wwPDB EM Map/Model Validation Report (i)

Jul 6, 2016 – 08:53 PM EDT

PDB ID	:	3JD5
EMDB ID:	:	EMD-5941
Title	:	Cryo-EM structure of the small subunit of the mammalian mitochondrial ribosome
Authors	:	Kaushal, P.S.; Sharma, M.R.; Booth, T.M.; Haque, E.M.; Tung, C.S.; Sanbonmatsu, K.Y.; Spremulli, L.L.; Agrawal, R.K.
Deposited on	:	2016-04-08
Resolution	:	7.00 Å(reported)
Based on PDB ID	:	3J9M, 5AJ3

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

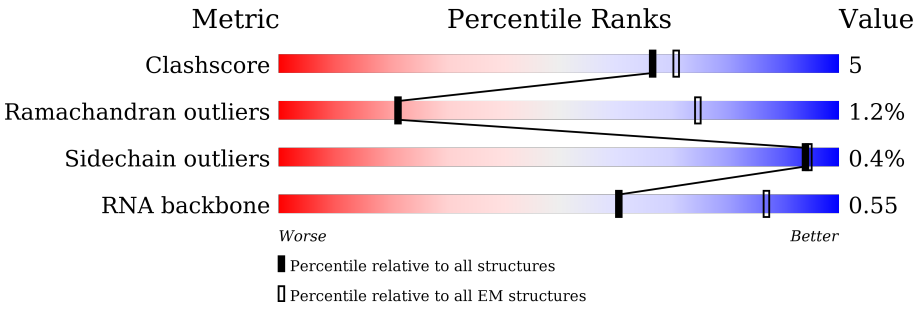
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.00 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
RNA backbone	3027	244

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	955	63% 33% •
2	B	293	65% 9% 26%
3	C	167	66% 13% 21%
4	E	430	65% 11% 24%
5	F	124	82% 16% •
6	G	242	78% 8% 14%
7	I	396	68% 10% 21%
8	J	201	50% 14% 36%

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Mol	Chain	Length	Quality of chain
9	K	197	56% 13% 31%
10	L	139	65% 12% 22%
11	N	128	62% 17% 21%
12	O	256	60% 7% 32%
13	P	135	74% 12% 14%
14	Q	130	74% 10% 16%
15	R	143	55% 13% 32%
16	U	87	90% 8%
17	a	359	80% 19%
18	b	190	69% 29%
19	c	173	96%
20	d	205	86% 14%
21	e	415	81% 17%
22	f	189	52% 48%
23	g	397	84% 15%
24	h	386	26% 73%
25	i	106	91% 8%
26	j	218	95%
27	k	325	83% 15%
28	m	118	100%
29	n	199	35% 64%
30	o	575	78% 20%
31	p	258	72% 28%
32	s	17	94% 6%
32	z	17	100%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 64319 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 RNA chain called 28S ribosomal RNA, mitochondial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	952	20256	9090	3685	6529	952	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	217	1726	1102	319	298	7	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	132	1072	692	197	179	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	328	2613	1634	494	474	11	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	124	991	627	179	179	6	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	208	1720	1093	313	301	13	0	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	311	Total	C	N	O	S	0	0
			2541	1608	454	467	12		

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	128	Total	C	N	O	S	0	0
			1049	676	180	190	3		

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	136	Total	C	N	O	S	0	0
			1001	628	193	177	3		

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	109	Total	C	N	O	S	0	0
			853	534	175	140	4		

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	101	Total	C	N	O	S	0	0
			861	538	178	140	5		

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	173	Total	C	N	O	S	0	0
			1421	904	258	250	9		

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	116	Total	C	N	O	S	0	0
			916	580	180	151	5		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	109	Total	C	N	O	S	0	0
			857	555	153	145	4		

- Molecule 15 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	97	Total	C	N	O	S	0	0
			788	507	136	138	7		

- Molecule 16 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	86	Total	C	N	O	S	0	0
			737	457	148	124	8		

- Molecule 17 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	289	Total	C	N	O	S	0	0
			2356	1505	400	443	8		

- Molecule 18 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	135	Total	C	N	O	S	0	0
			1108	717	195	194	2		

- Molecule 19 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	168	Total	C	N	O	S	0	0
			1374	878	246	241	9		

- Molecule 20 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	176	Total	C	N	O	S	0	0
			1463	899	290	272	2		

- Molecule 21 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	344	Total	C	N	O	S	0	0
			2822	1804	476	529	13		

- Molecule 22 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	f	98	Total	C	N	O	S	0	0
			775	493	135	143	4		

- Molecule 23 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	338	Total	C	N	O	S	0	0
			2754	1774	482	488	10		

- Molecule 24 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	h	103	Total	C	N	O	S	0	0
			871	566	141	161	3		

- Molecule 25 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	i	98	Total	C	N	O	S	0	0
			818	519	153	143	3		

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	213	Total	C	N	O	S	0	0
			1792	1132	346	309	5		

- Molecule 27 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	k	275	Total	C	N	O	S	0	0
			2227	1418	377	421	11		

- Molecule 28 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	m	118	Total	C	N	O	S	0	0
			945	587	185	164	9		

- Molecule 29 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	n	72	Total	C	N	O	S	0	0
			642	409	142	89	2		

- Molecule 30 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	o	461	Total	C	N	O	S	0	0
			3273	2082	573	605	13		

- Molecule 31 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	p	187	Total	C	N	O	S	0	0
			1531	968	288	267	8		

- Molecule 32 is a protein called unknown.

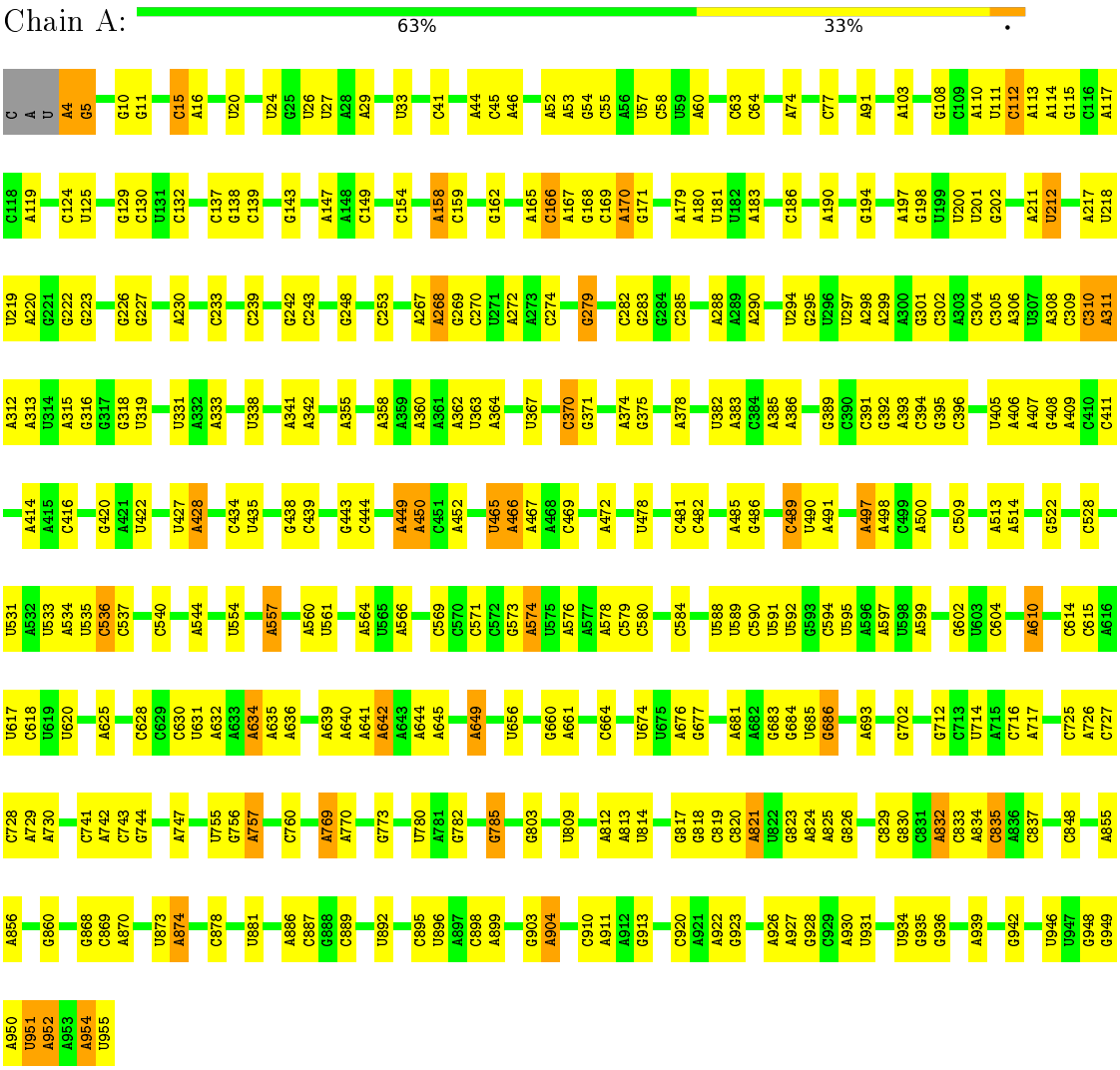
Mol	Chain	Residues	Atoms				AltConf	Trace
32	s	16	Total	C	N	O	0	0
			80	48	16	16		
32	z	17	Total	C	N	O	0	0
			86	51	17	18		

3 Residue-property plots (i)

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.

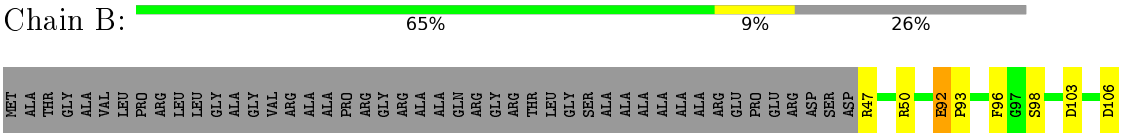
- Molecule 1: 28S ribosomal RNA, mitochondial

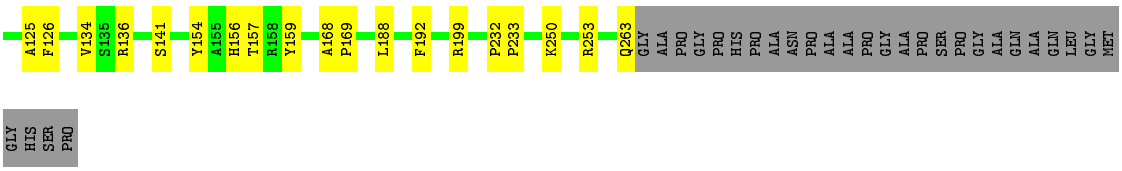
Chain A:



- Molecule 2: 28S ribosomal protein S2, mitochondrial

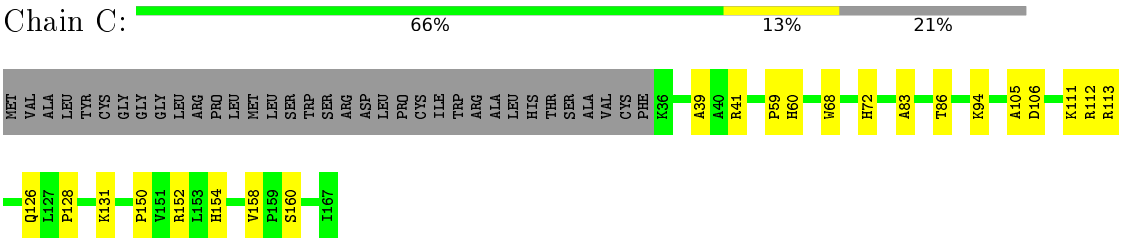
Chain B:





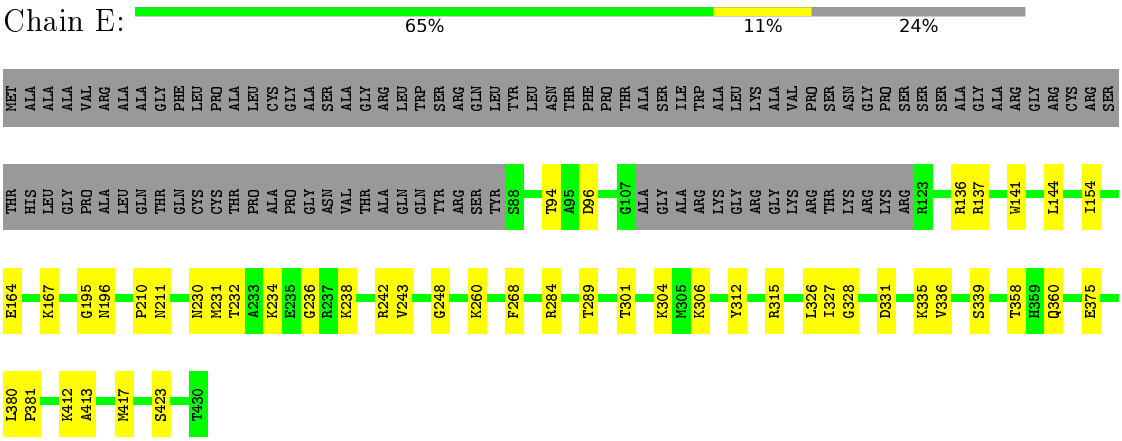
- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:



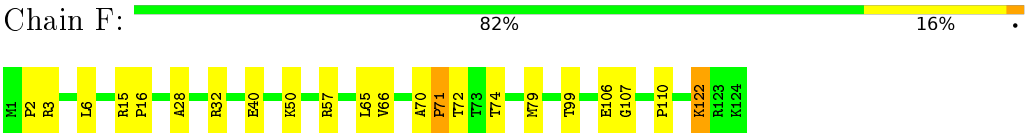
- Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain E:



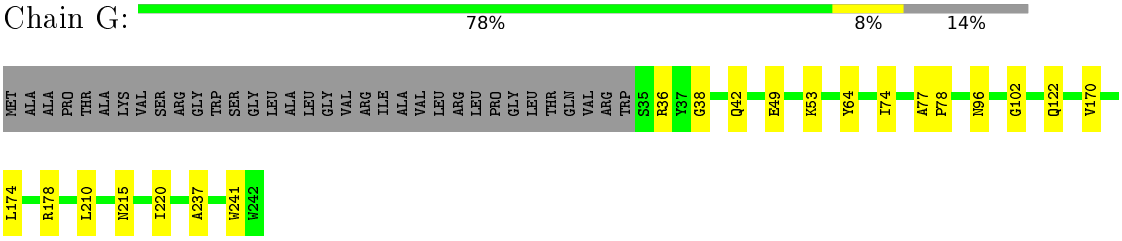
- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain F:



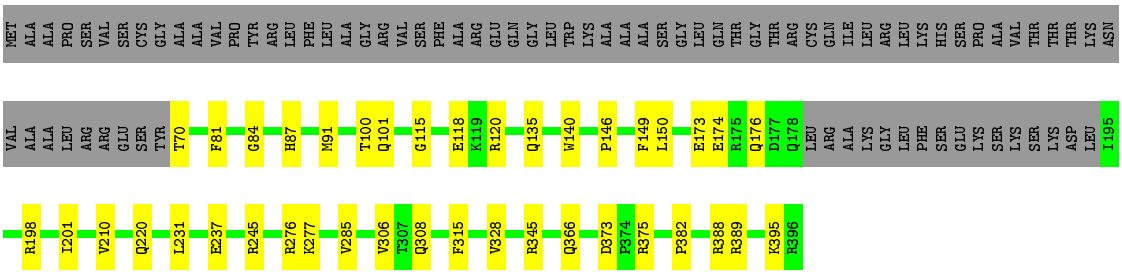
- Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain G:



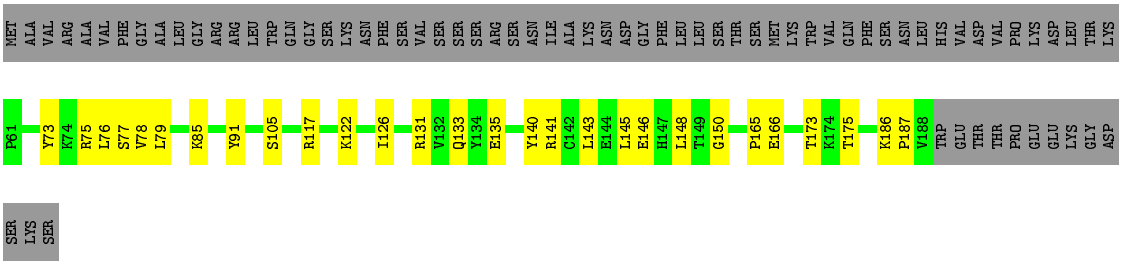
- Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain I:



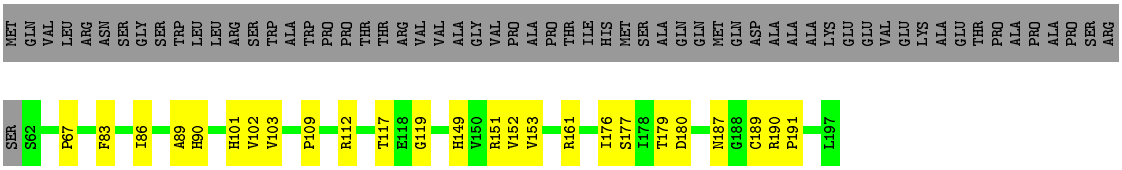
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain J:



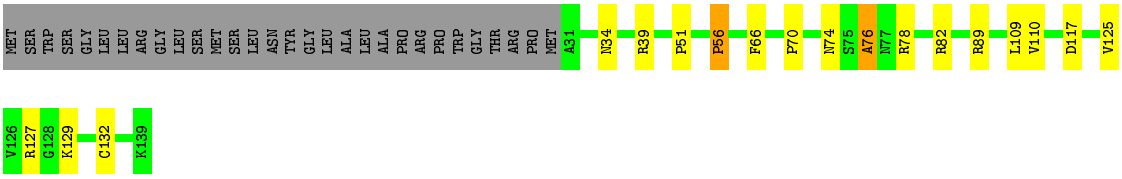
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain K:



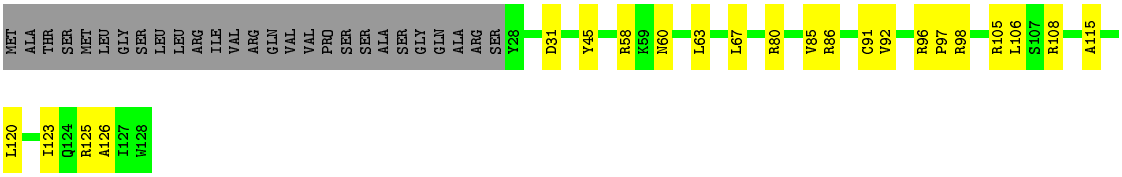
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain L:



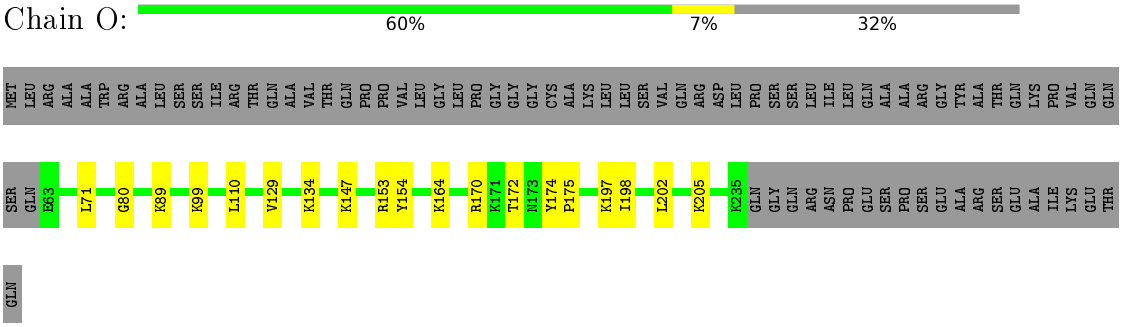
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain N:



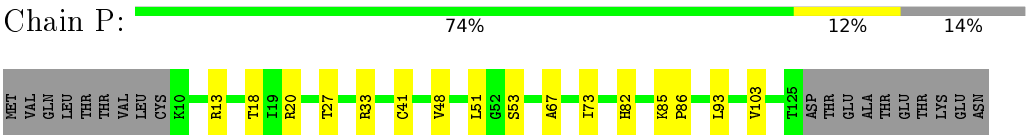
- Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain O:



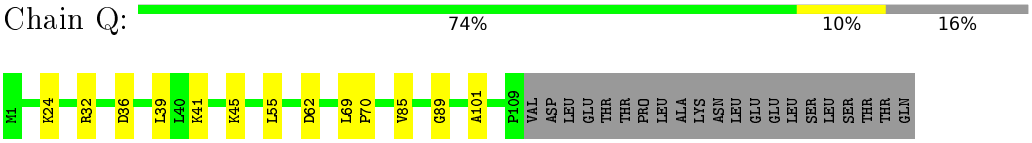
- Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain P:



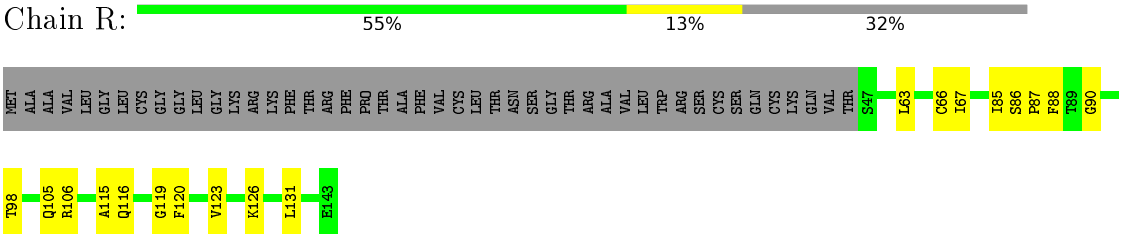
- Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain Q:



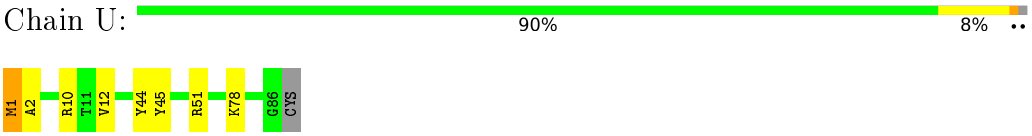
- Molecule 15: 28S ribosomal protein S18c, mitochondrial

Chain R:



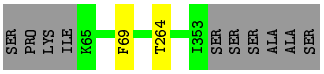
- Molecule 16: 28S ribosomal protein S21, mitochondrial

Chain U:



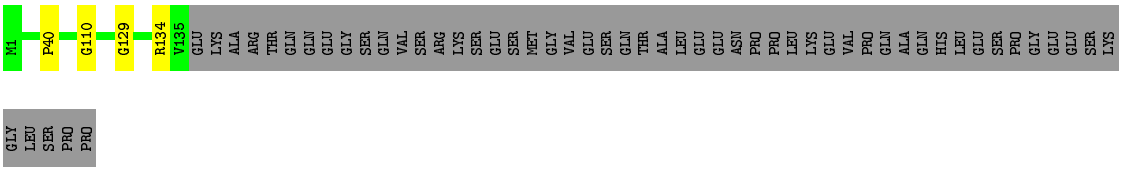
- Molecule 17: 28S ribosomal protein S22, mitochondrial

Chain a:



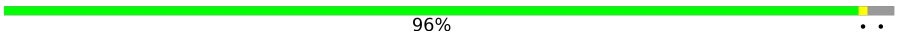
- Molecule 18: 28S ribosomal protein S23, mitochondrial

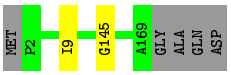
Chain b:



- Molecule 19: 28S ribosomal protein S25, mitochondrial

Chain c:



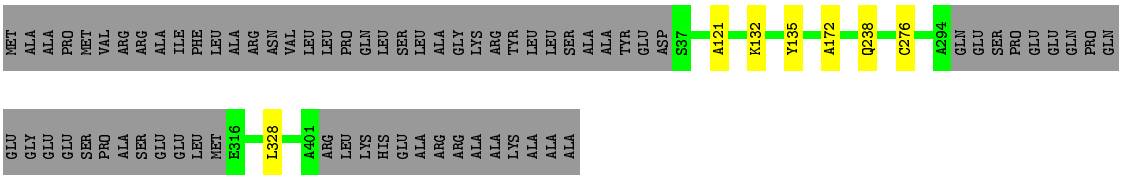


- Molecule 20: 28S ribosomal protein S26, mitochondrial

Chain d:

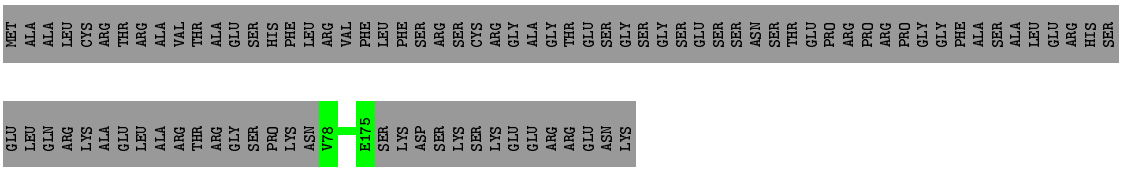
- Molecule 21: 28S ribosomal protein S27, mitochondrial

Chain e:



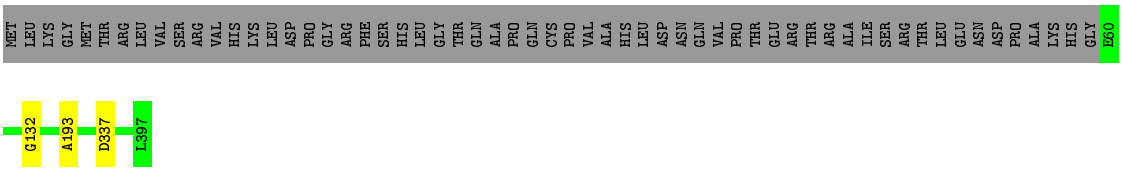
- Molecule 22: 28S ribosomal protein S28, mitochondrial

Chain f:



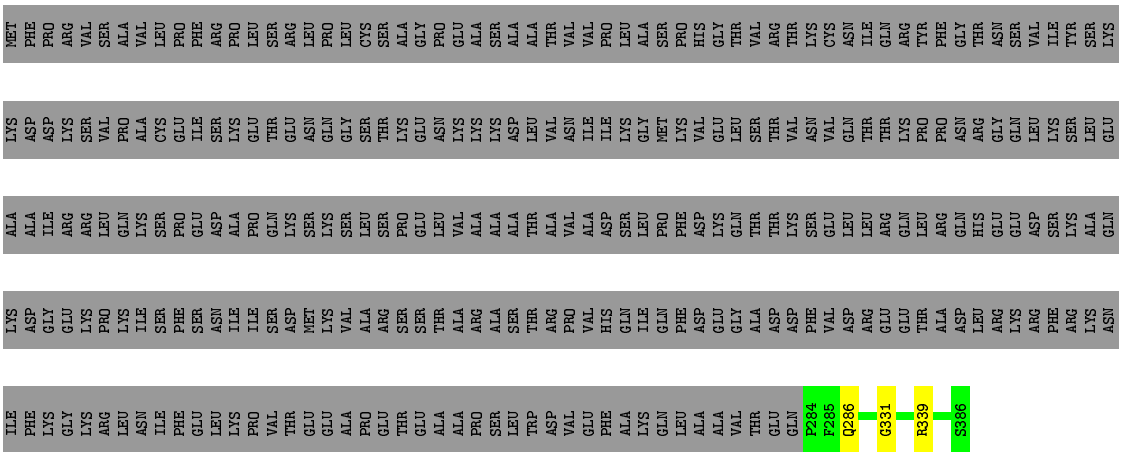
- Molecule 23: 28S ribosomal protein S29, mitochondrial

Chain g:



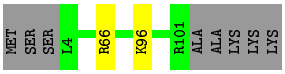
• Molecule 24: 28S ribosomal protein S31, mitochondrial

Chain h:



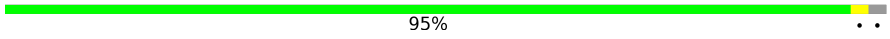
• Molecule 25: 28S ribosomal protein S33, mitochondrial

Chain i:



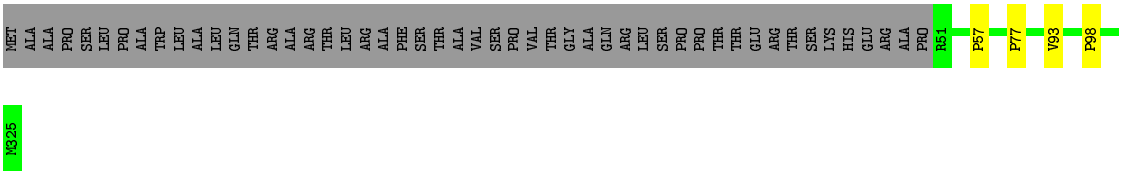
• Molecule 26: 28S ribosomal protein S34, mitochondrial

Chain j:



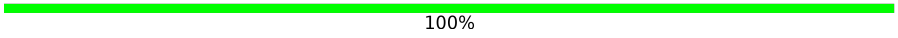
• Molecule 27: 28S ribosomal protein S35, mitochondrial

Chain k:



• Molecule 28: Coiled-coil-helix-coiled-coil-helix domain containing 1

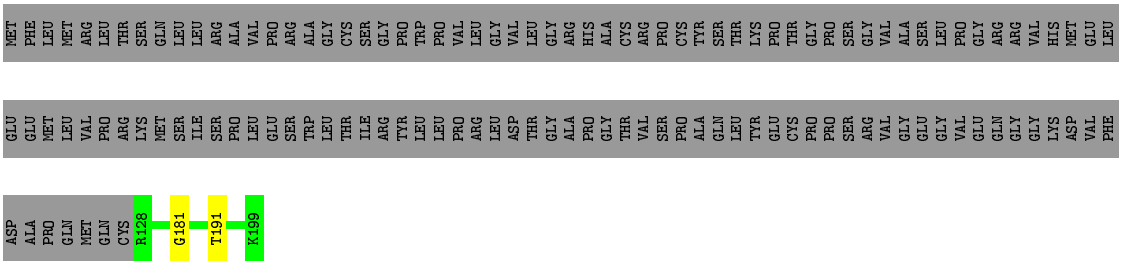
Chain m:



There are no outlier residues recorded for this chain.

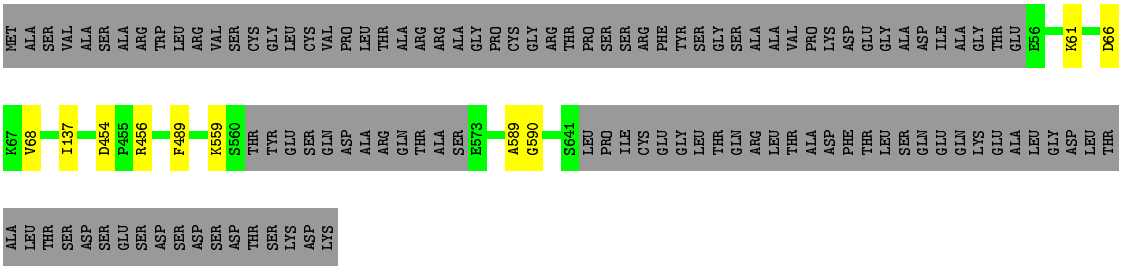
• Molecule 29: Aurora kinase A interacting protein 1

Chain n:



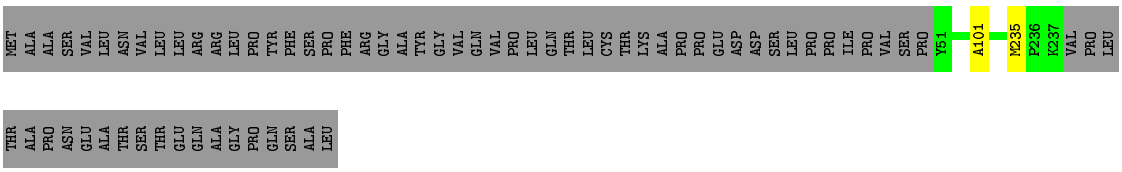
• Molecule 30: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain o:



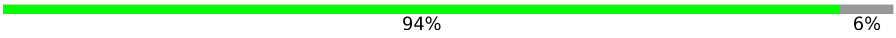
• Molecule 31: 28S ribosomal protein S18b, mitochondrial

Chain p:



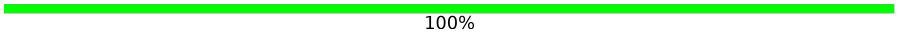
• Molecule 32: unknown

Chain s:



• Molecule 32: unknown

Chain z:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	307556	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	9.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	60000	Depositor
Image detector	GATAN UltraScan 1000 (2k x 2k)	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	0.10	0/22681	0.65	0/35318
10	L	0.23	0/872	0.40	0/1171
11	N	0.21	0/878	0.36	0/1179
12	O	0.23	0/1443	0.34	0/1927
13	P	0.23	0/937	0.38	0/1262
14	Q	0.23	0/874	0.42	0/1183
15	R	0.23	0/805	0.38	0/1082
16	U	0.22	0/748	0.36	0/995
17	a	0.23	0/2403	0.37	0/3246
18	b	0.24	0/1135	0.37	0/1528
19	c	0.24	0/1406	0.40	0/1894
2	B	0.24	0/1766	0.38	0/2392
20	d	0.23	0/1489	0.34	0/2008
21	e	0.23	0/2881	0.38	0/3893
22	f	0.24	0/787	0.42	0/1059
23	g	0.23	0/2819	0.39	0/3814
24	h	0.24	0/899	0.35	0/1209
25	i	0.22	0/834	0.36	0/1112
26	j	0.22	0/1841	0.39	0/2493
27	k	0.22	0/2275	0.36	0/3075
28	m	0.23	0/961	0.39	0/1284
29	n	0.21	0/654	0.34	0/862
3	C	0.23	0/1100	0.39	0/1487
30	o	0.24	0/2605	0.36	0/3526
31	p	0.23	0/1583	0.37	0/2149
4	E	0.23	0/2664	0.38	0/3578
5	F	0.23	0/1009	0.41	0/1362
6	G	0.23	0/1760	0.37	0/2366
7	I	0.23	0/2598	0.38	0/3490
8	J	0.23	0/1071	0.39	0/1447
9	K	0.24	0/1021	0.43	0/1380
All	All	0.20	0/66799	0.50	0/94771

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	20256	0	10258	151	0
2	B	1726	0	1747	16	0
3	C	1072	0	1091	15	0
4	E	2613	0	2638	29	0
5	F	991	0	1034	13	0
6	G	1720	0	1751	14	0
7	I	2541	0	2499	30	0
8	J	1049	0	1088	15	0
9	K	1001	0	1041	16	0
10	L	853	0	904	11	0
11	N	861	0	890	15	0
12	O	1421	0	1526	14	0
13	P	916	0	944	9	0
14	Q	857	0	920	7	0
15	R	788	0	823	17	0
16	U	737	0	759	7	0
17	a	2356	0	2371	0	0
18	b	1108	0	1124	0	0
19	c	1374	0	1395	0	0
20	d	1463	0	1438	0	0
21	e	2822	0	2816	0	0
22	f	775	0	793	0	0
23	g	2754	0	2793	0	0
24	h	871	0	814	0	0
25	i	818	0	845	0	0
26	j	1792	0	1810	0	0
27	k	2227	0	2267	0	0
28	m	945	0	984	0	0
29	n	642	0	718	0	0
30	o	3273	0	2695	0	0
31	p	1531	0	1495	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	s	80	0	18	0	0
32	z	86	0	19	0	0
All	All	64319	0	54308	302	0

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

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:A:H61	1:A:270:C:H42	1.41	0.67
8:J:76:LEU:HB2	8:J:145:LEU:HB2	1.79	0.64
1:A:190:A:H5'	13:P:20:ARG:HB2	1.79	0.64
1:A:299:A:H62	1:A:392:G:H21	1.45	0.64
1:A:416:C:N4	1:A:434:C:N3	2.46	0.63
8:J:77:SER:HB2	8:J:173:THR:HB	1.82	0.62
12:O:198:ILE:HA	12:O:202:LEU:HD23	1.83	0.61
1:A:528:C:H42	1:A:826:G:H1	1.49	0.60
1:A:628:C:H4'	4:E:210:PRO:HG3	1.83	0.60
1:A:295:G:O2'	12:O:153:ARG:NH2	2.34	0.60
1:A:309:C:N4	1:A:385:A:N1	2.49	0.60
7:I:173:GLU:HB2	7:I:231:LEU:HB2	1.84	0.59
1:A:395:G:H5"	12:O:197:LYS:HB2	1.84	0.59
13:P:33:ARG:HA	13:P:53:SER:HA	1.84	0.59
3:C:72:HIS:HE1	11:N:120:LEU:HA	1.66	0.59
15:R:86:SER:HB3	15:R:90:GLY:H	1.67	0.59
1:A:531:U:H3	1:A:823:G:H1	1.51	0.59
2:B:126:PHE:O	2:B:253:ARG:NH1	2.36	0.58
1:A:757:A:N1	11:N:80:ARG:NH2	2.51	0.58
1:A:597:A:N3	4:E:136:ARG:NH2	2.51	0.58
5:F:40:GLU:HB2	5:F:65:LEU:HB2	1.83	0.58
2:B:96:PHE:HB2	2:B:106:ASP:HB2	1.84	0.58
4:E:412:LYS:HG3	4:E:417:MET:HB2	1.85	0.58
13:P:20:ARG:NH2	13:P:41:CYS:SG	2.76	0.58
1:A:531:U:OP2	1:A:819:C:N4	2.37	0.58
11:N:60:ASN:HD22	11:N:63:LEU:H	1.51	0.58
11:N:91:CYS:SG	11:N:92:VAL:N	2.75	0.58
3:C:86:THR:HG21	11:N:106:LEU:HD21	1.86	0.57
6:G:215:ASN:HA	6:G:220:ILE:HG13	1.86	0.57
9:K:153:VAL:HG12	9:K:179:THR:HB	1.87	0.57
7:I:198:ARG:HH22	7:I:201:ILE:HD11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:A:N6	16:U:78:LYS:O	2.37	0.57
1:A:285:C:OP1	1:A:466:A:N6	2.38	0.57
15:R:116:GLN:HB3	15:R:123:VAL:HG22	1.87	0.57
1:A:331:U:O2'	9:K:112:ARG:NH2	2.37	0.56
4:E:230:ASN:HB3	4:E:238:LYS:HB3	1.86	0.56
1:A:360:A:O2'	16:U:51:ARG:NH1	2.38	0.56
1:A:610:A:H61	1:A:685:U:H3	1.53	0.56
3:C:111:LYS:HB3	8:J:166:GLU:HG2	1.88	0.56
7:I:276:ARG:HA	7:I:373:ASP:HB3	1.88	0.56
1:A:168:G:N2	1:A:202:G:O2'	2.38	0.56
1:A:112:C:N3	1:A:137:C:N4	2.43	0.56
11:N:96:ARG:NH1	11:N:98:ARG:O	2.39	0.55
1:A:414:A:N6	1:A:435:U:OP2	2.39	0.55
1:A:63:C:OP1	13:P:13:ARG:NH1	2.40	0.55
9:K:89:ALA:HB3	9:K:152:VAL:HA	1.88	0.55
1:A:465:U:OP2	2:B:50:ARG:NH2	53.10	0.55
1:A:243:C:H41	10:L:78:ARG:HH21	1.55	0.55
1:A:664:C:H1'	6:G:38:GLY:HA2	1.89	0.55
4:E:304:LYS:HB3	4:E:335:LYS:HB3	1.90	0.54
5:F:6:LEU:HB3	5:F:66:VAL:HB	1.88	0.54
1:A:744:G:N1	1:A:770:A:OP2	2.41	0.54
15:R:66:CYS:SG	15:R:67:ILE:N	2.80	0.54
1:A:743:C:OP2	1:A:769:A:N6	2.41	0.54
2:B:169:PRO:HG3	4:E:211:ASN:HA	1.89	0.54
1:A:166:C:O2	1:A:169:C:N4	2.40	0.54
1:A:154:C:OP1	1:A:158:A:N6	2.35	0.54
1:A:486:G:H1	1:A:509:C:H42	1.56	0.54
7:I:285:VAL:HG22	7:I:328:VAL:HG22	1.90	0.54
1:A:617:U:H3	1:A:674:U:H3	1.55	0.53
1:A:834:A:H5"	1:A:835:C:H2'	1.91	0.53
10:L:51:PRO:O	10:L:89:ARG:NH2	2.41	0.53
1:A:183:A:OP2	1:A:202:G:N1	2.38	0.53
7:I:382:PRO:HB2	8:J:131:ARG:HB2	1.89	0.53
1:A:382:U:H4'	5:F:72:THR:HG23	1.89	0.53
1:A:385:A:OP1	12:O:134:LYS:NZ	2.42	0.53
6:G:77:ALA:O	7:I:345:ARG:NH2	2.41	0.53
1:A:952:A:H5'	1:A:955:U:H3	1.72	0.53
9:K:102:VAL:H	9:K:112:ARG:HG2	1.74	0.53
1:A:873:U:H2'	1:A:874:A:H4'	1.91	0.53
6:G:64:TYR:HB2	7:I:366:GLN:HE22	1.74	0.53
1:A:642:A:OP1	7:I:220:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:G:H1	1:A:130:C:H42	1.55	0.52
8:J:133:GLN:HB2	11:N:126:ALA:HB2	1.90	0.52
1:A:267:A:H4'	1:A:269:G:H4'	1.90	0.52
4:E:289:THR:HG22	4:E:331:ASP:HB2	1.90	0.52
4:E:380:LEU:HD12	4:E:381:PRO:HD2	1.90	0.52
1:A:318:G:O2'	5:F:79:MET:SD	2.68	0.52
1:A:579:C:H42	11:N:85:VAL:HB	1.73	0.52
1:A:832:A:O2'	1:A:920:C:O2	2.28	0.52
2:B:136:ARG:HH21	2:B:159:TYR:HD1	1.58	0.52
1:A:5:G:H1	1:A:20:U:H3	1.57	0.52
10:L:34:ASN:OD1	14:Q:41:LYS:NZ	2.42	0.51
10:L:74:ASN:ND2	10:L:117:ASP:OD1	2.44	0.51
15:R:87:PRO:HA	15:R:126:LYS:HZ1	1.74	0.51
9:K:191:PRO:HD2	16:U:45:TYR:HB2	1.92	0.51
1:A:809:U:OP2	7:I:277:LYS:NZ	2.43	0.51
7:I:176:GLN:OE1	7:I:245:ARG:NH2	2.43	0.51
1:A:573:G:O3'	11:N:108:ARG:NH2	2.42	0.51
4:E:243:VAL:HG11	4:E:268:PHE:HE1	1.76	0.51
9:K:90:HIS:HB2	9:K:101:HIS:HB2	1.92	0.51
5:F:3:ARG:NH1	5:F:70:ALA:O	2.44	0.51
14:Q:69:LEU:HD12	14:Q:70:PRO:HD2	1.92	0.51
1:A:194:G:N2	1:A:197:A:OP2	2.44	0.51
1:A:930:A:N6	1:A:942:G:O6	2.43	0.51
12:O:110:LEU:HD23	12:O:129:VAL:HG13	1.93	0.51
7:I:118:GLU:HG3	7:I:120:ARG:H	1.76	0.51
1:A:227:G:OP1	4:E:196:ASN:ND2	2.44	0.51
1:A:308:A:H2'	1:A:309:C:H4'	1.93	0.50
4:E:284:ARG:NH1	4:E:327:ILE:O	2.44	0.50
7:I:84:GLY:HA2	7:I:87:HIS:HD2	1.76	0.50
9:K:103:VAL:HA	9:K:109:PRO:HA	1.93	0.50
4:E:136:ARG:HG3	4:E:137:ARG:HG2	1.93	0.50
5:F:28:ALA:O	5:F:32:ARG:NH1	2.44	0.50
1:A:26:U:OP1	1:A:212:U:O2'	2.27	0.50
1:A:319:U:H3	1:A:378:A:H61	1.59	0.50
3:C:83:ALA:HB2	11:N:105:ARG:HB2	1.93	0.50
7:I:174:GLU:HG2	7:I:237:GLU:HB3	1.94	0.50
1:A:481:C:N3	10:L:39:ARG:NH2	2.59	0.50
1:A:780:U:O2	7:I:389:ARG:NH1	2.39	0.50
6:G:42:GLN:HB2	6:G:74:ILE:HG22	1.93	0.50
1:A:77:C:OP1	1:A:149:C:O2'	2.25	0.49
4:E:242:ARG:HB3	4:E:260:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:284:ARG:HH11	4:E:328:GLY:HA3	1.76	0.49
7:I:149:PHE:HD1	7:I:150:LEU:HG	1.77	0.49
2:B:47:ARG:NH1	2:B:263:GLN:O	2.46	0.49
1:A:230:A:OP1	4:E:195:GLY:N	2.40	0.49
6:G:49:GLU:HB3	6:G:53:LYS:HE2	1.94	0.49
15:R:98:THR:OG1	15:R:105:GLN:OE1	2.26	0.49
3:C:60:HIS:HB3	11:N:125:ARG:HD2	1.94	0.49
1:A:374:A:H4'	1:A:450:A:H1'	1.94	0.49
6:G:36:ARG:HG3	7:I:375:ARG:HA	1.95	0.49
14:Q:36:ASP:OD2	14:Q:39:LEU:N	2.45	0.49
1:A:391:C:O2'	1:A:478:U:O2	2.31	0.49
1:A:485:A:O2'	1:A:514:A:O2'	2.29	0.49
1:A:594:C:H41	1:A:602:G:H5"	1.78	0.49
8:J:79:LEU:HD11	8:J:140:TYR:HB3	1.94	0.49
1:A:358:A:OP1	1:A:439:C:O2'	2.31	0.48
5:F:50:LYS:HG3	5:F:57:ARG:HH21	1.78	0.48
11:N:63:LEU:HB3	11:N:67:LEU:HD12	1.94	0.48
1:A:55:C:O2'	1:A:198:G:N2	2.46	0.48
3:C:68:TRP:HH2	7:I:115:GLY:HA3	1.78	0.48
1:A:580:C:H1'	11:N:86:ARG:HG2	1.94	0.48
6:G:170:VAL:HG12	6:G:237:ALA:HA	1.94	0.48
7:I:91:MET:O	9:K:117:THR:OG1	109.03	0.48
1:A:297:U:H5"	12:O:164:LYS:HD2	1.95	0.48
1:A:950:A:H5"	1:A:951:U:H5	1.78	0.48
4:E:358:THR:HG22	4:E:360:GLN:H	1.79	0.48
1:A:115:G:OP1	12:O:205:LYS:NZ	2.40	0.48
4:E:164:GLU:HA	4:E:167:LYS:HE2	1.96	0.48
9:K:189:CYS:SG	9:K:190:ARG:N	2.86	0.48
1:A:111:U:H3	1:A:491:A:H61	1.61	0.48
5:F:106:GLU:HG3	15:R:63:LEU:HB2	1.96	0.48
9:K:83:PHE:O	9:K:151:ARG:NH1	2.46	0.48
1:A:383:A:H5"	12:O:99:LYS:HD2	1.96	0.48
1:A:15:C:OP1	4:E:339:SER:OG	2.32	0.47
1:A:903:G:H2'	1:A:904:A:H8	1.79	0.47
1:A:27:U:H3	1:A:272:A:H61	1.60	0.47
1:A:574:A:N3	1:A:576:A:O2'	2.47	0.47
7:I:70:THR:HG21	7:I:135:GLN:HG3	1.96	0.47
1:A:367:U:O2	15:R:106:ARG:NH2	2.47	0.47
1:A:360:A:H2'	9:K:187:ASN:HD22	1.79	0.47
1:A:362:A:H62	15:R:123:VAL:HG12	1.80	0.47
1:A:820:C:H1'	6:G:241:TRP:HZ2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:42:GLN:H	6:G:74:ILE:HA	1.78	0.47
1:A:489:C:N4	1:A:931:U:OP2	2.44	0.47
6:G:174:LEU:HD22	6:G:178:ARG:HG2	1.97	0.47
1:A:634:A:H1'	4:E:260:LYS:HD3	1.97	0.47
1:A:656:U:O2'	7:I:118:GLU:OE1	2.33	0.47
1:A:630:C:HO2'	2:B:199:ARG:HH22	1.60	0.47
15:R:115:ALA:HB1	15:R:120:PHE:HB2	1.96	0.47
1:A:954:A:H3'	1:A:955:U:H5'	1.97	0.47
1:A:742:A:H61	1:A:773:G:H1	1.62	0.47
14:Q:24:LYS:HE2	14:Q:55:LEU:HA	1.97	0.47
1:A:414:A:O2'	1:A:942:G:O2'	2.32	0.46
4:E:306:LYS:NZ	4:E:413:ALA:O	2.46	0.46
8:J:85:LYS:HZ1	8:J:141:ARG:HE	1.62	0.46
10:L:76:ALA:HB3	10:L:78:ARG:HH12	1.80	0.46
15:R:85:ILE:HD11	15:R:126:LYS:HD3	1.96	0.46
1:A:631:U:O4	1:A:634:A:N6	2.49	0.46
16:U:1:MET:HA	16:U:2:ALA:HA	1.64	0.46
1:A:217:A:H61	1:A:268:A:H5'	1.80	0.46
1:A:283:G:H1	1:A:290:A:H2	1.63	0.46
1:A:625:A:O2'	1:A:649:A:N6	2.48	0.46
3:C:152:ARG:HB3	3:C:154:HIS:HE1	1.81	0.46
4:E:284:ARG:HD3	4:E:327:ILE:HG22	1.96	0.46
9:K:161:ARG:NH2	9:K:180:ASP:OD1	2.47	0.46
13:P:51:LEU:HD13	13:P:73:ILE:HG12	1.98	0.46
5:F:2:PRO:O	5:F:99:THR:OG1	2.34	0.46
9:K:67:PRO:HB3	15:R:131:LEU:HD23	1.98	0.46
1:A:615:C:H5'	8:J:122:LYS:HE2	1.98	0.46
1:A:712:G:O2'	1:A:803:G:OP1	2.31	0.46
1:A:301:G:O2'	1:A:478:U:OP1	2.26	0.46
1:A:544:A:O2'	1:A:712:G:OP2	2.33	0.46
8:J:186:LYS:HB2	8:J:187:PRO:HD3	1.98	0.46
13:P:85:LYS:HB2	13:P:86:PRO:HD3	1.96	0.46
3:C:41:ARG:HE	3:C:59:PRO:HD2	1.80	0.46
3:C:94:LYS:NZ	4:E:94:THR:OG1	2.49	0.46
8:J:75:ARG:HG3	8:J:146:GLU:HG2	1.97	0.46
2:B:168:ALA:H	2:B:169:PRO:HD2	1.81	0.46
4:E:301:THR:HG23	4:E:336:VAL:HG23	1.98	0.46
1:A:358:A:H1'	1:A:411:C:H42	1.81	0.46
5:F:107:GLY:HA3	15:R:63:LEU:HB3	1.97	0.45
12:O:174:TYR:HB3	12:O:175:PRO:HD3	1.98	0.45
3:C:113:ARG:HH21	8:J:165:PRO:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:373:ASP:OD1	7:I:375:ARG:NE	2.49	0.45
10:L:110:VAL:HG12	10:L:125:VAL:HG22	1.98	0.45
1:A:297:U:H2'	1:A:298:A:H8	1.82	0.45
1:A:685:U:H2'	1:A:686:G:H8	1.82	0.45
1:A:338:U:OP1	16:U:44:TYR:OH	2.33	0.45
11:N:91:CYS:HB3	11:N:96:ARG:H	1.81	0.45
13:P:93:LEU:HD21	13:P:103:VAL:HG11	1.97	0.45
10:L:127:ARG:HD2	10:L:132:CYS:HB3	1.98	0.45
1:A:534:A:H61	1:A:540:C:H1'	1.81	0.45
3:C:150:PRO:HB2	3:C:152:ARG:HH12	1.82	0.45
1:A:274:C:H1'	10:L:56:PRO:HG3	1.99	0.45
10:L:109:LEU:HD22	10:L:129:LYS:HD3	1.98	0.45
1:A:557:A:N6	1:A:702:G:O2'	2.50	0.45
2:B:125:ALA:HB1	2:B:250:LYS:HE2	1.98	0.45
2:B:92:GLU:HB2	2:B:93:PRO:HD3	1.97	0.45
1:A:310:C:O3'	15:R:106:ARG:NH1	2.47	0.45
1:A:443:G:O2'	1:A:497:A:N6	2.50	0.45
7:I:100:THR:HG22	7:I:101:GLN:H	1.81	0.45
1:A:614:C:H5'	3:C:39:ALA:HB2	1.99	0.44
5:F:15:ARG:HB3	5:F:16:PRO:HD3	2.00	0.44
1:A:560:A:O2'	1:A:584:C:O2	2.34	0.44
1:A:785:G:N2	1:A:812:A:O5'	2.46	0.44
1:A:469:C:OP1	5:F:122:LYS:NZ	2.48	0.44
1:A:566:A:O2'	7:I:395:LYS:O	2.36	0.44
1:A:113:A:N1	1:A:132:C:O2'	2.43	0.44
1:A:54:G:H4'	1:A:200:U:H1'	1.99	0.44
4:E:248:GLY:HA3	4:E:326:LEU:HB3	2.00	0.44
6:G:78:PRO:HA	7:I:276:ARG:HH22	1.83	0.44
2:B:141:SER:HA	2:B:157:THR:HG21	1.99	0.44
11:N:115:ALA:HB1	11:N:123:ILE:HG21	2.00	0.44
2:B:98:SER:HA	2:B:103:ASP:HA	2.00	0.43
1:A:311:A:OP2	15:R:106:ARG:NH2	2.36	0.43
2:B:188:LEU:HB3	2:B:192:PHE:HA	2.00	0.43
1:A:154:C:N3	1:A:162:G:N1	2.66	0.43
4:E:94:THR:HG22	4:E:96:ASP:H	1.84	0.43
1:A:406:A:H2'	1:A:407:A:C8	2.54	0.43
12:O:71:LEU:HD21	12:O:89:LYS:HE3	2.00	0.43
1:A:370:C:N4	1:A:371:G:O6	2.52	0.43
7:I:81:PHE:HZ	7:I:101:GLN:HE22	1.65	0.43
3:C:72:HIS:HA	3:C:112:ARG:HD3	2.01	0.43
2:B:134:VAL:HG13	2:B:156:HIS:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:U:OP1	1:A:564:A:N6	2.52	0.42
7:I:140:TRP:HA	7:I:146:PRO:HA	2.01	0.42
1:A:522:G:H21	1:A:837:C:H41	1.66	0.42
1:A:536:C:H2'	1:A:821:A:H2	1.85	0.42
1:A:898:C:H2'	1:A:899:A:C8	2.54	0.42
1:A:311:A:P	15:R:106:ARG:HH12	2.43	0.42
1:A:52:A:H5"	1:A:201:U:H4'	2.00	0.42
1:A:405:U:H2'	1:A:406:A:C8	2.53	0.42
1:A:683:G:H2'	1:A:684:G:C8	2.55	0.42
10:L:66:PHE:HE2	10:L:82:ARG:HB2	1.85	0.42
1:A:408:G:H2'	1:A:409:A:H8	1.84	0.42
1:A:449:A:N3	1:A:946:U:O2'	2.49	0.42
1:A:755:U:H2'	1:A:756:G:C8	2.54	0.42
1:A:785:G:H22	1:A:812:A:P	2.43	0.42
2:B:154:TYR:OH	7:I:146:PRO:O	2.33	0.42
14:Q:32:ARG:O	14:Q:45:LYS:N	2.48	0.42
1:A:443:G:OP2	12:O:147:LYS:NZ	2.45	0.42
5:F:71:PRO:HD2	5:F:74:THR:HB	2.02	0.42
1:A:295:G:O6	1:A:396:C:N4	2.52	0.42
1:A:371:G:O3'	12:O:154:TYR:OH	2.37	0.42
1:A:422:U:O2	1:A:428:A:N6	2.53	0.42
1:A:590:C:N4	1:A:591:U:O4	2.53	0.42
1:A:4:A:O2'	1:A:5:G:OP1	2.35	0.42
8:J:117:ARG:HG2	8:J:135:GLU:HG2	2.02	0.42
1:A:342:A:N3	1:A:420:G:O2'	2.40	0.42
1:A:490:U:H2'	1:A:491:A:H8	1.85	0.42
8:J:78:VAL:O	8:J:143:LEU:N	2.45	0.42
1:A:294:U:H2'	1:A:295:G:C8	2.55	0.42
1:A:785:G:O6	7:I:276:ARG:NH2	2.53	0.42
1:A:934:U:H2'	1:A:935:G:C8	2.55	0.42
3:C:128:PRO:HD2	3:C:131:LYS:HD2	2.01	0.42
4:E:312:TYR:HE2	4:E:315:ARG:HB2	1.85	0.42
9:K:86:ILE:HD13	9:K:176:ILE:HG13	2.01	0.42
1:A:11:G:H1'	4:E:231:MET:HB2	2.02	0.41
1:A:589:U:H2'	1:A:590:C:C6	2.55	0.41
1:A:782:G:H5'	7:I:388:ARG:HB3	2.02	0.41
1:A:813:A:OP1	6:G:96:ASN:ND2	2.46	0.41
6:G:122:GLN:HE21	6:G:210:LEU:HD13	1.85	0.41
1:A:4:A:H62	1:A:279:G:H5'	1.84	0.41
4:E:141:TRP:CD1	4:E:144:LEU:HD12	2.55	0.41
13:P:18:THR:HG23	13:P:82:HIS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:A:O2'	1:A:202:G:N2	2.52	0.41
12:O:174:TYR:HB2	14:Q:89:GLY:HA3	2.01	0.41
1:A:108:G:H1	1:A:139:C:H42	1.69	0.41
1:A:829:C:H2'	1:A:830:G:C8	2.55	0.41
9:K:149:HIS:HB3	9:K:176:ILE:HD11	2.02	0.41
1:A:716:C:H3'	1:A:717:A:H5'	2.02	0.41
9:K:177:SER:OG	16:U:12:VAL:O	2.35	0.41
1:A:45:C:H2'	1:A:46:A:C8	2.56	0.41
4:E:232:THR:HG22	4:E:234:LYS:H	1.86	0.41
1:A:220:A:N6	1:A:268:A:OP2	2.49	0.41
1:A:315:A:H2'	1:A:316:G:C8	2.56	0.41
1:A:154:C:H4'	1:A:167:A:H61	1.85	0.40
2:B:232:PRO:HB2	2:B:233:PRO:HD3	2.03	0.40
3:C:158:VAL:HG12	3:C:160:SER:H	1.84	0.40
13:P:53:SER:H	13:P:67:ALA:HB3	1.86	0.40
8:J:76:LEU:HD12	8:J:148:LEU:HD22	2.02	0.40
15:R:88:PHE:HB3	16:U:10:ARG:HA	2.03	0.40
1:A:171:G:OP1	1:A:180:A:O2'	2.34	0.40
1:A:358:A:O2'	1:A:438:G:N1	2.51	0.40
7:I:306:VAL:HG12	7:I:308:GLN:H	1.87	0.40
8:J:73:TYR:HE2	8:J:150:GLY:HA2	1.86	0.40
15:R:126:LYS:HZ1	15:R:131:LEU:HD13	1.86	0.40
1:A:222:G:H2'	1:A:223:G:C8	2.56	0.40
1:A:824:A:H2'	1:A:825:A:C8	2.57	0.40
12:O:172:THR:HB	14:Q:101:ALA:HB1	2.04	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
2	B	215/293 (73%)	197 (92%)	17 (8%)	1 (0%)	34 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	130/167 (78%)	108 (83%)	19 (15%)	3 (2%)	8 48
4	E	326/430 (76%)	280 (86%)	43 (13%)	3 (1%)	21 67
5	F	122/124 (98%)	106 (87%)	14 (12%)	2 (2%)	12 56
6	G	206/242 (85%)	188 (91%)	17 (8%)	1 (0%)	34 77
7	I	309/396 (78%)	277 (90%)	31 (10%)	1 (0%)	46 83
8	J	126/201 (63%)	105 (83%)	19 (15%)	2 (2%)	12 56
9	K	134/197 (68%)	119 (89%)	14 (10%)	1 (1%)	26 71
10	L	107/139 (77%)	86 (80%)	18 (17%)	3 (3%)	6 44
11	N	99/128 (77%)	89 (90%)	9 (9%)	1 (1%)	19 65
12	O	171/256 (67%)	158 (92%)	12 (7%)	1 (1%)	30 74
13	P	114/135 (84%)	101 (89%)	11 (10%)	2 (2%)	11 53
14	Q	107/130 (82%)	92 (86%)	14 (13%)	1 (1%)	21 67
15	R	95/143 (66%)	85 (90%)	9 (10%)	1 (1%)	17 63
16	U	84/87 (97%)	80 (95%)	4 (5%)	0	100 100
17	a	287/359 (80%)	260 (91%)	27 (9%)	0	100 100
18	b	133/190 (70%)	120 (90%)	10 (8%)	3 (2%)	8 48
19	c	166/173 (96%)	148 (89%)	16 (10%)	2 (1%)	16 61
20	d	174/205 (85%)	166 (95%)	8 (5%)	0	100 100
21	e	340/415 (82%)	287 (84%)	46 (14%)	7 (2%)	9 50
22	f	96/189 (51%)	93 (97%)	3 (3%)	0	100 100
23	g	334/397 (84%)	302 (90%)	29 (9%)	3 (1%)	21 67
24	h	101/386 (26%)	90 (89%)	9 (9%)	2 (2%)	9 51
25	i	96/106 (91%)	89 (93%)	6 (6%)	1 (1%)	19 65
26	j	211/218 (97%)	173 (82%)	33 (16%)	5 (2%)	7 47
27	k	273/325 (84%)	243 (89%)	26 (10%)	4 (2%)	13 57
28	m	116/118 (98%)	94 (81%)	22 (19%)	0	100 100
29	n	70/199 (35%)	66 (94%)	2 (3%)	2 (3%)	6 43
30	o	306/575 (53%)	273 (89%)	24 (8%)	9 (3%)	6 43
31	p	185/258 (72%)	154 (83%)	29 (16%)	2 (1%)	17 63
All	All	5233/7181 (73%)	4629 (88%)	541 (10%)	63 (1%)	21 61

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	N	97	PRO
5	F	71	PRO
5	F	110	PRO
6	G	102	GLY
10	L	56	PRO
15	R	119	GLY
23	g	193	ALA
27	k	77	PRO
27	k	98	PRO
29	n	181	GLY
30	o	489	PHE
30	o	559	LYS
31	p	101	ALA
3	C	105	ALA
10	L	70	PRO
13	P	27	THR
18	b	40	PRO
18	b	110	GLY
21	e	121	ALA
21	e	135	TYR
21	e	238	GLN
21	e	276	CYS
21	e	328	LEU
24	h	286	GLN
25	i	96	LYS
26	j	143	PRO
30	o	456	ARG
30	o	590	GLY
3	C	106	ASP
10	L	76	ALA
21	e	132	LYS
26	j	134	VAL
2	B	92	GLU
3	C	126	GLN
4	E	423	SER
8	J	105	SER
19	c	9	ILE
21	e	172	ALA
24	h	331	GLY
26	j	162	ARG
30	o	66	ASP
30	o	68	VAL
30	o	137	ILE

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Mol	Chain	Res	Type
30	o	454	ASP
31	p	235	MET
4	E	154	ILE
8	J	126	ILE
9	K	119	GLY
18	b	129	GLY
26	j	138	ASP
29	n	191	THR
30	o	589	ALA
13	P	48	VAL
23	g	132	GLY
23	g	337	ASP
4	E	236	GLY
7	I	210	VAL
12	O	80	GLY
27	k	93	VAL
14	Q	85	VAL
19	c	145	GLY
26	j	182	GLY
27	k	57	PRO

5.3.2 Protein sidechains (i)

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	
2	B	186/230 (81%)	186 (100%)	0	100	100
3	C	113/142 (80%)	113 (100%)	0	100	100
4	E	273/346 (79%)	272 (100%)	1 (0%)	93	96
5	F	109/109 (100%)	108 (99%)	1 (1%)	84	93
6	G	183/208 (88%)	183 (100%)	0	100	100
7	I	267/333 (80%)	266 (100%)	1 (0%)	93	96
8	J	118/182 (65%)	116 (98%)	2 (2%)	68	87
9	K	102/151 (68%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	L	94/118 (80%)	94 (100%)	0	100 100
11	N	91/113 (80%)	88 (97%)	3 (3%)	45 76
12	O	159/226 (70%)	158 (99%)	1 (1%)	90 95
13	P	95/113 (84%)	95 (100%)	0	100 100
14	Q	95/115 (83%)	94 (99%)	1 (1%)	80 91
15	R	89/126 (71%)	89 (100%)	0	100 100
16	U	77/78 (99%)	76 (99%)	1 (1%)	76 89
17	a	255/307 (83%)	253 (99%)	2 (1%)	86 94
18	b	115/163 (71%)	114 (99%)	1 (1%)	84 93
19	c	152/155 (98%)	152 (100%)	0	100 100
20	d	147/168 (88%)	147 (100%)	0	100 100
21	e	307/362 (85%)	307 (100%)	0	100 100
22	f	85/160 (53%)	85 (100%)	0	100 100
23	g	301/352 (86%)	301 (100%)	0	100 100
24	h	94/341 (28%)	93 (99%)	1 (1%)	80 91
25	i	88/94 (94%)	87 (99%)	1 (1%)	80 91
26	j	190/193 (98%)	190 (100%)	0	100 100
27	k	252/292 (86%)	252 (100%)	0	100 100
28	m	102/102 (100%)	102 (100%)	0	100 100
29	n	66/173 (38%)	66 (100%)	0	100 100
30	o	277/369 (75%)	276 (100%)	1 (0%)	93 96
31	p	166/226 (74%)	166 (100%)	0	100 100
All	All	4648/6047 (77%)	4631 (100%)	17 (0%)	94 96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	375	GLU
5	F	122	LYS
7	I	315	PHE
8	J	91	TYR
8	J	175	THR
11	N	31	ASP
11	N	45	TYR

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Mol	Chain	Res	Type
11	N	58	ARG
12	O	170	ARG
14	Q	62	ASP
16	U	1	MET
17	a	69	PHE
17	a	264	THR
18	b	134	ARG
24	h	339	ARG
25	i	66	ARG
30	o	61	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	ASN
2	B	123	HIS
2	B	139	GLN
2	B	186	HIS
2	B	243	GLN
2	B	255	GLN
3	C	72	HIS
3	C	154	HIS
4	E	155	GLN
4	E	415	GLN
5	F	100	GLN
6	G	122	GLN
6	G	227	HIS
7	I	87	HIS
7	I	127	HIS
7	I	178	GLN
7	I	255	HIS
7	I	296	ASN
7	I	366	GLN
8	J	147	HIS
9	K	99	GLN
9	K	101	HIS
9	K	149	HIS
10	L	106	HIS
11	N	60	ASN
11	N	66	HIS
11	N	68	GLN
12	O	199	HIS

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Mol	Chain	Res	Type
13	P	39	ASN
14	Q	44	ASN
14	Q	90	GLN
15	R	79	GLN
15	R	116	GLN
17	a	75	GLN
17	a	215	GLN
18	b	97	GLN
19	c	56	GLN
20	d	109	ASN
20	d	126	GLN
20	d	155	GLN
21	e	339	HIS
21	e	384	HIS
22	f	122	HIS
23	g	66	HIS
23	g	147	GLN
23	g	163	ASN
23	g	179	GLN
23	g	194	ASN
23	g	204	GLN
23	g	234	ASN
23	g	265	ASN
23	g	298	ASN
24	h	363	HIS
26	j	24	GLN
26	j	45	HIS
26	j	179	GLN
27	k	220	ASN
27	k	270	GLN
29	n	140	HIS
29	n	178	GLN
30	o	458	ASN
30	o	524	HIS
31	p	88	GLN
31	p	169	GLN
31	p	181	HIS
31	p	207	GLN
31	p	221	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	952/955 (99%)	170 (17%)	3 (0%)

All (170) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	G
1	A	10	G
1	A	16	A
1	A	24	U
1	A	33	U
1	A	41	C
1	A	44	A
1	A	53	A
1	A	57	U
1	A	58	C
1	A	60	A
1	A	64	C
1	A	74	A
1	A	91	A
1	A	103	A
1	A	110	A
1	A	112	C
1	A	114	A
1	A	117	A
1	A	119	A
1	A	124	C
1	A	125	U
1	A	129	G
1	A	138	G
1	A	143	G
1	A	147	A
1	A	158	A
1	A	159	C
1	A	165	A
1	A	166	C
1	A	170	A
1	A	179	A
1	A	181	U
1	A	186	C
1	A	211	A
1	A	212	U
1	A	218	U
1	A	219	U

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Mol	Chain	Res	Type
1	A	226	G
1	A	233	C
1	A	239	C
1	A	242	G
1	A	248	G
1	A	253	C
1	A	268	A
1	A	279	G
1	A	282	C
1	A	288	A
1	A	302	C
1	A	304	C
1	A	305	C
1	A	306	A
1	A	310	C
1	A	311	A
1	A	312	A
1	A	313	A
1	A	333	A
1	A	341	A
1	A	355	A
1	A	364	A
1	A	370	C
1	A	375	G
1	A	386	A
1	A	389	G
1	A	393	A
1	A	394	C
1	A	427	U
1	A	428	A
1	A	444	C
1	A	449	A
1	A	450	A
1	A	452	A
1	A	465	U
1	A	466	A
1	A	467	A
1	A	472	A
1	A	482	C
1	A	489	C
1	A	497	A
1	A	498	A

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Mol	Chain	Res	Type
1	A	500	A
1	A	513	A
1	A	533	U
1	A	535	U
1	A	536	C
1	A	537	C
1	A	557	A
1	A	561	U
1	A	569	C
1	A	571	C
1	A	574	A
1	A	578	A
1	A	588	U
1	A	592	U
1	A	595	U
1	A	599	A
1	A	604	C
1	A	610	A
1	A	618	C
1	A	620	U
1	A	632	A
1	A	634	A
1	A	635	A
1	A	636	A
1	A	639	A
1	A	640	A
1	A	641	A
1	A	642	A
1	A	644	A
1	A	645	A
1	A	649	A
1	A	660	G
1	A	661	A
1	A	676	A
1	A	677	G
1	A	681	A
1	A	686	G
1	A	693	A
1	A	714	U
1	A	725	C
1	A	726	A
1	A	727	C

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Mol	Chain	Res	Type
1	A	728	C
1	A	729	A
1	A	730	A
1	A	741	C
1	A	747	A
1	A	757	A
1	A	760	C
1	A	769	A
1	A	785	G
1	A	814	U
1	A	817	G
1	A	818	G
1	A	821	A
1	A	832	A
1	A	833	C
1	A	835	C
1	A	848	C
1	A	855	A
1	A	856	A
1	A	860	G
1	A	868	G
1	A	869	C
1	A	870	A
1	A	874	A
1	A	878	C
1	A	881	U
1	A	886	A
1	A	887	C
1	A	889	C
1	A	892	U
1	A	895	C
1	A	896	U
1	A	904	A
1	A	910	C
1	A	911	A
1	A	913	G
1	A	922	A
1	A	923	G
1	A	926	A
1	A	927	A
1	A	928	G
1	A	936	G

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Mol	Chain	Res	Type
1	A	939	A
1	A	948	G
1	A	949	G
1	A	951	U
1	A	952	A
1	A	954	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	4	A
1	A	15	C
1	A	363	U

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.