

wwPDB EM Validation Summary Report (i)

Nov 21, 2022 – 09:58 PM EST

PDB ID	:	3J46
EMDB ID	:	EMD-5693
Title	:	Structure of the SecY protein translocation channel in action
Authors	:	Akey, C.W.; Park, E.; Menetret, J.F.; Gumbart, J.C.; Ludtke, S.J.; Li, W.;
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Deposited on	:	2013-06-18
Resolution	:	10.10 Å(reported)
Based on initial models	:	3I8G, 2I2P, 3J01

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 10.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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	У	437	13%	20%	5% •			
2	Е	56	23% 46%	48%	5%			
3	G	67	10%	31%	7% •			
4	n	101	44% 59%	30%	6% 5%			
5	р	76	16%	50%	5%			
6	a	76	25%	36%	•			
7	5	234	14%	22%	•			

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Mol	Chain	Length		Quality of ch	ain		
0	т	100	17%				
8	1 T	100		88%		10	%•
			15%				
9	U	103		95%			••
			16%				
10	Y	63		95%			5%
11	1	63		76%		21%	•
12	2	36	•	72%		22%	•
13	3	44	45%		48%		7%
14	4	109	23%	50%		27%	



2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 17478 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 protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	У	437	Total 3361	C 2220	N 554	O 569	S 18	0	1

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
У	5	ACE	-	ACETYLATION	UNP P0AGA2
У	68	CYS	SER	ENGINEERED MUTATION	UNP P0AGA2
У	441	NH2	-	AMIDATION	UNP P0AGA2

• Molecule 2 is a protein called Preprotein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	Е	56	Total 433	C 283	N 76	O 73	S 1	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	73	ACE	-	ACETYLATION	UNP P0AG96
Е	128	NH2	-	AMIDATION	UNP P0AG96

• Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	G	67	Total 461	C 301	N 74	O 82	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	8	ACE	-	ACETYLATION	UNP P0AG99
G	74	NH2	-	AMIDATION	UNP P0AG99



• Molecule 4 is a protein called NC100.

Mol	Chain	Residues		At	oms			AltConf	Trace
4	n	101	Total 760	C 480	N 132	0 146	${ m S} { m 2}$	0	0

• Molecule 5 is a RNA chain called P-tRNA.

Mol	Chain	Residues		A	AltConf	Trace			
5	р	76	Total 1621	C 722	N 287	O 536	Р 76	0	0

• Molecule 6 is a RNA chain called A-tRNA.

Mol	Chain	Residues		Atoms						Trace
6	a	76	Total 1626	C 729	N 290	O 531	Р 75	S 1	0	0

• Molecule 7 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	234	Total 1733	C 1081	N 315	O 330	S 7	0	0

• Molecule 8 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	Т	100	Total	C	N 14C	0	S	0	0
			(87	496	140	143	2		

• Molecule 9 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	103	Total 789	C 498	N 148	0 143	0	0

• Molecule 10 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
10	V	63	Total	С	N	0	S	0	0
10	I	03	509	313	99	95	2	0	0

• Molecule 11 is a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues		\mathbf{A}	toms		Atoms					
11	1	63	Total 1350	C 603	N 245	O 439	Р 63	0	0			

• Molecule 12 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2	36	Total 775	C 345	N 142	O 252	Р 36	0	0

• Molecule 13 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
13	3	44	Total 948	C 423	N 180	O 301	Р 44	0	0

• Molecule 14 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	109	Total 2325	C 1038	N 409	O 769	Р 109	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: Protein translocase subunit SecY







Chain U:	%	95%		•	1
A1 A2 A2 V12 K18 K18 C19 C19	S23 S30 N33 N52 N33 N52 N52 N33 N52 N52 N33 N52 N33 N52 N33 N33 N33 N33 N33 N33 N33 N33 N33 N3	A62 164 A75 K78 B88 €91	KI 08		
• Molecule 10:	50S ribosomal pr	rotein L29P			
Chain Y:	5%	95%		5%	i -
M1 K2 L6 L6 L6 E17 E17	L22 N27 L28 R29 A32 A33 S34 S34	K 60 A 63			
• Molecule 11:	23S ribosomal R	NA			
Chain 1:		76%		21% •	
A52 A53 A53 G54 G55 C57 C57 G58 U59 G50 C61	A63 A64 A64 065 066 067 069 070 A71 A71 A74 A74	C76 C77 C79 C79 C79 C79 C79 C79 C81 A83 A83 A83 A83 C86 C86 C86 C86 C86 C86 C86 C86 C86 C87 C79 C79 C79 C79 C79 C77 C79 C77 C79 C77 C79 C77 C79 C77 C79 C77 C79 C77 C79 C77 C79 C77 C79 C77 C79 C77 C79 C79	G88 489 489 491 492 493 494 495 495 C96 C96 C97	430 1999 1100 1102 1102 1103 1104 1105 1105	6107 6108 6109 6110 A111
0112 0113 0114					
• Molecule 12:	23S ribosomal R	NA			
Chain 2: 🔽		72%		22% •	
A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 U1316 C1315	U1318 C1319 C1319 A1321 A1321 A1322 C1323 C1328 U1326 A1328 A1328 A1328 A1328 A1328	(1331) (1331) (1332) (1333) (1333) (1335) (1335) (1336) (1336) (1338) (1			
• Molecule 13:	23S ribosomal R	NA			
Chain 3:	45%		48%	7%	
A1515 G1516 G1517 G1517 C1518 01520 U1520 U1520 G1521 A1522 G1523 A1525 A1525	C1526 C1526 C1527 C1529 C1530 C1531 C1532 C1533 C1535 C1535 C1536 C1536 C1536 C1536 C1536 C1536	U15330 01540 01541 01542 01543 01544 01546 01546 01546 01548 01548 01548 01560	A1551 A1552 A1553 U1554 C1555 C1556 C1557 C1557 C1558		
• Molecule 14:	23S ribosomal R	NA			
Chain 4:	23%	50%		27%	
C2091 U2092 A2094 A2094 A2095 C2096 A2097 U2098 G2101 A2101	62102 62103 62103 72106 72106 72106 72109 72109 72110 72110 72111 72111 72111	A2115 G2115 G2115 G2116 G2119 G2121 G2122 G2125 G2125 G2125 G2125 G2125	G2127 G2128 G2128 U2130 U2130 U2131 U2131 G2133 A2134 A2136 G2135 G2135	0.213 0.2138 0.2139 0.2140 0.2140 0.2141 0.2143 0.2143 0.2145 0.2145	C2146 A2147 G2148 U2149 C2150
U2151 C2153 C2153 C2154 C2155 C2156 C2156 C2158 C2158 C2161 C2161	C2162 A2163 C2164 C2165 C2166 U2167 U2167 A2170 A2170 A2171 A2171 A2173	C2117 C2177 C2177 C2177 C2177 C2179 C2180 U2181 U2182 A2183 A2183 A2183 A2184 U2185 C2186 C2186 C2186 C2186 C2186 C2186 C2186 C2186 C2186 C2187 C2187 C2187 C2177 C2187 C2177 C2177 C2187 C2287	U2187 U2188 U2189 G2190 A2191 U2192 U2193 U2196 U2196 C2196	A2199	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	160	Depositor
Electron dose $(e^-/\text{\AA}^2)$	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	42000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	3.245	Depositor
Minimum map value	-0.464	Depositor
Average map value	0.072	Depositor
Map value standard deviation	0.294	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.12, 2.12, 2.12	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: MIA, ACE, NH2 $\,$

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	M_{ol} Chain B		Bond lengths		Bond angles		
MOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	у	1.71	27/3434~(0.8%)	2.07	97/4657~(2.1%)		
2	Е	1.70	3/437~(0.7%)	2.26	24/596~(4.0%)		
3	G	1.65	3/463~(0.6%)	2.12	17/622~(2.7%)		
4	n	1.63	2/774~(0.3%)	1.60	14/1048~(1.3%)		
5	р	3.30	222/1810~(12.3%)	3.82	397/2820~(14.1%)		
6	a	0.35	0/1783	0.77	4/2776~(0.1%)		
7	5	1.66	11/1748~(0.6%)	1.92	30/2355~(1.3%)		
8	Т	0.98	0/794	1.09	1/1060~(0.1%)		
9	U	0.96	0/797	1.04	0/1062		
10	Y	1.00	0/510	0.90	0/677		
11	1	1.62	1/1511~(0.1%)	2.50	178/2354~(7.6%)		
12	2	1.63	1/867~(0.1%)	2.45	97/1351~(7.2%)		
13	3	3.35	127/1062~(12.0%)	3.85	256/1655~(15.5%)		
14	4	3.46	373/2599~(14.4%)	3.88	636/4049~(15.7%)		
All	All	2.21	770/18589~(4.1%)	2.66	1751/27082~(6.5%)		

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	у	2	18
2	Е	0	2
3	G	0	1
4	n	3	0
5	р	0	29
6	a	0	1
7	5	0	3
9	U	0	1
11	1	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	2	0	2
13	3	0	19
14	4	0	63
All	All	5	141

The worst 5 of 770 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
4	n	99	ALA	C-N	31.42	1.89	1.33
13	3	1516	G	O3'-P	25.56	1.91	1.61
4	n	22	TYR	C-N	22.00	1.84	1.34
13	3	1551	А	O3'-P	17.96	1.82	1.61
14	4	2098	U	C2-N3	14.56	1.48	1.37

The worst 5 of 1751 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	р	19	G	N1-C6-O6	24.02	134.31	119.90
14	4	2108	А	N1-C6-N6	22.36	132.01	118.60
5	р	18	G	N1-C6-O6	20.82	132.39	119.90
5	р	37	А	N1-C6-N6	20.71	131.02	118.60
13	3	1535	А	N1-C6-N6	20.48	130.89	118.60

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	у	55	GLN	CA
1	у	56	GLN	CA
4	n	38	LEU	CA
4	n	39	HIS	CA
4	n	40	GLN	CA

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	У	22	ARG	Sidechain
1	У	34	ARG	Sidechain
1	у	38	PHE	Sidechain
1	У	45	ASP	Sidechain
1	У	57	ARG	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	У	3361	0	3514	0	0
2	Е	433	0	466	22	0
3	G	461	0	485	7	0
4	n	760	0	742	0	0
5	р	1621	0	818	0	0
6	а	1626	0	833	0	0
7	5	1733	0	1824	8	0
8	Т	787	0	844	20	0
9	U	789	0	847	0	0
10	Y	509	0	543	0	0
11	1	1350	0	678	2	0
12	2	775	0	389	0	0
13	3	948	0	478	0	0
14	4	2325	0	1168	8	0
All	All	17478	0	13629	45	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 20.

The worst 5 of 45 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)
2:E:81:LYS:HD2	8:T:93:LEU:CD1	1.30	1.62
2:E:81:LYS:CD	8:T:93:LEU:HD12	1.04	1.51
2:E:81:LYS:CD	8:T:93:LEU:CD1	1.94	1.21
2:E:81:LYS:HZ3	8:T:93:LEU:CG	1.57	1.17
2:E:81:LYS:CE	8:T:93:LEU:HD12	1.77	1.13

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	Per	centiles
1	У	435/437~(100%)	392 (90%)	18 (4%)	25~(6%)	1	18
2	E	54/56~(96%)	49 (91%)	4(7%)	1 (2%)	8	38
3	G	65/67~(97%)	57 (88%)	4 (6%)	4 (6%)	1	17
4	n	99/101~(98%)	42 (42%)	26 (26%)	31 (31%)	C	0
7	5	232/234~(99%)	198 (85%)	25~(11%)	9 (4%)	3	23
8	Т	98/100~(98%)	71 (72%)	20 (20%)	7 (7%)	1	14
9	U	101/103~(98%)	84 (83%)	14 (14%)	3(3%)	4	28
10	Y	61/63 (97%)	48 (79%)	11 (18%)	2(3%)	4	26
All	All	$1145/1161 \ (99\%)$	941 (82%)	122 (11%)	82 (7%)	2	14

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	У	45	ASP
1	у	56	GLN
1	у	258	TYR
1	у	266	PRO
1	у	298	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	У	353/353~(100%)	330~(94%)	23~(6%)	17 42	

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
2	Ε	47/47~(100%)	45~(96%)	2(4%)	29	53
3	G	46/46~(100%)	39~(85%)	7 (15%)	3	14
4	n	77/77~(100%)	61~(79%)	16 (21%)	1	6
7	5	$181/181 \ (100\%)$	170~(94%)	11 (6%)	18	44
8	Т	84/84~(100%)	79~(94%)	5~(6%)	19	44
9	U	84/84~(100%)	82~(98%)	2(2%)	49	69
10	Y	55/55~(100%)	54 (98%)	1 (2%)	59	77
All	All	927/927~(100%)	860 (93%)	67 (7%)	18	39

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5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	5	144	THR
8	Т	36	LYS
9	U	91	LYS
2	Е	94	THR
2	Е	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
7	5	165	ASN
7	5	168	ASN
9	U	52	ASN
8	Т	70	HIS
4	n	39	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	1	62/63~(98%)	13 (20%)	1 (1%)
12	2	35/36~(97%)	8 (22%)	1 (2%)
13	3	43/44~(97%)	7 (16%)	2(4%)
14	4	108/109~(99%)	39~(36%)	8 (7%)
5	р	75/76~(98%)	17 (22%)	0
6	a	74/76~(97%)	28 (37%)	0
All	All	397/404~(98%)	112 (28%)	12 (3%)



5 of 112 RNA backbone outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
5	р	2	С
5	р	4	G
5	р	5	G
5	р	7	А
5	р	8	U

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	4	2147	А
14	4	2152	G
14	4	2172	U
14	4	2157	G
13	3	1551	А

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

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	\mathbf{ths}	B	ond ang	les
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
6	MIA	a	37	6	24,31,32	1.85	4 (16%)	26,44,47	<mark>3.11</mark>	6 (23%)

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
6	MIA	a	37	6	-	2/11/33/34	0/3/3/3

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
6	a	37	MIA	C13-C14	6.42	1.50	1.32
6	a	37	MIA	C2-S10	4.22	1.79	1.75
6	a	37	MIA	C12-C13	-2.87	1.35	1.48
6	a	37	MIA	C8-N7	-2.06	1.31	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	a	37	MIA	C11-S10-C2	10.57	110.16	102.27
6	a	37	MIA	C12-N6-C6	-8.85	109.44	122.55
6	a	37	MIA	C5-C6-N1	-3.69	117.74	120.81
6	a	37	MIA	C2-N3-C4	-3.30	110.78	115.32
6	a	37	MIA	C12-C13-C14	-3.28	120.76	127.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	a	37	MIA	N6-C12-C13-C14
6	a	37	MIA	C3'-C4'-C5'-O5'

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
13	3	2
4	n	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	1516:G	O3'	1517:G	Р	1.91
1	n	99:ALA	С	100:GLY	Ν	1.89
1	n	22:TYR	С	23:GLU	Ν	1.84
1	3	1551:A	O3'	1552:A	Р	1.82



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5693. 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: 96

Y Index: 96



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: 103

Y Index: 99

Z Index: 89

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

This section was not generated.



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 3075 nm^3 ; this corresponds to an approximate mass of 2778 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 0.099 ${\rm \AA^{-1}}$



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-5693 and PDB model 3J46. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.8 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 (0.8).



9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.8085	0.0790	
1	0.9526	0.1260	1 0
2	0.9548	0.1000	1.0
3	0.9589	0.1440	
4	0.9630	0.0950	
5	0.8074	0.0590	
Е	0.7238	0.0410	
G	0.8581	0.0510	
Т	0.7276	0.0700	
U	0.8108	0.0750	
Y	0.7907	0.0870	0.0
a	0.6292	0.0690	<0.0
n	0.5294	-0.0090	
р	0.6582	0.0960	
у	0.8141	0.0630	

