



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:27 PM BST

PDB ID : 3J80  
EMDB ID: : EMD-2764  
Title : CryoEM structure of 40S-eIF1-eIF1A preinitiation complex  
Authors : Hussain, T.; Llacer, J.L.; Fernandez, I.S.; Savva, C.G.; Ramakrishnan, V.  
Deposited on : 2014-08-28  
Resolution : 3.75 Å(reported)  
Based on PDB ID : 3U5C, 3U5B

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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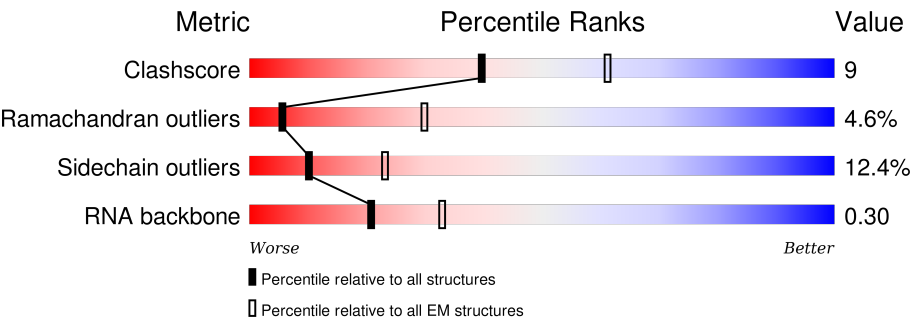
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.75 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  $\geq 3$ , 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	2	1799	<div><div>29%</div><div>52%</div><div>17%</div><div>.</div></div>
2	A	254	<div><div>52%</div><div>25%</div><div>5%</div><div>19%</div></div>
3	B	255	<div><div>59%</div><div>21%</div><div>.</div><div>.</div><div>16%</div></div>
4	C	259	<div><div>51%</div><div>27%</div><div>5%</div><div>16%</div></div>
5	E	261	<div><div>69%</div><div>25%</div><div>6%</div></div>
6	G	236	<div><div>69%</div><div>25%</div><div>.</div><div>.</div></div>
7	H	190	<div><div>63%</div><div>26%</div><div>7%</div><div>.</div></div>
8	I	201	<div><div>59%</div><div>30%</div><div>.</div><div>.</div><div>6%</div></div>





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Mol	Chain	Length	Quality of chain
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	D	237	
21	F	227	
22	K	106	
23	M	134	
24	P	140	
25	Q	143	
26	R	136	
27	S	146	
28	T	144	
29	U	117	
30	Z	108	
31	c	67	
32	d	56	
33	f	150	

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Mol	Chain	Length	Quality of chain
34	g	326	 91%6%
35	h	25	 88%12%
36	i	153	 58%5%37%
37	j	108	 74%6%20%

## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 77716 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1779	Total	C	N	O	P	0	0
			37775	16882	6653	12461	1779		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	206	Total	C	N	O	S	0	0
			1616	1035	285	294	2		

- Molecule 3 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	214	Total	C	N	O	S	0	0
			1722	1089	313	317	3		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 5 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 6 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 7 is a protein called eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 8 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total	C	N	O	S	0	0
			1493	926	301	265	1		

- Molecule 9 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 10 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 11 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 12 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 13 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 14 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 15 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 16 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 17 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	97	Total	C	N	O	S	0	0
			770	475	163	127	5		

- Molecule 18 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 19 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	53	Total	C	N	O	S	0	0
			428	268	87	72	1		

- Molecule 20 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 21 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 22 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 23 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	122	Total	C	N	O		0	0
			922	575	167	180			

- Molecule 24 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	123	Total	C	N	O	S	0	0
			980	628	179	168	5		

- Molecule 25 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	141	Total	C	N	O		0	0
			1105	709	204	192			

- Molecule 26 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	120	Total	C	N	O	S	0	0
			959	598	178	180	3		

- Molecule 27 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 28 is a protein called eS19.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 29 is a protein called uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	U	106	Total	C	N	O	S	0
			845	540	152	152	1	0

- Molecule 30 is a protein called eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Z	70	Total	C	N	O	S	0
			558	355	104	98	1	0

- Molecule 31 is a protein called eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	63	Total	C	N	O	S	0
			494	305	98	90	1	0

- Molecule 32 is a protein called uS14.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	d	53	Total	C	N	O	S	0
			446	280	89	76	1	0

- Molecule 33 is a protein called eS31.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	f	69	Total	C	N	O	S	0
			549	352	102	91	4	0

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	g	318	Total	C	N	O	S	0
			2466	1561	430	470	5	0

- Molecule 35 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 36 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	96	Total	C	N	O	S	0	0
			778	482	144	147	5		

- Molecule 37 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	86	Total	C	N	O	S	0	0
			695	439	128	124	4		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	67	Total	Mg	0
			67	67	

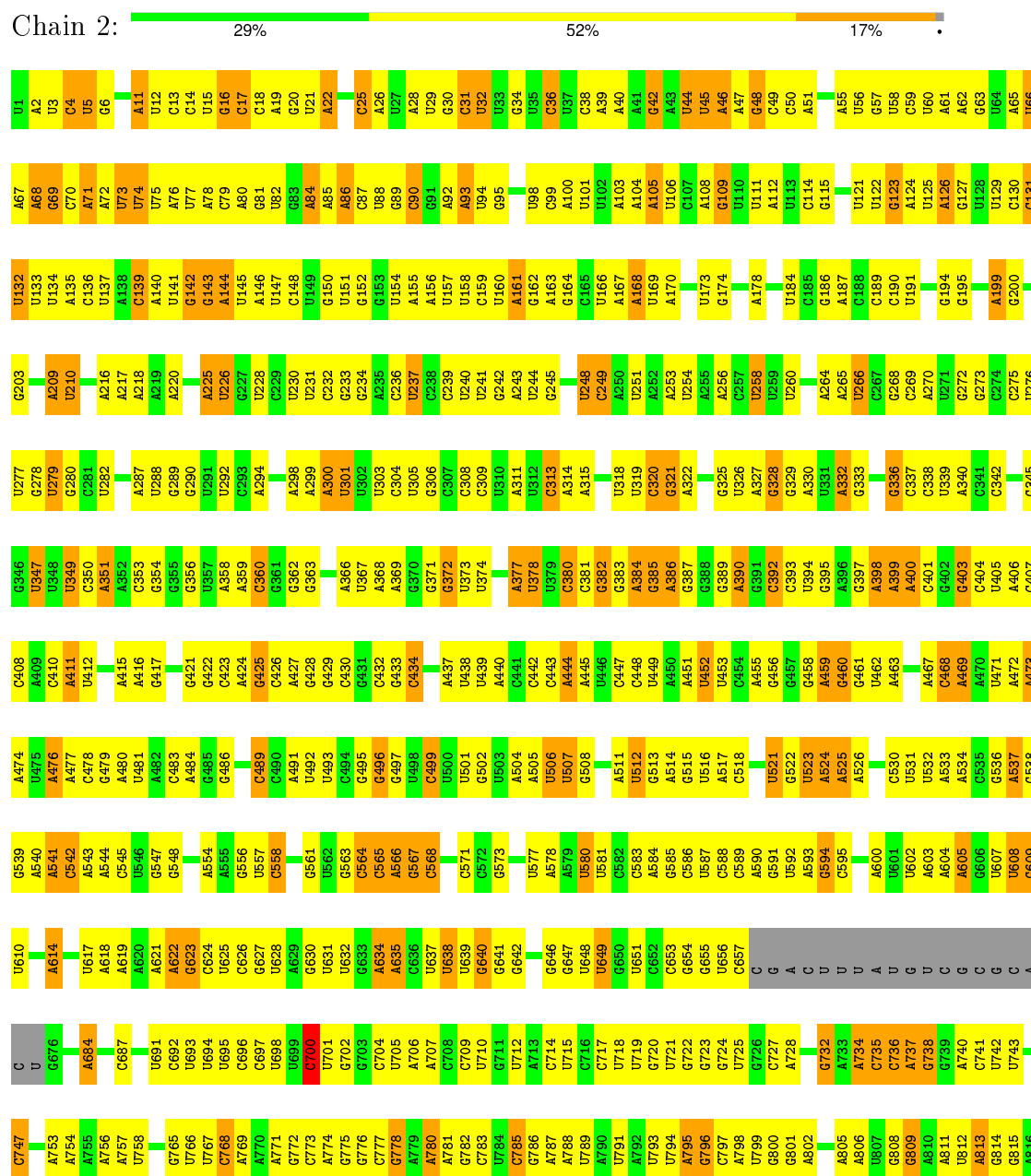
- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	b	1	Total	Zn	0
			1	1	
39	a	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

### 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: 18S rRNA

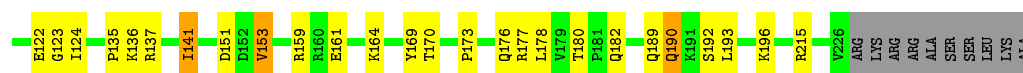
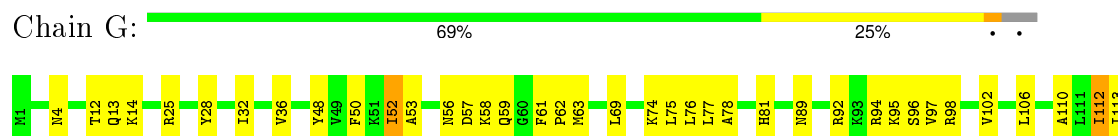


G1775	U1702	C1634	C1566	A1503	A1442	G1370	G1232	G1166	U1102	G1027	U959	U888	C817
G1778	C1703	C1635	A1567	G1504	G1443	A1371	A1233	U1167	U1103	U1028	U960	C889	G818
A1705	C1704	G1636	C1568	C1507	C1444	C1374	C1234	A1170	U1105	A1029	C961	U893	U819
U1706	A1705	C1637	C1569	G1508	C1445	U1378	G1235	G1171	G1106	U1030	A962	G894	U820
C1707	C1707	C1638	G1570	G1509	G1446	U1379	G1236	C1172	G1107	G1032	U963	U895	U821
U1708	U1708	U1641	G1572	G1510	C1449	A1380	U1239	C1173	G1108	G1033	A965	C896	G822
C1709	C1709	U1645	G1573	G1511	U1450	U1381	G1240	U1174	G1109	G1034	A966	A897	U825
G1710	A1710	A1646	A1574	A1512	G1451	G1381	G1241	G1175	G1110	A1035	U967	G898	C826
G1711	G1711	G1647	C1579	A1513	G1452	U1382	A1242	C1176	G1113	C1036	C968	U827	A828
A1712	A1712	U1648	A1580	A1514	G1453	G1383	G1243	G1177	U1114	U1037	A969	G900	U829
G1713	G1713	C1649	C1516	U1515	G1454	U1386	A1244	G1178	A1115	A1038	A970	G901	U830
U1718	U1718	C1650	U1517	C1516	C1455	C1387	G1244	G1179	U1116	G1039	A971	U904	U831
G1724	G1724	C1651	U1583	U1517	G1456	C1387	C1247	U1180	U1117	G1040	A972	A904	U832
G1725	A1725	G1652	A1584	G1519	C1457	U1388	U1248	U1181	G1117	A1041	C974	A906	U833
U1726	U1726	A1653	A1585	U1520	C1458	A1389	U1249	A1182	G1118	U1048	A978	U907	U837
C1727	G1727	G1654	G1586	G1521	G1459	U1390	U1250	A1183	U1119	G1049	G979	U908	U838
A1728	C1727	U1655	C1587	A1522	G1460	C1391	G1251	U1185	G1121	U1050	U980	U910	U839
U1729	A1728	G1656	U1588	A1523	C1461	G1392	U1252	U1186	G1125	G1056	U981	U911	U840
A1730	A1729	A1657	C1524	G1525	G1462	G1393	U1253	A1187	G1126	U1057	U982	G912	A843
U1733	U1730	G1658	A1590	C1525	G1463	C1396	A1254	A1188	C1127	C1052	A982	G913	G844
G1734	U1733	G1660	G1592	C1527	U1466	A1398	U1256	C1189	U1128	U1056	G984	A914	G845
U1737	G1734	G1661	U1593	C1528	A1467	A1399	U1257	A1193	U1129	U1057	G985	U915	A846
U1739	A1737	C1662	C1594	G1529	C1468	G1400	U1259	C1194	A1130	C1058	G986	U916	U853
U1740	U1739	U1663	A1595	U1530	A1469	G1403	G1263	A1195	A1131	U1059	A987	U917	A854
U1741	U1740	G1667	C1597	C1531	C1470	A1404	G1264	A1196	U1132	U1060	U988	U919	A855
A1742	A1741	A1668	G1599	U1535	U1471	U1408	U1265	G1197	C1133	A1061	C989	U920	U856
G1743	A1742	G1669	C1600	U1536	C1472	A1409	G1266	G1198	U1134	U1062	G990	U927	G857
G1744	G1743	U1670	U1601	G1537	C1475	A1409	G1267	G1199	A1135	G1065	A992	U931	U860
G1745	G1744	G1672	G1602	G1538	G1476	U1411	U1268	A1201	A1137	C1071	G993	U932	A861
G1746	G1745	C1673	G1603	G1539	C1477	A1412	G1269	A1202	A1138	A1080	U995	A932	A862
A1747	G1746	G1674	C1604	G1540	G1478	A1413	U1270	A1203	G1139	C1081	G996	C933	U863
U1750	A1747	U1675	U1605	A1541	C1479	U1414	G1272	U1205	G1140	A1074	A997	U934	A864
A1753	U1750	G1678	U1606	U1542	C1480	A1415	G1273	C1206	A1142	A1075	U998	G935	G865
U1754	A1753	A1679	G1608	G1544	A1481	G1416	G1276	A1207	U1143	U1079	C999	C936	G866
G1755	U1754	U1681	A1609	C1547	G1482	G1417	G1277	C1208	U1144	A1080	A1000	G937	G867
U1758	G1755	U1682	U1610	U1548	C1483	C1418	G1278	A1210	G1145	C1082	G1001	A938	A868
U1759	U1758	U1685	G1612	U1549	A1485	A1422	G1279	G1211	G1146	A1083	A1002	A940	C869
A1760	A1759	U1686	C1613	U1550	U1486	A1423	U1280	G1212	G1149	G1084	U1003	G941	G870
U1763	U1760	G1687	U1614	G1551	C1487	C1424	U1281	U1213	A1150	A1085	U1011	C942	G871
A1764	G1763	G1688	C1615	A1553	A1490	A1425	U1282	C1214	A1151	A1086	A1012	A943	U872
U1766	U1764	A1689	U1555	U1555	C1492	U1428	G1285	C1215	G1152	A1087	G1013	U944	C873
G1768	G1766	A1692	A1557	U1556	C1493	U1430	U1286	C1216	G1153	U1088	U1014	U945	G874
U1769	G1768	G1693	U1558	U1559	U1494	G1431	U1287	A1222	C1154	C1089	G1015	U946	G875
U1770	U1769	G1694	C1623	U1560	U1495	U1432	U1288	A1223	U1155	A1090	U1016	G947	G876
C1771	G1770	G1696	U1561	U1562	C1497	U1435	U1289	U1224	A1156	A1091	U1017	C948	G877
U1772	C1771	U1697	U1562	U1563	C1498	U1436	U1290	A1225	G1157	A1018	U1018	C949	C878
A1773	U1772	G1698	G1500	U1564	C1499	U1439	G1291	A1226	C1158	A1019	A1019	A950	C879
U1774	U1773	A1699	A1501	G1502	G1500	U1440	G1292	A1227	U1159	G1095	C1020	G953	U880
	A1774	A1633	G1502	U1565	U1502	U1441	G1293	G1227	C1160	U1096	C1021	G954	U881
					U1500		G1294	A1162	C1161	U1097	A1022	C955	A883
					A1501		G1295	G1163	U1162	G1099	A1024	G956	G884
					G1502		G1296	A1165	A1165	A1025	A1025	U957	U885
										A1026	A1026	U958	U887

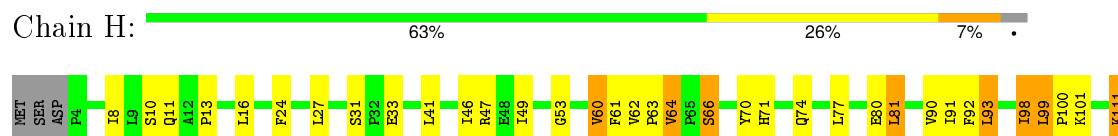
• Molecule 2: uS2

Chain A:  52% 25% 5% 19%

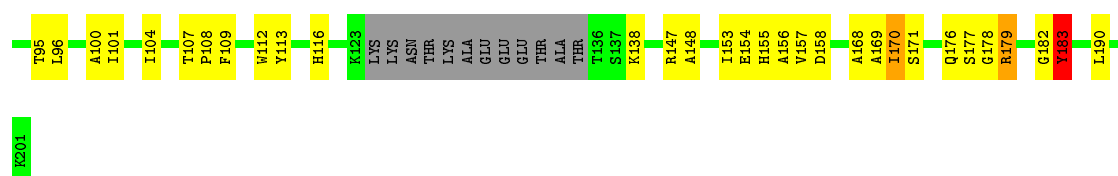
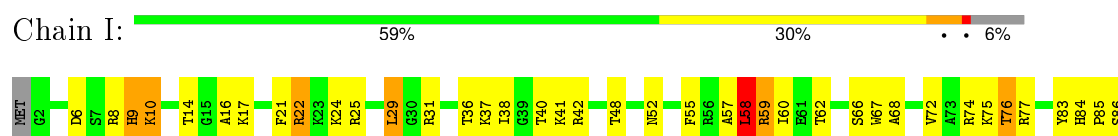




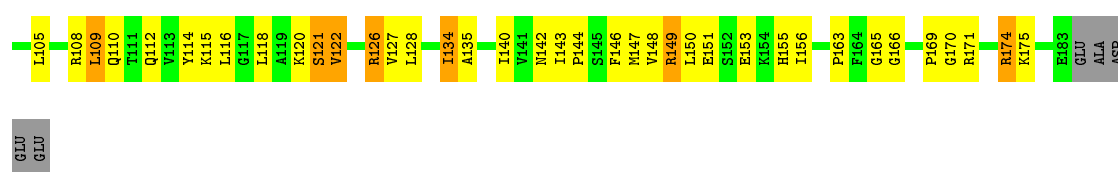
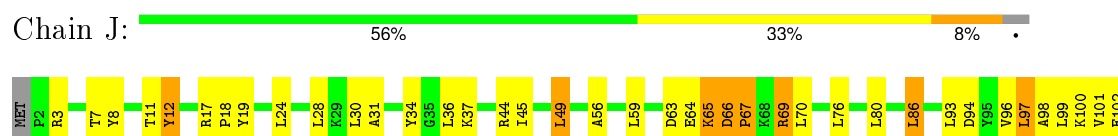
• Molecule 7: eS7



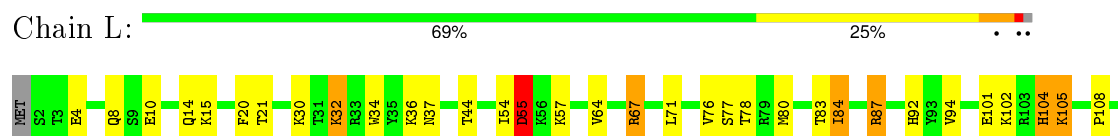
• Molecule 8: eS8



• Molecule 9: uS4



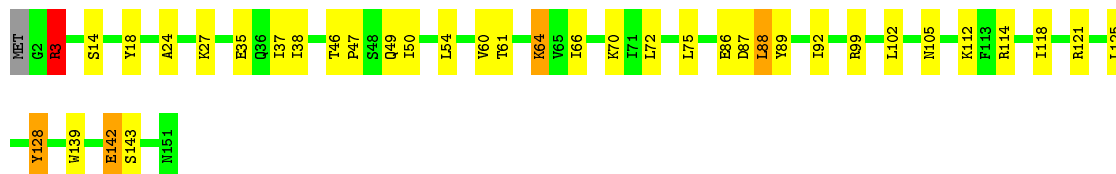
• Molecule 10: uS17





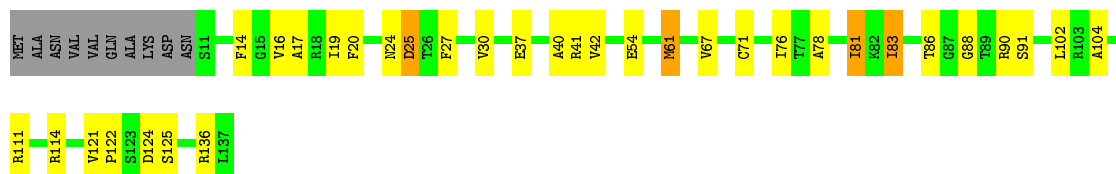
- Molecule 11: uS15

Chain N: 75% 21% ..



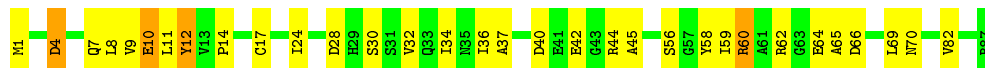
- Molecule 12: uS11

Chain O: 68% 22% 7%



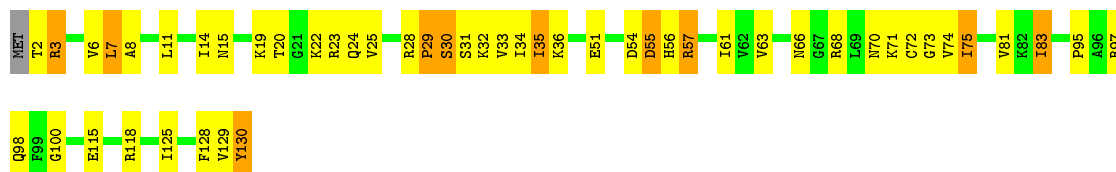
- Molecule 13: eS21

Chain V: 63% 32% 5%



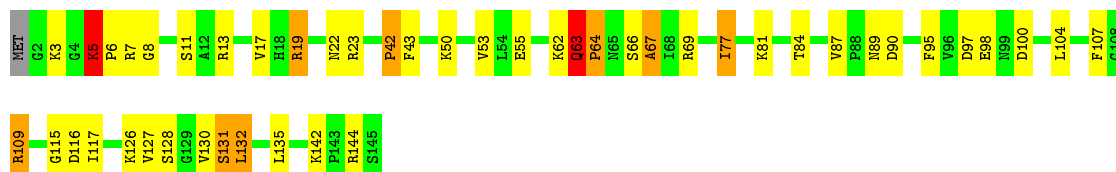
- Molecule 14: uS8

Chain W: 61% 31% 8%

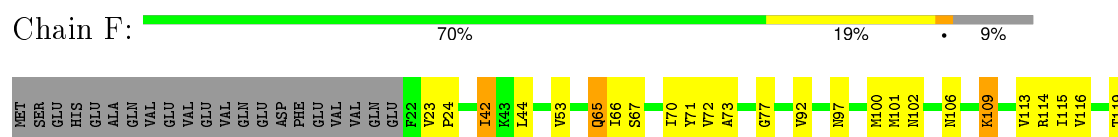


- Molecule 15: uS12

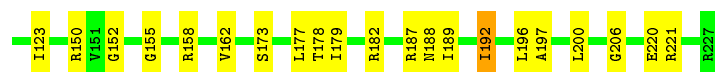
Chain X: 67% 26% 6%



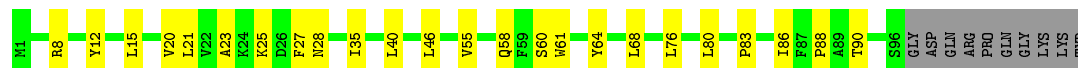
- Molecule 16: eS24



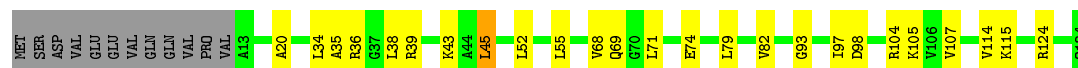




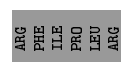
- Molecule 22: eS10



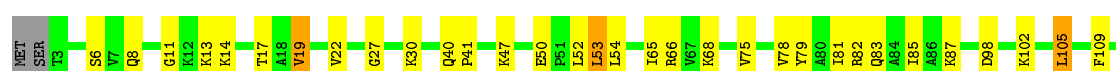
- Molecule 23: eS12



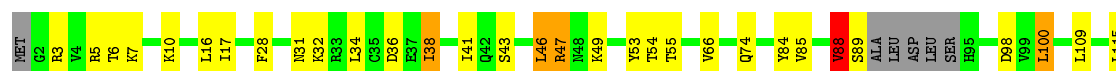
- Molecule 24: uS19



- Molecule 25: uS9

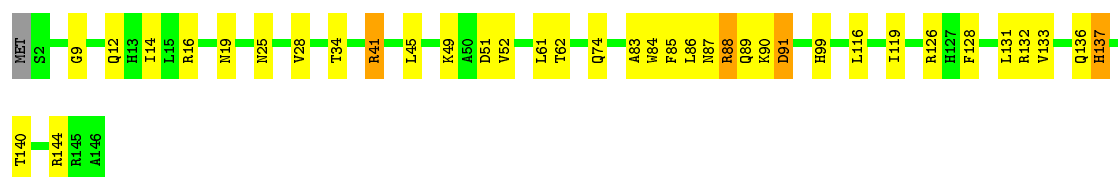


- Molecule 26: eS17



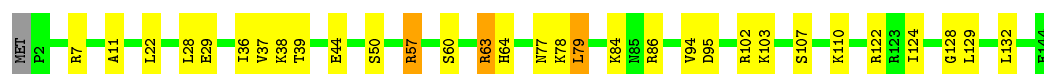
- Molecule 27: uS13





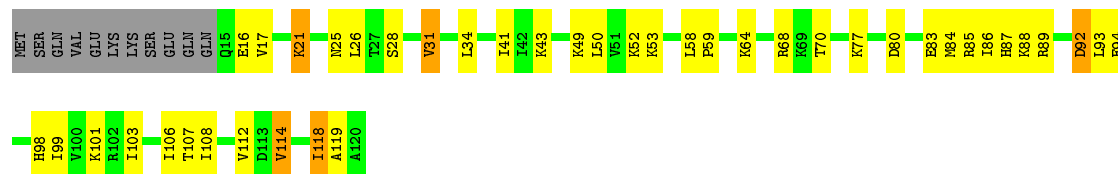
- Molecule 28: eS19

Chain T: 78% 19% ..



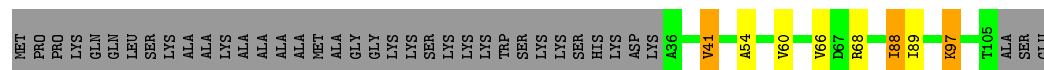
- Molecule 29: uS10

Chain U: 55% 32% • 9%



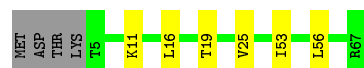
- Molecule 30: eS25

Chain Z: 57% 5% • 35%



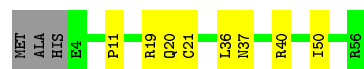
- Molecule 31: eS28

Chain c: 85% 9% 6%



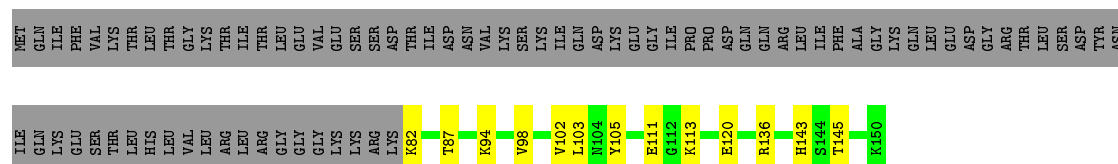
- Molecule 32: uS14

Chain d: 80% 14% 5%

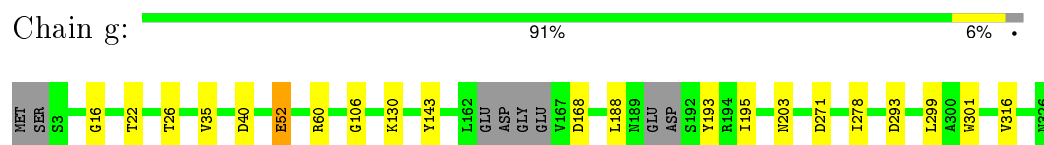


- Molecule 33: eS31

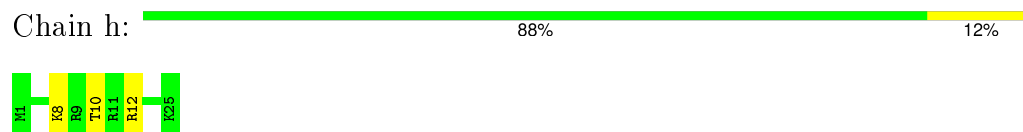
Chain f: 37% 9% 54%



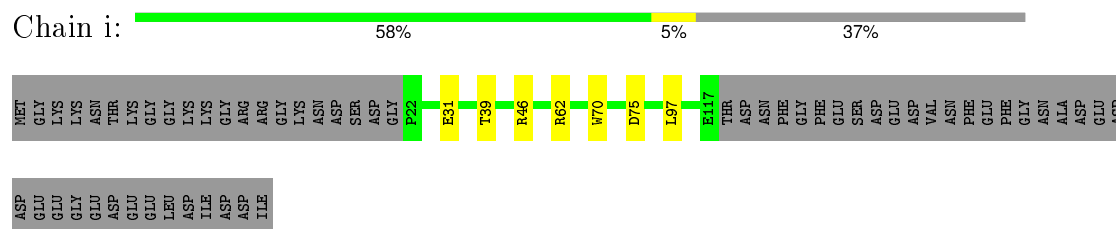
- Molecule 34: RACK1



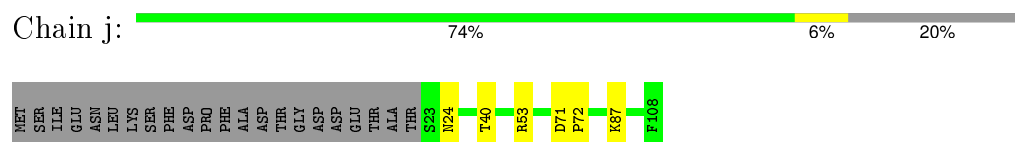
- Molecule 35: eL41



- Molecule 36: eIF1A



- Molecule 37: eIF1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	100709	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	2	0.30	0/42244	0.70	5/65823 (0.0%)
10	L	0.45	0/1276	0.70	0/1718
11	N	0.45	0/1210	0.78	1/1628 (0.1%)
12	O	0.40	0/953	0.72	0/1279
13	V	0.43	0/696	0.73	0/938
14	W	0.50	0/1039	0.82	0/1399
15	X	0.48	0/1137	0.80	0/1516
16	Y	0.42	0/1075	0.72	0/1433
17	a	0.44	0/782	0.82	0/1047
18	b	0.40	0/619	0.70	0/837
19	e	0.39	0/435	0.70	0/579
2	A	0.43	0/1656	0.78	0/2264
20	D	0.43	0/1769	0.70	0/2378
21	F	0.40	0/1628	0.71	0/2198
22	K	0.46	0/831	0.67	0/1123
23	M	0.40	0/929	0.69	0/1255
24	P	0.43	0/1000	0.65	0/1343
25	Q	0.41	0/1125	0.69	0/1510
26	R	0.44	0/969	0.73	0/1299
27	S	0.39	0/1212	0.68	0/1629
28	T	0.39	0/1129	0.68	0/1520
29	U	0.43	0/857	0.73	0/1158
3	B	0.40	0/1747	0.72	1/2353 (0.0%)
30	Z	0.43	0/567	0.64	0/762
31	c	0.39	0/496	0.72	0/666
32	d	0.47	0/457	0.66	0/607
33	f	0.47	0/562	0.65	0/751
34	g	0.41	0/2521	0.61	0/3431
35	h	0.39	0/234	0.81	0/300
36	i	0.38	0/788	0.62	0/1051
37	j	0.41	0/703	0.66	0/938
4	C	0.45	0/1659	0.79	3/2252 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
5	E	0.41	0/2122	0.71	1/2861 (0.0%)
6	G	0.39	0/1835	0.68	0/2451
7	H	0.43	0/1507	0.74	0/2028
8	I	0.44	0/1519	0.74	2/2033 (0.1%)
9	J	0.45	0/1495	0.82	2/2001 (0.1%)
All	All	0.37	0/82783	0.71	15/120359 (0.0%)

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
14	W	0	1
15	X	0	2
16	Y	0	1
17	a	0	1
25	Q	0	1
7	H	0	1
9	J	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1315	G	C2'-C3'-O3'	7.15	125.23	109.50
9	J	49	LEU	CA-CB-CG	7.12	131.67	115.30
4	C	139	LEU	CA-CB-CG	6.41	130.05	115.30
3	B	184	LEU	CA-CB-CG	6.33	129.86	115.30
8	I	29	LEU	CA-CB-CG	6.22	129.61	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	H	131	PHE	Peptide
9	J	12	TYR	Peptide
14	W	75	ILE	Peptide
15	X	11	SER	Peptide
15	X	63	GLN	Peptide

## 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	2	37775	0	19004	704	0
2	A	1616	0	1636	35	0
3	B	1722	0	1795	27	0
4	C	1629	0	1710	41	0
5	E	2078	0	2157	37	0
6	G	1812	0	1911	32	0
7	H	1483	0	1579	29	0
8	I	1493	0	1515	29	0
9	J	1471	0	1554	43	0
10	L	1248	0	1311	25	0
11	N	1187	0	1251	17	0
12	O	942	0	979	16	0
13	V	687	0	682	14	0
14	W	1021	0	1056	34	0
15	X	1119	0	1198	21	0
16	Y	1061	0	1111	17	0
17	a	770	0	822	0	0
18	b	609	0	631	0	0
19	e	428	0	468	0	0
20	D	1744	0	1826	27	0
21	F	1609	0	1679	18	0
22	K	809	0	810	10	0
23	M	922	0	953	9	0
24	P	980	0	1026	10	0
25	Q	1105	0	1170	20	0
26	R	959	0	1006	12	0
27	S	1193	0	1217	19	0
28	T	1110	0	1124	16	0
29	U	845	0	913	14	0
30	Z	558	0	585	2	0
31	c	494	0	534	0	0
32	d	446	0	436	0	0
33	f	549	0	564	0	0
34	g	2466	0	2406	0	0
35	h	233	0	284	0	0
36	i	778	0	779	0	0
37	j	695	0	729	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	67	0	0	0	0
39	a	1	0	0	0	0
39	b	1	0	0	0	0
39	f	1	0	0	0	0
All	All	77716	0	60411	1161	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 9.

The worst 5 of 1161 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)
1:2:1037:U:H3	1:2:1091:A:N6	1.23	1.32
1:2:1290:G:N2	1:2:1323:G:H22	1.28	1.28
1:2:991:A:N1	1:2:1011:U:O4	1.78	1.15
1:2:991:A:N1	1:2:1011:U:C4	2.17	1.12
1:2:1290:G:H22	1:2:1323:G:N2	1.56	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	204/254 (80%)	167 (82%)	24 (12%)	13 (6%)	2	26
3	B	212/255 (83%)	175 (82%)	25 (12%)	12 (6%)	2	28
4	C	215/259 (83%)	182 (85%)	23 (11%)	10 (5%)	3	33
5	E	258/261 (99%)	215 (83%)	36 (14%)	7 (3%)	6	48
6	G	224/236 (95%)	196 (88%)	24 (11%)	4 (2%)	11	56
7	H	182/190 (96%)	152 (84%)	15 (8%)	15 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	184/201 (92%)	146 (79%)	26 (14%)	12 (6%)	1	26
9	J	180/188 (96%)	148 (82%)	20 (11%)	12 (7%)	1	25
10	L	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	4	38
11	N	148/151 (98%)	127 (86%)	17 (12%)	4 (3%)	6	48
12	O	125/137 (91%)	98 (78%)	20 (16%)	7 (6%)	2	29
13	V	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1	18
14	W	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	4	38
15	X	142/145 (98%)	115 (81%)	13 (9%)	14 (10%)	1	13
16	Y	132/135 (98%)	114 (86%)	10 (8%)	8 (6%)	2	27
17	a	95/119 (80%)	64 (67%)	21 (22%)	10 (10%)	1	12
18	b	79/82 (96%)	62 (78%)	12 (15%)	5 (6%)	2	26
19	e	51/63 (81%)	47 (92%)	3 (6%)	1 (2%)	9	54
20	D	221/237 (93%)	197 (89%)	18 (8%)	6 (3%)	6	48
21	F	204/227 (90%)	169 (83%)	25 (12%)	10 (5%)	3	32
22	K	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	9	53
23	M	120/134 (90%)	96 (80%)	20 (17%)	4 (3%)	5	44
24	P	121/140 (86%)	99 (82%)	16 (13%)	6 (5%)	3	32
25	Q	139/143 (97%)	120 (86%)	15 (11%)	4 (3%)	6	46
26	R	116/136 (85%)	93 (80%)	18 (16%)	5 (4%)	3	36
27	S	143/146 (98%)	113 (79%)	23 (16%)	7 (5%)	3	32
28	T	141/144 (98%)	123 (87%)	15 (11%)	3 (2%)	9	53
29	U	104/117 (89%)	91 (88%)	5 (5%)	8 (8%)	1	20
30	Z	68/108 (63%)	53 (78%)	10 (15%)	5 (7%)	1	21
31	c	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
32	d	51/56 (91%)	41 (80%)	9 (18%)	1 (2%)	9	54
33	f	67/150 (45%)	43 (64%)	17 (25%)	7 (10%)	1	12
34	g	312/326 (96%)	256 (82%)	48 (15%)	8 (3%)	7	48
35	h	23/25 (92%)	23 (100%)	0	0	100	100
36	i	94/153 (61%)	86 (92%)	8 (8%)	0	100	100
37	j	84/108 (78%)	75 (89%)	8 (10%)	1 (1%)	16	63
All	All	4959/5572 (89%)	4127 (83%)	603 (12%)	229 (5%)	5	34

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	26	ALA
2	A	95	ALA
3	B	100	PHE
3	B	117	TRP
4	C	141	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	
2	A	174/211 (82%)	146 (84%)	28 (16%)	3	22
3	B	196/228 (86%)	176 (90%)	20 (10%)	9	43
4	C	176/203 (87%)	148 (84%)	28 (16%)	3	23
5	E	223/224 (100%)	189 (85%)	34 (15%)	3	25
6	G	192/200 (96%)	172 (90%)	20 (10%)	9	42
7	H	164/170 (96%)	140 (85%)	24 (15%)	4	27
8	I	148/159 (93%)	123 (83%)	25 (17%)	2	19
9	J	153/158 (97%)	129 (84%)	24 (16%)	3	24
10	L	136/137 (99%)	121 (89%)	15 (11%)	8	39
11	N	127/128 (99%)	114 (90%)	13 (10%)	9	43
12	O	96/104 (92%)	90 (94%)	6 (6%)	22	64
13	V	73/73 (100%)	59 (81%)	14 (19%)	2	13
14	W	110/111 (99%)	94 (86%)	16 (14%)	4	27
15	X	119/120 (99%)	104 (87%)	15 (13%)	5	32
16	Y	108/109 (99%)	88 (82%)	20 (18%)	2	15
17	a	82/100 (82%)	64 (78%)	18 (22%)	1	9
18	b	71/72 (99%)	60 (84%)	11 (16%)	3	24
19	e	47/55 (86%)	42 (89%)	5 (11%)	8	41
20	D	185/196 (94%)	161 (87%)	24 (13%)	5	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	F	174/194 (90%)	157 (90%)	17 (10%)	10	44
22	K	88/96 (92%)	79 (90%)	9 (10%)	9	43
23	M	97/109 (89%)	91 (94%)	6 (6%)	23	64
24	P	105/117 (90%)	92 (88%)	13 (12%)	6	33
25	Q	117/119 (98%)	102 (87%)	15 (13%)	5	32
26	R	109/124 (88%)	92 (84%)	17 (16%)	3	24
27	S	128/129 (99%)	110 (86%)	18 (14%)	4	29
28	T	117/118 (99%)	107 (92%)	10 (8%)	13	52
29	U	96/107 (90%)	82 (85%)	14 (15%)	4	27
30	Z	60/88 (68%)	57 (95%)	3 (5%)	30	70
31	c	55/59 (93%)	49 (89%)	6 (11%)	8	40
32	d	46/48 (96%)	39 (85%)	7 (15%)	3	25
33	f	58/133 (44%)	52 (90%)	6 (10%)	9	42
34	g	265/272 (97%)	251 (95%)	14 (5%)	28	69
35	h	23/23 (100%)	20 (87%)	3 (13%)	5	32
36	i	83/130 (64%)	76 (92%)	7 (8%)	14	53
37	j	77/96 (80%)	72 (94%)	5 (6%)	21	63
All	All	4278/4720 (91%)	3748 (88%)	530 (12%)	10	33

5 of 530 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	V	8	LEU
16	Y	81	ASP
32	d	20	GLN
13	V	59	ILE
15	X	19	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
11	N	49	GLN
14	W	24	GLN
32	d	10	HIS
12	O	99	GLN

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Mol	Chain	Res	Type
15	X	22	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1799 (98%)	836 (47%)	132 (7%)

5 of 836 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	11	A

5 of 132 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	747	C
1	2	1056	U
1	2	1655	U
1	2	812	U
1	2	896	C

## 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](#)

Of 70 ligands modelled in this entry, 70 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.