Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 10:15 PM EDT

PDB ID	:	5VFO / pdb_00005vfo
EMDB ID	:	EMD-8662
Title	:	Nucleotide-driven Triple-state Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome
Authors	:	Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y.
Deposited on	:	2017-04-08
Resolution	:	3.50 Å(reported)

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 ⓘ 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 ⓘ) were used in the production of this report:

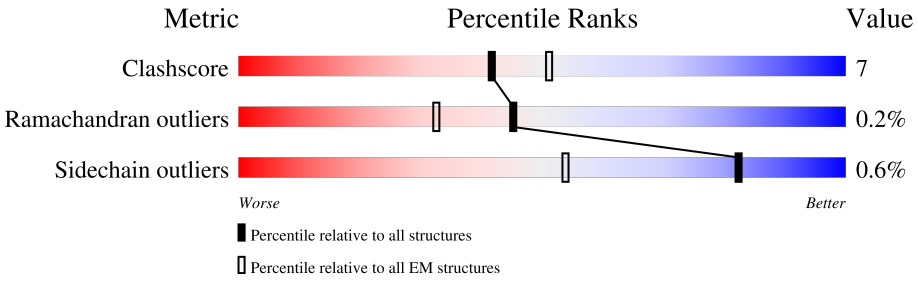
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	G	240	38% 82% 17%
1	g	240	50% 85% 15%
2	H	232	27% 81% 18%
2	h	232	46% 77% 23%
3	I	250	41% 76% 22%
3	i	250	56% 76% 22%
4	J	243	45% 80% 18%
4	j	243	60% 82% 16%

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Mol	Chain	Length	Quality of chain
5	K	234	41% 76% 20%
5	k	234	47% 79% 18%
6	L	238	28% 79% 20%
6	l	238	45% 86% 14%
7	M	245	39% 72% 26%
7	m	245	47% 80% 18%
8	N	191	24% 86% 13%
8	n	191	28% 87% 13%
9	O	220	29% 81% 18%
9	o	220	37% 81% 18%
10	P	204	19% 87% 13%
10	p	204	29% 83% 17%
11	Q	199	32% 79% 21%
11	q	199	31% 84% 15%
12	R	201	20% 80% 20%
12	r	201	25% 84% 16%
13	S	213	30% 85% 15%
13	s	213	26% 85% 15%
14	T	215	24% 89% 11%
14	t	215	24% 88% 12%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 47288 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		
1	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	230	Total	C	N	O	S	0	0
			1688	1070	284	329	5		
2	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
3	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
4	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	228	Total	C	N	O	S	0	0
			1729	1086	284	349	10		
5	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
6	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
7	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
8	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
9	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
11	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
12	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
13	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

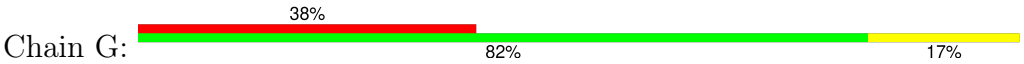
Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
14	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

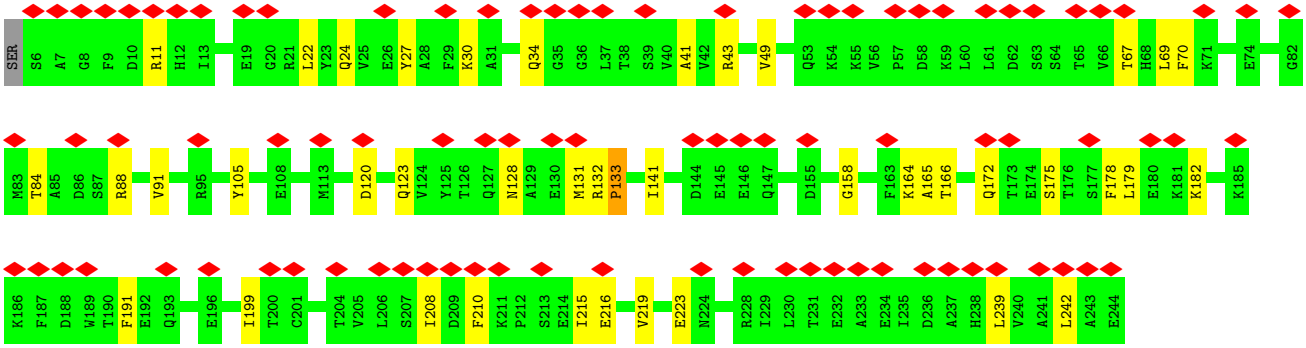
3 Residue-property plots (i)

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-6

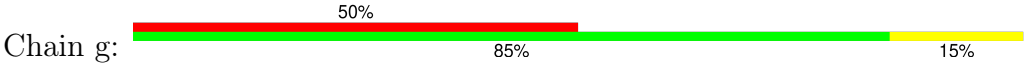
Chain G:

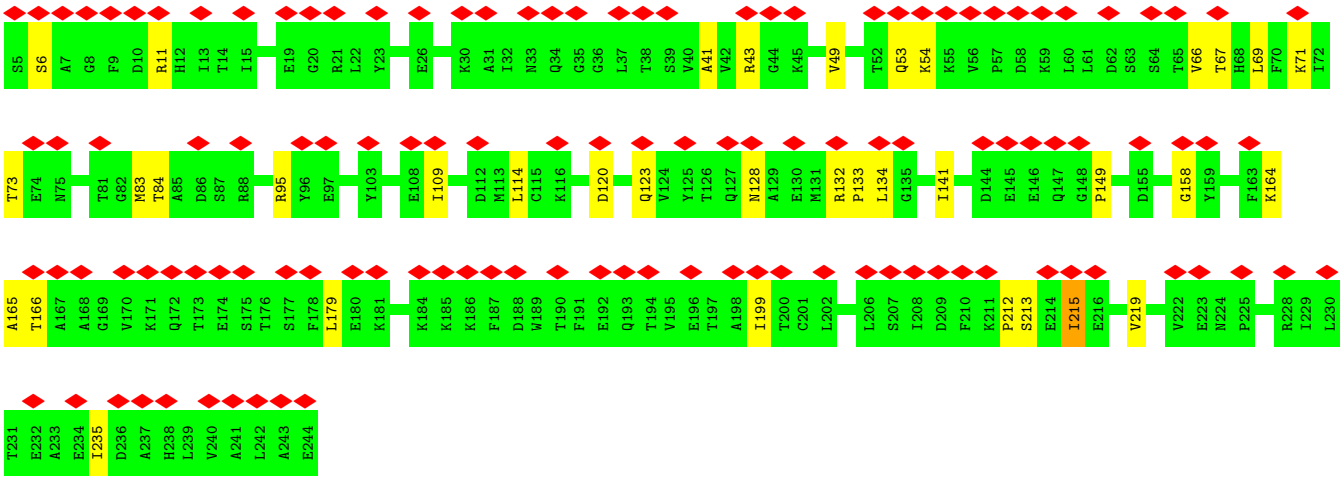




• Molecule 1: Proteasome subunit alpha type-6

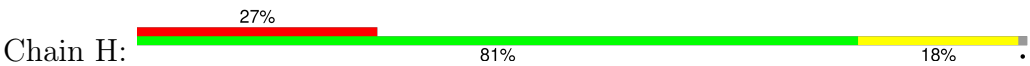
Chain g:

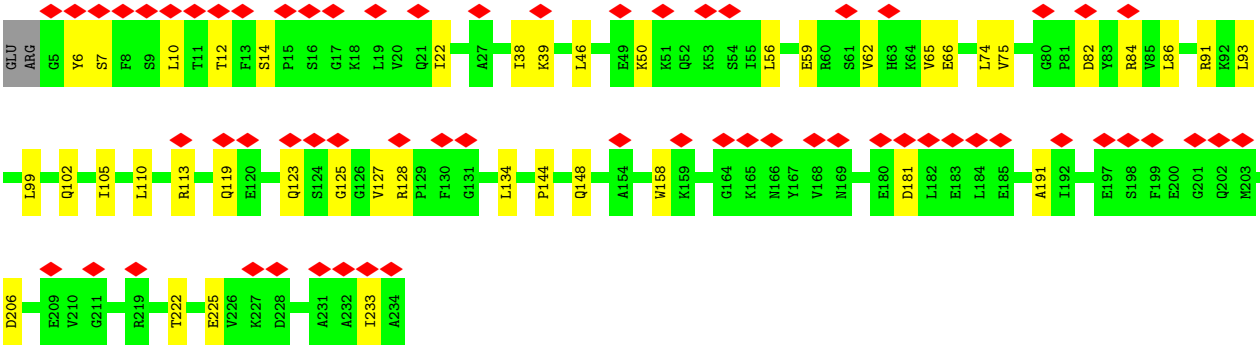




• Molecule 2: Proteasome subunit alpha type-2

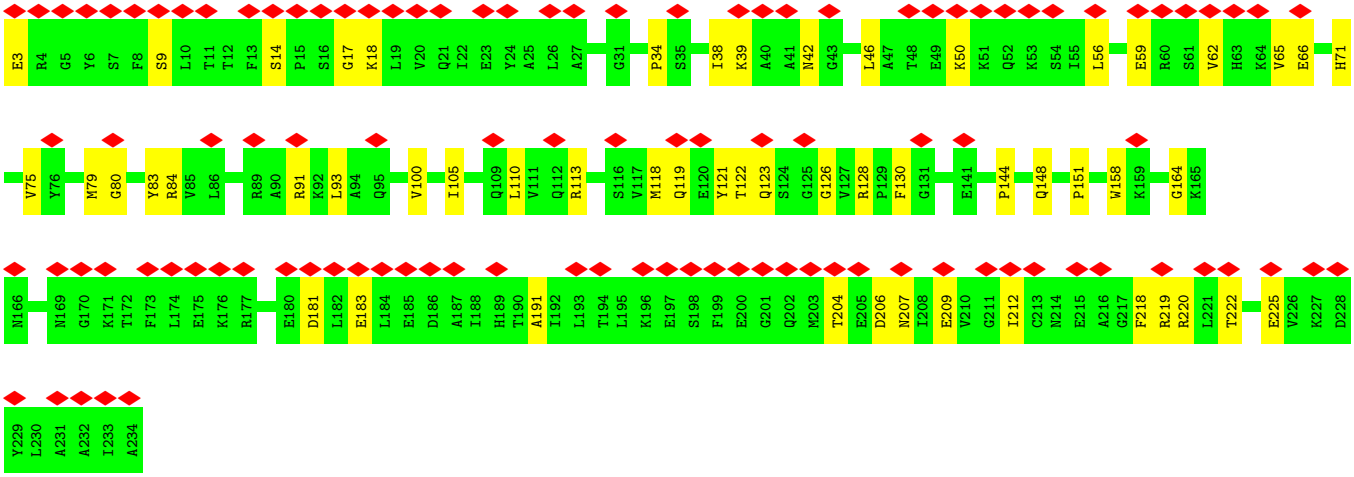
Chain H:





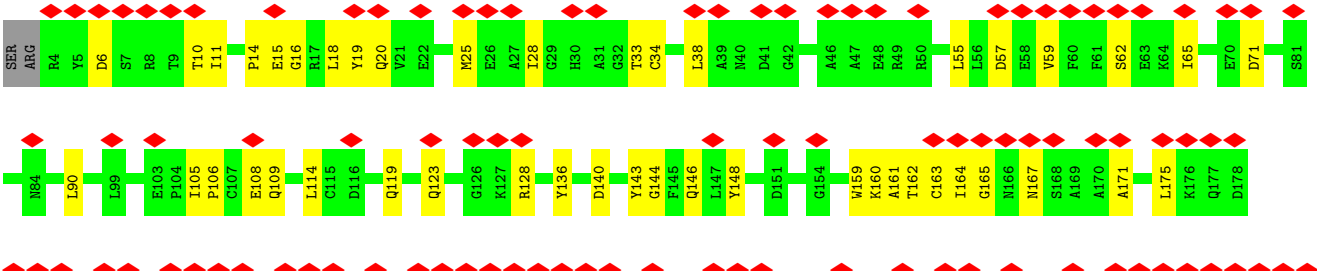
• Molecule 2: Proteasome subunit alpha type-2

Chain h:



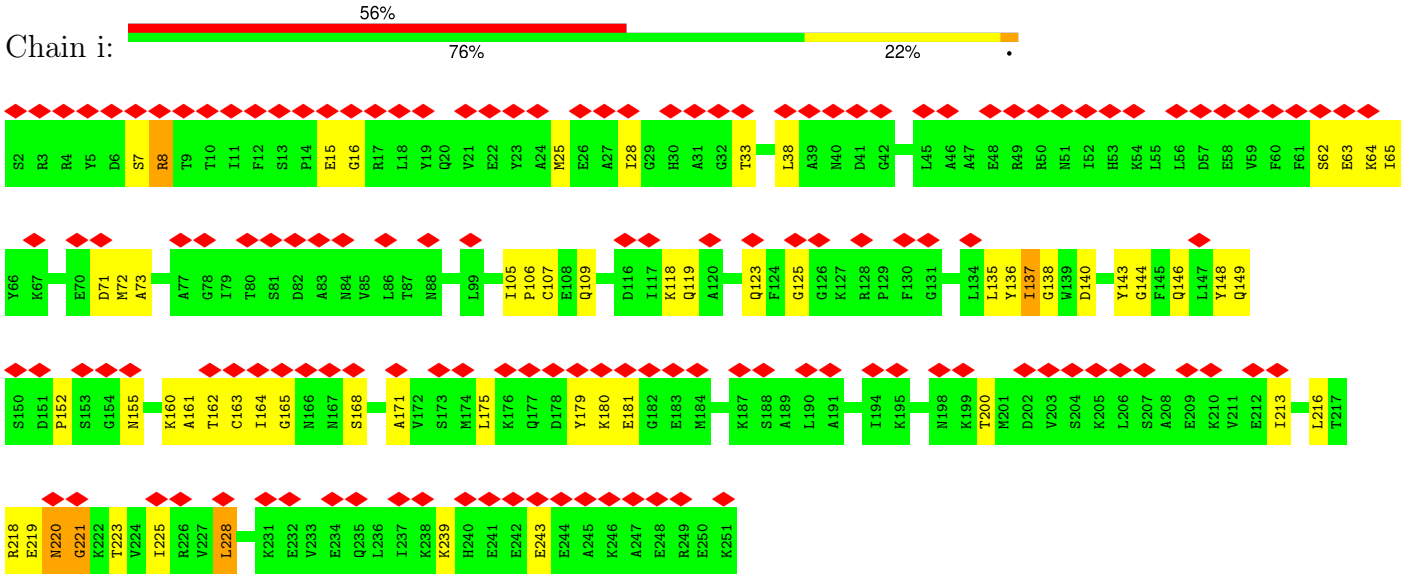
• Molecule 3: Proteasome subunit alpha type-4

Chain I:



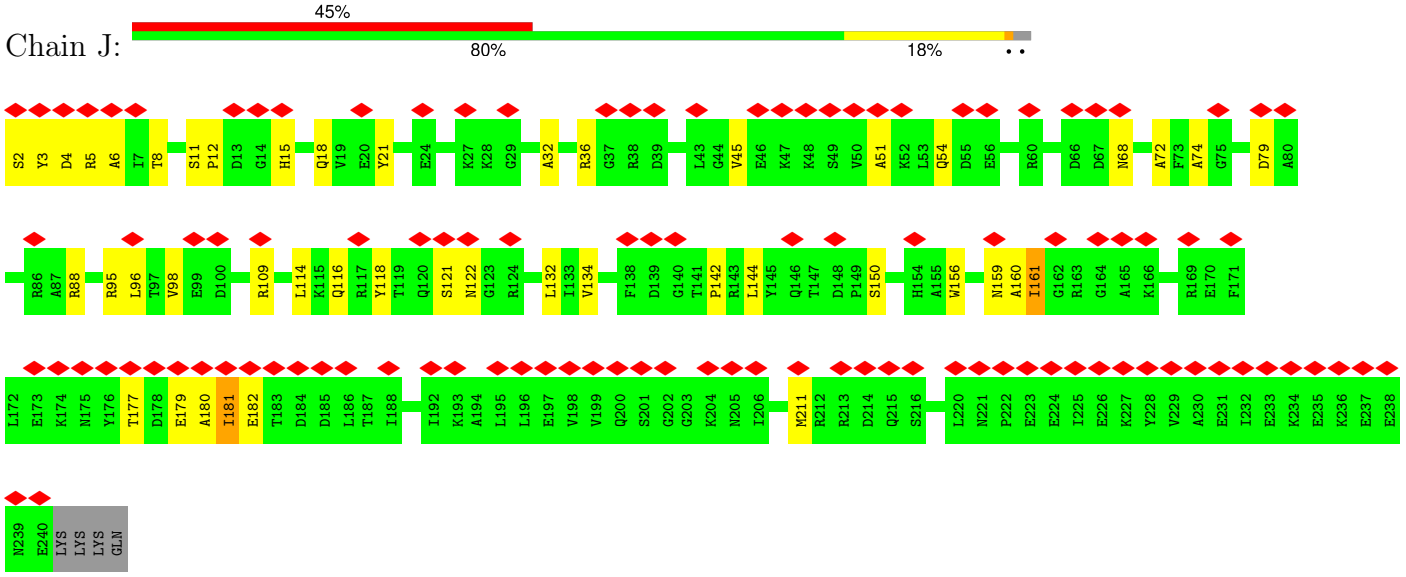
• Molecule 3: Proteasome subunit alpha type-4

Chain i:



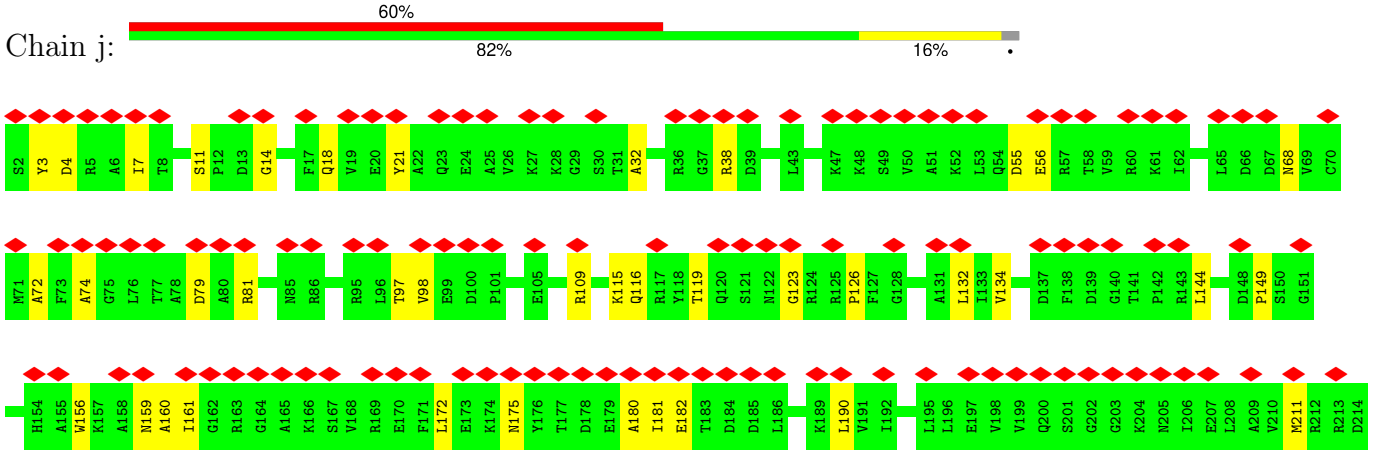
• Molecule 4: Proteasome subunit alpha type-7

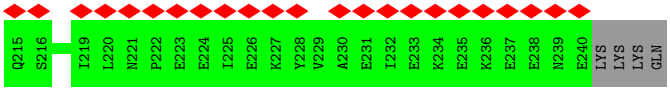
Chain J:



• Molecule 4: Proteasome subunit alpha type-7

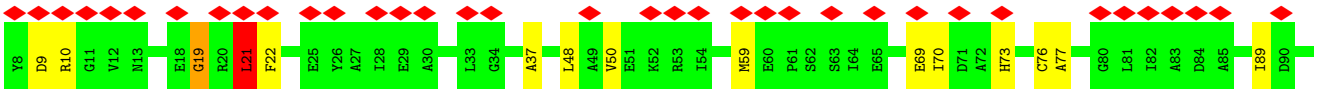
Chain j:

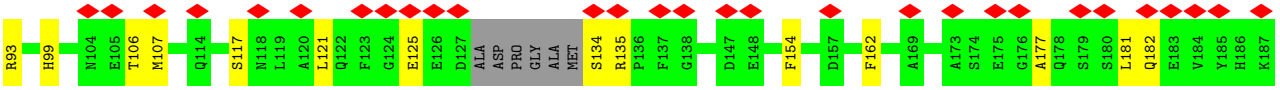


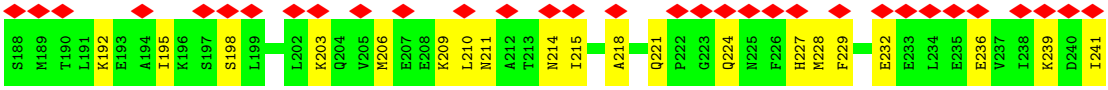


• Molecule 5: Proteasome subunit alpha type-5

Chain K:

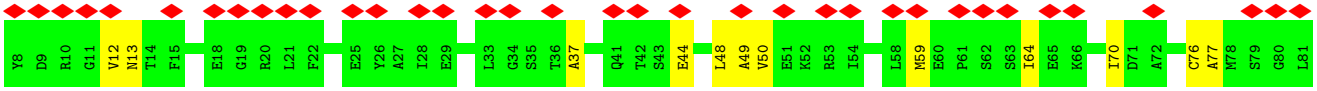


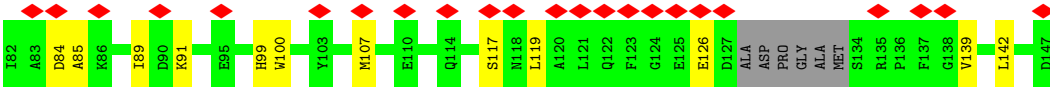


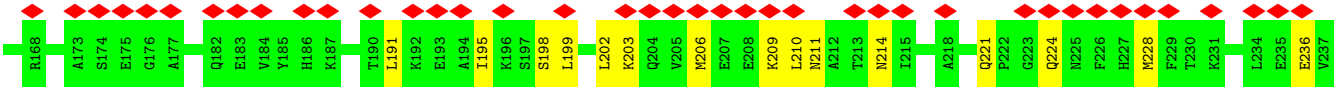


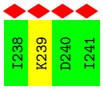
• Molecule 5: Proteasome subunit alpha type-5

Chain k:



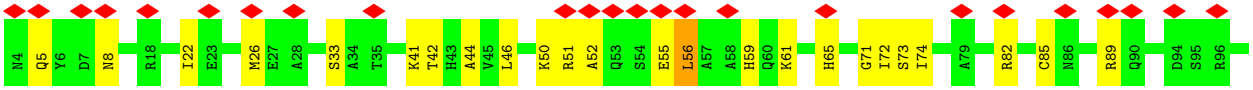


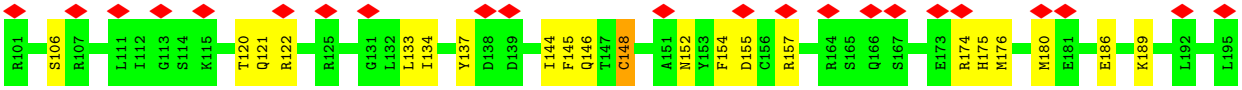


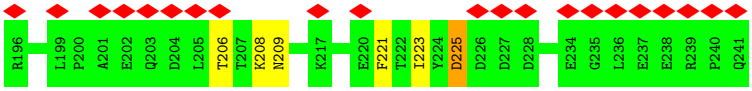


• Molecule 6: Proteasome subunit alpha type-1

Chain L:

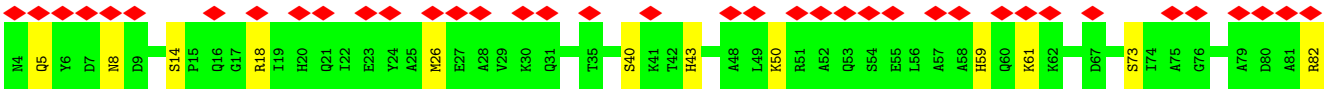


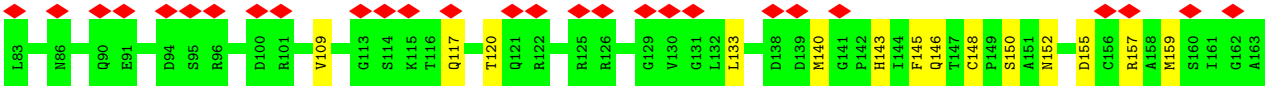


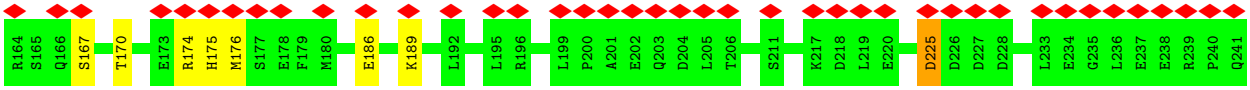


• Molecule 6: Proteasome subunit alpha type-1

Chain l:

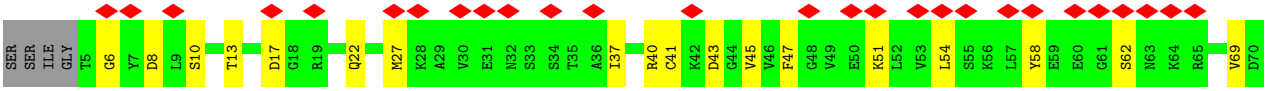


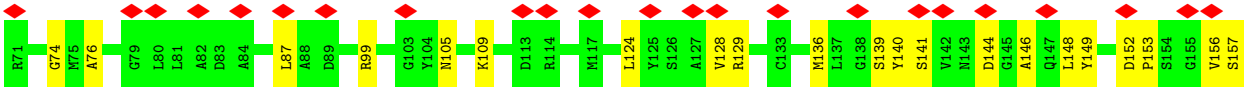


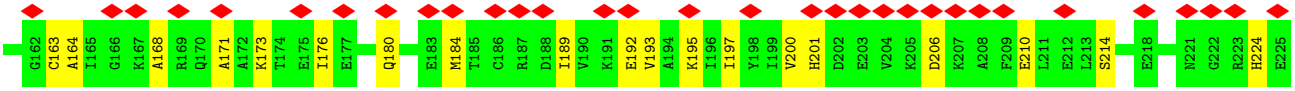


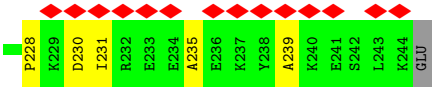
• Molecule 7: Proteasome subunit alpha type-3

Chain M:



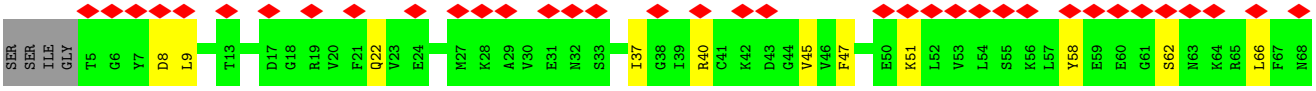


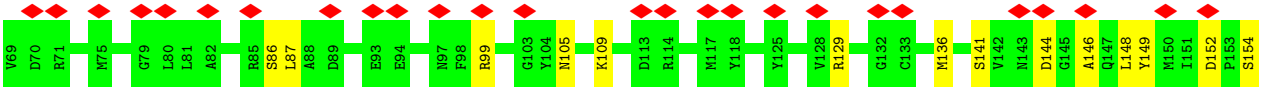


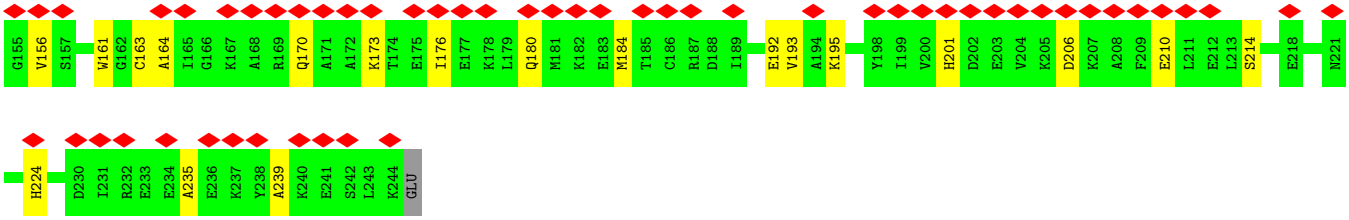


• Molecule 7: Proteasome subunit alpha type-3

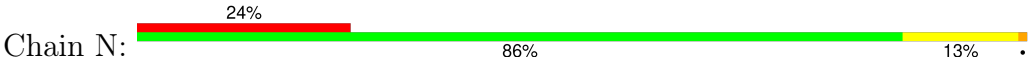
Chain m:

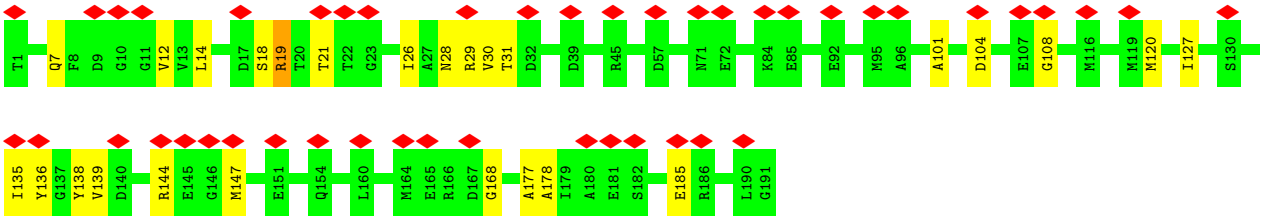




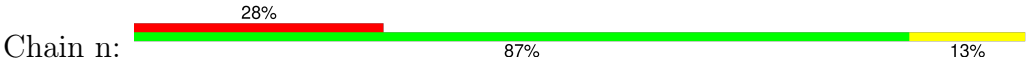


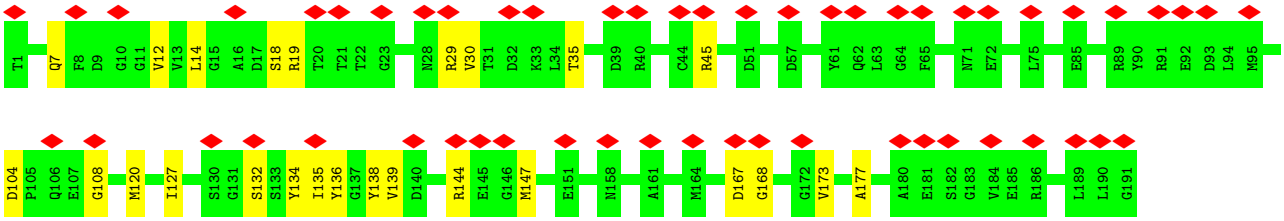
• Molecule 8: Proteasome subunit beta type-6



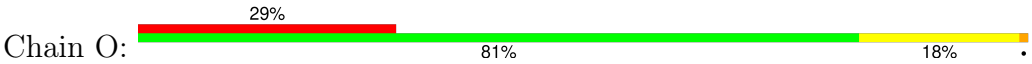


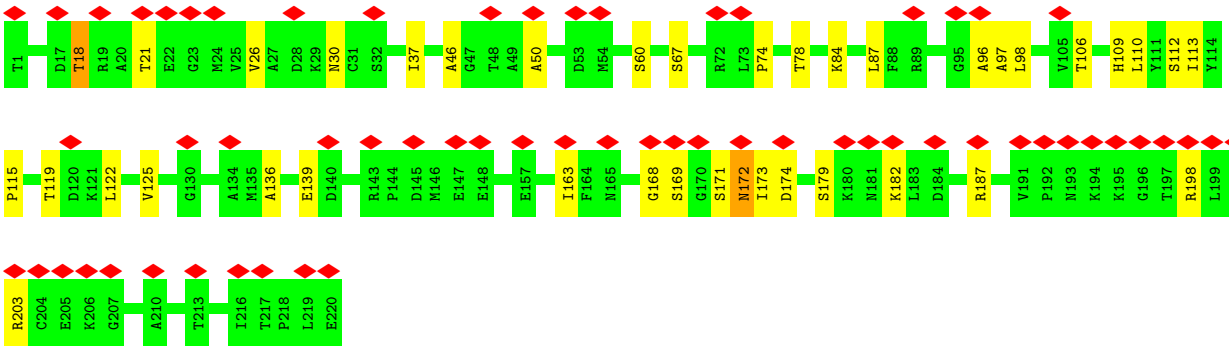
• Molecule 8: Proteasome subunit beta type-6



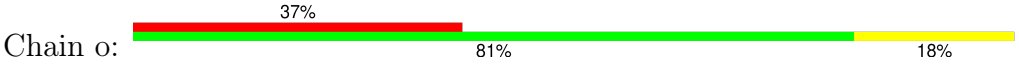


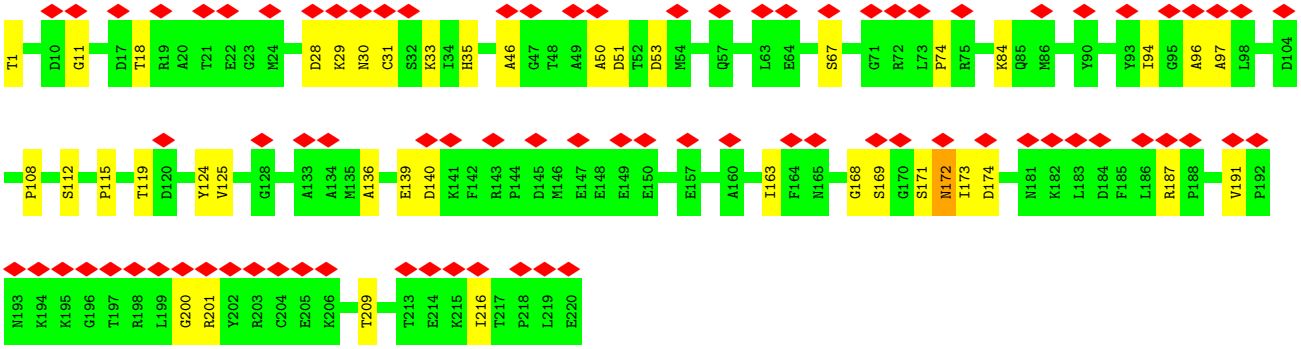
• Molecule 9: Proteasome subunit beta type-7



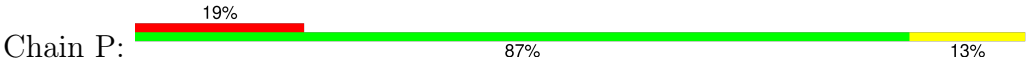


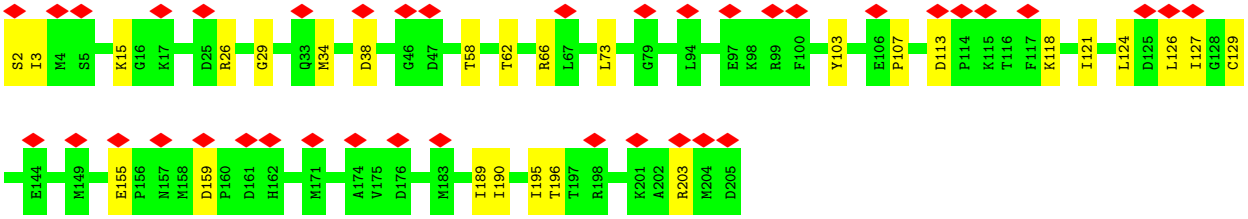
• Molecule 9: Proteasome subunit beta type-7



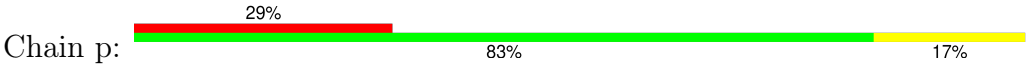


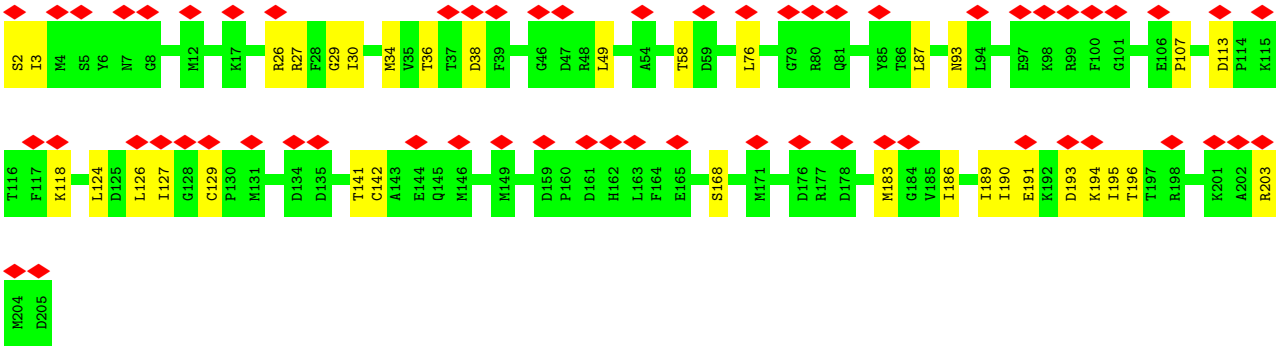
• Molecule 10: Proteasome subunit beta type-3



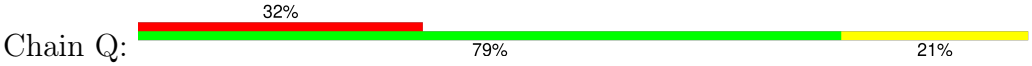


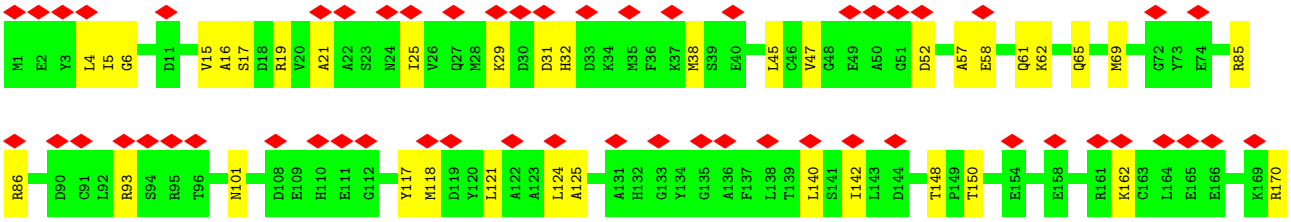
• Molecule 10: Proteasome subunit beta type-3

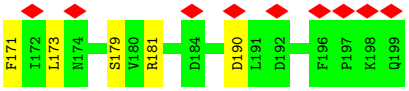




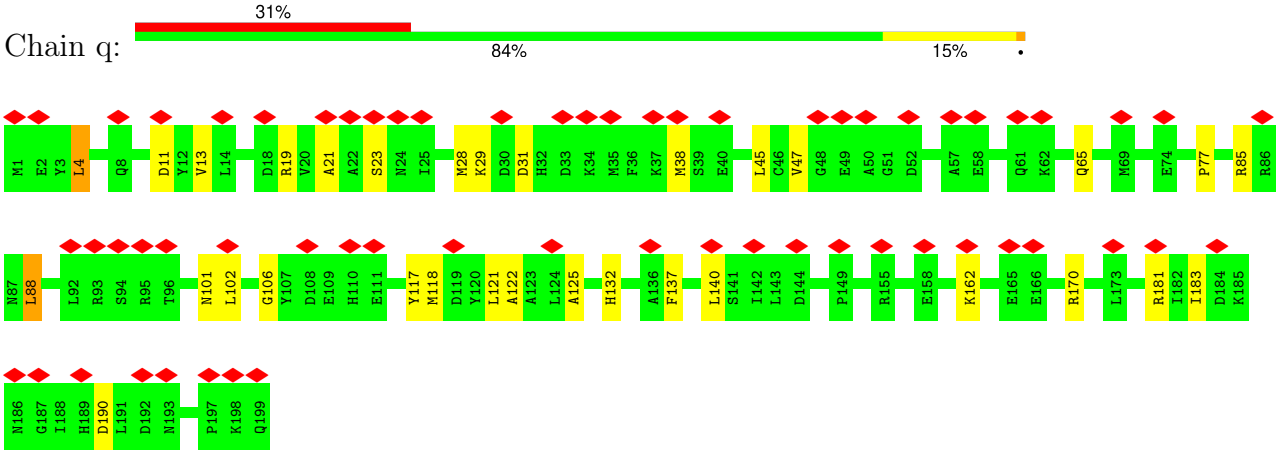
• Molecule 11: Proteasome subunit beta type-2



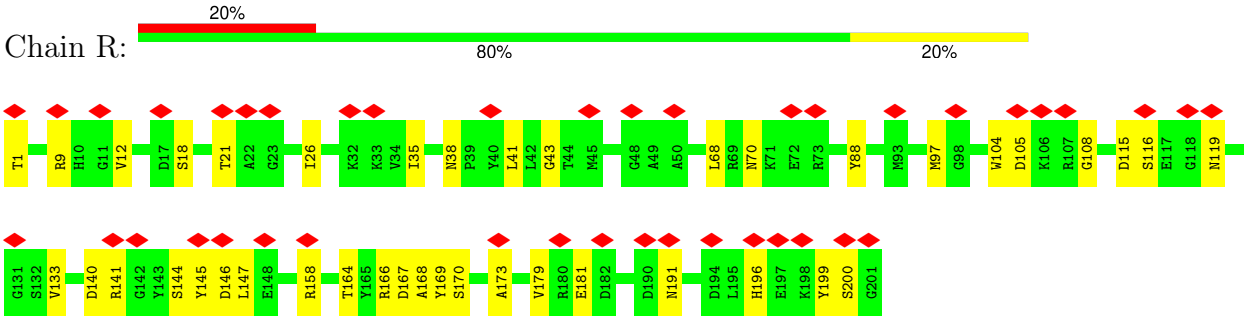




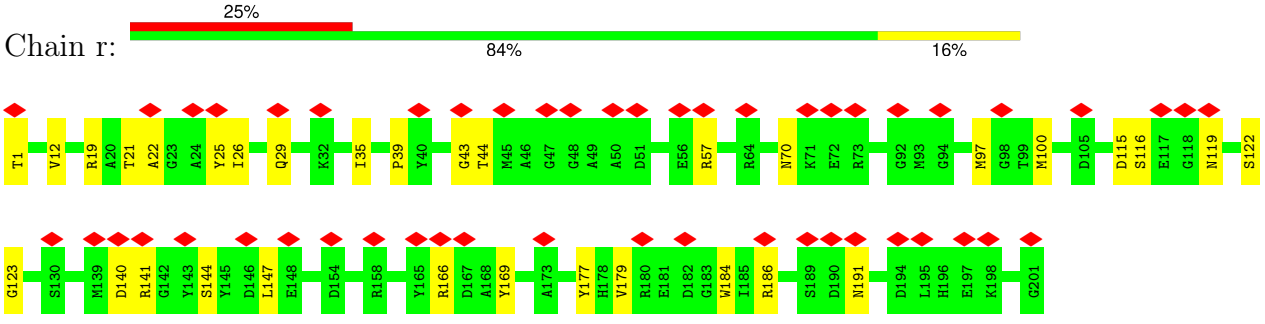
• Molecule 11: Proteasome subunit beta type-2



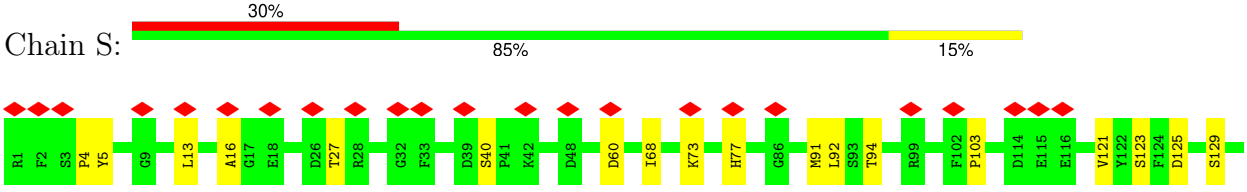
• Molecule 12: Proteasome subunit beta type-5

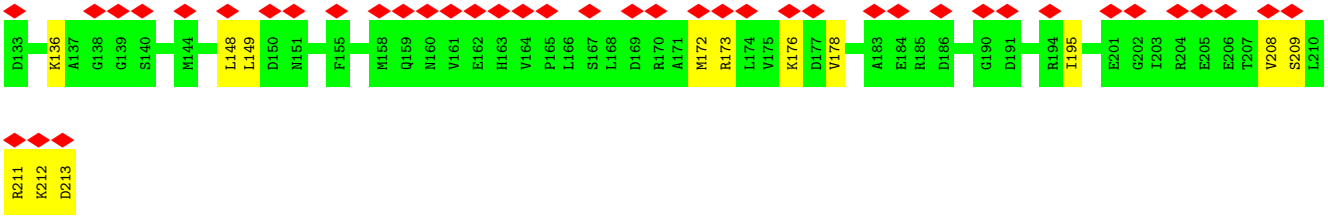


• Molecule 12: Proteasome subunit beta type-5

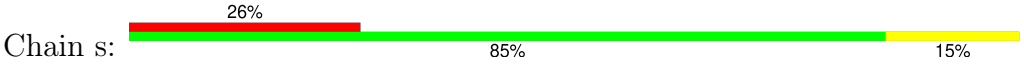


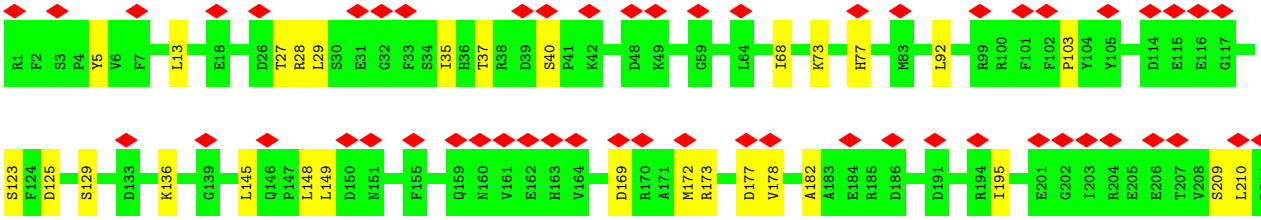
• Molecule 13: Proteasome subunit beta type-1



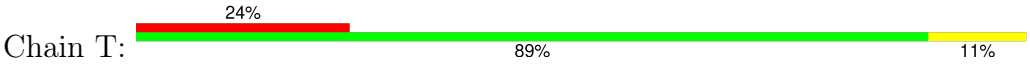


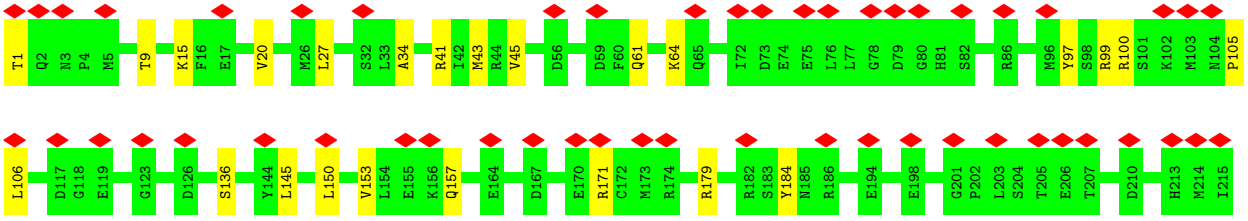
• Molecule 13: Proteasome subunit beta type-1



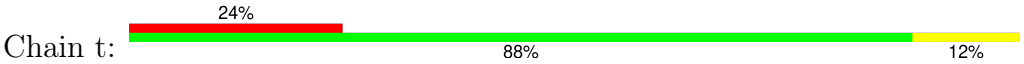


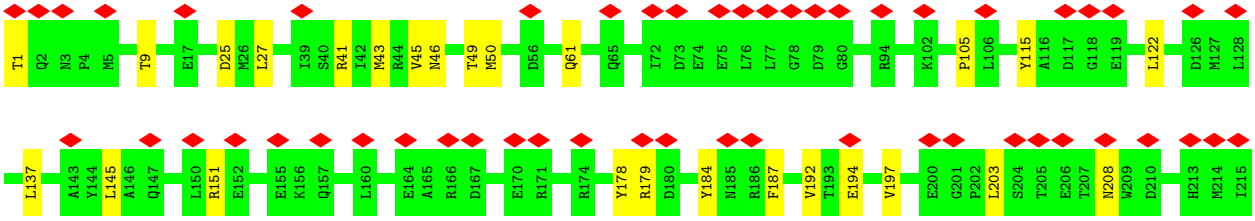
• Molecule 14: Proteasome subunit beta type-4





• Molecule 14: Proteasome subunit beta type-4





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	228086	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75, 0.75, 0.75	Depositor

5 Model quality

5.1 Standard geometry

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	G	0.40	0/1853	0.72	2/2515 (0.1%)
1	g	0.38	0/1859	0.65	1/2523 (0.0%)
2	H	0.40	0/1723	0.68	3/2346 (0.1%)
2	h	0.37	0/1743	0.61	2/2372 (0.1%)
3	I	0.42	0/1925	0.79	4/2606 (0.2%)
3	i	0.38	0/1942	0.70	2/2628 (0.1%)
4	J	0.40	0/1728	0.74	4/2358 (0.2%)
4	j	0.35	0/1728	0.59	0/2358
5	K	0.40	0/1755	0.79	4/2375 (0.2%)
5	k	0.36	0/1747	0.59	0/2364
6	L	0.43	0/1885	0.66	3/2552 (0.1%)
6	l	0.39	0/1885	0.63	2/2552 (0.1%)
7	M	0.41	0/1891	0.73	2/2552 (0.1%)
7	m	0.38	0/1891	0.64	0/2552
8	N	0.41	0/1454	0.63	0/1967
8	n	0.39	0/1454	0.60	0/1967
9	O	0.40	0/1670	0.61	2/2265 (0.1%)
9	o	0.38	0/1670	0.64	2/2265 (0.1%)
10	P	0.41	0/1614	0.54	0/2177
10	p	0.39	0/1614	0.56	2/2177 (0.1%)
11	Q	0.44	0/1603	0.65	0/2174
11	q	0.44	0/1603	0.67	0/2174
12	R	0.41	0/1579	0.55	0/2134
12	r	0.40	0/1579	0.54	0/2134
13	S	0.39	0/1671	0.56	0/2253
13	s	0.39	0/1671	0.56	0/2253
14	T	0.40	0/1700	0.58	0/2305
14	t	0.40	0/1700	0.59	0/2305
All	All	0.40	0/48137	0.64	35/65203 (0.1%)

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
3	I	0	3
3	i	0	2
4	j	0	1
5	K	0	4
9	O	0	2
9	o	0	1
All	All	0	13

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	21	LEU	CA-C-N	9.74	139.23	121.70
5	K	21	LEU	C-N-CA	9.74	139.23	121.70
1	G	223	GLU	N-CA-C	-9.38	103.93	114.62
7	M	6	GLY	CA-C-N	9.01	137.91	121.70
7	M	6	GLY	C-N-CA	9.01	137.91	121.70
5	K	19	GLY	CA-C-N	7.95	136.01	121.70
5	K	19	GLY	C-N-CA	7.95	136.01	121.70
3	I	15	GLU	N-CA-CB	-7.23	106.87	114.10
2	H	22	ILE	N-CA-C	-6.92	106.31	112.12
1	g	134	LEU	N-CA-C	6.56	119.22	111.02
2	h	79	MET	CA-C-N	6.42	125.81	121.13
2	h	79	MET	C-N-CA	6.42	125.81	121.13
4	J	182	GLU	CA-C-N	6.33	133.09	121.70
4	J	182	GLU	C-N-CA	6.33	133.09	121.70
6	L	148	CYS	N-CA-C	-6.30	102.55	108.22
2	H	7	SER	CA-C-N	6.14	132.75	121.70
2	H	7	SER	C-N-CA	6.14	132.75	121.70
9	o	171	SER	CA-C-N	6.04	133.07	121.54
9	o	171	SER	C-N-CA	6.04	133.07	121.54
9	O	172	ASN	CA-C-N	5.93	132.64	121.97
9	O	172	ASN	C-N-CA	5.93	132.64	121.97
4	J	181	ILE	CA-C-N	5.88	132.29	121.70
4	J	181	ILE	C-N-CA	5.88	132.29	121.70
6	l	225	ASP	CA-C-N	5.77	132.55	121.54
6	l	225	ASP	C-N-CA	5.77	132.55	121.54
3	I	15	GLU	CA-C-N	5.72	132.00	121.70
3	I	15	GLU	C-N-CA	5.72	132.00	121.70
3	I	15	GLU	N-CA-C	5.50	121.87	113.51
3	i	8	ARG	CA-C-N	5.39	131.84	121.54
3	i	8	ARG	C-N-CA	5.39	131.84	121.54
6	L	225	ASP	CA-C-N	5.26	131.58	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	225	ASP	C-N-CA	5.26	131.58	121.54
10	p	30	ILE	CA-C-N	5.25	128.70	120.82
10	p	30	ILE	C-N-CA	5.25	128.70	120.82
1	G	133	PRO	CA-C-O	-5.21	117.45	121.31

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	10	THR	Peptide
3	I	220	ASN	Peptide
3	I	221	GLY	Peptide
5	K	121	LEU	Peptide
5	K	19	GLY	Peptide
5	K	232	GLU	Peptide
5	K	9	ASP	Peptide
9	O	171	SER	Peptide
9	O	172	ASN	Peptide
3	i	220	ASN	Peptide
3	i	221	GLY	Peptide
4	j	180	ALA	Peptide
9	o	172	ASN	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	G	1820	0	1791	26	0
1	g	1826	0	1796	21	0
2	H	1688	0	1575	26	0
2	h	1708	0	1594	32	0
3	I	1895	0	1833	35	0
3	i	1912	0	1851	35	0
4	J	1704	0	1517	29	0
4	j	1704	0	1517	27	0
5	K	1729	0	1680	28	0
5	k	1722	0	1673	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	1850	0	1822	32	0
6	l	1850	0	1822	22	0
7	M	1856	0	1814	41	0
7	m	1856	0	1814	31	0
8	N	1430	0	1398	18	0
8	n	1430	0	1398	15	0
9	O	1643	0	1644	26	0
9	o	1643	0	1644	25	0
10	P	1585	0	1598	18	0
10	p	1585	0	1598	22	0
11	Q	1570	0	1547	30	0
11	q	1570	0	1547	20	0
12	R	1548	0	1499	28	0
12	r	1548	0	1499	22	0
13	S	1641	0	1618	17	0
13	s	1641	0	1618	17	0
14	T	1667	0	1628	15	0
14	t	1667	0	1628	18	0
All	All	47288	0	45963	615	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 7.

All (615) 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)
3:I:119:GLN:HE21	3:I:123:GLN:HE22	1.24	0.82
13:s:27:THR:HB	13:s:40:SER:H	1.53	0.73
13:S:27:THR:HB	13:S:40:SER:H	1.56	0.70
3:I:38:LEU:HG	3:I:160:LYS:HB3	1.75	0.68
5:k:91:LYS:HE2	5:k:119:LEU:HD11	1.75	0.67
6:l:186:GLU:HA	6:l:189:LYS:HG2	1.76	0.66
7:M:8:ASP:O	7:M:22:GLN:NE2	2.29	0.66
2:H:50:LYS:NZ	2:H:62:VAL:O	2.29	0.66
10:P:26:ARG:HH21	10:P:38:ASP:HA	1.60	0.65
11:Q:118:MET:HE1	11:Q:124:LEU:HD23	1.77	0.65
8:N:178:ALA:HB3	8:N:185:GLU:HB2	1.79	0.64
4:j:72:ALA:HB3	4:j:132:LEU:HB2	1.80	0.64
1:G:123:GLN:NE2	2:H:82:ASP:OD1	2.31	0.64
5:K:209:LYS:O	5:K:214:ASN:ND2	2.30	0.64
7:m:141:SER:HB3	7:m:144:ASP:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:157:ARG:HD2	6:l:176:MET:HE3	1.81	0.62
3:i:155:ASN:HA	4:j:81:ARG:HH22	1.63	0.62
11:Q:57:ALA:O	11:Q:61:GLN:HB3	2.00	0.62
4:j:109:ARG:NH2	12:r:70:ASN:OD1	2.32	0.62
7:M:40:ARG:NH1	7:M:146:ALA:O	2.33	0.62
11:Q:117:TYR:HB3	11:Q:125:ALA:HB3	1.82	0.62
13:S:123:SER:HB3	13:S:136:LYS:HG3	1.82	0.62
3:i:38:LEU:HG	3:i:160:LYS:HB3	1.82	0.62
3:i:106:PRO:HD2	3:i:109:GLN:HE21	1.65	0.62
14:t:9:THR:O	14:t:41:ARG:NH2	2.32	0.62
6:L:120:THR:O	7:M:129:ARG:NH1	2.31	0.61
9:o:96:ALA:H	9:o:115:PRO:HB3	1.65	0.61
1:g:41:ALA:HB3	1:g:166:THR:HB	1.83	0.61
3:I:25:MET:HA	3:I:28:ILE:HD12	1.82	0.61
7:m:47:PHE:HB2	7:m:214:SER:HB3	1.81	0.61
2:h:66:GLU:OE2	2:h:91:ARG:NH2	2.34	0.61
5:k:77:ALA:HB3	5:k:142:LEU:HB2	1.83	0.61
6:L:206:THR:H	6:L:209:ASN:HD21	1.49	0.60
7:m:214:SER:OG	7:m:224:HIS:NE2	2.33	0.60
6:L:157:ARG:HD2	6:L:176:MET:HE3	1.83	0.60
13:s:148:LEU:HD23	13:s:178:VAL:HG12	1.82	0.60
5:K:125:GLU:HG3	5:K:134:SER:HB2	1.83	0.60
7:M:141:SER:HB3	7:M:144:ASP:HB2	1.83	0.60
11:q:181:ARG:NH1	11:q:190:ASP:OD1	2.34	0.60
9:O:174:ASP:OD2	9:O:187:ARG:NH1	2.35	0.60
11:q:38:MET:O	11:q:65:GLN:NE2	2.35	0.60
7:M:27:MET:HA	7:M:153:PRO:HG2	1.82	0.60
5:k:76:CYS:SG	5:k:77:ALA:N	2.75	0.60
7:m:37:ILE:HD11	7:m:193:VAL:HG13	1.83	0.60
9:O:201:ARG:HD3	9:O:203:ARG:HE	1.67	0.60
9:o:174:ASP:OD2	9:o:187:ARG:NH1	2.35	0.60
6:L:41:LYS:NZ	6:L:180:MET:O	2.34	0.59
3:i:16:GLY:N	4:j:21:TYR:OH	2.35	0.59
7:m:8:ASP:O	7:m:22:GLN:NE2	2.33	0.59
14:t:43:MET:HE3	14:t:45:VAL:HG22	1.84	0.59
8:N:19:ARG:NH2	8:N:168:GLY:O	2.34	0.59
6:L:186:GLU:HA	6:L:189:LYS:HG2	1.83	0.59
13:S:148:LEU:HD23	13:S:178:VAL:HG12	1.85	0.59
7:m:40:ARG:NH1	7:m:146:ALA:O	2.35	0.59
14:T:9:THR:O	14:T:41:ARG:NH2	2.36	0.59
11:Q:142:ILE:HG21	12:r:141:ARG:HH21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:158:GLY:O	2:h:84:ARG:NH2	2.36	0.59
9:o:18:THR:HB	9:o:31:CYS:H	1.67	0.59
5:K:76:CYS:SG	5:K:77:ALA:N	2.76	0.59
14:t:1:THR:N	14:t:105:PRO:O	2.32	0.59
6:l:5:GLN:O	6:l:8:ASN:ND2	2.36	0.59
7:m:163:CYS:SG	7:m:164:ALA:N	2.76	0.58
4:J:74:ALA:HB2	4:J:161:ILE:HD13	1.85	0.58
3:I:143:TYR:HB2	3:I:146:GLN:HE21	1.68	0.58
11:q:21:ALA:HB3	11:q:29:LYS:HB3	1.85	0.58
1:G:67:THR:HG22	1:G:69:LEU:H	1.69	0.58
5:k:99:HIS:HB2	5:k:107:MET:HE3	1.85	0.58
8:n:144:ARG:H	8:n:147:MET:HE3	1.66	0.58
8:N:29:ARG:NH1	9:O:139:GLU:OE1	2.36	0.58
10:P:189:ILE:HG23	10:P:196:THR:HB	1.84	0.58
7:M:47:PHE:HB2	7:M:214:SER:HB3	1.84	0.58
7:m:192:GLU:HA	7:m:195:LYS:HE3	1.85	0.58
4:J:177:THR:OG1	4:J:179:GLU:O	2.21	0.58
5:K:117:SER:HB3	6:L:82:ARG:HH22	1.69	0.58
7:M:235:ALA:O	7:M:239:ALA:N	2.36	0.58
11:Q:21:ALA:HB3	11:Q:29:LYS:HB3	1.86	0.58
2:h:50:LYS:NZ	2:h:62:VAL:O	2.36	0.58
7:m:99:ARG:NH2	7:m:105:ASN:OD1	2.36	0.58
3:I:106:PRO:HD2	3:I:109:GLN:HE21	1.69	0.57
5:k:48:LEU:HD21	5:k:77:ALA:HB2	1.85	0.57
2:H:12:THR:OG1	3:I:20:GLN:NE2	2.37	0.57
3:i:143:TYR:HB2	3:i:146:GLN:HE21	1.69	0.57
1:g:165:ALA:HB1	1:g:179:LEU:HD13	1.86	0.57
1:g:165:ALA:HB3	2:h:56:LEU:HD22	1.85	0.57
7:M:99:ARG:NH2	7:M:105:ASN:OD1	2.38	0.57
13:S:173:ARG:NH1	9:o:200:GLY:O	2.38	0.57
4:J:116:GLN:NE2	4:J:150:SER:O	2.37	0.57
8:n:127:ILE:HB	8:n:132:SER:HB2	1.87	0.57
9:O:163:ILE:HA	9:O:168:GLY:HA3	1.87	0.57
8:N:21:THR:HG22	8:N:26:ILE:HG13	1.87	0.57
6:l:120:THR:O	7:m:129:ARG:NH1	2.32	0.57
4:J:109:ARG:NH2	12:R:70:ASN:OD1	2.37	0.56
10:p:58:THR:OG1	11:q:121:LEU:O	2.19	0.56
7:M:180:GLN:HB3	7:M:184:MET:HE3	1.87	0.56
12:R:1:THR:N	12:R:169:TYR:O	2.38	0.56
11:q:19:ARG:HH21	11:q:31:ASP:HB2	1.69	0.56
5:K:221:GLN:HB2	5:K:224:GLN:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:171:PHE:HB3	11:Q:173:LEU:H	1.69	0.56
14:T:27:LEU:HD22	14:T:184:TYR:HB2	1.86	0.56
10:p:113:ASP:HB2	10:p:118:LYS:HB3	1.87	0.56
7:M:37:ILE:HD11	7:M:193:VAL:HG13	1.88	0.56
7:M:214:SER:OG	7:M:224:HIS:NE2	2.39	0.56
9:O:21:THR:HG22	9:O:26:VAL:HA	1.88	0.56
2:h:42:ASN:ND2	2:h:183:GLU:OE1	2.38	0.56
3:i:123:GLN:NE2	4:j:79:ASP:OD1	2.39	0.56
4:j:7:ILE:HG22	4:j:18:GLN:HG3	1.86	0.56
6:l:50:LYS:HE2	6:l:61:LYS:HA	1.88	0.56
11:Q:19:ARG:HH21	11:Q:31:ASP:HB2	1.71	0.56
2:h:222:THR:OG1	2:h:225:GLU:OE1	2.22	0.56
11:Q:170:ARG:NE	12:r:140:ASP:OD2	2.35	0.56
5:k:37:ALA:HB2	5:k:50:VAL:HG23	1.88	0.56
3:I:34:CYS:H	3:I:164:ILE:HG13	1.71	0.56
3:I:171:ALA:HB2	3:I:200:THR:HG21	1.87	0.56
6:L:5:GLN:O	6:L:8:ASN:ND2	2.38	0.56
9:O:96:ALA:H	9:O:115:PRO:HB3	1.71	0.56
9:O:179:SER:HG	9:O:182:LYS:H	1.52	0.56
14:T:99:ARG:HG2	14:T:106:LEU:HG	1.87	0.56
2:h:71:HIS:HA	2:h:218:PHE:H	1.71	0.56
6:l:109:VAL:HG21	6:l:145:PHE:HD2	1.71	0.56
8:n:29:ARG:NH1	9:o:139:GLU:OE1	2.38	0.55
5:K:203:LYS:HA	5:K:206:MET:HG2	1.89	0.55
6:L:72:ILE:HG22	6:L:134:ILE:HG12	1.88	0.55
1:G:70:PHE:HD2	1:G:91:VAL:HG21	1.71	0.55
4:J:95:ARG:HG3	11:Q:62:LYS:HE3	1.89	0.55
7:M:51:LYS:O	7:M:210:GLU:N	2.38	0.55
10:p:189:ILE:HG23	10:p:196:THR:HB	1.88	0.55
14:t:145:LEU:HB3	14:t:179:ARG:HH21	1.72	0.55
7:m:51:LYS:O	7:m:210:GLU:N	2.39	0.55
9:o:35:HIS:NE2	9:o:53:ASP:OD1	2.40	0.55
2:H:6:TYR:HE2	2:H:14:SER:HA	1.69	0.55
9:O:198:ARG:NH1	10:P:155:GLU:OE2	2.35	0.55
2:H:39:LYS:HE2	2:H:144:PRO:HG2	1.87	0.55
13:s:169:ASP:OD2	13:s:173:ARG:NH2	2.39	0.55
5:K:48:LEU:HB3	5:K:218:ALA:HB3	1.89	0.55
14:T:43:MET:HE3	14:T:45:VAL:HG22	1.88	0.55
3:i:171:ALA:HB2	3:i:200:THR:HG21	1.89	0.55
3:i:216:LEU:HD12	3:i:225:ILE:HG12	1.89	0.54
13:S:16:ALA:HB2	13:S:121:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:o:163:ILE:HA	9:o:168:GLY:HA3	1.88	0.54
12:r:1:THR:N	12:r:169:TYR:O	2.40	0.54
12:r:19:ARG:HH21	12:r:29:GLN:HE22	1.55	0.54
6:L:33:SER:HA	6:L:51:ARG:HH22	1.73	0.54
5:k:100:TRP:O	12:r:57:ARG:NH2	2.41	0.54
12:r:12:VAL:HB	12:r:179:VAL:HB	1.88	0.54
3:I:123:GLN:NE2	4:J:79:ASP:OD1	2.40	0.54
10:p:36:THR:OG1	10:p:38:ASP:OD1	2.24	0.54
1:G:165:ALA:HB1	1:G:179:LEU:HD13	1.89	0.54
10:P:107:PRO:HG2	10:P:124:LEU:HB2	1.90	0.54
2:H:119:GLN:NE2	2:H:123:GLN:OE1	2.41	0.54
3:i:136:TYR:HB2	3:i:148:TYR:HB2	1.89	0.54
7:M:192:GLU:HA	7:M:195:LYS:HE3	1.90	0.54
9:o:50:ALA:HB2	10:p:129:CYS:HB2	1.90	0.54
4:J:72:ALA:HB3	4:J:132:LEU:HB2	1.89	0.53
11:q:117:TYR:HB3	11:q:125:ALA:HB3	1.88	0.53
14:T:171:ARG:NH2	9:o:140:ASP:OD1	2.40	0.53
5:k:228:MET:SD	5:k:228:MET:N	2.81	0.53
14:t:27:LEU:HD22	14:t:184:TYR:HB2	1.90	0.53
1:G:11:ARG:O	1:G:24:GLN:NE2	2.37	0.53
5:K:99:HIS:HB2	5:K:107:MET:HE3	1.90	0.53
2:H:10:LEU:O	3:I:128:ARG:NH2	2.42	0.53
4:J:11:SER:OG	4:J:15:HIS:N	2.41	0.53
7:m:40:ARG:HA	7:m:45:VAL:HA	1.91	0.53
7:m:180:GLN:HB3	7:m:184:MET:HE3	1.90	0.53
7:m:235:ALA:O	7:m:239:ALA:N	2.39	0.53
3:I:62:SER:OG	3:I:65:ILE:O	2.27	0.53
10:P:2:SER:OG	10:P:3:ILE:N	2.41	0.53
3:i:140:ASP:OD1	3:i:144:GLY:N	2.41	0.53
12:r:97:MET:O	12:r:116:SER:N	2.41	0.53
13:s:73:LYS:O	13:s:77:HIS:ND1	2.33	0.53
3:I:245:ALA:HA	3:I:248:GLU:HG2	1.91	0.53
5:k:203:LYS:HA	5:k:206:MET:HG2	1.90	0.53
7:m:40:ARG:HE	7:m:161:TRP:CD1	2.27	0.53
7:m:173:LYS:HA	7:m:176:ILE:HB	1.90	0.53
12:r:177:TYR:OH	12:r:186:ARG:NH2	2.42	0.53
2:h:181:ASP:OD1	2:h:181:ASP:N	2.40	0.52
11:Q:38:MET:O	11:Q:65:GLN:NE2	2.42	0.52
12:R:140:ASP:OD2	11:q:170:ARG:NE	2.41	0.52
13:S:4:PRO:O	14:T:100:ARG:NH2	2.43	0.52
5:k:117:SER:HB3	6:l:82:ARG:HH22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:n:18:SER:HB2	8:n:30:VAL:HA	1.91	0.52
1:G:131:MET:HE3	7:M:124:LEU:HD13	1.90	0.52
3:I:136:TYR:HB2	3:I:148:TYR:HB2	1.90	0.52
9:O:163:ILE:HG12	9:O:169:SER:H	1.74	0.52
1:G:27:TYR:HA	1:G:30:LYS:HZ3	1.75	0.52
2:H:74:LEU:HD21	2:H:134:LEU:HD22	1.92	0.52
3:I:33:THR:OG1	3:I:167:ASN:ND2	2.42	0.52
10:P:66:ARG:HH21	11:Q:86:ARG:HH22	1.56	0.52
9:o:163:ILE:HG12	9:o:169:SER:H	1.74	0.52
2:H:59:GLU:HG2	2:H:206:ASP:HB3	1.90	0.52
2:H:148:GLN:OE1	2:H:158:TRP:NE1	2.42	0.52
3:i:218:ARG:NH1	3:i:223:THR:OG1	2.40	0.52
4:j:74:ALA:HB2	4:j:161:ILE:HD13	1.92	0.52
7:M:173:LYS:HA	7:M:176:ILE:HB	1.91	0.52
2:h:39:LYS:HE2	2:h:144:PRO:HG2	1.91	0.52
8:n:35:THR:OG1	8:n:45:ARG:NH2	2.43	0.52
3:I:38:LEU:HB2	3:I:180:LYS:HE2	1.92	0.52
3:I:71:ASP:OD1	3:I:71:ASP:N	2.40	0.52
9:o:30:ASN:OD1	9:o:187:ARG:NH2	2.43	0.52
3:I:140:ASP:OD1	3:I:144:GLY:N	2.40	0.51
7:m:9:LEU:O	7:m:22:GLN:NE2	2.43	0.51
10:p:107:PRO:HG2	10:p:124:LEU:HB2	1.92	0.51
13:s:28:ARG:NH2	13:s:213:ASP:O	2.43	0.51
3:I:161:ALA:HB1	3:I:175:LEU:HD13	1.90	0.51
7:M:76:ALA:HB3	7:M:136:MET:HB2	1.92	0.51
1:g:53:GLN:HA	1:g:215:ILE:HA	1.92	0.51
1:g:120:ASP:OD1	2:h:84:ARG:NH1	2.43	0.51
2:h:212:ILE:HD11	2:h:219:ARG:HD3	1.92	0.51
9:o:209:THR:HG21	10:p:168:SER:HB3	1.92	0.51
10:P:29:GLY:HA3	10:P:34:MET:HA	1.92	0.51
10:P:58:THR:OG1	11:Q:121:LEU:O	2.17	0.51
5:k:85:ALA:HB2	5:k:139:VAL:HG21	1.92	0.51
6:l:26:MET:HE1	6:l:148:CYS:HB2	1.92	0.51
8:N:14:LEU:HD11	8:N:101:ALA:HB3	1.92	0.51
9:O:112:SER:HB3	9:O:125:VAL:HG11	1.93	0.51
14:T:27:LEU:HD11	14:T:34:ALA:HB1	1.91	0.51
2:h:9:SER:OG	2:h:123:GLN:O	2.21	0.51
7:m:152:ASP:OD1	7:m:156:VAL:N	2.43	0.51
5:K:37:ALA:HB2	5:K:50:VAL:HG23	1.92	0.51
5:k:209:LYS:O	5:k:214:ASN:ND2	2.43	0.51
4:j:134:VAL:HG22	4:j:144:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:68:ASN:HA	4:J:211:MET:HE1	1.93	0.51
1:g:67:THR:HG22	1:g:69:LEU:H	1.75	0.51
8:n:7:GLN:HA	8:n:12:VAL:HA	1.91	0.51
7:m:136:MET:HE3	7:m:148:LEU:HD11	1.91	0.51
11:q:88:LEU:HB3	11:q:122:ALA:HB2	1.93	0.51
5:k:157:ASP:OD2	5:k:159:SER:OG	2.27	0.51
3:i:62:SER:OG	3:i:65:ILE:O	2.29	0.50
12:r:22:ALA:N	12:r:25:TYR:O	2.42	0.50
13:s:13:LEU:HD11	13:s:149:LEU:HD11	1.92	0.50
5:K:154:PHE:HB3	5:K:162:PHE:HE1	1.75	0.50
4:j:116:GLN:NE2	5:k:84:ASP:OD1	2.44	0.50
9:O:30:ASN:OD1	9:O:187:ARG:NH2	2.44	0.50
11:Q:5:ILE:O	11:Q:16:ALA:N	2.44	0.50
14:T:153:VAL:O	14:T:157:GLN:N	2.43	0.50
1:G:158:GLY:O	2:H:84:ARG:NH2	2.44	0.50
10:P:159:ASP:N	10:P:159:ASP:OD1	2.42	0.50
13:s:172:MET:HE1	13:s:195:ILE:HG21	1.94	0.50
2:H:222:THR:OG1	2:H:225:GLU:OE1	2.24	0.50
5:K:21:LEU:HA	5:K:22:PHE:HB2	1.92	0.50
14:t:45:VAL:HB	14:t:49:THR:HG23	1.93	0.50
12:R:196:HIS:O	12:R:200:SER:CB	2.60	0.50
9:o:172:ASN:HB3	9:o:191:VAL:HG22	1.92	0.50
13:s:5:TYR:OH	13:s:103:PRO:O	2.24	0.50
14:t:46:ASN:OD1	14:t:46:ASN:N	2.45	0.50
7:M:43:ASP:OD1	7:M:43:ASP:N	2.45	0.49
10:P:15:LYS:HE3	10:P:121:ILE:HG12	1.94	0.49
3:i:161:ALA:HB1	3:i:175:LEU:HD13	1.94	0.49
6:l:40:SER:OG	6:l:43:HIS:N	2.42	0.49
9:O:46:ALA:HB3	9:O:97:ALA:HB3	1.93	0.49
11:Q:57:ALA:O	11:Q:61:GLN:CB	2.60	0.49
3:i:219:GLU:OE2	3:i:220:ASN:ND2	2.45	0.49
7:m:170:GLN:HA	7:m:173:LYS:HE2	1.93	0.49
5:k:70:ILE:HD11	5:k:89:ILE:HD12	1.93	0.49
9:o:124:TYR:OH	9:o:139:GLU:OE1	2.30	0.49
5:K:177:ALA:O	5:K:181:LEU:HB2	2.11	0.49
14:T:136:SER:HB2	14:T:150:LEU:HD13	1.95	0.49
8:n:18:SER:HB3	8:n:173:VAL:HG12	1.93	0.49
10:P:62:THR:OG1	11:Q:85:ARG:NH2	2.45	0.49
11:Q:47:VAL:O	11:Q:101:ASN:N	2.43	0.49
3:i:179:TYR:OH	3:i:181:GLU:OE1	2.29	0.49
6:L:146:GLN:HE21	6:L:154:PHE:HD2	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:181:ASP:OD1	2:H:181:ASP:N	2.45	0.49
6:l:148:CYS:SG	6:l:152:ASN:N	2.84	0.49
12:R:164:THR:HG22	12:R:170:SER:HB3	1.94	0.49
11:Q:181:ARG:NH1	11:Q:190:ASP:OD1	2.46	0.49
6:L:73:SER:HB3	6:L:133:LEU:HB2	1.95	0.48
13:S:68:ILE:HD11	13:S:92:LEU:HD13	1.94	0.48
1:g:84:THR:HB	7:m:156:VAL:HG22	1.94	0.48
3:i:149:GLN:OE1	3:i:162:THR:OG1	2.31	0.48
3:I:218:ARG:NH1	3:I:223:THR:OG1	2.42	0.48
9:O:110:LEU:HD21	9:O:125:VAL:HG22	1.95	0.48
6:l:117:GLN:HG2	7:m:86:SER:HB2	1.95	0.48
12:R:97:MET:O	12:R:116:SER:N	2.44	0.48
9:o:1:THR:HG23	9:o:33:LYS:HE3	1.95	0.48
5:K:93:ARG:NH1	12:R:68:LEU:O	2.45	0.48
8:n:19:ARG:NH2	8:n:168:GLY:O	2.46	0.48
8:n:127:ILE:HD13	8:n:136:TYR:HB2	1.94	0.48
10:P:203:ARG:HH12	12:r:191:ASN:HD21	1.61	0.48
12:R:21:THR:HG22	12:R:26:ILE:HG12	1.95	0.48
14:T:15:LYS:HG2	14:T:20:VAL:HG22	1.95	0.48
14:T:145:LEU:HB3	14:T:179:ARG:HH21	1.77	0.48
7:M:109:LYS:HA	7:M:149:TYR:HE2	1.78	0.48
1:g:54:LYS:NZ	1:g:213:SER:O	2.37	0.48
2:h:14:SER:OG	2:h:18:LYS:N	2.39	0.48
3:i:63:GLU:OE1	3:i:64:LYS:NZ	2.35	0.48
14:t:115:TYR:HE2	14:t:194:GLU:HB3	1.78	0.48
5:K:192:LYS:HA	5:K:195:ILE:HD12	1.95	0.48
5:K:195:ILE:O	5:K:198:SER:OG	2.32	0.48
5:K:236:GLU:HA	5:K:239:LYS:HE3	1.95	0.48
13:S:125:ASP:OD1	13:S:129:SER:N	2.43	0.48
2:h:65:VAL:HA	2:h:75:VAL:HG12	1.95	0.48
3:i:33:THR:HG23	3:i:168:SER:HB2	1.95	0.48
13:s:145:LEU:HD21	13:s:182:ALA:HB2	1.96	0.48
3:I:159:TRP:HA	4:J:54:GLN:HB2	1.96	0.48
4:J:134:VAL:HG22	4:J:144:LEU:HB2	1.95	0.48
4:j:175:ASN:HD21	4:j:190:LEU:HG	1.79	0.48
9:O:106:THR:OG1	9:O:109:HIS:NE2	2.36	0.48
9:O:136:ALA:HB2	14:t:179:ARG:HH22	1.79	0.48
11:Q:4:LEU:HD12	11:Q:45:LEU:HB3	1.95	0.48
11:Q:6:GLY:HA2	11:Q:15:VAL:HA	1.95	0.48
12:R:191:ASN:HD21	10:p:203:ARG:HH12	1.62	0.48
12:r:115:ASP:HB2	12:r:119:ASN:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:j:119:THR:HG22	4:j:126:PRO:HB3	1.96	0.48
13:s:209:SER:HG	13:s:212:LYS:HZ1	1.56	0.48
7:M:69:VAL:H	7:M:74:GLY:HA2	1.79	0.47
7:M:152:ASP:OD1	7:M:156:VAL:N	2.46	0.47
3:i:7:SER:OG	3:i:8:ARG:N	2.46	0.47
4:j:32:ALA:HB3	4:j:161:ILE:HD11	1.96	0.47
6:l:73:SER:HB3	6:l:133:LEU:HB2	1.97	0.47
8:n:14:LEU:HB2	8:n:177:ALA:HB3	1.96	0.47
9:o:84:LYS:HE2	9:o:119:THR:HG21	1.96	0.47
13:s:125:ASP:OD1	13:s:129:SER:N	2.45	0.47
1:G:178:PHE:O	1:G:182:LYS:HB2	2.14	0.47
2:H:93:LEU:HD11	2:H:113:ARG:HB3	1.96	0.47
7:M:201:HIS:HE1	7:M:206:ASP:HB2	1.79	0.47
8:N:18:SER:HB2	8:N:31:THR:H	1.78	0.47
1:g:71:LYS:O	1:g:95:ARG:NH2	2.47	0.47
5:k:211:ASN:OD1	5:k:214:ASN:ND2	2.47	0.47
4:J:88:ARG:NH1	11:Q:69:MET:O	2.48	0.47
5:K:210:LEU:HD11	5:K:215:ILE:HG12	1.96	0.47
6:L:44:ALA:HB1	6:L:144:ILE:HD11	1.97	0.47
10:P:190:ILE:HG22	10:P:195:ILE:HG23	1.97	0.47
6:L:50:LYS:HB3	6:L:59:HIS:HB3	1.97	0.47
10:p:26:ARG:HD3	10:p:186:ILE:HB	1.97	0.47
1:G:128:ASN:HA	2:H:127:VAL:HG12	1.95	0.47
1:G:208:ILE:HG22	1:G:210:PHE:HB3	1.96	0.47
4:J:32:ALA:HB2	4:J:45:VAL:HG23	1.97	0.47
14:T:179:ARG:HH22	9:o:136:ALA:HB2	1.79	0.47
3:i:105:ILE:HG13	3:i:107:CYS:H	1.78	0.47
10:p:58:THR:O	11:q:85:ARG:NH2	2.47	0.47
8:N:29:ARG:HH21	14:t:179:ARG:HB3	1.79	0.47
9:O:113:ILE:HG12	9:O:119:THR:HG22	1.96	0.47
3:i:25:MET:HA	3:i:28:ILE:HD12	1.95	0.47
3:i:162:THR:OG1	3:i:163:CYS:N	2.46	0.47
1:G:191:PHE:HE1	1:G:219:VAL:HG21	1.80	0.47
5:K:70:ILE:HD11	5:K:89:ILE:HD12	1.97	0.47
1:G:49:VAL:HG22	1:G:219:VAL:HG23	1.97	0.46
4:J:159:ASN:OD1	4:J:160:ALA:N	2.48	0.46
7:M:228:PRO:HB2	7:M:231:ILE:HB	1.97	0.46
2:h:148:GLN:OE1	2:h:158:TRP:NE1	2.48	0.46
12:r:144:SER:H	12:r:147:LEU:HD11	1.80	0.46
4:J:96:LEU:HA	11:Q:62:LYS:HE2	1.97	0.46
4:J:179:GLU:HG2	4:J:180:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:18:SER:OG	8:N:19:ARG:N	2.47	0.46
8:N:14:LEU:HB2	8:N:177:ALA:HB3	1.97	0.46
1:g:128:ASN:ND2	2:h:3:GLU:OE1	2.48	0.46
9:o:112:SER:HB3	9:o:125:VAL:HG11	1.96	0.46
10:p:49:LEU:HD21	10:p:87:LEU:HD22	1.96	0.46
8:n:104:ASP:N	8:n:108:GLY:O	2.47	0.46
11:q:13:VAL:HB	11:q:183:ILE:HD12	1.97	0.46
1:G:67:THR:HG23	1:G:216:GLU:HG2	1.97	0.46
3:i:228:LEU:H	3:i:228:LEU:HG	1.57	0.46
9:o:200:GLY:HA3	9:o:201:ARG:HA	1.63	0.46
1:G:43:ARG:HH21	1:G:164:LYS:HG2	1.79	0.46
4:J:5:ARG:HA	4:J:6:ALA:HA	1.75	0.46
3:i:71:ASP:OD1	3:i:71:ASP:N	2.48	0.46
6:l:146:GLN:HE22	6:l:159:MET:HE2	1.80	0.46
14:t:122:LEU:HG	14:t:137:LEU:HD12	1.97	0.46
9:O:50:ALA:HB2	10:P:129:CYS:HB2	1.97	0.46
10:P:103:TYR:HA	11:Q:93:ARG:HH12	1.80	0.46
2:h:46:LEU:HD13	2:h:75:VAL:HG13	1.96	0.46
7:m:8:ASP:OD1	7:m:8:ASP:N	2.46	0.46
11:q:11:ASP:N	11:q:11:ASP:OD1	2.47	0.46
3:i:38:LEU:HB2	3:i:180:LYS:HE2	1.98	0.46
3:i:119:GLN:HE21	3:i:123:GLN:HE22	1.62	0.46
4:j:172:LEU:HA	4:j:175:ASN:HB3	1.97	0.46
3:I:245:ALA:O	3:I:249:ARG:NH2	2.49	0.46
7:M:139:SER:OG	7:M:140:TYR:N	2.49	0.46
4:j:7:ILE:HG12	4:j:123:GLY:HA2	1.97	0.46
4:j:11:SER:OG	4:j:14:GLY:N	2.49	0.46
4:j:132:LEU:HD11	4:j:161:ILE:HG12	1.98	0.46
9:o:216:ILE:HG23	10:p:194:LYS:HD2	1.98	0.46
11:q:101:ASN:HB3	11:q:132:HIS:CD2	2.50	0.46
13:s:35:ILE:HB	14:t:151:ARG:HH12	1.81	0.46
13:s:68:ILE:HD11	13:s:92:LEU:HD13	1.98	0.46
2:H:46:LEU:HD13	2:H:75:VAL:HG13	1.97	0.46
6:L:46:LEU:HD13	6:L:73:SER:HB2	1.98	0.46
4:J:4:ASP:O	4:J:18:GLN:NE2	2.43	0.45
8:N:144:ARG:H	8:N:147:MET:HE3	1.80	0.45
2:h:80:GLY:HA2	2:h:83:TYR:HB3	1.96	0.45
4:J:51:ALA:HB3	4:J:54:GLN:HE22	1.82	0.45
11:Q:17:SER:OG	11:Q:179:SER:OG	2.34	0.45
3:I:164:ILE:HG22	3:I:165:GLY:H	1.82	0.45
6:L:85:CYS:SG	6:L:89:ARG:NE	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:43:ARG:NH1	1:g:149:PRO:O	2.48	0.45
12:r:35:ILE:N	12:r:43:GLY:O	2.49	0.45
1:g:83:MET:SD	1:g:132:ARG:NH1	2.82	0.45
12:R:97:MET:HB3	12:R:116:SER:HB3	1.99	0.45
14:t:25:ASP:HA	14:t:187:PHE:HA	1.98	0.45
8:N:120:MET:H	14:T:61:GLN:HE22	1.64	0.45
8:N:138:TYR:HB3	8:n:138:TYR:HB3	1.98	0.45
7:M:163:CYS:SG	7:M:164:ALA:N	2.90	0.45
9:O:202:TYR:OH	13:s:177:ASP:OD2	2.31	0.45
12:R:35:ILE:N	12:R:43:GLY:O	2.50	0.45
12:r:122:SER:OG	12:r:123:GLY:N	2.49	0.45
6:L:106:SER:HA	6:L:145:PHE:HE2	1.82	0.45
13:S:73:LYS:O	13:S:77:HIS:ND1	2.37	0.45
5:K:48:LEU:HD21	5:K:77:ALA:HB2	1.99	0.45
6:L:26:MET:HE1	6:L:148:CYS:HB2	1.99	0.45
8:N:127:ILE:HD13	8:N:136:TYR:HB2	1.99	0.45
7:m:109:LYS:HA	7:m:149:TYR:HE2	1.81	0.45
9:o:11:GLY:HA2	9:o:108:PRO:HB3	1.99	0.45
12:R:196:HIS:O	12:R:200:SER:HB3	2.16	0.45
13:s:209:SER:OG	13:s:210:LEU:N	2.50	0.45
6:L:225:ASP:N	6:L:225:ASP:OD1	2.48	0.44
13:S:209:SER:OG	13:S:212:LYS:NZ	2.41	0.44
3:i:239:LYS:NZ	3:i:243:GLU:OE2	2.47	0.44
6:l:155:ASP:HB3	7:m:62:SER:HB2	1.99	0.44
12:r:44:THR:HG21	12:r:100:MET:HE3	1.99	0.44
2:H:10:LEU:HD23	2:H:125:GLY:HA2	1.99	0.44
6:L:56:LEU:H	6:L:56:LEU:HG	1.64	0.44
9:O:84:LYS:HE2	9:O:119:THR:HG21	1.98	0.44
2:h:119:GLN:O	2:h:122:THR:OG1	2.26	0.44
6:L:52:ALA:HB2	6:L:59:HIS:CD2	2.52	0.44
2:h:100:VAL:HG13	10:p:93:ASN:HD22	1.81	0.44
9:o:67:SER:HB3	9:o:74:PRO:HG3	1.98	0.44
3:I:6:ASP:HB3	3:I:19:TYR:CZ	2.52	0.44
11:Q:4:LEU:HD22	11:Q:17:SER:HB2	2.00	0.44
13:S:60:ASP:OD1	14:T:97:TYR:OH	2.26	0.44
2:h:204:THR:N	2:h:207:ASN:OD1	2.49	0.44
6:l:140:MET:HE2	6:l:143:HIS:HE1	1.81	0.44
6:l:148:CYS:SG	6:l:150:SER:OG	2.68	0.44
1:G:34:GLN:NE2	7:M:17:ASP:O	2.42	0.44
12:R:144:SER:H	12:R:147:LEU:HD11	1.83	0.44
12:R:158:ARG:HH12	12:R:199:TYR:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:93:LEU:HD11	2:h:113:ARG:HB3	1.98	0.44
9:o:46:ALA:HB3	9:o:97:ALA:HB3	2.00	0.44
3:I:14:PRO:HB3	4:J:21:TYR:CE1	2.52	0.44
5:K:134:SER:OG	5:K:135:ARG:N	2.51	0.44
11:Q:52:ASP:OD1	12:R:88:TYR:OH	2.28	0.44
12:r:115:ASP:OD2	12:r:119:ASN:ND2	2.50	0.44
5:K:69:GLU:HG3	5:K:228:MET:HE1	2.00	0.44
12:R:133:VAL:HG21	11:q:137:PHE:HB3	2.00	0.44
12:R:141:ARG:HH22	11:q:162:LYS:C	2.25	0.44
5:k:44:GLU:OE1	5:k:191:LEU:N	2.50	0.44
8:N:28:ASN:HD21	9:O:122:LEU:HD21	1.82	0.44
13:S:172:MET:HE1	13:S:195:ILE:HG21	2.00	0.44
1:g:6:SER:HB2	1:g:11:ARG:HE	1.83	0.44
1:g:109:ILE:HD13	1:g:114:LEU:HD12	1.98	0.44
5:k:195:ILE:O	5:k:198:SER:OG	2.35	0.44
6:l:50:LYS:HB3	6:l:59:HIS:HB3	2.00	0.44
7:m:201:HIS:HE1	7:m:206:ASP:HB2	1.81	0.44
4:J:156:TRP:CD1	5:K:59:MET:HA	2.53	0.43
7:M:51:LYS:NZ	7:M:62:SER:O	2.50	0.43
12:R:12:VAL:HB	12:R:179:VAL:HB	2.00	0.43
2:h:118:MET:HE2	2:h:151:PRO:HA	2.00	0.43
1:G:120:ASP:OD1	2:H:84:ARG:NH1	2.51	0.43
7:M:37:ILE:HG12	7:M:197:ILE:HD11	2.00	0.43
9:O:98:LEU:HB2	9:O:113:ILE:HB	2.01	0.43
12:R:167:ASP:OD1	12:R:168:ALA:N	2.51	0.43
4:j:115:LYS:HD3	4:j:149:PRO:HA	2.01	0.43
4:j:159:ASN:OD1	4:j:160:ALA:N	2.51	0.43
8:n:134:TYR:HE2	8:n:167:ASP:HB2	1.82	0.43
4:J:8:THR:HG23	5:K:135:ARG:HB3	1.99	0.43
14:T:1:THR:N	14:T:105:PRO:O	2.39	0.43
9:o:51:ASP:HB3	9:o:94:ILE:HG23	2.00	0.43
10:p:29:GLY:HA3	10:p:34:MET:HA	2.00	0.43
10:p:190:ILE:HG22	10:p:195:ILE:HG23	2.01	0.43
14:t:178:TYR:OH	14:t:208:ASN:N	2.50	0.43
1:G:88:ARG:NH1	7:M:157:SER:O	2.39	0.43
10:p:191:GLU:HG3	10:p:193:ASP:H	1.84	0.43
1:G:84:THR:HB	7:M:156:VAL:HG22	1.99	0.43
2:H:99:LEU:O	2:H:102:GLN:NE2	2.51	0.43
3:I:105:ILE:HA	3:I:106:PRO:HD3	1.75	0.43
7:M:40:ARG:HA	7:M:45:VAL:HA	2.00	0.43
3:i:72:MET:HG2	3:i:138:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:73:ALA:HB3	3:i:137:ILE:HD11	1.99	0.43
10:p:141:THR:OG1	10:p:142:CYS:N	2.51	0.43
5:k:221:GLN:HB2	5:k:224:GLN:HB3	2.00	0.43
11:q:47:VAL:O	11:q:101:ASN:N	2.49	0.43
3:I:90:LEU:HD12	3:I:114:LEU:HD13	2.01	0.43
7:M:136:MET:HE3	7:M:148:LEU:HD11	2.01	0.43
13:S:176:LYS:HE2	13:S:208:VAL:HG21	2.01	0.43
9:o:28:ASP:OD1	9:o:29:LYS:N	2.52	0.43
3:I:14:PRO:C	3:I:16:GLY:HA2	2.44	0.43
6:l:157:ARG:NH2	7:m:58:TYR:O	2.51	0.43
2:H:66:GLU:OE2	2:H:91:ARG:NH2	2.52	0.43
7:M:58:TYR:CE1	7:M:62:SER:HB3	2.53	0.43
12:R:9:ARG:NH2	12:R:146:ASP:OD1	2.40	0.43
4:j:38:ARG:NH1	4:j:182:GLU:O	2.36	0.43
4:j:190:LEU:HD12	4:j:190:LEU:HA	1.84	0.43
9:O:37:ILE:HD13	9:O:60:SER:HB2	2.00	0.43
4:j:4:ASP:HB3	5:k:126:GLU:HB3	2.01	0.43
10:p:2:SER:OG	10:p:3:ILE:N	2.51	0.43
1:G:11:ARG:HE	1:G:27:TYR:HE2	1.67	0.42
1:G:165:ALA:HB3	2:H:56:LEU:HD22	2.00	0.42
3:I:18:LEU:HD23	3:I:18:LEU:HA	1.79	0.42
7:M:58:TYR:OH	7:M:62:SER:O	2.37	0.42
6:l:225:ASP:N	6:l:225:ASP:OD1	2.51	0.42
3:i:164:ILE:HG22	3:i:165:GLY:H	1.83	0.42
5:k:12:VAL:HG23	5:k:13:ASN:HB2	2.01	0.42
5:K:73:HIS:HE2	5:K:106:THR:HB	1.83	0.42
11:q:23:SER:HB2	11:q:28:MET:HE2	2.01	0.42
11:q:77:PRO:HB3	11:q:106:GLY:HA3	2.02	0.42
12:R:38:ASN:HB2	12:R:41:LEU:H	1.85	0.42
2:h:105:ILE:HG12	2:h:110:LEU:HD12	2.00	0.42
6:l:167:SER:O	6:l:170:THR:OG1	2.29	0.42
4:J:96:LEU:HG	11:Q:58:GLU:HB3	2.01	0.42
1:g:212:PRO:HB3	1:g:235:ILE:HG22	2.01	0.42
5:k:199:LEU:HA	5:k:202:LEU:HD12	2.01	0.42
7:m:152:ASP:OD2	7:m:154:SER:OG	2.31	0.42
1:G:105:TYR:HA	9:O:78:THR:HG23	2.01	0.42
1:G:132:ARG:HA	1:G:133:PRO:HD3	1.80	0.42
8:N:18:SER:OG	8:N:29:ARG:O	2.35	0.42
12:R:144:SER:HB3	12:R:147:LEU:HD21	2.01	0.42
6:l:14:SER:OG	6:l:18:ARG:O	2.33	0.42
12:r:21:THR:HG22	12:r:26:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:123:SER:HB3	13:s:136:LYS:HG3	2.01	0.42
2:H:38:ILE:HD12	2:H:191:ALA:HB2	2.02	0.42
4:J:114:LEU:O	4:J:118:TYR:HB2	2.20	0.42
1:g:49:VAL:HG22	1:g:219:VAL:HG23	2.01	0.42
7:M:10:SER:HB3	7:M:13:THR:HG23	2.01	0.42
1:g:43:ARG:HH21	1:g:164:LYS:HG2	1.84	0.42
2:h:9:SER:HA	2:h:126:GLY:H	1.85	0.42
4:J:2:SER:HA	4:J:12:PRO:HD3	2.01	0.42
5:K:241:ILE:HD12	5:K:241:ILE:HA	1.92	0.42
6:L:73:SER:OG	6:L:74:ILE:N	2.53	0.42
7:M:41:CYS:HB3	7:M:189:ILE:HG13	2.02	0.42
3:i:213:ILE:HB	3:i:228:LEU:HD11	2.00	0.42
5:k:49:ALA:HB1	5:k:202:LEU:HD11	2.02	0.42
14:t:49:THR:OG1	14:t:50:MET:N	2.53	0.42
12:R:104:TRP:CD2	12:R:181:GLU:HA	2.55	0.42
8:n:120:MET:H	14:t:61:GLN:HE22	1.68	0.42
6:L:71:GLY:HA3	6:L:221:PHE:CZ	2.55	0.41
3:i:125:GLY:O	4:j:3:TYR:OH	2.35	0.41
7:m:66:LEU:HD13	7:m:214:SER:HB2	2.00	0.41
11:q:102:LEU:HB2	11:q:118:MET:HB2	2.02	0.41
7:M:99:ARG:HH21	7:M:105:ASN:HA	1.84	0.41
8:N:7:GLN:HA	8:N:12:VAL:HA	2.02	0.41
8:N:104:ASP:N	8:N:108:GLY:O	2.49	0.41
11:Q:140:LEU:HD13	12:r:166:ARG:HH21	1.85	0.41
13:S:211:ARG:NE	13:S:213:ASP:OD1	2.47	0.41
4:J:2:SER:OG	4:J:3:TYR:N	2.53	0.41
6:L:50:LYS:HE2	6:L:61:LYS:HA	2.03	0.41
6:L:122:ARG:HG2	7:M:128:VAL:HG12	2.02	0.41
6:L:155:ASP:HB3	7:M:62:SER:HB2	2.01	0.41
2:h:14:SER:OG	2:h:17:GLY:N	2.53	0.41
13:s:29:LEU:HB3	13:s:37:THR:HG22	2.02	0.41
7:M:230:ASP:OD1	7:M:230:ASP:N	2.50	0.41
1:g:132:ARG:HA	1:g:133:PRO:HD3	1.83	0.41
4:j:116:GLN:O	4:j:119:THR:OG1	2.35	0.41
5:k:91:LYS:HB3	5:k:91:LYS:HE3	1.83	0.41
8:N:135:ILE:O	8:N:139:VAL:HB	2.21	0.41
11:Q:148:THR:HG22	11:Q:150:THR:H	1.85	0.41
12:R:105:ASP:HB3	12:R:108:GLY:H	1.85	0.41
13:S:13:LEU:HD11	13:S:149:LEU:HD11	2.02	0.41
13:S:91:MET:O	13:S:94:THR:OG1	2.32	0.41
2:h:38:ILE:HD12	2:h:191:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:121:TYR:CG	2:h:130:PHE:HE2	2.38	0.41
3:I:108:GLU:OE2	3:I:148:TYR:OH	2.30	0.41
4:J:36:ARG:HB2	4:J:142:PRO:HB2	2.03	0.41
6:L:59:HIS:ND1	6:L:208:LYS:O	2.54	0.41
9:O:18:THR:O	9:O:18:THR:OG1	2.25	0.41
2:h:59:GLU:HG2	2:h:206:ASP:HB3	2.02	0.41
7:m:58:TYR:HH	7:m:62:SER:C	2.25	0.41
12:r:39:PRO:HA	12:r:184:TRP:HE1	1.84	0.41
2:H:105:ILE:HG12	2:H:110:LEU:HD12	2.02	0.41
3:I:232:GLU:HA	3:I:235:GLN:HG2	2.03	0.41
11:Q:29:LYS:HE3	11:Q:32:HIS:HA	2.02	0.41
5:k:206:MET:HE1	5:k:210:LEU:HD13	2.01	0.41
3:I:55:LEU:HD23	3:I:55:LEU:HA	1.93	0.41
6:L:121:GLN:HA	7:M:129:ARG:NH1	2.36	0.41
6:L:174:ARG:HG3	6:L:175:HIS:ND1	2.35	0.41
9:O:67:SER:HB3	9:O:74:PRO:HG3	2.03	0.41
4:j:156:TRP:CD1	5:k:59:MET:HA	2.56	0.41
1:G:172:GLN:HA	1:G:175:SER:HB3	2.03	0.41
1:G:239:LEU:HD12	1:G:242:LEU:HD11	2.02	0.41
4:J:121:SER:OG	4:J:122:ASN:N	2.52	0.41
6:L:148:CYS:SG	6:L:152:ASN:N	2.88	0.41
12:R:115:ASP:HB2	12:R:119:ASN:H	1.86	0.41
12:R:144:SER:OG	12:R:145:TYR:N	2.54	0.41
12:R:166:ARG:HH21	11:q:140:LEU:HD12	1.86	0.41
8:n:135:ILE:O	8:n:139:VAL:HB	2.21	0.41
10:p:76:LEU:HD23	10:p:76:LEU:HA	1.88	0.41
10:p:113:ASP:N	10:p:118:LYS:O	2.51	0.41
10:p:126:LEU:HD12	10:p:127:ILE:HG23	2.03	0.41
12:r:19:ARG:HH21	12:r:29:GLN:NE2	2.19	0.41
3:I:164:ILE:HD12	3:I:164:ILE:HG23	1.90	0.41
3:I:228:LEU:H	3:I:228:LEU:HG	1.62	0.41
4:J:180:ALA:HA	4:J:181:ILE:HA	1.84	0.41
6:L:65:HIS:HB2	6:L:223:ILE:HD11	2.01	0.41
13:S:5:TYR:OH	13:S:103:PRO:O	2.31	0.41
2:h:34:PRO:HA	2:h:164:GLY:HA3	2.02	0.41
3:i:15:GLU:N	4:j:21:TYR:OH	2.54	0.41
4:j:55:ASP:OD1	4:j:56:GLU:N	2.54	0.41
6:l:174:ARG:HG3	6:l:175:HIS:ND1	2.36	0.41
11:q:4:LEU:HD22	11:q:45:LEU:HB3	2.02	0.41
2:H:65:VAL:HA	2:H:75:VAL:HG12	2.03	0.40
2:H:86:LEU:HD11	2:H:134:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:ARG:HH11	2:H:128:ARG:HD3	1.75	0.40
10:P:73:LEU:HD23	10:P:73:LEU:HA	1.92	0.40
11:Q:162:LYS:HB3	12:r:141:ARG:HH22	1.86	0.40
1:g:215:ILE:H	1:g:215:ILE:HG13	1.58	0.40
5:k:236:GLU:HA	5:k:239:LYS:HE3	2.02	0.40
3:I:57:ASP:HB3	3:I:59:VAL:HG13	2.03	0.40
5:K:227:HIS:NE2	5:K:229:PHE:O	2.54	0.40
7:M:168:ALA:HB1	7:M:171:ALA:HB3	2.03	0.40
9:O:87:LEU:HD23	9:O:87:LEU:HA	1.93	0.40
10:P:113:ASP:HB2	10:P:118:LYS:HB3	2.03	0.40
2:h:209:GLU:OE2	2:h:220:ARG:NH2	2.42	0.40
3:i:118:LYS:HE2	3:i:152:PRO:HA	2.04	0.40
1:g:123:GLN:OE1	2:h:128:ARG:NH2	2.54	0.40
4:j:68:ASN:HA	4:j:211:MET:HE1	2.04	0.40
7:m:58:TYR:CE1	7:m:62:SER:HB3	2.57	0.40
14:t:192:VAL:HG12	14:t:197:VAL:HG22	2.02	0.40
3:I:162:THR:OG1	3:I:163:CYS:N	2.55	0.40
5:K:182:GLN:NE2	6:L:55:GLU:OE1	2.53	0.40
6:L:42:THR:O	6:L:137:TYR:OH	2.37	0.40
12:R:18:SER:OG	12:R:173:ALA:N	2.55	0.40
10:p:27:ARG:HB2	10:p:183:MET:HB2	2.03	0.40
14:t:187:PHE:O	14:t:203:LEU:N	2.54	0.40
1:G:41:ALA:HB3	1:G:166:THR:HB	2.04	0.40
5:K:211:ASN:OD1	5:K:214:ASN:ND2	2.54	0.40
10:P:126:LEU:HD12	10:P:127:ILE:HG23	2.03	0.40
3:i:135:LEU:HD23	3:i:135:LEU:HA	1.89	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	G	237/240 (99%)	211 (89%)	26 (11%)	0	100	100
1	g	238/240 (99%)	217 (91%)	21 (9%)	0	100	100
2	H	228/232 (98%)	211 (92%)	16 (7%)	1 (0%)	30	64
2	h	230/232 (99%)	224 (97%)	6 (3%)	0	100	100
3	I	246/250 (98%)	220 (89%)	26 (11%)	0	100	100
3	i	248/250 (99%)	222 (90%)	25 (10%)	1 (0%)	30	64
4	J	237/243 (98%)	221 (93%)	15 (6%)	1 (0%)	30	64
4	j	237/243 (98%)	223 (94%)	11 (5%)	3 (1%)	10	41
5	K	224/234 (96%)	205 (92%)	18 (8%)	1 (0%)	30	64
5	k	224/234 (96%)	205 (92%)	19 (8%)	0	100	100
6	L	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
6	l	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
7	M	238/245 (97%)	218 (92%)	19 (8%)	1 (0%)	30	64
7	m	238/245 (97%)	222 (93%)	16 (7%)	0	100	100
8	N	189/191 (99%)	180 (95%)	8 (4%)	1 (0%)	25	59
8	n	189/191 (99%)	180 (95%)	9 (5%)	0	100	100
9	O	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	25	59
9	o	218/220 (99%)	205 (94%)	12 (6%)	1 (0%)	25	59
10	P	202/204 (99%)	188 (93%)	14 (7%)	0	100	100
10	p	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
11	Q	197/199 (99%)	181 (92%)	16 (8%)	0	100	100
11	q	197/199 (99%)	181 (92%)	16 (8%)	0	100	100
12	R	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
12	r	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
13	S	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
13	s	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
14	T	213/215 (99%)	200 (94%)	13 (6%)	0	100	100
14	t	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
All	All	6155/6250 (98%)	5749 (93%)	395 (6%)	11 (0%)	45	75

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	98	VAL
9	O	173	ILE
9	o	173	ILE
5	K	10	ARG
8	N	19	ARG
7	M	54	LEU
4	j	97	THR
4	j	181	ILE
2	H	233	ILE
4	j	98	VAL
3	i	221	GLY

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	G	192/205 (94%)	188 (98%)	4 (2%)	48 71
1	g	193/205 (94%)	188 (97%)	5 (3%)	41 66
2	H	162/190 (85%)	162 (100%)	0	100 100
2	h	164/190 (86%)	164 (100%)	0	100 100
3	I	191/210 (91%)	189 (99%)	2 (1%)	73 84
3	i	193/210 (92%)	191 (99%)	2 (1%)	73 84
4	J	152/207 (73%)	151 (99%)	1 (1%)	81 89
4	j	152/207 (73%)	152 (100%)	0	100 100
5	K	187/196 (95%)	186 (100%)	1 (0%)	86 93
5	k	186/196 (95%)	185 (100%)	1 (0%)	86 93
6	L	198/204 (97%)	196 (99%)	2 (1%)	73 84
6	l	198/204 (97%)	198 (100%)	0	100 100
7	M	192/202 (95%)	190 (99%)	2 (1%)	73 84
7	m	192/202 (95%)	191 (100%)	1 (0%)	86 93
8	N	148/148 (100%)	147 (99%)	1 (1%)	81 89
8	n	148/148 (100%)	148 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	O	177/181 (98%)	176 (99%)	1 (1%)	84 91
9	o	177/181 (98%)	177 (100%)	0	100 100
10	P	172/173 (99%)	172 (100%)	0	100 100
10	p	172/173 (99%)	172 (100%)	0	100 100
11	Q	164/170 (96%)	163 (99%)	1 (1%)	84 91
11	q	164/170 (96%)	162 (99%)	2 (1%)	67 82
12	R	153/156 (98%)	153 (100%)	0	100 100
12	r	153/156 (98%)	153 (100%)	0	100 100
13	S	174/178 (98%)	174 (100%)	0	100 100
13	s	174/178 (98%)	174 (100%)	0	100 100
14	T	175/178 (98%)	174 (99%)	1 (1%)	84 91
14	t	175/178 (98%)	175 (100%)	0	100 100
All	All	4878/5196 (94%)	4851 (99%)	27 (1%)	82 91

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	22	LEU
1	G	141	ILE
1	G	199	ILE
1	G	215	ILE
3	I	11	ILE
3	I	228	LEU
4	J	161	ILE
5	K	21	LEU
6	L	22	ILE
6	L	56	LEU
7	M	87	LEU
7	M	200	VAL
8	N	30	VAL
9	O	18	THR
11	Q	25	ILE
14	T	64	LYS
1	g	66	VAL
1	g	73	THR
1	g	141	ILE
1	g	199	ILE
1	g	215	ILE

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Mol	Chain	Res	Type
3	i	137	ILE
3	i	228	LEU
5	k	64	ILE
7	m	87	LEU
11	q	4	LEU
11	q	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	75	ASN
2	H	71	HIS
2	H	119	GLN
2	H	123	GLN
3	I	20	GLN
3	I	102	GLN
3	I	119	GLN
3	I	149	GLN
3	I	167	ASN
3	I	198	ASN
4	J	15	HIS
4	J	68	ASN
4	J	85	ASN
4	J	92	GLN
4	J	116	GLN
5	K	97	GLN
5	K	152	GLN
5	K	214	ASN
6	L	53	GLN
6	L	60	GLN
6	L	90	GLN
6	L	117	GLN
7	M	180	GLN
8	N	28	ASN
8	N	158	ASN
10	P	61	GLN
10	P	173	ASN
12	R	10	HIS
13	S	8	ASN
13	S	58	HIS
13	S	146	GLN
14	T	2	GLN

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Mol	Chain	Res	Type
14	T	61	GLN
14	T	69	GLN
1	g	75	ASN
2	h	95	GLN
3	i	20	GLN
3	i	119	GLN
3	i	146	GLN
3	i	167	ASN
3	i	198	ASN
4	j	116	GLN
4	j	122	ASN
4	j	175	ASN
5	k	114	GLN
5	k	214	ASN
6	l	8	ASN
6	l	20	HIS
6	l	53	GLN
6	l	90	GLN
6	l	117	GLN
6	l	146	GLN
7	m	110	HIS
9	o	116	HIS
10	p	18	ASN
10	p	61	GLN
10	p	93	ASN
11	q	132	HIS
12	r	85	ASN
13	s	146	GLN
13	s	157	ASN
14	t	2	GLN
14	t	61	GLN
14	t	69	GLN
14	t	89	HIS
14	t	213	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides 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.

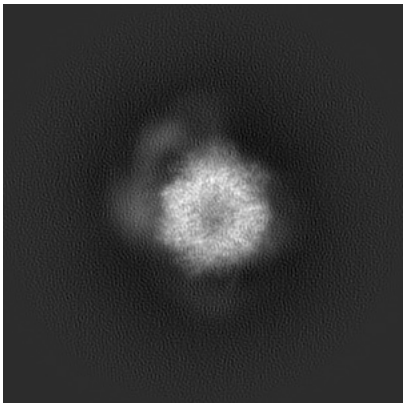
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8662. These allow visual inspection of the internal detail of the map and identification of artifacts.

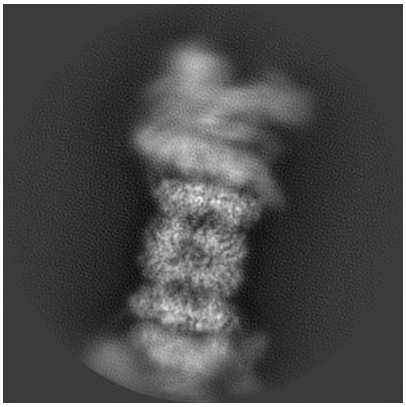
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

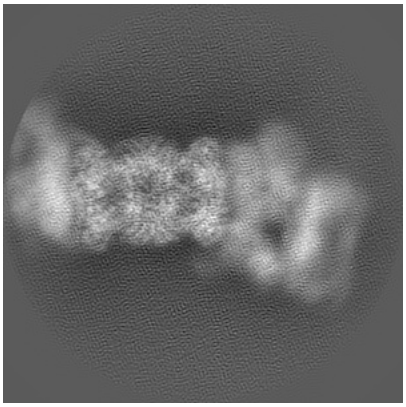
6.1.1 Primary map



X



Y

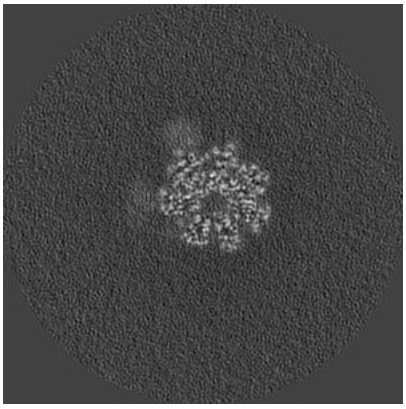


Z

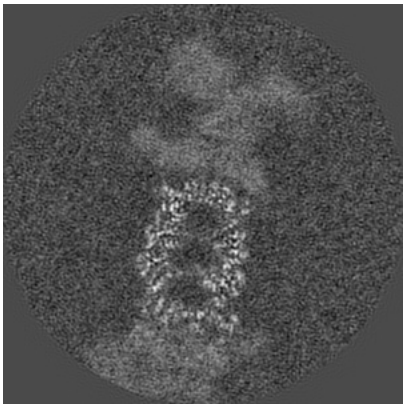
The images above show the map projected in three orthogonal directions.

6.2 Central slices

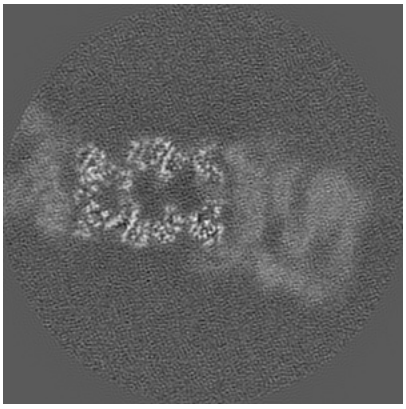
6.2.1 Primary map



X Index: 280



Y Index: 280

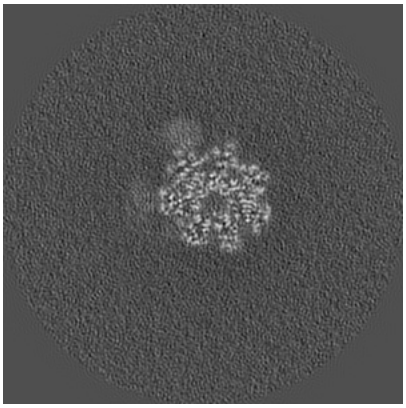


Z Index: 280

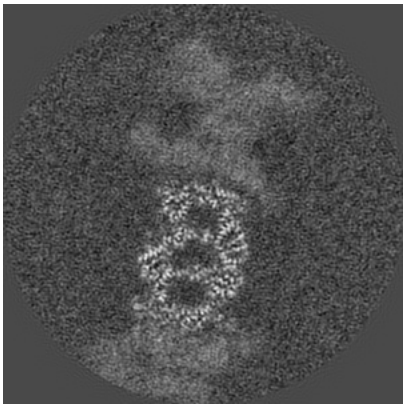
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

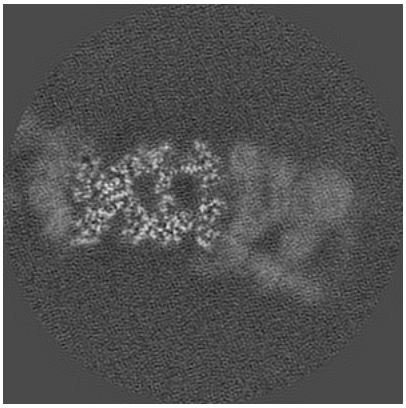
6.3.1 Primary map



X Index: 281



Y Index: 275

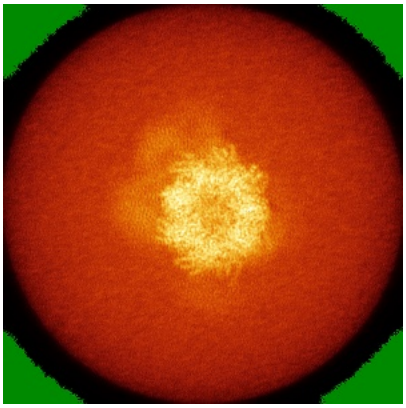


Z Index: 296

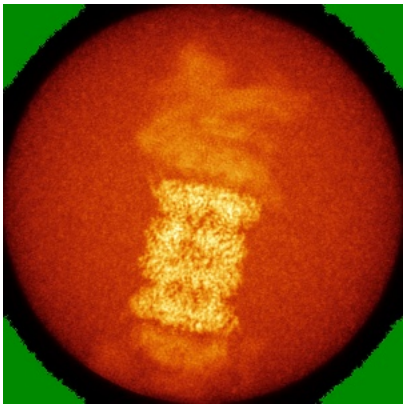
The images above show the largest variance slices of the map in three orthogonal directions.

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

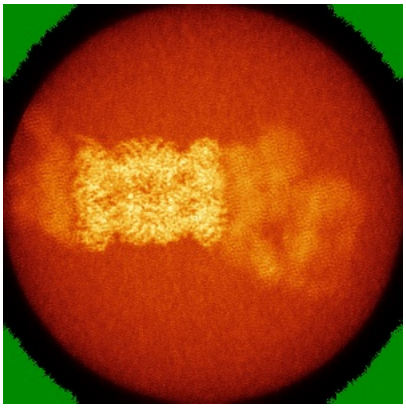
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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.

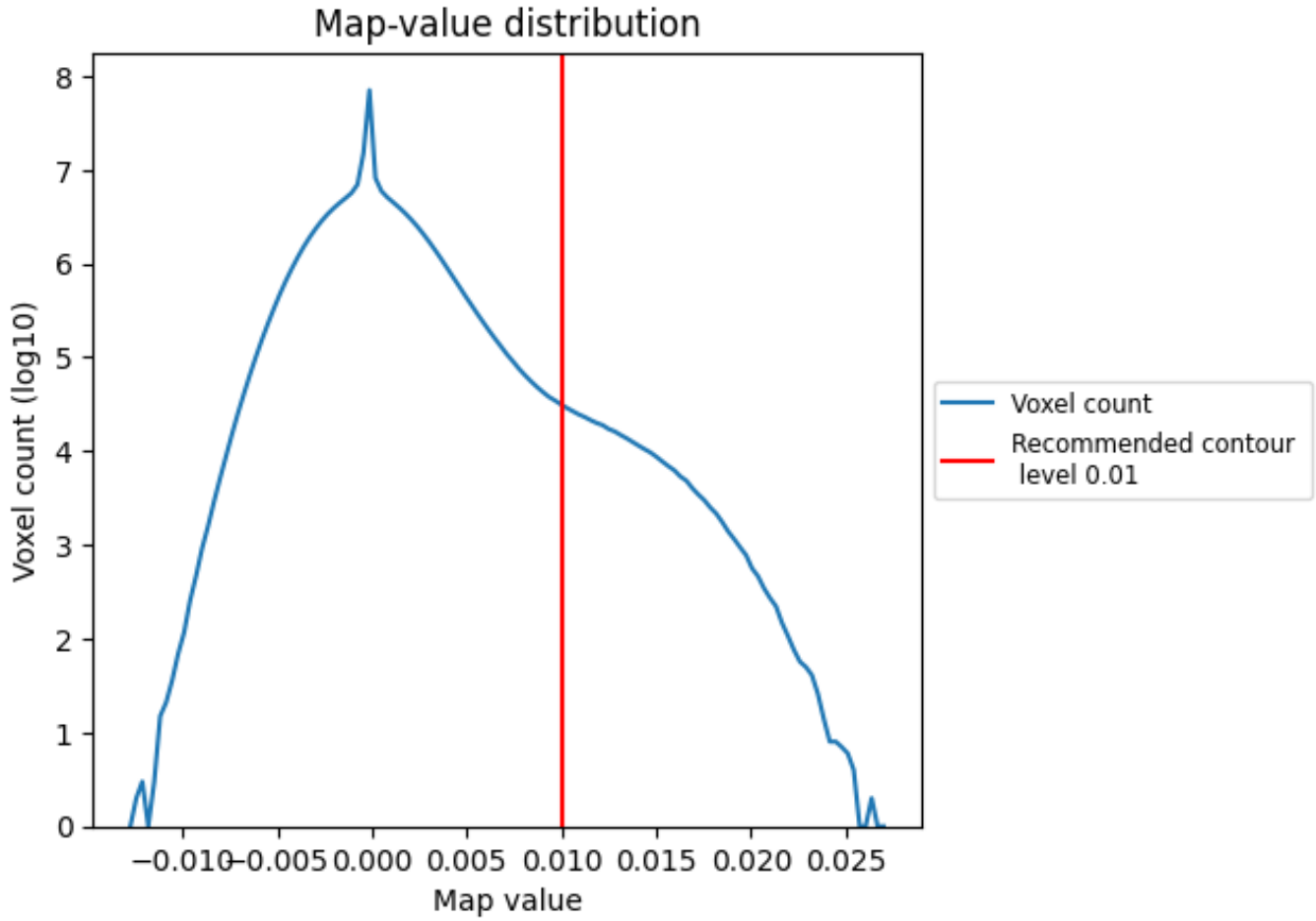
6.6 Mask visualisation (i)

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

7 Map analysis

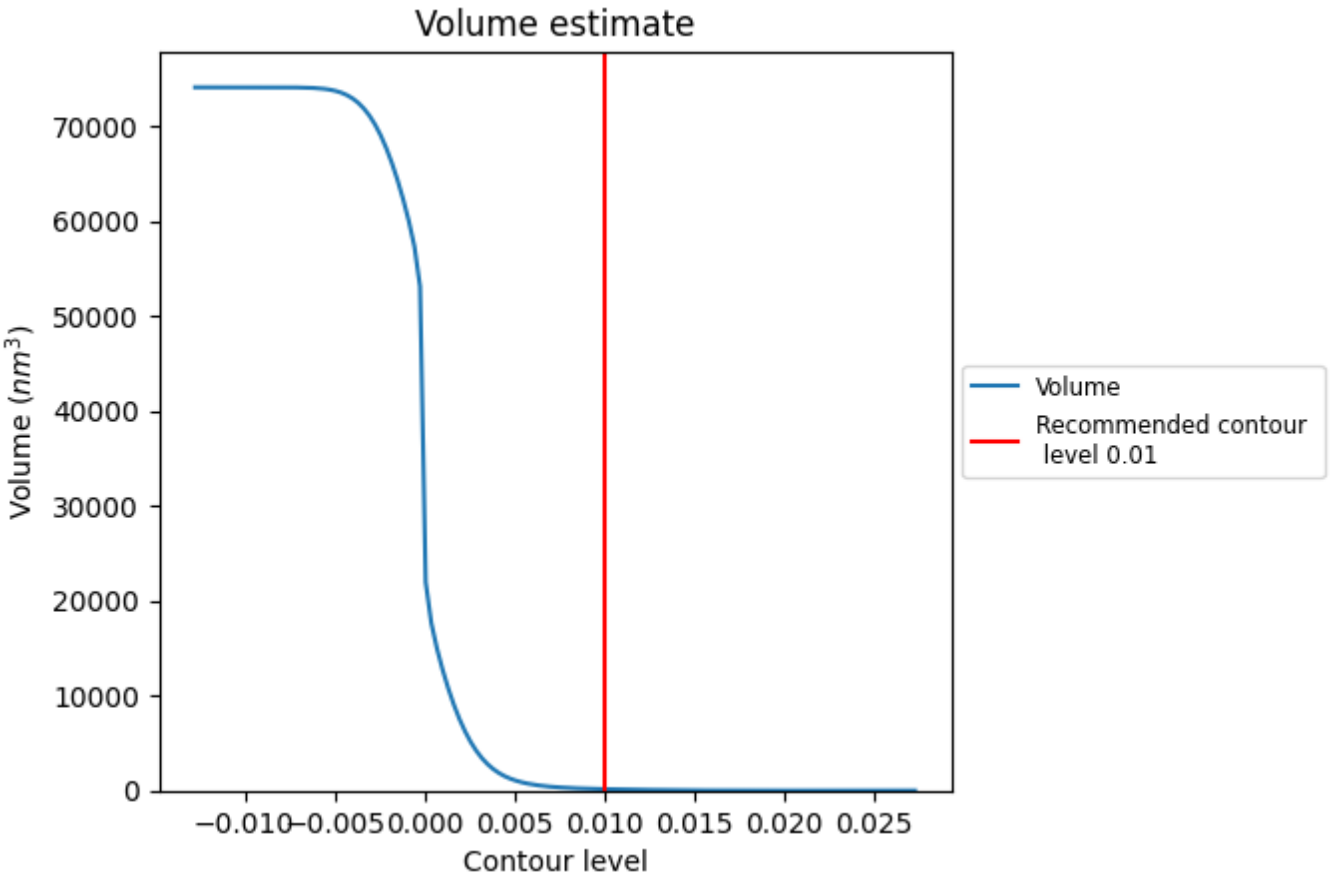
This section contains the results of statistical analysis of the map.

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.

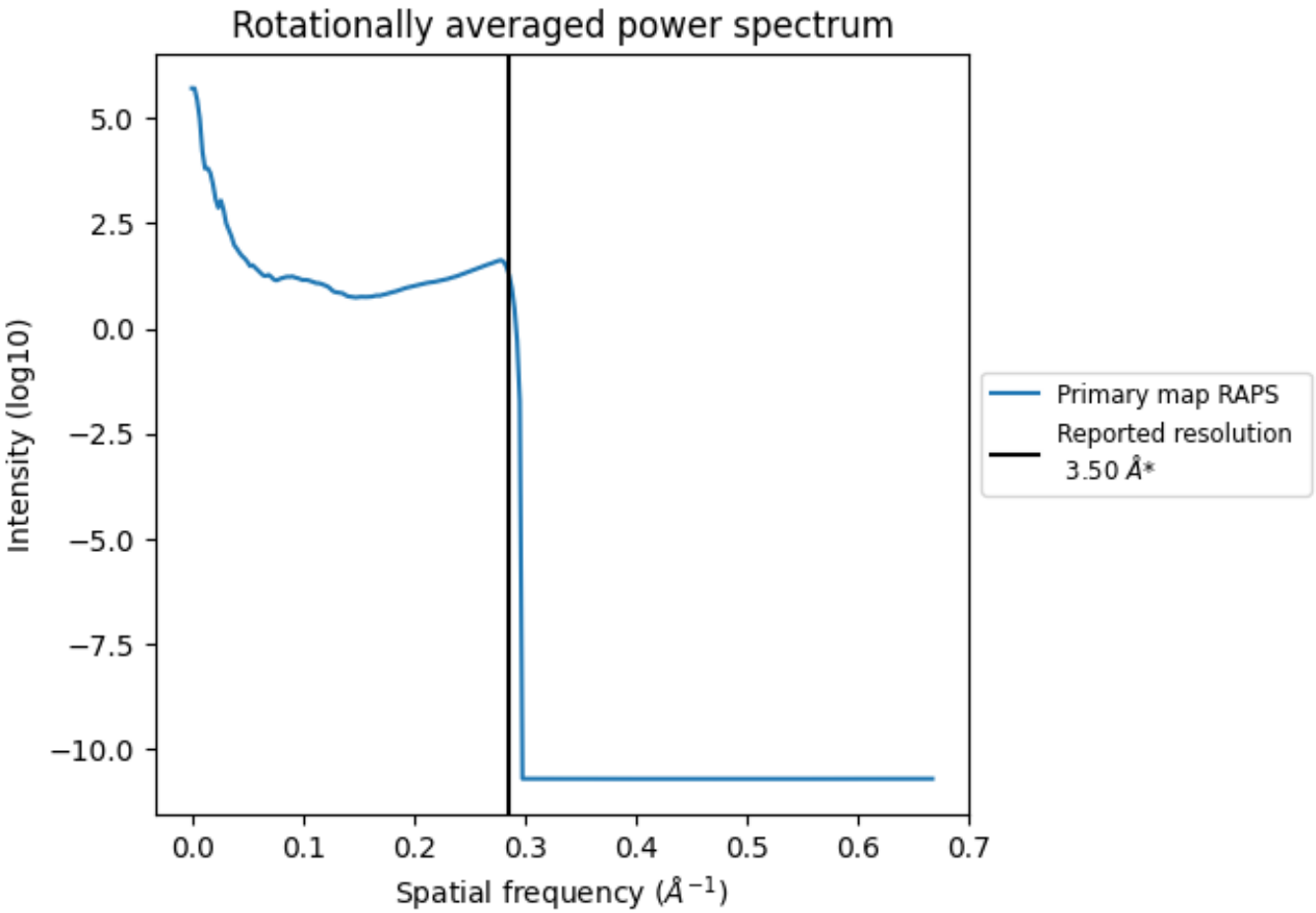
7.2 Volume estimate



The volume at the recommended contour level is 153 nm^3; this corresponds to an approximate mass of 138 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 0.286 $Å^{-1}$

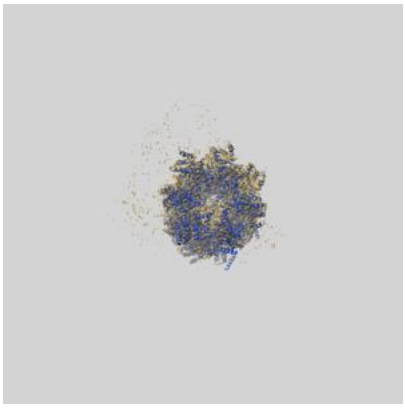
8 Fourier-Shell correlation

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

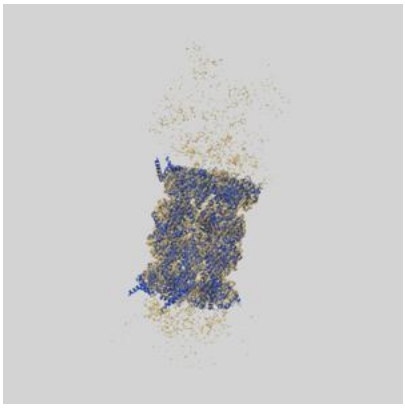
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8662 and PDB model 5VFO. Per-residue inclusion information can be found in section 3 on page 7.

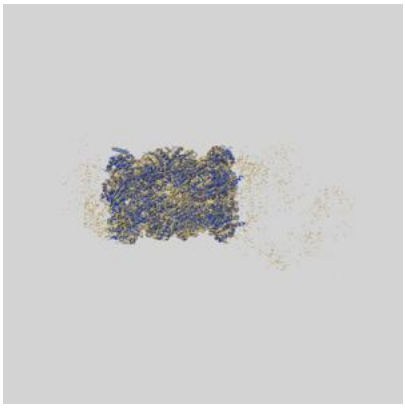
9.1 Map-model overlay



X



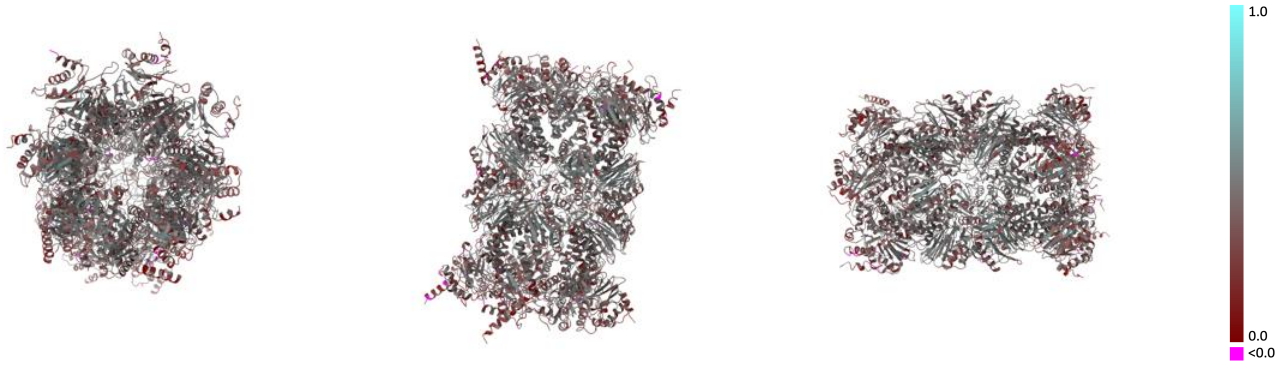
Y



Z

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

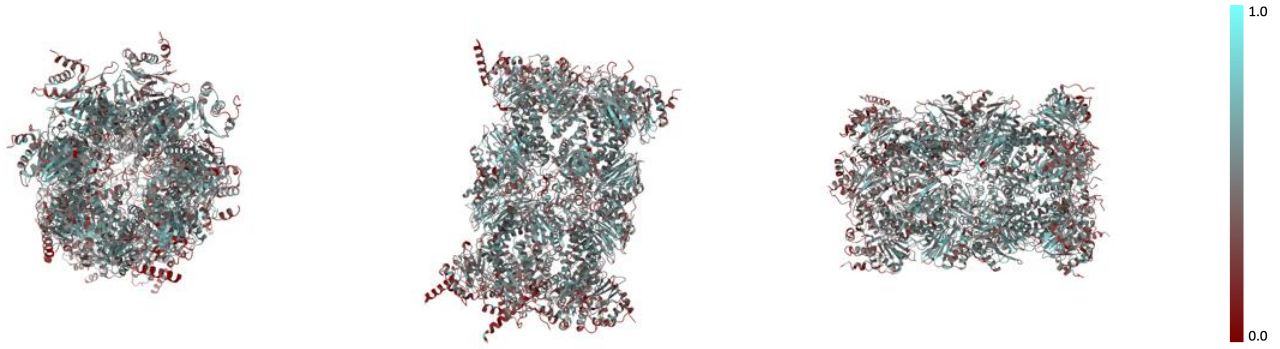
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

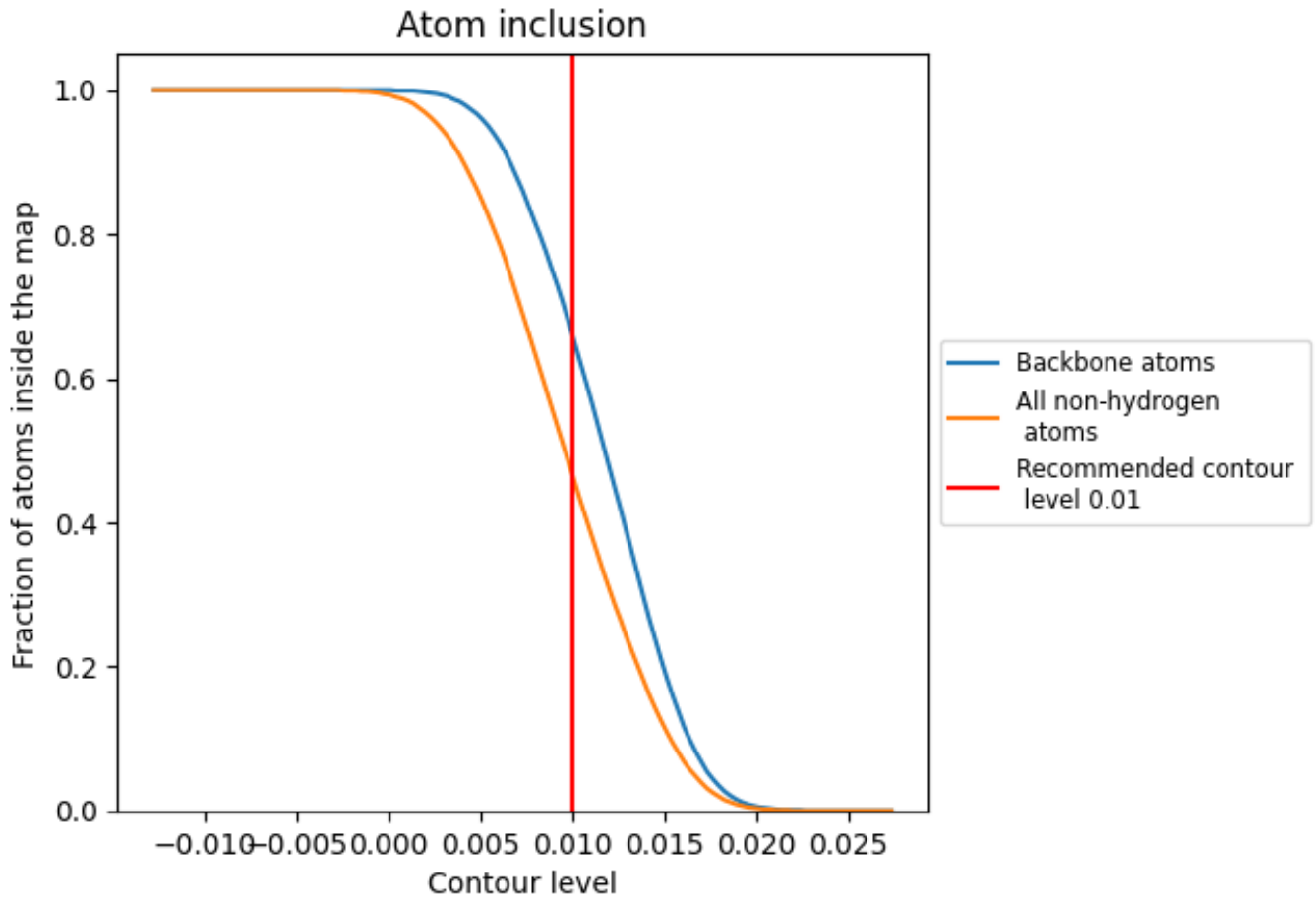
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 66% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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	Q-score
All	0.4630	0.3940
G	0.4560	0.3890
H	0.4900	0.4030
I	0.4460	0.3710
J	0.4190	0.3650
K	0.4330	0.3660
L	0.5000	0.4000
M	0.4610	0.3780
N	0.5280	0.4240
O	0.4820	0.4190
P	0.5290	0.4320
Q	0.4990	0.4000
R	0.5430	0.4240
S	0.4830	0.4210
T	0.5370	0.4340
g	0.3930	0.3730
h	0.4180	0.3770
i	0.3650	0.3470
j	0.3520	0.3370
k	0.4020	0.3530
l	0.4290	0.3610
m	0.4010	0.3560
n	0.5050	0.4230
o	0.4480	0.3950
p	0.4900	0.4220
q	0.5000	0.4190
r	0.5220	0.4220
s	0.4920	0.4300
t	0.5240	0.4240