

wwPDB EM Validation Summary Report (i)

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PDB ID	:	7TEJ
EMDB ID	:	EMD-25847
Title	:	Cryo-EM structure of the 20S Alpha 3 Deletion proteasome core particle
Authors	:	Walsh Jr., R.M.; Rawson, S.; Schnell, H.M.; Hanna, J.
Deposited on	:	2022-01-05
Resolution	:	2.74 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.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 2.74 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

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	1	241	76% 8%	16%
1	М	241	73% 11%	16%
2	2	266	73% 9%	18%
2	N	266	73% 9%	18%
3	А	252	86%	8% 6%
3	0	252	87%	6% 6%
4	В	250	85%	12% •
4	Р	250	90%	8% •



Mol	Chain	Length	Quality of chain		
5	С	254	79%	10% 1	1%
5	D	254	71% 76	% 22%	
5	Q	254	80%	9% 10	0%
5	R	254	69% 8%	22%	_
6	Е	260	56% 10%	34%	
6	S	260	57% 9%	34%	
7	F	234	82%	13%	5%
7	Т	234	83%	12%	5%
8	G	288	70% 10	0% 19%	_
8	U	288	69% 11	.% 19%	
9	Н	215	70%	14% 16%	, 0
9	V	215	71%	13% 16%	6
10	Ι	261	70% 8%	% 22%	
10	W	261	70% 7%	6 22%	_
11	J	205	89%	10	0% •
11	Х	205	• 84%	15%	•
12	K	198	89%	99	% •
12	Y	198	91%		7% •
13	L	287	63% 7%	30%	
13	Z	287	64% 6%	30%	

Continued from previous page...



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 91490 atoms, of which 45742 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 Proteasome subunit beta type-6.

Mol	Chain	Residues			AltConf	Trace				
1	1	202	Total	С	Η	Ν	Ο	S	0	0
	1 1	202	3163	1009	1568	276	306	4	0	0
1	М	202	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
	111	202	3163	1009	1568	276	306	4		

• Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues			AltConf	Trace				
2	2	218	Total	С	Н	Ν	0	S	0	0
_	-	-10	3412	1081	1706	291	328	6	Ŭ	Ŭ
2	N	218	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0
	IN	210	3412	1081	1706	291	328	6	0	0

• Molecule 3 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues			AltConf	Trace				
2	Λ	226	Total	С	Η	Ν	0	S	0	0
5	A	A 230	3732	1191	1863	313	357	8	0	0
2	0	226	Total	С	Η	Ν	0	S	0	0
5	0	230	3732	1191	1863	313	357	8	0	0

• Molecule 4 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues			AltConf	Trace				
4	В	244	Total	С	Η	Ν	0	S	0	0
4	D	244	3743	1188	1880	306	366	3	0	0
4	D	244	Total	С	Η	Ν	Ο	S	0	0
4	Ľ	244	3743	1188	1880	306	366	3	0	0

• Molecule 5 is a protein called Proteasome subunit alpha type-4.



Mol	Chain	Residues			Atom	S			AltConf	Trace
5	С	225	Total	С	Η	Ν	0	\mathbf{S}	0	0
0	U	220	3547	1108	1781	306	348	4	0	0
5	Л	107	Total	С	Η	Ν	0	S	0	0
0	D	197	3132	979	1579	268	302	4	0	0
5	0	228	Total	С	Η	Ν	0	S	0	0
0	Q	220	3596	1121	1806	312	353	4	0	0
5	В	107	Total	С	Н	Ν	0	S	0	0
5	п	191	3132	979	1579	268	302	4	0	U

• Molecule 6 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	171	Total	С	Η	Ν	0	\mathbf{S}	0	0
0 E	111	2656	839	1330	222	261	4	0	0	
6	C	171	Total	С	Η	Ν	0	S	0	0
0 2	S	1/1	2656	839	1330	222	261	4	U	U

• Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues				AltConf	Trace			
7	F	<u> </u>	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
1	I.	223	3438	1079	1728	297	330	4	0	0
7	т	222	Total	С	Η	Ν	0	S	0	0
· ·		223	3438	1079	1728	297	330	4	0	U

• Molecule 8 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
8	С	030	Total	С	Н	Ν	0	S	0	0
0	G	232	3608	1151	1804	314	335	4	0	0
0	T	020	Total	С	Η	Ν	0	S	0	0
0	U	232	3607	1151	1803	314	335	4	0	0

• Molecule 9 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
Q	н	181	Total	С	Η	Ν	Ο	S	0	0
9	11	101	2786	891	1383	232	273	7	0	0
0	V	191	Total	С	Η	Ν	Ο	S	0	0
9	v	101	2786	891	1383	232	273	7	0	0

• Molecule 10 is a protein called Proteasome subunit beta type-2.



Mol	Chain	Residues	Atoms						AltConf	Trace
10	т	203	Total	С	Η	Ν	0	S	0	0
10	1	205	3131	988	1574	270	293	6	0	0
10	W	203	Total	С	Η	Ν	0	S	0	0
10	vv	203	3131	988	1574	270	293	6	0	

• Molecule 11 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	т	202	Total	С	Η	Ν	0	S	0	0
	1	203	3142	1007	1567	257	303	8	0	0
11	v	202	Total	С	Η	Ν	0	S	0	0
11	Λ	205	3142	1007	1567	257	303	8	0	0

• Molecule 12 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
19	K	194	Total	С	Η	Ν	Ο	S	0	0
	Γ	194	3111	987	1558	263	298	5	0	0
19	v	104	Total	С	Η	Ν	Ο	S	0	0
12	I	194	3111	987	1558	263	298	5	0	

• Molecule 13 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
12	т	201	Total	С	Η	Ν	0	\mathbf{S}	0	0
10		201	3120	1010	1538	268	298	6	0	0
12	7	201	Total	С	Η	Ν	0	S	0	0
10		201	3120	1010	1538	268	298	6	0	U



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: Proteasome subunit beta type-6





• Molecule 3: Proteasome subunit alpha type-1



• Molecule 3: Proteasome subunit alpha type-1



• Molecule 4: Proteasome subunit alpha type-2



D230 R236 L250

• Molecule 4: Proteasome subunit alpha type-2



• Molecule 5: Proteasome subunit alpha type-4



• Molecule 5: Proteasome subunit alpha type-4

Chain D: 71% 7% 22%





• Molecule 5: Proteasome subunit alpha type-4



• Molecule 5: Proteasome subunit alpha type-4

Chain R:		6	9%			8%		22%			
MET SER CLY TYR ASP ASP ASP EER FILEU FILE PHE SER ASP CLY MIT	V20 L24	R29	V42	R48 ARG SER THR L52	D56 THR ARG ILE THR PRO SER K63	<mark>A</mark> 80 D81	L85	T121 GLN SER GLY GLY V126	V131	A136 G137	T163

N166 N167 N167 N167 N167 V171 V171 V171 V171 V171 V192 S198 S188 S198 S188 S198 S188 S188 S188 S188 S188

• Molecule 6: Proteasome subunit alpha type-5







• Molecule 7: Proteasome subunit alpha type-6



S205 L206 G227 V230 I234

• Molecule 7: Proteasome subunit alpha type-6



• Molecule 8: Proteasome subunit alpha type-7



• Molecule 9: Proteasome subunit beta type-1



Chain H:	70%	14%	16%
MET ALSO GLN CLN CLN CLN CLN ASP ASN ASN ASN ASN ASN CLN CLN CLN CLN CLN CLN CLN CLN CLN CL	T26 A35 A35 A35 A35 A35 A33 A33 T41 T41 T41 T41 T50 T41 C53 C56 C11 C12 C12 C12 C12 C12 C12 C12 C12 C12	ALA ASP THR Q72 A73 I74 VR9	v100 E103 E103 E104 E104 C105 GLU ASN LYS
ASP ASN LEU THR ALA 0115 1116 1116 1116 1116 1116 1116 1116	V195 1198 A199 E203 212		
• Molecule 9: Proteasome sub	unit beta type-1		
Chain V:	71%	13%	16%
MET ASN GLY GLY GLN CLU ASN ASN ASN ASN ASN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	T26 A35 A35 B36 B36 B37 T41 T41 T50 C63 C63 C63 C63 C63 C63 C63 C63 C63 C63	ASP Q72 Q79 E83	Y89 T96 S99 V100 F101 F101 E103 L104
C105 TYR GLU GLU GLU ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	V196 V196 V198 V212 V212		
• Molecule 10: Proteasome sub	ounit beta type-2		
Chain I:	70% 89	% 229	%
MET ALA ALA CLEU CLEU SER SER ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	LYNU ALLA THR STRR STRR STRR GET 132 ALS ALS ALS ALLA ALLA	ASP THR GLU GLU VAL THR GLU GLU	S107 S107 M111 M111 CLN GLN GLN CLY HIS HIS
GLY ALA ALA 126 133 134 133 1156 1156 1156 1156 1156 1156 1192 1192 1192 1192	V202 V202 V202 V202 V215 V215 V215 GLU GLU GLU GLU GLU GLU GLU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP		
• Molecule 10: Proteasome sub	ounit beta type-2		
Chain W:	70%	7% 22	2%
MET ALA ALA ALA CLEU CLEU SER PRE ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	LFNU ALA ALA ALA STRR STRR THR CLY CLY CLY CLY CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA	GLU ALA VAL THR GLN LB7 V119	GLY GLY HTS TLE GLY ALA ALA D133
8141 1142 11443 11443 11445 1155 1155 1155 1156 1156 1174 1192 1192 1192	v206 v206 v206 v219 v219 v219 v219 d1v d1v d1v d1v d1v d1v d1v d1v d1v d1v	ALA	
• Molecule 11: Proteasome sub	ounit beta type-3		
Chain J:	89%		10% •
MET MET SER SER SER 110 V11 V11 V12 C24 C24 C24 C24 C25 C25 C25 C25 C25 C25 C25 C25 C25 C25	V104 8131 8133 8133 8133 8133 8133 8133 8140 8141 8140 8144 117 0177 8180	D204	
• Molecule 11: Proteasome sub	ounit beta type-3		
Chain X:	84%		15% •
	WORLDWIDE PROTEIN DATA BANK		

K191

• Molecule 12: Proteasome subunit beta type-4

Chain K:	89%	9% •
MET 13 13 13 14 12 12 12	338 A46 E73 E73 831 1102 1102 1102 1102 1102 1102 1138 1138 1138 1138 1138 1138 1138 113	
• Molecule 12:	Proteasome subunit beta type-4	
Chain Y:	91%	7% •
MET 16 124 R35 S38 S38	E57 E53 S31 S31 S31 S31 738 7129 7138 7138 7138 7138 7138 7138 7138 7138	
• Molecule 13:	Proteasome subunit beta type-5	
Chain L:	63% 7%	30%
MET GLN ALA ALA ALA ASP SER PHE SER VAL VAL PRO	ASN ASN LEU VAL LEU CYS CLU CLEU CLEU CLEU CLEU CLEU CLEU CLEU	THR VAL PRO PRO PRO FILE SER PRO GIN GIN GIN ALA ALA ALA THR
ASP ASP SER ARG ASN PSN PSN ASP CYS LYS TLF LYS	LLE ALA ALA ALA ALA ALA T76 T76 T77 T78 T78 T78 T78 T78 T78 T78 T78 T78	dLY dLA dLA dLY dLY dLA dLA dLA dLA tL2 tC2 d t2 t2 t2 t2 t2 t2 t2 t2 t2 t2 t2 t2 t2
V268 F272 W273 W273 E277 E277 V285 I285 I285 G287		
• Molecule 13:	Proteasome subunit beta type-5	
Chain Z:	64% 6%	30%
MET GLN GLN ILE ALA ASP ASP SER PHE SER VAL VAL	ASN LEU VAL VAL CUU CUU CUU CUU CUU CUU CUU CUU CUU CU	THR PRO PRO PRO PRO PRO PRO PRO GLN GLN ARG ALA ARG ALA ARG THR THR
ASP ASP ASS ASS ASN ASN PRO CYS LYS LYS	LLE HLS HLA HLA HLA HLA CLY B1 F15 F12 GLY GLY GLY F129 F129 F129 F129 F129 F129 F129 F129	Y179 T180 A181 Y182 Y189 Y189 P200 P200 Y219 W260
W273 K276 E277 L226 U285 C285 C287 C287		



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	150227	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 $(e^-/\text{\AA}^2)$	53.85	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.451	Depositor
Minimum map value	-2.835	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.148	Depositor
Recommended contour level	0.385	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	1	0.29	0/1623	0.50	0/2183
1	М	0.30	0/1623	0.52	0/2183
2	2	0.28	0/1734	0.53	0/2353
2	Ν	0.28	0/1734	0.53	0/2353
3	А	0.30	0/1906	0.49	0/2581
3	0	0.30	0/1906	0.49	0/2581
4	В	0.30	0/1899	0.50	0/2571
4	Р	0.31	0/1899	0.49	0/2571
5	С	0.28	0/1792	0.52	0/2425
5	D	0.29	0/1573	0.53	0/2125
5	Q	0.28	0/1817	0.52	0/2460
5	R	0.28	0/1573	0.51	0/2125
6	Е	0.26	0/1340	0.49	0/1800
6	S	0.25	0/1340	0.49	0/1800
7	F	0.27	0/1735	0.50	0/2341
7	Т	0.26	0/1735	0.50	0/2341
8	G	0.31	0/1841	0.50	0/2484
8	U	0.30	0/1841	0.48	0/2484
9	Н	0.29	0/1429	0.51	0/1931
9	V	0.29	0/1429	0.50	0/1931
10	Ι	0.29	0/1585	0.51	0/2145
10	W	0.29	0/1585	0.51	0/2145
11	J	0.32	0/1605	0.50	0/2166
11	Х	0.32	0/1605	0.50	0/2166
12	К	0.31	0/1581	0.52	0/2132
12	Y	0.31	0/1581	0.53	0/2132
13	L	0.32	0/1617	0.52	0/2185
13	Ζ	0.31	0/1617	0.51	0/2185
All	All	0.29	0/46545	0.51	0/62879

There are no bond length outliers. There are no bond angle outliers.

There are no chirality outliers.



There are no planarity outliers.

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	1	1595	1568	1565	12	0
1	М	1595	1568	1565	17	0
2	2	1706	1706	1704	16	0
2	N	1706	1706	1704	16	0
3	А	1869	1863	1861	11	0
3	0	1869	1863	1861	10	0
4	В	1863	1880	1879	19	0
4	Р	1863	1880	1879	12	0
5	С	1766	1781	1778	19	0
5	D	1553	1579	1574	12	0
5	Q	1790	1806	1804	18	0
5	R	1553	1579	1574	15	0
6	Е	1326	1330	1323	19	0
6	S	1326	1330	1323	19	0
7	F	1710	1728	1725	20	0
7	Т	1710	1728	1725	20	0
8	G	1804	1804	1800	23	0
8	U	1804	1803	1800	22	0
9	Н	1403	1383	1380	20	0
9	V	1403	1383	1380	22	0
10	Ι	1557	1574	1571	13	0
10	W	1557	1574	1571	13	0
11	J	1575	1567	1566	12	0
11	Х	1575	1567	1566	21	0
12	K	1553	1558	1560	11	0
12	Y	1553	1558	1560	10	0
13	L	1582	1538	1535	14	0
13	Z	1582	1538	1535	11	0
All	All	45748	45742	45668	411	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 4.

The worst 5 of 411 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)
13:Z:82:ARG:NH1	13:Z:200:ASP:OD1	1.96	0.98
5:Q:14:ASP:O	5:R:29:ARG:NH1	2.06	0.88
6:S:197:GLU:OE2	6:S:231:TYR:OH	1.92	0.86
10:W:141:SER:OG	10:W:149:ASP:OD1	1.95	0.83
5:R:163:THR:HG21	5:R:171:VAL:HG13	1.59	0.83

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
1	1	196/241~(81%)	192 (98%)	4 (2%)	0	100	100
1	М	196/241~(81%)	192 (98%)	4(2%)	0	100	100
2	2	214/266~(80%)	209~(98%)	5(2%)	0	100	100
2	Ν	214/266~(80%)	209~(98%)	5(2%)	0	100	100
3	А	232/252~(92%)	230~(99%)	2(1%)	0	100	100
3	Ο	232/252~(92%)	230 (99%)	2(1%)	0	100	100
4	В	242/250~(97%)	242 (100%)	0	0	100	100
4	Р	242/250~(97%)	239 (99%)	3 (1%)	0	100	100
5	С	219/254~(86%)	216 (99%)	3 (1%)	0	100	100
5	D	187/254~(74%)	186 (100%)	1 (0%)	0	100	100
5	Q	224/254~(88%)	221 (99%)	3~(1%)	0	100	100
5	R	187/254~(74%)	185 (99%)	2(1%)	0	100	100
6	Ε	157/260~(60%)	157 (100%)	0	0	100	100
6	S	157/260~(60%)	157 (100%)	0	0	100	100
7	F	217/234~(93%)	213 (98%)	4 (2%)	0	100	100
7	Т	217/234~(93%)	216 (100%)	1 (0%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
8	G	226/288~(78%)	224~(99%)	2(1%)	0	100	100
8	U	226/288~(78%)	223~(99%)	3~(1%)	0	100	100
9	Н	175/215~(81%)	171 (98%)	4 (2%)	0	100	100
9	V	175/215~(81%)	172 (98%)	3 (2%)	0	100	100
10	Ι	197/261~(76%)	193~(98%)	4 (2%)	0	100	100
10	W	197/261~(76%)	194 (98%)	3 (2%)	0	100	100
11	J	201/205~(98%)	197 (98%)	4 (2%)	0	100	100
11	Х	201/205~(98%)	196 (98%)	5 (2%)	0	100	100
12	Κ	192/198~(97%)	187 (97%)	5 (3%)	0	100	100
12	Y	192/198~(97%)	186 (97%)	6(3%)	0	100	100
13	L	195/287~(68%)	194 (100%)	1 (0%)	0	100	100
13	Z	195/287~(68%)	194 (100%)	1 (0%)	0	100	100
All	All	5705/6930~(82%)	5625 (99%)	80 (1%)	0	100	100

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There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	1	169/201~(84%)	169 (100%)	0	100	100
1	М	169/201~(84%)	169 (100%)	0	100	100
2	2	186/224~(83%)	186 (100%)	0	100	100
2	Ν	186/224~(83%)	185 (100%)	1 (0%)	88	92
3	А	202/210~(96%)	202 (100%)	0	100	100
3	Ο	202/210~(96%)	202 (100%)	0	100	100
4	В	203/209~(97%)	202 (100%)	1 (0%)	88	92
4	Р	203/209~(97%)	203 (100%)	0	100	100
5	С	201/226~(89%)	201 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
5	D	176/226~(78%)	176 (100%)	0	100	100
5	Q	204/226~(90%)	204 (100%)	0	100	100
5	R	176/226~(78%)	176 (100%)	0	100	100
6	Ε	143/215~(66%)	143 (100%)	0	100	100
6	S	143/215~(66%)	143 (100%)	0	100	100
7	F	183/193~(95%)	183 (100%)	0	100	100
7	Т	183/193~(95%)	183 (100%)	0	100	100
8	G	191/239~(80%)	191 (100%)	0	100	100
8	U	191/239~(80%)	191 (100%)	0	100	100
9	Н	151/178~(85%)	151 (100%)	0	100	100
9	V	151/178~(85%)	151 (100%)	0	100	100
10	Ι	169/214~(79%)	169 (100%)	0	100	100
10	W	169/214~(79%)	169~(100%)	0	100	100
11	J	171/173~(99%)	171 (100%)	0	100	100
11	Х	171/173~(99%)	171 (100%)	0	100	100
12	Κ	172/175~(98%)	172 (100%)	0	100	100
12	Y	172/175~(98%)	172 (100%)	0	100	100
13	L	165/235~(70%)	165 (100%)	0	100	100
13	Ζ	165/235~(70%)	165 (100%)	0	100	100
All	All	4967/5836 (85%)	4965 (100%)	2 (0%)	100	100

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All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	В	50	LYS
2	Ν	137	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such side chains are listed below:

Mol	Chain	\mathbf{Res}	Type
13	L	141	HIS
1	М	114	HIS
6	S	188	HIS
6	Е	99	HIS



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type
10	Ι	201	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25847. 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: 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: 195

Y Index: 155

Z Index: 154

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

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

6.4.1 Primary map



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.385. 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 569 $\rm nm^3;$ this corresponds to an approximate mass of 514 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 0.365 \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-25847 and PDB model 7TEJ. 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 0.385 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 (0.385).



9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.385) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.5730
1	0.9500	0.5720
2	0.9720	0.5940
А	0.9560	0.5780
В	0.9590	0.5880
С	0.9500	0.5590
D	0.9490	0.5400
Ε	0.8740	0.4490
F	0.9490	0.5420
G	0.9570	0.5770
Н	0.9690	0.5920
Ι	0.9800	0.6080
J	0.9700	0.6160
K	0.9720	0.6050
L	0.9620	0.5900
Μ	0.9500	0.5720
Ν	0.9740	0.5930
О	0.9580	0.5800
Р	0.9630	0.5860
Q	0.9480	0.5500
R	0.9460	0.5410
S	0.8650	0.4450
Т	0.9410	0.5370
U	0.9570	0.5740
V	0.9720	0.5920
W	0.9780	0.6090
Х	0.9720	0.6120
Y	0.9740	0.6100
Z	0.9600	0.5880



1.0

