

wwPDB EM Validation Summary Report (i)

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PDB ID	:	6ZU9
EMDB ID	:	EMD-11439
Title	:	Structure of a yeast ABCE1-bound 48S initiation complex
Authors	:	Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.;
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Deposited on	:	2020-07-22
Resolution	:	6.20 Å(reported)

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. dev 92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
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 6.20 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.



Motric	Whole archive	EM structures		
	$(\# {\rm Entries})$	$(\# { m Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
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 >=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 <=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	2	1800	43% 39%	14% ••
2	Р	252	82%	18%
3	Q	255	88%	• 11%
4	R	254	85%	15%
5	S	261	97%	
6	Т	236	93%	• •
7	U	190	96%	
8	V	200	90%	• 6%



Mol	Chain	Length	Quality of chain	
9	W	197	92%	• 7%
10	Х	155	90%	• 8%
11	Y	151	• 98%	
12	Z	136	92%	• 7%
13	a	87	100%	
14	b	130	99%	
15	с	145	99%	••
16	d	135	99%	
17	е	119	82%	18%
18	f	82	18%	
19	g	63	8%	16%
20	Е	141	79% •	17%
21	В	240	92%	• 8%
22	С	225	92%	8%
23	D	105	86%	• 12%
24	F	143	81%	15%
25	Н	143	96%	••
26	Ι	136	88%	• 11%
27	J	146	97%	•••
28	K	144	97%	•••
29	L	121	83%	17%
30	М	108	7% . 2	24%
31	Ν	56	95%	5%
32	0	152	46% . 52%	
33	h	319	97%	••



Mol	Chain	Length			Quality	of chai	n		
34	i	67			94%				6%
35	1	347			84% 95%				5%
36	r	135		38% 39%			61%		
37	1	75	7%	51%			31%		16% •
38	m	405	13%	6%			64%		
39	0	964	—	54%		•		45%	
40	р	763	22%		83%			•	15%
41	q	812	—		77%				22%
42	3	8	12%	38%		38%		12%	12%
43	A	153	–	61%		5	% •	34%)
44	k	608	8%		94%				• 5%



2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 78384 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 ribosomal RNA.

Mol	Chain	Residues		1	AltConf	Trace			
1	2	1771	Total 37739	C 16872	N 6683	O 12413	Р 1771	0	0

• Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Р	206	Total 1020	C 608	N 206	O 206	0	0

• Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	226	Total 1119	C 667	N 226	O 226	0	0

• Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	R	216	Total 1058	C 626	N 216	O 216	0	0

• Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	258	Total 1267	C 751	N 258	O 258	0	0

• Molecule 6 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	Т	228	Total 1123	C 667	N 228	O 228	0	0



• Molecule 7 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
7	U	184	Total 913	C 545	N 184	0 184	0	0

• Molecule 8 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	V	187	Total	С	Ν	Ο	0	0
0	v	107	919	545	187	187	0	0

• Molecule 9 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
9	W	184	Total 910	C 542	N 184	0 184	0	0

• Molecule 10 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
10	Х	142	Total 702	C 418	N 142	O 142	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Х	147	ALA	GLY	conflict	UNP P0CX47

• Molecule 11 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues		Ato	AltConf	Trace		
11	Y	150	Total 742	C 442	N 150	O 150	0	0

• Molecule 12 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
12	Ζ	127	Total 620	C 366	N 127	O 127	0	0

• Molecule 13 is a protein called 40S ribosomal protein S21-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	a	87	Total 429	$\begin{array}{c} \mathrm{C} \\ 255 \end{array}$	N 87	O 87	0	0

• Molecule 14 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	b	129	Total 634	C 376	N 129	O 129	0	0

• Molecule 15 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
15	с	144	Total 704	C 416	N 144	0 144	0	0

• Molecule 16 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	d	134	Total 661	C 393	N 134	O 134	0	0

• Molecule 17 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
17	е	97	Total 482	C 288	N 97	O 97	0	0

• Molecule 18 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	f	81	Total 400	C 238	N 81	O 81	0	0

• Molecule 19 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	g	53	Total 261	C 155	N 53	O 53	0	0

• Molecule 20 is a protein called 40S ribosomal protein S15.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
20	Е	117	Total 576	C 342	N 117	0 117	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	137	SER	ARG	conflict	UNP Q01855

• Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	В	222	Total 1093	C 649	N 222	0 222	0	0

• Molecule 22 is a protein called Rps5p.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	С	206	Total 1020	C 608	N 206	O 206	0	0

• Molecule 23 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	D	92	Total 456	C 272	N 92	O 92	0	0

• Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	F	121	Total 595	C 353	N 121	O 121	0	0

• Molecule 25 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues		Atoms				Trace
25	Н	141	Total 693	C 411	N 141	0 141	0	0

• Molecule 26 is a protein called 40S ribosomal protein S17-A.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
26	Ι	121	Total 600	C 358	N 121	0 121	0	0

• Molecule 27 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	J	145	Total 715	C 425	N 145	0 145	0	0

• Molecule 28 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	K	143	Total 700	C 414	N 143	0 143	0	0

• Molecule 29 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	L	100	Total 496	C 296	N 100	O 100	0	0

• Molecule 30 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	М	82	Total 407	C 243	N 82	O 82	0	0

• Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Ν	53	Total 260	C 154	N 53	0 53	0	0
			200	104	55	55		

• Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	О	73	Total 361	C 215	N 73	0 73	0	0

• Molecule 33 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.



Mol	Chain	Residues	Atoms				AltConf	Trace
33	h	312	Total 1538	C 914	N 312	0 312	0	0

• Molecule 34 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
34	i	63	Total 310	C 184	N 63	O 63	0	0

• Molecule 35 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	1	330	Total 1624	C 964	N 330	O 330	0	0

• Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	r	53	Total 261	C 155	N 53	O 53	0	0

• Molecule 37 is a RNA chain called tRNA.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
37	1	75	Total 1639	C 734	N 298	0 531	Р 76	0	0

• Molecule 38 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	147	Total 726	C 432	N 147	0 147	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	183	LEU	PRO	conflict	UNP P38431

• Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit A.



Mol	Chain	Residues	Atoms				AltConf	Trace
39	О	529	Total 2632	C 1574	N 529	O 529	0	0

• Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues		Ator	ns		AltConf	Trace
40	р	646	Total 3201	C 1909	N 646	O 646	0	0

• Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues		Ator	ns		AltConf	Trace
41	q	636	Total 3169	C 1897	N 636	O 636	0	0

• Molecule 42 is a RNA chain called mRNA.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
42	3	8	Total 171	C 77	N 32	0 54	Р 8	0	0

• Molecule 43 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
43	А	101	Total 497	C 295	N 101	O 101	0	0

• Molecule 44 is a protein called Translation initiation factor RLI1.

Mol	Chain	Residues		Ator	ns		AltConf	Trace
44	k	579	Total 2860	C 1702	N 579	O 579	0	0

• Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
45	2	2	Total Mg 2 2	0
45	k	2	Total Mg 2 2	0

• Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	AltConf
46	Ν	1	Total Zn 1 1	0
46	О	1	Total Zn 1 1	0
46	m	1	Total Zn 1 1	0

• Molecule 47 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues		Ate	oms			AltConf
47	1.	1	Total	С	Ν	Ο	Р	0
47 K	K	1	27	10	5	10	2	0

• Molecule 48 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).





Mol	Chain	Residues		Ate	oms			AltConf
10	1.	1	Total	С	Ν	Ο	Р	0
48 K		31	10	5	13	3	U	



Mol	Chain	Residues	Atoms	AltConf
49	k	1	Total Fe S	0
-15	K	1	8 4 4	0
40	ŀ	1	Total Fe S	0
49	ĸ	I	8 4 4	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.

- Chain 2: 43% 39% 14%J73 J74 J75 A76 J77 V78 V78 V78 3712 4713 3714
- Molecule 1: 18S ribosomal RNA





 \bullet Molecule 2: 40S ribosomal protein S0-A

Chain P:





MET P2 P2 P2 P2 P2 P2 P2 P2 P2 P2 P2 P2 P2		
• Molecule 10: 40S ribosomal protein	S11-A	
Chain X:	90% •	8%
PHR THR THR A A A A A A A A A A A A A		
• Molecule 11: 40S ribosomal protein	S13	
Chain Y:	98%	••
MET C2 C3 C10 N151		
• Molecule 12: 40S ribosomal protein	S14-A	
Chain Z:	92%	• 7%
SER VAL VAL VAL ALA ALA ASP ASP ASP A101 L137		
• Molecule 13: 40S ribosomal protein	S21-A	
Chain a:	100%	
• Molecule 14: 40S ribesomel protein	l for this chain.	
• Molecule 14. 405 Hoosomai protein	522-A	
Chain b:	99%	
• Molecule 15: 40S ribosomal protein	S23-A	
Chain c:	99%	
MET 22 23 23 24 25 25 25 25 25 25 25 25 25 25 25 25 25		
• Molecule 16: 40S ribosomal protein	S24-A	
Chain d:	99%	





• Molecule 17: 40S ribosomal protein S26-A

Chain e:	82%	18%
P2 P2 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3 P3	VAL BER PRO ALA ALA ALA ALA ALA ALA LVS LVS LVS LLV	
• Molecule 18: 40S rib	oosomal protein S27-A	
Chain f:	99%	
MET V2 L3 V4 Q5 D6 L7 L8 H9 P10 P10 P10 K20	G27 G27 F47 K82 K82	
• Molecule 19: 40S rib	oosomal protein S30-A	
Chain g:	84%	16%
MET ALLA LYVS VAL HIS GLY GLY CL2 L2U L30 V50 V50 V51	SS1 VAL	
• Molecule 20: 40S rib	posomal protein S15	
Chain E:	79%	• 17%
SER GLN ALA ALA ALA ASN ASN ASN ASN ASS CYAL VAL VAL VAL VAL VAL VAL VAL VAL VAL V	V20 V20 M53 M53 M53 M53 M53 M53 M54 M54 M54 M54 M54 M54 M54 M54 M54 M54	
• Molecule 21: 40S rib	posomal protein S3	
Chain B:	92%	• 8%
MET A LA A LA A L4 L4 A 145 A	ALA ALA GLU CLU VAL ALA ALA ALA	
• Molecule 22: Rps5p		
Chain C:	92%	8%
MET ASP ASP ASP ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU VAL		

• Molecule 23: 40S ribosomal protein S10-A



Chain D:	86%	• 12%
M1 V55 L68 L68 L68 L68 L68 L68 L68 L18 Z10 T18 T18 ARC ARC ARC	ARG ARG TYR	
• Molecule 24: 40S rib	posomal protein S12	
Chain F:	81%	• 15%
MET SER ASP ASP ASP ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU VAL VAL	GLU GLN THR ALA ALA CLU VAL P82 B83 B82 B82 B82 B82 B82 B82 B82 B82 B82 B82	
• Molecule 25: 40S rib	posomal protein S16-A	
Chain H:	96%	
MET SER A 3 8 4 4 6 40 E 40 E 40 E 135 R143		
• Molecule 26: 40S rib	posomal protein S17-A	
Chain I:	88%	• 11%
MET C2 C2 R95 SER ASN VAL L100 L100 C1N A126 G1N A126 G1N A126 A126 A126 A126 A126 A126 A126 A126	TYR LLYS ARG VAL	
• Molecule 27: 40S rib	posomal protein S18-A	
Chain J:	97%	
MET 82 639 639 6135 8146 A146		
• Molecule 28: 40S rib	oosomal protein S19-A	
Chain K:	97%	••
MET P2 67.2 698 51.44		
• Molecule 29: 40S rib	posomal protein S20	
Chain L:	83%	17%
MET SER ASP ASP CILU CILU CILU CILU CILU CILU CILU CILU	GLN GLN 11LE 120 A119 SER ASN	
• Molecule 30: 40S rik	posomal protein S25-A	



Chain M:	7%74%		24%		
MET PRO PRO GLN GLN SER SER	LYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	w27 828 831 831 439 439 439 439 439 431 414 85 85 85 85 85 85 85 85 85 85 85 85 85			
• Molecule	31: 40S ribosomal protein	S29-A			
Chain N:		95%	5%		
ALA ALA 11S 24 26 26					
• Molecule	32: Ubiquitin-40S ribosom	nal protein S31			
Chain O:	46%	• 52%			
MET GLN ILE PHE LYS LYS LEU	THR CLYS LYS LYS THR THR THR CLU CLU CLU CLU ASP ASP ASP ASP ASP VAL	SER LYS TLE GLN ASP ASP CLU CLU CLU CLN CLN CLN CLN CLN CLN CLN CLN	PHE ALA GLY CLN CLN CLN CLN CLU CLU CLU CLU CLU CLU ASP CLY ARG CLY LEU	SER TYR ASN	
ILE GLN GLU SER THR LEU HIS HIS	LLEU VAL LLEU ARG ARG ARG GLY GLY CLEU FLO CLA CLA CLA CLA CLA CLA CLA CLA CLA CLA	A152			
• Molecule	33: Guanine nucleotide-bi	nding protein subunit	beta-like protein		
Chain h:		97%			
MET ALA SER ASN ASN B116 K117	<mark>ki3 16</mark> THR ALA ASN				
• Molecule	34: 40S ribosomal protein	S28-B			
Chain i:		94%	6%		
MET ASP SER LYS T5 R67					
• Molecule	35: Eukaryotic translation	n initiation factor 3 sul	bunit I		
Chain l:	849	% 95%	5%		
			4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4		57 56 60 61 62
E K H A K		******			
F63 T64 K65 V68 T69	670 871 872 875 875 875 875 875 875 876 879 881 882 882 882 883	C 200 C 200	H98 F101 F101 S102 P103 C104 G105 G105 Y107	F108 L109 A110 L112 L112 D113 N114 V115 M116 M116	N118 P119 G120 S121 1122 N123
	8 월 집 8 월 8 <mark>8 8 8 8 9 9 9 4 9 9 4 9 9 4 9 9 9 9 9 9 </mark>	ਸ਼ੵਜ਼ੵਸ਼ੵਗ਼ਗ਼ੵਲ਼ੵਜ਼ਗ਼ਲ਼ੑਖ਼ਲ਼ਲ਼► ●●●●●●●●●●	8 8 8 7 8 8 4 9 9 7 9 ◆◆◆◆◆ ◆◆◆◆◆◆	<u> </u>	- @ @ <u>@ </u>
111 Y12 E12 E12 E12 E12 R12	DI SI SI SI SI SI SI SI SI SI S	H14 K15 L14 L14 H15 B15 B15 C15 D15 D15 D15 D15 L15 L15 L15 L15 L15 L15 L15 L15 L15 L	V15 A16 A16 A16 A16 A16 A16 A16 A16 A16 A16	116 116 117 117 117 117 117 117 117 117	S11 S11 Y15 V18 U18 S18







• Molecule 39: Eukaryotic translation initiation factor 3 subunit A









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II $(4k \ge 4k)$	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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: SF4, H2U, ZN, 2MG, T6A, 1MG, RIA, ADP, ATP, 1MA, G7M, M2G, 5MC, 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		Bo	nd lengths	Bond angles		
MOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	2	0.66	2/42211~(0.0%)	1.50	865/65773~(1.3%)	
2	Р	0.32	0/1019	0.63	0/1419	
3	Q	0.34	0/1117	0.73	1/1554~(0.1%)	
4	R	0.33	0/1057	0.67	0/1465	
5	S	0.35	0/1266	0.72	1/1757~(0.1%)	
6	Т	0.33	0/1122	0.62	0/1559	
7	U	0.35	0/912	0.69	0/1271	
8	V	0.33	0/917	0.62	0/1271	
9	W	0.33	0/909	0.68	0/1265	
10	Х	0.34	0/701	0.69	0/975	
11	Y	0.33	0/741	0.64	1/1031~(0.1%)	
12	Ζ	0.34	0/619	0.72	0/856	
13	a	0.35	0/428	0.71	0/594	
14	b	0.32	0/633	0.69	0/878	
15	с	0.36	0/703	0.67	0/973	
16	d	0.34	0/660	0.63	0/917	
17	е	0.32	0/481	0.69	0/670	
18	f	0.40	0/399	0.95	0/554	
19	g	0.36	0/260	0.76	0/360	
20	Ε	0.34	0/575	0.66	0/798	
21	В	0.35	0/1092	0.71	1/1517~(0.1%)	
22	С	0.31	0/1019	0.64	0/1419	
23	D	0.33	0/455	0.73	0/633	
24	F	0.34	0/594	0.82	0/824	
25	Н	0.35	0/692	0.66	1/960~(0.1%)	
26	Ι	0.30	0/598	0.58	0/831	
27	J	0.34	0/714	0.65	0/992	
28	K	0.35	$0/\overline{699}$	0.64	0/968	
29	L	0.34	0/495	0.62	0/689	
30	М	0.33	0/406	0.74	0/565	
31	N	0.34	0/259	0.68	0/358	
32	0	0.37	0/360	0.87	0/500	



Mal	Chain	Bo	nd lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
33	h	0.34	0/1537	0.70	0/2137	
34	i	0.36	0/309	0.77	0/428	
35	1	0.31	0/1622	0.52	0/2252	
36	r	0.26	0/260	0.47	0/360	
37	1	0.35	1/1529~(0.1%)	0.67	0/2376	
38	m	0.38	0/725	0.56	0/1008	
39	0	0.40	0/2627	0.57	1/3662~(0.0%)	
40	р	0.40	0/3197	0.57	0/4452	
41	q	0.50	0/3163	0.58	0/4412	
42	3	0.57	1/191~(0.5%)	1.13	2/295~(0.7%)	
43	А	0.35	0/495	0.63	0/685	
44	k	0.57	0/2858	0.98	0/3977	
All	All	0.54	4/82626~(0.0%)	1.19	873/122240~(0.7%)	

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
7	U	0	1
24	F	0	2
25	Н	0	1
32	0	0	1
33	h	0	2
40	р	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
37	1	1	А	OP3-P	-10.01	1.49	1.61
42	3	28	А	O3'-P	6.59	1.69	1.61
1	2	1360	А	N9-C4	-5.79	1.34	1.37
1	2	1113	А	N9-C4	-5.39	1.34	1.37

The worst 5 of 873 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	2	1640	С	C5-C6-N1	14.40	128.20	121.00
1	2	1389	С	C2-N1-C1'	12.62	132.69	118.80
1	2	656	G	C8-N9-C1'	-12.23	111.09	127.00



	J	1	I J				
\mathbf{Mol}	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	2	1072	С	C6-N1-C2	-11.75	115.60	120.30
1	2	1527	С	C2-N1-C1'	11.68	131.64	118.80

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	F	110	GLY	Peptide
24	F	84	ASN	Peptide
25	Н	40	GLU	Peptide
32	0	144	CYS	Peptide
7	U	64	VAL	Peptide

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	2	37739	0	18984	347	0
2	Р	1020	0	474	0	0
3	Q	1119	0	501	0	0
4	R	1058	0	497	1	0
5	S	1267	0	571	2	0
6	Т	1123	0	514	7	0
7	U	913	0	400	1	0
8	V	919	0	450	3	0
9	W	910	0	420	1	0
10	Х	702	0	304	2	0
11	Y	742	0	345	1	0
12	Ζ	620	0	311	1	0
13	a	429	0	201	0	0
14	b	634	0	289	0	0
15	с	704	0	324	0	0
16	d	661	0	312	0	0
17	е	482	0	223	0	0
18	f	400	0	177	0	0
19	g	261	0	113	0	0
20	Ε	576	0	264	3	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	В	1093	0	520	1	0
22	С	1020	0	482	0	0
23	D	456	0	196	1	0
24	F	595	0	288	0	0
25	Н	693	0	323	2	0
26	Ι	600	0	259	1	0
27	J	715	0	318	4	0
28	K	700	0	334	3	0
29	L	496	0	207	0	0
30	М	407	0	182	1	0
31	N	260	0	112	0	0
32	0	361	0	162	1	0
33	h	1538	0	736	0	0
34	i	310	0	134	0	0
35	1	1624	0	727	0	0
36	r	261	0	122	0	0
37	1	1639	0	851	32	0
38	m	726	0	316	0	0
39	0	2632	0	1201	0	0
40	р	3201	0	1397	0	0
41	q	3169	0	1368	0	0
42	3	171	0	87	35	0
43	А	497	0	221	13	0
44	k	2860	0	1246	0	0
45	2	2	0	0	0	0
45	k	2	0	0	0	0
46	Ν	1	0	0	0	0
46	0	1	0	0	0	0
46	m	1	0	0	0	0
47	k	27	0	12	0	0
48	k	31	0	12	0	0
49	k	16	0	0	0	0
All	All	78384	0	37487	379	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 6.

The worst 5 of 379 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)
1:2:1637:C:O4'	42:3:31:G:C6	1.66	1.48



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1637:C:H4'	42:3:31:G:C5	1.82	1.13
1:2:1756:A:N1	43:A:67:LYS:HA	1.65	1.10
1:2:1637:C:C4'	42:3:31:G:C5	2.34	1.09
1:2:1637:C:C4	37:1:34:C:C2	2.42	1.07

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	Perce	ntiles
2	Р	204/252~(81%)	188 (92%)	16 (8%)	0	100	100
3	Q	222/255~(87%)	204 (92%)	17 (8%)	1 (0%)	29	69
4	R	214/254~(84%)	201 (94%)	13 (6%)	0	100	100
5	S	256/261~(98%)	237~(93%)	19 (7%)	0	100	100
6	Т	226/236~(96%)	214 (95%)	12 (5%)	0	100	100
7	U	182/190~(96%)	170 (93%)	12 (7%)	0	100	100
8	V	183/200~(92%)	174 (95%)	9 (5%)	0	100	100
9	W	182/197~(92%)	172 (94%)	10 (6%)	0	100	100
10	Х	140/155~(90%)	131 (94%)	9 (6%)	0	100	100
11	Y	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
12	Ζ	125/136~(92%)	111 (89%)	14 (11%)	0	100	100
13	a	85/87~(98%)	79~(93%)	6 (7%)	0	100	100
14	b	127/130~(98%)	117 (92%)	10 (8%)	0	100	100
15	с	142/145~(98%)	129 (91%)	12 (8%)	1 (1%)	22	63
16	d	132/135~(98%)	127 (96%)	5 (4%)	0	100	100
17	е	95/119~(80%)	89 (94%)	6 (6%)	0	100	100



Mol	Chain	Analysed	Favoured	Favoured Allowed		Perce	entiles
18	f	79/82~(96%)	71~(90%)	8 (10%)	0	100	100
19	g	51/63~(81%)	45 (88%)	6 (12%)	0	100	100
20	Е	115/141 (82%)	104 (90%)	11 (10%)	0	100	100
21	В	220/240~(92%)	211 (96%)	9 (4%)	0	100	100
22	С	204/225~(91%)	187 (92%)	17 (8%)	0	100	100
23	D	90/105~(86%)	76~(84%)	14 (16%)	0	100	100
24	F	119/143~(83%)	92~(77%)	24 (20%)	3(2%)	5	32
25	Н	139/143~(97%)	130 (94%)	9~(6%)	0	100	100
26	Ι	117/136~(86%)	113 (97%)	4 (3%)	0	100	100
27	J	143/146~(98%)	135 (94%)	8 (6%)	0	100	100
28	К	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
29	L	98/121 (81%)	90~(92%)	8 (8%)	0	100	100
30	М	80/108 (74%)	72 (90%)	8 (10%)	0	100	100
31	Ν	51/56~(91%)	51 (100%)	0	0	100	100
32	О	71/152~(47%)	51 (72%)	20 (28%)	0	100	100
33	h	310/319~(97%)	275~(89%)	35 (11%)	0	100	100
34	i	61/67~(91%)	58~(95%)	3 (5%)	0	100	100
35	1	326/347~(94%)	318 (98%)	8 (2%)	0	100	100
36	r	51/135~(38%)	48 (94%)	3 (6%)	0	100	100
38	m	145/405~(36%)	131 (90%)	13 (9%)	1 (1%)	22	63
39	О	519/964~(54%)	488 (94%)	26 (5%)	5 (1%)	15	54
40	р	638/763~(84%)	583 (91%)	43 (7%)	12 (2%)	8	38
41	q	624/812~(77%)	567~(91%)	45 (7%)	12 (2%)	8	38
43	А	97/153~(63%)	85(88%)	7 (7%)	5(5%)	2	19
44	k	575/608~(95%)	522 (91%)	47 (8%)	6 (1%)	15	54
All	All	7727/9481 (82%)	7123 (92%)	558 (7%)	46 (1%)	29	66

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	F	85	LYS
40	р	337	PRO
40	р	392	PRO



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Mol	Chain	Res	Type
40	р	690	GLN
43	А	31	GLU

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1800~(98%)	474~(26%)	39~(2%)
37	1	72/75~(96%)	28~(38%)	6 (8%)
42	3	7/8~(87%)	1 (14%)	1 (14%)
All	All	1847/1883~(98%)	503~(27%)	46 (2%)

5 of 503 RNA backbone outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	2	2	А
1	2	4	С
1	2	17	С
1	2	25	С
1	2	26	А

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1273	G
1	2	1633	А
1	2	1274	С
1	2	1430	U
1	2	1742	U

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

11 non-standard protein/DNA/RNA residues are 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



Mal	Trune	Chain	Dec	T in le	Bo	Bond lengths			ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	H2U	1	47	37	18,21,22	0.79	0	21,30,33	1.37	4 (19%)
37	M2G	1	26	37	20,27,28	1.75	3 (15%)	22,40,43	1.18	4 (18%)
37	RIA	1	64	37	31,38,39	0.53	0	39,57,60	0.65	0
37	H2U	1	16	37	18,21,22	0.80	1 (5%)	21,30,33	1.47	4 (19%)
37	T6A	1	37	37	27,34,35	1.04	2 (7%)	29,49,52	2.65	9 (31%)
37	1MA	1	58	37	16,25,26	1.81	3 (18%)	18,37,40	1.42	3 (16%)
37	1MG	1	9	37	18,26,27	0.99	0	19,39,42	1.48	4 (21%)
37	5MC	1	49	37	18,22,23	1.08	1 (5%)	26,32,35	1.33	5 (19%)
37	G7M	1	46	37	20,26,27	2.75	3 (15%)	17,39,42	1.01	1 (5%)
37	5MC	1	48	37	18,22,23	0.99	1 (5%)	26,32,35	1.31	4 (15%)
37	2MG	1	10	37	18,26,27	1.02	1 (5%)	16,38,41	1.19	2 (12%)

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. 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
37	H2U	1	47	37	-	5/7/38/39	0/2/2/2
37	M2G	1	26	37	-	6/7/29/30	0/3/3/3
37	RIA	1	64	37	-	3/13/51/52	0/4/4/4
37	H2U	1	16	37	-	1/7/38/39	0/2/2/2
37	T6A	1	37	37	-	8/19/41/42	0/3/3/3
37	1MA	1	58	37	-	0/3/25/26	0/3/3/3
37	1MG	1	9	37	-	2/3/25/26	0/3/3/3
37	5MC	1	49	37	-	2/7/25/26	0/2/2/2
37	G7M	1	46	37	-	1/3/25/26	0/3/3/3
37	5MC	1	48	37	-	3/7/25/26	0/2/2/2
37	2MG	1	10	37	_	2/5/27/28	0/3/3/3

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

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
	37	1	46	G7M	C8-N9	7.81	1.47	1.33



Contre	Continued from pretious page								
Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(A)	Ideal(Å)		
37	1	46	G7M	C8-N7	7.29	1.46	1.33		
37	1	26	M2G	C2-N3	5.69	1.37	1.30		
37	1	58	1MA	C2-N3	5.57	1.35	1.29		
37	1	46	G7M	C5-C4	4.76	1.48	1.39		

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
37	1	37	T6A	C12-N11-C10	8.55	136.18	121.94
37	1	37	T6A	C2-N1-C6	7.15	122.72	116.59
37	1	16	H2U	O4'-C1'-N1	3.92	114.64	109.30
37	1	37	T6A	C14-C12-C13	3.63	116.37	110.19
37	1	37	T6A	N3-C2-N1	-3.58	123.08	128.68

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
37	1	9	1MG	O4'-C4'-C5'-O5'
37	1	9	1MG	C3'-C4'-C5'-O5'
37	1	16	H2U	C4'-C5'-O5'-P
37	1	26	M2G	C3'-C4'-C5'-O5'
37	1	26	M2G	N1-C2-N2-CM1

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	1	37	T6A	8	0
37	1	9	1MG	1	0
37	1	48	5MC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.



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

Mal	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
	Type	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
49	SF4	k	705	-	0,12,12	-	-	-		
49	SF4	k	706	-	0,12,12	-	-	-		
47	ADP	k	701	45	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
48	ATP	k	703	45	26,33,33	0.93	1 (3%)	31,52,52	1.60	5 (16%)

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
49	SF4	k	705	-	-	-	0/6/5/5
49	SF4	k	706	-	-	-	0/6/5/5
47	ADP	k	701	45	-	5/12/32/32	0/3/3/3
48	ATP	k	703	45	-	2/18/38/38	0/3/3/3

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	k	703	ATP	C5-C4	2.50	1.47	1.40
47	k	701	ADP	C5-C4	2.47	1.47	1.40

All (2) bond length outliers are listed below:

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
47	k	701	ADP	PA-O3A-PB	-3.70	120.12	132.83
48	k	703	ATP	PB-O3B-PG	-3.64	120.35	132.83
48	k	703	ATP	PA-O3A-PB	-3.49	120.84	132.83
48	k	703	ATP	C3'-C2'-C1'	3.43	106.14	100.98
48	k	703	ATP	N3-C2-N1	-3.19	123.69	128.68

There are no chirality outliers.

5 of 7 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
47	k	701	ADP	C5'-O5'-PA-O1A
47	k	701	ADP	C5'-O5'-PA-O2A
48	k	703	ATP	O4'-C4'-C5'-O5'
47	k	701	ADP	PA-O3A-PB-O2B
47	k	701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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
41	q	2
37	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	16:H2U	O3'	18:G	Р	5.01
1	q	582:GLN	С	583:GLN	Ν	3.87
1	q	605:CYS	С	606:LEU	Ν	3.34



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11439. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 180





Z Index: 180

6.2.2 Raw map



X Index: 180

Y Index: 180



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: 174



Y Index: 160



Z Index: 154

6.3.2 Raw map



X Index: 174

Y Index: 159



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



6.4.2 Raw 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 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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 2020 nm^3 ; this corresponds to an approximate mass of 1824 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 0.161 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.161 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estim	Estimation criterion (FSC cut-off)				
Resolution estimate (A)	0.143	0.5	Half-bit			
Reported by author	6.20	-	-			
Author-provided FSC curve	6.19	8.92	6.41			
Unmasked-calculated*	8.35	15.70	9.13			

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.35 differs from the reported value 6.2 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11439 and PDB model 6ZU9. 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 0.009 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 (0.009).



9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.2200
1	0.9130	0.1270
2	0.9920	0.2340
3	0.8770	0.1710
А	0.9500	0.2640
В	0.9920	0.2580
С	0.9970	0.2500
D	1.0000	0.2660
Ε	0.9830	0.2310
F	0.9430	0.2140
Н	1.0000	0.2470
Ι	0.9970	0.2680
J	0.9900	0.2410
К	0.9910	0.2350
L	0.9980	0.2760
М	0.8920	0.2410
Ν	1.0000	0.2370
О	0.9590	0.2270
Р	0.9960	0.2790
Q	0.9950	0.2440
R	0.9960	0.2870
S	0.9980	0.2800
Т	0.9980	0.2560
U	0.9950	0.2700
V	0.9920	0.2680
W	0.9910	0.2580
Х	0.9860	0.2870
Y	0.9910	0.2590
Z	0.9950	0.2350
a	0.9980	0.2680
b	0.9970	0.2640
с	0.9900	0.2800
d	0.9800	0.2520
е	0.9860	0.2600
f	0.7850	0.0690



Chain	Atom inclusion	Q-score
g	0.9080	0.2430
h	0.9950	0.2360
i	0.9770	0.2290
k	0.8910	0.1740
1	0.1350	0.0260
m	0.6330	0.1700
0	0.9160	0.1460
р	0.7300	0.1280
q	0.9530	0.1670
r	0.0460	0.0810

