

wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 12:29 pm GMT

PDB ID : 6QM7

EMDB ID : EMD-4590

Title: Leishmania tarentolae proteasome 20S subunit complexed with GSK3494245

Authors : Rowland, P.; Goswami, P.

Deposited on : 2019-02-01

Resolution : 2.80 Å(reported)

Based on initial model : 4R3O

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 : 1.8.4, 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)

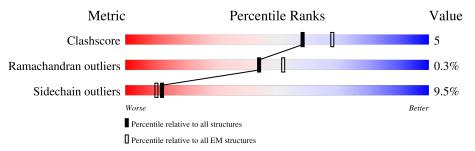
Validation Pipeline (wwPDB-VP) : 2.31.3

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 2.80 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
Metric	$(\# \mathrm{Entries})$	$(\# \mathrm{Entries})$
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	A	250	82%	14%	
1	О	250	82%	15%	•••
2	В	231	81%	16%	•••
2	Р	231	81%	16%	
3	С	285	80%	15%	•••
3	Q	285	79%	16%	•••
4	D	248	77%	8%	• •
4	R	248	76% 19	9%	

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Mol	Chain	Length	Quality of chain	
5	Е	344	57% 9%	• 33%
5	S	344	56% 10%	• 33%
6	F	428	47% 8% •	44%
6	Т	428	47% 8% •	44%
7	G	238	78%	15% • •
7	U	238	79%	16% • •
8	Н	283	67%	13% • 19%
8	V	283	67%	13% • 19%
9	I	254	68%	17% • 14%
9	W	254	69%	17% • 14%
10	J	205	83%	14% •
10	X	205	80%	18% •
11	K	206	82%	16% •
11	Y	206	81%	17% •
12	L	302	58% 9%	33%
12	Z	302	58% 9%	33%
13	M	339	46% 15% •	37%
13	a	339	56% 7%	37%
14	N	220	80%	17%
14	b	220	93%	6% •



2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 49518 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 alpha1 chain.

\mathbf{Mol}	Chain	Residues	Atoms					AltConf	Trace	
1	A	244		C 1169		_	S 12	0	0	
1	О	244	Total 1857	C 1169		O 353	S 12	0	0	

• Molecule 2 is a protein called Proteasome alpha2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	229		C 1112		_		0	0
2	Р	229	Total 1754	C 1112		_		0	0

• Molecule 3 is a protein called Proteasome alpha3 chain.

Mol	Chain	Residues		At	AltConf	Trace				
2	С	276	Total	С	N	О	S	0	0	
	210	2195	1379	382	422	12	0			
2	0	276	Total	С	N	О	S	0	0	
3	Q	Q 276	2195	1379	382	422	12	0		

• Molecule 4 is a protein called Proteasome alpha4 chain.

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
4	D	239		C 1180		_		0	0
4	R	239	Total 1873	C 1180		_	S 8	0	0

• Molecule 5 is a protein called Proteasome alpha5 chain.



Mol	Chain	Residues		At		AltConf	Trace			
5	E	229	Total	С	N	О	S	0	0	
5 E	229	1756	1094	302	347	13	U			
5	C	220	Total	С	N	О	S	0	0	
5	5	S 229	1756	1094	302	347	13	0		

• Molecule 6 is a protein called Proteasome alpha6 chain.

Mol	Chain	Residues		At		AltConf	Trace			
6	E	238	Total	С	N	О	S	0	0	
	230	1869	1173	325	359	12	0			
6	Т	220	Total	С	N	О	S	0	0	
0	1	T 238	1869	1173	325	359	12	0		

• Molecule 7 is a protein called Proteasome alpha7 chain.

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
7	G	228		C 1077		_	D	0	0
7	U	228	Total 1727	C 1077		0	S 10	0	0

• Molecule 8 is a protein called Proteasome beta1 chain.

Mol	Chain	Residues		At	AltConf	Trace		
8	Н	229		C 1062	O 341	\sim	0	0
8	V	229	Total 1710	C 1062		S 12	0	0

• Molecule 9 is a protein called Proteasome beta2 chain.

Mol	Chain	Residues	${f Atoms}$					AltConf	Trace	
O	Ţ	219	Total	С	N	О	S	0	0	
9	9 1	219	1659	1037	292	318	12	0		
0	7.7.7	219	Total	С	N	О	S	0	0	
	W	VV 219	1659	1037	292	318	12		U	

• Molecule 10 is a protein called Proteasome beta3 chain.

Mol	Chain	Residues		\mathbf{A}^{1}	toms			AltConf	Trace
10	J	204	Total 1557	C 980	N 259	O 302	S 16	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
10	X	204	Total 1557	C 980	N 259	O 302	S 16	0	0

• Molecule 11 is a protein called Proteasome beta4 chain.

Mol	Chain	Residues		${f Atoms}$			AltConf	Trace	
11	K	206		C 1012		O 304	S 16	0	0
11	Y	206	Total 1612	C 1012		O 304	S 16	0	0

• Molecule 12 is a protein called Proteasome beta5 chain.

Mol	Chain	Residues	Atoms			AltConf	Trace		
19	Т	202	Total	С	N	О	S	0	0
12	П	202	1579	998	277	297	7		
19	7	Z 202	Total	С	N	О	S	0	0
12	L		1579	998	277	297	7		

• Molecule 13 is a protein called Proteasome beta6 chain.

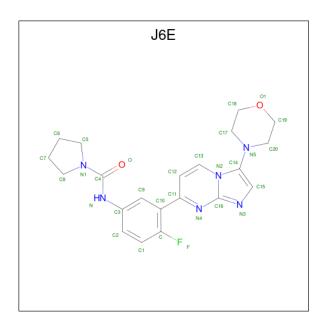
Mol	Chain	Residues	Atoms				AltConf	Trace	
13	М	214	Total 1702	C 1079	- '	O 324	~	0	0
13	a	214	Total 1702	C 1079		O 324	S 12	0	0

• Molecule 14 is a protein called Proteasome beta7 chain.

Mol	Chain	Residues	Atoms				AltConf	Trace	
14	N	218	Total 1712	C 1083			S 14	0	0
14	b	218	Total 1712	C 1083			S 14	0	0

• Molecule 15 is $\{N\}$ -[4-fluoranyl-3-(3-morpholin-4-ylimidazo[1,2-a]pyrimidin-7-yl)pheny l]pyrrolidine-1-carboxamide (three-letter code: J6E) (formula: $C_{21}H_{23}FN_6O_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			AltConf
15	Т	1	Total	С	F	N	О	0
10	Ъ	1	30	21	1	6	2	U
15	7	1	Total	С	F	N	О	0
1.0		1	30	21	1	6	2	

• Molecule 16 is water.

Mol	Chain	Residues	Atoms	AltConf
16	A	9	Total O 9 9	0
16	В	9	Total O 9 9	0
16	С	8	Total O 8 8	0
16	D	6	Total O 6 6	0
16	Е	8	Total O 8 8	0
16	F	8	Total O 8 8	0
16	G	12	Total O 12 12	0
16	Н	21	Total O 21 21	0
16	I	7	Total O 7 7	0
16	J	15	Total O 15 15	0

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Mol		$oxed{ \mathbf{Residues} }$	Atoms	AltConf
16	K	9	Total O 9 9	0
16	L	15	Total O 15 15	0
16	M	13	Total O 13 13	0
16	N	21	Total O 21 21	0
16	О	11	Total O 11 11	0
16	Р	13	Total O 13 13	0
16	Q	8	Total O 8 8	0
16	R	9	Total O 9 9	0
16	S	6	Total O 6 6	0
16	Т	8	Total O 8 8	0
16	U	5	Total O 5 5	0
16	V	19	Total O 19 19	0
16	W	15	Total O 15 15	0
16	X	23	Total O 23 23	0
16	Y	8	Total O 8 8	0
16	Z	17	Total O 17 17	0
16	a	11	Total O 11 11	0
16	b	20	Total O 20 20	0

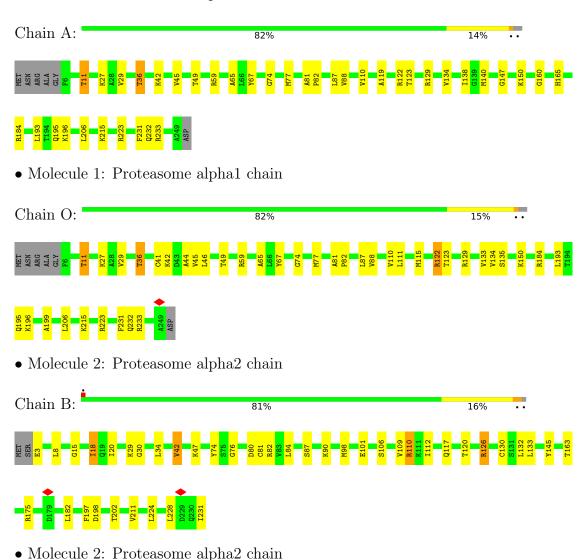


Chain P:

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 alpha1 chain



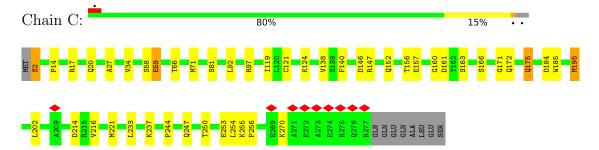
81%



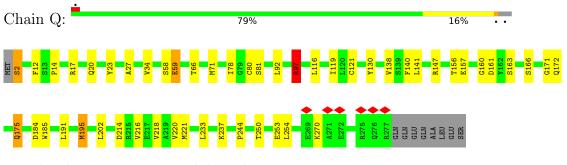
16%



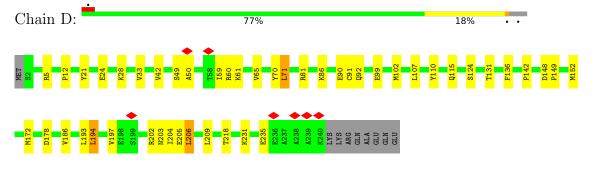
• Molecule 3: Proteasome alpha3 chain



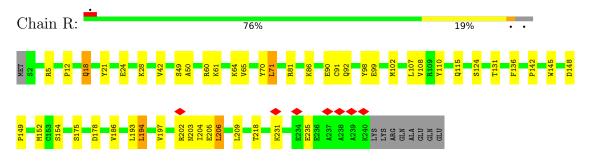
• Molecule 3: Proteasome alpha3 chain



• Molecule 4: Proteasome alpha4 chain

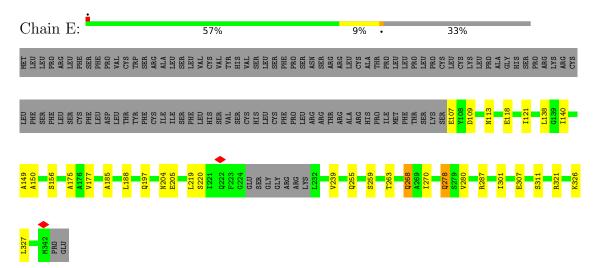


• Molecule 4: Proteasome alpha4 chain

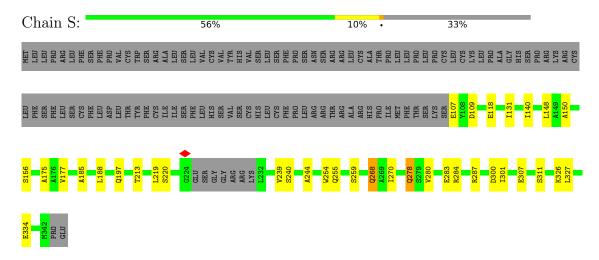




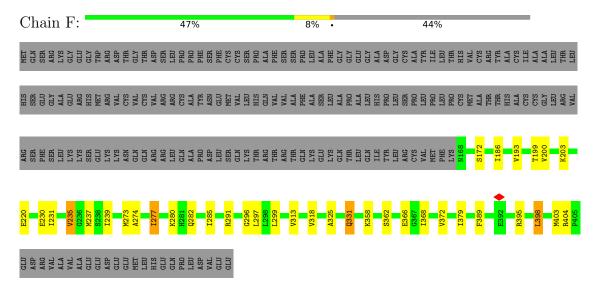
• Molecule 5: Proteasome alpha5 chain



• Molecule 5: Proteasome alpha5 chain

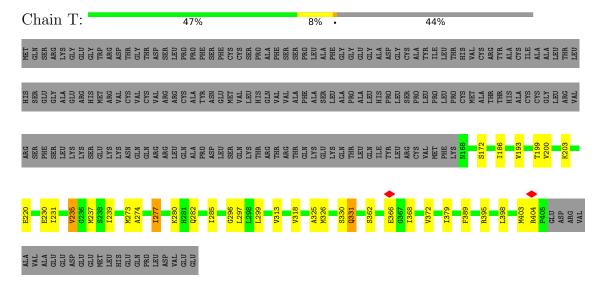


• Molecule 6: Proteasome alpha6 chain

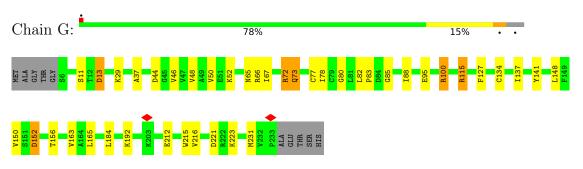




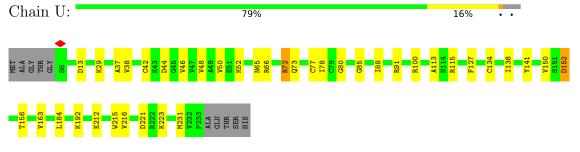
• Molecule 6: Proteasome alpha6 chain



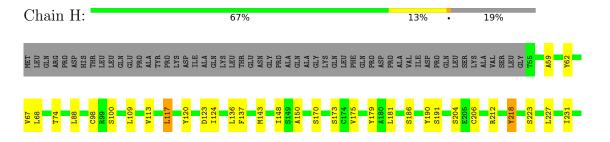
• Molecule 7: Proteasome alpha7 chain



• Molecule 7: Proteasome alpha7 chain



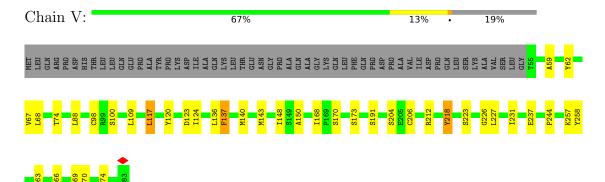
• Molecule 8: Proteasome beta1 chain



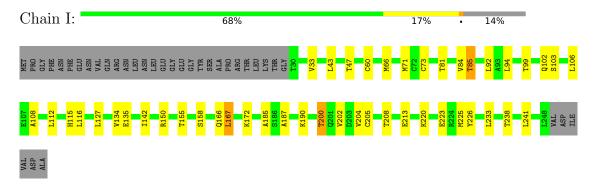




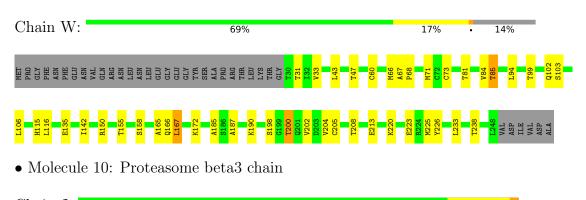
• Molecule 8: Proteasome beta1 chain

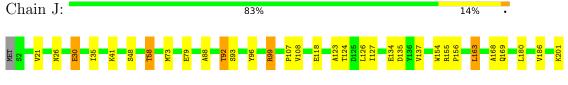


• Molecule 9: Proteasome beta2 chain



• Molecule 9: Proteasome beta2 chain

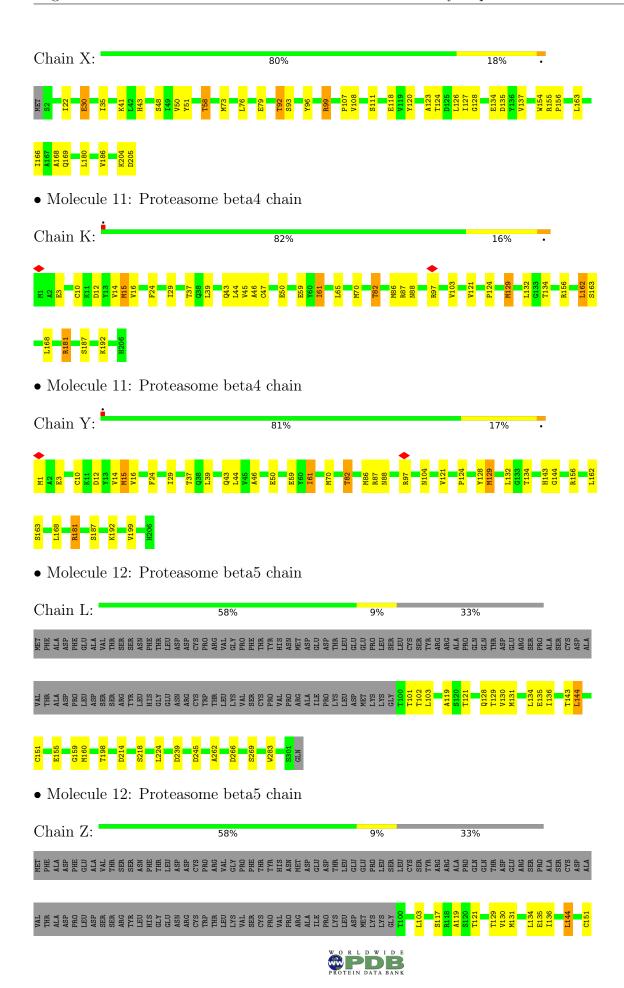






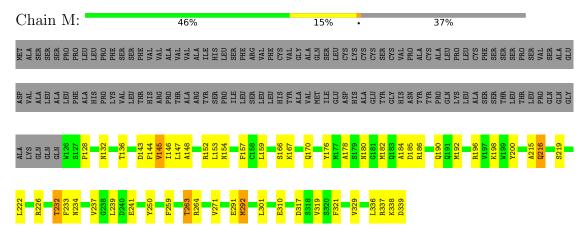
• Molecule 10: Proteasome beta3 chain



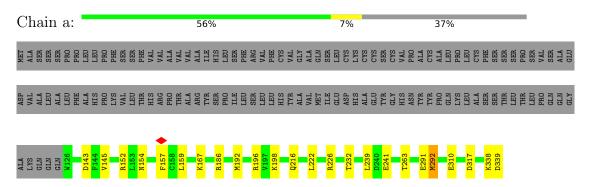




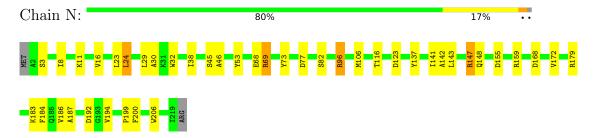
• Molecule 13: Proteasome beta6 chain



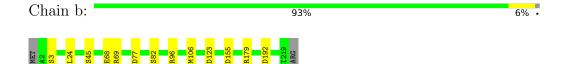
• Molecule 13: Proteasome beta6 chain



• Molecule 14: Proteasome beta7 chain



• Molecule 14: Proteasome beta7 chain





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182775	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 $(e^-/\text{Å}^2)$	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.622	Depositor
Minimum map value	-0.361	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0667	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: J6E

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	Bond	lengths	Во	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.61	0/1889	0.88	0/2562
1	О	0.60	0/1889	0.89	0/2562
2	В	0.61	0/1787	0.84	0/2421
2	Р	0.61	0/1787	0.84	0/2421
3	С	0.61	0/2242	0.86	0/3034
3	Q	0.61	0/2242	0.86	1/3034 (0.0%)
4	D	0.63	0/1902	0.87	0/2562
4	R	0.62	0/1902	0.87	0/2562
5	Е	0.63	0/1784	0.85	0/2414
5	S	0.63	0/1784	0.86	0/2414
6	F	0.62	0/1907	0.84	0/2575
6	Т	0.61	0/1907	0.84	0/2575
7	G	0.62	0/1759	0.85	1/2379~(0.0%)
7	U	0.62	0/1759	0.85	0/2379
8	Н	0.60	0/1742	0.89	2/2359 (0.1%)
8	V	0.61	0/1742	0.89	$1/2359 \ (0.0\%)$
9	I	0.59	0/1685	0.87	0/2284
9	W	0.59	0/1685	0.87	0/2284
10	J	0.60	0/1583	0.89	0/2135
10	X	0.61	0/1583	0.89	0/2135
11	K	0.60	0/1643	0.89	0/2222
11	Y	0.60	0/1643	0.89	0/2222
12	L	0.60	0/1613	0.87	0/2183
12	Z	0.59	0/1613	0.87	0/2183
13	M	0.58	0/1743	0.89	0/2354
13	a	0.58	0/1743	0.90	0/2354
14	N	0.60	0/1748	0.88	1/2363~(0.0%)
14	b	0.60	0/1748	0.87	0/2363
All	All	0.61	0/50054	0.87	$6/67694 \ (0.0\%)$

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
2	Р	0	1
3	С	0	2
3	Q	0	3
10	J	0	1
10	X	0	1
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
8	Н	218	TYR	CB-CG-CD1	6.96	125.17	121.00
8	V	218	TYR	CB-CG-CD1	6.79	125.08	121.00
8	Н	218	TYR	CB-CG-CD2	-5.65	117.61	121.00
3	Q	97	ARG	NE-CZ-NH1	5.28	122.94	120.30
14	N	147	ARG	NE-CZ-NH2	-5.22	117.69	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	С	140	PHE	Peptide
3	С	171	GLY	Peptide
10	J	204	LYS	Peptide
2	Р	132	LEU	Peptide
3	Q	130	TYR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1857	0	1871	17	0
1	О	1857	0	1871	17	0
2	В	1754	0	1741	15	0

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Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
2	Р	1754	0	1741	14	0
3	С	2195	0	2142	21	0
3	Q	2195	0	2142	26	0
4	D	1873	0	1868	16	0
4	R	1873	0	1868	21	0
5	Е	1756	0	1736	16	0
5	S	1756	0	1736	15	0
6	F	1869	0	1823	18	0
6	Т	1869	0	1823	17	0
7	G	1727	0	1691	23	0
7	U	1727	0	1691	17	0
8	Н	1710	0	1665	19	0
8	V	1710	0	1665	16	0
9	I	1659	0	1684	21	0
9	W	1659	0	1684	22	0
10	J	1557	0	1552	18	0
10	X	1557	0	1552	21	0
11	K	1612	0	1571	21	0
11	Y	1612	0	1571	22	0
12	L	1579	0	1538	13	0
12	Z	1579	0	1538	12	0
13	M	1702	0	1638	26	0
13	a	1702	0	1638	0	0
14	N	1712	0	1668	25	0
14	b	1712	0	1668	0	0
15	L	30	0	0	0	0
15	Z	30	0	0	0	0
16	A	9	0	0	1	0
16	В	9	0	0	0	0
16	С	8	0	0	0	0
16	D	6	0	0	0	0
16	Е	8	0	0	0	0
16	F	8	0	0	0	0
16	G	12	0	0	0	0
16	H	21	0	0	0	0
16	I	7	0	0	0	0
16	J	15	0	0	0	0
16	K	9	0	0	0	0
16	L	15	0	0	0	0
16	M	13	0	0	0	0
16	N	21	0	0	0	0
16	О	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Р	13	0	0	0	0
16	Q	8	0	0	0	0
16	R	9	0	0	0	0
16	S	6	0	0	0	0
16	Τ	8	0	0	0	0
16	U	5	0	0	0	0
16	V	19	0	0	0	0
16	W	15	0	0	1	0
16	X	23	0	0	0	0
16	Y	8	0	0	0	0
16	Z	17	0	0	0	0
16	a	11	0	0	0	0
16	b	20	0	0	0	0
All	All	49518	0	48376	436	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 5.

The worst 5 of 436 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
4:D:91:CYS:SG	4:D:107:LEU:HD13	2.20	0.82
1:O:36:THR:HG22	1:O:49:THR:HG23	1.62	0.82
5:E:185:ALA:HB2	5:E:239:VAL:HG21	1.66	0.78
1:A:36:THR:HG22	1:A:49:THR:HG23	1.67	0.77
8:V:68:LEU:HD23	8:V:98:CYS:SG	2.24	0.77

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	A	242/250 (97%)	233 (96%)	9 (4%)	0	100	100
1	О	242/250 (97%)	233 (96%)	9 (4%)	0	100	100
2	В	227/231 (98%)	216 (95%)	11 (5%)	0	100	100
2	Р	227/231 (98%)	218 (96%)	9 (4%)	0	100	100
3	С	274/285 (96%)	266 (97%)	8 (3%)	0	100	100
3	Q	274/285 (96%)	265 (97%)	9 (3%)	0	100	100
4	D	237/248 (96%)	228 (96%)	7 (3%)	2 (1%)	19	49
4	R	237/248 (96%)	226 (95%)	9 (4%)	2 (1%)	19	49
5	Е	225/344 (65%)	222 (99%)	3 (1%)	0	100	100
5	S	225/344 (65%)	221 (98%)	4 (2%)	0	100	100
6	F	236/428 (55%)	230 (98%)	5 (2%)	1 (0%)	34	66
6	Т	236/428 (55%)	229 (97%)	6 (2%)	1 (0%)	34	66
7	G	226/238 (95%)	218 (96%)	8 (4%)	0	100	100
7	U	226/238 (95%)	219 (97%)	7 (3%)	0	100	100
8	Н	227/283 (80%)	212 (93%)	14 (6%)	1 (0%)	34	66
8	V	227/283 (80%)	213 (94%)	13 (6%)	1 (0%)	34	66
9	I	217/254 (85%)	204 (94%)	10 (5%)	3 (1%)	11	34
9	W	217/254 (85%)	205 (94%)	9 (4%)	3 (1%)	11	34
10	J	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	29	61
10	X	202/205 (98%)	191 (95%)	10 (5%)	1 (0%)	29	61
11	K	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
11	Y	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
12	L	200/302 (66%)	188 (94%)	12 (6%)	0	100	100
12	Z	200/302 (66%)	188 (94%)	12 (6%)	0	100	100
13	М	212/339~(62%)	204 (96%)	5 (2%)	3 (1%)	11	34
13	a	212/339 (62%)	204 (96%)	5 (2%)	3 (1%)	11	34
14	N	216/220 (98%)	202 (94%)	14 (6%)	0	100	100
14	b	216/220 (98%)	204 (94%)	12 (6%)	0	100	100
All	All	6290/7666 (82%)	6020 (96%)	248 (4%)	22 (0%)	44	72

5 of 22 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
4	D	49	SER
4	R	49	SER
9	W	200	THR
9	I	200	THR
9	I	223	GLU

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	Perce	entiles
1	A	$193/197\ (98\%)$	177 (92%)	16 (8%)	11	32
1	О	$193/197\ (98\%)$	177 (92%)	16 (8%)	11	32
2	В	188/190~(99%)	164 (87%)	24 (13%)	4	13
2	Р	188/190~(99%)	164 (87%)	24 (13%)	4	13
3	C	233/241~(97%)	210 (90%)	23 (10%)	8	23
3	Q	$233/241\ (97\%)$	210 (90%)	23 (10%)	8	23
4	D	$200/208\ (96\%)$	175 (88%)	25 (12%)	4	14
4	R	$200/208\ (96\%)$	174 (87%)	26 (13%)	4	13
5	E	$193/301\ (64\%)$	178 (92%)	15 (8%)	12	35
5	S	$193/301\ (64\%)$	178 (92%)	15 (8%)	12	35
6	F	$200/363\ (55\%)$	184 (92%)	16 (8%)	12	34
6	Т	$200/363\ (55\%)$	185 (92%)	15 (8%)	13	37
7	G	184/190~(97%)	169 (92%)	15 (8%)	11	33
7	U	184/190~(97%)	167 (91%)	17 (9%)	9	27
8	Н	$184/229\ (80\%)$	170 (92%)	14 (8%)	13	36
8	V	$184/229\ (80\%)$	168 (91%)	16 (9%)	10	30
9	I	180/209 (86%)	163 (91%)	17 (9%)	8	26
9	W	180/209~(86%)	163 (91%)	17 (9%)	8	26
10	J	$167/168\ (99\%)$	153 (92%)	14 (8%)	11	31
10	X	$167/168\ (99\%)$	151 (90%)	16 (10%)	8	24

Continued on next page...



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
11	K	172/172 (100%)	153 (89%)	19 (11%)	6	19
11	Y	172/172 (100%)	154 (90%)	18 (10%)	7	20
12	L	163/253 (64%)	152 (93%)	11 (7%)	16	43
12	Z	163/253 (64%)	152 (93%)	11 (7%)	16	43
13	M	181/288 (63%)	156 (86%)	25 (14%)	3	11
13	a	181/288 (63%)	159 (88%)	22 (12%)	5	15
14	N	181/183 (99%)	166 (92%)	15 (8%)	11	32
14	b	181/183 (99%)	168 (93%)	13 (7%)	14	38
All	All	5238/6384 (82%)	4740 (90%)	498 (10%)	12	25

5 of 498 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	337	ARG
11	Y	88	ASN
2	Р	198	ASP
11	Y	59	GLU
13	a	198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
7	U	65	ASN
13	a	188	GLN
9	W	102	GLN
11	Y	143	HIS
9	I	247	GLN

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond 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).

Mol	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	J6E	Z	4000	-	29,34,34	0.64	0	34,48,48	0.74	2 (5%)
15	J6E	L	4000	-	29,34,34	0.66	0	34,48,48	0.86	1 (2%)

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
15	J6E	Z	4000	-	-	0/12/31/31	0/5/5/5
15	J6E	L	4000	-	=	0/12/31/31	0/5/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
15	L	4000	J6E	C13-C12-C11	2.89	120.13	118.03
15	Z	4000	J6E	C13-C12-C11	2.71	120.00	118.03
15	Z	4000	J6E	C12-C13-N2	-2.07	118.09	120.66

There are no chirality outliers.

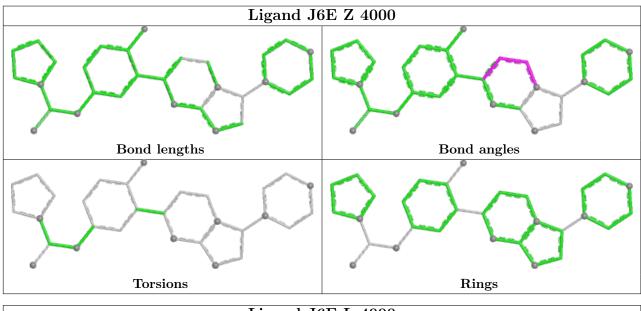
There are no torsion outliers.

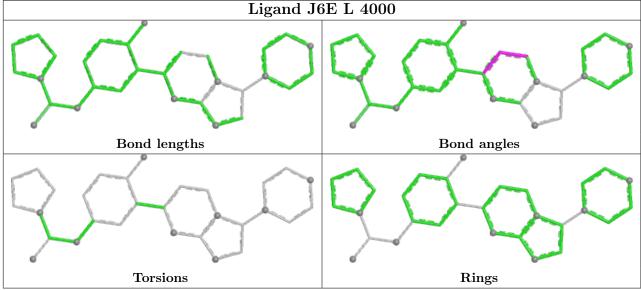
There are no ring outliers.

No monomer is involved in short contacts.



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







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



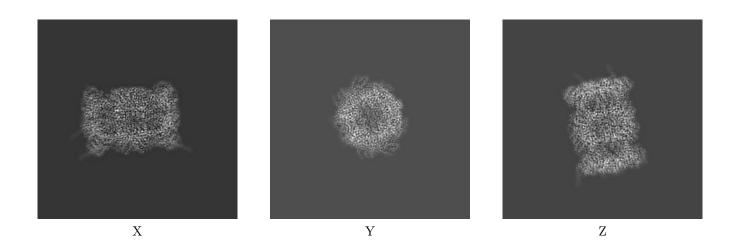
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4590. 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.

6.1 Orthogonal projections (i)

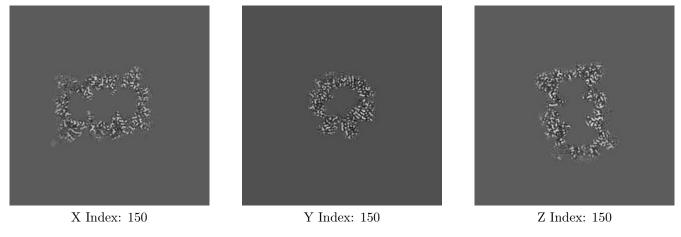
6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map

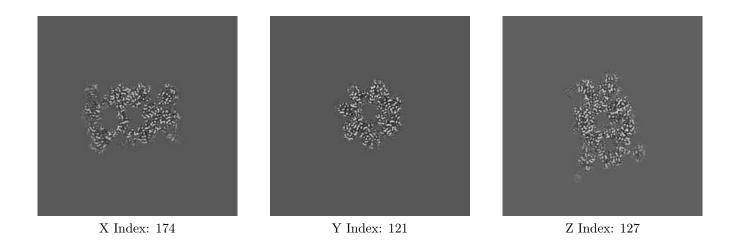




The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

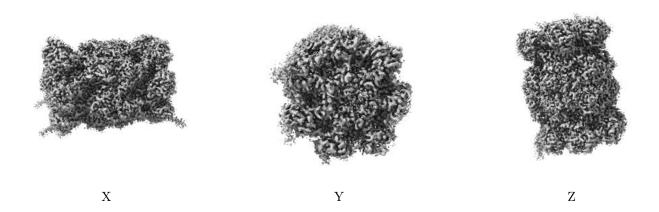
6.3.1 Primary map



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 0.0667. 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)

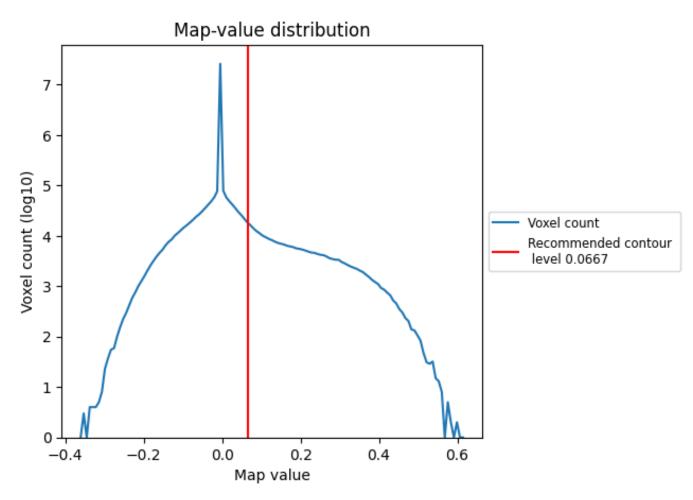
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

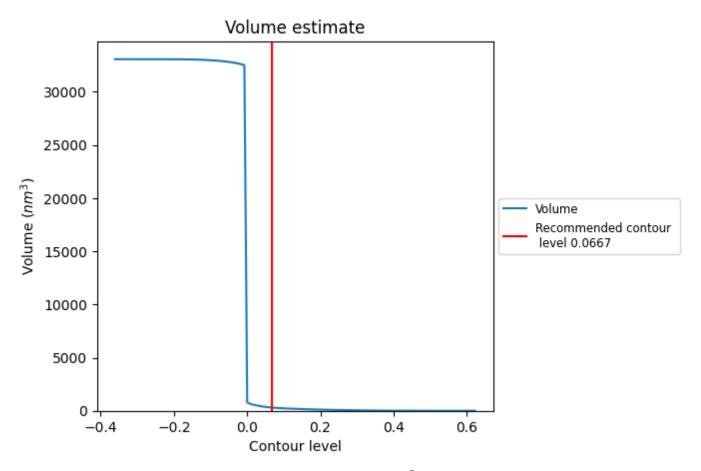
7.1 Map-value distribution (i)



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)

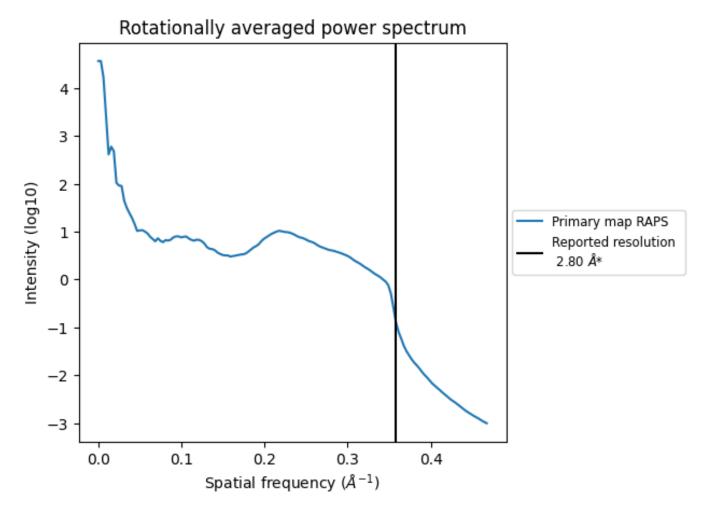


The volume at the recommended contour level is $306~\mathrm{nm}^3$; this corresponds to an approximate mass of $276~\mathrm{kDa}$.

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 0.357 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

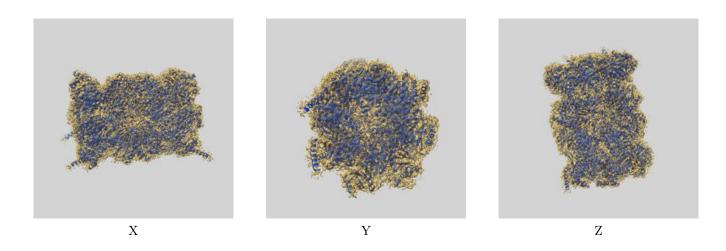
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4590 and PDB model 6QM7. Per-residue inclusion information can be found in section 3 on page 9.

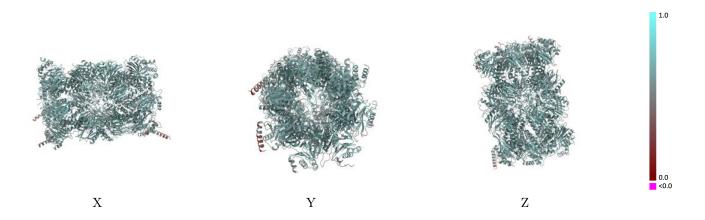
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0667 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.

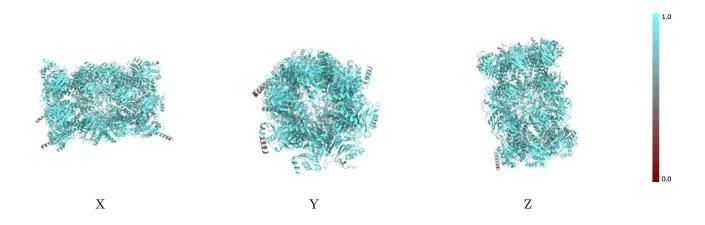


9.2 Q-score mapped to coordinate model (i)



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.

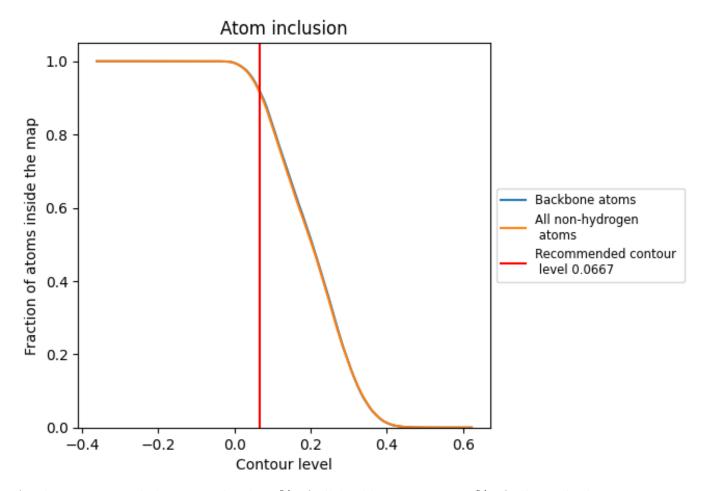
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0667).



9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.0667) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.6070
A	0.9098	0.6080
В	0.9067	0.6070
С	0.8768	0.5890
D	0.8670	0.5780
Е	0.8926	0.5980
F	0.9042	0.6040
G	0.9150	0.6100
Н	0.9606	0.6310
I	0.9274	0.6180
J	0.9431	0.6280
K	0.9353	0.6140
L	0.9495	0.6310
M	0.9442	0.6180
N	0.9401	0.6280
О	0.9147	0.6040
P	0.9125	0.6030
Q	0.8856	0.5750
R	0.8670	0.5680
S	0.9060	0.5930
Т	0.9037	0.5980
U	0.9145	0.6050
V	0.9504	0.6270
W	0.9268	0.6080
X	0.9287	0.6200
Y	0.9378	0.6110
Z	0.9411	0.6250
a	0.9316	0.6110
b	0.9305	0.6220



