Full wwPDB EM Validation Report

Jan 15, 2022 – 08:18 am GMT

PDB ID	:	7PXA
EMDB ID	:	EMD-13695
Title	:	Open-gate mycobacterium 20S CP proteasome in complex MPA - global 3D refinement
Authors	:	Jomaa, A.; Kavalchuk, M.; Weber-Ban, E.
Deposited on	:	2021-10-08
Resolution	:	2.80 Å(reported)
Based on initial model	:	5KWA

This is a 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 following versions of software and data (see references (1)) were used in the production of this report:

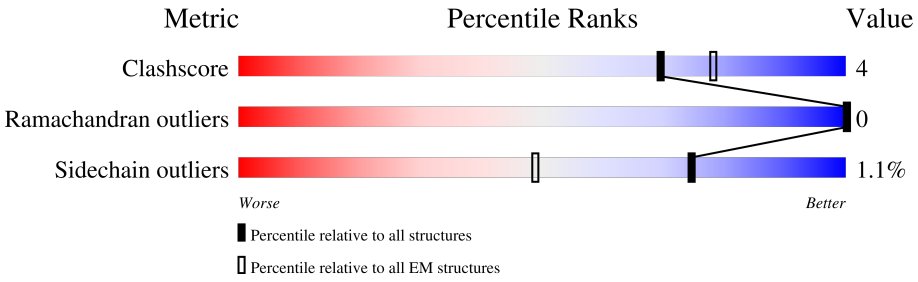
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 (#Entries)	EM structures (#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	0	248	6% 74% 12% • 13%
1	2	248	5% 75% 10% • 13%
1	4	248	6% 76% 10% 13%
1	6	248	7% 75% 11% 13%
1	8	248	6% 74% 12% 13%
1	I	248	22% 70% 16% • 14%
1	K	248	20% 75% 13% 12%
1	O	248	22% 72% 15% 13%

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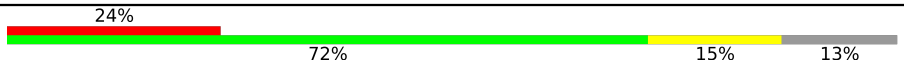
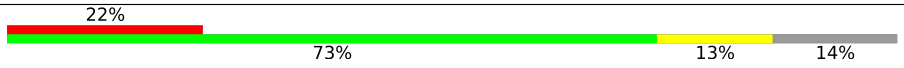
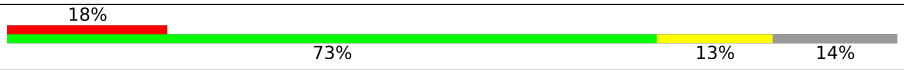
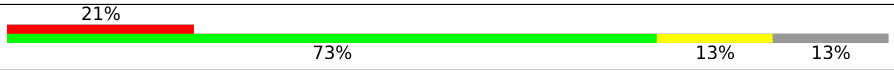
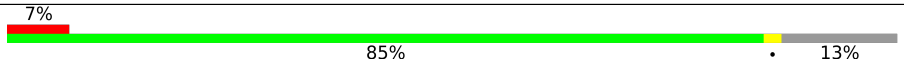
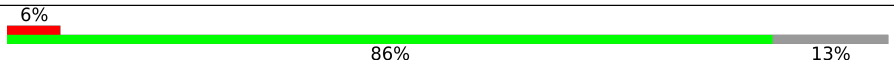
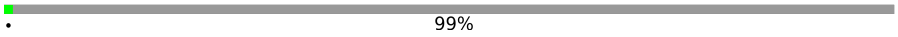
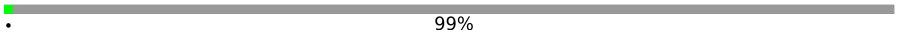
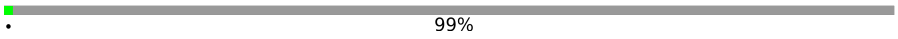
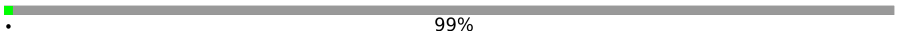
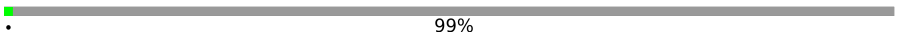
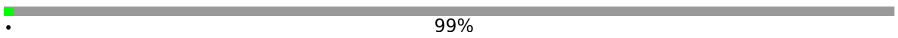
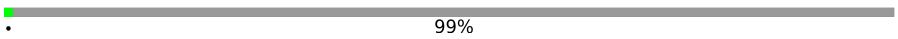
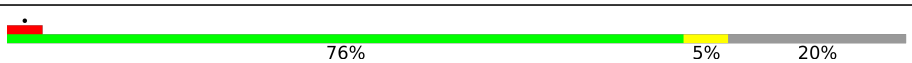
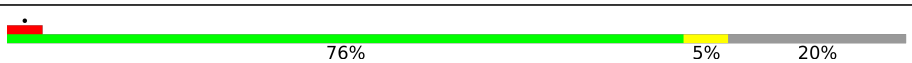
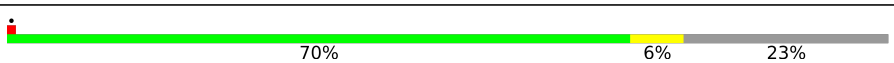
Mol	Chain	Length	Quality of chain
1	Q	248	
1	T	248	
1	X	248	
1	Z	248	
1	d	248	
1	f	248	
2	1	609	
2	A	609	
2	B	609	
2	C	609	
2	D	609	
2	E	609	
2	F	609	
3	H	291	
3	J	291	
3	L	291	
3	M	291	
3	N	291	
3	P	291	
3	R	291	
3	S	291	
3	U	291	
3	V	291	
3	W	291	
3	Y	291	

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Mol	Chain	Length	Quality of chain
3	a	291	
3	b	291	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 46614 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	2	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	4	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	6	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	8	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	I	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	K	217	Total	C	N	O	S	0	0
			1668	1044	305	316	3		
1	O	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	Q	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	T	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	X	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	Z	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	d	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	f	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		

- Molecule 2 is a protein called AAA ATPase forming ring-shaped complexes.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	5	Total	C	N	O	0	0
			42	28	6	8		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	5	Total	C	N	O	0	0
			42	28	6	8		
2	B	5	Total	C	N	O	0	0
			42	28	6	8		
2	C	7	Total	C	N	O	0	0
			56	35	9	12		
2	D	5	Total	C	N	O	0	0
			42	28	6	8		
2	E	7	Total	C	N	O	0	0
			56	35	9	12		
2	F	6	Total	C	N	O	0	0
			50	32	8	10		

- Molecule 3 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	J	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	L	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	M	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	N	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	P	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	R	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	S	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	U	234	Total	C	N	O	S	0	0
			1715	1072	295	343	5		
3	V	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	W	234	Total	C	N	O	S	0	0
			1715	1072	295	343	5		
3	Y	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	a	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		

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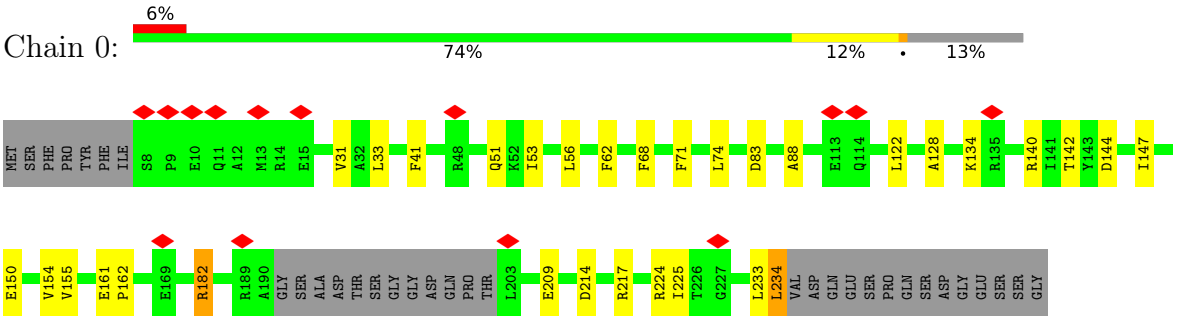
Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		

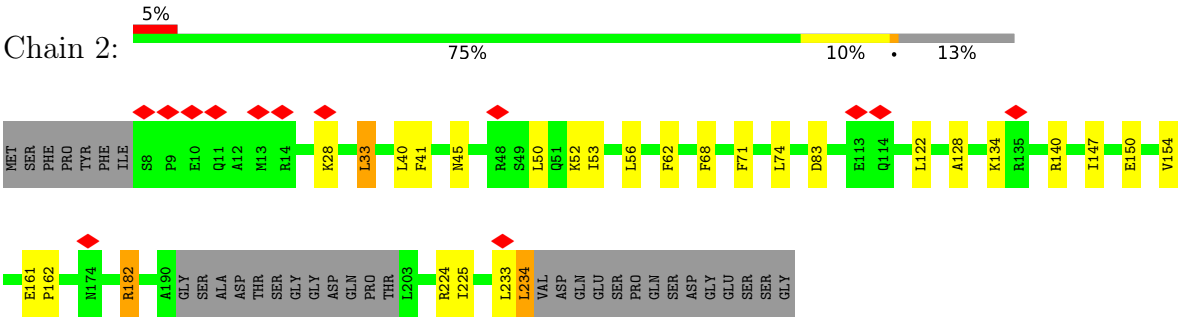
3 Residue-property plots (i)

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.

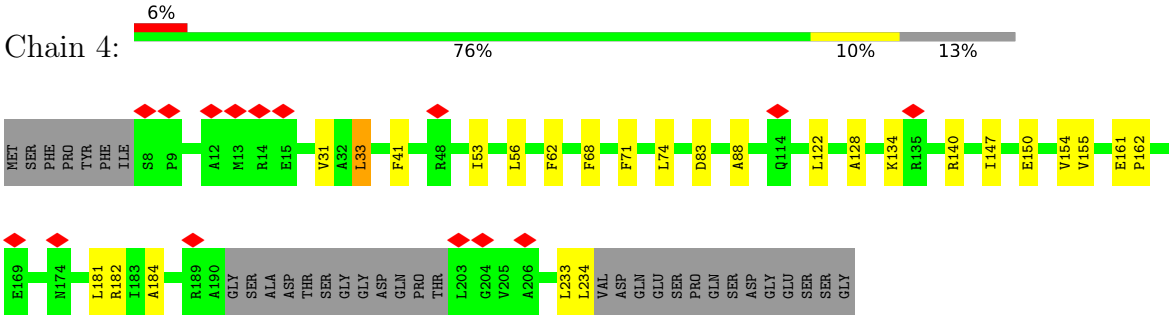
• Molecule 1: Proteasome subunit alpha



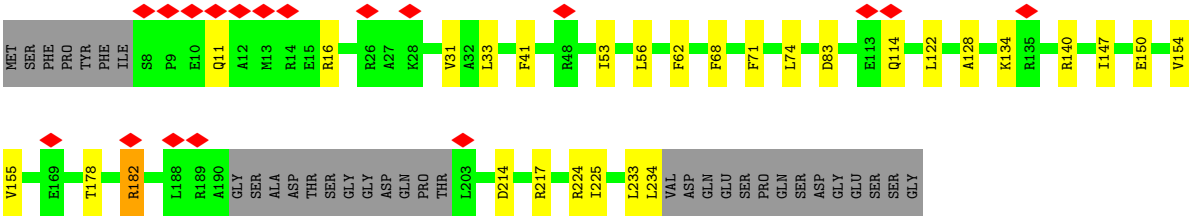
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

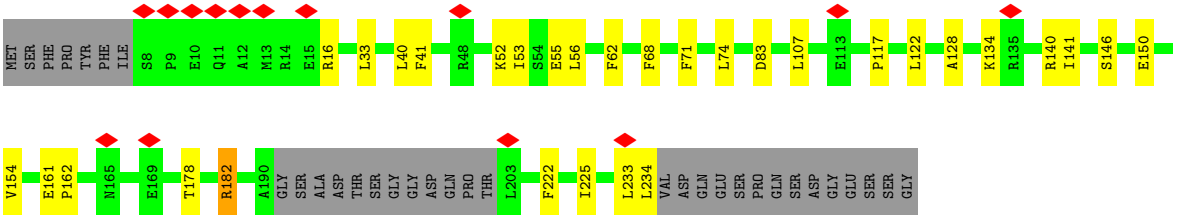


• Molecule 1: Proteasome subunit alpha



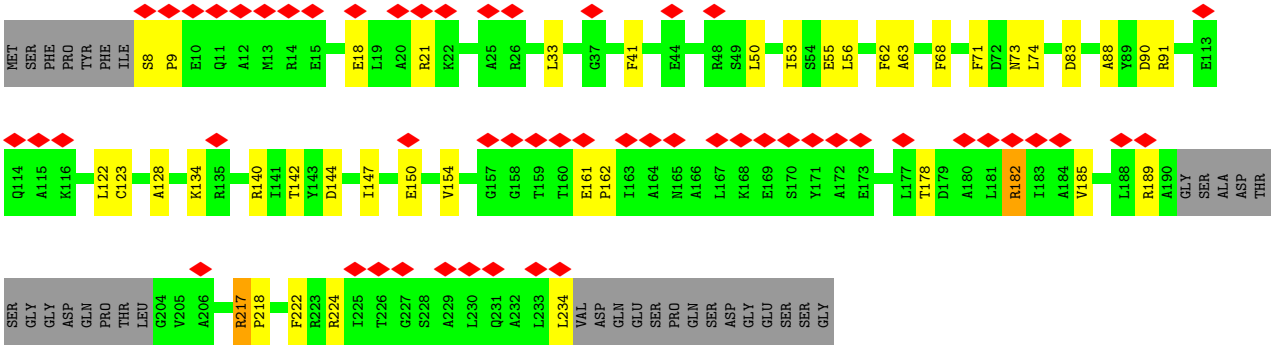
• Molecule 1: Proteasome subunit alpha

Chain 8:



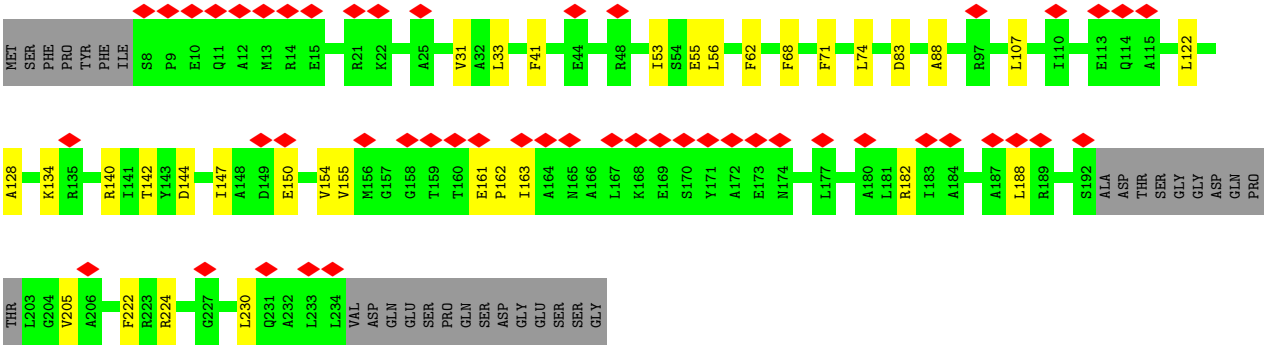
• Molecule 1: Proteasome subunit alpha

Chain I:



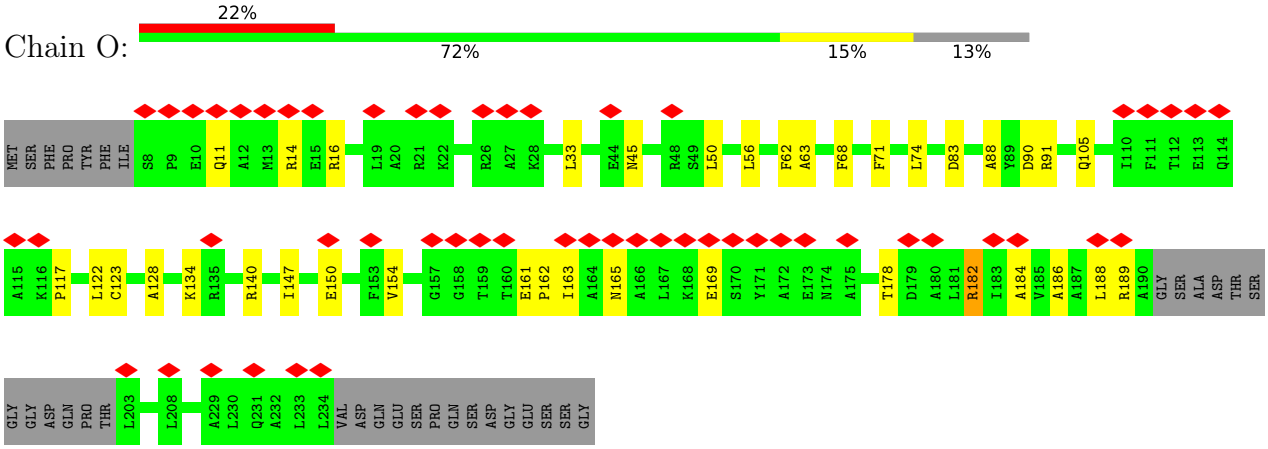
• Molecule 1: Proteasome subunit alpha

Chain K:



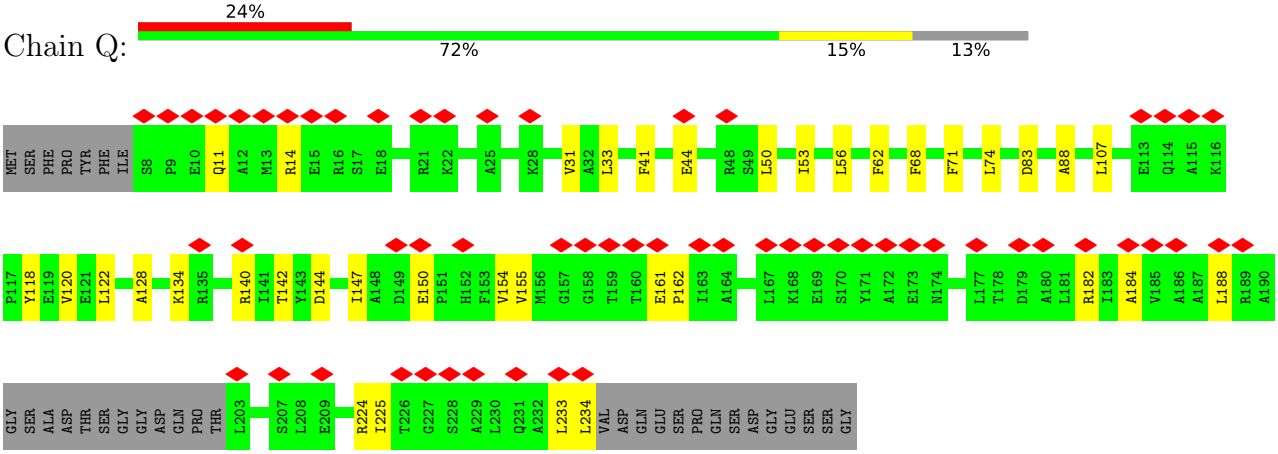
• Molecule 1: Proteasome subunit alpha

Chain O:



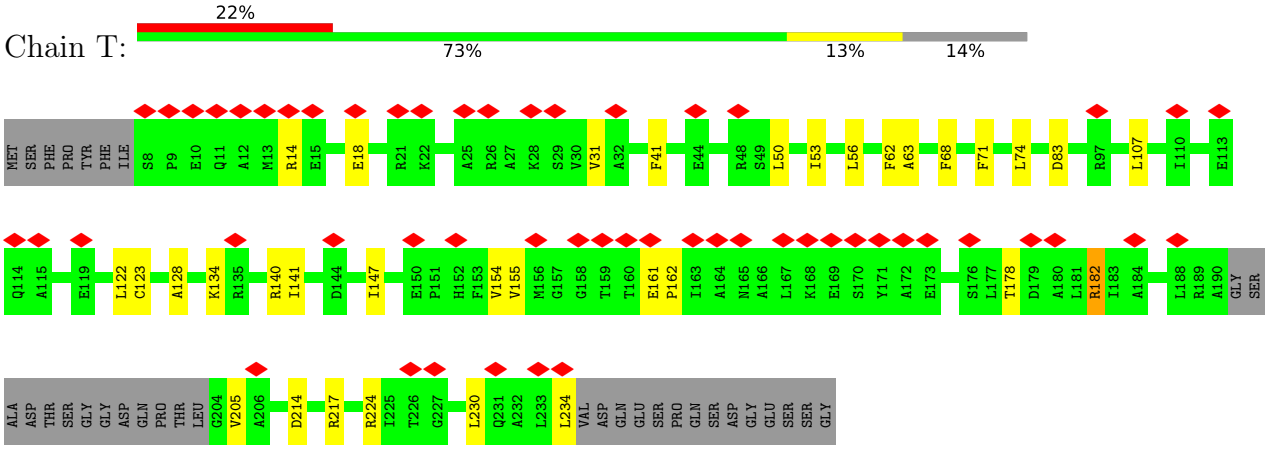
• Molecule 1: Proteasome subunit alpha

Chain Q:



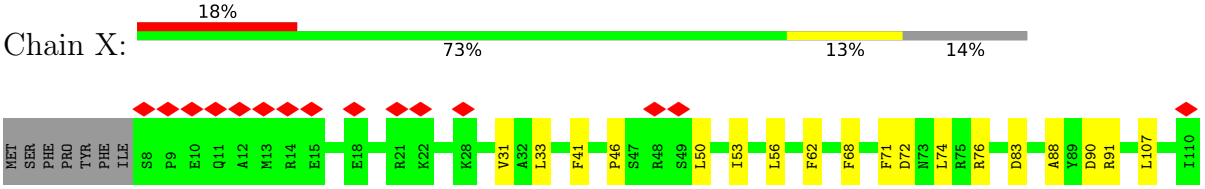
• Molecule 1: Proteasome subunit alpha

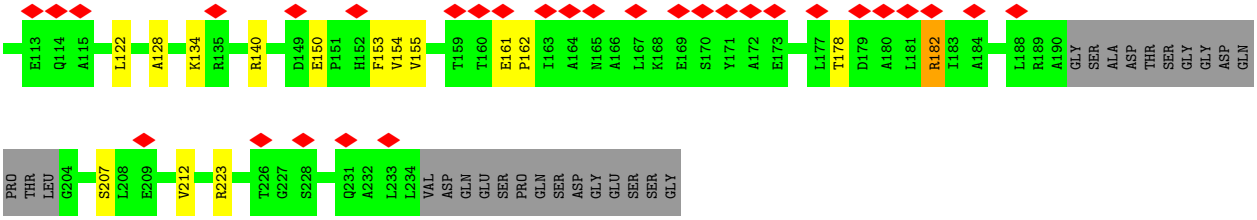
Chain T:



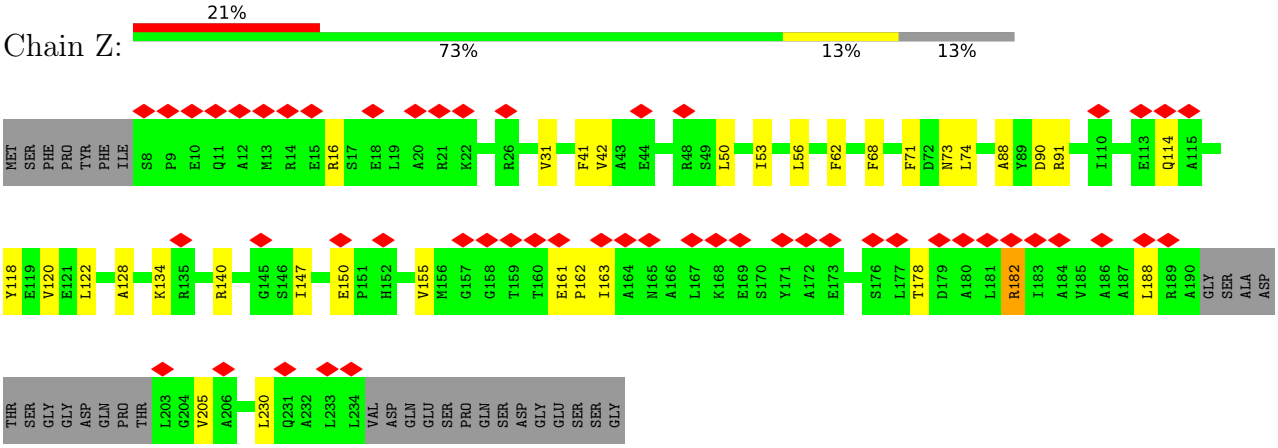
• Molecule 1: Proteasome subunit alpha

Chain X:

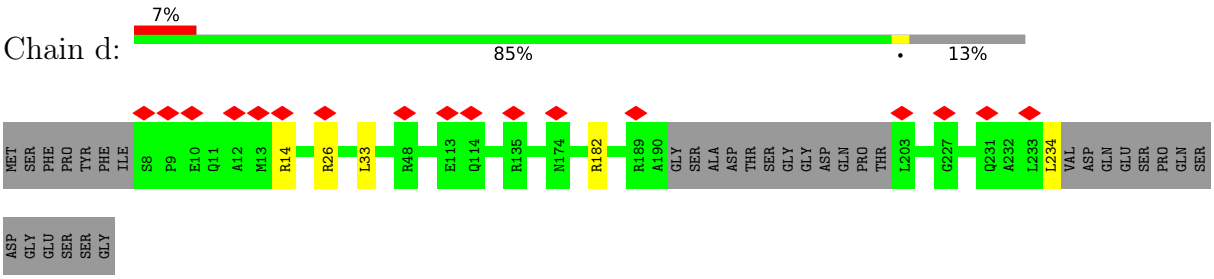




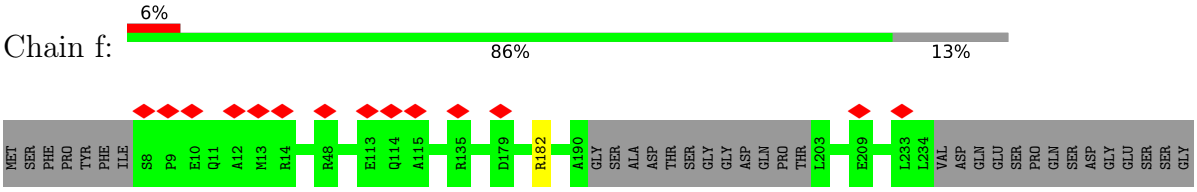
• Molecule 1: Proteasome subunit alpha



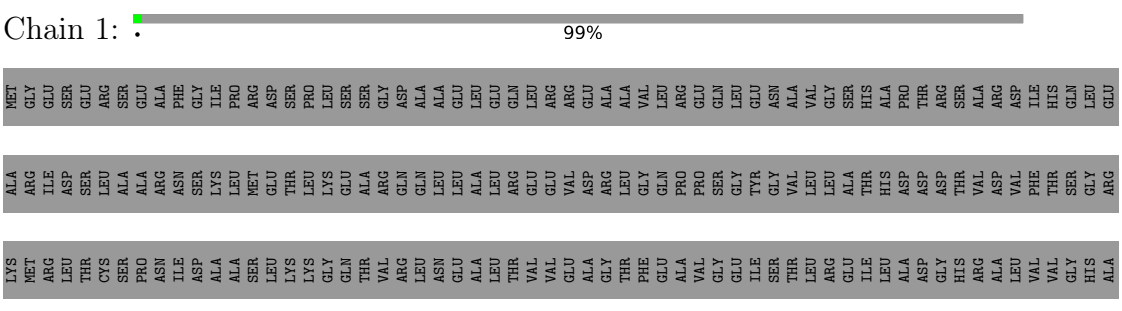
• Molecule 1: Proteasome subunit alpha

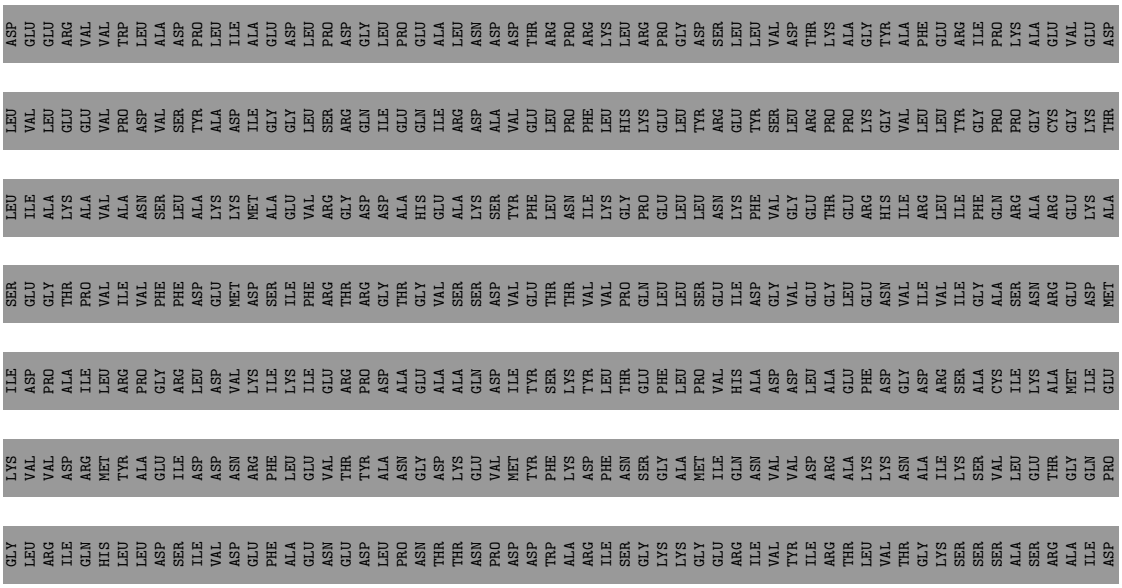


• Molecule 1: Proteasome subunit alpha



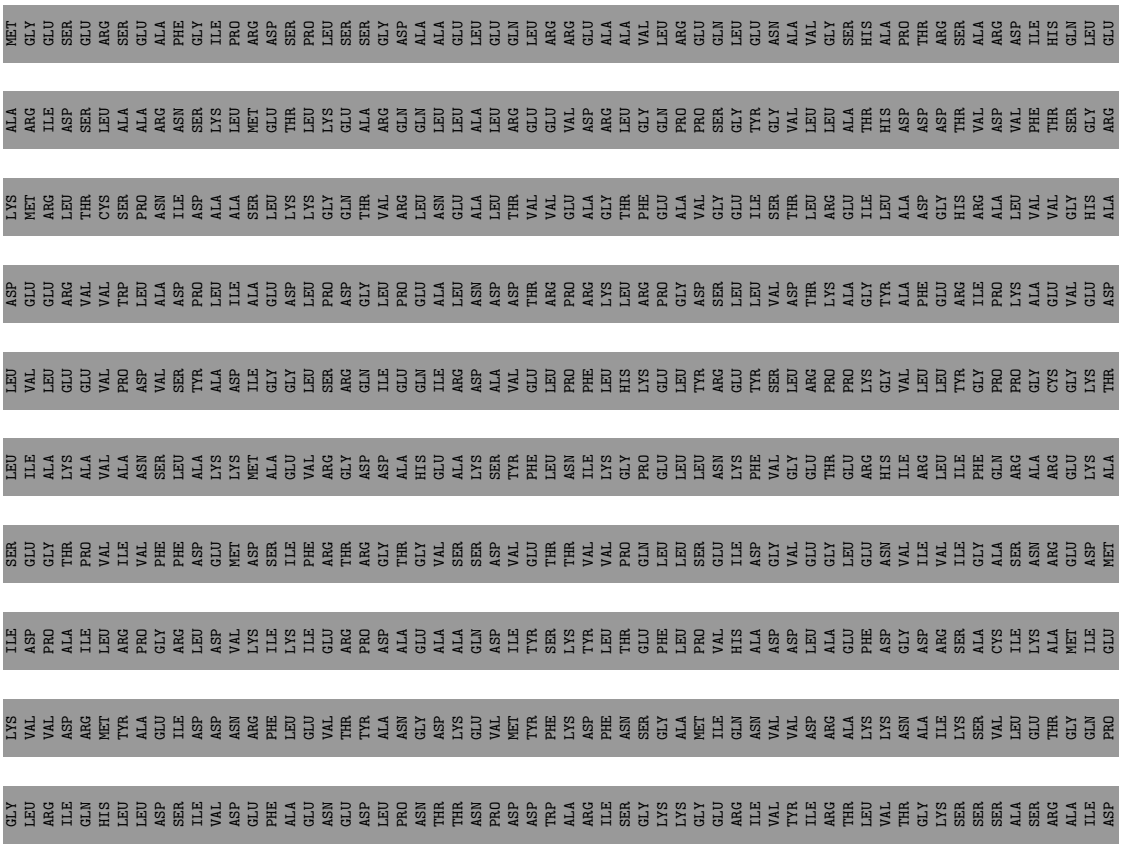
• Molecule 2: AAA ATPase forming ring-shaped complexes

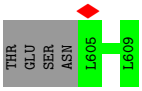




• Molecule 2: AAA ATPase forming ring-shaped complexes

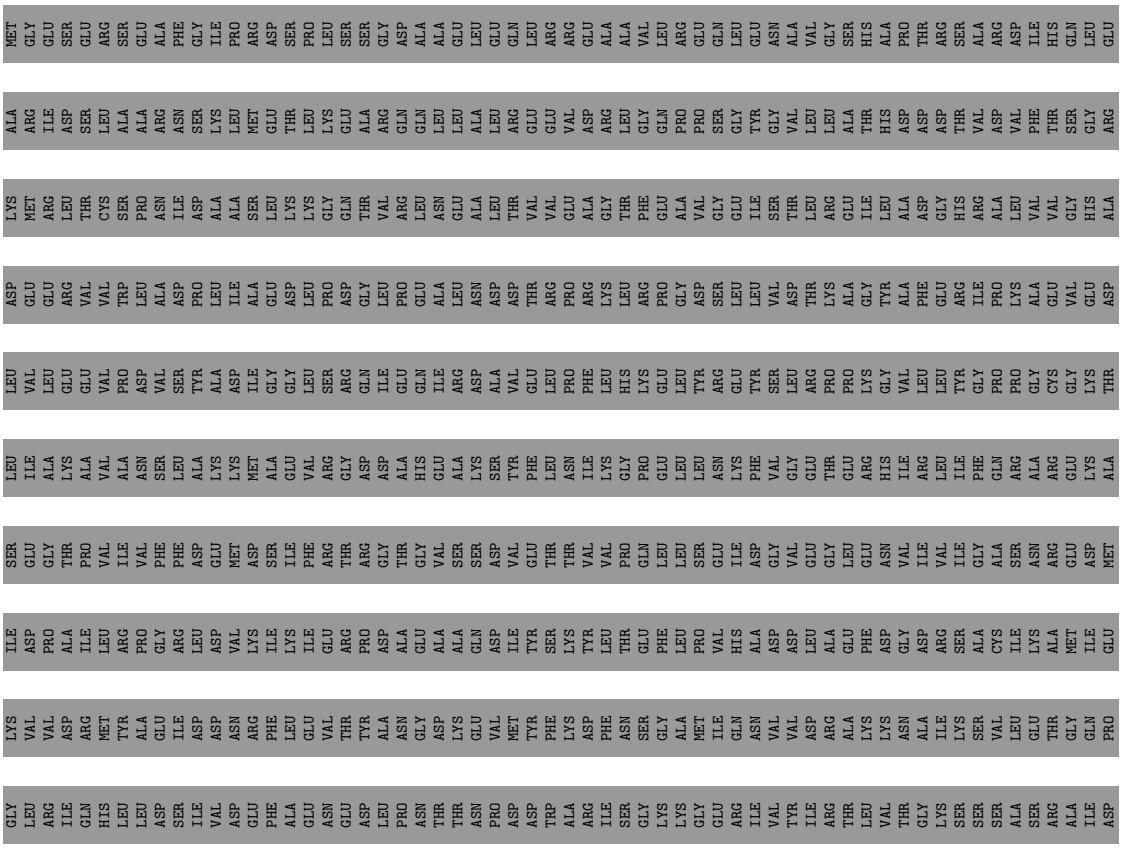
Chain A: 99%

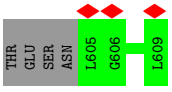




• Molecule 2: AAA ATPase forming ring-shaped complexes

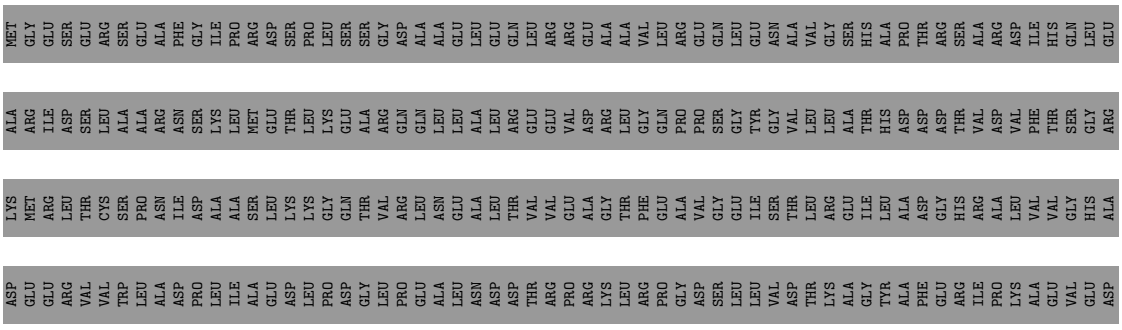
Chain B: 99%

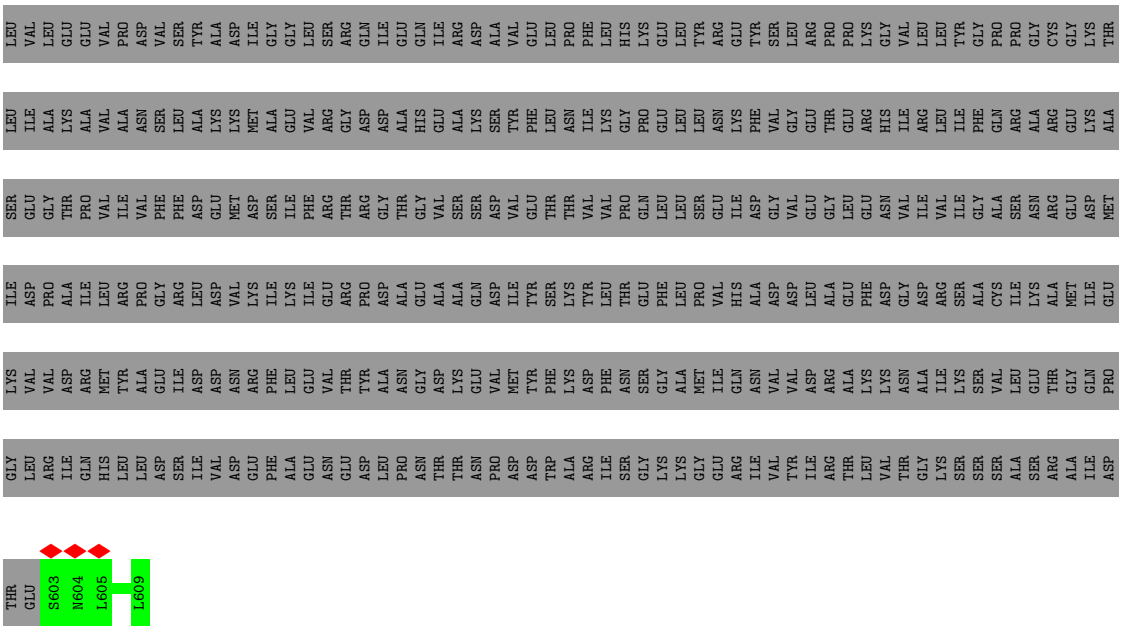




• Molecule 2: AAA ATPase forming ring-shaped complexes

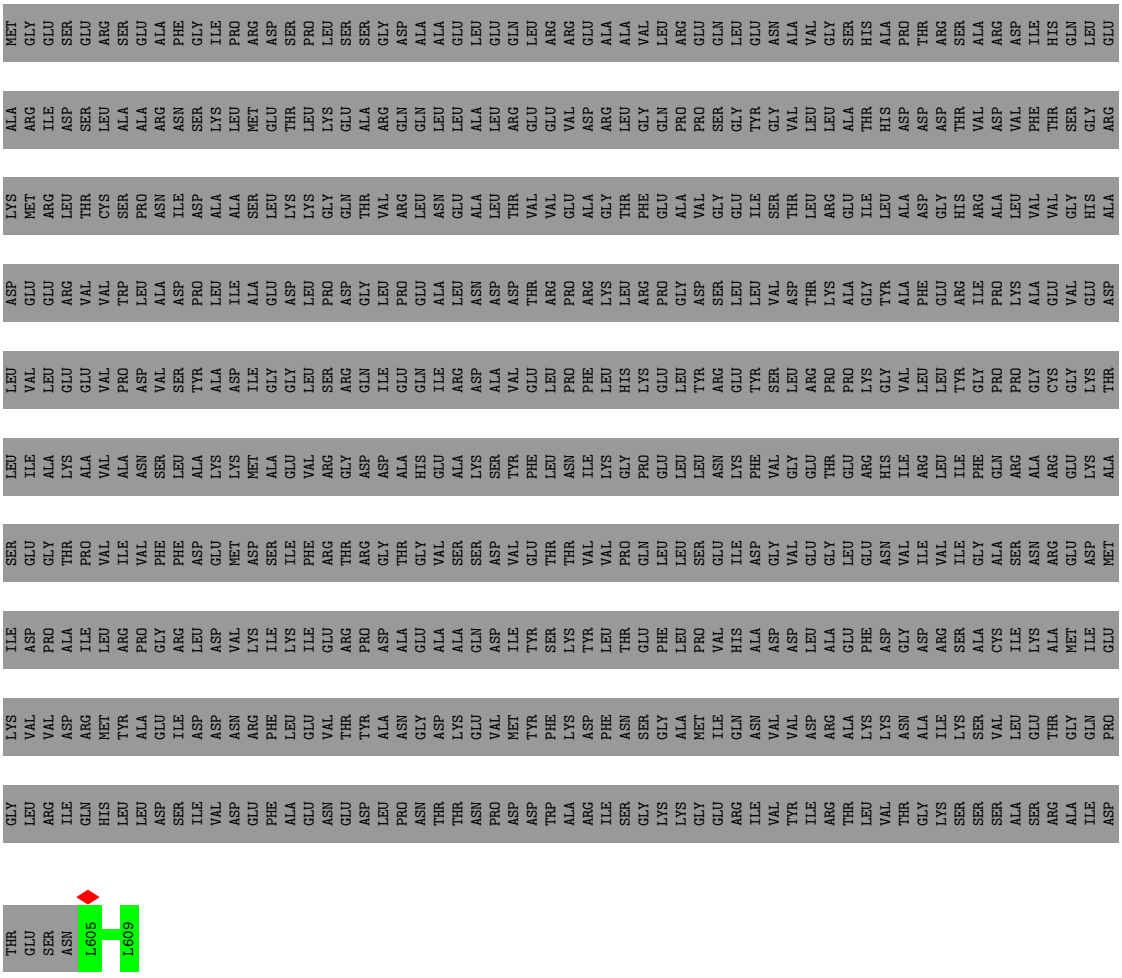
Chain C: 99%





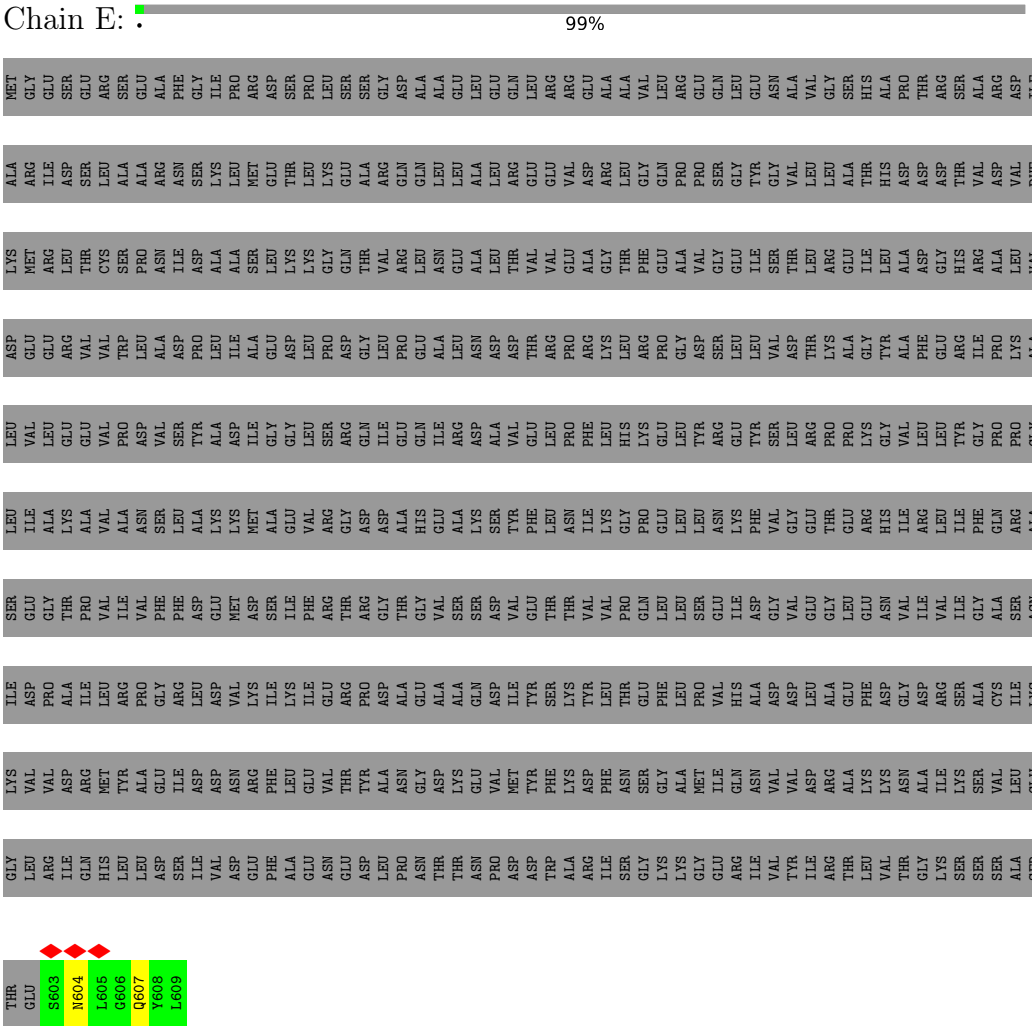
• Molecule 2: AAA ATPase forming ring-shaped complexes

Chain D: 99%



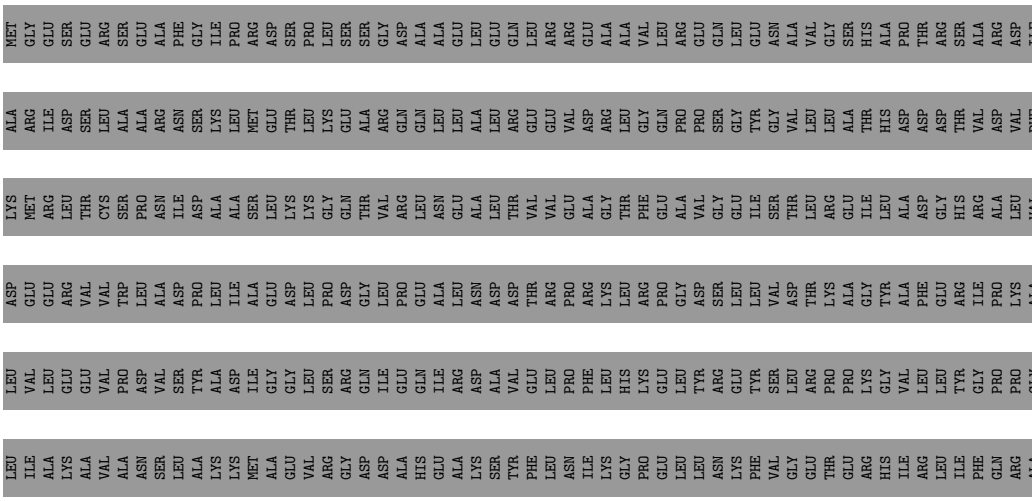
• Molecule 2: AAA ATPase forming ring-shaped complexes

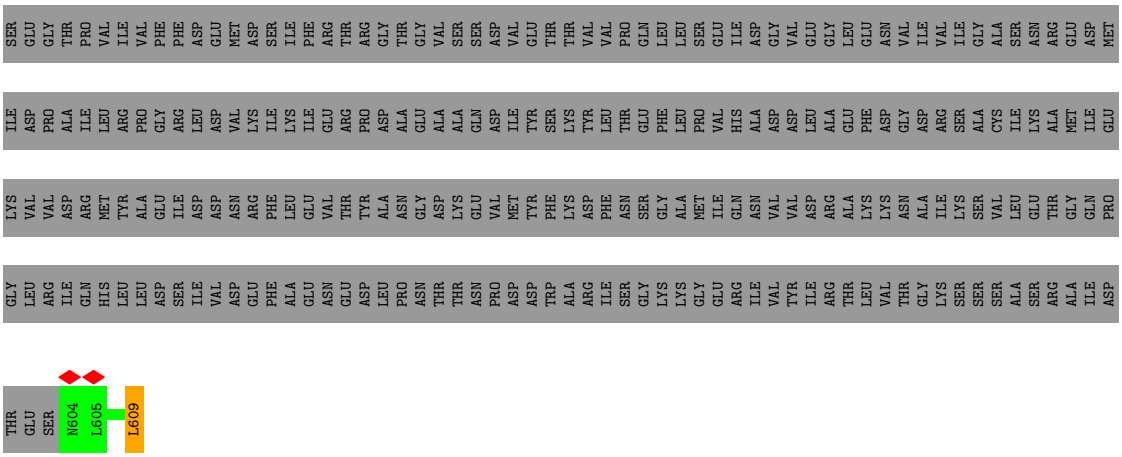
Chain E:



• Molecule 2: AAA ATPase forming ring-shaped complexes

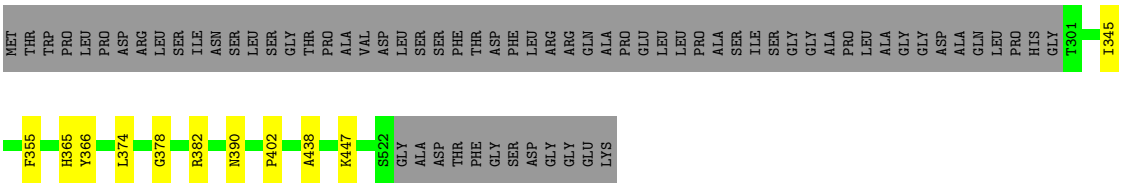
Chain F:





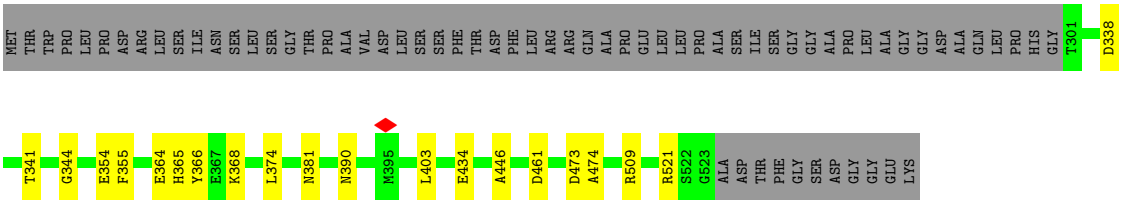
• Molecule 3: Proteasome subunit beta

Chain H:



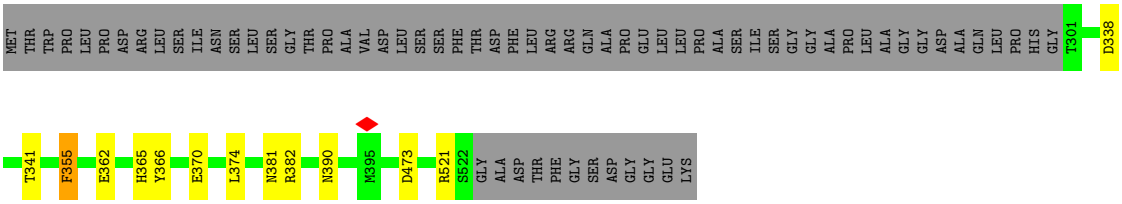
• Molecule 3: Proteasome subunit beta

Chain J:



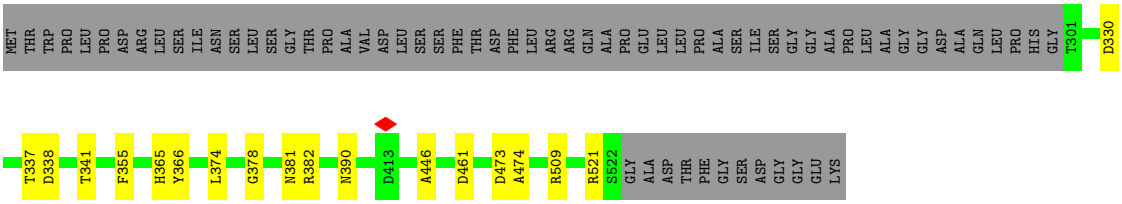
• Molecule 3: Proteasome subunit beta

Chain L:



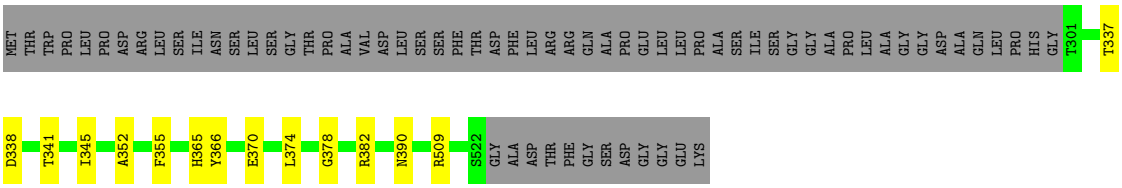
• Molecule 3: Proteasome subunit beta

Chain M:



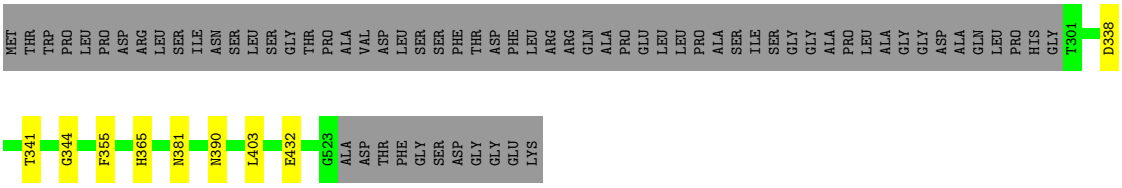
• Molecule 3: Proteasome subunit beta

Chain N:



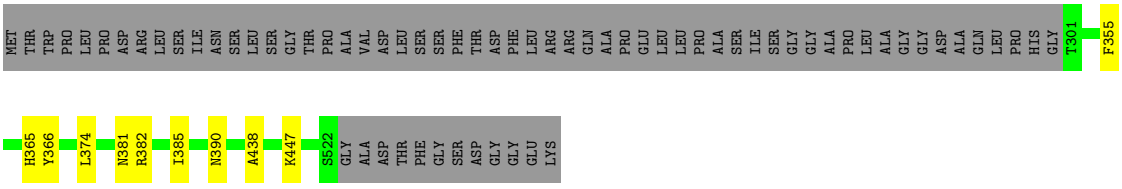
• Molecule 3: Proteasome subunit beta

Chain P:



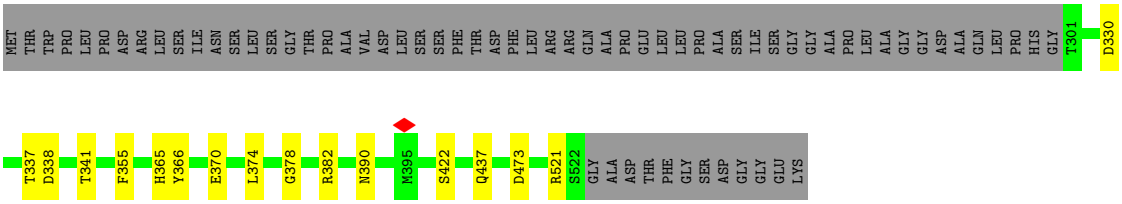
• Molecule 3: Proteasome subunit beta

Chain R:



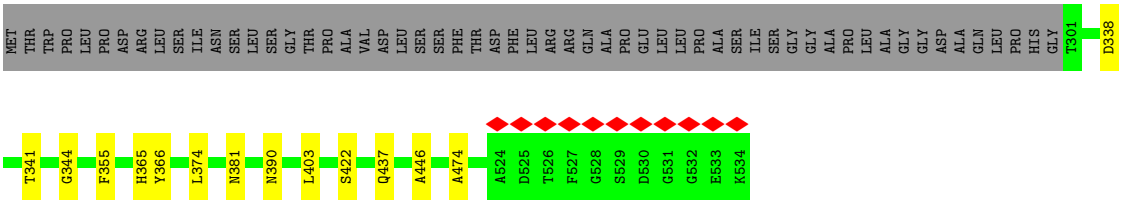
• Molecule 3: Proteasome subunit beta

Chain S:



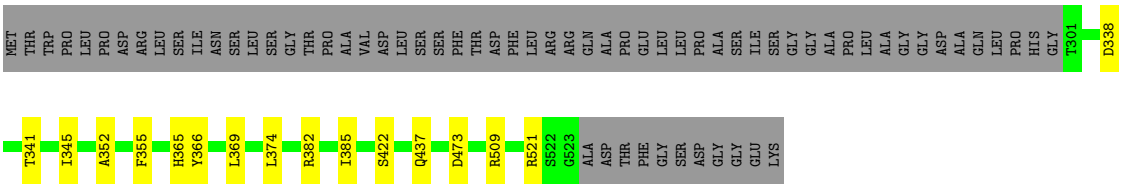
• Molecule 3: Proteasome subunit beta

Chain U:



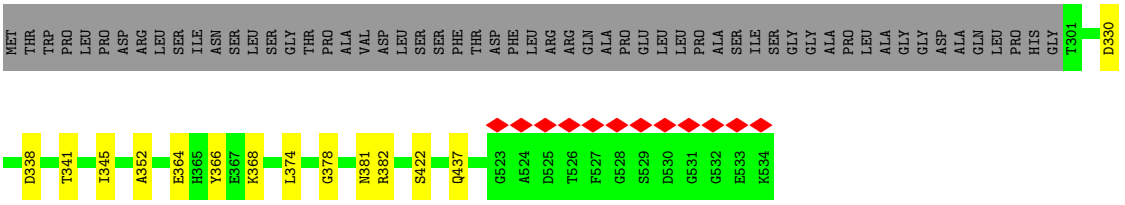
• Molecule 3: Proteasome subunit beta

Chain V:



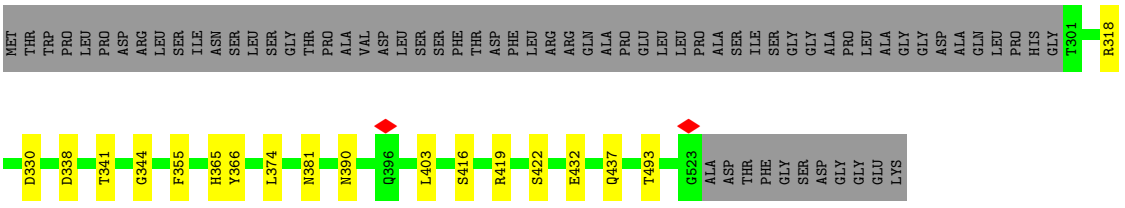
• Molecule 3: Proteasome subunit beta

Chain W:



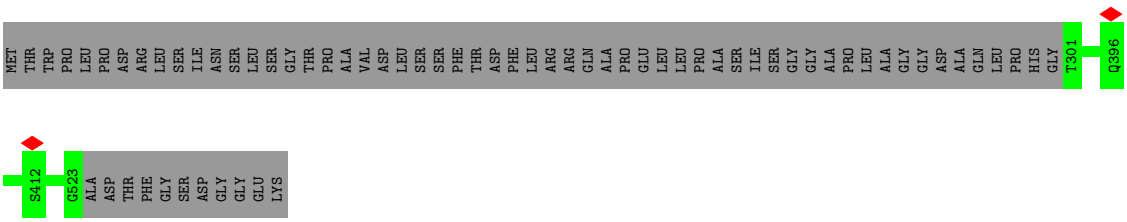
• Molecule 3: Proteasome subunit beta

Chain Y:



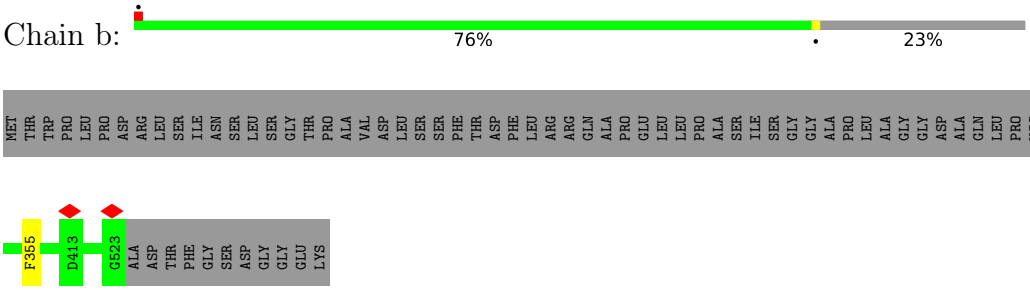
• Molecule 3: Proteasome subunit beta

Chain a:



• Molecule 3: Proteasome subunit beta

Chain b:


76%
23%
MET THR TRP PRO LEU PRO ASP ARG LEU SER ILE ASN SER LEU SER GLY THR PRO ALA VAL ASP LEU SER SER PHE THR ASP PHE LEU ARG ARG GLN ALA PRO GLU LEU LEU PRO ALA SER ILE SER GLY GLY ALA PRO LEU ALA GLY GLY ASP ALA GLN LEU PRO HIS GLY
T301
D330
F355
D413
G523
ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	222719	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0236	Depositor
Map size (Å)	430.144, 430.144, 430.144	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.222, 1.222, 1.222	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.24	0/1683	0.41	0/2274
1	2	0.24	0/1683	0.41	0/2274
1	4	0.24	0/1683	0.41	0/2274
1	6	0.24	0/1683	0.40	0/2274
1	8	0.24	0/1683	0.40	0/2274
1	I	0.24	0/1675	0.40	0/2263
1	K	0.24	0/1693	0.40	0/2287
1	O	0.24	0/1683	0.40	0/2274
1	Q	0.24	0/1683	0.40	0/2274
1	T	0.24	0/1675	0.40	0/2263
1	X	0.24	0/1675	0.40	0/2263
1	Z	0.24	0/1683	0.40	0/2274
1	d	0.24	0/1683	0.41	0/2274
1	f	0.24	0/1683	0.41	0/2274
2	1	0.23	0/42	0.43	0/54
2	A	0.23	0/42	0.43	0/54
2	B	0.26	0/42	0.43	0/54
2	C	0.25	0/56	0.51	0/73
2	D	0.23	0/42	0.43	0/54
2	E	0.24	0/56	0.43	0/73
2	F	0.26	0/50	0.41	0/65
3	H	0.24	0/1660	0.42	0/2251
3	J	0.24	0/1664	0.42	0/2256
3	L	0.24	0/1660	0.42	0/2251
3	M	0.24	0/1660	0.42	0/2251
3	N	0.24	0/1660	0.42	0/2251
3	P	0.24	0/1664	0.42	0/2256
3	R	0.24	0/1660	0.42	0/2251
3	S	0.24	0/1660	0.42	0/2251
3	U	0.24	0/1740	0.42	0/2357
3	V	0.24	0/1664	0.42	0/2256
3	W	0.24	0/1740	0.43	0/2357
3	Y	0.24	0/1664	0.42	0/2256
3	a	0.24	0/1664	0.42	0/2256

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	b	0.24	0/1664	0.43	0/2256
All	All	0.24	0/47302	0.41	0/63999

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1658	0	1659	18	0
1	2	1658	0	1659	16	0
1	4	1658	0	1659	13	0
1	6	1658	0	1659	14	0
1	8	1658	0	1659	17	0
1	I	1650	0	1648	25	0
1	K	1668	0	1667	18	0
1	O	1658	0	1659	22	0
1	Q	1658	0	1659	21	0
1	T	1650	0	1648	19	0
1	X	1650	0	1648	19	0
1	Z	1658	0	1659	18	0
1	d	1658	0	1659	0	0
1	f	1658	0	1659	0	0
2	1	42	0	41	1	0
2	A	42	0	41	0	0
2	B	42	0	41	0	0
2	C	56	0	52	0	0
2	D	42	0	41	0	0
2	E	56	0	52	2	0
2	F	50	0	47	1	0
3	H	1636	0	1625	7	0
3	J	1640	0	1628	10	0
3	L	1636	0	1625	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	1636	0	1625	10	0
3	N	1636	0	1625	8	0
3	P	1640	0	1628	5	0
3	R	1636	0	1625	6	0
3	S	1636	0	1625	9	0
3	U	1715	0	1690	8	0
3	V	1640	0	1628	8	0
3	W	1715	0	1690	7	0
3	Y	1640	0	1628	10	0
3	a	1640	0	1628	0	0
3	b	1640	0	1628	0	0
All	All	46614	0	46414	291	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:74:LEU:HD23	1:6:122:LEU:HD11	1.73	0.70
1:Z:74:LEU:HD23	1:Z:122:LEU:HD11	1.73	0.70
1:0:74:LEU:HD23	1:0:122:LEU:HD11	1.72	0.70
1:8:74:LEU:HD23	1:8:122:LEU:HD11	1.74	0.69
1:2:74:LEU:HD23	1:2:122:LEU:HD11	1.74	0.68
1:K:74:LEU:HD23	1:K:122:LEU:HD11	1.76	0.68
1:X:74:LEU:HD23	1:X:122:LEU:HD11	1.76	0.67
1:4:74:LEU:HD23	1:4:122:LEU:HD11	1.76	0.66
3:J:338:ASP:OD1	3:J:341:THR:OG1	2.15	0.65
1:O:186:ALA:HA	1:O:189:ARG:HD2	1.79	0.64
1:I:217:ARG:HG3	1:I:218:PRO:HD2	1.79	0.64
1:O:74:LEU:HD23	1:O:122:LEU:HD11	1.80	0.63
1:I:74:LEU:HD23	1:I:122:LEU:HD11	1.81	0.63
1:T:41:PHE:HB3	1:T:53:ILE:HD13	1.80	0.63
1:T:74:LEU:HD23	1:T:122:LEU:HD11	1.81	0.63
1:6:140:ARG:HH11	1:6:154:VAL:HG13	1.65	0.62
1:X:83:ASP:OD2	3:Y:365:HIS:ND1	2.31	0.62
1:8:52:LYS:HD2	2:F:609:LEU:HD22	1.81	0.62
1:K:140:ARG:HH11	1:K:154:VAL:HG13	1.65	0.61
1:K:205:VAL:HG13	1:K:230:LEU:HD23	1.83	0.60
1:Q:74:LEU:HD23	1:Q:122:LEU:HD11	1.82	0.60
1:X:140:ARG:HH11	1:X:154:VAL:HG13	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:53:ILE:O	1:T:224:ARG:NH2	2.33	0.60
1:6:83:ASP:OD2	3:N:365:HIS:ND1	2.32	0.60
1:8:83:ASP:OD2	3:V:365:HIS:ND1	2.32	0.59
3:M:338:ASP:OD1	3:M:341:THR:OG1	2.20	0.59
1:O:11:GLN:OE1	1:O:14:ARG:NH2	2.36	0.59
1:0:140:ARG:NH2	1:0:150:GLU:OE2	2.36	0.59
1:X:41:PHE:HB3	1:X:53:ILE:HD13	1.85	0.59
3:Y:432:GLU:OE2	3:Y:437:GLN:NE2	2.35	0.59
1:O:83:ASP:OD2	3:P:365:HIS:ND1	2.34	0.59
1:O:178:THR:HG22	1:O:182:ARG:HE	1.69	0.58
3:Y:381:ASN:ND2	1:Z:88:ALA:O	2.38	0.57
1:T:83:ASP:OD2	3:U:365:HIS:ND1	2.33	0.57
1:K:83:ASP:OD2	3:L:365:HIS:ND1	2.34	0.57
1:2:56:LEU:HG	1:2:62:PHE:HB2	1.87	0.57
1:T:182:ARG:NH1	1:T:234:LEU:O	2.37	0.56
1:2:41:PHE:HB3	1:2:53:ILE:HD13	1.86	0.56
1:8:16:ARG:HB3	1:8:117:PRO:HG3	1.87	0.56
1:8:140:ARG:HH11	1:8:154:VAL:HG13	1.69	0.56
1:Q:74:LEU:HD21	1:Q:107:LEU:HD21	1.88	0.56
1:K:53:ILE:O	1:K:224:ARG:NH2	2.38	0.56
3:M:473:ASP:OD1	3:M:521:ARG:NH1	2.36	0.56
1:2:128:ALA:HB2	1:2:134:LYS:HB3	1.88	0.56
1:O:140:ARG:HH11	1:O:154:VAL:HG13	1.70	0.56
1:I:53:ILE:O	1:I:224:ARG:NH2	2.35	0.56
1:I:83:ASP:OD2	3:J:365:HIS:ND1	2.33	0.56
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.88	0.55
1:8:41:PHE:HB3	1:8:53:ILE:HD13	1.87	0.55
1:8:140:ARG:NH2	1:8:150:GLU:OE2	2.39	0.55
1:Z:140:ARG:NH2	1:Z:150:GLU:OE2	2.36	0.55
1:4:56:LEU:HG	1:4:62:PHE:HB2	1.88	0.55
1:4:140:ARG:HH11	1:4:154:VAL:HG13	1.72	0.55
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.89	0.55
1:4:128:ALA:HB2	1:4:134:LYS:HB3	1.89	0.55
3:P:381:ASN:ND2	1:Q:88:ALA:O	2.40	0.54
3:L:381:ASN:ND2	1:X:88:ALA:O	2.41	0.54
1:6:41:PHE:HB3	1:6:53:ILE:HD13	1.88	0.54
1:6:53:ILE:O	1:6:224:ARG:NH2	2.35	0.54
1:T:178:THR:HG22	1:T:182:ARG:HE	1.73	0.54
3:J:461:ASP:OD1	3:J:509:ARG:NH2	2.41	0.54
1:8:128:ALA:HB2	1:8:134:LYS:HB3	1.91	0.53
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:128:ALA:HB2	1:T:134:LYS:HB3	1.90	0.53
1:6:140:ARG:NH2	1:6:150:GLU:OE2	2.42	0.53
1:8:56:LEU:HG	1:8:62:PHE:HB2	1.89	0.53
1:X:31:VAL:HG12	1:X:155:VAL:HG22	1.91	0.53
1:2:140:ARG:NH2	1:2:150:GLU:OE2	2.42	0.52
1:6:225:ILE:HG21	1:6:233:LEU:HD22	1.91	0.52
1:0:56:LEU:HG	1:0:62:PHE:HB2	1.90	0.52
3:L:355:PHE:HZ	3:L:390:ASN:HB2	1.73	0.52
3:S:355:PHE:HZ	3:S:390:ASN:HB2	1.75	0.52
1:I:128:ALA:HB2	1:I:134:LYS:HB3	1.92	0.52
1:0:41:PHE:HB3	1:0:53:ILE:HD13	1.92	0.51
1:8:68:PHE:HA	1:8:71:PHE:CE2	2.45	0.51
1:Z:163:ILE:HD13	1:Z:188:LEU:HD12	1.92	0.51
1:I:88:ALA:O	3:U:381:ASN:ND2	2.44	0.51
3:R:382:ARG:HH21	3:R:385:ILE:HD12	1.76	0.51
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.92	0.51
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.93	0.51
3:L:338:ASP:OD1	3:L:341:THR:OG1	2.19	0.51
3:Y:355:PHE:HZ	3:Y:390:ASN:HB2	1.76	0.51
1:0:53:ILE:O	1:0:224:ARG:NH2	2.37	0.51
1:I:185:VAL:HG21	1:I:234:LEU:HD11	1.93	0.51
3:P:338:ASP:OD1	3:P:341:THR:OG1	2.19	0.51
1:Q:53:ILE:O	1:Q:224:ARG:NH2	2.38	0.51
1:X:56:LEU:HG	1:X:62:PHE:HB2	1.94	0.51
1:K:140:ARG:NH2	1:K:150:GLU:OE2	2.44	0.50
1:K:68:PHE:HA	1:K:71:PHE:CE2	2.46	0.50
1:I:140:ARG:HH11	1:I:154:VAL:HG13	1.76	0.50
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.47	0.50
1:T:68:PHE:HA	1:T:71:PHE:CE2	2.46	0.50
1:K:56:LEU:HG	1:K:62:PHE:HB2	1.92	0.50
1:X:128:ALA:HB2	1:X:134:LYS:HB3	1.94	0.50
3:R:355:PHE:HZ	3:R:390:ASN:HB2	1.75	0.50
3:M:337:THR:HG1	3:M:341:THR:HG1	1.58	0.49
1:T:14:ARG:NH1	1:T:18:GLU:OE2	2.45	0.49
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.47	0.49
1:0:209:GLU:OE2	1:0:224:ARG:NH1	2.45	0.49
1:2:225:ILE:HG21	1:2:233:LEU:HD22	1.95	0.49
3:J:381:ASN:ND2	1:O:88:ALA:O	2.45	0.49
1:Z:31:VAL:HG12	1:Z:155:VAL:HG22	1.93	0.49
1:4:68:PHE:HA	1:4:71:PHE:CE2	2.47	0.49
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:604:ASN:OD1	2:E:604:ASN:N	2.46	0.49
1:K:88:ALA:O	3:R:381:ASN:ND2	2.45	0.49
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.95	0.48
1:2:53:ILE:O	1:2:224:ARG:NH2	2.46	0.48
1:6:16:ARG:NH2	1:6:114:GLN:O	2.42	0.48
1:6:68:PHE:HA	1:6:71:PHE:CE2	2.48	0.48
3:N:337:THR:OG1	3:N:341:THR:OG1	2.30	0.48
3:W:338:ASP:OD1	3:W:341:THR:OG1	2.20	0.48
3:M:355:PHE:HZ	3:M:390:ASN:HB2	1.77	0.48
1:6:56:LEU:HG	1:6:62:PHE:HB2	1.94	0.48
1:X:68:PHE:HA	1:X:71:PHE:CE2	2.49	0.48
1:Q:83:ASP:OD2	3:R:365:HIS:ND1	2.43	0.48
3:V:473:ASP:OD1	3:V:521:ARG:NH1	2.37	0.48
3:W:364:GLU:HG2	3:W:368:LYS:HE2	1.96	0.48
1:Z:68:PHE:HA	1:Z:71:PHE:CE2	2.49	0.48
1:2:68:PHE:HA	1:2:71:PHE:CE2	2.49	0.48
1:T:56:LEU:HG	1:T:62:PHE:HB2	1.96	0.48
3:U:355:PHE:HZ	3:U:390:ASN:HB2	1.79	0.48
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.96	0.47
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.95	0.47
1:T:31:VAL:HG12	1:T:155:VAL:HG22	1.95	0.47
3:W:345:ILE:HB	3:W:352:ALA:HB1	1.95	0.47
1:2:28:LYS:HB2	1:2:52:LYS:HZ2	1.80	0.47
1:2:182:ARG:NH1	1:2:234:LEU:O	2.48	0.47
1:I:140:ARG:NH2	1:I:150:GLU:OE2	2.47	0.47
3:M:461:ASP:OD1	3:M:509:ARG:NH2	2.47	0.47
1:O:50:LEU:HD11	1:Q:147:ILE:HG23	1.97	0.47
1:O:140:ARG:NH2	1:O:150:GLU:OE2	2.48	0.47
1:0:128:ALA:HB2	1:0:134:LYS:HB3	1.97	0.47
3:H:355:PHE:HZ	3:H:390:ASN:HB2	1.81	0.46
3:J:355:PHE:HZ	3:J:390:ASN:HB2	1.81	0.46
1:X:178:THR:HG22	1:X:182:ARG:HE	1.80	0.46
3:Y:338:ASP:OD1	3:Y:341:THR:OG1	2.20	0.46
1:0:83:ASP:OD2	3:S:365:HIS:ND1	2.32	0.46
1:I:185:VAL:O	1:I:189:ARG:HG3	2.16	0.46
1:X:212:VAL:HG21	1:X:223:ARG:HH21	1.80	0.46
1:6:128:ALA:HB2	1:6:134:LYS:HB3	1.96	0.46
1:Q:140:ARG:HH11	1:Q:154:VAL:HG13	1.80	0.46
1:I:73:ASN:ND2	1:O:105:GLN:OE1	2.49	0.46
3:V:338:ASP:OD1	3:V:341:THR:OG1	2.21	0.46
1:K:147:ILE:HG23	1:Q:50:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.97	0.45
1:Z:56:LEU:HG	1:Z:62:PHE:HB2	1.97	0.45
3:R:438:ALA:HB3	3:R:447:LYS:HG3	1.98	0.45
1:K:31:VAL:HG12	1:K:155:VAL:HG22	1.97	0.45
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.99	0.45
3:L:473:ASP:OD1	3:L:521:ARG:NH1	2.41	0.45
1:4:33:LEU:HD21	1:4:184:ALA:HB2	1.98	0.45
1:I:147:ILE:HG23	1:T:50:LEU:HD11	1.97	0.45
1:I:178:THR:HG22	1:I:182:ARG:HE	1.81	0.45
3:P:355:PHE:HZ	3:P:390:ASN:HB2	1.81	0.45
1:T:140:ARG:HH11	1:T:154:VAL:HG13	1.82	0.45
1:T:147:ILE:HG23	1:Z:50:LEU:HD11	1.99	0.45
1:0:140:ARG:HH11	1:0:154:VAL:HG13	1.82	0.45
1:0:182:ARG:NH1	1:0:234:LEU:O	2.50	0.44
1:Z:178:THR:HG22	1:Z:182:ARG:HE	1.81	0.44
1:Q:142:THR:OG1	1:Q:144:ASP:OD1	2.32	0.44
3:V:382:ARG:HH21	3:V:385:ILE:HD12	1.81	0.44
1:I:161:GLU:HB2	1:I:162:PRO:HD3	2.00	0.44
3:V:345:ILE:HB	3:V:352:ALA:HB1	1.99	0.44
1:8:146:SER:HA	2:E:607:GLN:HB2	1.98	0.44
3:H:438:ALA:HB3	3:H:447:LYS:HG3	2.00	0.44
1:X:46:PRO:HA	1:X:207:SER:HA	1.99	0.44
1:2:140:ARG:HH11	1:2:154:VAL:HG13	1.83	0.44
1:8:33:LEU:HD11	1:8:40:LEU:HD23	1.99	0.44
3:N:338:ASP:OD1	3:N:341:THR:OG1	2.20	0.44
1:Z:41:PHE:HB3	1:Z:53:ILE:HD13	1.99	0.44
1:I:50:LEU:HD11	1:O:147:ILE:HG23	1.99	0.44
1:O:16:ARG:HH11	1:O:117:PRO:HD3	1.83	0.44
3:S:473:ASP:OD1	3:S:521:ARG:NH1	2.39	0.44
3:Y:344:GLY:O	3:Y:403:LEU:N	2.51	0.44
1:X:161:GLU:HB2	1:X:162:PRO:HD3	2.00	0.44
1:Z:161:GLU:HB2	1:Z:162:PRO:HD3	1.99	0.44
1:0:68:PHE:HA	1:0:71:PHE:CE2	2.53	0.43
3:N:366:TYR:CD1	3:N:374:LEU:HG	2.53	0.43
1:T:107:LEU:HD12	1:T:141:ILE:HG22	2.01	0.43
1:I:63:ALA:HB3	1:I:123:CYS:HB3	2.01	0.43
3:J:364:GLU:HG2	3:J:368:LYS:HE2	2.00	0.43
3:J:473:ASP:OD1	3:J:521:ARG:NH1	2.45	0.43
1:O:90:ASP:OD1	1:O:91:ARG:N	2.52	0.43
1:4:41:PHE:HB3	1:4:53:ILE:HD13	2.00	0.43
3:J:344:GLY:O	3:J:403:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:225:ILE:HG21	1:0:233:LEU:HD22	2.01	0.43
3:N:355:PHE:HZ	3:N:390:ASN:HB2	1.82	0.43
1:T:63:ALA:HB3	1:T:123:CYS:HB3	2.01	0.43
1:X:72:ASP:O	1:X:76:ARG:HG3	2.19	0.43
3:P:344:GLY:O	3:P:403:LEU:N	2.51	0.43
3:L:362:GLU:OE2	3:L:382:ARG:NE	2.48	0.43
3:H:345:ILE:HA	3:H:402:PRO:HA	2.01	0.43
1:O:33:LEU:HD21	1:O:184:ALA:HB2	2.00	0.43
1:Q:33:LEU:HD21	1:Q:184:ALA:HB2	2.01	0.43
1:2:83:ASP:OD2	3:M:365:HIS:ND1	2.31	0.43
1:4:140:ARG:NH2	1:4:150:GLU:OE2	2.50	0.43
3:N:345:ILE:HB	3:N:352:ALA:HB1	2.01	0.43
3:S:337:THR:OG1	3:S:341:THR:OG1	2.37	0.43
3:U:338:ASP:OD1	3:U:341:THR:OG1	2.17	0.43
1:0:31:VAL:HG12	1:0:155:VAL:HG22	1.99	0.43
1:4:161:GLU:HB2	1:4:162:PRO:HD3	2.00	0.43
1:2:161:GLU:HB2	1:2:162:PRO:HD3	2.01	0.42
1:Q:161:GLU:HB2	1:Q:162:PRO:HD3	2.01	0.42
1:0:88:ALA:O	3:W:381:ASN:ND2	2.52	0.42
3:H:366:TYR:CD1	3:H:374:LEU:HG	2.54	0.42
1:I:142:THR:OG1	1:I:144:ASP:OD1	2.31	0.42
1:K:161:GLU:HB2	1:K:162:PRO:HD3	2.01	0.42
3:N:366:TYR:CZ	3:N:370:GLU:HG3	2.54	0.42
3:N:378:GLY:O	3:N:382:ARG:HG2	2.20	0.42
1:O:163:ILE:HD13	1:O:188:LEU:HD12	2.01	0.42
3:W:366:TYR:CD1	3:W:374:LEU:HG	2.55	0.42
1:Z:118:TYR:HB3	1:Z:120:VAL:HG22	2.02	0.42
1:Z:205:VAL:HG12	1:Z:230:LEU:HG	2.02	0.42
1:O:45:ASN:ND2	1:O:50:LEU:O	2.40	0.42
3:U:422:SER:HB3	3:U:437:GLN:HG2	2.02	0.42
3:Y:318:ARG:HD3	3:Y:493:THR:HG23	2.02	0.42
3:Y:416:SER:O	3:Y:419:ARG:NH1	2.44	0.42
1:0:161:GLU:HB2	1:0:162:PRO:HD3	2.02	0.42
1:8:55:GLU:HB2	1:8:222:PHE:CG	2.55	0.42
1:I:55:GLU:HB2	1:I:222:PHE:CG	2.54	0.42
1:K:142:THR:OG1	1:K:144:ASP:OD1	2.25	0.42
1:Q:44:GLU:HB2	1:Q:188:LEU:HD21	2.02	0.42
1:0:142:THR:OG1	1:0:144:ASP:OD1	2.27	0.42
1:2:45:ASN:ND2	1:2:50:LEU:O	2.38	0.42
1:4:181:LEU:HD23	1:4:233:LEU:HB3	2.00	0.42
1:O:63:ALA:HB3	1:O:123:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:338:ASP:OD1	3:S:341:THR:OG1	2.20	0.42
3:U:366:TYR:CD1	3:U:374:LEU:HG	2.55	0.42
3:Y:366:TYR:CD1	3:Y:374:LEU:HG	2.54	0.42
1:O:161:GLU:HB2	1:O:162:PRO:HD3	2.02	0.42
3:S:366:TYR:CD1	3:S:374:LEU:HG	2.55	0.42
3:U:446:ALA:HB2	3:U:474:ALA:HB2	2.01	0.42
3:V:366:TYR:CD1	3:V:374:LEU:HG	2.54	0.42
3:R:366:TYR:CD1	3:R:374:LEU:HG	2.54	0.42
1:Z:31:VAL:HG23	1:Z:42:VAL:HB	2.01	0.42
1:X:33:LEU:HB3	1:X:153:PHE:HB3	2.02	0.41
1:4:88:ALA:O	3:M:381:ASN:ND2	2.53	0.41
3:S:422:SER:HB3	3:S:437:GLN:HG2	2.01	0.41
1:Z:90:ASP:OD1	1:Z:91:ARG:N	2.53	0.41
1:0:214:ASP:HB3	1:0:217:ARG:HG2	2.02	0.41
1:X:107:LEU:HD23	1:X:107:LEU:HA	1.88	0.41
1:Z:16:ARG:NH1	1:Z:114:GLN:O	2.51	0.41
3:H:378:GLY:O	3:H:382:ARG:HG2	2.21	0.41
1:O:165:ASN:O	1:O:169:GLU:HG2	2.20	0.41
1:Q:140:ARG:NH2	1:Q:150:GLU:OE2	2.53	0.41
1:T:161:GLU:HB2	1:T:162:PRO:HD3	2.02	0.41
1:4:83:ASP:OD2	3:H:365:HIS:ND1	2.31	0.41
3:M:366:TYR:CD1	3:M:374:LEU:HG	2.56	0.41
3:J:446:ALA:HB2	3:J:474:ALA:HB2	2.03	0.41
1:Q:225:ILE:HG21	1:Q:233:LEU:HD22	2.03	0.41
1:8:225:ILE:HG21	1:8:233:LEU:HD22	2.01	0.41
3:L:366:TYR:CD1	3:L:374:LEU:HG	2.56	0.41
3:L:366:TYR:CZ	3:L:370:GLU:HG3	2.55	0.41
3:M:446:ALA:HB2	3:M:474:ALA:HB2	2.01	0.41
1:2:33:LEU:HD11	1:2:40:LEU:HD23	2.03	0.41
1:6:178:THR:HG22	1:6:182:ARG:HE	1.86	0.41
1:8:107:LEU:HD12	1:8:141:ILE:HG22	2.02	0.41
3:H:345:ILE:HG12	3:H:402:PRO:HB3	2.03	0.41
3:J:366:TYR:CD1	3:J:374:LEU:HG	2.56	0.41
1:K:107:LEU:HD23	1:K:107:LEU:HA	1.88	0.41
1:Q:118:TYR:HB3	1:Q:120:VAL:HG22	2.03	0.41
1:T:205:VAL:HG13	1:T:230:LEU:HD23	2.02	0.41
1:T:214:ASP:HB3	1:T:217:ARG:HG2	2.02	0.41
3:W:378:GLY:O	3:W:382:ARG:HG2	2.20	0.41
1:0:51:GLN:OE1	1:0:224:ARG:NH2	2.53	0.41
1:6:214:ASP:HB3	1:6:217:ARG:HG2	2.03	0.41
1:X:140:ARG:NH2	1:X:150:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:609:LEU:HD11	1:2:50:LEU:HD13	2.03	0.40
1:I:90:ASP:OD1	1:I:91:ARG:N	2.54	0.40
3:V:422:SER:HB3	3:V:437:GLN:HG2	2.03	0.40
1:Z:128:ALA:HB2	1:Z:134:LYS:HB3	2.03	0.40
1:8:161:GLU:HB2	1:8:162:PRO:HD3	2.02	0.40
1:8:178:THR:O	1:8:182:ARG:HD3	2.22	0.40
1:K:163:ILE:HD13	1:K:188:LEU:HD12	2.03	0.40
3:S:366:TYR:CZ	3:S:370:GLU:HG3	2.56	0.40
3:U:344:GLY:O	3:U:403:LEU:N	2.53	0.40
3:V:369:LEU:HD23	3:V:369:LEU:HA	1.95	0.40
1:X:50:LEU:HD11	1:Z:147:ILE:HG23	2.04	0.40
3:Y:422:SER:HB3	3:Y:437:GLN:HG2	2.02	0.40
1:I:8:SER:HB3	1:I:9:PRO:HD3	2.02	0.40
1:I:150:GLU:HG3	1:I:154:VAL:HG22	2.04	0.40
3:M:378:GLY:O	3:M:382:ARG:HG2	2.21	0.40
3:W:422:SER:HB3	3:W:437:GLN:HG2	2.03	0.40
1:Q:11:GLN:HG2	1:Q:14:ARG:HH22	1.86	0.40
3:S:378:GLY:O	3:S:382:ARG:HG2	2.21	0.40
1:X:90:ASP:OD1	1:X:91:ARG:N	2.55	0.40
1:4:31:VAL:HG12	1:4:155:VAL:HG22	2.02	0.40
1:6:31:VAL:HG12	1:6:155:VAL:HG22	2.03	0.40
1:I:18:GLU:OE1	1:I:21:ARG:NH2	2.39	0.40
1:K:55:GLU:HB2	1:K:222:PHE:CG	2.56	0.40

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	Percentiles	
1	0	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	2	211/248 (85%)	207 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	6	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
1	8	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
1	I	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
1	K	213/248 (86%)	209 (98%)	4 (2%)	0	100	100
1	O	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	Q	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	T	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
1	X	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
1	Z	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	d	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	f	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
2	1	3/609 (0%)	2 (67%)	1 (33%)	0	100	100
2	A	3/609 (0%)	2 (67%)	1 (33%)	0	100	100
2	B	3/609 (0%)	3 (100%)	0	0	100	100
2	C	5/609 (1%)	5 (100%)	0	0	100	100
2	D	3/609 (0%)	2 (67%)	1 (33%)	0	100	100
2	E	5/609 (1%)	4 (80%)	1 (20%)	0	100	100
2	F	4/609 (1%)	4 (100%)	0	0	100	100
3	H	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	J	221/291 (76%)	219 (99%)	2 (1%)	0	100	100
3	L	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	M	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	N	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	P	221/291 (76%)	220 (100%)	1 (0%)	0	100	100
3	R	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	S	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	U	232/291 (80%)	229 (99%)	3 (1%)	0	100	100
3	V	221/291 (76%)	219 (99%)	2 (1%)	0	100	100
3	W	232/291 (80%)	230 (99%)	2 (1%)	0	100	100
3	Y	221/291 (76%)	219 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	221/291 (76%)	219 (99%)	2 (1%)	0	100	100
3	b	221/291 (76%)	218 (99%)	3 (1%)	0	100	100
All	All	6089/11809 (52%)	5996 (98%)	93 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	165/192 (86%)	161 (98%)	4 (2%)	49	81
1	2	165/192 (86%)	161 (98%)	4 (2%)	49	81
1	4	165/192 (86%)	161 (98%)	4 (2%)	49	81
1	6	165/192 (86%)	160 (97%)	5 (3%)	41	75
1	8	165/192 (86%)	163 (99%)	2 (1%)	71	92
1	I	164/192 (85%)	161 (98%)	3 (2%)	59	86
1	K	166/192 (86%)	164 (99%)	2 (1%)	71	92
1	O	165/192 (86%)	164 (99%)	1 (1%)	86	96
1	Q	165/192 (86%)	163 (99%)	2 (1%)	71	92
1	T	164/192 (85%)	163 (99%)	1 (1%)	86	96
1	X	164/192 (85%)	163 (99%)	1 (1%)	86	96
1	Z	165/192 (86%)	163 (99%)	2 (1%)	71	92
1	d	165/192 (86%)	160 (97%)	5 (3%)	41	75
1	f	165/192 (86%)	164 (99%)	1 (1%)	86	96
2	1	4/511 (1%)	4 (100%)	0	100	100
2	A	4/511 (1%)	4 (100%)	0	100	100
2	B	4/511 (1%)	4 (100%)	0	100	100
2	C	6/511 (1%)	6 (100%)	0	100	100
2	D	4/511 (1%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	6/511 (1%)	6 (100%)	0	100 100
2	F	5/511 (1%)	4 (80%)	1 (20%)	1 4
3	H	164/217 (76%)	164 (100%)	0	100 100
3	J	164/217 (76%)	162 (99%)	2 (1%)	71 92
3	L	164/217 (76%)	163 (99%)	1 (1%)	86 96
3	M	164/217 (76%)	163 (99%)	1 (1%)	86 96
3	N	164/217 (76%)	163 (99%)	1 (1%)	86 96
3	P	164/217 (76%)	163 (99%)	1 (1%)	86 96
3	R	164/217 (76%)	164 (100%)	0	100 100
3	S	164/217 (76%)	163 (99%)	1 (1%)	86 96
3	U	171/217 (79%)	171 (100%)	0	100 100
3	V	164/217 (76%)	162 (99%)	2 (1%)	71 92
3	W	171/217 (79%)	170 (99%)	1 (1%)	86 96
3	Y	164/217 (76%)	163 (99%)	1 (1%)	86 96
3	a	164/217 (76%)	164 (100%)	0	100 100
3	b	164/217 (76%)	162 (99%)	2 (1%)	71 92
All	All	4651/9303 (50%)	4600 (99%)	51 (1%)	74 92

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	33	LEU
1	0	147	ILE
1	0	182	ARG
1	0	234	LEU
1	2	33	LEU
1	2	147	ILE
1	2	182	ARG
1	2	234	LEU
1	4	33	LEU
1	4	147	ILE
1	4	182	ARG
1	4	234	LEU
1	6	11	GLN
1	6	33	LEU
1	6	147	ILE

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Mol	Chain	Res	Type
1	6	182	ARG
1	6	234	LEU
1	8	182	ARG
1	8	234	LEU
2	F	609	LEU
1	I	33	LEU
1	I	182	ARG
1	I	217	ARG
3	J	354	GLU
3	J	434	GLU
1	K	33	LEU
1	K	182	ARG
3	L	355	PHE
3	M	330	ASP
3	N	509	ARG
1	O	182	ARG
3	P	432	GLU
1	Q	182	ARG
1	Q	234	LEU
3	S	330	ASP
1	T	182	ARG
3	V	355	PHE
3	V	509	ARG
3	W	330	ASP
1	X	182	ARG
3	Y	330	ASP
1	Z	73	ASN
1	Z	182	ARG
3	b	330	ASP
3	b	355	PHE
1	d	14	ARG
1	d	26	ARG
1	d	33	LEU
1	d	182	ARG
1	d	234	LEU
1	f	182	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	607	GLN
1	I	114	GLN

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Mol	Chain	Res	Type
1	K	114	GLN
1	O	114	GLN
1	Q	114	GLN
1	X	114	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)

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.

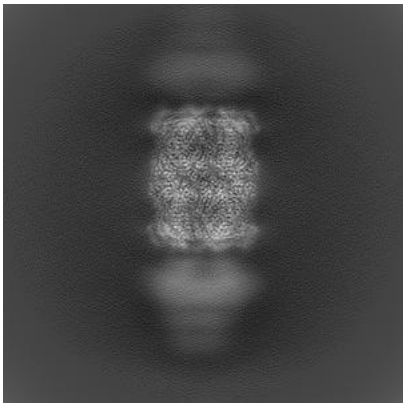
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13695. These allow visual inspection of the internal detail of the map and identification of artifacts.

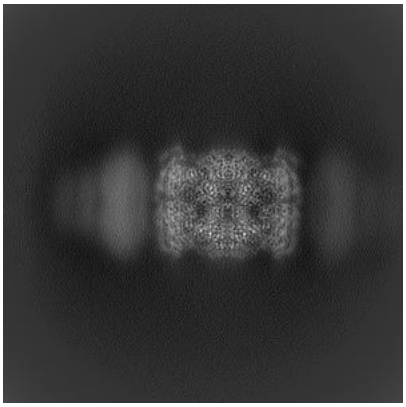
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

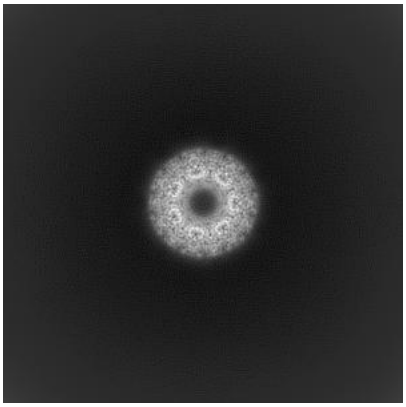
6.1.1 Primary map



X



Y

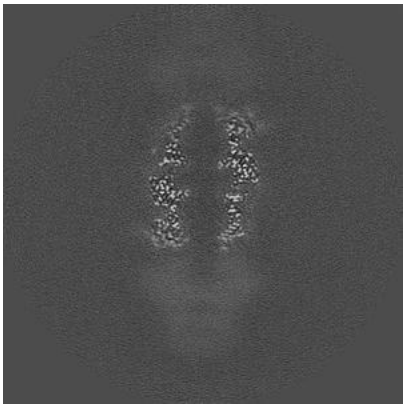


Z

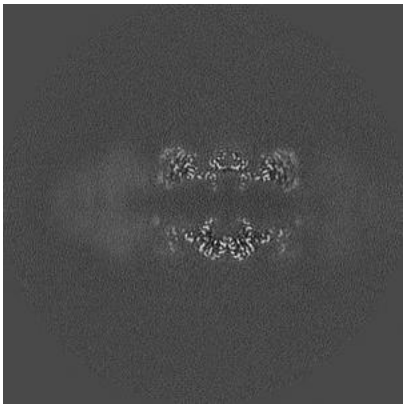
The images above show the map projected in three orthogonal directions.

6.2 Central slices

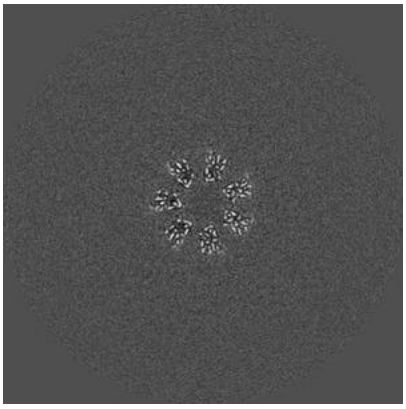
6.2.1 Primary map



X Index: 176



Y Index: 176

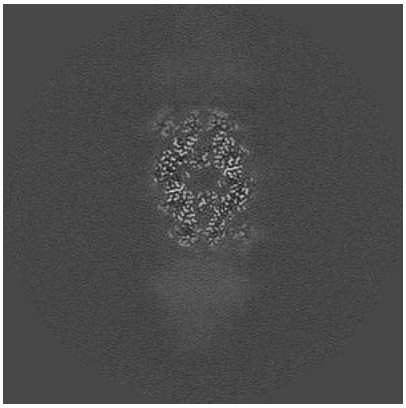


Z Index: 176

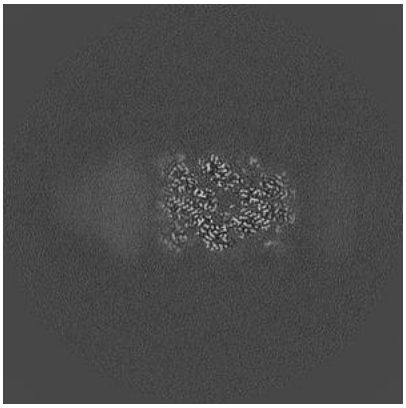
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

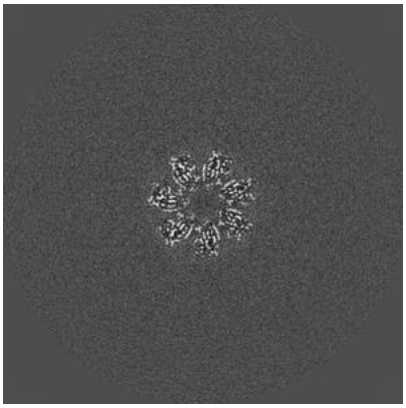
6.3.1 Primary map



X Index: 155



Y Index: 152



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

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0236. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

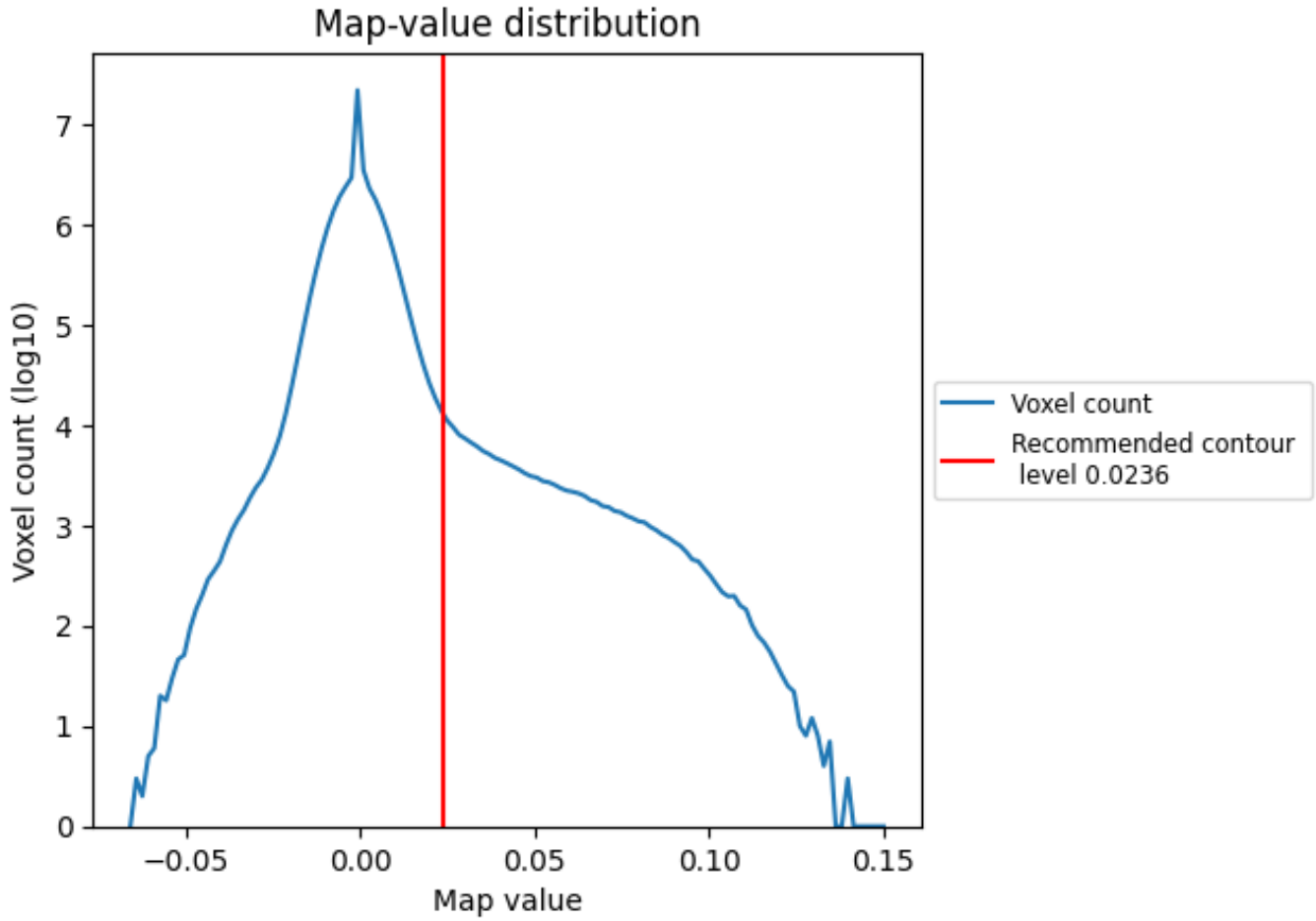
6.5 Mask visualisation (i)

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

7 Map analysis

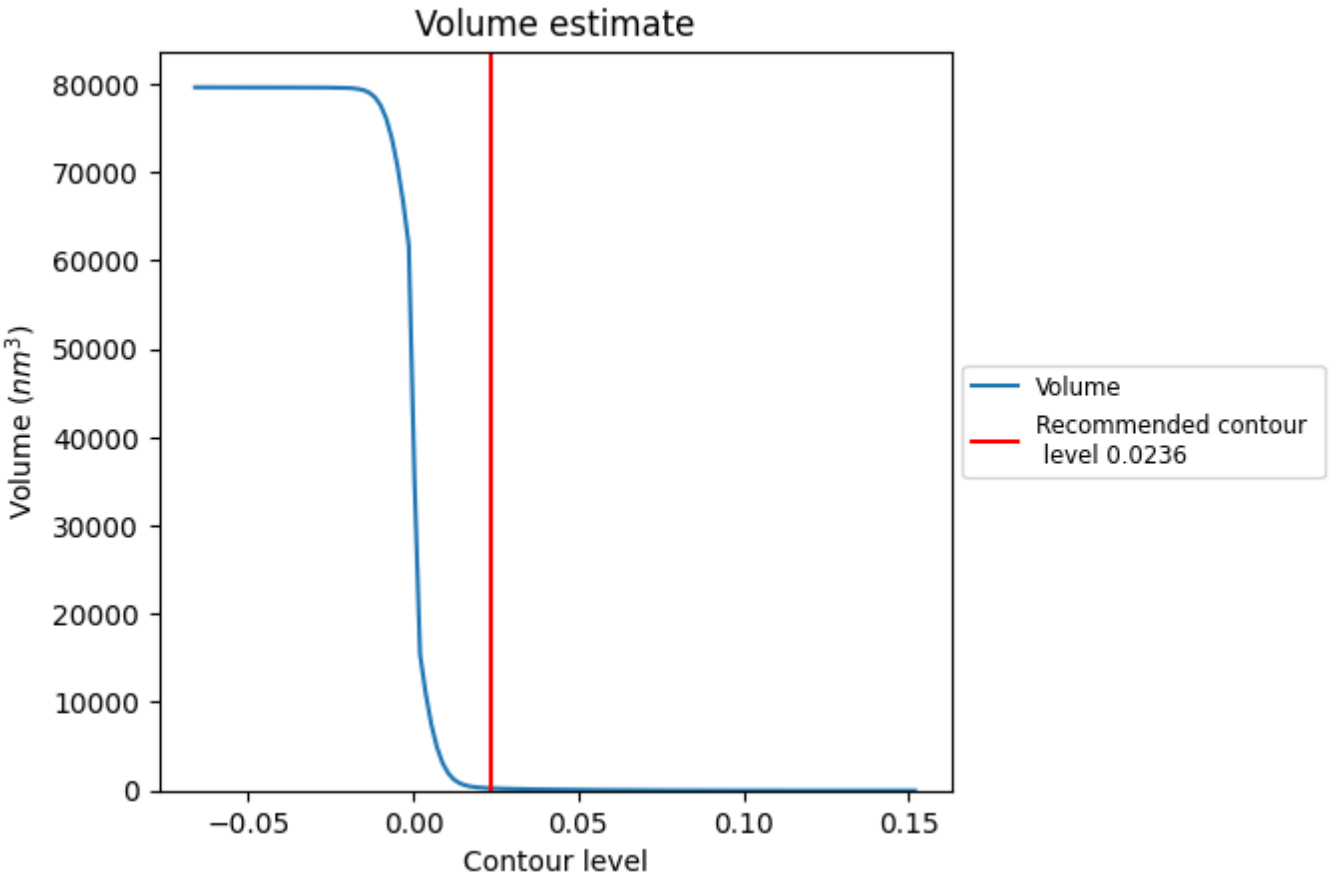
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

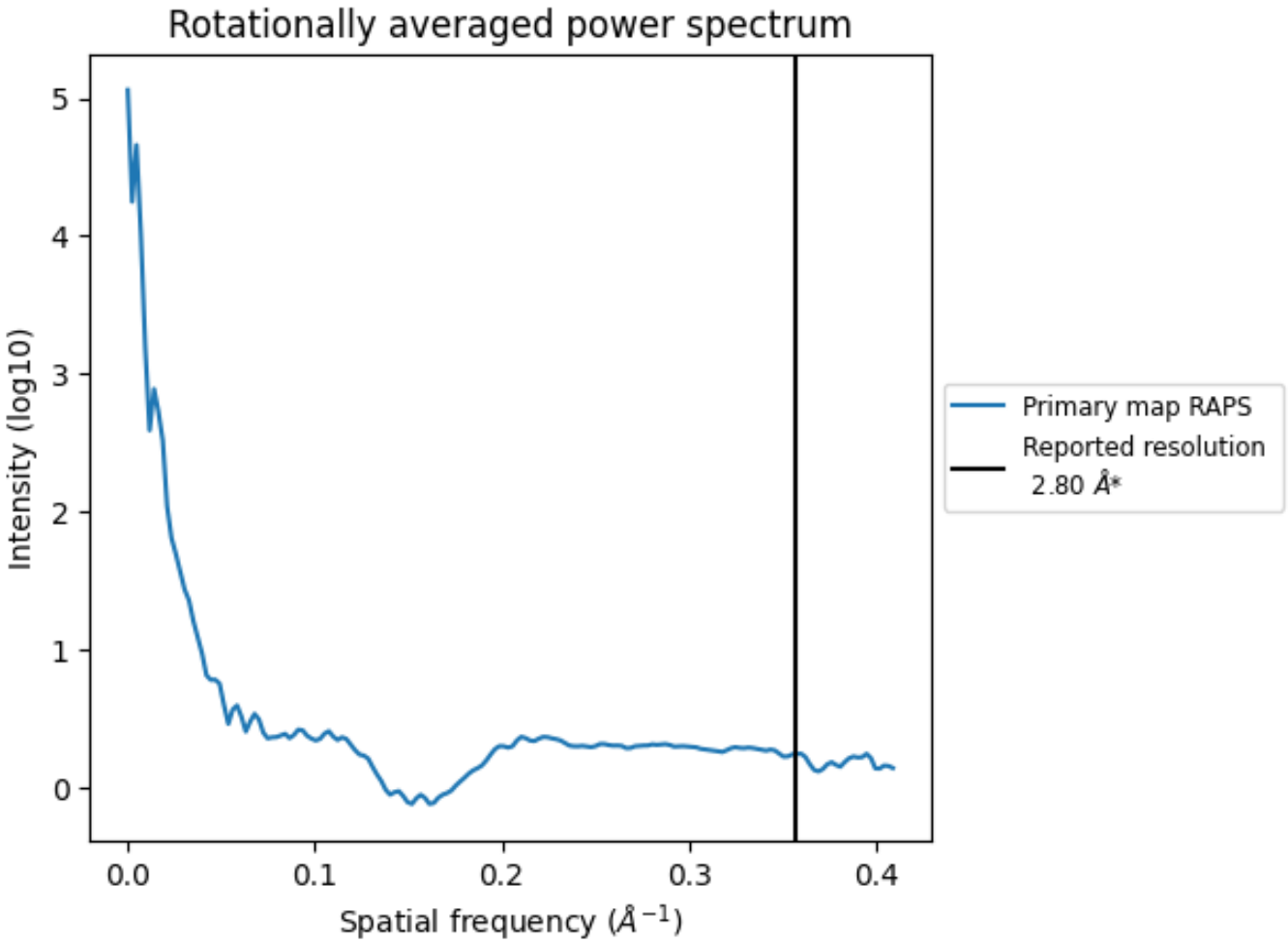
7.2 Volume estimate



The volume at the recommended contour level is 258 nm^3; this corresponds to an approximate mass of 233 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 $Å^{-1}$

8 Fourier-Shell correlation (i)

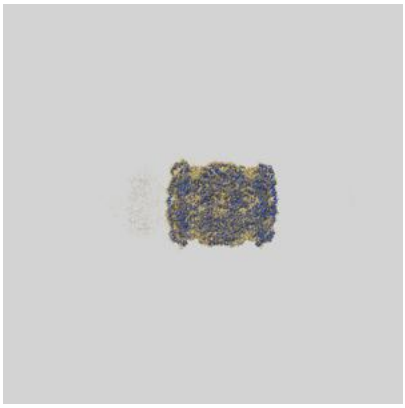
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

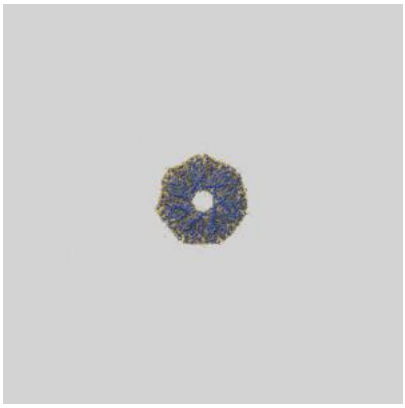
This section contains information regarding the fit between EMDB map EMD-13695 and PDB model 7PXA. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay

X



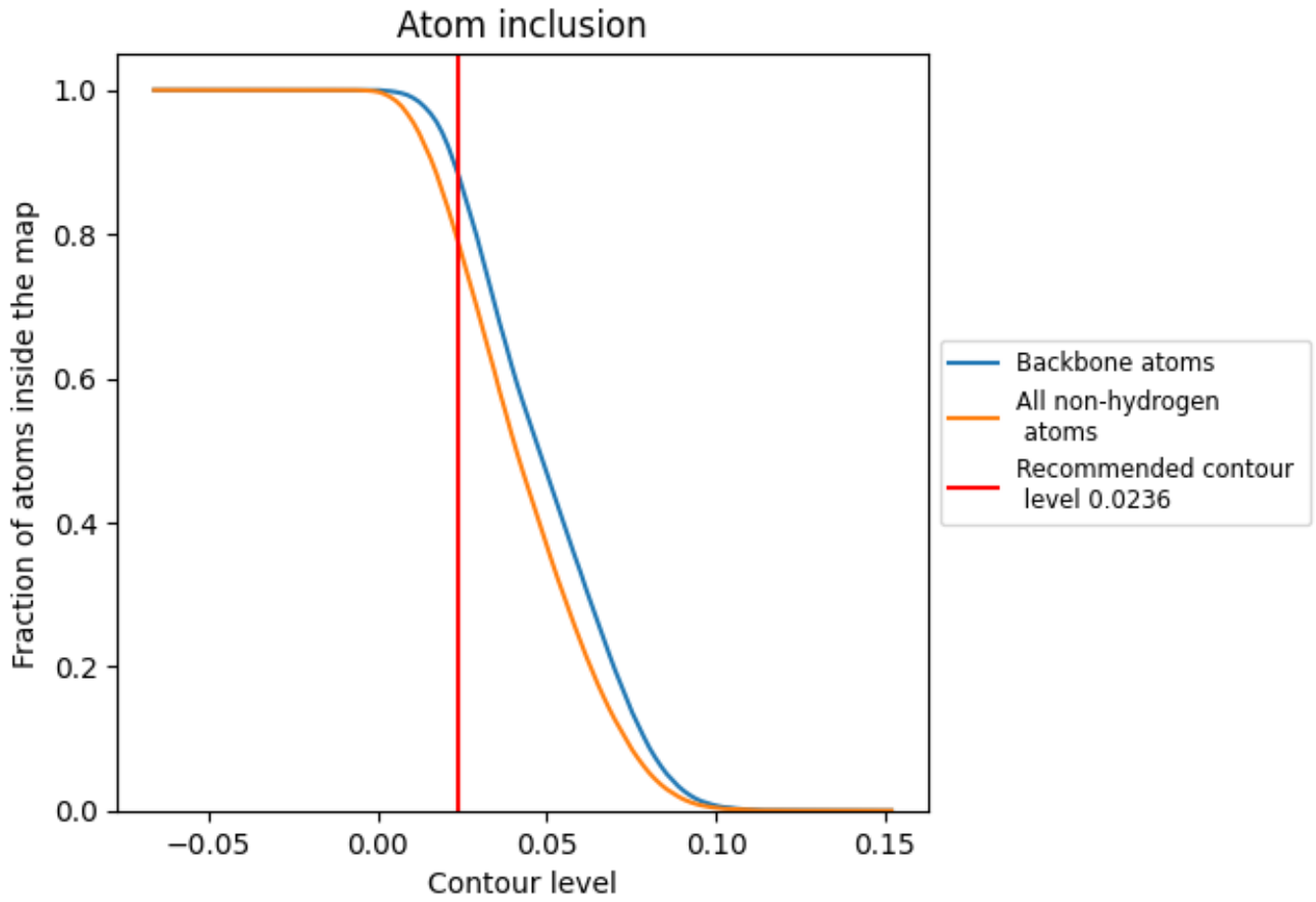
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0236 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 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.