28
2	C	102	THR	C-N-CA	5.49	127.64	120.28
1	N	448	ASP	CA-C-N	5.49	132.02	121.54
1	N	448	ASP	C-N-CA	5.49	132.02	121.54
1	M	225	ARG	CA-C-N	5.49	129.93	122.19
1	M	225	ARG	C-N-CA	5.49	129.93	122.19
1	S	444	GLN	CA-C-N	5.49	127.63	120.28
1	S	444	GLN	C-N-CA	5.49	127.63	120.28
2	H	95	TYR	CA-C-N	5.49	131.58	121.70
2	H	95	TYR	C-N-CA	5.49	131.58	121.70
1	4	259	ILE	CA-C-N	5.48	132.01	121.54
1	4	259	ILE	C-N-CA	5.48	132.01	121.54
1	M	202	VAL	N-CA-C	-5.48	100.70	108.65
1	N	89	HIS	ND1-CE1-NE2	5.48	113.88	108.40
1	S	432	ARG	CA-C-N	5.48	127.63	120.28
1	S	432	ARG	C-N-CA	5.48	127.63	120.28
2	H	98	LEU	CB-CA-C	-5.48	101.69	110.79
3	f	159	PRO	CA-C-N	5.48	127.94	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	f	159	PRO	C-N-CA	5.48	127.94	120.54
2	E	57	SER	CA-C-N	5.48	127.62	120.28
2	E	57	SER	C-N-CA	5.48	127.62	120.28
2	D	172	ASN	CA-CB-CG	-5.47	107.13	112.60
1	3	78	LEU	CA-C-N	5.47	124.66	118.97
1	3	78	LEU	C-N-CA	5.47	124.66	118.97
1	1	107	ARG	CB-CA-C	-5.47	102.29	110.88
1	S	222	CYS	CA-C-N	5.47	127.61	120.28
1	S	222	CYS	C-N-CA	5.47	127.61	120.28
1	4	429	HIS	ND1-CE1-NE2	5.47	113.87	108.40
1	M	423	VAL	CA-C-N	5.47	128.06	120.29
1	M	423	VAL	C-N-CA	5.47	128.06	120.29
3	f	132	PRO	CA-C-N	5.47	126.68	119.84
3	f	132	PRO	C-N-CA	5.47	126.68	119.84
1	M	162	SER	CA-C-N	5.47	127.61	120.28
1	M	162	SER	C-N-CA	5.47	127.61	120.28
1	4	73	VAL	CA-C-N	5.46	128.05	120.29
1	4	73	VAL	C-N-CA	5.46	128.05	120.29
1	O	205	VAL	CA-C-N	5.46	128.60	120.95
1	O	205	VAL	C-N-CA	5.46	128.60	120.95
1	Q	74	LEU	CA-C-N	5.46	127.60	120.28
1	Q	74	LEU	C-N-CA	5.46	127.60	120.28
1	1	393	ARG	CA-C-N	5.46	127.60	120.28
1	1	393	ARG	C-N-CA	5.46	127.60	120.28
3	k	89	ARG	N-CA-C	-5.46	100.80	109.59
1	P	374	ALA	CA-C-N	5.46	131.97	121.54
1	P	374	ALA	C-N-CA	5.46	131.97	121.54
2	D	98	LEU	CA-C-N	5.46	127.86	120.38
2	D	98	LEU	C-N-CA	5.46	127.86	120.38
3	f	151	ALA	CA-C-N	5.46	127.59	120.28
3	f	151	ALA	C-N-CA	5.46	127.59	120.28
2	G	186	LEU	CA-C-N	5.46	127.59	120.28
2	G	186	LEU	C-N-CA	5.46	127.59	120.28
2	I	118	TYR	N-CA-C	5.46	126.28	111.00
2	E	104	ASP	CA-C-N	5.46	128.04	120.29
2	E	104	ASP	C-N-CA	5.46	128.04	120.29
1	R	420	ASP	CA-C-N	5.45	128.59	120.31
1	R	420	ASP	C-N-CA	5.45	128.59	120.31
3	e	133	PRO	N-CA-C	-5.45	107.06	114.80
1	2	314	GLU	CA-C-N	5.45	128.99	120.82
1	2	314	GLU	C-N-CA	5.45	128.99	120.82
1	4	317	TYR	CA-C-N	5.45	127.52	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	317	TYR	C-N-CA	5.45	127.52	120.44
1	O	239	LYS	N-CA-C	-5.45	107.64	114.56
1	P	202	VAL	N-CA-C	-5.45	100.75	108.65
2	I	43	ARG	N-CA-C	-5.45	105.39	113.40
1	O	89	HIS	ND1-CE1-NE2	5.45	113.85	108.40
1	T	319	HIS	CA-CB-CG	5.45	119.25	113.80
1	R	349	HIS	ND1-CE1-NE2	5.44	113.84	108.40
1	O	395	ILE	CA-C-N	5.44	125.14	119.92
1	O	395	ILE	C-N-CA	5.44	125.14	119.92
1	P	125	SER	CA-C-N	5.43	125.79	121.61
1	P	125	SER	C-N-CA	5.43	125.79	121.61
1	T	195	PRO	CA-C-N	5.43	127.56	120.28
1	T	195	PRO	C-N-CA	5.43	127.56	120.28
1	R	70	ASP	CA-C-N	5.43	125.51	119.32
1	R	70	ASP	C-N-CA	5.43	125.51	119.32
1	N	134	ALA	N-CA-C	5.42	116.87	111.07
3	i	137	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
1	P	138	VAL	CA-C-N	5.42	127.55	120.28
1	P	138	VAL	C-N-CA	5.42	127.55	120.28
1	R	371	LYS	CA-C-N	5.42	131.89	121.54
1	R	371	LYS	C-N-CA	5.42	131.89	121.54
1	O	235	GLN	N-CA-C	-5.42	105.36	112.41
1	N	256	GLY	CA-C-N	5.42	127.54	120.28
1	N	256	GLY	C-N-CA	5.42	127.54	120.28
1	Q	202	VAL	N-CA-C	-5.42	100.80	108.65
1	Q	106	ALA	CA-C-N	5.41	127.53	120.28
1	Q	106	ALA	C-N-CA	5.41	127.53	120.28
1	S	393	ARG	N-CA-C	-5.41	106.60	114.12
1	P	89	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
2	F	91	ASP	CA-C-N	5.41	127.97	120.29
2	F	91	ASP	C-N-CA	5.41	127.97	120.29
3	f	136	LEU	CA-C-N	5.41	127.80	120.44
3	f	136	LEU	C-N-CA	5.41	127.80	120.44
1	O	70	ASP	CA-C-N	5.41	125.48	119.32
1	O	70	ASP	C-N-CA	5.41	125.48	119.32
1	M	328	ARG	CA-C-N	5.40	127.47	120.44
1	M	328	ARG	C-N-CA	5.40	127.47	120.44
1	1	310	VAL	N-CA-C	5.40	120.58	109.34
1	3	137	GLY	CA-C-N	5.40	128.09	120.42
1	3	137	GLY	C-N-CA	5.40	128.09	120.42
1	3	145	ARG	N-CA-CB	5.40	119.62	110.49
1	P	214	PRO	CA-C-N	5.40	127.36	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	214	PRO	C-N-CA	5.40	127.36	120.56
1	2	449	LEU	N-CA-CB	5.40	119.67	110.50
1	N	348	HIS	ND1-CE1-NE2	5.39	113.79	108.40
1	S	333	ILE	CA-C-N	5.39	127.45	120.44
1	S	333	ILE	C-N-CA	5.39	127.45	120.44
1	R	214	PRO	CA-C-N	5.39	127.85	120.46
1	R	214	PRO	C-N-CA	5.39	127.85	120.46
2	G	82	GLY	CA-C-O	-5.39	116.39	120.76
1	T	339	ASP	CB-CA-C	-5.39	110.38	116.63
2	A	66	TRP	CA-C-N	5.39	127.50	120.28
2	A	66	TRP	C-N-CA	5.39	127.50	120.28
1	T	82	ILE	N-CA-CB	5.39	117.86	110.54
1	P	362	GLU	CA-C-N	5.38	125.95	119.98
1	P	362	GLU	C-N-CA	5.38	125.95	119.98
2	L	172	ASN	N-CA-C	-5.38	104.50	111.71
1	4	395	ILE	N-CA-C	-5.38	100.00	107.80
2	F	172	ASN	CA-C-N	5.38	127.93	120.29
2	F	172	ASN	C-N-CA	5.38	127.93	120.29
2	A	60	ARG	CA-C-N	5.38	131.38	121.70
2	A	60	ARG	C-N-CA	5.38	131.38	121.70
3	l	59	VAL	CA-C-N	5.38	127.15	121.45
3	l	59	VAL	C-N-CA	5.38	127.15	121.45
1	P	118	PRO	CA-C-N	5.38	130.45	122.82
1	P	118	PRO	C-N-CA	5.38	130.45	122.82
3	f	162	GLY	CA-C-N	5.38	127.92	120.29
3	f	162	GLY	C-N-CA	5.38	127.92	120.29
1	M	360	TYR	N-CA-C	5.37	119.04	111.52
1	R	202	VAL	N-CA-C	-5.37	100.86	108.65
1	4	143	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	T	457	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
1	N	118	PRO	CA-C-N	5.37	129.98	122.36
1	N	118	PRO	C-N-CA	5.37	129.98	122.36
2	J	95	TYR	CA-C-N	5.37	131.36	121.70
2	J	95	TYR	C-N-CA	5.37	131.36	121.70
2	K	164	LYS	CA-C-N	5.37	130.30	122.41
2	K	164	LYS	C-N-CA	5.37	130.30	122.41
2	L	200	LEU	N-CA-C	-5.36	104.65	113.50
1	N	449	LEU	N-CA-C	-5.36	99.39	110.80
1	P	345	ASP	CA-C-O	-5.36	115.69	120.19
2	G	84	LEU	N-CA-C	5.36	118.73	111.17
3	g	137	HIS	CA-CB-CG	5.36	119.16	113.80
3	h	121	LYS	CA-C-N	5.36	127.72	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h	121	LYS	C-N-CA	5.36	127.72	120.38
2	J	135	LYS	N-CA-C	-5.36	100.57	109.46
1	1	308	CYS	CA-C-N	5.36	127.45	120.28
1	1	308	CYS	C-N-CA	5.36	127.45	120.28
1	2	236	ALA	CA-C-N	5.36	127.75	120.63
1	2	236	ALA	C-N-CA	5.36	127.75	120.63
1	O	298	THR	CA-C-O	-5.35	113.15	118.34
2	B	59	GLN	CA-C-N	5.35	131.32	121.70
2	B	59	GLN	C-N-CA	5.35	131.32	121.70
1	1	82	ILE	N-CA-C	5.34	116.07	110.62
1	1	244	VAL	N-CA-C	-5.34	108.07	113.47
2	I	125	VAL	N-CA-C	-5.34	100.62	108.85
2	D	108	GLU	CA-C-N	5.34	127.43	120.28
2	D	108	GLU	C-N-CA	5.34	127.43	120.28
3	g	71	ASP	CA-C-N	5.34	131.31	121.70
3	g	71	ASP	C-N-CA	5.34	131.31	121.70
2	H	88	GLY	CA-C-N	5.34	131.74	121.54
2	H	88	GLY	C-N-CA	5.34	131.74	121.54
1	P	159	VAL	CA-C-N	5.34	127.43	120.28
1	P	159	VAL	C-N-CA	5.34	127.43	120.28
1	2	114	ILE	N-CA-C	-5.33	106.66	113.22
2	A	188	ALA	CA-C-N	5.33	127.37	120.44
2	A	188	ALA	C-N-CA	5.33	127.37	120.44
2	D	205	TYR	N-CA-C	-5.33	104.70	113.50
1	S	328	ARG	CA-C-N	5.33	127.74	120.54
1	S	328	ARG	C-N-CA	5.33	127.74	120.54
2	D	127	PHE	N-CA-CB	5.33	119.56	110.50
3	f	86	VAL	N-CA-C	5.33	115.54	110.42
3	g	106	THR	N-CA-CB	5.33	117.74	110.01
3	a	80	ASP	N-CA-C	-5.33	101.31	109.41
1	P	368	MET	N-CA-CB	5.33	117.95	110.12
1	P	437	SER	N-CA-C	-5.33	101.33	109.64
1	T	408	PHE	CA-CB-CG	5.33	119.13	113.80
3	c	94	GLY	CA-C-N	5.33	127.37	120.44
3	c	94	GLY	C-N-CA	5.33	127.37	120.44
1	M	316	GLU	CA-C-N	5.33	127.36	120.44
1	M	316	GLU	C-N-CA	5.33	127.36	120.44
1	P	107	ARG	CA-C-N	5.33	127.42	120.28
1	P	107	ARG	C-N-CA	5.33	127.42	120.28
1	T	384	ALA	N-CA-CB	5.33	119.49	110.49
2	B	176	SER	N-CA-CB	5.32	119.48	110.49
2	L	74	TYR	N-CA-CB	5.32	119.48	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	349	HIS	CE1-NE2-CD2	-5.32	103.69	109.00
1	S	95	TYR	CA-C-N	5.31	125.88	119.98
1	S	95	TYR	C-N-CA	5.31	125.88	119.98
1	M	285	GLY	N-CA-C	-5.31	104.92	111.45
1	T	214	PRO	CA-C-N	5.31	127.73	120.46
1	T	214	PRO	C-N-CA	5.31	127.73	120.46
2	I	67	ASN	CA-C-N	5.31	127.73	120.46
2	I	67	ASN	C-N-CA	5.31	127.73	120.46
3	a	54	LYS	N-CA-C	-5.31	104.39	111.87
2	I	85	GLY	CA-C-N	5.31	131.25	121.70
2	I	85	GLY	C-N-CA	5.31	131.25	121.70
2	J	85	GLY	CA-C-N	5.31	131.25	121.70
2	J	85	GLY	C-N-CA	5.31	131.25	121.70
1	R	350	TYR	N-CA-C	-5.30	103.09	109.72
1	4	116	ALA	CA-C-N	5.30	126.36	119.78
1	4	116	ALA	C-N-CA	5.30	126.36	119.78
1	N	80	TYR	CA-C-N	5.30	128.12	120.38
1	N	80	TYR	C-N-CA	5.30	128.12	120.38
3	l	58	ASN	CA-C-N	5.30	131.52	121.97
3	l	58	ASN	C-N-CA	5.30	131.52	121.97
2	C	172	ASN	N-CA-C	-5.30	100.68	108.79
2	C	201	SER	N-CA-C	-5.30	104.75	113.50
3	j	58	ASN	CA-C-N	5.30	131.51	121.97
3	j	58	ASN	C-N-CA	5.30	131.51	121.97
1	M	148	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
3	k	137	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
1	1	333	ILE	CA-C-N	5.30	127.33	120.44
1	1	333	ILE	C-N-CA	5.30	127.33	120.44
2	J	98	LEU	N-CA-C	-5.30	104.76	113.50
1	P	146	LYS	N-CA-C	-5.29	99.66	108.34
1	R	413	PHE	N-CA-C	-5.29	105.67	113.61
2	C	85	GLY	CA-C-N	5.29	131.23	121.70
2	C	85	GLY	C-N-CA	5.29	131.23	121.70
1	M	133	ILE	CA-C-N	5.29	127.32	120.44
1	M	133	ILE	C-N-CA	5.29	127.32	120.44
3	j	158	GLU	O-C-N	-5.29	115.24	121.32
1	1	90	SER	CA-C-N	5.29	131.64	121.54
1	1	90	SER	C-N-CA	5.29	131.64	121.54
1	M	293	SER	N-CA-C	-5.29	100.69	108.99
1	M	403	HIS	ND1-CE1-NE2	5.29	113.69	108.40
1	N	239	LYS	N-CA-C	-5.29	108.08	114.75
1	4	112	SER	CA-C-N	5.29	127.37	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	112	SER	C-N-CA	5.29	127.37	120.28
3	e	166	LYS	N-CA-C	-5.29	108.09	114.75
1	Q	456	GLN	CA-C-N	5.29	131.22	121.70
1	Q	456	GLN	C-N-CA	5.29	131.22	121.70
1	N	271	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	Q	372	ASP	N-CA-CB	5.28	119.42	110.49
2	C	80	LYS	CA-C-N	5.28	131.21	121.70
2	C	80	LYS	C-N-CA	5.28	131.21	121.70
1	M	333	ILE	CA-C-N	5.28	127.30	120.44
1	M	333	ILE	C-N-CA	5.28	127.30	120.44
3	e	69	CYS	N-CA-C	-5.28	104.79	113.50
2	F	95	TYR	CA-C-N	5.27	131.19	121.70
2	F	95	TYR	C-N-CA	5.27	131.19	121.70
2	K	97	ARG	CA-C-N	5.27	127.34	120.28
2	K	97	ARG	C-N-CA	5.27	127.34	120.28
2	L	172	ASN	CA-C-N	5.27	131.61	121.54
2	L	172	ASN	C-N-CA	5.27	131.61	121.54
1	2	159	VAL	CA-C-N	5.27	127.34	120.28
1	2	159	VAL	C-N-CA	5.27	127.34	120.28
3	i	107	GLU	CA-C-N	5.27	129.03	120.60
3	i	107	GLU	C-N-CA	5.27	129.03	120.60
3	e	124	ASP	CA-CB-CG	-5.27	107.33	112.60
1	O	171	PHE	CA-C-N	5.27	130.08	122.44
1	O	171	PHE	C-N-CA	5.27	130.08	122.44
2	F	48	ALA	N-CA-C	-5.27	104.51	112.99
1	Q	181	SER	N-CA-C	-5.26	106.54	113.17
2	A	177	HIS	CG-CD2-NE2	5.26	112.46	107.20
1	4	328	ARG	CA-C-N	5.26	127.28	120.44
1	4	328	ARG	C-N-CA	5.26	127.28	120.44
3	a	163	GLU	CA-C-N	5.26	128.31	120.31
3	a	163	GLU	C-N-CA	5.26	128.31	120.31
1	2	446	GLY	CA-C-N	5.26	131.17	121.70
1	2	446	GLY	C-N-CA	5.26	131.17	121.70
1	T	122	ILE	N-CA-CB	5.26	118.40	111.25
1	O	407	ARG	N-CA-C	-5.26	99.72	108.34
1	T	309	GLU	CA-C-N	5.26	127.66	120.46
1	T	309	GLU	C-N-CA	5.26	127.66	120.46
1	1	218	ILE	CA-C-N	5.26	126.89	120.22
1	1	218	ILE	C-N-CA	5.26	126.89	120.22
3	g	121	LYS	CA-C-N	5.26	127.58	120.38
3	g	121	LYS	C-N-CA	5.26	127.58	120.38
2	D	117	PRO	CA-C-N	5.25	127.75	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	117	PRO	C-N-CA	5.25	127.75	120.29
2	I	45	ASP	N-CA-C	5.25	117.07	110.24
1	S	112	SER	CA-C-N	5.25	127.84	120.28
1	S	112	SER	C-N-CA	5.25	127.84	120.28
3	d	72	VAL	N-CA-C	-5.25	108.16	113.20
1	4	93	HIS	N-CA-C	-5.25	105.54	112.94
1	N	457	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
2	L	86	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	3	349	HIS	ND1-CE1-NE2	5.24	113.64	108.40
3	j	82	LYS	N-CA-C	-5.24	99.04	108.48
1	Q	368	MET	CB-CA-C	-5.24	102.09	110.79
2	I	56	SER	CA-C-N	5.24	127.73	120.29
2	I	56	SER	C-N-CA	5.24	127.73	120.29
3	i	91	LYS	O-C-N	-5.24	116.97	123.36
1	4	136	LYS	CB-CG-CD	5.24	123.34	111.30
1	N	268	ILE	N-CA-C	-5.24	100.70	108.45
1	N	424	GLU	CA-C-N	5.24	127.61	120.54
1	N	424	GLU	C-N-CA	5.24	127.61	120.54
2	A	55	ALA	CA-C-N	5.24	127.25	120.44
2	A	55	ALA	C-N-CA	5.24	127.25	120.44
3	b	91	LYS	N-CA-C	-5.24	100.07	108.55
2	J	193	ALA	CA-C-N	5.24	127.29	120.28
2	J	193	ALA	C-N-CA	5.24	127.29	120.28
1	M	328	ARG	NE-CZ-NH1	-5.23	116.27	121.50
3	j	99	ILE	N-CA-CB	5.23	116.67	110.55
1	3	453	LYS	CA-C-N	5.23	131.11	121.70
1	3	453	LYS	C-N-CA	5.23	131.11	121.70
1	N	84	TYR	N-CA-C	-5.23	104.64	112.54
1	Q	156	HIS	CG-CD2-NE2	5.23	112.43	107.20
1	P	319	HIS	ND1-CE1-NE2	5.23	113.63	108.40
1	1	120	GLU	N-CA-C	-5.22	106.49	112.92
1	3	308	CYS	CA-C-N	5.22	127.23	120.44
1	3	308	CYS	C-N-CA	5.22	127.23	120.44
2	D	183	HIS	ND1-CE1-NE2	5.22	113.62	108.40
2	E	105	SER	CA-C-N	5.22	127.23	120.44
2	E	105	SER	C-N-CA	5.22	127.23	120.44
3	j	131	LEU	CA-C-N	5.22	125.76	120.38
3	j	131	LEU	C-N-CA	5.22	125.76	120.38
1	3	449	LEU	CA-C-N	5.22	131.51	121.54
1	3	449	LEU	C-N-CA	5.22	131.51	121.54
1	N	136	LYS	CA-C-N	5.22	125.73	119.94
1	N	136	LYS	C-N-CA	5.22	125.73	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	359	ALA	N-CA-CB	5.22	119.31	110.49
1	1	185	ASP	CA-C-N	5.22	128.24	120.31
1	1	185	ASP	C-N-CA	5.22	128.24	120.31
1	T	416	GLU	CA-C-N	5.22	127.54	120.44
1	T	416	GLU	C-N-CA	5.22	127.54	120.44
2	L	112	ASP	CA-C-N	5.22	127.27	120.28
2	L	112	ASP	C-N-CA	5.22	127.27	120.28
1	1	303	GLY	CA-C-N	5.22	127.27	120.28
1	1	303	GLY	C-N-CA	5.22	127.27	120.28
2	C	177	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
3	1	137	HIS	CA-C-N	5.21	127.70	120.29
3	1	137	HIS	C-N-CA	5.21	127.70	120.29
2	E	66	TRP	CA-C-N	5.21	127.78	120.28
2	E	66	TRP	C-N-CA	5.21	127.78	120.28
2	F	84	LEU	CA-C-N	5.21	131.07	121.70
2	F	84	LEU	C-N-CA	5.21	131.07	121.70
2	J	50	CYS	N-CA-C	-5.21	99.70	110.80
2	E	93	THR	N-CA-C	-5.21	106.95	113.72
2	F	176	SER	N-CA-CB	5.21	119.29	110.49
1	N	450	LYS	N-CA-CB	5.21	117.92	110.06
1	2	244	VAL	N-CA-C	-5.20	107.23	112.17
1	M	180	LYS	N-CA-C	-5.20	106.61	113.17
1	Q	257	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
2	B	169	THR	N-CA-C	-5.20	106.17	112.88
3	j	109	VAL	N-CA-CB	5.20	117.62	110.54
1	1	281	LEU	N-CA-C	-5.20	101.01	108.60
1	1	200	VAL	N-CA-C	-5.20	100.58	108.17
1	2	449	LEU	CA-C-N	5.20	131.46	121.54
1	2	449	LEU	C-N-CA	5.20	131.46	121.54
3	a	139	SER	CA-C-N	5.20	127.76	120.28
3	a	139	SER	C-N-CA	5.20	127.76	120.28
2	H	108	GLU	CA-C-N	5.20	127.24	120.28
2	H	108	GLU	C-N-CA	5.20	127.24	120.28
1	1	139	ALA	N-CA-C	5.19	116.63	111.07
2	F	178	ASP	N-CA-C	-5.19	108.21	114.75
1	O	250	ASP	N-CA-C	-5.19	106.89	113.43
1	S	78	LEU	CA-C-O	-5.19	113.31	118.34
1	1	123	PHE	CA-CB-CG	-5.19	108.61	113.80
1	Q	393	ARG	N-CA-C	-5.19	106.91	114.12
3	a	142	ALA	CA-C-N	5.19	127.18	120.44
3	a	142	ALA	C-N-CA	5.19	127.18	120.44
1	N	415	THR	CA-C-N	5.19	128.19	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	415	THR	C-N-CA	5.19	128.19	120.31
1	O	195	PRO	CA-C-N	5.19	127.66	120.29
1	O	195	PRO	C-N-CA	5.19	127.66	120.29
3	i	121	LYS	CA-C-N	5.19	127.48	120.38
3	i	121	LYS	C-N-CA	5.19	127.48	120.38
1	2	350	TYR	N-CA-C	-5.18	102.03	109.24
2	H	46	ILE	CA-CB-CG1	5.18	119.22	110.40
1	N	395	ILE	N-CA-C	-5.18	100.85	108.11
1	O	357	SER	N-CA-CB	5.18	119.25	110.49
2	K	84	LEU	CA-C-N	5.18	131.03	121.70
2	K	84	LEU	C-N-CA	5.18	131.03	121.70
1	4	432	ARG	CA-C-N	5.18	127.17	120.44
1	4	432	ARG	C-N-CA	5.18	127.17	120.44
3	c	146	ILE	CA-C-N	5.18	127.22	120.28
3	c	146	ILE	C-N-CA	5.18	127.22	120.28
2	B	199	ASP	CA-CB-CG	-5.18	107.42	112.60
1	Q	235	GLN	N-CA-C	-5.18	106.28	112.59
3	d	54	LYS	N-CA-C	-5.17	106.65	113.17
1	3	140	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	O	157	LYS	CA-C-N	5.17	127.16	120.44
1	O	157	LYS	C-N-CA	5.17	127.16	120.44
2	F	201	SER	N-CA-C	-5.17	99.79	110.80
2	A	115	ASP	CA-C-N	5.17	127.58	120.39
2	A	115	ASP	C-N-CA	5.17	127.58	120.39
1	M	362	GLU	CA-C-N	5.17	125.72	119.98
1	M	362	GLU	C-N-CA	5.17	125.72	119.98
1	M	415	THR	N-CA-C	-5.17	101.55	109.41
1	O	423	VAL	CA-C-N	5.17	127.62	120.29
1	O	423	VAL	C-N-CA	5.17	127.62	120.29
3	c	139	SER	CB-CA-C	-5.17	101.90	110.68
1	P	200	VAL	N-CA-C	-5.16	100.63	108.17
1	Q	323	SER	CA-C-N	5.16	127.20	120.28
1	Q	323	SER	C-N-CA	5.16	127.20	120.28
1	1	275	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	2	278	VAL	O-C-N	-5.16	117.10	123.09
1	3	84	TYR	CB-CA-C	-5.16	102.12	110.79
1	3	424	GLU	CA-C-N	5.16	127.51	120.54
1	3	424	GLU	C-N-CA	5.16	127.51	120.54
1	M	140	ARG	CA-C-N	5.16	127.15	120.44
1	M	140	ARG	C-N-CA	5.16	127.15	120.44
2	A	106	LEU	CA-C-N	5.16	127.19	120.28
2	A	106	LEU	C-N-CA	5.16	127.19	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	122	ASN	CA-C-N	5.16	127.19	120.28
3	d	122	ASN	C-N-CA	5.16	127.19	120.28
3	e	136	LEU	N-CA-C	-5.16	106.22	112.88
1	P	281	LEU	CB-CA-C	-5.16	109.65	115.79
1	P	401	LEU	CA-C-N	5.16	127.19	120.28
1	P	401	LEU	C-N-CA	5.16	127.19	120.28
3	h	150	LEU	CA-C-N	5.16	127.19	120.28
3	h	150	LEU	C-N-CA	5.16	127.19	120.28
3	k	58	ASN	CA-C-N	5.16	131.25	121.97
3	k	58	ASN	C-N-CA	5.16	131.25	121.97
1	N	164	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	N	164	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	O	257	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
1	R	307	ALA	CA-C-N	5.16	127.61	120.29
1	R	307	ALA	C-N-CA	5.16	127.61	120.29
1	l	406	ILE	N-CA-C	5.15	115.90	108.48
3	k	150	LEU	CA-C-N	5.15	127.19	120.28
3	k	150	LEU	C-N-CA	5.15	127.19	120.28
3	l	122	ASN	CA-C-N	5.15	127.19	120.28
3	l	122	ASN	C-N-CA	5.15	127.19	120.28
1	N	89	HIS	CE1-NE2-CD2	-5.15	103.85	109.00
1	N	348	HIS	CG-CD2-NE2	5.15	112.35	107.20
1	T	381	CYS	N-CA-C	-5.15	106.68	113.17
2	H	58	ASN	N-CA-CB	5.15	117.78	110.16
2	F	125	VAL	CA-C-N	5.15	131.38	121.54
2	F	125	VAL	C-N-CA	5.15	131.38	121.54
2	G	80	LYS	CA-C-N	5.15	130.97	121.70
2	G	80	LYS	C-N-CA	5.15	130.97	121.70
1	3	74	LEU	CA-C-N	5.15	127.18	120.28
1	3	74	LEU	C-N-CA	5.15	127.18	120.28
1	R	368	MET	CB-CA-C	-5.15	102.80	110.88
1	1	279	GLU	CA-C-N	5.15	128.08	120.82
1	1	279	GLU	C-N-CA	5.15	128.08	120.82
1	N	277	ARG	N-CA-C	-5.15	105.29	112.03
2	A	48	ALA	N-CA-CB	5.15	119.19	110.49
2	D	86	HIS	CE1-NE2-CD2	-5.15	103.85	109.00
2	H	56	SER	CA-C-N	5.15	127.13	120.44
2	H	56	SER	C-N-CA	5.15	127.13	120.44
1	2	439	LEU	CA-C-N	5.14	127.59	120.29
1	2	439	LEU	C-N-CA	5.14	127.59	120.29
1	Q	413	PHE	N-CA-C	-5.14	107.00	113.28
1	4	243	ASP	N-CA-C	-5.14	101.48	109.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	398	ASP	N-CA-C	-5.14	102.55	109.95
3	c	113	THR	CA-C-N	5.14	127.51	120.46
3	c	113	THR	C-N-CA	5.14	127.51	120.46
1	1	316	GLU	CA-C-N	5.14	127.17	120.28
1	1	316	GLU	C-N-CA	5.14	127.17	120.28
1	2	415	THR	N-CA-C	-5.14	101.55	109.52
2	G	139	ASP	CA-C-N	5.14	127.12	120.44
2	G	139	ASP	C-N-CA	5.14	127.12	120.44
3	a	73	MET	CA-C-N	5.14	128.51	120.75
3	a	73	MET	C-N-CA	5.14	128.51	120.75
3	g	141	LEU	CA-C-N	5.14	127.17	120.28
3	g	141	LEU	C-N-CA	5.14	127.17	120.28
3	j	138	CYS	CA-C-N	5.14	127.17	120.28
3	j	138	CYS	C-N-CA	5.14	127.17	120.28
1	2	116	ALA	N-CA-CB	5.14	119.17	110.49
1	S	188	GLU	CA-C-N	5.14	127.12	120.44
1	S	188	GLU	C-N-CA	5.14	127.12	120.44
1	T	414	THR	CA-C-N	5.14	130.58	122.36
1	T	414	THR	C-N-CA	5.14	130.58	122.36
3	b	125	ILE	CA-C-N	5.14	127.12	120.44
3	b	125	ILE	C-N-CA	5.14	127.12	120.44
2	E	131	VAL	N-CA-C	-5.14	98.61	107.24
1	1	412	ARG	CA-C-N	5.13	127.97	119.35
1	1	412	ARG	C-N-CA	5.13	127.97	119.35
1	3	454	TRP	CA-C-N	5.13	130.94	121.70
1	3	454	TRP	C-N-CA	5.13	130.94	121.70
3	a	95	CYS	CA-C-N	5.13	126.56	120.14
3	a	95	CYS	C-N-CA	5.13	126.56	120.14
1	Q	359	ALA	CA-C-N	5.13	129.41	122.07
1	Q	359	ALA	C-N-CA	5.13	129.41	122.07
1	S	407	ARG	N-CA-C	-5.13	98.91	107.99
1	3	401	LEU	CA-C-N	5.13	127.11	120.44
1	3	401	LEU	C-N-CA	5.13	127.11	120.44
1	4	257	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
1	O	300	LEU	CA-C-N	5.13	127.48	120.46
1	O	300	LEU	C-N-CA	5.13	127.48	120.46
3	b	89	ARG	N-CA-CB	5.13	118.79	110.43
3	g	155	LEU	N-CA-C	-5.13	105.77	112.23
1	O	71	PRO	CA-C-N	5.12	127.15	120.28
1	O	71	PRO	C-N-CA	5.12	127.15	120.28
1	O	339	ASP	CA-CB-CG	-5.12	107.48	112.60
2	K	132	LEU	CB-CA-C	5.12	118.58	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	400	ASP	CA-C-N	5.12	127.14	120.28
1	1	400	ASP	C-N-CA	5.12	127.14	120.28
1	O	76	ALA	CA-C-N	5.12	127.56	120.29
1	O	76	ALA	C-N-CA	5.12	127.56	120.29
1	O	125	SER	N-CA-C	-5.12	104.74	112.99
2	H	207	GLY	CA-C-N	5.12	131.32	121.54
2	H	207	GLY	C-N-CA	5.12	131.32	121.54
2	L	116	LYS	CA-C-N	5.12	126.24	119.84
2	L	116	LYS	C-N-CA	5.12	126.24	119.84
2	D	99	ALA	N-CA-C	5.12	117.52	111.33
1	1	101	ALA	CA-C-N	5.12	127.14	120.28
1	1	101	ALA	C-N-CA	5.12	127.14	120.28
1	4	445	ASP	CA-C-N	5.11	125.66	119.98
1	4	445	ASP	C-N-CA	5.11	125.66	119.98
2	E	61	GLY	CA-C-N	5.11	131.31	121.54
2	E	61	GLY	C-N-CA	5.11	131.31	121.54
2	J	99	ALA	N-CA-C	-5.11	104.75	111.96
1	2	156	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	2	171	PHE	N-CA-CB	5.11	117.43	110.38
2	G	142	THR	O-C-N	-5.11	117.15	123.33
1	M	383	SER	N-CA-CB	5.11	119.12	110.49
1	Q	386	LEU	CA-C-N	5.11	127.49	120.39
1	Q	386	LEU	C-N-CA	5.11	127.49	120.39
1	2	261	GLY	CA-C-O	-5.10	114.22	121.52
1	4	96	GLY	CA-C-N	5.10	127.12	120.28
1	4	96	GLY	C-N-CA	5.10	127.12	120.28
1	M	388	PRO	CA-C-N	5.10	131.28	121.54
1	M	388	PRO	C-N-CA	5.10	131.28	121.54
1	N	400	ASP	CA-C-N	5.10	127.11	120.28
1	N	400	ASP	C-N-CA	5.10	127.11	120.28
1	R	273	ARG	N-CA-CB	5.10	119.45	110.37
2	A	195	LYS	CA-C-N	5.10	127.95	120.71
2	A	195	LYS	C-N-CA	5.10	127.95	120.71
3	l	99	ILE	N-CA-CB	5.10	117.48	110.54
1	2	371	LYS	CA-C-N	5.10	131.28	121.54
1	2	371	LYS	C-N-CA	5.10	131.28	121.54
1	N	165	SER	CA-C-N	5.10	127.11	120.28
1	N	165	SER	C-N-CA	5.10	127.11	120.28
1	T	181	SER	N-CA-C	-5.10	107.01	113.18
3	g	80	ASP	CA-CB-CG	-5.10	107.50	112.60
1	M	403	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
2	C	123	TYR	CA-C-N	5.10	131.28	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	123	TYR	C-N-CA	5.10	131.28	121.54
1	3	299	PRO	CA-C-N	5.10	127.36	120.38
1	3	299	PRO	C-N-CA	5.10	127.36	120.38
1	T	157	LYS	CA-C-N	5.10	127.06	120.44
1	T	157	LYS	C-N-CA	5.10	127.06	120.44
1	M	452	ILE	N-CA-C	-5.09	101.29	108.27
1	P	163	CYS	CA-C-N	5.09	127.11	120.28
1	P	163	CYS	C-N-CA	5.09	127.11	120.28
1	1	114	ILE	N-CA-C	5.09	117.45	111.09
1	P	372	ASP	CA-CB-CG	5.09	117.69	112.60
2	H	51	THR	CA-C-N	5.09	124.88	119.28
2	H	51	THR	C-N-CA	5.09	124.88	119.28
1	N	67	THR	CA-C-N	5.09	125.10	120.21
1	N	67	THR	C-N-CA	5.09	125.10	120.21
2	E	177	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
2	L	131	VAL	CB-CA-C	5.09	117.04	110.12
2	A	121	GLU	CA-C-N	5.09	128.00	120.82
2	A	121	GLU	C-N-CA	5.09	128.00	120.82
3	j	158	GLU	CA-C-O	-5.09	113.19	120.16
2	C	174	VAL	CA-C-N	5.08	127.09	120.28
2	C	174	VAL	C-N-CA	5.08	127.09	120.28
1	3	180	LYS	N-CA-C	-5.08	107.08	113.28
1	T	374	ALA	CA-C-N	5.08	130.85	121.70
1	T	374	ALA	C-N-CA	5.08	130.85	121.70
2	C	165	ARG	N-CA-C	-5.08	102.26	110.14
2	F	165	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	3	415	THR	N-CA-C	-5.08	101.57	109.14
2	H	153	GLN	N-CA-C	-5.08	101.69	109.41
2	I	181	SER	CA-C-N	5.08	127.09	120.28
2	I	181	SER	C-N-CA	5.08	127.09	120.28
1	1	98	GLU	CA-C-N	5.08	127.08	120.28
1	1	98	GLU	C-N-CA	5.08	127.08	120.28
1	R	357	SER	O-C-N	-5.07	117.08	123.27
2	F	113	LEU	CA-C-N	5.07	127.08	120.28
2	F	113	LEU	C-N-CA	5.07	127.08	120.28
2	K	95	TYR	CB-CG-CD2	-5.07	113.19	120.80
2	B	43	ARG	NE-CZ-NH2	5.07	123.76	119.20
2	E	162	GLY	CA-C-N	5.07	125.07	119.90
2	E	162	GLY	C-N-CA	5.07	125.07	119.90
1	T	456	GLN	CA-C-N	5.07	130.82	121.70
1	T	456	GLN	C-N-CA	5.07	130.82	121.70
2	F	148	GLN	CA-C-N	5.07	128.38	120.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	148	GLN	C-N-CA	5.07	128.38	120.68
3	i	89	ARG	N-CA-CB	5.07	119.26	111.46
1	Q	81	LEU	N-CA-C	5.06	116.80	111.28
3	d	138	CYS	CA-C-N	5.06	127.06	120.28
3	d	138	CYS	C-N-CA	5.06	127.06	120.28
3	f	127	LYS	N-CA-C	5.06	117.19	111.11
1	2	310	VAL	N-CA-C	5.06	115.78	110.62
1	1	89	HIS	N-CA-CB	5.06	119.04	110.49
1	P	172	GLN	N-CA-C	-5.06	99.02	108.02
2	C	98	LEU	CA-C-N	5.05	127.01	120.44
2	C	98	LEU	C-N-CA	5.05	127.01	120.44
2	G	105	SER	CA-C-N	5.05	127.05	120.28
2	G	105	SER	C-N-CA	5.05	127.05	120.28
1	1	364	GLU	N-CA-C	5.05	116.48	111.07
1	3	91	ARG	CA-C-N	5.05	131.19	121.54
1	3	91	ARG	C-N-CA	5.05	131.19	121.54
1	S	268	ILE	CA-CB-CG1	5.05	118.99	110.40
2	E	189	GLU	CA-C-N	5.05	127.05	120.28
2	E	189	GLU	C-N-CA	5.05	127.05	120.28
2	J	198	LEU	N-CA-CB	5.05	119.02	110.49
1	4	132	ASN	OD1-CG-ND2	5.05	127.65	122.60
1	R	346	PRO	N-CA-C	-5.05	108.91	114.92
1	4	250	ASP	CA-CB-CG	-5.04	107.56	112.60
1	M	214	PRO	CA-C-N	5.04	127.11	120.60
1	M	214	PRO	C-N-CA	5.04	127.11	120.60
3	h	122	ASN	CA-C-N	5.04	127.04	120.28
3	h	122	ASN	C-N-CA	5.04	127.04	120.28
1	1	318	ASP	CA-CB-CG	5.04	117.64	112.60
1	O	101	ALA	CA-C-N	5.04	127.04	120.28
1	O	101	ALA	C-N-CA	5.04	127.04	120.28
2	K	187	ALA	CA-C-N	5.04	127.03	120.28
2	K	187	ALA	C-N-CA	5.04	127.03	120.28
2	I	51	THR	CA-C-O	-5.04	116.60	121.08
1	M	298	THR	CA-C-O	-5.04	113.45	118.34
1	S	321	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	2	92	THR	N-CA-CB	5.04	119.00	110.49
1	4	89	HIS	CE1-NE2-CD2	-5.04	103.97	109.00
1	P	403	HIS	ND1-CE1-NE2	5.04	113.44	108.40
2	A	57	SER	CA-C-N	5.04	127.03	120.28
2	A	57	SER	C-N-CA	5.04	127.03	120.28
1	4	315	MET	N-CA-C	5.03	117.42	111.33
1	P	229	PHE	CA-CB-CG	5.03	118.83	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	365	SER	CA-C-N	5.03	126.98	120.44
1	R	365	SER	C-N-CA	5.03	126.98	120.44
3	b	139	SER	CA-C-N	5.03	127.53	120.28
3	b	139	SER	C-N-CA	5.03	127.53	120.28
2	D	70	LYS	N-CA-C	5.03	116.77	111.28
2	K	181	SER	CA-C-N	5.03	127.02	120.28
2	K	181	SER	C-N-CA	5.03	127.02	120.28
1	N	230	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
2	E	178	ASP	CB-CA-C	-5.03	102.59	109.28
2	A	83	THR	CA-C-N	5.03	131.15	121.54
2	A	83	THR	C-N-CA	5.03	131.15	121.54
1	2	322	ILE	N-CA-CB	5.03	118.12	110.58
1	M	93	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
3	c	159	PRO	CA-C-N	5.03	127.33	120.54
3	c	159	PRO	C-N-CA	5.03	127.33	120.54
2	F	181	SER	CA-C-N	5.03	127.02	120.28
2	F	181	SER	C-N-CA	5.03	127.02	120.28
1	N	106	ALA	CA-C-N	5.02	127.01	120.28
1	N	106	ALA	C-N-CA	5.02	127.01	120.28
2	C	112	ASP	CA-C-N	5.02	127.01	120.28
2	C	112	ASP	C-N-CA	5.02	127.01	120.28
3	j	159	PRO	CA-C-N	5.02	127.32	120.54
3	j	159	PRO	C-N-CA	5.02	127.32	120.54
1	N	419	VAL	CA-C-N	5.02	127.01	120.28
1	N	419	VAL	C-N-CA	5.02	127.01	120.28
3	h	130	CYS	N-CA-CB	5.02	118.98	110.49
2	D	60	ARG	CA-C-N	5.02	130.74	121.70
2	D	60	ARG	C-N-CA	5.02	130.74	121.70
1	3	442	MET	CA-C-N	5.02	127.33	120.46
1	3	442	MET	C-N-CA	5.02	127.33	120.46
2	K	203	LEU	CA-C-N	5.02	127.51	120.28
2	K	203	LEU	C-N-CA	5.02	127.51	120.28
1	1	429	HIS	CE1-NE2-CD2	-5.01	103.98	109.00
1	3	70	ASP	CA-CB-CG	5.01	117.61	112.60
1	3	154	THR	CA-C-N	5.01	128.32	120.75
1	3	154	THR	C-N-CA	5.01	128.32	120.75
1	N	70	ASP	CA-C-N	5.01	125.04	119.32
1	N	70	ASP	C-N-CA	5.01	125.04	119.32
1	Q	452	ILE	N-CA-C	-5.01	101.06	108.23
2	E	68	VAL	CA-C-N	5.01	126.96	120.44
2	E	68	VAL	C-N-CA	5.01	126.96	120.44
2	E	174	VAL	CA-C-N	5.01	127.93	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	174	VAL	C-N-CA	5.01	127.93	120.31
1	P	156	HIS	ND1-CE1-NE2	5.01	113.41	108.40
2	F	114	ALA	CA-C-N	5.01	127.93	120.31
2	F	114	ALA	C-N-CA	5.01	127.93	120.31
3	g	70	GLY	CA-C-N	5.01	131.11	121.54
3	g	70	GLY	C-N-CA	5.01	131.11	121.54
1	1	370	LEU	N-CA-C	5.01	118.97	113.21
3	d	126	ALA	CA-C-N	5.01	127.30	120.54
3	d	126	ALA	C-N-CA	5.01	127.30	120.54
1	4	222	CYS	CA-C-N	5.01	126.99	120.28
1	4	222	CYS	C-N-CA	5.01	126.99	120.28
2	I	46	ILE	N-CA-C	-5.01	108.24	113.10
1	O	381	CYS	N-CA-C	-5.00	100.14	110.80
2	L	67	ASN	CA-C-N	5.00	127.32	120.46
2	L	67	ASN	C-N-CA	5.00	127.32	120.46
1	2	89	HIS	ND1-CE1-NE2	5.00	113.40	108.40
1	3	112	SER	CA-C-N	5.00	127.48	120.28
1	3	112	SER	C-N-CA	5.00	127.48	120.28
2	K	50	CYS	N-CA-C	-5.00	101.69	109.24

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	121	ILE	Mainchain
1	1	260	TYR	Sidechain
1	1	269	TYR	Sidechain
1	2	175	TYR	Sidechain
1	2	269	TYR	Sidechain
1	2	350	TYR	Sidechain
1	3	228	TYR	Sidechain
1	3	260	TYR	Sidechain
1	4	412	ARG	Sidechain
1	4	80	TYR	Sidechain
2	G	175	TYR	Sidechain
2	H	54	ARG	Sidechain
2	I	110	PHE	Sidechain
2	J	95	TYR	Sidechain
1	M	421	TYR	Sidechain
1	P	85	TYR	Sidechain
1	Q	360	TYR	Sidechain
1	Q	84	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	R	228	TYR	Sidechain
1	T	390	TYR	Sidechain
1	T	84	TYR	Sidechain
1	T	93	HIS	Sidechain
3	a	153	TYR	Sidechain
3	d	153	TYR	Sidechain
3	g	153	TYR	Sidechain
3	h	153	TYR	Sidechain
3	k	153	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3040	0	3058	27	0
1	2	3040	0	3058	5	0
1	3	3040	0	3057	10	0
1	4	3040	0	3058	10	0
1	M	3040	0	3058	8	0
1	N	3040	0	3058	3	0
1	O	3040	0	3057	20	0
1	P	3040	0	3058	12	0
1	Q	3040	0	3057	14	0
1	R	3040	0	3058	5	0
1	S	3040	0	3058	2	0
1	T	3040	0	3058	7	0
2	A	1328	0	1302	2	0
2	B	1328	0	1302	3	0
2	C	1328	0	1302	9	0
2	D	1328	0	1302	9	0
2	E	1328	0	1302	40	0
2	F	1328	0	1302	0	0
2	G	1328	0	1302	3	0
2	H	1328	0	1302	5	0
2	I	1328	0	1302	2	0
2	J	1328	0	1302	2	0
2	K	1328	0	1301	28	0
2	L	1328	0	1302	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	a	872	0	917	1	0
3	b	872	0	917	1	0
3	c	872	0	917	0	0
3	d	872	0	917	1	0
3	e	872	0	917	0	0
3	f	872	0	916	1	0
3	g	872	0	917	1	0
3	h	872	0	917	3	0
3	i	872	0	917	3	0
3	j	872	0	917	9	0
3	k	872	0	917	0	0
3	l	872	0	917	1	0
All	All	62880	0	63319	216	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 2.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:126:SER:N	2:E:127:PHE:CD1	1.78	1.50
1:Q:95:TYR:OH	2:C:134:VAL:CG1	1.63	1.45
2:E:126:SER:N	2:E:127:PHE:HD1	1.01	1.43
2:E:126:SER:CA	2:E:127:PHE:HB2	1.71	1.20
2:E:126:SER:HA	2:E:127:PHE:CB	1.63	1.18
2:K:123:TYR:CD1	2:K:135:LYS:HB3	1.78	1.18
2:K:123:TYR:HD1	2:K:135:LYS:CB	1.55	1.17
3:j:81:GLU:HA	3:j:153:TYR:OH	1.43	1.16
2:E:127:PHE:HB3	2:E:132:LEU:HD22	1.15	1.14
1:T:95:TYR:OH	2:L:136:LEU:HA	1.46	1.13
1:Q:95:TYR:CZ	2:C:134:VAL:HG13	1.84	1.11
2:E:127:PHE:HB3	2:E:132:LEU:CD2	1.83	1.09
2:E:127:PHE:CB	2:E:132:LEU:HD22	1.83	1.08
2:K:123:TYR:HD1	2:K:135:LYS:HB3	1.02	1.06
1:T:95:TYR:OH	2:L:136:LEU:CA	2.03	1.05
2:K:123:TYR:CD1	2:K:135:LYS:CB	2.38	0.98
1:O:357:SER:HB2	1:O:358:PHE:HB2	1.42	0.98
2:E:127:PHE:CD2	2:E:133:THR:N	2.32	0.97
2:E:127:PHE:CZ	2:E:134:VAL:HA	2.02	0.94
1:T:95:TYR:OH	2:L:137:GLY:N	2.00	0.93
1:T:95:TYR:OH	2:L:136:LEU:C	2.13	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:125:VAL:HA	2:E:127:PHE:CE1	2.06	0.90
1:Q:95:TYR:CE1	2:C:134:VAL:HG22	2.07	0.90
2:E:125:VAL:C	2:E:127:PHE:HD1	1.79	0.89
2:E:124:ASP:O	2:E:127:PHE:HE1	1.56	0.88
2:E:127:PHE:HZ	2:E:134:VAL:HA	1.32	0.88
2:E:125:VAL:C	2:E:127:PHE:CD1	2.53	0.87
2:E:126:SER:CA	2:E:127:PHE:HD1	1.87	0.86
2:E:126:SER:CA	2:E:127:PHE:CD1	2.58	0.86
1:Q:95:TYR:OH	2:C:134:VAL:HG13	0.67	0.85
2:E:127:PHE:CE2	2:E:133:THR:N	2.40	0.84
1:O:357:SER:CB	1:O:358:PHE:HB2	2.05	0.83
3:j:81:GLU:CA	3:j:153:TYR:OH	2.24	0.83
2:E:126:SER:CA	2:E:127:PHE:CB	2.39	0.82
2:E:124:ASP:O	2:E:127:PHE:CE1	2.33	0.81
2:K:123:TYR:CD1	2:K:135:LYS:C	2.58	0.81
1:O:340:VAL:HA	1:O:358:PHE:HE1	1.47	0.80
2:E:127:PHE:HD2	2:E:133:THR:N	1.77	0.78
2:E:127:PHE:HD2	2:E:133:THR:H	1.30	0.75
2:D:201:SER:C	2:D:209:ASP:OD2	2.28	0.75
1:O:356:LEU:CA	1:O:358:PHE:HE2	1.99	0.75
2:E:126:SER:HA	2:E:127:PHE:HB2	0.80	0.75
1:T:95:TYR:HH	2:L:136:LEU:CA	2.00	0.74
2:K:123:TYR:HD1	2:K:135:LYS:HB2	1.51	0.74
2:E:125:VAL:CA	2:E:127:PHE:CE1	2.70	0.74
1:1:358:PHE:CG	1:1:406:ILE:HG13	2.23	0.70
2:K:123:TYR:CG	2:K:135:LYS:O	2.44	0.70
3:j:154:LYS:O	3:j:157:GLN:N	2.25	0.69
1:3:330:ILE:HD11	1:3:354:ILE:HD11	1.76	0.67
1:T:95:TYR:HH	2:L:136:LEU:C	2.01	0.67
1:Q:92:THR:HB	1:Q:95:TYR:HD1	1.58	0.67
2:K:136:LEU:N	2:K:136:LEU:HD12	2.10	0.66
2:E:124:ASP:C	2:E:127:PHE:HE1	2.02	0.66
2:K:203:LEU:HD23	2:K:204:ALA:H	1.60	0.66
1:O:356:LEU:HB3	1:O:358:PHE:CE2	2.31	0.65
2:K:136:LEU:O	2:K:137:GLY:O	2.15	0.64
2:E:126:SER:N	2:E:127:PHE:CG	2.58	0.64
2:E:127:PHE:CZ	2:E:134:VAL:CA	2.81	0.64
1:O:356:LEU:HB3	1:O:358:PHE:HE2	1.65	0.62
1:1:356:LEU:O	1:1:358:PHE:HD2	1.83	0.62
2:K:122:ASP:O	2:K:123:TYR:CG	2.52	0.62
2:K:123:TYR:OH	2:K:136:LEU:O	1.97	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:123:TYR:CD1	2:K:135:LYS:O	2.54	0.59
1:O:340:VAL:HA	1:O:358:PHE:CE1	2.33	0.59
1:O:356:LEU:CB	1:O:358:PHE:HE2	2.15	0.59
1:1:452:ILE:H	1:1:453:LYS:C	2.11	0.58
2:K:123:TYR:CE1	2:K:135:LYS:HB3	2.36	0.58
2:E:127:PHE:HB2	2:E:132:LEU:HD22	1.81	0.58
3:j:80:ASP:O	3:j:153:TYR:CZ	2.57	0.58
2:E:126:SER:CA	2:E:127:PHE:CG	2.87	0.58
1:P:298:THR:H	1:P:299:PRO:HD2	1.70	0.57
2:K:122:ASP:O	2:K:123:TYR:CD2	2.58	0.56
1:Q:92:THR:CB	1:Q:95:TYR:HD1	2.18	0.56
1:2:298:THR:H	1:2:299:PRO:HD2	1.70	0.56
2:E:127:PHE:HZ	2:E:134:VAL:CA	2.11	0.55
1:Q:95:TYR:CE1	2:C:134:VAL:CG2	2.86	0.55
1:Q:92:THR:HB	1:Q:95:TYR:CD1	2.41	0.55
1:1:357:SER:HA	1:1:358:PHE:HB2	1.89	0.55
1:T:95:TYR:CZ	2:L:136:LEU:HA	2.37	0.55
2:E:95:TYR:HB3	2:E:96:GLU:HA	1.88	0.54
2:C:85:GLY:H	2:C:86:HIS:CG	2.25	0.54
2:E:125:VAL:CA	2:E:127:PHE:CD1	2.90	0.54
3:h:72:VAL:HG23	3:h:73:MET:H	1.72	0.54
1:M:457:HIS:CE1	3:l:137:HIS:CE1	2.96	0.54
2:E:126:SER:C	2:E:127:PHE:CD1	2.86	0.54
1:P:271:ARG:HD2	1:P:273:ARG:H	1.73	0.54
1:4:429:HIS:CE1	3:d:90:PHE:CZ	2.96	0.54
1:O:447:ILE:HG23	1:O:448:ASP:H	1.73	0.54
2:D:201:SER:HB2	2:D:209:ASP:OD2	2.08	0.54
1:N:202:VAL:HG12	1:N:203:MET:H	1.73	0.53
1:1:132:ASN:HD21	1:1:158:CYS:HB2	1.74	0.52
2:D:208:LYS:O	2:D:209:ASP:OD1	2.28	0.52
1:3:354:ILE:HG22	1:3:355:ASN:N	2.19	0.52
3:h:79:VAL:HG12	3:h:80:ASP:H	1.75	0.52
2:I:85:GLY:HA3	2:I:86:HIS:CG	2.44	0.51
1:P:72:ARG:H	1:P:72:ARG:HD2	1.75	0.51
2:D:95:TYR:HB3	2:D:96:GLU:HA	1.92	0.51
3:g:69:CYS:HB2	3:g:137:HIS:CD2	2.46	0.51
1:1:358:PHE:CD2	1:1:406:ILE:CG1	2.91	0.51
1:1:119:ARG:HH22	1:1:276:VAL:H	1.58	0.50
2:H:66:TRP:CD1	2:H:67:ASN:H	2.29	0.50
2:K:136:LEU:N	2:K:136:LEU:CD1	2.73	0.50
2:G:93:THR:HA	3:i:122:ASN:HD21	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:153:TYR:O	3:j:156:LYS:HB2	2.12	0.50
2:E:125:VAL:CA	2:E:127:PHE:HE1	2.21	0.50
1:M:373:VAL:HG12	1:M:375:LEU:H	1.76	0.50
2:D:202:SER:N	2:D:209:ASP:OD2	2.45	0.50
1:N:121:ILE:HD12	1:N:121:ILE:H	1.77	0.50
1:Q:202:VAL:HG12	1:Q:203:MET:H	1.76	0.50
1:Q:373:VAL:HG12	1:Q:375:LEU:H	1.77	0.50
1:1:115:GLY:O	1:4:140:ARG:NH2	2.45	0.49
1:P:260:TYR:H	2:H:47:ASP:HB3	1.78	0.49
1:N:157:LYS:HZ3	1:N:389:SER:H	1.61	0.49
1:4:140:ARG:HH12	1:4:143:ARG:HH21	1.60	0.49
3:a:79:VAL:HG12	3:a:80:ASP:H	1.77	0.49
2:E:72:SER:HA	2:E:73:VAL:HG12	1.93	0.49
2:K:123:TYR:CD1	2:K:135:LYS:HB2	2.30	0.49
1:2:449:LEU:H	2:J:53:ARG:HA	1.77	0.49
1:O:302:VAL:HG12	1:O:306:ALA:H	1.78	0.49
1:1:105:ARG:HE	1:P:455:THR:H	1.61	0.49
3:j:81:GLU:HA	3:j:153:TYR:HH	1.71	0.48
3:j:154:LYS:O	3:j:155:LEU:C	2.56	0.48
2:E:127:PHE:CD2	2:E:132:LEU:C	2.91	0.48
1:R:93:HIS:CD2	1:R:96:GLY:HA3	2.49	0.48
1:3:330:ILE:CD1	1:3:354:ILE:HD11	2.43	0.47
2:K:122:ASP:C	2:K:123:TYR:CD2	2.92	0.47
1:M:357:SER:HA	1:M:358:PHE:CG	2.49	0.47
1:Q:97:TRP:HE1	2:C:118:TYR:HB3	1.78	0.47
2:K:136:LEU:O	2:K:137:GLY:C	2.56	0.47
1:1:212:LYS:H	1:1:349:HIS:HA	1.80	0.47
1:1:356:LEU:O	1:1:358:PHE:CD2	2.66	0.47
1:M:120:GLU:HA	1:M:270:ILE:HG23	1.96	0.47
1:O:304:LEU:HD12	1:O:304:LEU:H	1.79	0.47
1:1:447:ILE:HG13	1:1:448:ASP:H	1.80	0.47
2:K:123:TYR:CD1	2:K:135:LYS:CA	2.98	0.47
1:2:200:VAL:HG23	1:2:227:VAL:HG11	1.96	0.47
1:S:202:VAL:HG12	1:S:203:MET:H	1.79	0.47
1:3:452:ILE:H	1:3:453:LYS:HB2	1.80	0.47
1:R:71:PRO:HG2	3:b:113:THR:H	1.79	0.47
1:1:105:ARG:HG2	1:P:454:TRP:H	1.80	0.46
1:1:358:PHE:CD2	1:1:406:ILE:HG13	2.50	0.46
1:O:349:HIS:H	1:O:349:HIS:CD2	2.33	0.46
1:1:203:MET:HE3	1:1:206:ASN:HA	1.97	0.46
1:Q:367:LEU:HD13	1:Q:367:LEU:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:208:LYS:HG2	2:K:209:ASP:H	1.81	0.46
1:3:353:CYS:O	1:3:354:ILE:HG13	2.15	0.46
2:I:95:TYR:HB3	2:I:96:GLU:HA	1.96	0.46
1:M:415:THR:HG22	1:M:416:GLU:H	1.81	0.46
1:O:340:VAL:HG23	1:O:358:PHE:CZ	2.51	0.46
1:1:275:ARG:HE	1:4:275:ARG:HG3	1.81	0.46
2:E:127:PHE:CD2	2:E:132:LEU:HB3	2.51	0.46
2:H:175:TYR:HB3	2:H:179:GLY:H	1.81	0.46
1:P:357:SER:HA	1:P:358:PHE:HB2	1.98	0.46
2:K:60:ARG:HB3	2:K:61:GLY:HA3	1.99	0.45
1:1:450:LYS:H	1:1:450:LYS:HD2	1.82	0.45
2:K:46:ILE:HD13	2:K:46:ILE:H	1.82	0.45
1:P:202:VAL:HG12	1:P:203:MET:H	1.81	0.45
1:1:452:ILE:HB	1:1:453:LYS:HB2	1.99	0.45
1:2:212:LYS:H	1:2:349:HIS:HA	1.82	0.45
1:3:270:ILE:O	1:3:270:ILE:HG23	2.17	0.45
2:K:95:TYR:HB2	2:K:96:GLU:HA	1.99	0.45
1:M:202:VAL:HG12	1:M:203:MET:H	1.82	0.44
1:3:330:ILE:HG12	1:3:354:ILE:CD1	2.46	0.44
2:E:125:VAL:HA	2:E:127:PHE:CD1	2.47	0.44
1:1:355:ASN:HD22	1:1:407:ARG:HG3	1.82	0.44
1:4:89:HIS:CD2	2:A:127:PHE:HB2	2.53	0.44
3:j:153:TYR:HE2	3:j:157:GLN:HE21	1.63	0.44
2:E:127:PHE:HD2	2:E:132:LEU:CA	2.31	0.44
2:H:97:ARG:HH12	2:L:133:THR:HG22	1.83	0.44
1:O:457:HIS:H	2:A:195:LYS:HE2	1.83	0.44
3:h:68:ALA:H	3:h:70:GLY:H	1.64	0.44
2:K:70:LYS:H	2:K:70:LYS:HD2	1.82	0.43
2:K:136:LEU:C	2:K:137:GLY:O	2.61	0.43
1:O:287:GLN:H	1:R:119:ARG:H	1.65	0.43
3:i:87:ASP:CG	3:i:88:ALA:H	2.26	0.43
1:1:387:GLU:H	1:M:443:VAL:HG11	1.83	0.43
1:O:286:GLY:HA3	1:R:120:GLU:H	1.82	0.43
2:B:46:ILE:HD13	2:B:46:ILE:H	1.82	0.43
2:G:86:HIS:CD2	2:G:87:PRO:HA	2.53	0.43
2:G:151:ASN:HD21	2:H:150:PRO:HB2	1.83	0.43
1:P:371:LYS:HA	3:i:103:SER:HB3	1.99	0.43
1:4:81:LEU:C	1:4:83:ASN:H	2.27	0.43
2:E:127:PHE:HD2	2:E:132:LEU:C	2.27	0.43
1:1:279:GLU:HA	1:2:119:ARG:H	1.83	0.43
1:3:440:TRP:CD2	1:O:390:TYR:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:TRP:CD1	2:B:67:ASN:H	2.37	0.43
2:C:85:GLY:H	2:C:86:HIS:CD2	2.37	0.43
1:1:425:LYS:HG2	1:1:429:HIS:CE1	2.54	0.42
1:4:71:PRO:HG2	2:D:86:HIS:H	1.85	0.42
1:S:348:HIS:O	1:S:348:HIS:CG	2.72	0.42
2:D:90:LEU:HD13	2:D:90:LEU:HA	1.93	0.42
1:O:204:THR:HA	1:O:215:ILE:HD11	2.01	0.42
2:E:46:ILE:HD13	2:E:46:ILE:H	1.84	0.42
2:J:120:PHE:CG	2:J:121:GLU:N	2.87	0.42
1:Q:357:SER:HA	1:Q:358:PHE:HB2	2.02	0.42
1:4:136:LYS:HG2	1:P:457:HIS:CD2	2.55	0.42
1:Q:92:THR:CB	1:Q:95:TYR:CD1	3.01	0.42
2:L:126:SER:HA	2:L:127:PHE:HB2	2.01	0.42
1:O:129:GLU:HG3	1:R:105:ARG:HH12	1.85	0.42
1:1:454:TRP:HA	1:1:455:THR:HB	2.01	0.41
2:D:201:SER:CA	2:D:209:ASP:OD2	2.67	0.41
2:K:123:TYR:CE1	2:K:135:LYS:C	2.98	0.41
1:1:89:HIS:CE1	2:D:127:PHE:CZ	3.08	0.41
1:4:342:MET:HG2	1:4:344:GLY:H	1.85	0.41
2:L:175:TYR:HB3	2:L:179:GLY:H	1.85	0.41
1:1:118:PRO:HD3	1:P:457:HIS:CE1	2.55	0.41
1:3:330:ILE:HG12	1:3:354:ILE:HD13	2.01	0.41
2:B:95:TYR:HB3	2:B:96:GLU:HA	2.03	0.41
1:1:265:VAL:HG12	1:1:304:LEU:HD13	2.03	0.41
3:j:80:ASP:O	3:j:153:TYR:CE2	2.74	0.41
1:O:369:ALA:HA	3:f:100:ALA:HA	2.03	0.40
1:1:289:ARG:HD2	1:3:287:GLN:HE22	1.86	0.40
2:K:122:ASP:C	2:K:123:TYR:CG	2.99	0.40
2:C:173:TRP:HE1	2:C:182:LEU:H	1.69	0.40
1:4:454:TRP:CD1	1:P:156:HIS:CD2	3.10	0.40
1:M:228:TYR:CD1	1:M:276:VAL:HG12	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	389/391 (100%)	333 (86%)	30 (8%)	26 (7%)	1	12
1	2	389/391 (100%)	341 (88%)	27 (7%)	21 (5%)	1	15
1	3	389/391 (100%)	334 (86%)	37 (10%)	18 (5%)	2	17
1	4	389/391 (100%)	332 (85%)	34 (9%)	23 (6%)	1	13
1	M	389/391 (100%)	346 (89%)	30 (8%)	13 (3%)	3	21
1	N	389/391 (100%)	340 (87%)	40 (10%)	9 (2%)	5	28
1	O	389/391 (100%)	332 (85%)	35 (9%)	22 (6%)	1	14
1	P	389/391 (100%)	345 (89%)	29 (8%)	15 (4%)	2	19
1	Q	389/391 (100%)	343 (88%)	32 (8%)	14 (4%)	2	20
1	R	389/391 (100%)	342 (88%)	31 (8%)	16 (4%)	2	18
1	S	389/391 (100%)	335 (86%)	36 (9%)	18 (5%)	2	17
1	T	389/391 (100%)	341 (88%)	34 (9%)	14 (4%)	2	20
2	A	167/169 (99%)	124 (74%)	28 (17%)	15 (9%)	0	8
2	B	167/169 (99%)	140 (84%)	18 (11%)	9 (5%)	1	15
2	C	167/169 (99%)	125 (75%)	27 (16%)	15 (9%)	0	8
2	D	167/169 (99%)	126 (75%)	33 (20%)	8 (5%)	2	16
2	E	167/169 (99%)	133 (80%)	20 (12%)	14 (8%)	0	9
2	F	167/169 (99%)	134 (80%)	23 (14%)	10 (6%)	1	13
2	G	167/169 (99%)	135 (81%)	23 (14%)	9 (5%)	1	15
2	H	167/169 (99%)	133 (80%)	25 (15%)	9 (5%)	1	15
2	I	167/169 (99%)	130 (78%)	21 (13%)	16 (10%)	0	7
2	J	167/169 (99%)	132 (79%)	17 (10%)	18 (11%)	0	6
2	K	167/169 (99%)	137 (82%)	22 (13%)	8 (5%)	2	16
2	L	167/169 (99%)	125 (75%)	27 (16%)	15 (9%)	0	8
3	a	116/118 (98%)	94 (81%)	16 (14%)	6 (5%)	1	15
3	b	116/118 (98%)	102 (88%)	9 (8%)	5 (4%)	2	17
3	c	116/118 (98%)	97 (84%)	16 (14%)	3 (3%)	4	25
3	d	116/118 (98%)	97 (84%)	12 (10%)	7 (6%)	1	13
3	e	116/118 (98%)	97 (84%)	12 (10%)	7 (6%)	1	13
3	f	116/118 (98%)	98 (84%)	13 (11%)	5 (4%)	2	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	116/118 (98%)	95 (82%)	12 (10%)	9 (8%)	1	10
3	h	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	7	36
3	i	116/118 (98%)	96 (83%)	13 (11%)	7 (6%)	1	13
3	j	116/118 (98%)	86 (74%)	16 (14%)	14 (12%)	0	4
3	k	116/118 (98%)	99 (85%)	10 (9%)	7 (6%)	1	13
3	l	116/118 (98%)	99 (85%)	12 (10%)	5 (4%)	2	17
All	All	8064/8136 (99%)	6798 (84%)	834 (10%)	432 (5%)	2	15

All (432) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	88	PRO
1	1	89	HIS
1	1	98	GLU
1	1	119	ARG
1	1	298	THR
1	1	381	CYS
1	1	392	LEU
1	1	455	THR
1	2	68	PRO
1	2	116	ALA
1	2	118	PRO
1	2	273	ARG
1	2	292	ARG
1	2	372	ASP
1	2	387	GLU
1	3	92	THR
1	3	117	ASP
1	3	280	ALA
1	3	383	SER
1	3	450	LYS
1	3	451	SER
1	4	88	PRO
1	4	372	ASP
1	4	452	ILE
1	M	275	ARG
1	M	277	ARG
1	M	375	LEU
1	M	389	SER
1	N	357	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	373	VAL
1	N	456	GLN
1	O	358	PHE
1	O	361	VAL
1	O	362	GLU
1	O	449	LEU
1	P	282	GLN
1	P	358	PHE
1	P	375	LEU
1	P	450	LYS
1	P	452	ILE
1	Q	112	SER
1	Q	116	ALA
1	Q	358	PHE
1	R	273	ARG
1	R	372	ASP
1	S	89	HIS
1	S	119	ARG
1	S	273	ARG
1	S	372	ASP
1	S	447	ILE
1	T	87	ASN
1	T	359	ALA
1	T	384	ALA
2	A	48	ALA
2	A	73	VAL
2	A	84	LEU
2	A	121	GLU
3	a	130	CYS
3	b	130	CYS
2	C	60	ARG
2	C	119	THR
2	C	124	ASP
3	c	130	CYS
2	D	80	LYS
2	D	84	LEU
2	D	174	VAL
3	d	91	LYS
3	d	130	CYS
2	E	62	LEU
2	E	73	VAL
2	E	91	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	e	56	SER
3	e	130	CYS
2	F	126	SER
2	F	127	PHE
2	F	203	LEU
2	F	208	LYS
3	f	130	CYS
3	f	135	LYS
3	g	71	ASP
3	g	130	CYS
2	H	60	ARG
2	H	127	PHE
2	H	209	ASP
3	h	130	CYS
2	I	84	LEU
3	i	92	THR
3	i	130	CYS
2	J	50	CYS
2	J	198	LEU
3	j	112	LYS
3	j	113	THR
3	j	130	CYS
3	k	130	CYS
2	L	74	TYR
2	L	117	PRO
3	l	96	GLY
3	l	132	PRO
1	1	80	TYR
1	1	94	ALA
1	1	123	PHE
1	1	386	LEU
1	2	279	GLU
1	2	396	GLY
1	2	413	PHE
1	2	447	ILE
1	2	452	ILE
1	3	275	ARG
1	3	357	SER
1	3	358	PHE
1	4	81	LEU
1	4	260	TYR
1	4	294	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4	312	GLN
1	M	358	PHE
1	M	371	LYS
1	M	382	THR
1	M	383	SER
1	M	448	ASP
1	N	449	LEU
1	O	84	TYR
1	O	119	ARG
1	O	302	VAL
1	O	357	SER
1	O	383	SER
1	O	446	GLY
1	P	383	SER
1	Q	262	PRO
1	Q	375	LEU
1	R	116	ALA
1	R	276	VAL
1	R	358	PHE
1	R	447	ILE
1	S	452	ILE
1	T	90	SER
1	T	116	ALA
1	T	313	GLN
1	T	451	SER
2	A	47	ASP
2	A	141	GLY
2	A	203	LEU
2	A	206	SER
3	a	58	ASN
3	a	64	VAL
3	a	87	ASP
3	a	92	THR
2	B	84	LEU
2	B	126	SER
2	B	178	ASP
2	B	203	LEU
3	b	58	ASN
2	C	120	PHE
2	C	139	ASP
2	C	203	LEU
2	D	89	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	d	64	VAL
2	E	43	ARG
2	E	84	LEU
2	E	85	GLY
2	F	49	THR
2	F	62	LEU
2	F	79	ARG
3	f	58	ASN
2	G	97	ARG
2	G	177	HIS
3	g	68	ALA
3	g	120	ILE
2	H	62	LEU
2	H	80	LYS
2	H	91	ASP
2	H	208	LYS
3	h	73	MET
2	I	118	TYR
2	I	122	ASP
2	I	127	PHE
2	I	140	LEU
2	I	174	VAL
3	i	134	VAL
2	J	174	VAL
2	J	204	ALA
2	J	208	LYS
3	j	53	ASP
3	j	68	ALA
3	j	80	ASP
2	K	94	THR
2	K	137	GLY
2	L	91	ASP
2	L	97	ARG
2	L	127	PHE
2	L	143	TYR
2	L	173	TRP
2	L	178	ASP
3	l	59	VAL
1	1	91	ARG
1	1	115	GLY
1	1	214	PRO
1	1	264	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	279	GLU
1	1	292	ARG
1	2	257	HIS
1	2	293	SER
1	2	369	ALA
1	2	450	LYS
1	3	245	ASN
1	3	286	GLY
1	3	449	LEU
1	4	85	TYR
1	4	279	GLU
1	4	284	GLY
1	4	313	GLN
1	M	292	ARG
1	M	446	GLY
1	N	88	PRO
1	N	286	GLY
1	O	118	PRO
1	O	293	SER
1	O	385	SER
1	O	386	LEU
1	P	285	GLY
1	P	353	CYS
1	P	373	VAL
1	P	455	THR
1	Q	89	HIS
1	Q	264	GLY
1	Q	277	ARG
1	Q	286	GLY
1	Q	293	SER
1	Q	372	ASP
1	Q	385	SER
1	R	286	GLY
1	R	293	SER
1	R	294	GLY
1	R	297	PRO
1	R	377	SER
1	R	385	SER
1	S	84	TYR
1	S	277	ARG
1	S	451	SER
1	T	286	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	340	VAL
2	A	177	HIS
2	A	195	LYS
2	B	63	ASN
2	B	74	TYR
3	b	95	CYS
2	C	84	LEU
2	C	118	TYR
2	C	130	GLY
2	C	138	GLY
2	C	204	ALA
2	D	63	ASN
2	D	203	LEU
2	E	63	ASN
2	E	87	PRO
2	E	127	PHE
2	E	204	ALA
3	e	58	ASN
3	e	92	THR
2	F	130	GLY
2	F	176	SER
2	G	118	TYR
2	G	122	ASP
2	G	143	TYR
2	G	171	LYS
2	G	176	SER
3	g	65	GLY
3	g	93	PHE
2	I	138	GLY
2	I	176	SER
2	I	204	ALA
3	i	90	PHE
2	J	63	ASN
2	J	74	TYR
2	J	91	ASP
2	J	130	GLY
2	J	140	LEU
2	J	177	HIS
3	j	51	SER
2	K	72	SER
2	K	89	SER
2	K	127	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	177	HIS
3	k	68	ALA
2	L	47	ASP
2	L	152	LYS
3	l	68	ALA
1	1	87	ASN
1	1	93	HIS
1	3	91	ARG
1	3	145	ARG
1	3	386	LEU
1	3	447	ILE
1	4	87	ASN
1	4	90	SER
1	M	273	ARG
1	N	359	ALA
1	O	117	ASP
1	O	257	HIS
1	O	277	ARG
1	O	296	VAL
1	O	376	SER
1	O	454	TRP
1	P	361	VAL
1	R	279	GLU
1	S	92	THR
1	S	385	SER
1	S	448	ASP
1	T	91	ARG
1	T	245	ASN
1	T	360	TYR
1	T	362	GLU
1	T	447	ILE
2	A	120	PHE
2	A	126	SER
2	A	204	ALA
3	a	120	ILE
2	B	157	SER
3	b	69	CYS
2	C	81	SER
2	C	129	SER
2	C	176	SER
2	D	178	ASP
2	E	203	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	e	68	ALA
3	e	95	CYS
2	F	171	LYS
2	G	208	LYS
2	I	161	SER
2	I	177	HIS
2	I	195	LYS
3	i	129	LEU
2	J	129	SER
2	J	178	ASP
3	j	110	LYS
3	j	157	GLN
2	L	89	SER
2	L	118	TYR
2	L	141	GLY
1	1	83	ASN
1	1	312	GLN
1	1	448	ASP
1	2	145	ARG
1	2	298	THR
1	2	379	SER
1	3	88	PRO
1	4	92	THR
1	4	214	PRO
1	4	262	PRO
1	4	373	VAL
1	4	383	SER
1	4	389	SER
1	4	410	ILE
1	O	123	PHE
1	P	245	ASN
1	P	298	THR
1	Q	273	ARG
1	R	283	SER
1	R	289	ARG
1	S	214	PRO
1	S	384	ALA
1	S	453	LYS
2	A	90	LEU
2	B	129	SER
3	b	129	LEU
2	D	74	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	d	136	LEU
2	E	176	SER
3	e	129	LEU
2	G	201	SER
3	g	53	ASP
3	g	129	LEU
3	g	165	GLU
2	I	178	ASP
2	I	203	LEU
2	I	209	ASP
2	J	65	ILE
2	J	139	ASP
2	J	203	LEU
3	j	87	ASP
3	j	88	ALA
3	j	129	LEU
3	j	166	LYS
2	K	163	PRO
2	K	178	ASP
3	k	58	ASN
3	k	129	LEU
3	k	136	LEU
2	L	126	SER
3	l	133	PRO
1	1	117	ASP
1	1	179	GLN
1	1	310	VAL
1	2	359	ALA
1	4	297	PRO
1	N	283	SER
1	N	447	ILE
1	P	291	MET
1	S	90	SER
2	A	163	PRO
2	B	89	SER
2	C	126	SER
3	c	129	LEU
3	d	129	LEU
3	d	133	PRO
2	E	208	LYS
3	f	129	LEU
3	i	64	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	161	SER
2	J	196	THR
3	k	91	LYS
1	O	273	ARG
1	P	351	PRO
1	S	82	ILE
3	d	65	GLY
2	E	150	PRO
3	f	133	PRO
2	H	163	PRO
3	i	59	VAL
1	R	261	GLY
2	H	61	GLY
2	I	163	PRO
3	j	86	VAL
3	k	59	VAL
1	2	117	ASP
1	4	273	ARG
1	M	117	ASP
1	Q	79	PRO
2	L	87	PRO
1	3	244	VAL
1	4	299	PRO
1	S	117	ASP
3	c	96	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	1	333/333 (100%)	319 (96%)	14 (4%)	26	48
1	2	333/333 (100%)	317 (95%)	16 (5%)	23	44
1	3	333/333 (100%)	318 (96%)	15 (4%)	24	46
1	4	333/333 (100%)	318 (96%)	15 (4%)	24	46
1	M	333/333 (100%)	321 (96%)	12 (4%)	31	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	333/333 (100%)	321 (96%)	12 (4%)	31	52
1	O	333/333 (100%)	321 (96%)	12 (4%)	31	52
1	P	333/333 (100%)	321 (96%)	12 (4%)	31	52
1	Q	333/333 (100%)	322 (97%)	11 (3%)	33	55
1	R	333/333 (100%)	315 (95%)	18 (5%)	20	41
1	S	333/333 (100%)	324 (97%)	9 (3%)	39	61
1	T	333/333 (100%)	320 (96%)	13 (4%)	28	49
2	A	146/146 (100%)	140 (96%)	6 (4%)	27	49
2	B	146/146 (100%)	140 (96%)	6 (4%)	27	49
2	C	146/146 (100%)	139 (95%)	7 (5%)	23	44
2	D	146/146 (100%)	138 (94%)	8 (6%)	19	41
2	E	146/146 (100%)	135 (92%)	11 (8%)	12	33
2	F	146/146 (100%)	141 (97%)	5 (3%)	32	54
2	G	146/146 (100%)	139 (95%)	7 (5%)	23	44
2	H	146/146 (100%)	137 (94%)	9 (6%)	16	38
2	I	146/146 (100%)	135 (92%)	11 (8%)	12	33
2	J	146/146 (100%)	142 (97%)	4 (3%)	39	61
2	K	146/146 (100%)	133 (91%)	13 (9%)	9	28
2	L	146/146 (100%)	137 (94%)	9 (6%)	16	38
3	a	94/94 (100%)	86 (92%)	8 (8%)	10	29
3	b	94/94 (100%)	92 (98%)	2 (2%)	47	65
3	c	94/94 (100%)	87 (93%)	7 (7%)	13	33
3	d	94/94 (100%)	90 (96%)	4 (4%)	26	47
3	e	94/94 (100%)	91 (97%)	3 (3%)	34	56
3	f	94/94 (100%)	89 (95%)	5 (5%)	20	41
3	g	94/94 (100%)	91 (97%)	3 (3%)	34	56
3	h	94/94 (100%)	87 (93%)	7 (7%)	13	33
3	i	94/94 (100%)	86 (92%)	8 (8%)	10	29
3	j	94/94 (100%)	88 (94%)	6 (6%)	16	37
3	k	94/94 (100%)	94 (100%)	0	100	100
3	l	94/94 (100%)	88 (94%)	6 (6%)	16	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6876/6876 (100%)	6562 (95%)	314 (5%)	25	45

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	73	VAL
1	1	105	ARG
1	1	121	ILE
1	1	171	PHE
1	1	212	LYS
1	1	254	ILE
1	1	263	LYS
1	1	268	ILE
1	1	270	ILE
1	1	309	GLU
1	1	370	LEU
1	1	386	LEU
1	1	431	LYS
1	1	443	VAL
1	2	71	PRO
1	2	73	VAL
1	2	78	LEU
1	2	80	TYR
1	2	202	VAL
1	2	244	VAL
1	2	263	LYS
1	2	268	ILE
1	2	271	ARG
1	2	275	ARG
1	2	292	ARG
1	2	322	ILE
1	2	366	LEU
1	2	386	LEU
1	2	447	ILE
1	2	452	ILE
1	3	73	VAL
1	3	119	ARG
1	3	136	LYS
1	3	221	ILE
1	3	239	LYS
1	3	268	ILE
1	3	276	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	288	GLU
1	3	301	VAL
1	3	310	VAL
1	3	312	GLN
1	3	340	VAL
1	3	425	LYS
1	3	452	ILE
1	3	455	THR
1	4	81	LEU
1	4	82	ILE
1	4	89	HIS
1	4	129	GLU
1	4	136	LYS
1	4	166	LEU
1	4	263	LYS
1	4	268	ILE
1	4	270	ILE
1	4	281	LEU
1	4	292	ARG
1	4	408	PHE
1	4	415	THR
1	4	444	GLN
1	4	449	LEU
1	M	73	VAL
1	M	104	GLU
1	M	114	ILE
1	M	129	GLU
1	M	244	VAL
1	M	263	LYS
1	M	268	ILE
1	M	270	ILE
1	M	312	GLN
1	M	373	VAL
1	M	387	GLU
1	M	447	ILE
1	N	74	LEU
1	N	104	GLU
1	N	136	LYS
1	N	166	LEU
1	N	263	LYS
1	N	289	ARG
1	N	312	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	375	LEU
1	N	408	PHE
1	N	415	THR
1	N	431	LYS
1	N	447	ILE
1	O	74	LEU
1	O	83	ASN
1	O	84	TYR
1	O	245	ASN
1	O	263	LYS
1	O	271	ARG
1	O	272	ARG
1	O	275	ARG
1	O	312	GLN
1	O	372	ASP
1	O	382	THR
1	O	401	LEU
1	P	82	ILE
1	P	136	LYS
1	P	263	LYS
1	P	276	VAL
1	P	312	GLN
1	P	370	LEU
1	P	375	LEU
1	P	386	LEU
1	P	387	GLU
1	P	408	PHE
1	P	444	GLN
1	P	449	LEU
1	Q	92	THR
1	Q	114	ILE
1	Q	129	GLU
1	Q	166	LEU
1	Q	239	LYS
1	Q	263	LYS
1	Q	268	ILE
1	Q	367	LEU
1	Q	371	LYS
1	Q	373	VAL
1	Q	452	ILE
1	R	70	ASP
1	R	79	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	80	TYR
1	R	81	LEU
1	R	97	TRP
1	R	109	GLN
1	R	166	LEU
1	R	212	LYS
1	R	239	LYS
1	R	263	LYS
1	R	268	ILE
1	R	275	ARG
1	R	276	VAL
1	R	287	GLN
1	R	367	LEU
1	R	431	LYS
1	R	450	LYS
1	R	453	LYS
1	S	140	ARG
1	S	166	LEU
1	S	237	VAL
1	S	263	LYS
1	S	268	ILE
1	S	276	VAL
1	S	278	VAL
1	S	342	MET
1	S	356	LEU
1	T	74	LEU
1	T	81	LEU
1	T	166	LEU
1	T	239	LYS
1	T	263	LYS
1	T	268	ILE
1	T	312	GLN
1	T	366	LEU
1	T	415	THR
1	T	423	VAL
1	T	431	LYS
1	T	449	LEU
1	T	453	LYS
2	A	60	ARG
2	A	70	LYS
2	A	131	VAL
2	A	156	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	200	LEU
2	A	208	LYS
3	a	64	VAL
3	a	79	VAL
3	a	99	ILE
3	a	119	THR
3	a	129	LEU
3	a	155	LEU
3	a	158	GLU
3	a	166	LYS
2	B	46	ILE
2	B	51	THR
2	B	70	LYS
2	B	131	VAL
2	B	155	TRP
2	B	171	LYS
3	b	57	LYS
3	b	89	ARG
2	C	42	LEU
2	C	60	ARG
2	C	66	TRP
2	C	79	ARG
2	C	80	LYS
2	C	90	LEU
2	C	182	LEU
3	c	54	LYS
3	c	63	LEU
3	c	71	ASP
3	c	82	LYS
3	c	90	PHE
3	c	91	LYS
3	c	129	LEU
2	D	46	ILE
2	D	60	ARG
2	D	90	LEU
2	D	131	VAL
2	D	134	VAL
2	D	135	LYS
2	D	198	LEU
2	D	200	LEU
3	d	79	VAL
3	d	82	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	d	91	LYS
3	d	166	LYS
2	E	46	ILE
2	E	68	VAL
2	E	69	LYS
2	E	70	LYS
2	E	73	VAL
2	E	83	THR
2	E	84	LEU
2	E	131	VAL
2	E	152	LYS
2	E	171	LYS
2	E	200	LEU
3	e	74	LYS
3	e	77	ILE
3	e	114	VAL
2	F	83	THR
2	F	90	LEU
2	F	106	LEU
2	F	203	LEU
2	F	208	LYS
3	f	63	LEU
3	f	72	VAL
3	f	82	LYS
3	f	110	LYS
3	f	147	LYS
2	G	46	ILE
2	G	60	ARG
2	G	69	LYS
2	G	97	ARG
2	G	140	LEU
2	G	173	TRP
2	G	180	VAL
3	g	72	VAL
3	g	119	THR
3	g	141	LEU
2	H	46	ILE
2	H	62	LEU
2	H	79	ARG
2	H	80	LYS
2	H	90	LEU
2	H	102	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	127	PHE
2	H	136	LEU
2	H	177	HIS
3	h	63	LEU
3	h	73	MET
3	h	74	LYS
3	h	79	VAL
3	h	91	LYS
3	h	119	THR
3	h	158	GLU
2	I	75	LEU
2	I	97	ARG
2	I	116	LYS
2	I	118	TYR
2	I	120	PHE
2	I	125	VAL
2	I	127	PHE
2	I	132	LEU
2	I	145	ILE
2	I	174	VAL
2	I	208	LYS
3	i	77	ILE
3	i	90	PHE
3	i	91	LYS
3	i	92	THR
3	i	107	GLU
3	i	134	VAL
3	i	154	LYS
3	i	167	LYS
2	J	84	LEU
2	J	171	LYS
2	J	200	LEU
2	J	208	LYS
3	j	104	LEU
3	j	110	LYS
3	j	118	LEU
3	j	122	ASN
3	j	127	LYS
3	j	160	LYS
2	K	46	ILE
2	K	58	ASN
2	K	62	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	69	LYS
2	K	70	LYS
2	K	75	LEU
2	K	108	GLU
2	K	109	PHE
2	K	132	LEU
2	K	136	LEU
2	K	180	VAL
2	K	190	LEU
2	K	203	LEU
2	L	46	ILE
2	L	62	LEU
2	L	84	LEU
2	L	117	PRO
2	L	132	LEU
2	L	165	ARG
2	L	169	THR
2	L	195	LYS
2	L	208	LYS
3	l	63	LEU
3	l	79	VAL
3	l	99	ILE
3	l	132	PRO
3	l	135	LYS
3	l	150	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	89	HIS
1	1	109	GLN
1	1	131	ASN
1	1	132	ASN
1	1	148	HIS
1	1	156	HIS
1	1	207	ASN
1	1	230	HIS
1	1	245	ASN
1	1	282	GLN
1	1	287	GLN
1	1	355	ASN
1	1	429	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	444	GLN
1	2	83	ASN
1	2	131	ASN
1	2	206	ASN
1	2	245	ASN
1	2	257	HIS
1	2	312	GLN
1	2	319	HIS
1	2	355	ASN
1	2	403	HIS
1	2	428	GLN
1	3	156	HIS
1	3	206	ASN
1	3	207	ASN
1	3	245	ASN
1	3	282	GLN
1	3	287	GLN
1	3	313	GLN
1	3	319	HIS
1	3	429	HIS
1	3	444	GLN
1	4	89	HIS
1	4	93	HIS
1	4	132	ASN
1	4	153	GLN
1	4	257	HIS
1	4	287	GLN
1	4	313	GLN
1	4	343	ASN
1	4	349	HIS
1	4	403	HIS
1	4	429	HIS
1	4	444	GLN
1	4	456	GLN
1	4	457	HIS
1	M	93	HIS
1	M	131	ASN
1	M	153	GLN
1	M	156	HIS
1	M	235	GLN
1	M	245	ASN
1	M	282	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	312	GLN
1	M	319	HIS
1	M	349	HIS
1	M	429	HIS
1	M	456	GLN
1	N	87	ASN
1	N	109	GLN
1	N	132	ASN
1	N	148	HIS
1	N	213	GLN
1	N	230	HIS
1	N	287	GLN
1	N	312	GLN
1	N	349	HIS
1	N	444	GLN
1	N	456	GLN
1	O	83	ASN
1	O	109	GLN
1	O	132	ASN
1	O	148	HIS
1	O	206	ASN
1	O	230	HIS
1	O	312	GLN
1	O	313	GLN
1	O	349	HIS
1	O	403	HIS
1	P	87	ASN
1	P	93	HIS
1	P	131	ASN
1	P	148	HIS
1	P	156	HIS
1	P	172	GLN
1	P	230	HIS
1	P	312	GLN
1	P	319	HIS
1	P	348	HIS
1	P	355	ASN
1	P	428	GLN
1	P	429	HIS
1	P	457	HIS
1	Q	83	ASN
1	Q	89	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	108	GLN
1	Q	156	HIS
1	Q	207	ASN
1	Q	235	GLN
1	Q	257	HIS
1	Q	349	HIS
1	Q	403	HIS
1	R	83	ASN
1	R	131	ASN
1	R	132	ASN
1	R	153	GLN
1	R	230	HIS
1	R	235	GLN
1	R	282	GLN
1	R	287	GLN
1	R	312	GLN
1	R	348	HIS
1	R	355	ASN
1	R	444	GLN
1	S	87	ASN
1	S	93	HIS
1	S	109	GLN
1	S	132	ASN
1	S	148	HIS
1	S	153	GLN
1	S	235	GLN
1	S	282	GLN
1	S	287	GLN
1	S	349	HIS
1	S	403	HIS
1	S	429	HIS
1	T	83	ASN
1	T	109	GLN
1	T	131	ASN
1	T	132	ASN
1	T	156	HIS
1	T	207	ASN
1	T	230	HIS
1	T	235	GLN
1	T	312	GLN
1	T	319	HIS
1	T	349	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	428	GLN
2	A	183	HIS
2	B	58	ASN
2	B	59	GLN
3	b	122	ASN
3	b	157	GLN
2	C	67	ASN
2	C	71	GLN
3	c	137	HIS
3	c	157	GLN
2	D	59	GLN
2	D	77	ASN
2	D	86	HIS
2	D	146	ASN
2	D	183	HIS
3	d	58	ASN
3	d	122	ASN
3	d	137	HIS
2	E	67	ASN
2	E	148	GLN
3	e	78	GLN
3	e	137	HIS
2	F	58	ASN
2	F	59	GLN
2	F	86	HIS
2	F	151	ASN
2	F	172	ASN
2	F	177	HIS
2	F	183	HIS
3	f	76	GLN
3	f	78	GLN
3	f	122	ASN
2	G	77	ASN
2	G	86	HIS
2	G	146	ASN
2	G	151	ASN
2	G	153	GLN
2	G	172	ASN
2	G	183	HIS
3	g	137	HIS
2	H	59	GLN
2	H	67	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	71	GLN
2	H	77	ASN
2	H	172	ASN
2	H	177	HIS
3	h	137	HIS
3	h	157	GLN
2	I	63	ASN
2	I	64	GLN
2	I	67	ASN
2	I	148	GLN
3	i	122	ASN
3	i	157	GLN
2	J	59	GLN
2	J	64	GLN
2	J	172	ASN
3	j	122	ASN
3	j	137	HIS
2	K	146	ASN
2	K	177	HIS
2	L	59	GLN
2	L	64	GLN
2	L	71	GLN
3	l	137	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

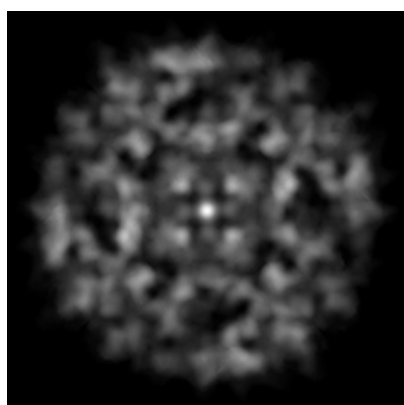
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8301. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

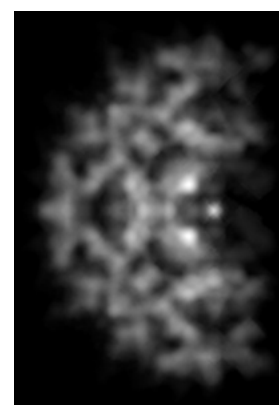
6.1.1 Primary map



X



Y

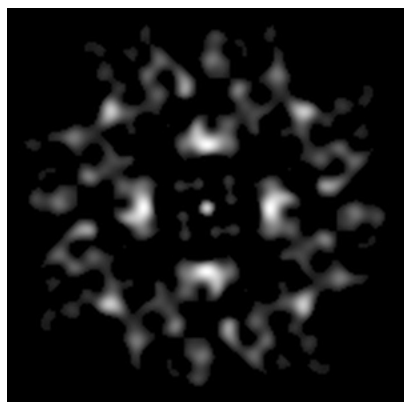


Z

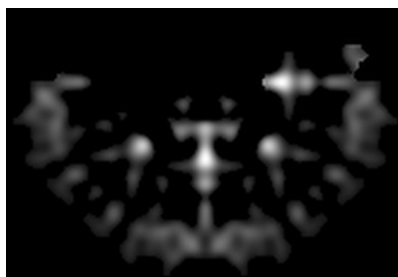
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

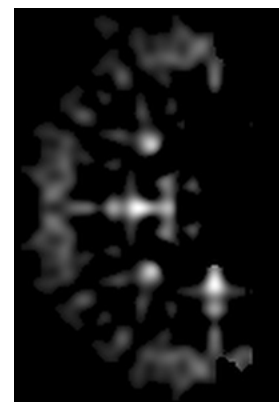
6.2.1 Primary map



X Index: 56



Y Index: 82

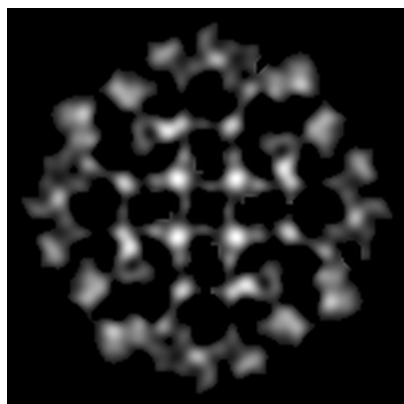


Z Index: 82

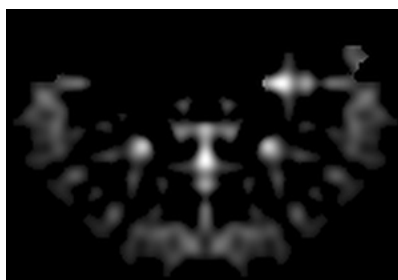
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

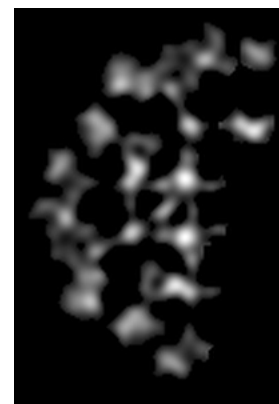
6.3.1 Primary map



X Index: 71



Y Index: 82

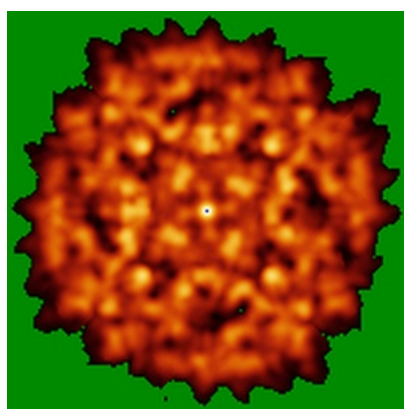


Z Index: 93

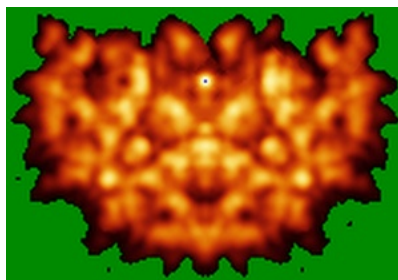
The images above show the largest variance slices of the map in three orthogonal directions.

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

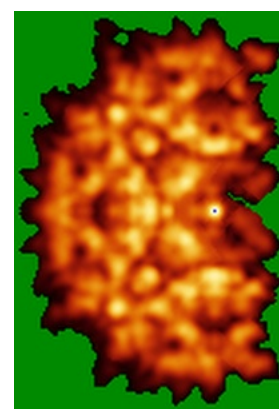
6.4.1 Primary map



X



Y

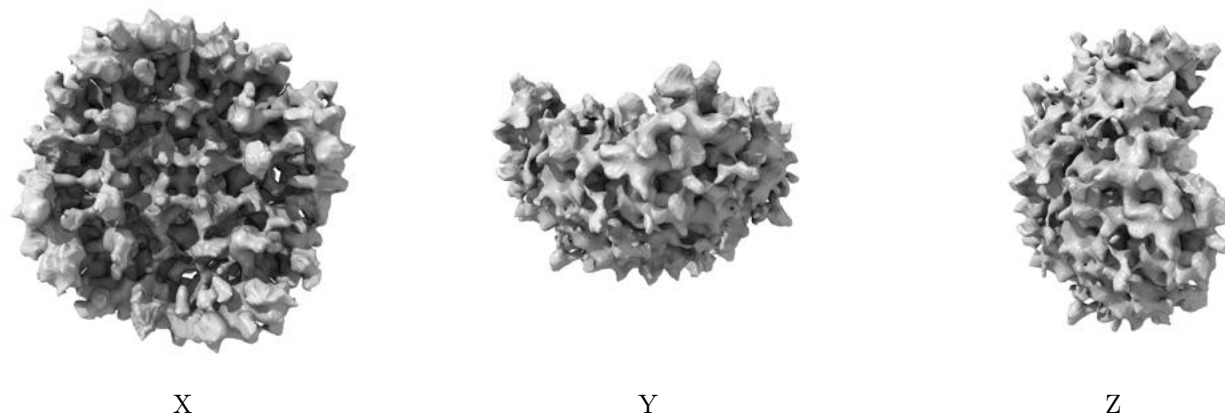


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

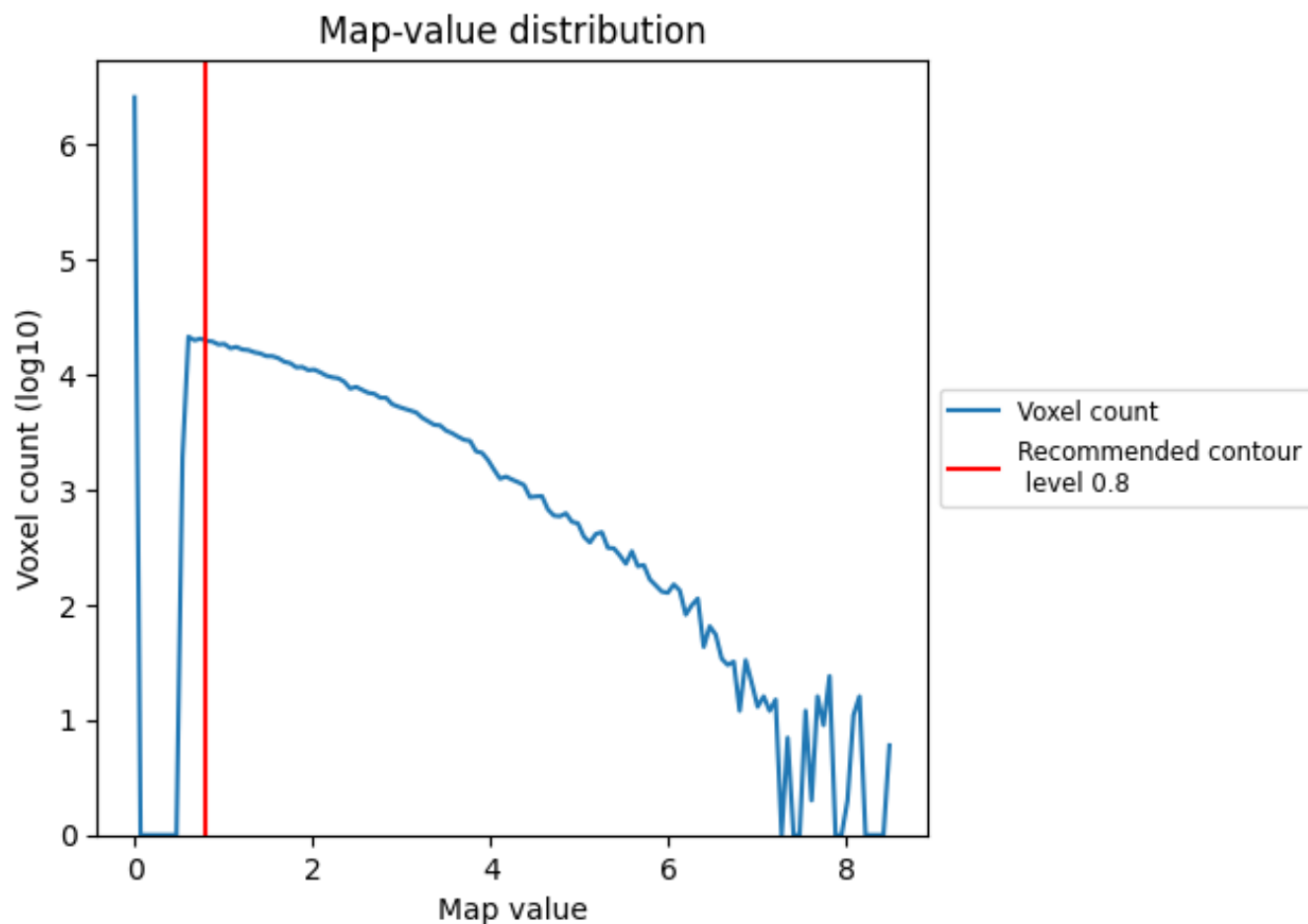
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

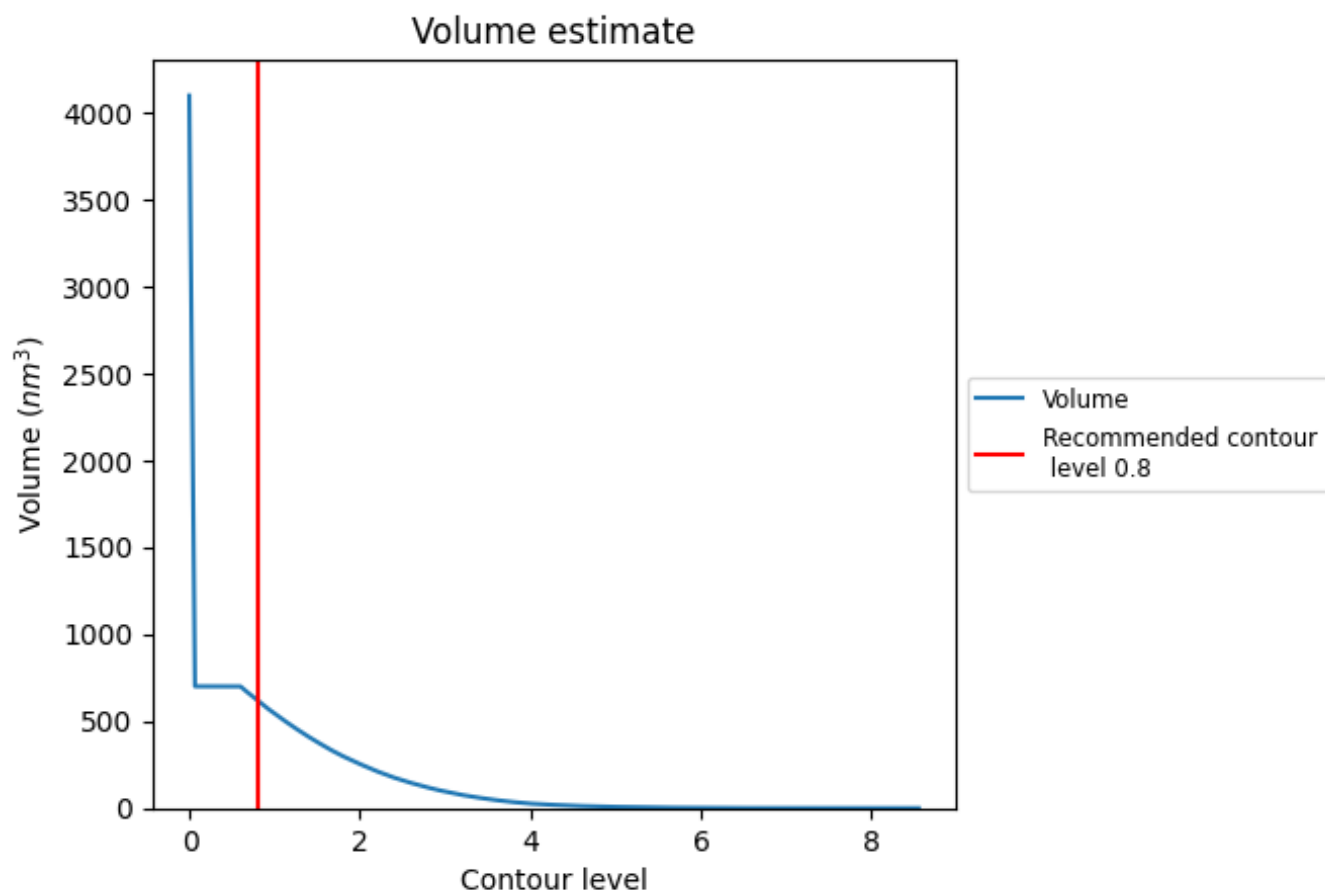
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 619 nm^3 ; this corresponds to an approximate mass of 559 kDa.

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

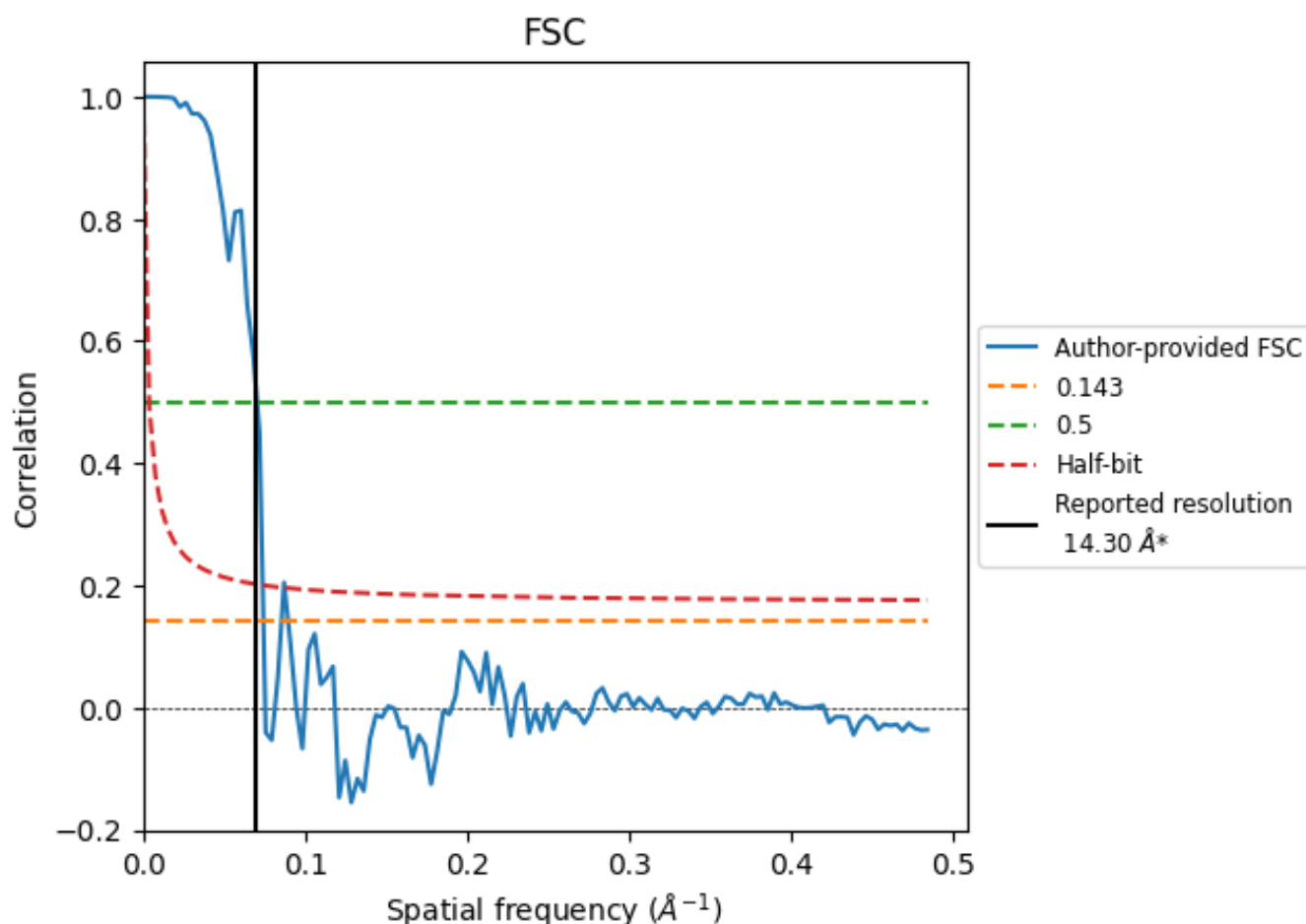
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.070 Å⁻¹

8.2 Resolution estimates [i](#)

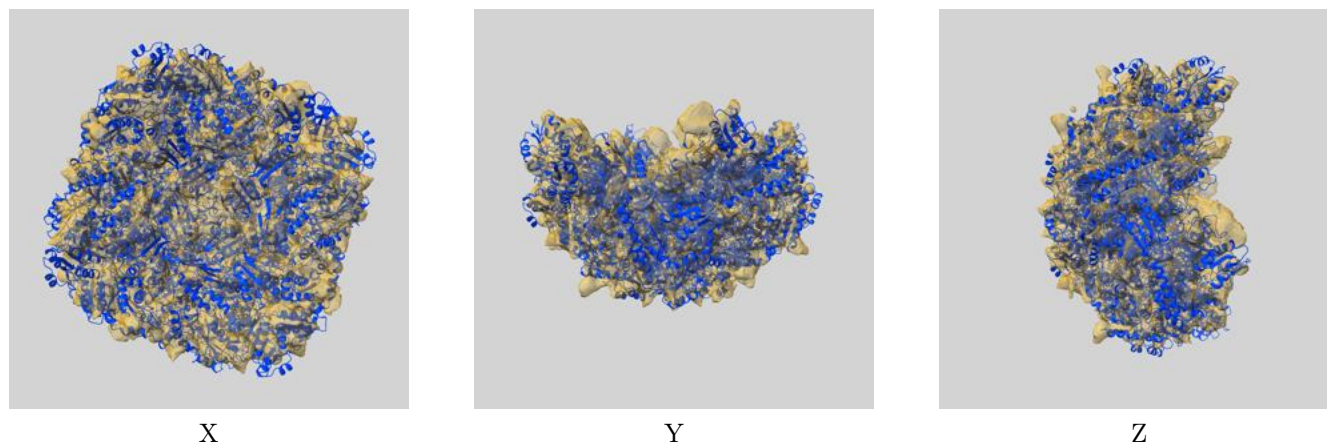
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	14.30	-	-
Author-provided FSC curve	13.50	14.22	13.57
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

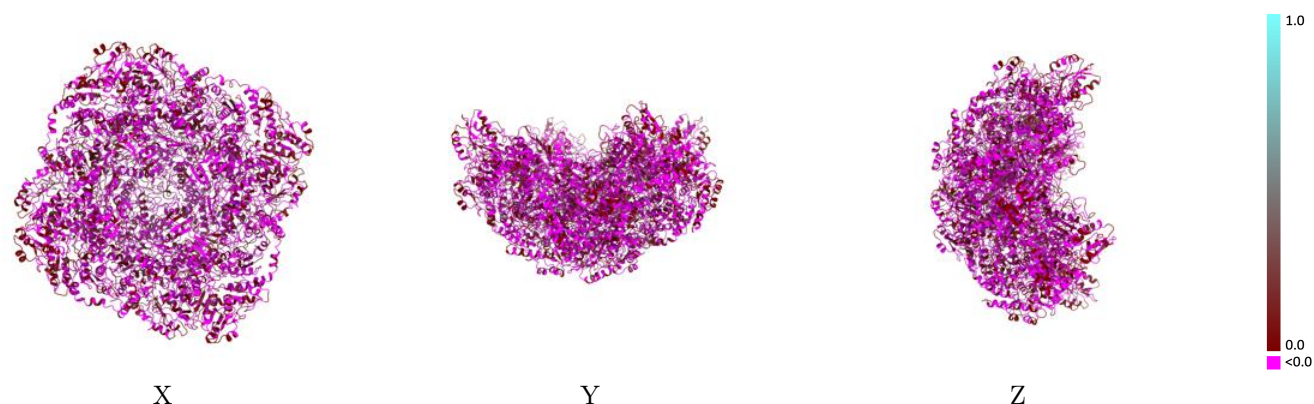
This section contains information regarding the fit between EMDB map EMD-8301 and PDB model 5KZ5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



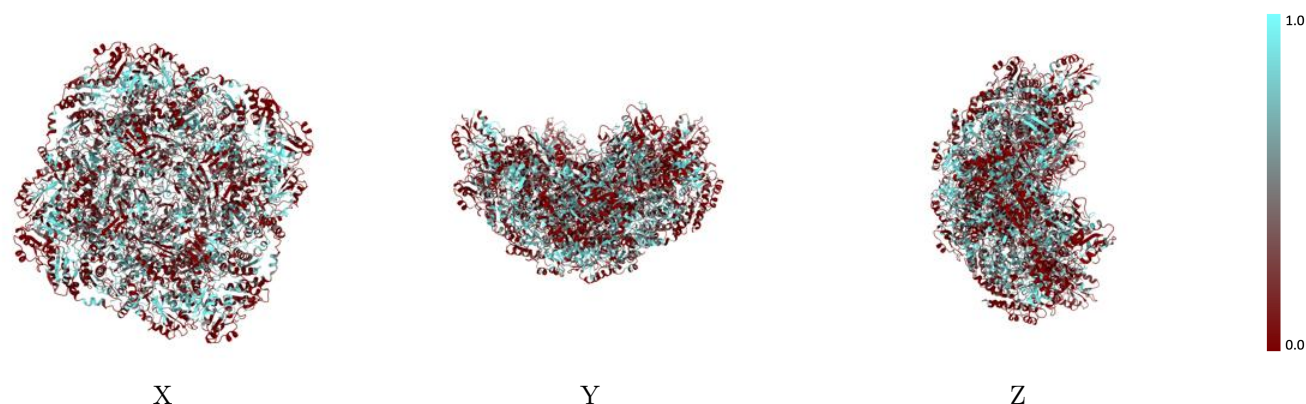
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



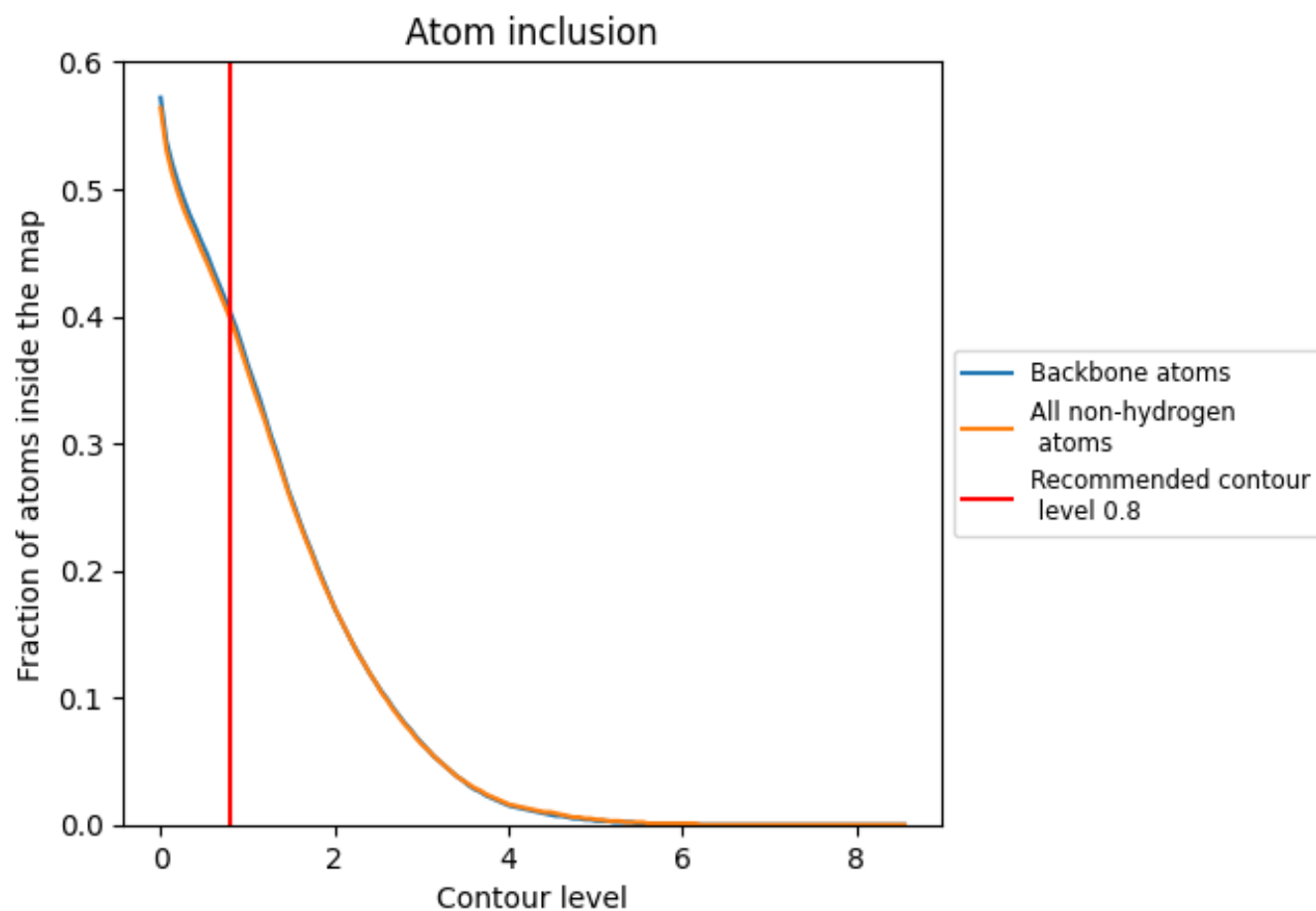
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion ⓘ



At the recommended contour level, 40% of all backbone atoms, 40% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3980	 -0.0200
1	 0.4510	 -0.0190
2	 0.4320	 -0.0250
3	 0.3890	 -0.0270
4	 0.4560	 -0.0160
A	 0.3990	 -0.0250
B	 0.4460	 -0.0140
C	 0.3460	 -0.0420
D	 0.4090	 -0.0230
E	 0.4230	 -0.0110
F	 0.3770	 -0.0470
G	 0.4240	 -0.0240
H	 0.4230	 -0.0290
I	 0.3990	 -0.0400
J	 0.4470	 -0.0220
K	 0.3990	 -0.0220
L	 0.3530	 -0.0460
M	 0.3810	 -0.0140
N	 0.3550	 -0.0180
O	 0.3420	 -0.0220
P	 0.3630	 -0.0040
Q	 0.3610	 -0.0150
R	 0.3530	 -0.0110
S	 0.3650	 -0.0090
T	 0.3330	 -0.0120
a	 0.4510	 -0.0170
b	 0.3490	 -0.0370
c	 0.5370	 -0.0150
d	 0.4720	 -0.0030
e	 0.3310	 -0.0300
f	 0.5320	 -0.0140
g	 0.4540	 -0.0370
h	 0.3920	 -0.0250
i	 0.4640	 -0.0260
j	 0.4410	 -0.0390



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.4390	 -0.0140
l	 0.4750	 -0.0200