

Feb 17, 2024 – 09:27 AM EST

]	PDB ID	:	7TEO
\mathbf{EN}	MDB ID	:	EMD-25848
	Title	:	Cryo-EM structure of the 20S Alpha 3 Deletion proteasome core particle in complex with FUB1
Depo	Authors sited on	:	Walsh Jr., R.M.; Rawson, S.; Schnell, H.M.; Hanna, J. 2022-01-05
Re	solution	:	2.97 Å(reported)
	This is	a F	full wwPDB EM Validation 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 2.97 Å.

Sidechain outliers

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	Percentile Ranks	Value
Ramachandran outliers		0
Sidechain outliers		0.0%
Worse		Better
Percentile relat	ive to all structures	
Percentile relat	ive to all EM structures	
Metric	Whole archive	EM structures
	(#Entries)	(#Entries)
Ramachandran outliers	154571	4023

154315

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 $\leq 5\%$ 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.

3826

Mol	Chain	Length	Quality of chain	
1	1	241	91%	8%
1	М	241	92%	8%
2	2	266	86%	14%
2	Ν	266	86%	14%
3	А	252	93%	7%
3	0	252	93%	7%
4	В	250	96%	•
4	Р	250	96%	•
5	С	254	87%	13%

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Mol	Chain	Length	Quality of chain	
5	D	254	82%	18%
5	Q	254	87%	13%
5	R	254	82%	18%
6	Е	260	80%	20%
6	S	260	80%	20%
7	F	234	99%	
7	Т	234	99%	·
8	G	288	84%	16%
8	U	288	84%	16%
9	Н	215	91%	9%
9	V	215	91%	9%
10	Ι	261	84%	16%
10	W	261	84%	16%
11	J	205	99%	
11	Х	205	99%	
12	K	198	98%	
12	Y	198	98%	
13	L	287	74%	26%
13	Z	287	74%	26%
14	a	250	1 32% 68%	
14	b	250	32% 68%	

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2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 97522 atoms, of which 48612 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	Atoms						AltConf	Trace
1	1	991	Total	С	Η	Ν	Ο	S	0	0
	1 1	221	3449	1110	1701	301	333	4	0	0
1	м	221	Total	С	Η	Ν	0	\mathbf{S}	0	0
	111	221	3449	1110	1701	301	333	4	0	0

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

Mol	Chain	Residues			AltConf	Trace				
2	2	230	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
2	2	230	3595	1137	1798	307	346	7	0	0
2	N	230	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
	1 N	230	3595	1137	1798	307	346	7	0	U

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

Mol	Chain	Residues			AltConf	Trace				
2	Λ	224	Total	С	Η	Ν	0	S	0	0
5	A	234	3687	1176	1841	308	354	8	0	0
2	0	224	Total	С	Η	Ν	0	S	0	0
5	0	204	3687	1176	1841	308	354	8	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	В	941	Total	С	Η	Ν	Ο	S	0	0
	D	241	3694	1170	1856	303	362	3	0	0
4	D	941	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
4	1	241	3694	1170	1856	303	362	3	0	0

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



Mol	Chain	Residues			Atom	5			AltConf	Trace
5	C	າາາ	Total	С	Η	Ν	0	\mathbf{S}	0	0
0	U		3521	1098	1771	304	344	4	0	0
5	П	208	Total	С	Η	Ν	0	S	0	0
0		208	3288	1025	1650	284	325	4	0	0
5	0	າາາ	Total	С	Η	Ν	0	S	0	0
0	Q		3521	1098	1771	304	344	4	0	0
5	D	208	Total	С	Н	Ν	0	S	0	0
5	n	200	3287	1025	1649	284	325	4	U	U

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

Mol	Chain	Residues				AltConf	Trace			
6	F	207	Total	С	Η	Ν	0	S	0	0
0 E	Ľ	201	3176	997	1583	266	324	6	0	0
6	C	207	Total	С	Η	Ν	0	S	0	0
0	S	207	3176	997	1583	266	324	6	0	U

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

Mol	Chain	Residues		Atoms						Trace
7	F	221	Total	С	Η	Ν	0	S	0	0
1	T,	231	3551	1114	1778	307	348	4	0	0
7	Т	021	Total	С	Η	Ν	0	S	0	0
		201	3551	1114	1778	307	348	4		U

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

Mol	Chain	Residues			Atoms	5			AltConf	Trace	
8	C	243	Total	С	Η	Ν	0	S	0	0	
0	G	240	3776	1203	1884	329	356	4	0	0	
0	T	242	Total	С	Η	Ν	0	S	0	0	
8	U	U	240	3776	1203	1884	329	356	4	0	0

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

Mol	Chain	Residues			Atom	s			AltConf	Trace
Q	н	106	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
9	11	190	2992	955	1480	250	300	7	0	0
0	V	106	Total	С	Η	Ν	Ο	S	0	0
9	v	190	2991	955	1479	250	300	7	0	U

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



Mol	Chain	Residues			AltConf	Trace				
10	т	220	Total	С	Η	Ν	0	S	0	0
10	1	220	3347	1054	1677	291	319	6	0	0
10	W	220	Total	С	Η	Ν	0	S	0	0
10	VV	220	3347	1054	1677	291	319	6	0	0

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

Mol	Chain	Residues		Atoms						Trace
11	Т	202	Total	С	Η	Ν	0	S	0	0
	II J	203	3142	1007	1567	257	303	8	0	
11	v	202	Total	С	Η	Ν	0	S	0	0
	Λ	203	3142	1007	1567	257	303	8		0

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

Mol	Chain	Residues			Atom	.s			AltConf	Trace
19	K	105	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
12	IX	195	3130	992	1569	264	299	6	0	0
19	V	105	Total	С	Η	Ν	0	S	0	0
12	Y	Y 195		992	1569	264	299	6	0	0

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

Mol	Chain	Residues		Atoms						Trace	
13	L	212	Total	С	Η	Ν	0	\mathbf{S}	0	0	
10	Б	212	3237	1045	1593	280	312	7	0		
12	7	010	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	
10		212	3237	1045	1593	280	312	7	0	0	

• Molecule 14 is a protein called Silencing boundary-establishment protein FUB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	0	Q1	Total	С	Η	Ν	0	S	0	0
14	a	01	1177	393	559	101	121	3	0	0
14	h	Q1	Total	С	Η	Ν	0	S	0	0
14	D	01	1177	393	559	101	121	3	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: Proteasome subunit beta type-6







- Molecule 6: Proteasome subunit alpha type-5 Chain E: 80% 20% ALA LEU PPHE GLY GLY GLY GLY GLV GLV GLV GLU SER ARG GLU SER ARG FRO PRO MET PHE LEU LEU ARG SER GLU TYR ASP GLN VAL GLU GLU SER SER LEU GLU GLU ALA ALA GLU SER PRO GLU GLU ALA MET • Molecule 6: Proteasome subunit alpha type-5 Chain S: 80% 20% MET PHE LEU THR ARG SER GLU ARG ASP GLY VAL GLN VAL GLU GLU SER SER LEU LEU GLU ALA ILE ALA GLU SER PRO GLU GLU ALA ASP VAL VAL CLU E E • Molecule 7: Proteasome subunit alpha type-6 Chain F: 99% MET PHE ARG • Molecule 7: Proteasome subunit alpha type-6 Chain T: 99% • Molecule 8: Proteasome subunit alpha type-7 Chain G: 84% 16% MET SER SER GLY GCLY A ASP A ASP GCLU A ASP GCLU A ASP ASP A ASP A ASP ASP ASP A ASP ASP ASP ASP ASP ASP ASP ASP ASP A • Molecule 8: Proteasome subunit alpha type-7 Chain U: 84% 16% AET SER LE
- Molecule 9: Proteasome subunit beta type-1



Chain H:	91%	9%
MET ASN GLY TILE GLN VAL ASP ASN ASN ASN LVS CLY GLU VAL		
• Molecule 9: Proteason	me subunit beta type-1	
Chain V:	91%	9%
MET ASN GLY TLLE TLLE GLN VAL ASD ASN ASN ASN ASN LLYS CLYS GLU VAL		
• Molecule 10: Protease	ome subunit beta type-2	
Chain I:	84%	16%
MET ALA GLY CLEU LEU EER PHE ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	ASN SER THR GLN CLN CLN CLN CLN CLN CLN CLN CLN CLN C	
• Molecule 10: Protease	ome subunit beta type-2	
Chain W:	84%	16%
MET ALA GLY LEU CLEU LEU ASR ASN ASN ASN ASN ASN ASN ALA ALA ALU	SER SER CIAR CIAR CIAR PRO PRO PRO PRO CIAR CIAR CIA CIA CIA CIA CIA CIA CIA CIA CIA CIA	
• Molecule 11: Protease	ome subunit beta type-3	
Chain J:	99%	
MET BER D205		
• Molecule 11: Protease	ome subunit beta type-3	
Chain X:	99%	
MET D3 D2 D2 D205		
• Molecule 12: Protease	ome subunit beta type-4	
Chain K:	98%	•
M1 F 196 GLN ALA GLN		

• Molecule 12: Proteasome subunit beta type-4



Chain Y:	98%	·
M1 F195 GLN ALA GLN		
• Molecule 13:	Proteasome subunit beta type-5	
Chain L:	74%	26%
MET GLN GLN ALA ALA ASP SER PHE SER VAL	ASN ASN VAL LEU LYS CLV CLV CLV ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	GLN ARG ARG ARG ARG ARG SER CEU PRO PRO PRO PRO CLN CLEU ARG CLN ALA ALA ALA ALA ALA ALA ALA ALA ALA A
ASP ASP SER SER ASN ASN PRO ASP CYS LYS LLYS ILLE	LLA ALA HIS GLY C287	
• Molecule 13:	Proteasome subunit beta type-5	
Chain Z:	74%	26%
MET GLN GLN ILE ALA ALA ASP SER PHE SER VAL	ASN ASN VAL LEU VAL LYS GLU CLU CLU CLU CLU CLU CLU CLU CLU CLU C	GLN ARG ALE U ALA ALA ALA FRU FRU FRU FRU FRU GLN GLN GLN GLN ALA ALA ALA ALA ALA ALA ALA ALA ALA
ASP ASP SER ASR ASR ASR PRO ASP CYS LYS ILLE ILLE	1115 ALA HIS GIY C287	
• Molecule 14:	Silencing boundary-establishment	protein FUB1
Chain a:	32%	68%
MET ILE GLU GLU ASN VAL CLU CLU LEU VAL CLU CLU	LEU VAL LEU GIU GIU GIU CIU ARC CIU CIU CIU CIU CIU CIU CIU CIU CIU CI	ARG ARG ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP
LEU ASP ASP ASP ASP ASP LYS TYR THR VAL VAL VAL	ARG HIS SER THR SER THR MET THR MET THR CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	LEU GLU GLU GLU GLU SER FLEU VAL PRO ASP PRO ASP TLEU TLEU TLEU TLEU CLN GLN GLN GLN GLN GLN CLN
R ALA K ALA E ASP E ASP E ASP 127 138 0139 C AN C AN	A144 14H 14H 164 164 168 168 168 178 178 168 178 178 178 178 178 178 178 17	P202 P202 ARG ARG ARG ARG CP20 CP20 CP20 CP20 CP20 CP20 CP20 CP20
• Molecule 14:	Silencing boundary-establishment	protein FUB1
Chain b:	32%	68%
MET TLF GLU GLU ASN LYS CLU CLU CLU CLU GLU	LER LUC CLUC CLUC CLUC CLUC CLUC CLUC CLUC	ART LITE LITE ARS ARS ARS ARS CLU LITE CLU ALLEU VALLEU VALLEU VALLEU VALLEU VALLEU VALLEU VALLEU VALLEU VALLEU VALLEU VALLEU VALLEU TAR
LEU ASP ASP ASP ASP ASP LYS TYR THR VAL VAL VAL	ARG HIS CLY THR THR THE THE THR VAL CVAL CVAL CVAL CVAL CVAL CVAL CVAL	LEU GLU GLU GLU GLU FLEU PLEU PLEU PLU CLU CLU CLU CLU CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN



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# 4 Experimental information (i)

| Property                           | Value                           | Source    |
|------------------------------------|---------------------------------|-----------|
| EM reconstruction method           | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                   | POINT, C2                       | Depositor |
| Number of particles used           | 56059                           | 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                  | 3.742                           | Depositor |
| Minimum map value                  | -1.746                          | Depositor |
| Average map value                  | 0.002                           | Depositor |
| Map value standard deviation       | 0.115                           | Depositor |
| Recommended contour level          | 0.306                           | 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   |
|-----|---------|------|----------|------|----------|
|     | Ullaili | RMSZ | # Z  > 5 | RMSZ | # Z  > 5 |
| 1   | 1       | 0.26 | 0/1786   | 0.51 | 0/2408   |
| 1   | М       | 0.26 | 0/1786   | 0.50 | 0/2408   |
| 2   | 2       | 0.25 | 0/1828   | 0.51 | 0/2480   |
| 2   | Ν       | 0.25 | 0/1828   | 0.51 | 0/2480   |
| 3   | А       | 0.26 | 0/1882   | 0.48 | 0/2549   |
| 3   | 0       | 0.27 | 0/1882   | 0.48 | 0/2549   |
| 4   | В       | 0.26 | 0/1873   | 0.47 | 0/2536   |
| 4   | Р       | 0.26 | 0/1873   | 0.48 | 0/2536   |
| 5   | С       | 0.25 | 0/1773   | 0.51 | 0/2396   |
| 5   | D       | 0.25 | 0/1660   | 0.50 | 0/2244   |
| 5   | Q       | 0.25 | 0/1773   | 0.51 | 0/2396   |
| 5   | R       | 0.26 | 0/1660   | 0.51 | 0/2244   |
| 6   | Е       | 0.24 | 0/1612   | 0.47 | 0/2171   |
| 6   | S       | 0.24 | 0/1612   | 0.47 | 0/2171   |
| 7   | F       | 0.24 | 0/1800   | 0.50 | 0/2433   |
| 7   | Т       | 0.25 | 0/1800   | 0.50 | 0/2433   |
| 8   | G       | 0.26 | 0/1932   | 0.47 | 0/2609   |
| 8   | U       | 0.26 | 0/1932   | 0.47 | 0/2609   |
| 9   | Н       | 0.26 | 0/1541   | 0.48 | 0/2087   |
| 9   | V       | 0.26 | 0/1541   | 0.49 | 0/2087   |
| 10  | Ι       | 0.25 | 0/1701   | 0.49 | 0/2307   |
| 10  | W       | 0.25 | 0/1701   | 0.49 | 0/2307   |
| 11  | J       | 0.26 | 0/1605   | 0.48 | 0/2166   |
| 11  | Х       | 0.27 | 0/1605   | 0.49 | 0/2166   |
| 12  | Κ       | 0.26 | 0/1589   | 0.50 | 0/2142   |
| 12  | Y       | 0.27 | 0/1589   | 0.50 | 0/2142   |
| 13  | L       | 0.27 | 0/1681   | 0.51 | 0/2274   |
| 13  | Ζ       | 0.27 | 0/1681   | 0.51 | 0/2274   |
| 14  | a       | 0.27 | 0/641    | 0.45 | 0/873    |
| 14  | b       | 0.25 | 0/641    | 0.44 | 0/873    |
| All | All     | 0.26 | 0/49808  | 0.49 | 0/67350  |

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 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     | 219/241~(91%)                | 214 (98%)  | 5(2%)   | 0        | 100   | 100    |
| 1   | М     | 219/241~(91%)                | 215 (98%)  | 4 (2%)  | 0        | 100   | 100    |
| 2   | 2     | 228/266~(86%)                | 223 (98%)  | 5(2%)   | 0        | 100   | 100    |
| 2   | Ν     | 228/266~(86%)                | 226 (99%)  | 2(1%)   | 0        | 100   | 100    |
| 3   | А     | 230/252~(91%)                | 228 (99%)  | 2(1%)   | 0        | 100   | 100    |
| 3   | Ο     | 230/252~(91%)                | 227 (99%)  | 3~(1%)  | 0        | 100   | 100    |
| 4   | В     | 239/250~(96%)                | 239 (100%) | 0       | 0        | 100   | 100    |
| 4   | Р     | 239/250~(96%)                | 239 (100%) | 0       | 0        | 100   | 100    |
| 5   | С     | 212/254~(84%)                | 209 (99%)  | 3~(1%)  | 0        | 100   | 100    |
| 5   | D     | 202/254~(80%)                | 198 (98%)  | 4 (2%)  | 0        | 100   | 100    |
| 5   | Q     | 212/254~(84%)                | 207 (98%)  | 5 (2%)  | 0        | 100   | 100    |
| 5   | R     | 202/254~(80%)                | 201 (100%) | 1 (0%)  | 0        | 100   | 100    |
| 6   | Ε     | 201/260~(77%)                | 197 (98%)  | 4 (2%)  | 0        | 100   | 100    |
| 6   | S     | 201/260~(77%)                | 200 (100%) | 1 (0%)  | 0        | 100   | 100    |
| 7   | F     | 229/234~(98%)                | 228 (100%) | 1 (0%)  | 0        | 100   | 100    |
| 7   | Т     | 229/234~(98%)                | 226 (99%)  | 3 (1%)  | 0        | 100   | 100    |
| 8   | G     | $24\overline{1/288}\ (84\%)$ | 236 (98%)  | 5 (2%)  | 0        | 100   | 100    |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Perce | entiles |
|-----|-------|-----------------|------------|---------|----------|-------|---------|
| 8   | U     | 241/288~(84%)   | 236~(98%)  | 5(2%)   | 0        | 100   | 100     |
| 9   | Н     | 194/215~(90%)   | 191 (98%)  | 3 (2%)  | 0        | 100   | 100     |
| 9   | V     | 194/215~(90%)   | 190 (98%)  | 4 (2%)  | 0        | 100   | 100     |
| 10  | Ι     | 218/261~(84%)   | 216 (99%)  | 2(1%)   | 0        | 100   | 100     |
| 10  | W     | 218/261 (84%)   | 214 (98%)  | 4 (2%)  | 0        | 100   | 100     |
| 11  | J     | 201/205~(98%)   | 194 (96%)  | 7 (4%)  | 0        | 100   | 100     |
| 11  | Х     | 201/205~(98%)   | 193 (96%)  | 8 (4%)  | 0        | 100   | 100     |
| 12  | Κ     | 193/198~(98%)   | 189 (98%)  | 4 (2%)  | 0        | 100   | 100     |
| 12  | Y     | 193/198~(98%)   | 189 (98%)  | 4 (2%)  | 0        | 100   | 100     |
| 13  | L     | 210/287~(73%)   | 207~(99%)  | 3 (1%)  | 0        | 100   | 100     |
| 13  | Z     | 210/287~(73%)   | 207~(99%)  | 3 (1%)  | 0        | 100   | 100     |
| 14  | a     | 73/250~(29%)    | 72~(99%)   | 1 (1%)  | 0        | 100   | 100     |
| 14  | b     | 73/250~(29%)    | 73 (100%)  | 0       | 0        | 100   | 100     |
| All | All   | 6180/7430~(83%) | 6084 (98%) | 96 (2%) | 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 | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | 1     | 184/201~(92%) | 183 (100%) | 1 (0%)   | 88          | 95  |
| 1   | М     | 184/201~(92%) | 184 (100%) | 0        | 100         | 100 |
| 2   | 2     | 196/224~(88%) | 196 (100%) | 0        | 100         | 100 |
| 2   | Ν     | 196/224~(88%) | 196 (100%) | 0        | 100         | 100 |
| 3   | А     | 200/210~(95%) | 200 (100%) | 0        | 100         | 100 |
| 3   | Ο     | 200/210~(95%) | 200 (100%) | 0        | 100         | 100 |
| 4   | В     | 200/209~(96%) | 200 (100%) | 0        | 100         | 100 |
| 4   | Р     | 200/209~(96%) | 200 (100%) | 0        | 100         | 100 |

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| 0 0 |       | r r · · · · · · · · · · · · · · · · · · |             |          |            |     |
|-----|-------|-----------------------------------------|-------------|----------|------------|-----|
| Mol | Chain | Analysed                                | Rotameric   | Outliers | Percentile |     |
| 5   | С     | 200/226~(88%)                           | 200 (100%)  | 0        | 100        | 100 |
| 5   | D     | 185/226~(82%)                           | 185 (100%)  | 0        | 100        | 100 |
| 5   | Q     | 200/226~(88%)                           | 200 (100%)  | 0        | 100        | 100 |
| 5   | R     | 185/226~(82%)                           | 185 (100%)  | 0        | 100        | 100 |
| 6   | Ε     | 172/215~(80%)                           | 172~(100%)  | 0        | 100        | 100 |
| 6   | S     | 172/215~(80%)                           | 172 (100%)  | 0        | 100        | 100 |
| 7   | F     | 190/193~(98%)                           | 190 (100%)  | 0        | 100        | 100 |
| 7   | Т     | 190/193~(98%)                           | 190 (100%)  | 0        | 100        | 100 |
| 8   | G     | 201/239~(84%)                           | 200 (100%)  | 1 (0%)   | 88         | 95  |
| 8   | U     | 201/239~(84%)                           | 201 (100%)  | 0        | 100        | 100 |
| 9   | Н     | 162/178~(91%)                           | 162 (100%)  | 0        | 100        | 100 |
| 9   | V     | 162/178~(91%)                           | 162 (100%)  | 0        | 100        | 100 |
| 10  | Ι     | 179/214 (84%)                           | 179 (100%)  | 0        | 100        | 100 |
| 10  | W     | 179/214 (84%)                           | 179 (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     | 173/175~(99%)                           | 173 (100%)  | 0        | 100        | 100 |
| 12  | Y     | 173/175~(99%)                           | 173 (100%)  | 0        | 100        | 100 |
| 13  | L     | 169/235~(72%)                           | 169 (100%)  | 0        | 100        | 100 |
| 13  | Z     | 169/235~(72%)                           | 169 (100%)  | 0        | 100        | 100 |
| 14  | a     | 64/207~(31%)                            | 64 (100%)   | 0        | 100        | 100 |
| 14  | b     | $\overline{64/207} \ (31\%)$            | 64 (100%)   | 0        | 100        | 100 |
| All | All   | 5292/6250~(85%)                         | 5290 (100%) | 2 (0%)   | 100        | 100 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 192 | LYS  |
| 8   | G     | 168 | ARG  |

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | Ε     | 73  | HIS  |
| 6   | Е     | 147 | HIS  |
| 7   | F     | 69  | HIS  |
| 7   | Т     | 69  | HIS  |

### 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-25848. 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.

#### Central slices (i) 6.2

#### 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: 173

Y Index: 164

Z Index: 155

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 0.306. 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 563  $\text{nm}^3$ ; this corresponds to an approximate mass of 508 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 0.337  ${\rm \AA^{-1}}$ 



# 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-25848 and PDB model 7TEO. 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 0.306 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 (0.306).



### 9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.306) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All   | 0.9270         | 0.5320  |
| 1     | 0.9480         | 0.5560  |
| 2     | 0.9490         | 0.5690  |
| А     | 0.9500         | 0.5350  |
| В     | 0.9270         | 0.5380  |
| С     | 0.8490         | 0.4300  |
| D     | 0.8740         | 0.4460  |
| Ε     | 0.8820         | 0.4610  |
| F     | 0.9370         | 0.5320  |
| G     | 0.9390         | 0.5350  |
| Н     | 0.9540         | 0.5640  |
| Ι     | 0.9630         | 0.5750  |
| J     | 0.9630         | 0.5790  |
| K     | 0.9590         | 0.5680  |
| L     | 0.9570         | 0.5740  |
| М     | 0.9520         | 0.5620  |
| Ν     | 0.9530         | 0.5700  |
| О     | 0.9530         | 0.5340  |
| Р     | 0.9290         | 0.5380  |
| Q     | 0.8430         | 0.4280  |
| R     | 0.8670         | 0.4400  |
| S     | 0.8820         | 0.4640  |
| Т     | 0.9290         | 0.5300  |
| U     | 0.9440         | 0.5330  |
| V     | 0.9580         | 0.5630  |
| W     | 0.9650         | 0.5790  |
| X     | 0.9600         | 0.5760  |
| Y     | 0.9560         | 0.5670  |
| Z     | 0.9630         | 0.5700  |
| a     | 0.8430         | 0.5100  |
| b     | 0.8650         | 0.5210  |

