



Full wwPDB EM Validation Report ⓘ

Mar 17, 2025 – 03:06 PM JST

PDB ID : 8W8M
EMDB ID : EMD-37355
Title : Cryo-EM structure of helical filament of MyD88 TIR
Authors : Kasai, K.; Imamura, K.; Narita, A.; Makino, F.; Miyata, T.; Kato, T.; Namba, K.; Onishi, H.; Tochio, H.
Deposited on : 2023-09-04
Resolution : 3.28 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

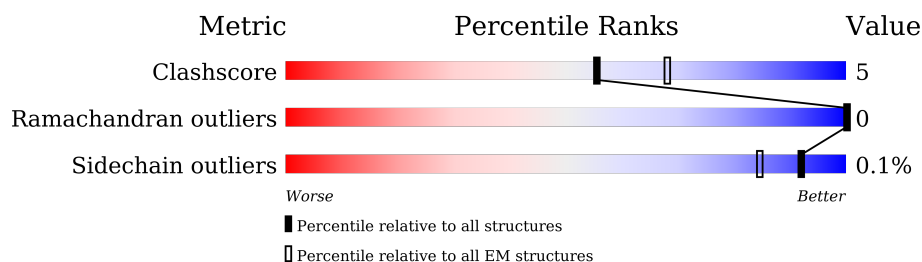
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

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 3.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1A	144	<div> <div>28%</div> <div>85%</div> <div>8%</div> <div>6%</div> </div>
1	1B	144	<div> <div>29%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	1C	144	<div> <div>27%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	1D	144	<div> <div>27%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	1E	144	<div> <div>28%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	1F	144	<div> <div>26%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	2A	144	<div> <div>29%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	2B	144	<div> <div>24%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	2C	144	<div> <div>28%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	2D	144	<div> <div>26%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	2E	144	<div> <div>24%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	2F	144	<div> <div>23%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	3A	144	<div> <div>23%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	3B	144	<div> <div>26%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	3C	144	<div> <div>26%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
1	3D	144	<div> <div>26%</div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
1	3E	144	<div> <div>27%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	3F	144	<div> <div>23%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	A1	144	<div> <div>32%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	A2	144	<div> <div>25%</div> <div>79%</div> <div>15%</div> <div>6%</div> </div>
1	A3	144	<div> <div>24%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	B1	144	<div> <div>31%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	B2	144	<div> <div>29%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	B3	144	<div> <div>24%</div> <div>80%</div> <div>13%</div> <div>6%</div> </div>
1	C1	144	<div> <div>31%</div> <div>85%</div> <div>8%</div> <div>6%</div> </div>
1	C2	144	<div> <div>28%</div> <div>79%</div> <div>15%</div> <div>6%</div> </div>
1	C3	144	<div> <div>23%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
1	D1	144	<div> <div>33%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	D2	144	<div> <div>28%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	D3	144	<div> <div>24%</div> <div>76%</div> <div>17%</div> <div>6%</div> </div>
1	E1	144	<div> <div>31%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	E2	144	<div> <div>31%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>
1	E3	144	<div> <div>24%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F1	144	<div> <div>32%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	F2	144	<div> <div>33%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
1	F3	144	<div> <div>24%</div> <div>78%</div> <div>16%</div> <div>6%</div> </div>
1	G1	144	<div> <div>29%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	G2	144	<div> <div>31%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	G3	144	<div> <div>26%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	H1	144	<div> <div>30%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	H2	144	<div> <div>31%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	H3	144	<div> <div>24%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	I1	144	<div> <div>30%</div> <div>74%</div> <div>20%</div> <div>6%</div> </div>
1	I2	144	<div> <div>32%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>
1	I3	144	<div> <div>21%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	J1	144	<div> <div>26%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	J2	144	<div> <div>28%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	J3	144	<div> <div>20%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	K1	144	<div> <div>24%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	K2	144	<div> <div>27%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
1	K3	144	<div> <div>16%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
1	L1	144	<div> <div>15%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	L2	144	<div> <div>26%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
1	L3	144	<div> <div>13%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
1	M1	144	<div> <div>14%</div> <div>77%</div> <div>17%</div> <div>6%</div> </div>
1	M2	144	<div> <div>13%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	M3	144	<div> <div>10%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	N1	144	<div> <div>12%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	N2	144	
1	N3	144	
1	O1	144	
1	O2	144	
1	O3	144	
1	P1	144	
1	P2	144	
1	P3	144	
1	Q1	144	
1	Q2	144	
1	Q3	144	
1	R1	144	
1	R2	144	
1	R3	144	
1	S1	144	
1	S2	144	
1	S3	144	
1	T1	144	
1	T2	144	
1	T3	144	
1	U1	144	
1	U2	144	
1	U3	144	
1	V1	144	
1	V2	144	

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Mol	Chain	Length	Quality of chain
1	V3	144	
1	W1	144	
1	W2	144	
1	W3	144	
1	X1	144	
1	X2	144	
1	X3	144	
1	Y1	144	
1	Y2	144	
1	Y3	144	
1	YD	144	
1	YE	144	
1	YF	144	
1	Z1	144	
1	Z2	144	
1	Z3	144	
1	ZD	144	
1	ZE	144	
1	ZF	144	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 113934 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 Myeloid differentiation primary response protein MyD88.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	D3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	E1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	E2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	E3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	F1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	F2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	F3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	D1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	A2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	A3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	B1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	B2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	B3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	C1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	C2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	C3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	J2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	J3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	K1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	K2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	K3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	L1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	L2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	L3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	J1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	G2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	G3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	H1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	H2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	H3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	I1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	I2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	I3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	G1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	M2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	M3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	N1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	N2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	N3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	O1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	O2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	O3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	M1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	P2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	P3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	Q1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	Q2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	Q3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	R1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	R2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	R3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	P1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	S2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	S3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	T1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	T2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	T3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	U1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	U2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	U3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	S1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	V2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	V3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	W1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	W2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	W3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	X1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	X2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	X3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	V1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	Y2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	Y3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	Z1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	Z2	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	Z3	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	1A	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	2A	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	3A	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y1	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	2B	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	3B	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	1C	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	2C	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	3C	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	1D	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	2D	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	3D	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	1B	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	ZD	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	YE	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	ZE	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	1E	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	YF	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	ZF	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	1F	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	YD	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	2E	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	3E	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		
1	2F	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		

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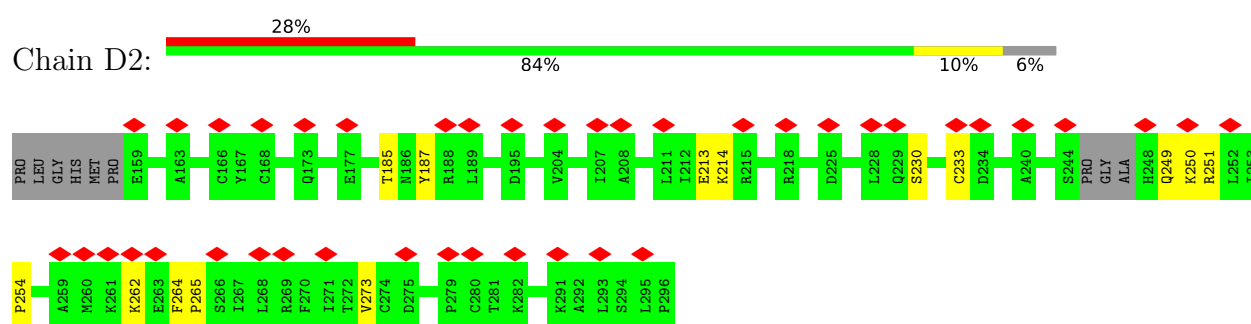
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3F	135	Total	C	N	O	S	0	0
			1117	719	190	197	11		

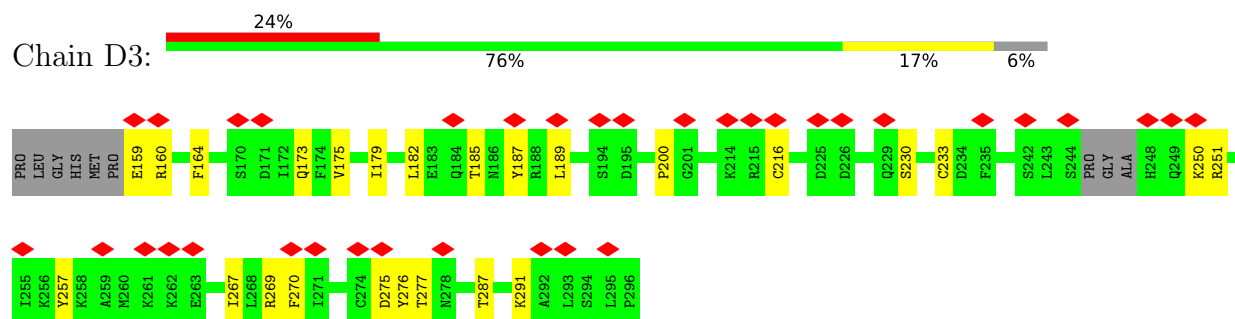
3 Residue-property plots

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.

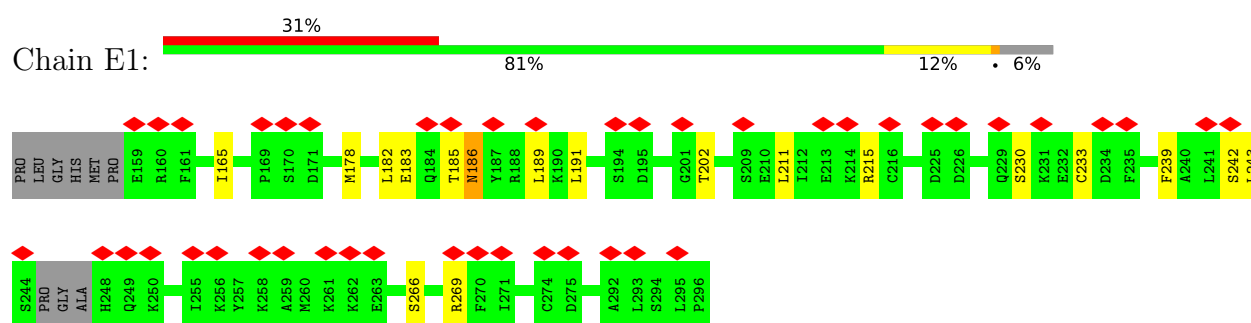
- Molecule 1: Myeloid differentiation primary response protein MyD88



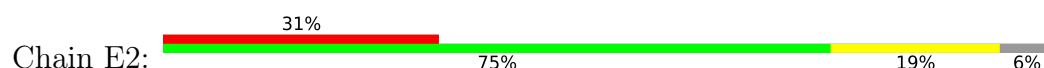
- Molecule 1: Myeloid differentiation primary response protein MyD88

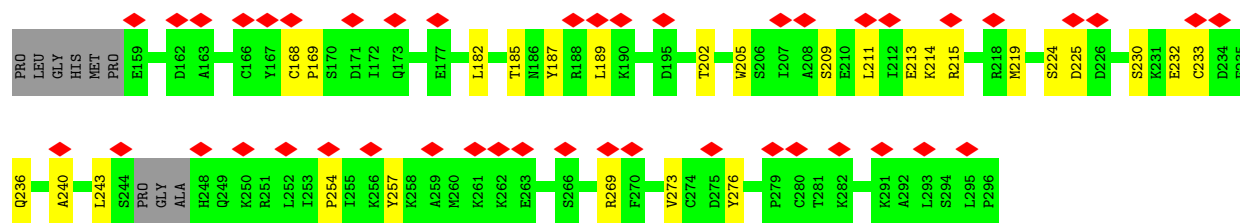


- Molecule 1: Myeloid differentiation primary response protein MyD88

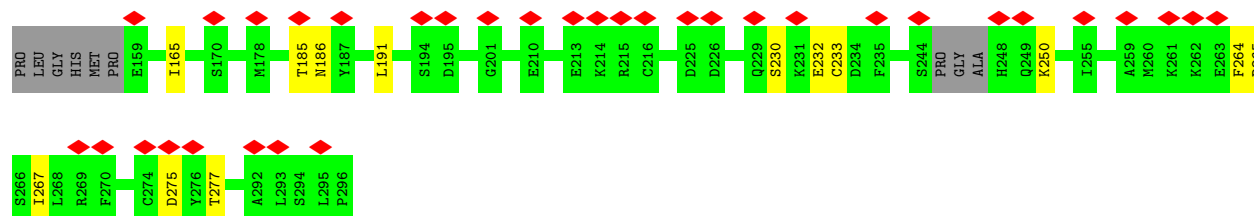
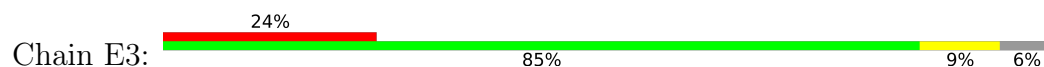


- Molecule 1: Myeloid differentiation primary response protein MyD88

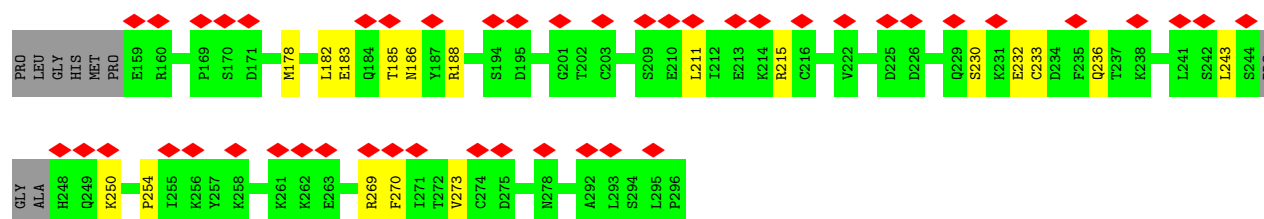
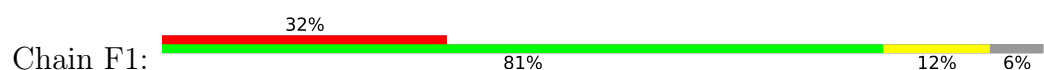




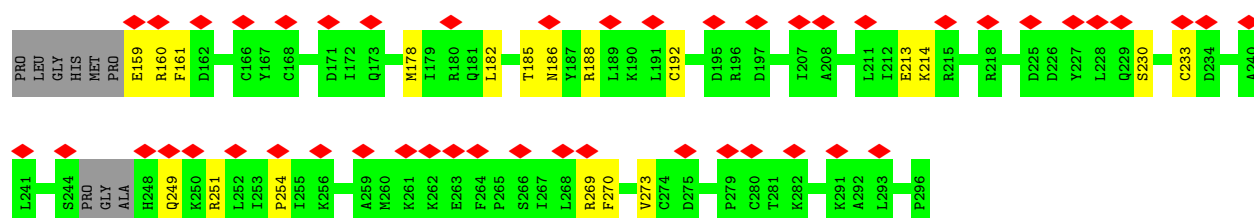
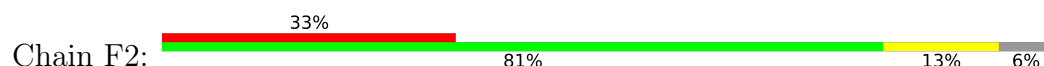
- Molecule 1: Myeloid differentiation primary response protein MyD88



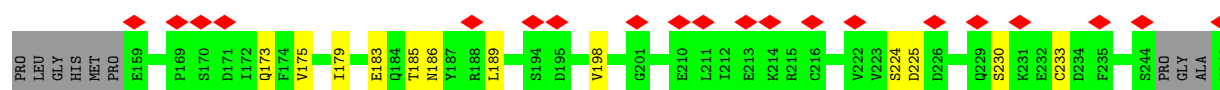
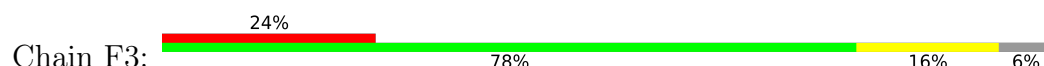
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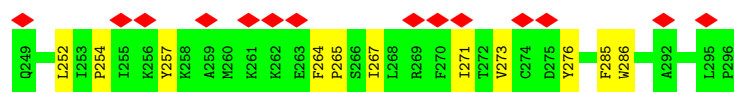


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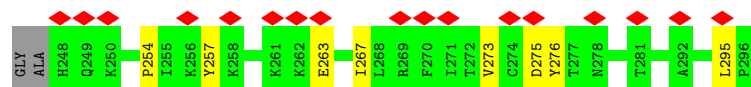
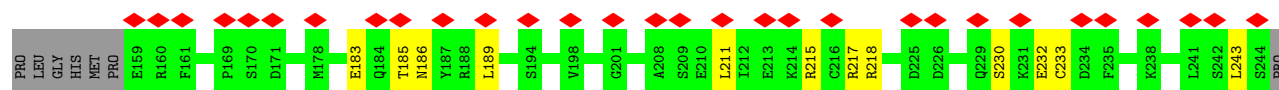
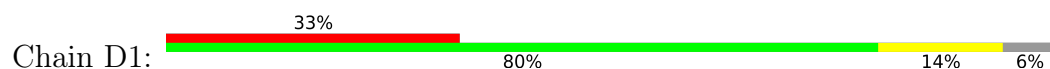


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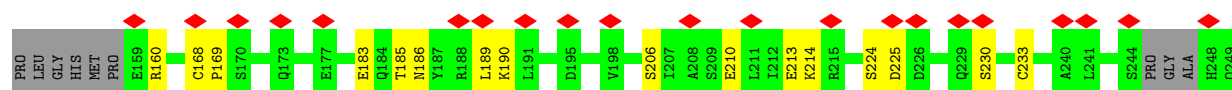
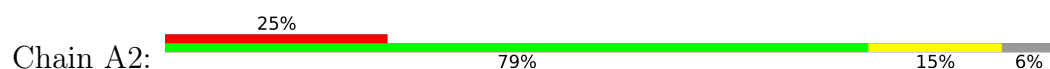




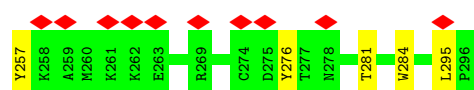
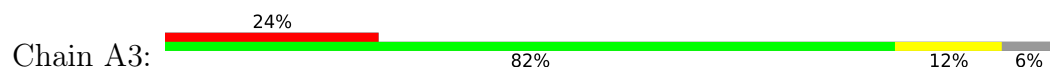
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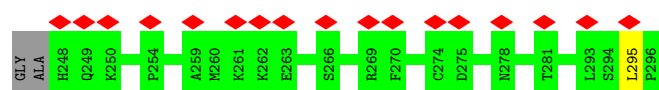
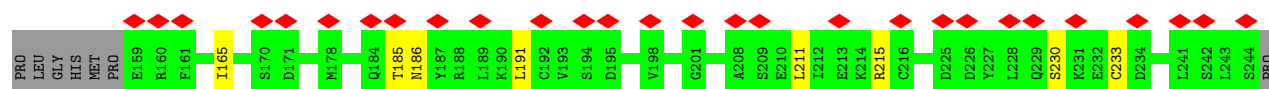
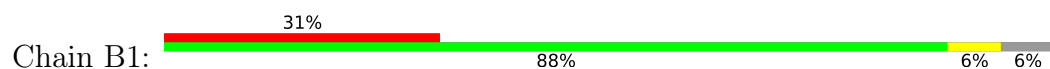
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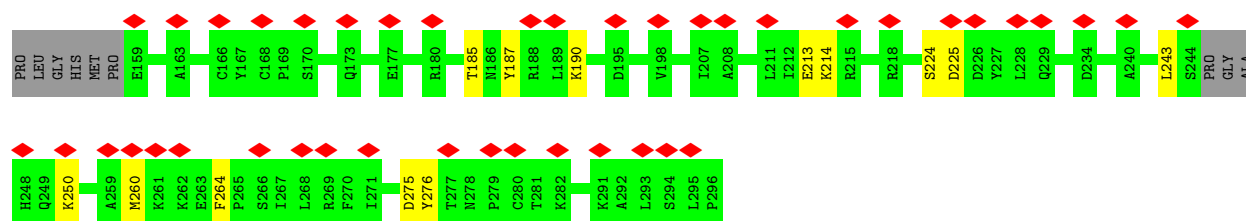


- Molecule 1: Myeloid differentiation primary response protein MyD88



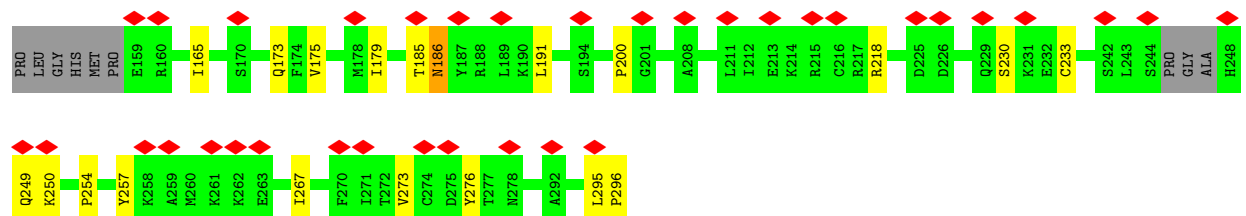
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain B2: 29% 85% 9% 6%



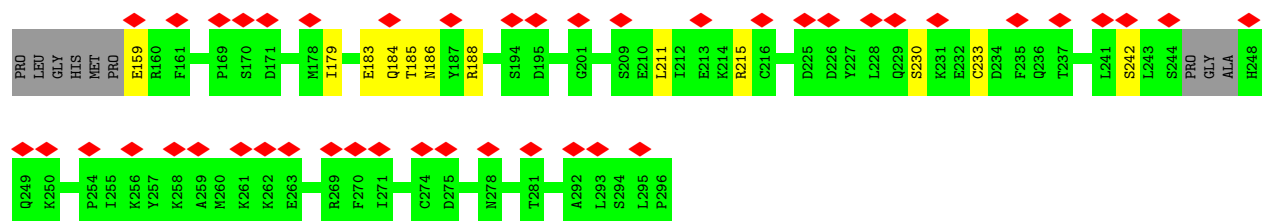
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain B3: 24% 80% 13% 6%



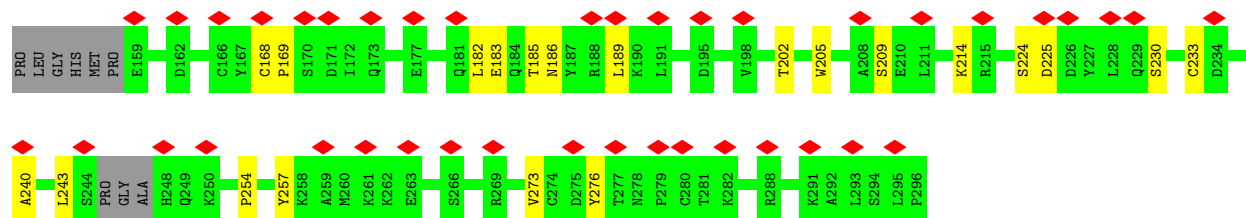
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain C1: 31% 85% 8% 6%



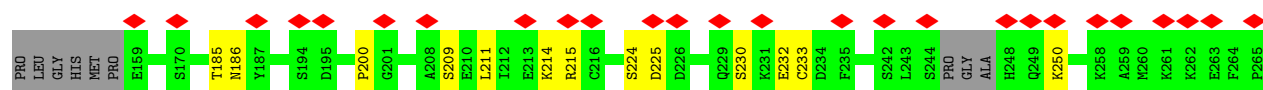
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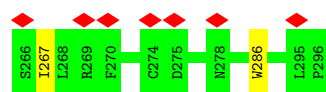
Chain C2: 28% 79% 15% 6%



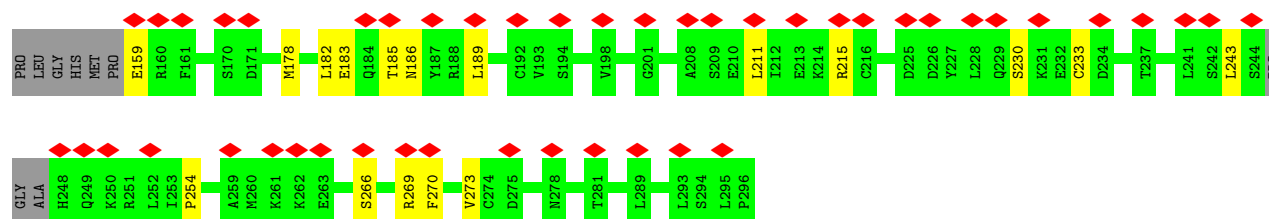
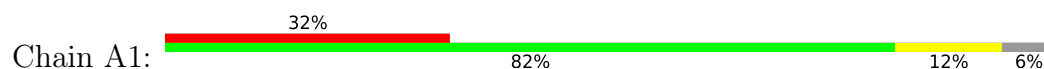
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain C3: 23% 83% 10% 6%

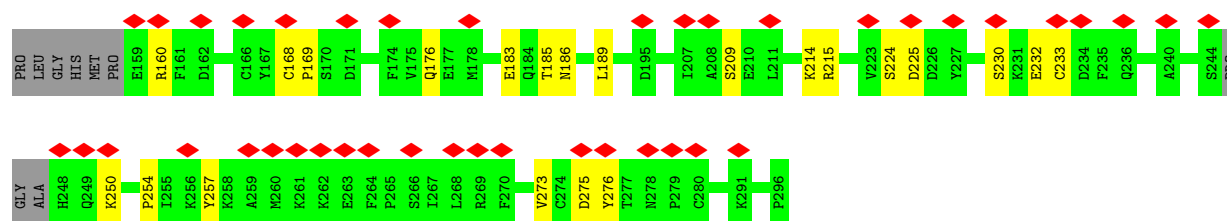
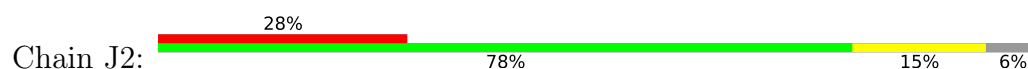




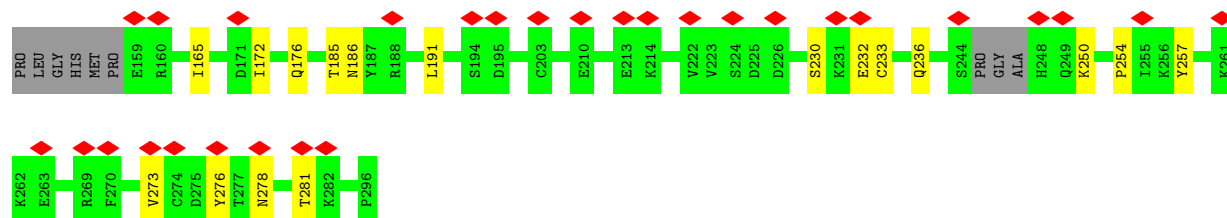
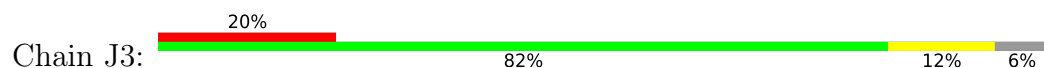
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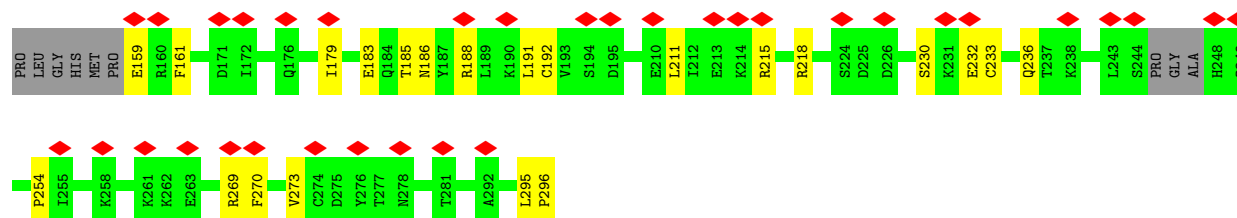
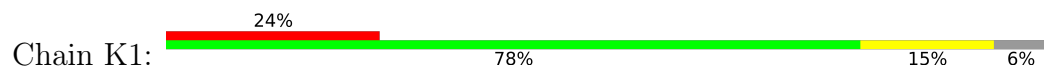
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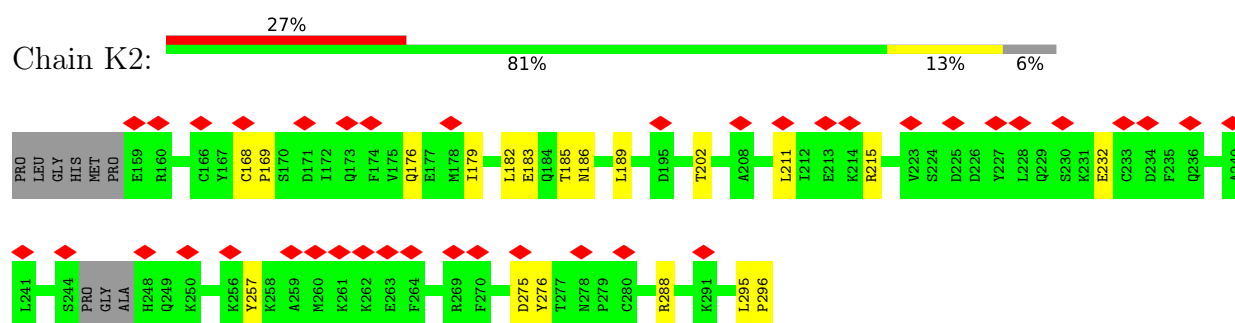
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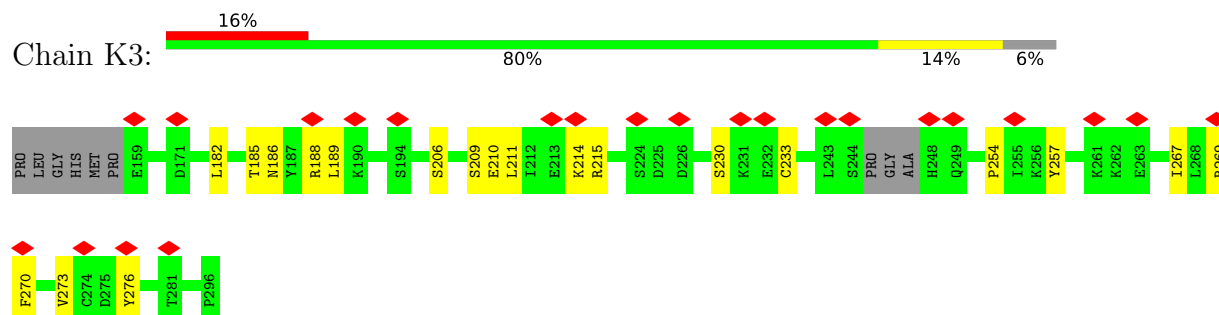
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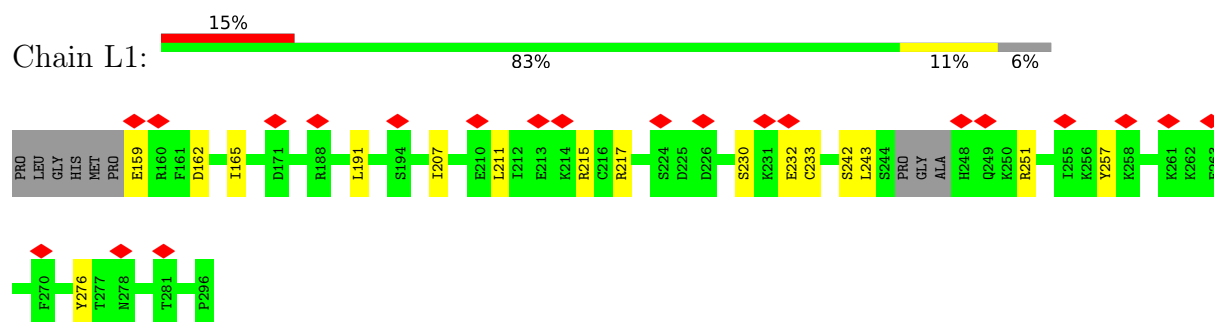
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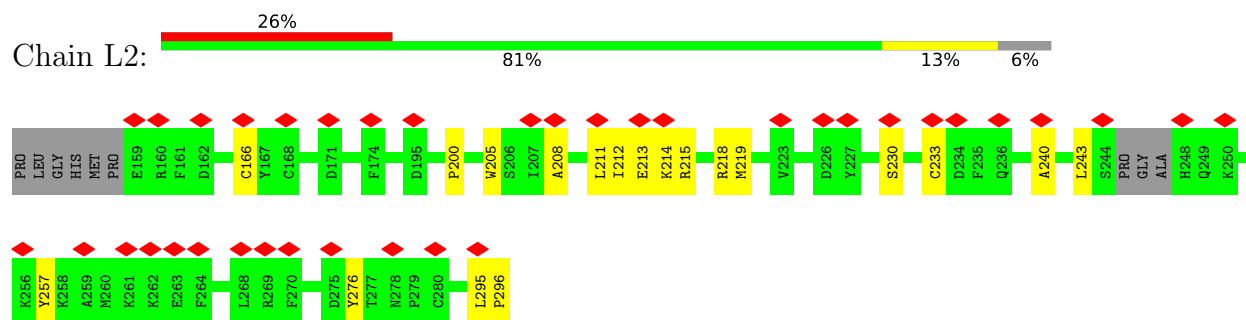
- Molecule 1: Myeloid differentiation primary response protein MyD88



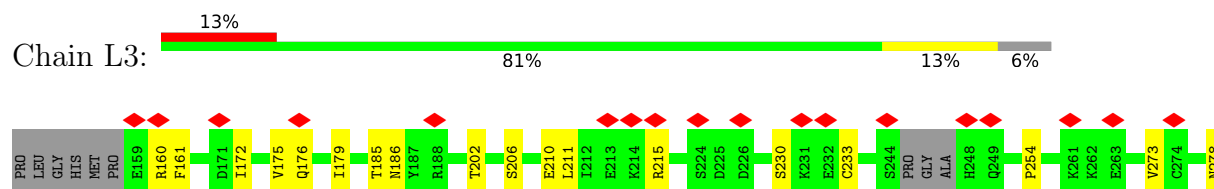
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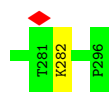


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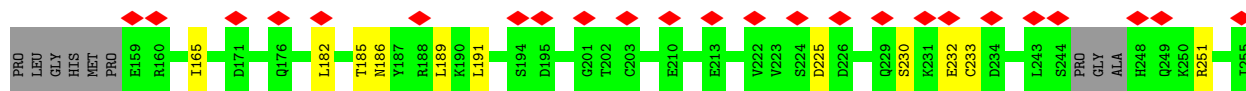
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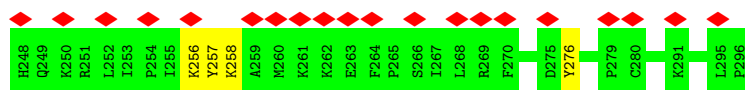
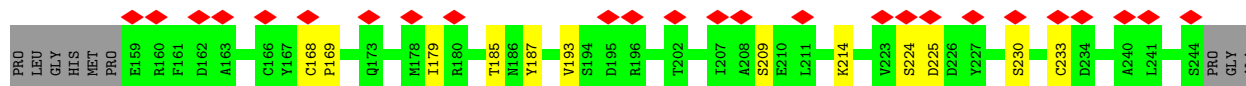
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain J1: 26% 81% 12% 6%



- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain G2: 31% 83% 11% 6%



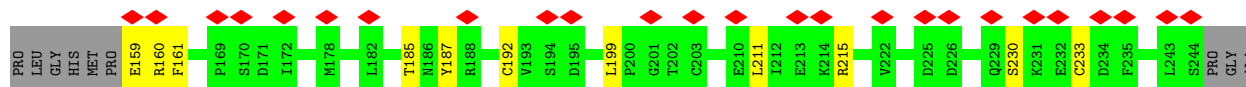
- Molecule 1: Myeloid differentiation primary response protein MyD88

Chain G3: 26% 78% 15% 6%

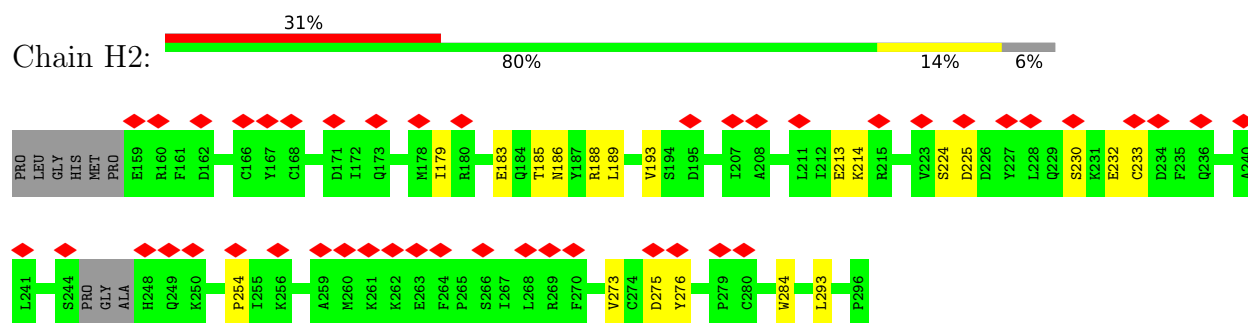


- Molecule 1: Myeloid differentiation primary response protein MyD88

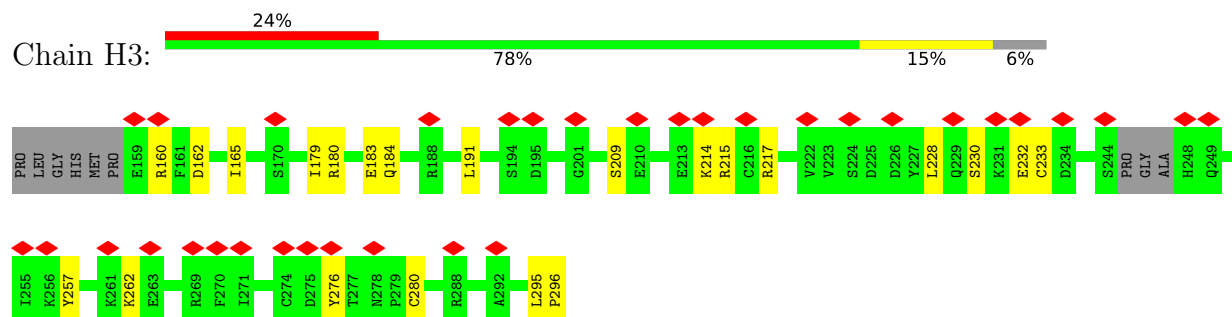
Chain H1: 30% 81% 12% 6%



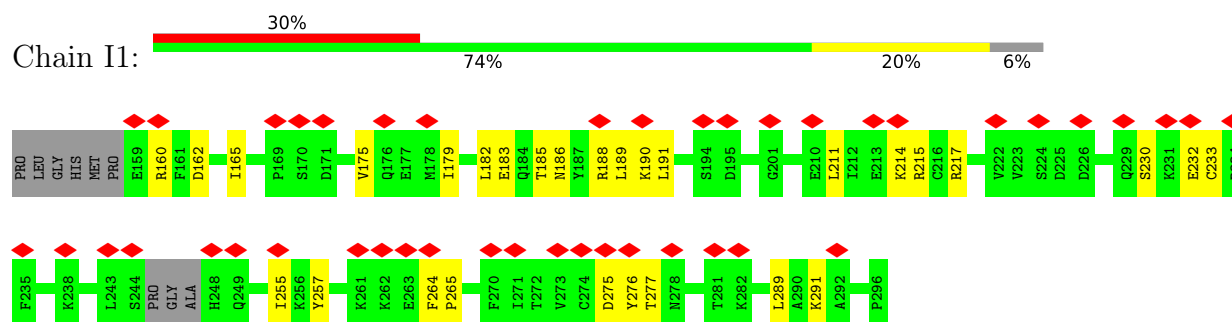
- Molecule 1: Myeloid differentiation primary response protein MyD88



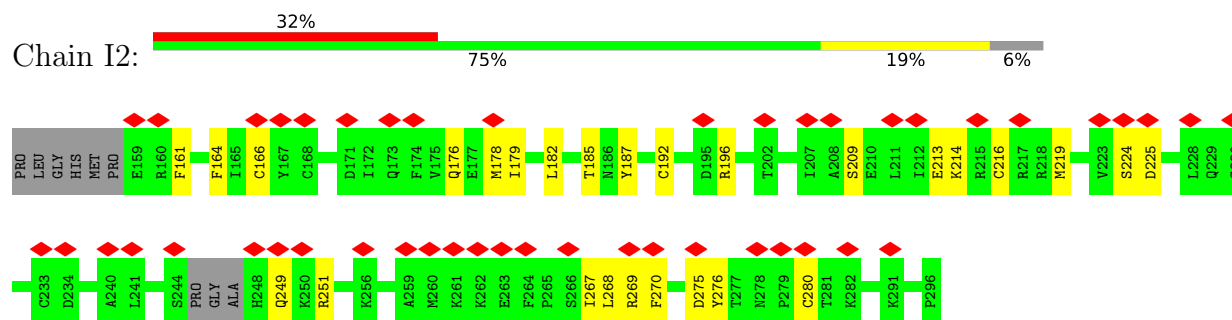
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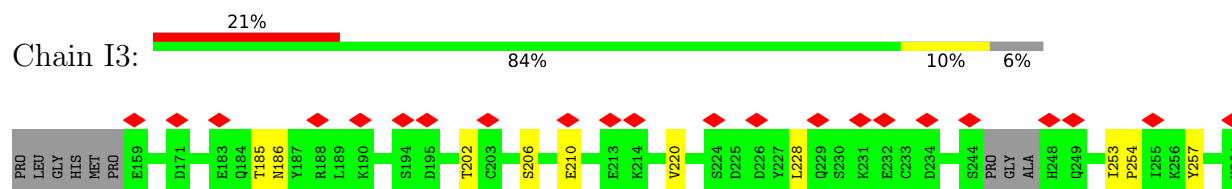
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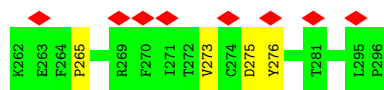


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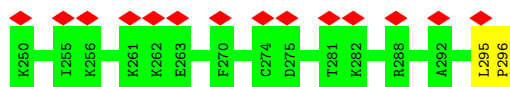
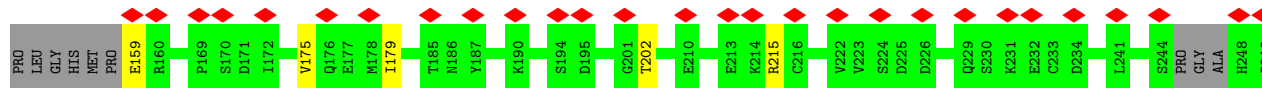
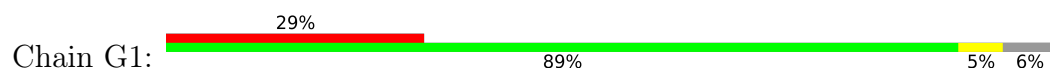


- Molecule 1: Myeloid differentiation primary response protein MyD88

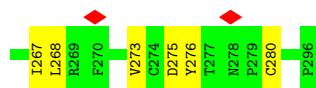
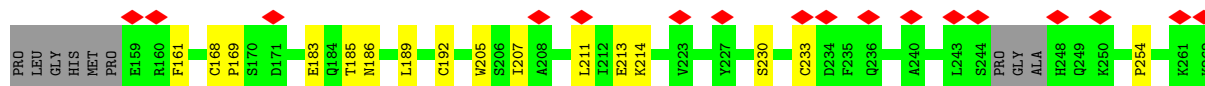
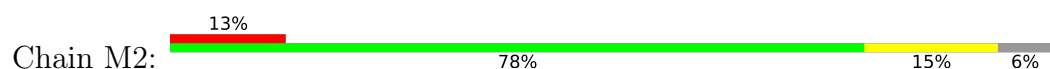




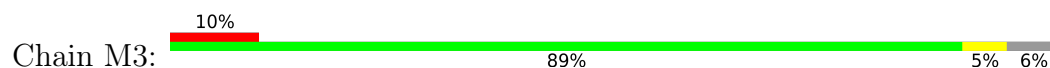
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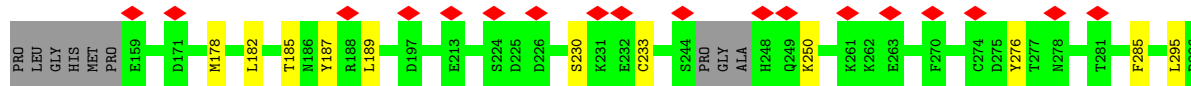
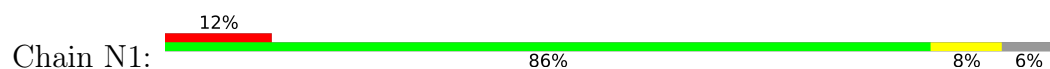
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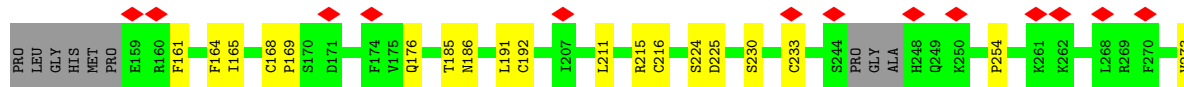
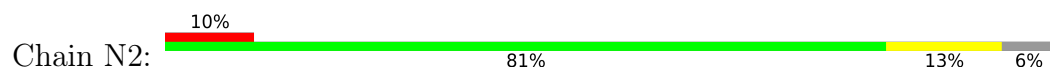
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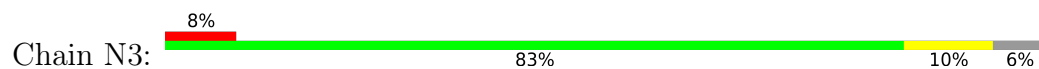


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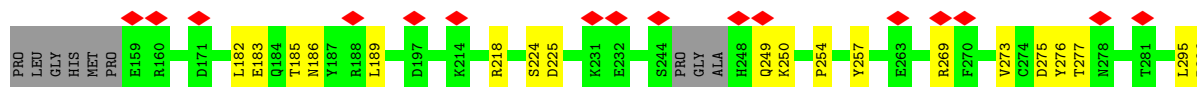
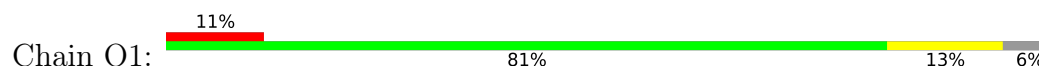




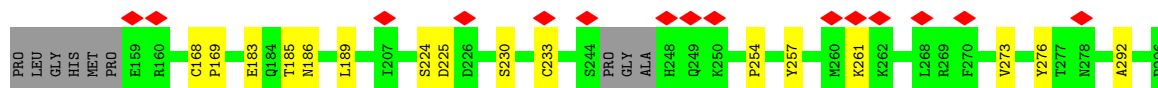
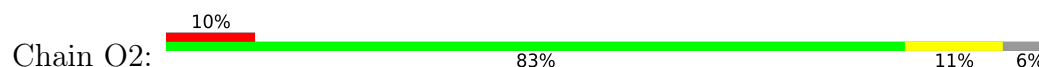
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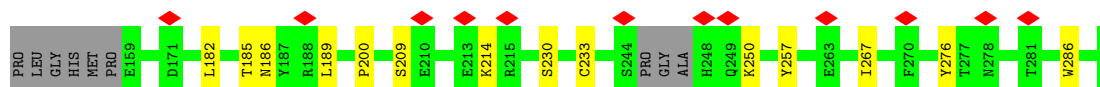
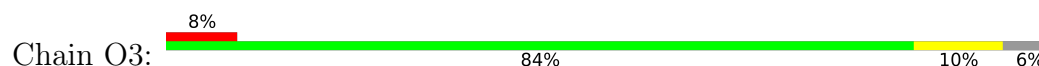
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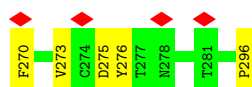
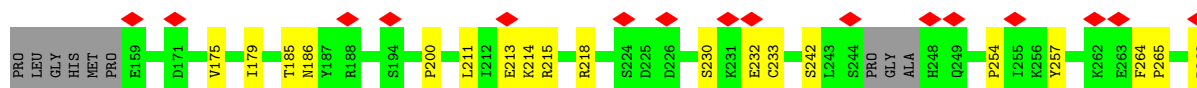
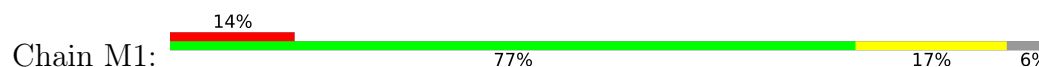
- Molecule 1: Myeloid differentiation primary response protein MyD88



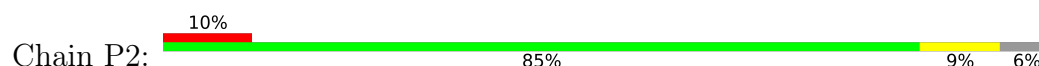
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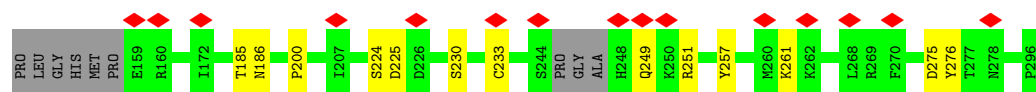


- Molecule 1: Myeloid differentiation primary response protein MyD88

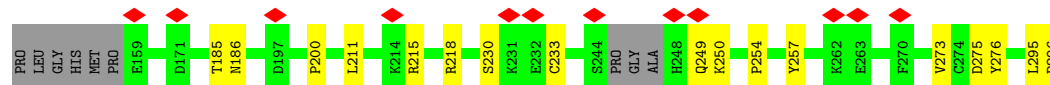
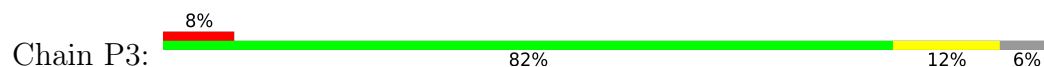


- Molecule 1: Myeloid differentiation primary response protein MyD88

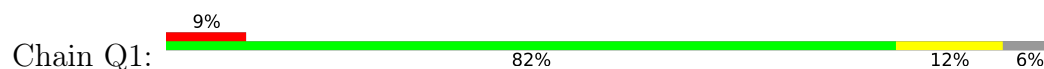




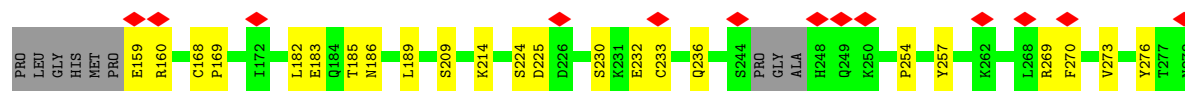
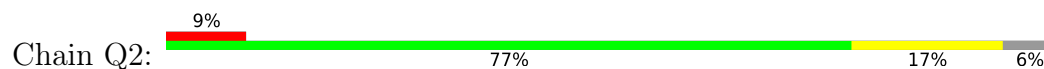
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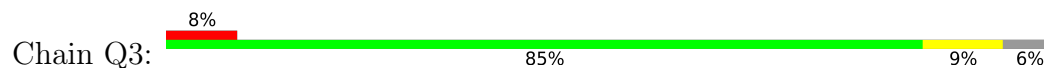
- Molecule 1: Myeloid differentiation primary response protein MyD88



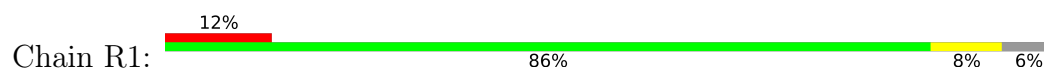
- Molecule 1: Myeloid differentiation primary response protein MyD88



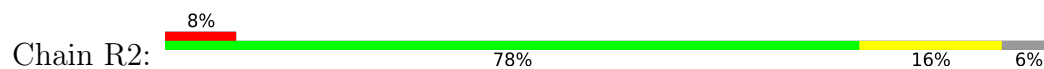
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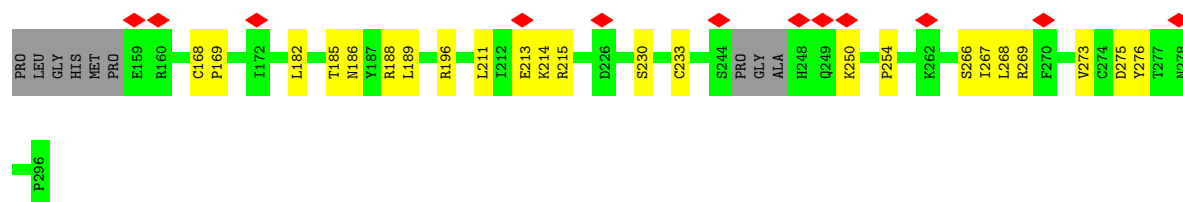


- Molecule 1: Myeloid differentiation primary response protein MyD88

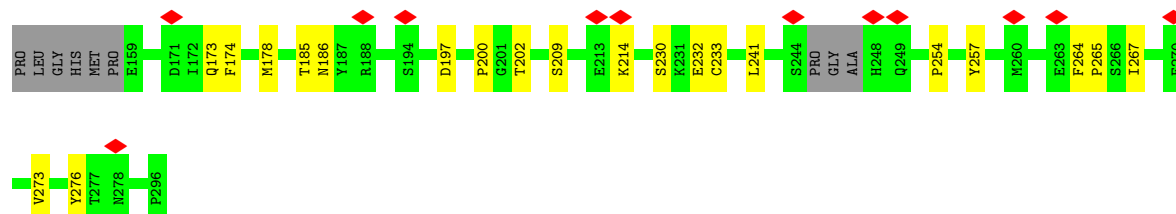
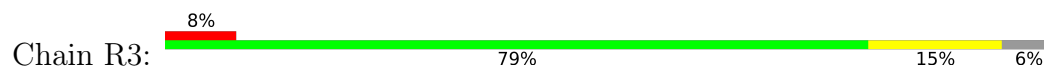


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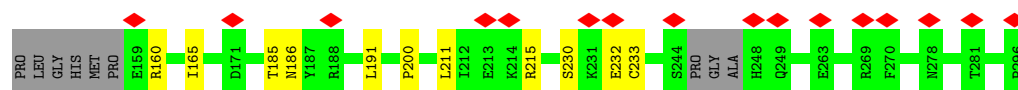
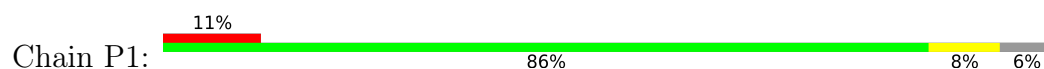




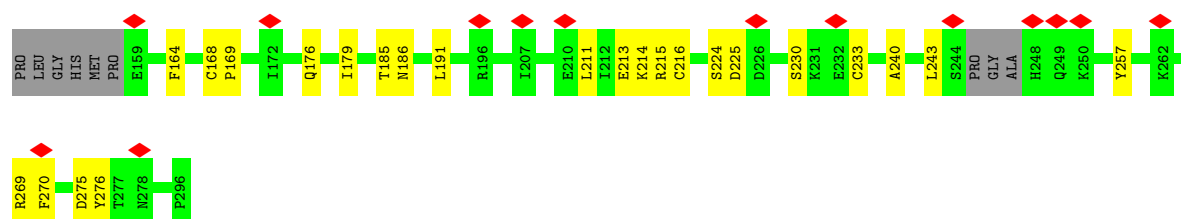
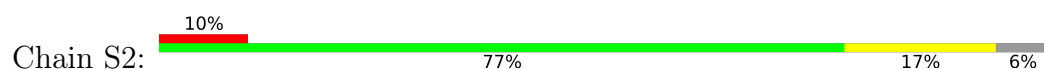
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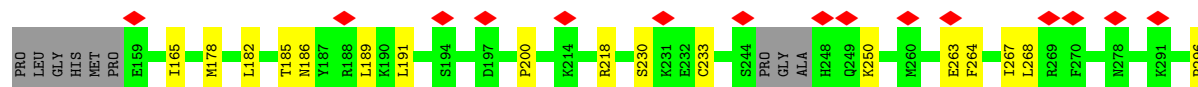
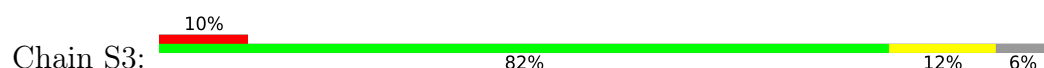
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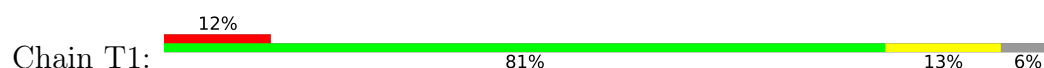
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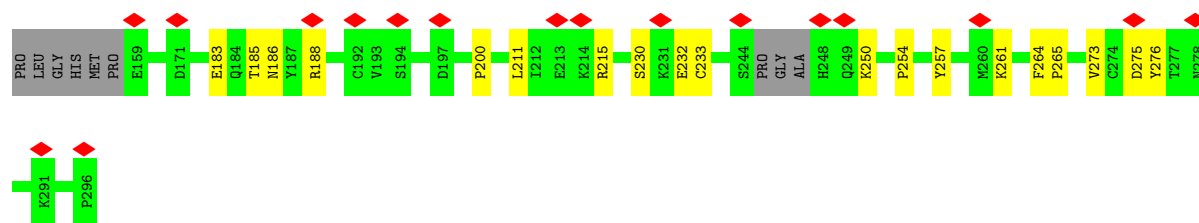


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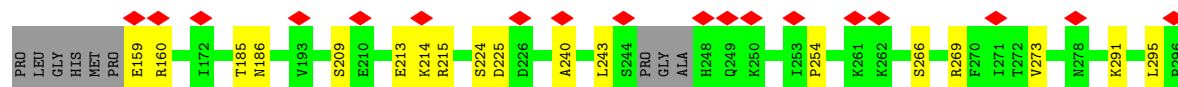
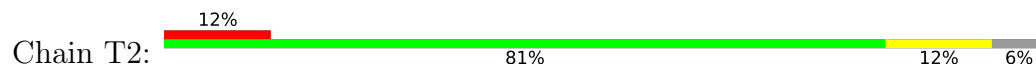


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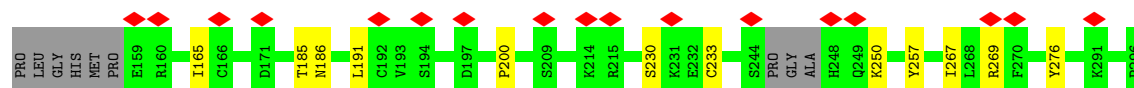
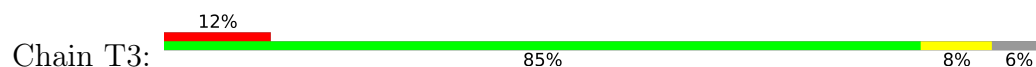




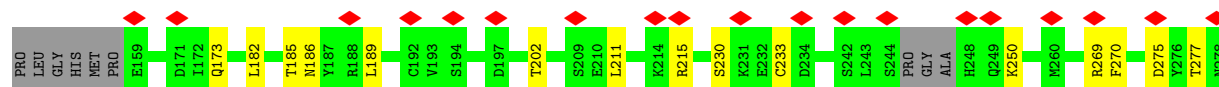
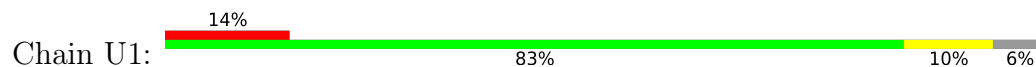
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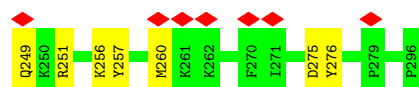
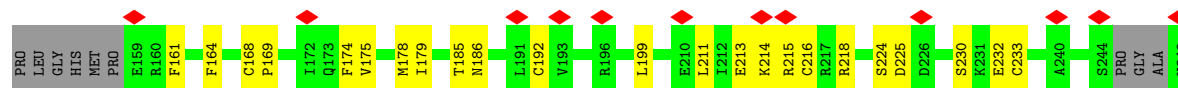
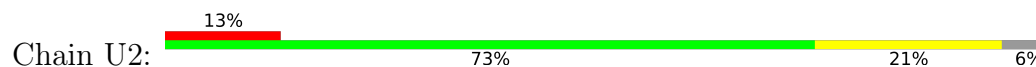
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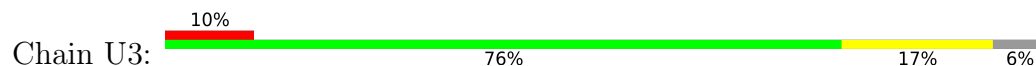
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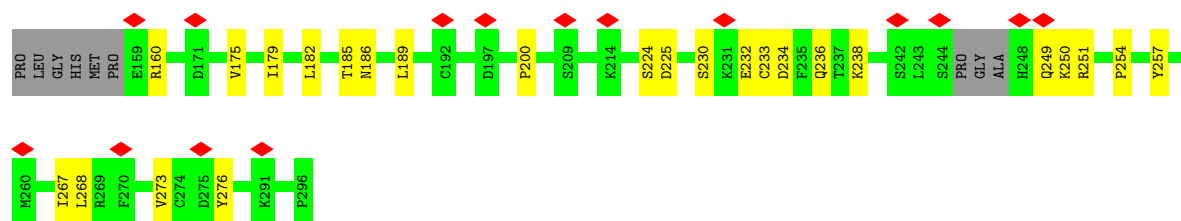


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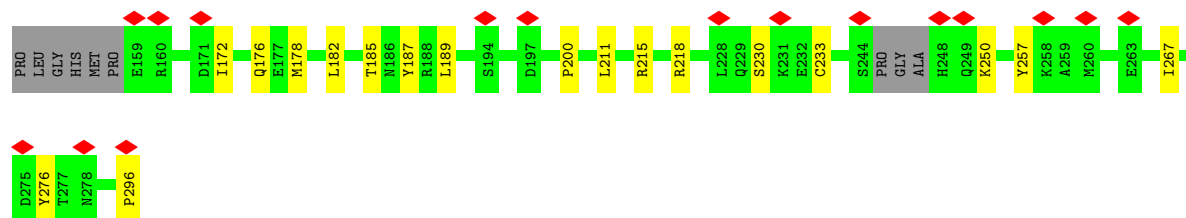
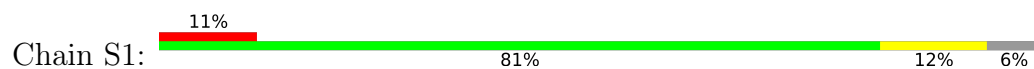


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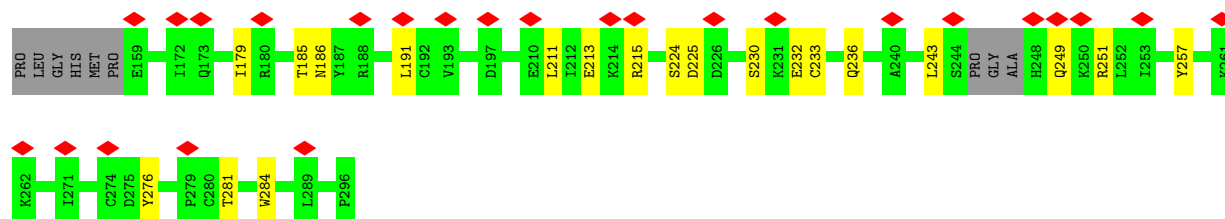
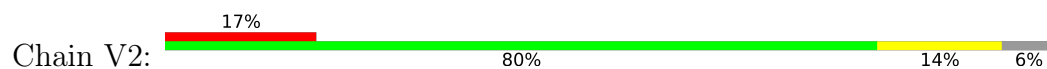




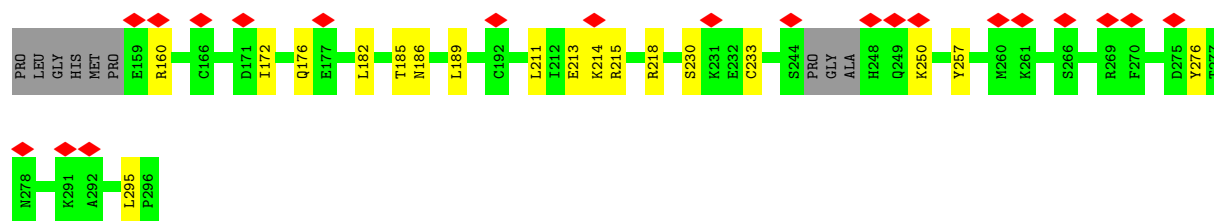
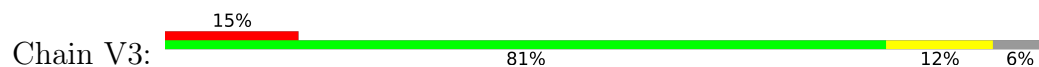
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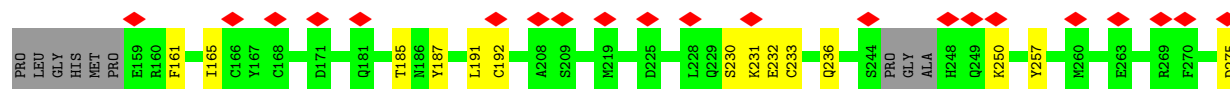
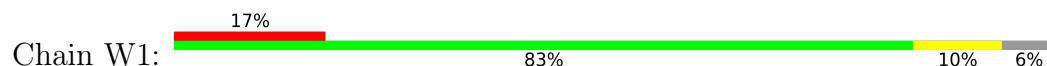
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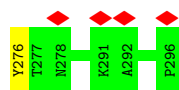


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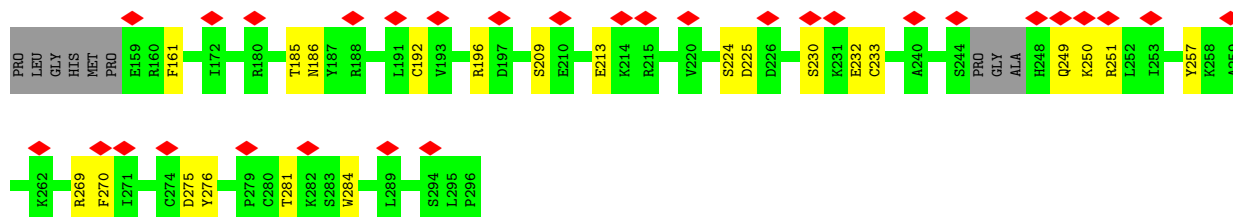
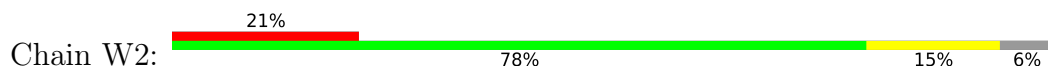


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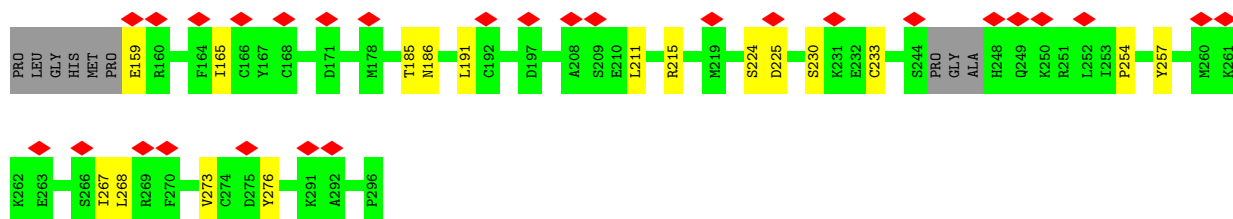
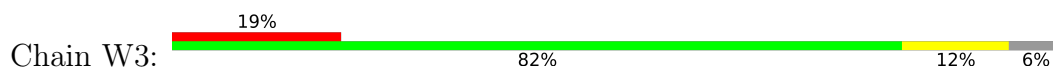




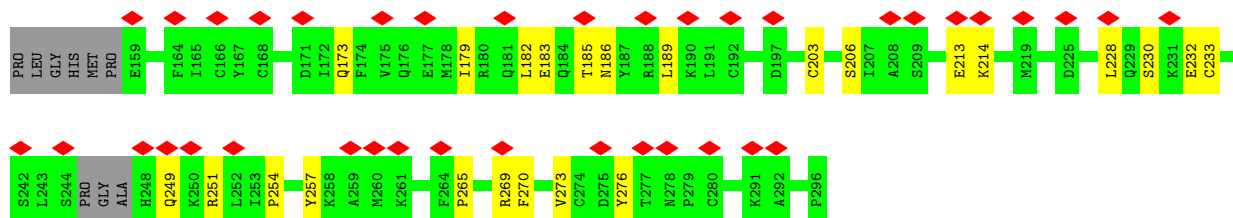
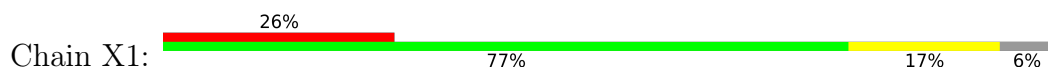
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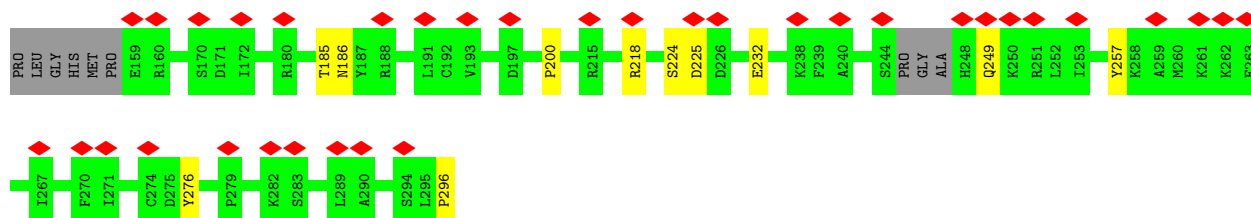
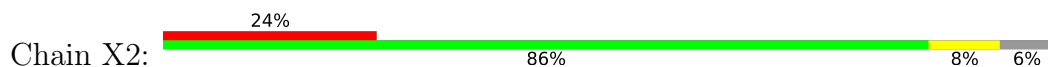
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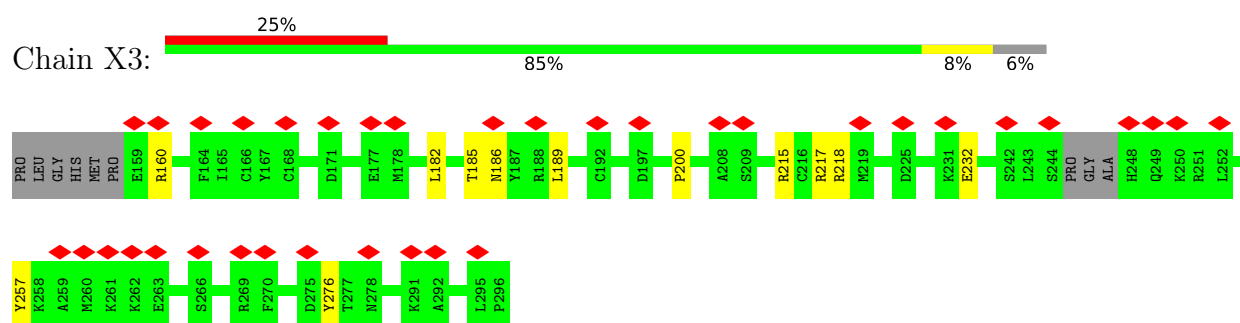
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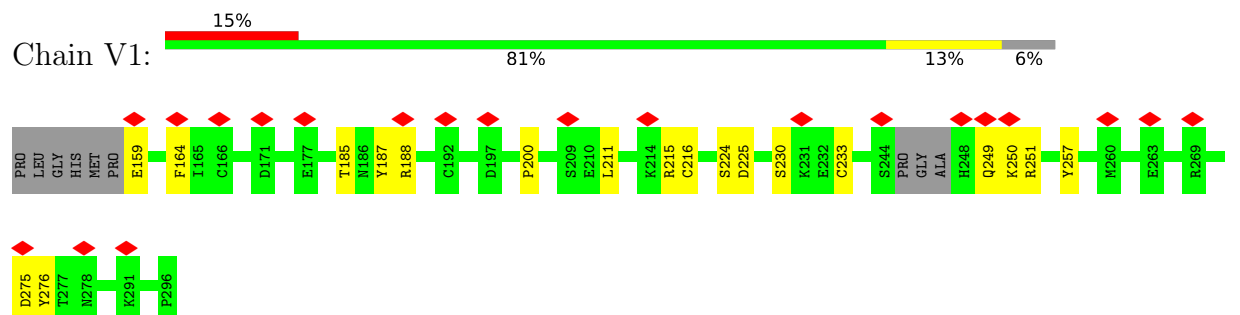
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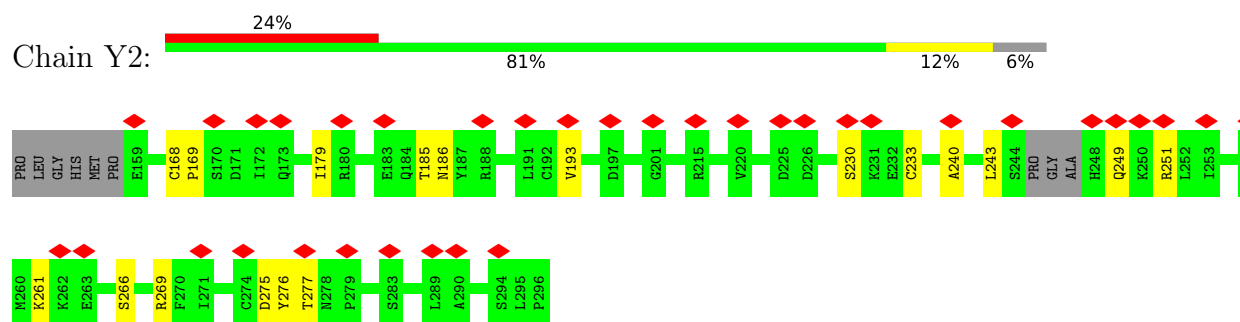
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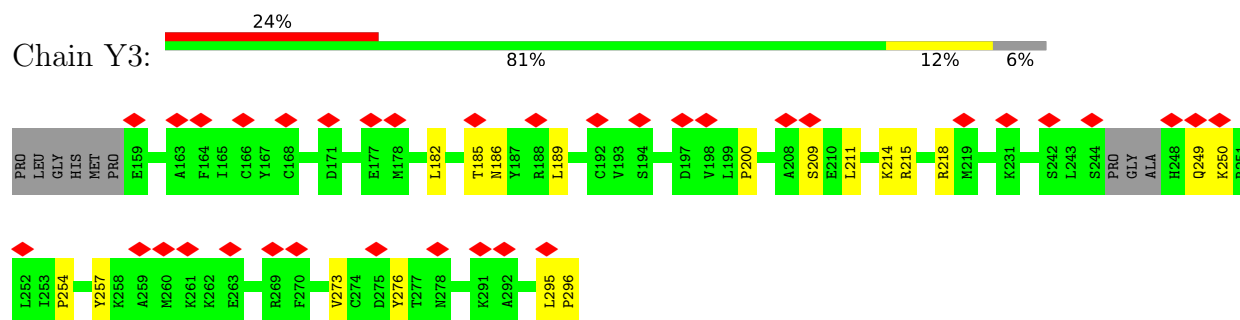
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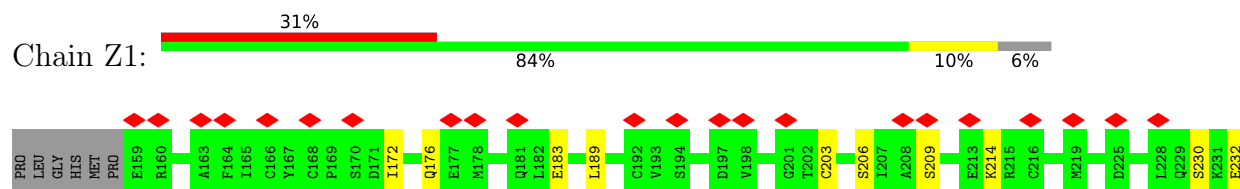
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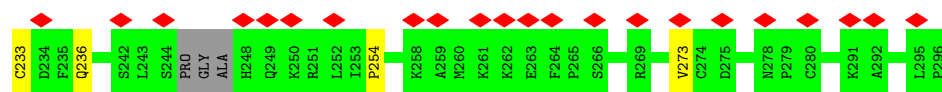


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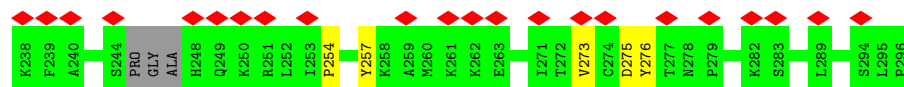
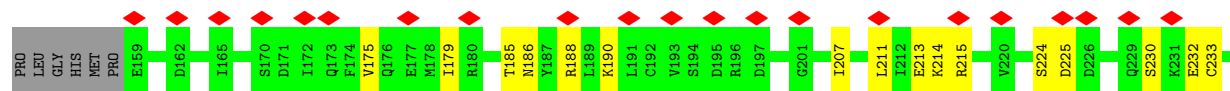
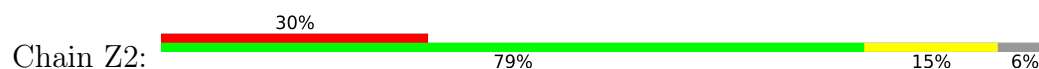


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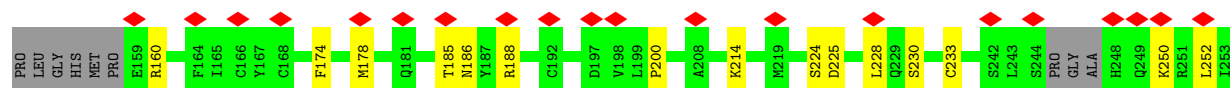
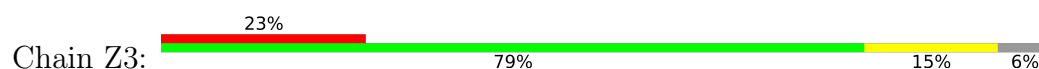




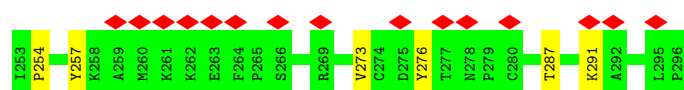
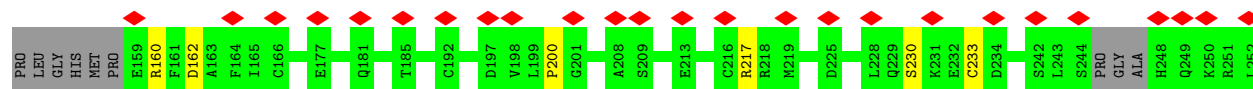
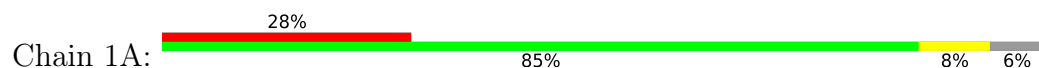
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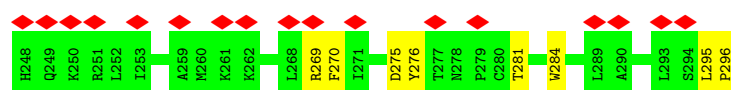
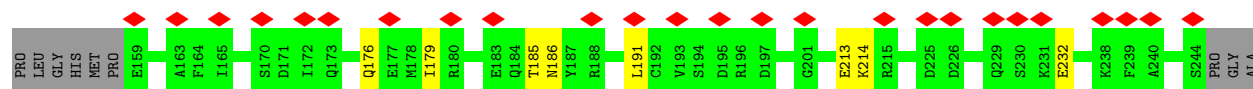
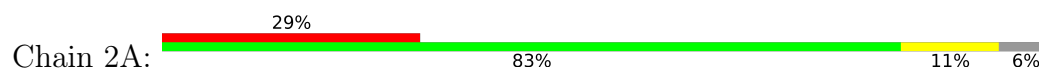
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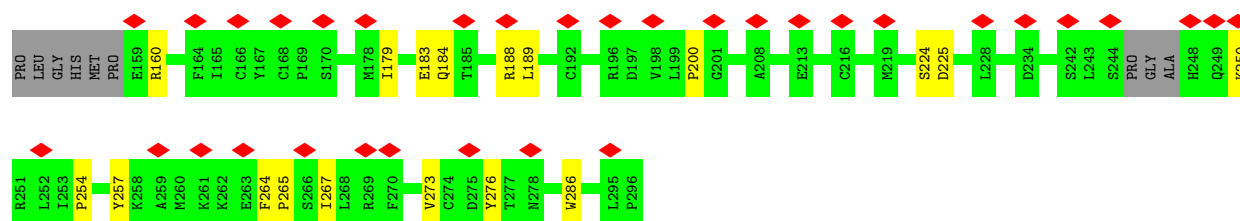
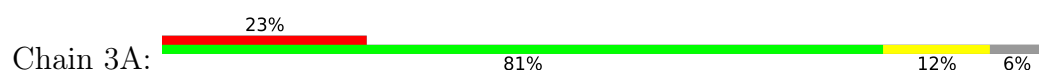
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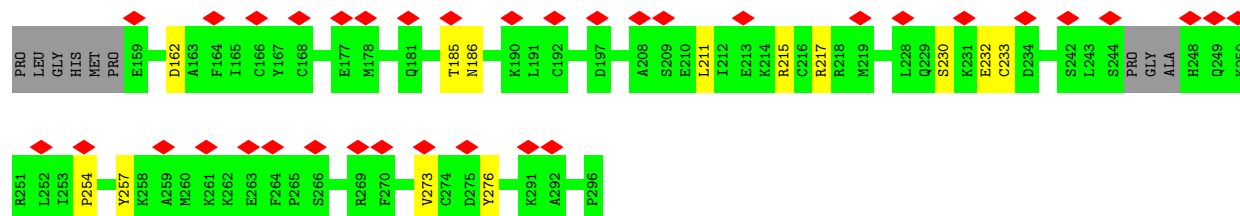
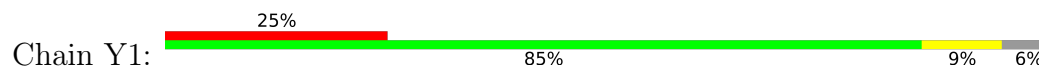
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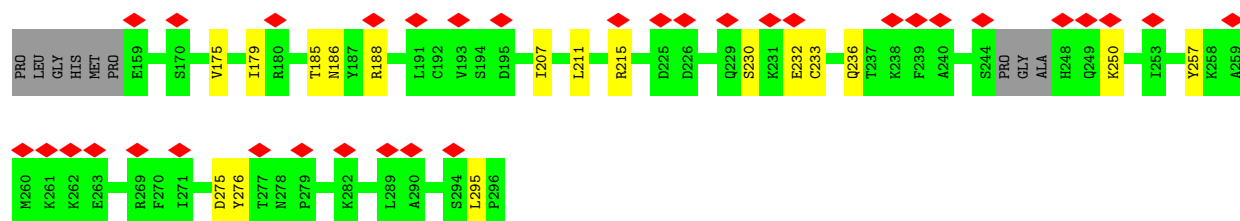
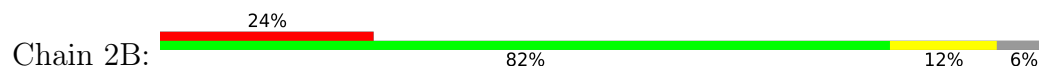
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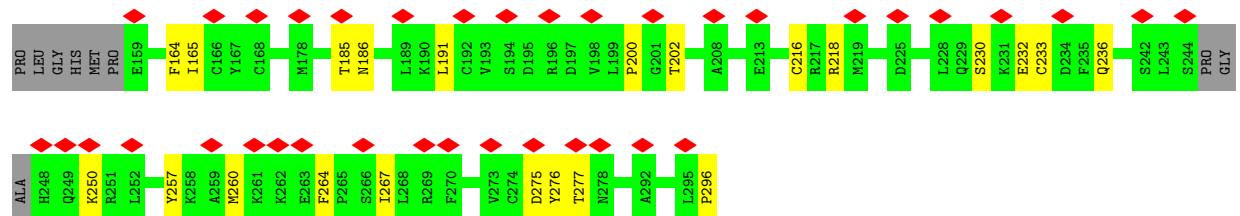
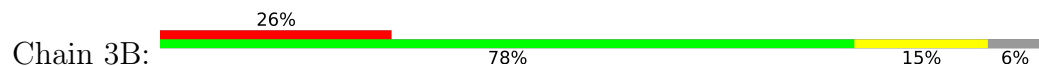
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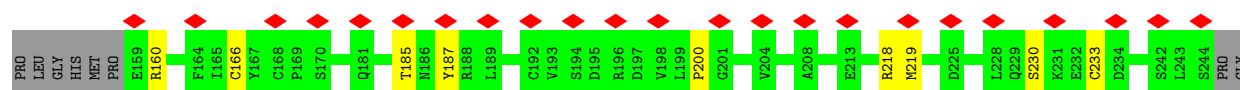
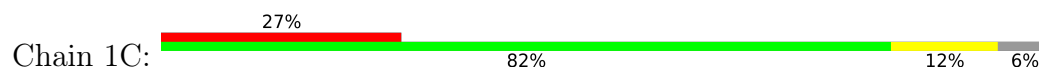
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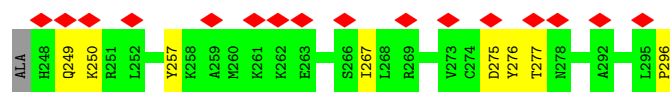


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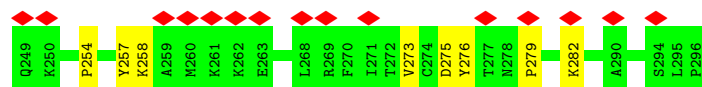
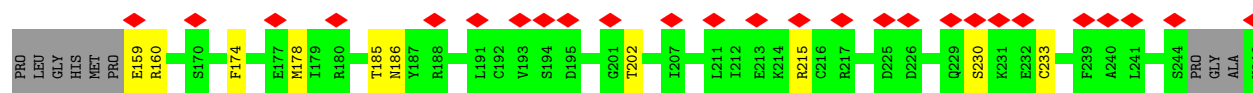
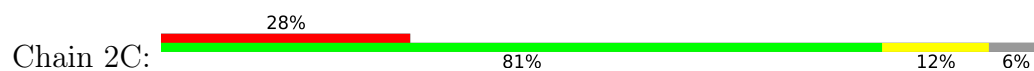


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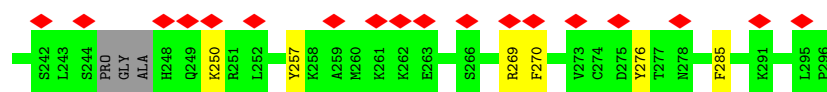
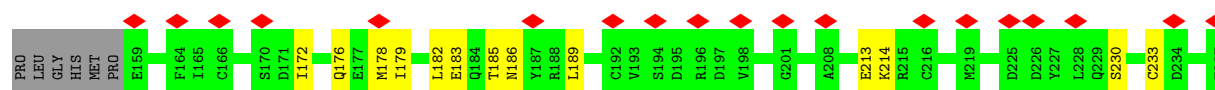
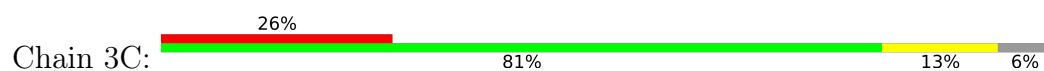




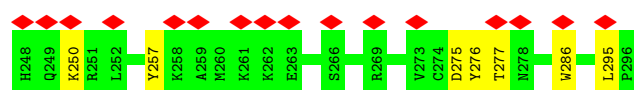
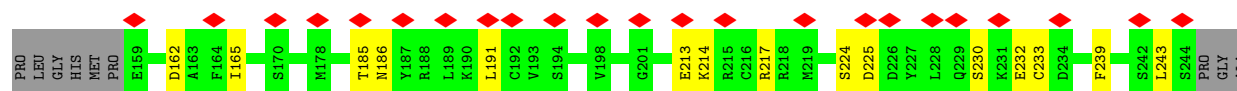
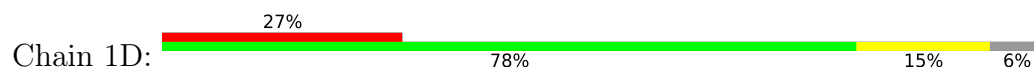
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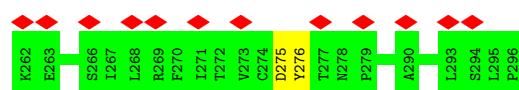
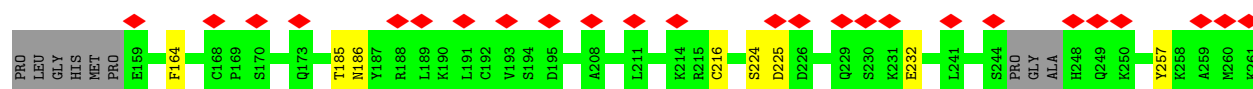
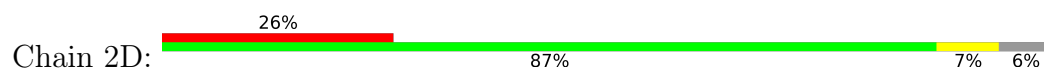
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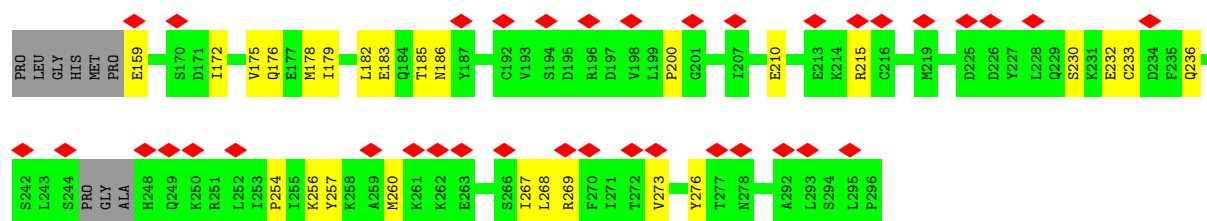
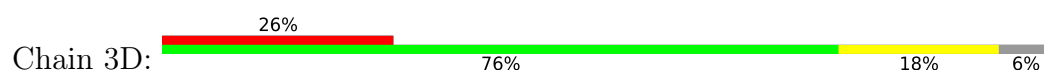
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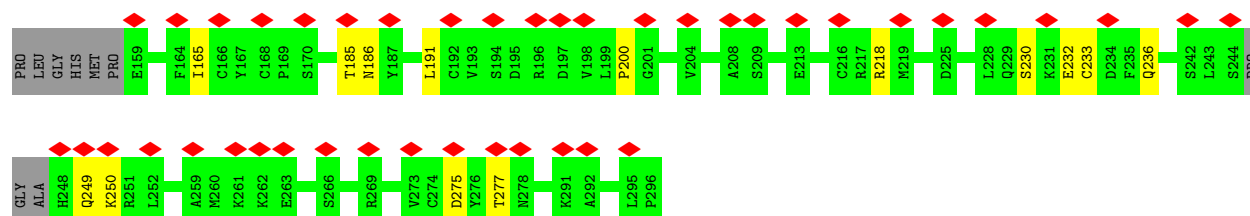
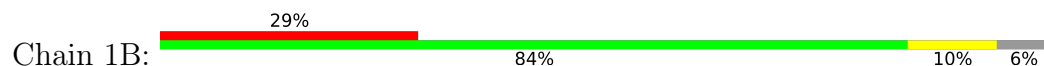
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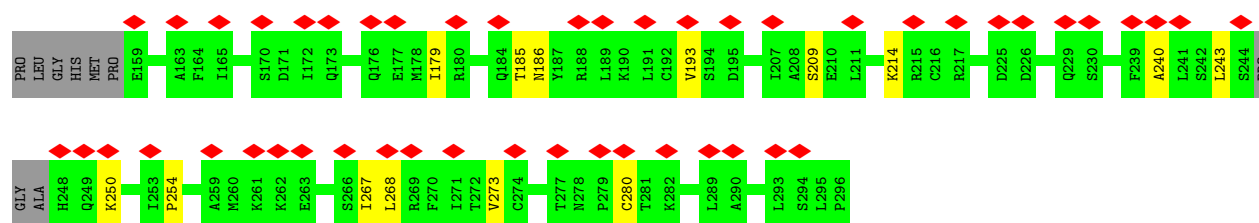
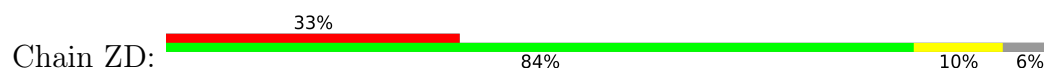
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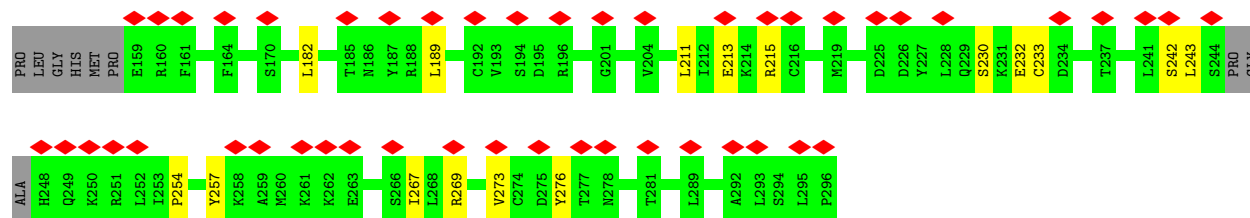
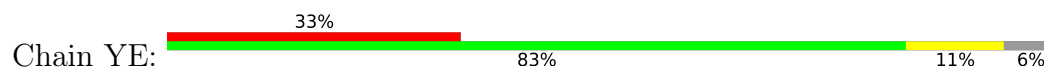
- Molecule 1: Myeloid differentiation primary response protein MyD88



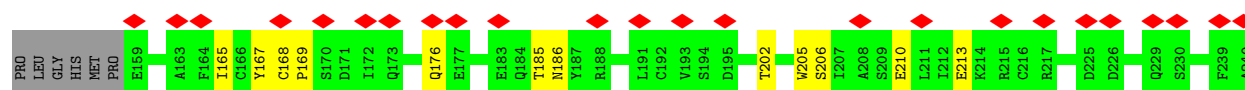
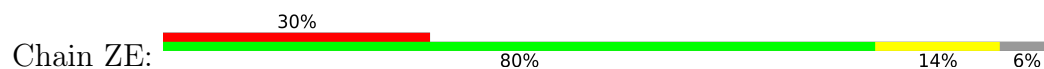
- Molecule 1: Myeloid differentiation primary response protein MyD88

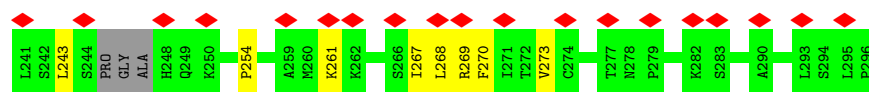


- Molecule 1: Myeloid differentiation primary response protein MyD88

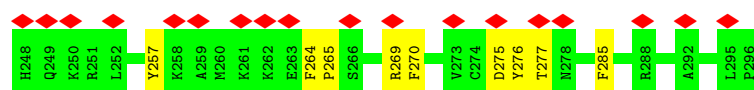
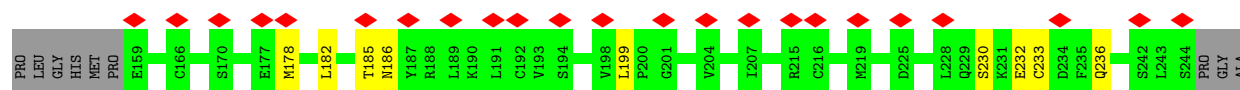
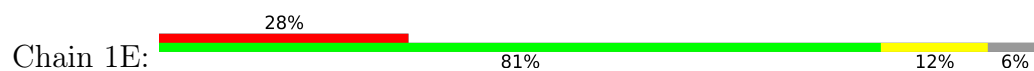


- Molecule 1: Myeloid differentiation primary response protein MyD88

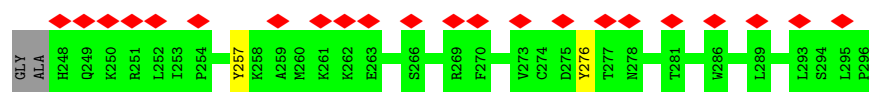
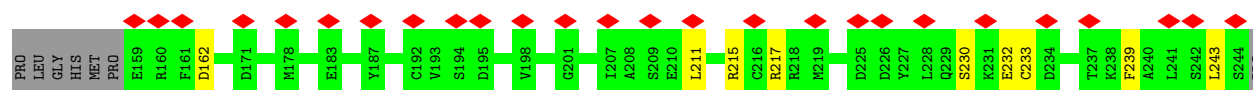
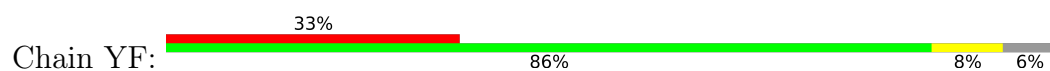




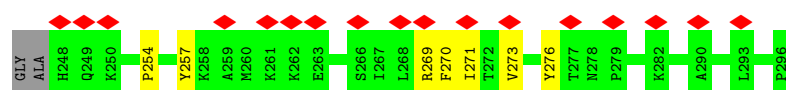
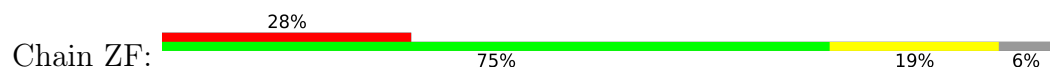
- Molecule 1: Myeloid differentiation primary response protein MyD88



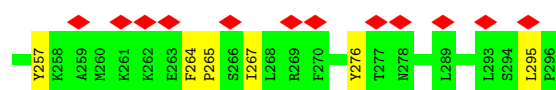
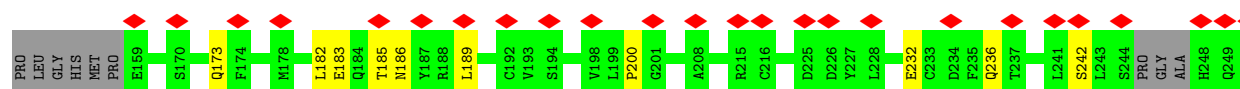
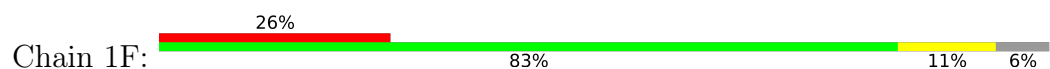
- Molecule 1: Myeloid differentiation primary response protein MyD88



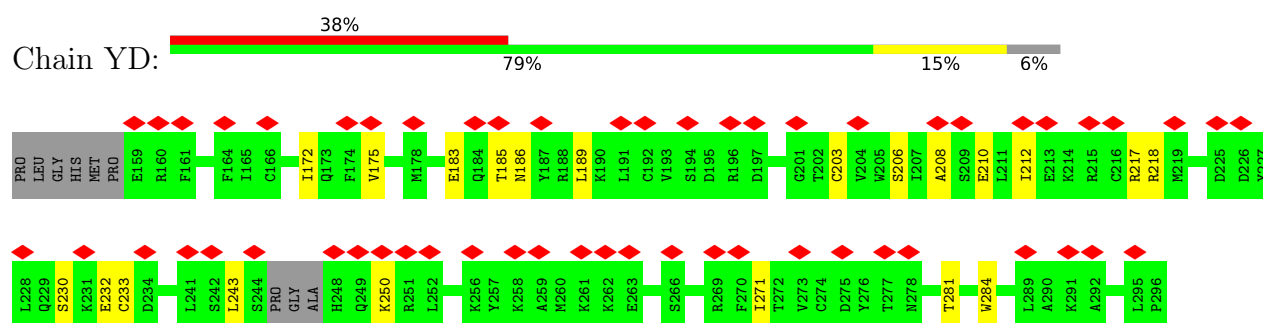
- Molecule 1: Myeloid differentiation primary response protein MyD88



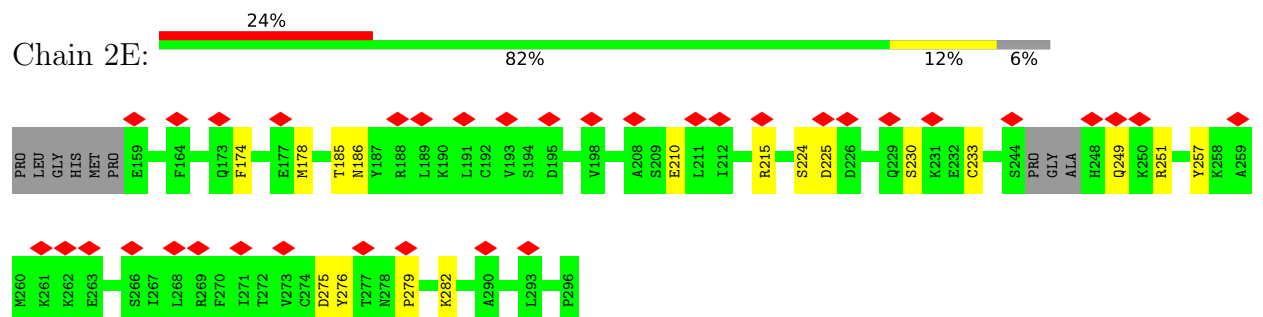
- Molecule 1: Myeloid differentiation primary response protein MyD88



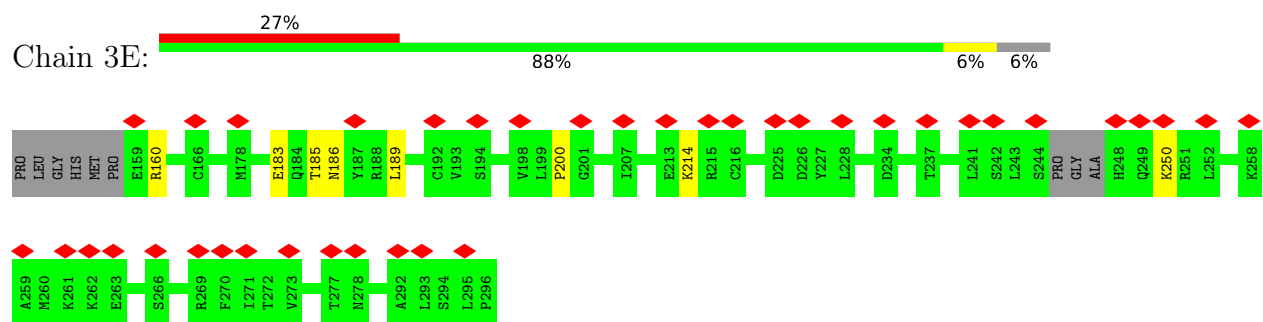
- Molecule 1: Myeloid differentiation primary response protein MyD88



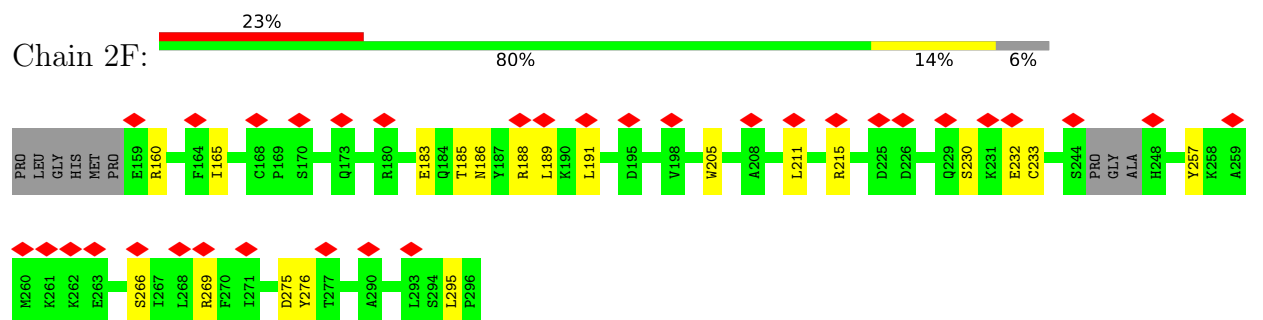
- Molecule 1: Myeloid differentiation primary response protein MyD88



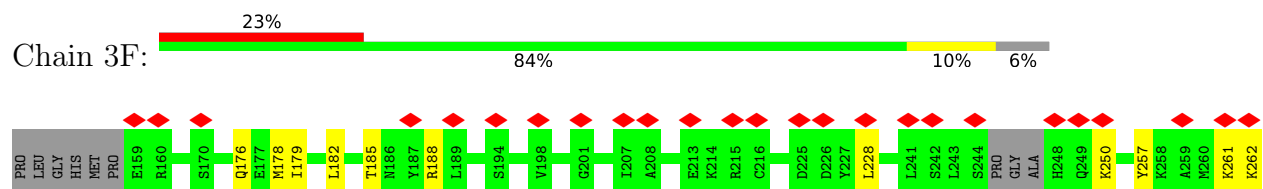
- Molecule 1: Myeloid differentiation primary response protein MyD88



- Molecule 1: Myeloid differentiation primary response protein MyD88



- Molecule 1: Myeloid differentiation primary response protein MyD88





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.506	Depositor
Minimum map value	-1.121	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.55	Depositor
Map size (\AA)	607.5, 607.5, 607.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	0.25	0/1141	0.48	0/1538
1	1B	0.24	0/1141	0.47	0/1538
1	1C	0.24	0/1141	0.48	0/1538
1	1D	0.25	0/1141	0.48	0/1538
1	1E	0.24	0/1141	0.48	0/1538
1	1F	0.25	0/1141	0.49	0/1538
1	2A	0.24	0/1141	0.48	0/1538
1	2B	0.25	0/1141	0.48	0/1538
1	2C	0.25	0/1141	0.49	0/1538
1	2D	0.24	0/1141	0.48	0/1538
1	2E	0.24	0/1141	0.49	0/1538
1	2F	0.24	0/1141	0.49	0/1538
1	3A	0.25	0/1141	0.49	0/1538
1	3B	0.25	0/1141	0.50	0/1538
1	3C	0.24	0/1141	0.48	0/1538
1	3D	0.25	0/1141	0.51	0/1538
1	3E	0.24	0/1141	0.48	0/1538
1	3F	0.24	0/1141	0.49	0/1538
1	A1	0.25	0/1141	0.48	0/1538
1	A2	0.24	0/1141	0.48	0/1538
1	A3	0.24	0/1141	0.49	0/1538
1	B1	0.24	0/1141	0.48	0/1538
1	B2	0.24	0/1141	0.49	0/1538
1	B3	0.26	0/1141	0.50	0/1538
1	C1	0.24	0/1141	0.48	0/1538
1	C2	0.24	0/1141	0.48	0/1538
1	C3	0.24	0/1141	0.48	0/1538
1	D1	0.24	0/1141	0.49	0/1538
1	D2	0.24	0/1141	0.48	0/1538
1	D3	0.25	0/1141	0.50	0/1538
1	E1	0.24	0/1141	0.48	0/1538
1	E2	0.25	0/1141	0.48	0/1538
1	E3	0.25	0/1141	0.49	0/1538
1	F1	0.24	0/1141	0.48	0/1538

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	F2	0.24	0/1141	0.50	0/1538
1	F3	0.24	0/1141	0.49	0/1538
1	G1	0.25	0/1141	0.50	0/1538
1	G2	0.24	0/1141	0.49	0/1538
1	G3	0.26	0/1141	0.52	0/1538
1	H1	0.24	0/1141	0.49	0/1538
1	H2	0.24	0/1141	0.50	0/1538
1	H3	0.25	0/1141	0.50	0/1538
1	I1	0.25	0/1141	0.50	0/1538
1	I2	0.24	0/1141	0.49	0/1538
1	I3	0.25	0/1141	0.50	0/1538
1	J1	0.24	0/1141	0.49	0/1538
1	J2	0.24	0/1141	0.48	0/1538
1	J3	0.24	0/1141	0.49	0/1538
1	K1	0.24	0/1141	0.49	0/1538
1	K2	0.24	0/1141	0.48	0/1538
1	K3	0.24	0/1141	0.48	0/1538
1	L1	0.24	0/1141	0.49	0/1538
1	L2	0.25	0/1141	0.50	0/1538
1	L3	0.25	0/1141	0.49	0/1538
1	M1	0.25	0/1141	0.49	0/1538
1	M2	0.24	0/1141	0.48	0/1538
1	M3	0.24	0/1141	0.48	0/1538
1	N1	0.24	0/1141	0.48	0/1538
1	N2	0.24	0/1141	0.48	0/1538
1	N3	0.24	0/1141	0.48	0/1538
1	O1	0.25	0/1141	0.50	0/1538
1	O2	0.25	0/1141	0.49	0/1538
1	O3	0.24	0/1141	0.49	0/1538
1	P1	0.25	0/1141	0.49	0/1538
1	P2	0.24	0/1141	0.49	0/1538
1	P3	0.24	0/1141	0.49	0/1538
1	Q1	0.25	0/1141	0.49	0/1538
1	Q2	0.24	0/1141	0.47	0/1538
1	Q3	0.25	0/1141	0.49	0/1538
1	R1	0.25	0/1141	0.49	0/1538
1	R2	0.24	0/1141	0.47	0/1538
1	R3	0.24	0/1141	0.49	0/1538
1	S1	0.24	0/1141	0.48	0/1538
1	S2	0.24	0/1141	0.48	0/1538
1	S3	0.24	0/1141	0.48	0/1538
1	T1	0.25	0/1141	0.49	0/1538
1	T2	0.25	0/1141	0.50	0/1538

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T3	0.24	0/1141	0.49	0/1538
1	U1	0.24	0/1141	0.48	0/1538
1	U2	0.24	0/1141	0.48	0/1538
1	U3	0.24	0/1141	0.47	0/1538
1	V1	0.25	0/1141	0.49	0/1538
1	V2	0.24	0/1141	0.49	0/1538
1	V3	0.24	0/1141	0.48	0/1538
1	W1	0.25	0/1141	0.48	0/1538
1	W2	0.25	0/1141	0.49	0/1538
1	W3	0.24	0/1141	0.50	0/1538
1	X1	0.24	0/1141	0.49	0/1538
1	X2	0.24	0/1141	0.47	0/1538
1	X3	0.25	0/1141	0.50	0/1538
1	Y1	0.25	0/1141	0.49	0/1538
1	Y2	0.24	0/1141	0.49	0/1538
1	Y3	0.24	0/1141	0.48	0/1538
1	YD	0.24	0/1141	0.49	0/1538
1	YE	0.25	0/1141	0.51	0/1538
1	YF	0.25	0/1141	0.48	0/1538
1	Z1	0.24	0/1141	0.48	0/1538
1	Z2	0.25	0/1141	0.48	0/1538
1	Z3	0.25	0/1141	0.50	0/1538
1	ZD	0.25	0/1141	0.48	0/1538
1	ZE	0.24	0/1141	0.49	0/1538
1	ZF	0.24	0/1141	0.48	0/1538
All	All	0.24	0/116382	0.49	0/156876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	1117	0	1136	7	0
1	1B	1117	0	1136	10	0
1	1C	1117	0	1136	12	0
1	1D	1117	0	1136	13	0
1	1E	1117	0	1136	11	0
1	1F	1117	0	1136	12	0
1	2A	1117	0	1136	11	0
1	2B	1117	0	1136	13	0
1	2C	1117	0	1136	11	0
1	2D	1117	0	1136	7	0
1	2E	1117	0	1136	9	0
1	2F	1117	0	1136	14	0
1	3A	1117	0	1136	12	0
1	3B	1117	0	1136	15	0
1	3C	1117	0	1136	12	0
1	3D	1117	0	1136	18	0
1	3E	1117	0	1136	6	0
1	3F	1117	0	1136	8	0
1	A1	1117	0	1136	12	0
1	A2	1117	0	1136	12	0
1	A3	1117	0	1136	12	0
1	B1	1117	0	1136	6	0
1	B2	1117	0	1136	8	0
1	B3	1117	0	1136	16	0
1	C1	1117	0	1136	9	0
1	C2	1117	0	1136	13	0
1	C3	1117	0	1136	11	0
1	D1	1117	0	1136	14	0
1	D2	1117	0	1136	8	0
1	D3	1117	0	1136	15	0
1	E1	1117	0	1136	13	0
1	E2	1117	0	1136	16	0
1	E3	1117	0	1136	8	0
1	F1	1117	0	1136	12	0
1	F2	1117	0	1136	13	0
1	F3	1117	0	1136	16	0
1	G1	1117	0	1136	4	0
1	G2	1117	0	1136	8	0
1	G3	1117	0	1136	14	0
1	H1	1117	0	1136	12	0
1	H2	1117	0	1136	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H3	1117	0	1136	12	0
1	I1	1117	0	1136	16	0
1	I2	1117	0	1136	16	0
1	I3	1117	0	1136	10	0
1	J1	1117	0	1136	12	0
1	J2	1117	0	1136	15	0
1	J3	1117	0	1136	11	0
1	K1	1117	0	1136	12	0
1	K2	1117	0	1136	13	0
1	K3	1117	0	1136	11	0
1	L1	1117	0	1136	9	0
1	L2	1117	0	1136	11	0
1	L3	1117	0	1136	13	0
1	M1	1117	0	1136	17	0
1	M2	1117	0	1136	12	0
1	M3	1117	0	1136	4	0
1	N1	1117	0	1136	7	0
1	N2	1117	0	1136	11	0
1	N3	1117	0	1136	9	0
1	O1	1117	0	1136	14	0
1	O2	1117	0	1136	11	0
1	O3	1117	0	1136	11	0
1	P1	1117	0	1136	7	0
1	P2	1117	0	1136	9	0
1	P3	1117	0	1136	11	0
1	Q1	1117	0	1136	11	0
1	Q2	1117	0	1136	15	0
1	Q3	1117	0	1136	8	0
1	R1	1117	0	1136	9	0
1	R2	1117	0	1136	14	0
1	R3	1117	0	1136	15	0
1	S1	1117	0	1136	12	0
1	S2	1117	0	1136	14	0
1	S3	1117	0	1136	11	0
1	T1	1117	0	1136	13	0
1	T2	1117	0	1136	11	0
1	T3	1117	0	1136	9	0
1	U1	1117	0	1136	9	0
1	U2	1117	0	1136	19	0
1	U3	1117	0	1136	15	0
1	V1	1117	0	1136	12	0
1	V2	1117	0	1136	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V3	1117	0	1136	12	0
1	W1	1117	0	1136	10	0
1	W2	1117	0	1136	14	0
1	W3	1117	0	1136	9	0
1	X1	1117	0	1136	14	0
1	X2	1117	0	1136	7	0
1	X3	1117	0	1136	8	0
1	Y1	1117	0	1136	8	0
1	Y2	1117	0	1136	11	0
1	Y3	1117	0	1136	11	0
1	YD	1117	0	1136	13	0
1	YE	1117	0	1136	10	0
1	YF	1117	0	1136	7	0
1	Z1	1117	0	1136	7	0
1	Z2	1117	0	1136	12	0
1	Z3	1117	0	1136	13	0
1	ZD	1117	0	1136	9	0
1	ZE	1117	0	1136	13	0
1	ZF	1117	0	1136	17	0
All	All	113934	0	115872	1095	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1095) 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:B3:186:ASN:O	1:B3:186:ASN:ND2	2.08	0.86
1:2B:185:THR:HG22	1:2B:186:ASN:H	1.50	0.77
1:Y2:240:ALA:HA	1:Y2:243:LEU:HD12	1.70	0.72
1:N2:185:THR:HG22	1:N2:186:ASN:H	1.56	0.71
1:P2:185:THR:HG22	1:P2:186:ASN:H	1.53	0.71
1:T2:240:ALA:HA	1:T2:243:LEU:HD12	1.71	0.71
1:L2:213:GLU:HG2	1:L2:214:LYS:HD3	1.71	0.71
1:A3:185:THR:HG22	1:A3:186:ASN:H	1.56	0.70
1:2A:295:LEU:HD12	1:2A:296:PRO:HD2	1.73	0.69
1:2F:185:THR:HG22	1:2F:186:ASN:H	1.56	0.69
1:U2:213:GLU:HG2	1:U2:214:LYS:HG2	1.75	0.69
1:X3:182:LEU:HD12	1:X3:189:LEU:HD12	1.74	0.68
1:K2:295:LEU:HD12	1:K2:296:PRO:HD2	1.75	0.68
1:S2:240:ALA:HA	1:S2:243:LEU:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y2:185:THR:HG22	1:Y2:186:ASN:H	1.57	0.68
1:K2:185:THR:HG22	1:K2:186:ASN:H	1.58	0.68
1:E1:185:THR:HG22	1:E1:186:ASN:H	1.59	0.68
1:V2:185:THR:HG22	1:V2:186:ASN:H	1.59	0.68
1:A2:185:THR:HG22	1:A2:186:ASN:H	1.59	0.67
1:K3:185:THR:HG22	1:K3:186:ASN:H	1.59	0.67
1:J2:185:THR:HG22	1:J2:186:ASN:H	1.60	0.67
1:B3:185:THR:HG22	1:B3:186:ASN:H	1.59	0.67
1:T1:200:PRO:O	1:U1:250:LYS:NZ	2.27	0.67
1:U2:185:THR:HG22	1:U2:186:ASN:H	1.60	0.67
1:I2:213:GLU:HG2	1:I2:214:LYS:HG3	1.77	0.67
1:W2:185:THR:HG22	1:W2:186:ASN:H	1.60	0.67
1:L3:160:ARG:NH2	1:L3:215:ARG:O	2.28	0.67
1:M2:185:THR:HG22	1:M2:186:ASN:H	1.59	0.67
1:2A:213:GLU:HG3	1:2A:214:LYS:HG3	1.76	0.67
1:ZF:182:LEU:HD12	1:ZF:189:LEU:HD12	1.76	0.66
1:L3:160:ARG:HE	1:L3:161:PHE:H	1.41	0.66
1:S2:185:THR:HG22	1:S2:186:ASN:H	1.60	0.66
1:D3:200:PRO:O	1:E3:250:LYS:NZ	2.28	0.66
1:K3:230:SER:OG	1:K3:233:CYS:SG	2.53	0.66
1:L2:295:LEU:HD12	1:L2:296:PRO:HD2	1.77	0.66
1:W1:250:LYS:NZ	1:V1:200:PRO:O	2.28	0.66
1:J3:185:THR:HG22	1:J3:186:ASN:H	1.60	0.66
1:H2:185:THR:HG22	1:H2:186:ASN:H	1.61	0.66
1:1D:185:THR:HG22	1:1D:186:ASN:H	1.61	0.66
1:1A:200:PRO:O	1:1B:250:LYS:NZ	2.29	0.66
1:H3:228:LEU:HD22	1:H3:262:LYS:HE3	1.77	0.65
1:B1:185:THR:HG22	1:B1:186:ASN:H	1.60	0.65
1:A1:185:THR:HG22	1:A1:186:ASN:H	1.61	0.65
1:K1:159:GLU:HA	1:K1:215:ARG:HH21	1.61	0.65
1:1C:218:ARG:NH1	1:1C:249:GLN:O	2.29	0.65
1:O1:218:ARG:NH1	1:O1:249:GLN:O	2.30	0.65
1:A3:200:PRO:O	1:B3:250:LYS:NZ	2.29	0.65
1:D1:185:THR:HG22	1:D1:186:ASN:H	1.62	0.64
1:N1:250:LYS:NZ	1:M1:200:PRO:O	2.30	0.64
1:M1:269:ARG:HH21	1:M1:270:PHE:HE2	1.45	0.64
1:ZF:185:THR:HG22	1:ZF:186:ASN:H	1.62	0.64
1:C2:209:SER:O	1:C2:214:LYS:NZ	2.28	0.64
1:E2:240:ALA:HA	1:E2:243:LEU:HD12	1.79	0.64
1:L3:185:THR:HG22	1:L3:186:ASN:H	1.61	0.64
1:R2:185:THR:HG22	1:R2:186:ASN:H	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z3:185:THR:O	1:Z3:188:ARG:NH1	2.31	0.64
1:F1:183:GLU:O	1:F1:188:ARG:NH2	2.31	0.64
1:Q3:185:THR:HG22	1:Q3:186:ASN:H	1.60	0.64
1:H1:185:THR:HG23	1:H1:187:TYR:H	1.63	0.64
1:U3:185:THR:HG22	1:U3:186:ASN:H	1.63	0.64
1:G3:203:CYS:HG	1:G3:206:SER:HG	1.43	0.64
1:K1:185:THR:HG22	1:K1:186:ASN:H	1.62	0.63
1:2E:185:THR:HG22	1:2E:186:ASN:H	1.61	0.63
1:C2:185:THR:HG22	1:C2:186:ASN:H	1.63	0.63
1:3C:185:THR:HG22	1:3C:186:ASN:H	1.61	0.63
1:I1:255:ILE:HD11	1:I1:289:LEU:HD11	1.79	0.63
1:U3:175:VAL:O	1:U3:179:ILE:HG13	1.98	0.63
1:W1:185:THR:HG23	1:W1:187:TYR:H	1.63	0.63
1:G1:175:VAL:O	1:G1:179:ILE:HD12	1.99	0.63
1:T3:185:THR:HG22	1:T3:186:ASN:H	1.64	0.63
1:Z3:185:THR:HG22	1:Z3:186:ASN:H	1.64	0.63
1:F3:175:VAL:O	1:F3:179:ILE:HD12	1.98	0.63
1:O3:185:THR:HG22	1:O3:186:ASN:H	1.64	0.62
1:Y3:218:ARG:NH2	1:Y3:295:LEU:O	2.31	0.62
1:ZD:185:THR:HG22	1:ZD:186:ASN:H	1.64	0.62
1:D3:230:SER:OG	1:D3:233:CYS:SG	2.56	0.62
1:O2:185:THR:HG22	1:O2:186:ASN:H	1.64	0.62
1:P3:185:THR:HG22	1:P3:186:ASN:H	1.63	0.62
1:R2:213:GLU:HG3	1:R2:214:LYS:HG3	1.80	0.62
1:2D:185:THR:HG22	1:2D:186:ASN:H	1.63	0.62
1:S3:185:THR:HG22	1:S3:186:ASN:H	1.62	0.62
1:X3:185:THR:HG22	1:X3:186:ASN:H	1.65	0.62
1:Z2:185:THR:HG22	1:Z2:186:ASN:H	1.63	0.62
1:3D:175:VAL:O	1:3D:179:ILE:HG13	1.99	0.62
1:S3:200:PRO:O	1:T3:250:LYS:NZ	2.33	0.62
1:A2:213:GLU:HG3	1:A2:214:LYS:HG3	1.82	0.62
1:A3:250:LYS:NZ	1:1F:200:PRO:O	2.32	0.62
1:2C:185:THR:HG22	1:2C:186:ASN:H	1.64	0.62
1:F1:185:THR:HG22	1:F1:186:ASN:H	1.63	0.62
1:ZE:185:THR:HG22	1:ZE:186:ASN:H	1.64	0.62
1:E1:186:ASN:ND2	1:E1:186:ASN:O	2.32	0.62
1:J3:230:SER:OG	1:J3:233:CYS:SG	2.57	0.62
1:3B:200:PRO:O	1:3C:250:LYS:NZ	2.33	0.62
1:P3:218:ARG:NH2	1:P3:295:LEU:O	2.33	0.61
1:Q2:185:THR:HG22	1:Q2:186:ASN:H	1.65	0.61
1:C3:185:THR:HG22	1:C3:186:ASN:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E3:185:THR:HG22	1:E3:186:ASN:H	1.64	0.61
1:U3:200:PRO:O	1:V3:250:LYS:NZ	2.33	0.61
1:V1:185:THR:HG23	1:V1:187:TYR:H	1.65	0.61
1:N2:230:SER:OG	1:N2:233:CYS:SG	2.58	0.61
1:D3:175:VAL:O	1:D3:179:ILE:HG13	2.00	0.61
1:O3:230:SER:OG	1:O3:233:CYS:SG	2.58	0.61
1:L2:218:ARG:NH2	1:L2:296:PRO:O	2.34	0.61
1:L3:175:VAL:O	1:L3:179:ILE:HG13	2.01	0.61
1:X2:185:THR:HG22	1:X2:186:ASN:H	1.65	0.61
1:R3:200:PRO:O	1:S3:250:LYS:NZ	2.33	0.61
1:2B:175:VAL:O	1:2B:179:ILE:HD12	1.99	0.60
1:YD:250:LYS:HE3	1:YD:271:ILE:HD11	1.82	0.60
1:G1:295:LEU:HD12	1:G1:296:PRO:HD2	1.83	0.60
1:Z3:174:PHE:O	1:Z3:178:MET:HG3	2.01	0.60
1:W2:230:SER:OG	1:W2:233:CYS:SG	2.60	0.60
1:M1:185:THR:HG22	1:M1:186:ASN:H	1.66	0.60
1:1C:200:PRO:O	1:1D:250:LYS:NZ	2.34	0.60
1:K3:267:ILE:HD12	1:K3:267:ILE:H	1.67	0.60
1:W3:185:THR:HG22	1:W3:186:ASN:H	1.66	0.60
1:W3:211:LEU:HD23	1:W3:215:ARG:HD3	1.84	0.60
1:L1:159:GLU:HA	1:L1:215:ARG:HH21	1.66	0.60
1:P3:218:ARG:NH2	1:P3:296:PRO:O	2.35	0.60
1:D3:185:THR:HG23	1:D3:187:TYR:H	1.66	0.60
1:H3:257:TYR:HA	1:H3:276:TYR:HB3	1.82	0.60
1:Q1:250:LYS:NZ	1:P1:200:PRO:O	2.30	0.60
1:R3:267:ILE:HD12	1:R3:267:ILE:H	1.67	0.60
1:ZD:250:LYS:HE3	1:ZE:202:THR:HG22	1.84	0.60
1:W3:230:SER:OG	1:W3:233:CYS:SG	2.59	0.59
1:B3:218:ARG:NH1	1:B3:249:GLN:O	2.35	0.59
1:E2:185:THR:HG23	1:E2:187:TYR:H	1.67	0.59
1:L3:230:SER:OG	1:L3:233:CYS:SG	2.60	0.59
1:H2:230:SER:OG	1:H2:233:CYS:SG	2.59	0.59
1:H3:209:SER:O	1:H3:214:LYS:NZ	2.35	0.59
1:U1:185:THR:HG22	1:U1:186:ASN:H	1.66	0.59
1:E1:230:SER:OG	1:E1:233:CYS:SG	2.61	0.59
1:T1:183:GLU:O	1:T1:188:ARG:NH2	2.35	0.59
1:B3:200:PRO:O	1:C3:250:LYS:NZ	2.36	0.59
1:2A:185:THR:HG22	1:2A:186:ASN:H	1.65	0.59
1:O1:218:ARG:NH2	1:O1:295:LEU:O	2.34	0.59
1:L3:211:LEU:HA	1:L3:215:ARG:HB2	1.85	0.59
1:G2:185:THR:HG23	1:G2:187:TYR:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G3:209:SER:O	1:G3:214:LYS:NZ	2.35	0.59
1:M3:230:SER:OG	1:M3:233:CYS:SG	2.61	0.59
1:3E:185:THR:HG22	1:3E:186:ASN:H	1.65	0.59
1:T1:250:LYS:NZ	1:S1:200:PRO:O	2.36	0.59
1:F2:185:THR:HG22	1:F2:186:ASN:H	1.68	0.59
1:X1:230:SER:OG	1:X1:233:CYS:SG	2.60	0.58
1:G3:267:ILE:HD12	1:G3:267:ILE:H	1.68	0.58
1:U1:230:SER:OG	1:U1:233:CYS:SG	2.61	0.58
1:D2:230:SER:OG	1:D2:233:CYS:SG	2.59	0.58
1:A3:230:SER:OG	1:A3:233:CYS:SG	2.60	0.58
1:L1:165:ILE:HD11	1:L1:191:LEU:HD23	1.84	0.58
1:T1:230:SER:OG	1:T1:233:CYS:SG	2.62	0.58
1:E2:230:SER:OG	1:E2:233:CYS:SG	2.61	0.58
1:S3:230:SER:OG	1:S3:233:CYS:SG	2.62	0.58
1:1F:185:THR:HG22	1:1F:186:ASN:H	1.66	0.58
1:O3:209:SER:O	1:O3:214:LYS:NZ	2.33	0.58
1:M1:218:ARG:NH1	1:M1:296:PRO:O	2.35	0.58
1:F2:213:GLU:HG3	1:F2:214:LYS:HG3	1.85	0.58
1:Y3:200:PRO:O	1:Z3:250:LYS:NZ	2.35	0.58
1:M2:213:GLU:HG3	1:M2:214:LYS:HG3	1.86	0.58
1:Q1:218:ARG:NH2	1:Q1:296:PRO:O	2.37	0.58
1:Q1:230:SER:OG	1:Q1:233:CYS:SG	2.61	0.58
1:Y3:218:ARG:NH2	1:Y3:296:PRO:O	2.37	0.58
1:Z1:230:SER:OG	1:Z1:233:CYS:SG	2.62	0.58
1:B3:218:ARG:NH2	1:B3:295:LEU:O	2.33	0.58
1:Z2:232:GLU:OE1	1:Z2:232:GLU:N	2.37	0.58
1:L1:207:ILE:HG13	1:L1:211:LEU:HD12	1.86	0.58
1:N1:185:THR:HG23	1:N1:187:TYR:H	1.68	0.58
1:R2:182:LEU:HD12	1:R2:189:LEU:HD12	1.86	0.58
1:L1:162:ASP:OD1	1:L1:217:ARG:NH2	2.36	0.57
1:W2:250:LYS:NZ	1:X2:200:PRO:O	2.36	0.57
1:B3:230:SER:OG	1:B3:233:CYS:SG	2.62	0.57
1:T3:230:SER:OG	1:T3:233:CYS:SG	2.62	0.57
1:T3:267:ILE:HD12	1:T3:267:ILE:H	1.68	0.57
1:S1:230:SER:OG	1:S1:233:CYS:SG	2.60	0.57
1:3A:200:PRO:O	1:3B:250:LYS:NZ	2.37	0.57
1:YF:230:SER:HG	1:YF:233:CYS:HG	1.52	0.57
1:U3:182:LEU:HD22	1:U3:189:LEU:HD12	1.84	0.57
1:2C:159:GLU:OE2	1:2C:215:ARG:NH2	2.37	0.57
1:K1:218:ARG:NH2	1:K1:295:LEU:O	2.38	0.57
1:R1:230:SER:OG	1:R1:233:CYS:SG	2.60	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:257:TYR:HA	1:3A:276:TYR:HB3	1.85	0.57
1:2B:211:LEU:HD23	1:2B:215:ARG:HD3	1.86	0.57
1:YD:230:SER:OG	1:YD:233:CYS:SG	2.63	0.57
1:F3:230:SER:OG	1:F3:233:CYS:SG	2.63	0.57
1:C3:267:ILE:HD12	1:C3:267:ILE:H	1.69	0.57
1:X1:185:THR:HG22	1:X1:186:ASN:H	1.70	0.57
1:J3:250:LYS:HZ2	1:I3:202:THR:HA	1.70	0.57
1:S1:182:LEU:HD22	1:S1:189:LEU:HD12	1.86	0.57
1:W2:232:GLU:N	1:W2:232:GLU:OE1	2.37	0.57
1:E3:267:ILE:HD12	1:E3:267:ILE:H	1.69	0.57
1:R1:200:PRO:O	1:S1:250:LYS:NZ	2.35	0.57
1:U2:232:GLU:OE1	1:U2:232:GLU:N	2.36	0.57
1:V3:230:SER:OG	1:V3:233:CYS:SG	2.62	0.56
1:U3:230:SER:OG	1:U3:233:CYS:SG	2.63	0.56
1:C1:185:THR:HG22	1:C1:186:ASN:H	1.71	0.56
1:L2:166:CYS:HB2	1:L2:219:MET:HE2	1.87	0.56
1:R3:257:TYR:HA	1:R3:276:TYR:HB3	1.86	0.56
1:U2:218:ARG:NH1	1:U2:249:GLN:O	2.38	0.56
1:W2:269:ARG:HH12	1:W2:270:PHE:HE2	1.54	0.56
1:Y1:230:SER:OG	1:Y1:233:CYS:SG	2.64	0.56
1:B3:218:ARG:NH2	1:B3:296:PRO:O	2.38	0.56
1:S1:257:TYR:HA	1:S1:276:TYR:HB3	1.87	0.56
1:2E:230:SER:HG	1:2E:233:CYS:HG	1.51	0.56
1:K1:218:ARG:NH2	1:K1:296:PRO:O	2.37	0.56
1:3E:200:PRO:O	1:3F:250:LYS:NZ	2.38	0.56
1:R2:230:SER:HG	1:R2:233:CYS:HG	1.54	0.56
1:2D:232:GLU:OE1	1:2D:232:GLU:N	2.38	0.56
1:R3:230:SER:OG	1:R3:233:CYS:SG	2.60	0.56
1:ZD:240:ALA:HA	1:ZD:243:LEU:HD12	1.88	0.56
1:F3:185:THR:HG22	1:F3:186:ASN:H	1.71	0.56
1:2C:254:PRO:HG2	1:2C:273:VAL:HA	1.88	0.56
1:1D:162:ASP:OD1	1:1D:217:ARG:NH2	2.36	0.56
1:S1:185:THR:HG23	1:S1:187:TYR:H	1.71	0.56
1:3B:257:TYR:HA	1:3B:276:TYR:HB3	1.88	0.56
1:1E:269:ARG:HH21	1:1E:270:PHE:HE2	1.54	0.56
1:O2:186:ASN:ND2	1:O3:286:TRP:HB3	2.21	0.55
1:3B:267:ILE:HD12	1:3B:267:ILE:H	1.70	0.55
1:1B:230:SER:OG	1:1B:233:CYS:SG	2.63	0.55
1:G2:179:ILE:HD11	1:G2:193:VAL:HG21	1.88	0.55
1:G3:175:VAL:O	1:G3:179:ILE:HG12	2.06	0.55
1:H2:254:PRO:HG2	1:H2:273:VAL:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q2:254:PRO:HG2	1:Q2:273:VAL:HA	1.88	0.55
1:A1:182:LEU:HB3	1:A1:189:LEU:HD12	1.89	0.55
1:V2:230:SER:OG	1:V2:233:CYS:SG	2.65	0.55
1:ZF:254:PRO:HG2	1:ZF:273:VAL:HA	1.87	0.55
1:C1:230:SER:OG	1:C1:233:CYS:SG	2.65	0.55
1:G2:256:LYS:NZ	1:G2:258:LYS:O	2.40	0.55
1:Y3:182:LEU:HB3	1:Y3:189:LEU:HD12	1.87	0.55
1:C3:230:SER:HG	1:C3:233:CYS:HG	1.55	0.55
1:Q1:211:LEU:HD23	1:Q1:215:ARG:HD3	1.89	0.55
1:F2:230:SER:OG	1:F2:233:CYS:SG	2.63	0.55
1:L3:206:SER:O	1:L3:210:GLU:HB2	2.06	0.55
1:3D:159:GLU:HA	1:3D:215:ARG:HH21	1.71	0.55
1:D3:250:LYS:NZ	1:C3:200:PRO:O	2.33	0.55
1:I1:182:LEU:HD22	1:I1:189:LEU:HD12	1.89	0.55
1:B2:185:THR:HG23	1:B2:187:TYR:H	1.72	0.54
1:C3:209:SER:O	1:C3:214:LYS:NZ	2.39	0.54
1:O1:185:THR:HG22	1:O1:186:ASN:H	1.71	0.54
1:S2:213:GLU:HG3	1:S2:214:LYS:HG3	1.88	0.54
1:Y3:218:ARG:NH1	1:Y3:249:GLN:O	2.40	0.54
1:1C:185:THR:HG23	1:1C:187:TYR:H	1.71	0.54
1:C2:240:ALA:HA	1:C2:243:LEU:HD12	1.90	0.54
1:V3:211:LEU:HD23	1:V3:215:ARG:HD3	1.89	0.54
1:R2:230:SER:OG	1:R2:233:CYS:SG	2.63	0.54
1:3D:185:THR:HG22	1:3D:186:ASN:H	1.73	0.54
1:F1:269:ARG:HG3	1:F1:270:PHE:HD1	1.73	0.54
1:I1:160:ARG:NH1	1:I1:214:LYS:O	2.40	0.54
1:D2:185:THR:HG23	1:D2:187:TYR:H	1.73	0.54
1:B1:230:SER:OG	1:B1:233:CYS:SG	2.65	0.54
1:J2:230:SER:OG	1:J2:233:CYS:SG	2.65	0.54
1:Z1:209:SER:O	1:Z1:214:LYS:NZ	2.39	0.54
1:3C:230:SER:OG	1:3C:233:CYS:SG	2.64	0.54
1:YE:211:LEU:HD23	1:YE:215:ARG:HG3	1.88	0.54
1:C2:230:SER:HG	1:C2:233:CYS:HG	1.55	0.54
1:U2:257:TYR:HA	1:U2:276:TYR:HB3	1.89	0.54
1:1C:230:SER:HG	1:1C:233:CYS:HG	1.54	0.54
1:D3:182:LEU:HB3	1:D3:189:LEU:HD12	1.89	0.54
1:E1:178:MET:HG2	1:E1:182:LEU:HD12	1.90	0.54
1:S2:230:SER:OG	1:S2:233:CYS:SG	2.63	0.54
1:1A:257:TYR:HA	1:1A:276:TYR:HB3	1.90	0.54
1:F2:178:MET:HG3	1:F2:182:LEU:HD12	1.88	0.54
1:O1:218:ARG:NH2	1:O1:296:PRO:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D3:269:ARG:HH21	1:D3:270:PHE:HE1	1.54	0.54
1:J1:269:ARG:HH21	1:J1:270:PHE:HE1	1.56	0.54
1:U2:175:VAL:O	1:U2:179:ILE:HG13	2.08	0.54
1:C3:230:SER:OG	1:C3:233:CYS:SG	2.66	0.53
1:V2:230:SER:HG	1:V2:233:CYS:HG	1.53	0.53
1:3D:230:SER:OG	1:3D:233:CYS:SG	2.66	0.53
1:YE:182:LEU:HB3	1:YE:189:LEU:HD12	1.90	0.53
1:S2:179:ILE:HG22	1:S2:191:LEU:HD12	1.90	0.53
1:L1:230:SER:OG	1:L1:233:CYS:SG	2.62	0.53
1:R1:211:LEU:HA	1:R1:215:ARG:HD3	1.90	0.53
1:H1:211:LEU:HD23	1:H1:215:ARG:HG3	1.89	0.53
1:I1:183:GLU:O	1:I1:188:ARG:NH2	2.42	0.53
1:L2:240:ALA:HA	1:L2:243:LEU:HD12	1.91	0.53
1:G3:218:ARG:HD2	1:G3:251:ARG:HA	1.91	0.53
1:H3:230:SER:OG	1:H3:233:CYS:SG	2.61	0.53
1:P3:230:SER:OG	1:P3:233:CYS:SG	2.67	0.53
1:S3:182:LEU:HD22	1:S3:189:LEU:HD12	1.89	0.53
1:1A:162:ASP:OD1	1:1A:217:ARG:NH2	2.37	0.53
1:F2:249:GLN:OE1	1:F2:251:ARG:HB2	2.09	0.53
1:B3:175:VAL:O	1:B3:179:ILE:HG13	2.07	0.53
1:I2:185:THR:HG23	1:I2:187:TYR:H	1.73	0.53
1:H2:179:ILE:HD11	1:H2:193:VAL:HG21	1.90	0.53
1:2F:186:ASN:ND2	1:3F:286:TRP:HB3	2.24	0.53
1:E2:213:GLU:HG2	1:E2:214:LYS:HD3	1.91	0.53
1:N3:165:ILE:HD11	1:N3:191:LEU:HD13	1.91	0.53
1:Y1:211:LEU:HD23	1:Y1:215:ARG:HD3	1.91	0.53
1:N1:230:SER:OG	1:N1:233:CYS:SG	2.58	0.52
1:Y1:162:ASP:OD1	1:Y1:217:ARG:NH2	2.42	0.52
1:V1:230:SER:OG	1:V1:233:CYS:SG	2.67	0.52
1:1A:230:SER:OG	1:1A:233:CYS:SG	2.67	0.52
1:2D:185:THR:HG22	1:2D:186:ASN:N	2.24	0.52
1:YE:230:SER:OG	1:YE:233:CYS:SG	2.65	0.52
1:3F:178:MET:HG2	1:3F:182:LEU:HD12	1.92	0.52
1:S1:218:ARG:NH2	1:S1:296:PRO:O	2.42	0.52
1:3D:178:MET:HG2	1:3D:182:LEU:HD12	1.91	0.52
1:3D:269:ARG:HG3	1:3D:269:ARG:HH11	1.74	0.52
1:ZF:224:SER:OG	1:ZF:225:ASP:N	2.42	0.52
1:F2:186:ASN:ND2	1:F3:286:TRP:HB3	2.24	0.52
1:H3:162:ASP:OD1	1:H3:217:ARG:NH1	2.43	0.52
1:1C:257:TYR:HA	1:1C:276:TYR:HB3	1.91	0.52
1:I1:230:SER:OG	1:I1:233:CYS:SG	2.65	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P3:200:PRO:O	1:Q3:250:LYS:NZ	2.43	0.52
1:R1:230:SER:HG	1:R1:233:CYS:HG	1.53	0.52
1:W1:257:TYR:HA	1:W1:276:TYR:HB3	1.91	0.52
1:A2:224:SER:OG	1:A2:225:ASP:N	2.42	0.52
1:H1:254:PRO:HG2	1:H1:273:VAL:HA	1.92	0.52
1:I3:228:LEU:HD21	1:I3:265:PRO:HG3	1.92	0.52
1:T1:185:THR:HG22	1:T1:186:ASN:H	1.73	0.52
1:1E:185:THR:HG22	1:1E:186:ASN:H	1.74	0.52
1:T2:209:SER:O	1:T2:214:LYS:NZ	2.40	0.52
1:1D:230:SER:OG	1:1D:233:CYS:SG	2.67	0.52
1:2F:230:SER:HG	1:2F:233:CYS:HG	1.52	0.52
1:D3:257:TYR:HA	1:D3:276:TYR:HB3	1.91	0.51
1:P3:218:ARG:NH1	1:P3:249:GLN:O	2.43	0.51
1:3F:185:THR:O	1:3F:188:ARG:NH1	2.40	0.51
1:W1:230:SER:OG	1:W1:233:CYS:SG	2.67	0.51
1:E3:165:ILE:HD11	1:E3:191:LEU:HD13	1.92	0.51
1:F1:230:SER:OG	1:F1:233:CYS:SG	2.69	0.51
1:P1:230:SER:OG	1:P1:233:CYS:SG	2.65	0.51
1:2B:230:SER:OG	1:2B:233:CYS:SG	2.69	0.51
1:E1:202:THR:HG22	1:F1:250:LYS:HE2	1.92	0.51
1:D1:230:SER:OG	1:D1:233:CYS:SG	2.69	0.51
1:D1:254:PRO:HG2	1:D1:273:VAL:HA	1.92	0.51
1:C1:159:GLU:HA	1:C1:215:ARG:HH21	1.76	0.51
1:M2:254:PRO:HG2	1:M2:273:VAL:HA	1.93	0.51
1:T3:200:PRO:O	1:U3:250:LYS:NZ	2.40	0.51
1:S2:224:SER:OG	1:S2:225:ASP:N	2.43	0.51
1:T1:254:PRO:HG2	1:T1:273:VAL:HA	1.92	0.51
1:Q1:182:LEU:HB3	1:Q1:189:LEU:HD12	1.93	0.51
1:2A:232:GLU:OE2	1:2A:232:GLU:N	2.42	0.51
1:3B:230:SER:OG	1:3B:233:CYS:SG	2.67	0.51
1:I1:162:ASP:OD1	1:I1:217:ARG:NH2	2.34	0.51
1:N1:178:MET:HG2	1:N1:182:LEU:HD12	1.93	0.51
1:W2:185:THR:HG22	1:W2:186:ASN:N	2.23	0.51
1:A1:269:ARG:HG3	1:A1:270:PHE:HD1	1.76	0.51
1:Q3:257:TYR:HA	1:Q3:276:TYR:HB3	1.93	0.51
1:U3:254:PRO:HG2	1:U3:273:VAL:HA	1.91	0.51
1:ZD:267:ILE:HG23	1:ZD:268:LEU:HG	1.93	0.51
1:M1:211:LEU:HA	1:M1:215:ARG:HD3	1.92	0.51
1:2D:257:TYR:HA	1:2D:276:TYR:HB3	1.92	0.51
1:ZE:213:GLU:HG3	1:ZE:243:LEU:HD11	1.92	0.51
1:A1:230:SER:OG	1:A1:233:CYS:SG	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F1:269:ARG:HG3	1:F1:270:PHE:CD1	2.47	0.50
1:Z2:175:VAL:O	1:Z2:179:ILE:HD12	2.11	0.50
1:1C:218:ARG:NH2	1:1C:296:PRO:O	2.43	0.50
1:3D:200:PRO:O	1:3E:250:LYS:NZ	2.42	0.50
1:1E:257:TYR:HA	1:1E:276:TYR:HB3	1.93	0.50
1:H3:160:ARG:NH2	1:H3:215:ARG:O	2.44	0.50
1:1C:230:SER:OG	1:1C:233:CYS:SG	2.65	0.50
1:YF:211:LEU:HD23	1:YF:215:ARG:HG3	1.93	0.50
1:T1:211:LEU:HD23	1:T1:215:ARG:HG3	1.91	0.50
1:T3:269:ARG:HG3	1:T3:269:ARG:HH11	1.75	0.50
1:K2:211:LEU:HD23	1:K2:215:ARG:HG3	1.94	0.50
1:U1:211:LEU:HD23	1:U1:215:ARG:HD3	1.94	0.50
1:2E:249:GLN:HG2	1:2E:251:ARG:HG3	1.94	0.50
1:H2:213:GLU:HG3	1:H2:214:LYS:HG3	1.94	0.50
1:Q3:224:SER:OG	1:Q3:225:ASP:N	2.44	0.50
1:R3:174:PHE:O	1:R3:178:MET:HG3	2.11	0.50
1:E2:257:TYR:HA	1:E2:276:TYR:HB3	1.92	0.50
1:Z3:160:ARG:NH1	1:Z3:214:LYS:O	2.45	0.50
1:E2:224:SER:OG	1:E2:225:ASP:N	2.45	0.50
1:F3:198:VAL:O	1:G3:288:ARG:NH1	2.44	0.50
1:U2:249:GLN:HE22	1:U2:251:ARG:HB2	1.76	0.50
1:K3:206:SER:O	1:K3:210:GLU:HB3	2.11	0.50
1:G2:224:SER:OG	1:G2:225:ASP:N	2.45	0.50
1:M1:211:LEU:HD23	1:M1:215:ARG:HD3	1.93	0.50
1:1A:254:PRO:HG2	1:1A:273:VAL:HA	1.94	0.50
1:YD:208:ALA:HA	1:YD:212:ILE:HD13	1.94	0.50
1:B2:213:GLU:HG2	1:B2:214:LYS:HG3	1.93	0.49
1:J3:165:ILE:HD11	1:J3:191:LEU:HD13	1.94	0.49
1:O2:183:GLU:HG3	1:O2:189:LEU:O	2.11	0.49
1:V3:185:THR:HG22	1:V3:186:ASN:H	1.77	0.49
1:Z3:257:TYR:HA	1:Z3:276:TYR:HB3	1.94	0.49
1:3B:185:THR:HG22	1:3B:186:ASN:N	2.28	0.49
1:2E:174:PHE:O	1:2E:178:MET:HG3	2.12	0.49
1:YE:269:ARG:HG3	1:YE:269:ARG:HH11	1.77	0.49
1:K1:183:GLU:O	1:K1:188:ARG:NH2	2.45	0.49
1:R2:211:LEU:HA	1:R2:215:ARG:HB2	1.95	0.49
1:V1:159:GLU:HA	1:V1:215:ARG:HH21	1.77	0.49
1:Y2:230:SER:OG	1:Y2:233:CYS:SG	2.67	0.49
1:2A:186:ASN:ND2	1:3A:286:TRP:HB3	2.28	0.49
1:C1:183:GLU:O	1:C1:188:ARG:NH1	2.45	0.49
1:Z2:207:ILE:HB	1:Z2:211:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:179:ILE:HG23	1:3A:183:GLU:OE1	2.13	0.49
1:Z3:230:SER:OG	1:Z3:233:CYS:SG	2.66	0.49
1:J2:254:PRO:HG2	1:J2:273:VAL:HA	1.95	0.49
1:I2:275:ASP:OD1	1:I2:276:TYR:N	2.45	0.49
1:S1:211:LEU:HD23	1:S1:215:ARG:HD3	1.95	0.49
1:V2:215:ARG:HG3	1:V2:215:ARG:HH11	1.77	0.49
1:Z2:213:GLU:HG2	1:Z2:214:LYS:HG3	1.95	0.49
1:E2:211:LEU:HD23	1:E2:215:ARG:HG3	1.93	0.49
1:F2:269:ARG:HH22	1:F2:270:PHE:HE2	1.61	0.49
1:Q3:230:SER:OG	1:Q3:233:CYS:SG	2.61	0.49
1:Y3:257:TYR:HA	1:Y3:276:TYR:HB3	1.94	0.49
1:Q1:172:ILE:O	1:Q1:176:GLN:HG2	2.12	0.49
1:U2:230:SER:OG	1:U2:233:CYS:SG	2.70	0.49
1:2E:224:SER:OG	1:2E:225:ASP:N	2.46	0.49
1:G3:176:GLN:NE2	1:H3:280:CYS:SG	2.86	0.49
1:R3:197:ASP:N	1:R3:197:ASP:OD1	2.46	0.49
1:Z2:254:PRO:HG2	1:Z2:273:VAL:HA	1.94	0.49
1:2C:279:PRO:HA	1:2C:282:LYS:HE2	1.95	0.49
1:YF:230:SER:OG	1:YF:233:CYS:SG	2.63	0.49
1:K2:185:THR:HG22	1:K2:186:ASN:N	2.26	0.49
1:P2:249:GLN:OE1	1:P2:251:ARG:HB2	2.13	0.49
1:Q2:230:SER:OG	1:Q2:233:CYS:SG	2.70	0.49
1:3B:185:THR:HG22	1:3B:186:ASN:H	1.78	0.49
1:3D:254:PRO:HG2	1:3D:273:VAL:HA	1.94	0.49
1:2E:257:TYR:HA	1:2E:276:TYR:HB3	1.93	0.49
1:G3:173:GLN:OE1	1:G3:173:GLN:N	2.40	0.48
1:V3:160:ARG:NH1	1:V3:214:LYS:O	2.46	0.48
1:I1:232:GLU:OE1	1:I1:232:GLU:N	2.42	0.48
1:Y2:185:THR:HG22	1:Y2:186:ASN:N	2.26	0.48
1:2F:275:ASP:OD1	1:2F:276:TYR:N	2.46	0.48
1:D1:232:GLU:OE2	1:D1:232:GLU:N	2.43	0.48
1:H2:189:LEU:HD13	1:H2:293:LEU:HD11	1.93	0.48
1:M1:230:SER:HG	1:M1:233:CYS:HG	1.61	0.48
1:T2:159:GLU:OE2	1:T2:215:ARG:NH2	2.46	0.48
1:2A:269:ARG:HH21	1:2A:270:PHE:HE2	1.59	0.48
1:1D:213:GLU:HG3	1:1D:214:LYS:HG3	1.95	0.48
1:R3:254:PRO:HG2	1:R3:273:VAL:HA	1.94	0.48
1:W3:257:TYR:HA	1:W3:276:TYR:HB3	1.95	0.48
1:YF:232:GLU:OE1	1:YF:232:GLU:N	2.43	0.48
1:I2:224:SER:OG	1:I2:225:ASP:N	2.47	0.48
1:N3:185:THR:HG22	1:N3:186:ASN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O2:224:SER:OG	1:O2:225:ASP:N	2.46	0.48
1:R3:185:THR:HG22	1:R3:186:ASN:H	1.77	0.48
1:P1:165:ILE:HD11	1:P1:191:LEU:HD13	1.96	0.48
1:Y3:211:LEU:HD23	1:Y3:215:ARG:HG3	1.95	0.48
1:3D:215:ARG:HG3	1:3D:215:ARG:HH11	1.79	0.48
1:A2:230:SER:OG	1:A2:233:CYS:SG	2.67	0.48
1:K1:211:LEU:HD23	1:K1:215:ARG:HG3	1.95	0.48
1:H1:230:SER:HG	1:H1:233:CYS:HG	1.58	0.48
1:V2:224:SER:OG	1:V2:225:ASP:N	2.47	0.48
1:V1:257:TYR:HA	1:V1:276:TYR:HB3	1.95	0.48
1:2A:281:THR:HG22	1:2A:284:TRP:HZ3	1.78	0.48
1:C2:224:SER:OG	1:C2:225:ASP:N	2.46	0.48
1:G1:159:GLU:O	1:G1:215:ARG:NE	2.39	0.48
1:3A:254:PRO:HG2	1:3A:273:VAL:HA	1.96	0.48
1:F1:211:LEU:HD23	1:F1:215:ARG:HG3	1.94	0.48
1:J2:224:SER:OG	1:J2:225:ASP:N	2.45	0.48
1:I3:254:PRO:HG2	1:I3:273:VAL:HA	1.96	0.48
1:N3:254:PRO:HG2	1:N3:273:VAL:HA	1.96	0.48
1:ZF:159:GLU:HA	1:ZF:215:ARG:HH21	1.78	0.48
1:D1:267:ILE:HD12	1:D1:267:ILE:H	1.79	0.48
1:V3:182:LEU:HD22	1:V3:189:LEU:HD12	1.96	0.48
1:2C:230:SER:HG	1:2C:233:CYS:HG	1.62	0.48
1:2D:275:ASP:OD1	1:2D:276:TYR:N	2.47	0.48
1:2E:275:ASP:OD1	1:2E:276:TYR:N	2.47	0.48
1:K1:179:ILE:HG22	1:K1:191:LEU:HD12	1.94	0.48
1:K1:269:ARG:HG3	1:K1:270:PHE:CD2	2.49	0.48
1:H1:230:SER:OG	1:H1:233:CYS:SG	2.66	0.48
1:U2:215:ARG:HG3	1:U2:215:ARG:HH11	1.77	0.48
1:ZD:280:CYS:SG	1:ZE:176:GLN:NE2	2.87	0.48
1:B3:165:ILE:HD11	1:B3:191:LEU:HD13	1.95	0.47
1:M2:230:SER:OG	1:M2:233:CYS:SG	2.69	0.47
1:X1:182:LEU:HB3	1:X1:189:LEU:HD12	1.96	0.47
1:2B:185:THR:HG22	1:2B:186:ASN:N	2.22	0.47
1:2B:257:TYR:HA	1:2B:276:TYR:HB3	1.95	0.47
1:ZF:211:LEU:HD23	1:ZF:215:ARG:HG3	1.96	0.47
1:T2:254:PRO:HG2	1:T2:273:VAL:HA	1.94	0.47
1:V1:188:ARG:HA	1:V1:188:ARG:HD3	1.75	0.47
1:D2:249:GLN:OE1	1:D2:251:ARG:HB2	2.15	0.47
1:A3:171:ASP:OD1	1:A3:257:TYR:OH	2.31	0.47
1:X2:257:TYR:HA	1:X2:276:TYR:HB3	1.97	0.47
1:3B:165:ILE:HD11	1:3B:191:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J2:176:GLN:NE2	1:I2:280:CYS:SG	2.88	0.47
1:2B:232:GLU:OE2	1:2B:232:GLU:N	2.47	0.47
1:2F:160:ARG:NH1	1:2F:215:ARG:O	2.48	0.47
1:2F:211:LEU:HA	1:2F:215:ARG:HB2	1.96	0.47
1:A3:202:THR:HG22	1:B3:250:LYS:HD2	1.97	0.47
1:C1:184:GLN:HA	1:C1:188:ARG:HH12	1.79	0.47
1:J2:257:TYR:HA	1:J2:276:TYR:HB3	1.96	0.47
1:H3:232:GLU:OE2	1:H3:232:GLU:N	2.47	0.47
1:W1:232:GLU:OE2	1:W1:232:GLU:N	2.43	0.47
1:X3:160:ARG:HE	1:X3:160:ARG:HA	1.80	0.47
1:Y3:209:SER:O	1:Y3:214:LYS:NZ	2.32	0.47
1:F1:254:PRO:HG2	1:F1:273:VAL:HA	1.97	0.47
1:F2:161:PHE:CG	1:F2:192:CYS:HB2	2.50	0.47
1:G2:209:SER:O	1:G2:214:LYS:NZ	2.36	0.47
1:I2:269:ARG:HE	1:I2:270:PHE:HE2	1.62	0.47
1:O1:182:LEU:HB3	1:O1:189:LEU:HD12	1.96	0.47
1:S3:267:ILE:HG23	1:S3:268:LEU:HG	1.97	0.47
1:3A:183:GLU:HG2	1:3A:189:LEU:O	2.15	0.47
1:2F:185:THR:HG22	1:2F:186:ASN:N	2.27	0.47
1:D1:211:LEU:HD23	1:D1:215:ARG:HG3	1.96	0.47
1:K1:254:PRO:HG2	1:K1:273:VAL:HA	1.96	0.47
1:L2:230:SER:OG	1:L2:233:CYS:SG	2.66	0.47
1:I2:209:SER:O	1:I2:214:LYS:NZ	2.45	0.47
1:N2:185:THR:HG22	1:N2:186:ASN:N	2.27	0.47
1:R2:275:ASP:OD1	1:R2:276:TYR:N	2.48	0.47
1:V1:211:LEU:HD23	1:V1:215:ARG:HG3	1.97	0.47
1:3C:178:MET:HG2	1:3C:182:LEU:HD12	1.97	0.47
1:1F:182:LEU:HD22	1:1F:189:LEU:HD12	1.97	0.47
1:E1:186:ASN:ND2	1:E1:186:ASN:C	2.68	0.47
1:A3:185:THR:HG22	1:A3:186:ASN:N	2.26	0.47
1:B2:260:MET:HE1	1:B2:264:PHE:HD1	1.80	0.47
1:B3:230:SER:HG	1:B3:233:CYS:HG	1.62	0.47
1:I2:267:ILE:HG23	1:I2:268:LEU:HG	1.97	0.47
1:T2:213:GLU:HG3	1:T2:243:LEU:HD21	1.97	0.47
1:1D:286:TRP:HB3	1:ZD:186:ASN:ND2	2.29	0.47
1:E2:182:LEU:HD22	1:E2:189:LEU:HD12	1.97	0.47
1:F3:183:GLU:HG2	1:F3:189:LEU:O	2.14	0.47
1:O1:269:ARG:HD2	1:O1:269:ARG:O	2.15	0.47
1:V3:218:ARG:NH1	1:V3:295:LEU:O	2.47	0.47
1:Y2:179:ILE:HD11	1:Y2:193:VAL:HG21	1.97	0.47
1:F3:230:SER:HG	1:F3:233:CYS:HG	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V2:249:GLN:OE1	1:V2:251:ARG:HB2	2.15	0.47
1:X2:232:GLU:OE1	1:X2:232:GLU:N	2.39	0.47
1:F2:185:THR:HG22	1:F2:186:ASN:N	2.29	0.46
1:C1:211:LEU:HD23	1:C1:215:ARG:HG3	1.97	0.46
1:J3:254:PRO:HG2	1:J3:273:VAL:HA	1.97	0.46
1:H1:199:LEU:HD11	1:I1:291:LYS:HD2	1.97	0.46
1:P1:160:ARG:HE	1:P1:160:ARG:HB3	1.58	0.46
1:S3:218:ARG:NH1	1:S3:296:PRO:O	2.39	0.46
1:3B:230:SER:HG	1:3B:233:CYS:HG	1.63	0.46
1:3F:228:LEU:HD21	1:3F:265:PRO:HG3	1.96	0.46
1:J2:168:CYS:SG	1:J2:169:PRO:HD2	2.56	0.46
1:O3:200:PRO:O	1:P3:250:LYS:NZ	2.46	0.46
1:U1:269:ARG:HH21	1:U1:270:PHE:HE1	1.63	0.46
1:V1:275:ASP:OD1	1:V1:276:TYR:N	2.48	0.46
1:L1:242:SER:HA	1:L2:205:TRP:HB3	1.98	0.46
1:H3:179:ILE:HG23	1:H3:183:GLU:OE2	2.15	0.46
1:R2:254:PRO:HG2	1:R2:273:VAL:HA	1.96	0.46
1:R2:267:ILE:HG23	1:R2:268:LEU:HG	1.97	0.46
1:Y2:266:SER:O	1:Y2:269:ARG:HG2	2.16	0.46
1:2F:232:GLU:OE2	1:2F:232:GLU:N	2.46	0.46
1:E2:254:PRO:HG2	1:E2:273:VAL:HA	1.97	0.46
1:J1:182:LEU:HB3	1:J1:189:LEU:HD12	1.97	0.46
1:I1:175:VAL:O	1:I1:179:ILE:HG13	2.14	0.46
1:3C:257:TYR:HA	1:3C:276:TYR:HB3	1.97	0.46
1:A2:254:PRO:HG2	1:A2:273:VAL:HA	1.97	0.46
1:N3:257:TYR:HA	1:N3:276:TYR:HB3	1.96	0.46
1:O2:261:LYS:HE3	1:O2:261:LYS:HB2	1.77	0.46
1:M1:213:GLU:HG2	1:M1:214:LYS:HZ2	1.79	0.46
1:M1:275:ASP:OD1	1:M1:276:TYR:N	2.49	0.46
1:U3:267:ILE:HG23	1:U3:268:LEU:HG	1.97	0.46
1:1A:287:THR:O	1:1A:291:LYS:HG3	2.14	0.46
1:ZE:165:ILE:HG22	1:ZE:167:TYR:HD1	1.81	0.46
1:1F:232:GLU:OE1	1:1F:232:GLU:N	2.46	0.46
1:K2:257:TYR:HA	1:K2:276:TYR:HB3	1.96	0.46
1:M2:207:ILE:HG23	1:M2:211:LEU:HD12	1.98	0.46
1:M1:232:GLU:OE1	1:M1:232:GLU:N	2.45	0.46
1:U3:230:SER:HG	1:U3:233:CYS:HG	1.55	0.46
1:Y1:232:GLU:OE1	1:Y1:232:GLU:N	2.42	0.46
1:I1:275:ASP:OD1	1:I1:277:THR:HG22	2.15	0.46
1:S2:257:TYR:HA	1:S2:276:TYR:HB3	1.97	0.46
1:2D:164:PHE:HB2	1:2D:216:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:182:LEU:HD22	1:C2:189:LEU:HD12	1.97	0.46
1:L1:243:LEU:HD11	1:L1:251:ARG:NH1	2.31	0.46
1:R3:232:GLU:OE1	1:R3:232:GLU:N	2.46	0.46
1:U2:211:LEU:HA	1:U2:215:ARG:HB2	1.96	0.46
1:2C:257:TYR:OH	1:2C:258:LYS:NZ	2.49	0.46
1:ZF:179:ILE:O	1:ZF:183:GLU:HB2	2.16	0.46
1:E1:186:ASN:C	1:E1:186:ASN:HD22	2.09	0.46
1:B3:257:TYR:HA	1:B3:276:TYR:HB3	1.97	0.46
1:J2:215:ARG:HG3	1:J2:215:ARG:HH11	1.80	0.46
1:G3:295:LEU:HD12	1:G3:296:PRO:HD2	1.98	0.46
1:P3:211:LEU:HD23	1:P3:215:ARG:HG3	1.98	0.46
1:V1:249:GLN:HB3	1:V1:251:ARG:HG3	1.98	0.46
1:H1:159:GLU:HA	1:H1:215:ARG:HH21	1.81	0.46
1:O3:182:LEU:HD22	1:O3:189:LEU:HD12	1.97	0.46
1:P2:224:SER:OG	1:P2:225:ASP:N	2.49	0.46
1:S2:211:LEU:HA	1:S2:215:ARG:HB2	1.98	0.46
1:T1:232:GLU:OE1	1:T1:232:GLU:N	2.45	0.46
1:W2:249:GLN:OE1	1:W2:251:ARG:HB2	2.16	0.46
1:X1:232:GLU:OE2	1:X1:232:GLU:N	2.43	0.46
1:F1:243:LEU:HD23	1:F1:243:LEU:HA	1.84	0.45
1:J1:185:THR:HG22	1:J1:186:ASN:H	1.82	0.45
1:3D:267:ILE:HG23	1:3D:268:LEU:HG	1.97	0.45
1:P3:254:PRO:HG2	1:P3:273:VAL:HA	1.97	0.45
1:V2:185:THR:HG22	1:V2:186:ASN:N	2.27	0.45
1:X2:224:SER:OG	1:X2:225:ASP:N	2.50	0.45
1:ZE:206:SER:O	1:ZE:210:GLU:HB2	2.17	0.45
1:ZF:186:ASN:O	1:ZF:188:ARG:NE	2.49	0.45
1:D2:213:GLU:HG3	1:D2:214:LYS:HG3	1.98	0.45
1:D3:251:ARG:HE	1:D3:251:ARG:HB3	1.53	0.45
1:K2:183:GLU:HG2	1:K2:189:LEU:O	2.15	0.45
1:O2:254:PRO:HG2	1:O2:273:VAL:HA	1.98	0.45
1:T2:266:SER:O	1:T2:269:ARG:HG2	2.15	0.45
1:1B:218:ARG:NH1	1:1B:249:GLN:O	2.49	0.45
1:ZD:209:SER:O	1:ZD:214:LYS:NZ	2.38	0.45
1:K3:254:PRO:HG2	1:K3:273:VAL:HA	1.99	0.45
1:K3:269:ARG:HG3	1:K3:270:PHE:CD1	2.52	0.45
1:I2:251:ARG:O	1:I2:251:ARG:HG2	2.16	0.45
1:I3:185:THR:HG22	1:I3:186:ASN:H	1.80	0.45
1:Q2:182:LEU:HD22	1:Q2:189:LEU:HD12	1.98	0.45
1:Q2:257:TYR:HA	1:Q2:276:TYR:HB3	1.98	0.45
1:Q2:269:ARG:HH22	1:Q2:270:PHE:HE2	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YE:257:TYR:HA	1:YE:276:TYR:HB3	1.98	0.45
1:J2:275:ASP:OD1	1:J2:276:TYR:N	2.49	0.45
1:I2:178:MET:HG2	1:I2:182:LEU:HD12	1.99	0.45
1:M3:257:TYR:HA	1:M3:276:TYR:HB3	1.99	0.45
1:P2:275:ASP:OD1	1:P2:276:TYR:N	2.50	0.45
1:1F:232:GLU:O	1:1F:236:GLN:HG3	2.16	0.45
1:2F:165:ILE:HD11	1:2F:191:LEU:HB3	1.98	0.45
1:B3:254:PRO:HG2	1:B3:273:VAL:HA	1.99	0.45
1:H2:224:SER:OG	1:H2:225:ASP:N	2.50	0.45
1:I1:185:THR:HG22	1:I1:186:ASN:H	1.82	0.45
1:R1:232:GLU:OE1	1:R1:232:GLU:N	2.44	0.45
1:S3:178:MET:HG2	1:S3:182:LEU:HD12	1.99	0.45
1:T2:185:THR:HG22	1:T2:186:ASN:N	2.32	0.45
1:V2:232:GLU:O	1:V2:236:GLN:HG3	2.16	0.45
1:Y1:230:SER:HG	1:Y1:233:CYS:HG	1.64	0.45
1:Y1:257:TYR:HA	1:Y1:276:TYR:HB3	1.99	0.45
1:YD:281:THR:HG22	1:YD:284:TRP:HZ3	1.81	0.45
1:K3:188:ARG:HA	1:K3:188:ARG:HD3	1.76	0.45
1:W2:275:ASP:OD2	1:W2:276:TYR:N	2.50	0.45
1:Z2:230:SER:OG	1:Z2:233:CYS:SG	2.68	0.45
1:H3:295:LEU:HD12	1:H3:296:PRO:HD2	1.99	0.45
1:I2:161:PHE:CG	1:I2:192:CYS:HB2	2.52	0.45
1:O3:257:TYR:HA	1:O3:276:TYR:HB3	1.98	0.45
1:Q3:264:PHE:CG	1:Q3:265:PRO:HD2	2.52	0.45
1:W3:159:GLU:HA	1:W3:215:ARG:HH21	1.81	0.45
1:3E:160:ARG:NH1	1:3E:214:LYS:O	2.43	0.45
1:P2:257:TYR:HA	1:P2:276:TYR:HB3	1.99	0.45
1:X3:257:TYR:HA	1:X3:276:TYR:HB3	1.98	0.45
1:B1:165:ILE:HD11	1:B1:191:LEU:HD13	1.98	0.45
1:J1:230:SER:OG	1:J1:233:CYS:SG	2.73	0.45
1:G3:257:TYR:HA	1:G3:276:TYR:HB3	1.98	0.45
1:O1:250:LYS:HB3	1:O1:250:LYS:HE2	1.81	0.45
1:S2:269:ARG:HH22	1:S2:270:PHE:HE2	1.65	0.45
1:T1:257:TYR:HA	1:T1:276:TYR:HB3	1.98	0.45
1:W2:257:TYR:HA	1:W2:276:TYR:HB3	1.98	0.45
1:2F:295:LEU:HD23	1:2F:295:LEU:HA	1.89	0.45
1:D1:230:SER:HG	1:D1:233:CYS:HG	1.60	0.44
1:L3:215:ARG:HG3	1:L3:215:ARG:HH11	1.81	0.44
1:M1:254:PRO:HG2	1:M1:273:VAL:HA	1.99	0.44
1:M1:269:ARG:HD2	1:M1:269:ARG:O	2.17	0.44
1:Q1:224:SER:OG	1:Q1:225:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R2:250:LYS:HB2	1:R2:250:LYS:HE2	1.77	0.44
1:X3:200:PRO:O	1:Y3:250:LYS:NZ	2.49	0.44
1:2A:185:THR:HG22	1:2A:186:ASN:N	2.32	0.44
1:3C:269:ARG:HH21	1:3C:270:PHE:HE1	1.64	0.44
1:3D:210:GLU:O	1:3D:215:ARG:HG2	2.18	0.44
1:J3:250:LYS:NZ	1:I3:202:THR:HG22	2.32	0.44
1:L2:211:LEU:HD23	1:L2:215:ARG:HG3	1.99	0.44
1:H2:183:GLU:HG2	1:H2:189:LEU:O	2.15	0.44
1:N2:165:ILE:HD11	1:N2:191:LEU:HD13	1.99	0.44
1:U1:173:GLN:H	1:U1:173:GLN:CD	2.20	0.44
1:W2:281:THR:HG22	1:W2:284:TRP:HZ3	1.81	0.44
1:X3:160:ARG:NH2	1:X3:215:ARG:HA	2.33	0.44
1:1F:257:TYR:HA	1:1F:276:TYR:HB3	1.98	0.44
1:B3:173:GLN:H	1:B3:173:GLN:CD	2.20	0.44
1:C2:186:ASN:ND2	1:C3:286:TRP:HB3	2.33	0.44
1:K1:232:GLU:O	1:K1:236:GLN:HG3	2.17	0.44
1:L2:208:ALA:HA	1:L2:212:ILE:HD12	1.99	0.44
1:L3:278:ASN:O	1:L3:282:LYS:HG3	2.17	0.44
1:P1:232:GLU:OE1	1:P1:232:GLU:N	2.44	0.44
1:V2:281:THR:HG22	1:V2:284:TRP:HZ3	1.83	0.44
1:W1:232:GLU:O	1:W1:236:GLN:HG3	2.16	0.44
1:X1:185:THR:HG22	1:X1:186:ASN:N	2.33	0.44
1:1A:160:ARG:HA	1:1A:160:ARG:HD2	1.73	0.44
1:2B:250:LYS:HD3	1:2C:202:THR:HA	1.99	0.44
1:D1:243:LEU:HD23	1:D1:243:LEU:HA	1.87	0.44
1:D1:257:TYR:HA	1:D1:276:TYR:HB3	1.99	0.44
1:C3:232:GLU:OE1	1:C3:232:GLU:N	2.43	0.44
1:N2:254:PRO:HG2	1:N2:273:VAL:HA	1.99	0.44
1:Q2:209:SER:O	1:Q2:214:LYS:NZ	2.43	0.44
1:Z2:257:TYR:HA	1:Z2:276:TYR:HB3	1.98	0.44
1:2B:275:ASP:OD1	1:2B:276:TYR:N	2.51	0.44
1:3D:256:LYS:HE3	1:3D:260:MET:HG3	1.98	0.44
1:1B:232:GLU:OE2	1:1B:232:GLU:N	2.44	0.44
1:YE:232:GLU:OE1	1:YE:232:GLU:N	2.45	0.44
1:3F:257:TYR:HA	1:3F:276:TYR:HB3	1.99	0.44
1:D2:262:LYS:HE3	1:D2:262:LYS:HB3	1.89	0.44
1:A2:183:GLU:HG3	1:A2:189:LEU:O	2.17	0.44
1:A3:281:THR:HG22	1:A3:284:TRP:HZ3	1.83	0.44
1:C2:254:PRO:HG2	1:C2:273:VAL:HA	1.99	0.44
1:J2:250:LYS:HD3	1:K2:202:THR:HG22	2.00	0.44
1:K2:182:LEU:HD22	1:K2:189:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I2:166:CYS:HB2	1:I2:219:MET:HE2	1.98	0.44
1:X1:173:GLN:H	1:X1:173:GLN:CD	2.20	0.44
1:Y3:185:THR:HG22	1:Y3:186:ASN:N	2.33	0.44
1:3B:218:ARG:NH1	1:3B:296:PRO:O	2.41	0.44
1:3C:179:ILE:HG23	1:3C:183:GLU:OE2	2.18	0.44
1:1F:173:GLN:H	1:1F:173:GLN:CD	2.19	0.44
1:A1:254:PRO:HG2	1:A1:273:VAL:HA	1.98	0.44
1:H1:160:ARG:HE	1:H1:160:ARG:HB3	1.61	0.44
1:N2:224:SER:OG	1:N2:225:ASP:N	2.51	0.44
1:3B:202:THR:HG22	1:3C:250:LYS:HD2	1.99	0.44
1:YD:185:THR:HG22	1:YD:186:ASN:N	2.32	0.44
1:F2:254:PRO:HG2	1:F2:273:VAL:HA	1.99	0.44
1:F3:257:TYR:HA	1:F3:276:TYR:HB3	1.99	0.44
1:D1:183:GLU:HG3	1:D1:189:LEU:O	2.18	0.44
1:J1:185:THR:HG22	1:J1:186:ASN:N	2.32	0.44
1:G3:160:ARG:HE	1:G3:160:ARG:HB2	1.60	0.44
1:Q2:168:CYS:SG	1:Q2:169:PRO:HD2	2.58	0.44
1:R3:209:SER:O	1:R3:214:LYS:NZ	2.43	0.44
1:U3:160:ARG:HD2	1:U3:160:ARG:HA	1.73	0.44
1:ZE:185:THR:HG22	1:ZE:186:ASN:N	2.32	0.44
1:1F:264:PHE:CG	1:1F:265:PRO:HD2	2.53	0.44
1:2F:183:GLU:HG3	1:2F:189:LEU:O	2.17	0.44
1:E3:264:PHE:CD1	1:E3:265:PRO:HD2	2.53	0.44
1:F1:232:GLU:O	1:F1:236:GLN:HG3	2.18	0.44
1:D1:217:ARG:HE	1:D1:218:ARG:NH1	2.16	0.44
1:B2:224:SER:OG	1:B2:225:ASP:N	2.50	0.44
1:C2:168:CYS:SG	1:C2:169:PRO:HD2	2.57	0.44
1:G2:168:CYS:SG	1:G2:169:PRO:HD2	2.58	0.44
1:I3:257:TYR:HA	1:I3:276:TYR:HB3	2.00	0.44
1:O1:254:PRO:HG2	1:O1:273:VAL:HA	2.00	0.44
1:P2:261:LYS:HE3	1:P2:261:LYS:HB2	1.82	0.44
1:S2:275:ASP:OD1	1:S2:276:TYR:N	2.51	0.44
1:ZE:269:ARG:HH21	1:ZE:270:PHE:HE2	1.65	0.44
1:2E:279:PRO:HA	1:2E:282:LYS:HE3	1.99	0.44
1:E2:168:CYS:SG	1:E2:169:PRO:HD2	2.58	0.44
1:A1:266:SER:O	1:A1:269:ARG:HG2	2.18	0.44
1:K3:182:LEU:HD12	1:K3:189:LEU:HD12	2.00	0.44
1:L3:202:THR:HG22	1:M3:250:LYS:NZ	2.33	0.44
1:U2:215:ARG:HG3	1:U2:215:ARG:NH1	2.33	0.44
1:W2:209:SER:HA	1:W2:213:GLU:HG3	1.99	0.44
1:X3:232:GLU:OE1	1:X3:232:GLU:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2D:224:SER:OG	1:2D:225:ASP:N	2.51	0.44
1:1E:185:THR:HG22	1:1E:186:ASN:N	2.33	0.44
1:1E:230:SER:OG	1:1E:233:CYS:SG	2.58	0.44
1:1F:183:GLU:HB3	1:1F:189:LEU:O	2.18	0.44
1:J1:251:ARG:HE	1:J1:251:ARG:HB3	1.61	0.43
1:O2:292:ALA:HB2	1:P2:200:PRO:HD2	2.00	0.43
1:U2:161:PHE:CG	1:U2:192:CYS:HB2	2.53	0.43
1:U2:224:SER:OG	1:U2:225:ASP:N	2.51	0.43
1:YD:185:THR:HG22	1:YD:186:ASN:H	1.84	0.43
1:YD:217:ARG:HH21	1:YD:218:ARG:HH12	1.65	0.43
1:A2:160:ARG:HD2	1:A2:160:ARG:HA	1.84	0.43
1:K3:209:SER:O	1:K3:214:LYS:NZ	2.51	0.43
1:I1:211:LEU:HD23	1:I1:215:ARG:HG3	1.99	0.43
1:I2:249:GLN:OE1	1:I2:251:ARG:HB2	2.18	0.43
1:I3:220:VAL:HG12	1:I3:253:ILE:HB	1.99	0.43
1:M2:161:PHE:CG	1:M2:192:CYS:HB2	2.53	0.43
1:M1:175:VAL:O	1:M1:179:ILE:HG13	2.18	0.43
1:R3:264:PHE:CG	1:R3:265:PRO:HD2	2.53	0.43
1:1D:224:SER:OG	1:1D:225:ASP:N	2.51	0.43
1:E1:242:SER:HA	1:E2:205:TRP:HB3	2.00	0.43
1:E3:232:GLU:OE1	1:E3:232:GLU:N	2.43	0.43
1:C3:224:SER:OG	1:C3:225:ASP:N	2.51	0.43
1:O2:168:CYS:SG	1:O2:169:PRO:HD2	2.58	0.43
1:P3:257:TYR:HA	1:P3:276:TYR:HB3	2.00	0.43
1:U3:224:SER:OG	1:U3:225:ASP:N	2.52	0.43
1:X2:218:ARG:NH2	1:X2:296:PRO:O	2.52	0.43
1:V1:224:SER:OG	1:V1:225:ASP:N	2.50	0.43
1:Z1:172:ILE:O	1:Z1:176:GLN:HG2	2.18	0.43
1:2A:275:ASP:OD1	1:2A:276:TYR:N	2.51	0.43
1:2B:250:LYS:HE2	1:2C:202:THR:HG22	1.99	0.43
1:1E:264:PHE:CD1	1:1E:265:PRO:HD2	2.53	0.43
1:ZF:213:GLU:HG2	1:ZF:214:LYS:HG3	2.00	0.43
1:ZF:257:TYR:HA	1:ZF:276:TYR:HB3	2.00	0.43
1:YD:183:GLU:HG2	1:YD:189:LEU:O	2.18	0.43
1:E1:183:GLU:HG3	1:E1:189:LEU:O	2.19	0.43
1:E2:219:MET:HE3	1:E2:236:GLN:HB3	1.99	0.43
1:D1:263:GLU:N	1:D1:263:GLU:OE1	2.51	0.43
1:A1:185:THR:HG22	1:A1:186:ASN:N	2.32	0.43
1:M2:168:CYS:SG	1:M2:169:PRO:HD2	2.58	0.43
1:V2:179:ILE:HG22	1:V2:191:LEU:HD12	1.99	0.43
1:1B:232:GLU:O	1:1B:236:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1E:232:GLU:O	1:1E:236:GLN:HG3	2.19	0.43
1:ZF:232:GLU:CD	1:ZF:232:GLU:H	2.22	0.43
1:F3:173:GLN:H	1:F3:173:GLN:CD	2.21	0.43
1:F3:224:SER:OG	1:F3:225:ASP:N	2.50	0.43
1:F3:264:PHE:CG	1:F3:265:PRO:HD2	2.54	0.43
1:I1:257:TYR:HA	1:I1:276:TYR:HB3	1.99	0.43
1:V2:213:GLU:HG3	1:V2:243:LEU:HD11	1.99	0.43
1:3A:224:SER:OG	1:3A:225:ASP:N	2.51	0.43
1:1D:257:TYR:HA	1:1D:276:TYR:HB3	1.99	0.43
1:E3:230:SER:OG	1:E3:233:CYS:SG	2.61	0.43
1:B1:211:LEU:HD23	1:B1:215:ARG:HG3	2.01	0.43
1:B2:250:LYS:NZ	1:C2:202:THR:HG22	2.34	0.43
1:B3:267:ILE:HD12	1:B3:267:ILE:H	1.84	0.43
1:L3:215:ARG:HG3	1:L3:215:ARG:NH1	2.33	0.43
1:H1:250:LYS:HE2	1:G1:202:THR:HG22	2.01	0.43
1:I1:165:ILE:HD11	1:I1:191:LEU:HD13	2.00	0.43
1:X1:269:ARG:HH22	1:X1:270:PHE:HE1	1.65	0.43
1:1D:232:GLU:OE1	1:1D:232:GLU:N	2.44	0.43
1:3D:257:TYR:HA	1:3D:276:TYR:HB3	2.00	0.43
1:1F:267:ILE:H	1:1F:267:ILE:HD12	1.83	0.43
1:D1:275:ASP:OD1	1:D1:276:TYR:N	2.51	0.43
1:O2:230:SER:OG	1:O2:233:CYS:SG	2.70	0.43
1:P2:185:THR:HG22	1:P2:186:ASN:N	2.27	0.43
1:Q2:232:GLU:O	1:Q2:236:GLN:HG3	2.19	0.43
1:S2:168:CYS:SG	1:S2:169:PRO:HD2	2.59	0.43
1:W1:165:ILE:HD11	1:W1:191:LEU:HD22	2.01	0.43
1:1C:250:LYS:NZ	1:1B:200:PRO:O	2.49	0.43
1:D2:264:PHE:CD1	1:D2:265:PRO:HD2	2.54	0.43
1:J1:165:ILE:HD11	1:J1:191:LEU:HD13	2.01	0.43
1:G3:232:GLU:O	1:G3:236:GLN:HG3	2.19	0.43
1:Z1:254:PRO:HG2	1:Z1:273:VAL:HA	2.00	0.43
1:Z3:252:LEU:HD23	1:Z3:271:ILE:HD13	2.01	0.43
1:ZD:254:PRO:HG2	1:ZD:273:VAL:HA	2.00	0.43
1:C2:183:GLU:HG3	1:C2:189:LEU:O	2.18	0.43
1:A1:159:GLU:HA	1:A1:215:ARG:HH21	1.84	0.43
1:N3:230:SER:OG	1:N3:233:CYS:SG	2.75	0.43
1:T1:264:PHE:CG	1:T1:265:PRO:HD2	2.54	0.43
1:T2:295:LEU:HD23	1:T2:295:LEU:HA	1.90	0.43
1:X2:218:ARG:NH1	1:X2:249:GLN:O	2.45	0.43
1:Y2:275:ASP:OD1	1:Y2:276:TYR:N	2.52	0.43
1:1D:165:ILE:HD11	1:1D:191:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZF:183:GLU:HG2	1:ZF:189:LEU:O	2.19	0.43
1:YD:203:CYS:SG	1:YD:206:SER:HB2	2.59	0.43
1:E2:232:GLU:CD	1:E2:232:GLU:H	2.23	0.43
1:F1:178:MET:HG2	1:F1:182:LEU:HD12	2.00	0.43
1:K2:275:ASP:OD1	1:K2:276:TYR:N	2.52	0.43
1:H2:232:GLU:H	1:H2:232:GLU:CD	2.22	0.43
1:I2:164:PHE:HB2	1:I2:216:CYS:SG	2.58	0.43
1:N1:182:LEU:HD22	1:N1:189:LEU:HD12	2.01	0.43
1:S3:165:ILE:HD11	1:S3:191:LEU:HD13	1.99	0.43
1:T3:269:ARG:HG3	1:T3:269:ARG:NH1	2.34	0.43
1:V2:215:ARG:HG3	1:V2:215:ARG:NH1	2.33	0.43
1:V3:172:ILE:O	1:V3:176:GLN:HG2	2.19	0.43
1:X3:217:ARG:HH21	1:X3:218:ARG:HH12	1.67	0.43
1:3A:264:PHE:CG	1:3A:265:PRO:HD2	2.54	0.43
1:R1:211:LEU:HD23	1:R1:215:ARG:HD3	2.01	0.42
1:T2:224:SER:OG	1:T2:225:ASP:N	2.52	0.42
1:U1:182:LEU:HD22	1:U1:189:LEU:HD12	2.01	0.42
1:W3:254:PRO:HG2	1:W3:273:VAL:HA	2.00	0.42
1:Z1:203:CYS:SG	1:Z1:206:SER:HB2	2.59	0.42
1:A2:295:LEU:HD23	1:A2:295:LEU:HA	1.91	0.42
1:A3:203:CYS:SG	1:A3:206:SER:HB2	2.59	0.42
1:J2:232:GLU:CD	1:J2:232:GLU:H	2.22	0.42
1:K3:257:TYR:HA	1:K3:276:TYR:HB3	2.01	0.42
1:M2:267:ILE:HG23	1:M2:268:LEU:HG	2.01	0.42
1:Q2:160:ARG:HE	1:Q2:160:ARG:HB2	1.65	0.42
1:Q2:224:SER:OG	1:Q2:225:ASP:N	2.52	0.42
1:3A:184:GLN:O	1:3A:188:ARG:NH1	2.51	0.42
1:3D:269:ARG:HG3	1:3D:269:ARG:NH1	2.34	0.42
1:ZF:269:ARG:HH22	1:ZF:270:PHE:HE1	1.65	0.42
1:E1:266:SER:HA	1:E1:269:ARG:HG3	2.02	0.42
1:H3:165:ILE:HD11	1:H3:191:LEU:HB3	2.01	0.42
1:Q1:211:LEU:HA	1:Q1:215:ARG:HD3	2.01	0.42
1:S3:263:GLU:OE2	1:S3:264:PHE:N	2.52	0.42
1:1C:166:CYS:HB2	1:1C:219:MET:HE2	2.00	0.42
1:J2:215:ARG:HG3	1:J2:215:ARG:NH1	2.35	0.42
1:O1:257:TYR:HA	1:O1:276:TYR:HB3	2.01	0.42
1:M1:257:TYR:HA	1:M1:276:TYR:HB3	2.01	0.42
1:2C:275:ASP:OD1	1:2C:276:TYR:N	2.52	0.42
1:ZE:267:ILE:HG23	1:ZE:268:LEU:HG	2.01	0.42
1:1E:276:TYR:HD1	1:1E:285:PHE:CG	2.38	0.42
1:ZF:168:CYS:SG	1:ZF:169:PRO:HD2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2F:266:SER:O	1:2F:269:ARG:HG2	2.19	0.42
1:I3:275:ASP:OD1	1:I3:276:TYR:N	2.52	0.42
1:R2:266:SER:O	1:R2:269:ARG:HG2	2.18	0.42
1:S2:164:PHE:HB2	1:S2:216:CYS:SG	2.59	0.42
1:U2:164:PHE:HB2	1:U2:216:CYS:SG	2.59	0.42
1:W2:224:SER:OG	1:W2:225:ASP:N	2.52	0.42
1:Y2:261:LYS:HE3	1:Y2:261:LYS:HB3	1.89	0.42
1:Z2:211:LEU:HD23	1:Z2:215:ARG:HD3	2.02	0.42
1:Z2:275:ASP:OD1	1:Z2:276:TYR:N	2.53	0.42
1:Y1:185:THR:HG22	1:Y1:186:ASN:N	2.34	0.42
1:3C:182:LEU:HD22	1:3C:189:LEU:HD12	2.02	0.42
1:ZE:168:CYS:SG	1:ZE:169:PRO:HD2	2.59	0.42
1:2F:257:TYR:HA	1:2F:276:TYR:HB3	2.00	0.42
1:B2:275:ASP:OD1	1:B2:276:TYR:N	2.52	0.42
1:C2:257:TYR:HA	1:C2:276:TYR:HB3	2.01	0.42
1:J1:257:TYR:HA	1:J1:276:TYR:HB3	2.02	0.42
1:H3:180:ARG:HA	1:H3:184:GLN:HG3	2.00	0.42
1:P3:275:ASP:OD1	1:P3:276:TYR:N	2.53	0.42
1:A1:211:LEU:HD23	1:A1:215:ARG:HG3	2.01	0.42
1:N3:232:GLU:O	1:N3:236:GLN:HG3	2.20	0.42
1:P2:230:SER:OG	1:P2:233:CYS:SG	2.77	0.42
1:Q1:218:ARG:NH2	1:Q1:295:LEU:O	2.53	0.42
1:U3:257:TYR:HA	1:U3:276:TYR:HB3	2.01	0.42
1:1D:295:LEU:HD23	1:1D:295:LEU:HA	1.93	0.42
1:YE:242:SER:HA	1:ZE:205:TRP:HB3	2.01	0.42
1:YF:162:ASP:OD1	1:YF:217:ARG:NH2	2.52	0.42
1:YD:212:ILE:HG22	1:YD:243:LEU:HD11	2.01	0.42
1:D3:173:GLN:H	1:D3:173:GLN:CD	2.20	0.42
1:E1:211:LEU:HD23	1:E1:215:ARG:HG3	2.01	0.42
1:F2:160:ARG:HE	1:F2:160:ARG:HB2	1.67	0.42
1:K2:232:GLU:H	1:K2:232:GLU:CD	2.23	0.42
1:L3:254:PRO:HG2	1:L3:273:VAL:HA	2.01	0.42
1:S2:176:GLN:HA	1:S2:179:ILE:HG12	2.02	0.42
1:W3:165:ILE:HD11	1:W3:191:LEU:HD13	2.02	0.42
1:X1:249:GLN:HB3	1:X1:251:ARG:HG3	2.01	0.42
1:X1:257:TYR:HA	1:X1:276:TYR:HB3	2.01	0.42
1:1D:275:ASP:OD1	1:1D:277:THR:HG22	2.20	0.42
1:A2:168:CYS:SG	1:A2:169:PRO:HD2	2.59	0.42
1:J2:209:SER:O	1:J2:214:LYS:NZ	2.52	0.42
1:J3:172:ILE:O	1:J3:176:GLN:HG2	2.20	0.42
1:O2:186:ASN:HB3	1:O3:185:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R1:241:LEU:HD23	1:R1:241:LEU:HA	1.91	0.42
1:S1:178:MET:HG3	1:S1:182:LEU:HD12	2.02	0.42
1:Y2:275:ASP:OD1	1:Y2:277:THR:HG22	2.20	0.42
1:Z2:224:SER:OG	1:Z2:225:ASP:N	2.53	0.42
1:ZD:179:ILE:HD11	1:ZD:193:VAL:HG21	2.00	0.42
1:YE:213:GLU:HG3	1:YE:243:LEU:HD11	2.02	0.42
1:YD:232:GLU:OE1	1:YD:232:GLU:N	2.42	0.42
1:K2:176:GLN:HA	1:K2:179:ILE:HG22	2.02	0.42
1:N2:164:PHE:HB2	1:N2:216:CYS:SG	2.60	0.42
1:Z2:190:LYS:HE2	1:Z2:190:LYS:HB2	1.95	0.42
1:2B:232:GLU:O	1:2B:236:GLN:HG3	2.19	0.42
1:1B:185:THR:HG22	1:1B:186:ASN:H	1.85	0.42
1:YE:267:ILE:H	1:YE:267:ILE:HD12	1.85	0.42
1:ZF:230:SER:HG	1:ZF:233:CYS:HG	1.64	0.42
1:D2:250:LYS:HE2	1:E2:202:THR:HG22	2.00	0.41
1:B1:185:THR:HG22	1:B1:186:ASN:N	2.32	0.41
1:M3:185:THR:HG22	1:M3:186:ASN:H	1.85	0.41
1:N2:168:CYS:SG	1:N2:169:PRO:HD2	2.60	0.41
1:O1:183:GLU:HG2	1:O1:189:LEU:O	2.20	0.41
1:O3:185:THR:HG22	1:O3:186:ASN:N	2.34	0.41
1:U1:275:ASP:OD1	1:U1:277:THR:HG22	2.20	0.41
1:3B:275:ASP:OD1	1:3B:277:THR:HG22	2.21	0.41
1:1F:242:SER:HA	1:2F:205:TRP:HB3	2.02	0.41
1:2E:210:GLU:OE2	1:2E:215:ARG:NH1	2.53	0.41
1:E2:209:SER:O	1:E2:214:LYS:NZ	2.43	0.41
1:F2:159:GLU:HB3	1:F2:160:ARG:H	1.67	0.41
1:A3:209:SER:O	1:A3:214:LYS:NZ	2.39	0.41
1:C1:185:THR:HG22	1:C1:186:ASN:N	2.33	0.41
1:J3:232:GLU:O	1:J3:236:GLN:HG3	2.20	0.41
1:H2:284:TRP:CE2	1:I2:196:ARG:HG3	2.55	0.41
1:U1:202:THR:HG22	1:V1:250:LYS:HE2	2.01	0.41
1:U2:275:ASP:OD1	1:U2:276:TYR:N	2.54	0.41
1:V3:213:GLU:HG3	1:V3:214:LYS:HG3	2.02	0.41
1:X1:213:GLU:HG3	1:X1:214:LYS:HG3	2.02	0.41
1:Z3:295:LEU:HD23	1:Z3:295:LEU:HA	1.92	0.41
1:3B:260:MET:HE1	1:3B:264:PHE:HD1	1.84	0.41
1:ZE:254:PRO:HG2	1:ZE:273:VAL:HA	2.02	0.41
1:ZF:190:LYS:HB2	1:ZF:190:LYS:HE3	1.89	0.41
1:3E:183:GLU:HG2	1:3E:189:LEU:O	2.20	0.41
1:A3:295:LEU:HD23	1:A3:295:LEU:HA	1.96	0.41
1:G3:228:LEU:HD21	1:G3:265:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N2:211:LEU:HA	1:N2:215:ARG:HB2	2.02	0.41
1:O2:257:TYR:HA	1:O2:276:TYR:HB3	2.01	0.41
1:R3:173:GLN:OE1	1:R3:173:GLN:N	2.51	0.41
1:W1:231:LYS:HA	1:W1:231:LYS:HD2	1.93	0.41
1:X1:179:ILE:HG23	1:X1:183:GLU:OE1	2.21	0.41
1:Z3:200:PRO:O	1:3A:250:LYS:NZ	2.51	0.41
1:3C:213:GLU:HG3	1:3C:214:LYS:HG3	2.02	0.41
1:YD:172:ILE:HA	1:YD:175:VAL:HG12	2.02	0.41
1:B2:190:LYS:HE3	1:B2:190:LYS:HB2	1.83	0.41
1:J1:232:GLU:H	1:J1:232:GLU:CD	2.23	0.41
1:T1:185:THR:HG22	1:T1:186:ASN:N	2.35	0.41
1:X1:228:LEU:HD21	1:X1:265:PRO:HG3	2.01	0.41
1:Y2:249:GLN:OE1	1:Y2:251:ARG:HB2	2.20	0.41
1:1B:165:ILE:HD11	1:1B:191:LEU:HD22	2.02	0.41
1:1E:275:ASP:OD1	1:1E:277:THR:HG22	2.21	0.41
1:3F:176:GLN:HA	1:3F:179:ILE:HD12	2.02	0.41
1:A2:257:TYR:HA	1:A2:276:TYR:HB3	2.02	0.41
1:B1:295:LEU:HD23	1:B1:295:LEU:HA	1.93	0.41
1:C3:211:LEU:HD23	1:C3:215:ARG:HD3	2.03	0.41
1:J2:160:ARG:HE	1:J2:160:ARG:HB2	1.73	0.41
1:J1:225:ASP:OD2	1:J1:260:MET:HB2	2.20	0.41
1:J1:275:ASP:OD1	1:J1:276:TYR:N	2.53	0.41
1:O1:275:ASP:OD1	1:O1:276:TYR:N	2.53	0.41
1:M1:230:SER:OG	1:M1:233:CYS:SG	2.71	0.41
1:Q2:284:TRP:CE2	1:R2:196:ARG:HG3	2.55	0.41
1:P1:185:THR:HG22	1:P1:186:ASN:N	2.36	0.41
1:S2:230:SER:HG	1:S2:233:CYS:HG	1.62	0.41
1:T1:275:ASP:OD1	1:T1:276:TYR:N	2.54	0.41
1:T3:257:TYR:HA	1:T3:276:TYR:HB3	2.01	0.41
1:Y3:254:PRO:HG2	1:Y3:273:VAL:HA	2.02	0.41
1:1B:185:THR:HG22	1:1B:186:ASN:N	2.35	0.41
1:E1:165:ILE:HD11	1:E1:191:LEU:HD13	2.03	0.41
1:L3:172:ILE:O	1:L3:176:GLN:HG3	2.20	0.41
1:I1:264:PHE:CG	1:I1:265:PRO:HD2	2.56	0.41
1:M2:280:CYS:SG	1:N2:176:GLN:NE2	2.93	0.41
1:Q3:209:SER:HA	1:Q3:213:GLU:HG3	2.02	0.41
1:T2:159:GLU:HB3	1:T2:160:ARG:H	1.75	0.41
1:U2:256:LYS:HE3	1:U2:260:MET:HG3	2.02	0.41
1:Y2:168:CYS:SG	1:Y2:169:PRO:HD2	2.59	0.41
1:1C:275:ASP:OD1	1:1C:277:THR:HG22	2.20	0.41
1:2C:174:PHE:O	1:2C:178:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3D:232:GLU:O	1:3D:236:GLN:HG3	2.20	0.41
1:1E:178:MET:HG2	1:1E:182:LEU:HD12	2.02	0.41
1:D2:254:PRO:HG2	1:D2:273:VAL:HA	2.02	0.41
1:D3:159:GLU:HB3	1:D3:160:ARG:H	1.72	0.41
1:D3:287:THR:O	1:D3:291:LYS:HG3	2.21	0.41
1:F3:185:THR:HG22	1:F3:186:ASN:N	2.35	0.41
1:F3:276:TYR:HB2	1:F3:285:PHE:CE1	2.56	0.41
1:A1:243:LEU:HD23	1:A1:243:LEU:HA	1.91	0.41
1:L1:232:GLU:H	1:L1:232:GLU:CD	2.24	0.41
1:L1:257:TYR:HA	1:L1:276:TYR:HB3	2.02	0.41
1:H2:275:ASP:OD1	1:H2:276:TYR:N	2.54	0.41
1:I2:176:GLN:HA	1:I2:179:ILE:HG22	2.03	0.41
1:N3:200:PRO:O	1:O3:250:LYS:HD3	2.21	0.41
1:V2:257:TYR:HA	1:V2:276:TYR:HB3	2.02	0.41
1:V3:160:ARG:HH11	1:V3:215:ARG:HA	1.85	0.41
1:X1:254:PRO:HG2	1:X1:273:VAL:HA	2.02	0.41
1:3D:215:ARG:HG3	1:3D:215:ARG:NH1	2.35	0.41
1:1E:199:LEU:HD13	1:1F:295:LEU:HD11	2.03	0.41
1:YF:239:PHE:O	1:YF:243:LEU:HG	2.21	0.41
1:K1:230:SER:OG	1:K1:233:CYS:SG	2.76	0.41
1:H1:275:ASP:OD1	1:H1:276:TYR:N	2.54	0.41
1:O1:275:ASP:OD1	1:O1:277:THR:HG22	2.21	0.41
1:Q1:203:CYS:SG	1:Q1:206:SER:HB2	2.60	0.41
1:Q2:159:GLU:HB3	1:Q2:160:ARG:H	1.64	0.41
1:Q2:269:ARG:HB3	1:Q2:269:ARG:NH1	2.36	0.41
1:R1:257:TYR:HA	1:R1:276:TYR:HB3	2.03	0.41
1:R1:275:ASP:OD1	1:R1:277:THR:HG22	2.21	0.41
1:R3:185:THR:HG22	1:R3:186:ASN:N	2.36	0.41
1:T2:291:LYS:HD2	1:U2:199:LEU:HD21	2.02	0.41
1:U3:249:GLN:HG2	1:U3:251:ARG:HG3	2.03	0.41
1:V3:185:THR:HG22	1:V3:186:ASN:N	2.35	0.41
1:2B:207:ILE:HB	1:2B:211:LEU:HD12	2.03	0.41
1:1C:267:ILE:H	1:1C:267:ILE:HD12	1.86	0.41
1:1D:239:PHE:O	1:1D:243:LEU:HG	2.20	0.41
1:E3:275:ASP:OD1	1:E3:277:THR:HG22	2.21	0.41
1:F1:185:THR:HG22	1:F1:186:ASN:N	2.34	0.41
1:F2:230:SER:HG	1:F2:233:CYS:HG	1.61	0.41
1:F3:252:LEU:HD22	1:F3:271:ILE:HD13	2.02	0.41
1:D1:295:LEU:HD23	1:D1:295:LEU:HA	1.90	0.41
1:J2:183:GLU:HG2	1:J2:189:LEU:O	2.21	0.41
1:J3:185:THR:HG22	1:J3:186:ASN:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J3:257:TYR:HA	1:J3:276:TYR:HB3	2.01	0.41
1:K1:161:PHE:CD2	1:K1:192:CYS:HB2	2.56	0.41
1:J1:293:LEU:HD23	1:J1:293:LEU:HA	1.94	0.41
1:G3:179:ILE:HG23	1:G3:183:GLU:OE2	2.21	0.41
1:I1:162:ASP:HB2	1:I1:190:LYS:O	2.21	0.41
1:I3:206:SER:O	1:I3:210:GLU:HB3	2.20	0.41
1:M2:183:GLU:HG2	1:M2:189:LEU:O	2.21	0.41
1:N1:276:TYR:HD1	1:N1:285:PHE:CG	2.39	0.41
1:R3:202:THR:HG23	1:S3:250:LYS:HZ3	1.86	0.41
1:P1:211:LEU:HA	1:P1:215:ARG:HD3	2.02	0.41
1:U2:168:CYS:SG	1:U2:169:PRO:HD2	2.61	0.41
1:V2:211:LEU:HD23	1:V2:215:ARG:HG3	2.02	0.41
1:W2:161:PHE:CG	1:W2:192:CYS:HB2	2.56	0.41
1:V1:164:PHE:HB2	1:V1:216:CYS:SG	2.61	0.41
1:Z1:183:GLU:HG2	1:Z1:189:LEU:O	2.21	0.41
1:2A:176:GLN:HA	1:2A:179:ILE:HG12	2.02	0.41
1:3B:164:PHE:HB2	1:3B:216:CYS:SG	2.61	0.41
1:3C:172:ILE:O	1:3C:176:GLN:HG2	2.21	0.41
1:3D:179:ILE:HG23	1:3D:183:GLU:OE2	2.20	0.41
1:3E:185:THR:HG22	1:3E:186:ASN:N	2.35	0.41
1:3F:261:LYS:HG3	1:3F:262:LYS:HZ2	1.85	0.41
1:E2:269:ARG:O	1:E2:269:ARG:HG2	2.21	0.41
1:C1:179:ILE:HG23	1:C1:183:GLU:OE1	2.21	0.41
1:A1:183:GLU:HG3	1:A1:189:LEU:O	2.21	0.41
1:N3:185:THR:HG22	1:N3:186:ASN:N	2.36	0.41
1:U2:174:PHE:O	1:U2:178:MET:HG3	2.21	0.41
1:V2:284:TRP:CE2	1:W2:196:ARG:HG3	2.56	0.41
1:X1:203:CYS:SG	1:X1:206:SER:HB2	2.61	0.41
1:Y1:254:PRO:HG2	1:Y1:273:VAL:HA	2.03	0.41
1:2B:295:LEU:HD23	1:2B:295:LEU:HA	1.95	0.41
1:E1:239:PHE:O	1:E1:243:LEU:HG	2.21	0.40
1:C1:242:SER:HA	1:C2:205:TRP:HB3	2.03	0.40
1:G2:230:SER:HG	1:G2:233:CYS:HG	1.58	0.40
1:H1:161:PHE:CD2	1:H1:192:CYS:HB2	2.56	0.40
1:N2:161:PHE:CG	1:N2:192:CYS:HB2	2.57	0.40
1:R2:168:CYS:SG	1:R2:169:PRO:HD2	2.61	0.40
1:R2:185:THR:HG22	1:R2:186:ASN:N	2.33	0.40
1:R3:241:LEU:HD23	1:R3:241:LEU:HA	1.97	0.40
1:T3:165:ILE:HD11	1:T3:191:LEU:HD13	2.01	0.40
1:U3:232:GLU:O	1:U3:236:GLN:HG3	2.22	0.40
1:W1:275:ASP:OD1	1:W1:276:TYR:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W3:267:ILE:HG23	1:W3:268:LEU:HG	2.02	0.40
1:Z3:228:LEU:HD21	1:Z3:265:PRO:HG3	2.03	0.40
1:Z3:267:ILE:H	1:Z3:267:ILE:HD12	1.85	0.40
1:3D:172:ILE:O	1:3D:176:GLN:HG3	2.21	0.40
1:YE:254:PRO:HG2	1:YE:273:VAL:HA	2.02	0.40
1:G2:257:TYR:HA	1:G2:276:TYR:HB3	2.02	0.40
1:H1:264:PHE:CG	1:H1:265:PRO:HD2	2.56	0.40
1:I3:185:THR:HG22	1:I3:186:ASN:N	2.35	0.40
1:Q3:185:THR:HG22	1:Q3:186:ASN:N	2.33	0.40
1:V3:257:TYR:HA	1:V3:276:TYR:HB3	2.03	0.40
1:Z3:224:SER:OG	1:Z3:225:ASP:N	2.52	0.40
1:2A:179:ILE:HG22	1:2A:191:LEU:HD12	2.03	0.40
1:3C:276:TYR:HB2	1:3C:285:PHE:CE1	2.56	0.40
1:1B:275:ASP:OD1	1:1B:277:THR:HG22	2.21	0.40
1:ZE:261:LYS:HB2	1:ZE:261:LYS:HE2	1.83	0.40
1:YF:257:TYR:HA	1:YF:276:TYR:HB3	2.03	0.40
1:ZF:254:PRO:HD3	1:ZF:271:ILE:HD12	2.03	0.40
1:D3:267:ILE:H	1:D3:267:ILE:HD12	1.86	0.40
1:F3:254:PRO:HG2	1:F3:273:VAL:HA	2.03	0.40
1:A2:206:SER:O	1:A2:210:GLU:HB2	2.22	0.40
1:A3:257:TYR:HA	1:A3:276:TYR:HB3	2.02	0.40
1:K2:288:ARG:HG2	1:L2:200:PRO:HD3	2.03	0.40
1:K3:211:LEU:HD23	1:K3:215:ARG:HG3	2.03	0.40
1:M2:205:TRP:HB3	1:M1:242:SER:HA	2.02	0.40
1:O3:267:ILE:HD12	1:O3:267:ILE:H	1.87	0.40
1:S1:172:ILE:O	1:S1:176:GLN:HG2	2.21	0.40
1:S1:267:ILE:H	1:S1:267:ILE:HD12	1.87	0.40
1:W3:224:SER:OG	1:W3:225:ASP:N	2.54	0.40
1:Z1:232:GLU:O	1:Z1:236:GLN:HG3	2.21	0.40
1:1C:160:ARG:HE	1:1C:160:ARG:HB2	1.65	0.40
1:YD:206:SER:O	1:YD:210:GLU:HB2	2.21	0.40
1:D3:164:PHE:HB2	1:D3:216:CYS:SG	2.62	0.40
1:A2:190:LYS:HE3	1:A2:190:LYS:HB2	1.89	0.40
1:A1:178:MET:HG2	1:A1:182:LEU:HD12	2.03	0.40
1:J3:278:ASN:ND2	1:J3:281:THR:HG23	2.36	0.40
1:K2:168:CYS:SG	1:K2:169:PRO:HD2	2.61	0.40
1:M2:275:ASP:OD1	1:M2:276:TYR:N	2.55	0.40
1:O1:224:SER:OG	1:O1:225:ASP:N	2.55	0.40
1:Q2:183:GLU:HG2	1:Q2:189:LEU:O	2.21	0.40
1:3A:267:ILE:H	1:3A:267:ILE:HD12	1.86	0.40
1:D3:275:ASP:OD1	1:D3:277:THR:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F3:267:ILE:HD12	1:F3:267:ILE:H	1.87	0.40
1:B2:243:LEU:HD23	1:B2:243:LEU:HA	1.91	0.40
1:L2:257:TYR:HA	1:L2:276:TYR:HB3	2.02	0.40
1:N1:295:LEU:HD23	1:N1:295:LEU:HA	1.98	0.40
1:N3:224:SER:OG	1:N3:225:ASP:N	2.54	0.40
1:O1:295:LEU:HD23	1:O1:295:LEU:HA	1.97	0.40
1:M1:264:PHE:CG	1:M1:265:PRO:HD2	2.56	0.40
1:Q1:267:ILE:H	1:Q1:267:ILE:HD12	1.87	0.40
1:T1:261:LYS:HE2	1:T1:261:LYS:HB2	1.89	0.40
1:U3:234:ASP:O	1:U3:238:LYS:HG3	2.21	0.40
1:S1:230:SER:HG	1:S1:233:CYS:HG	1.60	0.40
1:W1:161:PHE:CD2	1:W1:192:CYS:HB2	2.56	0.40
1:3A:160:ARG:HD3	1:3A:160:ARG:HA	1.92	0.40
1:3B:232:GLU:O	1:3B:236:GLN:HG3	2.20	0.40
1:2C:160:ARG:HE	1:2C:160:ARG:HB3	1.69	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	1A	131/144 (91%)	123 (94%)	8 (6%)	0	100	100
1	1B	131/144 (91%)	128 (98%)	3 (2%)	0	100	100
1	1C	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	1D	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	1E	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	1F	131/144 (91%)	129 (98%)	2 (2%)	0	100	100
1	2A	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	2B	131/144 (91%)	124 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2C	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	2D	131/144 (91%)	123 (94%)	8 (6%)	0	100	100
1	2E	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	2F	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	3A	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	3B	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	3C	131/144 (91%)	128 (98%)	3 (2%)	0	100	100
1	3D	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	3E	131/144 (91%)	128 (98%)	3 (2%)	0	100	100
1	3F	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	A1	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	A2	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	A3	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	B1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	B2	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	B3	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	C1	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	C2	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	C3	131/144 (91%)	128 (98%)	3 (2%)	0	100	100
1	D1	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	D2	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	D3	131/144 (91%)	122 (93%)	9 (7%)	0	100	100
1	E1	131/144 (91%)	128 (98%)	3 (2%)	0	100	100
1	E2	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	E3	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	F1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	F2	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	F3	131/144 (91%)	123 (94%)	8 (6%)	0	100	100
1	G1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	G2	131/144 (91%)	123 (94%)	8 (6%)	0	100	100
1	G3	131/144 (91%)	127 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	H2	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	H3	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	I1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	I2	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	I3	131/144 (91%)	128 (98%)	3 (2%)	0	100	100
1	J1	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	J2	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	J3	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	K1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	K2	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	K3	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	L1	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	L2	131/144 (91%)	122 (93%)	9 (7%)	0	100	100
1	L3	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	M1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	M2	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	M3	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	N1	131/144 (91%)	129 (98%)	2 (2%)	0	100	100
1	N2	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	N3	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	O1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	O2	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	O3	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	P1	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	P2	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	P3	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	Q1	131/144 (91%)	128 (98%)	3 (2%)	0	100	100
1	Q2	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	Q3	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	R1	131/144 (91%)	129 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R2	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	R3	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	S1	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	S2	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	S3	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	T1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	T2	131/144 (91%)	123 (94%)	8 (6%)	0	100	100
1	T3	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	U1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	U2	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	U3	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	V1	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	V2	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	V3	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	W1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	W2	131/144 (91%)	123 (94%)	8 (6%)	0	100	100
1	W3	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	X1	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	X2	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	X3	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	Y1	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	Y2	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	Y3	131/144 (91%)	124 (95%)	7 (5%)	0	100	100
1	YD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
1	YE	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	YF	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
1	Z1	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	Z2	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	Z3	131/144 (91%)	122 (93%)	9 (7%)	0	100	100
1	ZD	131/144 (91%)	125 (95%)	6 (5%)	0	100	100
1	ZE	131/144 (91%)	127 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ZF	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
All	All	13362/14688 (91%)	12835 (96%)	527 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1A	128/134 (96%)	128 (100%)	0	100	100
1	1B	128/134 (96%)	128 (100%)	0	100	100
1	1C	128/134 (96%)	128 (100%)	0	100	100
1	1D	128/134 (96%)	128 (100%)	0	100	100
1	1E	128/134 (96%)	128 (100%)	0	100	100
1	1F	128/134 (96%)	128 (100%)	0	100	100
1	2A	128/134 (96%)	128 (100%)	0	100	100
1	2B	128/134 (96%)	127 (99%)	1 (1%)	79	87
1	2C	128/134 (96%)	128 (100%)	0	100	100
1	2D	128/134 (96%)	128 (100%)	0	100	100
1	2E	128/134 (96%)	128 (100%)	0	100	100
1	2F	128/134 (96%)	127 (99%)	1 (1%)	79	87
1	3A	128/134 (96%)	128 (100%)	0	100	100
1	3B	128/134 (96%)	128 (100%)	0	100	100
1	3C	128/134 (96%)	128 (100%)	0	100	100
1	3D	128/134 (96%)	128 (100%)	0	100	100
1	3E	128/134 (96%)	128 (100%)	0	100	100
1	3F	128/134 (96%)	128 (100%)	0	100	100
1	A1	128/134 (96%)	128 (100%)	0	100	100
1	A2	128/134 (96%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A3	128/134 (96%)	128 (100%)	0	100	100
1	B1	128/134 (96%)	128 (100%)	0	100	100
1	B2	128/134 (96%)	128 (100%)	0	100	100
1	B3	128/134 (96%)	127 (99%)	1 (1%)	79	87
1	C1	128/134 (96%)	128 (100%)	0	100	100
1	C2	128/134 (96%)	128 (100%)	0	100	100
1	C3	128/134 (96%)	128 (100%)	0	100	100
1	D1	128/134 (96%)	128 (100%)	0	100	100
1	D2	128/134 (96%)	128 (100%)	0	100	100
1	D3	128/134 (96%)	128 (100%)	0	100	100
1	E1	128/134 (96%)	127 (99%)	1 (1%)	79	87
1	E2	128/134 (96%)	128 (100%)	0	100	100
1	E3	128/134 (96%)	128 (100%)	0	100	100
1	F1	128/134 (96%)	128 (100%)	0	100	100
1	F2	128/134 (96%)	127 (99%)	1 (1%)	79	87
1	F3	128/134 (96%)	128 (100%)	0	100	100
1	G1	128/134 (96%)	128 (100%)	0	100	100
1	G2	128/134 (96%)	128 (100%)	0	100	100
1	G3	128/134 (96%)	128 (100%)	0	100	100
1	H1	128/134 (96%)	128 (100%)	0	100	100
1	H2	128/134 (96%)	127 (99%)	1 (1%)	79	87
1	H3	128/134 (96%)	128 (100%)	0	100	100
1	I1	128/134 (96%)	128 (100%)	0	100	100
1	I2	128/134 (96%)	128 (100%)	0	100	100
1	I3	128/134 (96%)	128 (100%)	0	100	100
1	J1	128/134 (96%)	128 (100%)	0	100	100
1	J2	128/134 (96%)	128 (100%)	0	100	100
1	J3	128/134 (96%)	128 (100%)	0	100	100
1	K1	128/134 (96%)	128 (100%)	0	100	100
1	K2	128/134 (96%)	128 (100%)	0	100	100
1	K3	128/134 (96%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L1	128/134 (96%)	128 (100%)	0	100	100
1	L2	128/134 (96%)	128 (100%)	0	100	100
1	L3	128/134 (96%)	128 (100%)	0	100	100
1	M1	128/134 (96%)	128 (100%)	0	100	100
1	M2	128/134 (96%)	128 (100%)	0	100	100
1	M3	128/134 (96%)	128 (100%)	0	100	100
1	N1	128/134 (96%)	128 (100%)	0	100	100
1	N2	128/134 (96%)	128 (100%)	0	100	100
1	N3	128/134 (96%)	128 (100%)	0	100	100
1	O1	128/134 (96%)	128 (100%)	0	100	100
1	O2	128/134 (96%)	128 (100%)	0	100	100
1	O3	128/134 (96%)	128 (100%)	0	100	100
1	P1	128/134 (96%)	128 (100%)	0	100	100
1	P2	128/134 (96%)	128 (100%)	0	100	100
1	P3	128/134 (96%)	128 (100%)	0	100	100
1	Q1	128/134 (96%)	128 (100%)	0	100	100
1	Q2	128/134 (96%)	128 (100%)	0	100	100
1	Q3	128/134 (96%)	128 (100%)	0	100	100
1	R1	128/134 (96%)	128 (100%)	0	100	100
1	R2	128/134 (96%)	127 (99%)	1 (1%)	79	87
1	R3	128/134 (96%)	128 (100%)	0	100	100
1	S1	128/134 (96%)	128 (100%)	0	100	100
1	S2	128/134 (96%)	128 (100%)	0	100	100
1	S3	128/134 (96%)	128 (100%)	0	100	100
1	T1	128/134 (96%)	128 (100%)	0	100	100
1	T2	128/134 (96%)	128 (100%)	0	100	100
1	T3	128/134 (96%)	128 (100%)	0	100	100
1	U1	128/134 (96%)	128 (100%)	0	100	100
1	U2	128/134 (96%)	128 (100%)	0	100	100
1	U3	128/134 (96%)	128 (100%)	0	100	100
1	V1	128/134 (96%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V2	128/134 (96%)	128 (100%)	0	100	100
1	V3	128/134 (96%)	128 (100%)	0	100	100
1	W1	128/134 (96%)	128 (100%)	0	100	100
1	W2	128/134 (96%)	128 (100%)	0	100	100
1	W3	128/134 (96%)	128 (100%)	0	100	100
1	X1	128/134 (96%)	128 (100%)	0	100	100
1	X2	128/134 (96%)	128 (100%)	0	100	100
1	X3	128/134 (96%)	128 (100%)	0	100	100
1	Y1	128/134 (96%)	128 (100%)	0	100	100
1	Y2	128/134 (96%)	128 (100%)	0	100	100
1	Y3	128/134 (96%)	128 (100%)	0	100	100
1	YD	128/134 (96%)	128 (100%)	0	100	100
1	YE	128/134 (96%)	128 (100%)	0	100	100
1	YF	128/134 (96%)	128 (100%)	0	100	100
1	Z1	128/134 (96%)	128 (100%)	0	100	100
1	Z2	128/134 (96%)	127 (99%)	1 (1%)	79	87
1	Z3	128/134 (96%)	128 (100%)	0	100	100
1	ZD	128/134 (96%)	128 (100%)	0	100	100
1	ZE	128/134 (96%)	128 (100%)	0	100	100
1	ZF	128/134 (96%)	128 (100%)	0	100	100
All	All	13056/13668 (96%)	13048 (100%)	8 (0%)	92	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E1	186	ASN
1	F2	188	ARG
1	B3	186	ASN
1	H2	188	ARG
1	R2	188	ARG
1	Z2	188	ARG
1	2B	188	ARG
1	2F	188	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	E1	186	ASN
1	B3	186	ASN
1	G3	176	GLN
1	O2	186	ASN
1	U2	249	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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.

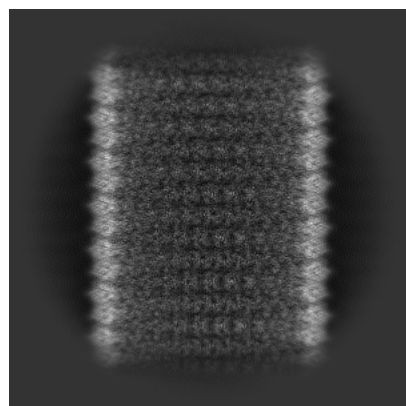
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37355. These allow visual inspection of the internal detail of the map and identification of artifacts.

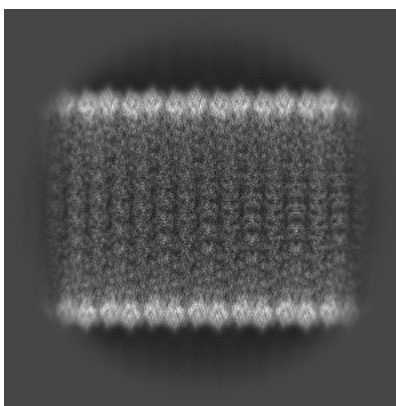
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

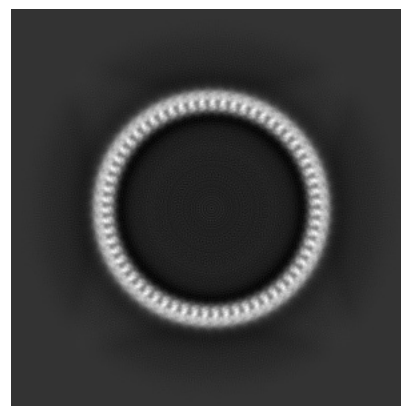
6.1.1 Primary map



X

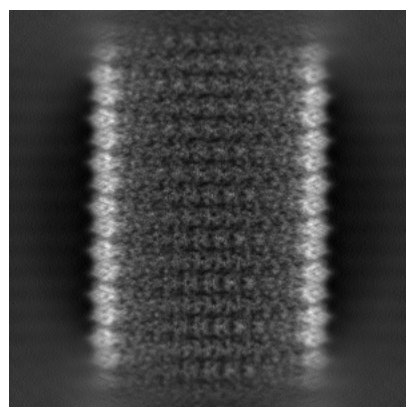


Y

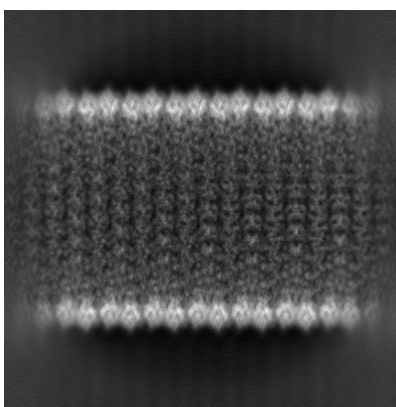


Z

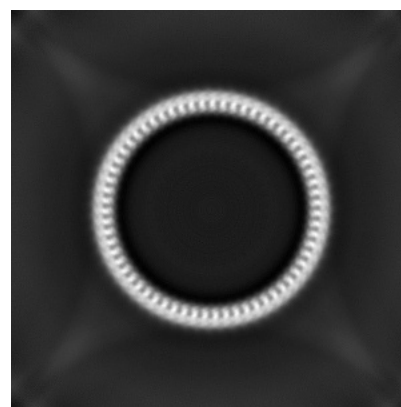
6.1.2 Raw map



X



Y

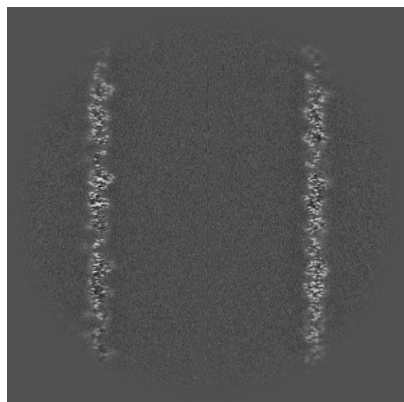


Z

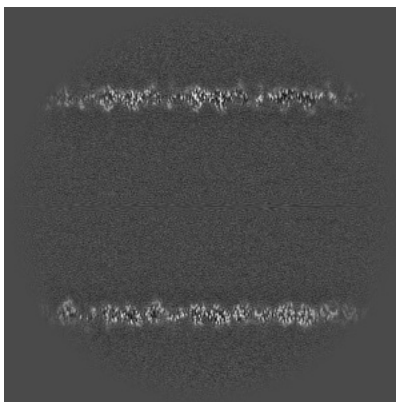
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

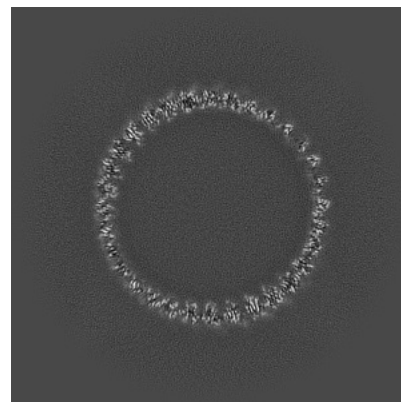
6.2.1 Primary map



X Index: 225

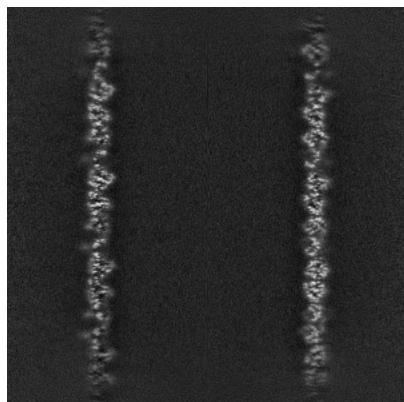


Y Index: 225

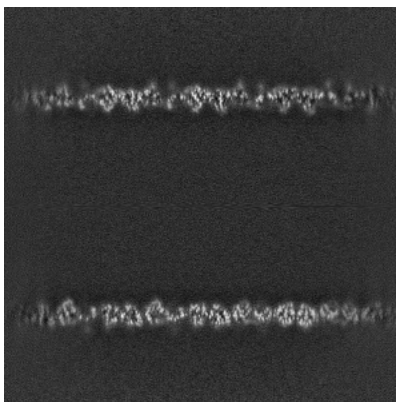


Z Index: 225

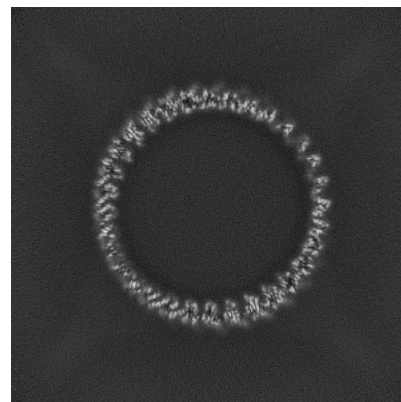
6.2.2 Raw map



X Index: 225



Y Index: 225

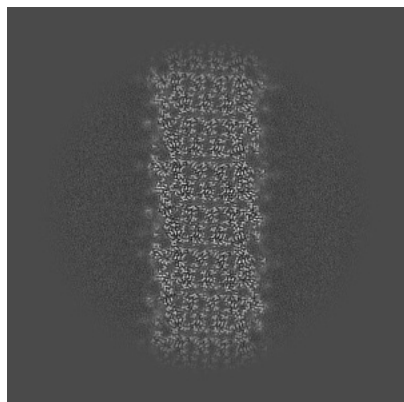


Z Index: 225

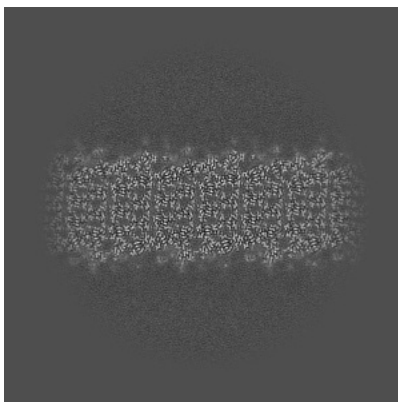
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

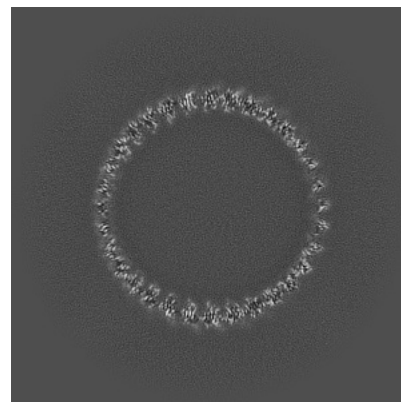
6.3.1 Primary map



X Index: 342

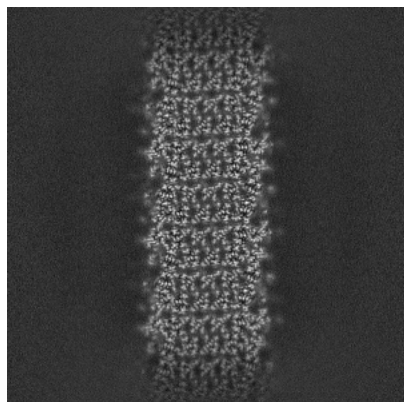


Y Index: 343

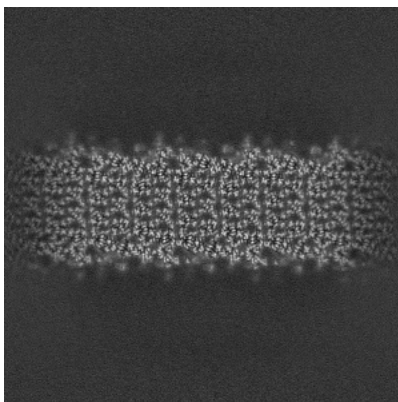


Z Index: 229

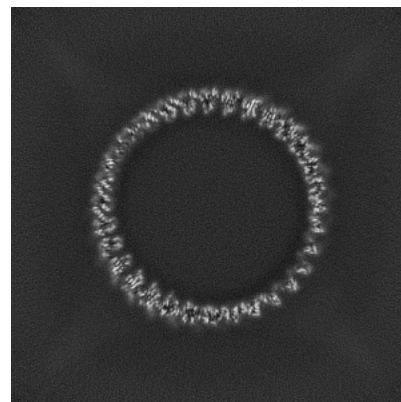
6.3.2 Raw map



X Index: 110



Y Index: 109

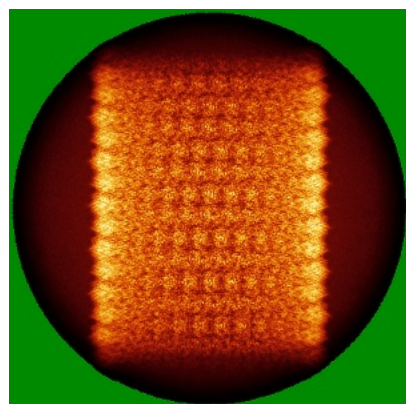


Z Index: 234

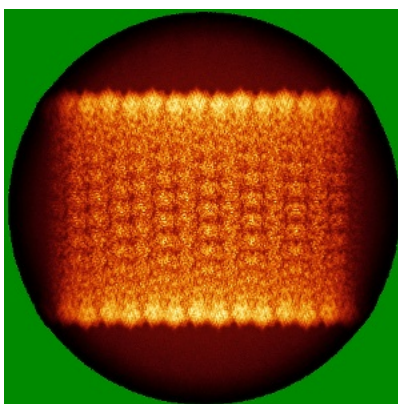
The images above show the largest variance slices of the map in three orthogonal directions.

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

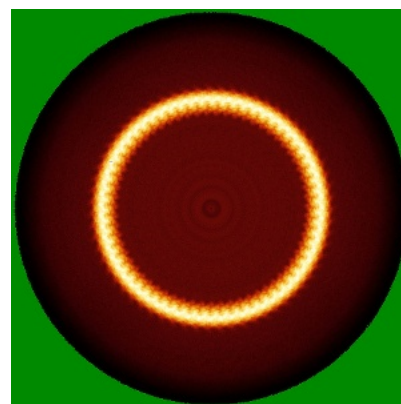
6.4.1 Primary map



X

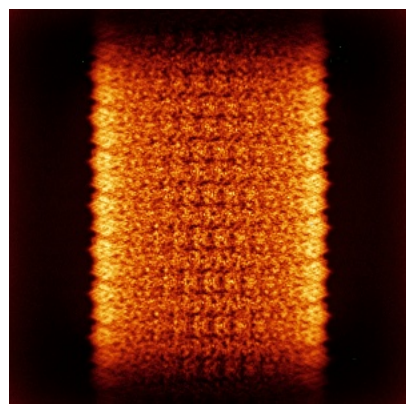


Y

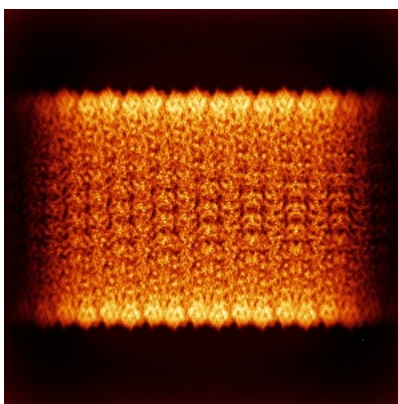


Z

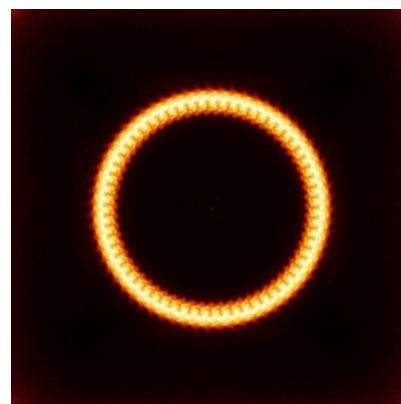
6.4.2 Raw map



X



Y

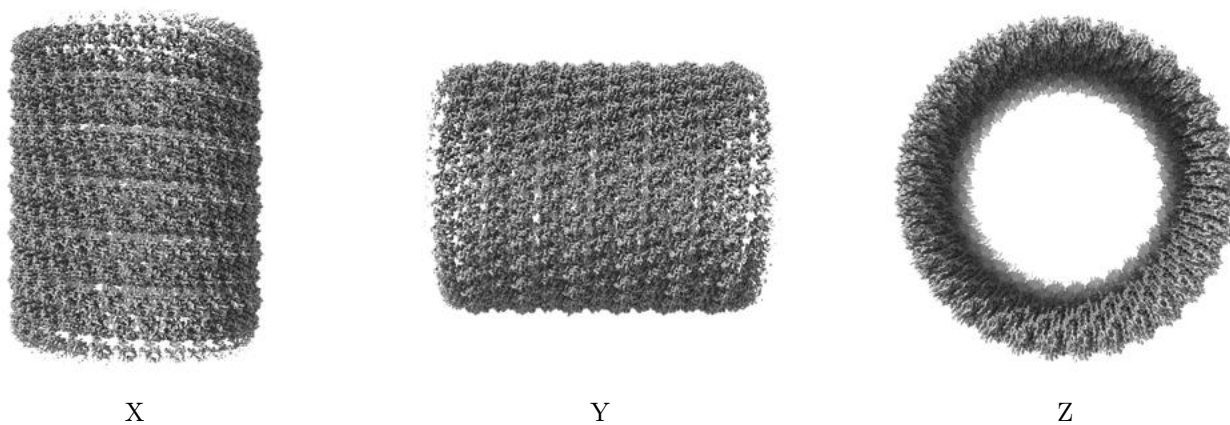


Z

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.

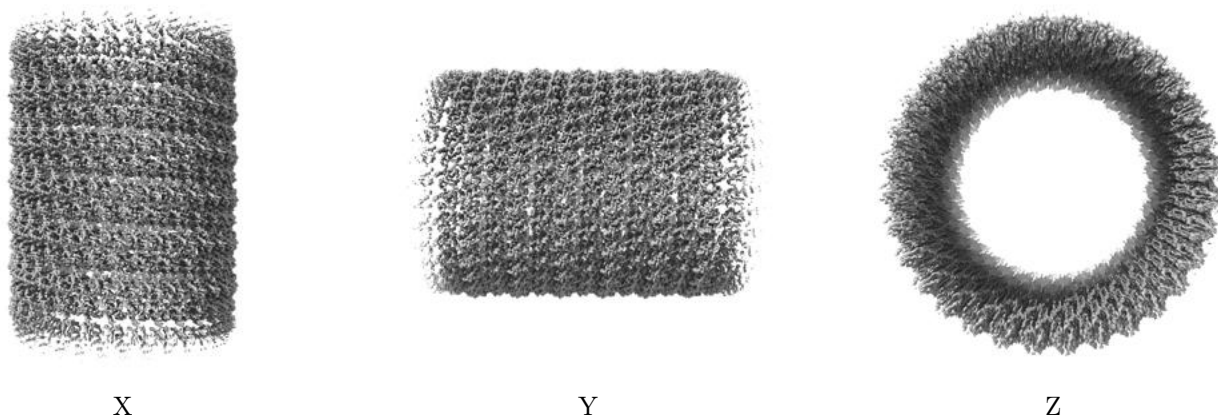
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

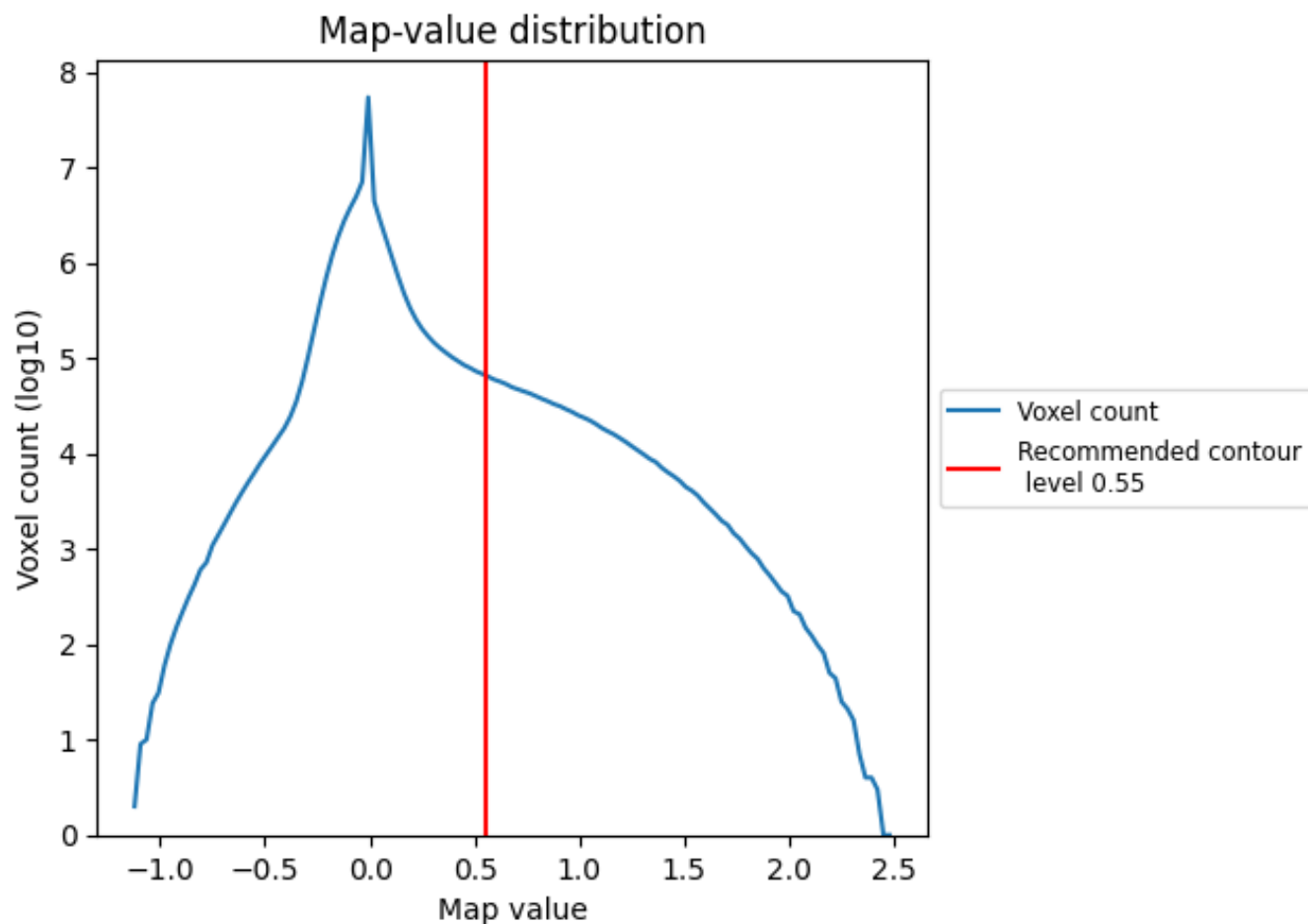
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

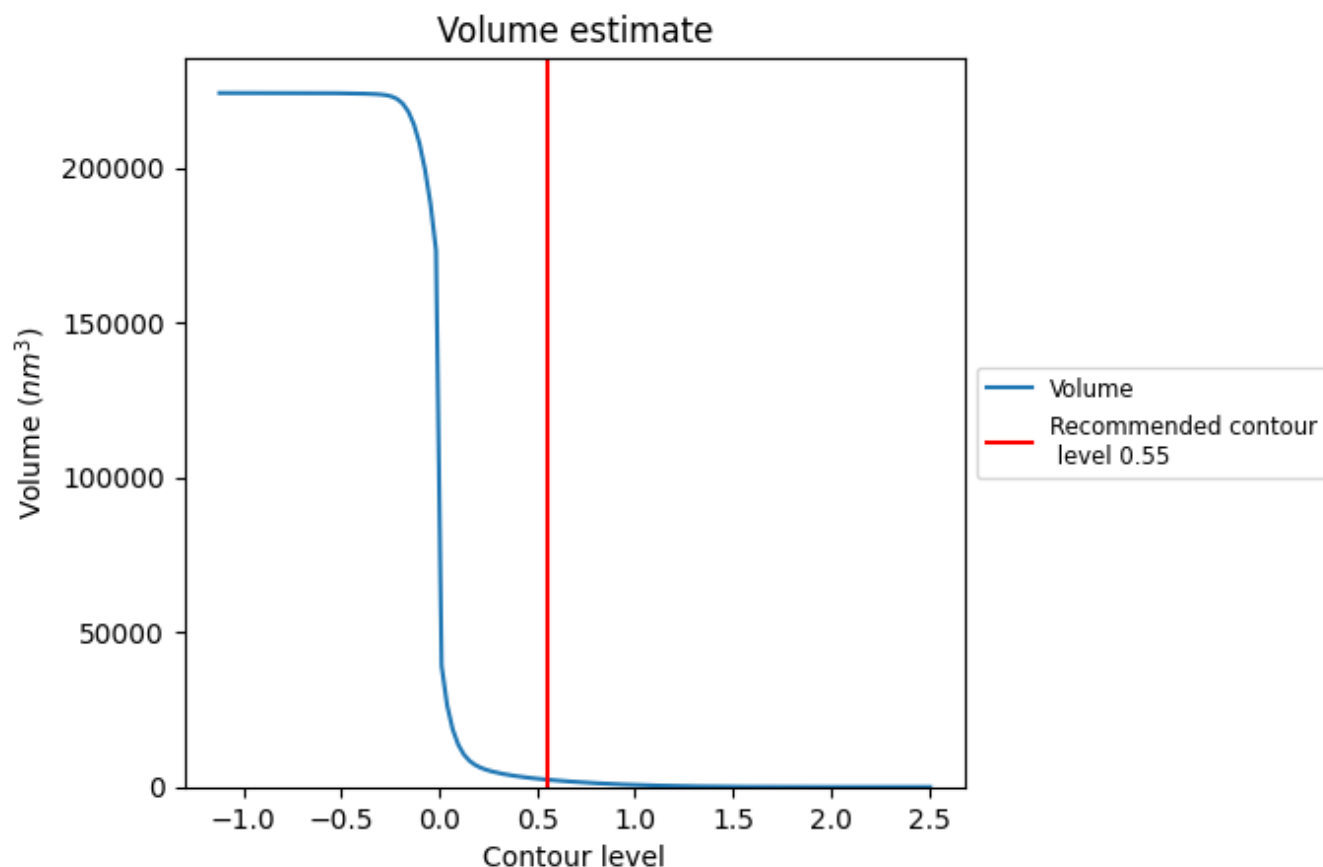
This section contains the results of statistical analysis of the map.

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.

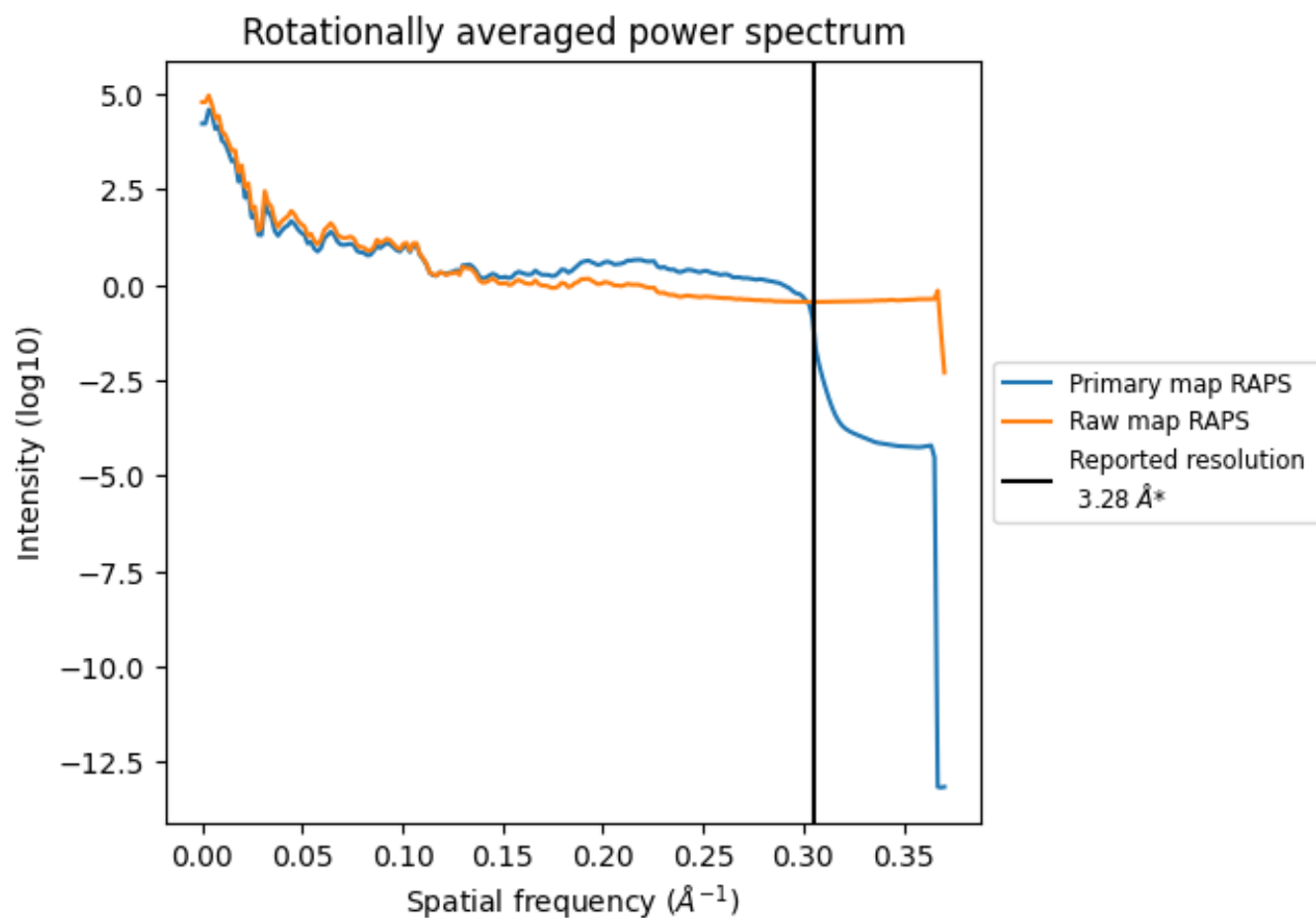
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2361 nm³; this corresponds to an approximate mass of 2133 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 ⓘ

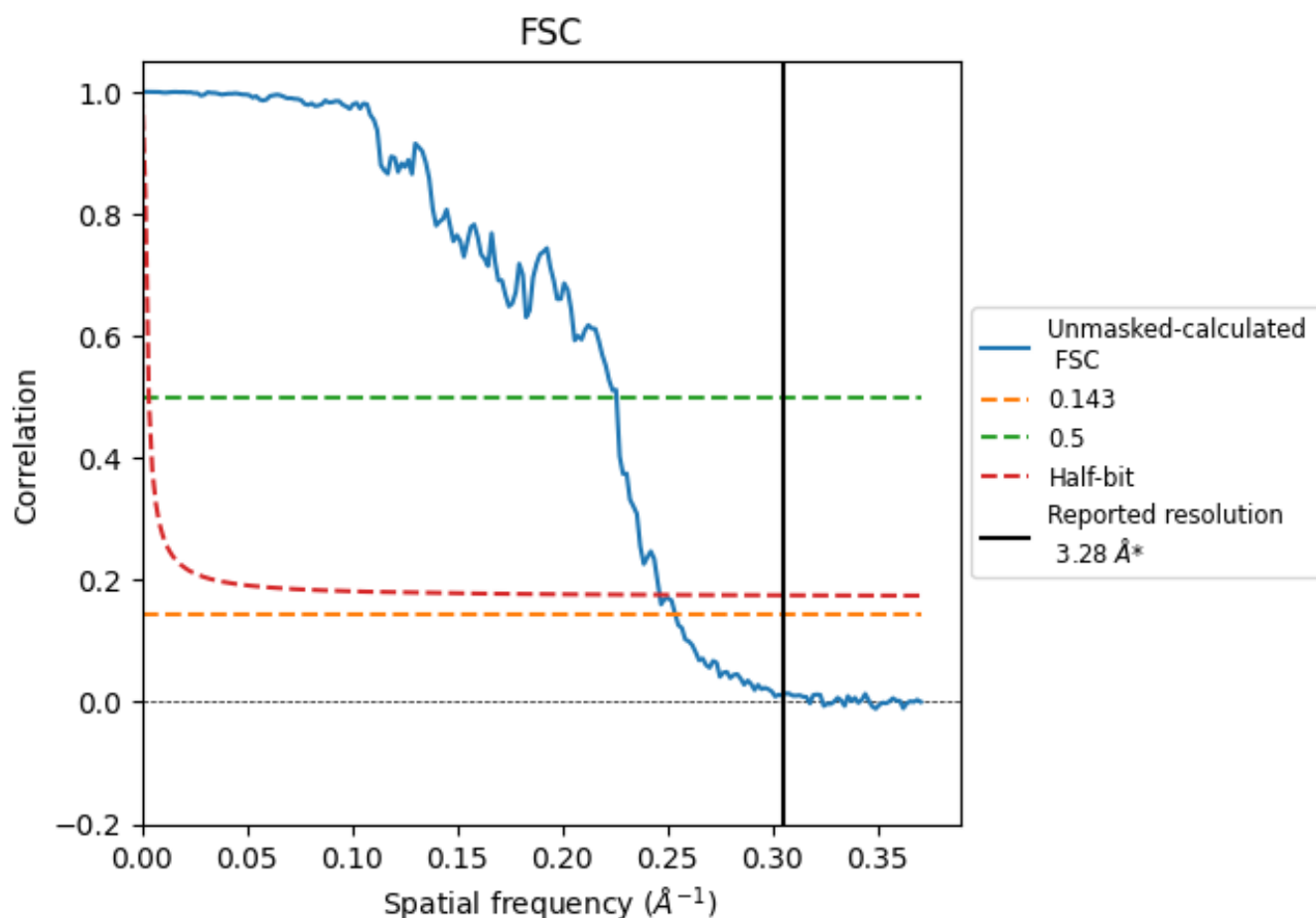


*Reported resolution corresponds to spatial frequency of 0.305 \AA^{-1}

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 0.305 Å⁻¹

8.2 Resolution estimates [i](#)

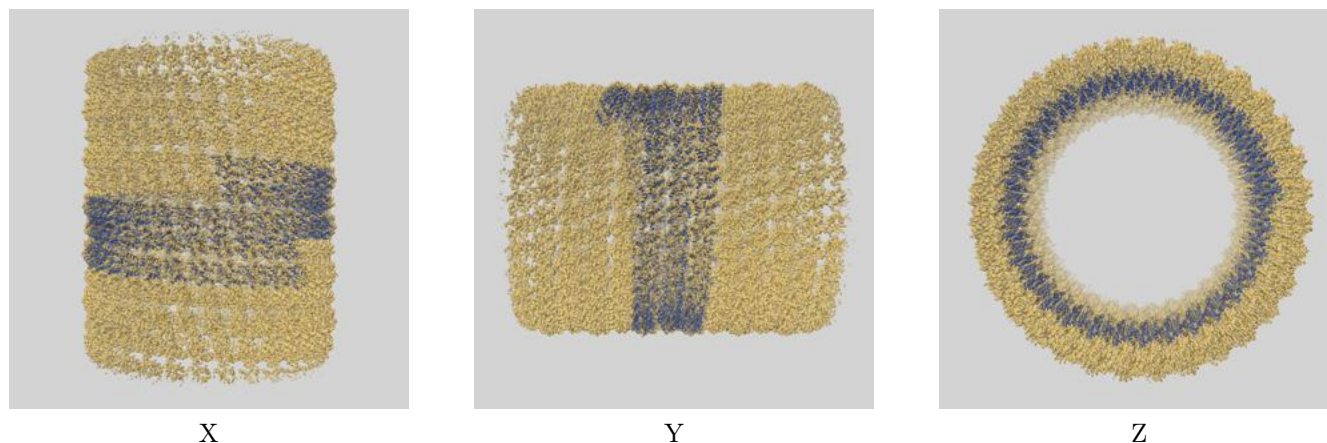
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	4.43	4.06

*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 3.94 differs from the reported value 3.28 by more than 10 %

9 Map-model fit [i](#)

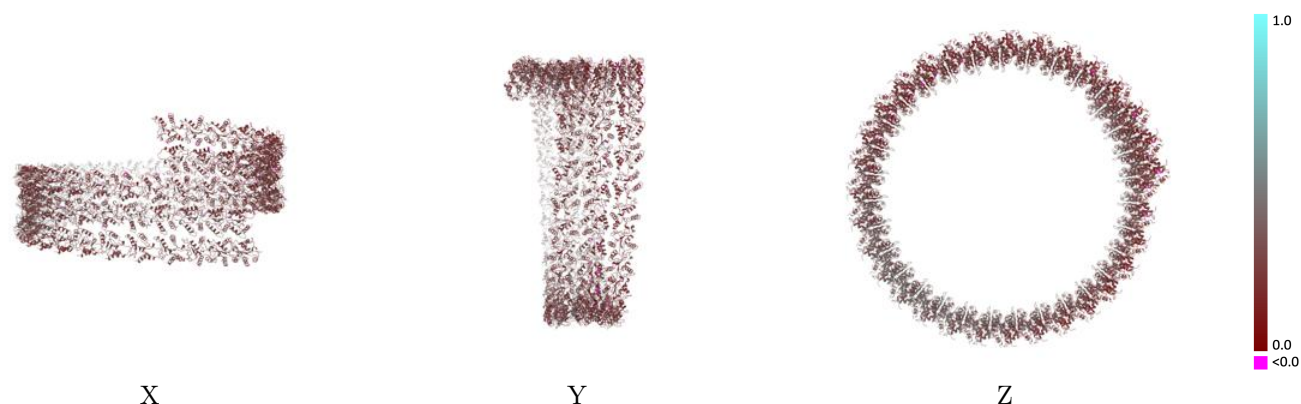
This section contains information regarding the fit between EMDB map EMD-37355 and PDB model 8W8M. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



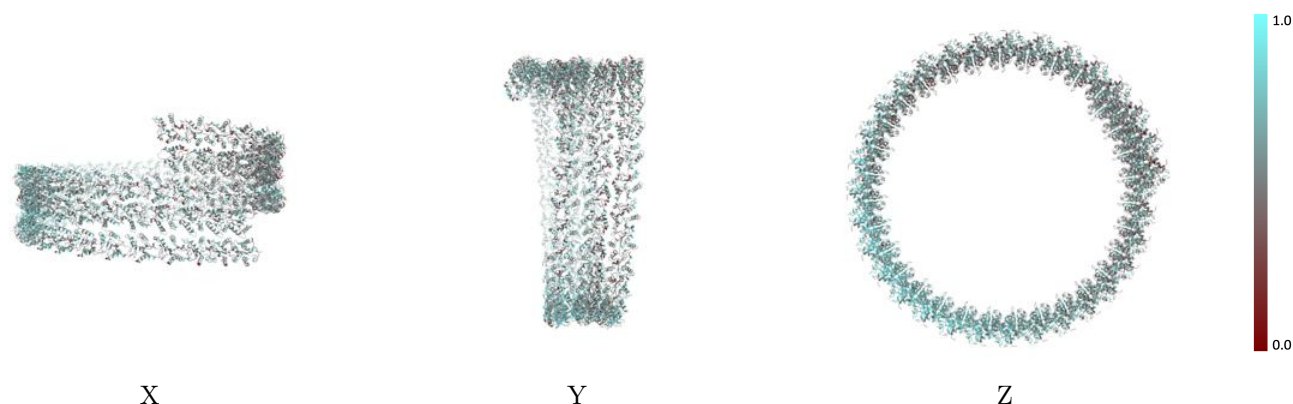
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



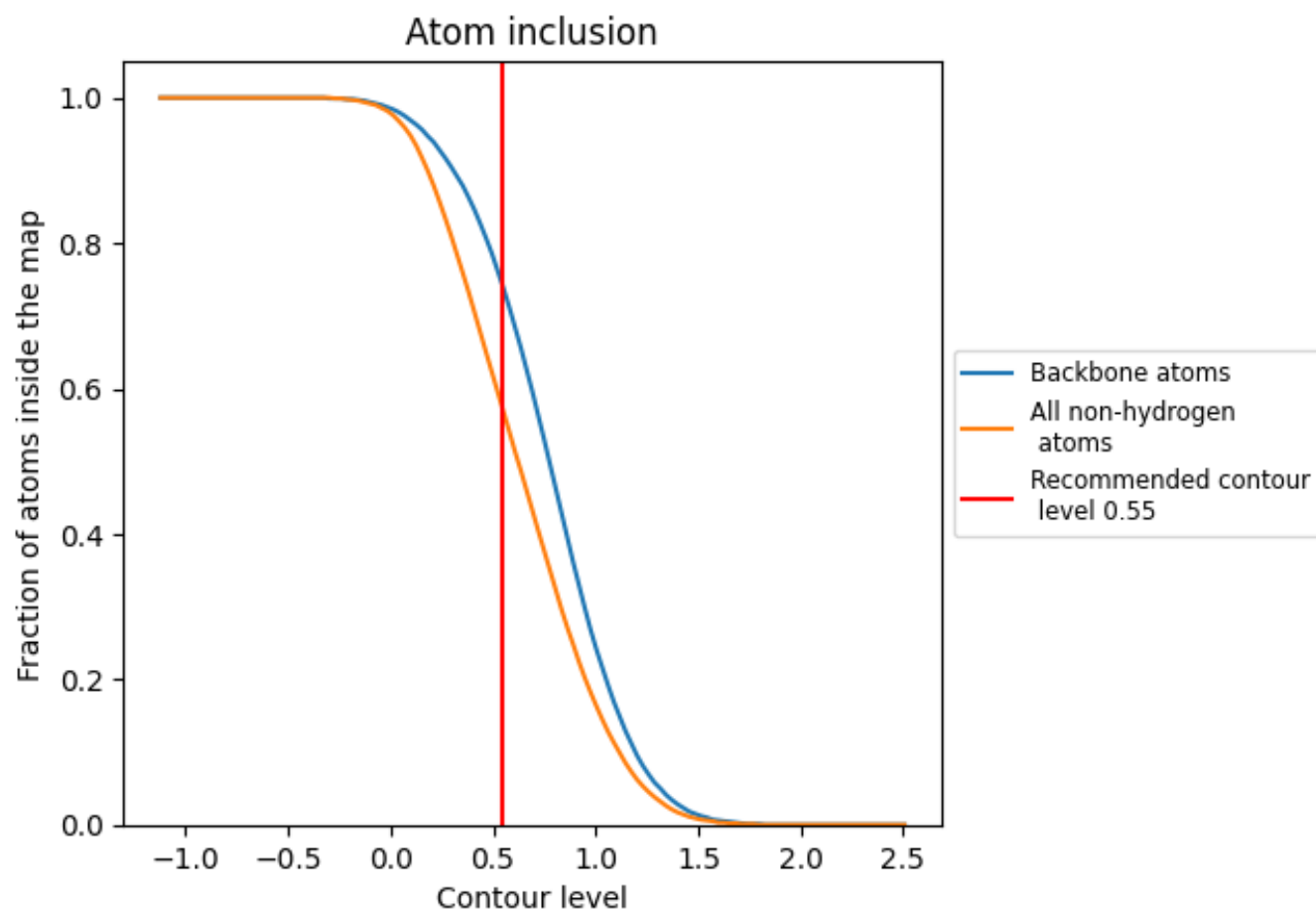
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5690	 0.2960
1A	 0.5370	 0.2500
1B	 0.5260	 0.2500
1C	 0.5350	 0.2530
1D	 0.5330	 0.2530
1E	 0.5390	 0.2680
1F	 0.5330	 0.2600
2A	 0.5420	 0.2770
2B	 0.5450	 0.2780
2C	 0.5300	 0.2840
2D	 0.5510	 0.2900
2E	 0.5520	 0.2940
2F	 0.5560	 0.2950
3A	 0.5460	 0.2830
3B	 0.5420	 0.2780
3C	 0.5410	 0.2880
3D	 0.5330	 0.2900
3E	 0.5470	 0.2980
3F	 0.5560	 0.2980
A1	 0.4970	 0.2300
A2	 0.5200	 0.2440
A3	 0.5410	 0.2710
B1	 0.4990	 0.2290
B2	 0.5110	 0.2540
B3	 0.5480	 0.2740
C1	 0.5040	 0.2360
C2	 0.5290	 0.2540
C3	 0.5440	 0.2820
D1	 0.5020	 0.2310
D2	 0.5200	 0.2500
D3	 0.5240	 0.2840
E1	 0.5020	 0.2370
E2	 0.5170	 0.2450
E3	 0.5310	 0.2760
F1	 0.5000	 0.2360























































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Chain	Atom inclusion	Q-score
F2	0.5060	0.2440
F3	0.5360	0.2770
G1	0.5080	0.2350
G2	0.5110	0.2510
G3	0.5360	0.2730
H1	0.5090	0.2370
H2	0.5180	0.2530
H3	0.5480	0.2810
I1	0.5070	0.2330
I2	0.5290	0.2580
I3	0.5710	0.2850
J1	0.5330	0.2530
J2	0.5300	0.2760
J3	0.5720	0.2900
K1	0.5570	0.2650
K2	0.5760	0.2970
K3	0.6000	0.3170
L1	0.5800	0.2870
L2	0.5940	0.3080
L3	0.6210	0.3330
M1	0.5980	0.3050
M2	0.6230	0.3420
M3	0.6490	0.3670
N1	0.6230	0.3320
N2	0.6380	0.3580
N3	0.6660	0.3850
O1	0.6400	0.3570
O2	0.6570	0.3840
O3	0.6790	0.4120
P1	0.6470	0.3650
P2	0.6650	0.3980
P3	0.6940	0.4170
Q1	0.6500	0.3810
Q2	0.6640	0.4010
Q3	0.6810	0.4240
R1	0.6510	0.3730
R2	0.6680	0.3960
R3	0.6880	0.4150
S1	0.6460	0.3690
S2	0.6610	0.3770
S3	0.6700	0.3950
T1	0.6320	0.3440

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Chain	Atom inclusion	Q-score
T2	 0.6340	 0.3610
T3	 0.6570	 0.3790
U1	 0.6200	 0.3210
U2	 0.6180	 0.3370
U3	 0.6490	 0.3500
V1	 0.5960	 0.2990
V2	 0.5920	 0.3120
V3	 0.6140	 0.3280
W1	 0.5800	 0.2780
W2	 0.5820	 0.2960
W3	 0.5850	 0.3090
X1	 0.5530	 0.2690
X2	 0.5610	 0.2840
X3	 0.5690	 0.2920
Y1	 0.5470	 0.2510
Y2	 0.5440	 0.2760
Y3	 0.5560	 0.2850
YD	 0.4830	 0.2160
YE	 0.4950	 0.2290
YF	 0.4900	 0.2250
Z1	 0.5270	 0.2510
Z2	 0.5380	 0.2760
Z3	 0.5460	 0.2790
ZD	 0.5010	 0.2470
ZE	 0.5200	 0.2500
ZF	 0.5170	 0.2540