

wwPDB EM Validation Summary Report (i)

Feb 22, 2024 – 08:02 PM EST

PDB ID 4V66: EMDB ID : EMD-1056 Title : Structure of the E. coli ribosome and the tRNAs in Post-accommodation state Authors Devkota, B.; Caulfield, T.R.; Tan, R.-Z.; Harvey, S.C. : Deposited on 2008-08-03 : 9.00 Å(reported) Resolution : Based on initial models 1EHZ, 2I2P :

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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
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

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 9.00 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	EM structures
	(#Entries)	(#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							
				64%	-						
1	AA	76	22%	37	39%	•					
				54%							
1	AE	76	22%		62%		16%				
				57%							
1	AP	76	21%		53%		25% •				
			10%								
2	AM	20	15%	30%		55%					
				66%							
3	A1	1530	15%	47%		3	8%				
				70%							
4	AB	241		61%		23%	5% 10%				
				46%							
5	AC	129		57%		26%	5% • 9%				



Conti	nued from	n previous f	page		
Mol	Chain	Length	Quality of	chain	
			73%		
6	AD	124	56% 53%	31%	10% ••
7	AF	118	53%	35%	8% • •
8	AG	101	65%	24%	• • 5%
9	AH	89	62%	30%	6% ••
10	AI	82	57%	34%	9%
11	AJ	84	56%	30%	8% • 5%
12	AK	75	25% 36% 29%	8%	27%
13	AL	92	51%	24% 9%	. 14%
1/	AN	87	57%		- 17/0 60/
15		01	28%	20%	0% •
10	AO	233	61% 42%	23%	•• 12%
16	AQ	71	37% 27% 53%	7% •	28%
17	AR	206	64%	28%	7%
18	AS	159	62% 53%	25%	8% 6%
19	AT	135	42% 24%	6 7% .	26%
20	AU	179	48%	29% 6% •	16%
21	AV	130	62%	31%	5% ••
22	AW	130	58%	29%	9% ••
23	AX	103	59%	27%	8% • 5%
24	BA	117	66% 20% 44%	36%	
25	BB	2903	55% 15% 43%	42%	
26	BC	94	72% 67%	31%	, 0 •
27	BD	123	57%	32%	
28	BE	144	60%	210/	129/
20		190	63%	31%	12% •
29	BF	136	55% 39%	29%	12% •
30	BG	127	55%	36%	9%



Mol	Chain	Length	Quality of a	chain	
31	BH	117	55%	33%	
			52%	5570	
32	BI	115	61%	28%	9% ••
33	BJ	118	58%	28%	13% ••
34	BK	103	92%	200/	1.00/
- 04	DR	105	50% 46%	39%	10% •
35	BL	110	59%	30%	10% •
36	BM	99	60%	30%	7% •
97	DN	270	59%		
- 57	DN	270	50%	36%	11% ••
38	BO	103	53%	29%	15% ••
39	BP	85	46%	45%	7% ••
40	DO	6.2	51%		
40	BQ	63	<u> </u>	29%	8% •
41	BR	59	63%	25%	7% • •
42	BS	70		33%	7%
			44%	5570	770
43	BT	57	44%	39%	12% • •
44	BU	54	65%	26%	9%
45	BV	46	50%	20%	0%
10	DV	10	69%	5078	578 •
46	BW	64	45%	33% 16	% 6%
47	BX	38	55%	34%	11%
18	BV	200	38%	20%	00/
40	DI	209	58%	30%	9% •
49	BZ	213	68% 72%	25%	6% •
50	B1	201	54%	33%	11% •
51	Do	170	33%		
- 51	D2	178	58%	33%	8% •
52	B3	177	67%	27%	• ••
53	B4	149	70%	26%	·
F 4	Dr	140	38%		
54	R2	142	70%	23%	5% ••
55	B6	140	57%	26%	14% •





2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 149248 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 A/T, P and E-site tRNAs.

Mol	Chain	Residues		A	toms		AltConf	Trace	
1	AA	75	Total	C 715	N 288	0 523	Р 74	0	0
1	AP	75	Total 1600	715 C 715	200 N 288	$\begin{array}{r} 523 \\ \hline 0 \\ 523 \end{array}$	74 P 74	0	0
1	AE	76	Total 1622	C 725	N 293	0 529	Р 75	0	0

• Molecule 2 is a RNA chain called mRNA model.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AM	20	Total 397	C 180	N 40	0 158	Р 19	0	0

• Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues		I		AltConf	Trace		
3	A1	1530	Total 32828	C 14642	N 6024	O 10633	Р 1529	0	0

• Molecule 4 is a protein called 30S ribosomal protein S2.

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

• Molecule 5 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
5	AC	117	Total 876	C 540	N 174	0 159	${ m S} { m 3}$	0	0

• Molecule 6 is a protein called 30S ribosomal protein S12.



Mol	Chain	Residues		At	oms	AltConf	Trace		
6	AD	123	Total 954	C 590	N 196	O 164	$\frac{S}{4}$	0	0

• Molecule 7 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	AF	114	Total 883	C 546	N 178	0 156	${ m S} { m 3}$	0	0

• Molecule 8 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues		At	oms		AltConf	Trace	
8	AG	96	Total 773	C 483	N 160	0 127	$\frac{S}{3}$	0	0

• Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	AH	88	Total 715	C 440	N 146	0 128	S 1	0	0

• Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
10	AI	82	Total 648	C 406	N 128	0 113	S 1	0	0

• Molecule 11 is a protein called 30S ribosomal protein S17.

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

• Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
12	AK	55	Total 455	C 288	N 86	0 81	0	0

• Molecule 13 is a protein called 30S ribosomal protein S19.



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

• Molecule 14 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues		At	oms	AltConf	Trace		
14	AN	85	Total 664	C 411	N 137	0 113	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
15	AO	206	Total 1624	C 1028	N 305	0 288	$\frac{S}{3}$	0	0

• Molecule 16 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
16	AQ	51	Total 425	C 265	N 86	O 73	S 1	0	0

• Molecule 17 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues		At	AltConf	Trace			
17	AR	205	Total 1642	C 1026	N 315	O 297	$\frac{S}{4}$	0	0

• Molecule 18 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues		At	oms	Atoms					
18	AS	150	Total 1105	C 687	N 211	O 201	S 6	0	0		

• Molecule 19 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	AT	100	Total 817	C 515	N 148	0 148	S 6	0	0

• Molecule 20 is a protein called 30S ribosomal protein S7.



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

• Molecule 21 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms			AltConf	Trace
21	AV	129	Total 978	C 616	N 173	0 183	S 6	0	0

• Molecule 22 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues		At	oms			AltConf	Trace
22	AW	127	Total 1021	C 634	N 206	0 178	$\frac{S}{3}$	0	0

• Molecule 23 is a protein called 30S ribosomal protein S10.

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

• Molecule 24 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
24	BA	117	Total 2504	C 1116	N 459	0 813	Р 116	0	0

• Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
25	BB	2903	Total 62317	C 27801	N 11467	O 20147	Р 2902	0	0

• Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
26	BC	94	Total 752	C 479	N 137	0 133	${ m S} { m 3}$	0	0

• Molecule 27 is a protein called 50S ribosomal protein L14.



Mol	Chain	Residues		At	oms			AltConf	Trace
27	BD	121	Total 930	C 582	N 179	O 164	${ m S}{ m 5}$	0	0

• Molecule 28 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms	AltConf	Trace		
28	BE	144	Total 1052	C 654	N 207	0 189	${S \over 2}$	0	0

• Molecule 29 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	BF	136	Total 1073	C 686	N 205	0 176	S 6	0	0

• Molecule 30 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	BG	127	Total 1007	C 621	N 204	0 177	${ m S}{ m 5}$	0	0

• Molecule 31 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	BH	117	Total 899	$\begin{array}{c} \mathrm{C} \\ 557 \end{array}$	N 179	O 162	S 1	0	0

• Molecule 32 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
32	BI	114	Total 916	С 574	N 179	0 162	S 1	0	0

• Molecule 33 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
33	BJ	117	Total 946	C 604	N 192	O 150	0	0

• Molecule 34 is a protein called 50S ribosomal protein L21.



Mol	Chain	Residues		At	oms			AltConf	Trace
34	BK	103	Total 815	C 516	N 153	0 144	${ m S} { m 2}$	0	0

• Molecule 35 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	AltConf	Trace			
35	BL	110	Total 856	C 532	N 166	0 155	${f S}\ 3$	0	0

• Molecule 36 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	BM	99	Total 777	C 491	N 145	0 139	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		At	AltConf	Trace			
37	BN	267	Total 2053	C 1271	N 416	O 359	${ m S} 7$	0	0

• Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
38	BO	102	Total 779	C 492	N 146	0 141	0	0

• Molecule 39 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	BP	84	Total 633	C 391	N 129	0 112	S 1	0	0

• Molecule 40 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
40	BQ	63	Total 508	C 313	N 99	0 94	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 41 is a protein called 50S ribosomal protein L30.



Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
41	BR	58	Total 448	C 281	N 87	O 78	${ m S} { m 2}$	0	0

• Molecule 42 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
42	BS	70	Total 548	C 339	N 104	O 99	S 6	0	0

• Molecule 43 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
43	BT	56	Total 443	C 269	N 94	O 79	S 1	0	0

• Molecule 44 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
44	BU	54	Total 440	C 284	N 81	O 75	0	0

• Molecule 45 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
45	BV	46	Total 376	C 228	N 90	O 56	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 46 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
46	BW	64	Total 503	C 323	N 105	O 73	${ m S} { m 2}$	0	0

• Molecule 47 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
47	BX	38	Total 301	C 185	N 65	0 47	${S \atop 4}$	0	0

• Molecule 48 is a protein called 50S ribosomal protein L3.



Mol	Chain	Residues		At	oms			AltConf	Trace
48	BY	209	Total 1564	C 979	N 288	O 293	$\frac{S}{4}$	0	0

• Molecule 49 is a protein called 50S ribosomal protein L1P.

Mol	Chain	Residues		Ate	AltConf	Trace			
49	BZ	213	Total 1687	C 1078	N 300	O 308	S 1	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BZ	1	MET	-	insertion	UNP P35024
BZ	?	-	MET	deletion	UNP P35024
BZ	70	SER	PHE	conflict	UNP P35024
BZ	82	LYS	ASN	conflict	UNP P35024
BZ	?	-	MET	deletion	UNP P35024
BZ	?	-	MET	deletion	UNP P35024
BZ	?	-	MET	deletion	UNP P35024

• Molecule 50 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	AltConf	Trace			
50	B1	201	Total 1551	C 974	N 283	O 289	${ m S}{ m 5}$	0	0

• Molecule 51 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
51	B2	178	Total 1419	C 905	N 251	0 257	S 6	0	0

• Molecule 52 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			AltConf	Trace
52	B3	176	Total 1322	C 832	N 243	0 245	${S \over 2}$	0	0

• Molecule 53 is a protein called 50S ribosomal protein L9.



Mol	Chain	Residues		At	oms			AltConf	Trace
53	B4	149	Total 1110	C 699	N 197	0 213	S 1	0	0

 $\bullet\,$ Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues		At	AltConf	Trace			
54	B5	141	Total 1031	C 651	N 179	O 195	S 6	0	0

• Molecule 55 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B6	140	Total 1112	C 704	N 210	0 194	${S \atop 4}$	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: A/T, P and E-site tRNAs







• Molecule 3: 16S rRNA



PROTEIN DATA BANK







• Molecule 7: 30S ribosomal protein S13















GLY ASP SER GLU GLU GLU GLU GLU GLU GLU



• Molecule 23: 30S ribosomal protein S10

71% Chain AX: 59% 27% 8% • 5%









PROTEIN DATA BANK





• Molecule 27: 50S ribosomal protein L14





• Molecule 28: 50S ribosomal protein L15



• Molecule 29: 50S ribosomal protein L16





















• Molecule 50: 50S ribosomal protein L4









 \bullet Molecule 51: 50S ribosomal protein L5



• Molecule 54: 50S ribosomal protein L11





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52181	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	15	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	250.773	Depositor
Minimum map value	-142.587	Depositor
Average map value	1.513	Depositor
Map value standard deviation	24.331	Depositor
Recommended contour level	43.4	Depositor
Map size (Å)	366.6, 366.6, 366.6	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.82, 2.82, 2.82	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AA	3.40	236/1789~(13.2%)	4.38	561/2788~(20.1%)	
1	AE	3.39	235/1814~(13.0%)	4.16	549/2827~(19.4%)	
1	AP	4.04	200/1789~(11.2%)	4.62	517/2788~(18.5%)	
2	AM	2.83	38/436~(8.7%)	3.84	119/672~(17.7%)	
3	A1	3.49	4705/36759~(12.8%)	4.27	10939/57346~(19.1%)	
4	AB	1.61	8/1735~(0.5%)	2.18	57/2338~(2.4%)	
5	AC	1.67	7/892~(0.8%)	2.45	47/1205~(3.9%)	
6	AD	1.69	12/968~(1.2%)	2.37	39/1300~(3.0%)	
7	AF	1.58	5/892~(0.6%)	2.47	46/1193~(3.9%)	
8	AG	1.66	9/785~(1.1%)	2.56	33/1046~(3.2%)	
9	AH	1.80	12/723~(1.7%)	2.44	37/966~(3.8%)	
10	AI	1.65	6/658~(0.9%)	2.62	33/884~(3.7%)	
11	AJ	1.59	5/657~(0.8%)	2.37	33/881~(3.7%)	
12	AK	1.77	5/462~(1.1%)	2.48	33/621~(5.3%)	
13	AL	1.63	3/652~(0.5%)	2.09	19/877~(2.2%)	
14	AN	1.53	3/670~(0.4%)	2.09	21/888~(2.4%)	
15	AO	1.66	19/1651~(1.2%)	2.22	58/2225~(2.6%)	
16	AQ	1.74	6/430~(1.4%)	2.77	30/570~(5.3%)	
17	AR	1.65	17/1664~(1.0%)	2.37	81/2227~(3.6%)	
18	AS	1.67	10/1118~(0.9%)	2.31	38/1504~(2.5%)	
19	AT	1.63	5/835~(0.6%)	2.30	36/1128~(3.2%)	
20	AU	1.68	10/1187~(0.8%)	2.46	56/1591~(3.5%)	
21	AV	1.64	7/988~(0.7%)	2.27	43/1326~(3.2%)	
22	AW	1.78	14/1033~(1.4%)	2.59	48/1375~(3.5%)	
23	AX	1.57	4/796~(0.5%)	2.46	38/1077~(3.5%)	
24	BA	3.32	357/2800~(12.8%)	4.36	854/4367~(19.6%)	
25	BB	15.87	8884/69795~(12.7%)	4.40	21260/108884~(19.5%)	
26	BC	1.63	10/765~(1.3%)	2.11	24/1025~(2.3%)	
27	BD	1.69	$7/939~\overline{(0.7\%)}$	2.47	44/1258~(3.5%)	
28	BE	1.68	9/1061~(0.8%)	2.33	$3\overline{7}/1413~(2.6\%)$	
29	BF	1.62	6/1092~(0.5%)	2.24	37/1460~(2.5%)	
30	BG	1.70	10/1020~(1.0%)	2.53	58/1364~(4.3%)	
31	BH	1.69	11/909~(1.2%)	2.40	43/1219~(3.5%)	
32	BI	1.71	8/928~(0.9%)	2.37	36/1242~(2.9%)	



Mal	Chain		Bond lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
33	BJ	1.71	15/959~(1.6%)	2.50	62/1278~(4.9%)	
34	BK	1.62	5/828~(0.6%)	2.36	35/1107~(3.2%)	
35	BL	1.52	4/863~(0.5%)	2.38	33/1156~(2.9%)	
36	BM	1.54	4/784~(0.5%)	2.16	28/1048~(2.7%)	
37	BN	1.74	26/2092~(1.2%)	2.34	97/2813~(3.4%)	
38	BO	1.59	2/787~(0.3%)	2.39	37/1051~(3.5%)	
39	BP	1.71	7/641~(1.1%)	2.42	28/848~(3.3%)	
40	BQ	1.67	5/509~(1.0%)	2.16	15/677~(2.2%)	
41	BR	1.60	5/452~(1.1%)	2.10	15/605~(2.5%)	
42	BS	1.65	8/558~(1.4%)	2.43	20/745~(2.7%)	
43	BT	1.77	7/449~(1.6%)	2.34	22/599~(3.7%)	
44	BU	1.61	3/447~(0.7%)	2.19	18/594~(3.0%)	
45	BV	1.74	3/379~(0.8%)	2.64	22/498~(4.4%)	
46	BW	1.55	3/512~(0.6%)	2.18	20/676~(3.0%)	
47	BX	1.56	2/302~(0.7%)	2.90	18/397~(4.5%)	
48	BY	1.69	11/1585~(0.7%)	2.23	58/2134~(2.7%)	
49	ΒZ	1.57	8/1711~(0.5%)	2.13	57/2305~(2.5%)	
50	B1	1.66	15/1570~(1.0%)	2.30	70/2113~(3.3%)	
51	B2	1.67	11/1443~(0.8%)	2.29	62/1937~(3.2%)	
52	B3	1.60	9/1342~(0.7%)	2.13	50/1816~(2.8%)	
53	B4	1.61	$11/1121 \ (1.0\%)$	2.08	27/1515~(1.8%)	
54	B5	1.51	4/1045~(0.4%)	2.16	$3\overline{5}/1410~(2.5\%)$	
55	B6	1.69	9/1135~(0.8%)	2.39	60/1529~(3.9%)	
All	All	10.61	$1506\overline{0}/162206~(9.3\%)$	3.93	36793/242726~(15.2%)	

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	52
1	AE	0	46
1	AP	2	51
2	AM	0	12
3	A1	4	995
4	AB	0	8
5	AC	0	4
6	AD	0	9
7	AF	0	8
8	AG	0	3
9	AH	0	2



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Mol	Chain	#Chirality outliers	#Planarity outliers
10	AI	0	9
11	AJ	0	4
12	AK	0	3
13	AL	0	8
14	AN	1	0
15	AO	0	9
16	AQ	0	5
17	AR	0	5
18	AS	0	2
19	AT	0	9
20	AU	0	8
21	AV	0	4
22	AW	0	9
23	AX	0	2
24	BA	0	81
25	BB	3	1853
26	BC	0	2
27	BD	0	4
28	BE	0	5
29	BF	0	9
30	BG	0	5
31	BH	0	7
32	BI	0	6
33	BJ	0	3
34	BK	0	11
35	BL	0	4
36	BM	0	3
37	BN	0	12
38	BO	0	4
39	BP	0	7
41	BR	0	4
42	BS	0	7
43	BT	0	3
44	BU	0	3
45	BV	0	4
46	BW	0	7
47	BX	0	1
48	BY	0	8
49	BZ	0	9
50	B1	0	9
51	B2	0	7
52	B3	0	7



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Mol	Chain	#Chirality outliers	#Planarity outliers
53	B4	0	3
54	B5	0	3
55	B6	0	12
All	All	10	3370

The worst 5 of 15060 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BB	995	C	C4-C5	2385.00	20.50	1.43
25	BB	995	С	C2-N3	2363.63	20.26	1.35
25	BB	995	С	C4-N4	2355.33	22.53	1.33
3	A1	1429	А	P-O5'	178.05	3.37	1.59
3	A1	1340	A	C3'-O3'	103.07	2.86	1.42

The worst 5 of 36793 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
25	BB	995	С	C5-C4-N4	-167.42	3.01	120.20
25	BB	995	С	C4-C5-C6	-165.92	34.44	117.40
25	BB	995	С	N1-C2-N3	-110.87	41.59	119.20
1	AP	74	С	P-O3'-C3'	-90.94	10.58	119.70
25	BB	995	С	N3-C4-C5	-73.62	92.45	121.90

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AP	31	А	C1',C2'
3	A1	13	U	C1',C2'
3	A1	1198	G	C4'
3	A1	1483	А	C2'
14	AN	13	SER	CA

5 of 3370 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1	G	Sidechain
1	AA	3	G	Sidechain
1	AA	4	G	Sidechain
1	AA	5	А	Sidechain
1	AA	6	U	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	1600	0	754	13	0
1	AE	1622	0	773	5	0
1	AP	1600	0	756	42	0
2	AM	397	0	202	4	0
3	A1	32828	0	15398	147	0
4	AB	1704	0	1732	7	0
5	AC	876	0	887	5	0
6	AD	954	0	1019	5	0
7	AF	883	0	944	5	0
8	AG	773	0	824	4	0
9	AH	715	0	742	3	0
10	AI	648	0	666	0	0
11	AJ	648	0	691	2	0
12	AK	455	0	478	1	0
13	AL	637	0	665	5	0
14	AN	664	0	714	5	0
15	AO	1624	0	1699	2	0
16	AQ	425	0	449	1	0
17	AR	1642	0	1710	6	0
18	AS	1105	0	1148	3	0
19	AT	817	0	808	2	0
20	AU	1174	0	1230	0	0
21	AV	978	0	1034	3	0
22	AW	1021	0	1070	0	0
23	AX	786	0	828	7	0
24	BA	2504	0	1160	13	0
25	BB	62317	0	29301	262	0
26	BC	752	0	780	2	0
27	BD	930	0	1000	1	0
28	BE	1052	0	1129	6	0
29	BF	1073	0	1157	8	0
30	BG	1007	0	1045	5	0
31	BH	899	0	935	2	0
32	BI	916	0	965	6	0
33	BJ	946	0	1022	3	0
34	BK	815	0	839	5	0
35	BL	856	0	922	2	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BM	777	0	840	5	0
37	BN	2053	0	2122	10	0
38	BO	779	0	834	8	0
39	BP	633	0	656	0	0
40	BQ	508	0	543	5	0
41	BR	448	0	491	0	0
42	BS	548	0	552	0	0
43	BT	443	0	461	1	0
44	BU	440	0	485	1	0
45	BV	376	0	418	5	0
46	BW	503	0	574	3	0
47	BX	301	0	343	0	0
48	BY	1564	0	1616	7	0
49	ΒZ	1687	0	1814	4	0
50	B1	1551	0	1619	6	0
51	B2	1419	0	1460	6	0
52	B3	1322	0	1374	4	0
53	B4	1110	0	1148	1	0
54	B5	1031	0	1088	2	0
55	B6	1112	0	1147	1	0
All	All	149248	0	97061	544	0

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The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 544 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)
25:BB:1687:G:C2'	25:BB:1687:G:C3'	1.94	1.42
25:BB:1687:G:C2'	25:BB:1687:G:C1'	1.98	1.40
1:AP:31:A:C2'	3:A1:1340:A:H3'	1.50	1.40
25:BB:1687:G:C3'	25:BB:1687:G:C4'	1.99	1.37
1:AP:31:A:C2'	1:AP:31:A:C1'	2.04	1.35

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	Perc	entiles
4	AB	216/241~(90%)	173 (80%)	35~(16%)	8 (4%)	3	24
5	AC	115/129~(89%)	85 (74%)	26~(23%)	4 (4%)	3	25
6	AD	121/124~(98%)	71 (59%)	35~(29%)	15 (12%)	0	5
7	AF	112/118~(95%)	76 (68%)	27~(24%)	9 (8%)	1	12
8	AG	94/101~(93%)	71 (76%)	18 (19%)	5 (5%)	2	19
9	AH	86/89~(97%)	67 (78%)	14 (16%)	5 (6%)	1	18
10	AI	80/82~(98%)	56 (70%)	15 (19%)	9 (11%)	0	7
11	AJ	78/84~(93%)	51 (65%)	22~(28%)	5~(6%)	1	16
12	AK	53/75~(71%)	40 (76%)	9~(17%)	4 (8%)	1	13
13	AL	77/92~(84%)	57 (74%)	13 (17%)	7 (9%)	1	11
14	AN	83/87~(95%)	68 (82%)	12 (14%)	3 (4%)	3	25
15	AO	204/233~(88%)	157 (77%)	33 (16%)	14 (7%)	1	15
16	AQ	49/71~(69%)	38 (78%)	7 (14%)	4 (8%)	1	12
17	AR	203/206~(98%)	165 (81%)	29~(14%)	9 (4%)	2	22
18	AS	148/159~(93%)	111 (75%)	26~(18%)	11 (7%)	1	14
19	AT	98/135~(73%)	76 (78%)	15~(15%)	7 (7%)	1	14
20	AU	148/179~(83%)	118 (80%)	20 (14%)	10 (7%)	1	15
21	AV	127/130~(98%)	102 (80%)	17 (13%)	8 (6%)	1	17
22	AW	125/130~(96%)	96 (77%)	22~(18%)	7~(6%)	2	19
23	AX	96/103~(93%)	73 (76%)	15 (16%)	8 (8%)	1	12
26	BC	92/94~(98%)	70 (76%)	16 (17%)	6 (6%)	1	16
27	BD	119/123~(97%)	84 (71%)	25 (21%)	10 (8%)	1	12
28	BE	142/144~(99%)	90 (63%)	27 (19%)	25 (18%)	0	3
29	BF	134/136~(98%)	74 (55%)	37 (28%)	23 (17%)	0	3
30	BG	125/127~(98%)	82 (66%)	32 (26%)	11 (9%)	1	11



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	BH	115/117~(98%)	78~(68%)	27~(24%)	10 (9%)	1 11
32	BI	112/115~(97%)	67~(60%)	32 (29%)	13 (12%)	0 6
33	BJ	115/118 (98%)	84 (73%)	19 (16%)	12 (10%)	0 8
34	BK	101/103 (98%)	57 (56%)	32 (32%)	12 (12%)	0 6
35	BL	108/110 (98%)	71 (66%)	18 (17%)	19 (18%)	0 3
36	BM	97/99~(98%)	70 (72%)	19 (20%)	8 (8%)	1 12
37	BN	265/270~(98%)	167 (63%)	49 (18%)	49 (18%)	0 2
38	BO	100/103~(97%)	51 (51%)	31 (31%)	18 (18%)	0 3
39	BP	82/85~(96%)	42 (51%)	26 (32%)	14 (17%)	0 3
40	BQ	61/63~(97%)	44 (72%)	13 (21%)	4 (7%)	1 16
41	BR	56/59~(95%)	39 (70%)	10 (18%)	7 (12%)	0 5
42	BS	68/70~(97%)	47 (69%)	14 (21%)	7 (10%)	0 8
43	BT	54/57~(95%)	37 (68%)	11 (20%)	6 (11%)	0 7
44	BU	52/54~(96%)	35~(67%)	14 (27%)	3 (6%)	1 18
45	BV	44/46~(96%)	33~(75%)	9 (20%)	2(4%)	2 22
46	BW	62/64~(97%)	31 (50%)	16 (26%)	15 (24%)	0 1
47	BX	36/38~(95%)	23~(64%)	6 (17%)	7~(19%)	0 2
48	BY	207/209~(99%)	120 (58%)	54 (26%)	33 (16%)	0 3
49	BZ	211/213 (99%)	169 (80%)	33 (16%)	9 (4%)	2 22
50	B1	199/201~(99%)	117 (59%)	53 (27%)	29 (15%)	0 4
51	B2	176/178~(99%)	125 (71%)	35 (20%)	16 (9%)	1 11
52	B3	174/177~(98%)	145 (83%)	19 (11%)	10 (6%)	1 18
53	B4	147/149~(99%)	109 (74%)	31 (21%)	7 (5%)	2 21
54	B5	139/142~(98%)	116 (84%)	17 (12%)	6 (4%)	2 22
55	B6	138/140 (99%)	78 (56%)	40 (29%)	20 (14%)	0 4
All	All	5844/6172~(95%)	4106 (70%)	1175 (20%)	563 (10%)	1 10

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5 of 563 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AB	21	TYR
4	AB	97	GLY
4	AB	169	HIS



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Mol	Chain	Res	Type
5	AC	118	ASN
6	AD	15	VAL

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
4	AB	180/199~(90%)	167~(93%)	13~(7%)	14	39
5	AC	90/99~(91%)	81 (90%)	9~(10%)	7	26
6	AD	103/104~(99%)	91~(88%)	12~(12%)	5	21
7	AF	92/96~(96%)	82~(89%)	10 (11%)	6	23
8	AG	79/84~(94%)	76~(96%)	3~(4%)	33	57
9	AH	76/77~(99%)	71~(93%)	5(7%)	16	41
10	AI	65/65~(100%)	61 (94%)	4~(6%)	18	43
11	AJ	74/78~(95%)	69~(93%)	5(7%)	16	41
12	AK	48/66~(73%)	42 (88%)	6(12%)	4	19
13	AL	70/79~(89%)	62~(89%)	8 (11%)	5	21
14	AN	65/66~(98%)	58~(89%)	7 (11%)	6	23
15	AO	170/190~(90%)	158 (93%)	12 (7%)	14	39
16	AQ	44/61~(72%)	39~(89%)	5 (11%)	5	21
17	AR	172/173~(99%)	156 (91%)	16 (9%)	9	28
18	AS	113/119~(95%)	97~(86%)	16 (14%)	3	16
19	AT	87/116~(75%)	78~(90%)	9 (10%)	7	25
20	AU	123/147~(84%)	109 (89%)	14 (11%)	5	21
21	AV	104/105~(99%)	98 (94%)	6 (6%)	20	45
22	AW	105/107~(98%)	95~(90%)	10 (10%)	8	27
23	AX	86/90~(96%)	81 (94%)	5 (6%)	20	45
26	BC	78/78~(100%)	76~(97%)	2 (3%)	46	66
27	BD	102/104~(98%)	94 (92%)	8 (8%)	12	36



α \cdot \cdot \cdot	C		
Continued	from	previous	page

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
28	BE	103/103~(100%)	84 (82%)	19 (18%)	1	9
29	BF	109/109~(100%)	94 (86%)	15 (14%)	3	17
30	BG	103/103~(100%)	94 (91%)	9~(9%)	10	31
31	BH	87/87~(100%)	82 (94%)	5 (6%)	20	45
32	BI	99/100~(99%)	95~(96%)	4 (4%)	31	55
33	BJ	89/90~(99%)	79~(89%)	10 (11%)	6	22
34	BK	84/84 (100%)	73 (87%)	11 (13%)	4	18
35	BL	93/93~(100%)	83 (89%)	10 (11%)	6	23
36	BM	83/83 (100%)	71 (86%)	12 (14%)	3	15
37	BN	213/215~(99%)	188 (88%)	25 (12%)	5	21
38	BO	83/84~(99%)	74 (89%)	9 (11%)	6	23
39	BP	62/63~(98%)	53 (86%)	9 (14%)	3	15
40	BQ	55/55~(100%)	45 (82%)	10 (18%)	1	10
41	BR	48/49~(98%)	45 (94%)	3 (6%)	18	43
42	BS	62/62~(100%)	58 (94%)	4 (6%)	17	42
43	BT	47/48~(98%)	34 (72%)	13 (28%)	0	3
44	BU	48/48 (100%)	43 (90%)	5 (10%)	7	24
45	BV	38/38~(100%)	32 (84%)	6 (16%)	2	13
46	BW	51/51~(100%)	41 (80%)	10 (20%)	1	8
47	BX	34/34~(100%)	32 (94%)	2(6%)	19	45
48	BY	164/164~(100%)	150 (92%)	14 (8%)	10	33
49	BZ	187/187~(100%)	172 (92%)	15 (8%)	12	35
50	B1	165/165~(100%)	143 (87%)	22 (13%)	4	18
51	B2	149/149~(100%)	133 (89%)	16 (11%)	6	23
52	B3	137/138 (99%)	123 (90%)	14 (10%)	7	25
53	B4	114/114 (100%)	104 (91%)	10 (9%)	10	31
54	B5	109/110~(99%)	100 (92%)	9 (8%)	11	34
55	B6	$114/114 \ (100\%)$	102 (90%)	12 (10%)	7	24
All	All	4856/5043 (96%)	4368 (90%)	488 (10%)	11	26

 $5~{\rm of}~488$ residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
31	BH	54	VAL
52	B3	21	GLN
37	BN	66	PHE
51	B2	146	ASP
54	B5	117	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such side chains are listed below:

Mol	Chain	Res	Type
37	BN	162	GLN
55	B6	76	HIS
43	BT	3	GLN
30	BG	16	HIS
37	BN	114	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	75/76~(98%)	21 (28%)	10 (13%)
1	AE	75/76~(98%)	12 (16%)	5~(6%)
1	AP	74/76~(97%)	10 (13%)	9(12%)
2	AM	20/20~(100%)	10 (50%)	8 (40%)
24	BA	116/117~(99%)	36 (31%)	18 (15%)
25	BB	2901/2903~(99%)	1500 (51%)	494 (17%)
3	A1	1529/1530~(99%)	730 (47%)	270 (17%)
All	All	4790/4798~(99%)	2319 (48%)	814 (16%)

5 of 2319 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	С
1	AA	3	G
1	AA	10	G
1	AA	16	U
1	AA	17	U

5 of 814 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BB	814	С
25	BB	1497	U



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Mol	Chain	Res	Type
25	BB	2799	А
25	BB	958	U
25	BB	811	U

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 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
25	BB	1
1	AP	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BB	1959:G	O3'	1960:A	Р	3.49
1	AP	74:C	O3'	75:C	Р	1.29



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1056. 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.

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 65



Y Index: 65



Z Index: 65



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: 68

Y Index: 68

Z Index: 58

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 43.4. 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 2462 nm^3 ; this corresponds to an approximate mass of 2224 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 0.111 ${\rm \AA^{-1}}$



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-1056 and PDB model 4V66. 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 43.4 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 (43.4).



9.4 Atom inclusion (i)



At the recommended contour level, 36% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (43.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3630	-0.0040
A1	0.3040	-0.0060
AA	0.3110	0.0030
AB	0.2260	-0.0120
AC	0.4430	0.0120
AD	0.2320	-0.0130
AE	0.4020	-0.0090
AF	0.4050	-0.0120
AG	0.1040	-0.0300
AH	0.1730	0.0060
AI	0.0000	-0.0250
AJ	0.2610	-0.0340
AK	0.6440	0.0240
AL	0.0370	-0.0070
AM	0.7100	0.0400
AN	0.4180	0.0020
AO	0.6430	0.0220
AP	0.3780	-0.0140
AQ	0.3890	-0.0540
AR	0.4320	-0.0070
AS	0.5970	-0.0040
AT	0.2310	0.0030
AU	0.5160	-0.0040
AV	0.4660	0.0180
AW	0.1320	0.0180
AX	0.2560	-0.0200
B1	0.2470	-0.0070
B2	0.6610	0.0260
B3	0.1920	-0.0360
B4	0.0750	-0.0060
B5	0.5770	-0.0120
B6	0.5010	0.0050
BA	0.3050	-0.0250
BB	0.4050	-0.0030
BC	0.2330	-0.0090

0.0 <0.0

1.0



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Chain	Atom inclusion	Q-score
BD	0.3820	-0.0020
BE	0.3730	-0.0020
BF	0.3480	-0.0040
BG	0.5840	-0.0030
BH	0.4220	0.0030
BI	0.4100	-0.0180
BJ	0.1770	-0.0330
BK	0.0770	0.0020
BL	0.4600	0.0040
BM	0.2620	-0.0100
BN	0.3830	0.0020
BO	0.0010	-0.0340
BP	0.5960	0.0340
BQ	0.4780	0.0290
BR	0.4430	-0.0030
BS	0.2920	0.0010
BT	0.4890	-0.0090
BU	0.1710	-0.0080
BV	0.4440	0.0120
BW	0.2550	-0.0220
BX	0.2890	-0.0030
BY	0.5370	0.0070
BZ	0.0450	-0.0170

