



wwPDB EM Map/Model Validation Report ⓘ

Oct 10, 2016 – 02:06 PM EDT

PDB ID : 5KZ5
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 wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

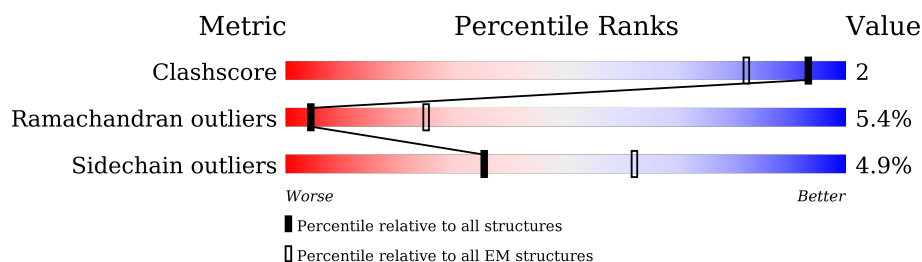
1 Overall quality at a glance

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.




















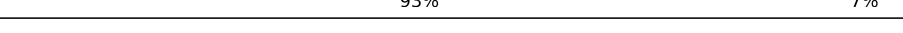
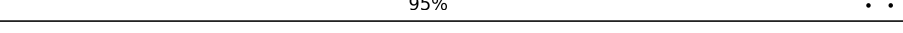




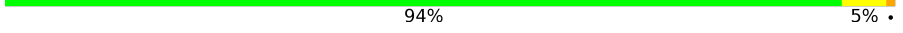

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	391	81% 15% .
1	2	391	87% 11% .
1	3	391	86% 10% .
1	4	391	86% 12% .
1	M	391	88% 11% .
1	N	391	91% 9% .
1	O	391	85% 13% .
1	P	391	88% 10% .
1	Q	391	90% 9% .

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Mol	Chain	Length	Quality of chain
1	R	391	 88% 11% .
1	S	391	 90% 10%
1	T	391	 89% 9% .
2	A	169	 79% 18% .
2	B	169	 88% 9% .
2	C	169	 82% 15% .
2	D	169	 85% 12% .
2	E	169	 79% 16% . .
2	F	169	 87% 10% . .
2	G	169	 86% 11% . .
2	H	169	 86% 11% . .
2	I	169	 80% 16% . .
2	J	169	 83% 16% .
2	K	169	 80% 16% .
2	L	169	 80% 17% . .
3	a	118	 89% 10% .
3	b	118	 93% 7%
3	c	118	 95% . .
3	d	118	 92% 8% .
3	e	118	 92% 8% .
3	f	118	 90% 10%
3	g	118	 88% 12%
3	h	118	 94% 5% .
3	i	118	 91% 6% . .
3	j	118	 83% 16% .

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Mol	Chain	Length	Quality of chain
3	k	118	<div><div></div><div>92%</div><div>7%</div><div></div></div>
3	l	118	<div><div></div><div>90%</div><div>9%</div><div></div></div>

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	C	N	O	S	0	0
			3040	1905	540	576	19		
1	2	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	3	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	4	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	M	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	N	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	O	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	P	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	Q	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	R	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	S	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		
1	T	391	Total	C	N	O	S	0	0
			3040	1905	540	576	19		

- Molecule 2 is a protein called Frataxin, mitochondrial.

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

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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		

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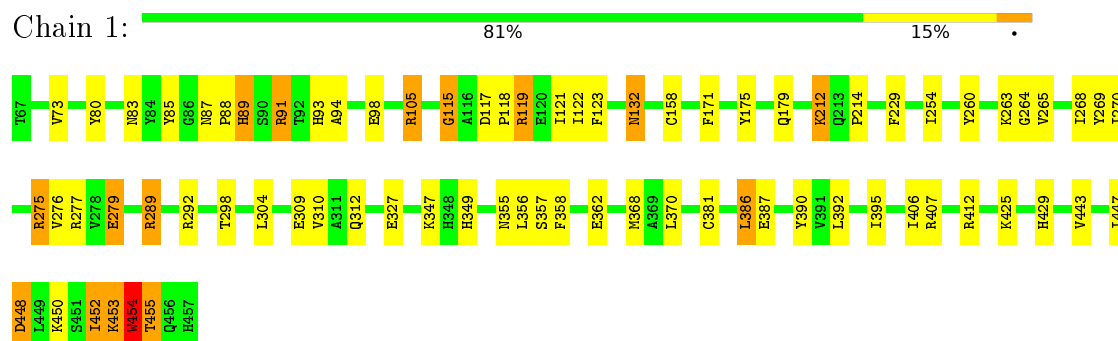
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	k	118	Total	C	N	O	S	0	0
			872	549	147	170	6		
3	l	118	Total	C	N	O	S	0	0
			872	549	147	170	6		

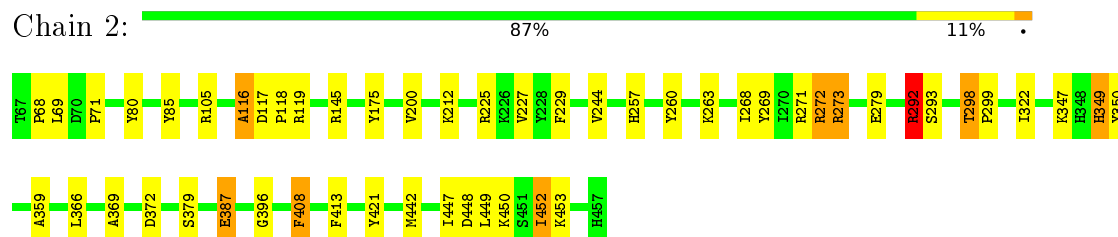
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

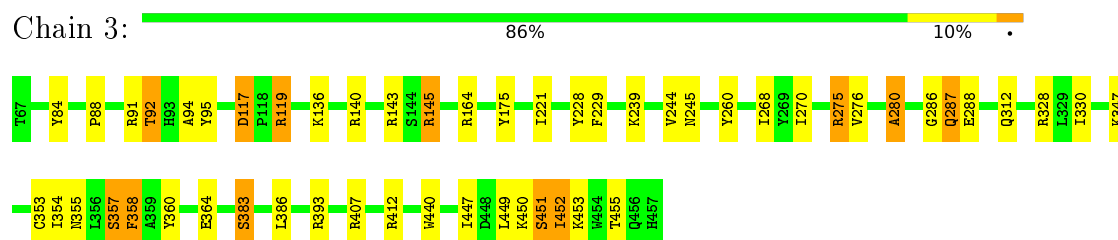
- Molecule 1: Cysteine desulfurase, mitochondrial



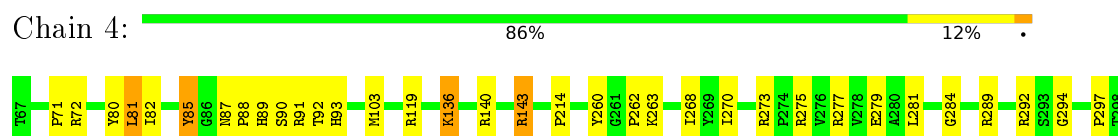
- Molecule 1: Cysteine desulfurase, mitochondrial



- Molecule 1: Cysteine desulfurase, mitochondrial



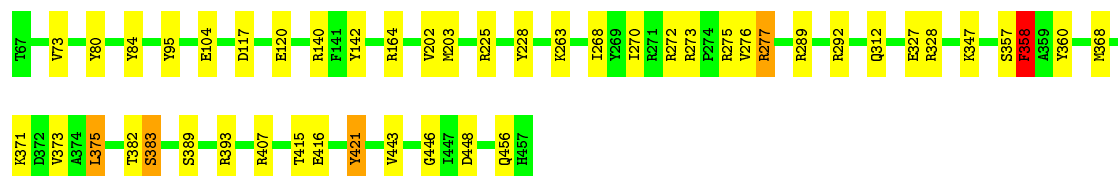
- Molecule 1: Cysteine desulfurase, mitochondrial





- Molecule 1: Cysteine desulfurase, mitochondrial

Chain M: 88% 11% .



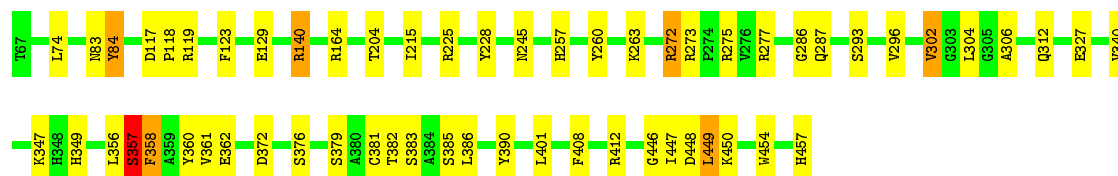
- Molecule 1: Cysteine desulfurase, mitochondrial

Chain N: 91% 9% .



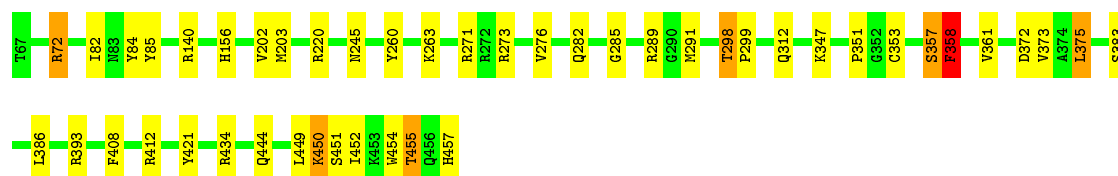
- Molecule 1: Cysteine desulfurase, mitochondrial

Chain O: 85% 13% .



- Molecule 1: Cysteine desulfurase, mitochondrial

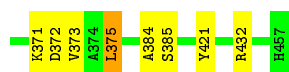
Chain P: 88% 10% .



- Molecule 1: Cysteine desulfurase, mitochondrial

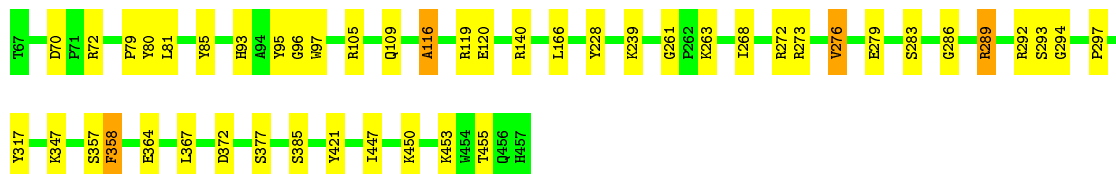
Chain Q: 90% 9% .





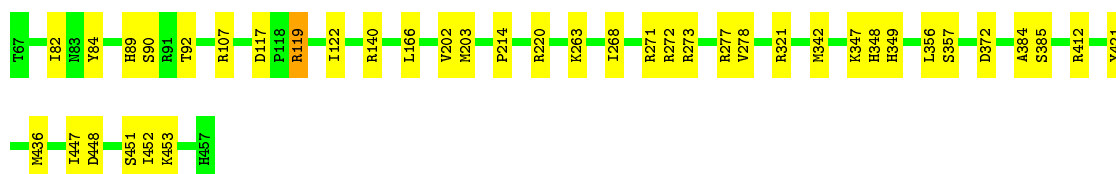
- Molecule 1: Cysteine desulfurase, mitochondrial

Chain R: 88% 11%



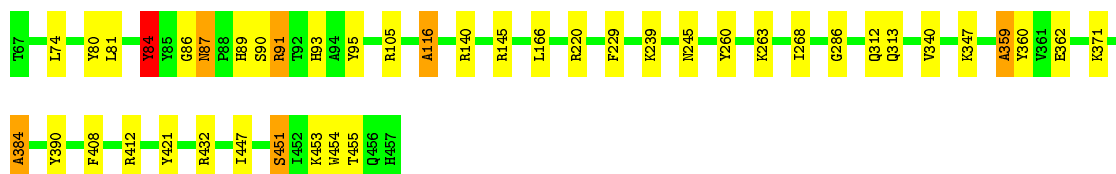
- Molecule 1: Cysteine desulfurase, mitochondrial

Chain S: 90% 10%



- Molecule 1: Cysteine desulfurase, mitochondrial

Chain T: 89% 9%



- Molecule 2: Frataxin, mitochondrial

Chain A: 79% 18%



- Molecule 2: Frataxin, mitochondrial

Chain B: 88% 9%



- Molecule 2: Frataxin, mitochondrial

Chain C: 82% 15%



- Molecule 2: Frataxin, mitochondrial

Chain D: 85% 12% .



- Molecule 2: Frataxin, mitochondrial

Chain E: 79% 16% . .



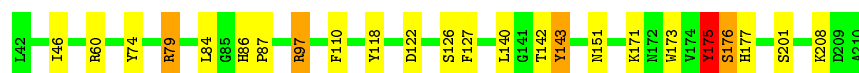
- Molecule 2: Frataxin, mitochondrial

Chain F: 87% 10% . .



- Molecule 2: Frataxin, mitochondrial

Chain G: 86% 11% . .



- Molecule 2: Frataxin, mitochondrial

Chain H: 86% 11% . .



- Molecule 2: Frataxin, mitochondrial

Chain I: 80% 16% . .

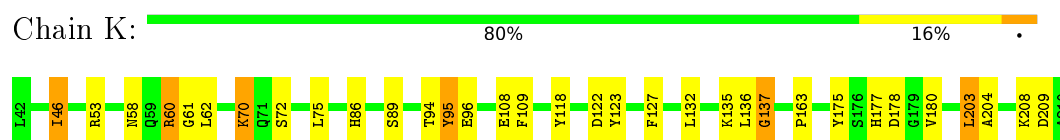


- Molecule 2: Frataxin, mitochondrial

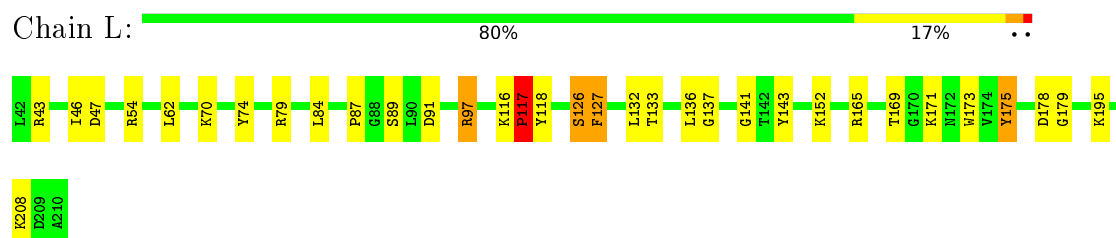
Chain J: 83% 16% .



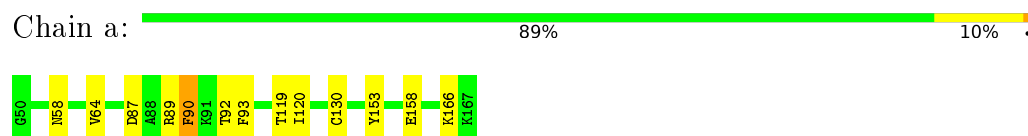
- Molecule 2: Frataxin, mitochondrial



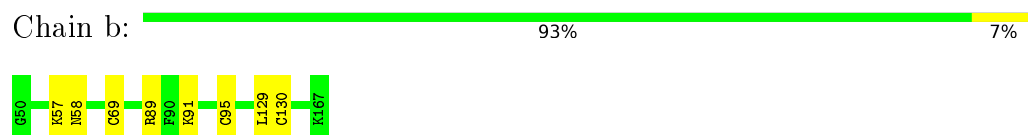
- Molecule 2: Frataxin, mitochondrial



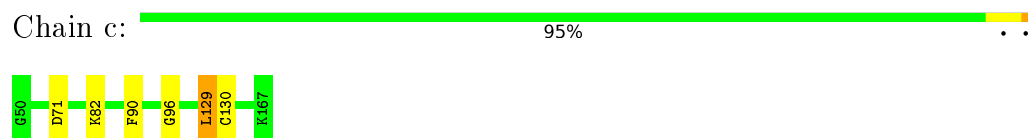
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



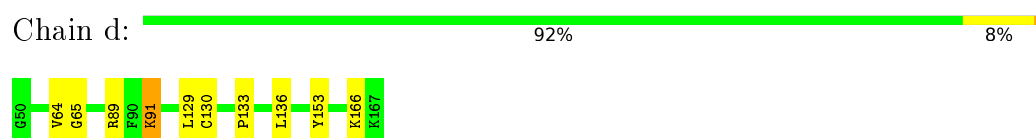
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



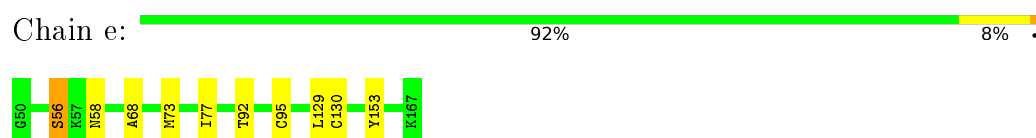
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



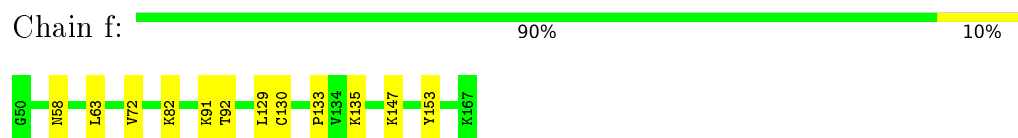
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



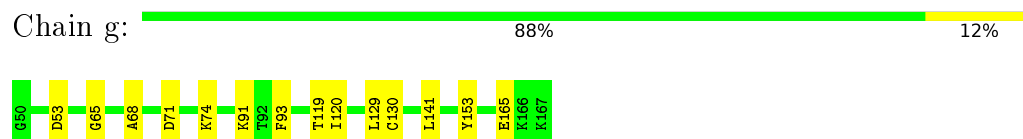
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



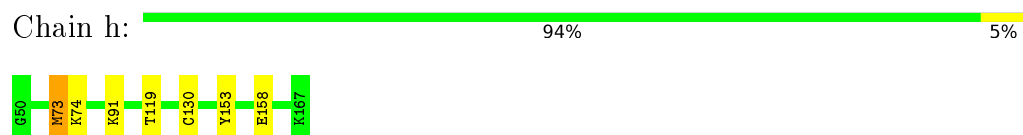
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



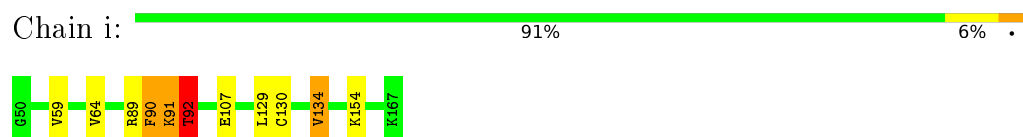
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



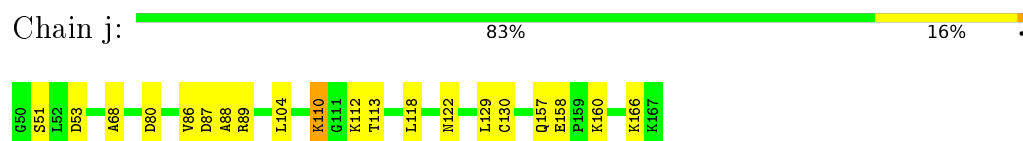
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



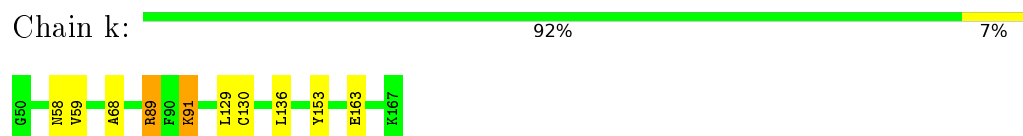
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



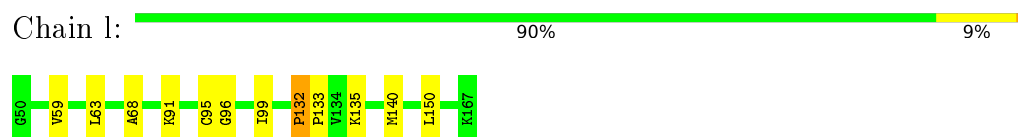
- Molecule 3: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



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



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



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	4124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	210	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	115000	Depositor
Image detector	Not provided	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 >2	RMSZ	# Z >2
1	1	1.09	0/3096	1.27	10/4185 (0.2%)
1	2	1.10	0/3096	1.31	21/4185 (0.5%)
1	3	1.13	1/3096 (0.0%)	1.31	27/4185 (0.6%)
1	4	1.09	0/3096	1.28	11/4185 (0.3%)
1	M	1.12	0/3096	1.27	18/4185 (0.4%)
1	N	1.11	0/3096	1.24	12/4185 (0.3%)
1	O	1.12	1/3096 (0.0%)	1.32	16/4185 (0.4%)
1	P	1.12	0/3096	1.26	13/4185 (0.3%)
1	Q	1.10	0/3096	1.25	15/4185 (0.4%)
1	R	1.13	2/3096 (0.1%)	1.28	13/4185 (0.3%)
1	S	1.13	0/3096	1.24	8/4185 (0.2%)
1	T	1.14	1/3096 (0.0%)	1.25	18/4185 (0.4%)
2	A	1.08	0/1356	1.35	11/1838 (0.6%)
2	B	1.09	0/1356	1.32	7/1838 (0.4%)
2	C	1.11	2/1356 (0.1%)	1.41	12/1838 (0.7%)
2	D	1.10	0/1356	1.34	9/1838 (0.5%)
2	E	1.11	0/1356	1.33	11/1838 (0.6%)
2	F	1.12	0/1356	1.37	10/1838 (0.5%)
2	G	1.12	1/1356 (0.1%)	1.36	10/1838 (0.5%)
2	H	1.11	0/1356	1.36	9/1838 (0.5%)
2	I	1.08	0/1356	1.35	13/1838 (0.7%)
2	J	1.08	0/1356	1.34	8/1838 (0.4%)
2	K	1.09	0/1356	1.35	7/1838 (0.4%)
2	L	1.05	0/1356	1.32	8/1838 (0.4%)
3	a	0.99	0/881	1.27	4/1181 (0.3%)
3	b	0.96	0/881	1.13	0/1181
3	c	0.98	0/881	1.18	0/1181
3	d	1.00	0/881	1.22	1/1181 (0.1%)
3	e	0.96	0/881	1.20	3/1181 (0.3%)
3	f	0.97	0/881	1.20	2/1181 (0.2%)
3	g	0.99	0/881	1.22	1/1181 (0.1%)
3	h	0.99	0/881	1.19	0/1181
3	i	0.99	0/881	1.22	3/1181 (0.3%)
3	j	0.98	0/881	1.24	2/1181 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	k	1.00	0/881	1.19	1/1181 (0.1%)
3	l	0.97	0/881	1.18	1/1181 (0.1%)
All	All	1.09	8/63996 (0.0%)	1.28	315/86448 (0.4%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	53	ARG	NE-CZ	5.92	1.40	1.33
1	3	275	ARG	NE-CZ	5.59	1.40	1.33
1	T	105	ARG	NE-CZ	5.42	1.40	1.33
1	R	289	ARG	NE-CZ	5.40	1.40	1.33
2	G	79	ARG	CD-NE	5.28	1.55	1.46
1	O	164	ARG	NE-CZ	5.22	1.39	1.33
2	C	60	ARG	NE-CZ	5.15	1.39	1.33
1	R	292	ARG	NE-CZ	5.00	1.39	1.33

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	95	TYR	CB-CG-CD2	-13.02	113.19	121.00
1	R	95	TYR	CB-CG-CD1	11.22	127.73	121.00
1	R	95	TYR	CB-CG-CD2	-11.09	114.35	121.00
2	K	95	TYR	CB-CG-CD1	10.23	127.14	121.00
1	R	85	TYR	CB-CG-CD2	-10.20	114.88	121.00
1	P	434	ARG	NE-CZ-NH1	-9.80	115.40	120.30
1	2	80	TYR	CB-CG-CD1	9.69	126.82	121.00
1	O	228	TYR	CB-CG-CD2	-9.31	115.42	121.00
1	P	289	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	Q	85	TYR	CB-CG-CD2	-8.92	115.65	121.00
1	O	228	TYR	CB-CG-CD1	8.86	126.31	121.00
1	4	119	ARG	NE-CZ-NH1	-8.68	115.96	120.30
2	D	127	PHE	CB-CG-CD1	8.43	126.70	120.80
1	Q	421	TYR	CB-CG-CD2	-8.43	115.94	121.00
1	P	84	TYR	CB-CG-CD2	-8.30	116.02	121.00
3	a	90	PHE	CB-CG-CD2	-8.26	115.02	120.80
2	E	166	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	M	328	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	O	260	TYR	CB-CG-CD1	-7.98	116.21	121.00
1	2	85	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	2	408	PHE	CB-CG-CD1	7.94	126.36	120.80
1	O	260	TYR	CB-CG-CD2	7.92	125.75	121.00
1	N	164	ARG	NE-CZ-NH1	-7.91	116.34	120.30
1	2	80	TYR	CB-CG-CD2	-7.90	116.26	121.00
2	G	110	PHE	CB-CG-CD1	7.83	126.28	120.80
3	i	91	LYS	C-N-CA	7.77	141.11	121.70
2	K	118	TYR	CB-CG-CD1	7.75	125.65	121.00
2	E	72	SER	C-N-CA	7.68	140.90	121.70
1	S	321	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	Q	421	TYR	CB-CG-CD1	7.63	125.58	121.00
2	B	175	TYR	CB-CG-CD2	-7.61	116.44	121.00
3	a	90	PHE	CB-CG-CD1	7.58	126.11	120.80
3	e	153	TYR	CB-CG-CD2	-7.56	116.47	121.00
1	P	358	PHE	N-CA-CB	7.54	124.17	110.60
1	M	421	TYR	CB-CG-CD2	-7.54	116.48	121.00
1	2	260	TYR	CB-CG-CD1	7.52	125.51	121.00
2	C	175	TYR	CB-CG-CD2	-7.49	116.50	121.00
1	4	143	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	O	381	CYS	C-N-CA	7.46	140.35	121.70
2	B	175	TYR	CB-CG-CD1	7.45	125.47	121.00
1	M	421	TYR	CB-CG-CD1	7.38	125.43	121.00
3	a	93	PHE	CB-CG-CD1	7.36	125.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	85	TYR	CB-CG-CD1	7.36	125.41	121.00
1	N	271	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	T	87	ASN	N-CA-CB	7.23	123.62	110.60
2	E	84	LEU	C-N-CA	7.20	137.43	122.30
3	i	92	THR	N-CA-CB	7.17	123.92	110.30
2	K	118	TYR	CB-CG-CD2	-7.12	116.73	121.00
1	3	140	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	T	84	TYR	CB-CG-CD1	7.11	125.26	121.00
1	M	84	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	P	220	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	Q	358	PHE	CB-CG-CD1	7.09	125.77	120.80
1	1	275	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	N	164	ARG	NE-CZ-NH2	7.08	123.84	120.30
2	E	110	PHE	CB-CG-CD1	-7.05	115.86	120.80
1	R	116	ALA	N-CA-CB	7.03	119.94	110.10
1	3	94	ALA	C-N-CA	7.01	139.23	121.70
1	R	421	TYR	CB-CG-CD1	7.01	125.21	121.00
1	1	454	TRP	C-N-CA	6.98	139.16	121.70
1	3	358	PHE	N-CA-CB	6.98	123.16	110.60
2	I	117	PRO	C-N-CA	6.98	139.14	121.70
1	R	289	ARG	NE-CZ-NH1	-6.95	116.82	120.30
2	F	165	ARG	NE-CZ-NH2	6.95	123.77	120.30
2	F	54	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	G	110	PHE	CB-CG-CD2	-6.94	115.94	120.80
1	M	289	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	Q	358	PHE	N-CA-CB	6.93	123.07	110.60
2	B	43	ARG	NE-CZ-NH2	6.93	123.76	120.30
1	Q	107	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	I	60	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	3	383	SER	N-CA-CB	6.88	120.81	110.50
1	3	117	ASP	N-CA-CB	6.87	122.96	110.60
1	N	271	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	2	408	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	R	85	TYR	CB-CG-CD1	6.83	125.10	121.00
1	3	119	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	3	452	ILE	C-N-CA	6.79	138.68	121.70
2	C	117	PRO	C-N-CA	6.78	138.64	121.70
2	J	43	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	M	95	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	T	384	ALA	N-CA-CB	6.71	119.49	110.10
1	T	412	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	S	122	ILE	N-CA-C	-6.65	93.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	143	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	S	107	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	J	109	PHE	CB-CG-CD2	-6.61	116.18	120.80
1	2	225	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	3	451	SER	N-CA-CB	6.59	120.39	110.50
1	O	450	LYS	C-N-CA	6.59	138.16	121.70
1	P	393	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	T	359	ALA	N-CA-CB	6.58	119.31	110.10
1	T	455	THR	C-N-CA	6.57	138.12	121.70
1	R	455	THR	C-N-CA	6.55	138.08	121.70
1	S	421	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	T	421	TYR	CB-CG-CD2	-6.54	117.08	121.00
2	D	97	ARG	N-CA-CB	6.52	122.33	110.60
1	M	95	TYR	CB-CG-CD1	6.52	124.91	121.00
1	1	452	ILE	C-N-CA	6.52	137.99	121.70
1	T	421	TYR	CB-CG-CD1	6.50	124.90	121.00
1	3	229	PHE	CB-CG-CD1	6.50	125.35	120.80
2	L	79	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	3	328	ARG	NE-CZ-NH2	6.50	123.55	120.30
2	A	48	ALA	N-CA-CB	6.49	119.19	110.10
1	2	116	ALA	N-CA-CB	6.48	119.17	110.10
2	E	85	GLY	C-N-CA	6.47	137.87	121.70
3	k	89	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	J	120	PHE	CB-CG-CD1	6.46	125.32	120.80
1	2	421	TYR	CB-CG-CD1	-6.45	117.13	121.00
2	C	175	TYR	CB-CG-CD1	6.42	124.85	121.00
1	T	451	SER	N-CA-CB	6.41	120.11	110.50
1	P	84	TYR	CB-CG-CD1	6.39	124.84	121.00
1	3	229	PHE	CB-CG-CD2	-6.37	116.34	120.80
1	R	421	TYR	CB-CG-CD2	-6.37	117.18	121.00
2	D	127	PHE	CB-CG-CD2	-6.33	116.37	120.80
1	M	142	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	3	358	PHE	CB-CG-CD1	6.31	125.22	120.80
2	L	79	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	B	60	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	M	289	ARG	NE-CZ-NH2	6.28	123.44	120.30
2	I	127	PHE	N-CA-CB	6.27	121.89	110.60
1	Q	225	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	R	317	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	P	450	LYS	N-CA-CB	6.26	121.86	110.60
1	4	408	PHE	CB-CG-CD2	-6.25	116.42	120.80
2	A	118	TYR	CB-CG-CD2	-6.25	117.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	360	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	S	107	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	O	449	LEU	C-N-CA	6.21	137.22	121.70
2	I	126	SER	C-N-CA	6.20	137.20	121.70
2	G	143	TYR	N-CA-CB	6.19	121.75	110.60
1	Q	357	SER	C-N-CA	6.17	137.12	121.70
1	1	175	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	P	357	SER	C-N-CA	6.14	137.05	121.70
2	A	72	SER	C-N-CA	6.12	137.00	121.70
1	3	357	SER	C-N-CA	6.10	136.95	121.70
2	F	175	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	T	432	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	T	91	ARG	NE-CZ-NH2	-6.07	117.27	120.30
2	H	126	SER	C-N-CA	6.06	136.85	121.70
1	4	277	ARG	NE-CZ-NH2	6.05	123.32	120.30
3	j	89	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	O	272	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	T	80	TYR	CB-CG-CD2	-5.99	117.41	121.00
2	B	176	SER	N-CA-CB	5.99	119.48	110.50
1	M	407	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	1	368	MET	CG-SD-CE	-5.95	90.69	100.20
2	J	143	TYR	CB-CG-CD1	5.94	124.56	121.00
1	P	421	TYR	CB-CG-CD1	5.94	124.56	121.00
2	F	60	ARG	C-N-CA	5.94	134.77	122.30
1	N	140	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	3	94	ALA	CB-CA-C	5.93	119.00	110.10
2	A	71	GLN	C-N-CA	5.93	136.52	121.70
1	S	220	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	T	145	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	Q	119	ARG	NE-CZ-NH2	-5.91	117.34	120.30
3	a	93	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	M	80	TYR	CB-CG-CD1	5.88	124.53	121.00
2	F	127	PHE	N-CA-CB	5.88	121.18	110.60
1	2	260	TYR	CB-CG-CD2	-5.87	117.48	121.00
3	f	92	THR	N-CA-CB	5.86	121.44	110.30
2	F	176	SER	N-CA-CB	5.86	119.29	110.50
1	N	269	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	O	357	SER	N-CA-CB	5.83	119.25	110.50
1	R	358	PHE	N-CA-CB	5.83	121.10	110.60
1	O	408	PHE	CB-CG-CD2	-5.82	116.73	120.80
3	l	95	CYS	C-N-CA	5.81	134.51	122.30
1	4	91	ARG	NE-CZ-NH2	-5.80	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	358	PHE	CB-CG-CD2	-5.80	116.74	120.80
1	M	456	GLN	C-N-CA	5.79	136.19	121.70
2	L	97	ARG	N-CA-CB	5.79	121.02	110.60
1	3	84	TYR	CB-CG-CD1	5.78	124.47	121.00
1	Q	107	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	Q	432	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	1	91	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	M	383	SER	N-CA-CB	5.75	119.12	110.50
2	L	175	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	K	60	ARG	CA-C-N	5.74	127.67	116.20
2	C	143	TYR	CB-CG-CD1	5.72	124.43	121.00
2	C	127	PHE	N-CA-CB	5.72	120.89	110.60
1	2	448	ASP	C-N-CA	5.70	135.94	121.70
2	H	83	THR	C-N-CA	5.69	135.93	121.70
2	I	166	TYR	CB-CG-CD1	5.69	124.41	121.00
2	C	60	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	H	127	PHE	N-CA-CB	5.67	120.80	110.60
1	O	140	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	T	86	GLY	C-N-CA	5.66	135.85	121.70
2	I	118	TYR	N-CA-C	5.66	126.28	111.00
2	I	166	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	3	84	TYR	CB-CG-CD2	-5.64	117.62	121.00
2	G	142	THR	C-N-CA	5.63	135.77	121.70
2	B	126	SER	C-N-CA	5.63	135.76	121.70
2	K	53	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	P	451	SER	C-N-CA	5.60	135.71	121.70
2	L	43	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	2	272	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	2	105	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	3	140	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	4	368	MET	CG-SD-CE	-5.59	91.26	100.20
1	3	358	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	3	92	THR	N-CA-CB	5.58	120.91	110.30
2	L	43	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	g	74	LYS	N-CA-C	-5.57	95.95	111.00
2	I	120	PHE	CB-CG-CD1	5.57	124.70	120.80
2	F	95	TYR	CB-CG-CD1	5.57	124.34	121.00
1	O	225	ARG	NE-CZ-NH2	5.56	123.08	120.30
2	G	176	SER	N-CA-CB	5.56	118.84	110.50
1	N	95	TYR	CB-CG-CD1	5.56	124.33	121.00
1	T	220	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	Q	317	TYR	CB-CG-CD2	-5.54	117.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	273	ARG	N-CA-CB	5.53	120.56	110.60
1	O	381	CYS	CB-CA-C	5.49	121.39	110.40
2	J	120	PHE	CB-CG-CD2	-5.49	116.96	120.80
2	H	74	TYR	CB-CG-CD1	-5.49	117.71	121.00
2	C	84	LEU	C-N-CA	5.48	133.81	122.30
1	N	350	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	I	120	PHE	CB-CG-CD2	-5.44	117.00	120.80
1	1	395	ILE	N-CA-C	-5.43	96.33	111.00
1	N	225	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	2	387	GLU	CA-C-N	5.43	132.30	117.10
1	2	442	MET	CG-SD-CE	-5.42	91.52	100.20
1	M	80	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	4	119	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	M	225	ARG	NE-CZ-NH1	-5.41	117.59	120.30
2	C	143	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	4	72	ARG	NE-CZ-NH1	-5.41	117.60	120.30
2	L	117	PRO	CA-C-N	5.38	129.04	117.20
1	3	95	TYR	CB-CG-CD1	-5.37	117.78	121.00
2	G	175	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	M	225	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	P	289	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	1	453	LYS	CA-C-N	5.35	128.97	117.20
1	3	175	TYR	CB-CG-CD1	5.35	124.21	121.00
1	N	105	ARG	NE-CZ-NH1	-5.33	117.63	120.30
2	E	118	TYR	CB-CG-CD1	-5.33	117.80	121.00
2	I	86	HIS	N-CA-CB	5.33	120.19	110.60
2	D	95	TYR	C-N-CA	5.33	135.01	121.70
2	D	84	LEU	C-N-CA	5.32	133.48	122.30
2	C	135	LYS	N-CA-CB	5.32	120.17	110.60
2	E	176	SER	N-CA-CB	5.32	118.48	110.50
2	H	209	ASP	N-CA-CB	5.31	120.16	110.60
1	R	357	SER	C-N-CA	5.31	134.97	121.70
1	M	393	ARG	NE-CZ-NH2	5.29	122.95	120.30
2	B	95	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	F	208	LYS	N-CA-CB	5.28	120.11	110.60
2	G	74	TYR	CB-CG-CD2	5.28	124.17	121.00
1	3	407	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	T	229	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	2	292	ARG	N-CA-CB	5.26	120.07	110.60
2	A	43	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	T	260	TYR	CB-CG-CD2	-5.26	117.85	121.00
1	1	122	ILE	N-CA-C	-5.25	96.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	209	ASP	CB-CG-OD2	5.25	123.02	118.30
2	G	126	SER	C-N-CA	5.25	134.81	121.70
1	3	280	ALA	N-CA-CB	5.23	117.42	110.10
2	A	85	GLY	N-CA-C	-5.23	100.03	113.10
2	I	84	LEU	N-CA-CB	5.23	120.85	110.40
3	d	89	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	N	456	GLN	N-CA-CB	5.21	119.99	110.60
2	H	177	HIS	CA-CB-CG	5.21	122.46	113.60
2	A	109	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	4	412	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	Q	328	ARG	NE-CZ-NH1	-5.20	117.70	120.30
2	K	175	TYR	CB-CG-CD2	-5.19	117.88	121.00
1	1	229	PHE	CB-CG-CD1	5.19	124.44	120.80
1	Q	384	ALA	N-CA-CB	5.19	117.37	110.10
3	f	153	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	2	229	PHE	CB-CG-CD2	-5.19	117.17	120.80
2	C	176	SER	N-CA-CB	5.18	118.28	110.50
2	D	77	ASN	N-CA-C	-5.17	97.03	111.00
1	2	421	TYR	CB-CG-CD2	5.17	124.10	121.00
1	S	119	ARG	N-CA-CB	5.17	119.90	110.60
1	P	220	ARG	NE-CZ-NH2	5.16	122.88	120.30
3	j	158	GLU	CA-C-N	5.16	131.54	117.10
2	C	126	SER	C-N-CA	5.15	134.58	121.70
2	I	84	LEU	C-N-CA	5.15	133.12	122.30
2	H	165	ARG	NE-CZ-NH1	-5.15	117.72	120.30
2	C	60	ARG	N-CA-CB	5.15	119.86	110.60
1	R	292	ARG	NE-CZ-NH1	-5.15	117.73	120.30
2	E	166	TYR	CB-CG-CD1	5.14	124.08	121.00
1	O	381	CYS	CA-C-N	5.13	128.49	117.20
2	J	118	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	3	360	TYR	CB-CG-CD2	5.13	124.08	121.00
3	e	73	MET	CG-SD-CE	-5.12	92.01	100.20
2	G	127	PHE	CB-CG-CD1	5.12	124.38	120.80
2	A	206	SER	N-CA-CB	5.11	118.17	110.50
2	A	80	LYS	C-N-CA	5.11	134.47	121.70
2	F	66	TRP	CB-CG-CD2	-5.11	119.96	126.60
2	E	165	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	3	94	ALA	CA-C-N	5.08	128.39	117.20
1	O	379	SER	C-N-CA	5.08	134.41	121.70
2	D	74	TYR	CB-CG-CD1	-5.08	117.95	121.00
2	I	118	TYR	CB-CG-CD1	5.08	124.05	121.00
2	A	71	GLN	CB-CA-C	5.07	120.54	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	360	TYR	N-CA-CB	5.07	119.72	110.60
1	N	95	TYR	CB-CG-CD2	-5.06	117.96	121.00
2	F	166	TYR	CB-CG-CD1	5.06	124.04	121.00
1	2	69	LEU	CB-CG-CD1	5.06	119.60	111.00
2	H	127	PHE	N-CA-C	-5.06	97.35	111.00
2	A	95	TYR	CB-CG-CD2	-5.06	117.97	121.00
2	L	97	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	J	43	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	4	85	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	T	116	ALA	N-CA-CB	5.04	117.16	110.10
2	E	80	LYS	C-N-CA	5.04	134.30	121.70
1	4	421	TYR	CB-CG-CD1	5.04	124.02	121.00
2	H	175	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	3	143	ARG	NE-CZ-NH1	-5.03	117.78	120.30
3	i	91	LYS	CA-C-N	5.03	128.27	117.20
2	D	126	SER	C-N-CA	5.02	134.25	121.70
1	S	357	SER	C-N-CA	5.02	134.25	121.70
2	G	127	PHE	CB-CG-CD2	-5.02	117.29	120.80
3	e	56	SER	N-CA-CB	5.01	118.02	110.50
1	3	145	ARG	N-CA-CB	5.01	119.62	110.60
2	E	95	TYR	CB-CG-CD1	-5.01	118.00	121.00

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

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Mol	Chain	Res	Type	Group
1	Q	360	TYR	Sidechain
1	Q	84	TYR	Sidechain
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	26	0
1	2	3040	0	3058	5	0
1	3	3040	0	3057	10	0
1	4	3040	0	3058	8	0
1	M	3040	0	3058	7	0
1	N	3040	0	3058	3	0
1	O	3040	0	3057	19	0
1	P	3040	0	3058	11	0
1	Q	3040	0	3057	14	0
1	R	3040	0	3058	4	0
1	S	3040	0	3058	2	0
1	T	3040	0	3058	8	0
2	A	1328	0	1302	2	0
2	B	1328	0	1302	2	0
2	C	1328	0	1302	9	0
2	D	1328	0	1302	9	0
2	E	1328	0	1302	39	0
2	F	1328	0	1302	0	0
2	G	1328	0	1302	2	0
2	H	1328	0	1302	4	0
2	I	1328	0	1302	2	0
2	J	1328	0	1302	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1328	0	1301	25	0
2	L	1328	0	1302	11	0
3	a	872	0	917	0	0
3	b	872	0	917	0	0
3	c	872	0	917	0	0
3	d	872	0	917	0	0
3	e	872	0	917	0	0
3	f	872	0	916	0	0
3	g	872	0	917	0	0
3	h	872	0	917	0	0
3	i	872	0	917	0	0
3	j	872	0	917	0	0
3	k	872	0	917	0	0
3	l	872	0	917	0	0
All	All	62880	0	63319	188	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 (188) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:125:VAL:HA	2:E:127:PHE:CE1	2.06	0.90
2:E:127:PHE:CE2	2:E:133:THR:N	2.40	0.90
1:Q:95:TYR:CE1	2:C:134:VAL:HG22	2.07	0.90
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
1:T:95:TYR:OH	2:L:136:LEU:C	2.13	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:125:VAL:C	2:E:127:PHE:HD1	1.79	0.84
1:O:357:SER:CB	1:O:358:PHE:HB2	2.05	0.83
2:E:126:SER:CA	2:E:127:PHE:CB	2.39	0.82
2:E:125:VAL:C	2:E:127:PHE:CD1	2.53	0.82
2:E:124:ASP:O	2:E:127:PHE:CE1	2.33	0.81
1:O:340:VAL:HA	1:O:358:PHE:HE1	1.47	0.80
1:T:95:TYR:HH	2:L:136:LEU:CA	1.93	0.79
2:E:127:PHE:HD2	2:E:133:THR:N	1.77	0.78
2:K:123:TYR:CD1	2:K:135:LYS:C	2.58	0.77
2:E:127:PHE:HD2	2:E:133:THR:H	1.30	0.75
2:E:126:SER:HA	2:E:127:PHE:HB2	0.80	0.75
1:O:356:LEU:CA	1:O:358:PHE:HE2	1.99	0.75
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:D:201:SER:C	2:D:209:ASP:OD2	2.28	0.70
2:K:123:TYR:CG	2:K:135:LYS:O	2.44	0.70
1:3:330:ILE:HD11	1:3:354:ILE:HD11	1.76	0.67
1:Q:92:THR:HB	1:Q:95:TYR:HD1	1.58	0.67
2:K:136:LEU:HD12	2:K:136:LEU:N	2.10	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:T:95:TYR:HH	2:L:136:LEU:C	2.01	0.62
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:E:124:ASP:C	2:E:127:PHE:HE1	2.02	0.61
2:K:123:TYR:OH	2:K:136:LEU:O	1.97	0.61
2:K:123:TYR:CD1	2:K:135:LYS:O	2.54	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:T:95:TYR:HH	2:L:136:LEU:HA	1.60	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
1:1:452:ILE:H	1:1:453:LYS:C	2.11	0.54
1:P:271:ARG:HD2	1:P:273:ARG:H	1.73	0.54
2:D:201:SER:HB2	2:D:209:ASP:OD2	2.08	0.54
1:O:447:ILE:HG23	1:O:448:ASP:H	1.73	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
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
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:K:136:LEU:N	2:K:136:LEU:CD1	2.73	0.50
2:E:125:VAL:CA	2:E:127:PHE:HE1	2.21	0.50
2:D:202:SER:N	2:D:209:ASP:OD2	2.45	0.50
1:M:373:VAL:HG12	1:M:375:LEU:H	1.76	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
1:4:140:ARG:HH12	1:4:143:ARG:HH21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:126:SER:C	2:E:127:PHE:CD1	2.86	0.49
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
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
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
1:1:105: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:Q:367:LEU:O	1:Q:367:LEU:HD13	2.15	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:127:PHE:HD2	2:E:132:LEU:CA	2.31	0.44
1:N:157:LYS:HZ3	1:N:389:SER:H	1.66	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
2:K:70:LYS:H	2:K:70:LYS:HD2	1.82	0.43
1:O:287:GLN:H	1:R:119:ARG:H	1.65	0.43
2:E:127:PHE:CD2	2:E:132:LEU:C	2.91	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
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:G:151:ASN:HD21	2:H:150:PRO:HB2	1.83	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
2:C:85:GLY:H	2:C:86:HIS:CD2	2.37	0.43
2:D:201:SER:CA	2:D:209:ASP:OD2	2.67	0.42
1:S:348:HIS:CG	1:S:348:HIS:O	2.72	0.42
1:1:425:LYS:HG2	1:1:429:HIS:CE1	2.54	0.42
2:K:136:LEU:O	2:K:137:GLY:C	2.56	0.42
1:4:71:PRO:HG2	2:D:86:HIS:H	1.85	0.42
2:D:90:LEU:HD13	2:D:90:LEU:HA	1.93	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:O:204:THR:HA	1:O:215:ILE:HD11	2.01	0.42
2:K:122:ASP:C	2:K:123:TYR:CD2	2.92	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
2:L:126:SER:HA	2:L:127:PHE:HB2	2.01	0.42
1:Q:92:THR:CB	1:Q:95:TYR:CD1	3.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:265:VAL:HG12	1:1:304:LEU:HD13	2.03	0.41
1:1:289:ARG:HD2	1:3:287:GLN:HE22	1.86	0.40
2:C:173:TRP:HE1	2:C:182:LEU:H	1.69	0.40
1:M:228:TYR:CD1	1:M:276:VAL:HG12	2.56	0.40
1:4:454:TRP:CD1	1:P:156:HIS:CD2	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	389/391 (100%)	333 (86%)	30 (8%)	26 (7%)	1	24
1	2	389/391 (100%)	341 (88%)	27 (7%)	21 (5%)	2	29
1	3	389/391 (100%)	334 (86%)	37 (10%)	18 (5%)	3	33
1	4	389/391 (100%)	332 (85%)	34 (9%)	23 (6%)	2	27
1	M	389/391 (100%)	346 (89%)	30 (8%)	13 (3%)	5	40
1	N	389/391 (100%)	340 (87%)	40 (10%)	9 (2%)	8	48
1	O	389/391 (100%)	332 (85%)	35 (9%)	22 (6%)	2	28
1	P	389/391 (100%)	345 (89%)	29 (8%)	15 (4%)	4	36
1	Q	389/391 (100%)	343 (88%)	32 (8%)	14 (4%)	4	38
1	R	389/391 (100%)	342 (88%)	31 (8%)	16 (4%)	3	35
1	S	389/391 (100%)	335 (86%)	36 (9%)	18 (5%)	3	33
1	T	389/391 (100%)	341 (88%)	34 (9%)	14 (4%)	4	38
2	A	167/169 (99%)	124 (74%)	28 (17%)	15 (9%)	1	17
2	B	167/169 (99%)	140 (84%)	18 (11%)	9 (5%)	2	29
2	C	167/169 (99%)	125 (75%)	27 (16%)	15 (9%)	1	17
2	D	167/169 (99%)	126 (75%)	33 (20%)	8 (5%)	3	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	167/169 (99%)	133 (80%)	20 (12%)	14 (8%)	1	18
2	F	167/169 (99%)	134 (80%)	23 (14%)	10 (6%)	2	26
2	G	167/169 (99%)	135 (81%)	23 (14%)	9 (5%)	2	29
2	H	167/169 (99%)	133 (80%)	25 (15%)	9 (5%)	2	29
2	I	167/169 (99%)	130 (78%)	21 (13%)	16 (10%)	1	15
2	J	167/169 (99%)	132 (79%)	17 (10%)	18 (11%)	0	11
2	K	167/169 (99%)	137 (82%)	22 (13%)	8 (5%)	3	32
2	L	167/169 (99%)	125 (75%)	27 (16%)	15 (9%)	1	17
3	a	116/118 (98%)	94 (81%)	16 (14%)	6 (5%)	2	30
3	b	116/118 (98%)	102 (88%)	9 (8%)	5 (4%)	3	34
3	c	116/118 (98%)	97 (84%)	16 (14%)	3 (3%)	7	45
3	d	116/118 (98%)	97 (84%)	12 (10%)	7 (6%)	2	26
3	e	116/118 (98%)	97 (84%)	12 (10%)	7 (6%)	2	26
3	f	116/118 (98%)	98 (84%)	13 (11%)	5 (4%)	3	34
3	g	116/118 (98%)	95 (82%)	12 (10%)	9 (8%)	1	20
3	h	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	11	55
3	i	116/118 (98%)	96 (83%)	13 (11%)	7 (6%)	2	26
3	j	116/118 (98%)	86 (74%)	16 (14%)	14 (12%)	0	8
3	k	116/118 (98%)	99 (85%)	10 (9%)	7 (6%)	2	26
3	l	116/118 (98%)	99 (85%)	12 (10%)	5 (4%)	3	34
All	All	8064/8136 (99%)	6798 (84%)	834 (10%)	432 (5%)	4	29

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	L	74	TYR
2	L	117	PRO
3	1	96	GLY
3	1	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	311 (93%)	22 (7%)	21	57
1	2	333/333 (100%)	319 (96%)	14 (4%)	36	70
1	3	333/333 (100%)	318 (96%)	15 (4%)	34	69
1	4	333/333 (100%)	314 (94%)	19 (6%)	25	62
1	M	333/333 (100%)	320 (96%)	13 (4%)	39	72
1	N	333/333 (100%)	316 (95%)	17 (5%)	29	66
1	O	333/333 (100%)	318 (96%)	15 (4%)	34	69
1	P	333/333 (100%)	319 (96%)	14 (4%)	36	70
1	Q	333/333 (100%)	323 (97%)	10 (3%)	48	77
1	R	333/333 (100%)	314 (94%)	19 (6%)	25	62
1	S	333/333 (100%)	320 (96%)	13 (4%)	39	72
1	T	333/333 (100%)	318 (96%)	15 (4%)	34	69
2	A	146/146 (100%)	134 (92%)	12 (8%)	14	49
2	B	146/146 (100%)	140 (96%)	6 (4%)	37	71
2	C	146/146 (100%)	140 (96%)	6 (4%)	37	71
2	D	146/146 (100%)	140 (96%)	6 (4%)	37	71
2	E	146/146 (100%)	137 (94%)	9 (6%)	23	60
2	F	146/146 (100%)	138 (94%)	8 (6%)	27	63
2	G	146/146 (100%)	138 (94%)	8 (6%)	27	63
2	H	146/146 (100%)	138 (94%)	8 (6%)	27	63
2	I	146/146 (100%)	135 (92%)	11 (8%)	17	53
2	J	146/146 (100%)	142 (97%)	4 (3%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	146/146 (100%)	135 (92%)	11 (8%)	17	53
2	L	146/146 (100%)	133 (91%)	13 (9%)	12	44
3	a	94/94 (100%)	89 (95%)	5 (5%)	28	64
3	b	94/94 (100%)	91 (97%)	3 (3%)	46	76
3	c	94/94 (100%)	90 (96%)	4 (4%)	35	70
3	d	94/94 (100%)	92 (98%)	2 (2%)	61	84
3	e	94/94 (100%)	93 (99%)	1 (1%)	80	91
3	f	94/94 (100%)	89 (95%)	5 (5%)	28	64
3	g	94/94 (100%)	91 (97%)	3 (3%)	46	76
3	h	94/94 (100%)	89 (95%)	5 (5%)	28	64
3	i	94/94 (100%)	87 (93%)	7 (7%)	17	54
3	j	94/94 (100%)	89 (95%)	5 (5%)	28	64
3	k	94/94 (100%)	91 (97%)	3 (3%)	46	76
3	l	94/94 (100%)	87 (93%)	7 (7%)	17	54
All	All	6876/6876 (100%)	6538 (95%)	338 (5%)	35	67

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	73	VAL
1	1	85	TYR
1	1	105	ARG
1	1	132	ASN
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	277	ARG
1	1	289	ARG
1	1	309	GLU
1	1	327	GLU
1	1	347	LYS
1	1	362	GLU
1	1	370	LEU
1	1	386	LEU

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Mol	Chain	Res	Type
1	1	390	TYR
1	1	412	ARG
1	1	443	VAL
1	1	454	TRP
1	2	71	PRO
1	2	244	VAL
1	2	263	LYS
1	2	268	ILE
1	2	271	ARG
1	2	272	ARG
1	2	292	ARG
1	2	322	ILE
1	2	347	LYS
1	2	349	HIS
1	2	366	LEU
1	2	408	PHE
1	2	452	ILE
1	2	453	LYS
1	3	119	ARG
1	3	136	LYS
1	3	164	ARG
1	3	221	ILE
1	3	239	LYS
1	3	268	ILE
1	3	276	VAL
1	3	287	GLN
1	3	288	GLU
1	3	312	GLN
1	3	347	LYS
1	3	364	GLU
1	3	393	ARG
1	3	412	ARG
1	3	455	THR
1	4	81	LEU
1	4	82	ILE
1	4	93	HIS
1	4	103	MET
1	4	136	LYS
1	4	263	LYS
1	4	268	ILE
1	4	270	ILE
1	4	281	LEU

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Mol	Chain	Res	Type
1	4	289	ARG
1	4	292	ARG
1	4	347	LYS
1	4	349	HIS
1	4	368	MET
1	4	372	ASP
1	4	393	ARG
1	4	408	PHE
1	4	415	THR
1	4	444	GLN
1	M	73	VAL
1	M	104	GLU
1	M	140	ARG
1	M	164	ARG
1	M	263	LYS
1	M	268	ILE
1	M	272	ARG
1	M	277	ARG
1	M	312	GLN
1	M	327	GLU
1	M	347	LYS
1	M	358	PHE
1	M	368	MET
1	N	74	LEU
1	N	104	GLU
1	N	136	LYS
1	N	140	ARG
1	N	166	LEU
1	N	263	LYS
1	N	272	ARG
1	N	287	GLN
1	N	289	ARG
1	N	312	GLN
1	N	347	LYS
1	N	358	PHE
1	N	393	ARG
1	N	408	PHE
1	N	415	THR
1	N	444	GLN
1	N	447	ILE
1	O	74	LEU
1	O	83	ASN

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Mol	Chain	Res	Type
1	O	84	TYR
1	O	140	ARG
1	O	245	ASN
1	O	263	LYS
1	O	272	ARG
1	O	275	ARG
1	O	312	GLN
1	O	327	GLU
1	O	347	LYS
1	O	372	ASP
1	O	382	THR
1	O	401	LEU
1	O	412	ARG
1	P	72	ARG
1	P	82	ILE
1	P	140	ARG
1	P	263	LYS
1	P	276	VAL
1	P	312	GLN
1	P	347	LYS
1	P	372	ASP
1	P	375	LEU
1	P	386	LEU
1	P	408	PHE
1	P	412	ARG
1	P	444	GLN
1	P	449	LEU
1	Q	92	THR
1	Q	114	ILE
1	Q	239	LYS
1	Q	263	LYS
1	Q	268	ILE
1	Q	277	ARG
1	Q	347	LYS
1	Q	364	GLU
1	Q	367	LEU
1	Q	371	LYS
1	R	70	ASP
1	R	72	ARG
1	R	79	PRO
1	R	80	TYR
1	R	81	LEU

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Mol	Chain	Res	Type
1	R	97	TRP
1	R	109	GLN
1	R	140	ARG
1	R	166	LEU
1	R	239	LYS
1	R	263	LYS
1	R	268	ILE
1	R	272	ARG
1	R	276	VAL
1	R	347	LYS
1	R	364	GLU
1	R	367	LEU
1	R	450	LYS
1	R	453	LYS
1	S	140	ARG
1	S	166	LEU
1	S	263	LYS
1	S	268	ILE
1	S	271	ARG
1	S	272	ARG
1	S	278	VAL
1	S	342	MET
1	S	347	LYS
1	S	349	HIS
1	S	356	LEU
1	S	412	ARG
1	S	436	MET
1	T	74	LEU
1	T	81	LEU
1	T	84	TYR
1	T	89	HIS
1	T	140	ARG
1	T	166	LEU
1	T	239	LYS
1	T	263	LYS
1	T	268	ILE
1	T	312	GLN
1	T	347	LYS
1	T	371	LYS
1	T	408	PHE
1	T	453	LYS
1	T	454	TRP

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Mol	Chain	Res	Type
2	A	47	ASP
2	A	53	ARG
2	A	60	ARG
2	A	70	LYS
2	A	79	ARG
2	A	98	LEU
2	A	110	PHE
2	A	156	LEU
2	A	173	TRP
2	A	200	LEU
2	A	208	LYS
2	A	209	ASP
3	a	89	ARG
3	a	90	PHE
3	a	119	THR
3	a	158	GLU
3	a	166	LYS
2	B	46	ILE
2	B	70	LYS
2	B	155	TRP
2	B	164	LYS
2	B	171	LYS
2	B	175	TYR
3	b	57	LYS
3	b	89	ARG
3	b	91	LYS
2	C	42	LEU
2	C	66	TRP
2	C	79	ARG
2	C	80	LYS
2	C	90	LEU
2	C	175	TYR
3	c	71	ASP
3	c	82	LYS
3	c	90	PHE
3	c	129	LEU
2	D	45	ASP
2	D	46	ILE
2	D	60	ARG
2	D	135	LYS
2	D	198	LEU
2	D	200	LEU

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Mol	Chain	Res	Type
3	d	91	LYS
3	d	166	LYS
2	E	46	ILE
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	77	ILE
2	F	45	ASP
2	F	90	LEU
2	F	97	ARG
2	F	106	LEU
2	F	116	LYS
2	F	171	LYS
2	F	203	LEU
2	F	208	LYS
3	f	63	LEU
3	f	72	VAL
3	f	82	LYS
3	f	91	LYS
3	f	147	LYS
2	G	46	ILE
2	G	60	ARG
2	G	79	ARG
2	G	84	LEU
2	G	97	ARG
2	G	140	LEU
2	G	173	TRP
2	G	175	TYR
3	g	91	LYS
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	127	PHE

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Mol	Chain	Res	Type
2	H	136	LEU
2	H	177	HIS
3	h	73	MET
3	h	74	LYS
3	h	91	LYS
3	h	119	THR
3	h	158	GLU
2	I	75	LEU
2	I	97	ARG
2	I	115	ASP
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	174	VAL
2	I	208	LYS
3	i	89	ARG
3	i	90	PHE
3	i	91	LYS
3	i	92	THR
3	i	107	GLU
3	i	134	VAL
3	i	154	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	160	LYS
2	K	46	ILE
2	K	58	ASN
2	K	62	LEU
2	K	70	LYS
2	K	75	LEU
2	K	86	HIS
2	K	108	GLU
2	K	109	PHE

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Mol	Chain	Res	Type
2	K	132	LEU
2	K	180	VAL
2	K	203	LEU
3	k	89	ARG
3	k	91	LYS
3	k	163	GLU
2	L	46	ILE
2	L	54	ARG
2	L	62	LEU
2	L	70	LYS
2	L	84	LEU
2	L	116	LYS
2	L	117	PRO
2	L	132	LEU
2	L	165	ARG
2	L	169	THR
2	L	171	LYS
2	L	195	LYS
2	L	208	LYS
3	l	63	LEU
3	l	91	LYS
3	l	99	ILE
3	l	132	PRO
3	l	135	LYS
3	l	140	MET
3	l	150	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	89	HIS
1	1	132	ASN
1	1	148	HIS
1	1	156	HIS
1	1	355	ASN
1	1	429	HIS
1	2	132	ASN
1	2	206	ASN
1	2	348	HIS
1	3	156	HIS
1	3	207	ASN
1	3	230	HIS

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Mol	Chain	Res	Type
1	3	287	GLN
1	3	349	HIS
1	3	429	HIS
1	4	93	HIS
1	4	132	ASN
1	4	148	HIS
1	4	257	HIS
1	4	403	HIS
1	4	429	HIS
1	M	156	HIS
1	N	230	HIS
1	N	349	HIS
1	O	148	HIS
1	O	230	HIS
1	O	349	HIS
1	P	132	ASN
1	P	156	HIS
1	P	355	ASN
1	P	457	HIS
1	Q	89	HIS
1	Q	108	GLN
1	Q	257	HIS
1	Q	403	HIS
1	R	83	ASN
1	R	109	GLN
1	R	132	ASN
1	R	230	HIS
1	R	282	GLN
1	R	312	GLN
1	S	132	ASN
1	S	349	HIS
1	S	444	GLN
2	A	183	HIS
2	B	58	ASN
2	B	148	GLN
3	c	78	GLN
3	c	137	HIS
3	c	157	GLN
3	e	137	HIS
3	e	157	GLN
2	F	71	GLN
2	F	151	ASN

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Mol	Chain	Res	Type
2	G	151	ASN
3	g	137	HIS
2	H	172	ASN
2	H	177	HIS
2	I	172	ASN
3	i	122	ASN
3	j	122	ASN
2	K	177	HIS
2	L	63	ASN
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 carbohydrates 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.