

wwPDB EM Validation Summary Report (i)

Nov 20, 2022 - 12:59 am GMT

PDB ID	:	6FVV
EMDB ID	:	EMD-4321
Title	:	26S proteasome, s3 state
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Deposited on	:	2018-03-05
Resolution	:	5.40 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 43
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	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 5.40 Å.

Ramachandran outliers

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.



154571

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 $<=5\%$
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.

4023

3826

Mol	Chain	Length	Quality of chain	
1	А	241	99%	•
1	a	241	80% 1	7% •
2	В	249	98%	•
2	b	249	40% 82%	16% •
3	С	244	99%	•
3	с	244	76% 23	% •
4	D	251	92%	• 6%
4	d	251	80%	.8% •
5	Ε	244	95%	5%



Conti	nued fron	n previous	page	
Mol	Chain	Length	Quality of chain	
5	е	244	42% 78%	20% ·
6	F	231	97%	•
6	f	231	74%	21% •
7	G	242	96%	•
7	g	242	74%	21% 5%
8	1	196	• 82%	15% •
8	h	196	• • 75%	21% •
9	2	226	83%	16% ·
9	i	226	80%	16% •
10	3	204	76%	22% •
10	j	204	77%	20% •
11	4	195	• 79%	19% •
11	k	195	75%	21% •
12	5	212	75%	23% •
12	1	212	77%	21% •
13	6	222	74%	23% •
13	m	222	74%	23% •
14	7	232	70%	25% ••
14	n	232	76%	18% 6%
15	W	197	76%	20% • •
16	V	289	75%	21% •
17	Т	266	81%	17% •
18	Х	127	73%	22% •
19	Y	89	46%	19% •
20	Z	970	59% 86%	6% • 7%



Mol	Chain	Length	Quality of chain	
01	N	022	12%	
<u></u>	IN	922	81%	16% •
22	S	475	78%	18% •
23	Р	440	• 81%	17% •
24	Q	434	7%	18% •
25	R	405	7%	20% •
26	II	304	14%	170/
20	0	004	7%	1770 •
27	Ο	388	76%	21% ••
28	Н	417	74%	23% •
29	Ι	385	78%	19% •
30	K	394	18%	23% • •
			13%	
31	L	388	77%	18% • •
32	М	421	78%	19% ·
	-	107	23%	
33	J	405	74%	21% • •



2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 110420 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues		Ate	AltConf	Trace			
1	a	241	Total 1908	C 1214	N 320	O 366	S 8	0	0
1	А	241	Total 1908	C 1214	N 320	O 366	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	249	Total 1907	C 1214	N 314	0 376	${ m S} { m 3}$	0	0
2	В	249	Total 1907	C 1214	N 314	O 376	${ m S} { m 3}$	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	244	Total	С	Ν	0	S	0	0
- З – С	C	244	1905	1201	321	380	3	0	0
3 C	244	Total	С	Ν	0	S	0	0	
	U	244	1905	1201	321	380	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	251	Total 1982	C 1235	N 350	O 393	${S \atop 4}$	0	0
4	D	237	Total 1859	C 1164	N 325	O 366	${}^{\mathrm{S}}_{4}$	0	0

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



Mol	Chain	Residues	Atoms					AltConf	Trace
5	5 0	944	Total	С	Ν	Ο	\mathbf{S}	0	0
0 6	С	244	1883	1176	316	384	7		0
5	5 E	244	Total	С	Ν	0	\mathbf{S}	0	0
0		244	1883	1176	316	384	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	021	Total	С	Ν	0	S	0	0
0 1	1	201	1773	1114	307	348	4	0	0
6	F	021	Total	С	Ν	0	S	0	0
0	Г	231	1773	1114	307	348	4	0	0

• Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	g	242	Total 1886	C 1199	N 328	O 355	${S \atop 4}$	0	0
7	G	242	Total 1886	C 1199	N 328	O 355	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	h	106	Total	С	Ν	0	S	0	0
0	11	190	1512	955	250	300	7	0	0
0	1	106	Total	С	Ν	0	S	0	0
0		190	1512	955	250	300	7		

• Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues		Ate		AltConf	Trace		
9	i	226	Total 1720	C 1082	N 298	O 333	${ m S} 7$	0	0
9	2	226	Total 1720	C 1082	N 298	O 333	${ m S} 7$	0	0

• Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues		At	AltConf	Trace			
10	j	204	Total 1581	C 1010	N 258	O 305	S 8	0	0



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Mol	Chain	Residues		At	oms			AltConf	Trace
10	3	204	Total 1581	C 1010	N 258	O 305	S 8	0	0

• Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	ŀ	105	Total	С	Ν	0	S	0	0
11	K	195	1562	992	264	300	6	0	0
11	4	105	Total	С	Ν	0	S	0	0
	4	195	1562	992	264	300	6	0	0

• Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues		At	oms		AltConf	Trace	
19	1	919	Total	С	Ν	0	\mathbf{S}	0	0
12	1	212	1644	1045	280	312	7	0	0
19	F	919	Total	С	Ν	0	\mathbf{S}	0	0
	5	212	1644	1045	280	312	$\overline{7}$	0	0

• Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues		Ate	oms		AltConf	Trace	
13	m	222	Total 1757	C 1115	N 303	O 335	S 4	0	0
13	6	222	Total 1757	C 1115	N 303	O 335	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues		At	oms		AltConf	Trace	
14	n	232	Total 1816	C 1148	N 311	O 350	${f S}{7}$	0	0
14	7	229	Total 1790	C 1133	N 306	0 344	${f S}7$	0	0

• Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	W	197	Total 1535	C 962	N 269	O 301	${ m S} { m 3}$	0	0

• Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.



Mol	Chain	Residues		At	oms			AltConf	Trace
16	V	289	Total 2274	C 1425	N 389	O 446	S 14	0	0

• Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues		Ate	AltConf	Trace			
17	Т	266	Total 2193	C 1405	N 349	0 433	S 6	0	0

• Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	Х	127	Total 1033	C 664	N 169	0 196	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0

• Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	Y	89	Total 731	C 447	N 119	0 164	S 1	0	0

• Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues		Α	toms			AltConf	Trace
20	Ζ	906	Total 7006	C 4416	N 1150	0 1410	S 30	0	0

• Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues		Α	toms			AltConf	Trace
21	N	099	Total	С	Ν	Ο	\mathbf{S}	0	0
		922	7158	4536	1205	1389	28		U

• Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues		At	oms			AltConf	Trace
22	S	475	Total 3895	C 2488	N 653	0 739	S 15	0	0

• Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.



Mol	Chain	Residues		At	oms			AltConf	Trace
23	Р	440	Total 3609	C 2297	N 604	O 698	S 10	0	0

• Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues		At	AltConf	Trace			
24	Q	434	Total 3499	C 2225	N 577	O 681	S 16	0	0

• Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues		At	AltConf	Trace			
25	R	405	Total 3259	C 2077	N 535	0 637	S 10	0	0

• Molecule 26 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	304	Total 2427	C 1529	N 414	0 477	${f S}7$	0	0

• Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues		At	oms			AltConf	Trace
27	О	388	Total 3186	C 2051	N 519	O 608	S 8	0	0

• Molecule 28 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues		At	oms			AltConf	Trace
28	Н	417	Total 3234	C 2008	N 578	O 632	S 16	0	0

• Molecule 29 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues		At		AltConf	Trace		
29	Ι	385	Total 3022	C 1899	N 508	O 598	S 17	0	0

• Molecule 30 is a protein called 26S proteasome regulatory subunit 6B homolog.



Mol	Chain	Residues	Atoms			AltConf	Trace		
30	K	394	Total 3113	C 1951	N 548	O 604	S 10	0	0

• Molecule 31 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	L	388	Total 3083	C 1942	N 548	0 581	S 12	0	0

• Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues		At	oms			AltConf	Trace
32	М	421	Total 3285	C 2043	N 573	O 656	S 13	0	0

• Molecule 33 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues		At	oms			AltConf	Trace
33	J	405	Total 3171	C 1995	N 565	O 593	S 18	0	0

• Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues		Ate	oms			AltConf
34	Н	1	Total	С	Ν	Ο	Р	0
01		-	27	10	5	10	2	Ŭ



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Mol	Chain	Residues		Ate	oms			AltConf
34	М	1	Total 27	C 10	N 5	O 10	Р 2	0

• Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
35	Н	1	Total Mg 1 1	0
35	Ι	1	Total Mg 1 1	0
35	К	1	Total Mg 1 1	0
35	${ m L}$	1	Total Mg 1 1	0
35	М	1	Total Mg 1 1	0
35	J	1	Total Mg 1 1	0

• Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues		Ate	oms			AltConf
26	Т	1	Total	С	Ν	Ο	Р	0
90	1	1	31	10	5	13	3	0
26	V	1	Total	С	Ν	Ο	Р	0
- 30	Γ	1	31	10	5	13	3	0



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Mol	Chain	Residues		Ate	oms			AltConf	
26	т	1	Total	С	Ν	Ο	Р	0	
- 30	Ľ	1	31	10	5	13	3	0	
26	т	1	Total	С	Ν	Ο	Р	0	
30	1	1	31	10	5	13	3	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 alpha type-1





• Molecule 2: Proteasome subunit alpha type-2

Chain B: 98% T2 D3 Y5 • Molecule 3: Proteasome subunit alpha type-3 37% Chain c: 76% 23% R5 Υ6 24 D202 S203 S204 A205 A206 T207 Y208 P209 D209 D209 C211 E211 E212 F213 T245 • Molecule 3: Proteasome subunit alpha type-3 Chain C: 99% G2 S3 R4 • Molecule 4: Proteasome subunit alpha type-4 38% Chain d: 80% 18%

• Molecule 4: Proteasome subunit alpha type-4









D1966 T30 L1366 445 L1316 445 V2065 445 V216 445 V216 445 V218 848 V219 475 V224 466 V223 181 V224 181 N223 181 N224 190 V224 190 N223 181 N224 191 N223 191 N224 191 N223 191 N224 110 N224 114 P235 1142 N119 1142 N119 114 V3 1142 N119 1142 N119 1142 N119 1142 N119 1143 N116 1143 N116 1143 N116 1142 N116 1143 N116 1143 N116 1143 N149 1175 N149 1175 N149 1175 N149 1175 N149 1134 N149

• Molecule 9: Proteasome subunit beta type-2





• Molecule 10: Proteasome subunit beta type-3



• Molecule 10: Proteasome subunit beta type-3







F210 F210 F210 F210 F216 S217 S217 S249 S246 S250 S270 S270

• Molecule 12: Proteasome subunit beta type-5

Chain 5:	75%	23% •
176 1882 1882 1985 1985 1986 196 196 196 196 1196 1119	M120 A124 F129 F129 M133 M133 M133 R144 E145 E145 F145 F145 K165 Y165 Y165	M175 M175 M175 1186 1186 1186 1186 1188 1188 1188 118

1201 7202 7203 7204 7204 7204 7205 7210

• Molecule 13: Proteasome subunit beta type-6





• Molecule 13: Proteasome subunit beta type-6 Chain 6: 74% 23% • Molecule 14: Proteasome subunit beta type-7 6% Chain n: 76% 18% 6% • Molecule 14: Proteasome subunit beta type-7 Chain 7: 70% 25% . GLN GLN LYS • Molecule 15: 26S proteasome regulatory subunit RPN10 18% Chain W: 76% 20%





• Molecule 20: 26S proteasome regulatory subunit RPN1



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• Molecule 21: 26S proteasome regulatory subunit RPN2







1481 1333 1487 1487 1487 1487 1487 1487 1487 1487 1487 1487 1487 1486 1487 1338 1487 1336 1487 1336 1488 1336 1496 1356 1337 1346 1337 1346 1337 1346 1337 1346 1337 1346 1337 1377 1337 1377 1337 1349 1337 1377 1337 1343 1338 1346 1341 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1377 1378 13406 1440</td

• Molecule 23: 26S proteasome regulatory subunit RPN5









• Molecule 26: 26S proteasome regulatory subunit RPN8



• Molecule 27: 26S proteasome regulatory subunit RPN9









• Molecule 31: 26S proteasome subunit RPT4











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	292279	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 $(e^-/\text{\AA}^2)$	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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: ADP, ATP, 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		B	ond lengths	-	Bond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.93	0/1946	0.97	2/2634~(0.1%)
1	a	1.71	14/1946~(0.7%)	1.88	37/2634~(1.4%)
2	В	0.91	0/1944	0.96	1/2632~(0.0%)
2	b	1.73	15/1944~(0.8%)	1.90	44/2632~(1.7%)
3	С	0.94	0/1935	0.96	4/2618~(0.2%)
3	с	1.77	20/1935~(1.0%)	2.02	58/2618~(2.2%)
4	D	0.96	0/1888	0.96	2/2557~(0.1%)
4	d	1.75	19/2012~(0.9%)	1.93	38/2718~(1.4%)
5	Ε	1.70	2/1909~(0.1%)	1.32	7/2571~(0.3%)
5	е	1.71	23/1909~(1.2%)	1.86	34/2571~(1.3%)
6	F	0.95	0/1800	0.97	3/2433~(0.1%)
6	f	1.76	23/1800~(1.3%)	1.99	52/2433~(2.1%)
7	G	0.93	0/1926	1.20	6/2599~(0.2%)
7	g	1.73	21/1926~(1.1%)	2.10	54/2599~(2.1%)
8	1	1.72	16/1541~(1.0%)	1.85	25/2087~(1.2%)
8	h	1.73	14/1541~(0.9%)	1.90	41/2087~(2.0%)
9	2	1.74	21/1751~(1.2%)	1.87	31/2373~(1.3%)
9	i	1.75	17/1751~(1.0%)	1.93	35/2373~(1.5%)
10	3	1.74	18/1611~(1.1%)	1.94	42/2174~(1.9%)
10	j	1.71	10/1611~(0.6%)	1.94	41/2174~(1.9%)
11	4	1.73	9/1590~(0.6%)	1.90	28/2142~(1.3%)
11	k	1.76	19/1590~(1.2%)	1.95	39/2142~(1.8%)
12	5	1.75	23/1681~(1.4%)	1.92	41/2274~(1.8%)
12	1	1.77	16/1681~(1.0%)	2.05	48/2274~(2.1%)
13	6	1.76	16/1795~(0.9%)	2.00	51/2420~(2.1%)
13	m	1.74	20/1795~(1.1%)	2.05	52/2420~(2.1%)
14	7	1.72	15/1821~(0.8%)	2.03	61/2470~(2.5%)
14	n	1.73	18/1847~(1.0%)	2.07	52/2503~(2.1%)
15	W	1.71	16/1558~(1.0%)	1.94	39/2111~(1.8%)
16	V	1.69	$21\overline{/2309}~(0.9\%)$	1.95	$61\overline{/3115}~(2.0\%)$
17	Т	1.70	16/2236~(0.7%)	1.89	44/3017~(1.5%)
18	Х	1.74	6/1059~(0.6%)	1.98	33/1432~(2.3%)



Mal	Chain	E	Bond lengths		Bond angles
10101	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
19	Y	1.65	4/741~(0.5%)	1.98	15/1000~(1.5%)
20	Ζ	1.34	16/7123~(0.2%)	1.29	62/9645~(0.6%)
21	Ν	1.71	48/7273~(0.7%)	1.89	159/9822~(1.6%)
22	S	1.69	32/3967~(0.8%)	1.87	81/5355~(1.5%)
23	Р	1.66	25/3664~(0.7%)	1.87	71/4940~(1.4%)
24	Q	1.70	30/3556~(0.8%)	1.93	88/4787~(1.8%)
25	R	1.72	26/3314~(0.8%)	1.97	93/4469~(2.1%)
26	U	1.67	16/2461~(0.7%)	1.82	42/3327~(1.3%)
27	0	1.70	30/3247~(0.9%)	1.95	82/4380~(1.9%)
28	Н	1.73	29/3282~(0.9%)	1.94	88/4423~(2.0%)
29	Ι	1.69	28/3059~(0.9%)	1.87	66/4115~(1.6%)
30	K	1.75	37/3156~(1.2%)	2.19	89/4261~(2.1%)
31	L	1.73	33/3128~(1.1%)	2.22	90/4201~(2.1%)
32	М	2.68	30/3323~(0.9%)	2.13	81/4478~(1.8%)
33	J	1.91	44/3212 (1.4%)	2.14	86/4316~(2.0%)
All	All	1.68	856/112094 (0.8%)	1.84	2299/151356~(1.5%)

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	a	0	9
2	b	0	3
3	с	0	5
4	D	0	1
4	d	0	5
5	е	0	3
6	F	0	1
6	f	0	6
7	G	0	2
7	g	0	12
8	1	0	6
8	h	0	8
9	2	0	4
9	i	0	6
10	3	0	4
10	j	0	4
11	4	0	6
11	k	0	4
12	5	0	6



Mol	Chain	#Chirality outliers	#Planarity outliers
12	1	0	5
13	6	0	9
13	m	0	6
14	7	0	5
14	n	0	12
15	W	0	7
16	V	0	6
17	Т	0	10
18	Х	0	2
19	Y	0	1
20	Ζ	0	9
21	N	0	24
22	S	0	18
23	Р	0	16
24	Q	0	13
25	R	0	11
26	U	0	6
27	0	0	9
28	Н	0	13
29	Ι	0	9
30	K	0	19
31	L	0	18
32	М	0	13
33	J	0	15
All	All	0	351

The worst 5 of 856 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
5	Ε	20	ARG	NE-CZ	62.28	2.14	1.33
32	М	433	TYR	CE2-CZ	51.52	2.05	1.38
32	М	433	TYR	CG-CD1	51.22	2.05	1.39
32	М	433	TYR	CG-CD2	50.39	2.04	1.39
32	М	433	TYR	CE1-CZ	48.44	2.01	1.38

The worst 5 of 2299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
31	L	185	GLY	O-C-N	-66.69	16.00	122.70
30	K	167	PRO	O-C-N	-47.18	47.21	122.70
33	J	211	ILE	O-C-N	-47.12	47.31	122.70
32	М	338	LEU	O-C-N	-33.56	69.00	122.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
20	Ζ	728	LYS	CG-CD-CE	-29.48	23.45	111.90

There are no chirality outliers.

5 of 351 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	а	105	ARG	Sidechain
1	а	128	TYR	Sidechain
1	a	131	ARG	Sidechain
1	а	30	TYR	Sidechain
1	a	46	ARG	Sidechain

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	entiles
1	А	239/241~(99%)	223~(93%)	16 (7%)	0	100	100
1	a	239/241~(99%)	226~(95%)	11 (5%)	2 (1%)	19	60
2	В	247/249~(99%)	232 (94%)	15 (6%)	0	100	100
2	b	247/249~(99%)	231 (94%)	14 (6%)	2 (1%)	19	60
3	С	242/244~(99%)	232~(96%)	10 (4%)	0	100	100
3	с	242/244~(99%)	230~(95%)	12 (5%)	0	100	100
4	D	235/251~(94%)	222 (94%)	13 (6%)	0	100	100
4	d	249/251~(99%)	229 (92%)	14 (6%)	6 (2%)	6	35
5	E	242/244~(99%)	225 (93%)	11 (4%)	6 (2%)	5	34



α \cdots 1	c		
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	1	p	P

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
5	е	242/244~(99%)	222 (92%)	17 (7%)	3~(1%)	13	50
6	F	229/231~(99%)	219~(96%)	9 (4%)	1 (0%)	34	72
6	f	229/231~(99%)	211 (92%)	13 (6%)	5 (2%)	6	37
7	G	240/242~(99%)	229 (95%)	11 (5%)	0	100	100
7	g	240/242~(99%)	229~(95%)	10 (4%)	1 (0%)	34	72
8	1	194/196~(99%)	185 (95%)	8 (4%)	1 (0%)	29	69
8	h	194/196~(99%)	177 (91%)	12 (6%)	5 (3%)	5	33
9	2	224/226~(99%)	215 (96%)	7 (3%)	2 (1%)	17	56
9	i	224/226~(99%)	206 (92%)	15 (7%)	3 (1%)	12	48
10	3	202/204~(99%)	187 (93%)	14 (7%)	1 (0%)	29	69
10	j	202/204~(99%)	185 (92%)	11 (5%)	6 (3%)	4	30
11	4	193/195~(99%)	183 (95%)	7 (4%)	3 (2%)	9	44
11	k	193/195~(99%)	176 (91%)	13 (7%)	4 (2%)	7	37
12	5	210/212 (99%)	197 (94%)	12 (6%)	1 (0%)	29	69
12	1	210/212 (99%)	195 (93%)	15 (7%)	0	100	100
13	6	220/222 (99%)	204 (93%)	12 (6%)	4 (2%)	8	41
13	m	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	11	46
14	7	227/232~(98%)	205 (90%)	18 (8%)	4 (2%)	8	41
14	n	230/232~(99%)	214 (93%)	14 (6%)	2 (1%)	17	56
15	W	195/197~(99%)	178 (91%)	11 (6%)	6 (3%)	4	30
16	V	287/289~(99%)	260 (91%)	20 (7%)	7 (2%)	6	35
17	Т	264/266~(99%)	248 (94%)	14 (5%)	2 (1%)	19	60
18	Х	125/127~(98%)	105 (84%)	15 (12%)	5 (4%)	3	25
19	Y	87/89~(98%)	72 (83%)	10 (12%)	5 (6%)	1	19
20	Z	902/970~(93%)	820 (91%)	59 (6%)	23 (2%)	5	34
21	N	920/922~(100%)	865 (94%)	41 (4%)	14 (2%)	10	46
22	S	473/475 (100%)	445 (94%)	19 (4%)	9 (2%)	8	39
23	Р	438/440 (100%)	415 (95%)	16 (4%)	7 (2%)	9	44
24	Q	432/434 (100%)	394 (91%)	26 (6%)	12 (3%)	5	32
25	R	403/405~(100%)	388 (96%)	10 (2%)	5 (1%)	13	50
26	U	302/304~(99%)	288 (95%)	13 (4%)	1 (0%)	41	76



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	rce	entiles
27	Ο	386/388~(100%)	371 (96%)	10 (3%)	5 (1%)	1	.2	48
28	Н	415/417~(100%)	364 (88%)	39 (9%)	12 (3%)	4	4	31
29	Ι	379/385~(98%)	353~(93%)	18 (5%)	8 (2%)	ľ	7	37
30	Κ	392/394~(100%)	353~(90%)	28 (7%)	11 (3%)		5	32
31	L	384/388~(99%)	360~(94%)	18 (5%)	6 (2%)		9	44
32	М	419/421~(100%)	376~(90%)	30 (7%)	13 (3%)	4	4	30
33	J	403/405~(100%)	362 (90%)	22(6%)	19 (5%)	1	2	23
All	All	13911/14094~(99%)	12913 (93%)	763 (6%)	235 (2%)	1	3	43

5 of 235 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	31	THR
4	d	50	SER
6	f	14	SER
5	Е	16	SER
13	6	27	ASP

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	А	206/206~(100%)	204 (99%)	2 (1%)	76 86
1	a	206/206~(100%)	201~(98%)	5 (2%)	49 69
2	В	208/208~(100%)	205~(99%)	3 (1%)	67 81
2	b	208/208~(100%)	203~(98%)	5 (2%)	49 69
3	С	203/203~(100%)	202 (100%)	1 (0%)	88 93
3	с	203/203~(100%)	199~(98%)	4 (2%)	55 73
4	D	210/224~(94%)	207~(99%)	3 (1%)	67 81
4	d	224/224~(100%)	217 (97%)	7 (3%)	40 62
5	Ε	200/200~(100%)	196 (98%)	4 (2%)	55 73



Mol	Chain	Analysed	Rotameric	Outliers Per		ntiles
5	е	200/200~(100%)	192~(96%)	8 (4%)	31	56
6	F	190/190~(100%)	188~(99%)	2(1%)	73	85
6	f	190/190~(100%)	181~(95%)	9~(5%)	26	52
7	G	200/200~(100%)	196 (98%)	4 (2%)	55	73
7	g	200/200~(100%)	189 (94%)	11 (6%)	21	48
8	1	162/162~(100%)	157 (97%)	5 (3%)	40	62
8	h	162/162~(100%)	159~(98%)	3 (2%)	57	75
9	2	185/185~(100%)	180 (97%)	5 (3%)	44	65
9	i	185/185~(100%)	178 (96%)	7 (4%)	33	57
10	3	172/172~(100%)	168 (98%)	4 (2%)	50	70
10	j	172/172~(100%)	168 (98%)	4 (2%)	50	70
11	4	173/173~(100%)	168 (97%)	5 (3%)	42	64
11	k	173/173~(100%)	170 (98%)	3 (2%)	60	78
12	5	169/169~(100%)	166 (98%)	3 (2%)	59	77
12	1	169/169~(100%)	161 (95%)	8 (5%)	26	52
13	6	185/185~(100%)	182 (98%)	3 (2%)	62	79
13	m	185/185~(100%)	178 (96%)	7 (4%)	33	57
14	7	195/198~(98%)	186 (95%)	9(5%)	27	53
14	n	198/198~(100%)	188 (95%)	10 (5%)	24	50
15	W	171/171~(100%)	165~(96%)	6 (4%)	36	60
16	V	253/253~(100%)	249 (98%)	4 (2%)	62	79
17	Т	249/249~(100%)	243 (98%)	6 (2%)	49	69
18	Х	116/116~(100%)	112 (97%)	4 (3%)	37	60
19	Y	81/81 (100%)	78~(96%)	3 (4%)	34	58
20	Ζ	773/828~(93%)	746 (96%)	27 (4%)	36	60
21	Ν	776/776~(100%)	758~(98%)	18 (2%)	50	70
22	S	447/447~(100%)	433 (97%)	14 (3%)	40	62
23	Р	412/412 (100%)	405 (98%)	7 (2%)	60	78
24	Q	391/391~(100%)	380~(97%)	11 (3%)	43	65
25	R	356/356~(100%)	350~(98%)	6 (2%)	60	78
26	U	277/277~(100%)	268 (97%)	9 (3%)	39	61



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
27	Ο	363/363~(100%)	348~(96%)	15 (4%)	30	55
28	Н	352/352~(100%)	343~(97%)	9(3%)	46	67
29	Ι	342/342~(100%)	329~(96%)	13 (4%)	33	57
30	Κ	346/346~(100%)	329~(95%)	17 (5%)	25	51
31	L	332/332~(100%)	321~(97%)	11 (3%)	38	61
32	М	364/364~(100%)	357~(98%)	7 (2%)	57	75
33	J	352/352~(100%)	339~(96%)	13 (4%)	34	58
All	All	12086/12158~(99%)	11742 (97%)	344 (3%)	46	65

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	Р	435	LYS
29	Ι	112	ILE
24	Q	170	ASP
27	0	58	ARG
30	Κ	161	MET

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such side chains are listed below:

Mol	Chain	Res	Type
17	Т	123	HIS
31	L	189	GLN
21	Ν	613	HIS
31	L	67	HIS
33	J	123	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)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
INIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
36	ATP	L	501	35	26,33,33	1.30	3 (11%)	31,52,52	1.61	5 (16%)
36	ATP	J	501	35	26,33,33	1.21	3 (11%)	31,52,52	1.91	6 (19%)
36	ATP	Ι	501	35	26,33,33	1.37	3 (11%)	31,52,52	1.61	6 (19%)
36	ATP	K	501	35	26,33,33	1.37	3 (11%)	31,52,52	1.61	6 (19%)
34	ADP	Н	501	35	24,29,29	1.27	3 (12%)	29,45,45	2.41	6 (20%)
34	ADP	М	501	35	24,29,29	2.00	6 (25%)	29,45,45	2.33	6 (20%)

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
36	ATP	L	501	35	-	5/18/38/38	0/3/3/3
36	ATP	J	501	35	-	4/18/38/38	0/3/3/3
36	ATP	Ι	501	35	-	5/18/38/38	0/3/3/3
36	ATP	К	501	35	-	4/18/38/38	0/3/3/3
34	ADP	Н	501	35	-	4/12/32/32	0/3/3/3
34	ADP	М	501	35	-	4/12/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
34	М	501	ADP	C4-N3	-5.43	1.28	1.35



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
34	М	501	ADP	O4'-C4'	4.85	1.55	1.45
36	L	501	ATP	C2-N3	4.26	1.39	1.32
36	Κ	501	ATP	C2-N3	4.26	1.39	1.32
36	Ι	501	ATP	C2-N3	4.25	1.38	1.32

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
34	М	501	ADP	PA-O3A-PB	10.20	167.84	132.83
34	Н	501	ADP	PA-O3A-PB	8.49	161.96	132.83
36	J	501	ATP	PB-O3B-PG	5.53	151.80	132.83
36	J	501	ATP	PA-O3A-PB	5.00	149.97	132.83
34	Н	501	ADP	N3-C2-N1	4.95	136.41	128.68

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
34	Н	501	ADP	C5'-O5'-PA-O2A
34	Н	501	ADP	C5'-O5'-PA-O3A
34	М	501	ADP	C5'-O5'-PA-O1A
36	Ι	501	ATP	PB-O3B-PG-O2G
36	Κ	501	ATP	PB-O3B-PG-O2G

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 sufficient 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
29	Ι	2
32	М	2
33	J	2
31	L	1
30	Κ	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	180:PHE	С	181:ASP	Ν	2.67
1	Ι	183:ASP	С	184:ILE	Ν	2.58
1	Ι	186:GLY	С	187:LEU	Ν	2.56
1	М	338:LEU	С	339:ARG	Ν	1.69
1	J	212:ARG	С	213:VAL	Ν	1.68



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4321. 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: 192

Y Index: 192



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: 122

Y Index: 213

Z Index: 182

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 0.01. 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. 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 1039 nm^3 ; this corresponds to an approximate mass of 938 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 0.185 \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-4321 and PDB model 6FVV. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.01 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 (0.01).



9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 61% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.6137	0.1490
1	0.7305	0.1860
2	0.7209	0.1970
3	0.6851	0.1880
4	0.7142	0.1830
5	0.7396	0.1850
6	0.7096	0.1840
7	0.7228	0.1830
А	0.7003	0.1800
В	0.6814	0.1950
С	0.6883	0.1850
D	0.7001	0.1870
E	0.6742	0.1750
F	0.7096	0.1830
G	0.7101	0.1820
Н	0.5848	0.1240
I	0.5764	0.1380
J	0.5794	0.1250
K	0.5986	0.1410
L	0.6451	0.1490
М	0.5988	0.1300
N	0.6509	0.1540
0	0.6891	0.1520
P	0.7388	0.1520
Q	0.6927	0.1450
R	0.6898	0.1450
S	0.6218	0.1380
T	0.6385	0.1340
U	0.6133	0.1490
V	0.6502	0.1610
W	0.6015	0.1360
X	0.2613	0.0510
Y	0.4136	0.0670
Z	0.3348	0.0590
a	0.5005	0.1460



Chain	Atom inclusion	Q-score
b	0.4422	0.1550
С	0.4705	0.1370
d	0.4515	0.1300
е	0.4498	0.1420
f	0.5227	0.1570
g	0.5167	0.1430
h	0.6954	0.1650
i	0.6779	0.1790
j	0.6600	0.1750
k	0.6763	0.1760
l	0.6874	0.1680
m	0.6527	0.1690
n	0.6639	0.1710

