



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 08:39 AM UTC

PDB ID : 6MUX / pdb_00006mux
EMDB ID : EMD-9259
Title : The structure of the Plasmodium falciparum 20S proteasome in complex with one PA28 activator
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 : 3.90 Å (reported)
Based on initial models : 6MUW, 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:

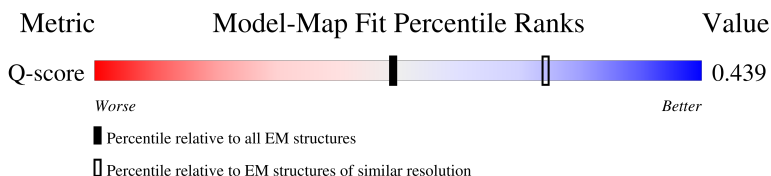
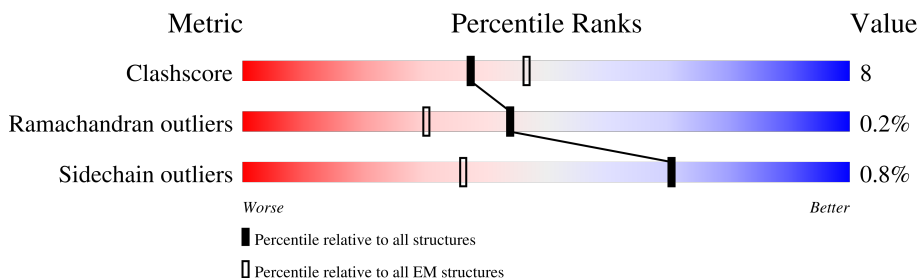
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.90 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	8855 (3.40 - 4.40)

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	11% 80% 14% 6%
1	O	260	19% 76% 18% 6%
2	B	235	7% 79% 16% 5%
2	P	235	9% 76% 21% .

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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	61% 53% 15% 32%
15	e	279	59% 56% 11% 33%
15	f	279	59% 57% 11% 32%
15	g	279	53% 55% 13% 32%
15	h	279	48% 57% 11% 32%
15	i	279	42% 58% 10% 32%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 60284 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	244	Total	C	N	O	S	0	0
			1928	1213	323	377	15		
1	O	244	Total	C	N	O	S	0	0
			1928	1213	323	377	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	229	Total	C	N	O	S	0	0
			1826	1175	298	347	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
			1918	1230	308	377	3		
3	Q	245	Total	C	N	O	S	0	0
			1965	1258	319	385	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	233	Total	C	N	O	S	0	0
			1845	1178	312	347	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	228	Total	C	N	O	S	0	0
			1767	1115	292	349	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	235	Total	C	N	O	S	0	0
			1870	1191	308	361	10		
6	T	234	Total	C	N	O	S	0	0
			1858	1182	307	359	10		

- 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	194	Total	C	N	O	S	0	0
			1547	978	265	292	12		
8	V	194	Total	C	N	O	S	0	0
			1547	978	265	292	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	188	Total	C	N	O	S	0	0
			1578	1019	261	295	3		
15	d	190	Total	C	N	O	S	0	0
			1595	1029	265	298	3		

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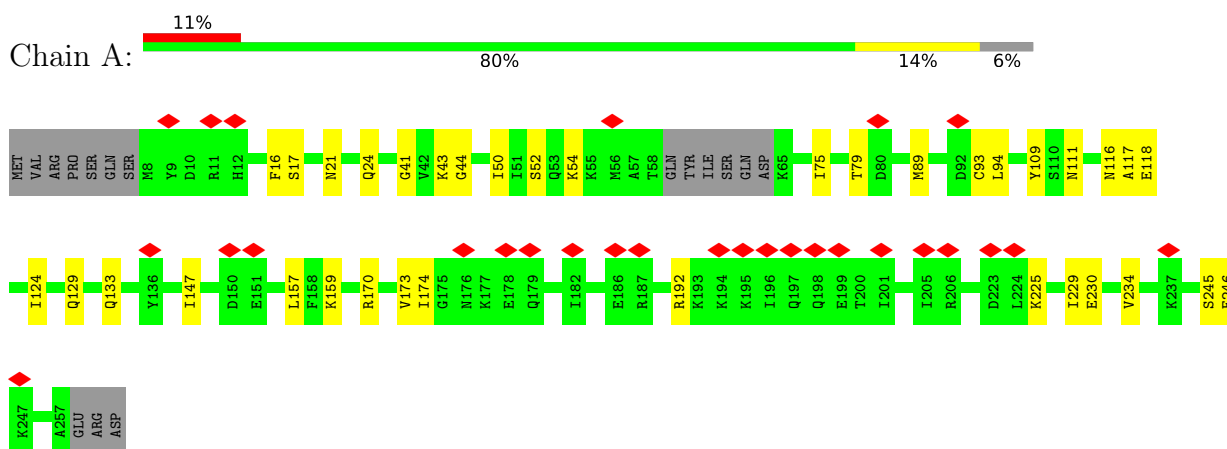
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Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	187	Total 1571	C 1014	N 260	O 294	S 3	0	0
15	f	190	Total 1595	C 1029	N 265	O 298	S 3	0	0
15	g	190	Total 1595	C 1029	N 265	O 298	S 3	0	0
15	h	190	Total 1595	C 1029	N 265	O 298	S 3	0	0
15	i	190	Total 1595	C 1029	N 265	O 298	S 3	0	0

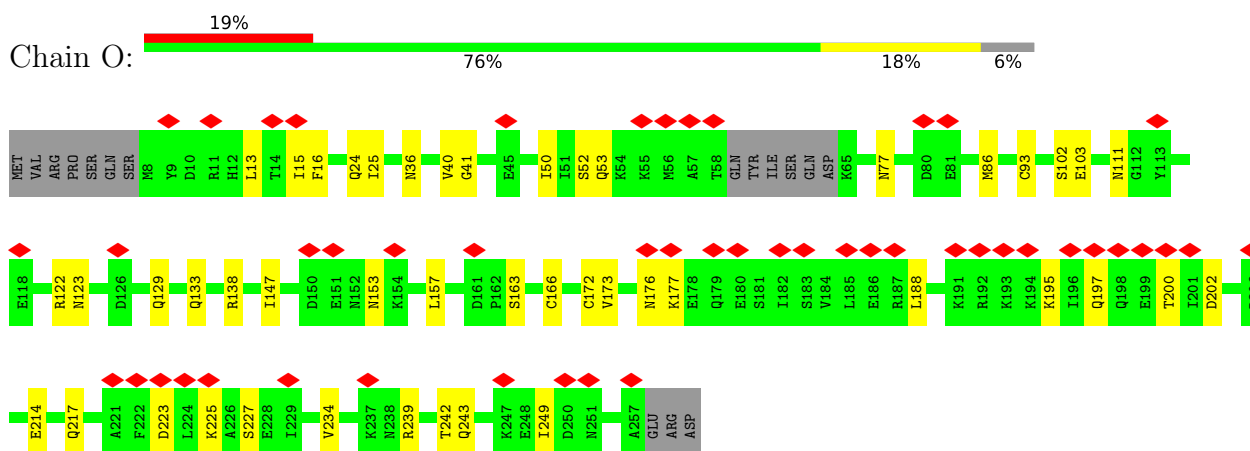
3 Residue-property plots

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.

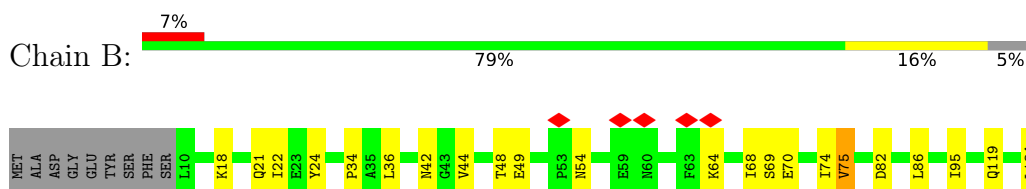
- Molecule 1: 20S proteasome alpha-1 subunit

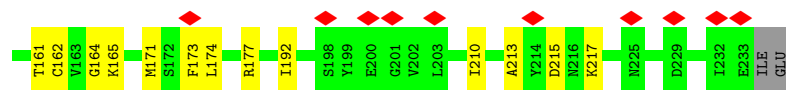


- Molecule 1: 20S proteasome alpha-1 subunit

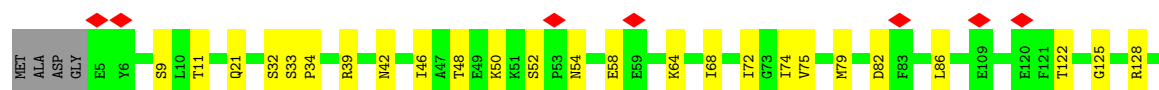
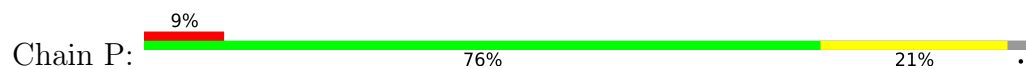


- Molecule 2: 20S proteasome alpha-2 subunit

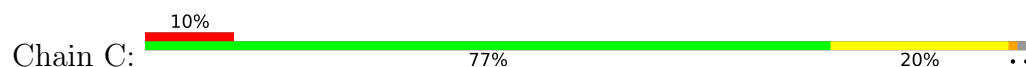




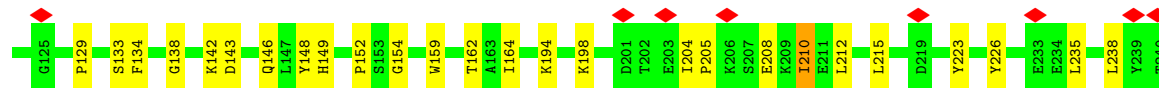
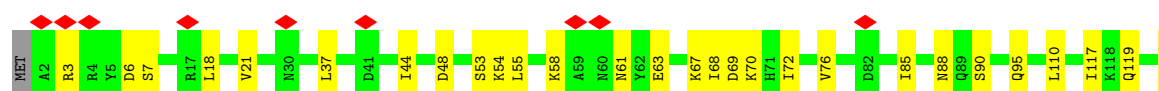
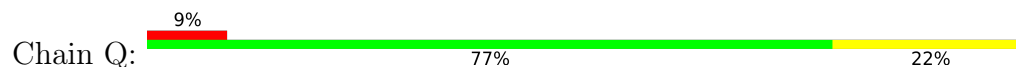
- Molecule 2: 20S proteasome alpha-2 subunit



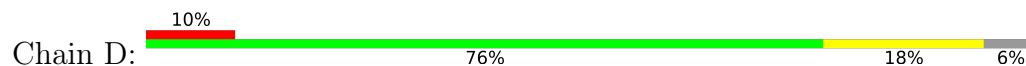
- Molecule 3: 20S proteasome alpha-3 subunit

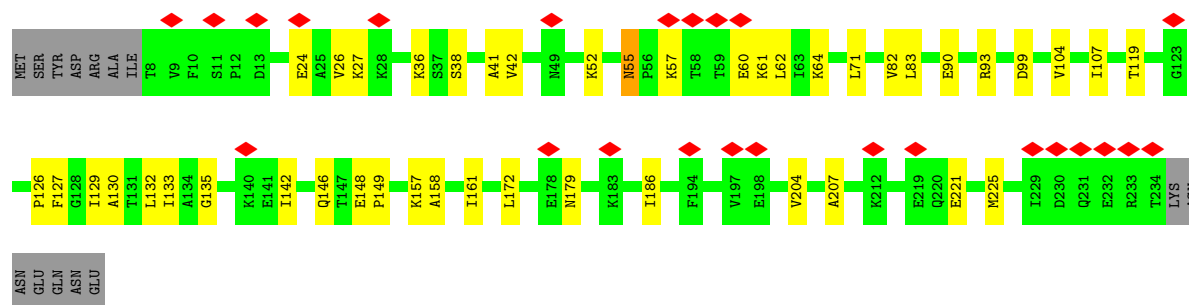


- Molecule 3: 20S proteasome alpha-3 subunit

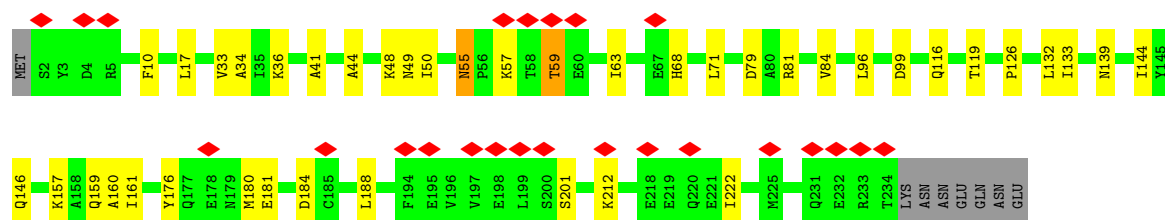
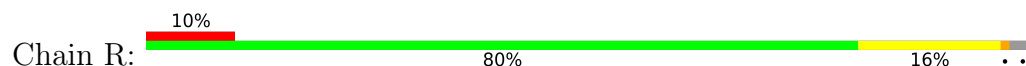


- Molecule 4: 20S proteasome alpha-4 subunit

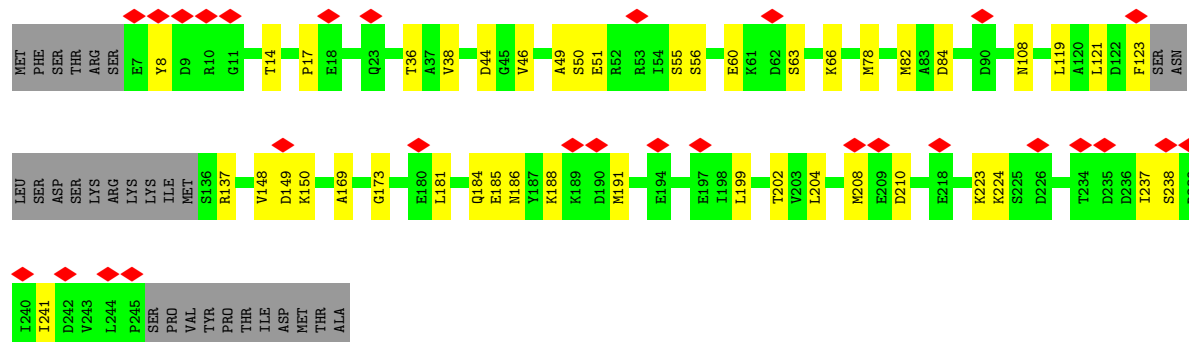




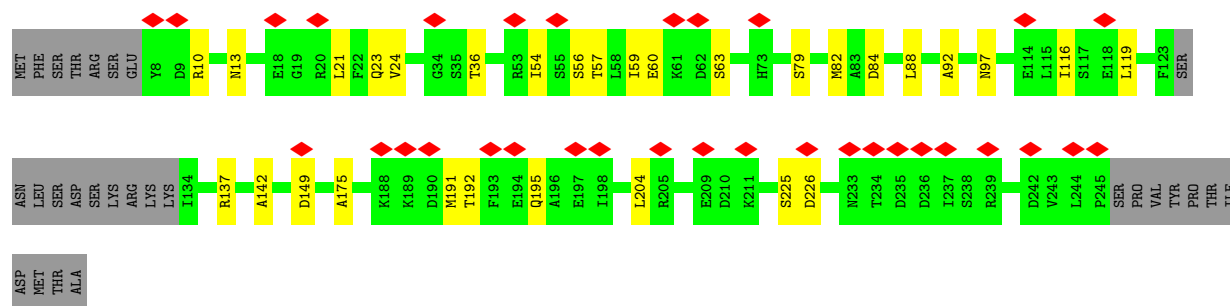
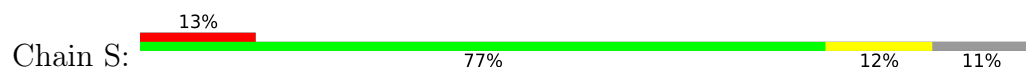
- Molecule 4: 20S proteasome alpha-4 subunit



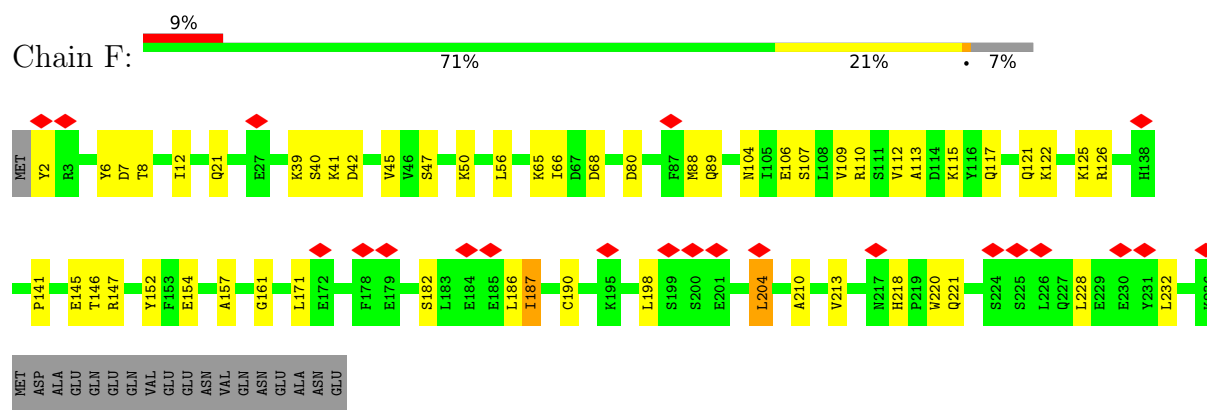
- Molecule 5: 20S proteasome alpha-5 subunit



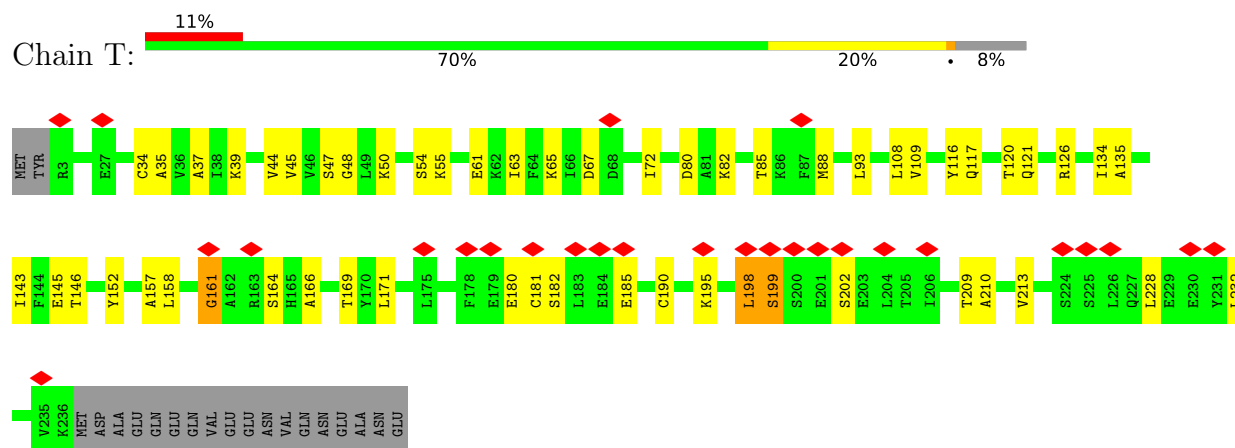
- Molecule 5: 20S proteasome alpha-5 subunit



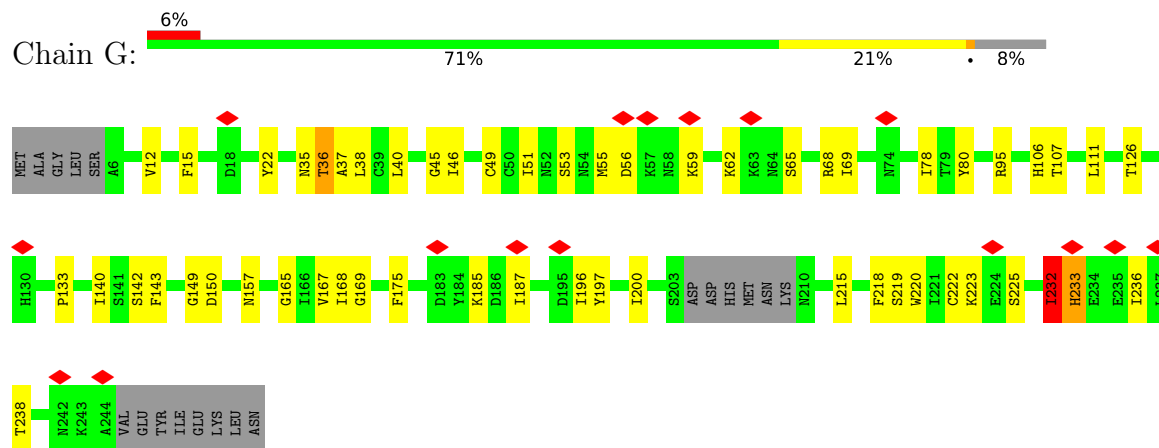
- Molecule 6: 20S proteasome alpha-6 subunit



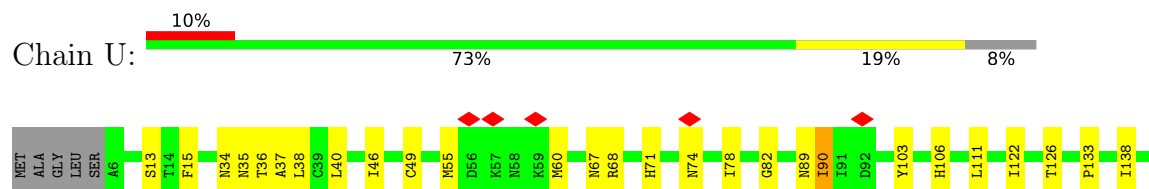
- Molecule 6: 20S proteasome alpha-6 subunit

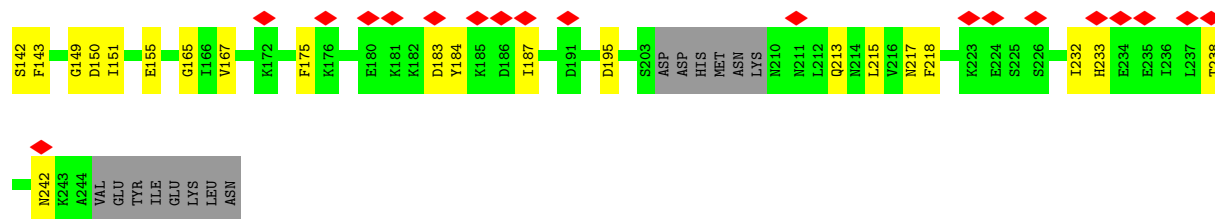


- Molecule 7: 20S proteasome alpha-7 subunit

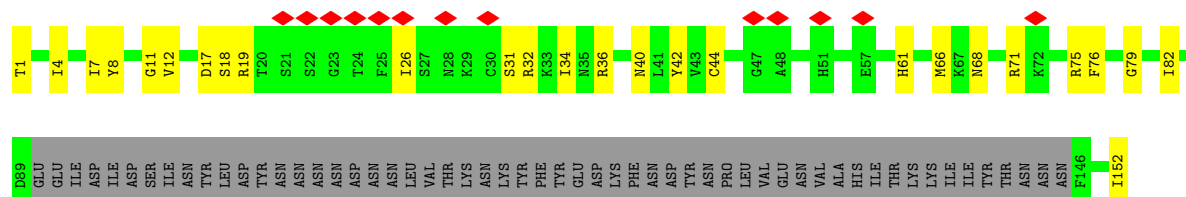


- Molecule 7: 20S proteasome alpha-7 subunit

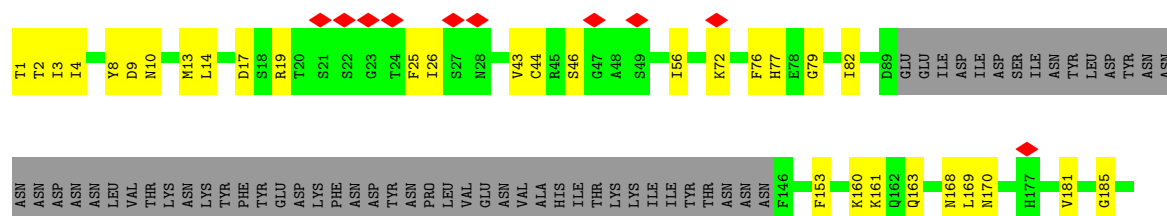




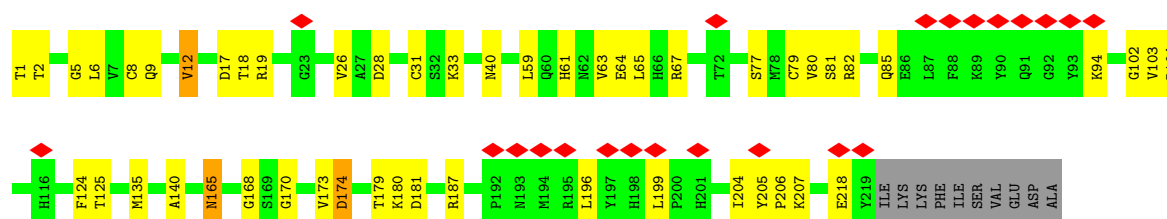
- Molecule 8: 20S proteasome beta-1 subunit



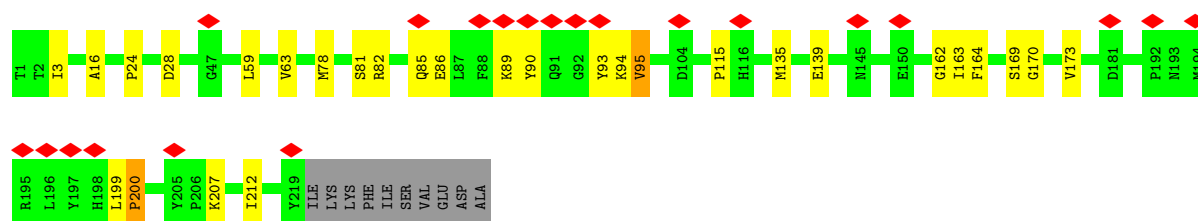
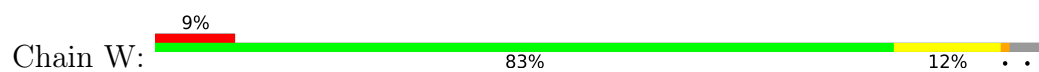
- Molecule 8: 20S proteasome beta-1 subunit



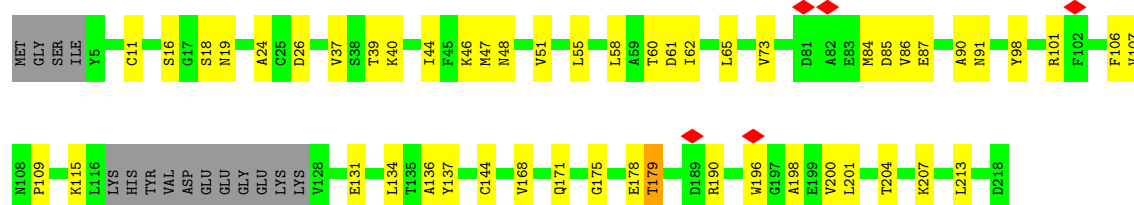
- Molecule 9: 20S proteasome beta-2 subunit



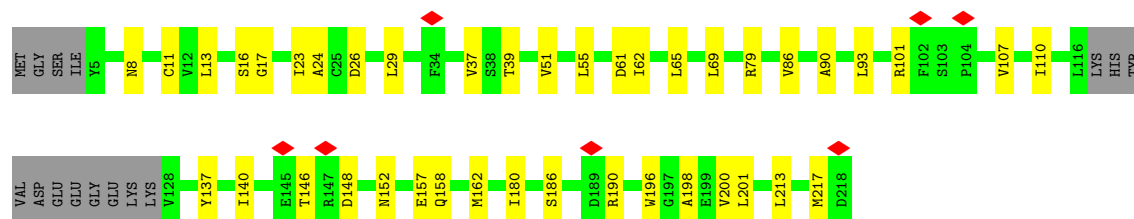
- Molecule 9: 20S proteasome beta-2 subunit



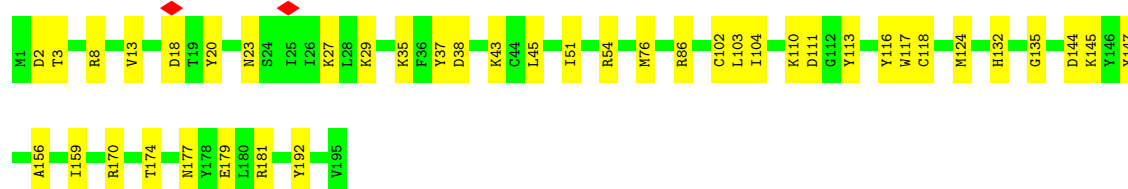
- Molecule 10: 20S proteasome beta-3 subunit



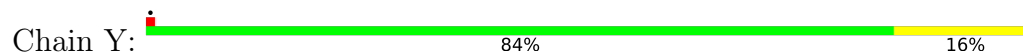
- Molecule 10: 20S proteasome beta-3 subunit



- Molecule 11: 20S proteasome beta-4 subunit



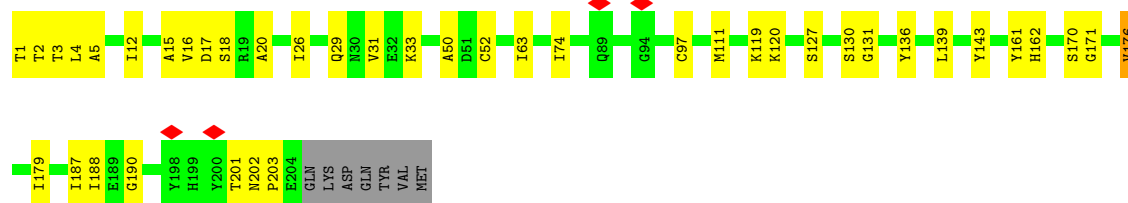
- Molecule 11: 20S proteasome beta-4 subunit



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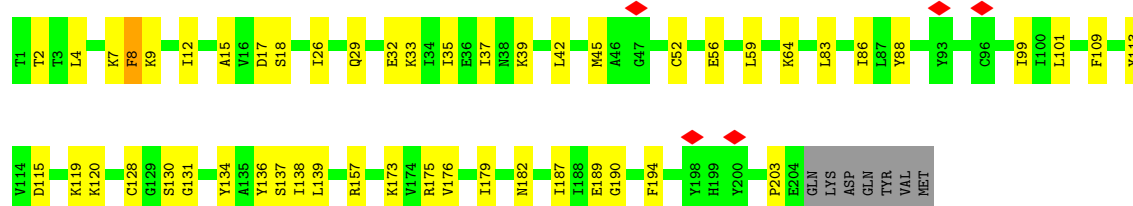
- Molecule 12: 20S proteasome beta-5 subunit

Chain L:  77% 19%



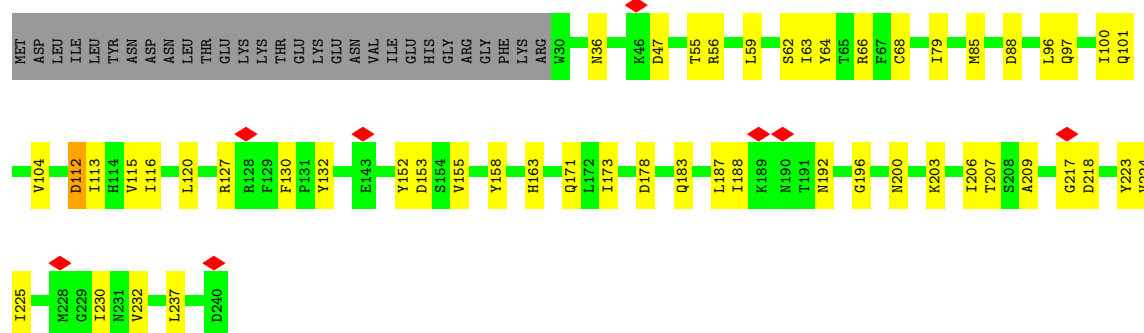
- Molecule 12: 20S proteasome beta-5 subunit

Chain Z:  73% 24%



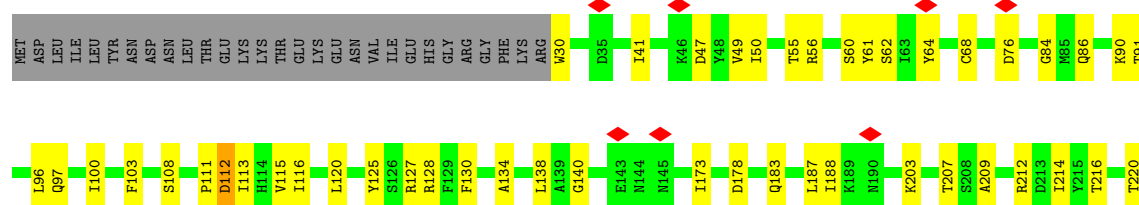
- Molecule 13: 20S proteasome beta-6 subunit

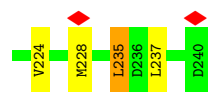
Chain M:  66% 21% 12%



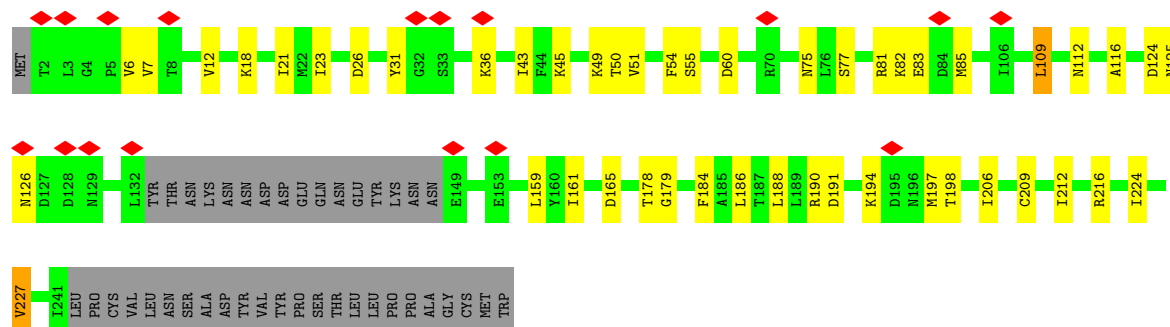
- Molecule 13: 20S proteasome beta-6 subunit

Chain a:  67% 20% 12%

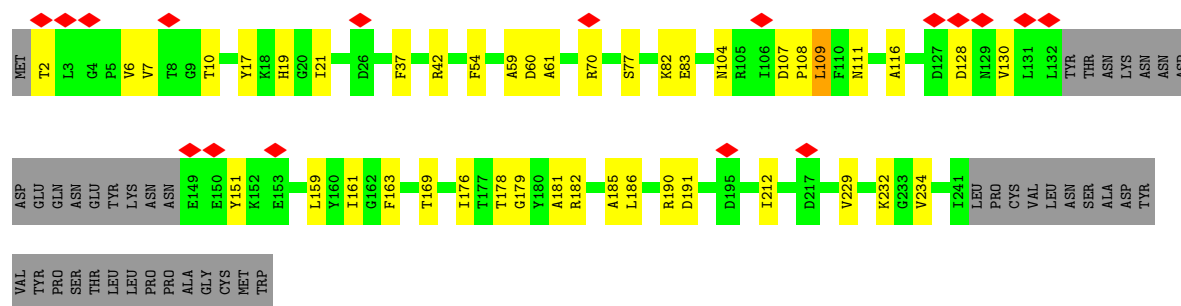




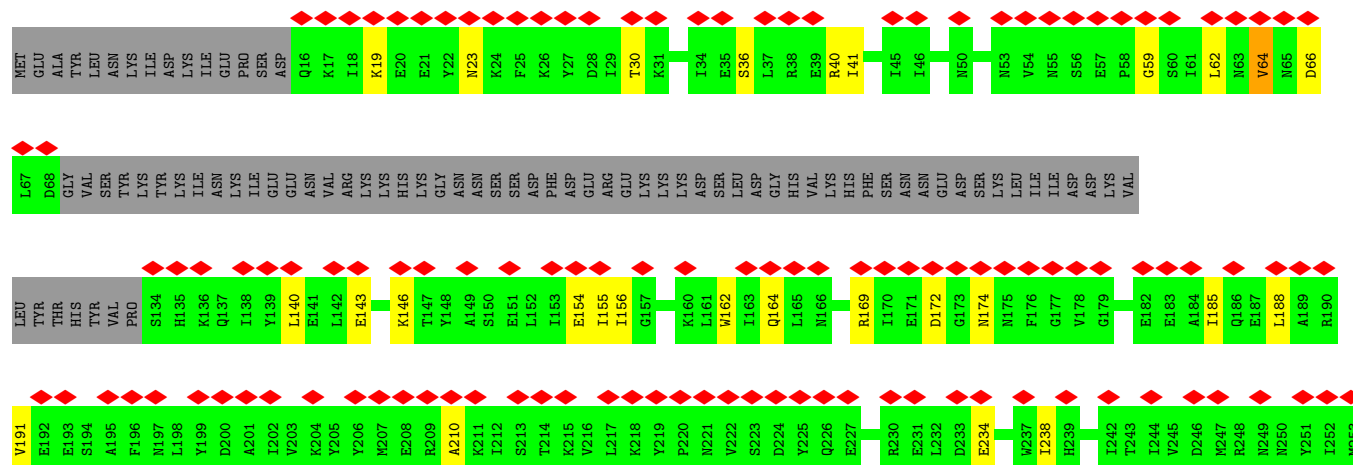
• Molecule 14: 20S proteasome beta-7 subunit

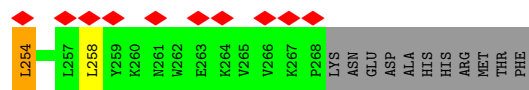


• Molecule 14: 20S proteasome beta-7 subunit

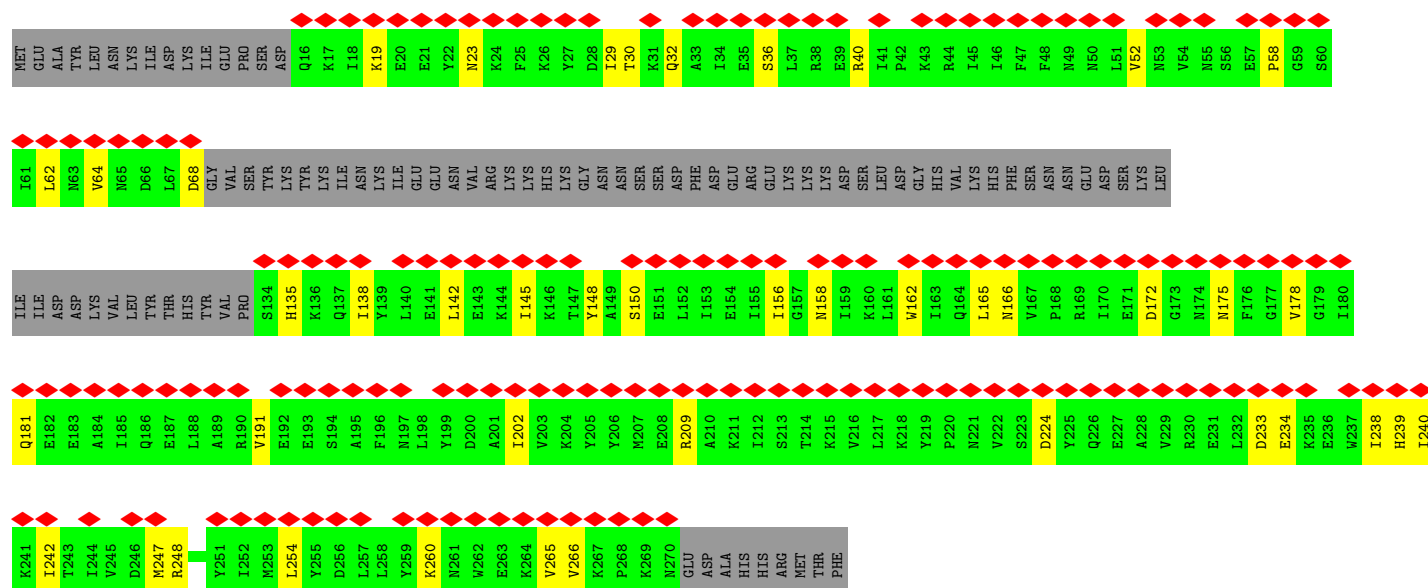


• Molecule 15: Proteasome activator PA28

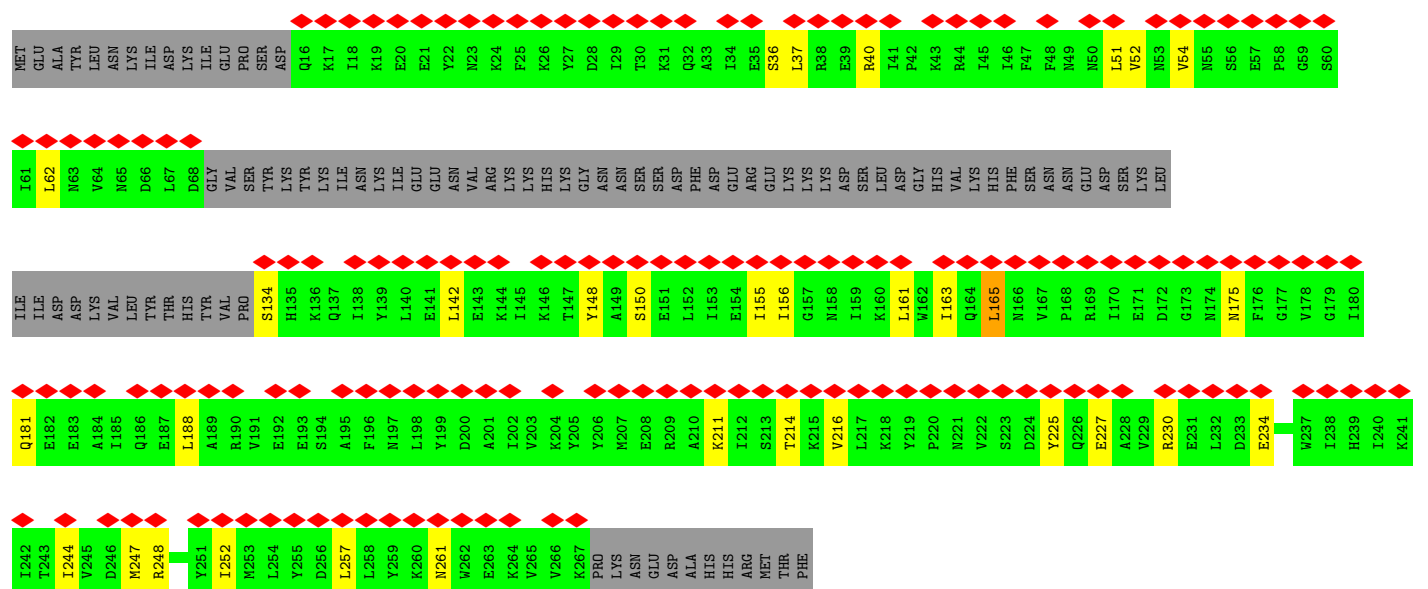




• Molecule 15: Proteasome activator PA28

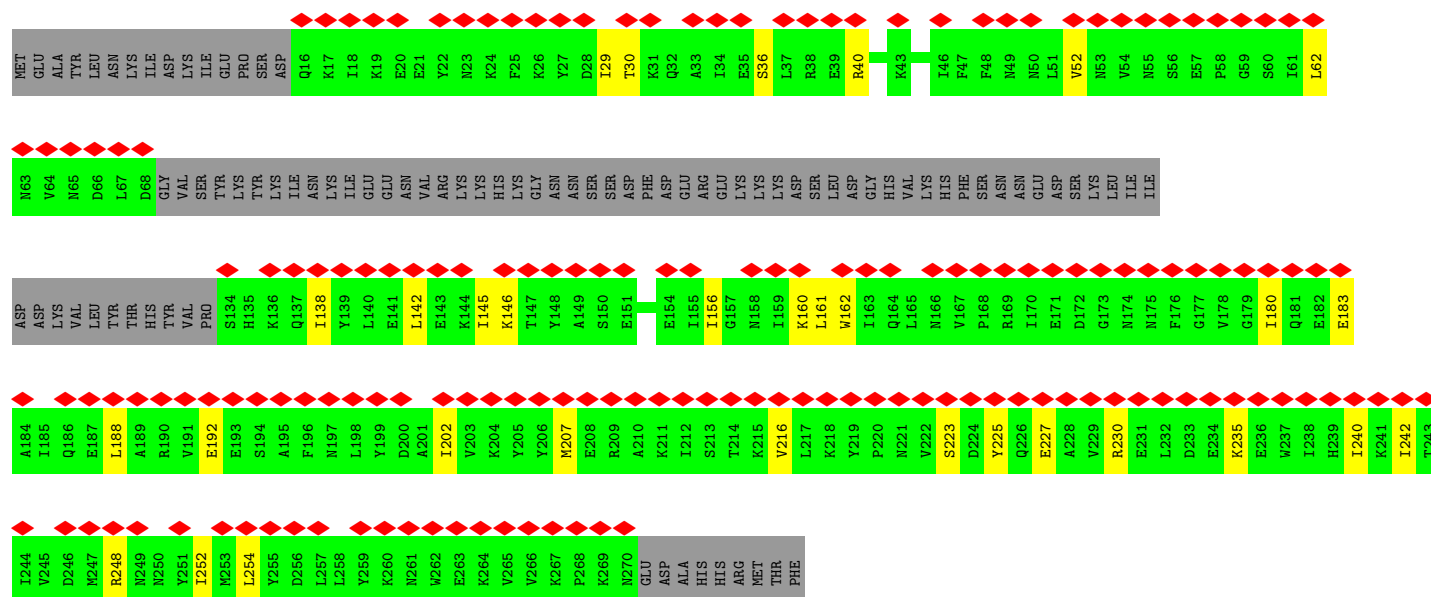


• Molecule 15: Proteasome activator PA28

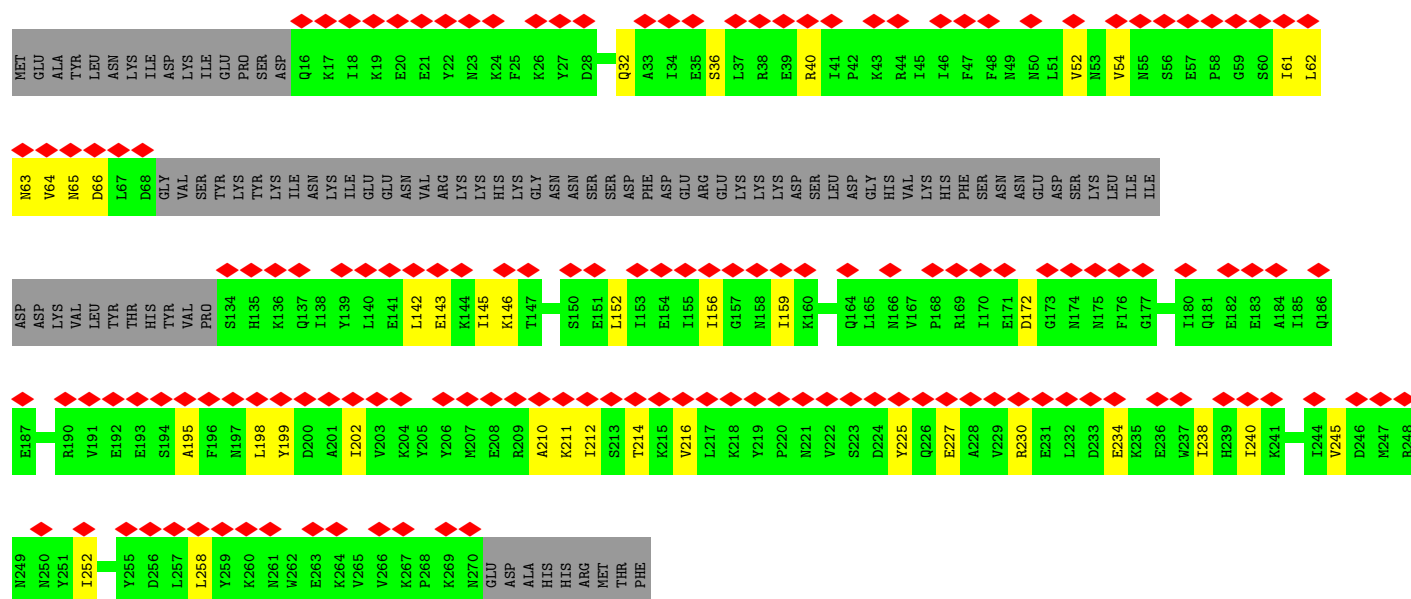


• Molecule 15: Proteasome activator PA28

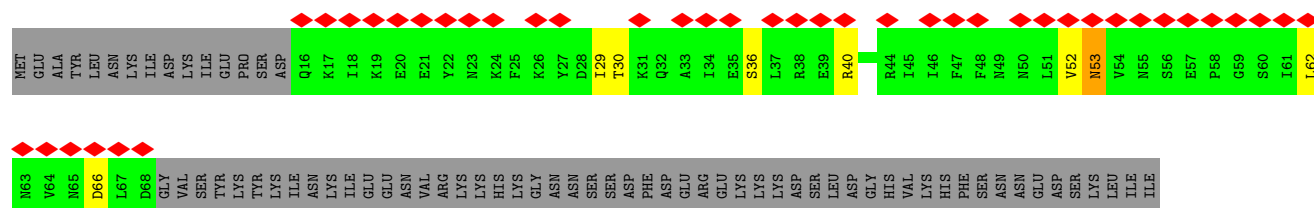


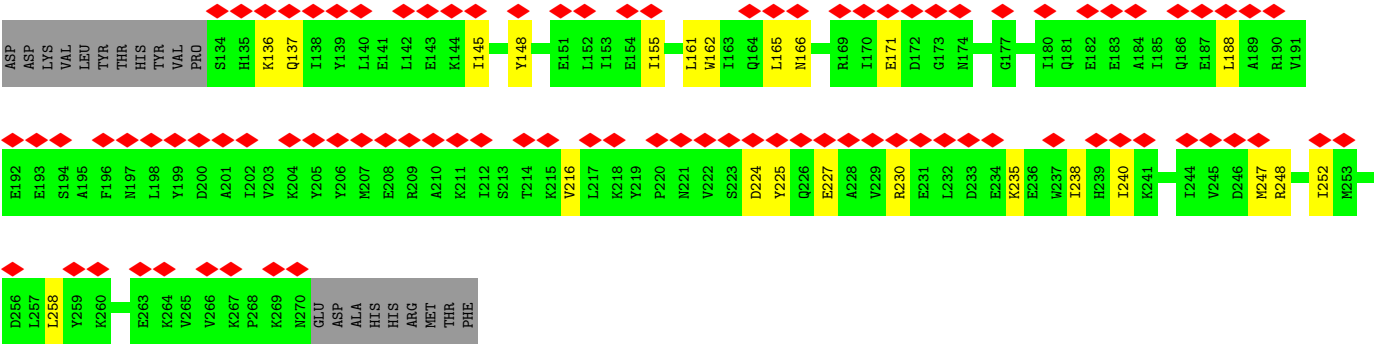


• Molecule 15: Proteasome activator PA28

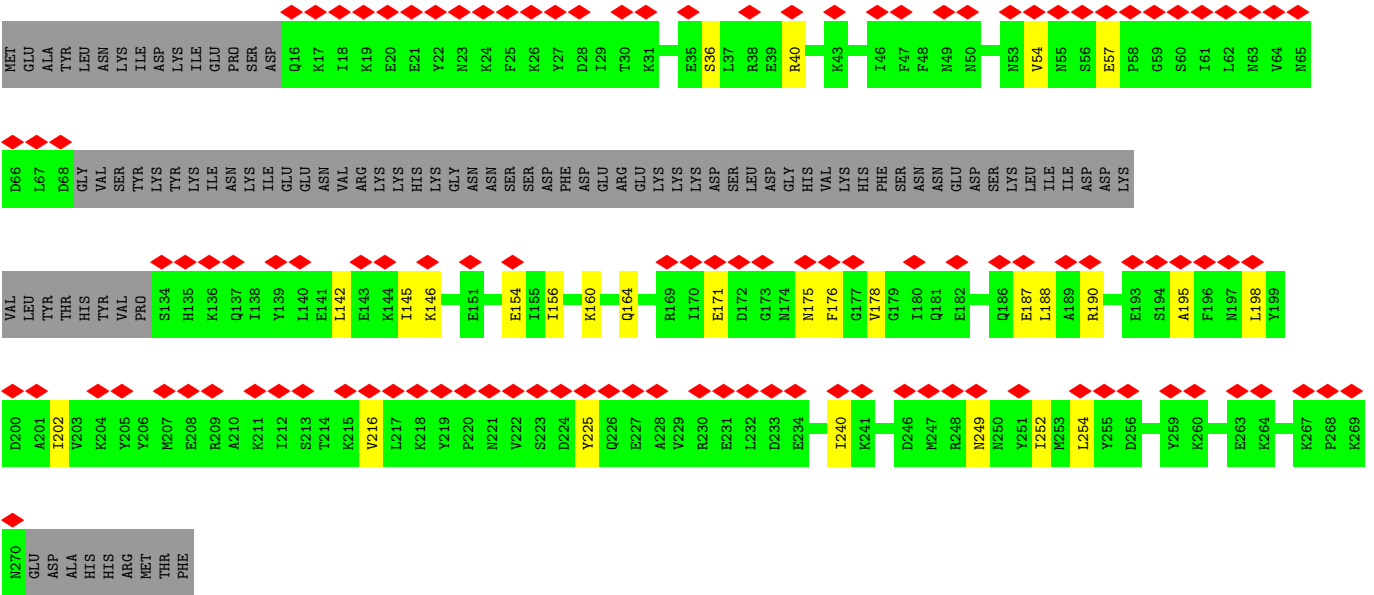
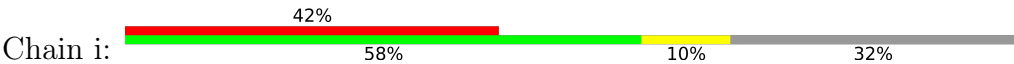


• Molecule 15: Proteasome activator PA28





● Molecule 15: Proteasome activator PA28



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57337	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	33.420	Depositor
Minimum map value	-19.000	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	0.36	0/1953	0.69	0/2632
1	O	0.34	0/1953	0.72	0/2632
2	B	0.37	0/1814	0.63	0/2450
2	P	0.35	0/1860	0.70	1/2512 (0.0%)
3	C	0.41	0/1953	0.71	3/2643 (0.1%)
3	Q	0.39	0/2001	0.73	3/2707 (0.1%)
4	D	0.37	0/1824	0.70	2/2461 (0.1%)
4	R	0.35	0/1875	0.66	0/2530
5	E	0.32	0/1784	0.63	0/2410
5	S	0.32	0/1791	0.61	0/2419
6	F	0.39	0/1905	0.75	1/2566 (0.0%)
6	T	0.37	0/1892	0.75	3/2548 (0.1%)
7	G	0.41	0/1947	0.87	5/2631 (0.2%)
7	U	0.38	0/1947	0.82	3/2631 (0.1%)
8	H	0.43	0/1571	0.83	3/2105 (0.1%)
8	V	0.39	0/1571	0.74	0/2105
9	I	0.40	0/1712	0.73	1/2328 (0.0%)
9	W	0.38	0/1712	0.74	3/2328 (0.1%)
10	J	0.48	0/1621	0.72	0/2189
10	X	0.47	0/1621	0.70	0/2189
11	K	0.48	0/1649	0.73	0/2223
11	Y	0.49	0/1649	0.71	0/2223
12	L	0.44	0/1633	0.81	3/2202 (0.1%)
12	Z	0.48	0/1633	0.79	3/2202 (0.1%)
13	M	0.43	0/1708	0.74	4/2314 (0.2%)
13	a	0.45	0/1708	0.76	1/2314 (0.0%)
14	N	0.38	0/1882	0.73	4/2538 (0.2%)
14	b	0.38	0/1882	0.68	1/2538 (0.0%)
15	c	0.31	0/1606	0.77	0/2166
15	d	0.30	0/1623	0.77	0/2188
15	e	0.30	0/1598	0.77	0/2154
15	f	0.30	0/1623	0.77	1/2188 (0.0%)
15	g	0.31	0/1623	0.75	0/2188
15	h	0.31	0/1623	0.74	0/2188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	i	0.31	0/1623	0.73	1/2188 (0.0%)
All	All	0.39	0/61370	0.73	46/82830 (0.1%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	188	ILE	N-CA-C	12.83	122.75	110.30
9	W	200	PRO	CA-C-N	9.20	134.40	121.61
9	W	200	PRO	C-N-CA	9.20	134.40	121.61
7	U	90	ILE	N-CA-C	-8.61	104.35	112.96
6	T	161	GLY	N-CA-C	7.14	130.10	113.18
7	G	232	ILE	CA-C-N	7.09	135.08	121.54
7	G	232	ILE	C-N-CA	7.09	135.08	121.54
4	D	57	LYS	CA-C-N	6.42	133.79	121.54
4	D	57	LYS	C-N-CA	6.42	133.79	121.54
9	I	199	LEU	N-CA-C	6.29	123.72	109.81
7	G	185	LYS	CA-C-N	6.13	133.26	121.54
7	G	185	LYS	C-N-CA	6.13	133.26	121.54
9	W	199	LEU	N-CA-C	6.10	123.29	109.81
14	N	109	LEU	CA-CB-CG	6.07	137.54	116.30
14	N	54	PHE	CA-C-N	5.81	134.55	122.41
14	N	54	PHE	C-N-CA	5.81	134.55	122.41
8	H	178	ASP	CA-C-N	5.75	129.88	121.31
8	H	178	ASP	C-N-CA	5.75	129.88	121.31
14	N	124	ASP	N-CA-C	5.68	119.05	110.64
13	a	115	VAL	N-CA-C	-5.63	107.33	112.96
14	b	109	LEU	CA-CB-CG	5.63	136.00	116.30
6	F	161	GLY	N-CA-C	5.55	118.57	110.63
3	C	208	GLU	CA-C-N	5.38	131.82	121.54
3	C	208	GLU	C-N-CA	5.38	131.82	121.54
7	U	238	THR	CA-C-N	-5.33	113.17	119.84
7	U	238	THR	C-N-CA	-5.33	113.17	119.84
7	G	165	GLY	N-CA-C	-5.29	100.65	113.18
3	Q	208	GLU	CA-C-N	5.24	131.54	121.54
3	Q	208	GLU	C-N-CA	5.24	131.54	121.54
15	f	254	LEU	CA-CB-CG	5.21	134.54	116.30
2	P	138	GLY	N-CA-C	5.18	118.06	111.37
3	Q	208	GLU	N-CA-C	-5.18	105.42	112.26
3	C	208	GLU	N-CA-C	-5.16	105.44	112.26
13	M	130	PHE	N-CA-C	-5.15	99.99	108.75
6	T	198	LEU	CA-C-N	5.09	131.25	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	198	LEU	C-N-CA	5.09	131.25	121.54
15	i	57	GLU	CA-CB-CG	5.07	124.24	114.10
13	M	115	VAL	N-CA-C	-5.05	107.91	112.96
12	Z	190	GLY	CA-C-N	5.04	131.18	121.54
12	Z	190	GLY	C-N-CA	5.04	131.18	121.54
12	L	190	GLY	CA-C-N	5.04	131.16	121.54
12	L	190	GLY	C-N-CA	5.04	131.16	121.54
8	H	165	TYR	CA-CB-CG	5.03	122.95	113.90
12	Z	8	PHE	CB-CA-C	-5.03	101.19	113.15
13	M	36	ASN	CA-C-N	5.02	131.24	121.41
13	M	36	ASN	C-N-CA	5.02	131.24	121.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1928	0	1933	23	0
1	O	1928	0	1933	30	0
2	B	1782	0	1810	29	0
2	P	1826	0	1844	33	0
3	C	1918	0	1918	32	0
3	Q	1965	0	1962	39	0
4	D	1795	0	1831	27	0
4	R	1845	0	1878	29	0
5	E	1760	0	1752	26	0
5	S	1767	0	1766	21	0
6	F	1870	0	1869	37	0
6	T	1858	0	1860	36	0
7	G	1906	0	1859	33	0
7	U	1906	0	1859	31	0
8	H	1547	0	1549	37	0
8	V	1547	0	1549	32	0
9	I	1676	0	1674	36	0
9	W	1676	0	1674	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1595	0	1584	34	0
10	X	1595	0	1584	28	0
11	K	1614	0	1584	31	0
11	Y	1614	0	1584	26	0
12	L	1600	0	1558	28	0
12	Z	1600	0	1558	33	0
13	M	1676	0	1681	34	0
13	a	1676	0	1681	38	0
14	N	1845	0	1814	29	0
14	b	1845	0	1814	34	0
15	c	1578	0	1602	20	0
15	d	1595	0	1621	32	0
15	e	1571	0	1595	22	0
15	f	1595	0	1621	23	0
15	g	1595	0	1621	26	0
15	h	1595	0	1621	22	0
15	i	1595	0	1621	17	0
All	All	60284	0	60264	905	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 8.

All (905) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:PHE:H	2:P:21:GLN:HE22	1.31	0.78
15:i:145:ILE:HG13	15:i:240:ILE:HD12	1.68	0.76
15:f:145:ILE:HG13	15:f:240:ILE:HD11	1.73	0.70
2:B:34:PRO:HA	2:B:164:GLY:HA3	1.74	0.70
14:N:186:LEU:HD21	14:N:190:ARG:HH21	1.59	0.68
1:O:50:ILE:HG12	1:O:147:ILE:HD12	1.75	0.68
10:J:48:ASN:HD21	10:J:84:MET:H	1.41	0.68
2:P:34:PRO:HA	2:P:164:GLY:HA3	1.76	0.67
2:B:75:VAL:HG22	2:B:135:LEU:HB2	1.76	0.67
15:f:29:ILE:HG12	15:g:54:VAL:HG21	1.76	0.67
8:H:34:ILE:HG13	8:H:44:CYS:HB3	1.76	0.66
14:b:21:ILE:HD11	14:b:159:LEU:HB3	1.77	0.66
9:I:174:ASP:HB3	9:I:187:ARG:HD3	1.78	0.65
4:R:68:HIS:HB3	4:R:212:LYS:HA	1.78	0.65
15:c:36:SER:HA	15:c:40:ARG:HB2	1.78	0.64
15:f:52:VAL:O	15:f:248:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:77:HIS:HE1	8:V:153:PHE:HB3	1.63	0.64
15:h:62:LEU:HD12	15:h:238:ILE:HG13	1.79	0.64
15:i:216:VAL:HG22	15:i:225:TYR:HB3	1.79	0.64
1:A:129:GLN:NE2	2:B:82:ASP:OD1	2.30	0.63
9:W:81:SER:O	9:W:85:GLN:NE2	2.30	0.63
3:Q:48:ASP:HA	3:Q:210:ILE:HG22	1.79	0.63
15:c:191:VAL:HG11	15:c:254:LEU:HD21	1.81	0.63
14:N:216:ARG:NH1	9:W:135:MET:SD	2.72	0.63
4:R:181:GLU:H	4:R:184:ASP:HB3	1.64	0.63
4:D:119:THR:HG22	4:D:126:PRO:HB3	1.81	0.63
6:T:109:VAL:O	6:T:152:TYR:OH	2.15	0.63
10:X:65:LEU:HD22	10:X:107:VAL:HG21	1.81	0.62
6:T:109:VAL:HG23	6:T:134:ILE:HD12	1.80	0.62
5:E:36:THR:HA	5:E:173:GLY:HA3	1.82	0.62
7:G:68:ARG:HD3	7:G:80:TYR:HB2	1.81	0.62
14:N:43:ILE:HG21	14:N:227:VAL:HG11	1.82	0.62
11:Y:38:ASP:OD2	11:Y:181:ARG:NH1	2.32	0.62
12:Z:83:LEU:HD12	12:Z:101:LEU:HD11	1.81	0.62
11:Y:156:ALA:HA	11:Y:159:ILE:HD12	1.82	0.62
12:L:63:ILE:HD12	12:L:74:ILE:HG21	1.82	0.62
13:M:183:GLN:HG3	13:M:188:ILE:HG23	1.82	0.62
15:d:64:VAL:HG21	15:d:234:GLU:HG3	1.81	0.61
1:A:54:LYS:HE3	1:A:230:GLU:HG3	1.82	0.61
9:I:81:SER:O	9:I:85:GLN:NE2	2.34	0.61
4:D:158:ALA:HB1	4:D:172:LEU:HD13	1.82	0.61
5:S:191:MET:HE2	5:S:195:GLN:HB3	1.83	0.61
7:U:35:ASN:HB2	7:U:68:ARG:HH12	1.66	0.61
7:U:49:CYS:HA	7:U:218:PHE:HB3	1.82	0.61
15:g:36:SER:HA	15:g:40:ARG:HB2	1.83	0.61
8:V:17:ASP:HB2	8:V:225:GLY:HA3	1.83	0.60
8:V:4:ILE:HG22	8:V:181:VAL:HG23	1.82	0.60
10:X:146:THR:HG22	10:X:148:ASP:H	1.67	0.60
10:J:44:ILE:HD12	10:J:201:LEU:HD22	1.84	0.60
1:O:24:GLN:HE22	7:U:15:PHE:H	1.49	0.59
11:Y:125:ASP:OD1	11:Y:125:ASP:N	2.35	0.59
12:Z:4:LEU:HD22	12:Z:139:LEU:HD11	1.84	0.59
3:C:135:LEU:HD21	3:C:162:THR:HB	1.83	0.59
8:H:19:ARG:HB2	8:H:225:GLY:HA2	1.82	0.59
9:W:90:TYR:HB3	9:W:93:TYR:HB2	1.84	0.59
3:C:76:VAL:HA	3:C:134:PHE:HB3	1.84	0.59
12:L:1:THR:HA	12:L:33:LYS:HZ1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:136:TYR:OH	11:Y:170:ARG:NH1	2.36	0.59
14:b:10:THR:O	14:b:42:ARG:NH2	2.36	0.59
15:g:52:VAL:HG13	15:g:61:ILE:HD13	1.85	0.59
5:E:14:THR:HG21	6:F:8:THR:HG23	1.84	0.59
7:G:106:HIS:HB2	8:H:82:ILE:HG21	1.83	0.59
15:e:165:LEU:HD21	15:f:252:ILE:HD12	1.83	0.59
6:F:122:LYS:HD2	6:F:125:LYS:HD2	1.84	0.59
13:M:96:LEU:HD13	13:M:120:LEU:HD13	1.84	0.59
10:J:11:CYS:N	10:J:26:ASP:OD1	2.35	0.59
5:E:121:LEU:HD23	5:E:123:PHE:H	1.67	0.58
5:S:92:ALA:HB2	5:S:116:ILE:HD11	1.84	0.58
8:V:216:TYR:O	8:V:220:ASN:ND2	2.36	0.58
2:P:79:MET:HE3	2:P:82:ASP:HB2	1.86	0.58
15:d:145:ILE:HD11	15:d:240:ILE:HG23	1.86	0.58
15:f:216:VAL:HG22	15:f:225:TYR:HB3	1.85	0.58
7:U:36:THR:OG1	7:U:37:ALA:N	2.35	0.58
8:H:19:ARG:NE	8:H:224:SER:O	2.29	0.58
10:J:198:ALA:HB3	10:J:213:LEU:HB2	1.86	0.58
4:R:55:ASN:N	4:R:55:ASN:OD1	2.36	0.58
12:L:161:TYR:OH	10:X:217:MET:SD	2.60	0.57
11:Y:86:ARG:HG2	11:Y:122:SER:HB2	1.86	0.57
3:C:103:GLU:OE2	11:K:110:LYS:NZ	2.37	0.57
9:I:103:VAL:HG21	9:I:180:LYS:HA	1.86	0.57
13:a:228:MET:SD	13:a:228:MET:N	2.75	0.57
10:X:196:TRP:HD1	10:X:217:MET:HA	1.70	0.57
12:L:3:THR:HA	12:L:16:VAL:HG12	1.87	0.57
15:c:155:ILE:HD11	15:d:58:PRO:HG3	1.85	0.57
1:A:159:LYS:HD2	1:A:174:ILE:HD13	1.85	0.57
13:M:173:ILE:HD11	13:M:209:ALA:HB2	1.85	0.57
4:R:96:LEU:HB2	11:Y:63:LYS:HG3	1.86	0.57
3:C:58:LYS:HG3	3:C:60:ASN:H	1.69	0.57
3:C:115:CYS:HA	3:C:118:LYS:HD2	1.86	0.57
6:F:228:LEU:HA	6:F:232:LEU:HD12	1.87	0.57
10:J:16:SER:HB3	10:J:134:LEU:HD13	1.87	0.57
11:K:38:ASP:OD1	11:K:181:ARG:NH1	2.38	0.57
11:K:104:ILE:HB	11:K:116:TYR:HB2	1.87	0.57
13:a:173:ILE:HD11	13:a:209:ALA:HB2	1.87	0.57
8:H:8:TYR:OH	8:H:232:ASN:ND2	2.38	0.57
15:d:181:GLN:NE2	15:d:265:VAL:O	2.37	0.57
6:F:157:ALA:HB1	6:F:171:LEU:HD13	1.86	0.57
15:f:146:LYS:NZ	15:g:234:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1:THR:N	9:I:168:GLY:O	2.38	0.56
10:X:55:LEU:HB3	10:X:62:ILE:HD12	1.85	0.56
3:Q:18:LEU:HB2	3:Q:21:VAL:HG12	1.87	0.56
14:b:186:LEU:HD21	14:b:190:ARG:HH21	1.69	0.56
15:f:30:THR:HG22	15:f:162:TRP:HE1	1.69	0.56
2:B:119:GLN:NE2	3:C:82:ASP:OD1	2.39	0.56
5:E:108:ASN:HD21	5:E:150:LYS:HB2	1.71	0.56
10:X:24:ALA:HB2	10:X:200:VAL:HG23	1.87	0.56
7:G:69:ILE:HG21	7:G:219:SER:HB2	1.87	0.56
2:P:9:SER:HA	2:P:125:GLY:HA2	1.87	0.56
12:Z:115:ASP:HB2	12:Z:119:LYS:HG3	1.88	0.56
14:b:107:ASP:OD1	14:b:107:ASP:N	2.39	0.56
6:T:117:GLN:OE1	6:T:121:GLN:NE2	2.39	0.56
3:C:146:GLN:NE2	3:C:148:TYR:OH	2.39	0.56
8:H:17:ASP:HB2	8:H:225:GLY:HA3	1.87	0.56
6:F:145:GLU:OE2	6:F:147:ARG:NH1	2.39	0.56
6:T:157:ALA:HB1	6:T:171:LEU:HD13	1.87	0.56
14:b:2:THR:N	14:b:60:ASP:OD1	2.39	0.56
4:D:36:LYS:HD3	4:D:157:LYS:HG2	1.88	0.56
6:F:7:ASP:O	6:F:21:GLN:NE2	2.38	0.56
6:F:65:LYS:O	6:F:89:GLN:NE2	2.39	0.56
11:K:43:LYS:HZ1	11:K:76:MET:HB3	1.71	0.56
13:a:50:ILE:HG12	13:a:224:VAL:HG22	1.88	0.56
15:d:148:TYR:HB3	15:d:247:MET:HE2	1.88	0.56
8:H:40:ASN:ND2	8:H:156:TYR:O	2.39	0.56
11:K:156:ALA:HA	11:K:159:ILE:HD12	1.88	0.56
5:S:54:ILE:HG23	5:S:59:ILE:HB	1.88	0.56
15:e:257:LEU:O	15:e:261:ASN:ND2	2.39	0.56
7:G:95:ARG:NE	14:N:77:SER:OG	2.38	0.55
1:O:36:ASN:OD1	1:O:176:ASN:ND2	2.36	0.55
15:c:62:LEU:HD12	15:c:238:ILE:HG23	1.87	0.55
15:g:64:VAL:HG11	15:g:234:GLU:HG2	1.87	0.55
9:I:174:ASP:OD1	9:I:174:ASP:N	2.36	0.55
6:T:181:CYS:SG	6:T:182:SER:N	2.78	0.55
5:E:84:ASP:OD2	5:E:137:ARG:NH2	2.39	0.55
6:F:182:SER:O	6:F:186:LEU:N	2.39	0.55
7:G:36:THR:OG1	7:G:37:ALA:N	2.37	0.55
2:P:179:ASN:H	2:P:182:ILE:HD11	1.71	0.55
13:a:49:VAL:HG21	13:a:140:GLY:H	1.71	0.55
14:N:82:LYS:HB3	14:N:126:ASN:HD22	1.70	0.55
6:T:80:ASP:OD2	6:T:126:ARG:NH1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:GLN:NE2	4:D:148:GLU:OE2	2.39	0.55
8:H:189:ILE:HD13	8:H:217:ALA:HB2	1.89	0.55
3:Q:69:ASP:OD2	3:Q:95:GLN:NE2	2.38	0.55
4:R:10:PHE:H	5:S:23:GLN:HE22	1.55	0.55
14:b:6:VAL:HG13	14:b:7:VAL:HG23	1.87	0.55
1:O:217:GLN:NE2	1:O:223:ASP:O	2.40	0.55
15:e:134:SER:N	15:f:223:SER:HG	2.05	0.55
3:C:119:GLN:HG2	4:D:82:VAL:HG21	1.88	0.55
5:S:149:ASP:N	5:S:149:ASP:OD2	2.36	0.55
7:U:106:HIS:HB2	8:V:82:ILE:HG21	1.89	0.55
14:N:75:ASN:HD21	14:N:85:MET:HA	1.72	0.55
9:W:93:TYR:O	10:X:101:ARG:NH2	2.40	0.55
9:I:59:LEU:HD21	9:I:79:CYS:HB3	1.88	0.55
15:g:216:VAL:HG22	15:g:225:TYR:HB3	1.89	0.55
13:M:55:THR:HB	13:M:68:CYS:H	1.71	0.55
14:b:42:ARG:HD2	14:b:54:PHE:HB2	1.89	0.54
1:A:225:LYS:HD3	1:A:229:ILE:HG13	1.90	0.54
13:a:84:GLY:HA3	13:a:134:ALA:HA	1.90	0.54
9:W:85:GLN:O	9:W:89:LYS:NZ	2.40	0.54
2:B:173:PHE:O	2:B:177:ARG:NH1	2.40	0.54
7:G:150:ASP:OD1	7:G:150:ASP:N	2.40	0.54
2:P:74:ILE:HD11	2:P:134:LEU:HD13	1.89	0.54
4:D:90:GLU:OE1	4:D:93:ARG:NH1	2.40	0.54
2:P:39:ARG:HD3	2:P:159:MET:HG2	1.88	0.54
15:h:29:ILE:HG12	15:i:54:VAL:HG21	1.89	0.54
3:C:198:LYS:HE2	3:C:245:LYS:HE2	1.89	0.54
11:Y:194:THR:HG23	11:Y:195:VAL:HG23	1.88	0.54
2:P:206:LYS:HE3	2:P:228:LYS:HB2	1.89	0.54
6:T:45:VAL:HG22	6:T:213:VAL:HG12	1.89	0.54
10:X:51:VAL:HG22	10:X:86:VAL:HG22	1.89	0.54
12:Z:7:LYS:HA	12:Z:12:ILE:HG12	1.89	0.54
15:d:142:LEU:HA	15:d:145:ILE:HD12	1.88	0.54
3:C:184:THR:OG1	3:C:187:GLU:OE1	2.26	0.54
8:V:2:THR:HG22	8:V:185:GLY:HA3	1.89	0.54
15:d:30:THR:HG22	15:d:162:TRP:HE1	1.72	0.54
1:O:86:MET:HB3	1:O:93:CYS:HB2	1.90	0.54
7:U:46:ILE:HD11	7:U:149:GLY:HA3	1.90	0.54
8:V:13:MET:HE3	8:V:232:ASN:HD22	1.72	0.54
6:F:154:GLU:OE1	7:G:62:LYS:NZ	2.37	0.54
4:R:41:ALA:HB1	4:R:144:ILE:HD11	1.90	0.54
15:c:64:VAL:HG11	15:c:234:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:d:52:VAL:O	15:d:248:ARG:NH1	2.41	0.54
1:A:43:LYS:HE2	1:A:170:ARG:HA	1.89	0.53
4:D:55:ASN:OD1	4:D:55:ASN:N	2.41	0.53
10:J:190:ARG:NH2	13:a:178:ASP:OD2	2.39	0.53
10:X:162:MET:SD	10:X:186:SER:OG	2.66	0.53
3:Q:146:GLN:NE2	3:Q:148:TYR:OH	2.41	0.53
8:V:198:LYS:H	8:V:201:MET:HE3	1.74	0.53
2:B:95:ILE:HG23	9:I:61:HIS:HB3	1.90	0.53
12:Z:32:GLU:HG3	12:Z:175:ARG:HH12	1.73	0.53
12:Z:4:LEU:HD12	12:Z:15:ALA:HB3	1.90	0.53
15:g:156:ILE:HA	15:g:159:ILE:HG22	1.90	0.53
10:J:51:VAL:HG22	10:J:86:VAL:HG22	1.91	0.53
11:K:23:ASN:HB2	11:K:29:LYS:HG2	1.90	0.53
7:G:22:TYR:OH	15:h:171:GLU:OE2	2.26	0.53
8:V:170:ASN:HB2	14:b:59:ALA:HB1	1.91	0.53
8:V:204:LYS:O	8:V:208:ASN:ND2	2.41	0.53
13:a:127:ARG:NH2	14:b:104:ASN:OD1	2.41	0.53
3:Q:3:ARG:NH2	5:S:10:ARG:O	2.42	0.53
13:a:56:ARG:NH1	13:a:214:ILE:O	2.42	0.53
15:e:51:LEU:HD22	15:e:244:ILE:HG21	1.91	0.53
9:I:204:ILE:HB	9:I:207:LYS:HE3	1.90	0.53
5:E:149:ASP:N	5:E:149:ASP:OD1	2.39	0.53
9:W:86:GLU:OE2	9:W:94:LYS:NZ	2.42	0.53
15:d:36:SER:HA	15:d:40:ARG:HB2	1.89	0.53
9:I:104:ASP:O	9:I:180:LYS:NZ	2.41	0.52
10:J:98:TYR:OH	10:J:101:ARG:NH1	2.40	0.52
8:H:165:TYR:HB3	8:H:175:GLU:HB2	1.92	0.52
1:O:195:LYS:O	1:O:197:GLN:NE2	2.43	0.52
7:U:67:ASN:HA	7:U:217:ASN:HD21	1.73	0.52
15:h:145:ILE:HG13	15:h:240:ILE:HD12	1.91	0.52
10:J:115:LYS:HB3	10:J:131:GLU:HB2	1.90	0.52
12:L:50:ALA:HB3	13:M:155:VAL:HG12	1.91	0.52
13:a:41:ILE:HD12	13:a:173:ILE:HG21	1.91	0.52
7:U:38:LEU:HB3	7:U:49:CYS:HB2	1.91	0.52
7:U:126:THR:HG22	7:U:133:PRO:HB3	1.91	0.52
6:F:117:GLN:OE1	6:F:121:GLN:NE2	2.43	0.52
14:N:21:ILE:HD12	14:N:161:ILE:HD11	1.92	0.52
6:T:146:THR:HG22	6:T:152:TYR:HE1	1.73	0.52
15:d:142:LEU:HD11	15:d:202:ILE:HG12	1.91	0.52
8:H:169:LEU:HD12	14:N:6:VAL:HG21	1.92	0.52
13:M:113:ILE:HA	13:M:116:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LEU:HD12	2:B:149:ILE:HD12	1.92	0.52
3:C:15:GLU:N	15:d:172:ASP:OD2	2.42	0.52
3:C:26:GLU:HA	3:C:29:ASN:HD22	1.72	0.52
6:F:42:ASP:OD1	6:F:42:ASP:N	2.42	0.52
7:G:46:ILE:HD11	7:G:149:GLY:HA3	1.90	0.52
4:R:34:ALA:HB2	4:R:132:LEU:HD13	1.92	0.52
11:Y:51:ILE:HG12	11:Y:54:ARG:HH22	1.74	0.52
15:d:29:ILE:HG13	15:d:158:ASN:HD21	1.75	0.52
15:g:199:TYR:HB3	15:h:235:LYS:HD2	1.91	0.52
15:h:30:THR:HG22	15:h:162:TRP:HE1	1.74	0.52
14:N:60:ASP:HB3	14:N:109:LEU:HB2	1.91	0.52
14:b:181:ALA:HB1	14:b:185:ALA:HB3	1.91	0.52
15:d:19:LYS:O	15:d:23:ASN:ND2	2.43	0.52
2:B:69:SER:OG	2:B:70:GLU:N	2.41	0.52
14:N:178:THR:OG1	14:N:179:GLY:N	2.43	0.52
14:N:191:ASP:OD1	14:N:191:ASP:N	2.43	0.52
10:X:137:TYR:O	10:X:152:ASN:ND2	2.40	0.52
8:H:40:ASN:HB3	8:H:75:ARG:HH21	1.75	0.51
1:O:122:ARG:NE	1:O:166:CYS:SG	2.83	0.51
15:d:32:GLN:HG3	15:e:54:VAL:HG12	1.91	0.51
1:A:109:TYR:HB2	8:H:61:HIS:HB2	1.92	0.51
6:F:218:HIS:ND1	6:F:221:GLN:OE1	2.43	0.51
8:H:19:ARG:HH11	8:H:26:ILE:HG21	1.75	0.51
3:Q:88:ASN:OD1	10:X:79:ARG:NH2	2.43	0.51
2:B:192:ILE:HD11	2:B:210:ILE:HD11	1.92	0.51
3:C:52:ILE:HG22	3:C:56:ILE:HD11	1.92	0.51
6:F:6:TYR:HA	6:F:12:ILE:HD12	1.91	0.51
10:J:87:GLU:OE2	10:J:91:ASN:ND2	2.41	0.51
1:O:111:ASN:OD1	9:W:82:ARG:NH2	2.40	0.51
12:Z:2:THR:N	12:Z:17:ASP:OD1	2.43	0.51
1:A:50:ILE:HG12	1:A:147:ILE:HD12	1.92	0.51
10:J:55:LEU:HB3	10:J:62:ILE:HG12	1.91	0.51
10:J:85:ASP:OD1	10:J:85:ASP:N	2.38	0.51
12:L:2:THR:N	12:L:17:ASP:OD2	2.42	0.51
1:O:25:ILE:HD13	1:O:163:SER:HB3	1.92	0.51
4:R:33:VAL:HB	4:R:44:ALA:HB3	1.92	0.51
6:F:68:ASP:O	6:F:220:TRP:N	2.43	0.51
15:g:145:ILE:HG13	15:g:240:ILE:HD12	1.91	0.51
7:G:55:MET:HB2	7:G:215:LEU:HD11	1.93	0.51
2:P:75:VAL:HB	2:P:135:LEU:HB2	1.93	0.51
8:H:18:SER:O	8:H:18:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:191:ASP:OD1	14:b:191:ASP:N	2.44	0.51
6:F:198:LEU:HD21	6:F:204:LEU:HB2	1.93	0.51
1:O:52:SER:OG	1:O:53:GLN:N	2.44	0.51
4:R:180:MET:SD	4:R:180:MET:N	2.84	0.51
6:T:116:TYR:O	6:T:120:THR:OG1	2.29	0.51
13:a:113:ILE:HA	13:a:116:ILE:HG22	1.93	0.51
13:a:127:ARG:NH1	13:a:130:PHE:O	2.43	0.51
15:g:210:ALA:HB2	15:h:224:ASP:HB2	1.93	0.51
3:C:155:ASN:OD1	3:C:155:ASN:N	2.39	0.51
4:D:83:LEU:HD23	4:D:129:ILE:HD11	1.93	0.51
7:G:223:LYS:HG3	7:G:225:SER:HB3	1.93	0.51
9:I:204:ILE:HG22	9:I:206:PRO:HD2	1.92	0.51
9:I:6:LEU:HA	9:I:124:PHE:HA	1.94	0.50
15:f:160:LYS:NZ	15:f:192:GLU:OE2	2.38	0.50
12:L:176:VAL:HG13	12:L:187:ILE:HB	1.93	0.50
6:T:50:LYS:HE2	6:T:210:ALA:HB2	1.93	0.50
15:d:191:VAL:HG11	15:d:254:LEU:HD11	1.93	0.50
15:i:156:ILE:HG23	15:i:188:LEU:HD22	1.93	0.50
8:H:76:PHE:HD2	8:H:79:GLY:H	1.59	0.50
13:M:66:ARG:NH2	9:W:164:PHE:O	2.44	0.50
13:M:178:ASP:OD2	10:X:190:ARG:NH2	2.41	0.50
13:a:47:ASP:OD1	13:a:47:ASP:N	2.45	0.50
13:M:196:GLY:O	13:M:200:ASN:ND2	2.45	0.50
2:P:48:THR:HG21	2:P:64:LYS:HB2	1.93	0.50
3:Q:122:THR:HG22	3:Q:129:PRO:HB3	1.93	0.50
10:J:65:LEU:HD22	10:J:107:VAL:HG21	1.93	0.50
2:P:68:ILE:HB	2:P:72:ILE:HB	1.93	0.50
3:Q:198:LYS:HE3	3:Q:245:LYS:HD3	1.93	0.50
8:V:19:ARG:HG2	8:V:26:ILE:HD12	1.93	0.50
6:F:80:ASP:OD1	6:F:126:ARG:NH1	2.37	0.50
13:M:187:LEU:HB2	9:W:207:LYS:HZ2	1.77	0.50
14:N:206:ILE:HA	14:N:209:CYS:HB3	1.93	0.50
15:e:36:SER:HA	15:e:40:ARG:HB2	1.92	0.50
3:C:35:ILE:HD11	3:C:175:LEU:HD11	1.93	0.50
9:I:64:GLU:HA	9:I:67:ARG:HG2	1.93	0.50
10:J:18:SER:OG	10:J:19:ASN:N	2.45	0.50
2:P:11:THR:OG1	2:P:122:THR:O	2.28	0.50
13:a:62:SER:OG	14:b:182:ARG:NH2	2.41	0.50
3:C:176:LYS:HG2	4:D:52:LYS:HD2	1.94	0.50
7:G:45:GLY:HA3	7:G:222:CYS:HB2	1.94	0.50
8:H:19:ARG:HD2	8:H:26:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:N	9:I:17:ASP:OD1	2.44	0.50
5:E:50:SER:OG	5:E:51:GLU:N	2.45	0.50
4:R:139:ASN:OD1	4:R:139:ASN:N	2.43	0.50
4:R:176:TYR:HA	4:R:188:LEU:HD21	1.93	0.50
6:T:199:SER:OG	6:T:202:SER:O	2.30	0.50
12:Z:35:ILE:HD13	12:Z:56:GLU:HG3	1.94	0.50
15:d:166:ASN:HD21	15:d:266:VAL:HG23	1.77	0.50
3:C:33:ILE:HD11	3:C:163:ALA:HB1	1.94	0.49
10:J:204:THR:OG1	10:J:207:LYS:O	2.27	0.49
13:M:112:ASP:OD1	13:M:112:ASP:N	2.34	0.49
8:V:4:ILE:HD11	8:V:210:ILE:HG23	1.93	0.49
14:b:178:THR:OG1	14:b:179:GLY:N	2.41	0.49
15:f:36:SER:HA	15:f:40:ARG:HB2	1.94	0.49
2:B:139:VAL:HG23	2:B:213:ALA:HB1	1.94	0.49
7:G:49:CYS:HA	7:G:218:PHE:HB3	1.93	0.49
10:J:136:ALA:HB3	10:J:144:CYS:HB2	1.94	0.49
13:M:171:GLN:HB2	10:X:157:GLU:HG2	1.94	0.49
3:Q:154:GLY:O	4:R:81:ARG:NH2	2.45	0.49
3:Q:194:LYS:HE2	3:Q:238:LEU:HD11	1.94	0.49
4:R:99:ASP:OD2	12:Z:120:LYS:NZ	2.45	0.49
5:S:192:THR:HG23	5:S:195:GLN:HE21	1.76	0.49
10:X:198:ALA:HB3	10:X:213:LEU:HB2	1.93	0.49
15:g:211:LYS:O	15:g:214:THR:OG1	2.26	0.49
6:F:47:SER:OG	6:F:190:CYS:SG	2.66	0.49
9:I:18:THR:HG1	9:I:31:CYS:H	1.60	0.49
11:K:102:CYS:O	11:K:132:HIS:NE2	2.43	0.49
2:P:32:SER:OG	2:P:33:SER:N	2.45	0.49
10:X:16:SER:OG	10:X:17:GLY:N	2.46	0.49
12:Z:182:ASN:OD1	12:Z:182:ASN:N	2.45	0.49
15:e:148:TYR:HB3	15:e:247:MET:HE2	1.94	0.49
2:B:36:LEU:HD11	2:B:174:LEU:HD11	1.94	0.49
8:H:12:VAL:HG21	8:H:164:LEU:HB2	1.94	0.49
8:H:31:SER:OG	8:H:32:ARG:N	2.46	0.49
2:P:196:LYS:NZ	2:P:233:GLU:O	2.46	0.49
9:W:28:ASP:OD1	9:W:28:ASP:N	2.45	0.49
11:Y:104:ILE:HB	11:Y:116:TYR:HB2	1.94	0.49
1:O:41:GLY:HA3	1:O:50:ILE:HD13	1.94	0.49
2:B:18:LYS:NZ	15:c:172:ASP:O	2.45	0.49
3:C:194:LYS:HE2	3:C:238:LEU:HD11	1.94	0.49
12:Z:130:SER:OG	12:Z:131:GLY:N	2.45	0.49
8:H:152:ILE:HD11	8:H:182:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:203:LYS:O	13:M:207:THR:OG1	2.31	0.49
10:X:8:ASN:HD21	10:X:29:LEU:HG	1.77	0.49
4:R:201:SER:HB2	4:R:222:ILE:HG22	1.94	0.49
5:S:56:SER:OG	5:S:57:THR:N	2.45	0.49
8:V:9:ASP:OD1	8:V:10:ASN:ND2	2.45	0.49
3:C:48:ASP:HA	3:C:210:ILE:HG22	1.93	0.49
5:E:55:SER:OG	5:E:56:SER:N	2.45	0.49
11:K:111:ASP:OD1	11:K:111:ASP:N	2.44	0.49
5:S:192:THR:H	5:S:195:GLN:HB2	1.77	0.49
5:E:188:LYS:HB2	5:E:191:MET:HG3	1.93	0.49
15:i:160:LYS:HG2	15:i:164:GLN:HE21	1.78	0.49
10:J:87:GLU:O	10:J:91:ASN:ND2	2.42	0.48
13:a:220:THR:HG23	13:a:237:LEU:HD11	1.95	0.48
15:g:52:VAL:HG13	15:g:61:ILE:HG21	1.95	0.48
10:X:11:CYS:N	10:X:26:ASP:OD2	2.36	0.48
15:d:156:ILE:HD12	15:d:191:VAL:HG13	1.96	0.48
15:i:171:GLU:O	15:i:175:ASN:ND2	2.45	0.48
5:E:44:ASP:OD1	5:E:44:ASP:N	2.44	0.48
9:I:63:VAL:O	9:I:67:ARG:N	2.44	0.48
3:Q:212:LEU:HB2	3:Q:226:TYR:HD2	1.79	0.48
11:Y:86:ARG:HG3	11:Y:124:MET:HB3	1.94	0.48
15:c:30:THR:HG22	15:c:162:TRP:HE1	1.78	0.48
1:A:24:GLN:HE22	7:G:15:PHE:H	1.59	0.48
13:M:64:TYR:OH	14:N:165:ASP:OD2	2.26	0.48
7:U:150:ASP:OD1	7:U:150:ASP:N	2.44	0.48
2:B:48:THR:HG21	2:B:64:LYS:HB2	1.95	0.48
9:I:140:ALA:HB2	14:b:212:ILE:HD11	1.94	0.48
5:E:169:ALA:HB3	6:F:56:LEU:HD13	1.96	0.48
13:M:218:ASP:HA	13:M:237:LEU:HB2	1.96	0.48
14:N:49:LYS:HE3	14:N:125:ASN:HD22	1.78	0.48
11:Y:19:THR:HB	11:Y:32:ASP:H	1.79	0.48
12:Z:113:TYR:OH	12:Z:128:CYS:SG	2.64	0.48
15:h:66:ASP:O	15:h:137:GLN:NE2	2.36	0.48
4:D:26:VAL:HG21	4:D:130:ALA:HB3	1.95	0.48
4:D:130:ALA:HB2	4:D:149:PRO:HD3	1.96	0.48
4:D:132:LEU:HA	4:D:146:GLN:HA	1.96	0.48
12:L:170:SER:OG	12:L:171:GLY:N	2.47	0.48
7:U:55:MET:HG3	7:U:213:GLN:HE22	1.78	0.48
8:V:1:THR:N	8:V:223:SER:O	2.46	0.48
15:e:216:VAL:HG22	15:e:225:TYR:HB3	1.94	0.48
3:C:143:ASP:OD1	3:C:143:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:77:ASN:HD22	8:V:72:LYS:HE2	1.79	0.48
8:V:8:TYR:OH	8:V:232:ASN:ND2	2.46	0.48
15:e:227:GLU:OE1	15:e:230:ARG:NH2	2.37	0.48
4:D:71:LEU:HD12	4:D:133:ILE:HG12	1.96	0.48
10:J:175:GLY:O	10:J:179:THR:OG1	2.29	0.48
12:L:201:THR:HA	9:W:212:ILE:HD11	1.96	0.48
2:P:11:THR:HG22	2:P:21:GLN:HG3	1.96	0.48
4:R:63:ILE:HD12	4:R:84:VAL:HG21	1.95	0.48
6:T:180:GLU:OE1	6:T:182:SER:OG	2.31	0.48
2:B:161:THR:OG1	2:B:162:CYS:N	2.47	0.48
7:G:167:VAL:HG21	7:G:175:PHE:HB2	1.95	0.48
9:I:207:LYS:HE2	13:a:187:LEU:HB2	1.96	0.48
10:J:55:LEU:HD11	10:J:65:LEU:HD23	1.95	0.48
2:P:154:CYS:SG	2:P:155:TYR:N	2.87	0.48
3:Q:143:ASP:N	3:Q:143:ASP:OD1	2.46	0.48
9:W:63:VAL:HG22	9:W:78:MET:HE1	1.96	0.48
12:Z:134:TYR:O	12:Z:137:SER:OG	2.31	0.48
15:f:142:LEU:HD21	15:f:202:ILE:HD12	1.96	0.48
1:A:245:SER:OG	1:A:246:GLU:N	2.46	0.47
6:F:2:TYR:HA	15:g:172:ASP:HA	1.96	0.47
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.96	0.47
2:B:42:ASN:HB2	2:B:215:ASP:HB3	1.95	0.47
6:F:146:THR:HG22	6:F:152:TYR:HE1	1.78	0.47
13:M:152:TYR:HB3	13:M:158:TYR:HA	1.95	0.47
14:N:26:ASP:OD1	14:N:26:ASP:N	2.37	0.47
5:S:88:LEU:HD12	5:S:119:LEU:HD23	1.96	0.47
6:T:161:GLY:N	6:T:164:SER:OG	2.47	0.47
13:a:76:ASP:OD2	13:a:76:ASP:N	2.42	0.47
13:a:112:ASP:OD1	13:a:112:ASP:N	2.37	0.47
13:a:183:GLN:HG3	13:a:188:ILE:HG23	1.96	0.47
14:b:163:PHE:HB2	14:b:176:ILE:HG21	1.96	0.47
15:h:148:TYR:HB3	15:h:247:MET:HE2	1.95	0.47
7:G:62:LYS:HB2	7:G:65:SER:HB3	1.95	0.47
8:H:1:THR:N	8:H:223:SER:O	2.48	0.47
10:J:55:LEU:HD13	10:J:109:PRO:HB3	1.95	0.47
1:O:138:ARG:HB2	7:U:13:SER:HA	1.94	0.47
7:U:74:ASN:HD22	14:b:130:VAL:HB	1.79	0.47
15:e:163:ILE:HD11	15:e:181:GLN:HG2	1.96	0.47
4:D:107:ILE:HG22	4:D:133:ILE:HD13	1.96	0.47
6:F:45:VAL:HG12	6:F:213:VAL:HG22	1.96	0.47
9:I:28:ASP:OD1	9:I:28:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:3:ILE:HD13	8:V:44:CYS:HB3	1.96	0.47
8:V:160:LYS:HB3	8:V:163:GLN:HE22	1.80	0.47
6:F:47:SER:HG	6:F:190:CYS:HG	1.55	0.47
4:D:221:GLU:HG3	4:D:225:MET:HE2	1.96	0.47
7:G:142:SER:OG	7:G:143:PHE:N	2.47	0.47
9:I:179:THR:OG1	9:I:180:LYS:N	2.48	0.47
6:T:47:SER:OG	6:T:190:CYS:SG	2.64	0.47
2:B:95:ILE:HG21	9:I:65:LEU:HD12	1.96	0.47
3:C:161:ALA:HB1	3:C:175:LEU:HD13	1.96	0.47
4:D:24:GLU:HA	4:D:27:LYS:HD2	1.96	0.47
5:E:148:VAL:HG21	5:E:224:LYS:HA	1.96	0.47
1:O:177:LYS:HA	1:O:177:LYS:HD3	1.70	0.47
2:P:160:ALA:HB3	3:Q:55:LEU:HD21	1.96	0.47
3:Q:70:LYS:HD2	3:Q:70:LYS:HA	1.69	0.47
7:U:34:ASN:ND2	7:U:82:GLY:O	2.48	0.47
15:e:52:VAL:O	15:e:248:ARG:NH1	2.48	0.47
14:N:55:SER:HB3	14:N:112:ASN:HB2	1.96	0.47
2:P:52:SER:OG	2:P:54:ASN:O	2.33	0.47
2:P:54:ASN:N	2:P:54:ASN:OD1	2.47	0.47
3:Q:142:LYS:NZ	11:Y:74:THR:OG1	2.43	0.47
4:R:57:LYS:HG3	4:R:59:THR:H	1.80	0.47
6:T:72:ILE:HG21	6:T:88:MET:HE1	1.95	0.47
14:b:186:LEU:HG	14:b:190:ARG:HE	1.79	0.47
15:d:68:ASP:O	15:d:135:HIS:NE2	2.47	0.47
15:h:165:LEU:HD21	15:i:252:ILE:HG12	1.97	0.47
1:A:16:PHE:H	2:B:21:GLN:HE22	1.61	0.47
7:U:40:LEU:HA	7:U:165:GLY:HA2	1.96	0.47
15:c:164:GLN:HE21	15:c:185:ILE:HG21	1.79	0.47
15:g:52:VAL:HG11	15:g:245:VAL:HG22	1.97	0.47
15:g:63:ASN:ND2	15:g:65:ASN:OD1	2.48	0.47
1:A:116:ASN:ND2	1:A:118:GLU:OE1	2.48	0.47
6:F:113:ALA:HB2	6:F:152:TYR:CZ	2.50	0.47
8:V:76:PHE:HD2	8:V:79:GLY:H	1.63	0.47
15:c:19:LYS:O	15:c:23:ASN:ND2	2.48	0.47
15:d:247:MET:HE3	15:d:247:MET:HB3	1.80	0.47
8:H:188:TYR:O	8:V:191:SER:OG	2.30	0.46
6:T:182:SER:OG	6:T:182:SER:O	2.33	0.46
11:Y:13:VAL:HG11	11:Y:105:ALA:HB1	1.96	0.46
13:a:203:LYS:O	13:a:207:THR:OG1	2.29	0.46
15:h:36:SER:HA	15:h:40:ARG:HB2	1.96	0.46
5:E:60:GLU:O	5:E:63:SER:OG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:SER:HB3	6:F:186:LEU:HD22	1.97	0.46
3:Q:72:ILE:HG21	3:Q:110:LEU:HD23	1.97	0.46
13:a:56:ARG:NH1	13:a:216:THR:O	2.48	0.46
13:a:138:LEU:HD23	13:a:138:LEU:HA	1.79	0.46
1:A:89:MET:HG2	7:G:157:ASN:HD21	1.80	0.46
2:B:22:ILE:HD13	2:B:22:ILE:HA	1.81	0.46
13:M:62:SER:OG	13:M:63:ILE:N	2.48	0.46
13:M:223:TYR:HE1	13:M:232:VAL:HG13	1.79	0.46
1:O:13:LEU:HB2	1:O:24:GLN:HG2	1.98	0.46
7:U:90:ILE:HD13	7:U:122:ILE:HD11	1.96	0.46
8:V:160:LYS:HB3	8:V:163:GLN:NE2	2.29	0.46
8:V:161:LYS:HA	8:V:161:LYS:HD3	1.79	0.46
15:g:32:GLN:HE22	15:g:40:ARG:HH22	1.64	0.46
15:i:175:ASN:HB2	15:i:178:VAL:HG22	1.97	0.46
4:D:42:VAL:HG21	4:D:186:ILE:HG12	1.97	0.46
9:I:8:CYS:SG	9:I:9:GLN:N	2.86	0.46
13:M:153:ASP:OD1	13:M:153:ASP:N	2.42	0.46
4:R:116:GLN:NE2	5:S:84:ASP:OD1	2.47	0.46
15:g:227:GLU:HG2	15:g:230:ARG:HH21	1.81	0.46
1:A:79:THR:HA	8:H:68:ASN:HD21	1.81	0.46
10:J:61:ASP:OD2	10:J:106:PHE:N	2.42	0.46
14:N:216:ARG:NE	9:W:139:GLU:OE2	2.47	0.46
8:V:201:MET:HE1	8:V:209:LEU:HD13	1.97	0.46
12:Z:18:SER:O	12:Z:18:SER:OG	2.31	0.46
15:f:180:ILE:HA	15:f:183:GLU:HG2	1.98	0.46
15:g:195:ALA:HA	15:g:198:LEU:HD23	1.96	0.46
8:H:198:LYS:HA	8:H:198:LYS:HD3	1.72	0.46
12:L:1:THR:HG1	12:L:130:SER:H	1.63	0.46
14:N:31:TYR:HB2	14:N:36:LYS:HB2	1.97	0.46
4:R:159:GLN:OE1	4:R:160:ALA:N	2.49	0.46
8:V:19:ARG:HB2	8:V:225:GLY:HA2	1.97	0.46
2:B:54:ASN:N	2:B:54:ASN:OD1	2.47	0.46
5:E:119:LEU:HD23	5:E:119:LEU:HA	1.79	0.46
12:L:4:LEU:HD12	12:L:15:ALA:HB3	1.97	0.46
12:L:16:VAL:HG21	12:L:33:LYS:HB2	1.97	0.46
3:Q:58:LYS:HD2	3:Q:58:LYS:HA	1.76	0.46
8:V:3:ILE:HD12	8:V:46:SER:HB3	1.98	0.46
15:c:143:GLU:HA	15:c:146:LYS:HE3	1.97	0.46
15:i:36:SER:HA	15:i:40:ARG:HB2	1.96	0.46
11:K:43:LYS:NZ	11:K:76:MET:O	2.40	0.46
12:L:139:LEU:O	12:L:143:TYR:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:36:LYS:HE2	4:R:157:LYS:HA	1.98	0.46
15:g:66:ASP:OD1	15:g:66:ASP:N	2.39	0.46
15:g:142:LEU:HD12	15:g:202:ILE:HD12	1.98	0.46
1:A:41:GLY:HA3	1:A:50:ILE:HD13	1.97	0.46
12:L:2:THR:OG1	12:L:131:GLY:O	2.29	0.46
12:L:12:ILE:HB	12:L:179:ILE:HD12	1.97	0.46
5:S:60:GLU:O	5:S:63:SER:OG	2.27	0.46
8:V:168:ASN:HD21	14:b:37:PHE:HZ	1.64	0.46
5:E:199:LEU:HA	5:E:202:THR:HG22	1.98	0.46
15:e:211:LYS:O	15:e:214:THR:OG1	2.31	0.46
15:i:142:LEU:HD22	15:i:202:ILE:HD12	1.98	0.46
1:A:111:ASN:OD1	9:I:82:ARG:NH2	2.49	0.45
1:A:129:GLN:HE22	1:A:133:GLN:HE21	1.64	0.45
3:C:160:PHE:CZ	4:D:55:ASN:HB3	2.51	0.45
6:F:106:GLU:OE2	6:F:110:ARG:NH2	2.41	0.45
9:I:5:GLY:O	9:I:125:THR:N	2.44	0.45
11:K:86:ARG:HD2	11:K:124:MET:HB3	1.97	0.45
6:T:37:ALA:HB1	6:T:143:ILE:HD13	1.97	0.45
13:a:60:SER:OG	13:a:61:TYR:N	2.48	0.45
7:G:111:LEU:HD12	7:G:111:LEU:HA	1.78	0.45
8:H:7:ILE:HA	8:H:12:VAL:HG23	1.98	0.45
12:L:203:PRO:O	10:X:39:THR:OG1	2.34	0.45
5:S:13:ASN:HB2	6:T:126:ARG:HD3	1.97	0.45
5:S:97:ASN:HD21	12:Z:64:LYS:HB3	1.81	0.45
7:U:142:SER:OG	7:U:143:PHE:N	2.50	0.45
13:a:97:GLN:HA	13:a:100:ILE:HG22	1.98	0.45
14:b:229:VAL:HG22	14:b:234:VAL:HG13	1.97	0.45
14:N:81:ARG:NE	14:N:83:GLU:OE1	2.49	0.45
2:P:50:LYS:NZ	2:P:58:GLU:O	2.46	0.45
3:Q:138:GLY:HA2	3:Q:215:LEU:HD11	1.99	0.45
15:h:235:LYS:HA	15:h:235:LYS:HD3	1.57	0.45
10:J:24:ALA:HB2	10:J:200:VAL:HG23	1.98	0.45
3:Q:68:ILE:HD12	3:Q:90:SER:HB3	1.99	0.45
7:U:167:VAL:HG11	7:U:175:PHE:HB2	1.98	0.45
14:b:60:ASP:HB3	14:b:109:LEU:HB2	1.97	0.45
14:b:151:TYR:HE1	14:b:232:LYS:HE2	1.82	0.45
15:i:254:LEU:HD23	15:i:254:LEU:HA	1.76	0.45
7:G:35:ASN:HB2	7:G:68:ARG:HH22	1.81	0.45
2:P:42:ASN:OD1	2:P:42:ASN:N	2.49	0.45
3:C:70:LYS:HA	3:C:70:LYS:HD3	1.81	0.45
11:K:170:ARG:NH1	12:Z:136:TYR:OH	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:206:ILE:HG23	13:M:237:LEU:HD11	1.98	0.45
3:Q:53:SER:OG	3:Q:54:LYS:N	2.50	0.45
8:V:169:LEU:HD12	14:b:6:VAL:HG21	1.99	0.45
12:Z:194:PHE:HD1	12:Z:194:PHE:HA	1.72	0.45
15:d:62:LEU:HD12	15:d:238:ILE:HG23	1.99	0.45
8:H:8:TYR:HB2	8:H:11:GLY:H	1.82	0.45
8:H:198:LYS:H	8:H:201:MET:HE3	1.81	0.45
11:K:179:GLU:HG3	11:K:192:TYR:HB3	1.99	0.45
13:M:97:GLN:HA	13:M:100:ILE:HG22	1.99	0.45
4:R:48:LYS:HD2	4:R:48:LYS:HA	1.72	0.45
6:T:117:GLN:HG3	7:U:89:ASN:HD22	1.82	0.45
6:T:145:GLU:HB2	6:T:158:LEU:HD11	1.98	0.45
12:Z:39:LYS:HE2	12:Z:39:LYS:HB3	1.85	0.45
15:f:142:LEU:HD23	15:f:146:LYS:HE2	1.98	0.45
7:U:46:ILE:HD12	7:U:151:ILE:HD11	1.98	0.45
9:W:162:GLY:O	9:W:169:SER:OG	2.31	0.45
3:C:82:ASP:OD2	3:C:128:ARG:NH1	2.48	0.45
7:G:56:ASP:HA	7:G:59:LYS:HE2	1.99	0.45
13:M:171:GLN:OE1	10:X:158:GLN:NE2	2.50	0.45
4:R:119:THR:HG22	4:R:126:PRO:HB3	1.98	0.45
5:S:21:LEU:HB2	5:S:24:VAL:HB	1.98	0.45
10:X:23:ILE:HG23	10:X:201:LEU:HB3	1.98	0.45
12:Z:83:LEU:HD23	12:Z:86:ILE:HD11	1.98	0.45
15:c:156:ILE:HG23	15:c:188:LEU:HD22	1.97	0.45
4:D:62:LEU:HD13	4:D:207:ALA:HB2	1.99	0.44
13:M:47:ASP:OD1	13:M:47:ASP:N	2.49	0.44
3:Q:149:HIS:CE1	3:Q:164:ILE:HG21	2.52	0.44
6:T:34:CYS:SG	6:T:35:ALA:N	2.90	0.44
15:i:195:ALA:HA	15:i:198:LEU:HD13	1.99	0.44
6:F:50:LYS:HE3	6:F:210:ALA:HB2	1.99	0.44
6:F:152:TYR:HD1	6:F:152:TYR:HA	1.62	0.44
6:F:154:GLU:HB3	7:G:65:SER:HB2	2.00	0.44
7:G:197:TYR:HA	7:G:200:ILE:HD12	1.99	0.44
6:T:157:ALA:HB3	7:U:60:MET:HE2	1.99	0.44
8:V:43:VAL:HG21	8:V:56:ILE:HD12	1.99	0.44
10:X:37:VAL:HG21	11:Y:117:TRP:CH2	2.53	0.44
11:K:103:LEU:HD23	11:K:103:LEU:HA	1.84	0.44
1:O:102:SER:O	1:O:102:SER:OG	2.35	0.44
13:a:64:TYR:HE1	14:b:182:ARG:HG2	1.81	0.44
15:g:143:GLU:HA	15:g:146:LYS:HE3	1.99	0.44
2:B:48:THR:OG1	2:B:49:GLU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:GLU:HB2	4:D:61:LYS:HD2	2.00	0.44
5:E:38:VAL:HG13	5:E:49:ALA:HB3	1.99	0.44
12:L:26:ILE:HD13	12:L:29:GLN:HE21	1.82	0.44
14:N:6:VAL:HG13	14:N:7:VAL:HG23	1.98	0.44
1:O:153:ASN:HD22	1:O:239:ARG:HH12	1.64	0.44
4:R:146:GLN:HE21	4:R:161:ILE:HG21	1.82	0.44
2:B:171:MET:HE3	3:C:55:LEU:HD23	1.98	0.44
13:M:96:LEU:HD22	13:M:120:LEU:HD22	1.99	0.44
15:c:154:GLU:HG2	15:d:62:LEU:HD23	2.00	0.44
2:B:165:LYS:HB3	2:B:165:LYS:HE2	1.83	0.44
3:C:171:ALA:HB2	3:C:199:SER:HB3	1.99	0.44
9:I:19:ARG:HD2	9:I:170:GLY:N	2.32	0.44
6:T:48:GLY:O	6:T:209:THR:OG1	2.31	0.44
7:U:78:ILE:HG23	7:U:138:ILE:HG23	1.98	0.44
15:f:138:ILE:HD12	15:f:138:ILE:HA	1.90	0.44
5:E:8:TYR:HE2	5:E:17:PRO:HD3	1.81	0.44
6:F:88:MET:HE2	6:F:112:VAL:HG21	1.98	0.44
5:S:36:THR:HB	5:S:175:ALA:HB3	1.98	0.44
7:U:103:TYR:OH	14:b:70:ARG:NE	2.38	0.44
9:W:3:ILE:HG23	9:W:16:ALA:HB2	2.00	0.44
13:a:203:LYS:HG2	13:a:235:LEU:HD13	1.99	0.44
15:c:210:ALA:HB2	15:d:224:ASP:HB2	2.00	0.44
15:h:155:ILE:HD12	15:h:155:ILE:HA	1.81	0.44
5:E:204:LEU:HD23	5:E:204:LEU:HA	1.85	0.44
11:K:174:THR:OG1	11:Y:174:THR:O	2.30	0.44
5:S:79:SER:OG	5:S:142:ALA:O	2.35	0.44
7:U:111:LEU:HD12	7:U:111:LEU:HA	1.82	0.44
12:Z:157:ARG:HE	12:Z:157:ARG:HB3	1.65	0.44
11:K:8:ARG:O	11:K:147:TYR:OH	2.25	0.44
12:L:111:MET:HE2	12:L:111:MET:HB3	1.83	0.44
14:N:23:ILE:HD11	14:N:116:ALA:HB3	2.00	0.44
8:V:17:ASP:HA	8:V:228:ILE:HG22	1.99	0.44
15:d:142:LEU:HD21	15:d:202:ILE:HG23	2.00	0.44
6:F:187:ILE:H	6:F:187:ILE:HG12	1.61	0.43
11:K:51:ILE:HB	12:L:119:LYS:HG2	2.00	0.43
4:R:71:LEU:HD12	4:R:133:ILE:HG12	1.99	0.43
11:Y:124:MET:HE3	11:Y:124:MET:HB2	1.84	0.43
12:Z:26:ILE:HD13	12:Z:29:GLN:HE21	1.83	0.43
5:E:66:LYS:HA	5:E:78:MET:HE2	1.99	0.43
9:I:33:LYS:HD3	9:I:33:LYS:HA	1.85	0.43
12:L:20:ALA:HB2	12:L:31:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:18:LYS:HE3	14:N:198:THR:HA	1.99	0.43
3:Q:68:ILE:HG21	3:Q:110:LEU:HD21	1.99	0.43
6:T:228:LEU:HA	6:T:232:LEU:HD12	2.00	0.43
15:c:234:GLU:OE1	15:i:146:LYS:NZ	2.41	0.43
5:E:208:MET:HG3	5:E:210:ASP:H	1.83	0.43
2:P:46:ILE:HD11	2:P:219:PHE:HZ	1.82	0.43
2:P:144:TYR:OH	2:P:216:ASN:ND2	2.52	0.43
3:Q:242:LYS:HD2	3:Q:242:LYS:HA	1.78	0.43
11:Y:2:ASP:OD1	11:Y:2:ASP:N	2.51	0.43
7:G:40:LEU:HD21	7:G:196:ILE:HD11	2.00	0.43
10:X:61:ASP:HB3	10:X:107:VAL:HG13	2.00	0.43
15:d:150:SER:HA	15:e:62:LEU:HD23	2.00	0.43
15:e:156:ILE:HG23	15:e:188:LEU:HD22	2.00	0.43
15:e:247:MET:HE3	15:e:247:MET:HB3	1.77	0.43
1:O:172:CYS:SG	1:O:173:VAL:N	2.92	0.43
7:U:71:HIS:CE1	14:b:77:SER:HA	2.54	0.43
11:Y:168:LYS:HG3	11:Y:176:ILE:HG22	2.00	0.43
12:Z:33:LYS:HD2	12:Z:45:MET:HG3	2.00	0.43
15:e:150:SER:HA	15:f:62:LEU:HD23	2.01	0.43
3:C:105:GLN:NE2	3:C:109:GLN:O	2.52	0.43
8:H:161:LYS:HA	8:H:161:LYS:HD3	1.75	0.43
11:K:3:THR:HG22	11:K:135:GLY:HA3	2.01	0.43
3:Q:76:VAL:HA	3:Q:134:PHE:HB3	2.00	0.43
13:a:86:GLN:HB3	14:b:169:THR:HG23	1.99	0.43
15:g:62:LEU:HD11	15:g:238:ILE:HG23	2.01	0.43
15:h:52:VAL:O	15:h:248:ARG:NH1	2.52	0.43
15:h:171:GLU:HA	15:i:176:PHE:HZ	1.81	0.43
1:A:44:GLY:HA2	1:A:192:ARG:HH22	1.84	0.43
4:D:83:LEU:HD13	4:D:127:PHE:HE2	1.83	0.43
6:F:109:VAL:O	6:F:152:TYR:OH	2.24	0.43
7:G:78:ILE:HG12	7:G:140:ILE:HG12	2.01	0.43
8:H:17:ASP:N	8:H:17:ASP:OD1	2.51	0.43
11:K:145:LYS:HD2	12:Z:138:ILE:HG23	2.00	0.43
1:O:40:VAL:HG23	1:O:173:VAL:HB	2.01	0.43
1:O:147:ILE:HG13	1:O:157:LEU:HD13	2.00	0.43
15:c:41:ILE:HD13	15:c:41:ILE:HA	1.90	0.43
15:d:138:ILE:HG13	15:d:240:ILE:HD11	2.01	0.43
15:d:165:LEU:HD11	15:e:252:ILE:HG13	2.01	0.43
15:f:227:GLU:HG3	15:f:230:ARG:HH21	1.84	0.43
1:A:116:ASN:OD1	1:A:117:ALA:N	2.52	0.43
3:C:153:SER:OG	3:C:155:ASN:OD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:18:SER:O	12:L:18:SER:OG	2.32	0.43
1:O:227:SER:O	1:O:227:SER:OG	2.30	0.43
2:P:157:ASN:HD21	3:Q:61:ASN:HB2	1.84	0.43
6:T:44:VAL:HG11	6:T:135:ALA:HB1	2.01	0.43
13:a:90:LYS:HA	13:a:90:LYS:HD2	1.75	0.43
4:D:41:ALA:HB2	4:D:142:ILE:HG21	2.01	0.43
4:D:132:LEU:HD22	4:D:161:ILE:HD11	2.01	0.43
5:E:82:MET:HE3	5:E:82:MET:HB2	1.91	0.43
7:G:233:HIS:HB2	7:G:236:ILE:HG12	2.00	0.43
6:T:166:ALA:O	6:T:169:THR:OG1	2.36	0.43
14:b:82:LYS:NZ	14:b:83:GLU:OE2	2.45	0.43
15:d:32:GLN:HE22	15:d:40:ARG:HH22	1.67	0.43
6:F:109:VAL:HB	6:F:152:TYR:CZ	2.54	0.43
7:G:38:LEU:HB3	7:G:49:CYS:HB2	2.01	0.43
8:H:66:MET:HE1	8:H:76:PHE:H	1.84	0.43
9:I:181:ASP:N	9:I:181:ASP:OD1	2.51	0.43
13:M:59:LEU:HD12	13:M:59:LEU:HA	1.83	0.43
5:S:204:LEU:HD23	5:S:204:LEU:HA	1.89	0.43
9:W:59:LEU:HD12	9:W:59:LEU:HA	1.86	0.43
12:Z:12:ILE:HD11	12:Z:109:PHE:HB3	2.00	0.43
15:f:161:LEU:HD21	15:g:252:ILE:HD11	2.00	0.43
15:g:212:ILE:HD12	15:g:212:ILE:HA	1.75	0.43
1:A:124:ILE:HD13	1:A:124:ILE:HA	1.92	0.42
4:D:38:SER:HB2	4:D:179:ASN:HB3	2.01	0.42
12:L:52:CYS:HB3	12:L:97:CYS:HB2	2.01	0.42
5:S:225:SER:OG	5:S:226:ASP:N	2.52	0.42
15:d:175:ASN:HB3	15:d:178:VAL:HG22	2.02	0.42
9:I:94:LYS:HE3	10:J:101:ARG:HH12	1.85	0.42
2:P:157:ASN:OD1	2:P:157:ASN:N	2.37	0.42
11:Y:110:LYS:HE3	11:Y:110:LYS:HB2	1.88	0.42
13:a:64:TYR:O	14:b:190:ARG:NH2	2.45	0.42
13:a:108:SER:O	13:a:108:SER:OG	2.32	0.42
6:F:39:LYS:NZ	6:F:141:PRO:O	2.39	0.42
8:H:211:LEU:HD11	8:H:244:VAL:HG11	2.02	0.42
8:H:234:THR:OG1	8:H:235:LYS:N	2.52	0.42
9:I:135:MET:HE3	9:I:135:MET:HB2	1.89	0.42
14:N:26:ASP:HA	14:N:224:ILE:HA	2.02	0.42
2:P:171:MET:HE2	2:P:171:MET:HB3	1.84	0.42
3:Q:119:GLN:NE2	4:R:79:ASP:OD1	2.49	0.42
4:R:33:VAL:HG13	4:R:160:ALA:HB2	2.00	0.42
7:U:155:GLU:H	7:U:155:GLU:HG2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:14:LEU:HB2	8:V:231:VAL:HG22	2.01	0.42
14:N:194:LYS:HG3	14:N:197:MET:HG2	2.02	0.42
1:O:225:LYS:HE2	1:O:225:LYS:HB2	1.81	0.42
2:P:192:ILE:HD11	2:P:210:ILE:HD11	2.01	0.42
3:Q:133:SER:HB2	3:Q:152:PRO:HD3	2.01	0.42
6:T:39:LYS:HB2	6:T:143:ILE:HD12	2.02	0.42
6:T:93:LEU:HD23	6:T:93:LEU:HA	1.90	0.42
10:X:90:ALA:O	10:X:137:TYR:OH	2.27	0.42
15:c:164:GLN:HE21	15:c:185:ILE:HD13	1.84	0.42
1:A:17:SER:OG	1:A:21:ASN:O	2.36	0.42
11:K:37:TYR:HB2	11:K:45:LEU:HB3	2.00	0.42
12:L:162:HIS:HE1	11:Y:145:LYS:HG3	1.84	0.42
3:Q:37:LEU:HB3	3:Q:44:ILE:HG12	2.02	0.42
7:U:67:ASN:OD1	7:U:217:ASN:ND2	2.52	0.42
15:f:142:LEU:HD11	15:f:202:ILE:HB	2.01	0.42
15:f:156:ILE:HD12	15:f:156:ILE:HA	1.86	0.42
15:h:136:LYS:HE3	15:h:136:LYS:HB2	1.79	0.42
3:C:149:HIS:HB3	3:C:159:TRP:CD1	2.54	0.42
10:J:37:VAL:HG21	11:K:117:TRP:CZ3	2.55	0.42
10:J:171:GLN:HE22	10:J:179:THR:HG21	1.85	0.42
11:K:20:TYR:HE1	11:K:177:ASN:HD22	1.66	0.42
13:M:79:ILE:HG12	13:M:225:ILE:HD11	2.01	0.42
1:O:188:LEU:HD21	1:O:214:GLU:HG3	2.01	0.42
10:X:13:LEU:HD23	10:X:180:ILE:HG13	2.01	0.42
14:N:116:ALA:HB2	14:N:161:ILE:HG23	2.01	0.42
7:U:242:ASN:OD1	7:U:242:ASN:N	2.52	0.42
8:V:218:MET:HG2	8:V:224:SER:HA	2.01	0.42
13:a:116:ILE:HD12	13:a:116:ILE:HA	1.88	0.42
15:d:239:HIS:HA	15:d:242:ILE:HG22	2.01	0.42
15:f:240:ILE:HD12	15:f:240:ILE:HA	1.79	0.42
11:K:35:LYS:HA	11:K:54:ARG:NH1	2.34	0.42
3:Q:194:LYS:HA	3:Q:194:LYS:HD3	1.84	0.42
13:a:103:PHE:HE2	13:a:111:PRO:HB3	1.85	0.42
7:U:184:TYR:OH	7:U:195:ASP:OD2	2.30	0.42
9:W:95:VAL:HA	9:W:115:PRO:HB3	2.02	0.42
15:c:59:GLY:N	15:i:154:GLU:OE1	2.39	0.42
10:J:196:TRP:CZ3	12:Z:203:PRO:HD2	2.54	0.42
4:R:132:LEU:HA	4:R:146:GLN:HA	2.01	0.42
11:Y:59:GLU:HG3	11:Y:63:LYS:HE2	2.02	0.42
15:h:53:ASN:OD1	15:h:53:ASN:N	2.52	0.42
1:A:52:SER:HB3	1:A:75:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:12:VAL:HG11	9:I:102:GLY:HA2	2.03	0.41
11:K:174:THR:O	11:Y:174:THR:OG1	2.38	0.41
13:M:187:LEU:HD12	9:W:207:LYS:HD2	2.01	0.41
13:M:225:ILE:HG12	13:M:230:ILE:HG22	2.02	0.41
14:N:188:LEU:HD22	14:N:212:ILE:HD11	2.02	0.41
1:O:242:THR:OG1	1:O:243:GLN:N	2.53	0.41
3:Q:85:ILE:HD13	3:Q:85:ILE:HA	1.86	0.41
3:Q:212:LEU:HB2	3:Q:226:TYR:CD2	2.55	0.41
7:U:183:ASP:OD2	7:U:183:ASP:N	2.45	0.41
2:B:217:LYS:HB3	2:B:217:LYS:HE2	1.76	0.41
7:G:232:ILE:HB	7:G:233:HIS:H	1.65	0.41
13:M:101:GLN:HA	13:M:104:VAL:HG12	2.02	0.41
2:P:195:LEU:HD23	2:P:195:LEU:HA	1.90	0.41
4:R:17:LEU:HD13	4:R:17:LEU:HA	1.94	0.41
15:d:209:ARG:NH1	15:d:233:ASP:OD2	2.53	0.41
15:h:216:VAL:HG22	15:h:225:TYR:HB3	2.00	0.41
6:F:66:ILE:HG23	6:F:89:GLN:HG3	2.01	0.41
10:J:39:THR:OG1	12:Z:203:PRO:O	2.37	0.41
14:N:21:ILE:HD11	14:N:159:LEU:HB3	2.01	0.41
1:O:103:GLU:OE2	1:O:123:ASN:ND2	2.49	0.41
3:Q:67:LYS:HD3	3:Q:223:TYR:HE2	1.85	0.41
14:b:61:ALA:HB2	14:b:111:ASN:HD21	1.83	0.41
15:g:142:LEU:O	15:g:146:LYS:HG3	2.20	0.41
2:B:24:TYR:HE1	15:c:174:ASN:HA	1.86	0.41
6:F:115:LYS:HD2	6:F:115:LYS:HA	1.85	0.41
8:H:4:ILE:HG12	8:H:181:VAL:HG23	2.02	0.41
9:I:165:ASN:N	9:I:165:ASN:OD1	2.51	0.41
11:K:144:ASP:OD1	11:K:144:ASP:N	2.53	0.41
4:R:180:MET:HB3	4:R:184:ASP:HB3	2.03	0.41
6:T:182:SER:HB2	6:T:185:GLU:HB3	2.01	0.41
11:Y:52:GLY:O	12:Z:88:TYR:OH	2.32	0.41
13:a:55:THR:HG1	13:a:68:CYS:H	1.67	0.41
15:e:211:LYS:HB2	15:e:211:LYS:HE2	1.84	0.41
1:A:93:CYS:SG	1:A:94:LEU:N	2.93	0.41
2:B:44:VAL:H	2:B:213:ALA:HB3	1.86	0.41
6:F:104:ASN:OD1	6:F:107:SER:N	2.53	0.41
7:G:126:THR:HG22	7:G:133:PRO:HB3	2.02	0.41
9:I:218:GLU:OE2	10:J:46:LYS:NZ	2.43	0.41
13:M:163:HIS:NE2	13:M:178:ASP:OD1	2.53	0.41
6:T:50:LYS:HD3	6:T:61:GLU:HA	2.02	0.41
15:e:155:ILE:HD12	15:e:155:ILE:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:e:230:ARG:NH1	15:e:234:GLU:OE1	2.54	0.41
15:f:62:LEU:HD22	15:f:242:ILE:HD11	2.02	0.41
4:D:64:LYS:HB3	4:D:64:LYS:HE2	1.81	0.41
5:E:223:LYS:HE2	5:E:223:LYS:HB2	1.95	0.41
9:I:205:TYR:HA	10:J:178:GLU:HG3	2.03	0.41
11:K:27:LYS:H	11:K:27:LYS:HG2	1.73	0.41
2:P:82:ASP:HB3	2:P:132:LEU:HD23	2.02	0.41
2:P:161:THR:OG1	2:P:162:CYS:N	2.53	0.41
4:R:49:ASN:ND2	4:R:50:ILE:O	2.53	0.41
10:X:93:LEU:HD23	10:X:93:LEU:HA	1.88	0.41
12:Z:52:CYS:HB2	12:Z:99:ILE:HD11	2.03	0.41
15:e:161:LEU:HD12	15:f:252:ILE:HD11	2.01	0.41
15:h:227:GLU:OE1	15:h:230:ARG:NH2	2.39	0.41
3:C:209:LYS:HD2	3:C:209:LYS:HA	1.81	0.41
4:D:99:ASP:OD1	12:L:120:LYS:NZ	2.54	0.41
4:D:104:VAL:HG21	4:D:135:GLY:H	1.86	0.41
7:G:35:ASN:OD1	7:G:53:SER:N	2.54	0.41
7:G:36:THR:HG23	7:G:51:ILE:HB	2.03	0.41
8:H:36:ARG:NH1	8:H:42:TYR:OH	2.54	0.41
8:H:71:ARG:HD3	8:H:71:ARG:HA	1.88	0.41
9:I:196:LEU:HD11	13:a:235:LEU:HD11	2.03	0.41
11:K:2:ASP:HB2	11:K:18:ASP:HB3	2.03	0.41
6:T:82:LYS:HA	6:T:85:THR:HG22	2.03	0.41
12:Z:173:LYS:HD3	12:Z:189:GLU:HG2	2.02	0.41
14:b:128:ASP:OD1	14:b:128:ASP:N	2.54	0.41
15:c:169:ARG:HA	15:d:260:LYS:HD3	2.03	0.41
15:f:207:MET:HE1	15:g:212:ILE:HG12	2.03	0.41
15:h:247:MET:HE3	15:h:247:MET:HB3	1.84	0.41
7:G:220:TRP:HE1	7:G:223:LYS:HG2	1.85	0.41
8:H:177:HIS:HB3	8:H:178:ASP:H	1.61	0.41
10:J:47:MET:HG3	10:J:73:VAL:HG11	2.02	0.41
11:K:174:THR:OG1	11:Y:174:THR:OG1	2.27	0.41
6:T:63:ILE:HD12	6:T:63:ILE:HA	1.92	0.41
10:X:110:ILE:HD11	10:X:152:ASN:HB2	2.03	0.41
14:b:116:ALA:HB2	14:b:161:ILE:HG23	2.01	0.41
15:c:66:ASP:OD1	15:c:66:ASP:N	2.40	0.41
2:B:86:LEU:HA	2:B:86:LEU:HD12	1.82	0.41
2:B:95:ILE:HD13	2:B:95:ILE:HA	1.89	0.41
3:C:86:LEU:HD23	3:C:86:LEU:HA	1.73	0.41
5:E:237:ILE:HD12	5:E:237:ILE:HA	1.95	0.41
8:H:232:ASN:OD1	8:H:233:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:29:LYS:NZ	12:L:127:SER:O	2.54	0.41
1:O:200:THR:HG22	1:O:202:ASP:H	1.85	0.41
2:P:86:LEU:HA	2:P:86:LEU:HD12	1.76	0.41
3:Q:69:ASP:OD1	3:Q:70:LYS:N	2.48	0.41
3:Q:117:ILE:HD12	3:Q:117:ILE:HA	1.89	0.41
3:Q:159:TRP:CG	3:Q:162:THR:HG1	2.39	0.41
11:Y:43:LYS:HG2	11:Y:81:PHE:CD2	2.56	0.41
12:Z:176:VAL:HG13	12:Z:187:ILE:HB	2.02	0.41
15:d:172:ASP:OD1	15:d:172:ASP:N	2.29	0.41
15:e:51:LEU:HD23	15:e:52:VAL:HG13	2.03	0.41
5:E:185:GLU:O	5:E:186:ASN:ND2	2.54	0.41
10:J:40:LYS:HD2	10:J:40:LYS:HA	1.87	0.41
13:M:127:ARG:HD3	13:M:132:TYR:CE1	2.55	0.41
10:X:69:LEU:HD22	10:X:93:LEU:HD21	2.03	0.41
12:Z:8:PHE:HB3	12:Z:9:LYS:H	1.71	0.41
2:B:64:LYS:HE2	2:B:64:LYS:HB3	1.92	0.40
5:E:181:LEU:HA	5:E:184:GLN:HG3	2.04	0.40
11:K:13:VAL:HG23	11:K:113:TYR:HB3	2.03	0.40
12:L:201:THR:HG22	12:L:202:ASN:H	1.85	0.40
3:Q:6:ASP:OD1	3:Q:7:SER:N	2.54	0.40
3:Q:204:ILE:HD11	3:Q:235:LEU:HG	2.02	0.40
10:X:140:ILE:HD12	10:X:140:ILE:HA	1.94	0.40
5:E:238:SER:HA	5:E:241:ILE:HG12	2.03	0.40
10:J:51:VAL:HG13	10:J:86:VAL:HG13	2.03	0.40
11:K:2:ASP:OD1	11:K:35:LYS:NZ	2.46	0.40
11:K:102:CYS:HB2	11:K:118:CYS:HB2	2.04	0.40
13:M:192:ASN:OD1	13:M:192:ASN:N	2.53	0.40
3:Q:63:GLU:H	3:Q:63:GLU:HG2	1.72	0.40
3:Q:204:ILE:HD12	3:Q:205:PRO:HD2	2.03	0.40
6:T:54:SER:OG	6:T:55:LYS:N	2.53	0.40
7:U:215:LEU:HD23	7:U:215:LEU:HA	1.94	0.40
15:h:161:LEU:HD13	15:i:249:ASN:HB2	2.03	0.40
15:i:187:GLU:OE1	15:i:190:ARG:NH2	2.54	0.40
2:B:68:ILE:HD11	2:B:74:ILE:HG21	2.03	0.40
6:F:41:LYS:HA	6:F:41:LYS:HD3	1.82	0.40
7:G:36:THR:HA	7:G:169:GLY:HA3	2.03	0.40
13:M:56:ARG:NE	13:M:217:GLY:HA2	2.37	0.40
13:M:85:MET:HG3	13:M:88:ASP:H	1.86	0.40
1:O:77:ASN:N	1:O:77:ASN:OD1	2.51	0.40
6:T:65:LYS:NZ	6:T:67:ASP:O	2.45	0.40
6:T:195:LYS:HA	6:T:198:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:42:LEU:HG	12:Z:179:ILE:HD11	2.03	0.40
14:b:17:TYR:CE2	14:b:19:HIS:HB2	2.56	0.40
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.91	0.40
3:C:242:LYS:HA	3:C:242:LYS:HD3	1.79	0.40
9:I:26:VAL:N	13:a:212:ARG:O	2.52	0.40
9:I:40:ASN:HB2	9:I:103:VAL:HG23	2.02	0.40
10:J:58:LEU:HG	10:J:60:THR:HG22	2.04	0.40
12:L:5:ALA:HB1	12:L:111:MET:SD	2.61	0.40
1:O:129:GLN:HE22	1:O:133:GLN:NE2	2.20	0.40
2:P:135:LEU:HD23	2:P:135:LEU:HA	1.85	0.40
11:Y:59:GLU:O	11:Y:63:LYS:HG2	2.22	0.40
12:Z:37:ILE:HG21	12:Z:59:LEU:HD23	2.04	0.40
13:a:30:TRP:CE2	14:b:108:PRO:HG3	2.56	0.40
13:a:96:LEU:HD22	13:a:120:LEU:HD11	2.03	0.40
8:H:216:TYR:HD1	8:H:216:TYR:HA	1.80	0.40
9:I:77:SER:HA	9:I:80:VAL:HG12	2.03	0.40
10:J:90:ALA:O	10:J:137:TYR:OH	2.31	0.40
14:N:45:LYS:HG3	14:N:51:VAL:HG12	2.04	0.40
14:N:184:PHE:HZ	8:V:25:PHE:HE1	1.70	0.40
1:O:249:ILE:HD13	1:O:249:ILE:HA	1.94	0.40
2:P:79:MET:HE1	2:P:128:ARG:HH12	1.87	0.40
5:S:82:MET:HE3	5:S:82:MET:HB3	1.99	0.40
5:S:84:ASP:OD2	5:S:137:ARG:NH1	2.50	0.40
6:T:88:MET:HG2	6:T:108:LEU:HD11	2.04	0.40
13:a:120:LEU:HA	13:a:120:LEU:HD23	1.90	0.40
13:a:125:TYR:CE1	13:a:128:ARG:HG3	2.57	0.40
14:b:21:ILE:HD12	14:b:161:ILE:HD11	2.03	0.40
15:h:252:ILE:HD13	15:h:252:ILE:HA	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/260 (92%)	214 (89%)	26 (11%)	0	100	100
1	O	240/260 (92%)	211 (88%)	29 (12%)	0	100	100
2	B	222/235 (94%)	203 (91%)	19 (9%)	0	100	100
2	P	227/235 (97%)	205 (90%)	22 (10%)	0	100	100
3	C	238/246 (97%)	217 (91%)	20 (8%)	1 (0%)	30	64
3	Q	243/246 (99%)	218 (90%)	24 (10%)	1 (0%)	30	64
4	D	225/241 (93%)	200 (89%)	25 (11%)	0	100	100
4	R	231/241 (96%)	211 (91%)	20 (9%)	0	100	100
5	E	223/256 (87%)	197 (88%)	26 (12%)	0	100	100
5	S	224/256 (88%)	200 (89%)	24 (11%)	0	100	100
6	F	233/254 (92%)	195 (84%)	37 (16%)	1 (0%)	30	64
6	T	232/254 (91%)	204 (88%)	27 (12%)	1 (0%)	30	64
7	G	229/252 (91%)	189 (82%)	37 (16%)	3 (1%)	9	40
7	U	229/252 (91%)	197 (86%)	29 (13%)	3 (1%)	9	40
8	H	190/252 (75%)	159 (84%)	29 (15%)	2 (1%)	11	43
8	V	190/252 (75%)	162 (85%)	28 (15%)	0	100	100
9	I	217/229 (95%)	175 (81%)	42 (19%)	0	100	100
9	W	217/229 (95%)	190 (88%)	26 (12%)	1 (0%)	24	59
10	J	199/218 (91%)	175 (88%)	24 (12%)	0	100	100
10	X	199/218 (91%)	176 (88%)	23 (12%)	0	100	100
11	K	193/195 (99%)	171 (89%)	22 (11%)	0	100	100
11	Y	193/195 (99%)	168 (87%)	25 (13%)	0	100	100
12	L	202/211 (96%)	166 (82%)	36 (18%)	0	100	100
12	Z	202/211 (96%)	171 (85%)	31 (15%)	0	100	100
13	M	209/240 (87%)	184 (88%)	25 (12%)	0	100	100
13	a	209/240 (87%)	178 (85%)	31 (15%)	0	100	100
14	N	220/265 (83%)	189 (86%)	31 (14%)	0	100	100
14	b	220/265 (83%)	192 (87%)	28 (13%)	0	100	100
15	c	184/279 (66%)	178 (97%)	6 (3%)	0	100	100
15	d	186/279 (67%)	180 (97%)	6 (3%)	0	100	100
15	e	183/279 (66%)	177 (97%)	6 (3%)	0	100	100
15	f	186/279 (67%)	179 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	g	186/279 (67%)	180 (97%)	6 (3%)	0	100	100
15	h	186/279 (67%)	179 (96%)	7 (4%)	0	100	100
15	i	186/279 (67%)	180 (97%)	6 (3%)	0	100	100
All	All	7393/8661 (85%)	6570 (89%)	810 (11%)	13 (0%)	44	74

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	233	HIS
8	H	178	ASP
6	T	199	SER
6	F	204	LEU
7	G	232	ILE
7	U	233	HIS
3	C	210	ILE
8	H	179	PHE
3	Q	210	ILE
7	U	232	ILE
7	G	187	ILE
7	U	187	ILE
9	W	24	PRO

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	215/231 (93%)	213 (99%)	2 (1%)	70	75
1	O	215/231 (93%)	213 (99%)	2 (1%)	70	75
2	B	196/205 (96%)	195 (100%)	1 (0%)	81	82
2	P	201/205 (98%)	201 (100%)	0	100	100
3	C	208/213 (98%)	206 (99%)	2 (1%)	68	75
3	Q	212/213 (100%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	194/207 (94%)	192 (99%)	2 (1%)	68	75
4	R	199/207 (96%)	197 (99%)	2 (1%)	68	75
5	E	195/223 (87%)	194 (100%)	1 (0%)	81	82
5	S	196/223 (88%)	196 (100%)	0	100	100
6	F	210/227 (92%)	209 (100%)	1 (0%)	81	82
6	T	209/227 (92%)	209 (100%)	0	100	100
7	G	212/229 (93%)	207 (98%)	5 (2%)	43	63
7	U	212/229 (93%)	212 (100%)	0	100	100
8	H	174/231 (75%)	174 (100%)	0	100	100
8	V	174/231 (75%)	173 (99%)	1 (1%)	78	80
9	I	185/194 (95%)	181 (98%)	4 (2%)	45	64
9	W	185/194 (95%)	182 (98%)	3 (2%)	55	69
10	J	178/191 (93%)	176 (99%)	2 (1%)	65	74
10	X	178/191 (93%)	178 (100%)	0	100	100
11	K	174/174 (100%)	174 (100%)	0	100	100
11	Y	174/174 (100%)	174 (100%)	0	100	100
12	L	169/176 (96%)	168 (99%)	1 (1%)	78	80
12	Z	169/176 (96%)	169 (100%)	0	100	100
13	M	189/216 (88%)	187 (99%)	2 (1%)	65	74
13	a	189/216 (88%)	186 (98%)	3 (2%)	55	69
14	N	201/239 (84%)	198 (98%)	3 (2%)	57	70
14	b	201/239 (84%)	201 (100%)	0	100	100
15	c	175/261 (67%)	171 (98%)	4 (2%)	44	63
15	d	177/261 (68%)	177 (100%)	0	100	100
15	e	174/261 (67%)	170 (98%)	4 (2%)	44	63
15	f	177/261 (68%)	175 (99%)	2 (1%)	65	74
15	g	177/261 (68%)	175 (99%)	2 (1%)	65	74
15	h	177/261 (68%)	173 (98%)	4 (2%)	44	63
15	i	177/261 (68%)	177 (100%)	0	100	100
All	All	6648/7739 (86%)	6595 (99%)	53 (1%)	70	77

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
1	A	234	VAL
2	B	75	VAL
3	C	43	VAL
3	C	155	ASN
4	D	55	ASN
4	D	204	VAL
5	E	46	VAL
6	F	187	ILE
7	G	12	VAL
7	G	36	THR
7	G	107	THR
7	G	168	ILE
7	G	238	THR
9	I	12	VAL
9	I	165	ASN
9	I	173	VAL
9	I	174	ASP
10	J	168	VAL
10	J	179	THR
12	L	176	VAL
13	M	112	ASP
13	M	224	VAL
14	N	12	VAL
14	N	50	THR
14	N	227	VAL
1	O	15	ILE
1	O	234	VAL
4	R	55	ASN
4	R	59	THR
8	V	234	THR
9	W	95	VAL
9	W	173	VAL
9	W	200	PRO
13	a	91	THR
13	a	112	ASP
13	a	235	LEU
15	c	64	VAL
15	c	140	LEU
15	c	254	LEU
15	c	258	LEU
15	e	37	LEU
15	e	142	LEU

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Mol	Chain	Res	Type
15	e	165	LEU
15	e	175	ASN
15	f	188	LEU
15	f	235	LYS
15	g	152	LEU
15	g	258	LEU
15	h	53	ASN
15	h	166	ASN
15	h	188	LEU
15	h	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	133	GLN
1	A	153	ASN
1	A	251	ASN
2	B	21	GLN
3	C	29	ASN
3	C	146	GLN
3	C	149	HIS
3	C	168	ASN
4	D	15	HIS
4	D	21	HIS
4	D	69	ASN
4	D	159	GLN
4	D	223	ASN
5	E	23	GLN
5	E	98	HIS
5	E	164	ASN
5	E	186	ASN
5	E	206	GLN
6	F	121	GLN
7	G	54	ASN
7	G	104	ASN
7	G	130	HIS
7	G	157	ASN
7	G	171	ASN
8	H	163	GLN
8	H	219	HIS
8	H	220	ASN

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Mol	Chain	Res	Type
8	H	222	ASN
10	J	171	GLN
10	J	182	GLN
11	K	69	GLN
11	K	88	ASN
11	K	101	ASN
11	K	150	ASN
11	K	177	ASN
11	K	186	ASN
12	L	29	GLN
12	L	89	GLN
12	L	162	HIS
12	L	180	HIS
12	L	202	ASN
13	M	171	GLN
13	M	183	GLN
13	M	185	ASN
14	N	19	HIS
14	N	38	GLN
14	N	65	HIS
14	N	72	ASN
14	N	75	ASN
14	N	92	HIS
14	N	125	ASN
14	N	126	ASN
1	O	24	GLN
1	O	133	GLN
1	O	153	ASN
1	O	179	GLN
2	P	21	GLN
2	P	71	HIS
2	P	100	GLN
2	P	170	ASN
2	P	189	HIS
2	P	216	ASN
3	Q	89	GLN
3	Q	146	GLN
3	Q	217	ASN
4	R	77	ASN
4	R	146	GLN
4	R	179	ASN
5	S	23	GLN

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Mol	Chain	Res	Type
5	S	43	ASN
5	S	97	ASN
5	S	195	GLN
5	S	206	GLN
6	T	60	GLN
6	T	95	HIS
6	T	121	GLN
6	T	217	ASN
7	U	64	ASN
7	U	89	ASN
7	U	104	ASN
7	U	157	ASN
7	U	213	GLN
7	U	217	ASN
8	V	163	GLN
8	V	168	ASN
8	V	208	ASN
8	V	219	HIS
8	V	220	ASN
8	V	232	ASN
9	W	35	HIS
9	W	69	ASN
9	W	71	ASN
9	W	85	GLN
9	W	172	ASN
9	W	193	ASN
10	X	80	GLN
10	X	158	GLN
11	Y	56	GLN
11	Y	73	ASN
11	Y	88	ASN
11	Y	101	ASN
11	Y	123	ASN
11	Y	186	ASN
12	Z	29	GLN
12	Z	110	ASN
12	Z	158	ASN
12	Z	178	HIS
12	Z	180	HIS
13	a	93	HIS
13	a	183	GLN
13	a	186	GLN

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Mol	Chain	Res	Type
14	b	38	GLN
14	b	62	GLN
14	b	112	ASN
15	c	32	GLN
15	c	158	ASN
15	c	164	GLN
15	c	175	ASN
15	d	55	ASN
15	d	158	ASN
15	d	164	GLN
15	d	166	ASN
15	d	174	ASN
15	e	16	GLN
15	e	23	ASN
15	e	32	GLN
15	e	49	ASN
15	e	261	ASN
15	f	23	ASN
15	f	65	ASN
15	f	197	ASN
15	f	239	HIS
15	g	49	ASN
15	g	50	ASN
15	g	53	ASN
15	g	63	ASN
15	g	65	ASN
15	g	158	ASN
15	g	186	GLN
15	g	250	ASN
15	h	32	GLN
15	h	166	ASN
15	h	250	ASN
15	i	50	ASN
15	i	164	GLN

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.

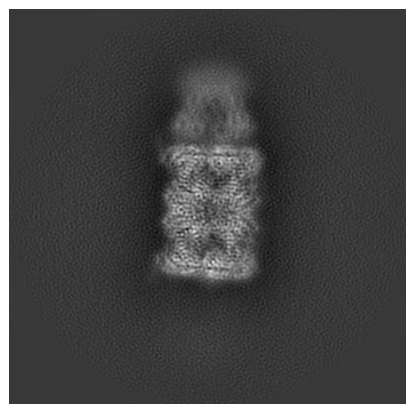
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9259. These allow visual inspection of the internal detail of the map and identification of artifacts.

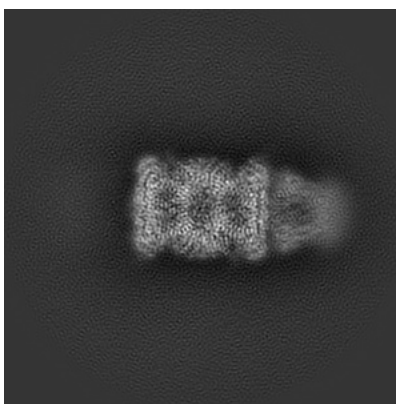
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

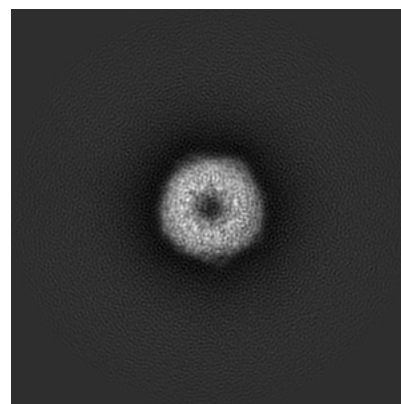
6.1.1 Primary map



X

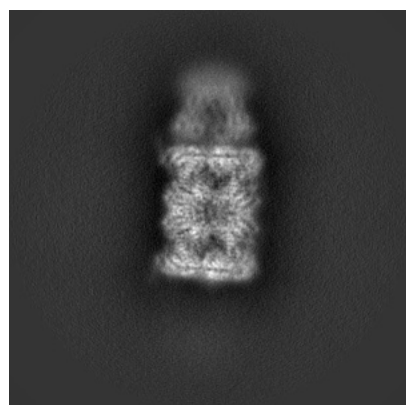


Y

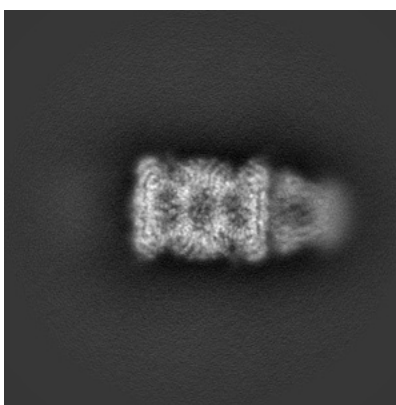


Z

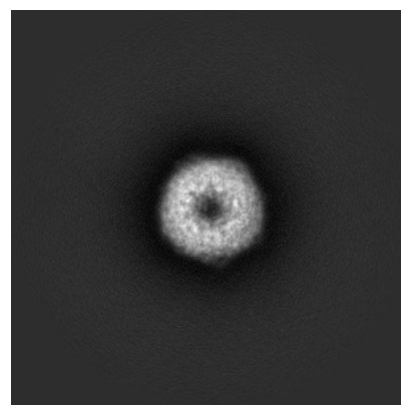
6.1.2 Raw map



X



Y



Z

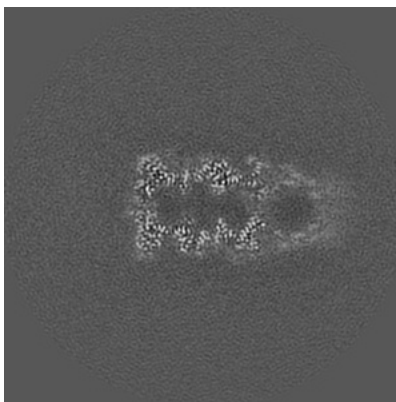
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

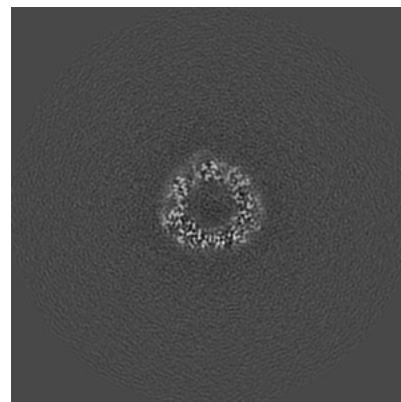
6.2.1 Primary map



X Index: 172

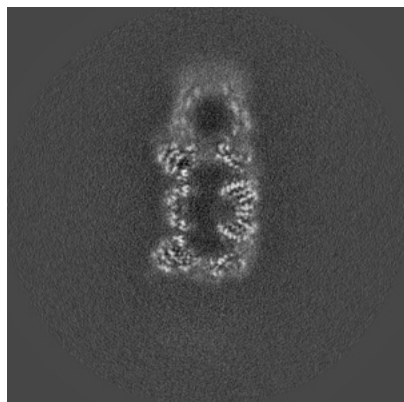


Y Index: 172

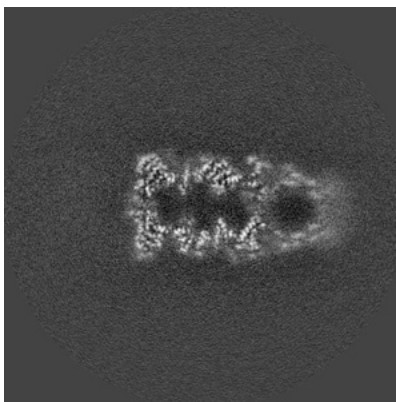


Z Index: 172

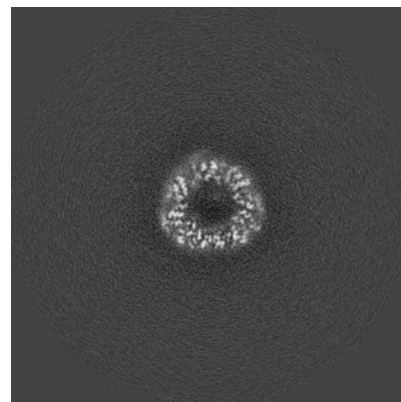
6.2.2 Raw map



X Index: 172



Y Index: 172

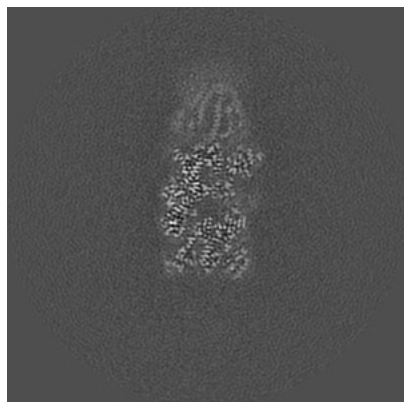


Z Index: 172

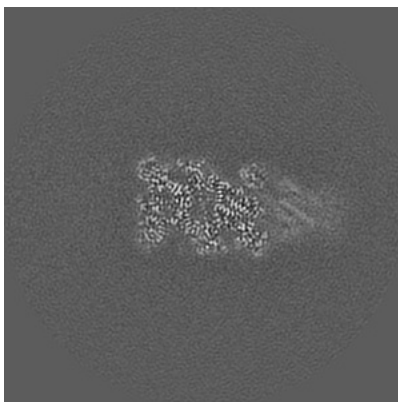
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

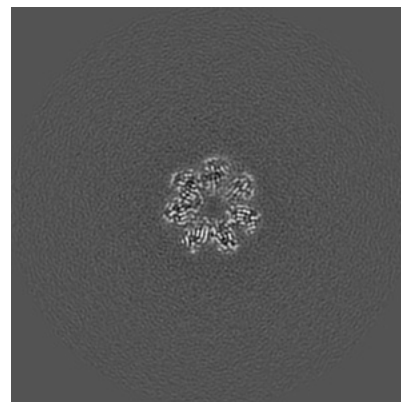
6.3.1 Primary map



X Index: 154

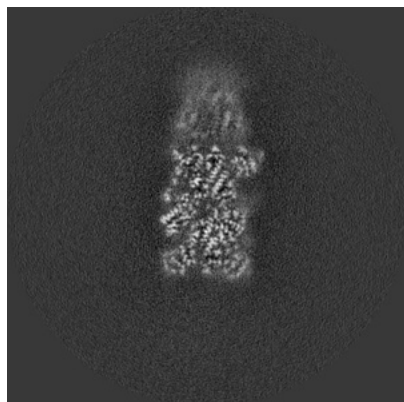


Y Index: 152

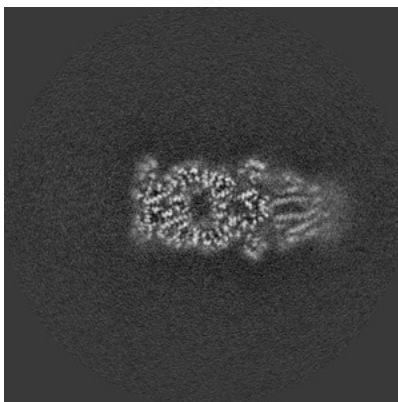


Z Index: 156

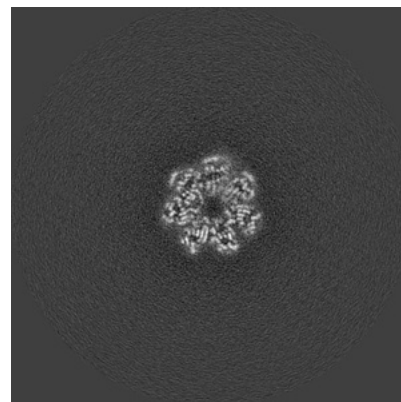
6.3.2 Raw map



X Index: 151



Y Index: 190

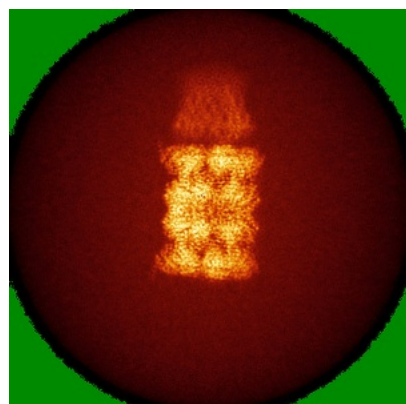


Z Index: 156

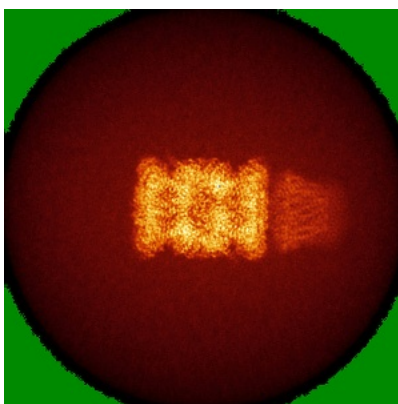
The images above show the largest variance slices of the map in three orthogonal directions.

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

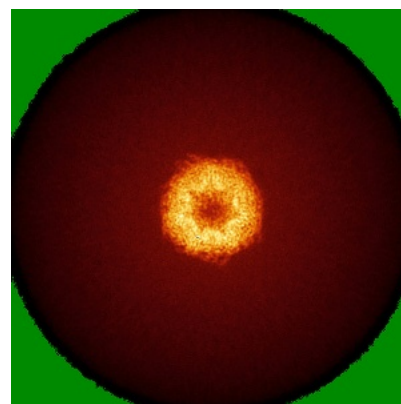
6.4.1 Primary map



X

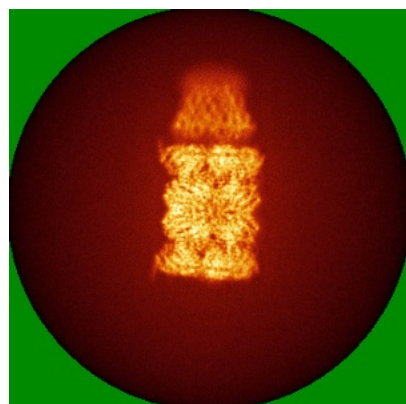


Y

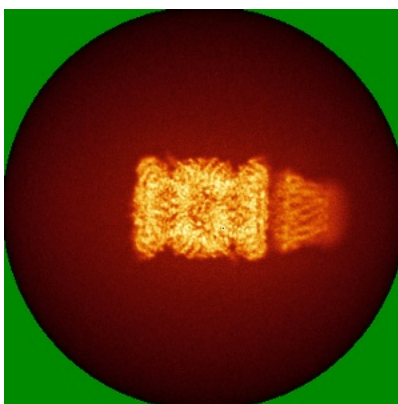


Z

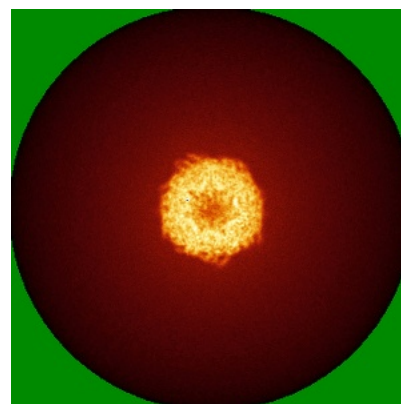
6.4.2 Raw map



X



Y

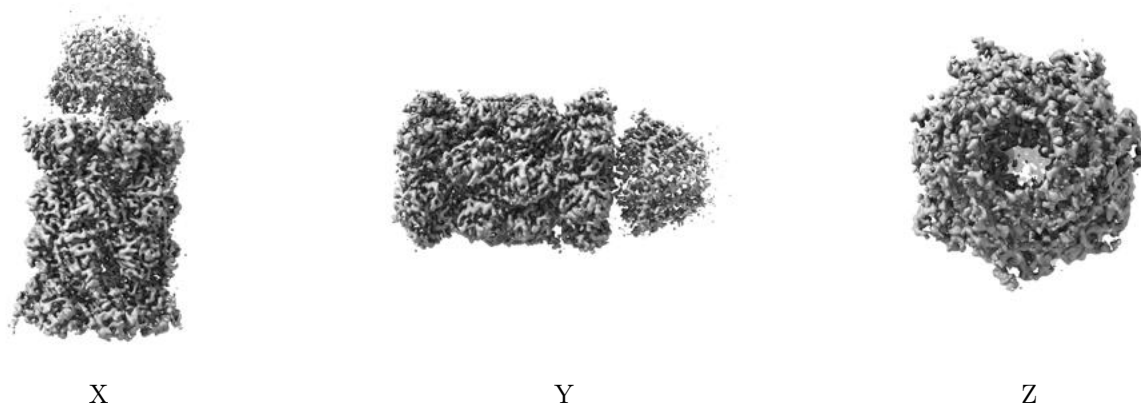


Z

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.

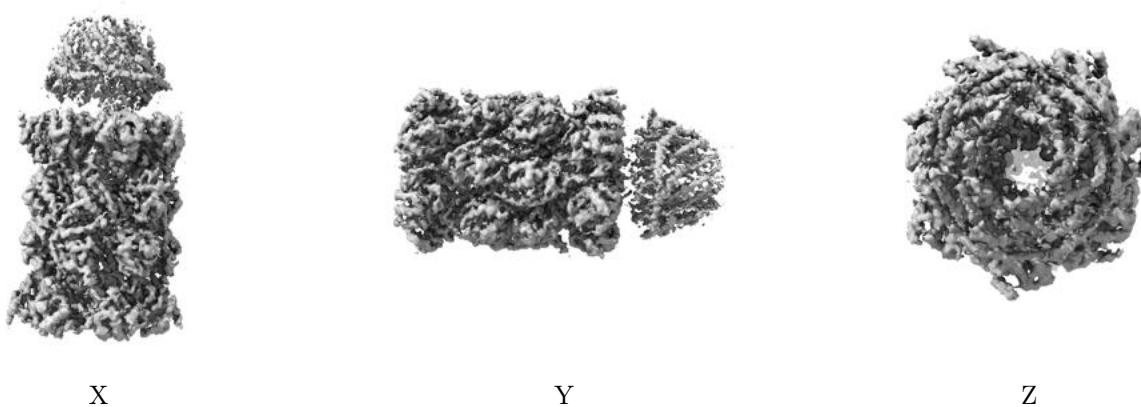
6.5 Orthogonal surface views [i](#)

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.

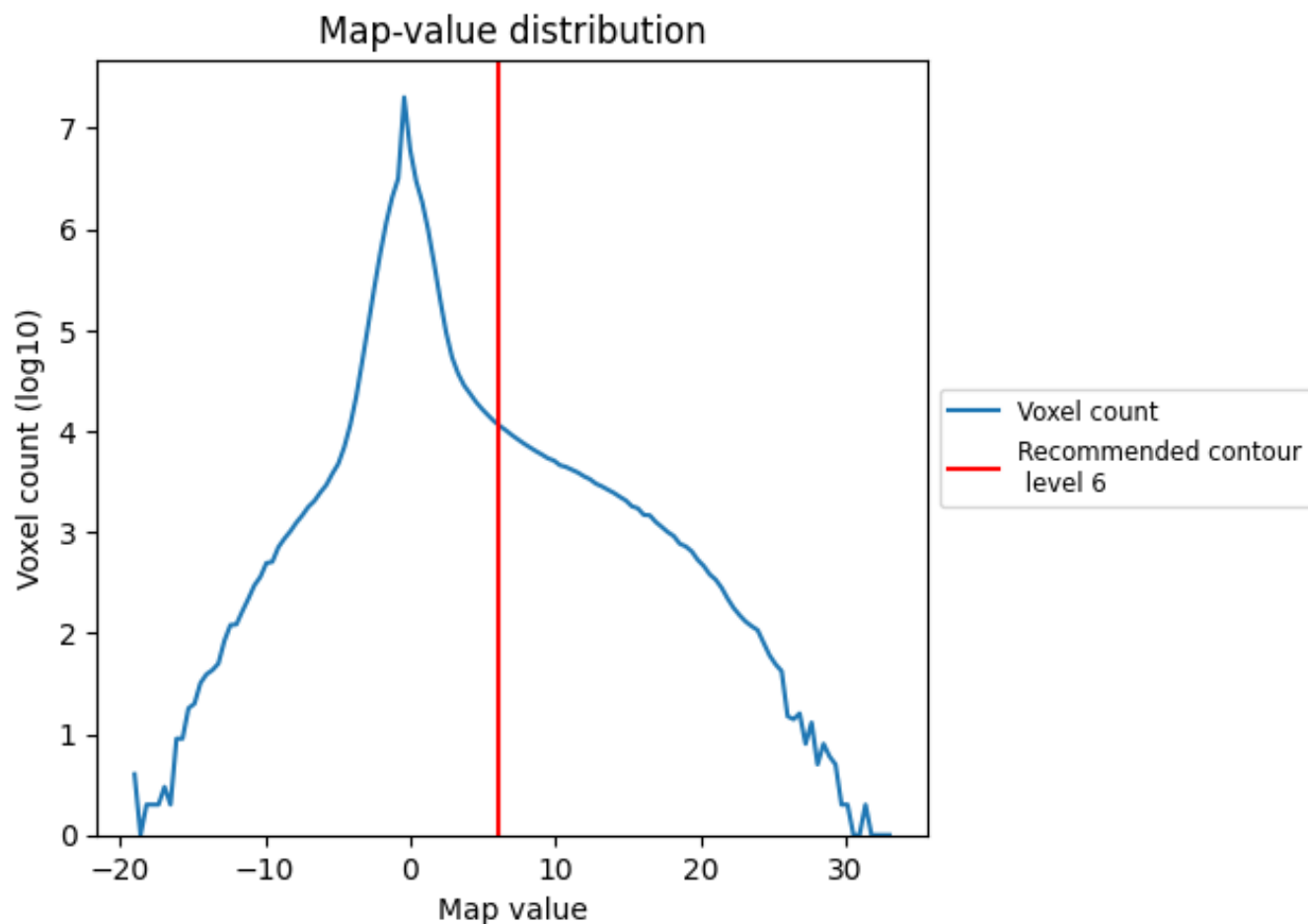
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

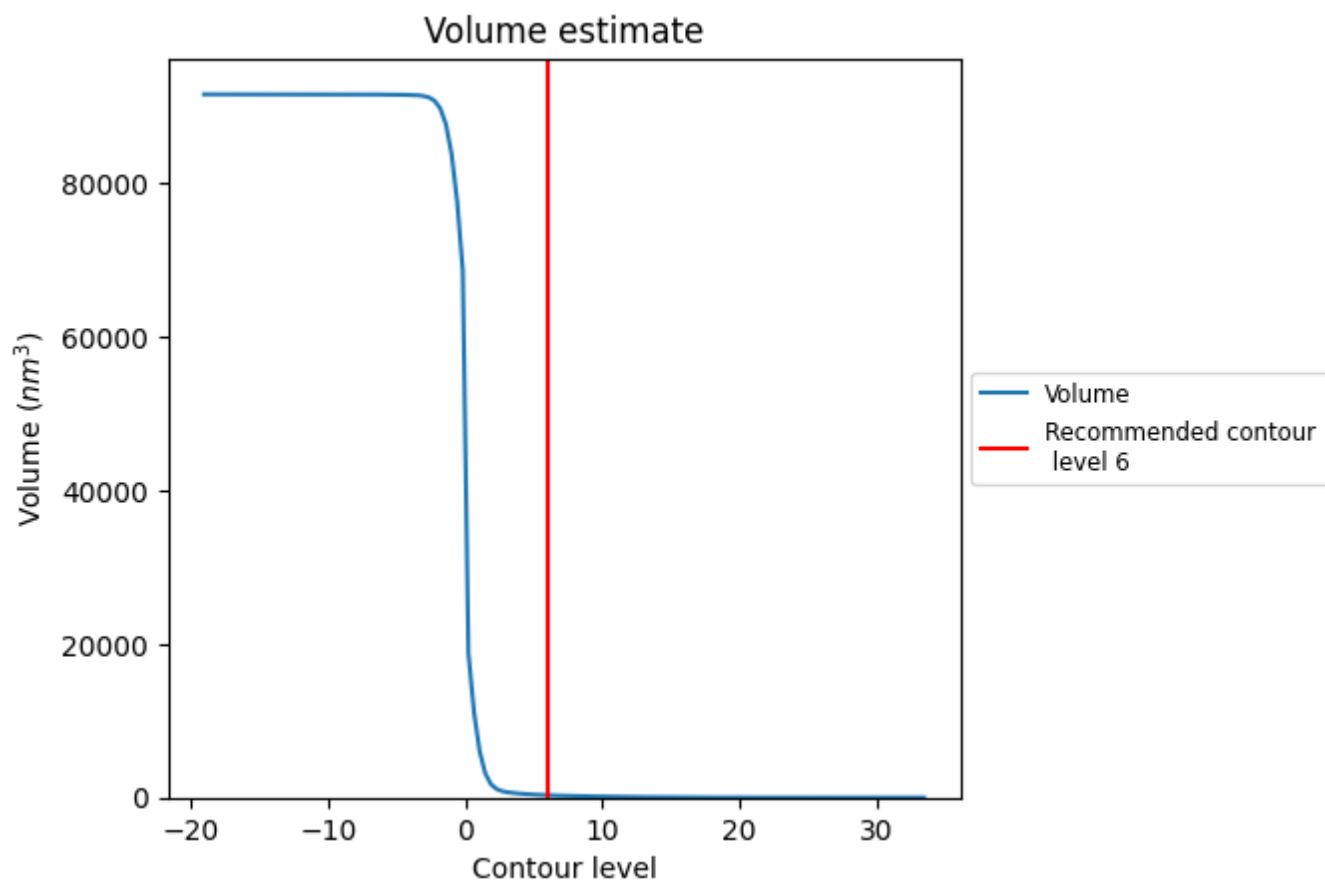
This section contains the results of statistical analysis of the map.

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.

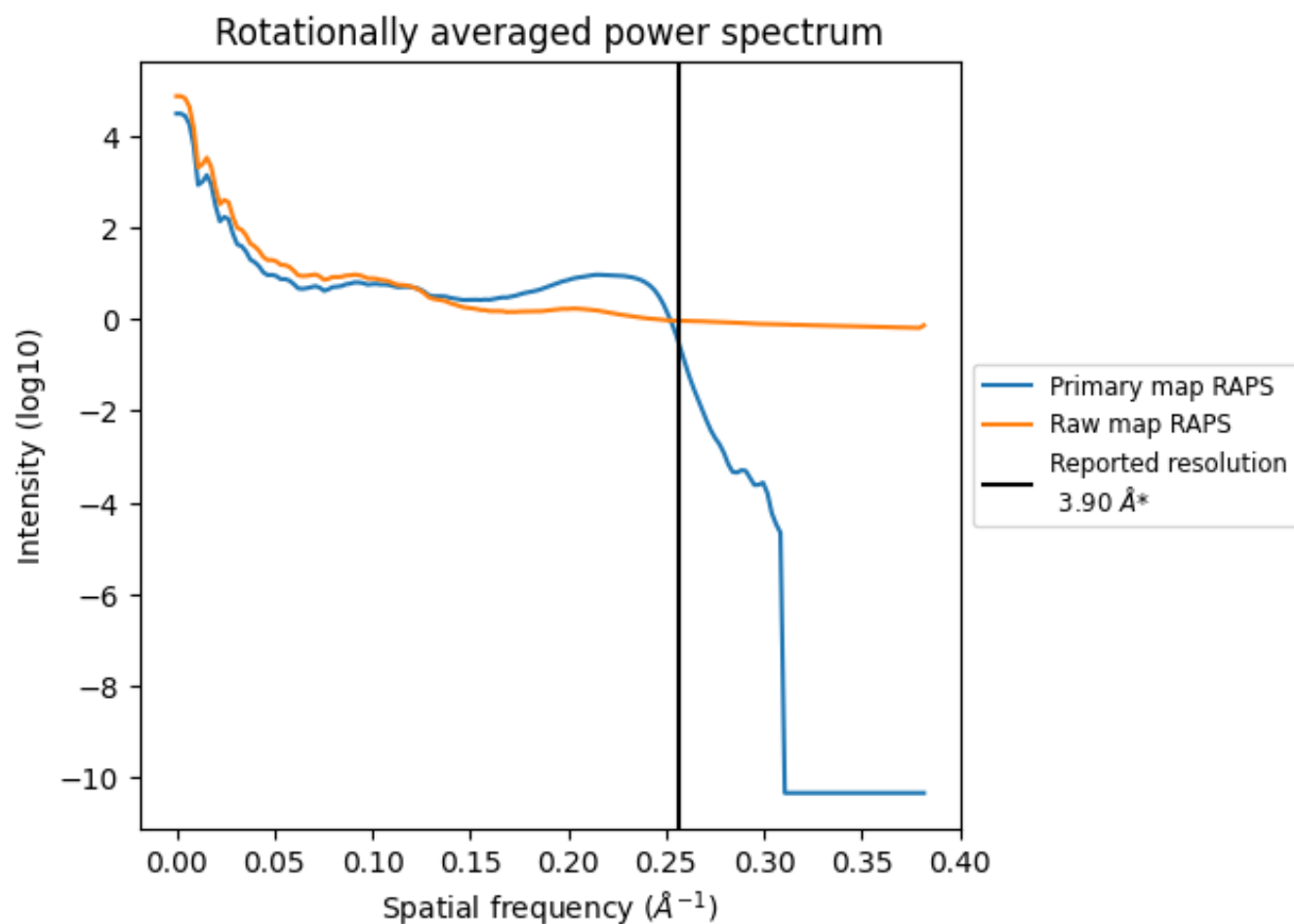
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm³; this corresponds to an approximate mass of 277 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 ⓘ

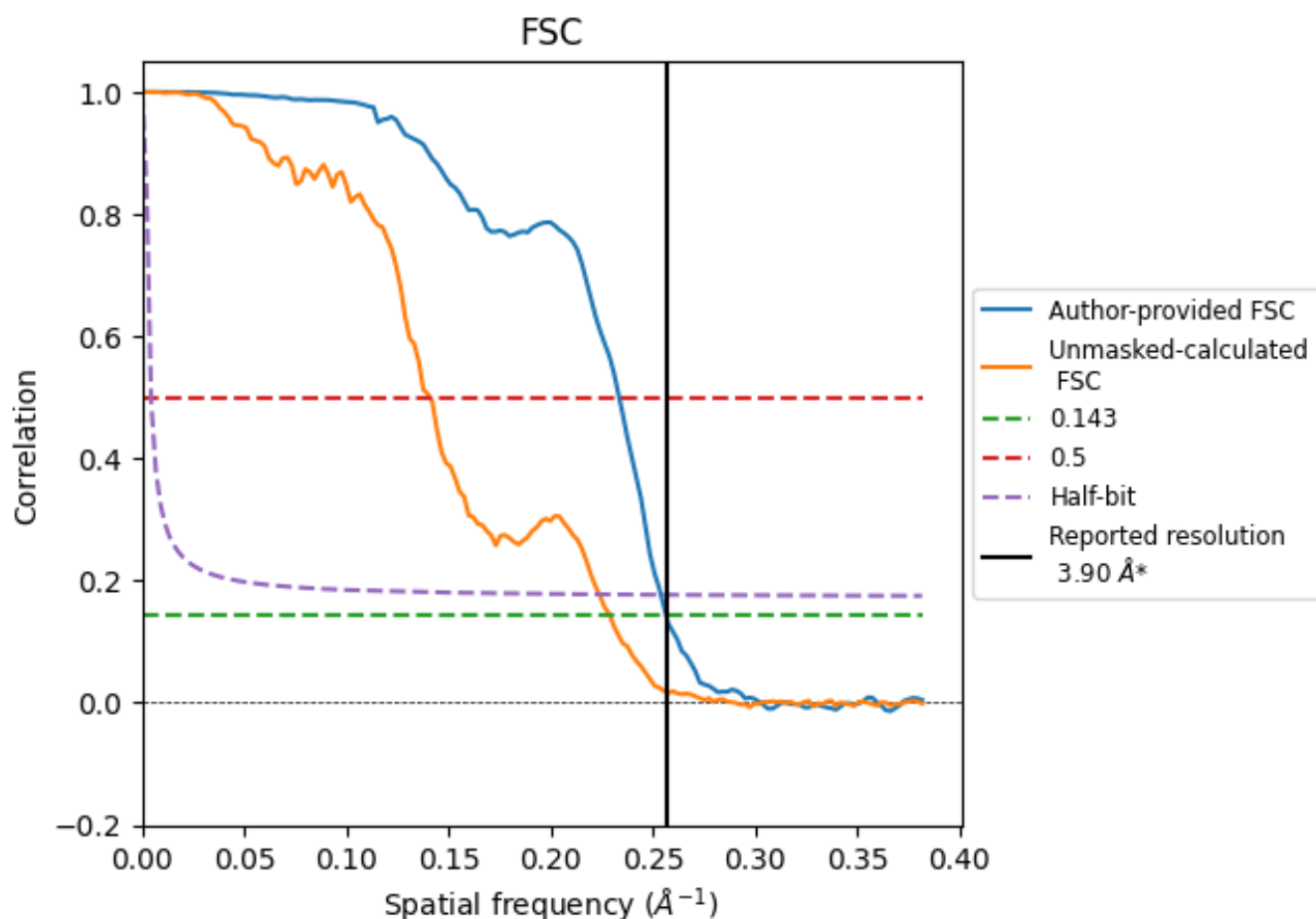


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

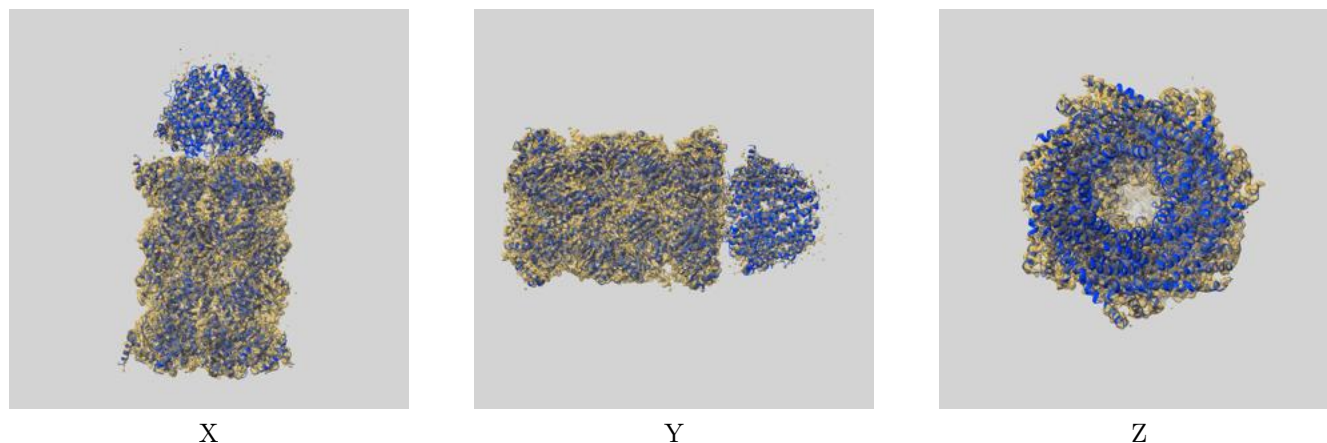
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.90	4.28	3.94
Unmasked-calculated*	4.37	7.11	4.47

*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 4.37 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

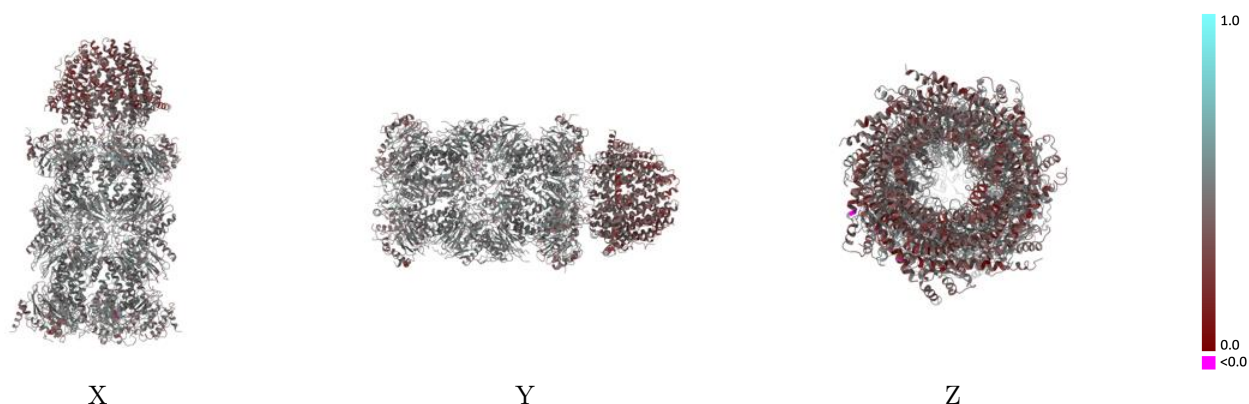
This section contains information regarding the fit between EMDB map EMD-9259 and PDB model 6MUX. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



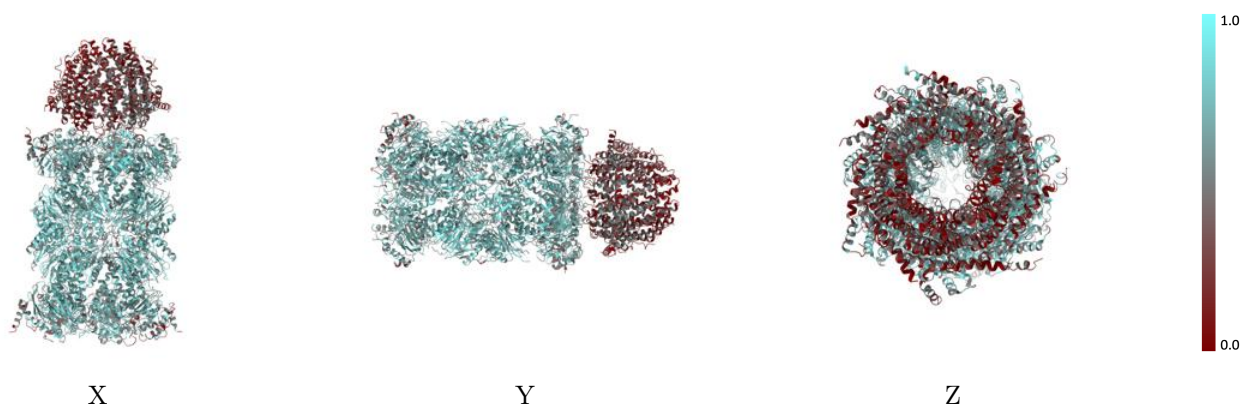
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



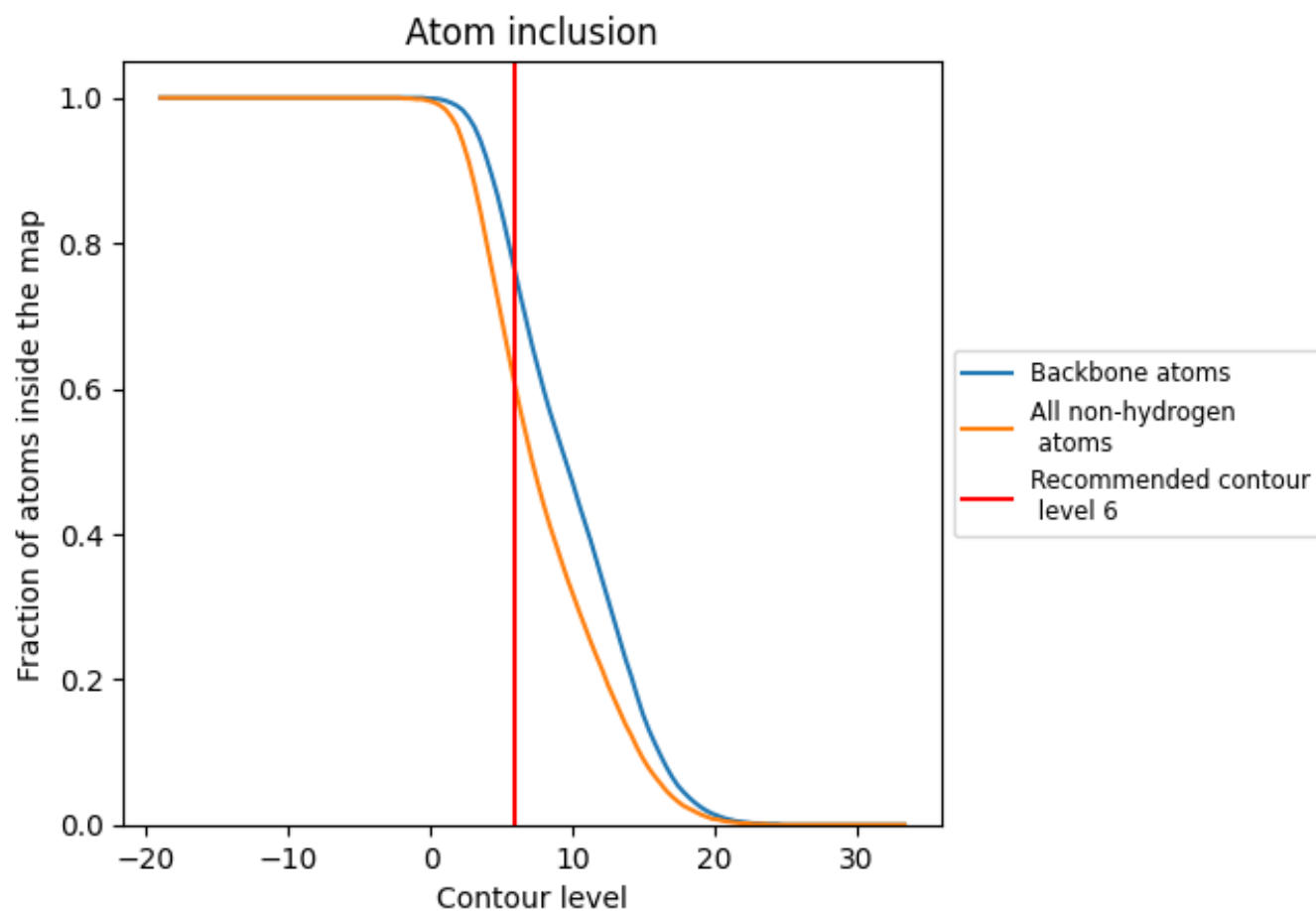
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 76% of all backbone atoms, 60% 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	 0.6020	 0.4390
A	 0.6440	 0.4620
B	 0.6640	 0.4590
C	 0.6660	 0.4550
D	 0.6240	 0.4530
E	 0.6050	 0.4530
F	 0.6620	 0.4540
G	 0.6960	 0.4640
H	 0.6900	 0.4470
I	 0.6730	 0.4500
J	 0.7520	 0.4800
K	 0.7720	 0.4800
L	 0.7520	 0.4750
M	 0.7210	 0.4800
N	 0.6820	 0.4760
O	 0.5940	 0.4450
P	 0.6340	 0.4550
Q	 0.6690	 0.4520
R	 0.6290	 0.4560
S	 0.6170	 0.4450
T	 0.6600	 0.4500
U	 0.6750	 0.4610
V	 0.6830	 0.4530
W	 0.6710	 0.4560
X	 0.7420	 0.4760
Y	 0.7590	 0.4770
Z	 0.7570	 0.4720
a	 0.7380	 0.4840
b	 0.6990	 0.4760
c	 0.3030	 0.3570
d	 0.2000	 0.3330
e	 0.1730	 0.3040
f	 0.2000	 0.3210
g	 0.2630	 0.3390
h	 0.3150	 0.3550
i	 0.3340	 0.3640

