



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:11 PM BST

PDB ID : 5A5T
EMDB ID: : EMD-3056
Title : Structure of mammalian eIF3 in the context of the 43S preinitiation complex
Authors : des-Georges, A.; Dhote, V.; Kuhn, L.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.; Hashem, Y.
Deposited on : 2015-06-21
Resolution : 6.00 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) : trunk27241

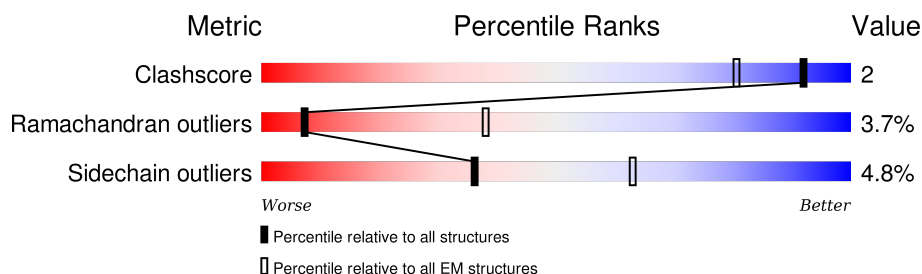
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	A	1362	38% 5% • 56%
2	C	843	57% 7% • 34%
3	E	445	78% 13% • • 6%
4	F	364	65% 9% • 25%
5	H	352	78% 12% • • 8%
6	K	218	93% 6% •
7	L	564	57% 7% • 34%
8	M	374	84% 12% • •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25432 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 EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	1
			4935	3107	893	914	21		

- Molecule 2 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	558	Total	C	N	O	S	0	1
			4529	2842	805	849	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	577	TYR	ALA	CONFLICT	UNP G1U971

- Molecule 3 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT E.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	420	Total	C	N	O	S	0	1
			3466	2220	587	639	20		

- Molecule 4 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

- Molecule 5 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT H.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 6 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT K.

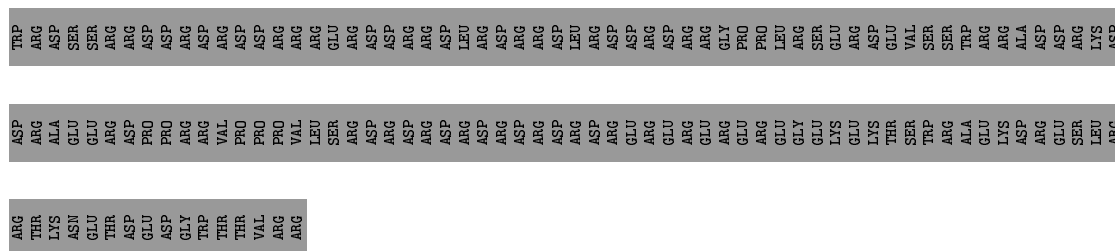
Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	216	Total	C	N	O	S	0	1
			1738	1109	286	330	13		

- Molecule 7 is a protein called UNCHARACTERIZED PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	373	Total	C	N	O	S	0	1
			3110	2010	520	563	17		

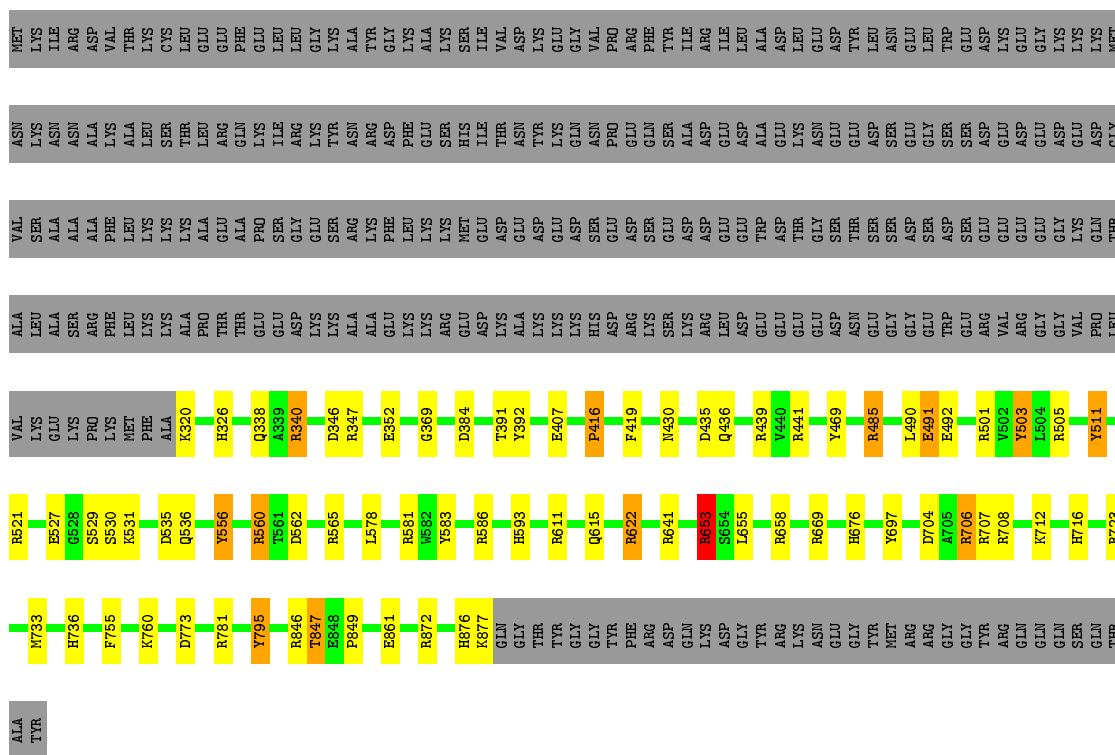
- Molecule 8 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT M.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	366	Total	C	N	O	S	0	1
			2919	1850	494	558	17		



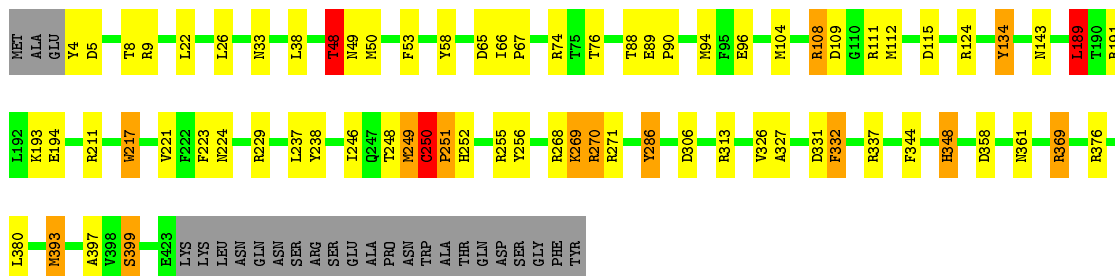
● Molecule 2: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT C

Chain C:  57% 7% 34%



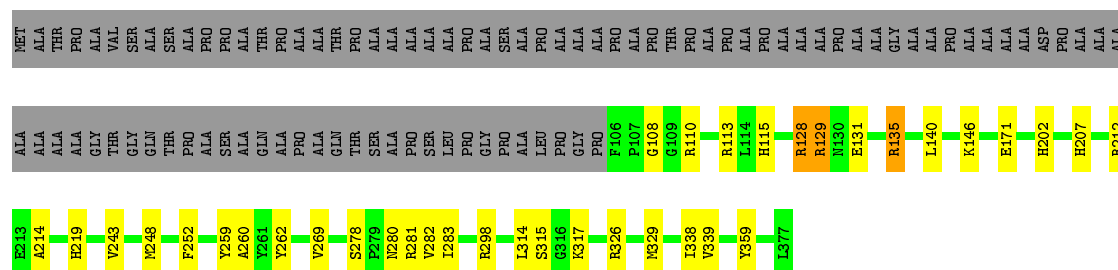
● Molecule 3: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT E

Chain E:  78% 13% • • 6%



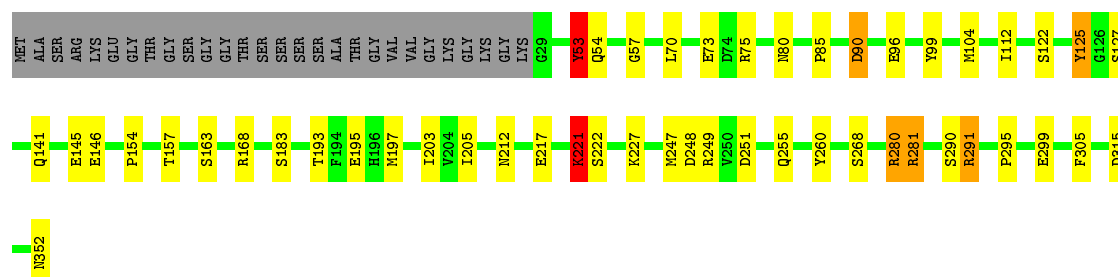
• Molecule 4: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT F

Chain F: 



• Molecule 5: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT H

Chain H: 78% 12% 8%



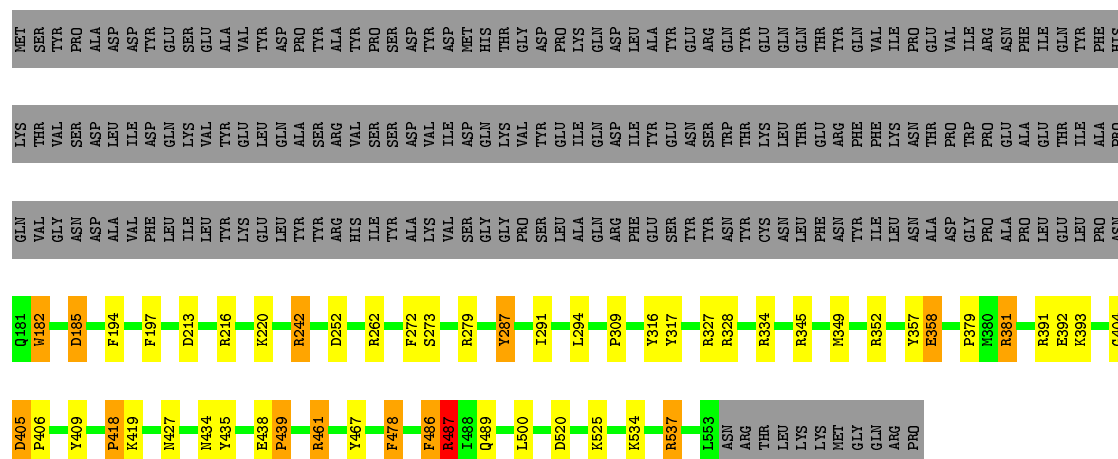
• Molecule 6: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT K

Chain K: 93% 6%



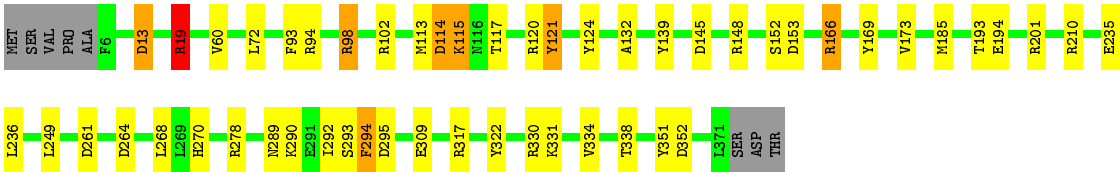
• Molecule 7: UNCHARACTERIZED PROTEIN

Chain L: 57% 7% 34%



• Molecule 8: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT M

Chain M: 84% 12% 2%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (4K X 4K)	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	A	0.70	0/5021	1.22	40/6781 (0.6%)
2	C	0.70	0/4608	1.19	35/6219 (0.6%)
3	E	1.61	8/3539 (0.2%)	1.29	43/4788 (0.9%)
4	F	0.69	0/2149	1.23	14/2920 (0.5%)
5	H	0.71	0/2675	1.09	7/3609 (0.2%)
6	K	0.69	0/1773	1.09	5/2398 (0.2%)
7	L	0.74	0/3186	1.18	28/4298 (0.7%)
8	M	0.70	0/2964	1.20	19/4000 (0.5%)
All	All	0.88	8/25915 (0.0%)	1.20	191/35013 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	22
2	C	1	18
3	E	1	11
4	F	0	6
5	H	1	8
6	K	0	4
7	L	2	12
8	M	1	13
All	All	6	94

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	189	LEU	CB-CG	53.28	3.07	1.52
3	E	217	TRP	CD2-CE3	30.41	1.85	1.40
3	E	217	TRP	CD2-CE2	30.28	1.77	1.41
3	E	217	TRP	CE2-CZ2	28.28	1.87	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	217	TRP	CE3-CZ3	22.94	1.77	1.38
3	E	217	TRP	CZ3-CH2	22.09	1.75	1.40
3	E	217	TRP	CZ2-CH2	22.06	1.79	1.37
3	E	251	PRO	C-N	14.84	1.68	1.34

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	128	ARG	NE-CZ-NH1	14.34	127.47	120.30
3	E	251	PRO	CA-C-N	-13.42	87.67	117.20
3	E	251	PRO	C-N-CA	11.49	150.42	121.70
3	E	251	PRO	CA-C-O	11.39	147.53	120.20
3	E	189	LEU	CB-CG-CD1	11.26	130.14	111.00
1	A	74	TYR	CB-CG-CD2	-10.24	114.85	121.00
3	E	189	LEU	CB-CG-CD2	9.90	127.83	111.00
1	A	74	TYR	CB-CG-CD1	9.82	126.89	121.00
2	C	503	TYR	CB-CG-CD2	-9.57	115.26	121.00
4	F	128	ARG	NE-CZ-NH2	-9.42	115.59	120.30
2	C	441	ARG	NE-CZ-NH1	9.12	124.86	120.30
3	E	369	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	62	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	C	872	ARG	NE-CZ-NH1	8.89	124.74	120.30
8	M	210	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	353	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	335	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	335	ARG	NE-CZ-NH1	8.40	124.50	120.30
4	F	212	ARG	NE-CZ-NH1	8.39	124.50	120.30
3	E	256	TYR	CB-CG-CD2	-8.39	115.97	121.00
4	F	259	TYR	CB-CG-CD2	-8.31	116.01	121.00
5	H	168	ARG	NE-CZ-NH1	8.31	124.45	120.30
2	C	795	TYR	CB-CG-CD1	8.21	125.93	121.00
2	C	795	TYR	CB-CG-CD2	-8.20	116.08	121.00
6	K	54	TYR	CB-CG-CD2	-8.12	116.12	121.00
1	A	190	ARG	NE-CZ-NH1	8.11	124.35	120.30
3	E	256	TYR	CB-CG-CD1	8.06	125.84	121.00
1	A	578	ARG	NE-CZ-NH2	-8.01	116.29	120.30
8	M	98	ARG	NE-CZ-NH2	-7.93	116.33	120.30
3	E	250	CYS	CA-C-O	-7.89	103.52	120.10
3	E	250	CYS	O-C-N	-7.82	106.24	121.10
8	M	98	ARG	NE-CZ-NH1	7.59	124.10	120.30
3	E	189	LEU	CA-CB-CG	7.54	132.64	115.30
7	L	279	ARG	NE-CZ-NH1	7.51	124.05	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	706	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	239	SER	N-CA-CB	7.43	121.65	110.50
2	C	505	ARG	NE-CZ-NH1	7.33	123.97	120.30
2	C	503	TYR	CB-CG-CD1	7.22	125.33	121.00
4	F	259	TYR	CB-CG-CD1	7.22	125.33	121.00
8	M	330	ARG	NE-CZ-NH1	7.21	123.91	120.30
2	C	391	THR	C-N-CA	7.20	139.70	121.70
7	L	381	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	172	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	158	ARG	NE-CZ-NH1	7.15	123.88	120.30
2	C	653	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	C	511	TYR	CB-CG-CD2	-7.12	116.72	121.00
3	E	268	ARG	C-N-CA	7.11	139.47	121.70
7	L	328	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	304	ARG	NE-CZ-NH2	-7.10	116.75	120.30
7	L	279	ARG	NE-CZ-NH2	-7.05	116.77	120.30
8	M	330	ARG	NE-CZ-NH2	-7.05	116.77	120.30
3	E	313	ARG	NE-CZ-NH1	6.99	123.80	120.30
6	K	54	TYR	CB-CG-CD1	6.97	125.18	121.00
7	L	216	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	C	581	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	195	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	157	TYR	CB-CG-CD2	-6.87	116.88	121.00
2	C	511	TYR	CB-CG-CD1	6.83	125.10	121.00
4	F	129	ARG	NE-CZ-NH1	6.79	123.69	120.30
3	E	332	PHE	CB-CG-CD1	6.78	125.55	120.80
2	C	847	THR	O-C-N	-6.78	111.85	122.70
1	A	469	ARG	NE-CZ-NH1	6.76	123.68	120.30
4	F	252	PHE	CB-CG-CD1	6.68	125.48	120.80
2	C	847	THR	C-N-CA	6.67	138.37	121.70
3	E	217	TRP	CG-CD1-NE1	6.67	116.77	110.10
7	L	185	ASP	CB-CG-OD1	6.65	124.29	118.30
3	E	211	ARG	NE-CZ-NH1	6.65	123.62	120.30
2	C	622	ARG	NE-CZ-NH2	-6.64	116.98	120.30
8	M	120	ARG	NE-CZ-NH1	6.62	123.61	120.30
7	L	391	ARG	NE-CZ-NH1	6.61	123.60	120.30
7	L	316	TYR	CB-CG-CD2	-6.59	117.05	121.00
3	E	143	ASN	C-N-CA	6.54	138.04	121.70
1	A	367	ARG	NE-CZ-NH1	6.53	123.57	120.30
8	M	124	TYR	CB-CG-CD2	-6.53	117.08	121.00
4	F	262	TYR	CB-CG-CD2	-6.52	117.09	121.00
3	E	108	ARG	NE-CZ-NH1	6.52	123.56	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	332	PHE	CB-CG-CD2	-6.45	116.29	120.80
1	A	202	ARG	NE-CZ-NH2	-6.39	117.11	120.30
4	F	110	ARG	NE-CZ-NH1	6.37	123.48	120.30
8	M	294	PHE	CB-CG-CD2	-6.34	116.36	120.80
2	C	586	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	E	337	ARG	NE-CZ-NH1	6.33	123.47	120.30
2	C	658	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	406	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	298	ARG	NE-CZ-NH1	6.28	123.44	120.30
7	L	478	PHE	CB-CG-CD1	6.28	125.19	120.80
5	H	53	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	62	ARG	NE-CZ-NH2	-6.26	117.17	120.30
7	L	327	ARG	NE-CZ-NH1	6.25	123.43	120.30
7	L	316	TYR	CB-CG-CD1	6.23	124.74	121.00
3	E	271	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	157	TYR	CB-CG-CD1	6.22	124.73	121.00
1	A	502	ARG	NE-CZ-NH1	6.15	123.37	120.30
7	L	357	TYR	CB-CG-CD2	-6.15	117.31	121.00
4	F	135	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	275	TYR	CB-CG-CD2	-6.12	117.33	121.00
3	E	268	ARG	O-C-N	-6.05	113.01	122.70
4	F	359	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	143	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	91	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	C	622	ARG	NE-CZ-NH1	6.00	123.30	120.30
3	E	143	ASN	O-C-N	-5.99	113.12	122.70
1	A	194	PHE	CB-CG-CD1	5.98	124.99	120.80
4	F	252	PHE	CB-CG-CD2	-5.98	116.61	120.80
7	L	478	PHE	CB-CG-CD2	-5.97	116.62	120.80
3	E	313	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	C	501	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	260	PHE	CB-CG-CD1	5.90	124.93	120.80
3	E	229	ARG	NE-CZ-NH2	-5.89	117.35	120.30
6	K	20	ARG	NE-CZ-NH1	5.89	123.25	120.30
3	E	217	TRP	CE2-CD2-CG	-5.89	102.59	107.30
8	M	322	TYR	CB-CG-CD2	-5.89	117.47	121.00
7	L	194	PHE	CB-CG-CD1	5.88	124.91	120.80
1	A	194	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	A	489	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	260	PHE	CB-CG-CD2	-5.82	116.72	120.80
2	C	755	PHE	CB-CG-CD1	5.82	124.88	120.80
1	A	438	ARG	NE-CZ-NH1	5.82	123.21	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	C	340	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	C	669	ARG	NE-CZ-NH2	-5.75	117.42	120.30
8	M	19	ARG	NE-CZ-NH1	5.71	123.16	120.30
7	L	461	ARG	NE-CZ-NH1	5.71	123.15	120.30
3	E	223	PHE	CB-CG-CD1	5.68	124.78	120.80
5	H	197	MET	CG-SD-CE	-5.68	91.12	100.20
7	L	272	PHE	CB-CG-CD1	5.65	124.75	120.80
7	L	334	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	C	755	PHE	CB-CG-CD2	-5.64	116.86	120.80
1	A	376	ARG	NE-CZ-NH1	5.63	123.11	120.30
7	L	379	PRO	C-N-CA	5.63	135.78	121.70
3	E	191	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	C	641	ARG	NE-CZ-NH2	-5.59	117.50	120.30
8	M	201	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	C	441	ARG	NE-CZ-NH2	-5.57	117.51	120.30
3	E	223	PHE	CB-CG-CD2	-5.55	116.91	120.80
8	M	114	ASP	N-CA-CB	-5.55	100.61	110.60
2	C	521	ARG	NE-CZ-NH1	5.54	123.07	120.30
6	K	8	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	C	723	ARG	NE-CZ-NH1	5.50	123.05	120.30
3	E	58	TYR	CB-CG-CD2	-5.49	117.70	121.00
3	E	189	LEU	CD1-CG-CD2	-5.46	94.11	110.50
3	E	9	ARG	NE-CZ-NH2	-5.46	117.57	120.30
3	E	53	PHE	CB-CG-CD2	-5.44	116.99	120.80
7	L	486	PHE	C-N-CA	5.44	135.30	121.70
3	E	9	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	571	ARG	NE-CZ-NH1	5.38	122.99	120.30
5	H	221	LYS	C-N-CA	5.36	135.10	121.70
6	K	155	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	E	399	SER	N-CA-CB	5.35	118.52	110.50
2	C	669	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	C	847	THR	CA-C-N	5.33	128.92	117.20
7	L	272	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	A	182	PHE	CB-CG-CD1	5.32	124.53	120.80
3	E	53	PHE	CB-CG-CD1	5.32	124.52	120.80
2	C	560	ARG	NE-CZ-NH2	-5.30	117.65	120.30
7	L	194	PHE	CB-CG-CD2	-5.30	117.09	120.80
8	M	148	ARG	NE-CZ-NH1	5.29	122.95	120.30
7	L	537	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	275	TYR	CB-CG-CD1	5.26	124.16	121.00
7	L	197	PHE	CB-CG-CD2	-5.26	117.12	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	124	ARG	NE-CZ-NH1	5.25	122.92	120.30
7	L	197	PHE	CB-CG-CD1	5.24	124.47	120.80
7	L	328	ARG	NE-CZ-NH2	-5.22	117.69	120.30
3	E	74	ARG	NE-CZ-NH1	5.22	122.91	120.30
8	M	322	TYR	CB-CG-CD1	5.22	124.13	121.00
8	M	115	LYS	C-N-CA	5.21	134.73	121.70
8	M	317	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	C	435	ASP	N-CA-CB	5.19	119.94	110.60
2	C	485	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	483	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	C	391	THR	O-C-N	-5.17	114.42	122.70
7	L	486	PHE	O-C-N	-5.17	114.42	122.70
8	M	166	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	427	TYR	CB-CG-CD2	-5.14	117.92	121.00
5	H	247	MET	CG-SD-CE	-5.12	92.01	100.20
2	C	490	LEU	C-N-CA	5.10	134.44	121.70
1	A	182	PHE	CB-CG-CD2	-5.09	117.24	120.80
8	M	124	TYR	CB-CG-CD1	5.09	124.05	121.00
8	M	294	PHE	CB-CG-CD1	5.06	124.34	120.80
1	A	489	ARG	NE-CZ-NH1	5.06	122.83	120.30
4	F	212	ARG	NE-CZ-NH2	-5.06	117.77	120.30
3	E	104	MET	CG-SD-CE	-5.06	92.11	100.20
5	H	53	TYR	CB-CG-CD1	5.05	124.03	121.00
3	E	211	ARG	NE-CZ-NH2	-5.04	117.78	120.30
3	E	48	THR	N-CA-CB	5.03	119.86	110.30
3	E	268	ARG	CA-C-N	5.03	128.26	117.20
7	L	409	TYR	CB-CG-CD2	-5.02	117.99	121.00
4	F	262	TYR	CB-CG-CD1	5.01	124.01	121.00
5	H	280	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	E	393	MET	CG-SD-CE	-5.01	92.18	100.20
7	L	487	ARG	NE-CZ-NH1	5.00	122.80	120.30

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	513	LYS	CA
3	E	67	PRO	CA
5	H	223	ALA	CA
7	L	418	PRO	CA
7	L	439	PRO	CA
8	M	115	LYS	CA

All (94) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	190	ARG	Sidechain
1	A	195	ARG	Sidechain
1	A	202	ARG	Sidechain
1	A	300	TYR	Sidechain
1	A	307	ARG	Sidechain
1	A	317	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	367	ARG	Sidechain
1	A	438	ARG	Sidechain
1	A	454	ARG	Sidechain
1	A	469	ARG	Sidechain
1	A	483	ARG	Sidechain
1	A	489	ARG	Sidechain
1	A	502	ARG	Sidechain
1	A	514	MET	Peptide
1	A	578	ARG	Sidechain
1	A	581	ARG	Sidechain
1	A	589	ARG	Sidechain
1	A	597	ARG	Sidechain
1	A	91	ARG	Sidechain
2	C	320	LYS	Peptide
2	C	347	ARG	Sidechain
2	C	439	ARG	Sidechain
2	C	469	TYR	Sidechain
2	C	485	ARG	Sidechain
2	C	503	TYR	Sidechain
2	C	531	LYS	Peptide
2	C	536	GLN	Peptide
2	C	556	TYR	Sidechain
2	C	565	ARG	Sidechain
2	C	583	TYR	Sidechain
2	C	611	ARG	Sidechain
2	C	622	ARG	Sidechain
2	C	653	ARG	Sidechain
2	C	697	TYR	Sidechain
2	C	708	ARG	Sidechain
2	C	781	ARG	Sidechain
2	C	846	ARG	Sidechain
3	E	108	ARG	Sidechain
3	E	250	CYS	Mainchain,Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	E	255	ARG	Sidechain
3	E	270	ARG	Sidechain
3	E	286	TYR	Sidechain
3	E	369	ARG	Sidechain
3	E	376	ARG	Sidechain
3	E	4	TYR	Sidechain
3	E	49	ASN	Peptide
3	E	66	ILE	Peptide
4	F	113	ARG	Sidechain
4	F	128	ARG	Sidechain,Peptide
4	F	135	ARG	Sidechain
4	F	298	ARG	Sidechain
4	F	326	ARG	Sidechain
5	H	122	SER	Peptide
5	H	125	TYR	Sidechain
5	H	249	ARG	Sidechain
5	H	281	ARG	Sidechain
5	H	290	SER	Peptide
5	H	291	ARG	Sidechain
5	H	75	ARG	Sidechain
5	H	99	TYR	Sidechain
6	K	100	ARG	Sidechain
6	K	139	ARG	Sidechain
6	K	8	ARG	Sidechain
6	K	97	ARG	Sidechain
7	L	242	ARG	Sidechain
7	L	262	ARG	Sidechain
7	L	287	TYR	Sidechain
7	L	317	TYR	Sidechain
7	L	345	ARG	Sidechain
7	L	352	ARG	Sidechain
7	L	405	ASP	Peptide
7	L	434	ASN	Peptide
7	L	438	GLU	Peptide
7	L	467	TYR	Sidechain
7	L	487	ARG	Peptide
7	L	537	ARG	Sidechain
8	M	102	ARG	Sidechain
8	M	114	ASP	Peptide
8	M	121	TYR	Sidechain
8	M	13	ASP	Peptide
8	M	166	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	M	169	TYR	Sidechain
8	M	19	ARG	Sidechain
8	M	249	LEU	Peptide
8	M	278	ARG	Sidechain
8	M	289	ASN	Peptide
8	M	351	TYR	Sidechain
8	M	94	ARG	Sidechain
8	M	98	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4935	0	5017	3	0
2	C	4529	0	4533	5	0
3	E	3466	0	3446	74	0
4	F	2111	0	2105	2	0
5	H	2624	0	2592	5	0
6	K	1738	0	1706	3	0
7	L	3110	0	3084	5	0
8	M	2919	0	2950	1	0
All	All	25432	0	25433	94	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 (94) 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)
3:E:217:TRP:CE3	3:E:217:TRP:CZ3	1.77	1.71
3:E:217:TRP:CH2	3:E:217:TRP:CZ3	1.75	1.62
3:E:217:TRP:CE2	3:E:217:TRP:CZ2	1.87	1.60
3:E:217:TRP:CH2	3:E:217:TRP:CZ2	1.79	1.59
3:E:217:TRP:CE3	3:E:217:TRP:CD2	1.86	1.59
3:E:217:TRP:CD2	3:E:217:TRP:CE2	1.77	1.52
3:E:189:LEU:HG	3:E:217:TRP:CD2	1.43	1.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:38:LEU:CD1	3:E:251:PRO:HD3	1.36	1.52
3:E:38:LEU:HD13	3:E:251:PRO:CD	1.43	1.46
3:E:251:PRO:C	3:E:252:HIS:N	1.68	1.45
3:E:189:LEU:HG	3:E:217:TRP:CE3	1.76	1.21
3:E:38:LEU:CD1	3:E:251:PRO:CD	2.10	1.18
3:E:189:LEU:CG	3:E:217:TRP:CE2	2.28	1.14
3:E:189:LEU:CB	3:E:217:TRP:CD2	2.30	1.13
3:E:189:LEU:CG	3:E:217:TRP:CD2	2.31	1.12
3:E:189:LEU:CB	3:E:217:TRP:CE2	2.31	1.12
3:E:189:LEU:CG	3:E:217:TRP:CE3	2.34	1.09
3:E:251:PRO:HB2	3:E:286:TYR:CE1	1.87	1.09
3:E:189:LEU:CG	3:E:217:TRP:CZ2	2.38	1.07
3:E:189:LEU:CG	3:E:217:TRP:CH2	2.38	1.06
3:E:251:PRO:N	3:E:252:HIS:H	1.53	1.06
3:E:189:LEU:CB	3:E:217:TRP:CZ2	2.39	1.06
3:E:189:LEU:CG	3:E:217:TRP:CZ3	2.41	1.03
3:E:251:PRO:CA	3:E:252:HIS:N	2.21	1.03
3:E:189:LEU:CB	3:E:217:TRP:CE3	2.42	1.02
3:E:189:LEU:CB	3:E:217:TRP:CZ3	2.43	1.01
3:E:189:LEU:CB	3:E:217:TRP:CH2	2.45	0.98
3:E:251:PRO:CD	3:E:252:HIS:H	1.77	0.96
3:E:251:PRO:HD2	3:E:252:HIS:HB2	1.43	0.95
3:E:189:LEU:HG	3:E:217:TRP:CE2	2.04	0.92
3:E:189:LEU:HB2	3:E:217:TRP:CE3	2.05	0.92
3:E:251:PRO:N	3:E:252:HIS:N	2.18	0.92
3:E:189:LEU:HB3	3:E:217:TRP:CH2	2.06	0.89
3:E:251:PRO:CD	3:E:252:HIS:HB2	2.05	0.85
3:E:38:LEU:HD13	3:E:251:PRO:CG	2.07	0.85
3:E:38:LEU:HD11	3:E:251:PRO:CD	2.04	0.84
3:E:189:LEU:CD1	3:E:217:TRP:CZ3	2.63	0.81
3:E:251:PRO:HB2	3:E:286:TYR:CZ	2.14	0.81
3:E:189:LEU:CD2	3:E:217:TRP:CZ2	2.67	0.77
3:E:38:LEU:CD1	3:E:251:PRO:HD2	2.15	0.77
3:E:38:LEU:HD13	3:E:251:PRO:HD3	0.76	0.76
3:E:189:LEU:CA	3:E:217:TRP:CE2	2.69	0.75
3:E:251:PRO:CG	3:E:252:HIS:HB2	2.18	0.74
3:E:251:PRO:HD2	3:E:252:HIS:CB	2.17	0.74
3:E:251:PRO:CB	3:E:286:TYR:CE1	2.70	0.74
3:E:189:LEU:CD2	3:E:217:TRP:CE2	2.70	0.74
3:E:189:LEU:HB3	3:E:217:TRP:CZ3	2.24	0.73
3:E:251:PRO:CG	3:E:252:HIS:N	2.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:189:LEU:HB2	3:E:217:TRP:CD2	2.22	0.73
3:E:38:LEU:HD11	3:E:251:PRO:HD2	1.71	0.68
3:E:251:PRO:CG	3:E:252:HIS:H	2.07	0.67
3:E:251:PRO:HG2	3:E:252:HIS:HB2	1.78	0.66
3:E:251:PRO:HG2	3:E:252:HIS:N	2.10	0.64
3:E:189:LEU:HD22	3:E:217:TRP:CZ2	2.36	0.59
7:L:358:GLU:CD	7:L:358:GLU:H	2.04	0.58
3:E:251:PRO:HB2	3:E:286:TYR:HE1	1.63	0.58
3:E:189:LEU:HA	3:E:217:TRP:CE2	2.38	0.58
3:E:189:LEU:HD23	3:E:217:TRP:CE2	2.39	0.56
3:E:251:PRO:CB	3:E:286:TYR:CZ	2.88	0.54
5:H:227:LYS:HD2	5:H:227:LYS:H	1.72	0.54
3:E:251:PRO:HG2	3:E:252:HIS:CB	2.38	0.53
3:E:250:CYS:N	3:E:251:PRO:HA	2.26	0.51
3:E:189:LEU:CD1	3:E:217:TRP:CH2	2.94	0.50
6:K:217:SER:N	7:L:534:LYS:NZ	2.60	0.50
3:E:189:LEU:CD1	3:E:217:TRP:CE3	2.94	0.50
1:A:285:LYS:HG2	1:A:292:HIS:CD2	2.46	0.50
3:E:249:MET:SD	3:E:251:PRO:HB3	2.53	0.49
6:K:196:ILE:HG13	6:K:197:LYS:H	1.77	0.48
3:E:189:LEU:C	3:E:217:TRP:CZ2	2.86	0.48
3:E:38:LEU:HD13	3:E:251:PRO:HG3	1.94	0.48
4:F:207:HIS:HE1	4:F:219:HIS:CE1	2.31	0.48
5:H:195:GLU:CD	5:H:195:GLU:H	2.17	0.48
3:E:344:PHE:CE1	3:E:348:HIS:CE1	3.01	0.48
3:E:251:PRO:CB	3:E:252:HIS:N	2.77	0.47
6:K:217:SER:N	7:L:534:LYS:HZ3	2.12	0.47
3:E:251:PRO:HG2	3:E:252:HIS:CA	2.45	0.47
3:E:112:MET:HA	3:E:115:ASP:HB2	1.98	0.46
1:A:353:ARG:HH11	5:H:90:ASP:CG	2.19	0.46
2:C:733:MET:HA	2:C:736:HIS:CD2	2.52	0.44
2:C:340:ARG:HE	2:C:384:ASP:CG	2.21	0.44
2:C:527:GLU:H	2:C:527:GLU:CD	2.22	0.43
7:L:242:ARG:HA	7:L:427:ASN:HD21	1.83	0.43
3:E:189:LEU:CA	3:E:217:TRP:CZ2	3.01	0.43
2:C:369:GLY:HA3	2:C:419:PHE:CG	2.54	0.42
2:C:877:LYS:N	5:H:280:ARG:NH2	2.66	0.42
3:E:96:GLU:CD	3:E:96:GLU:H	2.22	0.42
3:E:251:PRO:CD	3:E:252:HIS:CB	2.87	0.42
3:E:189:LEU:HD13	3:E:217:TRP:CZ3	2.54	0.42
5:H:217:GLU:CD	5:H:221:LYS:HZ1	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:HIS:CD2	1:A:488:SER:H	2.39	0.41
4:F:207:HIS:CE1	4:F:219:HIS:CE1	3.09	0.40
8:M:309:GLU:CD	8:M:331:LYS:HZ1	2.24	0.40
3:E:111:ARG:HB3	3:E:134:TYR:CZ	2.56	0.40
7:L:381:ARG:HH22	7:L:520:ASP:CG	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/1362 (44%)	544 (91%)	36 (6%)	18 (3%)	5	42
2	C	556/843 (66%)	512 (92%)	28 (5%)	16 (3%)	6	43
3	E	418/445 (94%)	362 (87%)	37 (9%)	19 (4%)	3	33
4	F	270/364 (74%)	234 (87%)	20 (7%)	16 (6%)	2	26
5	H	322/352 (92%)	277 (86%)	29 (9%)	16 (5%)	3	30
6	K	214/218 (98%)	200 (94%)	12 (6%)	2 (1%)	21	66
7	L	371/564 (66%)	331 (89%)	26 (7%)	14 (4%)	4	37
8	M	364/374 (97%)	320 (88%)	30 (8%)	14 (4%)	4	37
All	All	3113/4522 (69%)	2780 (89%)	218 (7%)	115 (4%)	7	37

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	136	ASP
1	A	166	ASN
1	A	478	CYS
1	A	539	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	392	TYR
2	C	416	PRO
2	C	430	ASN
2	C	712	LYS
3	E	67	PRO
3	E	76	THR
3	E	246	ILE
3	E	399	SER
4	F	214	ALA
4	F	243	VAL
4	F	248	MET
4	F	339	VAL
5	H	154	PRO
5	H	183	SER
5	H	222	SER
7	L	273	SER
7	L	406	PRO
7	L	439	PRO
7	L	489	GLN
7	L	500	LEU
8	M	115	LYS
8	M	117	THR
8	M	268	LEU
8	M	290	LYS
8	M	334	VAL
1	A	21	VAL
1	A	163	LEU
1	A	188	TYR
1	A	311	THR
1	A	501	THR
2	C	326	HIS
2	C	530	SER
2	C	704	ASP
2	C	847	THR
3	E	26	LEU
3	E	88	THR
3	E	238	TYR
3	E	326	VAL
4	F	260	ALA
4	F	315	SER
4	F	338	ILE
5	H	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	H	127	SER
5	H	291	ARG
7	L	294	LEU
8	M	173	VAL
8	M	193	THR
8	M	194	GLU
8	M	292	ILE
8	M	338	THR
1	A	135	GLU
1	A	239	SER
2	C	346	ASP
2	C	529	SER
3	E	48	THR
3	E	50	MET
3	E	237	LEU
3	E	249	MET
3	E	269	LYS
3	E	327	ALA
3	E	397	ALA
4	F	129	ARG
4	F	146	LYS
4	F	314	LEU
4	F	317	LYS
5	H	53	TYR
5	H	57	GLY
5	H	125	TYR
5	H	205	ILE
5	H	305	PHE
7	L	404	GLY
7	L	435	TYR
7	L	486	PHE
8	M	113	MET
1	A	421	GLU
1	A	480	LEU
2	C	655	LEU
2	C	849	PRO
3	E	90	PRO
3	E	380	LEU
5	H	112	ILE
5	H	193	THR
7	L	418	PRO
7	L	487	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	65	HIS
2	C	491	GLU
2	C	653	ARG
3	E	22	LEU
3	E	221	VAL
4	F	131	GLU
4	F	280	ASN
7	L	349	MET
8	M	132	ALA
1	A	344	MET
2	C	707	ARG
5	H	203	ILE
6	K	201	ILE
7	L	182	TRP
8	M	236	LEU
4	F	278	SER
6	K	202	VAL
1	A	514	MET
2	C	436	GLN
4	F	108	GLY
8	M	60	VAL
5	H	295	PRO
5	H	85	PRO
7	L	291	ILE
1	A	417	GLN
4	F	282	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	551/1245 (44%)	528 (96%)	23 (4%)	36	70
2	C	503/750 (67%)	480 (95%)	23 (5%)	33	68
3	E	384/406 (95%)	361 (94%)	23 (6%)	24	61
4	F	239/282 (85%)	231 (97%)	8 (3%)	45	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	293/311 (94%)	270 (92%)	23 (8%)	16	52
6	K	190/193 (98%)	188 (99%)	2 (1%)	80	91
7	L	342/516 (66%)	325 (95%)	17 (5%)	30	66
8	M	327/335 (98%)	309 (94%)	18 (6%)	27	64
All	All	2829/4038 (70%)	2692 (95%)	137 (5%)	36	67

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	16	ASN
1	A	45	LYS
1	A	110	GLN
1	A	136	ASP
1	A	162	ASP
1	A	170	VAL
1	A	179	GLN
1	A	209	GLN
1	A	261	SER
1	A	300	TYR
1	A	309	ASN
1	A	323	LEU
1	A	335	ARG
1	A	372	ASN
1	A	397	GLU
1	A	419	GLU
1	A	420	LYS
1	A	434	ASN
1	A	521	ASN
1	A	546	LYS
1	A	583	GLU
1	A	593	GLU
2	C	338	GLN
2	C	352	GLU
2	C	407	GLU
2	C	416	PRO
2	C	491	GLU
2	C	492	GLU
2	C	511	TYR
2	C	535	ASP
2	C	556	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	560	ARG
2	C	562	ASP
2	C	578	LEU
2	C	593	HIS
2	C	615	GLN
2	C	653	ARG
2	C	676	HIS
2	C	706	ARG
2	C	716	HIS
2	C	760	LYS
2	C	773	ASP
2	C	795	TYR
2	C	861	GLU
2	C	876	HIS
3	E	5	ASP
3	E	8	THR
3	E	33	ASN
3	E	48	THR
3	E	65	ASP
3	E	89	GLU
3	E	94	MET
3	E	109	ASP
3	E	134	TYR
3	E	189	LEU
3	E	193	LYS
3	E	194	GLU
3	E	224	ASN
3	E	248	THR
3	E	269	LYS
3	E	270	ARG
3	E	306	ASP
3	E	331	ASP
3	E	332	PHE
3	E	348	HIS
3	E	358	ASP
3	E	361	ASN
3	E	393	MET
4	F	115	HIS
4	F	140	LEU
4	F	171	GLU
4	F	202	HIS
4	F	269	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	281	ARG
4	F	283	ILE
4	F	329	MET
5	H	53	TYR
5	H	70	LEU
5	H	73	GLU
5	H	80	ASN
5	H	90	ASP
5	H	96	GLU
5	H	104	MET
5	H	141	GLN
5	H	145	GLU
5	H	146	GLU
5	H	157	THR
5	H	163	SER
5	H	212	ASN
5	H	221	LYS
5	H	248	ASP
5	H	251	ASP
5	H	255	GLN
5	H	260	TYR
5	H	268	SER
5	H	281	ARG
5	H	299	GLU
5	H	315	ASP
5	H	352	ASN
6	K	34	GLU
6	K	183	GLU
7	L	182	TRP
7	L	185	ASP
7	L	213	ASP
7	L	220	LYS
7	L	252	ASP
7	L	287	TYR
7	L	309	PRO
7	L	358	GLU
7	L	392	GLU
7	L	393	LYS
7	L	405	ASP
7	L	418	PRO
7	L	419	LYS
7	L	439	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	L	461	ARG
7	L	478	PHE
7	L	525	LYS
8	M	13	ASP
8	M	19	ARG
8	M	72	LEU
8	M	93	PHE
8	M	121	TYR
8	M	139	TYR
8	M	145	ASP
8	M	152	SER
8	M	153	ASP
8	M	185	MET
8	M	235	GLU
8	M	261	ASP
8	M	264	ASP
8	M	270	HIS
8	M	293	SER
8	M	294	PHE
8	M	295	ASP
8	M	352	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	HIS
2	C	326	HIS
2	C	572	HIS
2	C	840	GLN
3	E	85	GLN
3	E	216	HIS
3	E	349	GLN
4	F	207	HIS
5	H	328	GLN
7	L	546	GLN
8	M	205	HIS
8	M	348	GLN

5.3.3 RNA ⓘ

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.