

# wwPDB EM Validation Summary Report (i)

Apr 29, 2024 – 06:38 am BST

PDB ID	:	4V5H
EMDB ID	:	EMD-1657
Title	:	E.Coli 70s Ribosome Stalled During Translation Of Thac Leader Peptide.
Authors	:	Seidelt, B.; Innis, C.A.; Wilson, D.N.; Gartmann, M.; Armache, J.; Villa, E.;
		Trabuco, L.G.; Becker, T.; Mielke, T.; Schulten, K.; Steitz, T.A.; Beckmann,
		R.
Deposited on	:	2009-10-26
Resolution	:	5.80  Å(reported)
Based on initial models	:	3FIH. 3FIK

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 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 5.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		
RNA backbone	4643	859		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq=3, 2, 1$  and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain							
1	AA	1530	• 35%	47%	18%					
2	AB	218	54% 68%	28	3% •					
3	AC	206	37% 65%	25%	9% •					
4	AD	205	43% 67%	24%	8%					
5	AE	150	29% 65%	28%	7% •					
6	AF	100	65%	28%	6% •					
7	AG	150	<u>39%</u> 67%	25%	7% •					



Conti	nued fron	n previous p	page	
Mol	Chain	Length	Quality of	chain
			29%	
8	AH	129	71%	26% •
0	АТ	107	38%	
9	AI	127	59%	33% 7% •
10	ΔΙ	08	65% E 40/	429/
10	110	50	30%	42%
11	AK	117	70%	26% ••
			37%	
12	AL	123	66%	25% 8% •
			28%	
13	AM	113	60%	28% 9% •
14	A NI	06	27%	
14	AN	90	64%	27% 9%
15	AO	88	67%	25% 7%
10	110			23/0 170 •
16	AP	80	64%	32% ••
			25%	
17	AQ	80	65%	26% 8% •
10	1.5	~~	20%	
18	AR	55	64%	27% 9%
10	٨S	70	25%	200/
19	Ab	19	31%	30% 10%
20	AT	85	73%	22% • •
			57%	
21	AU	51	65%	27% 8%
			26%	
22	AV	77	58%	29% 13%
0.0	٨v	11	64%	
23	АЛ	11	<u>9% 18% 27%</u>	45%
24	ΑZ	20	80%	20%
21	112	20	26%	2070
25	B0	77	70%	25% 5%
			25%	
26	B1	63	65%	32% •
07		<b>F</b> 0	22%	
27	B2	58	76%	24%
28	B3	56	5270	250/ 70/
20	D0		26%	25% 7% •
29	B4	50	66%	30% •
			99%	
30	B5	234	77%	20% •
			37%	
31	B6	46	59%	20% 20% •
20	D7	C 4	23%	
- 32	В(	04	59%	39% •



Mol	Chain	Length	Quality of chain		
33	B8	38	76%	24	4%
34	BA	117	42% 43%		14% •
35	BB	2903	2200 1500		17%
00		2500	27%		1776
36	BC	271	68%	25%	6% •
37	BD	209	67%	23%	8% •
38	BE	201	66%	27%	6%
39	BF	178	63%	26%	10% •
40	BG	176	72%	22%	6% •
41	BH	149	71%	21%	5%
42	BI	141	75%		6%
43	BJ	142	18%	21%	8%
10	BK	191	33%	2170	
-11	DR	121	30%	20%	0% •
45	BL	143	67% 24%	29%	•
46	BM	136	68%	29%	•••
47	BN	120	67%	27%	7%
48	BO	116	74%	22%	•
49	BP	114	68%	25%	7%
50	BQ	117	60%	31%	7% •
51	BR	103	59%	32%	7% •
52	BS	110	61%	27%	12%
53	BT	93	56%	39%	5%
51	BII	109	19%	200	
- 54	DU	102	62%	20%	<u>ه</u> ، ښم
55	BW	94	61%	31%	7% •
56	BY	79	63%	27%	6% •



# 2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 145960 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 16S RIBOSOMAL RNA.

Mol	Chain	Residues		1	AltConf	Trace			
1	AA	1530	Total 32831	C 14642	N 6024	O 10635	Р 1530	0	0

• Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total 1704	C 1081	N 305	0 311	${ m S} 7$	0	0

• Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total 1624	C 1028	N 305	0 288	${ m S} { m 3}$	0	0

• Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total 1643	C 1026	N 315	O 298	${f S}$ $4$	0	0

• Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total 1105	C 687	N 211	O 201	${ m S}{ m 6}$	0	0

• Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total 817	C 515	N 148	0 148	S 6	0	0



• Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	AG	150	Total 1174	C 730	N 226	0 214	$\frac{S}{4}$	0	0

• Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	AH	129	Total 979	C 616	N 173	0 184	S 6	0	0

• Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	AI	127	Total 1022	C 634	N 206	0 179	${ m S} { m 3}$	0	0

• Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	AJ	98	Total 786	C 493	N 150	0 142	S 1	0	0

• Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	AK	117	Total 877	C 540	N 174	0 160	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	AL	123	Total 955	C 590	N 196	0 165	${S \atop 4}$	0	0

• Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	AM	113	Total 876	C 541	N 177	0 155	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	AN	96	Total 774	C 483	N 160	O 128	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	AO	88	Total 716	C 440	N 146	0 129	S 1	0	0

• Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues		At	oms			AltConf	Trace
16	AP	80	Total 638	C 400	N 126	0 111	S 1	0	0

• Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
17	AQ	80	Total 648	C 411	N 121	0 113	${ m S} { m 3}$	0	0

• Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues		Aton	ns		AltConf	Trace
18	AR	55	Total 455	C 288	N 86	0 81	0	0

• Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	AS	79	Total 637	C 408	N 120	O 107	${ m S} { m 2}$	0	0

• Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues		At	oms			AltConf	Trace
20	AT	85	Total 665	C 411	N 137	0 114	${ m S} { m 3}$	0	0

• Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
21	AU	51	Total 425	C 265	N 86	O 73	S 1	0	0

• Molecule 22 is a RNA chain called P-SITE TRNA.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
22	AV	77	Total 1649	C 733	N 297	0 542	Р 77	0	0

• Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues		Ate	$\mathbf{oms}$	AltConf	Trace		
23	AX	11	Total 236	C 106	N 46	O 73	Р 11	0	0

• Molecule 24 is a protein called POLY-ALA NASCENT CHAIN.

Mol	Chain	Residues	1	Ator	ns	AltConf	Trace	
24	AZ	20	Total 100	C 60	N 20	O 20	0	0

• Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
25	B0	77	Total 625	C 388	N 129	O 106	${ m S} { m 2}$	0	0

• Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues		Atc	ms	AltConf	Trace		
26	B1	63	Total 509	C 313	N 99	O 95	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
27	Bo	58	Total	С	Ν	Ο	$\mathbf{S}$	0	0
21	$D_{2}$	50	449	281	87	79	2	0	0

• Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L32.



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
28	B3	56	Total 444	C 269	N 94	O 80	S 1	0	0

• Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
29	Β4	50	Total 409	C 263	N 75	O 71	0	0

• Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues		At	AltConf	Trace			
30	B5	234	Total 1733	C 1081	N 315	O 330	S 7	0	0

• Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
31	B6	46	Total 377	C 228	N 90	O 57	$\frac{S}{2}$	0	0

• Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
32	Β7	64	Total 504	C 323	N 105	0 74	${S \over 2}$	0	0

• Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
33	B8	38	Total 302	C 185	N 65	0 48	$\frac{S}{4}$	0	0

• Molecule 34 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues		$\mathbf{A}$		AltConf	Trace		
34	BA	115	Total 2464	C 1097	N 451	0 801	Р 115	0	0

• Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.



Mol	Chain	Residues			AltConf	Trace			
35	BB	2903	Total 62321	C 27801	N 11467	O 20150	Р 2903	0	0

• Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues		Ate	AltConf	Trace			
36	BC	271	Total 2082	C 1288	N 423	0 364	${ m S} 7$	0	0

• Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	BD	209	Total 1565	C 979	N 288	0 294	$\frac{S}{4}$	0	0

• Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
38	BE	201	Total 1552	C 974	N 283	O 290	${ m S}{ m 5}$	0	0

• Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	BF	178	Total 1420	C 905	N 251	0 258	S 6	0	0

• Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	BG	175	Total 1316	C 827	N 242	0 245	${ m S} { m 2}$	0	0

• Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues		At	oms	AltConf	Trace		
41	BH	149	Total 1111	C 699	N 197	0 214	S 1	0	0

• Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L11.



Mol	Chain	Residues		At	oms	AltConf	Trace		
42	BI	141	Total 1032	C 651	N 179	O 196	S 6	0	0

• Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	BJ	142	Total 1129	С 714	N 212	O 199	$\frac{S}{4}$	0	0

• Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues		At	oms	AltConf	Trace		
44	BK	121	Total 930	C 582	N 179	0 163	S 6	0	0

• Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
45	BL	143	Total 1045	C 649	N 206	0 189	S 1	0	0

• Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues		At	oms			AltConf	Trace
46	BM	136	Total 1074	C 686	N 205	0 177	S 6	0	0

• Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
47	BN	120	Total 960	C 593	N 196	O 166	${ m S}{ m 5}$	0	0

• Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
48	BO	116	Total 892	C 552	N 178	O 162	0	0

 $\bullet\,$  Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L19.



Mol	Chain	Residues		At	oms	AltConf	Trace		
49	BP	114	Total 917	C 574	N 179	0 163	S 1	0	0

• Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
50	BQ	117	Total 947	C 604	N 192	O 151	0	0

• Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues		At	AltConf	Trace			
51	BR	103	Total 816	C 516	N 153	0 145	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues		At	oms			AltConf	Trace
52	BS	110	Total 857	C 532	N 166	0 156	${ m S} { m 3}$	0	0

• Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues		At	oms			AltConf	Trace
53	BT	93	Total 738	C 466	N 139	0 131	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
54	BU	99	Total 755	C 479	N 140	O 136	0	0

• Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues		At	oms			AltConf	Trace
55	BW	94	Total 753	C 479	N 137	0 134	${ m S} { m 3}$	0	0

• Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L27.



Mol	Chain	Residues		At	oms			AltConf	Trace
56	BY	79	Total 596	C 367	N 120	0 108	S 1	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S RIBOSOMAL RNA







• Molecule 2: 30S RIBOSOMAL PROTEIN S2



#### 













PROTEIN DATA BANK











• Molecule 35: 23S RIBOSOMAL RNA





C961	G962 U963	C964	C965	6966 11967	C968	G969	0370 6971	A972	A973	4975 4975	G976	G977	G978 A979	A980	A981	C982 A983	A984	C985	C987	A988	(1989 1000	A990 C991	C992	G993 7004	C995	A996	6997 0998	0000	A1000	G1002	G1003	01004 C1005	C1006	C1007 A1008	A1009	A1010	G1011 U1012	C1013	A1014 11015	G1016 G1016	G1017	U1018 111019	A1020	
A1021	G1022 U1023	G1024	G1025	G1026 A1027	A1028	A1029	G1031	A1032	01033	61034 01035	G1036	G1037	G1038 A1039	A1040	G1041	G1042 C1043	C1044	C1045	A1046 G1047	A1048	C1049	G1051	C1052	C1053	A1054 G1055	G1056	A1057	U1058	U1060	U1061	G1062 G1063	C1064	U1065	U1066	A1067 C1068	A1069	A1070	G1071 C1072	A1073	G1074	C1075	A1077	U1078	A1080
U1081	U1082 U1083	A1084	A1085	A1086 G1087	A1088	A1089	A1090	C1092	G1093	U1094	A1095	A1096	01097 A1098	G1099	C1 100	C1102	A1103	C1104	01105 C1106	G1107	U1108	C1109 G1110	A1111	G1112	C1113 C1114	G1115	G1116 C1117	C1118 C1118	U1119	G1120 C1121	G1122	C1123 G1124	G1125	A1126 A1127	G1128	A1129	U1130 C1131	U1132	A1133	A1134 C1135	G1136	G1137	61139 G1139	C1140
U1141	A1142 A1143	A1144	C1145	C1146 A1147	U1148	G1149		C1152	C1153	41155 A1155	A1156	G1157	C1158 11159	G1160	C1161	G1162 G1163	C1164	A1165	G1167	<mark>G1168</mark>	A1169	G1171	C1172	U1173	01174		G1177	C1178 C1170	U1180	U1181	G1182 U1183	U1184	G1185 G1186	G1187	U1188	61190	G1191	G1192 C1103	A1194	G1195	C1196 C1197	U1198	U1199 C1200	
U1201	G1202 111203	A1204	A1205	G1206 C1207	C1208	U1209	G1210 C1211	G1212	A1213	A1214 G1215	G1216	U1217	G1218 111219	G1220	C1221	01222 G1223	U1224	G1225	61227 G1227	G1228	C1229	N1230 U1231	G1232	C1233	G1235	G1236	A1237 C1238	G1239	U1240	A1 241 U1 242	C1243	A1244 G1245	A1246	A1247 G1248	U1249	G1250	G1251 G1252	A1253	A1254	01233 G1256	C1257	U1258 G1259	A1260	
C1261	A1262 U1263	A1264	A1265	G1 266 111 267	A1268	A1269 C1970	G1271	A1272	U1273	A1275 A1275	A1276	G1277	C1278 C1279	G1280	G1281	01282 G1283	A1284	A1285	A1287	G1288	C1289 C1200	C1290 C1291	G1292	C1293	C1295	G1296	C1297 C1298	G1299	G1300	A1301 A1302	G1303	A1304 C1305	C1306	A1307 A1308	G1309	G1310	G1311 U1312	U1313	C1314	U1316	G1317	01318 C1319	C1320	
A1321	A1322 C1323	G1324	U1325	01326 41327	A1328	U1329	61331 G1331	G1332	G1333	G1335 C1335	A1336	G1337	G1338 C1330	U1340	G1341	A1342 G1343	<b>U1344</b>	C1345	61340 A1347	C1348	C1349	C1351	U1352	A1353 A1354	G1355	G1356	C1357 C1358	A1359	G1360	01362 01362	C1363	61364 A1365	A1366	A1367 G1368	G1369	C1370	G1371 U1372	A1373	G1374 11275	C1376	G1377	A1378 11379	G1380	
G1381	G1382 A1383	A1384	A1385	C1386 A1387	G1388	G1389 111200	01390 01391	A1392	A1393	01394 A1395	U1396	U1397	C1398 C1399	U1400	G1401	01402 A1403	C1404	U1405	01406 G1407	G1408	U1409	61410 U1411	U1412	A1413	01415 U1415	G1416	C1417 G1418	A1419	A1420	G1421 G1422	G1423	G1424 G1425	G1426	A1427 C1428	G1429	G1430	A1431 G1432	A1433	A1434	G1435 G1436	C1437	01438 41439	01440	
G1441	U1442 U1443	G1444	G1445	C1446 C1447	G1448	G1449	G1450 C1451	G1452	A1453	G1455 G1455	G1456	<b>U1457</b>	01458 C1459	U1460	C1461	C1462 C1463	G1464	G1465	01460 01467	U1468	A1469	A14/0 G1471	C1472	G1473 111474	G1475	U1476	A1477 G1478	G1479	C1480	01401 G1482	G1483	01484 01485	U1486	01487 C1488	C1489	A1490	G1491 G1492	C1493	A1494	A1430 A1496	U1497	C1498 C1499	G1500	
G1501	A1502 A1503	A1504	A1505	01506 C1507	A1508	A1509	G1511	C1512	U1513	41515 A1515	G1516	G1517	C1518 C1519	U1520	G1521	A1522 U1523	G1524	A1525	G1527	A1528	G1529 C1520	C1531	A1532	C1533	A1535	C1536	G1537 C1538	U1539	G1540	01542 01542	G1543	A1545 A1545	G1546	C1547 A1548	A1549	C1550	A1552 A1552	A1553	01554 01555	G1556	C1557	C1558	01559	
C1561	U1562 U1563	C1564	C1565	A1567 G1567	G1568	A1569	A1571 A1571	A1572	G1573	C1575	U1576	C1577	01578 01579	A1580	G1581	C1582 A1583	U1584	C1585	A1586	G1588	U1589	A1590 A1591	C1592	A1593	01594 C1595	A1596	A1597	A1598 U1599	C1600	G1601 111602	A1603	C1604	C1606	C1607	A1609 A1609	A1610	C1611	G1613	A1614	C1615 A1616	C1617	A1618	G1619 G1620	
U1621	G1622 G1623	U1624	C1625	A1626 G1627	G1628	U1629	G1631	A1632	G1633	A1635	U1636	A1637	C1638 C1639	A1640	A1641	G1642 G1643	C1644	G1645	01647 U1647	U1648	G1649	G1651	A1652	G1653 A165A	A1055 A1655	C1656	01657 C1658	G1659	G1660	01662 U1662	G1663	A1664 A1665	G1666	G1667 A1668	A1669	C1670	01671 A1672	G1673	G1674	A1676	A1677	A1678 A1679	U1680	
G1681	G1682 U1683	G1684	C1685	C1686 G1687	U1688	A1689	A1690 C1691	U1692	U1693	G1695	G1696	G1697	A1698 C1699	A1700	A1701	G1702 G1703	C1704	A1705	C1706	C1708	U1709	G1710	01712	A1713	01714 C1715	U1716	A1717	G1/18 G1719	U1720	G1721	G1723	G1724 111706	C1726	C1727	01728 01729	C1730	G1731	G1733 G1733	G1734	A1735	G1737	G1738	A1739 G1740	
C1741	U1742 G1743	A1744	A1745	A1/46 111747	C1748	A1749	01751 01751	C1752	G1753	A1755	G1756	A1757	U1758 41759	C1760	C1761	A1762 G1763	C1764	U1765	G1767	C1768	U1769	C1771	A1772	A1773	U1775	G1776	01777 01778	U1779	A1780	U1/01 U1782	A1783	A1/84 A1785	A1786	A1787 C1788	A1789	C1790	A1/91 G1792	C1793	A1794	U1796	G1797	01798 01799	C1800	
A1801	A1802 A1803	C1804	A1805	C1806 G1807	A1808	A1809	61811	U1812	G1813 61814	41815 A1815	C1816	<mark>G1817</mark>	U1818 41819	U1820	A1821	C1822 G1823	G1824	U1825	01827	G1828	A1829	61831	C1832	C1833	01834 61835	C1836	C1837	C1838 G1839	G1840	U1841 C1842	C1843	C1844	G1846	A1847	A1848 G1849	G1850	U1851	01852 A1853	A1854	U1855 11956	01000 G1857	A1858	01859 G1860	



G1861	G1862 G1863	U1864	A1866	G1867 C1868	G1869	A1871	A1872 G1873	C1874	A1876	A1877	C1879	U1880	C1881 111882	U1883	G1884	A1885 U1886	C1887	G1888 A1889	A1890	G1891 C1892	C1893	C1894 C1895	G1896 G1897	U1898	A1699 A1900	A1901 C1902	G1903	G1904 C1905	G1906	G1908 C1908	C1909 61910	U1911	A1912 A1913	C1914	A1916	U1917 A1918	A1919	C1920				
G1921	01922 01923	C1924	01926 U1926	A1927 A1928	G1929	01931	A1932 G1933	C1934	41936 A1936	A1937	A1936 U1939	U1940	C1941	C1942 U1943	U1944	G1945	01940 C1947	G1948	G1950	U1951	A1953 A1953	G1954 U1955	U1956	C1957 C1958	G1959 A1960	C1961	01902 U1963	G1964 C1065	A1966	C1967 G1968	A1969	A1970 U1971	G1972 C1973	C1974	G1975 U1976	A1977	A1978 U1979	G1980				
A1981	01982 G1983	G1984	C1986	A1987 G1988	G1989	U1991	G1992 U1993	C1994	C1996	C1997	A1996 C1999	C2000	C2001 G2002	A2003	G2004	A 2005 C 2006	U2007	C2008 A2009	G2010	U2011 G2012	A2013	A2014 A2015	U2016 112017	G2018	A2019 A2020	C2021 112022	C2023	G2024 C2025	U2026	62027 U2028	G2029 A 2030	A2031	G2032 A2033	U2034	C2036	A2037	u2039	G2040				
U2041	A2042 C2043	C2044	G2046	C2047 G2048	G2049	A2051	A2052 G2053	A2054	G2056	G2057	A2058 A2059	A2060	G2061 A2062	C2063	C2064	C2066	G2067	U2068 G2069	A2070	A2071 C2072	C2073	U20/4 U2075	U2076 A2077	C2078	020/9 A2080	U2081 A2082	G2083	C2084 U2085	U2086	4208/ A2088	C2089 42090	C2091	U2092 G2093	A2094	C2096	A2097	U2099	G2100				
A2101		C2104	U2105	G2107	A2108 U2109	G2110	U2111 G2112	U2113 A2114	G2115	G2116	A2117		G2120	G2121	U2122	62123	G2125	A2126	G2127	G2128	C2129	U2131	U2132 G2133	A2134	A2135	U2137	G2138	U2139	G2140	A2142	C2143	C2145	C2146	A2147	U2149	C2150	U2151	G2152 C9153	A2154	U2155 G2156	G2157	A2158
C2161	G2162 A2163	C2164	C2165	U2167	G2168	A2169	A2171	A2173	C2174	C2175	C2177	C2178	C2179	U2180	U2181	02102 A2183	A2184	U2185	U2187	U2188 II2189	G2190	A2191 U2192	G2193	U2195	C2196 U2197	A2198	C2200	G2201	U2203	G2204 A2205	C2206	C2208	G2209 U2210	A2211	A2212	02213 C2214	C2215	G2216 G2217	G2218	U2220		
G2221	G2223 G2223	G2224	C2226	A2227 G2228	U2229	U2231	C2232 U2233	G2234	u2236	G2237	G2239	U2240	A2241 G2242	U2243	U2244	0.2246 G.2246	A2247	C2248 U2249	G2250	G2251 G2252	G2253	G2255	G2256 112257	C2258	02260 C2260	C2261 112262	C2263	C2264 U2265	A2266	A226/ A2268	G2269 A2270	G2271	U2272 A2273	A2274	G2276	G2277	G2279	<mark>G2280</mark>				
A2281	G2283 C2283	A2284	G2286	A2287 A2288	G2289	U2291	U2292 G2293	G2294	U2296	A2297	A2298 U2299	C2300	C2301 U2302	G2303	G2304	02306 C2306	62307	G2308 A2309	C2310	A2311	C2313	A2314 G2315	G2316	A2317 G2318	G2319 U2320	U2321	A2322 G2323	U2324 C2325	C2326	A2327 A2328	U2329	G2331 G2331	C2332 40333	U2334	A2335 A2336	G2337	C2338 C2339	A2340				
G2341 A2281	U2342 G2282 U2343 C2283	U2344 A2284	42346 G2286	C2347 A2287 U2348 A2288	G2349 G2349 G2289	G2351 U2291	A2352 U2292 G2353 G2293	C2354 G2294	U2356 U2296	G2357 A2297	A2300 A2290 C2359 U2299	G2360 C2300	G2361 C2301 C2362 II2302	G2363 G2303	C2364 G2304	G2366 C2306 C2306	G2367 G2307	C2368 C2308 A2369 A2309	G2370 C2310	G2371 A2311 U2372 HD217	G2373 C2313	C2374 A2314 G2375 G2315	A2376 G2316 A2377	A2378 G2318 G2318	G2380 G2319 C2380 U2320	A2381 U2321 (2382 02382	G2383 G2323	U2384 C2385 C2385	A2386 C2326	U238/ A2327 A2388 A2328	G2389 U2329 112390	G2391 G2331	A2392 C2332 U2393 A7333	C2394 U2334	G2396 A2336 G2396 A2336	G2397 112308	G2399 C2338 C2339 C2339	G2400 A2340				
U2401 G2341 A2281	U2402 C2342 U2343 C283	U2404 U2344 A2284	G2405 G2345 G2286 A2346 G2286	A2407 C2347 A2287 TT2A66 U2348 A2288	(22409 (22409 (22409) (22409) (22249) (22289) (22289) (22289) (22289) (22289)	G2410 C2200 G2350 A2411 G2351 U2291	A2412 A2852 U2292 C2413 G2353 G2293	G2414 C2354 G2294	C2415 C2350 C2290 C2290 C2290 C2290 C2296 C2216 C2216 C2216 C2216 C2216 C2216 C2296	C2417 G2357 A2297	A2418 A2556 A2256 119419 C2359 U2299	C2420 G2860 C2300	G2421 G2361 C2301 C2302 C2367 119302	C2422 12423 G2363 G2303	C2424 C2364 G2304	A2425 G2365 U2305 A2366 C2306	62367 C2427 G2367	G2428 C2368 G2308 C2369 A2309	42429 A2430 G2370 C2310	U2431 G2371 A2311 10430 U2372 III0310	A2433 G2373 C2313	A2434 C2374 A2314 A2435 G2375 G2315	G2436 A2376 G2316 A2377 A2377	02437 A2378 A2318 A2318 A2318	A2439 42379 62319 C2440 C2380 U2320	U2441 A2381 U2321 00440 G2382 02382	C2443 C2383 C2323	C2444 U2384 U2324 C2345 C2385 C2335	C2326 C2446 W0007	G2447 02387 A2327 A2448 A2388 A2328	U2449 4 C2389 U2329	A2450 G2391 G2331 A2451 G2331	C2452 A2392 C2332 C2452 U2393 A7333	A2453 C2394 U2334 G2454 C2394 U2334	G2455 C2399 A2335 Contes G2396 A2336	U2457 G2397 G2337	G2458 G2339 C2338 A2459 G2399 C2339	U2460 G2400 A2340				
A2461 U2401 G2341 A2281	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2464 U2404 U2344 A2284 C2345	C2466 C2406 A2346 C2286	C2467 A2407 C2347 A2287 A2468 TTAAAS U2348 A2288	A2469 02400 02349 02289 02469 022409 02249 02289	42471 62410 62351 02291 42291 02291	G2472         A2412         A2352         U2292           U2473         C2413         G2353         G2293	U2474 G2414 C2354 G2294	42476 G2415 42399 42399 42299 A2476 C2416 U2356 U2296	U2477 C2417 G2357 A2297	A2476 A2418 A2306 A2298 U2479 IID419 C2359 U2299	C2480 C2420 G2360 C2300	G2481 G2421 G2361 C2301 A2482 C2301 G2362 C2301	C2483 C2423 C2363 C2303	G2484 C2424 C2364 G2304	(22485 A2425 (22565 02305 (22486 A2366 C2306	G2487 C2427 G2367 G2307	G2488 G2428 C2368 G2308 U2489 A2309 A2369 A2309	G2490 A2430 G2370 C2310	U2491 U2431 G2371 A2311 U2492 Acres U2372 Horder	U2493 A2433 G2373 C2313	<sup>62494</sup> A2434 C2374 A2314 G2495 A2435 G2375 G2315	C2496 G2436 A2376 G2316 A2497 A2377 A2377	C2498 U2438 A2378 G2318 G2318	U2500 C2440 C2380 U2320	C2501 U2441 A2381 U2321 (22502 02441 G2382 02321	A2503 C2443 G2383 G2323 G2323	02504 G2444 02384 02324 02324 02324 02324 02325 02325	U2506 4 G2446 A2386 C2326	C2607 C2647 U238/ A2327 C2508 A2448 A238 A2328	G2509 U2449 ♦ G2389 U2329 U2329 U2329 U2329	C2510 A2450 C2510 G2331 G2331 G2331 G2331	C2512 C2452 A2392 C2332 A2513 C2452 U2393 A2833	U2514 C2454 C2394 U2334	C2515 C2455 C2395 A2335 A2516 Connee C2396 A2336	C2517 U2457 G2397 G2337 U2457 U2457 G2337	A2518 C2458 C2338 U2519 A2459 C2339 C2339 C2339	C2520 02460 G2400 A2340				
C2521 A2461 U2401 C2521 A2281	U2522 C2452 U2402 U2402 C2342 G2282 G2523 C2463 C9463	G2524 G2464 U2404 U2344 A2284	02526 02406 02406 02286 02286 02286	C2527 C2467 A2407 C2347 A2287 U2528 A2468 TDAA00 U2548 A2288	(2252) A2469 (22409 (2249) (2289) (2289) (22409 (22409) (22409	A2531 A2471 A2411 G2410 C2291 U2291	G2632         G2472         A2412         A2352         U2292           U2633         U2473         C20413         G2353         G2293	A2534 U2474 02414 C2354 G2294	G2536 A2476 C2415 U2356 U2296	U2537 U2477 C2417 G2357 A2297	C2539 A2479 A2418 A2356 A2295 C2539 U2479 IID419 C2559 U2299	C2540 C2480 C2420 G2360 C2300	A2541 G2481 G2421 G2361 C2301 42542 A2482 C2302 C2362 ID302	G2543 C2483 U2423 G2363 G2303	G2544 G2484 C2424 C2364 G2304	G2545 G2485 A2425 G2365 U2305 112546 C2486 C2486 C2306	A2547 G2487 C2427 G2367 G2307	U2548 G2488 G2428 C2368 G2308 G2549 U2489 G2428 A2309	G2550 G2490 A2430 G2370 C2310	C2551 U2491 U2431 G2371 A2311 U2552 U2492 A3745 U2872 H1940	C2553 U2493 A2433 C2373 C2313 C2313	02554 62494 A2434 C2374 A2314 02555 G2495 A2435 G2315 G2315	C2556 C2496 C2436 A2376 C2316 (2557 A2497 C2436 A2377 C2316	C2558 C2498 U2438 A2378 G2318 G2318	42560 U2500 C2499 A2439 42579 G2319 A2560 U2500 C2440 C2380 U2320	U2661 C2501 U2441 A2381 U2321 U2662 C2502 C2440 C2382 C2440	U2563 A2503 C2443 G2383 G2323	A2564 U2504 C2444 U2384 U2324 A2565 C2505 C2445 C2385 C3355	A2566 U2506 C2446 A2386 C2326	G2557 G2447 U2587 A2327 U2568 G2508 A2448 A2388 A2328	(2569 (2569 U2449 ♦ (2389 U2329 U23	U2571 U2511 A2450 C2391 C2330 U2571 U2511 A2451 C2331 C2331	A2572 C2512 C2452 A2392 C2332 C2573 A2513 C2452 U2393 A3543	C2574 U2514 C2454 C2394 U2334	02513         02515         02455         02395         A2335           62576         A2516         72356         A2336         A2335	A2577 C2517 C2517 U2457 C2397 C2337	C2579 02519 02458 02339 02338 02539 02339 022339 022339 022339 022339 022339 022339 022339 022339 022339 022339	U2580 C2520 U2460 A2340				
G2581 C2521 A2461 U2401 G2341 A2281	G2583 G2623 C2463 U2402 C2342 U2283 G2583 G2623 C2463 C2463 C2483	U2584 C2524 C2464 U2404 U2344 A2284	U2585 V 42625 C2466 A2405 42296 G2286 U2586	A2687 C25627 C2467 A2407 C2347 A2287 C2562 A2468 T02348 A2288 A2288	42600 (2529 (2469 (22409 (2289 (2289 (2289 (22289 (22289 (222409 (2228)))))))))))))))))	A2590 A2500 4250 42410 62351 42471 42411 62351 U2291	G2592         G2472         A2412         A2452         U2292           ΠΡ693         U2533         U2473         C2413         G2353         G293	C2594 A2584 U2474 C2414 C2354 C2294 c2294 c2294 c2294 c2294	Q2595         V2510         V2510         Q2415         V2300         V2230           117566         Q2536         A2476         C2416         U2356         U2296	C2597         U2637         U2477         C2417         C2367         A2267           C2597         00170         00170         00170         00000	A2598 U2536 A2476 A2418 A2596 A2296 C2539 U2479 I17419 C2359 U229	A2600 C2540 C2480 C2420 C2450 C2300	C2601 A2641 G2481 G2421 G2361 C2301 A262 A2482 C2421 G2362 ID302	A2602         C2643         C2483         C2483         C2483         C2483         C2283         C22803	U2604 G2544 G2484 G2424 G2364 G2304	U2605 G22455 A2425 G2260 U2605 00000 112646 C2486 0000 A2366 C2306	C2000 A2547 G2487 C2427 G2367 G2307	C2608 U2548 C2488 C2428 C2368 C2368 C2308 100000 C2549 U2489 C2400 A2369 A2309	C2610 C2550 C2490 A2430 C2310 C2310	C2611 C2651 U2491 U2431 G2371 A2311 02622 U2492 A2420 U2432 U2492	U2613 U2493 A2433 G2573 C2313 C2313	A2614 U2554 U2554 U2554 A2434 U2515 U2515 G2315 U2515 U2555 G2495 A2435 G2375 G2315	C2616 C2656 C2496 C2436 A2376 C2316 (22616 A247 A247 A247 A247 A247	02517 02517 02518 02498 02438 A2317 02318 02318	C2619 C2509 C2499 A2439 G2319 C2620 A2560 U2500 C2440 C2380 U2320	C2621         U2561         C2501         U2441         A2381         U2321           mmon         17562         C2502         mmon         C2382         mmon	02022 U2563 A2508 C2443 G2388 G2323	C2624 A2564 U2504 C2444 U2384 U2324 C2625 G2505 C2415 C2385 C2335	C2626 A2566 U2506 C2446 A2386 C2326	C2627 U2567 C2607 C2447 U2587 A237 C2628 C2568 C2568 A248 A2388 A2328	U2629 C2569 C2569 U2449 C2389 U2329 C2570 C2569 U2449 C2389 U2329	G2631 U2571 U2511 A2450 G2391 G2331 G2331 G2331	A2632 A2572 C2612 C2452 A2392 C2332 C2633 C2673 A2513 C2452 U2393 D9483	A2634 C24514 C2464 C2394 U2334	A2635 C2019 C2515 C2455 C2396 A2335 C2636 C2576 A2516 C2455 C2396 A2336	U2637 A2577 C2517 U2457 C2397 G2337 C2578 C2517 U2457 C2397 G2337	C2638 C2579 C2579 C2519 C2458 C2339 C2338 C2339 C2339 C2339 C2339 C2339	G2640 U2580 C2520 U2460 A2340				









• Molecule 46: 50S RIBOSOMAL PROTEIN L16







 $\bullet$  Molecule 55: 50S RIBOSOMAL PROTEIN L25







# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	263000	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	38900	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.760	Depositor
Minimum map value	-0.510	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	361.62, 363.82498, 361.62	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.2375, 1.23	Depositor



# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:  $5\mathrm{MU}$ 

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).

Mal	Chain		Bond lengths		Bond angles
NIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	AA	3.37	4837/36762~(13.2%)	3.72	8282/57350~(14.4%)
2	AB	1.71	14/1735~(0.8%)	2.05	53/2338~(2.3%)
3	AC	1.73	20/1651~(1.2%)	2.05	55/2225~(2.5%)
4	AD	1.80	24/1665~(1.4%)	2.05	48/2227~(2.2%)
5	AE	1.73	17/1118~(1.5%)	1.97	27/1504~(1.8%)
6	AF	1.77	7/835~(0.8%)	1.96	17/1128~(1.5%)
7	AG	1.82	18/1187~(1.5%)	2.01	40/1591~(2.5%)
8	AH	1.79	10/989~(1.0%)	2.07	29/1326~(2.2%)
9	AI	1.97	21/1034~(2.0%)	2.09	33/1375~(2.4%)
10	AJ	1.78	11/796~(1.4%)	1.89	15/1077~(1.4%)
11	AK	1.75	7/893~(0.8%)	1.96	18/1205~(1.5%)
12	AL	1.85	13/969~(1.3%)	1.98	28/1300~(2.2%)
13	AM	1.73	12/884~(1.4%)	2.02	28/1181~(2.4%)
14	AN	1.80	6/785~(0.8%)	1.92	19/1043~(1.8%)
15	AO	1.77	11/724~(1.5%)	1.90	24/966~(2.5%)
16	AP	1.84	9/648~(1.4%)	2.16	26/870~(3.0%)
17	AQ	1.73	4/657~(0.6%)	1.93	18/881~(2.0%)
18	AR	1.74	6/462~(1.3%)	2.28	16/621~(2.6%)
19	AS	1.78	8/652~(1.2%)	2.15	26/877~(3.0%)
20	AT	1.66	4/671~(0.6%)	1.93	17/888~(1.9%)
21	AU	1.82	6/430~(1.4%)	2.16	13/570~(2.3%)
22	AV	2.38	76/1820~(4.2%)	2.84	256/2836~(9.0%)
23	AX	1.81	4/264~(1.5%)	2.14	19/407~(4.7%)
24	AZ	1.97	1/99~(1.0%)	1.94	5/137~(3.6%)
25	B0	1.75	7/635~(1.1%)	2.27	19/848~(2.2%)
26	B1	1.72	5/510~(1.0%)	1.94	14/677~(2.1%)
27	B2	1.75	4/453~(0.9%)	1.86	10/605~(1.7%)
28	B3	1.82	6/450~(1.3%)	2.19	16/599~(2.7%)
29	B4	1.63	4/416~(1.0%)	2.02	13/554~(2.3%)
30	B5	1.56	11/1748~(0.6%)	1.95	40/2355~(1.7%)
31	B6	1.85	4/380 (1.1%)	2.31	17/498(3.4%)
32	B7	1.68	4/513~(0.8%)	2.03	12/676~(1.8%)



Mal	Chain	-	Bond lengths	Bond angles $\# Z  > 5$		
WIOI	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
33	B8	1.83	4/303~(1.3%)	2.01	7/397~(1.8%)	
34	BA	3.34	356/2753~(12.9%)	3.78	615/4288~(14.3%)	
35	BB	3.39	9308/69800~(13.3%)	3.73	15832/108892~(14.5%)	
36	BC	1.81	24/2121~(1.1%)	2.05	60/2852~(2.1%)	
37	BD	1.77	16/1586~(1.0%)	2.01	31/2134~(1.5%)	
38	BE	1.69	8/1571~(0.5%)	1.97	41/2113~(1.9%)	
39	BF	1.73	14/1444~(1.0%)	2.17	40/1937~(2.1%)	
40	BG	1.76	13/1335~(1.0%)	2.04	28/1803~(1.6%)	
41	BH	1.74	11/1122~(1.0%)	2.05	35/1515~(2.3%)	
42	BI	0.62	2/1046~(0.2%)	0.56	1/1410~(0.1%)	
43	BJ	1.77	12/1152~(1.0%)	2.04	30/1551~(1.9%)	
44	BK	1.76	13/939~(1.4%)	1.99	23/1257~(1.8%)	
45	BL	1.78	10/1054~(0.9%)	1.94	28/1403~(2.0%)	
46	BM	1.83	9/1093~(0.8%)	2.07	30/1460~(2.1%)	
47	BN	1.76	12/973~(1.2%)	2.22	32/1301~(2.5%)	
48	BO	1.79	15/902~(1.7%)	2.02	24/1209~(2.0%)	
49	BP	1.68	5/929~(0.5%)	2.03	20/1242~(1.6%)	
50	BQ	1.89	15/960~(1.6%)	2.11	29/1278~(2.3%)	
51	BR	1.80	11/829~(1.3%)	2.03	23/1107~(2.1%)	
52	BS	1.71	7/864~(0.8%)	2.16	34/1156~(2.9%)	
53	BT	1.69	5/744~(0.7%)	1.99	18/994~(1.8%)	
54	BU	1.73	3/761~(0.4%)	2.02	25/1013~(2.5%)	
55	BW	1.79	$1\overline{3}/766~(1.7\%)$	2.05	18/1025~(1.8%)	
56	BY	1.73	3/603~(0.5%)	2.11	$\overline{23/797}$ (2.9%)	
All	All	2.98	$1508\overline{0}/158485~(9.5\%)$	3.34	26300/236869~(11.1%)	

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	AA	0	740
2	AB	0	5
3	AC	0	7
4	AD	0	11
5	AE	0	5
6	AF	0	3
7	AG	0	3
8	AH	0	3
9	AI	0	7
10	AJ	0	6



a 1	C		
Continued	trom	previous	page
• • • • • • • • • • •	J	<i>r</i> · · · · · · · · · · · · · · · · · · ·	r ~g ····

Mol	Chain	#Chirality outliers	#Planarity outliers
11	AK	0	3
12	AL	0	5
13	AM	0	9
14	AN	0	3
15	AO	0	6
16	AP	0	4
17	AQ	0	1
18	AR	0	5
19	AS	0	4
20	AT	0	3
22	AV	0	13
23	AX	0	4
25	B0	0	4
26	B1	0	1
28	B3	0	2
29	B4	0	3
30	B5	0	6
31	B6	0	3
32	B7	0	1
34	BA	0	50
35	BB	0	1343
36	BC	0	8
37	BD	0	6
38	BE	0	5
39	BF	0	10
40	BG	0	3
41	BH	0	1
43	BJ	0	4
44	BK	0	5
45	BL	0	1
46	BM	0	3
47	BN	0	5
48	BO	0	2
49	BP	0	5
50	BQ	0	5
51	BR	0	3
52	BS	0	1
53	BT	0	1
54	BU	0	2
55	BW	0	4
56	BY	0	5
All	All	0	2342



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BB	1403	A	N9-C4	21.34	1.50	1.37
35	BB	1301	A	N7-C5	-20.38	1.27	1.39
1	AA	930	С	N1-C6	19.80	1.49	1.37
1	AA	816	А	N7-C5	-19.29	1.27	1.39
35	BB	1821	А	N9-C4	19.18	1.49	1.37

The worst 5 of 15080 bond length outliers are listed below:

The worst 5 of 26300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	AA	753	A	N1-C6-N6	30.52	136.91	118.60
35	BB	666	А	N1-C6-N6	26.10	134.26	118.60
35	BB	533	G	N1-C6-O6	25.90	135.44	119.90
1	AA	242	G	C5-C6-O6	-25.60	113.24	128.60
35	BB	1014	A	N1-C6-N6	25.57	133.94	118.60

There are no chirality outliers.

5 of 2342 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	11	G	Sidechain
1	AA	12	U	Sidechain
1	AA	5	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	A	Sidechain

## 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16502	183	0
2	AB	1704	0	1732	3	0
3	AC	1624	0	1699	12	0
4	AD	1643	0	1710	5	0
5	AE	1105	0	1148	6	0
6	AF	817	0	808	7	0
7	AG	1174	0	1230	5	0



Conti	nuea fron	<i>i</i> previous	page			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	979	0	1034	1	0
9	AI	1022	0	1070	9	0
10	AJ	786	0	828	3	0
11	AK	877	0	887	9	0
12	AL	955	0	1019	2	0
13	AM	876	0	937	7	0
14	AN	774	0	827	2	0
15	AO	716	0	742	3	0
16	AP	638	0	656	0	0
17	AQ	648	0	691	4	0
18	AR	455	0	478	1	0
19	AS	637	0	665	5	0
20	AT	665	0	714	4	0
21	AU	425	0	449	2	0
22	AV	1649	0	832	21	0
23	AX	236	0	121	10	0
24	AZ	100	0	99	0	0
25	B0	625	0	655	1	0
26	B1	509	0	543	1	0
27	B2	449	0	491	1	0
28	B3	444	0	461	3	0
29	B4	409	0	440	0	0
30	B5	1733	0	1824	4	0
31	B6	377	0	418	3	0
32	B7	504	0	574	5	0
33	B8	302	0	343	0	0
34	BA	2464	0	1246	8	0
35	BB	62321	0	31294	336	0
36	BC	2082	0	2157	14	0
37	BD	1565	0	1616	8	0
38	BE	1552	0	1619	9	0
39	BF	1420	0	1460	9	0
40	BG	1316	0	1364	4	0
41	BH	1111	0	1148	1	0
42	BI	1032	0	1088	118	0
43	BJ	1129	0	1162	8	0
44	BK	930	0	1003	6	0
45	BL	1045	0	1117	6	0
46	BM	1074	0	1157	4	0
47	BN	960	0	1000	2	0
48	BO	892	0	923	2	0
49	BP	917	0	965	4	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BQ	947	0	1022	8	0
51	BR	816	0	839	8	0
52	BS	857	0	922	3	0
53	BT	738	0	807	5	0
54	BU	755	0	807	10	0
55	BW	753	0	780	5	0
56	BY	596	0	610	1	0
All	All	145960	0	98733	840	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 3.

The worst 5 of 840 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
22:AV:35:G:N2	23:AX:18:C:C2	2.08	1.22
42:BI:11:GLN:HG2	42:BI:55:PRO:HB3	1.51	0.91
42:BI:140:GLU:O	42:BI:141:ASP:OXT	1.91	0.89
42:BI:27:LEU:HD23	42:BI:27:LEU:H	1.43	0.82
42:BI:121:ILE:HD13	42:BI:121:ILE:H	1.44	0.82

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	AB	216/218~(99%)	159 (74%)	41 (19%)	16 (7%)	1 13
3	AC	204/206~(99%)	158 (78%)	31 (15%)	15 (7%)	1 13
4	AD	203/205~(99%)	160 (79%)	34 (17%)	9 (4%)	2 22
5	AE	148/150~(99%)	110 (74%)	27 (18%)	11 (7%)	1 13



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erce	entiles	3
6	AF	98/100~(98%)	73 (74%)	18 (18%)	7 (7%)		1	14	
7	AG	148/150~(99%)	109 (74%)	33 (22%)	6 (4%)		3	22	
8	AH	127/129~(98%)	94 (74%)	27 (21%)	6 (5%)		2	21	
9	AI	125/127~(98%)	99 (79%)	21 (17%)	5 (4%)		3	23	
10	AJ	96/98~(98%)	71 (74%)	14 (15%)	11 (12%)		0	6	
11	AK	115/117~(98%)	96 (84%)	14 (12%)	5 (4%)		2	22	
12	AL	121/123~(98%)	100 (83%)	12 (10%)	9 (7%)		1	13	
13	AM	111/113 (98%)	80 (72%)	19 (17%)	12 (11%)		0	7	
14	AN	92/96~(96%)	57 (62%)	22 (24%)	13 (14%)		0	4	
15	AO	86/88~(98%)	73 (85%)	11 (13%)	2 (2%)		6	33	
16	AP	78/80~(98%)	62 (80%)	10 (13%)	6 (8%)		1	12	
17	AQ	78/80~(98%)	65 (83%)	7 (9%)	6 (8%)		1	12	
18	AR	53/55~(96%)	42 (79%)	8 (15%)	3 (6%)		1	17	
19	AS	77/79~(98%)	61 (79%)	13 (17%)	3 (4%)		3	23	
20	AT	83/85~(98%)	68 (82%)	13 (16%)	2 (2%)		6	33	
21	AU	49/51~(96%)	41 (84%)	5 (10%)	3 (6%)		1	16	
24	AZ	18/20~(90%)	16 (89%)	1 (6%)	1 (6%)		2	18	
25	B0	75/77~(97%)	52 (69%)	20 (27%)	3 (4%)		3	23	
26	B1	61/63~(97%)	45 (74%)	14 (23%)	2(3%)		4	26	
27	B2	56/58~(97%)	49 (88%)	7~(12%)	0	1	.00	100	
28	B3	54/56~(96%)	42 (78%)	9~(17%)	3~(6%)		2	18	
29	B4	48/50~(96%)	39 (81%)	7~(15%)	2 (4%)		3	22	
30	B5	232/234~(99%)	190 (82%)	37~(16%)	5 (2%)		6	35	
31	B6	44/46~(96%)	29~(66%)	11 (25%)	4 (9%)		1	10	
32	B7	62/64~(97%)	52 (84%)	5 (8%)	5 (8%)		1	12	
33	B8	36/38~(95%)	30 (83%)	4 (11%)	2(6%)		2	18	
36	BC	269/271~(99%)	209 (78%)	47 (18%)	13 (5%)		2	20	
37	BD	207/209 (99%)	149 (72%)	37 (18%)	21 (10%)		0	9	
38	BE	199/201~(99%)	161 (81%)	23 (12%)	15 (8%)		1	13	
39	BF	176/178~(99%)	131 (74%)	26 (15%)	19 (11%)		0	7	
40	BG	171/176 (97%)	134 (78%)	28 (16%)	9 (5%)		2	19	-



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erc	entiles
41	BH	147/149~(99%)	111 (76%)	31 (21%)	5(3%)		3	26
42	BI	139/141~(99%)	113 (81%)	21 (15%)	5 (4%)		3	25
43	BJ	140/142~(99%)	106 (76%)	24 (17%)	10 (7%)		1	14
44	BK	119/121~(98%)	95~(80%)	14 (12%)	10 (8%)		1	11
45	BL	141/143~(99%)	115 (82%)	16 (11%)	10 (7%)		1	14
46	BM	134/136~(98%)	105 (78%)	21 (16%)	8 (6%)		1	16
47	BN	118/120~(98%)	96 (81%)	16 (14%)	6 (5%)		<b>2</b>	19
48	BO	114/116~(98%)	98 (86%)	14 (12%)	2(2%)		8	40
49	BP	112/114~(98%)	85 (76%)	19 (17%)	8 (7%)		1	14
50	BQ	115/117~(98%)	84 (73%)	21 (18%)	10 (9%)		1	11
51	BR	101/103~(98%)	80 (79%)	13 (13%)	8 (8%)		1	12
52	BS	108/110~(98%)	76 (70%)	21 (19%)	11 (10%)		0	8
53	BT	91/93~(98%)	60 (66%)	25 (28%)	6 (7%)		1	15
54	BU	94/102~(92%)	71 (76%)	16 (17%)	7 (7%)		1	13
55	BW	92/94~(98%)	76 (83%)	10 (11%)	6 (6%)		1	15
56	BY	77/79~(98%)	46 (60%)	18 (23%)	13 (17%)		0	3
All	All	5858/5971 (98%)	4523 (77%)	956 (16%)	379 (6%)		2	15

5 of 379 Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
3	AC	17	TRP
3	AC	116	ALA
5	AE	11	GLN
5	AE	17	VAL
9	AI	58	GLU

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	entiles
2	AB	180/180~(100%)	171~(95%)	9~(5%)	24	49
3	AC	170/170~(100%)	158 (93%)	12 (7%)	14	39
4	AD	172/172~(100%)	165~(96%)	7 (4%)	30	55
5	AE	113/113 (100%)	103 (91%)	10 (9%)	10	31
6	AF	87/87~(100%)	85~(98%)	2(2%)	50	70
7	AG	123/123~(100%)	120 (98%)	3(2%)	49	69
8	AH	104/104~(100%)	99~(95%)	5(5%)	25	51
9	AI	105/105~(100%)	100 (95%)	5(5%)	25	51
10	AJ	86/86~(100%)	81 (94%)	5~(6%)	20	45
11	AK	90/90~(100%)	86 (96%)	4 (4%)	28	53
12	AL	103/103~(100%)	98~(95%)	5 (5%)	25	50
13	AM	91/91~(100%)	89~(98%)	2(2%)	52	71
14	AN	79/79~(100%)	76~(96%)	3 (4%)	33	57
15	AO	76/76~(100%)	69~(91%)	7 (9%)	9	29
16	AP	65/65~(100%)	62~(95%)	3~(5%)	27	52
17	AQ	74/74~(100%)	68~(92%)	6 (8%)	11	35
18	AR	48/48 (100%)	44 (92%)	4 (8%)	11	34
19	AS	70/70~(100%)	64 (91%)	6 (9%)	10	32
20	AT	65/65~(100%)	64 (98%)	1 (2%)	65	80
21	AU	44/44~(100%)	38~(86%)	6 (14%)	3	17
25	B0	67/67~(100%)	65~(97%)	2(3%)	41	63
26	B1	55/55~(100%)	50 (91%)	5 (9%)	9	30
27	B2	48/48 (100%)	47 (98%)	1 (2%)	53	72
28	B3	47/47~(100%)	46 (98%)	1 (2%)	53	72
29	B4	45/45~(100%)	42 (93%)	3 (7%)	16	40
30	B5	181/181 (100%)	175 (97%)	6(3%)	38	61
31	B6	38/38~(100%)	33~(87%)	5 (13%)	4	18
32	B7	51/51~(100%)	48 (94%)	3~(6%)	19	45
33	B8	34/34~(100%)	34 (100%)	0	100	100
36	BC	216/216~(100%)	204 (94%)	12 (6%)	21	46
37	BD	164/164~(100%)	146 (89%)	18 (11%)	6	22
38	BE	165/165~(100%)	157~(95%)	8 (5%)	25	51



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
39	BF	149/149~(100%)	143~(96%)	6 (4%)	31	55
40	BG	136/137~(99%)	125~(92%)	11 (8%)	11	35
41	BH	114/114~(100%)	110 (96%)	4 (4%)	36	59
42	BI	109/109~(100%)	104~(95%)	5 (5%)	27	52
43	BJ	116/116~(100%)	112~(97%)	4 (3%)	37	60
44	BK	102/102~(100%)	92~(90%)	10 (10%)	8	26
45	BL	102/102~(100%)	98~(96%)	4 (4%)	32	56
46	BM	109/109~(100%)	104~(95%)	5 (5%)	27	52
47	BN	100/100~(100%)	96~(96%)	4 (4%)	31	55
48	BO	86/86~(100%)	84 (98%)	2 (2%)	50	70
49	BP	99/99~(100%)	96~(97%)	3(3%)	41	63
50	BQ	89/89~(100%)	83~(93%)	6 (7%)	16	40
51	BR	84/84~(100%)	76~(90%)	8 (10%)	8	28
52	BS	93/93~(100%)	87~(94%)	6 (6%)	17	42
53	BT	80/80~(100%)	68~(85%)	12 (15%)	3	15
54	BU	81/83~(98%)	76~(94%)	5 (6%)	18	43
55	BW	78/78~(100%)	73~(94%)	5~(6%)	17	42
56	BY	59/59~(100%)	54 (92%)	5 (8%)	10	33
All	All	4842/4845~(100%)	4568 (94%)	274 (6%)	24	45

5 of 274 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	BQ	40	LYS
51	BR	78	ARG
54	BU	14	THR
19	AS	60	PHE
19	AS	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
43	BJ	40	HIS
51	BR	91	GLN
43	BJ	80	HIS



Continued from previous page...

Mol	Chain	Res	Type
49	BP	76	HIS
54	BU	39	ASN

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1530~(99%)	269~(17%)	34~(2%)
22	AV	76/77~(98%)	15 (19%)	0
23	AX	10/11~(90%)	8 (80%)	0
34	BA	112/117~(95%)	16 (14%)	2(1%)
35	BB	2902/2903~(99%)	471 (16%)	56 (1%)
All	All	4629/4638 (99%)	779~(16%)	92 (1%)

5 of 779 RNA backbone outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	AA	7	А
1	AA	9	G
1	AA	15	G
1	AA	31	G
1	AA	32	А

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BB	1332	G
35	BB	2131	U
35	BB	1459	G
35	BB	1808	А
35	BB	2145	С

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection.



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	$\mathbf{les}$
WIOI	wor Type Chain Kes	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
22	5MU	AV	54	22	18,21,23	0.64	0	26,30,35	0.71	1 (3%)

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
22	AV	54	5MU	O4'-C1'-N1	2.42	113.90	108.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:



Mol	Chain	Number of breaks
54	BU	1
14	AN	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BU	4:ILE	С	6:ARG	Ν	4.65
1	AN	35:ALA	С	40:ARG	Ν	4.56



#### Map visualisation (i) 6

This section contains visualisations of the EMDB entry EMD-1657. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

#### Orthogonal projections (i) 6.1

#### 6.1.1Primary map



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

#### 6.2Central slices (i)

#### 6.2.1Primary map



X Index: 147

Y Index: 147



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

### 6.3 Largest variance slices (i)

### 6.3.1 Primary map



X Index: 152

Y Index: 155

Z Index: 136

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

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

### 6.4.1 Primary map



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



### 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.6 Mask visualisation (i)

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



# 7 Map analysis (i)

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

## 7.1 Map-value distribution (i)



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



### 7.2 Volume estimate (i)



The volume at the recommended contour level is  $1327 \text{ nm}^3$ ; this corresponds to an approximate mass of 1198 kDa.

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



### 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.172  $\text{\AA}^{-1}$ 



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1657 and PDB model 4V5H. Per-residue inclusion information can be found in section 3 on page 14.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



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



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).



### 9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

$\mathbf{Chain}$	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.6880	0.1890
AA	0.7560	0.2050
AB	0.3910	0.1500
AC	0.4960	0.1420
AD	0.4610	0.1350
AE	0.5320	0.1500
AF	0.6060	0.1760
AG	0.4700	0.1610
AH	0.5290	0.1450
AI	0.4710	0.1220
AJ	0.3250	0.1070
AK	0.5430	0.1610
AL	0.5160	0.1630
AM	0.5490	0.1550
AN	0.5610	0.1400
AO	0.5640	0.1650
AP	0.5310	0.1390
AQ	0.5680	0.1720
AR	0.5870	0.1720
AS	0.5860	0.1570
AT	0.5280	0.1460
AU	0.3500	0.1570
AV	0.5620	0.1430
AX	0.2630	0.1480
AZ	0.4900	0.3070
BO	0.5410	0.1620
B1	0.5510	0.1390
B2	0.5810	0.1740
B3	0.5650	0.1600
B4	0.5760	0.1680
B5	0.0180	-0.0010
B6	0.4650	0.1340
B7	0.5580	0.1530
B8	0.5620	0.1810
BA	0.8170	0.2140



Chain	Atom inclusion	Q-score
BB	0.7850	0.2140
BC	0.5570	0.1700
BD	0.5980	0.1590
BE	0.4930	0.1400
BF	0.5940	0.1600
BG	0.6720	0.1850
BH	0.2460	0.1340
BI	0.2170	0.0320
BJ	0.6080	0.1750
BK	0.5070	0.1660
BL	0.5340	0.1610
BM	0.5540	0.1740
BN	0.5570	0.1360
BO	0.6230	0.1600
BP	0.5640	0.1720
BQ	0.5560	0.1160
BR	0.6200	0.1840
BS	0.5420	0.1360
BT	0.5230	0.1380
BU	0.5570	0.1560
BW	0.6440	0.1700
BY	0.5190	0.1080

