



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:58 AM UTC

PDB ID : 6MUV / pdb_00006muv
EMDB ID : EMD-9257
Title : The structure of the Plasmodium falciparum 20S proteasome in complex with two PA28 activators
Authors : Metcalfe, R.D.; Xie, S.C.; Hanssen, E.; Gillett, D.L.; Leis, A.P.; Tilley, L.; Griffin, M.D.W.
Deposited on : 2018-10-23
Resolution : 3.80 Å (reported)
Based on initial model : 6DFK

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:

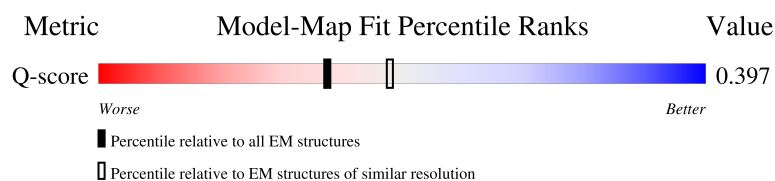
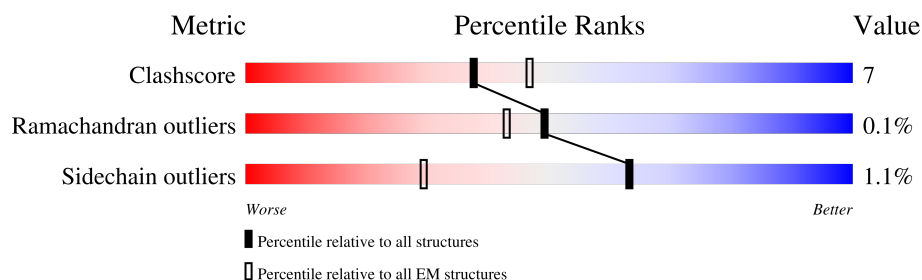
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	10% 75% 19% 5%
1	O	260	11% 75% 19% 5%
2	B	235	9% 74% 21% 5%
2	P	235	8% 75% 20% 5%

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Mol	Chain	Length	Quality of chain
3	C	246	
3	Q	246	
4	D	241	
4	R	241	
5	E	256	
5	S	256	
6	F	254	
6	T	254	
7	G	252	
7	U	252	
8	H	252	
8	V	252	
9	I	229	
9	W	229	
10	J	218	
10	X	218	
11	K	195	
11	Y	195	
12	L	211	
12	Z	211	
13	M	240	
13	a	240	
14	N	265	
14	b	265	
15	c	279	

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Mol	Chain	Length	Quality of chain
15	d	279	57% 53% 14% 33%
15	e	279	51% 51% 16% 33%
15	f	279	42% 60% 9% 31%
15	g	279	42% 58% 9% 32%
15	h	279	43% 59% 7% 33%
15	i	279	53% 54% 12% 33%
15	j	279	41% 59% 10% 31%
15	k	279	43% 57% 10% 32%
15	l	279	45% 58% 8% 33%
15	m	279	57% 52% 14% 33%
15	n	279	54% 54% 12% 33%
15	o	279	57% 55% 12% 33%
15	p	279	49% 54% 13% 33%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 71112 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 20S proteasome alpha-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	246	Total	C	N	O	S	0	0
			1943	1221	326	381	15		
1	O	246	Total	C	N	O	S	0	0
			1943	1221	326	381	15		

- Molecule 2 is a protein called 20S proteasome alpha-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1782	1146	293	337	6		
2	P	224	Total	C	N	O	S	0	0
			1782	1146	293	337	6		

- Molecule 3 is a protein called 20S proteasome alpha-3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	240	Total	C	N	O	S	0	0
			1917	1230	308	376	3		
3	Q	240	Total	C	N	O	S	0	0
			1917	1230	308	376	3		

- Molecule 4 is a protein called 20S proteasome alpha-4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	227	Total	C	N	O	S	0	0
			1795	1147	303	337	8		
4	R	227	Total	C	N	O	S	0	0
			1795	1147	303	337	8		

- Molecule 5 is a protein called 20S proteasome alpha-5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	227	Total	C	N	O	S	0	0
			1760	1109	291	350	10		
5	S	227	Total	C	N	O	S	0	0
			1760	1109	291	350	10		

- Molecule 6 is a protein called 20S proteasome alpha-6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	236	Total	C	N	O	S	0	0
			1878	1196	309	362	11		
6	T	236	Total	C	N	O	S	0	0
			1878	1196	309	362	11		

- Molecule 7 is a protein called 20S proteasome alpha-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1906	1215	319	360	12		
7	U	233	Total	C	N	O	S	0	0
			1906	1215	319	360	12		

- Molecule 8 is a protein called 20S proteasome beta-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	193	Total	C	N	O	S	0	0
			1536	969	264	291	12		
8	V	193	Total	C	N	O	S	0	0
			1536	969	264	291	12		

- Molecule 9 is a protein called 20S proteasome beta-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1676	1058	291	313	14		
9	W	219	Total	C	N	O	S	0	0
			1676	1058	291	313	14		

- Molecule 10 is a protein called 20S proteasome beta-3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	203	Total	C	N	O	S	0	0
			1595	1017	258	306	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	203	Total	C	N	O	S	0	0
			1595	1017	258	306	14		

- Molecule 11 is a protein called 20S proteasome beta-4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	195	Total	C	N	O	S	0	0
			1614	1042	266	298	8		
11	Y	195	Total	C	N	O	S	0	0
			1614	1042	266	298	8		

- Molecule 12 is a protein called 20S proteasome beta-5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	204	Total	C	N	O	S	0	0
			1600	1021	265	307	7		
12	Z	204	Total	C	N	O	S	0	0
			1600	1021	265	307	7		

- Molecule 13 is a protein called 20S proteasome beta-6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	211	Total	C	N	O	S	0	0
			1676	1073	277	319	7		
13	a	211	Total	C	N	O	S	0	0
			1676	1073	277	319	7		

- Molecule 14 is a protein called 20S proteasome beta-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	224	Total	C	N	O	S	0	0
			1845	1177	313	348	7		
14	b	224	Total	C	N	O	S	0	0
			1845	1177	313	348	7		

- Molecule 15 is a protein called Proteasome activator PA28.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	187	Total	C	N	O	S	0	0
			1568	1015	259	291	3		
15	d	187	Total	C	N	O	S	0	0
			1568	1015	259	291	3		

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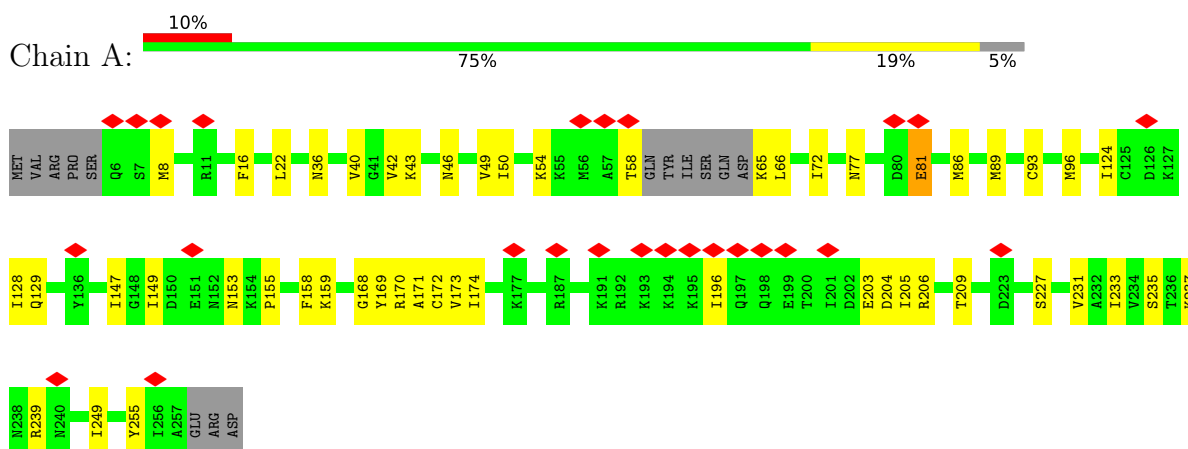
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Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	188	Total	C	N	O	S	0	0
			1576	1019	261	293	3		
15	f	193	Total	C	N	O	S	0	0
			1618	1043	270	302	3		
15	g	189	Total	C	N	O	S	0	0
			1585	1024	262	296	3		
15	h	186	Total	C	N	O	S	0	0
			1559	1009	257	290	3		
15	i	186	Total	C	N	O	S	0	0
			1559	1009	257	290	3		
15	j	193	Total	C	N	O	S	0	0
			1618	1043	270	302	3		
15	k	189	Total	C	N	O	S	0	0
			1585	1024	262	296	3		
15	l	186	Total	C	N	O	S	0	0
			1559	1009	257	290	3		
15	m	187	Total	C	N	O	S	0	0
			1568	1015	259	291	3		
15	n	186	Total	C	N	O	S	0	0
			1559	1009	257	290	3		
15	o	187	Total	C	N	O	S	0	0
			1568	1015	259	291	3		
15	p	188	Total	C	N	O	S	0	0
			1576	1019	261	293	3		

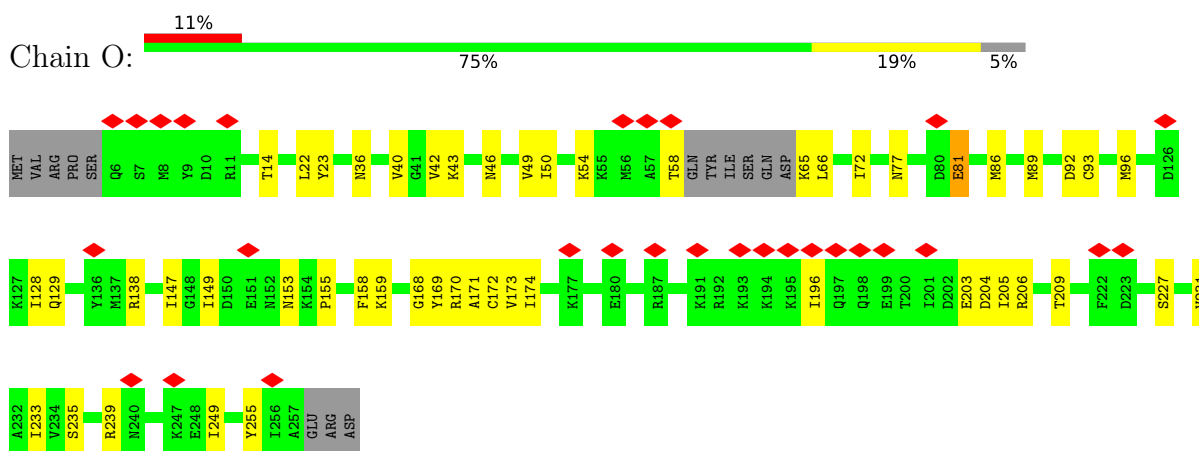
3 Residue-property plots

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.

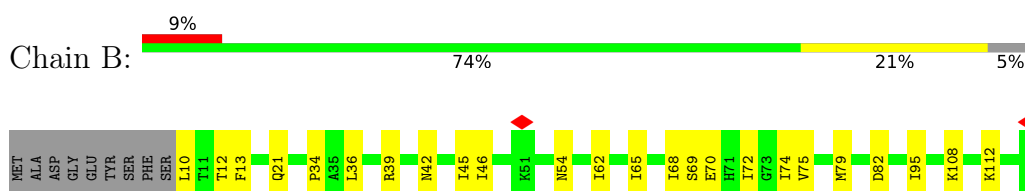
- Molecule 1: 20S proteasome alpha-1 subunit

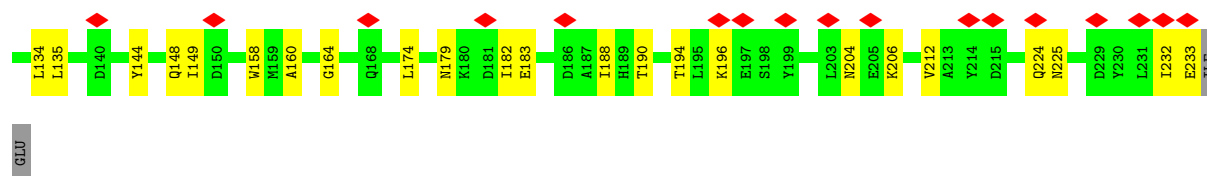


- Molecule 1: 20S proteasome alpha-1 subunit

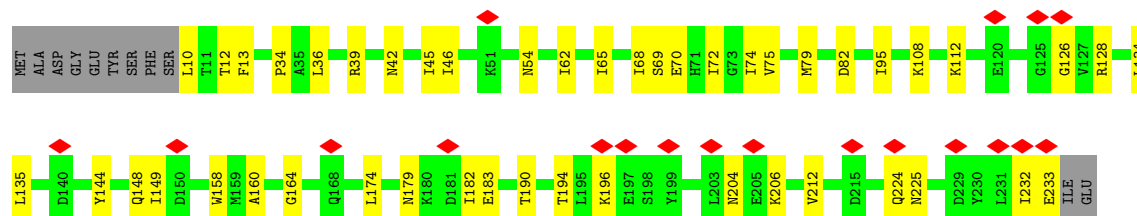
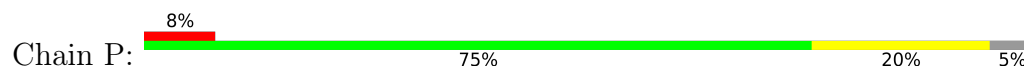


- Molecule 2: 20S proteasome alpha-2 subunit

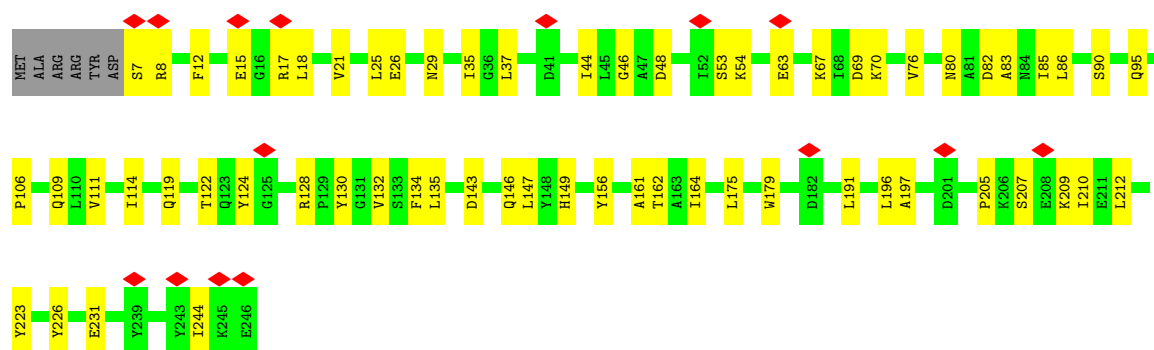
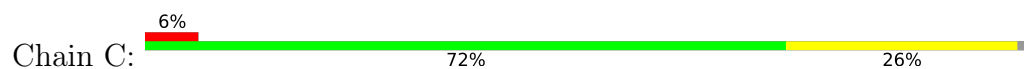




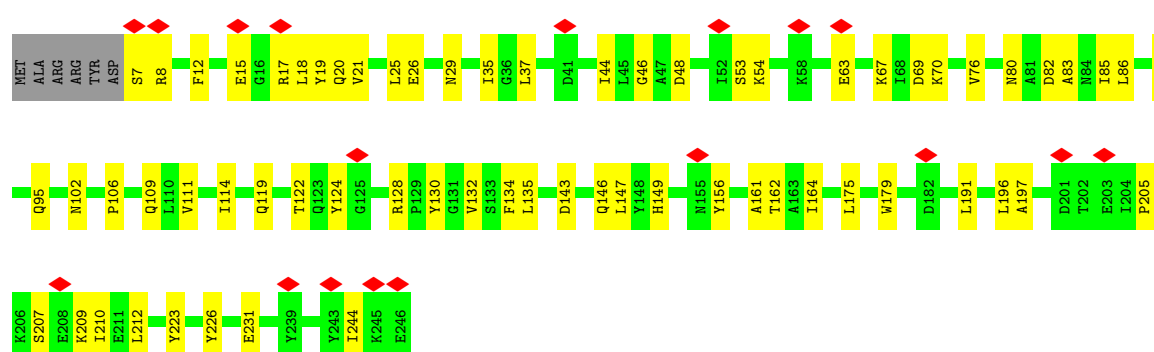
- Molecule 2: 20S proteasome alpha-2 subunit



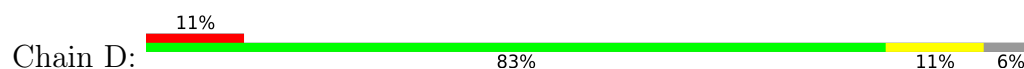
- Molecule 3: 20S proteasome alpha-3 subunit

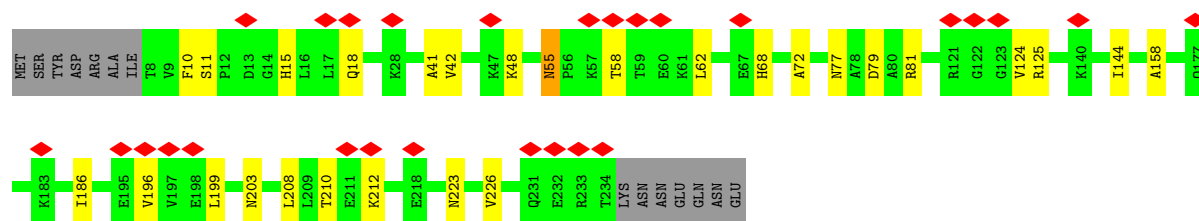


- Molecule 3: 20S proteasome alpha-3 subunit

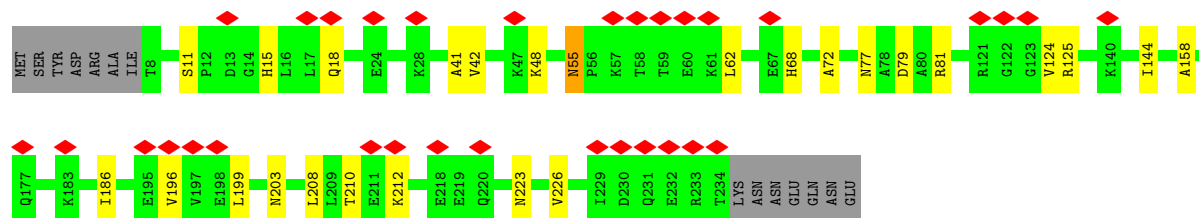
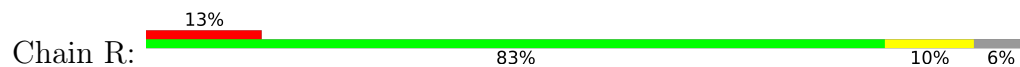


- Molecule 4: 20S proteasome alpha-4 subunit

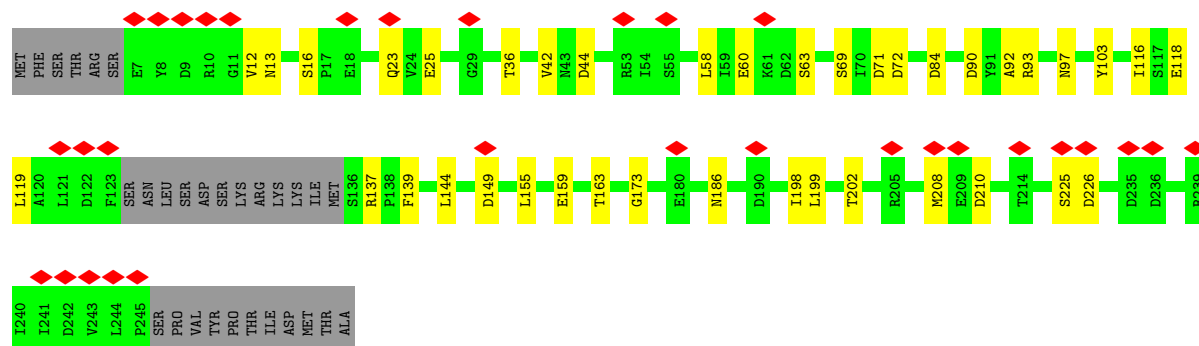
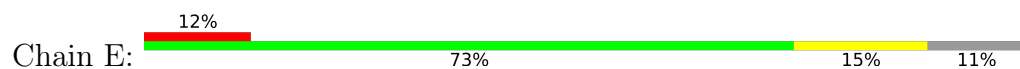




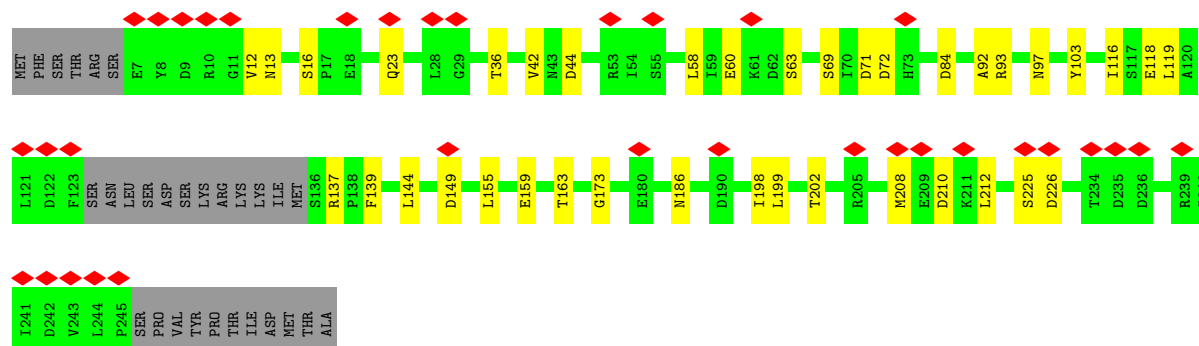
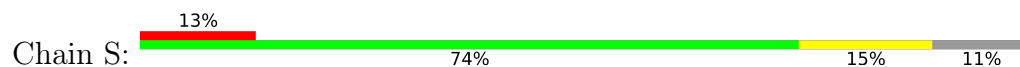
• Molecule 4: 20S proteasome alpha-4 subunit



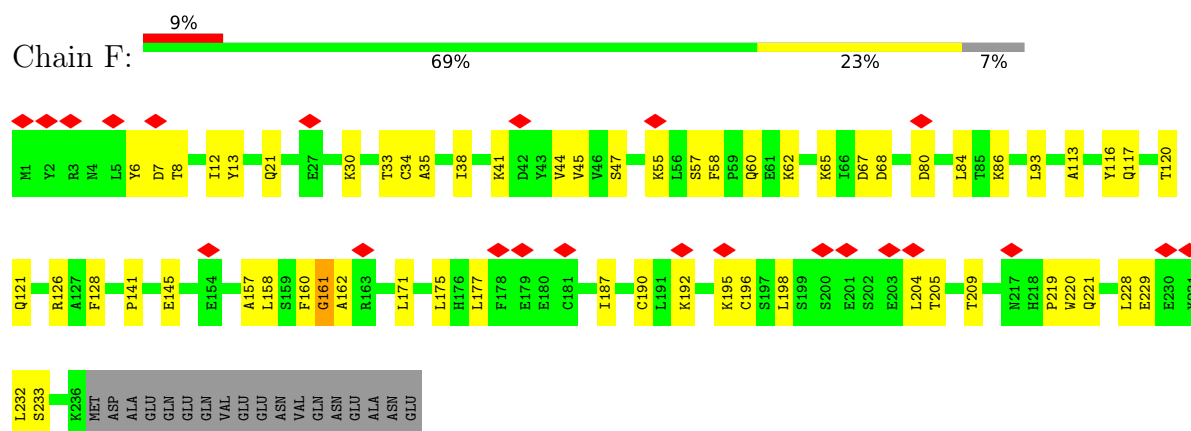
• Molecule 5: 20S proteasome alpha-5 subunit



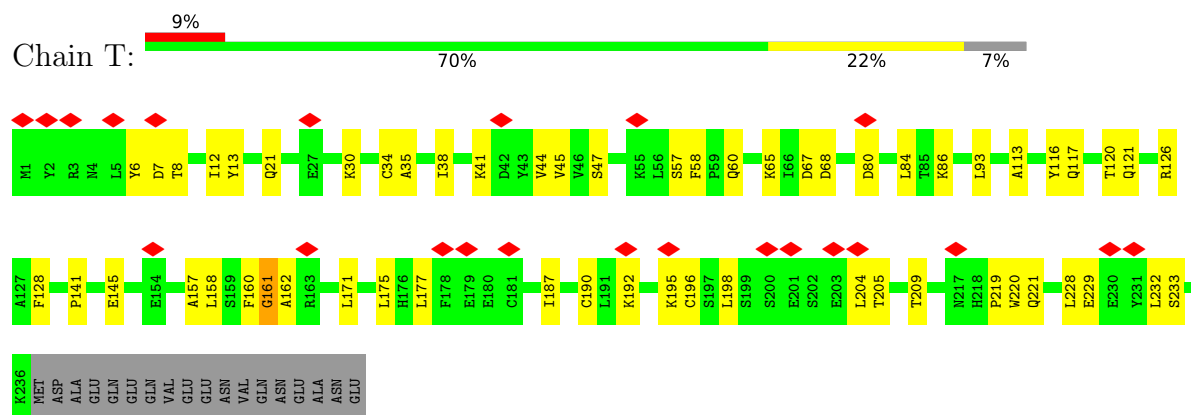
• Molecule 5: 20S proteasome alpha-5 subunit



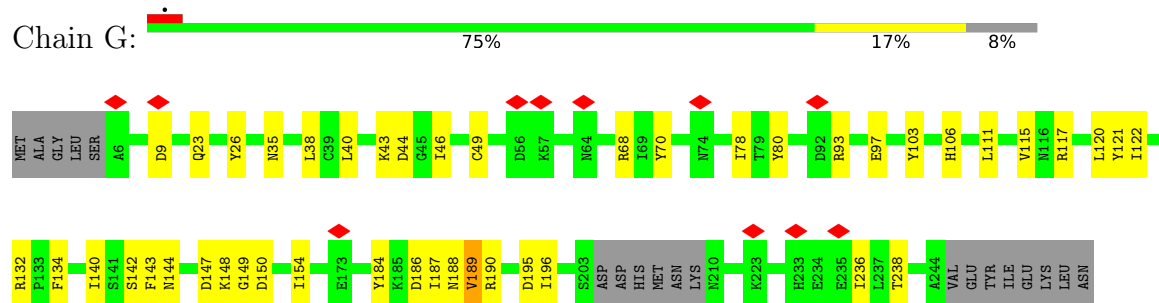
• Molecule 6: 20S proteasome alpha-6 subunit



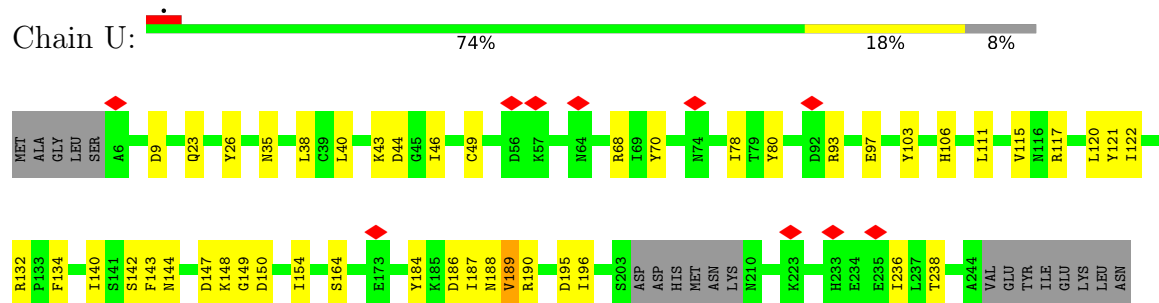
- Molecule 6: 20S proteasome alpha-6 subunit



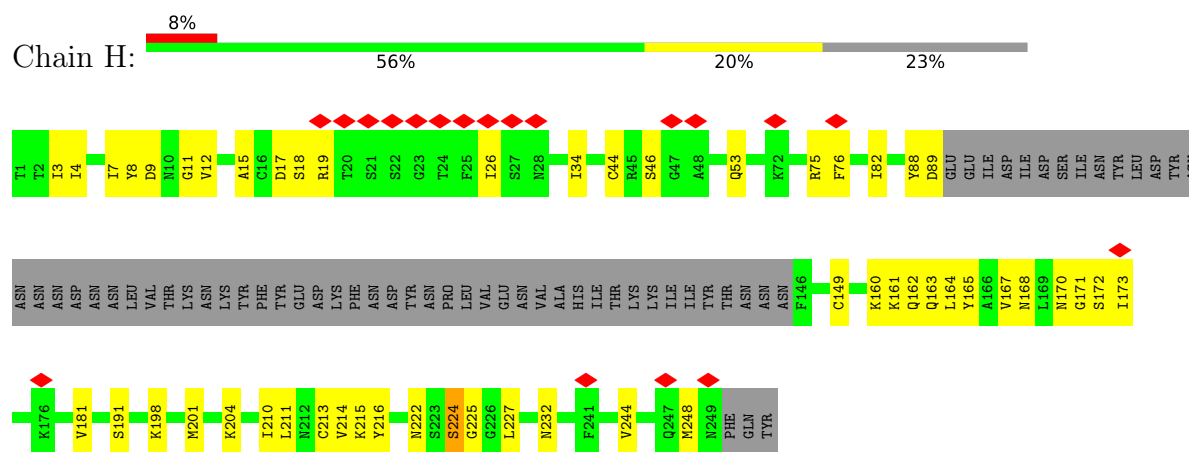
- Molecule 7: 20S proteasome alpha-7 subunit



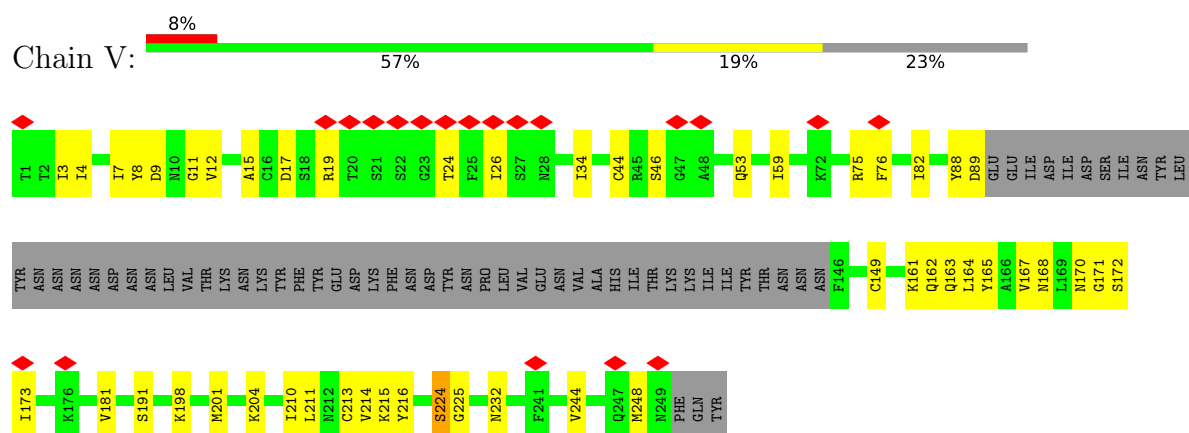
- Molecule 7: 20S proteasome alpha-7 subunit



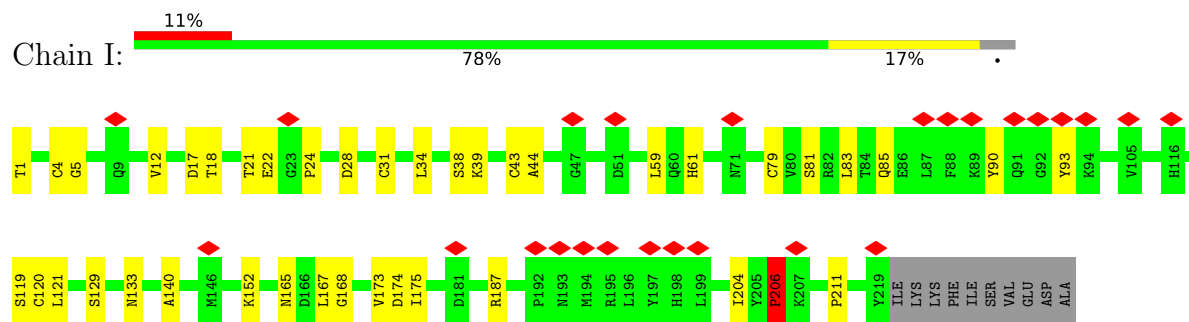
- Molecule 8: 20S proteasome beta-1 subunit



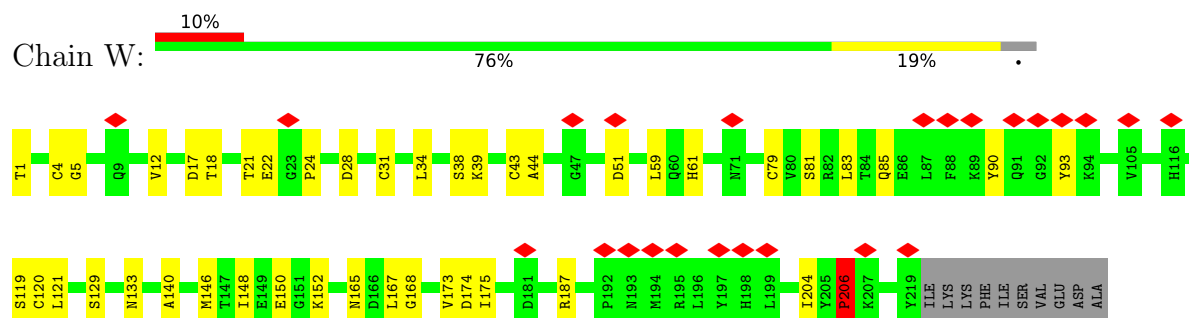
• Molecule 8: 20S proteasome beta-1 subunit



• Molecule 9: 20S proteasome beta-2 subunit

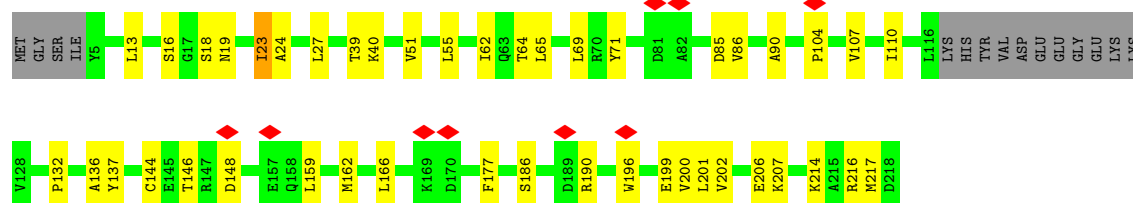


• Molecule 9: 20S proteasome beta-2 subunit



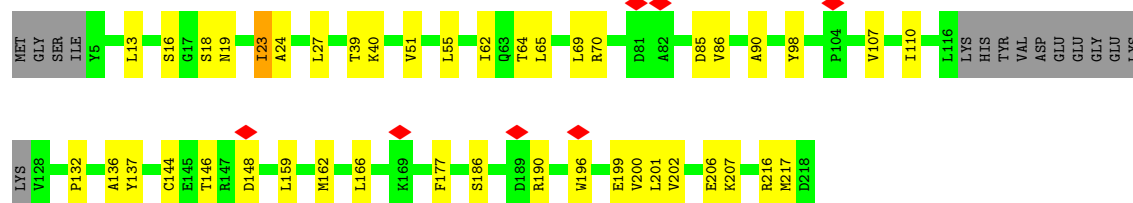
- Molecule 10: 20S proteasome beta-3 subunit

Chain J:  73% 20% 7%



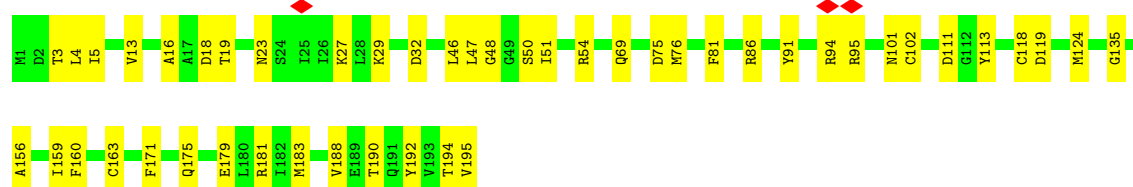
- Molecule 10: 20S proteasome beta-3 subunit

Chain X:  73% 19% 7%



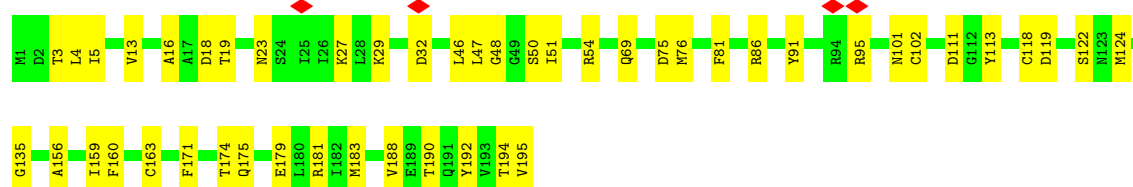
- Molecule 11: 20S proteasome beta-4 subunit

Chain K:  76% 24%



- Molecule 11: 20S proteasome beta-4 subunit

Chain Y:  75% 25%



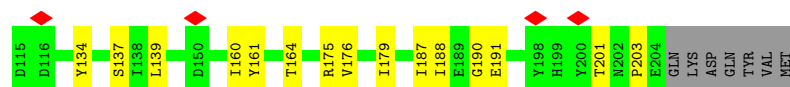
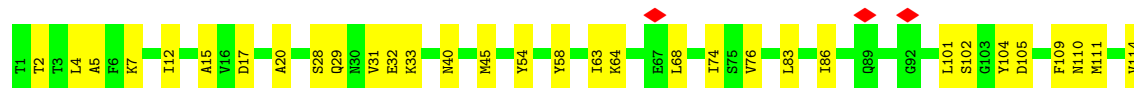
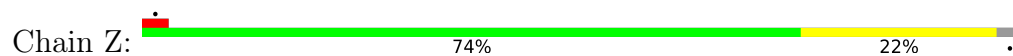
- Molecule 12: 20S proteasome beta-5 subunit

Chain L:  73% 23%

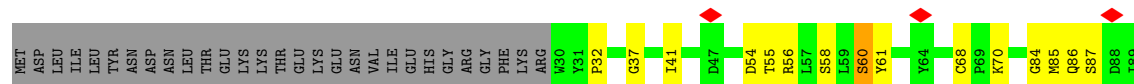




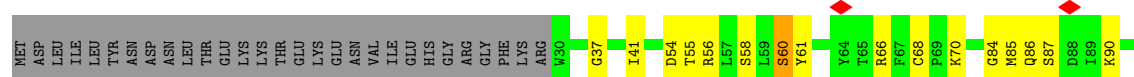
- Molecule 12: 20S proteasome beta-5 subunit



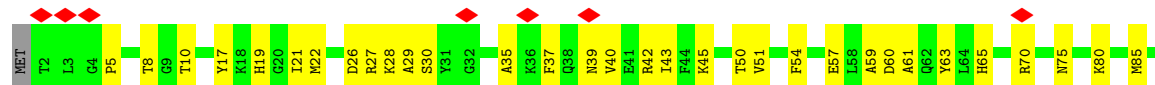
- Molecule 13: 20S proteasome beta-6 subunit

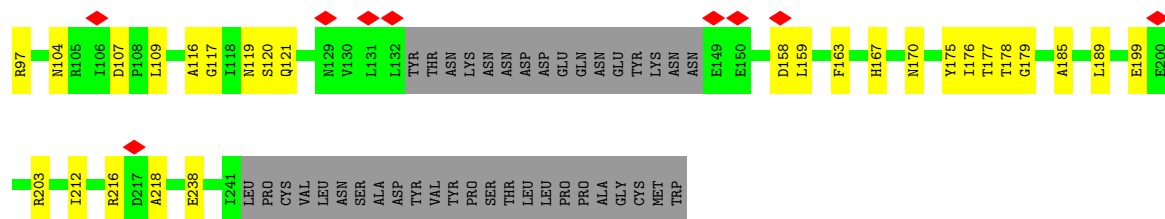


- Molecule 13: 20S proteasome beta-6 subunit

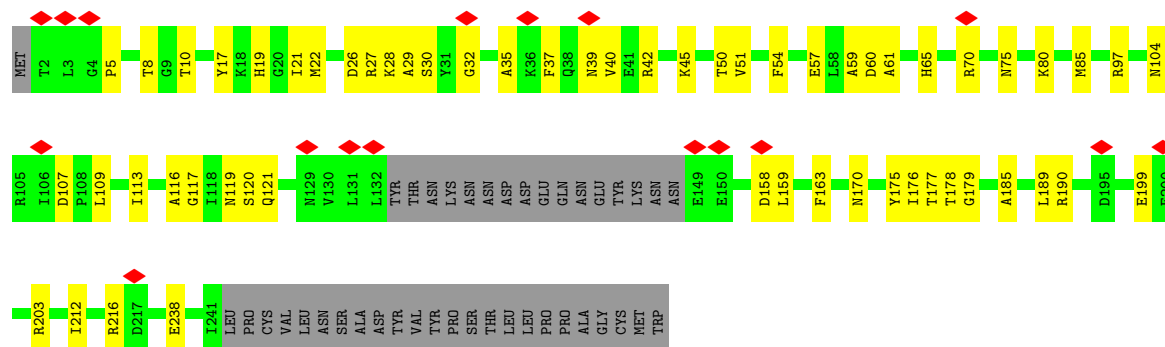


- Molecule 14: 20S proteasome beta-7 subunit

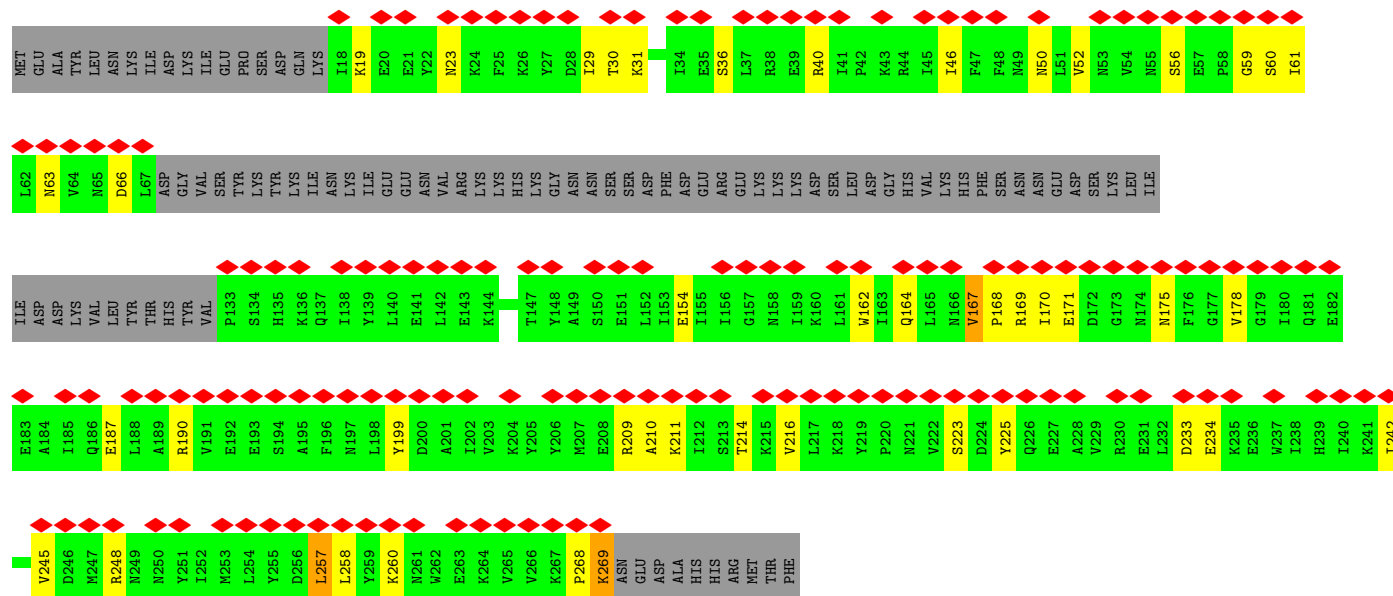




• Molecule 14: 20S proteasome beta-7 subunit



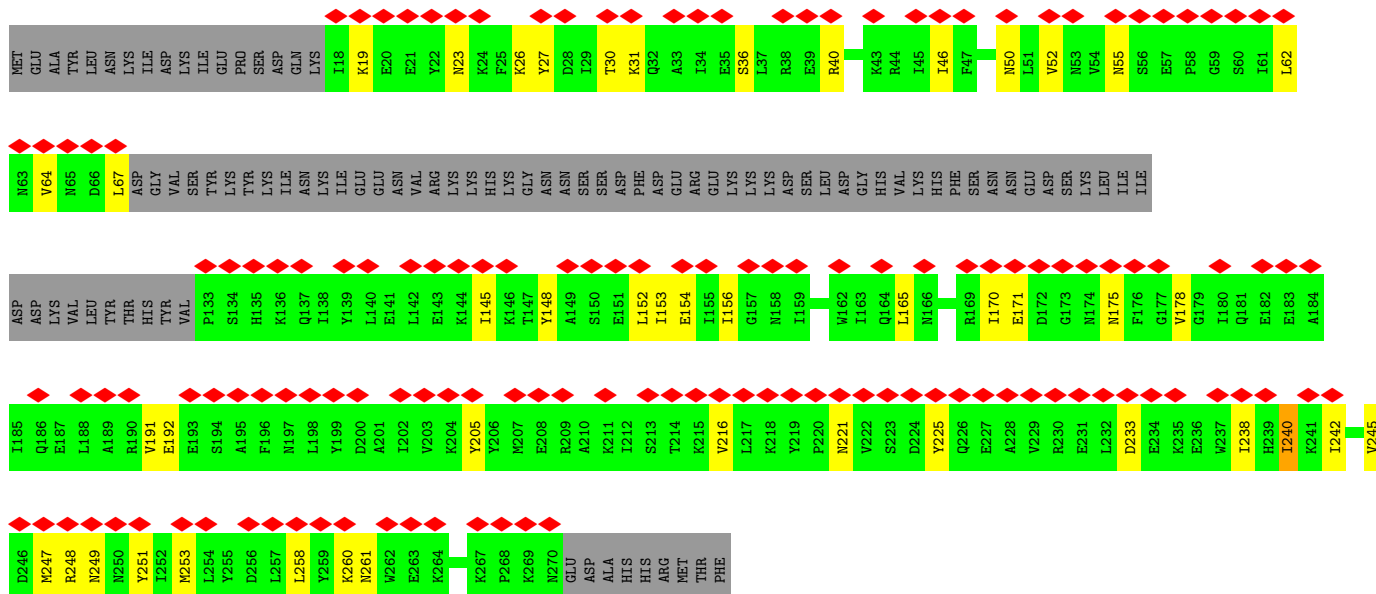
• Molecule 15: Proteasome activator PA28



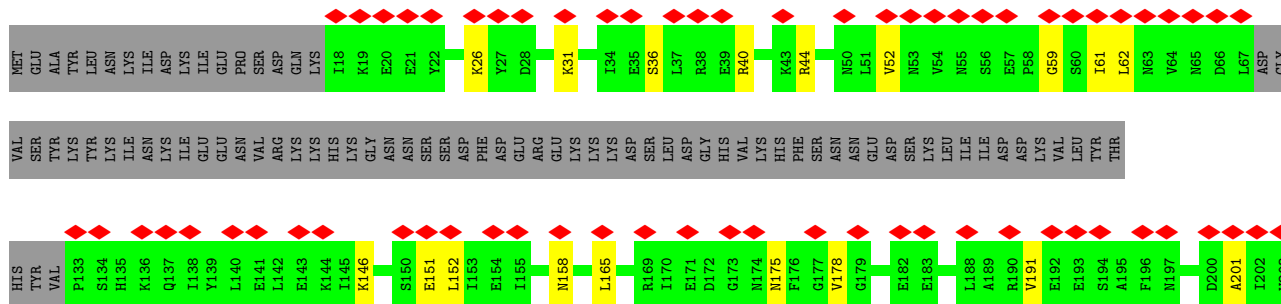
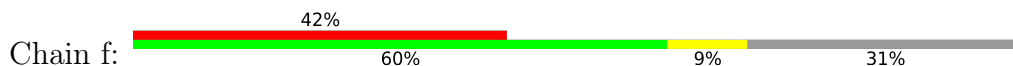
• Molecule 15: Proteasome activator PA28

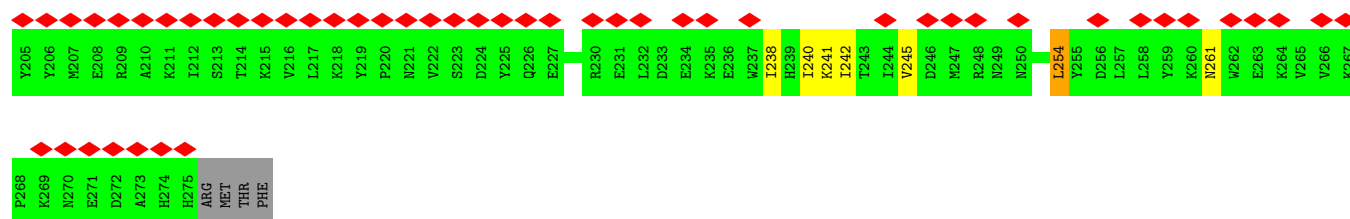


- Molecule 15: Proteasome activator PA28

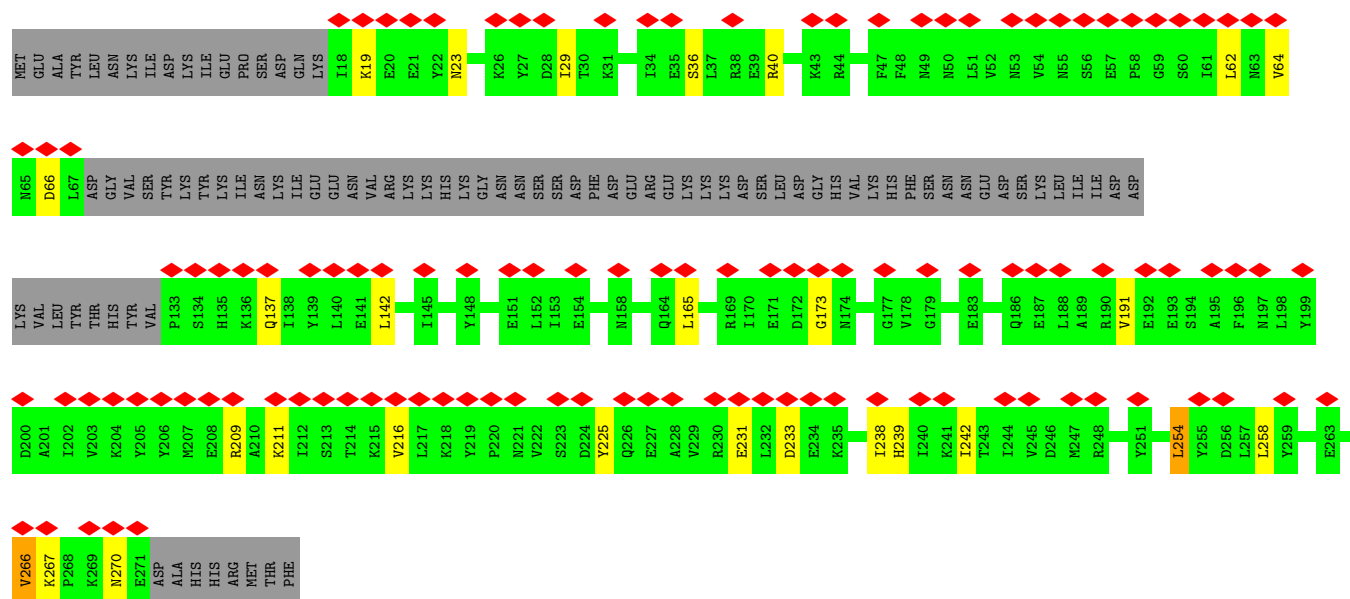
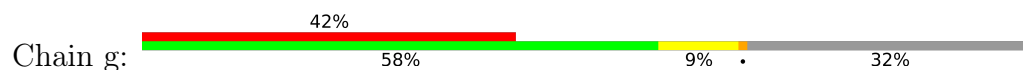


- Molecule 15: Proteasome activator PA28

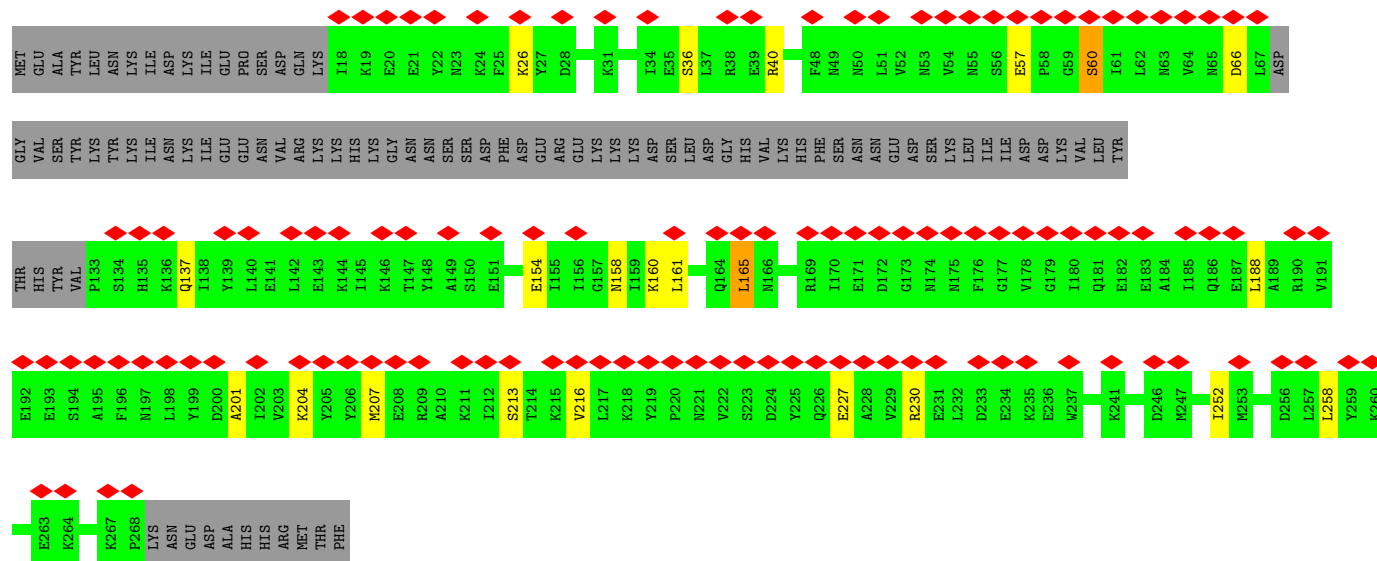
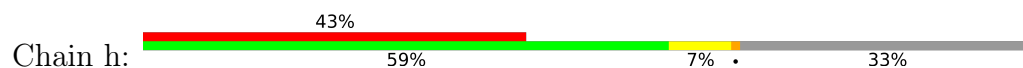




• Molecule 15: Proteasome activator PA28

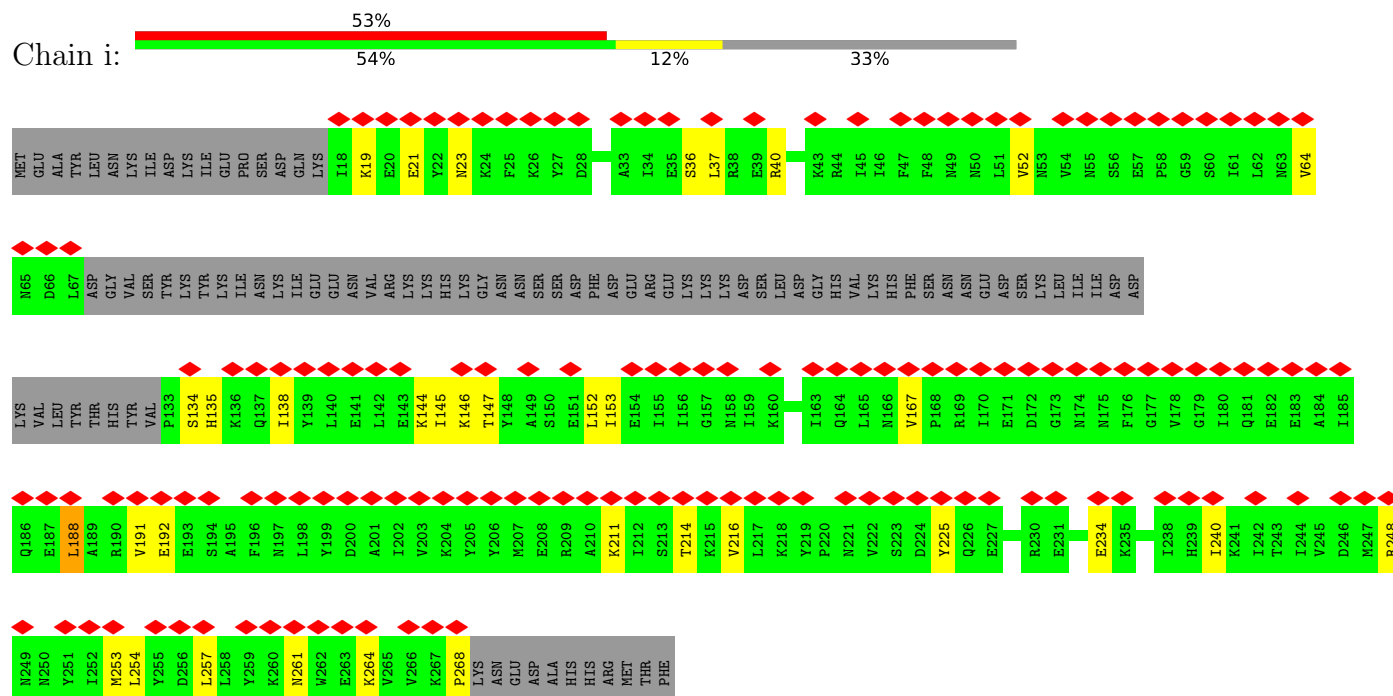


• Molecule 15: Proteasome activator PA28



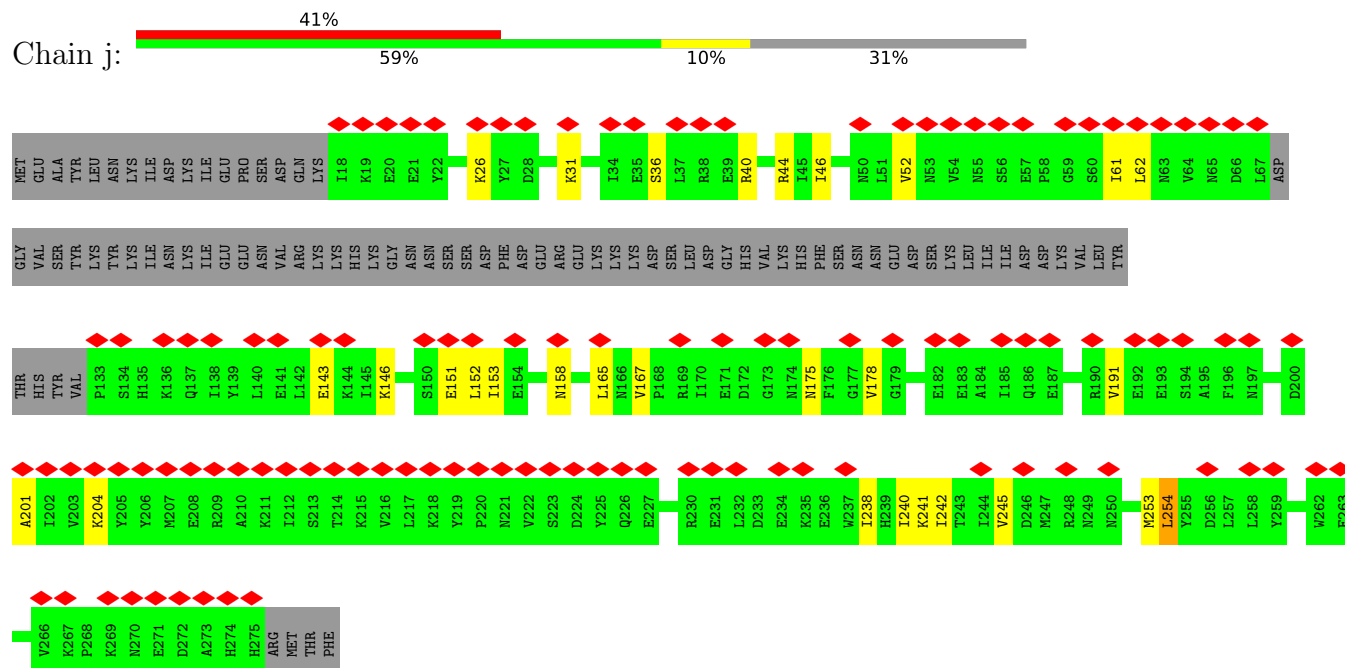
- Molecule 15: Proteasome activator PA28

Chain i:



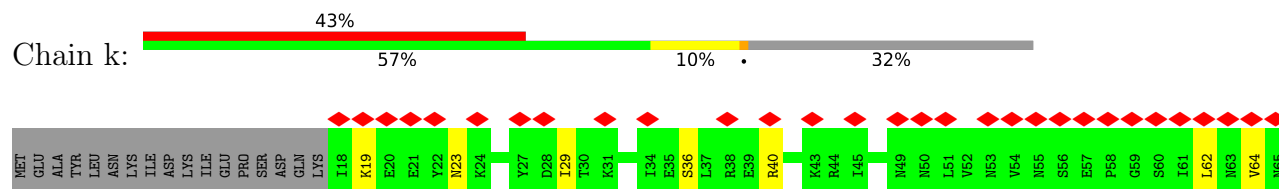
- Molecule 15: Proteasome activator PA28

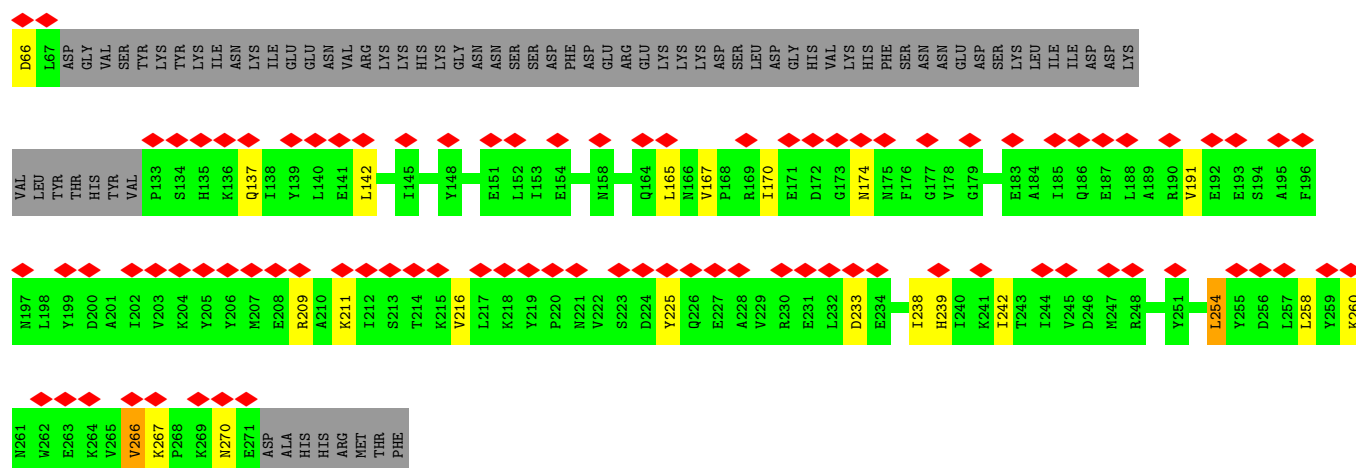
Chain j:



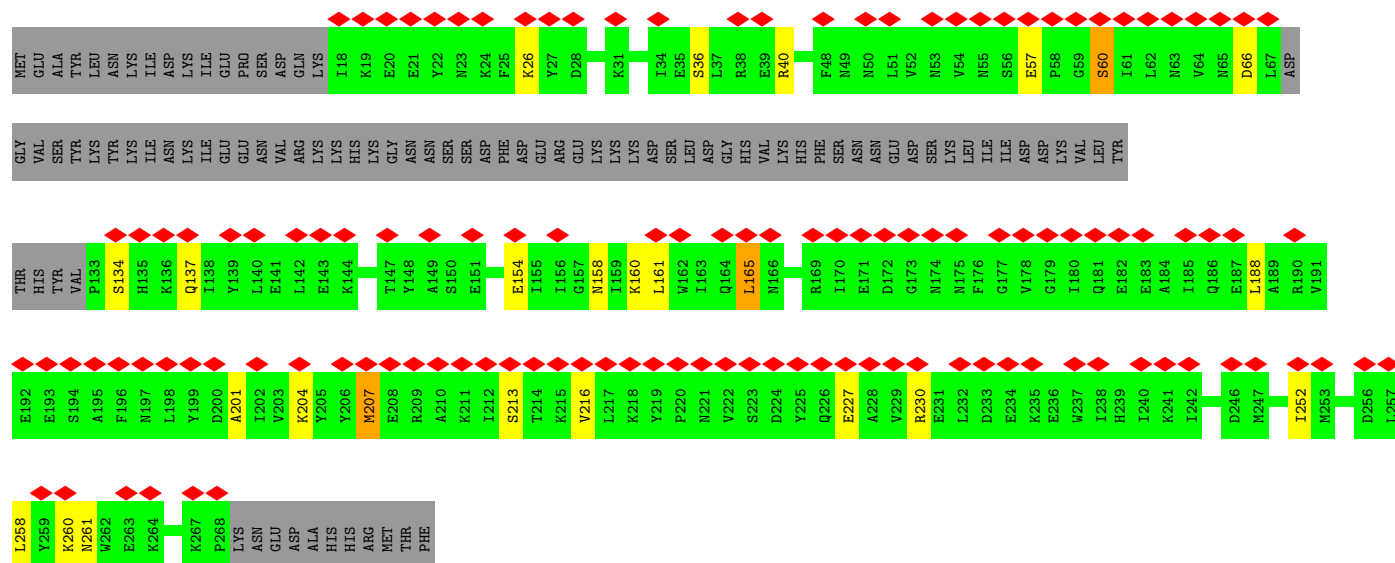
- Molecule 15: Proteasome activator PA28

Chain k:

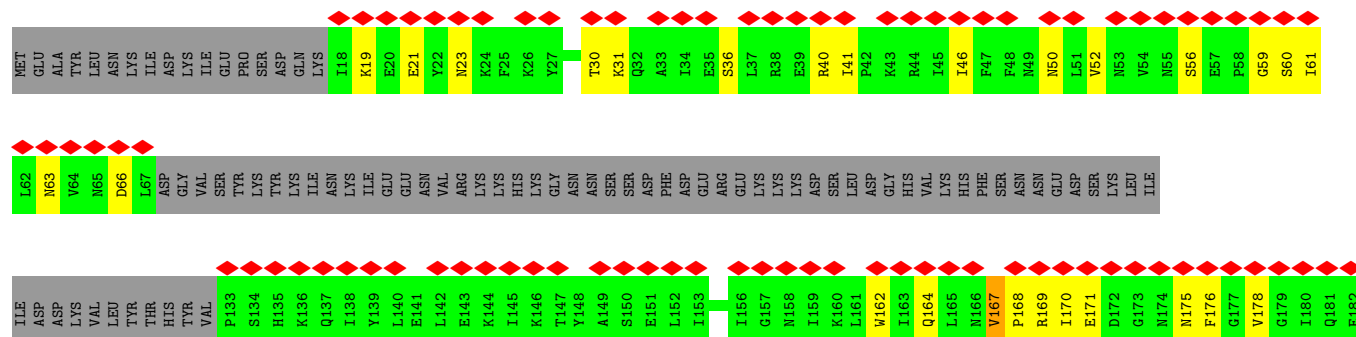


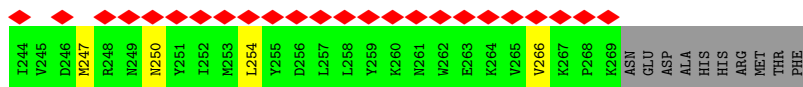


• Molecule 15: Proteasome activator PA28

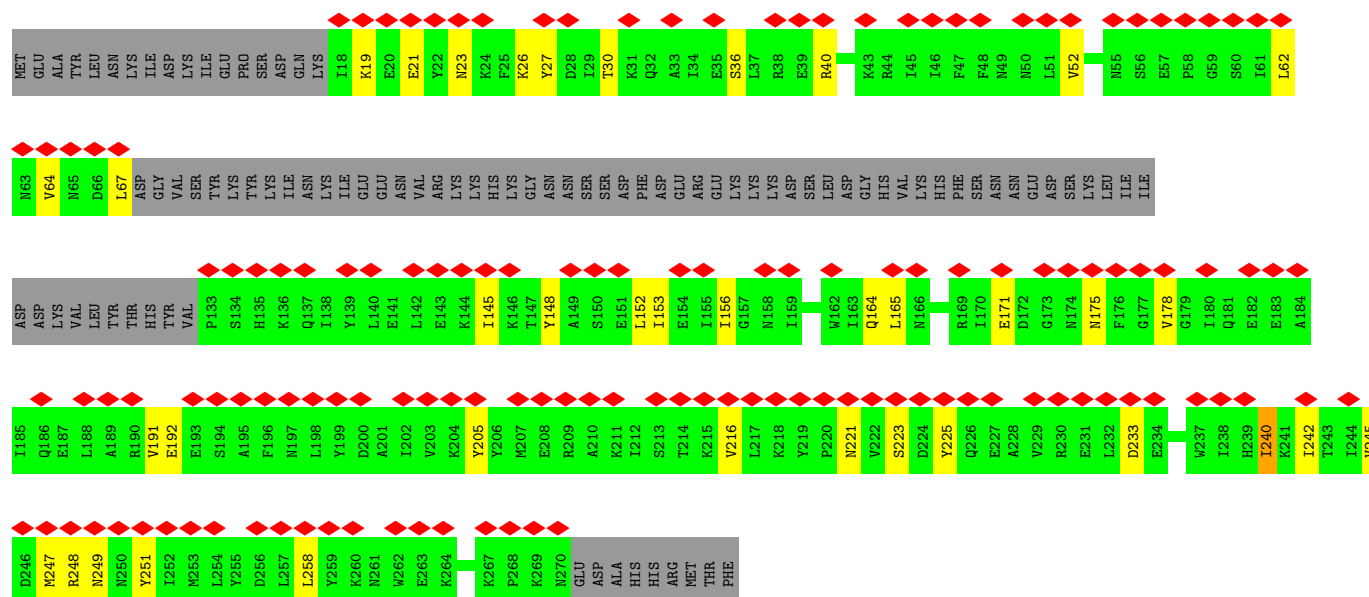


• Molecule 15: Proteasome activator PA28





Chain p:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	27516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	29.237	Depositor
Minimum map value	-16.919	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	450.63998, 450.63998, 450.63998	wwPDB
Map dimensions	344, 344, 344	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.31, 1.31, 1.31	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	A	0.40	0/1968	0.73	0/2652
1	O	0.39	0/1968	0.73	0/2652
2	B	0.39	0/1814	0.66	0/2450
2	P	0.39	0/1814	0.66	0/2450
3	C	0.43	0/1952	0.76	0/2643
3	Q	0.43	0/1952	0.76	0/2643
4	D	0.39	0/1824	0.72	0/2461
4	R	0.39	0/1824	0.72	0/2461
5	E	0.35	0/1784	0.63	0/2410
5	S	0.35	0/1784	0.63	0/2410
6	F	0.42	0/1913	0.71	4/2576 (0.2%)
6	T	0.42	0/1913	0.71	4/2576 (0.2%)
7	G	0.43	0/1947	0.78	3/2631 (0.1%)
7	U	0.43	0/1947	0.78	3/2631 (0.1%)
8	H	0.42	0/1559	0.78	2/2089 (0.1%)
8	V	0.42	0/1559	0.78	2/2089 (0.1%)
9	I	0.37	0/1712	0.67	2/2328 (0.1%)
9	W	0.37	0/1712	0.67	2/2328 (0.1%)
10	J	0.49	0/1621	0.73	0/2189
10	X	0.49	0/1621	0.74	0/2189
11	K	0.53	0/1649	0.71	0/2223
11	Y	0.53	0/1649	0.72	0/2223
12	L	0.48	0/1633	0.76	3/2202 (0.1%)
12	Z	0.48	0/1633	0.76	3/2202 (0.1%)
13	M	0.45	0/1708	0.75	2/2314 (0.1%)
13	a	0.45	0/1708	0.75	2/2314 (0.1%)
14	N	0.38	0/1882	0.71	3/2538 (0.1%)
14	b	0.38	0/1882	0.71	3/2538 (0.1%)
15	c	0.31	0/1597	0.78	1/2154 (0.0%)
15	d	0.31	0/1597	0.77	0/2154
15	e	0.31	0/1605	0.76	0/2165
15	f	0.31	0/1649	0.76	0/2225
15	g	0.32	0/1614	0.79	0/2177
15	h	0.31	0/1588	0.78	0/2143

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	i	0.31	0/1588	0.78	0/2143
15	j	0.31	0/1649	0.76	0/2225
15	k	0.32	0/1614	0.79	0/2177
15	l	0.31	0/1588	0.78	0/2143
15	m	0.30	0/1597	0.78	1/2154 (0.0%)
15	n	0.31	0/1588	0.78	0/2143
15	o	0.31	0/1597	0.77	0/2154
15	p	0.31	0/1605	0.76	0/2165
All	All	0.39	0/72408	0.74	40/97734 (0.0%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	232	VAL	CA-CB-CG1	7.08	122.44	110.40
13	a	232	VAL	CA-CB-CG1	7.07	122.42	110.40
6	T	161	GLY	N-CA-C	6.87	129.47	113.18
6	F	161	GLY	N-CA-C	6.85	129.42	113.18
12	Z	188	ILE	N-CA-C	6.71	123.29	109.34
12	L	188	ILE	N-CA-C	6.69	123.26	109.34
8	H	75	ARG	CA-C-N	6.68	134.31	121.54
8	H	75	ARG	C-N-CA	6.68	134.31	121.54
8	V	75	ARG	CA-C-N	6.67	134.28	121.54
8	V	75	ARG	C-N-CA	6.67	134.28	121.54
7	U	238	THR	CA-C-N	-6.57	111.69	120.96
7	U	238	THR	C-N-CA	-6.57	111.69	120.96
7	G	238	THR	CA-C-N	-6.56	111.70	120.96
7	G	238	THR	C-N-CA	-6.56	111.70	120.96
6	F	160	PHE	N-CA-C	5.96	117.15	107.32
13	a	232	VAL	CB-CA-C	5.95	121.05	111.29
13	M	232	VAL	CB-CA-C	5.94	121.03	111.29
6	T	160	PHE	N-CA-C	5.93	117.11	107.32
14	N	109	LEU	CA-CB-CG	5.70	136.24	116.30
14	b	109	LEU	CA-CB-CG	5.68	136.19	116.30
14	N	54	PHE	CA-C-N	5.63	132.29	121.54
14	N	54	PHE	C-N-CA	5.63	132.29	121.54
14	b	54	PHE	CA-C-N	5.62	132.28	121.54
14	b	54	PHE	C-N-CA	5.62	132.28	121.54
15	c	257	LEU	CA-CB-CG	5.50	135.57	116.30
15	m	257	LEU	CA-CB-CG	5.50	135.55	116.30
12	L	190	GLY	CA-C-N	5.31	131.68	121.54
12	L	190	GLY	C-N-CA	5.31	131.68	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	190	GLY	CA-C-N	5.31	131.68	121.54
12	Z	190	GLY	C-N-CA	5.31	131.68	121.54
9	I	206	PRO	CA-C-N	5.17	133.22	122.41
9	I	206	PRO	C-N-CA	5.17	133.22	122.41
9	W	206	PRO	CA-C-N	5.16	133.19	122.41
9	W	206	PRO	C-N-CA	5.16	133.19	122.41
6	T	8	THR	CA-C-N	5.12	131.31	121.54
6	T	8	THR	C-N-CA	5.12	131.31	121.54
6	F	8	THR	CA-C-N	5.11	131.31	121.54
6	F	8	THR	C-N-CA	5.11	131.31	121.54
7	U	189	VAL	N-CA-C	-5.09	107.78	111.90
7	G	189	VAL	N-CA-C	-5.07	107.80	111.90

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	A	1943	0	1946	33	0
1	O	1943	0	1946	32	0
2	B	1782	0	1810	31	0
2	P	1782	0	1810	30	0
3	C	1917	0	1918	41	0
3	Q	1917	0	1918	43	0
4	D	1795	0	1831	20	0
4	R	1795	0	1831	19	0
5	E	1760	0	1752	28	0
5	S	1760	0	1752	25	0
6	F	1878	0	1881	36	0
6	T	1878	0	1881	34	0
7	G	1906	0	1859	30	0
7	U	1906	0	1859	32	0
8	H	1536	0	1540	40	0
8	V	1536	0	1540	35	0
9	I	1676	0	1674	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	1676	0	1674	27	0
10	J	1595	0	1584	32	0
10	X	1595	0	1584	30	0
11	K	1614	0	1584	28	0
11	Y	1614	0	1584	29	0
12	L	1600	0	1558	35	0
12	Z	1600	0	1558	33	0
13	M	1676	0	1681	32	0
13	a	1676	0	1681	32	0
14	N	1845	0	1814	41	0
14	b	1845	0	1814	40	0
15	c	1568	0	1598	31	0
15	d	1568	0	1598	30	0
15	e	1576	0	1604	29	0
15	f	1618	0	1633	15	0
15	g	1585	0	1610	14	0
15	h	1559	0	1585	12	0
15	i	1559	0	1585	19	0
15	j	1618	0	1633	17	0
15	k	1585	0	1610	17	0
15	l	1559	0	1585	16	0
15	m	1568	0	1598	25	0
15	n	1559	0	1585	19	0
15	o	1568	0	1598	23	0
15	p	1576	0	1604	24	0
All	All	71112	0	71290	1062	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 (1062) 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)
15:c:164:GLN:HG3	15:d:253:MET:HG2	1.50	0.93
2:B:34:PRO:HA	2:B:164:GLY:HA3	1.72	0.71
2:P:34:PRO:HA	2:P:164:GLY:HA3	1.72	0.71
15:l:26:LYS:HE3	15:l:165:LEU:HD12	1.72	0.70
15:h:26:LYS:HE3	15:h:165:LEU:HD12	1.72	0.70
5:S:97:ASN:HD21	12:Z:64:LYS:HB3	1.58	0.68
5:E:97:ASN:HD21	12:L:64:LYS:HB3	1.58	0.68
15:c:216:VAL:HG22	15:c:225:TYR:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:m:216:VAL:HG22	15:m:225:TYR:HB3	1.77	0.67
15:i:216:VAL:HG22	15:i:225:TYR:HB3	1.76	0.66
8:H:88:TYR:HH	8:H:149:CYS:HG	1.44	0.66
14:N:50:THR:HG22	14:N:117:GLY:HA3	1.78	0.66
15:n:216:VAL:HG22	15:n:225:TYR:HB3	1.76	0.66
14:b:50:THR:HG22	14:b:117:GLY:HA3	1.78	0.66
15:d:216:VAL:HG22	15:d:225:TYR:HB3	1.78	0.65
15:o:216:VAL:HG22	15:o:225:TYR:HB3	1.78	0.65
4:R:18:GLN:HE22	3:Q:12:PHE:H	1.44	0.64
8:V:88:TYR:HH	8:V:149:CYS:HG	1.46	0.63
13:a:55:THR:HB	13:a:68:CYS:H	1.63	0.63
6:F:229:GLU:HA	6:F:233:SER:HB2	1.79	0.63
6:T:229:GLU:HA	6:T:233:SER:HB2	1.79	0.63
13:M:55:THR:HB	13:M:68:CYS:H	1.63	0.63
15:i:145:ILE:HG13	15:i:240:ILE:HD12	1.81	0.62
15:n:145:ILE:HG13	15:n:240:ILE:HD12	1.81	0.62
2:P:179:ASN:H	2:P:182:ILE:HD11	1.64	0.62
8:V:15:ALA:HB2	8:V:210:ILE:HD12	1.81	0.62
2:B:179:ASN:H	2:B:182:ILE:HD11	1.65	0.62
8:H:15:ALA:HB2	8:H:210:ILE:HD12	1.81	0.62
15:c:29:ILE:HD13	15:d:54:VAL:HG21	1.79	0.62
15:o:153:ILE:HD12	15:p:242:ILE:HD11	1.81	0.62
11:K:23:ASN:HB2	11:K:29:LYS:HG2	1.81	0.61
12:L:32:GLU:HA	12:L:175:ARG:HH12	1.65	0.61
12:L:63:ILE:HD12	12:L:74:ILE:HG21	1.81	0.61
12:Z:32:GLU:HA	12:Z:175:ARG:HH12	1.65	0.61
12:Z:63:ILE:HD12	12:Z:74:ILE:HG21	1.81	0.61
7:G:38:LEU:HB3	7:G:49:CYS:HB3	1.80	0.61
4:D:55:ASN:OD1	4:D:55:ASN:N	2.33	0.61
9:I:18:THR:HB	9:I:31:CYS:H	1.65	0.61
4:R:55:ASN:OD1	4:R:55:ASN:N	2.33	0.61
9:W:18:THR:HB	9:W:31:CYS:H	1.65	0.61
8:H:198:LYS:H	8:H:201:MET:HE3	1.63	0.61
8:V:198:LYS:H	8:V:201:MET:HE3	1.63	0.61
11:Y:23:ASN:HB2	11:Y:29:LYS:HG2	1.81	0.61
7:U:38:LEU:HB3	7:U:49:CYS:HB3	1.80	0.61
10:J:64:THR:OG1	11:K:86:ARG:NH2	2.34	0.61
6:F:192:LYS:NZ	6:F:196:CYS:SG	2.73	0.61
11:K:5:ILE:HB	11:K:16:ALA:HB3	1.82	0.61
15:e:216:VAL:HG22	15:e:225:TYR:HB3	1.82	0.61
13:M:37:GLY:O	13:M:70:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:5:ILE:HB	11:Y:16:ALA:HB3	1.82	0.61
13:a:37:GLY:O	13:a:70:LYS:NZ	2.33	0.61
15:c:260:LYS:NZ	15:i:167:VAL:O	2.31	0.61
15:p:216:VAL:HG22	15:p:225:TYR:HB3	1.82	0.61
6:T:192:LYS:NZ	6:T:196:CYS:SG	2.73	0.61
15:d:171:GLU:O	15:d:175:ASN:ND2	2.34	0.60
15:o:171:GLU:O	15:o:175:ASN:ND2	2.34	0.60
7:G:190:ARG:HH12	7:G:236:ILE:HD12	1.67	0.60
7:U:190:ARG:HH12	7:U:236:ILE:HD12	1.67	0.60
5:E:36:THR:HA	5:E:173:GLY:HA3	1.83	0.60
5:S:13:ASN:HB3	6:T:126:ARG:HB3	1.84	0.60
14:b:107:ASP:OD1	14:b:107:ASP:N	2.34	0.60
14:N:107:ASP:OD1	14:N:107:ASP:N	2.34	0.60
5:S:36:THR:HA	5:S:173:GLY:HA3	1.83	0.60
3:Q:90:SER:HB2	3:Q:114:ILE:HD12	1.83	0.60
5:E:208:MET:HG3	5:E:210:ASP:H	1.67	0.59
3:C:90:SER:HB2	3:C:114:ILE:HD12	1.83	0.59
8:H:8:TYR:OH	8:H:232:ASN:ND2	2.34	0.59
2:P:232:ILE:HG13	2:P:233:GLU:HG3	1.84	0.59
5:S:208:MET:HG3	5:S:210:ASP:H	1.67	0.59
15:k:267:LYS:HG2	15:k:270:ASN:HD22	1.67	0.59
8:V:8:TYR:OH	8:V:232:ASN:ND2	2.34	0.59
6:F:13:TYR:OH	7:G:132:ARG:NH1	2.35	0.59
2:B:232:ILE:HG13	2:B:233:GLU:HG3	1.84	0.59
3:C:18:LEU:HB2	3:C:21:VAL:HG12	1.85	0.59
3:Q:18:LEU:HB2	3:Q:21:VAL:HG12	1.85	0.59
15:g:267:LYS:HG2	15:g:270:ASN:HD22	1.67	0.59
15:f:36:SER:HA	15:f:40:ARG:HB2	1.84	0.59
15:j:36:SER:HA	15:j:40:ARG:HB2	1.84	0.59
1:O:50:ILE:HG12	1:O:147:ILE:HD12	1.85	0.59
1:A:50:ILE:HG12	1:A:147:ILE:HD12	1.85	0.58
12:L:33:LYS:HD3	12:L:45:MET:HG3	1.83	0.58
14:N:28:LYS:HE2	14:N:30:SER:HB3	1.86	0.58
12:Z:33:LYS:HD3	12:Z:45:MET:HG3	1.83	0.58
2:P:82:ASP:OD1	1:O:129:GLN:NE2	2.37	0.58
14:b:28:LYS:HE2	14:b:30:SER:HB3	1.86	0.58
15:c:154:GLU:OE1	15:d:59:GLY:N	2.29	0.58
15:g:19:LYS:O	15:g:23:ASN:ND2	2.36	0.58
3:C:122:THR:O	4:D:125:ARG:NH1	2.36	0.58
9:I:81:SER:O	9:I:85:GLN:NE2	2.36	0.58
6:F:34:CYS:SG	6:F:35:ALA:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:106:HIS:HB2	8:H:82:ILE:HG21	1.85	0.58
14:N:178:THR:OG1	14:N:179:GLY:N	2.36	0.58
6:T:34:CYS:SG	6:T:35:ALA:N	2.77	0.58
5:S:12:VAL:HG13	5:S:23:GLN:HG2	1.84	0.58
14:b:178:THR:OG1	14:b:179:GLY:N	2.36	0.58
12:Z:83:LEU:HD12	12:Z:101:LEU:HD11	1.86	0.58
5:E:12:VAL:HG13	5:E:23:GLN:HG2	1.84	0.58
5:E:149:ASP:N	5:E:149:ASP:OD1	2.36	0.58
12:L:83:LEU:HD12	12:L:101:LEU:HD11	1.86	0.58
5:S:149:ASP:OD1	5:S:149:ASP:N	2.36	0.58
9:W:81:SER:O	9:W:85:GLN:NE2	2.36	0.58
7:G:43:LYS:HB3	7:G:186:ASP:HA	1.84	0.58
13:M:127:ARG:NH1	13:M:130:PHE:O	2.37	0.58
13:a:127:ARG:NH1	13:a:130:PHE:O	2.37	0.58
15:e:19:LYS:O	15:e:23:ASN:ND2	2.35	0.58
15:p:19:LYS:O	15:p:23:ASN:ND2	2.35	0.58
12:L:12:ILE:HD11	12:L:109:PHE:HB3	1.84	0.58
14:N:216:ARG:NH1	8:V:26:ILE:O	2.37	0.58
7:U:43:LYS:HB3	7:U:186:ASP:HA	1.84	0.58
14:b:29:ALA:HB3	14:b:37:PHE:HB2	1.85	0.57
12:Z:12:ILE:HD11	12:Z:109:PHE:HB3	1.84	0.57
14:N:29:ALA:HB3	14:N:37:PHE:HB2	1.85	0.57
7:G:103:TYR:OH	14:N:70:ARG:NE	2.32	0.57
8:V:17:ASP:HB2	8:V:225:GLY:HA3	1.85	0.57
15:c:210:ALA:HB2	15:d:224:ASP:HB2	1.86	0.57
4:D:79:ASP:OD2	4:D:125:ARG:NH2	2.38	0.57
8:H:17:ASP:HB2	8:H:225:GLY:HA3	1.85	0.57
14:N:45:LYS:HA	14:N:51:VAL:HG12	1.86	0.57
4:R:79:ASP:OD2	4:R:125:ARG:NH2	2.38	0.57
14:b:45:LYS:HA	14:b:51:VAL:HG12	1.86	0.57
14:N:27:ARG:NH1	14:N:238:GLU:OE2	2.37	0.57
5:S:42:VAL:HG23	5:S:44:ASP:H	1.70	0.57
5:E:42:VAL:HG23	5:E:44:ASP:H	1.70	0.57
7:G:40:LEU:HD21	7:G:196:ILE:HD11	1.87	0.57
11:K:51:ILE:HG12	11:K:54:ARG:HH21	1.70	0.57
12:L:12:ILE:HB	12:L:179:ILE:HD12	1.86	0.57
11:Y:51:ILE:HG12	11:Y:54:ARG:HH21	1.70	0.57
14:b:27:ARG:NH1	14:b:238:GLU:OE2	2.37	0.57
3:C:212:LEU:HB2	3:C:226:TYR:HD2	1.69	0.57
10:X:85:ASP:N	10:X:85:ASP:OD1	2.37	0.57
12:Z:12:ILE:HB	12:Z:179:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:40:LEU:HD21	7:U:196:ILE:HD11	1.87	0.57
11:K:76:MET:HE2	11:K:81:PHE:HA	1.87	0.57
11:Y:76:MET:HE2	11:Y:81:PHE:HA	1.87	0.57
15:d:19:LYS:O	15:d:23:ASN:ND2	2.37	0.57
15:k:19:LYS:O	15:k:23:ASN:ND2	2.36	0.57
3:Q:212:LEU:HB2	3:Q:226:TYR:HD2	1.69	0.57
1:A:129:GLN:NE2	2:B:82:ASP:OD1	2.38	0.57
10:J:85:ASP:OD1	10:J:85:ASP:N	2.37	0.57
15:g:165:LEU:HD21	15:h:252:ILE:HG12	1.87	0.57
15:o:19:LYS:O	15:o:23:ASN:ND2	2.37	0.57
9:I:174:ASP:HB3	9:I:187:ARG:HG2	1.87	0.56
9:W:174:ASP:HB3	9:W:187:ARG:HG2	1.87	0.56
13:M:183:GLN:HG3	13:M:188:ILE:HG23	1.86	0.56
4:R:79:ASP:OD2	3:Q:119:GLN:NE2	2.38	0.56
13:a:183:GLN:HG3	13:a:188:ILE:HG23	1.87	0.56
15:c:19:LYS:O	15:c:23:ASN:ND2	2.38	0.56
14:b:17:TYR:HE1	14:b:22:MET:HB2	1.71	0.56
2:B:39:ARG:NH2	2:B:144:TYR:O	2.39	0.56
2:B:42:ASN:ND2	2:B:183:GLU:OE2	2.38	0.56
14:N:17:TYR:HE1	14:N:22:MET:HB2	1.71	0.56
2:P:39:ARG:NH2	2:P:144:TYR:O	2.39	0.56
15:o:36:SER:HA	15:o:40:ARG:HB2	1.88	0.56
8:H:19:ARG:HB2	8:H:225:GLY:HA2	1.88	0.56
8:V:19:ARG:HB2	8:V:225:GLY:HA2	1.88	0.56
15:d:36:SER:HA	15:d:40:ARG:HB2	1.88	0.56
2:P:42:ASN:ND2	2:P:183:GLU:OE2	2.38	0.56
15:c:36:SER:HA	15:c:40:ARG:HB2	1.88	0.56
6:T:13:TYR:OH	7:U:132:ARG:NH1	2.38	0.56
8:H:34:ILE:HG13	8:H:44:CYS:HB3	1.88	0.56
8:H:167:VAL:HG22	8:H:172:SER:HB2	1.87	0.56
8:V:167:VAL:HG22	8:V:172:SER:HB2	1.87	0.56
3:C:156:TYR:HH	4:D:58:THR:HG1	1.53	0.56
14:N:26:ASP:OD1	14:N:42:ARG:NH2	2.39	0.56
8:V:34:ILE:HG13	8:V:44:CYS:HB3	1.88	0.56
8:V:82:ILE:HG21	7:U:106:HIS:HB2	1.86	0.56
15:m:36:SER:HA	15:m:40:ARG:HB2	1.88	0.56
15:m:19:LYS:O	15:m:23:ASN:ND2	2.38	0.56
14:b:26:ASP:OD1	14:b:42:ARG:NH2	2.39	0.56
4:R:81:ARG:HE	3:Q:156:TYR:HE1	1.55	0.55
15:c:46:ILE:O	15:c:50:ASN:ND2	2.37	0.55
14:b:177:THR:HG21	14:b:185:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:GLU:OE1	3:C:80:ASN:ND2	2.39	0.55
13:M:196:GLY:O	13:M:200:ASN:ND2	2.39	0.55
14:N:177:THR:HG21	14:N:185:ALA:HB3	1.87	0.55
13:a:196:GLY:O	13:a:200:ASN:ND2	2.39	0.55
3:Q:63:GLU:OE1	3:Q:80:ASN:ND2	2.39	0.55
6:F:47:SER:OG	6:F:190:CYS:SG	2.64	0.55
8:V:168:ASN:ND2	8:V:171:GLY:O	2.38	0.55
6:T:47:SER:OG	6:T:190:CYS:SG	2.64	0.55
8:H:168:ASN:ND2	8:H:171:GLY:O	2.38	0.55
12:L:4:LEU:HD12	12:L:15:ALA:HB3	1.87	0.55
2:P:69:SER:OG	2:P:70:GLU:N	2.40	0.55
4:R:158:ALA:HB3	5:S:58:LEU:HD13	1.89	0.55
9:W:17:ASP:OD1	9:W:17:ASP:N	2.40	0.55
11:Y:118:CYS:SG	11:Y:119:ASP:N	2.79	0.55
12:Z:4:LEU:HD12	12:Z:15:ALA:HB3	1.87	0.55
2:B:69:SER:OG	2:B:70:GLU:N	2.40	0.55
2:B:148:GLN:OE1	2:B:158:TRP:NE1	2.39	0.55
11:K:118:CYS:SG	11:K:119:ASP:N	2.79	0.55
15:p:52:VAL:HG11	15:p:245:VAL:HG22	1.89	0.55
1:A:36:ASN:ND2	1:A:58:THR:OG1	2.35	0.55
2:B:36:LEU:HD11	2:B:174:LEU:HD11	1.88	0.55
3:C:161:ALA:HB1	3:C:175:LEU:HD13	1.87	0.55
9:I:17:ASP:OD1	9:I:17:ASP:N	2.40	0.55
15:d:52:VAL:HG23	15:d:61:ILE:HG21	1.88	0.55
15:g:266:VAL:HG22	15:g:267:LYS:HG3	1.88	0.55
15:o:52:VAL:HG23	15:o:61:ILE:HG21	1.88	0.55
2:P:36:LEU:HD11	2:P:174:LEU:HD11	1.88	0.55
2:P:148:GLN:OE1	2:P:158:TRP:NE1	2.39	0.55
15:e:52:VAL:HG11	15:e:245:VAL:HG22	1.89	0.55
15:k:266:VAL:HG22	15:k:267:LYS:HG3	1.88	0.55
3:Q:161:ALA:HB1	3:Q:175:LEU:HD13	1.87	0.55
4:D:199:LEU:HD13	4:D:226:VAL:HG22	1.89	0.54
10:J:51:VAL:HG22	10:J:86:VAL:HG22	1.90	0.54
11:K:3:THR:HG22	11:K:135:GLY:HA3	1.89	0.54
11:K:111:ASP:OD1	11:K:111:ASP:N	2.39	0.54
11:Y:3:THR:HG22	11:Y:135:GLY:HA3	1.89	0.54
11:Y:111:ASP:N	11:Y:111:ASP:OD1	2.39	0.54
4:R:199:LEU:HD13	4:R:226:VAL:HG22	1.89	0.54
15:k:170:ILE:H	15:l:261:ASN:HD21	1.55	0.54
10:X:51:VAL:HG22	10:X:86:VAL:HG22	1.90	0.54
13:M:127:ARG:NH2	14:N:104:ASN:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:5:PRO:HB2	14:N:8:THR:HG22	1.89	0.54
15:k:36:SER:HA	15:k:40:ARG:HB2	1.90	0.54
15:m:46:ILE:O	15:m:50:ASN:ND2	2.37	0.54
2:B:75:VAL:HB	2:B:135:LEU:HB2	1.89	0.54
4:R:125:ARG:NH1	3:Q:122:THR:O	2.40	0.54
15:e:67:LEU:HD21	15:e:233:ASP:HB3	1.89	0.54
15:h:36:SER:HA	15:h:40:ARG:HB2	1.88	0.54
10:J:40:LYS:NZ	10:J:199:GLU:OE2	2.40	0.54
15:g:36:SER:HA	15:g:40:ARG:HB2	1.90	0.54
15:j:152:LEU:HD21	15:j:191:VAL:HG12	1.88	0.54
14:b:5:PRO:HB2	14:b:8:THR:HG22	1.89	0.54
1:O:36:ASN:ND2	1:O:58:THR:OG1	2.35	0.54
9:I:38:SER:OG	9:I:39:LYS:N	2.41	0.54
2:P:75:VAL:HB	2:P:135:LEU:HB2	1.89	0.54
15:f:152:LEU:HD21	15:f:191:VAL:HG12	1.88	0.54
15:h:66:ASP:O	15:h:137:GLN:NE2	2.41	0.54
15:l:36:SER:HA	15:l:40:ARG:HB2	1.88	0.54
15:p:67:LEU:HD21	15:p:233:ASP:HB3	1.89	0.54
10:X:40:LYS:NZ	10:X:199:GLU:OE2	2.40	0.54
11:Y:183:MET:HG2	11:Y:188:VAL:HG12	1.89	0.54
9:I:59:LEU:HD21	9:I:79:CYS:HB2	1.89	0.54
4:D:77:ASN:O	4:D:81:ARG:NH1	2.40	0.54
10:J:217:MET:SD	12:Z:161:TYR:OH	2.65	0.54
11:K:183:MET:HG2	11:K:188:VAL:HG12	1.89	0.54
4:R:77:ASN:O	4:R:81:ARG:NH1	2.40	0.54
15:l:66:ASP:O	15:l:137:GLN:NE2	2.41	0.54
3:C:12:PHE:H	4:D:18:GLN:HE22	1.55	0.53
9:W:59:LEU:HD21	9:W:79:CYS:HB2	1.90	0.53
3:C:25:LEU:O	3:C:29:ASN:ND2	2.42	0.53
2:P:95:ILE:HD12	9:W:61:HIS:HB3	1.89	0.53
13:a:66:ARG:HH12	14:b:190:ARG:HD3	1.73	0.53
3:Q:25:LEU:O	3:Q:29:ASN:ND2	2.42	0.53
2:B:108:LYS:HE2	2:B:112:LYS:HD2	1.91	0.53
10:J:146:THR:HG22	10:J:148:ASP:H	1.73	0.53
15:f:191:VAL:HG21	15:f:254:LEU:HD21	1.91	0.53
15:j:191:VAL:HG21	15:j:254:LEU:HD21	1.91	0.53
3:C:143:ASP:OD2	3:C:146:GLN:NE2	2.41	0.53
6:F:117:GLN:OE1	6:F:121:GLN:NE2	2.38	0.53
2:P:108:LYS:HE2	2:P:112:LYS:HD2	1.91	0.53
15:m:52:VAL:O	15:m:248:ARG:NH1	2.40	0.53
15:m:209:ARG:NH1	15:m:233:ASP:OD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:159:LYS:HD2	1:O:174:ILE:HD13	1.90	0.53
6:F:68:ASP:O	6:F:220:TRP:N	2.42	0.53
5:S:16:SER:OG	15:o:172:ASP:OD2	2.26	0.53
15:c:52:VAL:O	15:c:248:ARG:NH1	2.40	0.53
3:Q:143:ASP:OD2	3:Q:146:GLN:NE2	2.41	0.53
6:T:68:ASP:O	6:T:220:TRP:N	2.42	0.53
1:A:159:LYS:HD2	1:A:174:ILE:HD13	1.90	0.53
14:N:212:ILE:HD11	9:W:140:ALA:HB2	1.91	0.53
10:X:146:THR:HG22	10:X:148:ASP:H	1.74	0.53
6:T:117:GLN:OE1	6:T:121:GLN:NE2	2.38	0.53
15:m:168:PRO:HB3	15:m:268:PRO:HB2	1.90	0.53
15:c:209:ARG:NH1	15:c:233:ASP:OD2	2.41	0.52
15:k:209:ARG:NH1	15:k:233:ASP:OD2	2.42	0.52
7:G:111:LEU:HD22	7:G:142:SER:HB3	1.91	0.52
5:S:118:GLU:OE1	6:T:86:LYS:NZ	2.41	0.52
7:U:111:LEU:HD22	7:U:142:SER:HB3	1.91	0.52
13:a:173:ILE:HD11	13:a:209:ALA:HB2	1.92	0.52
15:i:52:VAL:O	15:i:248:ARG:NH1	2.42	0.52
15:k:66:ASP:O	15:k:137:GLN:NE2	2.36	0.52
15:n:52:VAL:O	15:n:248:ARG:NH1	2.42	0.52
13:M:173:ILE:HD11	13:M:209:ALA:HB2	1.92	0.52
15:d:167:VAL:O	15:e:260:LYS:NZ	2.29	0.52
15:e:154:GLU:OE1	15:f:59:GLY:N	2.36	0.52
15:h:36:SER:OG	15:h:40:ARG:NH1	2.40	0.52
10:X:23:ILE:HG13	10:X:201:LEU:HB3	1.92	0.52
3:Q:130:TYR:HB3	3:Q:132:VAL:HG12	1.92	0.52
1:O:77:ASN:OD1	1:O:77:ASN:N	2.43	0.52
3:C:130:TYR:HB3	3:C:132:VAL:HG12	1.92	0.52
9:I:1:THR:HG23	9:I:129:SER:H	1.74	0.52
10:J:23:ILE:HG13	10:J:201:LEU:HB3	1.92	0.52
12:L:28:SER:OG	12:L:29:GLN:N	2.43	0.52
12:Z:28:SER:OG	12:Z:29:GLN:N	2.43	0.52
1:A:77:ASN:OD1	1:A:77:ASN:N	2.43	0.52
3:C:7:SER:OG	3:C:8:ARG:N	2.42	0.52
1:A:16:PHE:H	2:B:21:GLN:HE22	1.57	0.52
12:L:105:ASP:OD1	12:L:110:ASN:ND2	2.42	0.52
9:W:1:THR:HG23	9:W:129:SER:H	1.75	0.52
15:c:168:PRO:HB3	15:c:268:PRO:HB2	1.90	0.52
3:Q:7:SER:OG	3:Q:8:ARG:N	2.42	0.52
11:K:4:LEU:HD23	11:K:46:LEU:HG	1.91	0.52
13:M:56:ARG:NH1	13:M:216:THR:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:66:ASP:O	15:g:137:GLN:NE2	2.36	0.52
15:g:209:ARG:NH1	15:g:233:ASP:OD2	2.42	0.52
12:Z:105:ASP:OD1	12:Z:110:ASN:ND2	2.42	0.52
1:A:54:LYS:NZ	1:A:72:ILE:O	2.36	0.52
7:G:97:GLU:OE1	7:G:117:ARG:NH1	2.41	0.52
13:a:56:ARG:NH1	13:a:216:THR:O	2.43	0.52
15:l:36:SER:OG	15:l:40:ARG:NH1	2.40	0.52
14:N:10:THR:OG1	14:N:42:ARG:NH2	2.42	0.52
11:Y:4:LEU:HD23	11:Y:46:LEU:HG	1.91	0.52
7:U:97:GLU:OE1	7:U:117:ARG:NH1	2.41	0.52
11:K:23:ASN:HD22	11:K:27:LYS:HE2	1.75	0.51
2:P:206:LYS:O	2:P:224:GLN:NE2	2.43	0.51
15:k:62:LEU:HD12	15:k:238:ILE:HG23	1.93	0.51
14:b:10:THR:OG1	14:b:42:ARG:NH2	2.43	0.51
7:G:150:ASP:OD1	7:G:150:ASP:N	2.41	0.51
4:R:223:ASN:HA	4:R:226:VAL:HG12	1.91	0.51
11:Y:23:ASN:HD22	11:Y:27:LYS:HE2	1.76	0.51
15:g:62:LEU:HD12	15:g:238:ILE:HG23	1.93	0.51
4:D:223:ASN:HA	4:D:226:VAL:HG12	1.91	0.51
14:N:75:ASN:HD21	14:N:85:MET:HA	1.75	0.51
15:l:207:MET:HE1	15:n:228:ALA:HB1	1.92	0.51
7:U:184:TYR:OH	7:U:195:ASP:OD2	2.26	0.51
2:B:206:LYS:O	2:B:224:GLN:NE2	2.43	0.51
9:I:120:CYS:SG	9:I:121:LEU:N	2.84	0.51
10:J:16:SER:HB2	10:J:132:PRO:HB3	1.92	0.51
11:Y:86:ARG:NH2	10:X:64:THR:OG1	2.44	0.51
14:b:75:ASN:HD21	14:b:85:MET:HA	1.75	0.51
1:O:54:LYS:NZ	1:O:72:ILE:O	2.36	0.51
3:C:111:VAL:HA	3:C:114:ILE:HG22	1.93	0.51
10:J:190:ARG:HG2	13:a:175:PRO:HG3	1.93	0.51
11:K:91:TYR:O	11:K:95:ARG:NH2	2.44	0.51
11:Y:91:TYR:O	11:Y:95:ARG:NH2	2.44	0.51
10:X:16:SER:HB2	10:X:132:PRO:HB3	1.92	0.51
3:Q:111:VAL:HA	3:Q:114:ILE:HG22	1.93	0.51
7:U:150:ASP:OD1	7:U:150:ASP:N	2.41	0.51
7:G:184:TYR:OH	7:G:195:ASP:OD2	2.26	0.51
8:H:7:ILE:HA	8:H:12:VAL:HG23	1.92	0.51
10:J:65:LEU:HD22	10:J:107:VAL:HG21	1.93	0.51
6:T:228:LEU:HA	6:T:232:LEU:HD12	1.93	0.51
1:A:86:MET:HB3	1:A:93:CYS:HB2	1.93	0.51
8:V:7:ILE:HA	8:V:12:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:j:61:ILE:O	15:j:241:LYS:NZ	2.39	0.51
10:X:65:LEU:HD22	10:X:107:VAL:HG21	1.93	0.51
6:F:80:ASP:HB3	6:F:128:PHE:HD1	1.76	0.51
6:F:228:LEU:HA	6:F:232:LEU:HD12	1.93	0.51
15:k:165:LEU:HD21	15:l:252:ILE:HG12	1.91	0.51
15:m:175:ASN:HB2	15:m:178:VAL:HG22	1.93	0.51
6:T:45:VAL:HG21	6:T:187:ILE:HG22	1.91	0.51
4:D:42:VAL:HG21	4:D:186:ILE:HG12	1.92	0.51
8:H:26:ILE:O	14:b:216:ARG:NH1	2.43	0.51
4:R:42:VAL:HG21	4:R:186:ILE:HG12	1.91	0.51
3:Q:76:VAL:HA	3:Q:134:PHE:HB3	1.93	0.51
1:O:86:MET:HB3	1:O:93:CYS:HB2	1.93	0.51
6:F:45:VAL:HG21	6:F:187:ILE:HG22	1.92	0.51
5:S:72:ASP:N	5:S:72:ASP:OD1	2.43	0.51
6:T:80:ASP:HB3	6:T:128:PHE:HD1	1.76	0.51
3:C:76:VAL:HA	3:C:134:PHE:HB3	1.93	0.50
5:E:72:ASP:OD1	5:E:72:ASP:N	2.43	0.50
12:L:83:LEU:HD23	12:L:86:ILE:HD11	1.92	0.50
9:W:120:CYS:SG	9:W:121:LEU:N	2.84	0.50
12:Z:83:LEU:HD23	12:Z:86:ILE:HD11	1.92	0.50
10:J:136:ALA:HB3	10:J:144:CYS:HB3	1.93	0.50
15:e:171:GLU:O	15:e:175:ASN:ND2	2.45	0.50
15:p:26:LYS:HE3	15:p:165:LEU:HD11	1.93	0.50
15:p:171:GLU:O	15:p:175:ASN:ND2	2.45	0.50
10:X:136:ALA:HB3	10:X:144:CYS:HB3	1.93	0.50
11:K:156:ALA:HA	11:K:159:ILE:HD12	1.94	0.50
9:W:204:ILE:HG23	9:W:206:PRO:HD3	1.92	0.50
3:C:15:GLU:HG3	3:C:17:ARG:H	1.76	0.50
9:W:1:THR:N	9:W:168:GLY:O	2.44	0.50
15:e:26:LYS:HE3	15:e:165:LEU:HD11	1.93	0.50
15:n:188:LEU:HD12	15:n:254:LEU:HD22	1.94	0.50
9:I:204:ILE:HG23	9:I:206:PRO:HD3	1.92	0.50
10:J:39:THR:OG1	12:Z:203:PRO:O	2.29	0.50
3:Q:15:GLU:HG3	3:Q:17:ARG:H	1.76	0.50
1:A:49:VAL:HG11	1:A:209:THR:HG22	1.93	0.50
9:I:1:THR:N	9:I:168:GLY:O	2.44	0.50
2:P:12:THR:OG1	2:P:13:PHE:N	2.43	0.50
2:P:12:THR:OG1	3:Q:20:GLN:OE1	2.30	0.50
9:W:38:SER:OG	9:W:39:LYS:N	2.41	0.50
11:Y:156:ALA:HA	11:Y:159:ILE:HD12	1.94	0.50
15:f:242:ILE:HA	15:f:245:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:i:188:LEU:HD12	15:i:254:LEU:HD22	1.94	0.50
7:G:44:ASP:HB3	7:G:189:VAL:HG23	1.93	0.50
4:R:41:ALA:HB1	4:R:144:ILE:HD11	1.92	0.50
9:W:43:CYS:SG	9:W:44:ALA:N	2.84	0.50
15:c:175:ASN:HB2	15:c:178:VAL:HG22	1.93	0.50
15:k:216:VAL:HG22	15:k:225:TYR:HB3	1.94	0.50
5:E:118:GLU:OE1	6:F:86:LYS:NZ	2.44	0.50
2:P:10:LEU:HG	2:P:126:GLY:H	1.76	0.50
15:n:144:LYS:O	15:n:147:THR:OG1	2.27	0.50
15:p:148:TYR:HB3	15:p:247:MET:HE2	1.94	0.50
1:O:49:VAL:HG11	1:O:209:THR:HG22	1.93	0.50
7:U:44:ASP:HB3	7:U:189:VAL:HG23	1.93	0.50
4:D:41:ALA:HB1	4:D:144:ILE:HD11	1.92	0.50
15:e:148:TYR:HB3	15:e:247:MET:HE2	1.94	0.50
15:i:144:LYS:O	15:i:147:THR:OG1	2.27	0.50
15:j:62:LEU:HD23	15:j:238:ILE:HG13	1.93	0.50
15:j:242:ILE:HA	15:j:245:VAL:HG12	1.92	0.50
2:B:54:ASN:N	2:B:54:ASN:OD1	2.43	0.49
6:F:116:TYR:O	6:F:120:THR:OG1	2.30	0.49
8:H:163:GLN:HE21	8:H:165:TYR:HD1	1.59	0.49
9:I:43:CYS:SG	9:I:44:ALA:N	2.84	0.49
15:f:62:LEU:HD23	15:f:238:ILE:HG13	1.93	0.49
15:g:216:VAL:HG22	15:g:225:TYR:HB3	1.94	0.49
6:F:145:GLU:HG2	6:F:158:LEU:HD11	1.93	0.49
7:G:35:ASN:HB2	7:G:68:ARG:HH22	1.78	0.49
6:T:116:TYR:O	6:T:120:THR:OG1	2.30	0.49
7:U:35:ASN:HB2	7:U:68:ARG:HH22	1.77	0.49
2:B:10:LEU:HG	2:B:126:GLY:H	1.76	0.49
6:F:195:LYS:HG2	6:F:204:LEU:HD12	1.93	0.49
5:S:103:TYR:HB3	13:a:115:VAL:HG23	1.93	0.49
6:T:145:GLU:HG2	6:T:158:LEU:HD11	1.93	0.49
2:B:12:THR:OG1	2:B:13:PHE:N	2.43	0.49
13:M:152:TYR:HB3	13:M:158:TYR:HA	1.94	0.49
4:R:124:VAL:HG12	3:Q:124:TYR:HB3	1.94	0.49
8:V:53:GLN:NE2	9:W:119:SER:O	2.45	0.49
6:T:195:LYS:HG2	6:T:204:LEU:HD12	1.93	0.49
8:V:163:GLN:HE21	8:V:165:TYR:HD1	1.60	0.49
13:a:152:TYR:HB3	13:a:158:TYR:HA	1.94	0.49
15:i:264:LYS:HD3	15:i:268:PRO:HA	1.93	0.49
15:n:264:LYS:HD3	15:n:268:PRO:HA	1.93	0.49
12:L:7:LYS:H	12:L:12:ILE:HG23	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:134:TYR:O	12:L:137:SER:OG	2.28	0.49
2:P:54:ASN:N	2:P:54:ASN:OD1	2.43	0.49
12:Z:7:LYS:H	12:Z:12:ILE:HG23	1.77	0.49
7:U:9:ASP:OD2	7:U:26:TYR:OH	2.26	0.49
7:U:78:ILE:HG12	7:U:140:ILE:HG12	1.94	0.49
14:N:21:ILE:HD11	14:N:159:LEU:HB3	1.95	0.49
9:W:28:ASP:OD1	9:W:28:ASP:N	2.43	0.49
15:l:134:SER:H	15:n:223:SER:HB3	1.78	0.49
12:Z:134:TYR:O	12:Z:137:SER:OG	2.28	0.49
7:G:78:ILE:HG12	7:G:140:ILE:HG12	1.94	0.49
8:H:170:ASN:HB2	14:N:59:ALA:HB1	1.95	0.49
9:I:28:ASP:OD1	9:I:28:ASP:N	2.43	0.49
14:b:21:ILE:HD11	14:b:159:LEU:HB3	1.95	0.49
13:M:85:MET:HE2	13:M:87:SER:HB2	1.94	0.49
9:W:133:ASN:ND2	9:W:165:ASN:O	2.45	0.49
7:G:9:ASP:OD2	7:G:26:TYR:OH	2.27	0.48
15:f:44:ARG:NE	15:f:151:GLU:OE1	2.40	0.48
13:a:85:MET:HE2	13:a:87:SER:HB2	1.94	0.48
15:j:44:ARG:NE	15:j:151:GLU:OE1	2.40	0.48
12:Z:176:VAL:HG13	12:Z:187:ILE:HB	1.95	0.48
5:E:97:ASN:HD22	12:L:65:ILE:HG13	1.77	0.48
9:I:133:ASN:ND2	9:I:165:ASN:O	2.45	0.48
10:J:24:ALA:HB2	10:J:200:VAL:HG23	1.96	0.48
12:L:176:VAL:HG13	12:L:187:ILE:HB	1.95	0.48
10:X:24:ALA:HB2	10:X:200:VAL:HG23	1.96	0.48
5:E:103:TYR:HB3	13:M:115:VAL:HG23	1.94	0.48
15:c:56:SER:OG	15:c:60:SER:OG	2.30	0.48
5:S:84:ASP:OD2	5:S:137:ARG:NH1	2.43	0.48
5:E:13:ASN:HB3	6:F:126:ARG:HB3	1.95	0.48
9:I:34:LEU:HD23	9:I:44:ALA:HB2	1.96	0.48
12:L:4:LEU:HD22	12:L:139:LEU:HD11	1.95	0.48
4:D:42:VAL:HB	4:D:208:LEU:HD13	1.96	0.48
1:O:42:VAL:HA	1:O:171:ALA:HA	1.96	0.48
4:D:158:ALA:HB3	5:E:58:LEU:HD13	1.95	0.48
14:N:17:TYR:HE2	14:N:19:HIS:HB2	1.78	0.48
2:P:196:LYS:HB2	2:P:204:ASN:HD22	1.79	0.48
4:R:42:VAL:HB	4:R:208:LEU:HD13	1.96	0.48
9:W:34:LEU:HD23	9:W:44:ALA:HB2	1.96	0.48
14:b:17:TYR:HE2	14:b:19:HIS:HB2	1.78	0.48
12:Z:4:LEU:HD22	12:Z:139:LEU:HD11	1.95	0.48
1:A:42:VAL:HA	1:A:171:ALA:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:LYS:HB2	2:B:204:ASN:HD22	1.79	0.48
3:C:35:ILE:HG12	3:C:196:LEU:HD13	1.96	0.48
6:F:57:SER:OG	6:F:58:PHE:N	2.47	0.48
8:H:222:ASN:ND2	14:b:32:GLY:O	2.47	0.48
3:Q:35:ILE:HG12	3:Q:196:LEU:HD13	1.96	0.48
6:T:57:SER:OG	6:T:58:PHE:N	2.47	0.48
12:L:102:SER:HB2	12:L:111:MET:HG3	1.96	0.47
5:S:225:SER:OG	5:S:226:ASP:N	2.47	0.47
15:f:146:LYS:NZ	15:g:231:GLU:OE2	2.45	0.47
15:m:56:SER:OG	15:m:60:SER:OG	2.30	0.47
12:Z:102:SER:HB2	12:Z:111:MET:HG3	1.96	0.47
5:E:225:SER:OG	5:E:226:ASP:N	2.47	0.47
14:N:163:PHE:HB2	14:N:176:ILE:HG21	1.95	0.47
14:b:163:PHE:HB2	14:b:176:ILE:HG21	1.95	0.47
9:W:21:THR:OG1	9:W:22:GLU:N	2.47	0.47
15:e:36:SER:HA	15:e:40:ARG:HB2	1.95	0.47
9:I:59:LEU:HD22	9:I:83:LEU:HD21	1.97	0.47
9:W:59:LEU:HD22	9:W:83:LEU:HD21	1.96	0.47
13:a:127:ARG:NH2	14:b:104:ASN:OD1	2.46	0.47
15:h:154:GLU:O	15:h:158:ASN:ND2	2.48	0.47
15:p:36:SER:HA	15:p:40:ARG:HB2	1.95	0.47
11:K:13:VAL:HG23	11:K:113:TYR:HB3	1.97	0.47
15:c:169:ARG:NH2	15:c:171:GLU:OE2	2.45	0.47
15:f:201:ALA:HA	15:f:204:LYS:HZ2	1.79	0.47
15:j:201:ALA:HA	15:j:204:LYS:HZ2	1.80	0.47
15:l:154:GLU:O	15:l:158:ASN:ND2	2.48	0.47
11:Y:13:VAL:HG23	11:Y:113:TYR:HB3	1.97	0.47
15:m:59:GLY:O	15:m:63:ASN:ND2	2.47	0.47
6:T:13:TYR:HB2	7:U:23:GLN:HE22	1.79	0.47
3:C:46:GLY:HA2	3:C:212:LEU:HD23	1.97	0.47
6:F:34:CYS:HB2	6:F:162:ALA:HB3	1.97	0.47
9:I:174:ASP:OD1	9:I:174:ASP:N	2.46	0.47
12:L:203:PRO:O	10:X:39:THR:OG1	2.32	0.47
15:c:59:GLY:O	15:c:63:ASN:ND2	2.47	0.47
15:c:234:GLU:OE1	15:i:146:LYS:NZ	2.36	0.47
15:p:175:ASN:HB2	15:p:178:VAL:HG22	1.97	0.47
3:Q:46:GLY:HA2	3:Q:212:LEU:HD23	1.97	0.47
6:T:34:CYS:HB2	6:T:162:ALA:HB3	1.97	0.47
1:A:237:LYS:HB3	1:A:237:LYS:HE3	1.83	0.47
5:E:93:ARG:HD3	12:L:68:LEU:HB3	1.97	0.47
13:M:146:LYS:HA	13:M:146:LYS:HD2	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:204:LYS:HA	8:V:204:LYS:HD3	1.73	0.47
15:e:175:ASN:HB2	15:e:178:VAL:HG22	1.97	0.47
15:k:191:VAL:HG11	15:k:254:LEU:HD21	1.97	0.47
15:l:227:GLU:OE1	15:l:230:ARG:NH2	2.43	0.47
15:m:66:ASP:OD1	15:m:66:ASP:N	2.41	0.47
15:p:145:ILE:HG13	15:p:240:ILE:HD11	1.97	0.47
8:H:53:GLN:HE22	9:I:119:SER:H	1.62	0.47
9:W:174:ASP:OD1	9:W:174:ASP:N	2.46	0.47
15:g:191:VAL:HG11	15:g:254:LEU:HD21	1.97	0.47
15:o:211:LYS:O	15:o:214:THR:OG1	2.29	0.47
14:b:170:ASN:N	14:b:170:ASN:OD1	2.48	0.47
7:U:142:SER:OG	7:U:143:PHE:N	2.47	0.47
8:H:9:ASP:OD1	8:H:9:ASP:N	2.42	0.47
8:H:191:SER:HB2	8:V:216:TYR:HB3	1.96	0.47
11:K:181:ARG:NE	11:K:190:THR:OG1	2.46	0.47
14:N:170:ASN:OD1	14:N:170:ASN:N	2.48	0.47
11:Y:181:ARG:NE	11:Y:190:THR:OG1	2.46	0.47
15:c:52:VAL:HG23	15:c:61:ILE:HD13	1.97	0.47
15:e:145:ILE:HG13	15:e:240:ILE:HD11	1.97	0.47
1:O:158:PHE:HA	1:O:168:GLY:HA2	1.97	0.47
1:A:158:PHE:HA	1:A:168:GLY:HA2	1.97	0.46
14:N:27:ARG:NE	14:N:39:ASN:OD1	2.49	0.46
11:Y:160:PHE:HA	11:Y:163:CYS:HB3	1.97	0.46
15:c:199:TYR:HD1	15:d:235:LYS:HZ3	1.64	0.46
15:m:169:ARG:NH2	15:m:171:GLU:OE2	2.45	0.46
14:b:70:ARG:NE	7:U:103:TYR:OH	2.42	0.46
2:B:74:ILE:HD11	2:B:134:LEU:HD13	1.97	0.46
7:G:142:SER:OG	7:G:143:PHE:N	2.47	0.46
8:H:53:GLN:NE2	9:I:119:SER:O	2.47	0.46
2:P:45:ILE:HG22	2:P:212:VAL:HG12	1.97	0.46
2:P:74:ILE:HD11	2:P:134:LEU:HD13	1.97	0.46
13:a:146:LYS:HD2	13:a:146:LYS:HA	1.69	0.46
15:d:211:LYS:O	15:d:214:THR:OG1	2.29	0.46
14:b:27:ARG:NE	14:b:39:ASN:OD1	2.49	0.46
14:b:120:SER:HB2	14:b:158:ASP:HB3	1.98	0.46
5:E:92:ALA:HB2	5:E:116:ILE:HD13	1.98	0.46
8:H:210:ILE:HA	8:H:213:CYS:HB2	1.96	0.46
9:I:140:ALA:HB2	14:b:212:ILE:HD11	1.96	0.46
11:K:160:PHE:HA	11:K:163:CYS:HB3	1.97	0.46
14:N:120:SER:O	14:N:121:GLN:NE2	2.48	0.46
14:N:120:SER:HB2	14:N:158:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:210:ILE:HA	8:V:213:CYS:HB2	1.96	0.46
11:Y:86:ARG:HB2	11:Y:124:MET:HE3	1.97	0.46
2:B:45:ILE:HG22	2:B:212:VAL:HG12	1.97	0.46
8:H:216:TYR:HB3	8:V:191:SER:HB2	1.97	0.46
5:S:92:ALA:HB2	5:S:116:ILE:HD13	1.98	0.46
15:d:191:VAL:HG13	15:d:250:ASN:HD22	1.80	0.46
15:h:227:GLU:OE1	15:h:230:ARG:NH2	2.43	0.46
15:m:52:VAL:HG23	15:m:61:ILE:HD13	1.97	0.46
15:o:191:VAL:HG13	15:o:250:ASN:HD22	1.80	0.46
14:b:120:SER:O	14:b:121:GLN:NE2	2.48	0.46
4:D:10:PHE:H	5:E:23:GLN:NE2	2.13	0.46
11:K:3:THR:OG1	11:K:18:ASP:OD1	2.33	0.46
11:K:47:LEU:HD23	11:K:102:CYS:HB3	1.97	0.46
11:K:86:ARG:HB2	11:K:124:MET:HE3	1.97	0.46
13:M:86:GLN:HE21	13:M:90:LYS:HE2	1.80	0.46
14:N:175:TYR:HB2	14:N:189:LEU:HD21	1.97	0.46
14:b:175:TYR:HB2	14:b:189:LEU:HD21	1.97	0.46
1:A:204:ASP:OD1	1:A:204:ASP:N	2.46	0.46
13:M:114:HIS:NE2	13:M:142:ASP:OD2	2.48	0.46
14:N:10:THR:OG1	14:N:26:ASP:OD1	2.23	0.46
14:N:61:ALA:O	14:N:65:HIS:N	2.49	0.46
2:P:79:MET:SD	2:P:128:ARG:NH1	2.89	0.46
11:Y:47:LEU:HD23	11:Y:102:CYS:HB3	1.97	0.46
11:Y:69:GLN:HG2	11:Y:75:ASP:HA	1.97	0.46
13:a:86:GLN:HE21	13:a:90:LYS:HE2	1.80	0.46
13:a:114:HIS:NE2	13:a:142:ASP:OD2	2.48	0.46
15:c:223:SER:HB3	15:i:134:SER:H	1.80	0.46
14:b:28:LYS:HE3	14:b:35:ALA:HB2	1.97	0.46
14:b:61:ALA:O	14:b:65:HIS:N	2.49	0.46
1:O:204:ASP:OD1	1:O:204:ASP:N	2.47	0.46
2:B:79:MET:SD	2:B:128:ARG:NH1	2.89	0.46
2:B:134:LEU:HB2	2:B:149:ILE:HB	1.98	0.46
11:K:69:GLN:HG2	11:K:75:ASP:HA	1.97	0.46
15:j:175:ASN:HB2	15:j:178:VAL:HG22	1.97	0.46
2:B:46:ILE:HD12	2:B:65:ILE:HD12	1.97	0.46
3:C:95:GLN:HB3	10:J:71:TYR:HD1	1.81	0.46
6:F:6:TYR:HA	6:F:12:ILE:HD12	1.96	0.46
14:N:28:LYS:HE3	14:N:35:ALA:HB2	1.97	0.46
15:h:160:LYS:HB2	15:h:188:LEU:HD22	1.98	0.46
15:j:26:LYS:HG2	15:j:165:LEU:HD11	1.98	0.46
15:l:160:LYS:HB2	15:l:188:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:n:19:LYS:O	15:n:23:ASN:ND2	2.48	0.46
7:U:68:ARG:HD3	7:U:80:TYR:HB2	1.96	0.46
13:M:90:LYS:HD3	13:M:90:LYS:HA	1.71	0.46
15:c:223:SER:HB3	15:i:134:SER:N	2.31	0.46
15:i:19:LYS:O	15:i:23:ASN:ND2	2.48	0.46
14:b:10:THR:OG1	14:b:26:ASP:OD1	2.23	0.46
6:T:6:TYR:HA	6:T:12:ILE:HD12	1.96	0.46
1:O:22:LEU:HD23	1:O:22:LEU:HA	1.75	0.46
7:U:186:ASP:N	7:U:186:ASP:OD1	2.49	0.46
3:C:114:ILE:HD13	3:C:134:PHE:HZ	1.81	0.46
7:G:68:ARG:HD3	7:G:80:TYR:HB2	1.96	0.46
8:H:204:LYS:HD3	8:H:204:LYS:HA	1.73	0.46
9:I:167:LEU:HD11	13:a:58:SER:HB2	1.96	0.46
2:P:46:ILE:HD12	2:P:65:ILE:HD12	1.97	0.46
5:S:93:ARG:HD3	12:Z:68:LEU:HB3	1.98	0.46
15:c:167:VAL:O	15:d:260:LYS:NZ	2.39	0.46
15:f:26:LYS:HG2	15:f:165:LEU:HD11	1.98	0.46
15:f:175:ASN:HB2	15:f:178:VAL:HG22	1.97	0.46
15:g:239:HIS:HA	15:g:242:ILE:HG22	1.97	0.46
15:j:167:VAL:O	15:k:260:LYS:NZ	2.42	0.46
15:p:205:TYR:OH	15:p:233:ASP:OD1	2.34	0.46
10:X:177:PHE:HB2	10:X:202:VAL:HG21	1.97	0.46
3:Q:37:LEU:HD21	3:Q:191:LEU:HD23	1.98	0.46
3:C:26:GLU:HA	3:C:29:ASN:HD22	1.81	0.45
7:G:186:ASP:OD1	7:G:186:ASP:N	2.49	0.45
8:H:17:ASP:OD1	8:H:17:ASP:N	2.40	0.45
9:I:21:THR:OG1	9:I:22:GLU:N	2.47	0.45
10:J:177:PHE:HB2	10:J:202:VAL:HG21	1.97	0.45
15:e:205:TYR:OH	15:e:233:ASP:OD1	2.34	0.45
15:j:143:GLU:OE2	15:j:146:LYS:NZ	2.48	0.45
3:Q:114:ILE:HD13	3:Q:134:PHE:HZ	1.81	0.45
1:A:233:ILE:HG22	1:A:235:SER:H	1.82	0.45
3:C:37:LEU:HD21	3:C:191:LEU:HD23	1.98	0.45
2:P:134:LEU:HB2	2:P:149:ILE:HB	1.98	0.45
13:a:54:ASP:N	13:a:54:ASP:OD1	2.49	0.45
3:Q:106:PRO:HB2	3:Q:109:GLN:HG3	1.98	0.45
6:T:93:LEU:HD23	6:T:93:LEU:HA	1.84	0.45
3:C:106:PRO:HB2	3:C:109:GLN:HG3	1.98	0.45
3:C:149:HIS:CE1	3:C:164:ILE:HG21	2.51	0.45
13:M:54:ASP:N	13:M:54:ASP:OD1	2.49	0.45
13:a:90:LYS:HD3	13:a:90:LYS:HA	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:66:ASP:OD1	15:c:66:ASP:N	2.41	0.45
15:k:239:HIS:HA	15:k:242:ILE:HG22	1.97	0.45
3:Q:26:GLU:HA	3:Q:29:ASN:HD22	1.81	0.45
1:O:233:ILE:HG22	1:O:235:SER:H	1.82	0.45
3:C:53:SER:OG	3:C:54:LYS:N	2.49	0.45
15:d:153:ILE:HD12	15:e:242:ILE:HD11	1.99	0.45
3:Q:53:SER:OG	3:Q:54:LYS:N	2.49	0.45
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.75	0.45
12:L:203:PRO:HD2	10:X:196:TRP:CZ3	2.52	0.45
5:S:159:GLU:OE1	5:S:163:THR:OG1	2.35	0.45
8:V:4:ILE:HG13	8:V:181:VAL:HG23	1.99	0.45
13:a:206:ILE:HD13	13:a:206:ILE:HA	1.83	0.45
3:Q:149:HIS:CE1	3:Q:164:ILE:HG21	2.51	0.45
5:E:159:GLU:OE1	5:E:163:THR:OG1	2.35	0.45
8:H:4:ILE:HG13	8:H:181:VAL:HG23	1.99	0.45
8:V:17:ASP:OD1	8:V:17:ASP:N	2.40	0.45
2:B:225:ASN:N	2:B:225:ASN:OD1	2.49	0.45
4:D:11:SER:OG	4:D:15:HIS:N	2.50	0.45
6:F:93:LEU:HD23	6:F:93:LEU:HA	1.84	0.45
7:G:38:LEU:O	7:G:49:CYS:N	2.50	0.45
9:I:90:TYR:HB3	9:I:93:TYR:HB2	1.98	0.45
10:J:13:LEU:HD13	10:J:159:LEU:HD22	1.99	0.45
13:M:58:SER:HB2	9:W:167:LEU:HD11	1.98	0.45
14:N:119:ASN:N	14:N:158:ASP:O	2.46	0.45
14:b:119:ASN:N	14:b:158:ASP:O	2.46	0.45
10:X:13:LEU:HD13	10:X:159:LEU:HD22	1.99	0.45
7:U:38:LEU:O	7:U:49:CYS:N	2.50	0.45
7:G:46:ILE:HD11	7:G:149:GLY:HA3	1.98	0.45
7:G:93:ARG:NH1	7:G:97:GLU:OE2	2.50	0.45
13:M:206:ILE:HD13	13:M:206:ILE:HA	1.83	0.45
2:P:225:ASN:OD1	2:P:225:ASN:N	2.49	0.45
9:W:90:TYR:HB3	9:W:93:TYR:HB2	1.98	0.45
15:e:152:LEU:HD13	15:e:251:TYR:CZ	2.52	0.45
15:p:152:LEU:HD13	15:p:251:TYR:CZ	2.52	0.45
14:b:113:ILE:H	14:b:113:ILE:HG12	1.61	0.45
7:U:93:ARG:NH1	7:U:97:GLU:OE2	2.50	0.45
5:E:199:LEU:HA	5:E:202:THR:HG22	1.99	0.45
8:H:211:LEU:HD11	8:H:244:VAL:HG11	1.99	0.45
10:J:216:ARG:NH1	12:Z:191:GLU:O	2.43	0.45
4:R:11:SER:OG	4:R:15:HIS:N	2.50	0.45
8:V:211:LEU:HD11	8:V:244:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:k:167:VAL:O	15:l:260:LYS:NZ	2.40	0.45
15:m:187:GLU:OE2	15:m:190:ARG:NH2	2.47	0.45
7:U:46:ILE:HD11	7:U:149:GLY:HA3	1.98	0.45
7:G:120:LEU:HD23	7:G:120:LEU:HA	1.83	0.45
14:N:21:ILE:HG21	14:N:116:ALA:HB1	1.98	0.45
5:S:199:LEU:HA	5:S:202:THR:HG22	1.99	0.45
8:V:12:VAL:HG21	8:V:164:LEU:HB2	1.99	0.45
11:Y:86:ARG:HG3	11:Y:124:MET:HB2	1.99	0.45
15:m:176:PHE:HZ	15:n:171:GLU:HA	1.82	0.45
2:B:95:ILE:HD12	9:I:61:HIS:HB3	1.98	0.44
10:J:55:LEU:HB3	10:J:62:ILE:HG12	2.00	0.44
11:K:19:THR:HB	11:K:32:ASP:HA	1.98	0.44
5:S:69:SER:OG	5:S:71:ASP:O	2.34	0.44
11:Y:19:THR:HB	11:Y:32:ASP:HA	1.98	0.44
15:i:64:VAL:HG11	15:i:234:GLU:HG2	1.98	0.44
14:b:21:ILE:HG21	14:b:116:ALA:HB1	1.98	0.44
6:T:60:GLN:H	6:T:60:GLN:HG2	1.60	0.44
3:C:69:ASP:OD1	3:C:95:GLN:NE2	2.50	0.44
7:G:122:ILE:HG12	7:G:134:PHE:HD2	1.82	0.44
8:H:12:VAL:HG21	8:H:164:LEU:HB2	2.00	0.44
11:K:86:ARG:HG3	11:K:124:MET:HB2	2.00	0.44
11:K:194:THR:HG23	11:K:195:VAL:HG23	2.00	0.44
11:Y:194:THR:HG23	11:Y:195:VAL:HG23	2.00	0.44
10:X:55:LEU:HB3	10:X:62:ILE:HG12	2.00	0.44
2:B:68:ILE:HB	2:B:72:ILE:HB	1.99	0.44
8:H:88:TYR:O	14:N:63:TYR:OH	2.34	0.44
12:L:161:TYR:OH	10:X:217:MET:SD	2.69	0.44
2:P:68:ILE:HB	2:P:72:ILE:HB	1.99	0.44
13:a:225:ILE:HG12	13:a:230:ILE:HG22	2.00	0.44
15:e:240:ILE:HD12	15:e:240:ILE:HA	1.72	0.44
15:k:211:LYS:HB2	15:k:211:LYS:HE3	1.83	0.44
15:n:64:VAL:HG11	15:n:234:GLU:HG2	1.98	0.44
3:Q:69:ASP:OD1	3:Q:95:GLN:NE2	2.50	0.44
7:U:122:ILE:HG12	7:U:134:PHE:HD2	1.82	0.44
1:A:153:ASN:ND2	1:A:239:ARG:HH22	2.15	0.44
5:E:69:SER:OG	5:E:71:ASP:O	2.34	0.44
12:L:2:THR:N	12:L:17:ASP:OD1	2.49	0.44
13:M:225:ILE:HG12	13:M:230:ILE:HG22	2.00	0.44
13:a:120:LEU:HD12	13:a:138:LEU:HD11	2.00	0.44
15:o:152:LEU:HB2	15:o:247:MET:HE1	2.00	0.44
1:O:153:ASN:ND2	1:O:239:ARG:HH22	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:196:TRP:CZ3	12:Z:203:PRO:HD2	2.52	0.44
15:d:152:LEU:HB2	15:d:247:MET:HE1	2.00	0.44
15:g:211:LYS:HB2	15:g:211:LYS:HE3	1.83	0.44
12:Z:2:THR:N	12:Z:17:ASP:OD1	2.49	0.44
5:E:84:ASP:HB3	5:E:139:PHE:HD1	1.83	0.44
5:E:84:ASP:OD2	5:E:137:ARG:NH1	2.43	0.44
6:F:44:VAL:HG23	6:F:141:PRO:HB2	1.99	0.44
6:F:60:GLN:H	6:F:60:GLN:HG2	1.60	0.44
8:H:18:SER:OG	8:H:227:LEU:O	2.35	0.44
13:M:120:LEU:HD12	13:M:138:LEU:HD11	2.00	0.44
15:d:166:ASN:HD21	15:d:266:VAL:HA	1.83	0.44
15:p:240:ILE:HD12	15:p:240:ILE:HA	1.71	0.44
6:T:41:LYS:HA	6:T:41:LYS:HD3	1.76	0.44
7:U:120:LEU:HD23	7:U:120:LEU:HA	1.83	0.44
12:L:40:ASN:HD21	12:L:104:TYR:HB3	1.81	0.44
8:V:8:TYR:HB3	8:V:9:ASP:H	1.66	0.44
15:m:211:LYS:O	15:m:214:THR:OG1	2.31	0.44
15:m:242:ILE:HA	15:m:245:VAL:HG12	2.00	0.44
15:n:211:LYS:O	15:n:214:THR:OG1	2.33	0.44
15:o:166:ASN:HD21	15:o:266:VAL:HA	1.83	0.44
6:F:41:LYS:HA	6:F:41:LYS:HD3	1.76	0.44
13:M:84:GLY:HA3	13:M:134:ALA:HA	2.00	0.44
2:P:190:THR:O	2:P:194:THR:OG1	2.33	0.44
11:Y:179:GLU:HG3	11:Y:192:TYR:HB3	1.99	0.44
13:a:84:GLY:HA3	13:a:134:ALA:HA	2.00	0.44
15:c:187:GLU:OE2	15:c:190:ARG:NH2	2.47	0.44
15:i:211:LYS:O	15:i:214:THR:OG1	2.33	0.44
8:H:3:ILE:HD12	8:H:46:SER:HB3	2.00	0.44
12:L:54:TYR:HE1	13:M:122:VAL:HG12	1.82	0.44
13:M:41:ILE:HD12	13:M:173:ILE:HG21	1.98	0.44
4:R:48:LYS:HD3	4:R:203:ASN:HD21	1.83	0.44
5:S:84:ASP:HB3	5:S:139:PHE:HD1	1.83	0.44
13:a:41:ILE:HD12	13:a:173:ILE:HG21	1.98	0.44
15:d:164:GLN:HG3	15:e:253:MET:HG2	1.98	0.44
6:T:44:VAL:HG23	6:T:141:PRO:HB2	1.99	0.44
12:Z:40:ASN:HD21	12:Z:104:TYR:HB3	1.81	0.44
3:C:37:LEU:HB3	3:C:44:ILE:HG12	1.99	0.43
3:C:119:GLN:NE2	4:D:79:ASP:OD2	2.51	0.43
7:G:148:LYS:HA	7:G:148:LYS:HD3	1.78	0.43
11:K:179:GLU:HG3	11:K:192:TYR:HB3	1.99	0.43
11:Y:174:THR:O	11:Y:174:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:242:ILE:HA	15:c:245:VAL:HG12	2.00	0.43
12:Z:83:LEU:HB3	12:Z:114:VAL:HG11	2.00	0.43
1:A:96:MET:HE3	1:A:96:MET:HB3	1.81	0.43
4:D:48:LYS:HD3	4:D:203:ASN:HD21	1.83	0.43
6:F:7:ASP:O	6:F:21:GLN:NE2	2.51	0.43
8:H:53:GLN:NE2	9:I:119:SER:H	2.16	0.43
9:I:204:ILE:HG21	13:a:187:LEU:HD22	2.00	0.43
12:L:83:LEU:HB3	12:L:114:VAL:HG11	2.00	0.43
14:N:29:ALA:HB2	14:N:40:VAL:HG11	2.00	0.43
8:V:3:ILE:HD12	8:V:46:SER:HB3	2.00	0.43
13:a:113:ILE:HA	13:a:116:ILE:HG22	2.00	0.43
15:p:247:MET:HE3	15:p:247:MET:HB3	1.85	0.43
14:b:97:ARG:HA	14:b:97:ARG:HD2	1.82	0.43
6:T:7:ASP:O	6:T:21:GLN:NE2	2.51	0.43
7:U:148:LYS:HA	7:U:148:LYS:HD3	1.78	0.43
14:N:97:ARG:HA	14:N:97:ARG:HD2	1.82	0.43
15:d:170:ILE:HG12	15:e:261:ASN:HD21	1.83	0.43
15:e:247:MET:HE3	15:e:247:MET:HB3	1.85	0.43
15:e:248:ARG:HH21	15:e:249:ASN:HD21	1.65	0.43
15:o:52:VAL:HG23	15:o:61:ILE:HD13	2.00	0.43
15:o:134:SER:N	15:p:223:SER:OG	2.51	0.43
15:p:248:ARG:HH21	15:p:249:ASN:HD21	1.65	0.43
14:b:29:ALA:HB2	14:b:40:VAL:HG11	2.00	0.43
10:X:206:GLU:HG2	10:X:207:LYS:HG3	2.00	0.43
3:Q:37:LEU:HB3	3:Q:44:ILE:HG12	1.99	0.43
3:Q:143:ASP:N	3:Q:143:ASP:OD1	2.50	0.43
2:B:190:THR:O	2:B:194:THR:OG1	2.33	0.43
3:C:143:ASP:OD1	3:C:143:ASP:N	2.50	0.43
13:M:60:SER:OG	13:M:61:TYR:N	2.49	0.43
13:M:113:ILE:HA	13:M:116:ILE:HG22	2.00	0.43
13:a:60:SER:OG	13:a:61:TYR:N	2.49	0.43
15:c:30:THR:HG22	15:c:162:TRP:HE1	1.84	0.43
15:d:52:VAL:HG23	15:d:61:ILE:HD13	2.00	0.43
6:F:38:ILE:HD12	6:F:177:LEU:HD13	2.00	0.43
7:G:187:ILE:HG23	7:G:188:ASN:H	1.84	0.43
10:J:206:GLU:HG2	10:J:207:LYS:HG3	2.00	0.43
12:L:54:TYR:O	12:L:58:TYR:N	2.48	0.43
13:a:153:ASP:OD2	13:a:157:SER:OG	2.31	0.43
15:c:31:LYS:HE2	15:c:31:LYS:HB3	1.87	0.43
15:m:30:THR:HG22	15:m:162:TRP:HE1	1.84	0.43
14:b:57:GLU:HG2	14:b:60:ASP:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:187:ILE:HG23	7:U:188:ASN:H	1.84	0.43
4:D:48:LYS:HA	4:D:48:LYS:HD2	1.74	0.43
6:F:205:THR:HG22	6:F:209:THR:HG21	2.00	0.43
7:G:70:TYR:O	7:G:78:ILE:N	2.47	0.43
13:M:153:ASP:OD2	13:M:157:SER:OG	2.32	0.43
14:N:57:GLU:HG2	14:N:60:ASP:H	1.83	0.43
5:S:144:LEU:HG	5:S:155:LEU:HD11	2.00	0.43
15:c:211:LYS:O	15:c:214:THR:OG1	2.31	0.43
15:i:135:HIS:ND1	15:i:138:ILE:HG12	2.33	0.43
6:T:38:ILE:HD12	6:T:177:LEU:HD13	2.01	0.43
12:Z:54:TYR:O	12:Z:58:TYR:N	2.49	0.43
2:B:62:ILE:HD13	2:B:62:ILE:HA	1.89	0.43
4:D:62:LEU:HD23	4:D:72:ALA:HB2	2.01	0.43
8:H:8:TYR:HB3	8:H:9:ASP:H	1.66	0.43
4:R:62:LEU:HD23	4:R:72:ALA:HB2	2.01	0.43
13:a:206:ILE:HG22	13:a:237:LEU:HD11	2.01	0.43
3:C:86:LEU:O	3:C:90:SER:N	2.47	0.43
3:C:209:LYS:HA	3:C:209:LYS:HD2	1.93	0.43
10:J:166:LEU:HD23	10:J:166:LEU:HA	1.88	0.43
13:M:206:ILE:HG22	13:M:237:LEU:HD11	2.01	0.43
2:P:62:ILE:HD13	2:P:62:ILE:HA	1.89	0.43
11:Y:3:THR:OG1	11:Y:18:ASP:OD1	2.33	0.43
15:n:135:HIS:ND1	15:n:138:ILE:HG12	2.33	0.43
15:n:152:LEU:HD21	15:n:191:VAL:HG12	2.01	0.43
6:T:205:THR:HG22	6:T:209:THR:HG21	2.00	0.43
1:O:46:ASN:HA	1:O:155:PRO:HD3	2.00	0.43
1:A:46:ASN:HA	1:A:155:PRO:HD3	2.01	0.43
6:F:30:LYS:HA	6:F:161:GLY:HA3	2.00	0.43
15:d:32:GLN:NE2	15:e:55:ASN:OD1	2.52	0.43
15:f:61:ILE:O	15:f:241:LYS:NZ	2.39	0.43
15:i:152:LEU:HD21	15:i:191:VAL:HG12	2.01	0.43
3:Q:209:LYS:HA	3:Q:209:LYS:HD2	1.93	0.43
6:T:30:LYS:HA	6:T:161:GLY:HA3	2.00	0.43
5:E:144:LEU:HG	5:E:155:LEU:HD11	2.00	0.43
15:c:46:ILE:HD12	15:i:21:GLU:HG3	2.00	0.43
15:m:46:ILE:HD12	15:n:21:GLU:HG3	2.00	0.43
15:o:235:LYS:HA	15:o:235:LYS:HD3	1.80	0.43
10:X:110:ILE:HD13	10:X:110:ILE:HA	1.82	0.43
3:Q:86:LEU:O	3:Q:90:SER:N	2.47	0.43
1:O:96:MET:HE3	1:O:96:MET:HB3	1.81	0.43
7:U:70:TYR:O	7:U:78:ILE:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:HE2	1:A:170:ARG:HA	2.00	0.42
3:C:76:VAL:HG21	3:C:83:ALA:HB1	2.00	0.42
5:E:116:ILE:HD12	5:E:116:ILE:HA	1.80	0.42
6:F:157:ALA:HB1	6:F:171:LEU:HD13	2.01	0.42
15:h:213:SER:HA	15:h:216:VAL:HG12	2.01	0.42
15:l:213:SER:HA	15:l:216:VAL:HG12	2.01	0.42
3:Q:76:VAL:HG21	3:Q:83:ALA:HB1	2.00	0.42
5:E:25:GLU:HB3	15:d:174:ASN:HD21	1.83	0.42
8:H:215:LYS:HB3	8:H:248:MET:HG2	2.01	0.42
10:J:196:TRP:CD2	10:J:217:MET:HG3	2.53	0.42
9:W:152:LYS:HE2	9:W:175:ILE:HD11	2.00	0.42
15:j:46:ILE:HD12	15:p:21:GLU:HG3	2.01	0.42
10:X:90:ALA:O	10:X:137:TYR:OH	2.31	0.42
10:X:162:MET:SD	10:X:186:SER:OG	2.72	0.42
10:X:166:LEU:HD23	10:X:166:LEU:HA	1.88	0.42
10:X:196:TRP:CD2	10:X:217:MET:HG3	2.53	0.42
6:T:157:ALA:HB1	6:T:171:LEU:HD13	2.01	0.42
1:A:206:ARG:NH1	1:A:255:TYR:OH	2.52	0.42
6:F:13:TYR:HB2	7:G:23:GLN:HE22	1.84	0.42
9:I:152:LYS:HE2	9:I:175:ILE:HD11	2.00	0.42
10:J:69:LEU:HD12	10:J:69:LEU:HA	1.89	0.42
10:J:90:ALA:O	10:J:137:TYR:OH	2.31	0.42
10:J:162:MET:SD	10:J:186:SER:OG	2.72	0.42
4:R:48:LYS:HA	4:R:48:LYS:HD2	1.74	0.42
15:j:52:VAL:HG23	15:j:61:ILE:HG21	2.01	0.42
1:O:231:VAL:HG22	1:O:249:ILE:HD11	2.01	0.42
1:A:16:PHE:HB2	2:B:21:GLN:HE22	1.85	0.42
1:A:81:GLU:OE1	1:A:239:ARG:HB3	2.18	0.42
8:V:161:LYS:HD3	8:V:161:LYS:HA	1.83	0.42
8:V:215:LYS:HB3	8:V:248:MET:HG2	2.02	0.42
15:f:52:VAL:HG23	15:f:61:ILE:HG21	2.02	0.42
10:X:70:ARG:NH2	3:Q:102:ASN:OD1	2.50	0.42
3:Q:135:LEU:HD11	3:Q:162:THR:HB	2.01	0.42
1:O:159:LYS:HB3	1:O:169:TYR:HE2	1.85	0.42
1:O:206:ARG:NH1	1:O:255:TYR:OH	2.52	0.42
1:A:159:LYS:HB3	1:A:169:TYR:HE2	1.85	0.42
1:A:231:VAL:HG22	1:A:249:ILE:HD11	2.01	0.42
10:J:18:SER:OG	10:J:19:ASN:N	2.52	0.42
5:S:116:ILE:HD12	5:S:116:ILE:HA	1.80	0.42
13:a:116:ILE:HD12	13:a:116:ILE:HA	1.88	0.42
13:a:184:LYS:HD2	13:a:184:LYS:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:18:SER:OG	10:X:19:ASN:N	2.52	0.42
1:O:43:LYS:HE2	1:O:170:ARG:HA	2.00	0.42
1:O:81:GLU:OE1	1:O:239:ARG:HB3	2.19	0.42
3:C:135:LEU:HD11	3:C:162:THR:HB	2.01	0.42
8:H:161:LYS:HD3	8:H:161:LYS:HA	1.83	0.42
10:J:110:ILE:HD13	10:J:110:ILE:HA	1.83	0.42
15:k:174:ASN:HB2	1:O:23:TYR:CE1	2.55	0.42
15:p:27:TYR:O	15:p:30:THR:OG1	2.37	0.42
14:b:80:LYS:HE2	14:b:80:LYS:HB3	1.82	0.42
10:X:69:LEU:HD12	10:X:69:LEU:HA	1.89	0.42
3:Q:82:ASP:OD1	3:Q:128:ARG:NH1	2.52	0.42
1:A:8:MET:SD	15:g:173:GLY:HA2	2.60	0.42
3:C:82:ASP:OD1	3:C:128:ARG:NH1	2.52	0.42
3:C:135:LEU:HD12	3:C:147:LEU:HD11	2.02	0.42
10:J:27:LEU:HD23	10:J:40:LYS:HA	2.02	0.42
11:K:48:GLY:N	11:K:101:ASN:O	2.52	0.42
12:L:63:ILE:HD13	12:L:63:ILE:HA	1.88	0.42
15:d:235:LYS:HA	15:d:235:LYS:HD3	1.80	0.42
15:e:27:TYR:O	15:e:30:THR:OG1	2.37	0.42
15:e:153:ILE:HG13	15:e:192:GLU:HG3	2.02	0.42
15:l:57:GLU:O	15:l:60:SER:OG	2.32	0.42
15:o:150:SER:OG	15:p:62:LEU:O	2.35	0.42
15:p:153:ILE:HG13	15:p:192:GLU:HG3	2.02	0.42
10:X:27:LEU:HD23	10:X:40:LYS:HA	2.02	0.42
8:H:89:ASP:OD1	8:H:89:ASP:N	2.52	0.42
10:J:104:PRO:HB2	11:K:94:ARG:HH21	1.83	0.42
13:M:116:ILE:HD12	13:M:116:ILE:HA	1.88	0.42
14:N:218:ALA:HB3	8:V:24:THR:HG23	2.01	0.42
8:V:170:ASN:HB2	14:b:59:ALA:HB1	2.02	0.42
11:Y:48:GLY:N	11:Y:101:ASN:O	2.52	0.42
6:F:219:PRO:HD2	6:F:221:GLN:HE21	1.85	0.42
7:G:115:VAL:HG13	7:G:154:ILE:HD11	2.02	0.42
12:L:191:GLU:O	10:X:216:ARG:NH1	2.47	0.42
13:M:184:LYS:HD2	13:M:184:LYS:HA	1.79	0.42
14:b:26:ASP:OD1	14:b:26:ASP:N	2.47	0.42
6:T:219:PRO:HD2	6:T:221:GLN:HE21	1.85	0.42
3:C:37:LEU:HD11	3:C:179:TRP:HD1	1.85	0.42
3:C:67:LYS:HG3	3:C:223:TYR:HE2	1.84	0.42
15:h:57:GLU:O	15:h:60:SER:OG	2.32	0.42
3:Q:135:LEU:HD12	3:Q:147:LEU:HD11	2.02	0.42
6:T:113:ALA:HA	6:T:116:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:63:ILE:HD13	12:Z:63:ILE:HA	1.88	0.42
7:U:115:VAL:HG13	7:U:154:ILE:HD11	2.02	0.42
6:F:113:ALA:HA	6:F:116:TYR:HD2	1.84	0.41
8:H:19:ARG:NE	8:H:224:SER:O	2.33	0.41
12:L:160:ILE:O	12:L:164:THR:N	2.53	0.41
14:N:80:LYS:HE2	14:N:80:LYS:HB3	1.82	0.41
8:V:19:ARG:NE	8:V:224:SER:O	2.33	0.41
15:c:171:GLU:OE1	15:c:269:LYS:NZ	2.53	0.41
15:e:221:ASN:OD1	15:e:221:ASN:N	2.53	0.41
15:j:253:MET:HE2	15:p:164:GLN:HG3	2.01	0.41
15:p:221:ASN:OD1	15:p:221:ASN:N	2.53	0.41
3:Q:37:LEU:HD11	3:Q:179:TRP:HD1	1.85	0.41
3:Q:67:LYS:HG3	3:Q:223:TYR:HE2	1.84	0.41
6:T:175:LEU:HD12	6:T:175:LEU:HA	1.92	0.41
12:Z:160:ILE:O	12:Z:164:THR:N	2.52	0.41
2:B:160:ALA:HB1	2:B:174:LEU:HD13	2.02	0.41
3:C:124:TYR:HB3	4:D:124:VAL:HG12	2.01	0.41
5:E:16:SER:OG	15:d:172:ASP:OD2	2.38	0.41
5:E:90:ASP:OD1	12:L:69:ARG:NE	2.52	0.41
14:N:26:ASP:OD1	14:N:26:ASP:N	2.47	0.41
9:W:148:ILE:HD13	9:W:148:ILE:HA	1.93	0.41
8:H:4:ILE:HD13	8:H:214:VAL:HG22	2.02	0.41
10:J:40:LYS:HA	10:J:40:LYS:HD2	1.91	0.41
2:P:160:ALA:HB1	2:P:174:LEU:HD13	2.02	0.41
1:O:66:LEU:HD22	7:U:164:SER:HB2	2.02	0.41
6:F:175:LEU:HD12	6:F:175:LEU:HA	1.91	0.41
10:J:196:TRP:HZ3	12:Z:203:PRO:HD2	1.85	0.41
12:L:76:VAL:HG23	12:L:105:ASP:HB3	2.02	0.41
5:S:60:GLU:OE2	5:S:63:SER:N	2.54	0.41
8:V:89:ASP:OD1	8:V:89:ASP:N	2.52	0.41
15:m:21:GLU:HB3	15:o:46:ILE:HD12	2.02	0.41
15:o:175:ASN:OD1	15:o:175:ASN:N	2.53	0.41
12:Z:76:VAL:HG23	12:Z:105:ASP:HB3	2.02	0.41
7:U:93:ARG:HG2	7:U:121:TYR:CG	2.55	0.41
5:E:60:GLU:OE2	5:E:63:SER:N	2.54	0.41
7:G:93:ARG:HG2	7:G:121:TYR:CG	2.55	0.41
8:H:19:ARG:HD3	8:H:19:ARG:HA	1.70	0.41
12:L:64:LYS:HA	12:L:64:LYS:HD2	1.84	0.41
8:V:4:ILE:HD13	8:V:214:VAL:HG22	2.03	0.41
8:V:11:GLY:O	8:V:162:GLN:NE2	2.53	0.41
15:d:149:ALA:O	15:d:153:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:d:175:ASN:OD1	15:d:175:ASN:N	2.53	0.41
15:m:206:TYR:CE2	15:o:231:GLU:HG3	2.55	0.41
10:X:40:LYS:HA	10:X:40:LYS:HD2	1.91	0.41
1:A:203:GLU:HG3	1:A:206:ARG:HB2	2.01	0.41
4:D:68:HIS:ND1	4:D:212:LYS:HB3	2.35	0.41
6:F:84:LEU:HD23	6:F:84:LEU:HA	1.89	0.41
8:H:11:GLY:O	8:H:162:GLN:NE2	2.53	0.41
4:R:68:HIS:ND1	4:R:212:LYS:HB3	2.35	0.41
15:d:145:ILE:HG13	15:d:240:ILE:HD12	2.02	0.41
15:m:31:LYS:HE2	15:m:31:LYS:HB3	1.88	0.41
15:o:145:ILE:HG13	15:o:240:ILE:HD12	2.03	0.41
15:o:149:ALA:O	15:o:153:ILE:HG12	2.20	0.41
14:b:199:GLU:OE2	14:b:203:ARG:NH2	2.53	0.41
1:O:172:CYS:SG	1:O:173:VAL:N	2.93	0.41
1:O:203:GLU:HG3	1:O:206:ARG:HB2	2.01	0.41
12:Z:64:LYS:HA	12:Z:64:LYS:HD2	1.84	0.41
3:C:197:ALA:HB2	3:C:205:PRO:HG3	2.02	0.41
14:N:199:GLU:OE2	14:N:203:ARG:NH2	2.53	0.41
8:V:211:LEU:HD12	8:V:211:LEU:HA	1.82	0.41
15:m:171:GLU:OE1	15:m:269:LYS:NZ	2.53	0.41
15:n:36:SER:HA	15:n:40:ARG:HB2	2.02	0.41
3:Q:197:ALA:HB2	3:Q:205:PRO:HG3	2.02	0.41
6:T:84:LEU:HD23	6:T:84:LEU:HA	1.89	0.41
1:A:172:CYS:SG	1:A:173:VAL:N	2.93	0.41
6:F:198:LEU:HD12	6:F:198:LEU:HA	1.90	0.41
11:K:48:GLY:O	11:K:101:ASN:N	2.53	0.41
13:M:142:ASP:OD1	13:M:142:ASP:N	2.48	0.41
11:Y:48:GLY:O	11:Y:101:ASN:N	2.53	0.41
15:c:164:GLN:O	15:c:167:VAL:HG22	2.20	0.41
15:i:36:SER:HA	15:i:40:ARG:HB2	2.02	0.41
15:m:164:GLN:O	15:m:167:VAL:HG22	2.20	0.41
6:F:55:LYS:HD2	6:F:55:LYS:HA	1.95	0.41
12:L:161:TYR:HA	12:L:164:THR:HG22	2.03	0.41
13:M:32:PRO:HA	14:N:167:HIS:HE1	1.86	0.41
13:M:175:PRO:HG3	10:X:190:ARG:HG2	2.03	0.41
14:N:43:ILE:HD13	14:N:43:ILE:HA	1.88	0.41
13:a:142:ASP:OD1	13:a:142:ASP:N	2.48	0.41
15:d:188:LEU:HD13	15:d:254:LEU:HD13	2.03	0.41
15:f:31:LYS:HE2	15:f:31:LYS:HB3	1.90	0.41
15:h:158:ASN:HA	15:h:161:LEU:HD12	2.03	0.41
15:n:173:GLY:HA3	3:Q:19:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:85:ILE:HD13	3:Q:85:ILE:HA	1.91	0.41
6:T:65:LYS:NZ	6:T:67:ASP:O	2.46	0.41
1:O:92:ASP:OD1	1:O:138:ARG:NH2	2.43	0.41
1:O:149:ILE:HG22	1:O:155:PRO:HA	2.02	0.41
12:Z:161:TYR:HA	12:Z:164:THR:HG22	2.03	0.41
1:A:65:LYS:HB2	1:A:66:LEU:H	1.75	0.41
1:A:89:MET:HE3	1:A:89:MET:HB2	1.95	0.41
3:C:85:ILE:HD13	3:C:85:ILE:HA	1.91	0.41
15:h:201:ALA:O	15:h:204:LYS:HG3	2.20	0.41
15:i:257:LEU:O	15:i:261:ASN:ND2	2.41	0.41
15:l:201:ALA:O	15:l:204:LYS:HG3	2.20	0.41
15:o:188:LEU:HD13	15:o:254:LEU:HD13	2.03	0.41
1:O:65:LYS:HB2	1:O:66:LEU:H	1.75	0.41
1:A:128:ILE:HD13	1:A:128:ILE:HA	1.92	0.40
1:A:149:ILE:HG22	1:A:155:PRO:HA	2.02	0.40
2:B:95:ILE:HG23	9:I:61:HIS:HB3	2.03	0.40
3:C:207:SER:OG	3:C:231:GLU:OE2	2.33	0.40
6:F:65:LYS:NZ	6:F:67:ASP:O	2.46	0.40
7:G:144:ASN:HD22	7:G:147:ASP:H	1.69	0.40
9:I:4:CYS:SG	9:I:5:GLY:N	2.95	0.40
9:I:211:PRO:HD3	10:J:214:LYS:HB2	2.02	0.40
5:S:186:ASN:HB3	5:S:199:LEU:HD11	2.03	0.40
9:W:4:CYS:SG	9:W:5:GLY:N	2.95	0.40
15:d:175:ASN:HB2	15:d:178:VAL:HG12	2.04	0.40
15:e:31:LYS:HE2	15:e:31:LYS:HB3	1.95	0.40
15:e:170:ILE:HG22	15:f:261:ASN:ND2	2.36	0.40
15:l:158:ASN:HA	15:l:161:LEU:HD12	2.04	0.40
3:Q:70:LYS:HA	3:Q:70:LYS:HD3	1.87	0.40
1:O:205:ILE:HA	1:O:209:THR:HG23	2.04	0.40
1:A:205:ILE:HA	1:A:209:THR:HG23	2.04	0.40
5:E:186:ASN:HB3	5:E:199:LEU:HD11	2.03	0.40
2:P:128:ARG:HB2	1:O:14:THR:HB	2.02	0.40
8:V:19:ARG:HD3	8:V:19:ARG:HA	1.70	0.40
15:d:190:ARG:O	15:d:194:SER:OG	2.38	0.40
15:e:46:ILE:O	15:e:50:ASN:ND2	2.38	0.40
15:m:41:ILE:HD13	15:m:41:ILE:HA	1.86	0.40
15:n:153:ILE:HG13	15:n:192:GLU:HG2	2.03	0.40
15:o:175:ASN:HB2	15:o:178:VAL:HG12	2.04	0.40
15:o:190:ARG:O	15:o:194:SER:OG	2.38	0.40
6:T:198:LEU:HD12	6:T:198:LEU:HA	1.90	0.40
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:160:LYS:HE3	8:H:160:LYS:HB3	1.77	0.40
8:H:211:LEU:HD12	8:H:211:LEU:HA	1.82	0.40
11:K:171:PHE:HE2	11:K:175:GLN:HE22	1.69	0.40
12:L:5:ALA:HB1	12:L:111:MET:SD	2.62	0.40
12:L:20:ALA:HB2	12:L:31:VAL:HG21	2.02	0.40
9:W:51:ASP:OD1	10:X:98:TYR:OH	2.27	0.40
11:Y:171:PHE:HE2	11:Y:175:GLN:HE22	1.69	0.40
15:e:156:ILE:HD12	15:e:191:VAL:HG13	2.02	0.40
15:i:153:ILE:HG13	15:i:192:GLU:HG2	2.04	0.40
15:j:31:LYS:HE2	15:j:31:LYS:HB3	1.90	0.40
15:j:153:ILE:HD11	15:k:62:LEU:HG	2.03	0.40
3:Q:207:SER:OG	3:Q:231:GLU:OE2	2.33	0.40
1:O:128:ILE:HD13	1:O:128:ILE:HA	1.92	0.40
7:U:144:ASN:HD22	7:U:147:ASP:H	1.69	0.40
1:A:124:ILE:HD13	1:A:124:ILE:HA	1.95	0.40
2:B:188:ILE:HD13	2:B:188:ILE:HA	1.90	0.40
3:C:70:LYS:HA	3:C:70:LYS:HD3	1.87	0.40
9:W:146:MET:HB3	9:W:150:GLU:HB3	2.04	0.40
11:Y:86:ARG:HG2	11:Y:122:SER:HB2	2.03	0.40
15:n:257:LEU:O	15:n:261:ASN:ND2	2.41	0.40
15:p:156:ILE:HD12	15:p:191:VAL:HG13	2.03	0.40
1:O:89:MET:HE3	1:O:89:MET:HB2	1.95	0.40
12:Z:5:ALA:HB1	12:Z:111:MET:SD	2.62	0.40
6:F:33:THR:OG1	6:F:62:LYS:NZ	2.41	0.40
2:P:134:LEU:HD23	2:P:134:LEU:HA	1.92	0.40
5:S:208:MET:HE2	5:S:212:LEU:HD23	2.04	0.40
8:V:59:ILE:HD13	8:V:59:ILE:HA	1.84	0.40
15:e:62:LEU:HD12	15:e:238:ILE:HG23	2.04	0.40
7:U:111:LEU:HD12	7:U:111:LEU:HA	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	242/260 (93%)	211 (87%)	31 (13%)	0	100	100
1	O	242/260 (93%)	211 (87%)	31 (13%)	0	100	100
2	B	222/235 (94%)	207 (93%)	15 (7%)	0	100	100
2	P	222/235 (94%)	207 (93%)	15 (7%)	0	100	100
3	C	238/246 (97%)	217 (91%)	19 (8%)	2 (1%)	16	48
3	Q	238/246 (97%)	217 (91%)	19 (8%)	2 (1%)	16	48
4	D	225/241 (93%)	207 (92%)	18 (8%)	0	100	100
4	R	225/241 (93%)	207 (92%)	18 (8%)	0	100	100
5	E	223/256 (87%)	206 (92%)	17 (8%)	0	100	100
5	S	223/256 (87%)	206 (92%)	17 (8%)	0	100	100
6	F	234/254 (92%)	205 (88%)	29 (12%)	0	100	100
6	T	234/254 (92%)	205 (88%)	29 (12%)	0	100	100
7	G	229/252 (91%)	200 (87%)	29 (13%)	0	100	100
7	U	229/252 (91%)	200 (87%)	29 (13%)	0	100	100
8	H	189/252 (75%)	158 (84%)	30 (16%)	1 (0%)	24	57
8	V	189/252 (75%)	158 (84%)	30 (16%)	1 (0%)	24	57
9	I	217/229 (95%)	188 (87%)	27 (12%)	2 (1%)	14	45
9	W	217/229 (95%)	188 (87%)	27 (12%)	2 (1%)	14	45
10	J	199/218 (91%)	177 (89%)	22 (11%)	0	100	100
10	X	199/218 (91%)	176 (88%)	23 (12%)	0	100	100
11	K	193/195 (99%)	170 (88%)	23 (12%)	0	100	100
11	Y	193/195 (99%)	170 (88%)	23 (12%)	0	100	100
12	L	202/211 (96%)	175 (87%)	27 (13%)	0	100	100
12	Z	202/211 (96%)	175 (87%)	27 (13%)	0	100	100
13	M	209/240 (87%)	179 (86%)	29 (14%)	1 (0%)	24	57
13	a	209/240 (87%)	179 (86%)	29 (14%)	1 (0%)	24	57
14	N	220/265 (83%)	189 (86%)	31 (14%)	0	100	100
14	b	220/265 (83%)	189 (86%)	31 (14%)	0	100	100
15	c	183/279 (66%)	176 (96%)	7 (4%)	0	100	100
15	d	183/279 (66%)	177 (97%)	6 (3%)	0	100	100
15	e	184/279 (66%)	178 (97%)	6 (3%)	0	100	100
15	f	189/279 (68%)	181 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	g	185/279 (66%)	176 (95%)	9 (5%)	0	100	100
15	h	182/279 (65%)	176 (97%)	6 (3%)	0	100	100
15	i	182/279 (65%)	176 (97%)	6 (3%)	0	100	100
15	j	189/279 (68%)	181 (96%)	8 (4%)	0	100	100
15	k	185/279 (66%)	176 (95%)	9 (5%)	0	100	100
15	l	182/279 (65%)	176 (97%)	6 (3%)	0	100	100
15	m	183/279 (66%)	176 (96%)	7 (4%)	0	100	100
15	n	182/279 (65%)	176 (97%)	6 (3%)	0	100	100
15	o	183/279 (66%)	177 (97%)	6 (3%)	0	100	100
15	p	184/279 (66%)	178 (97%)	6 (3%)	0	100	100
All	All	8660/10614 (82%)	7857 (91%)	791 (9%)	12 (0%)	49	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	76	PHE
8	V	76	PHE
3	C	210	ILE
3	Q	210	ILE
9	I	206	PRO
9	W	206	PRO
9	I	24	PRO
13	M	146	LYS
9	W	24	PRO
13	a	146	LYS
3	C	244	ILE
3	Q	244	ILE

5.3.2 Protein sidechains ⓘ

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	A	217/231 (94%)	213 (98%)	4 (2%)	51	67
1	O	217/231 (94%)	213 (98%)	4 (2%)	51	67
2	B	196/205 (96%)	196 (100%)	0	100	100
2	P	196/205 (96%)	196 (100%)	0	100	100
3	C	208/213 (98%)	207 (100%)	1 (0%)	81	81
3	Q	208/213 (98%)	207 (100%)	1 (0%)	81	81
4	D	194/207 (94%)	191 (98%)	3 (2%)	57	69
4	R	194/207 (94%)	191 (98%)	3 (2%)	57	69
5	E	195/223 (87%)	193 (99%)	2 (1%)	68	74
5	S	195/223 (87%)	193 (99%)	2 (1%)	68	74
6	F	211/227 (93%)	211 (100%)	0	100	100
6	T	211/227 (93%)	211 (100%)	0	100	100
7	G	212/229 (93%)	212 (100%)	0	100	100
7	U	212/229 (93%)	212 (100%)	0	100	100
8	H	173/231 (75%)	171 (99%)	2 (1%)	63	72
8	V	173/231 (75%)	171 (99%)	2 (1%)	63	72
9	I	185/194 (95%)	183 (99%)	2 (1%)	65	73
9	W	185/194 (95%)	183 (99%)	2 (1%)	65	73
10	J	178/191 (93%)	177 (99%)	1 (1%)	78	79
10	X	178/191 (93%)	177 (99%)	1 (1%)	78	79
11	K	174/174 (100%)	173 (99%)	1 (1%)	78	79
11	Y	174/174 (100%)	173 (99%)	1 (1%)	78	79
12	L	169/176 (96%)	168 (99%)	1 (1%)	78	79
12	Z	169/176 (96%)	168 (99%)	1 (1%)	78	79
13	M	189/216 (88%)	187 (99%)	2 (1%)	65	73
13	a	189/216 (88%)	187 (99%)	2 (1%)	65	73
14	N	201/239 (84%)	201 (100%)	0	100	100
14	b	201/239 (84%)	201 (100%)	0	100	100
15	c	174/261 (67%)	169 (97%)	5 (3%)	37	58
15	d	174/261 (67%)	174 (100%)	0	100	100
15	e	175/261 (67%)	172 (98%)	3 (2%)	53	67
15	f	179/261 (69%)	176 (98%)	3 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	g	176/261 (67%)	170 (97%)	6 (3%)	32	55
15	h	173/261 (66%)	169 (98%)	4 (2%)	44	63
15	i	173/261 (66%)	170 (98%)	3 (2%)	53	67
15	j	179/261 (69%)	176 (98%)	3 (2%)	53	67
15	k	176/261 (67%)	170 (97%)	6 (3%)	32	55
15	l	173/261 (66%)	169 (98%)	4 (2%)	44	63
15	m	174/261 (67%)	169 (97%)	5 (3%)	37	58
15	n	173/261 (66%)	170 (98%)	3 (2%)	53	67
15	o	174/261 (67%)	174 (100%)	0	100	100
15	p	175/261 (67%)	172 (98%)	3 (2%)	53	67
All	All	7852/9566 (82%)	7766 (99%)	86 (1%)	63	73

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	81	GLU
1	A	196	ILE
1	A	227	SER
3	C	48	ASP
4	D	55	ASN
4	D	196	VAL
4	D	210	THR
5	E	119	LEU
5	E	198	ILE
8	H	173	ILE
8	H	224	SER
9	I	12	VAL
9	I	173	VAL
10	J	23	ILE
11	K	50	SER
12	L	201	THR
13	M	60	SER
13	M	232	VAL
4	R	55	ASN
4	R	196	VAL
4	R	210	THR
5	S	119	LEU

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Mol	Chain	Res	Type
5	S	198	ILE
8	V	173	ILE
8	V	224	SER
9	W	12	VAL
9	W	173	VAL
11	Y	50	SER
13	a	60	SER
13	a	232	VAL
15	c	167	VAL
15	c	170	ILE
15	c	257	LEU
15	c	258	LEU
15	c	269	LYS
15	e	64	VAL
15	e	240	ILE
15	e	258	LEU
15	f	158	ASN
15	f	240	ILE
15	f	254	LEU
15	g	29	ILE
15	g	64	VAL
15	g	142	LEU
15	g	254	LEU
15	g	258	LEU
15	g	266	VAL
15	h	60	SER
15	h	165	LEU
15	h	207	MET
15	h	258	LEU
15	i	37	LEU
15	i	188	LEU
15	i	253	MET
15	j	158	ASN
15	j	240	ILE
15	j	254	LEU
15	k	29	ILE
15	k	64	VAL
15	k	142	LEU
15	k	254	LEU
15	k	258	LEU
15	k	266	VAL
15	l	60	SER

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Mol	Chain	Res	Type
15	l	165	LEU
15	l	207	MET
15	l	258	LEU
15	m	167	VAL
15	m	170	ILE
15	m	257	LEU
15	m	258	LEU
15	m	269	LYS
15	n	37	LEU
15	n	188	LEU
15	n	253	MET
15	p	64	VAL
15	p	240	ILE
15	p	258	LEU
10	X	23	ILE
3	Q	48	ASP
1	O	40	VAL
1	O	81	GLU
1	O	196	ILE
1	O	227	SER
12	Z	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	36	ASN
1	A	129	GLN
1	A	134	HIS
1	A	153	ASN
1	A	207	ASN
2	B	21	GLN
2	B	67	GLN
2	B	157	ASN
2	B	207	ASN
2	B	224	GLN
3	C	29	ASN
3	C	71	HIS
3	C	89	GLN
3	C	100	ASN
3	C	113	GLN
4	D	18	GLN

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Mol	Chain	Res	Type
4	D	21	HIS
4	D	203	ASN
4	D	220	GLN
5	E	23	GLN
5	E	97	ASN
5	E	186	ASN
5	E	206	GLN
6	F	117	GLN
6	F	121	GLN
6	F	189	HIS
7	G	23	GLN
7	G	32	ASN
7	G	34	ASN
7	G	54	ASN
7	G	58	ASN
7	G	104	ASN
7	G	157	ASN
7	G	211	ASN
8	H	40	ASN
8	H	68	ASN
8	H	163	GLN
8	H	212	ASN
8	H	219	HIS
8	H	249	ASN
9	I	62	ASN
9	I	69	ASN
9	I	153	ASN
9	I	172	ASN
10	J	6	ASN
10	J	74	ASN
10	J	182	GLN
11	K	23	ASN
11	K	40	HIS
11	K	72	ASN
12	L	40	ASN
12	L	71	ASN
12	L	85	ASN
12	L	146	ASN
12	L	148	ASN
13	M	86	GLN
13	M	151	ASN
13	M	183	GLN

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Mol	Chain	Res	Type
13	M	200	ASN
14	N	38	GLN
14	N	62	GLN
14	N	75	ASN
14	N	89	GLN
14	N	92	HIS
2	P	21	GLN
2	P	67	GLN
2	P	157	ASN
2	P	207	ASN
2	P	224	GLN
4	R	18	GLN
4	R	203	ASN
4	R	220	GLN
5	S	23	GLN
5	S	97	ASN
5	S	186	ASN
5	S	206	GLN
8	V	40	ASN
8	V	68	ASN
8	V	163	GLN
8	V	212	ASN
8	V	219	HIS
8	V	249	ASN
9	W	62	ASN
9	W	69	ASN
9	W	153	ASN
9	W	172	ASN
11	Y	23	ASN
11	Y	40	HIS
11	Y	72	ASN
11	Y	88	ASN
13	a	86	GLN
13	a	151	ASN
13	a	183	GLN
13	a	200	ASN
15	c	166	ASN
15	c	197	ASN
15	c	261	ASN
15	d	32	GLN
15	d	53	ASN
15	d	181	GLN

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Mol	Chain	Res	Type
15	d	250	ASN
15	d	261	ASN
15	e	166	ASN
15	e	249	ASN
15	e	250	ASN
15	f	261	ASN
15	f	275	HIS
15	g	49	ASN
15	g	270	ASN
15	h	55	ASN
15	h	158	ASN
15	h	250	ASN
15	h	261	ASN
15	i	32	GLN
15	i	174	ASN
15	j	261	ASN
15	k	49	ASN
15	k	50	ASN
15	k	55	ASN
15	k	270	ASN
15	l	158	ASN
15	l	250	ASN
15	l	261	ASN
15	m	55	ASN
15	m	166	ASN
15	m	197	ASN
15	m	261	ASN
15	n	32	GLN
15	o	32	GLN
15	o	53	ASN
15	o	181	GLN
15	o	250	ASN
15	o	261	ASN
15	p	49	ASN
15	p	166	ASN
15	p	197	ASN
15	p	249	ASN
15	p	250	ASN
14	b	62	GLN
14	b	75	ASN
14	b	89	GLN
14	b	92	HIS

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Mol	Chain	Res	Type
14	b	121	GLN
10	X	74	ASN
10	X	182	GLN
3	Q	29	ASN
3	Q	71	HIS
3	Q	89	GLN
3	Q	100	ASN
3	Q	113	GLN
6	T	117	GLN
6	T	121	GLN
1	O	12	HIS
1	O	36	ASN
1	O	129	GLN
1	O	134	HIS
1	O	153	ASN
1	O	207	ASN
12	Z	40	ASN
12	Z	71	ASN
12	Z	85	ASN
12	Z	146	ASN
12	Z	148	ASN
12	Z	158	ASN
12	Z	162	HIS
7	U	23	GLN
7	U	32	ASN
7	U	34	ASN
7	U	54	ASN
7	U	58	ASN
7	U	104	ASN
7	U	123	HIS
7	U	144	ASN
7	U	211	ASN

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.

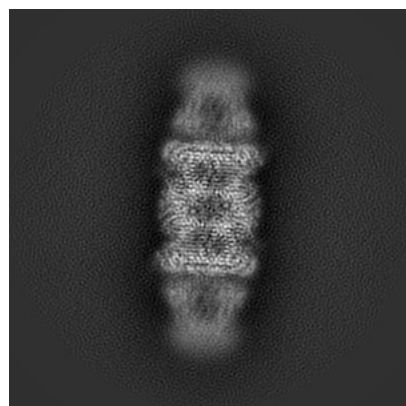
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9257. These allow visual inspection of the internal detail of the map and identification of artifacts.

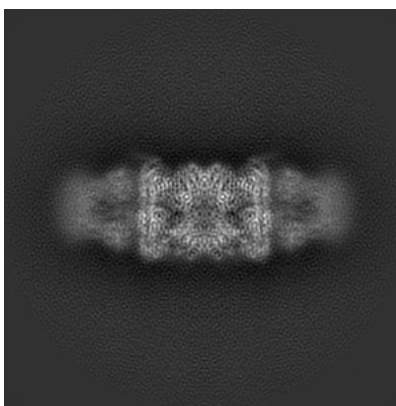
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

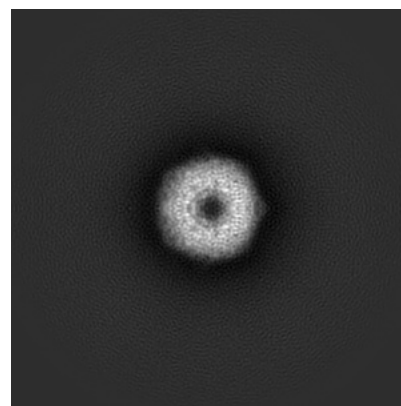
6.1.1 Primary map



X

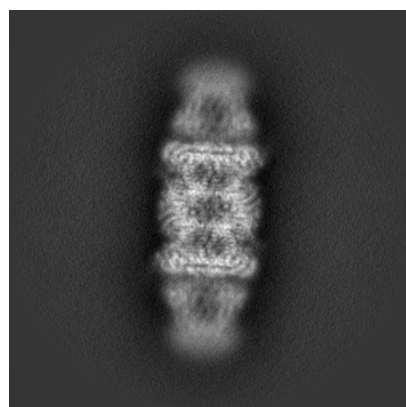


Y

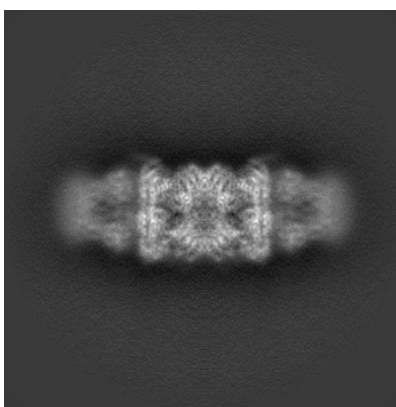


Z

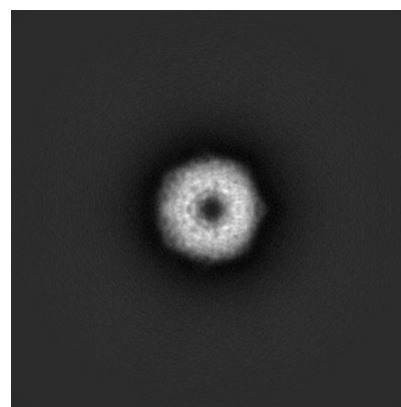
6.1.2 Raw map



X



Y

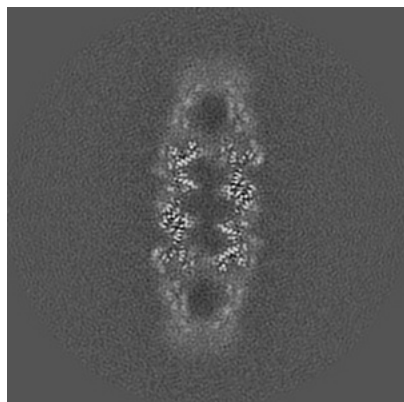


Z

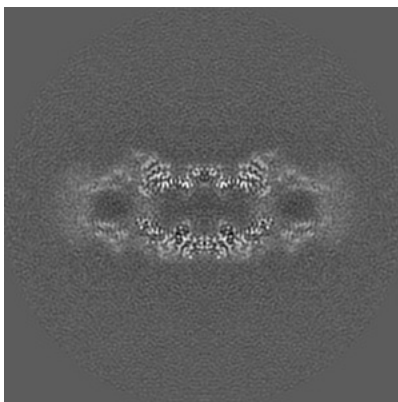
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

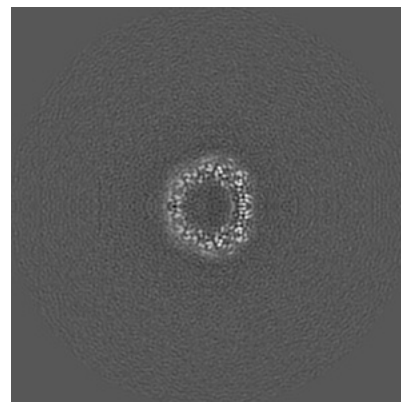
6.2.1 Primary map



X Index: 172

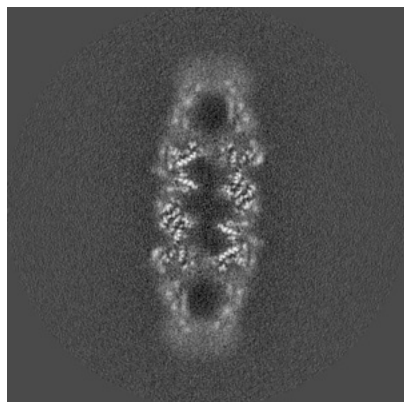


Y Index: 172

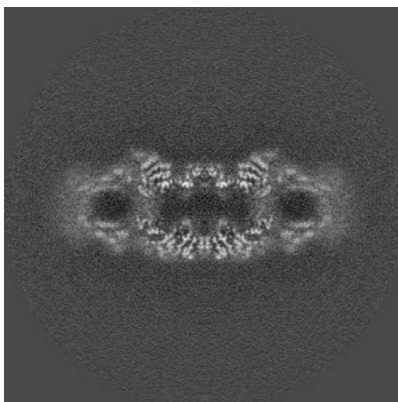


Z Index: 172

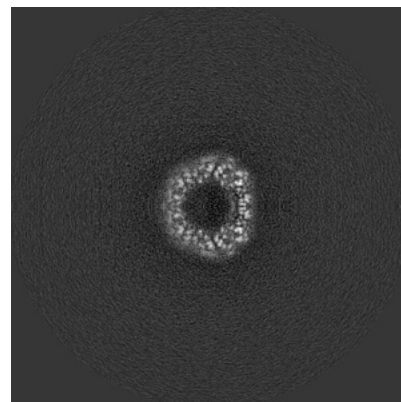
6.2.2 Raw map



X Index: 172



Y Index: 172

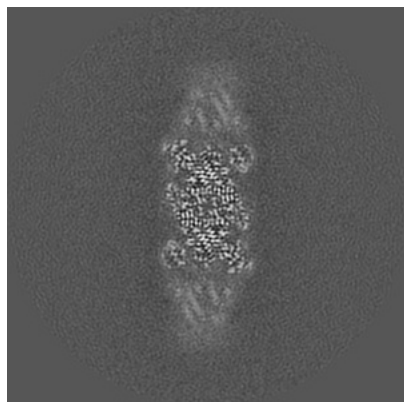


Z Index: 172

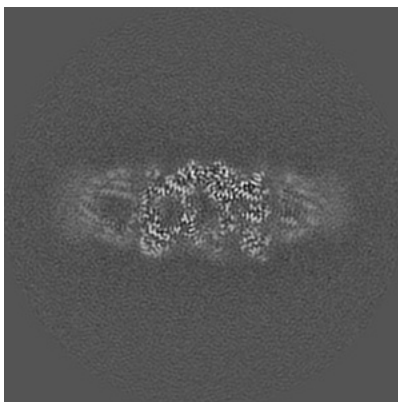
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

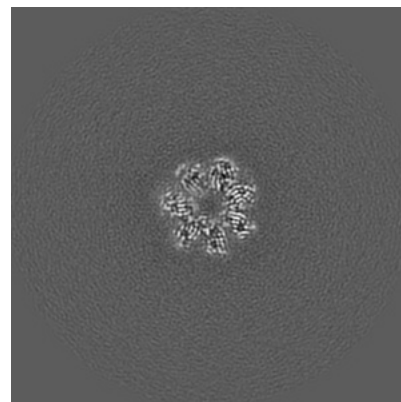
6.3.1 Primary map



X Index: 193

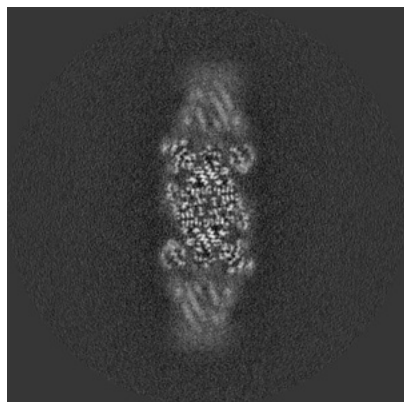


Y Index: 156

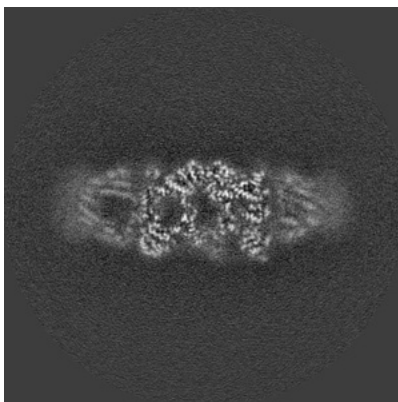


Z Index: 158

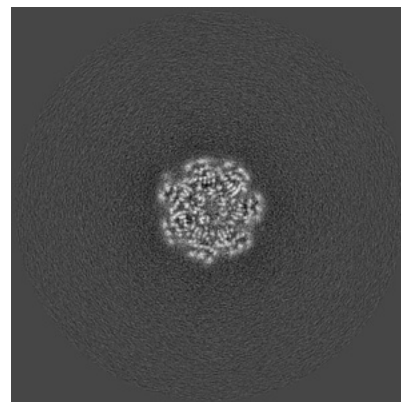
6.3.2 Raw map



X Index: 193



Y Index: 156

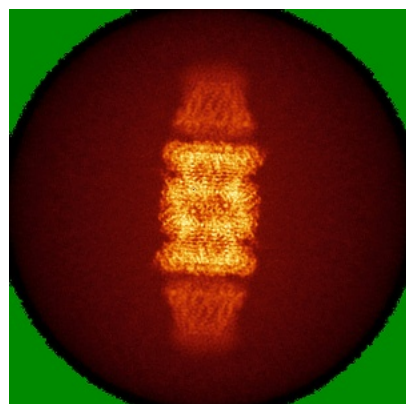


Z Index: 128

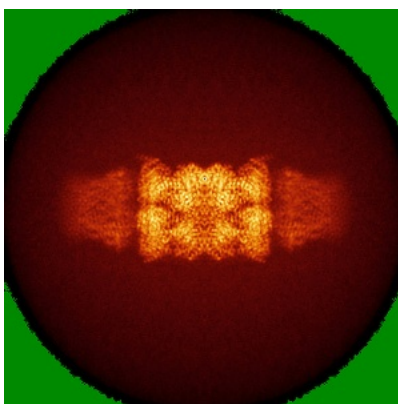
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

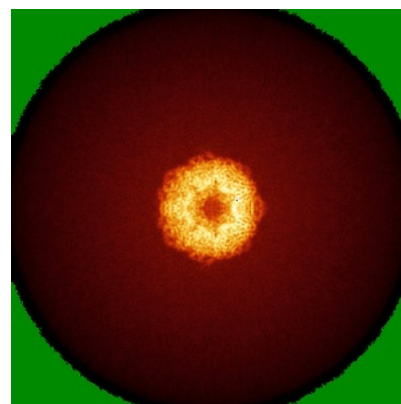
6.4.1 Primary map



X

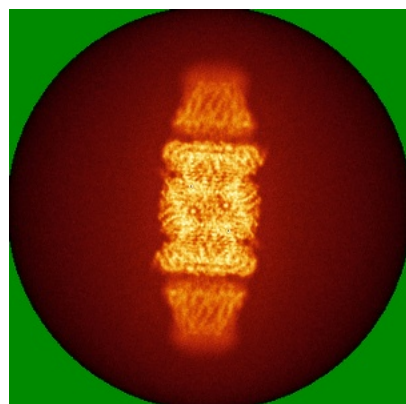


Y

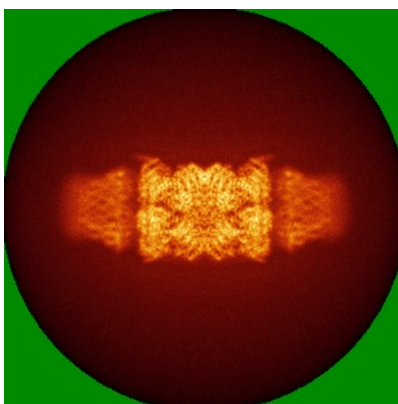


Z

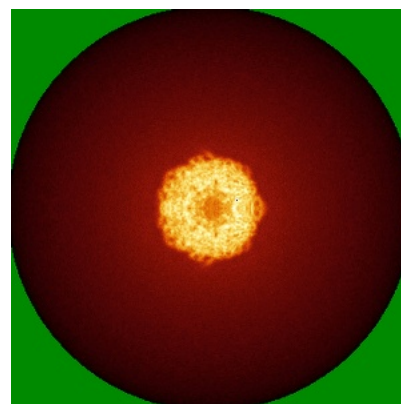
6.4.2 Raw map



X



Y

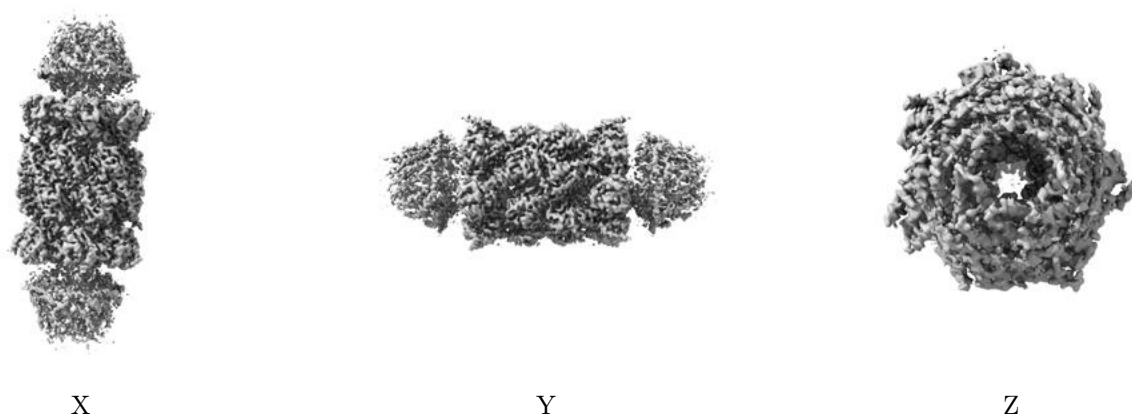


Z

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.

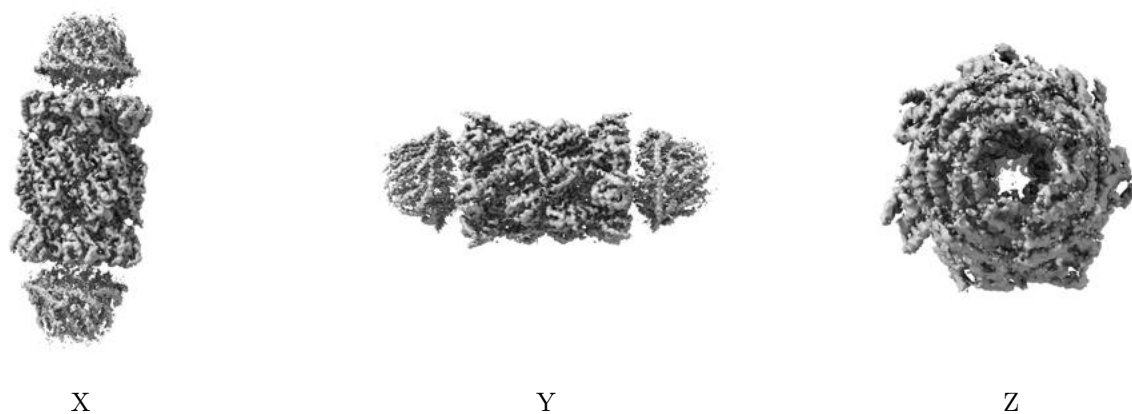
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

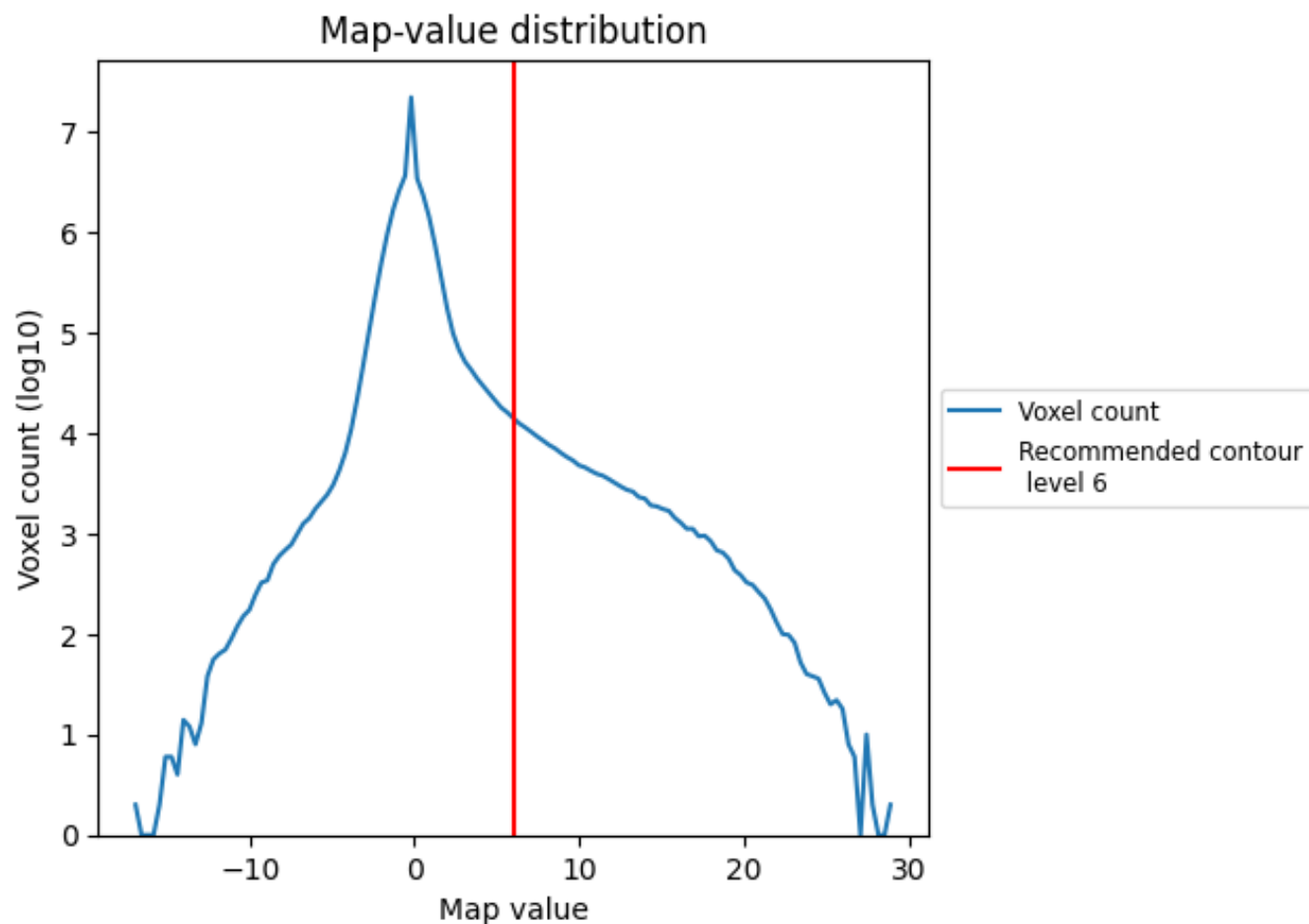
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

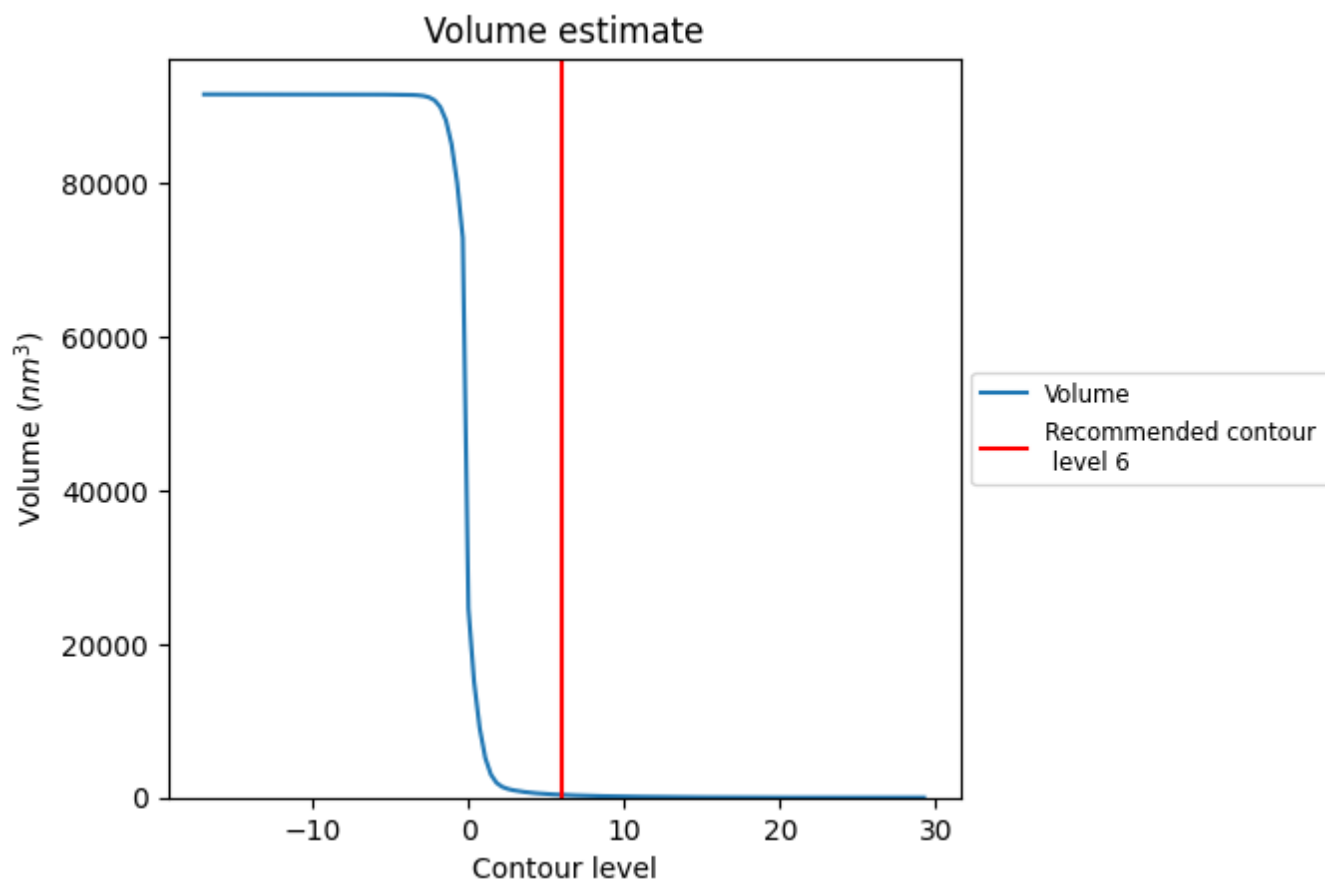
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

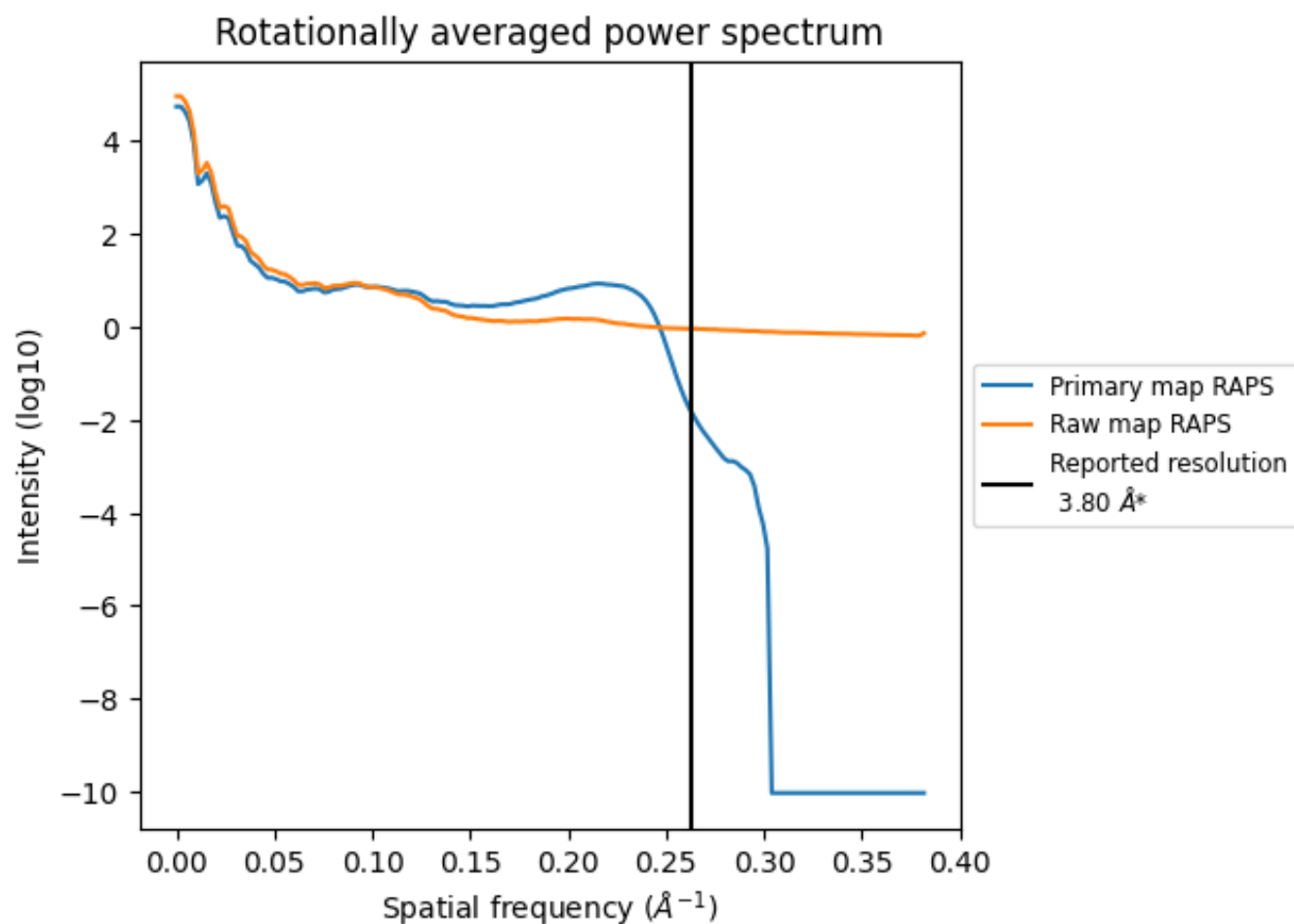
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 355 nm³; this corresponds to an approximate mass of 321 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 ⓘ

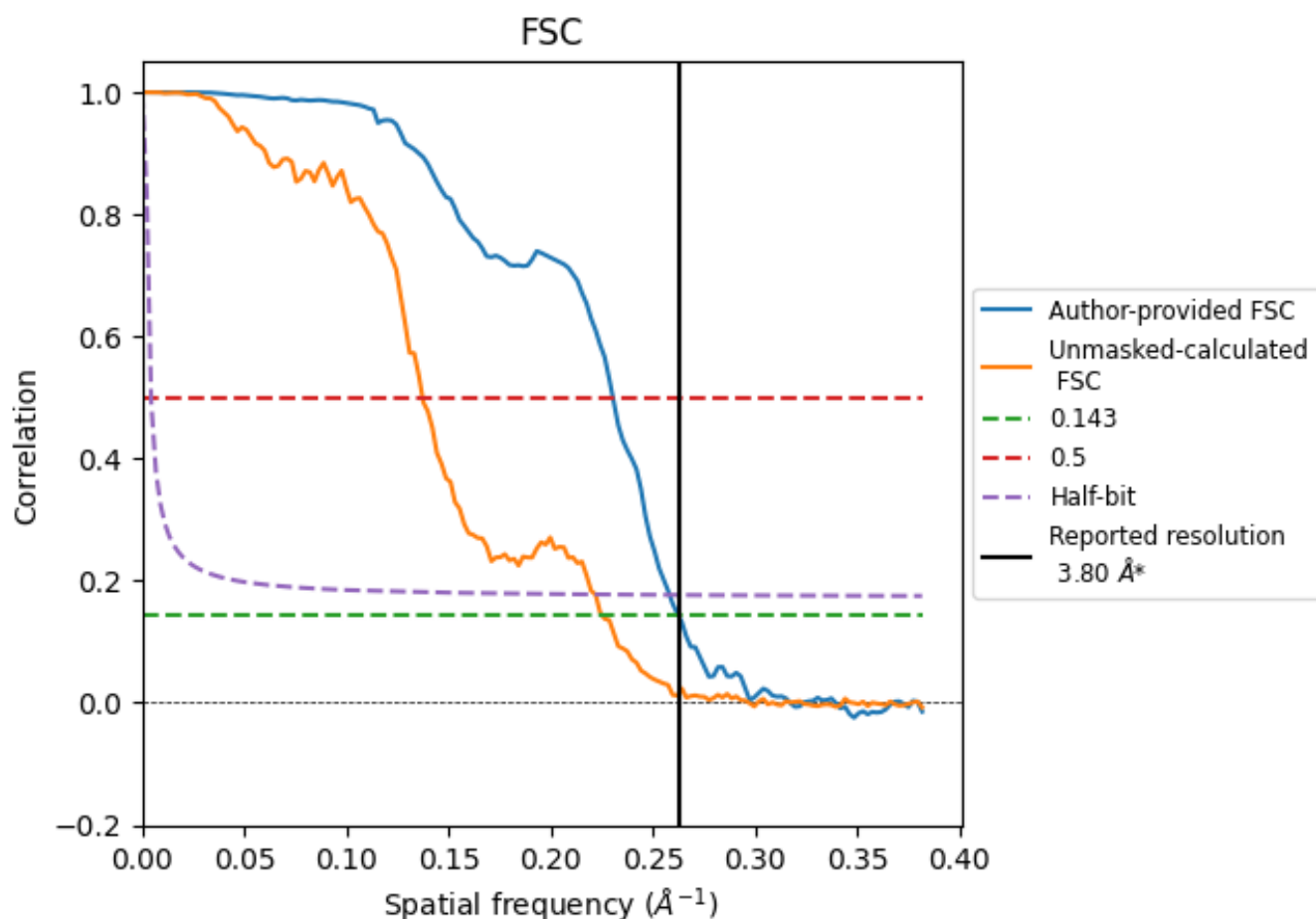


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

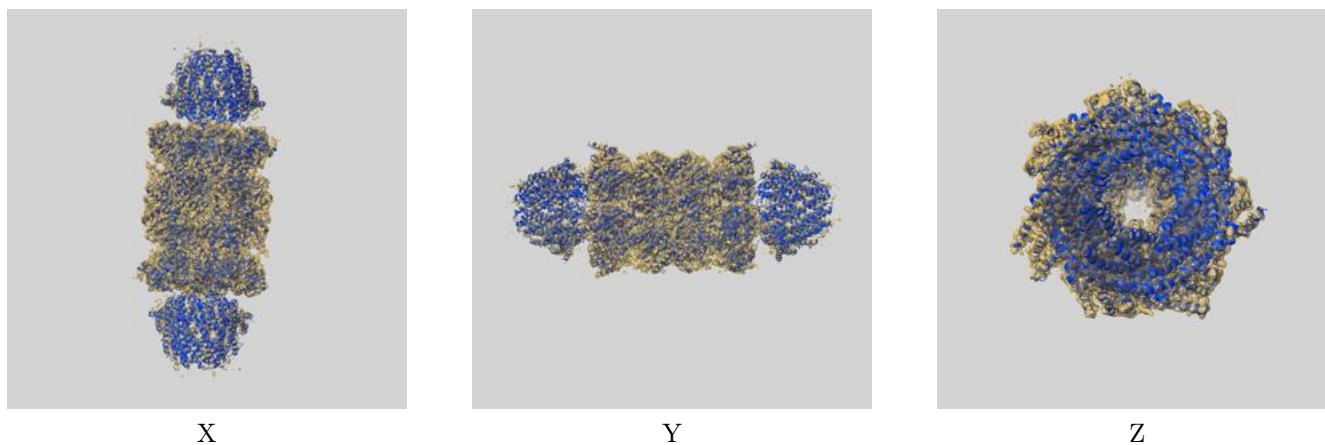
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.34	3.87
Unmasked-calculated*	4.44	7.29	4.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

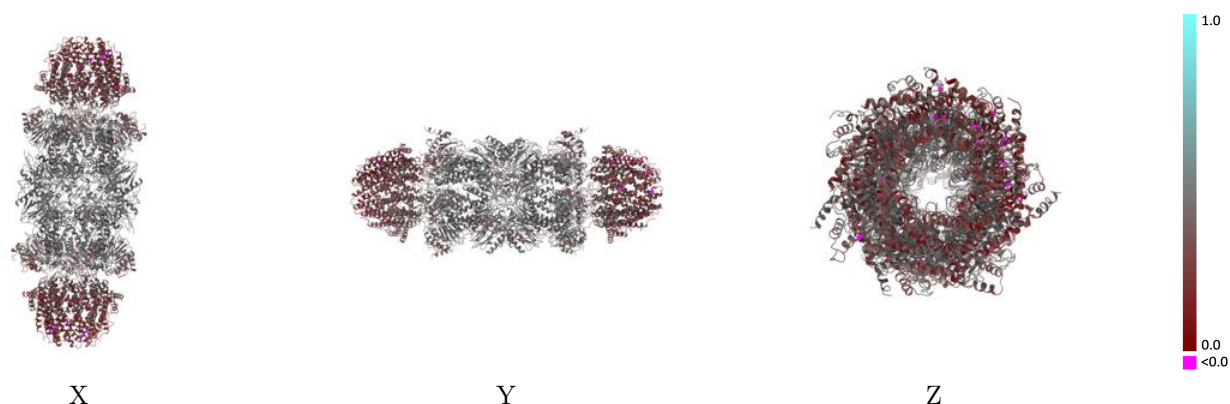
This section contains information regarding the fit between EMDB map EMD-9257 and PDB model 6MUV. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



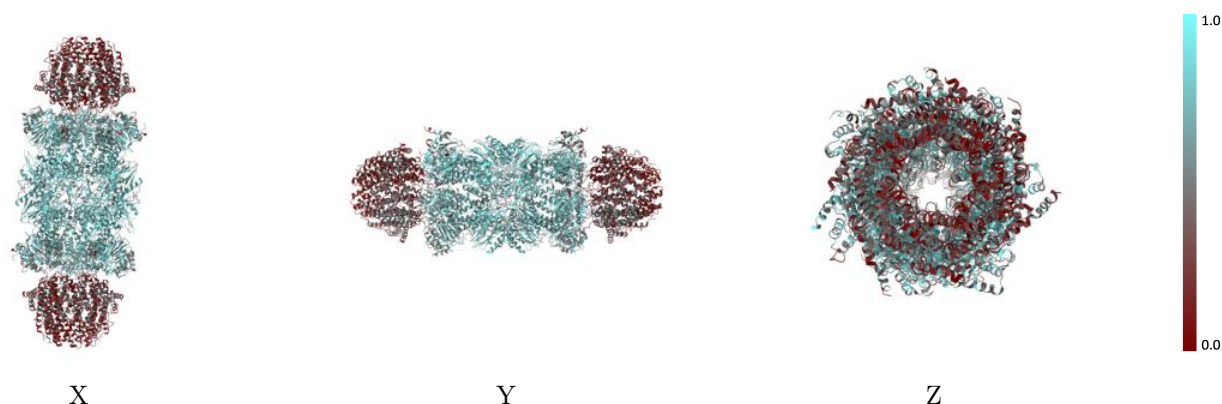
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



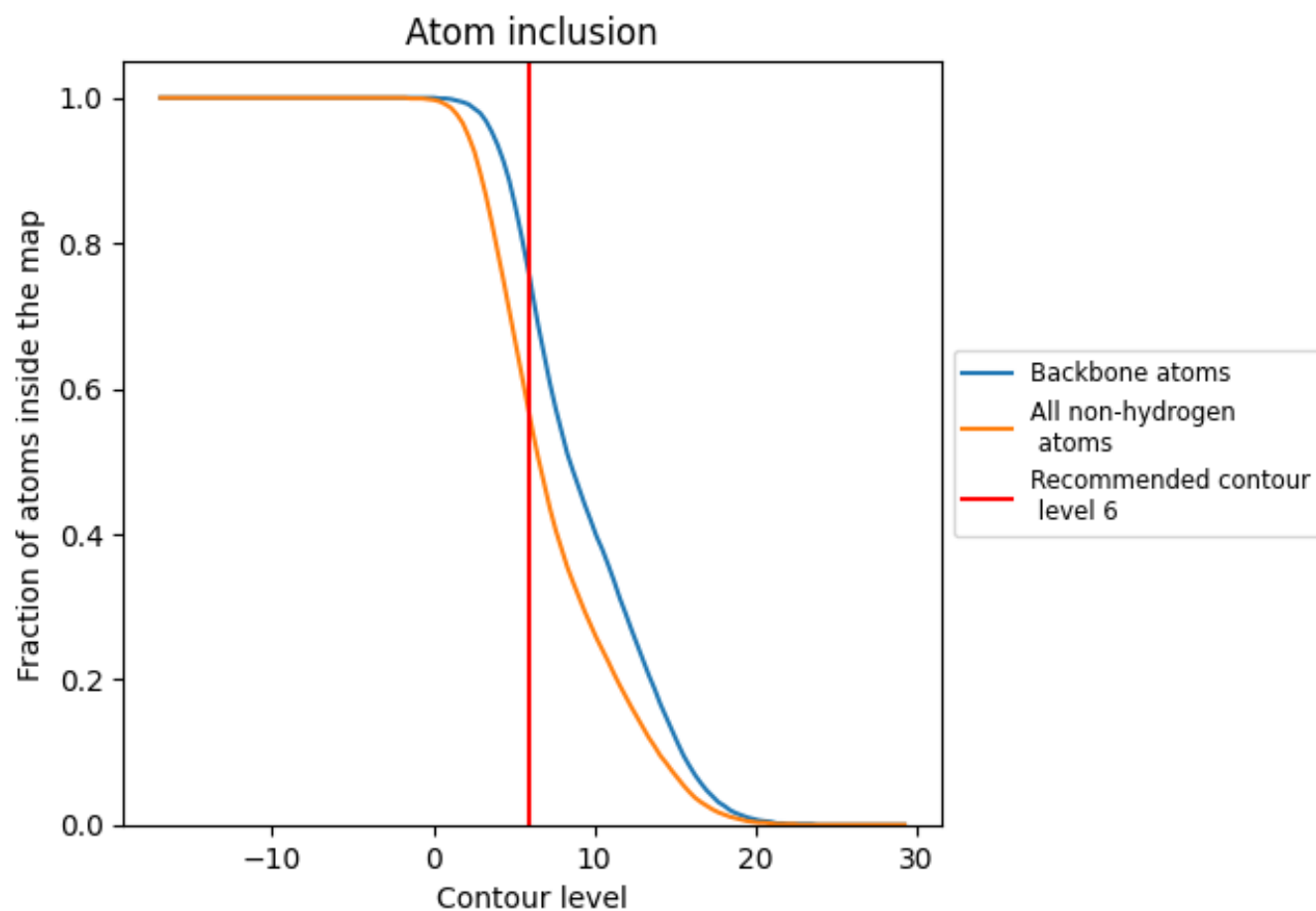
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 56% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5600	 0.3970
A	 0.6380	 0.4320
B	 0.6650	 0.4380
C	 0.6910	 0.4350
D	 0.6430	 0.4280
E	 0.6060	 0.4220
F	 0.6680	 0.4400
G	 0.6820	 0.4430
H	 0.6790	 0.4250
I	 0.6590	 0.4200
J	 0.7480	 0.4560
K	 0.7770	 0.4560
L	 0.7520	 0.4530
M	 0.7290	 0.4620
N	 0.6860	 0.4520
O	 0.6370	 0.4320
P	 0.6690	 0.4380
Q	 0.6900	 0.4360
R	 0.6420	 0.4270
S	 0.6040	 0.4200
T	 0.6690	 0.4390
U	 0.6810	 0.4430
V	 0.6750	 0.4240
W	 0.6580	 0.4220
X	 0.7490	 0.4570
Y	 0.7750	 0.4560
Z	 0.7550	 0.4520
a	 0.7260	 0.4600
b	 0.6890	 0.4520
c	 0.2330	 0.2640
d	 0.2060	 0.2730
e	 0.2870	 0.2960
f	 0.3380	 0.3290
g	 0.3350	 0.3340
h	 0.3200	 0.3230



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Chain	Atom inclusion	Q-score
i	 0.2470	 0.2860
j	 0.3380	 0.3300
k	 0.3420	 0.3320
l	 0.3200	 0.3240
m	 0.2320	 0.2800
n	 0.2410	 0.2880
o	 0.2140	 0.2740
p	 0.2800	 0.2950