Full wwPDB EM Validation Report

Nov 28, 2022 – 11:52 AM EST

PDB ID	:	7SPI
EMDB ID	:	EMD-24771
Title	:	Models for C13 reconstruction of Outer Membrane Core Complex (OMCC) of Type IV Secretion System (T4SS) encoded by a plasmid overproducing TraV, TraK and TraB of pED208
Authors	:	Liu, X.; Khara, P.; Baker, M.L.; Christie, P.J.; Hu, B.
Deposited on	:	2021-11-02
Resolution	:	2.97 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 (i) 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 (i)) were used in the production of this report:

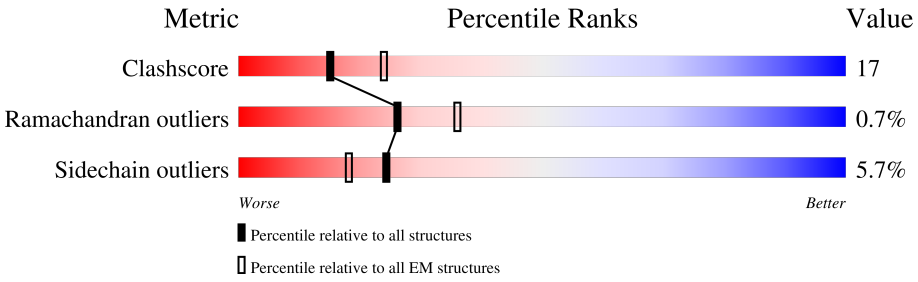
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.97 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A1	204	19% 8% 73%
1	A10	204	19% 8% 73%
1	A11	204	19% 8% 73%
1	A12	204	19% 8% 73%
1	A13	204	19% 8% 73%
1	A2	204	19% 8% 73%
1	A3	204	19% 8% 73%
1	A4	204	19% 8% 73%

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Mol	Chain	Length	Quality of chain
1	A5	204	19% 8% 73%
1	A6	204	19% 8% 73%
1	A7	204	19% 8% 73%
1	A8	204	19% 8% 73%
1	A9	204	19% 8% 73%
1	B1	204	22% 10% 68%
1	B10	204	5% 22% 10% 68%
1	B11	204	5% 22% 10% 68%
1	B12	204	22% 10% 68%
1	B13	204	5% 22% 10% 68%
1	B2	204	5% 22% 10% 68%
1	B3	204	5% 22% 10% 68%
1	B4	204	22% 10% 68%
1	B5	204	22% 10% 68%
1	B6	204	5% 22% 10% 68%
1	B7	204	5% 22% 10% 68%
1	B8	204	22% 10% 68%
1	B9	204	5% 22% 10% 68%
2	C1	246	65% 23% 12%
2	C10	246	65% 23% 12%
2	C11	246	65% 24% 12%
2	C12	246	65% 23% 12%
2	C13	246	65% 24% 12%
2	C2	246	65% 23% 12%
2	C3	246	65% 24% 12%

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Mol	Chain	Length	Quality of chain
2	C4	246	65% 23% 12%
2	C5	246	65% 24% 12%
2	C6	246	65% 23% 12%
2	C7	246	66% 22% 12%
2	C8	246	65% 23% 12%
2	C9	246	65% 24% 12%
2	D1	246	14% 65% 21% 12%
2	D10	246	14% 66% 20% 12%
2	D11	246	13% 65% 21% 12%
2	D12	246	14% 63% 23% 12%
2	D13	246	13% 65% 21% 12%
2	D2	246	13% 65% 22% 12%
2	D3	246	13% 65% 21% 12%
2	D4	246	13% 67% 20% 12%
2	D5	246	14% 67% 20% 12%
2	D6	246	14% 65% 22% 12%
2	D7	246	13% 66% 20% 12%
2	D8	246	13% 64% 22% 12%
2	D9	246	13% 66% 20% 12%
3	E1	453	98%
3	E10	453	98%
3	E11	453	98%
3	E12	453	98%
3	E13	453	98%
3	E2	453	98%

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Mol	Chain	Length	Quality of chain
3	E3	453	98%
3	E4	453	98%
3	E5	453	98%
3	E6	453	98%
3	E7	453	98%
3	E8	453	98%
3	E9	453	98%
3	F1	453	98%
3	F10	453	98%
3	F11	453	98%
3	F12	453	98%
3	F13	453	98%
3	F2	453	98%
3	F3	453	98%
3	F4	453	98%
3	F5	453	98%
3	F6	453	98%
3	F7	453	98%
3	F8	453	98%
3	F9	453	98%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 57408 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 TraV.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A2	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A3	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A4	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A5	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A6	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A7	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A8	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A9	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A10	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A11	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A12	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	A13	55	Total	C	N	O	S	0	0
			436	275	83	77	1		
1	B1	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B2	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B3	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B4	65	Total	C	N	O	S	0	0
			498	314	92	91	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	B5	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B6	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B7	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B8	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B9	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B10	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B11	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B12	65	Total	C	N	O	S	0	0
			498	314	92	91	1		
1	B13	65	Total	C	N	O	S	0	0
			498	314	92	91	1		

- Molecule 2 is a protein called TraK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C1	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C2	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C3	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C4	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C5	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C6	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C7	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C8	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C9	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C10	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	C11	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C12	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	C13	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D1	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D2	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D3	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D4	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D5	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D6	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D7	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D8	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D9	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D10	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D11	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D12	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		
2	D13	217	Total	C	N	O	S	0	0
			1654	1041	299	308	6		

- Molecule 3 is a protein called TraB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E1	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E2	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E3	11	Total	C	N	O	S	0	0
			87	52	15	18	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	E4	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E5	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E6	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E7	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E8	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E9	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E10	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E11	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E12	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	E13	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F1	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F2	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F3	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F4	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F5	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F6	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F7	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F8	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F9	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F10	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F11	11	Total	C	N	O	S	0	0
			87	52	15	18	2		

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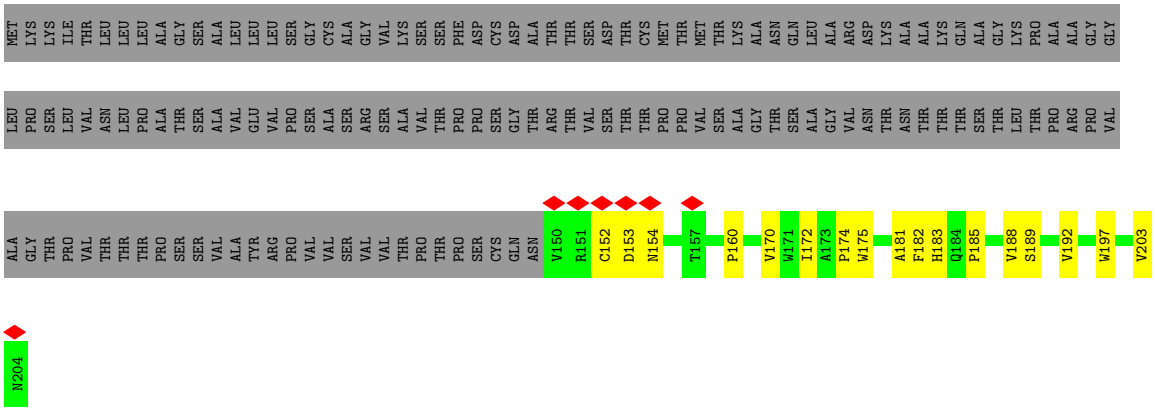
Mol	Chain	Residues	Atoms					AltConf	Trace
3	F12	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F13	11	Total	C	N	O	S	0	0
			87	52	15	18	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

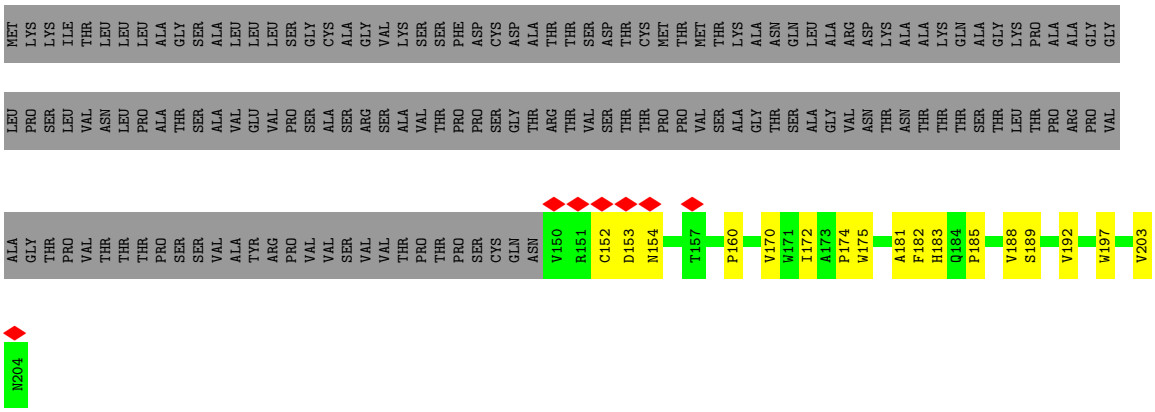
- Molecule 1: TraV

Chain A1:



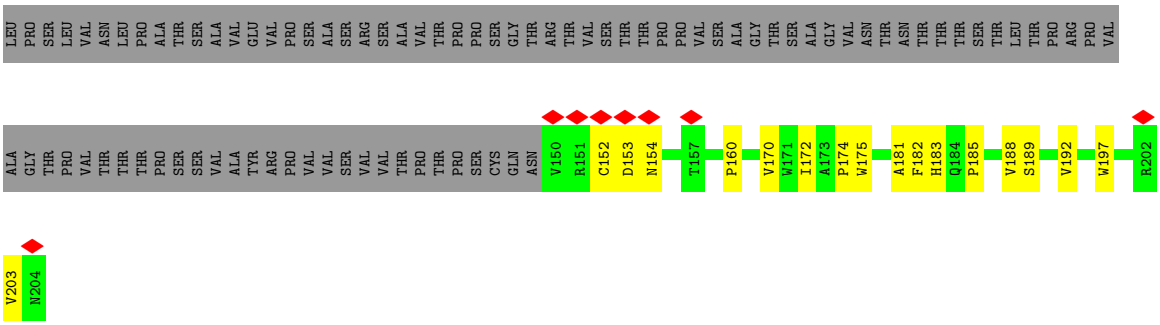
- Molecule 1: TraV

Chain A2:



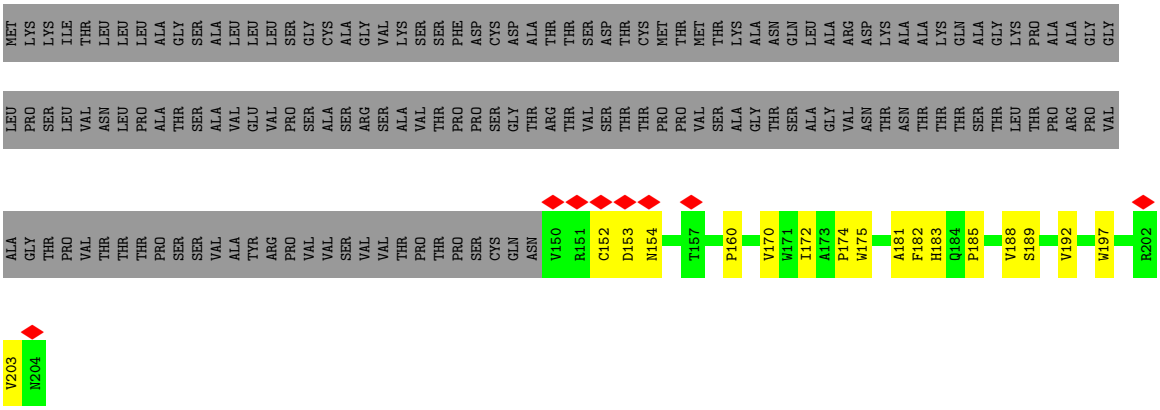
- Molecule 1: TraV

Chain A3:



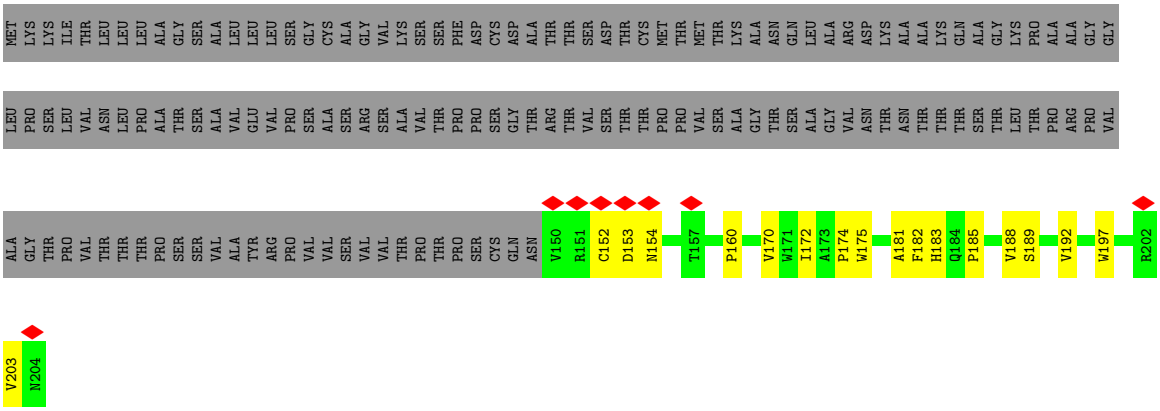
• Molecule 1: TraV

Chain A4:



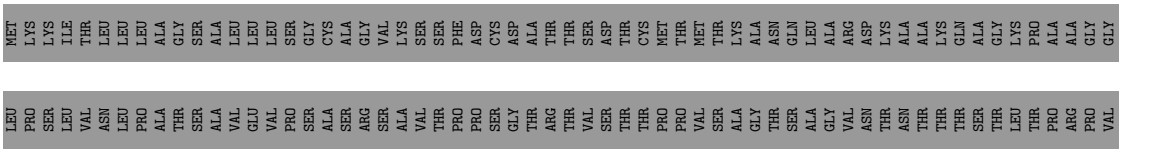
• Molecule 1: TraV

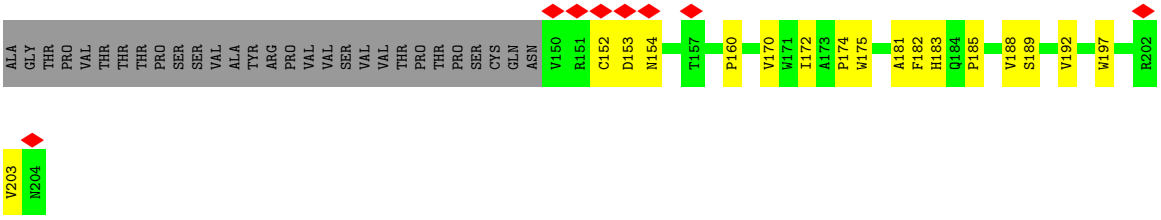
Chain A5:



• Molecule 1: TraV

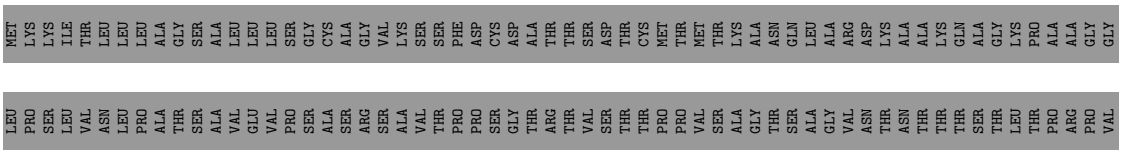
Chain A6:

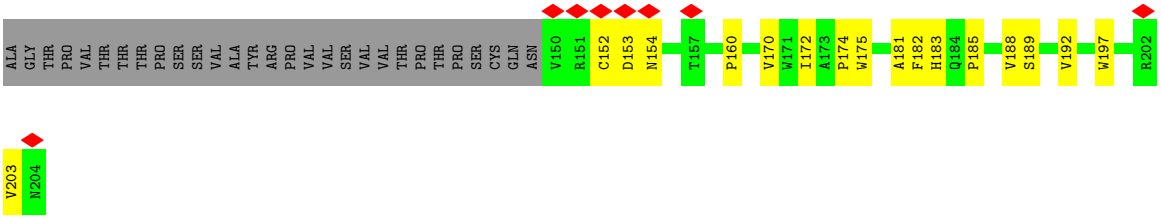




• Molecule 1: TraV

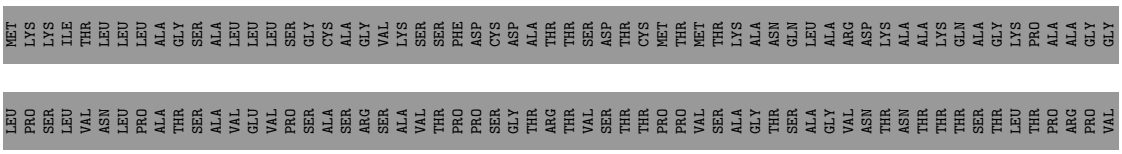
Chain A7:

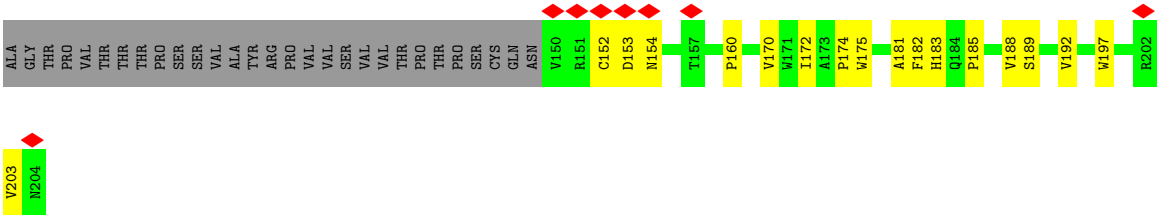




• Molecule 1: TraV

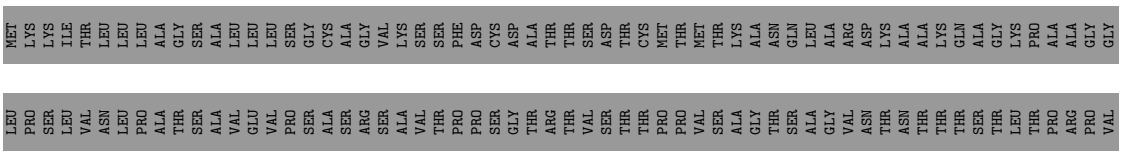
Chain A8:

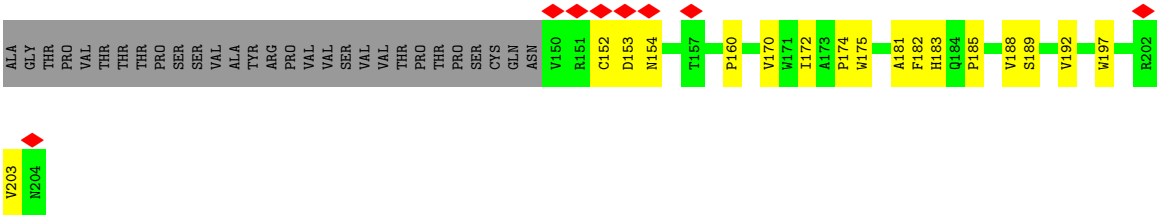




• Molecule 1: TraV

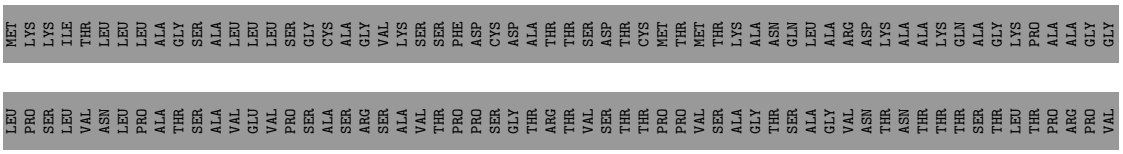
Chain A9:

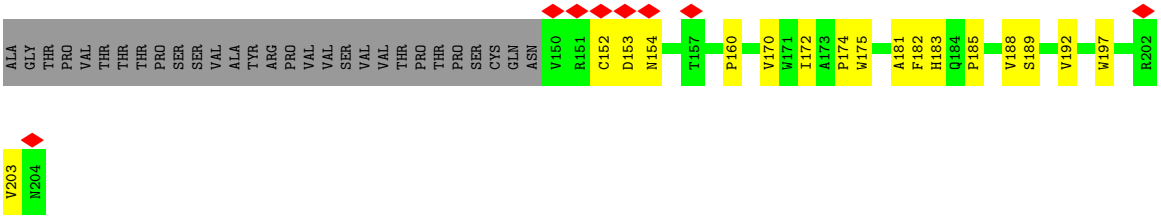




• Molecule 1: TraV

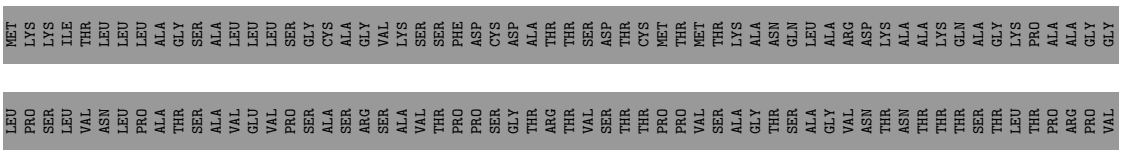
Chain A10:

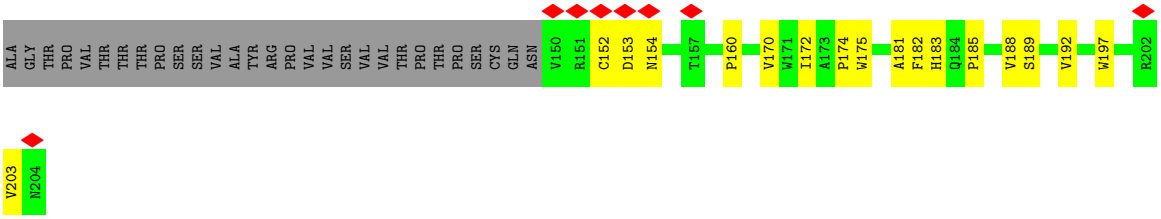




• Molecule 1: TraV

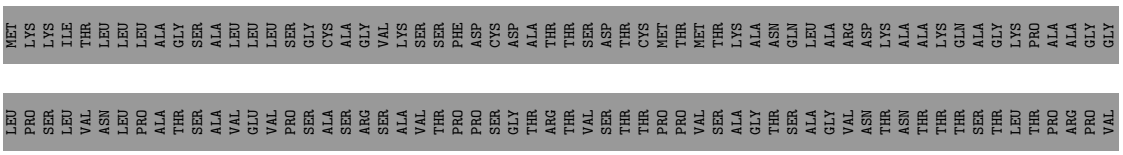
Chain A11:

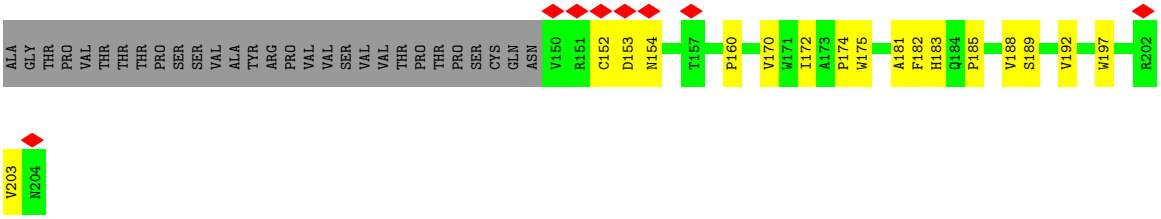




• Molecule 1: TraV

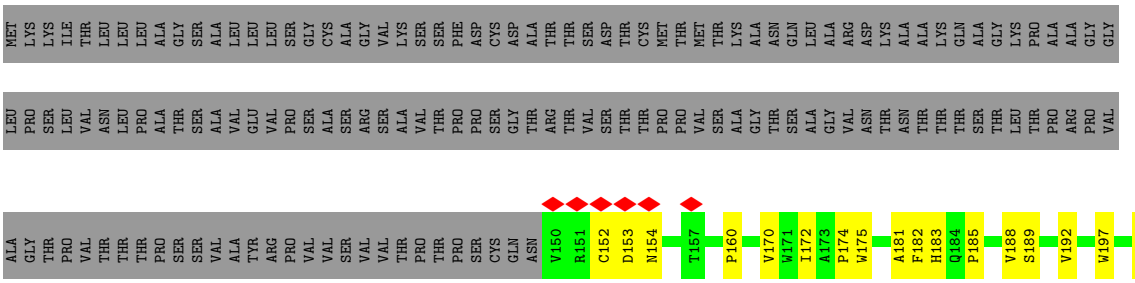
Chain A12:





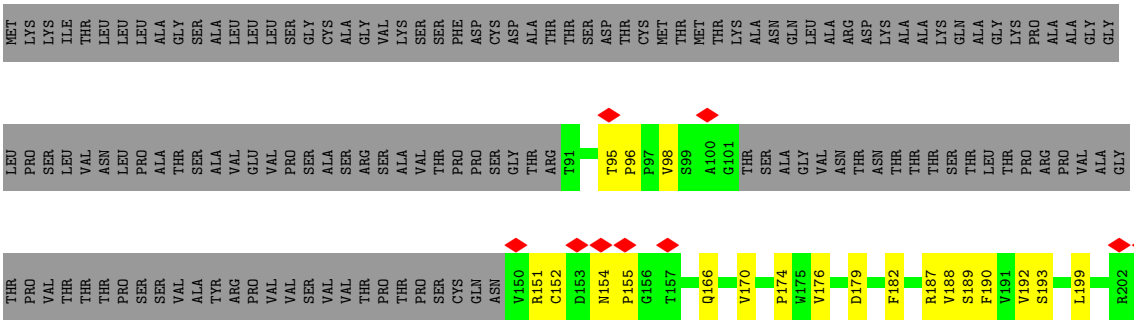
• Molecule 1: TraV

Chain A13:



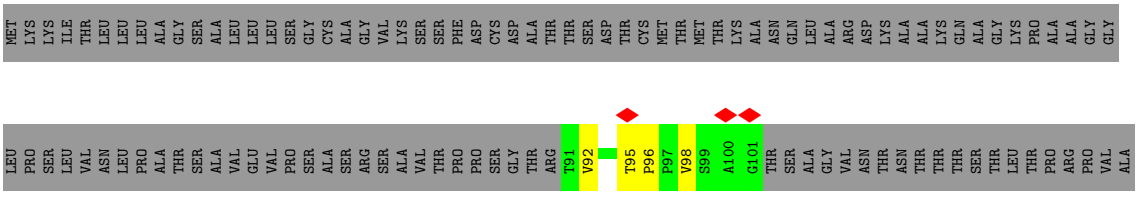
• Molecule 1: TraV

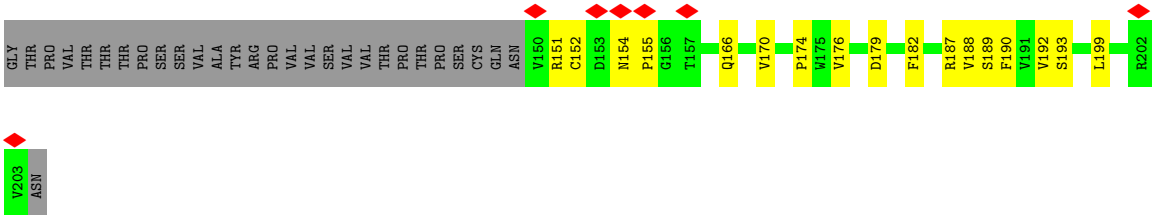
Chain B1:



• Molecule 1: TraV

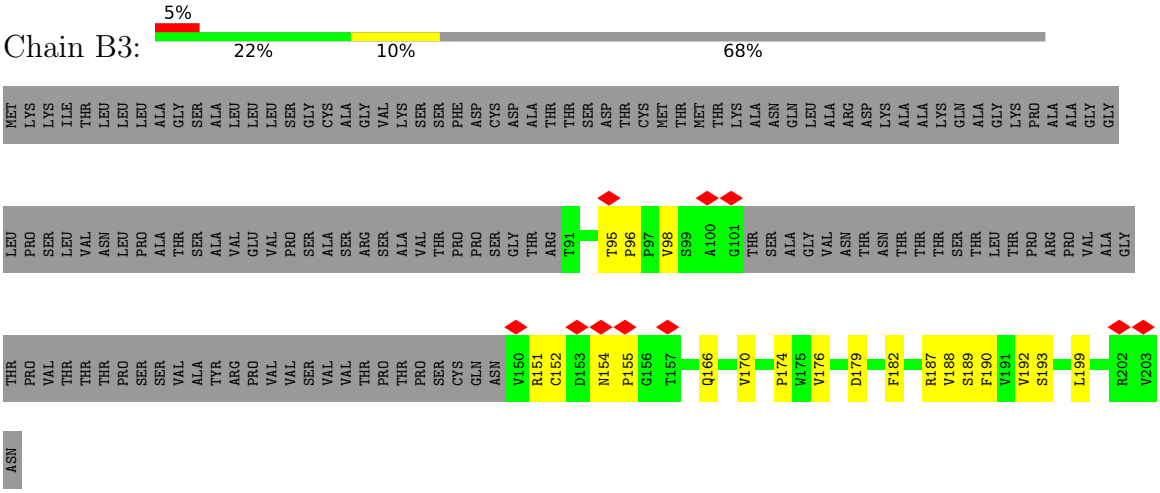
Chain B2:





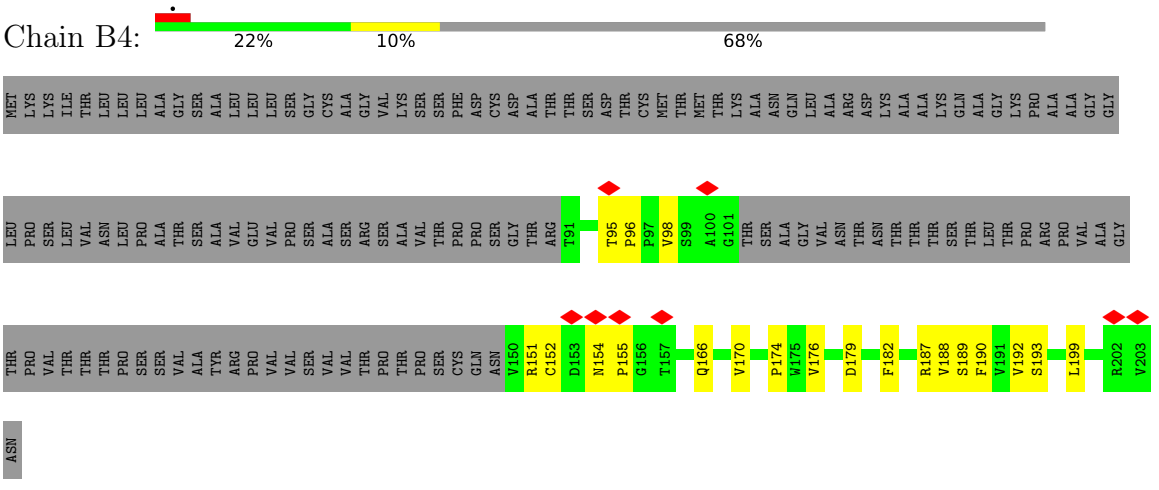
• Molecule 1: TraV

Chain B3:



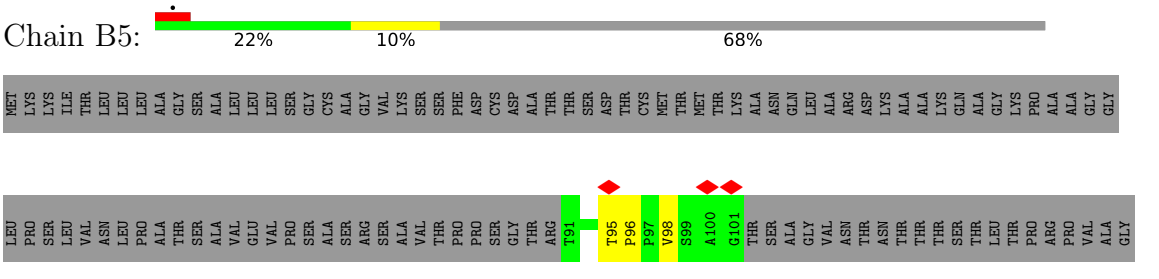
• Molecule 1: TraV

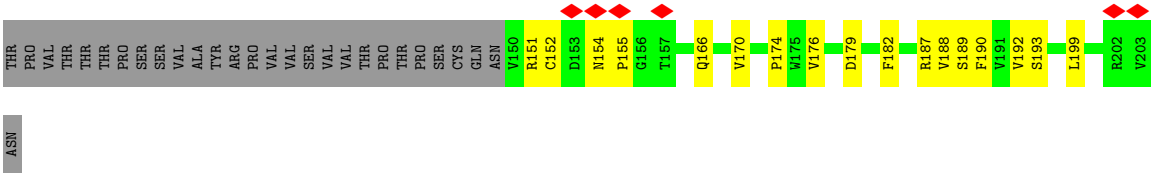
Chain B4:



• Molecule 1: TraV

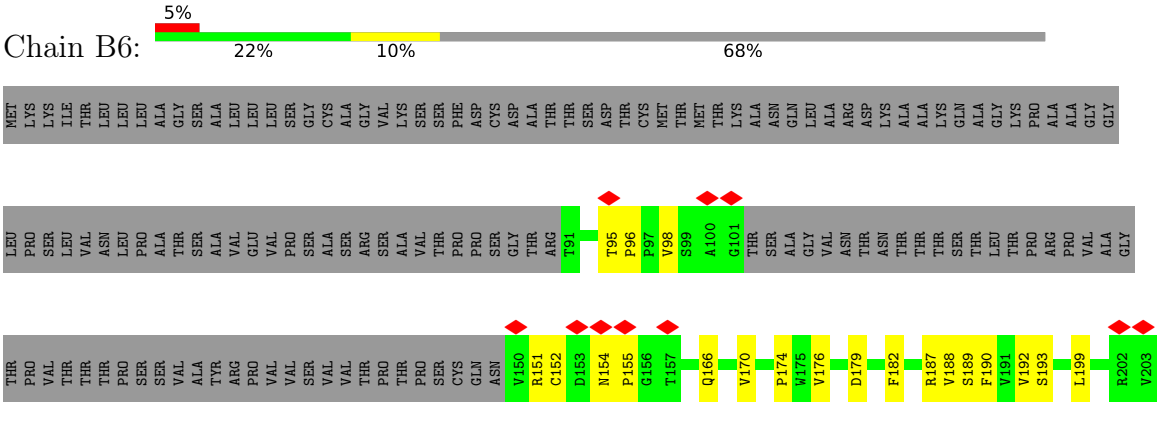
Chain B5:





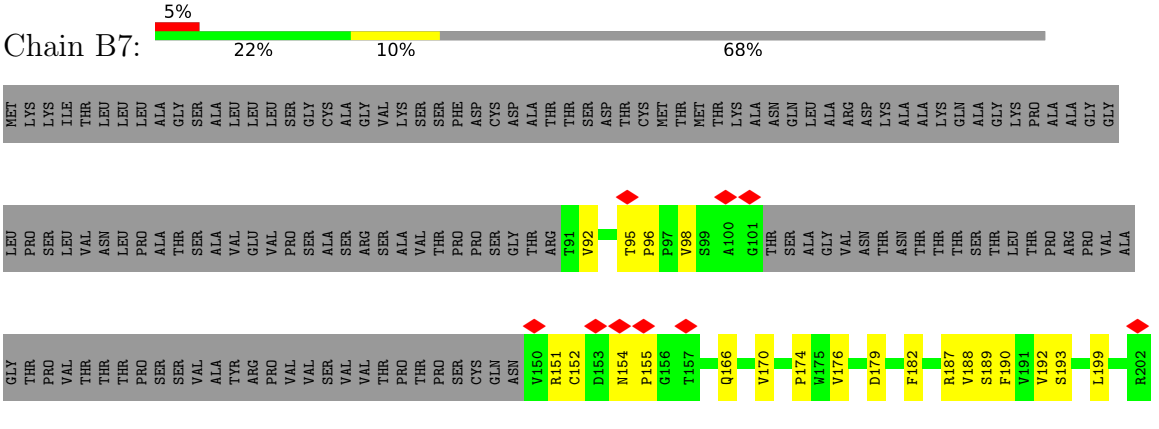
- Molecule 1: TraV

Chain B6:



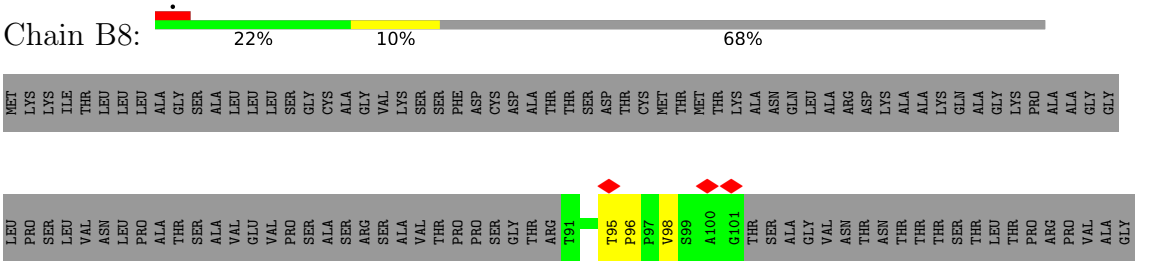
- Molecule 1: TraV

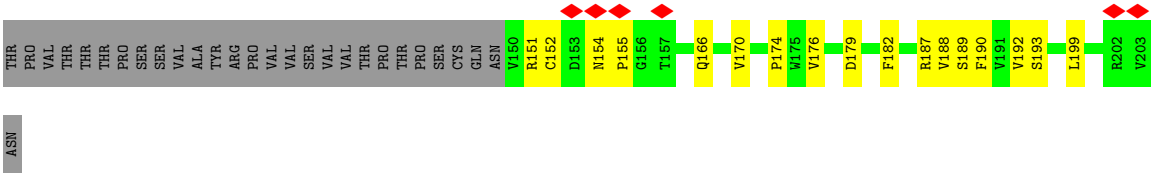
Chain B7:



- Molecule 1: TraV

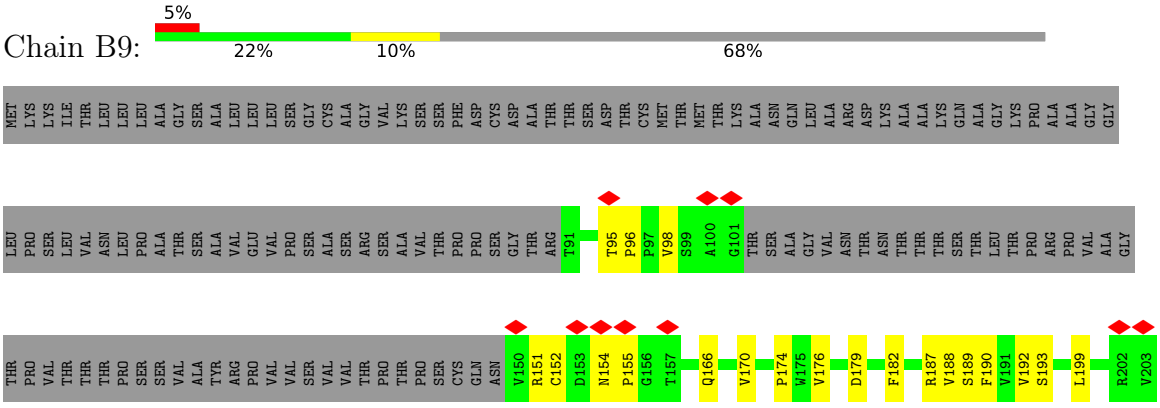
Chain B8:





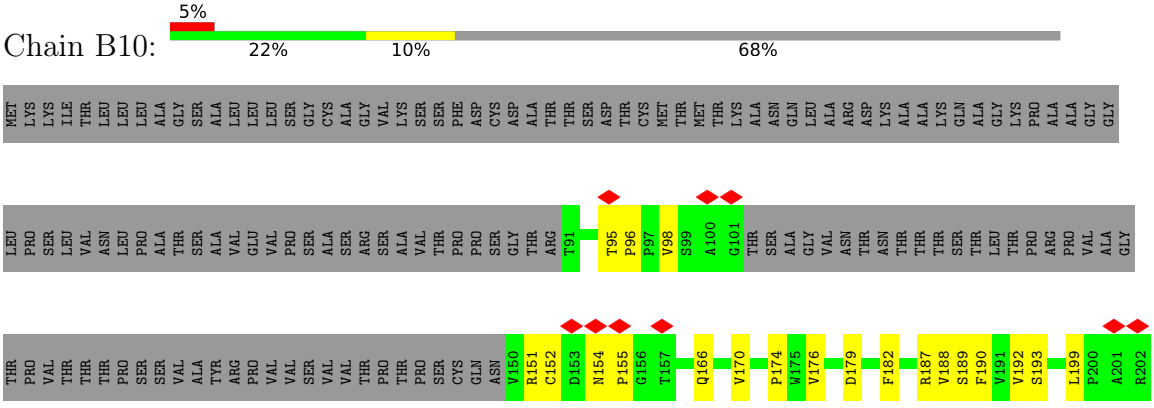
• Molecule 1: TraV

Chain B9:



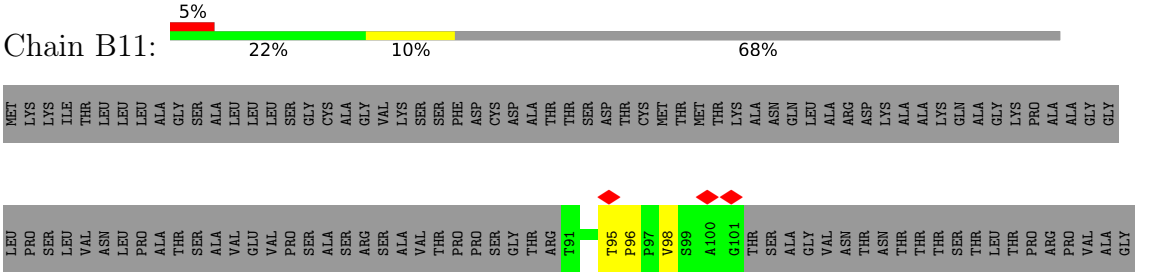
• Molecule 1: TraV

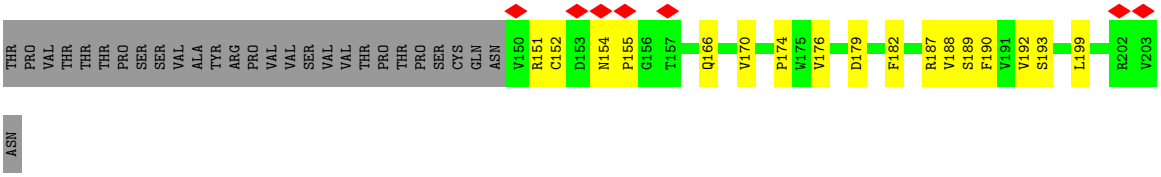
Chain B10:



• Molecule 1: TraV

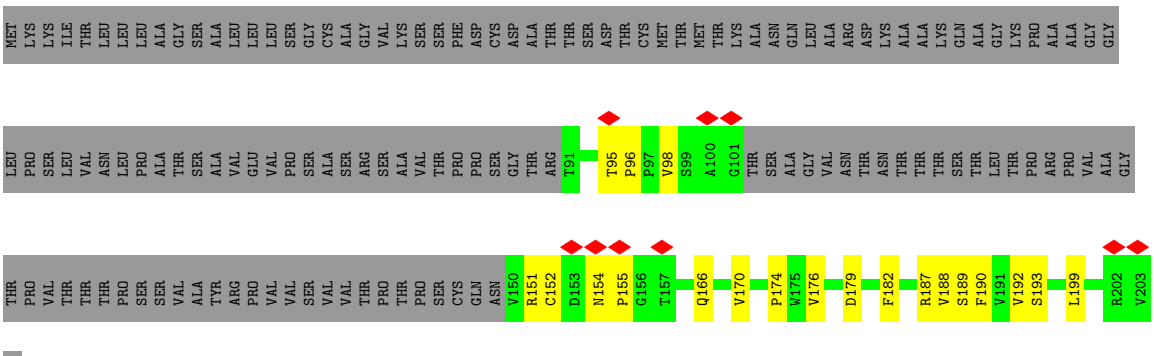
Chain B11:





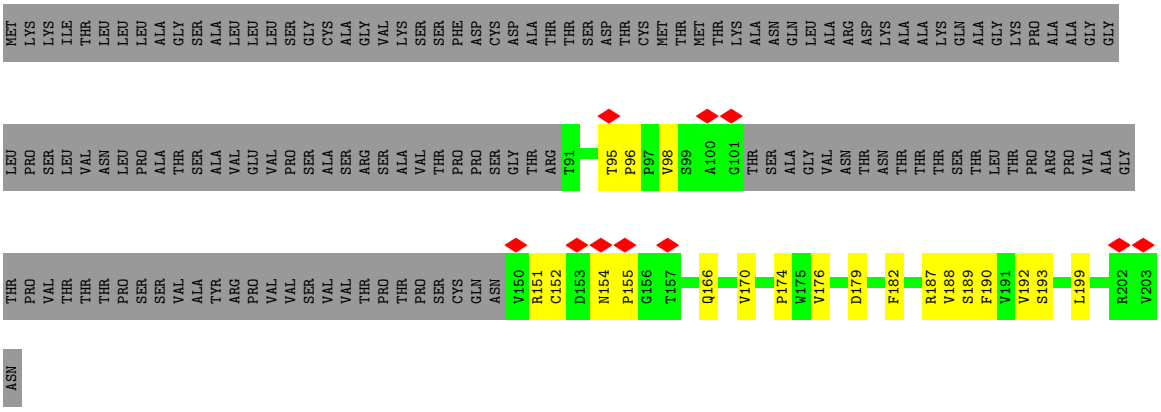
• Molecule 1: TraV

Chain B12:



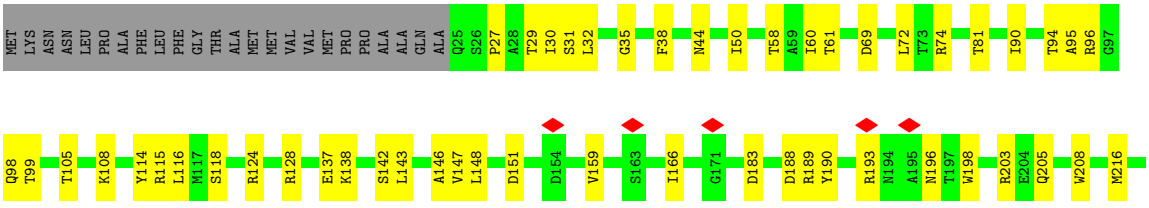
• Molecule 1: TraV

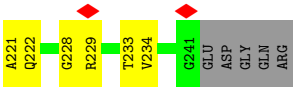
Chain B13:



• Molecule 2: TraK

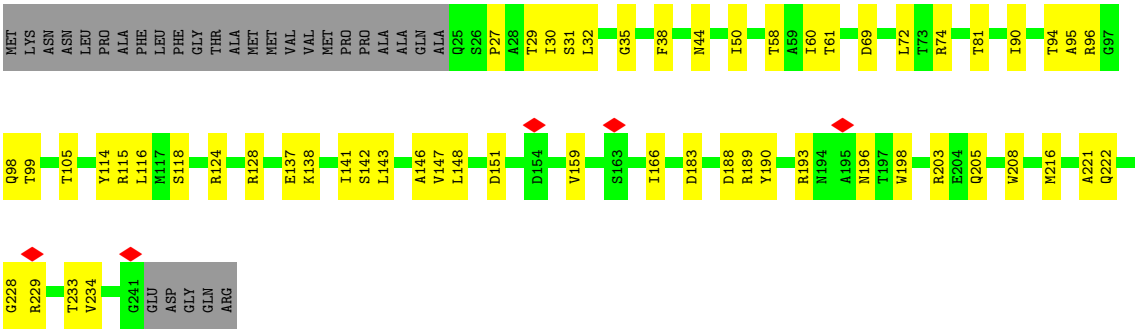
Chain C1:





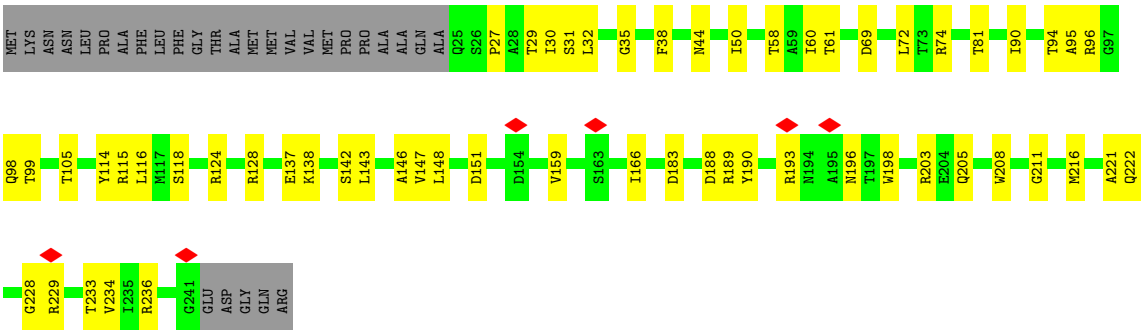
• Molecule 2: TraK

Chain C2:



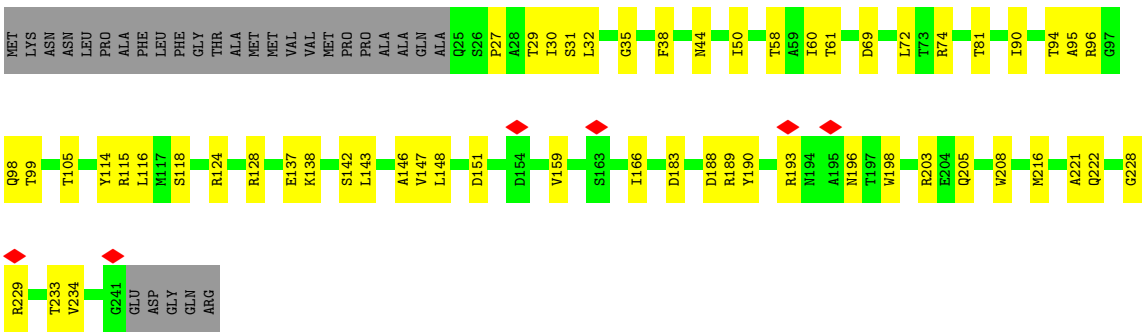
• Molecule 2: TraK

Chain C3:



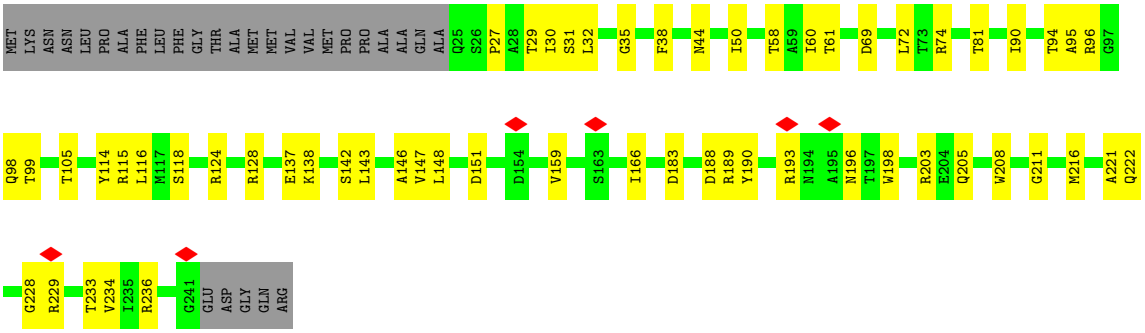
• Molecule 2: TraK

Chain C4:



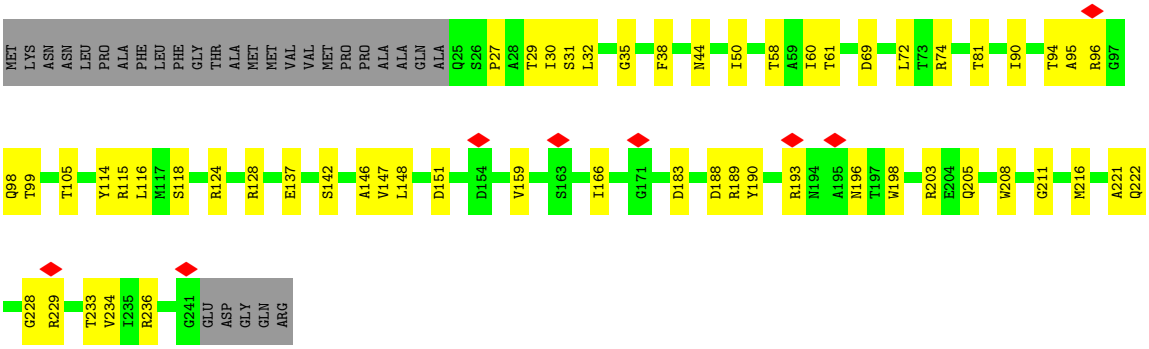
• Molecule 2: TraK

Chain C5:



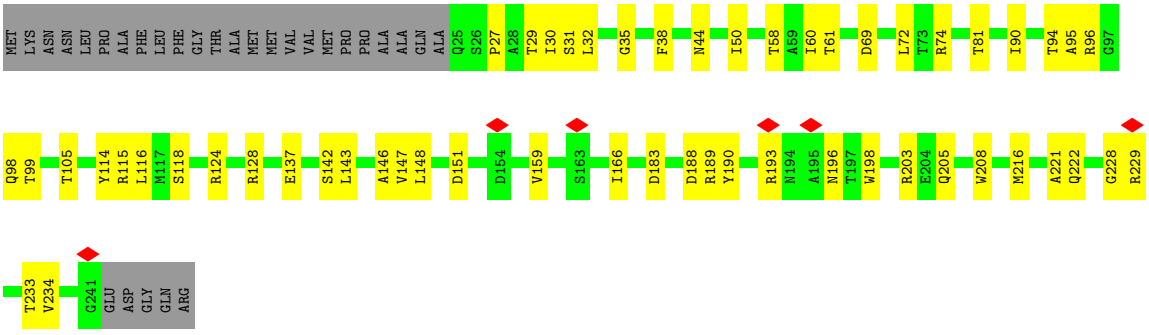
• Molecule 2: TraK

Chain C6:



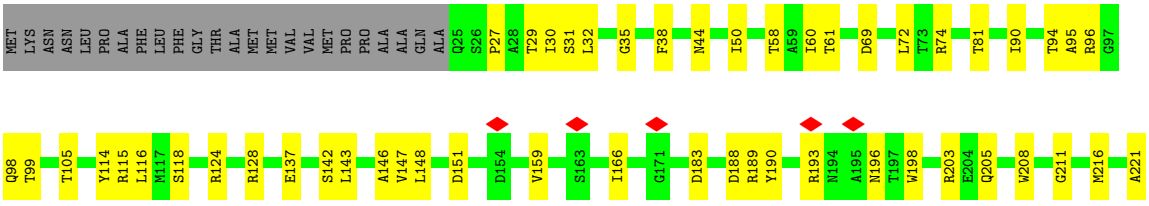
• Molecule 2: TraK

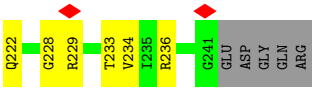
Chain C7:



• Molecule 2: TraK

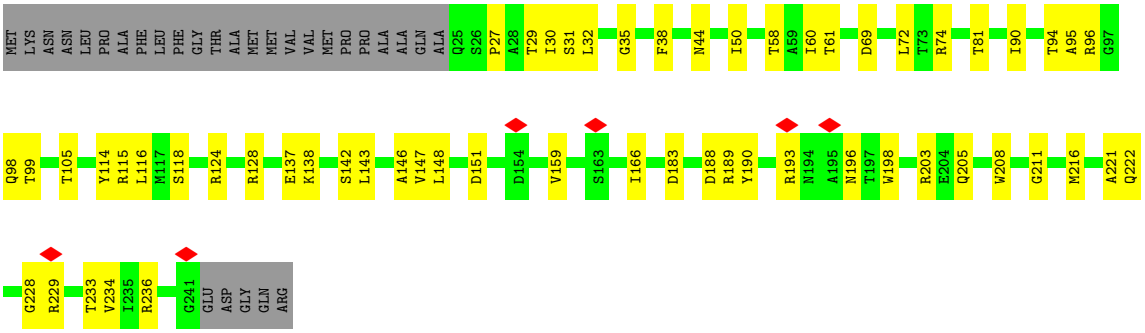
Chain C8:





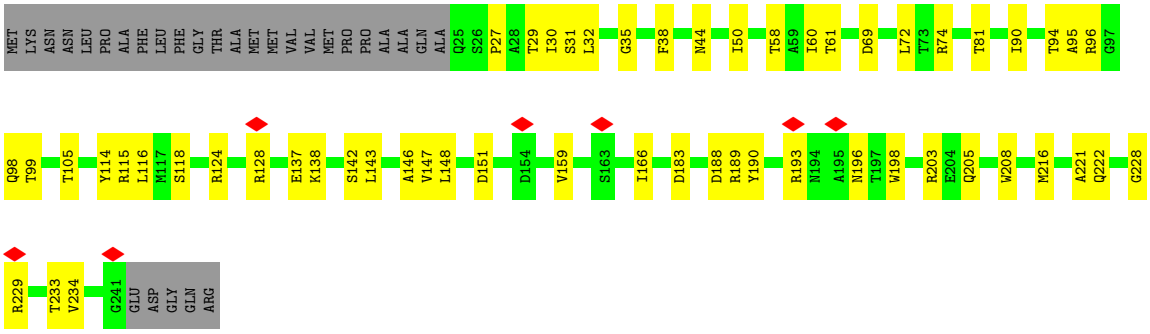
• Molecule 2: TraK

Chain C9:



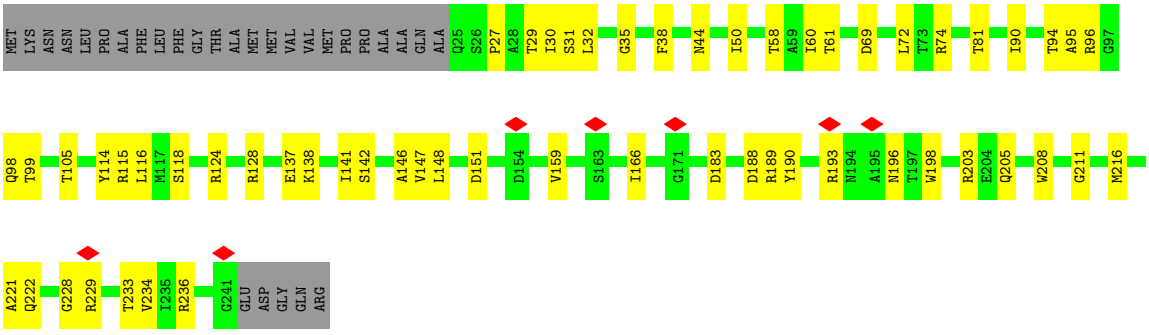
• Molecule 2: TraK

Chain C10:



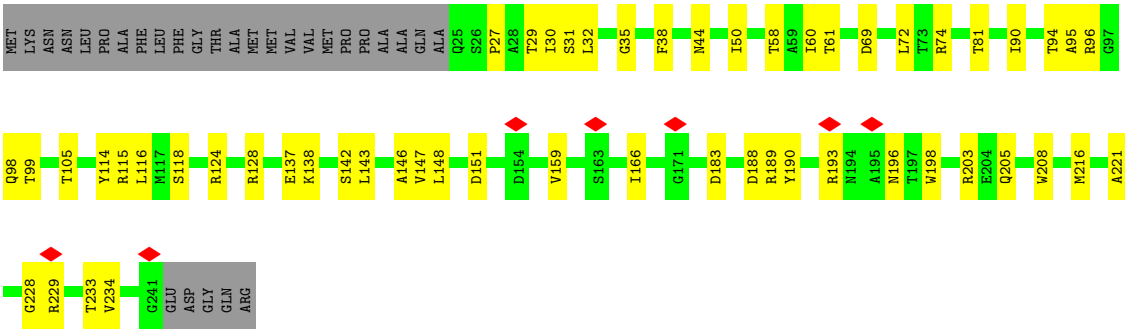
• Molecule 2: TraK

Chain C11:



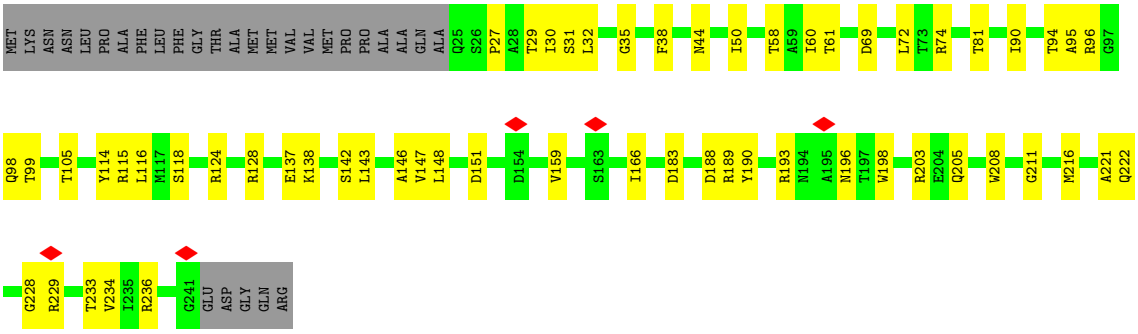
• Molecule 2: TraK

Chain C12:



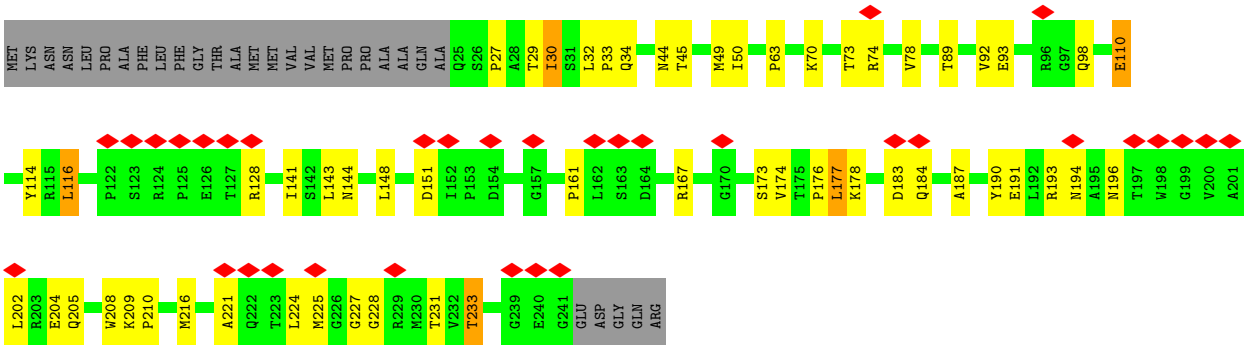
• Molecule 2: TraK

Chain C13:



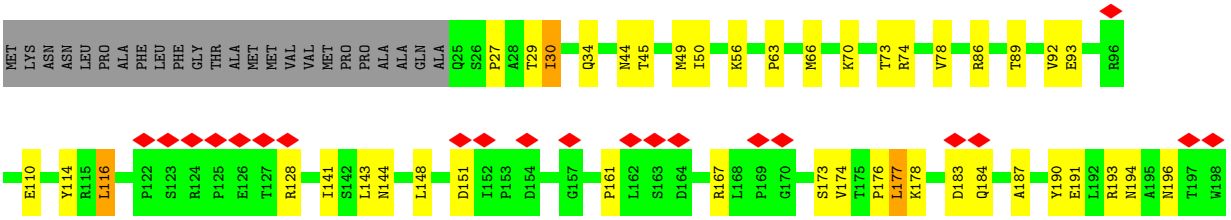
• Molecule 2: TraK

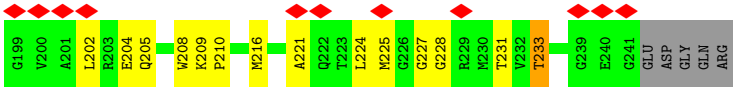
Chain D1:



• Molecule 2: TraK

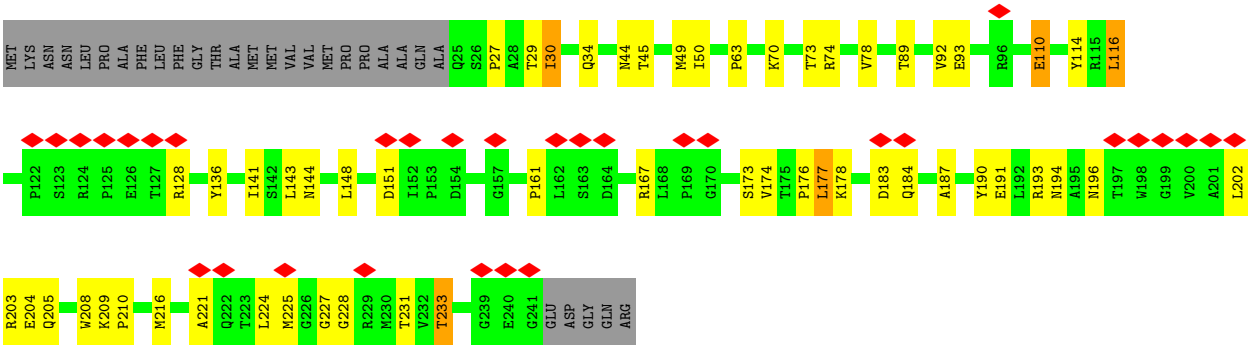
Chain D2:





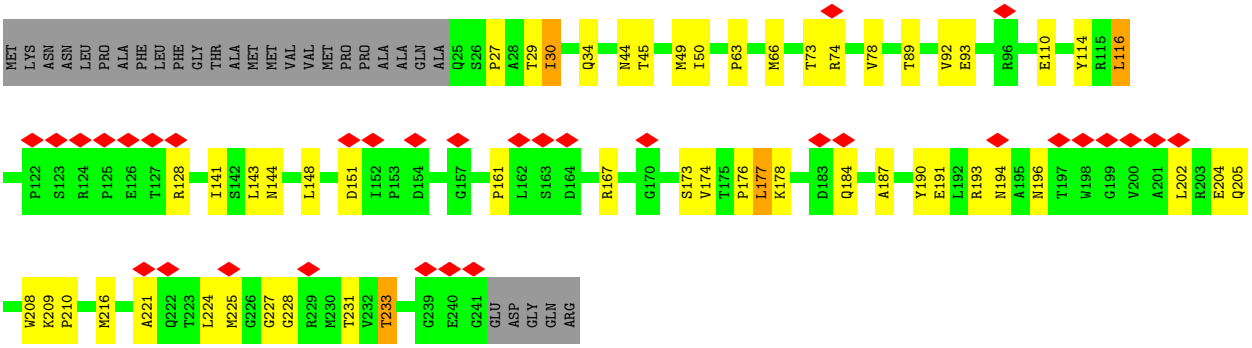
• Molecule 2: TraK

Chain D3:



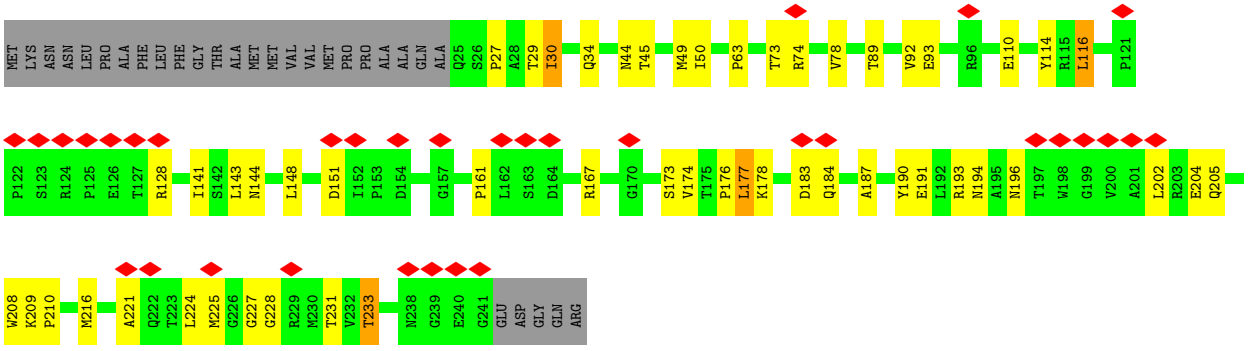
• Molecule 2: TraK

Chain D4:



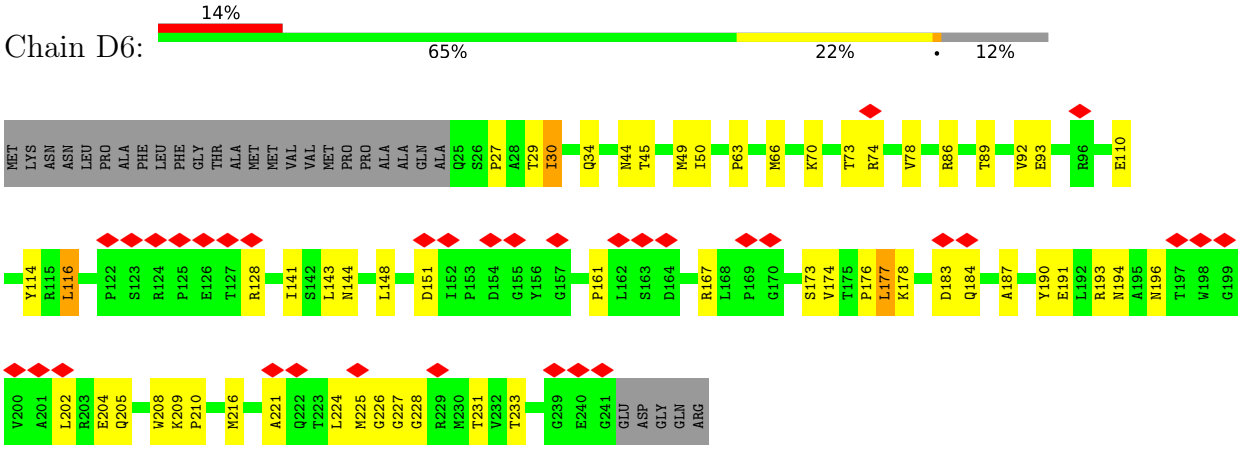
• Molecule 2: TraK

Chain D5:



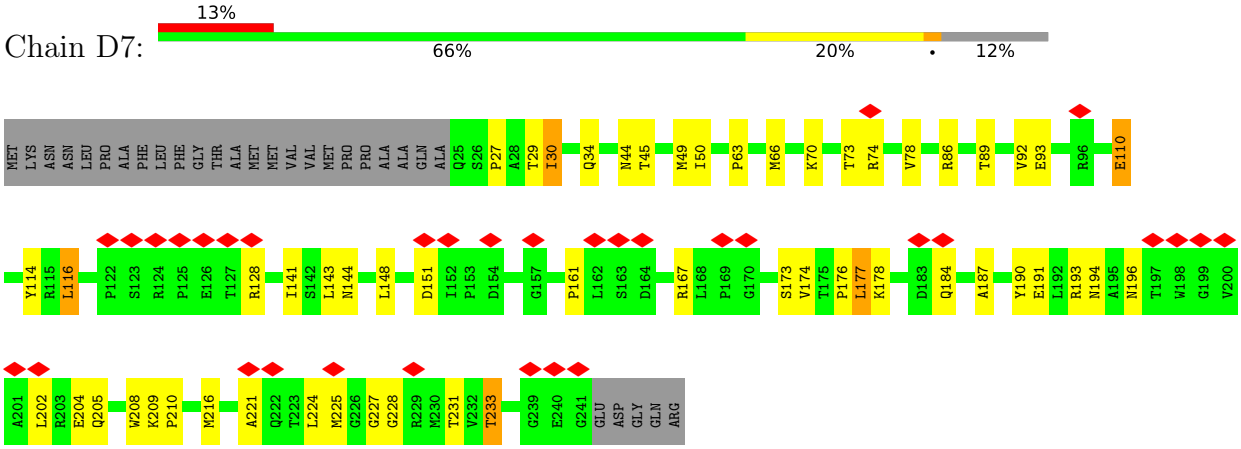
• Molecule 2: TraK

Chain D6:



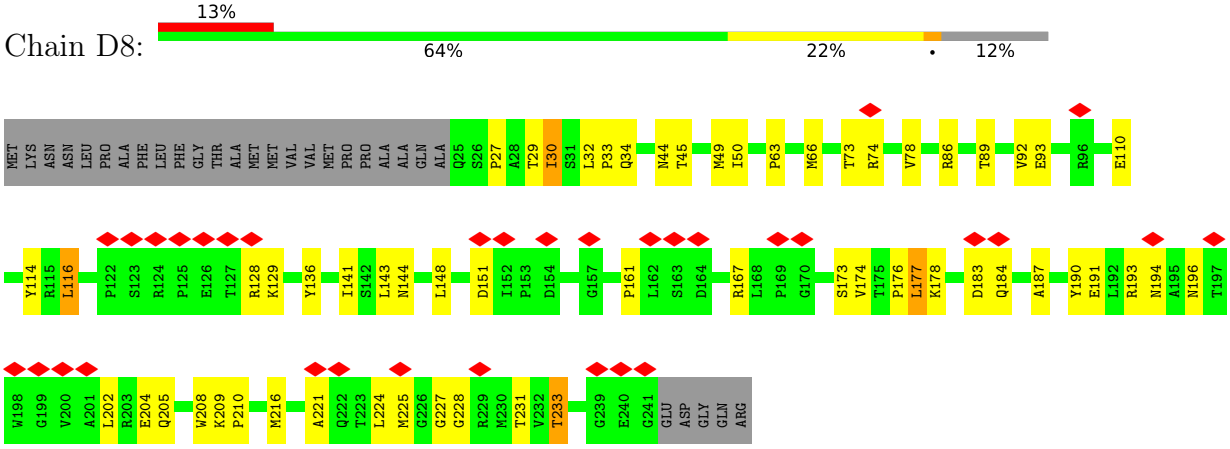
• Molecule 2: TraK

Chain D7:



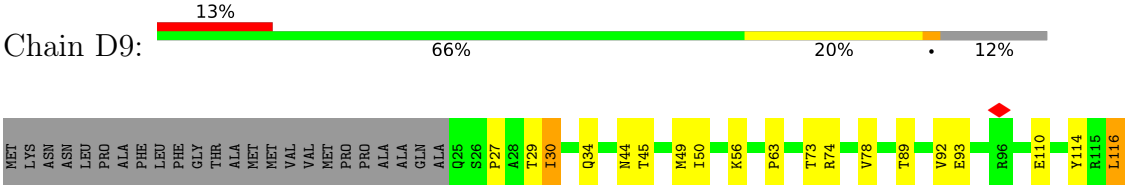
• Molecule 2: TraK

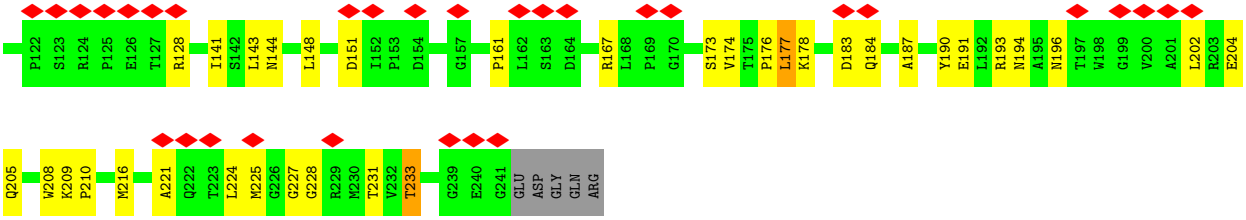
Chain D8:



• Molecule 2: TraK

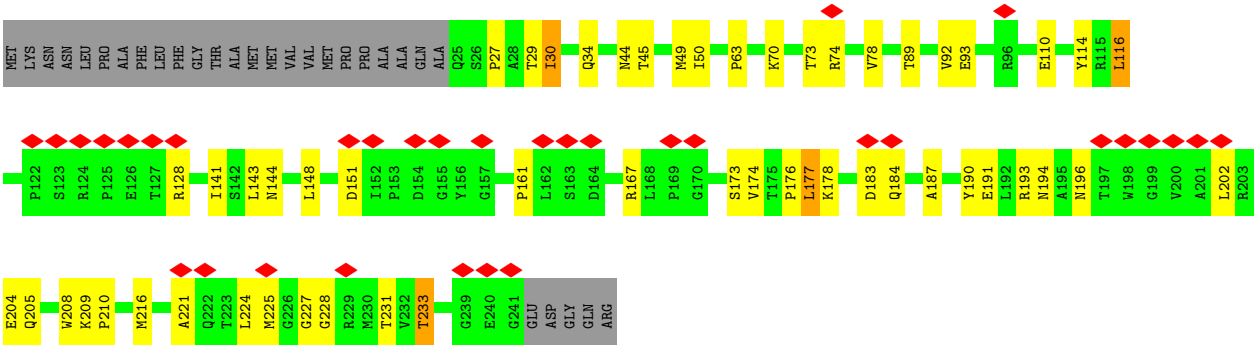
Chain D9:





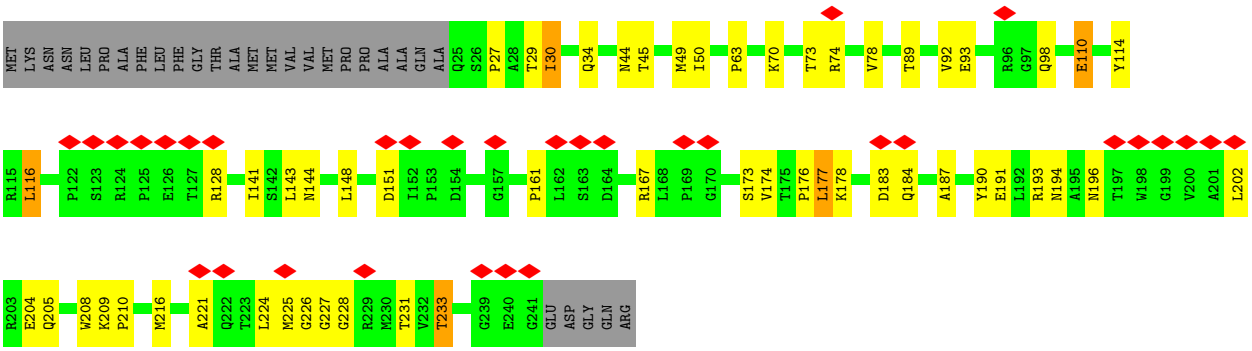
- Molecule 2: TraK

Chain D10:



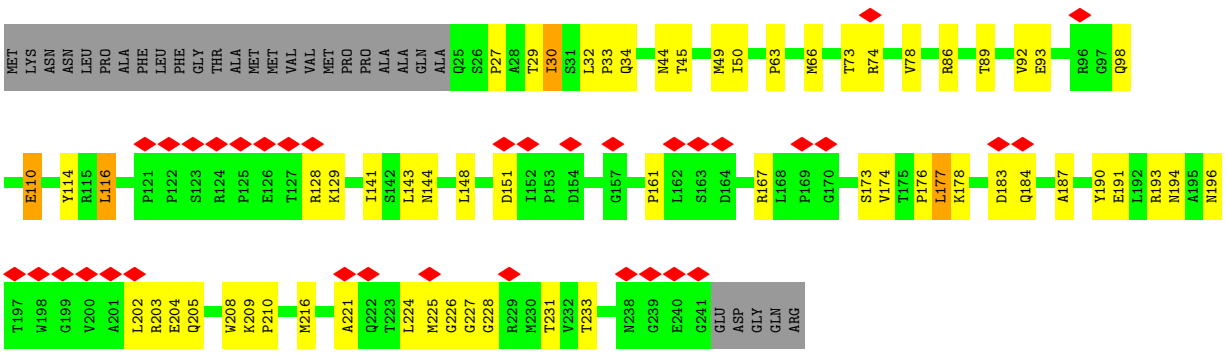
- Molecule 2: TraK

Chain D11:



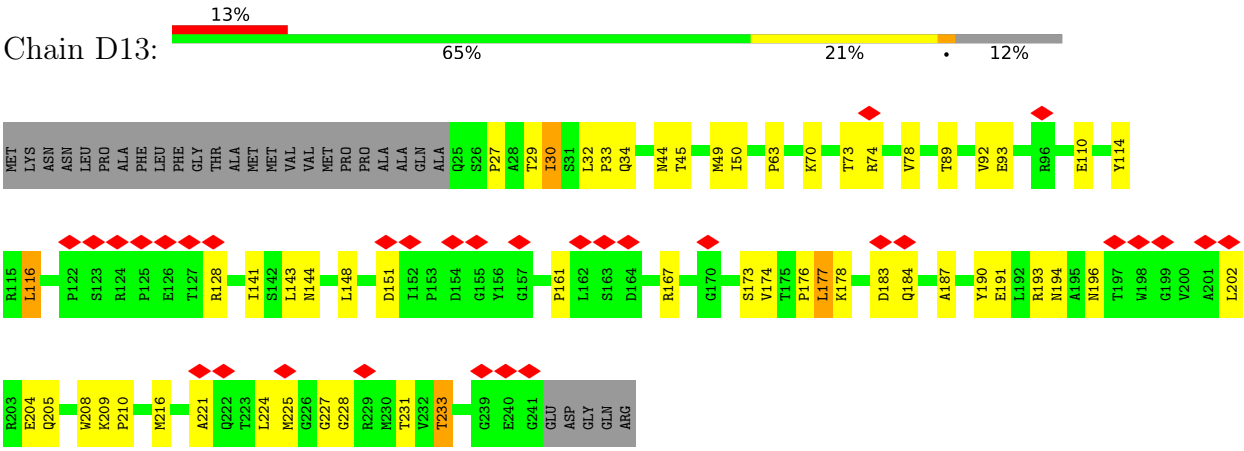
- Molecule 2: TraK

Chain D12:



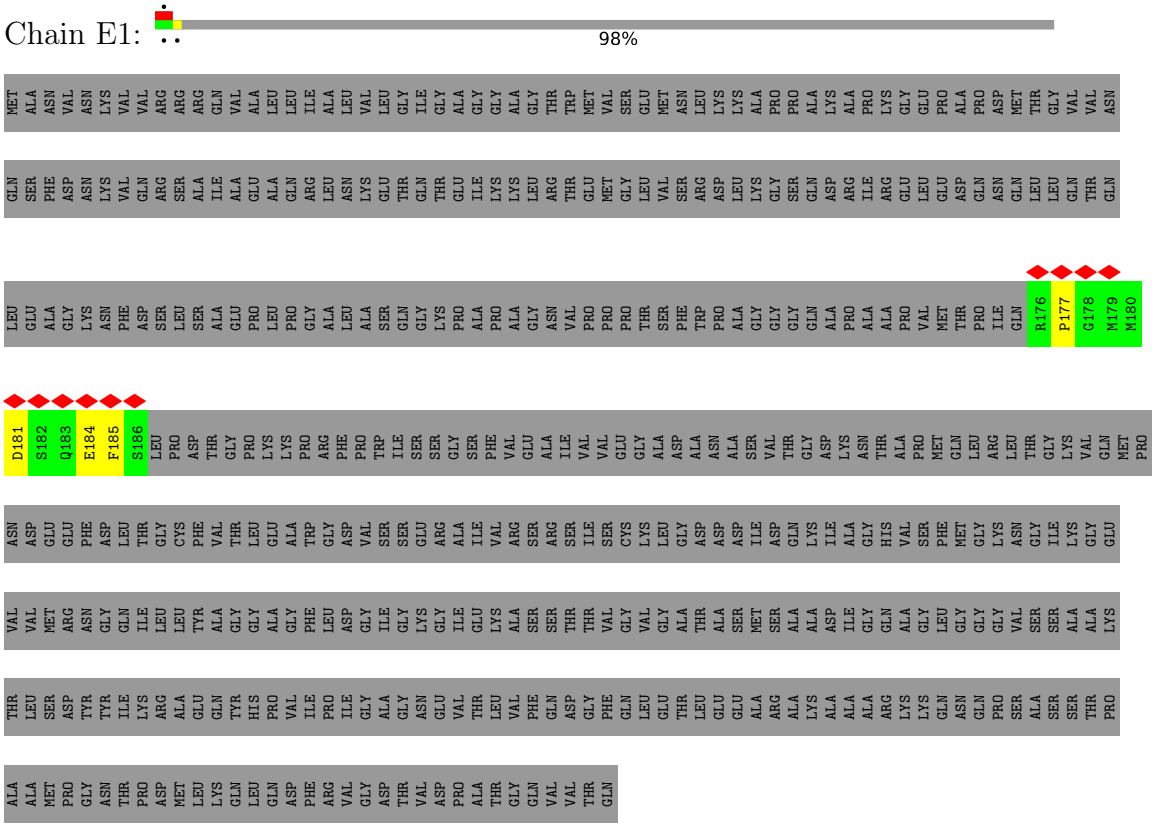
• Molecule 2: TraK

Chain D13:



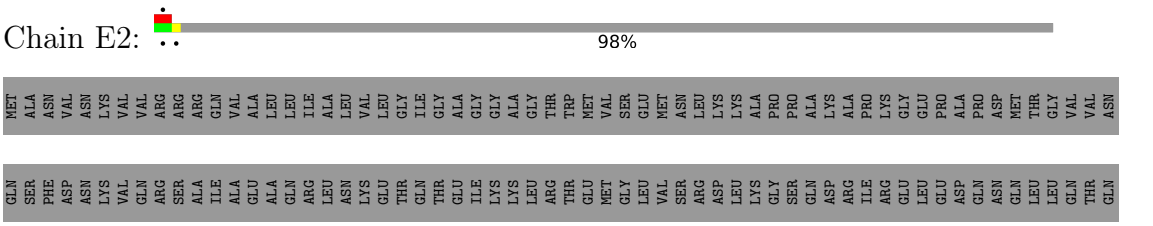
• Molecule 3: TraB

Chain E1:



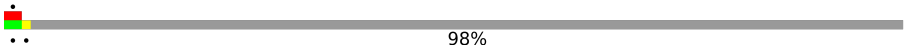
• Molecule 3: TraB

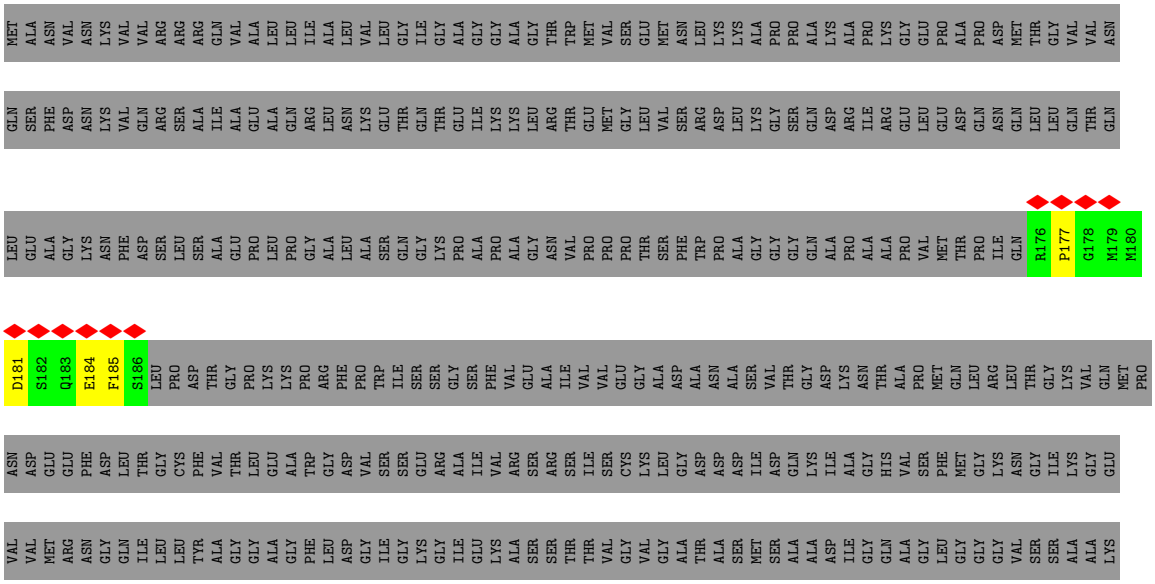
Chain E2:



• Molecule 3: TraB

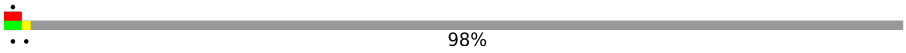
Chain E3:

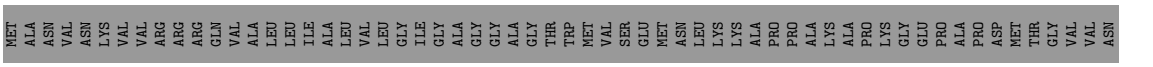




• Molecule 3: TraB

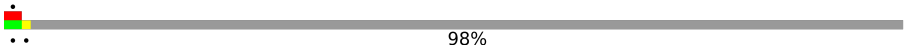
Chain E4:





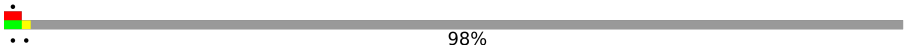
• Molecule 3: TraB

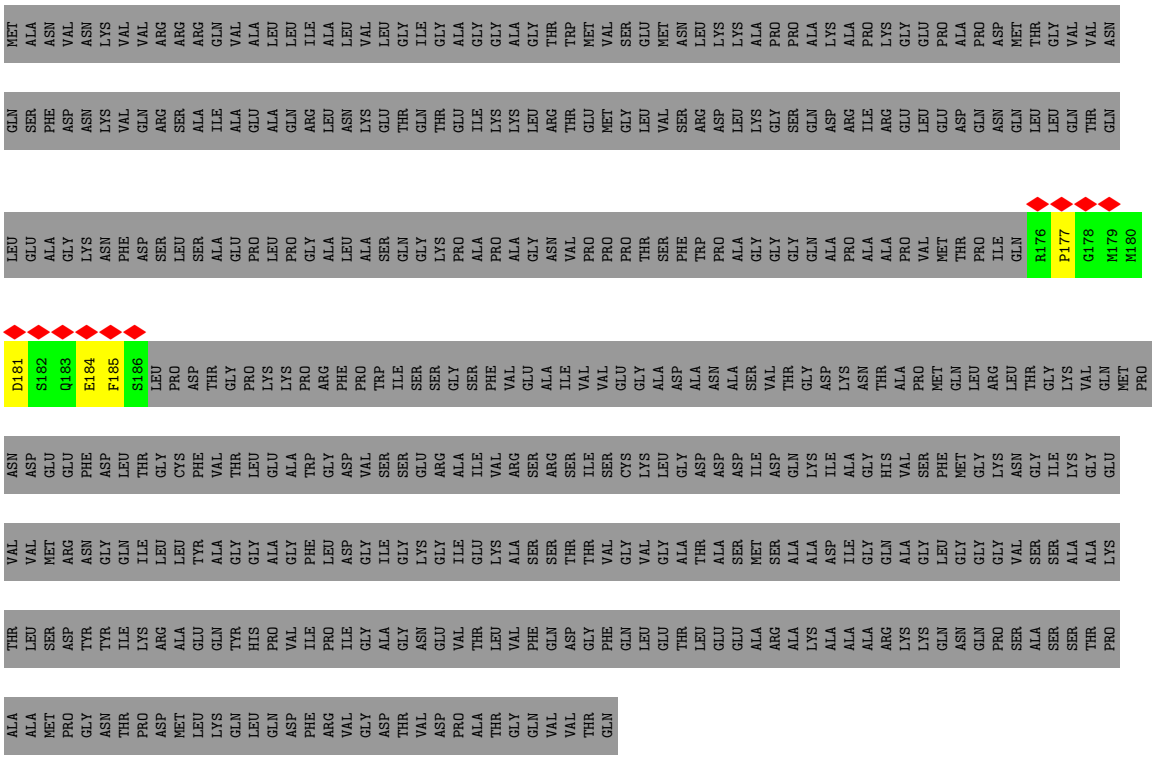
Chain E5:



• Molecule 3: TraB

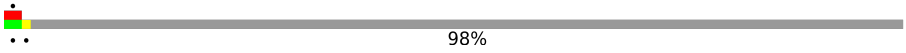
Chain E6:

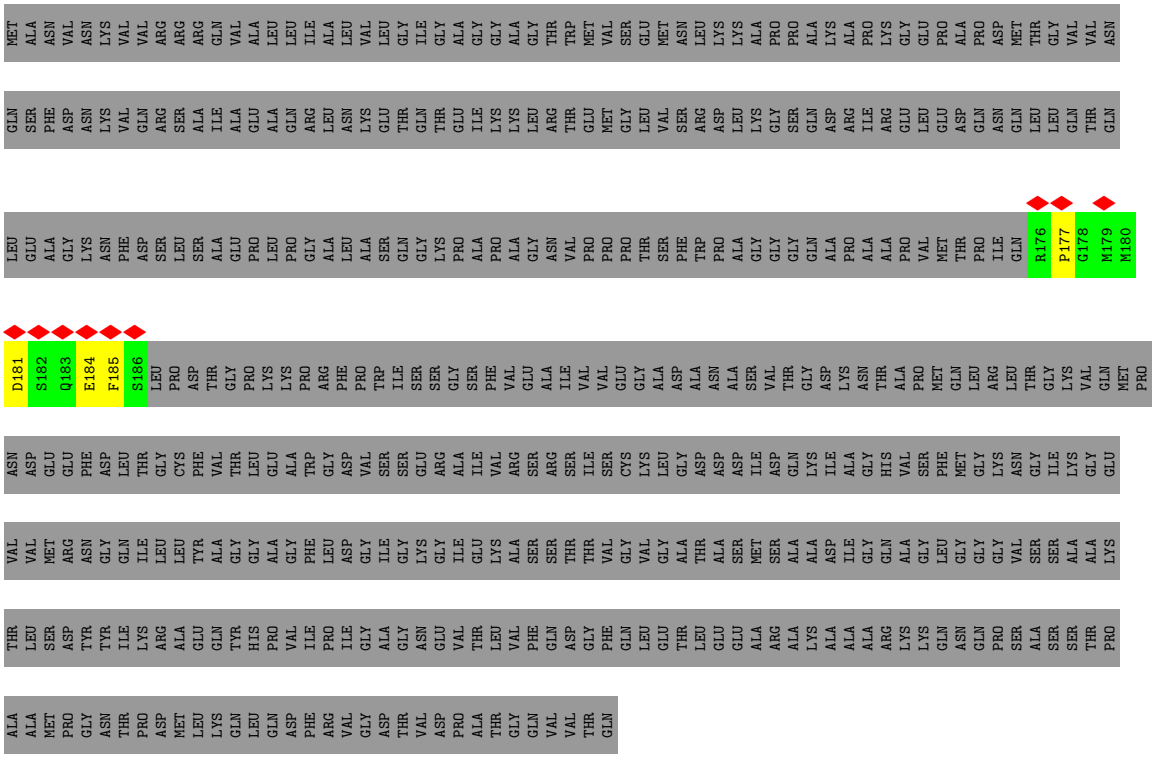




• Molecule 3: TraB

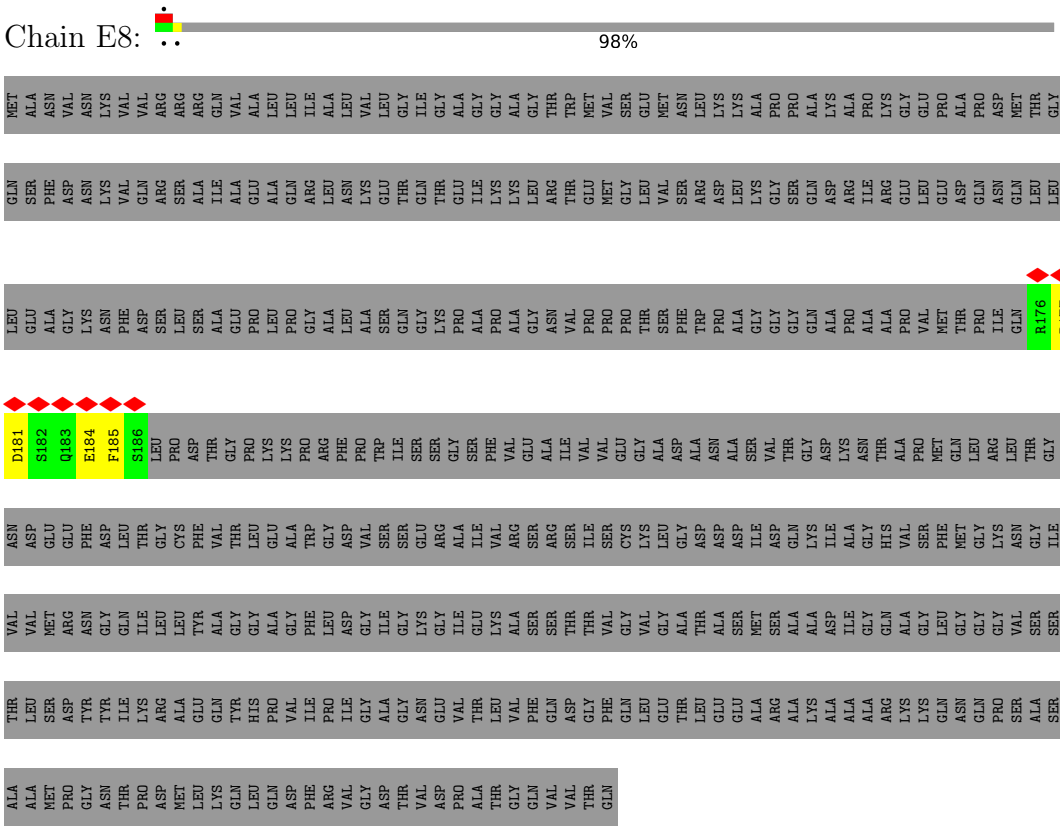
Chain E7:





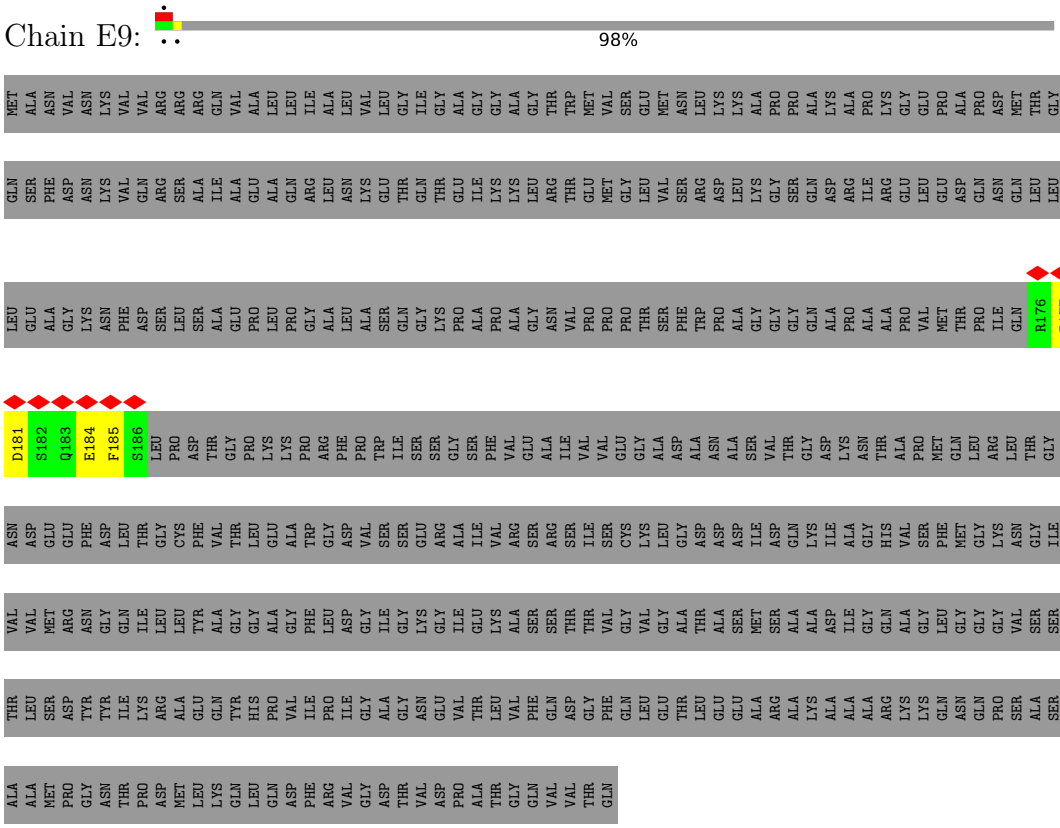
• Molecule 3: TraB

Chain E8:



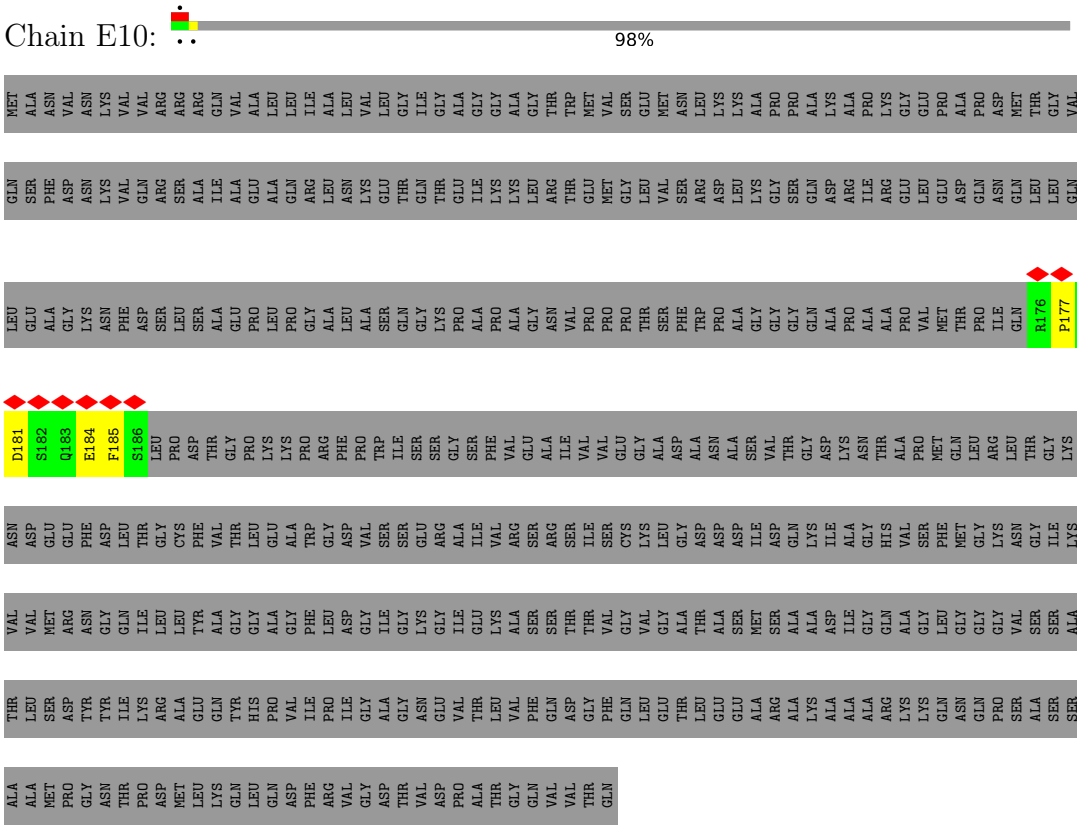
• Molecule 3: TraB

Chain E9:



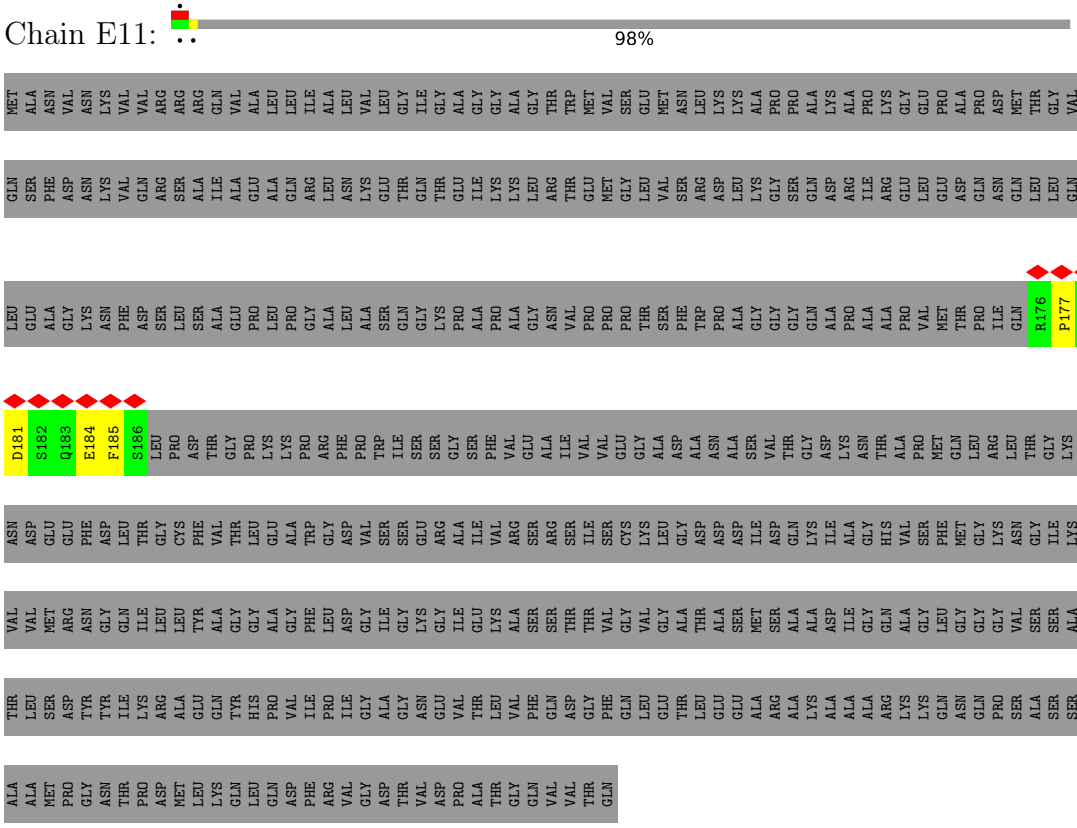
- Molecule 3: TraB

Chain E10:



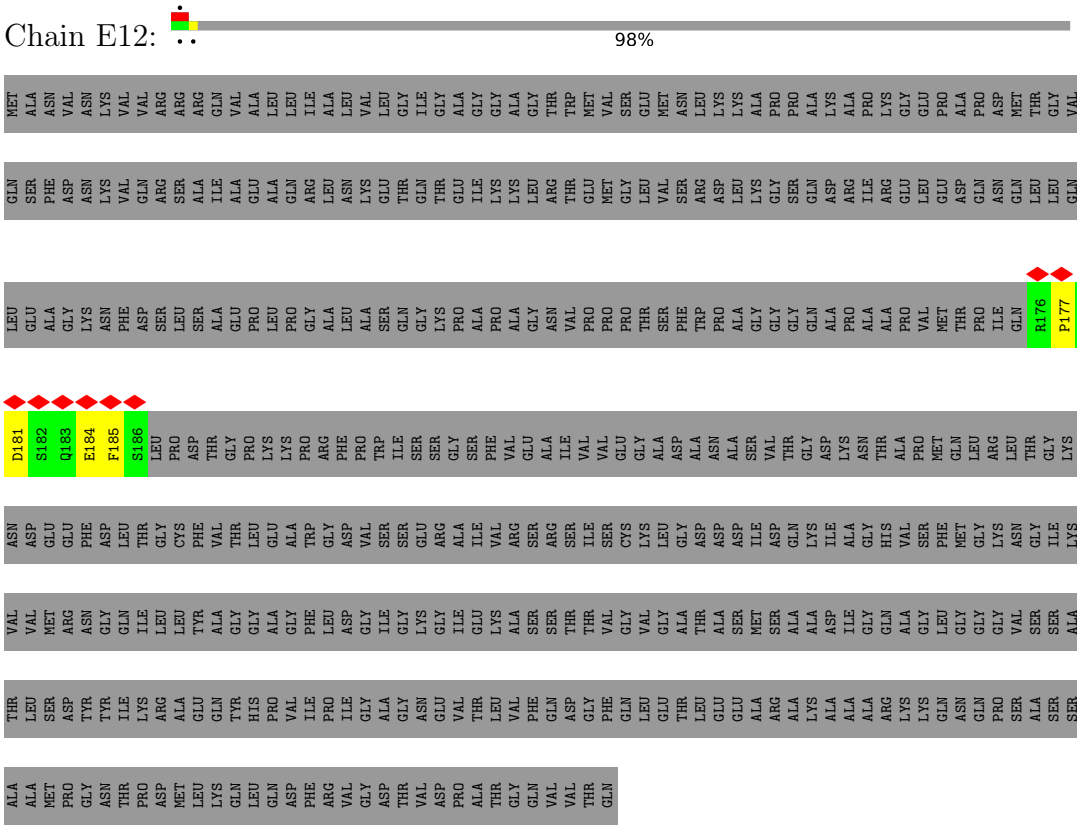
- Molecule 3: TraB

Chain E11:



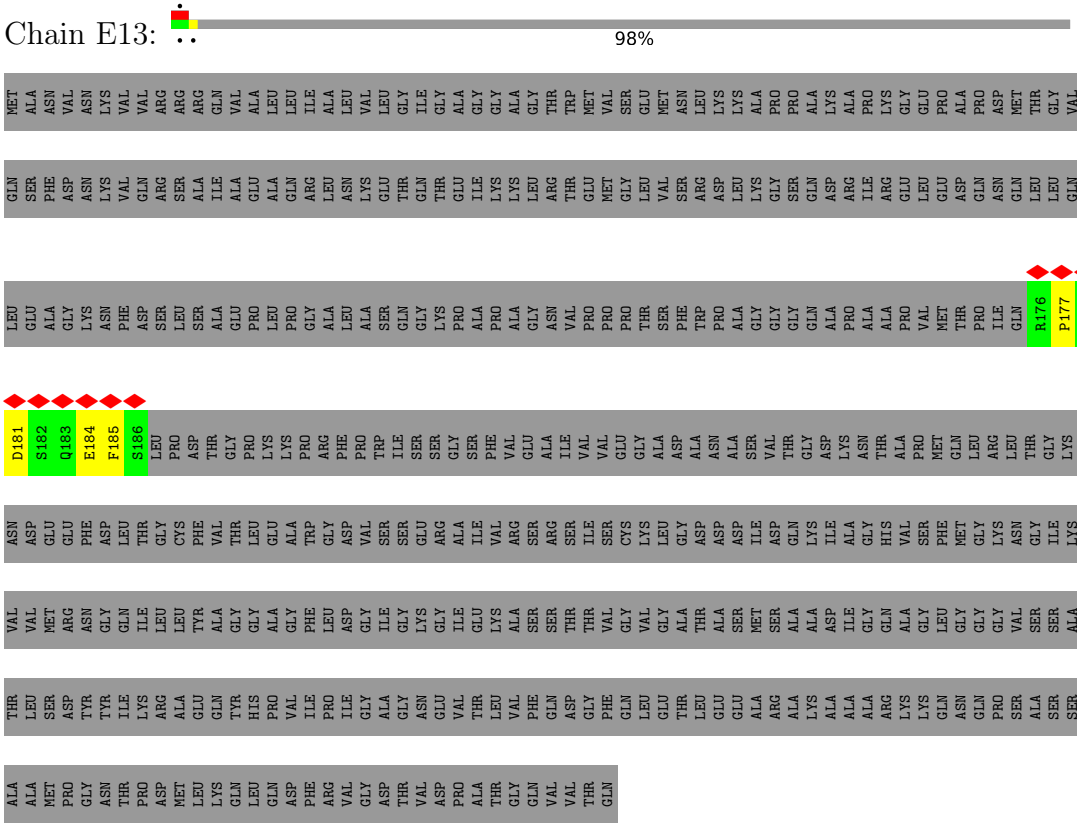
- Molecule 3: TraB

Chain E12:



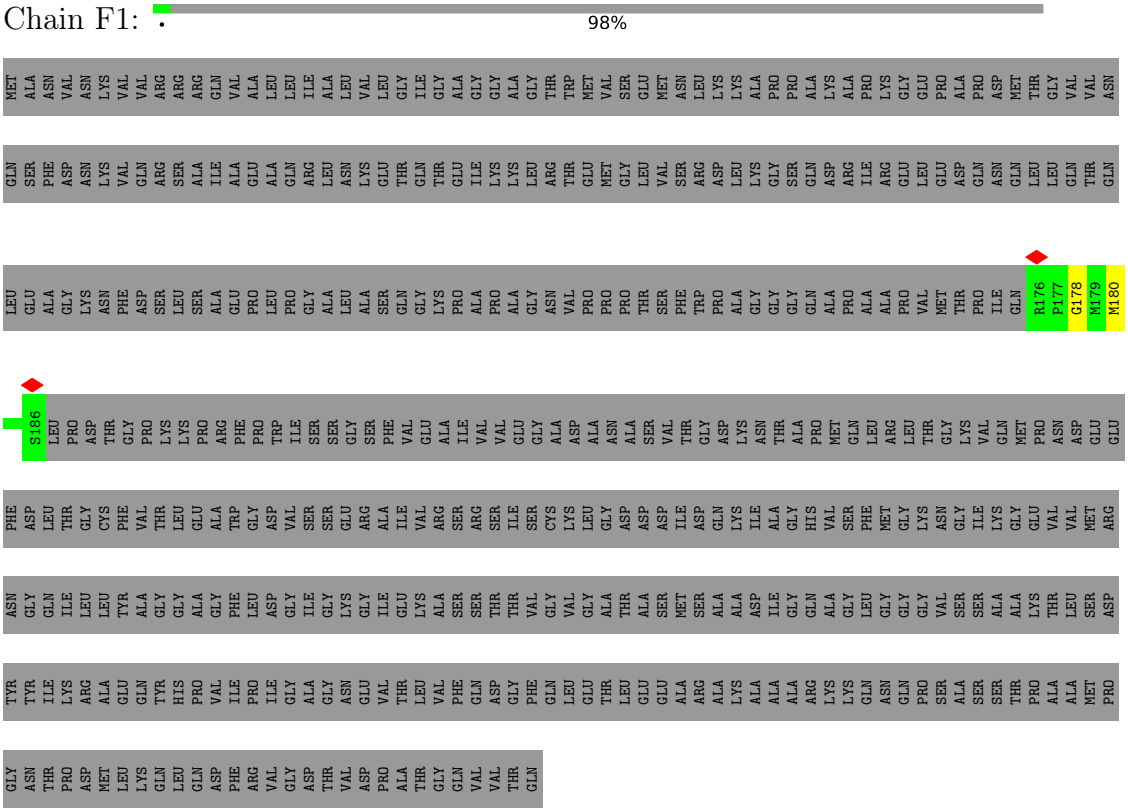
- Molecule 3: TraB

Chain E13:



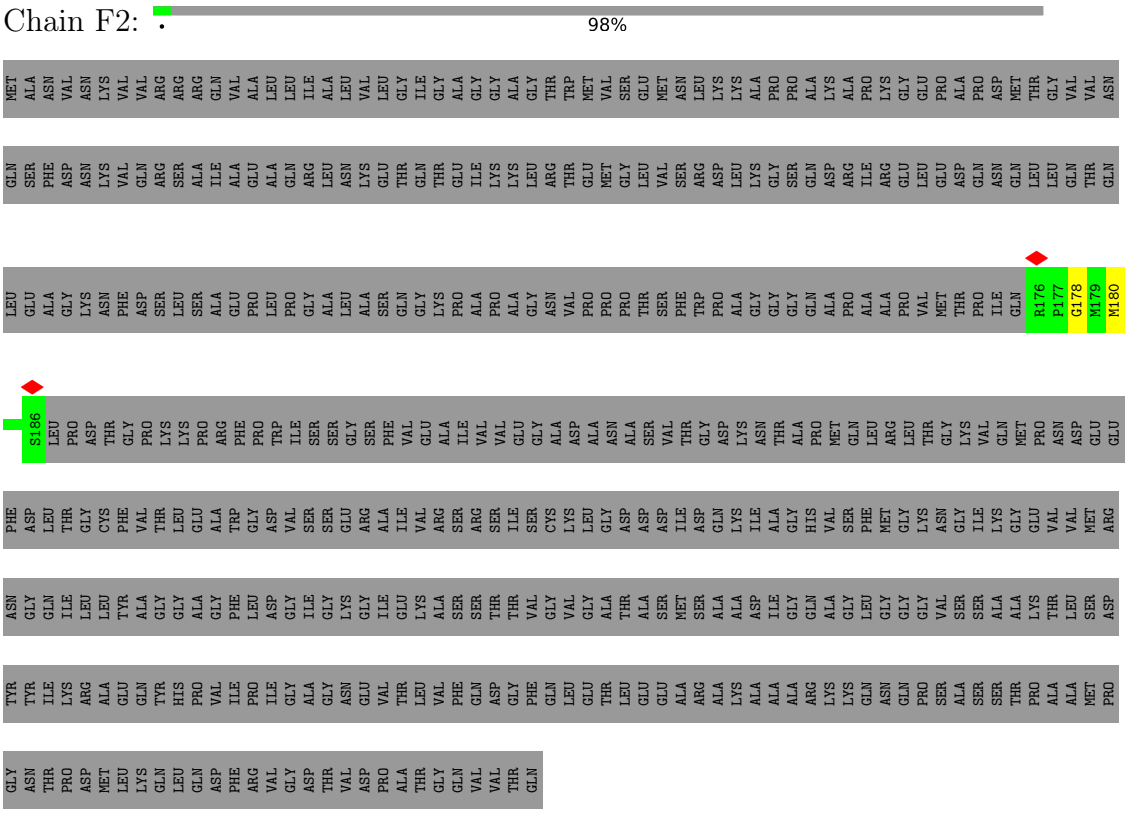
- Molecule 3: TraB

Chain F1:



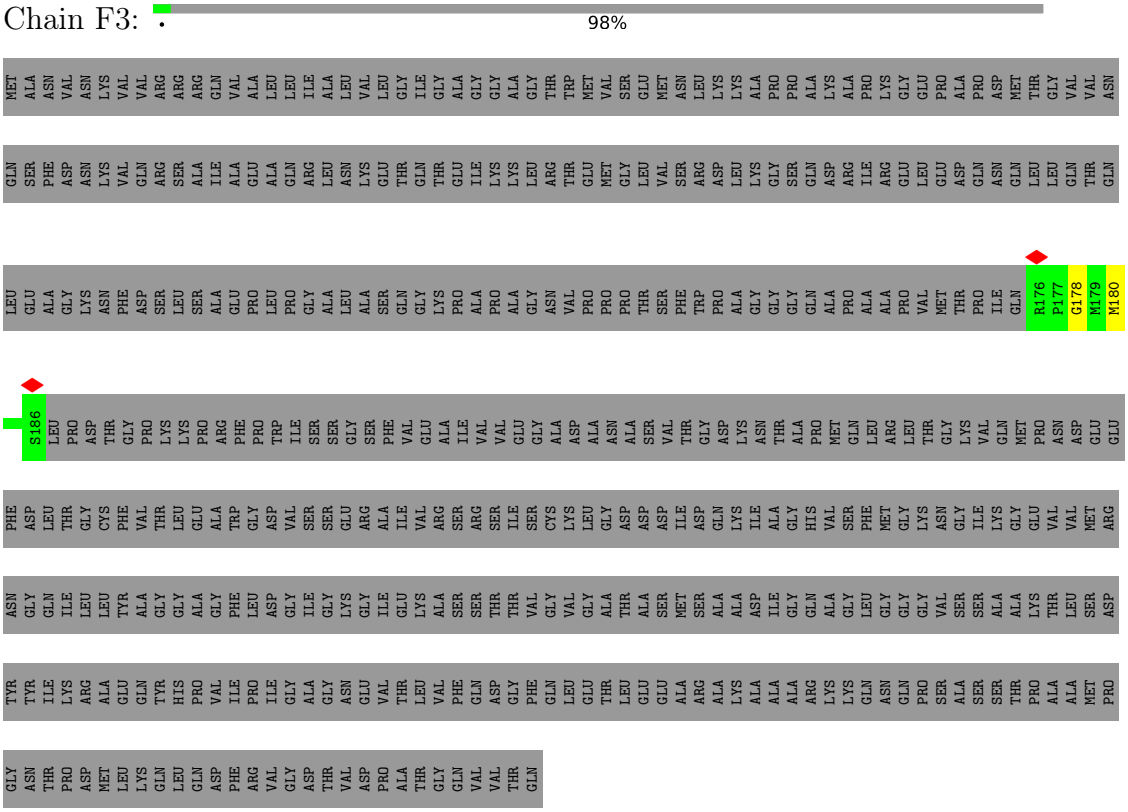
- Molecule 3: TraB

Chain F2:



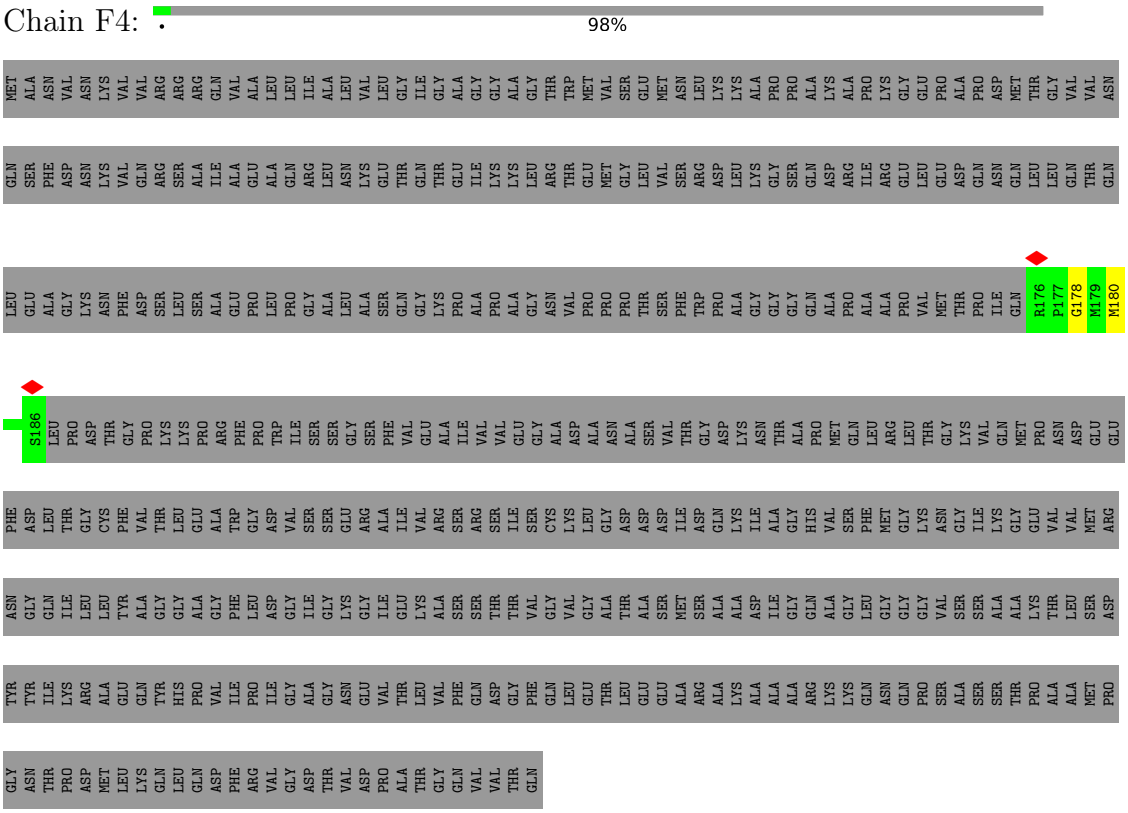
- Molecule 3: TraB

Chain F3:



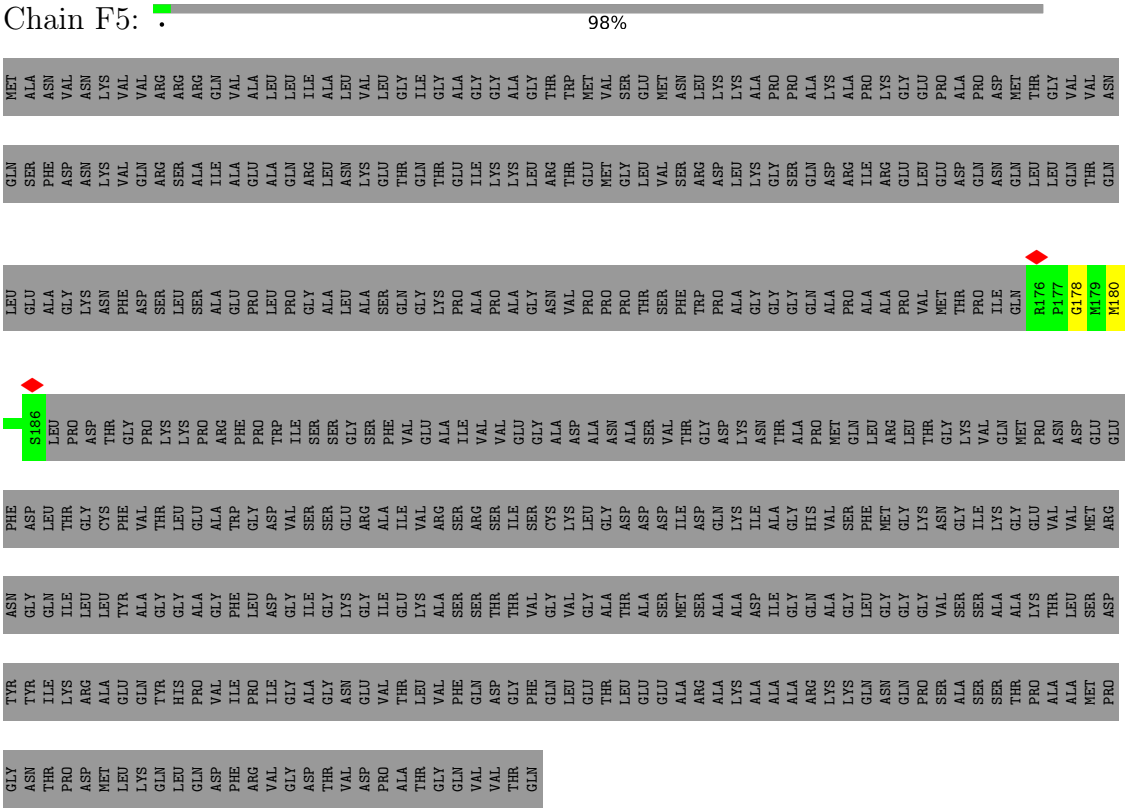
- Molecule 3: TraB

Chain F4:



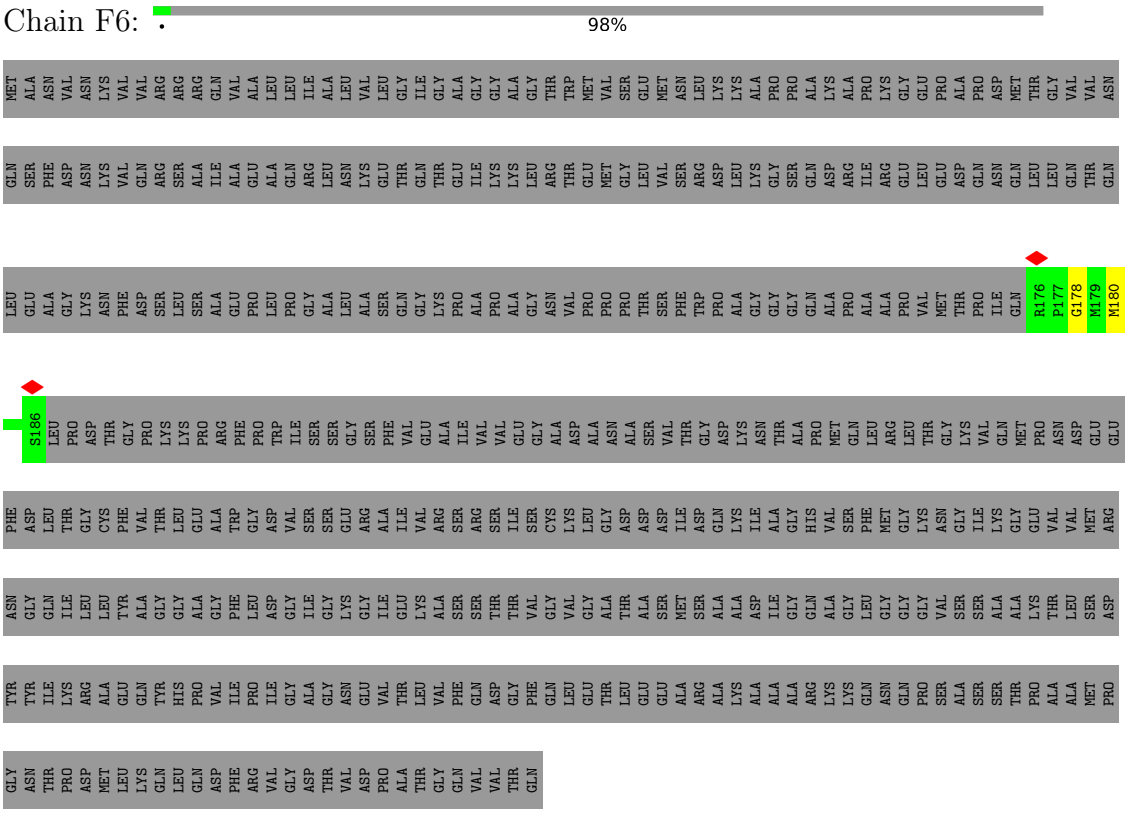
- Molecule 3: TraB

Chain F5:



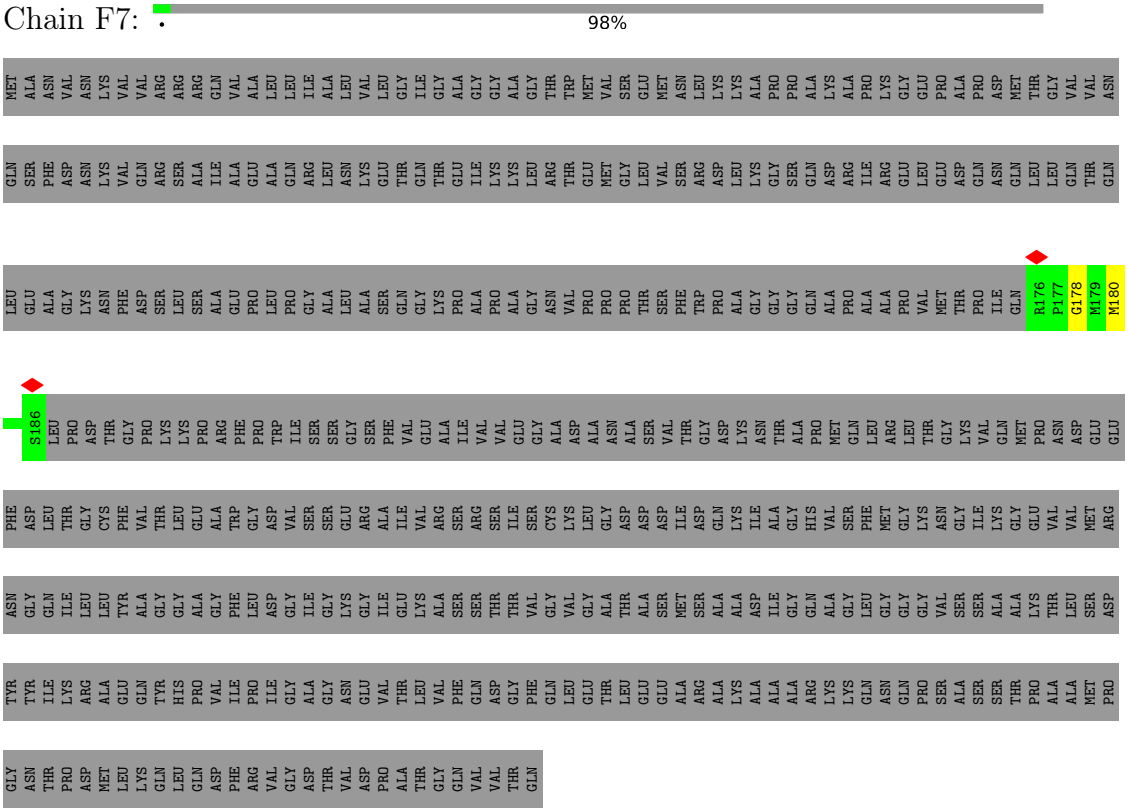
- Molecule 3: TraB

Chain F6:



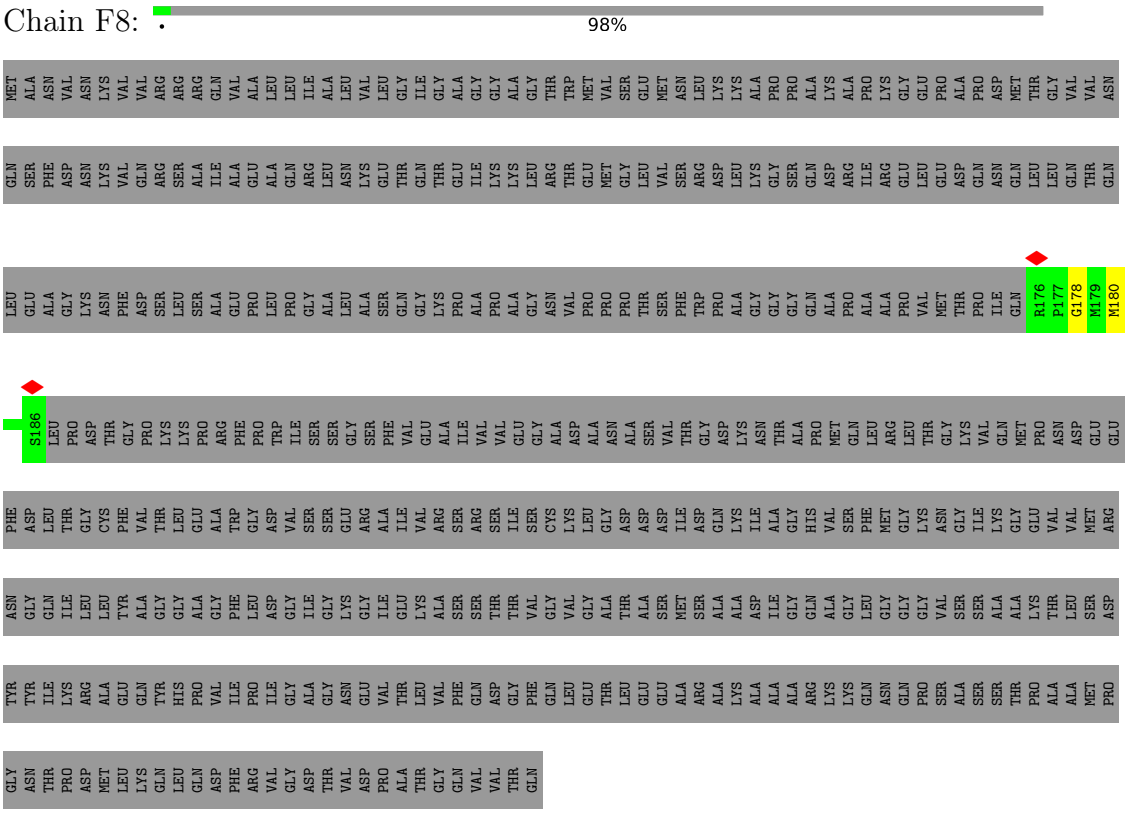
- Molecule 3: TraB

Chain F7:



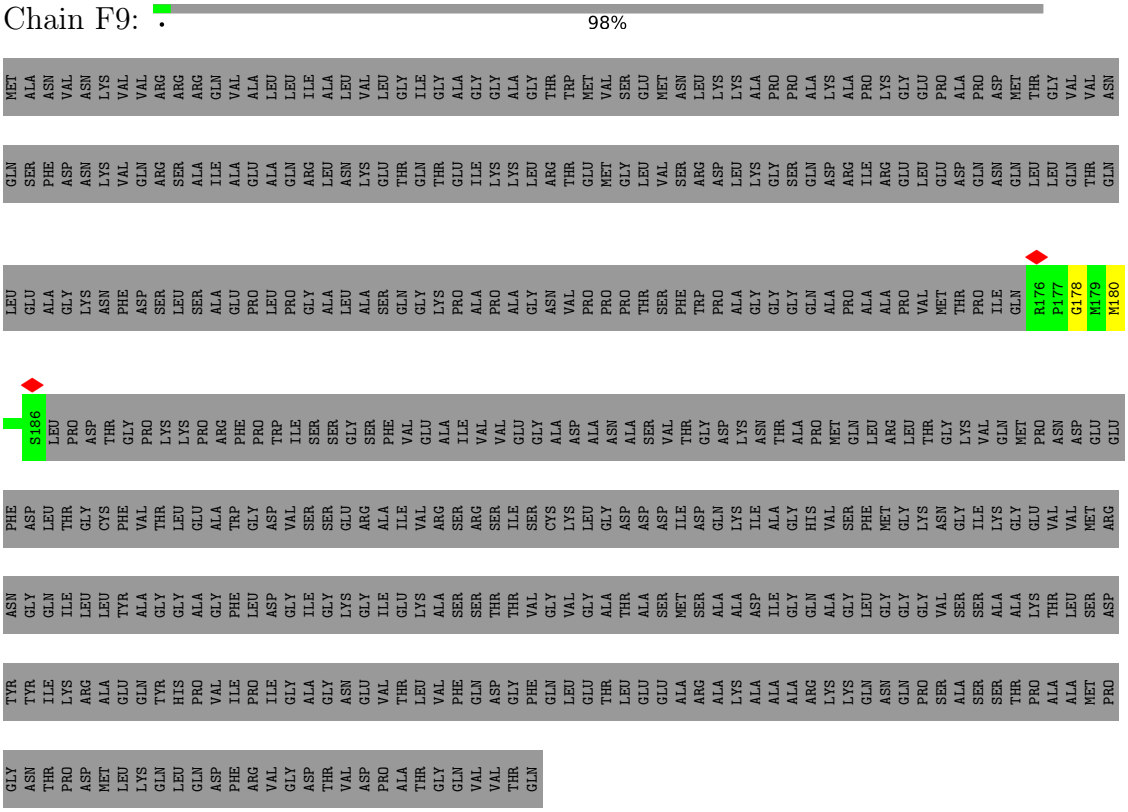
- Molecule 3: TraB

Chain F8:



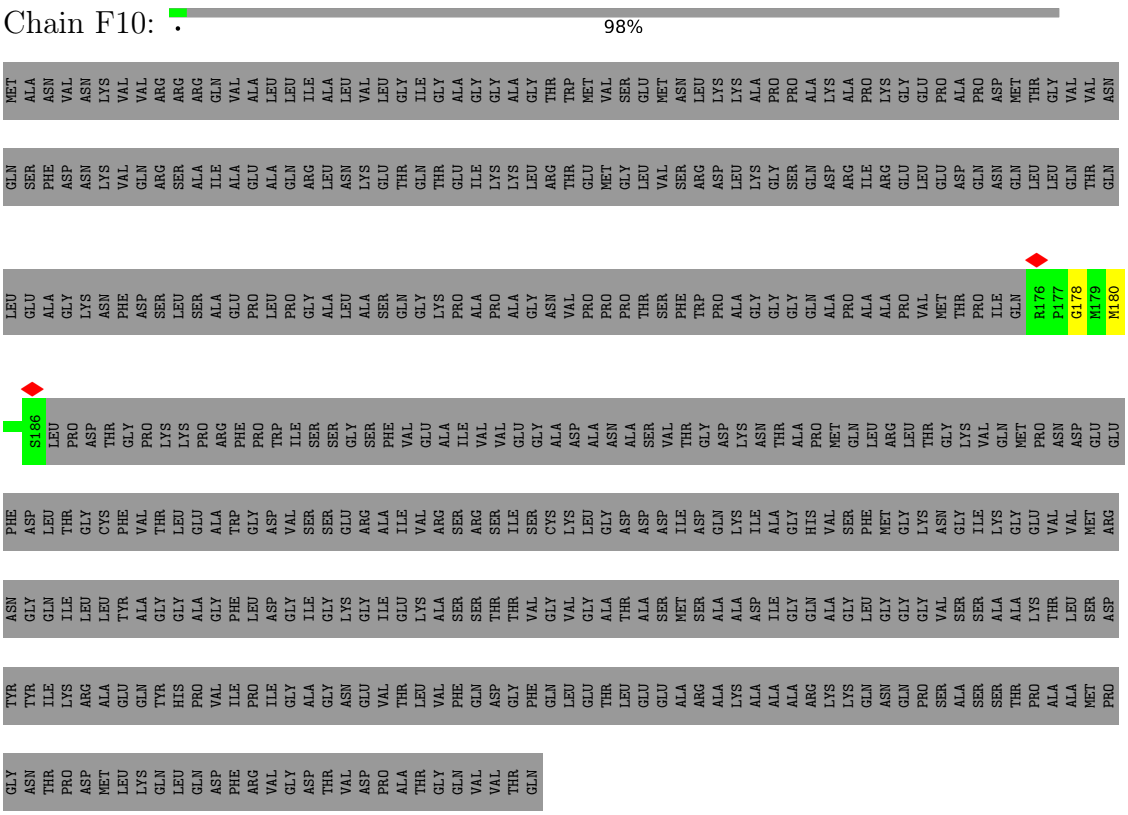
- Molecule 3: TraB

Chain F9:



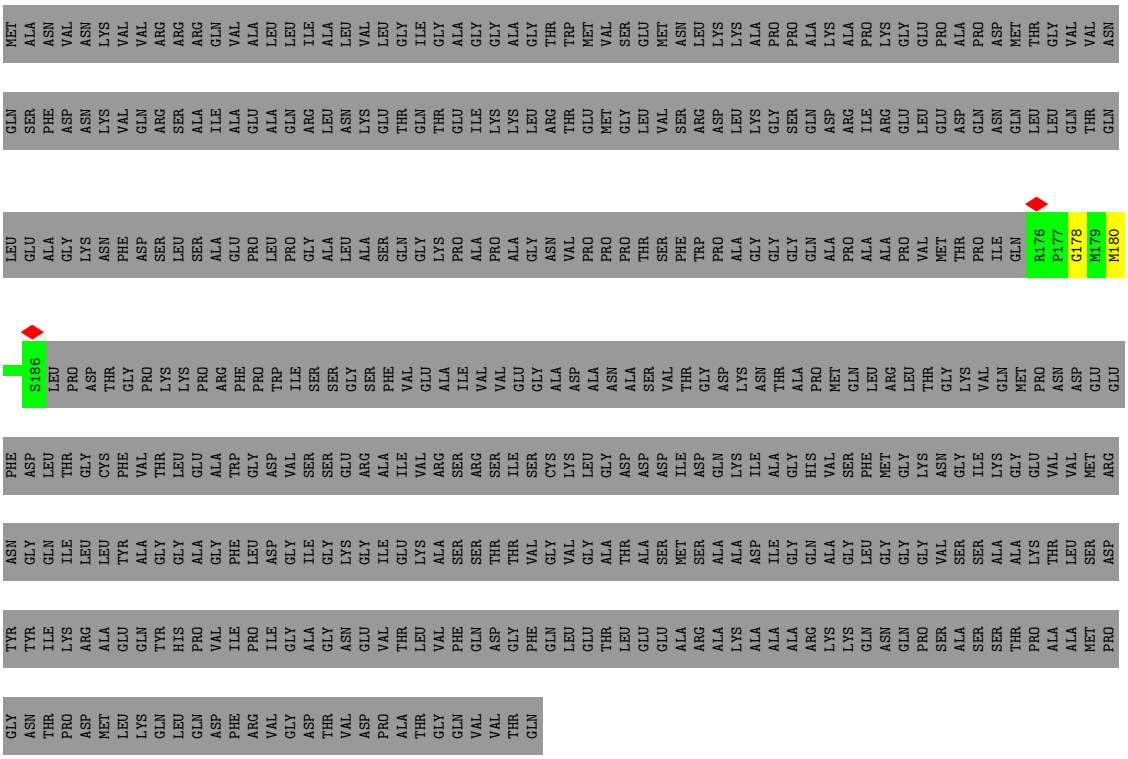
- Molecule 3: TraB

Chain F10:



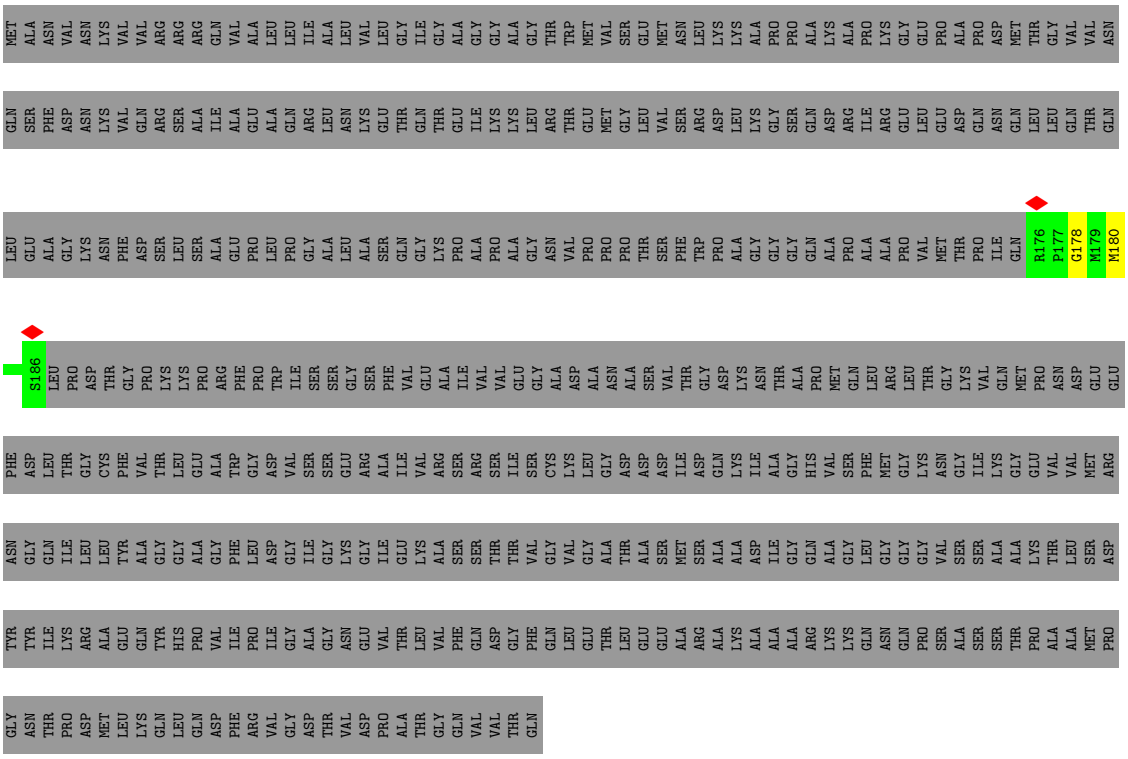
• Molecule 3: TraB

Chain F11: 98%



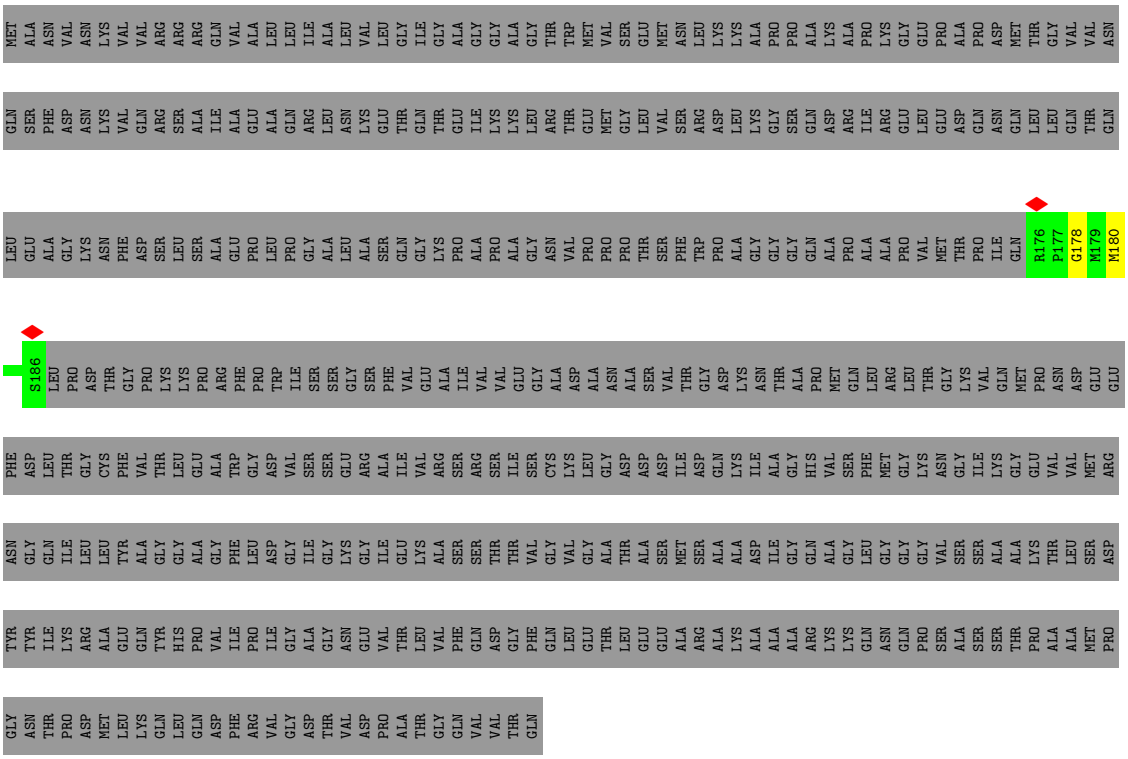
• Molecule 3: TraB

Chain F12: 98%



• Molecule 3: TraB

Chain F13: 98%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C13	Depositor
Number of particles used	148000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.160	Depositor
Minimum map value	-1.854	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	426.08, 426.08, 426.08	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0652, 1.0652, 1.0652	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A1	0.37	0/451	0.61	0/622
1	A10	0.37	0/451	0.61	0/622
1	A11	0.37	0/451	0.61	0/622
1	A12	0.37	0/451	0.61	0/622
1	A13	0.37	0/451	0.61	0/622
1	A2	0.37	0/451	0.61	0/622
1	A3	0.37	0/451	0.61	0/622
1	A4	0.37	0/451	0.61	0/622
1	A5	0.37	0/451	0.61	0/622
1	A6	0.37	0/451	0.61	0/622
1	A7	0.37	0/451	0.61	0/622
1	A8	0.37	0/451	0.61	0/622
1	A9	0.37	0/451	0.61	0/622
1	B1	0.38	0/514	0.61	0/710
1	B10	0.38	0/514	0.61	0/710
1	B11	0.38	0/514	0.61	0/710
1	B12	0.38	0/514	0.61	0/710
1	B13	0.38	0/514	0.61	0/710
1	B2	0.38	0/514	0.61	0/710
1	B3	0.38	0/514	0.61	0/710
1	B4	0.38	0/514	0.61	0/710
1	B5	0.38	0/514	0.61	0/710
1	B6	0.38	0/514	0.61	0/710
1	B7	0.38	0/514	0.61	0/710
1	B8	0.38	0/514	0.61	0/710
1	B9	0.38	0/514	0.61	0/710
2	C1	0.52	0/1688	0.70	0/2290
2	C10	0.52	0/1688	0.70	0/2290
2	C11	0.52	0/1688	0.70	0/2290
2	C12	0.52	0/1688	0.70	0/2290
2	C13	0.52	0/1688	0.70	0/2290
2	C2	0.52	0/1688	0.70	0/2290
2	C3	0.52	0/1688	0.70	0/2290
2	C4	0.52	0/1688	0.70	0/2290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	C5	0.52	0/1688	0.70	0/2290
2	C6	0.52	0/1688	0.70	0/2290
2	C7	0.52	0/1688	0.70	0/2290
2	C8	0.52	0/1688	0.70	0/2290
2	C9	0.52	0/1688	0.70	0/2290
2	D1	0.40	0/1688	0.65	0/2290
2	D10	0.40	0/1688	0.65	0/2290
2	D11	0.40	0/1688	0.65	0/2290
2	D12	0.40	0/1688	0.65	0/2290
2	D13	0.40	0/1688	0.65	0/2290
2	D2	0.40	0/1688	0.65	0/2290
2	D3	0.40	0/1688	0.65	0/2290
2	D4	0.40	0/1688	0.65	0/2290
2	D5	0.40	0/1688	0.65	0/2290
2	D6	0.40	0/1688	0.65	0/2290
2	D7	0.40	0/1688	0.65	0/2290
2	D8	0.40	0/1688	0.65	0/2290
2	D9	0.40	0/1688	0.65	0/2290
3	E1	0.48	0/88	0.56	0/115
3	E10	0.48	0/88	0.56	0/115
3	E11	0.48	0/88	0.56	0/115
3	E12	0.48	0/88	0.56	0/115
3	E13	0.48	0/88	0.56	0/115
3	E2	0.48	0/88	0.56	0/115
3	E3	0.48	0/88	0.56	0/115
3	E4	0.48	0/88	0.56	0/115
3	E5	0.48	0/88	0.56	0/115
3	E6	0.48	0/88	0.56	0/115
3	E7	0.48	0/88	0.56	0/115
3	E8	0.48	0/88	0.56	0/115
3	E9	0.48	0/88	0.56	0/115
3	F1	0.47	0/88	0.71	0/115
3	F10	0.47	0/88	0.71	0/115
3	F11	0.46	0/88	0.71	0/115
3	F12	0.47	0/88	0.71	0/115
3	F13	0.47	0/88	0.71	0/115
3	F2	0.46	0/88	0.71	0/115
3	F3	0.47	0/88	0.71	0/115
3	F4	0.47	0/88	0.71	0/115
3	F5	0.47	0/88	0.71	0/115
3	F6	0.46	0/88	0.71	0/115
3	F7	0.46	0/88	0.71	0/115
3	F8	0.47	0/88	0.71	0/115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	F9	0.47	0/88	0.71	0/115
All	All	0.45	0/58721	0.66	0/79846

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	436	0	414	26	0
1	A10	436	0	414	27	0
1	A11	436	0	414	26	0
1	A12	436	0	414	27	0
1	A13	436	0	414	26	0
1	A2	436	0	414	27	0
1	A3	436	0	414	25	0
1	A4	436	0	414	27	0
1	A5	436	0	414	26	0
1	A6	436	0	414	27	0
1	A7	436	0	414	27	0
1	A8	436	0	414	26	0
1	A9	436	0	414	26	0
1	B1	498	0	478	68	0
1	B10	498	0	478	69	0
1	B11	498	0	478	70	0
1	B12	498	0	478	69	0
1	B13	498	0	478	69	0
1	B2	498	0	478	69	0
1	B3	498	0	478	70	0
1	B4	498	0	478	69	0
1	B5	498	0	478	69	0
1	B6	498	0	478	68	0
1	B7	498	0	478	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B8	498	0	478	69	0
1	B9	498	0	478	70	0
2	C1	1654	0	1664	64	0
2	C10	1654	0	1664	62	0
2	C11	1654	0	1664	64	0
2	C12	1654	0	1664	63	0
2	C13	1654	0	1664	64	0
2	C2	1654	0	1664	64	0
2	C3	1654	0	1664	62	0
2	C4	1654	0	1664	63	0
2	C5	1654	0	1664	63	0
2	C6	1654	0	1664	63	0
2	C7	1654	0	1664	61	0
2	C8	1654	0	1664	61	0
2	C9	1654	0	1664	63	0
2	D1	1654	0	1664	57	0
2	D10	1654	0	1664	54	0
2	D11	1654	0	1664	57	0
2	D12	1654	0	1664	60	0
2	D13	1654	0	1664	55	0
2	D2	1654	0	1664	56	0
2	D3	1654	0	1664	57	0
2	D4	1654	0	1664	51	0
2	D5	1654	0	1664	52	0
2	D6	1654	0	1664	55	0
2	D7	1654	0	1664	54	0
2	D8	1654	0	1664	56	0
2	D9	1654	0	1664	53	0
3	E1	87	0	77	25	0
3	E10	87	0	77	25	0
3	E11	87	0	77	25	0
3	E12	87	0	77	25	0
3	E13	87	0	77	25	0
3	E2	87	0	77	25	0
3	E3	87	0	77	23	0
3	E4	87	0	77	25	0
3	E5	87	0	77	25	0
3	E6	87	0	77	25	0
3	E7	87	0	77	25	0
3	E8	87	0	77	24	0
3	E9	87	0	77	24	0
3	F1	87	0	77	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F10	87	0	77	2	0
3	F11	87	0	77	2	0
3	F12	87	0	77	2	0
3	F13	87	0	77	2	0
3	F2	87	0	77	2	0
3	F3	87	0	77	2	0
3	F4	87	0	77	2	0
3	F5	87	0	77	2	0
3	F6	87	0	77	2	0
3	F7	87	0	77	2	0
3	F8	87	0	77	2	0
3	F9	87	0	77	2	0
All	All	57408	0	56862	1904	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 17.

All (1904) 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)
2:C10:72:LEU:HD22	3:E10:185:PHE:CB	1.77	1.15
2:C9:72:LEU:HD22	3:E9:185:PHE:CB	1.77	1.14
2:C11:72:LEU:HD22	3:E11:185:PHE:CB	1.77	1.14
2:C1:72:LEU:HD22	3:E1:185:PHE:CB	1.77	1.14
2:C2:72:LEU:HD22	3:E2:185:PHE:CB	1.77	1.14
2:C6:72:LEU:HD22	3:E6:185:PHE:CB	1.77	1.14
2:C7:72:LEU:HD22	3:E7:185:PHE:CB	1.77	1.13
2:C3:72:LEU:HD22	3:E3:185:PHE:CB	1.77	1.13
2:C5:72:LEU:HD22	3:E5:185:PHE:CB	1.77	1.13
2:C8:72:LEU:HD22	3:E8:185:PHE:CB	1.77	1.13
2:C6:72:LEU:HD13	3:E6:185:PHE:CE2	1.84	1.12
2:C12:72:LEU:HD22	3:E12:185:PHE:CB	1.77	1.12
2:C13:72:LEU:HD22	3:E13:185:PHE:CB	1.77	1.13
2:C2:72:LEU:HD13	3:E2:185:PHE:CE2	1.84	1.12
2:C5:72:LEU:HD13	3:E5:185:PHE:CE2	1.84	1.12
2:C8:72:LEU:HD13	3:E8:185:PHE:CE2	1.84	1.12
2:C4:72:LEU:HD22	3:E4:185:PHE:CB	1.77	1.12
2:C3:72:LEU:HD13	3:E3:185:PHE:CE2	1.84	1.12
2:C1:72:LEU:HD13	3:E1:185:PHE:CE2	1.84	1.11
2:C4:72:LEU:HD13	3:E4:185:PHE:CE2	1.84	1.11
2:C9:72:LEU:HD13	3:E9:185:PHE:CE2	1.84	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C12:72:LEU:HD13	3:E12:185:PHE:CE2	1.84	1.11
2:C7:72:LEU:HD13	3:E7:185:PHE:CE2	1.84	1.11
2:C11:72:LEU:HD13	3:E11:185:PHE:CE2	1.84	1.10
2:C10:72:LEU:HD13	3:E10:185:PHE:CE2	1.84	1.10
2:C13:72:LEU:HD13	3:E13:185:PHE:CE2	1.84	1.10
2:C13:72:LEU:HD22	3:E13:185:PHE:HB3	1.34	1.09
2:C1:72:LEU:HD22	3:E1:185:PHE:HB3	1.34	1.09
2:C5:72:LEU:HD22	3:E5:185:PHE:HB3	1.34	1.09
2:C4:72:LEU:HD22	3:E4:185:PHE:HB3	1.34	1.08
2:C12:72:LEU:HD22	3:E12:185:PHE:HB3	1.34	1.08
1:A13:170:VAL:HG22	2:C13:216:MET:HB2	1.36	1.08
1:A1:170:VAL:HG22	2:C1:216:MET:HB2	1.36	1.07
2:C11:72:LEU:CD1	3:E11:185:PHE:CD2	2.37	1.07
2:C12:72:LEU:CD1	3:E12:185:PHE:CD2	2.37	1.07
1:A12:170:VAL:HG22	2:C12:216:MET:HB2	1.36	1.07
2:C6:72:LEU:CD1	3:E6:185:PHE:CD2	2.37	1.07
2:C7:72:LEU:CD1	3:E7:185:PHE:CD2	2.37	1.07
2:C8:72:LEU:CD1	3:E8:185:PHE:CD2	2.37	1.07
2:C10:72:LEU:CD1	3:E10:185:PHE:CD2	2.37	1.07
2:C5:72:LEU:CD1	3:E5:185:PHE:CD2	2.37	1.07
2:C13:72:LEU:CD1	3:E13:185:PHE:CD2	2.37	1.07
2:C9:72:LEU:CD1	3:E9:185:PHE:CD2	2.37	1.07
2:C2:72:LEU:HD22	3:E2:185:PHE:HB3	1.34	1.06
2:C4:72:LEU:CD1	3:E4:185:PHE:CD2	2.37	1.06
2:C12:72:LEU:CD1	3:E12:185:PHE:CE2	2.38	1.06
2:C1:72:LEU:CD1	3:E1:185:PHE:CE2	2.38	1.06
2:C7:72:LEU:CD1	3:E7:185:PHE:CE2	2.38	1.06
2:C8:72:LEU:CD1	3:E8:185:PHE:CE2	2.38	1.06
2:C11:72:LEU:CD1	3:E11:185:PHE:CE2	2.38	1.06
1:A2:170:VAL:HG22	2:C2:216:MET:HB2	1.36	1.06
2:C3:72:LEU:CD1	3:E3:185:PHE:CD2	2.37	1.06
2:C9:72:LEU:CD1	3:E9:185:PHE:CE2	2.38	1.06
2:C10:72:LEU:CD1	3:E10:185:PHE:CE2	2.38	1.06
2:C13:72:LEU:CD1	3:E13:185:PHE:CE2	2.38	1.06
1:B7:155:PRO:HD2	2:D8:205:GLN:CG	1.86	1.06
1:B9:155:PRO:HD2	2:D10:205:GLN:CG	1.86	1.06
2:C1:72:LEU:CD1	3:E1:185:PHE:CD2	2.37	1.06
2:C2:72:LEU:CD1	3:E2:185:PHE:CD2	2.37	1.06
2:C4:72:LEU:CD1	3:E4:185:PHE:CE2	2.38	1.06
2:C6:72:LEU:HD22	3:E6:185:PHE:HB3	1.34	1.06
1:B8:155:PRO:HD2	2:D9:205:GLN:CG	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C3:72:LEU:CD1	3:E3:185:PHE:CE2	2.38	1.06
1:A11:170:VAL:HG22	2:C11:216:MET:HB2	1.36	1.05
2:C5:72:LEU:CD1	3:E5:185:PHE:CE2	2.38	1.05
2:C6:72:LEU:CD1	3:E6:185:PHE:CE2	2.38	1.05
1:B6:155:PRO:HD2	2:D7:205:GLN:CG	1.86	1.05
1:B11:155:PRO:HD2	2:D12:205:GLN:CG	1.86	1.05
2:C9:72:LEU:HD22	3:E9:185:PHE:HB3	1.34	1.05
1:B10:155:PRO:HD2	2:D11:205:GLN:CG	1.86	1.05
2:C2:72:LEU:CD1	3:E2:185:PHE:CE2	2.38	1.05
2:C3:72:LEU:HD22	3:E3:185:PHE:HB3	1.34	1.05
2:C10:72:LEU:HD22	3:E10:185:PHE:HB3	1.34	1.05
2:C12:72:LEU:HD22	3:E12:185:PHE:CG	1.92	1.05
1:B4:155:PRO:HD2	2:D5:205:GLN:CG	1.86	1.05
1:B12:155:PRO:HD2	2:D13:205:GLN:CG	1.86	1.05
2:C8:72:LEU:HD22	3:E8:185:PHE:CG	1.92	1.05
2:C11:72:LEU:HD22	3:E11:185:PHE:CG	1.92	1.05
1:B3:155:PRO:HD2	2:D4:205:GLN:CG	1.86	1.04
2:C7:72:LEU:HD22	3:E7:185:PHE:CG	1.92	1.04
2:C8:72:LEU:HD22	3:E8:185:PHE:HB3	1.34	1.04
2:C2:72:LEU:HD22	3:E2:185:PHE:CG	1.92	1.04
2:C5:72:LEU:HD22	3:E5:185:PHE:CG	1.92	1.04
2:C13:72:LEU:HD22	3:E13:185:PHE:CG	1.92	1.04
1:B2:155:PRO:HD2	2:D3:205:GLN:CG	1.86	1.04
2:C9:72:LEU:HD22	3:E9:185:PHE:CG	1.92	1.04
1:A3:170:VAL:HG22	2:C3:216:MET:HB2	1.36	1.04
2:C1:72:LEU:HD22	3:E1:185:PHE:CG	1.92	1.04
2:C4:72:LEU:HD22	3:E4:185:PHE:CG	1.92	1.04
1:B5:155:PRO:HD2	2:D6:205:GLN:CG	1.86	1.03
1:B13:155:PRO:HD2	2:D1:205:GLN:CG	1.86	1.03
2:C10:72:LEU:HD22	3:E10:185:PHE:CG	1.92	1.03
1:A6:170:VAL:HG22	2:C6:216:MET:HB2	1.36	1.03
1:A7:170:VAL:HG22	2:C7:216:MET:HB2	1.36	1.03
2:C3:72:LEU:HD22	3:E3:185:PHE:CG	1.92	1.03
2:C11:72:LEU:HD22	3:E11:185:PHE:HB3	1.34	1.03
1:A8:170:VAL:HG22	2:C8:216:MET:HB2	1.36	1.03
1:B1:155:PRO:HD2	2:D2:205:GLN:CG	1.86	1.03
2:C6:72:LEU:HD22	3:E6:185:PHE:CG	1.92	1.03
1:A5:170:VAL:HG22	2:C5:216:MET:HB2	1.36	1.02
1:A10:170:VAL:HG22	2:C10:216:MET:HB2	1.36	1.02
1:A9:170:VAL:HG22	2:C9:216:MET:HB2	1.36	1.01
2:C7:72:LEU:HD22	3:E7:185:PHE:HB3	1.34	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:170:VAL:HG22	2:C4:216:MET:HB2	1.36	1.01
2:C9:72:LEU:HD13	3:E9:185:PHE:CD2	1.96	1.00
2:C5:72:LEU:HD13	3:E5:185:PHE:CD2	1.96	1.00
2:C2:72:LEU:HD13	3:E2:185:PHE:CD2	1.96	1.00
2:C1:72:LEU:HD13	3:E1:185:PHE:CD2	1.96	1.00
2:C6:72:LEU:HD13	3:E6:185:PHE:CD2	1.96	1.00
2:C10:72:LEU:HD13	3:E10:185:PHE:CZ	1.97	1.00
2:C3:72:LEU:HD13	3:E3:185:PHE:CZ	1.97	0.99
2:C4:72:LEU:HD13	3:E4:185:PHE:CD2	1.96	0.99
2:C11:72:LEU:HD13	3:E11:185:PHE:CZ	1.97	0.99
2:C12:72:LEU:CD2	3:E12:185:PHE:CB	2.40	0.99
2:C13:72:LEU:CD2	3:E13:185:PHE:CB	2.40	0.99
2:C1:72:LEU:HD13	3:E1:185:PHE:CZ	1.97	0.99
2:C3:72:LEU:HD13	3:E3:185:PHE:CD2	1.96	0.99
2:C8:72:LEU:HD13	3:E8:185:PHE:CD2	1.96	0.99
2:C9:72:LEU:HD13	3:E9:185:PHE:CZ	1.97	0.99
2:C13:72:LEU:HD13	3:E13:185:PHE:CD2	1.96	0.99
2:C6:72:LEU:HD13	3:E6:185:PHE:CZ	1.97	0.99
2:C1:72:LEU:CD2	3:E1:185:PHE:CB	2.40	0.99
2:C7:72:LEU:HD13	3:E7:185:PHE:CZ	1.97	0.99
2:C11:72:LEU:CD2	3:E11:185:PHE:CB	2.40	0.99
2:C5:72:LEU:CD2	3:E5:185:PHE:CB	2.40	0.99
2:C12:72:LEU:HD13	3:E12:185:PHE:CZ	1.97	0.99
2:C5:72:LEU:HD13	3:E5:185:PHE:CZ	1.97	0.99
2:C2:72:LEU:CD2	3:E2:185:PHE:CB	2.40	0.99
2:C4:72:LEU:CD2	3:E4:185:PHE:CB	2.40	0.99
2:C6:72:LEU:CD2	3:E6:185:PHE:CB	2.40	0.99
2:C10:72:LEU:CD2	3:E10:185:PHE:CB	2.40	0.99
2:C12:72:LEU:HD13	3:E12:185:PHE:CD2	1.96	0.99
2:C3:72:LEU:CD2	3:E3:185:PHE:CB	2.40	0.98
2:C8:72:LEU:HD13	3:E8:185:PHE:CZ	1.97	0.98
2:C7:72:LEU:HD13	3:E7:185:PHE:CD2	1.96	0.98
2:C7:72:LEU:CD2	3:E7:185:PHE:CB	2.40	0.98
2:C2:72:LEU:HD13	3:E2:185:PHE:CZ	1.97	0.98
2:C4:72:LEU:HD13	3:E4:185:PHE:CZ	1.97	0.98
2:C9:72:LEU:CD2	3:E9:185:PHE:CB	2.40	0.98
2:C13:72:LEU:HD13	3:E13:185:PHE:CZ	1.97	0.98
2:C8:72:LEU:CD2	3:E8:185:PHE:CB	2.40	0.98
1:B8:155:PRO:HD2	2:D9:205:GLN:HG3	1.46	0.98
1:B9:155:PRO:HD2	2:D10:205:GLN:HG3	1.46	0.97
2:C10:72:LEU:HD13	3:E10:185:PHE:CD2	1.96	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C11:72:LEU:HD13	3:E11:185:PHE:CD2	1.96	0.97
1:B7:155:PRO:HD2	2:D8:205:GLN:HG3	1.46	0.97
1:B10:155:PRO:HD2	2:D11:205:GLN:HG3	1.46	0.96
1:B6:155:PRO:HD2	2:D7:205:GLN:HG3	1.46	0.96
2:C6:74:ARG:HB2	2:D5:93:GLU:OE2	1.66	0.96
2:C8:74:ARG:HB2	2:D7:93:GLU:OE2	1.66	0.96
1:B1:155:PRO:HD2	2:D2:205:GLN:HG3	1.46	0.96
2:C9:74:ARG:HB2	2:D8:93:GLU:OE2	1.66	0.96
2:C11:74:ARG:HB2	2:D10:93:GLU:OE2	1.66	0.96
1:B13:155:PRO:HD2	2:D1:205:GLN:HG3	1.46	0.95
2:C7:74:ARG:HB2	2:D6:93:GLU:OE2	1.66	0.95
2:C10:74:ARG:HB2	2:D9:93:GLU:OE2	1.66	0.95
1:B2:155:PRO:HD2	2:D3:205:GLN:HG3	1.46	0.95
1:B3:155:PRO:HD2	2:D4:205:GLN:HG3	1.46	0.95
1:B4:155:PRO:HD2	2:D5:205:GLN:HG3	1.45	0.95
2:C13:74:ARG:HB2	2:D12:93:GLU:OE2	1.66	0.95
2:C3:74:ARG:HB2	2:D2:93:GLU:OE2	1.66	0.95
1:B12:155:PRO:HD2	2:D13:205:GLN:HG3	1.46	0.95
1:B11:155:PRO:HD2	2:D12:205:GLN:HG3	1.46	0.94
2:C5:74:ARG:HB2	2:D4:93:GLU:OE2	1.66	0.94
2:C4:74:ARG:HB2	2:D3:93:GLU:OE2	1.66	0.94
1:B5:155:PRO:HD2	2:D6:205:GLN:HG3	1.46	0.94
2:C1:74:ARG:HB2	2:D13:93:GLU:OE2	1.66	0.94
2:C2:74:ARG:HB2	2:D1:93:GLU:OE2	1.66	0.94
2:C11:72:LEU:HD11	3:E11:185:PHE:CD2	2.03	0.94
2:C12:72:LEU:HD11	3:E12:185:PHE:CD2	2.03	0.94
2:C12:74:ARG:HB2	2:D11:93:GLU:OE2	1.66	0.93
2:C5:72:LEU:HD11	3:E5:185:PHE:CD2	2.03	0.93
2:C6:72:LEU:HD11	3:E6:185:PHE:CD2	2.03	0.93
2:C10:72:LEU:HD11	3:E10:185:PHE:CD2	2.03	0.93
2:C8:72:LEU:HD11	3:E8:185:PHE:CD2	2.03	0.93
2:C7:72:LEU:HD11	3:E7:185:PHE:CD2	2.03	0.93
2:C9:72:LEU:HD11	3:E9:185:PHE:CD2	2.03	0.93
2:C13:72:LEU:HD11	3:E13:185:PHE:CD2	2.03	0.93
2:C4:72:LEU:HD11	3:E4:185:PHE:CD2	2.03	0.93
2:C1:72:LEU:HD11	3:E1:185:PHE:CD2	2.03	0.92
1:B6:95:THR:HG22	1:B7:176:VAL:HG23	1.51	0.92
1:B7:95:THR:HG22	1:B8:176:VAL:HG23	1.51	0.92
2:C2:72:LEU:HD11	3:E2:185:PHE:CD2	2.03	0.91
2:C3:72:LEU:HD11	3:E3:185:PHE:CD2	2.03	0.91
1:B5:95:THR:HG22	1:B6:176:VAL:HG23	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B8:95:THR:HG22	1:B9:176:VAL:HG23	1.51	0.91
1:B12:95:THR:HG22	1:B13:176:VAL:HG23	1.51	0.91
1:B1:176:VAL:HG23	1:B13:95:THR:HG22	1.51	0.91
2:D9:74:ARG:NH2	3:E9:184:GLU:HG3	1.86	0.91
2:D8:74:ARG:NH2	3:E8:184:GLU:HG3	1.86	0.90
2:D2:74:ARG:NH2	3:E2:184:GLU:HG3	1.86	0.90
1:B1:95:THR:HG22	1:B2:176:VAL:HG23	1.51	0.90
1:B11:95:THR:HG22	1:B12:176:VAL:HG23	1.51	0.90
2:D3:74:ARG:NH2	3:E3:184:GLU:HG3	1.86	0.90
2:D10:74:ARG:NH2	3:E10:184:GLU:HG3	1.86	0.90
2:D1:74:ARG:NH2	3:E1:184:GLU:HG3	1.86	0.90
1:B2:95:THR:HG22	1:B3:176:VAL:HG23	1.51	0.90
1:B4:95:THR:HG22	1:B5:176:VAL:HG23	1.51	0.90
1:B6:95:THR:HG22	1:B7:176:VAL:CG2	2.02	0.90
1:B8:170:VAL:HG11	2:D8:144:ASN:ND2	1.87	0.90
1:B9:95:THR:HG22	1:B10:176:VAL:CG2	2.02	0.90
2:D7:74:ARG:NH2	3:E7:184:GLU:HG3	1.87	0.90
1:B3:95:THR:HG22	1:B4:176:VAL:CG2	2.02	0.90
1:B4:95:THR:HG22	1:B5:176:VAL:CG2	2.02	0.90
1:B9:170:VAL:HG11	2:D9:144:ASN:ND2	1.87	0.90
2:D4:74:ARG:NH2	3:E4:184:GLU:HG3	1.86	0.90
2:D11:74:ARG:NH2	3:E11:184:GLU:HG3	1.86	0.89
1:B7:95:THR:HG22	1:B8:176:VAL:CG2	2.02	0.89
1:B10:95:THR:HG22	1:B11:176:VAL:HG23	1.51	0.89
1:B1:176:VAL:CG2	1:B13:95:THR:HG22	2.02	0.89
1:B5:170:VAL:HG11	2:D5:144:ASN:ND2	1.87	0.89
2:D6:74:ARG:NH2	3:E6:184:GLU:HG3	1.86	0.89
2:D13:74:ARG:NH2	3:E13:184:GLU:HG3	1.86	0.89
1:B1:95:THR:HG22	1:B2:176:VAL:CG2	2.02	0.89
1:B7:170:VAL:HG11	2:D7:144:ASN:ND2	1.87	0.89
1:B8:95:THR:HG22	1:B9:176:VAL:CG2	2.02	0.89
1:B10:95:THR:HG22	1:B11:176:VAL:CG2	2.02	0.89
2:D5:74:ARG:NH2	3:E5:184:GLU:HG3	1.86	0.89
1:B3:95:THR:HG22	1:B4:176:VAL:HG23	1.51	0.89
1:B9:95:THR:HG22	1:B10:176:VAL:HG23	1.51	0.89
1:B12:170:VAL:HG11	2:D12:144:ASN:ND2	1.87	0.89
1:B6:170:VAL:HG11	2:D6:144:ASN:ND2	1.87	0.89
1:B12:95:THR:HG22	1:B13:176:VAL:CG2	2.02	0.89
1:B5:95:THR:HG22	1:B6:176:VAL:CG2	2.02	0.89
1:B11:170:VAL:HG11	2:D11:144:ASN:ND2	1.87	0.89
2:D12:74:ARG:NH2	3:E12:184:GLU:HG3	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B2:170:VAL:HG11	2:D2:144:ASN:ND2	1.87	0.89
1:B2:95:THR:HG22	1:B3:176:VAL:CG2	2.02	0.88
1:B10:170:VAL:HG11	2:D10:144:ASN:ND2	1.87	0.88
1:B4:170:VAL:HG11	2:D4:144:ASN:ND2	1.87	0.88
1:B4:96:PRO:HG3	1:B5:174:PRO:HB2	1.56	0.88
1:B11:95:THR:HG22	1:B12:176:VAL:CG2	2.02	0.88
1:B2:96:PRO:HG3	1:B3:174:PRO:HB2	1.56	0.88
1:B1:170:VAL:HG11	2:D1:144:ASN:ND2	1.87	0.88
1:B1:96:PRO:HG3	1:B2:174:PRO:HB2	1.56	0.88
1:B3:96:PRO:HG3	1:B4:174:PRO:HB2	1.56	0.88
1:B3:170:VAL:HG11	2:D3:144:ASN:ND2	1.87	0.88
1:B13:170:VAL:HG11	2:D13:144:ASN:ND2	1.87	0.88
2:C5:72:LEU:CD2	3:E5:185:PHE:CG	2.57	0.88
1:B1:174:PRO:HB2	1:B13:96:PRO:HG3	1.56	0.87
2:C6:72:LEU:CD2	3:E6:185:PHE:CG	2.57	0.87
1:B5:96:PRO:HG3	1:B6:174:PRO:HB2	1.56	0.87
1:B8:95:THR:CG2	1:B9:176:VAL:CG2	2.53	0.87
1:B5:95:THR:CG2	1:B6:176:VAL:CG2	2.53	0.87
1:B6:96:PRO:HG3	1:B7:174:PRO:HB2	1.56	0.87
2:C4:72:LEU:CD2	3:E4:185:PHE:CG	2.57	0.87
2:C10:72:LEU:CD2	3:E10:185:PHE:CG	2.57	0.87
2:C1:72:LEU:CD2	3:E1:185:PHE:CG	2.57	0.87
2:C3:72:LEU:CD2	3:E3:185:PHE:CG	2.57	0.87
2:C9:72:LEU:CD2	3:E9:185:PHE:CG	2.57	0.87
2:C13:72:LEU:CD2	3:E13:185:PHE:CG	2.57	0.87
1:B7:95:THR:CG2	1:B8:176:VAL:CG2	2.53	0.87
2:C2:72:LEU:CD2	3:E2:185:PHE:CG	2.57	0.87
1:B12:96:PRO:HG3	1:B13:174:PRO:HB2	1.56	0.87
1:B6:95:THR:CG2	1:B7:176:VAL:CG2	2.53	0.87
1:B1:95:THR:CG2	1:B2:176:VAL:CG2	2.53	0.87
1:B2:95:THR:CG2	1:B3:176:VAL:CG2	2.53	0.86
1:B10:95:THR:CG2	1:B11:176:VAL:CG2	2.53	0.86
2:C7:72:LEU:CD2	3:E7:185:PHE:CG	2.57	0.86
2:C11:72:LEU:CD2	3:E11:185:PHE:CG	2.57	0.86
2:C12:72:LEU:CD2	3:E12:185:PHE:CG	2.57	0.86
1:B11:95:THR:CG2	1:B12:176:VAL:CG2	2.53	0.86
1:B12:95:THR:CG2	1:B13:176:VAL:CG2	2.53	0.86
2:C8:72:LEU:CD2	3:E8:185:PHE:CG	2.57	0.86
1:B3:95:THR:CG2	1:B4:176:VAL:CG2	2.53	0.86
1:B8:96:PRO:HG3	1:B9:174:PRO:HB2	1.56	0.86
1:B9:95:THR:CG2	1:B10:176:VAL:CG2	2.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:176:VAL:CG2	1:B13:95:THR:CG2	2.53	0.86
1:B7:96:PRO:HG3	1:B8:174:PRO:HB2	1.56	0.86
1:B1:155:PRO:HD2	2:D2:205:GLN:HG2	1.58	0.86
1:B4:95:THR:CG2	1:B5:176:VAL:CG2	2.53	0.86
1:B10:96:PRO:HG3	1:B11:174:PRO:HB2	1.56	0.86
1:B11:96:PRO:HG3	1:B12:174:PRO:HB2	1.56	0.86
1:B2:155:PRO:HD2	2:D3:205:GLN:HG2	1.58	0.85
1:B13:155:PRO:HD2	2:D1:205:GLN:HG2	1.58	0.85
2:C13:35:GLY:HA3	2:D13:27:PRO:HD3	1.58	0.85
2:C12:35:GLY:HA3	2:D12:27:PRO:HD3	1.58	0.85
1:B8:187:ARG:HH11	2:D8:204:GLU:CD	1.80	0.85
1:B9:96:PRO:HG3	1:B10:174:PRO:HB2	1.56	0.85
1:A13:152:CYS:SG	1:B11:151:ARG:N	2.50	0.85
1:B12:187:ARG:HH11	2:D12:204:GLU:CD	1.80	0.85
1:A12:152:CYS:SG	1:B10:151:ARG:N	2.50	0.85
1:B3:155:PRO:HD2	2:D4:205:GLN:HG2	1.58	0.85
1:B12:155:PRO:HD2	2:D13:205:GLN:HG2	1.58	0.85
1:A11:152:CYS:SG	1:B9:151:ARG:N	2.50	0.85
1:A1:152:CYS:SG	1:B12:151:ARG:N	2.50	0.85
1:B2:187:ARG:HH11	2:D2:204:GLU:CD	1.80	0.85
2:C1:35:GLY:HA3	2:D1:27:PRO:HD3	1.58	0.85
1:B13:187:ARG:HH11	2:D13:204:GLU:CD	1.80	0.84
1:B7:187:ARG:HH11	2:D7:204:GLU:CD	1.80	0.84
1:A10:152:CYS:SG	1:B8:151:ARG:N	2.50	0.84
1:B11:187:ARG:HH11	2:D11:204:GLU:CD	1.80	0.84
2:C11:35:GLY:HA3	2:D11:27:PRO:HD3	1.59	0.84
1:A2:152:CYS:SG	1:B13:151:ARG:N	2.50	0.84
1:B3:187:ARG:HH11	2:D3:204:GLU:CD	1.80	0.84
1:B9:187:ARG:HH11	2:D9:204:GLU:CD	1.80	0.84
1:B11:155:PRO:HD2	2:D12:205:GLN:HG2	1.58	0.84
1:B4:155:PRO:HD2	2:D5:205:GLN:HG2	1.58	0.84
2:C4:35:GLY:HA3	2:D4:27:PRO:HD3	1.59	0.84
1:A9:152:CYS:SG	1:B7:151:ARG:N	2.50	0.84
2:C5:35:GLY:HA3	2:D5:27:PRO:HD3	1.58	0.83
2:C2:72:LEU:CD2	3:E2:185:PHE:HB3	2.07	0.83
2:C9:72:LEU:CD2	3:E9:185:PHE:HB3	2.07	0.83
1:A3:152:CYS:SG	1:B1:151:ARG:N	2.50	0.83
1:A5:152:CYS:SG	1:B3:151:ARG:N	2.50	0.83
1:B6:187:ARG:HH11	2:D6:204:GLU:CD	1.80	0.83
2:C3:35:GLY:HA3	2:D3:27:PRO:HD3	1.59	0.83
1:B1:187:ARG:HH11	2:D1:204:GLU:CD	1.80	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B10:155:PRO:HD2	2:D11:205:GLN:HG2	1.58	0.83
1:B10:187:ARG:HH11	2:D10:204:GLU:CD	1.80	0.83
1:A6:152:CYS:SG	1:B4:151:ARG:N	2.50	0.83
2:C6:35:GLY:HA3	2:D6:27:PRO:HD3	1.58	0.83
1:A8:152:CYS:SG	1:B6:151:ARG:N	2.50	0.83
1:B5:187:ARG:HH11	2:D5:204:GLU:CD	1.80	0.83
2:C2:35:GLY:HA3	2:D2:27:PRO:HD3	1.59	0.83
2:C3:72:LEU:CD2	3:E3:185:PHE:HB3	2.07	0.83
1:B5:155:PRO:HD2	2:D6:205:GLN:HG2	1.58	0.83
2:C7:35:GLY:HA3	2:D7:27:PRO:HD3	1.59	0.83
2:C10:35:GLY:HA3	2:D10:27:PRO:HD3	1.58	0.83
1:A4:152:CYS:SG	1:B2:151:ARG:N	2.50	0.82
1:B4:187:ARG:HH11	2:D4:204:GLU:CD	1.80	0.82
1:A12:160:PRO:HG3	1:B11:189:SER:OG	1.80	0.82
1:B9:155:PRO:HD2	2:D10:205:GLN:HG2	1.58	0.82
1:A3:160:PRO:HG3	1:B2:189:SER:OG	1.80	0.82
1:A4:160:PRO:HG3	1:B3:189:SER:OG	1.80	0.82
1:A7:152:CYS:SG	1:B5:151:ARG:N	2.50	0.82
1:B6:155:PRO:HD2	2:D7:205:GLN:HG2	1.58	0.82
2:C8:35:GLY:HA3	2:D8:27:PRO:HD3	1.59	0.82
1:A2:160:PRO:HG3	1:B1:189:SER:OG	1.80	0.82
1:B7:155:PRO:HD2	2:D8:205:GLN:HG2	1.58	0.82
1:B8:155:PRO:HD2	2:D9:205:GLN:HG2	1.58	0.82
1:A10:160:PRO:HG3	1:B9:189:SER:OG	1.80	0.82
1:A1:160:PRO:HG3	1:B13:189:SER:OG	1.80	0.82
1:A6:160:PRO:HG3	1:B5:189:SER:OG	1.79	0.82
1:A11:160:PRO:HG3	1:B10:189:SER:OG	1.80	0.82
2:C9:35:GLY:HA3	2:D9:27:PRO:HD3	1.58	0.81
2:C4:72:LEU:CD2	3:E4:185:PHE:HB3	2.07	0.81
1:A13:160:PRO:HG3	1:B12:189:SER:OG	1.80	0.81
1:A8:160:PRO:HG3	1:B7:189:SER:OG	1.79	0.81
1:A5:160:PRO:HG3	1:B4:189:SER:OG	1.80	0.81
2:C11:72:LEU:CD2	3:E11:185:PHE:HB3	2.07	0.81
1:A9:160:PRO:HG3	1:B8:189:SER:OG	1.80	0.80
2:C10:72:LEU:CD2	3:E10:185:PHE:HB3	2.07	0.80
2:C12:72:LEU:CD2	3:E12:185:PHE:HB3	2.07	0.80
1:A7:160:PRO:HG3	1:B6:189:SER:OG	1.80	0.80
2:C3:72:LEU:HD13	3:E3:185:PHE:CE1	2.17	0.80
2:C12:72:LEU:HD13	3:E12:185:PHE:CE1	2.17	0.80
2:C7:72:LEU:CD2	3:E7:185:PHE:HB3	2.07	0.80
2:C8:72:LEU:CD2	3:E8:185:PHE:HB3	2.07	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:160:PRO:HG3	1:B6:189:SER:CB	2.12	0.80
1:A8:160:PRO:HG3	1:B7:189:SER:CB	2.12	0.80
1:B1:96:PRO:CG	1:B2:174:PRO:HB2	2.12	0.80
1:B2:96:PRO:CG	1:B3:174:PRO:HB2	2.12	0.80
2:C2:72:LEU:HD13	3:E2:185:PHE:CE1	2.17	0.80
2:C9:72:LEU:HD13	3:E9:185:PHE:CE1	2.17	0.80
2:C11:72:LEU:HD13	3:E11:185:PHE:CE1	2.17	0.80
1:A9:160:PRO:HG3	1:B8:189:SER:CB	2.12	0.80
1:B1:174:PRO:HB2	1:B13:96:PRO:CG	2.12	0.80
1:B3:96:PRO:CG	1:B4:174:PRO:HB2	2.12	0.80
2:C6:72:LEU:HD13	3:E6:185:PHE:CE1	2.17	0.80
2:C13:72:LEU:HD13	3:E13:185:PHE:CE1	2.17	0.80
2:C13:72:LEU:CD2	3:E13:185:PHE:HB3	2.07	0.80
1:A6:160:PRO:HG3	1:B5:189:SER:CB	2.12	0.79
1:A10:160:PRO:HG3	1:B9:189:SER:CB	2.12	0.79
1:B4:96:PRO:CG	1:B5:174:PRO:HB2	2.12	0.79
2:C5:72:LEU:CD2	3:E5:185:PHE:HB3	2.07	0.79
1:B5:96:PRO:CG	1:B6:174:PRO:HB2	2.12	0.79
1:B12:96:PRO:CG	1:B13:174:PRO:HB2	2.12	0.79
2:C4:72:LEU:HD13	3:E4:185:PHE:CE1	2.17	0.79
2:C8:72:LEU:HD13	3:E8:185:PHE:CE1	2.17	0.79
1:A5:160:PRO:HG3	1:B4:189:SER:CB	2.12	0.79
1:A11:160:PRO:HG3	1:B10:189:SER:CB	2.12	0.79
2:C5:72:LEU:HD13	3:E5:185:PHE:CE1	2.17	0.79
1:A5:203:VAL:HG23	2:C4:208:TRP:CE3	2.18	0.79
1:A6:203:VAL:HG23	2:C5:208:TRP:CE3	2.18	0.79
1:B6:96:PRO:CG	1:B7:174:PRO:HB2	2.12	0.79
2:C10:72:LEU:HD13	3:E10:185:PHE:CE1	2.17	0.79
1:A4:203:VAL:HG23	2:C3:208:TRP:CE3	2.18	0.79
1:A7:203:VAL:HG23	2:C6:208:TRP:CE3	2.18	0.79
1:B11:96:PRO:CG	1:B12:174:PRO:HB2	2.12	0.79
1:B4:192:VAL:HG11	2:D4:148:LEU:HD23	1.65	0.79
1:B5:192:VAL:HG11	2:D5:148:LEU:HD23	1.65	0.79
2:C1:72:LEU:HD13	3:E1:185:PHE:CE1	2.17	0.79
1:A2:160:PRO:HG3	1:B1:189:SER:CB	2.12	0.78
1:A4:160:PRO:HG3	1:B3:189:SER:CB	2.12	0.78
1:A8:203:VAL:HG23	2:C7:208:TRP:CE3	2.18	0.78
1:A12:160:PRO:HG3	1:B11:189:SER:CB	2.12	0.78
1:B2:192:VAL:HG11	2:D2:148:LEU:HD23	1.66	0.78
1:B3:192:VAL:HG11	2:D3:148:LEU:HD23	1.66	0.78
1:B9:96:PRO:CG	1:B10:174:PRO:HB2	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C7:72:LEU:HD13	3:E7:185:PHE:CE1	2.17	0.78
1:A1:160:PRO:HG3	1:B13:189:SER:CB	2.12	0.78
1:A3:203:VAL:HG23	2:C2:208:TRP:CE3	2.18	0.78
1:B1:192:VAL:HG11	2:D1:148:LEU:HD23	1.66	0.78
1:B10:96:PRO:CG	1:B11:174:PRO:HB2	2.12	0.78
1:B13:192:VAL:HG11	2:D13:148:LEU:HD23	1.65	0.78
1:A3:160:PRO:HG3	1:B2:189:SER:CB	2.12	0.78
1:A9:203:VAL:HG23	2:C8:208:TRP:CE3	2.18	0.78
1:B6:192:VAL:HG11	2:D6:148:LEU:HD23	1.65	0.78
1:B7:96:PRO:CG	1:B8:174:PRO:HB2	2.12	0.78
1:B8:96:PRO:CG	1:B9:174:PRO:HB2	2.12	0.78
1:A2:203:VAL:HG23	2:C1:208:TRP:CE3	2.18	0.78
2:C1:72:LEU:CD2	3:E1:185:PHE:HB3	2.07	0.78
2:C9:72:LEU:HD13	3:E9:185:PHE:CG	2.19	0.78
1:A13:160:PRO:HG3	1:B12:189:SER:CB	2.12	0.78
2:C8:72:LEU:HD13	3:E8:185:PHE:CG	2.19	0.78
1:A11:203:VAL:HG23	2:C10:208:TRP:CE3	2.18	0.78
1:B12:192:VAL:HG11	2:D12:148:LEU:HD23	1.65	0.78
2:C10:72:LEU:HD13	3:E10:185:PHE:CG	2.19	0.78
1:A1:203:VAL:HG23	2:C13:208:TRP:CE3	2.18	0.78
1:A10:203:VAL:HG23	2:C9:208:TRP:CE3	2.18	0.78
1:A13:203:VAL:HG23	2:C12:208:TRP:CE3	2.18	0.78
1:B10:192:VAL:HG11	2:D10:148:LEU:HD23	1.65	0.78
1:B11:192:VAL:HG11	2:D11:148:LEU:HD23	1.65	0.78
2:C1:72:LEU:HD13	3:E1:185:PHE:CG	2.19	0.78
1:B7:192:VAL:HG11	2:D7:148:LEU:HD23	1.65	0.77
2:C2:72:LEU:HD13	3:E2:185:PHE:CG	2.19	0.77
1:A12:203:VAL:HG23	2:C11:208:TRP:CE3	2.18	0.77
1:B9:192:VAL:HG11	2:D9:148:LEU:HD23	1.65	0.77
2:C6:72:LEU:CD2	3:E6:185:PHE:HB3	2.07	0.77
1:B8:192:VAL:HG11	2:D8:148:LEU:HD23	1.65	0.77
2:C7:72:LEU:HD13	3:E7:185:PHE:CG	2.19	0.77
2:C11:72:LEU:HD13	3:E11:185:PHE:CG	2.19	0.77
2:C13:72:LEU:HD13	3:E13:185:PHE:CG	2.19	0.77
2:C3:72:LEU:HD13	3:E3:185:PHE:CG	2.19	0.77
2:C5:72:LEU:HD13	3:E5:185:PHE:CG	2.19	0.77
2:C4:72:LEU:HD13	3:E4:185:PHE:CG	2.19	0.76
2:D4:173:SER:OG	2:D4:193:ARG:HB2	1.86	0.76
2:C6:72:LEU:HD13	3:E6:185:PHE:CG	2.19	0.76
2:D3:173:SER:OG	2:D3:193:ARG:HB2	1.86	0.76
2:D7:173:SER:OG	2:D7:193:ARG:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D13:173:SER:OG	2:D13:193:ARG:HB2	1.86	0.76
2:D8:173:SER:OG	2:D8:193:ARG:HB2	1.86	0.76
2:D1:173:SER:OG	2:D1:193:ARG:HB2	1.86	0.76
2:C12:72:LEU:HD13	3:E12:185:PHE:CG	2.19	0.76
2:D10:173:SER:OG	2:D10:193:ARG:HB2	1.86	0.76
2:D5:173:SER:OG	2:D5:193:ARG:HB2	1.86	0.76
2:D11:173:SER:OG	2:D11:193:ARG:HB2	1.86	0.75
2:D2:173:SER:OG	2:D2:193:ARG:HB2	1.86	0.75
2:D6:173:SER:OG	2:D6:193:ARG:HB2	1.86	0.75
2:D12:173:SER:OG	2:D12:193:ARG:HB2	1.86	0.75
2:C1:147:VAL:HG11	2:C1:233:THR:HG21	1.70	0.74
2:C11:147:VAL:HG11	2:C11:233:THR:HG21	1.70	0.74
2:C2:147:VAL:HG11	2:C2:233:THR:HG21	1.69	0.74
2:C12:147:VAL:HG11	2:C12:233:THR:HG21	1.70	0.74
2:C13:147:VAL:HG11	2:C13:233:THR:HG21	1.70	0.74
2:D9:173:SER:OG	2:D9:193:ARG:HB2	1.86	0.74
2:C9:147:VAL:HG11	2:C9:233:THR:HG21	1.70	0.74
2:C10:147:VAL:HG11	2:C10:233:THR:HG21	1.70	0.74
1:B5:188:VAL:HG11	2:D5:141:ILE:HD11	1.70	0.74
1:B10:188:VAL:HG11	2:D10:141:ILE:HD11	1.70	0.74
1:B6:188:VAL:HG11	2:D6:141:ILE:HD11	1.70	0.74
1:B12:188:VAL:HG11	2:D12:141:ILE:HD11	1.70	0.74
1:A6:170:VAL:HG22	2:C6:216:MET:CB	2.18	0.74
1:B3:188:VAL:HG11	2:D3:141:ILE:HD11	1.70	0.74
1:B4:188:VAL:HG11	2:D4:141:ILE:HD11	1.70	0.74
1:B11:188:VAL:HG11	2:D11:141:ILE:HD11	1.70	0.74
2:C3:147:VAL:HG11	2:C3:233:THR:HG21	1.70	0.74
1:B1:188:VAL:HG11	2:D1:141:ILE:HD11	1.70	0.74
1:B13:188:VAL:HG11	2:D13:141:ILE:HD11	1.70	0.74
1:B2:188:VAL:HG11	2:D2:141:ILE:HD11	1.70	0.73
1:A10:170:VAL:HG22	2:C10:216:MET:CB	2.18	0.73
1:B9:188:VAL:HG11	2:D9:141:ILE:HD11	1.70	0.73
1:B7:188:VAL:HG11	2:D7:141:ILE:HD11	1.70	0.73
1:A11:170:VAL:HG22	2:C11:216:MET:CB	2.18	0.73
2:C4:147:VAL:HG11	2:C4:233:THR:HG21	1.70	0.73
2:C7:147:VAL:HG11	2:C7:233:THR:HG21	1.70	0.73
1:B8:188:VAL:HG11	2:D8:141:ILE:HD11	1.70	0.73
2:C5:147:VAL:HG11	2:C5:233:THR:HG21	1.70	0.73
2:C8:147:VAL:HG11	2:C8:233:THR:HG21	1.70	0.73
1:A3:170:VAL:HG22	2:C3:216:MET:CB	2.18	0.73
1:A9:170:VAL:HG22	2:C9:216:MET:CB	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C5:72:LEU:HD11	3:E5:185:PHE:CE2	2.23	0.72
2:C6:147:VAL:HG11	2:C6:233:THR:HG21	1.70	0.72
1:A1:170:VAL:HG22	2:C1:216:MET:CB	2.18	0.72
1:A13:170:VAL:HG22	2:C13:216:MET:CB	2.18	0.72
1:A5:170:VAL:HG22	2:C5:216:MET:CB	2.18	0.72
2:C12:72:LEU:HD11	3:E12:185:PHE:CE2	2.23	0.72
1:A10:189:SER:OG	1:B10:182:PHE:HB3	1.90	0.71
2:C2:69:ASP:OD2	3:F1:180:MET:HG2	1.91	0.71
1:A1:189:SER:OG	1:B1:182:PHE:HB3	1.91	0.71
1:A7:189:SER:OG	1:B7:182:PHE:HB3	1.91	0.71
2:C4:69:ASP:OD2	3:F3:180:MET:HG2	1.91	0.71
2:C6:69:ASP:OD2	3:F5:180:MET:HG2	1.90	0.71
1:A8:189:SER:OG	1:B8:182:PHE:HB3	1.91	0.71
2:C3:69:ASP:OD2	3:F2:180:MET:HG2	1.91	0.71
2:C7:69:ASP:OD2	3:F6:180:MET:HG2	1.91	0.71
2:C11:69:ASP:OD2	3:F10:180:MET:HG2	1.91	0.71
1:A2:170:VAL:HG22	2:C2:216:MET:CB	2.18	0.71
1:A5:189:SER:OG	1:B5:182:PHE:HB3	1.90	0.71
2:C12:69:ASP:OD2	3:F11:180:MET:HG2	1.90	0.71
1:A4:189:SER:OG	1:B4:182:PHE:HB3	1.91	0.71
1:A13:189:SER:OG	1:B13:182:PHE:HB3	1.90	0.71
2:C5:69:ASP:OD2	3:F4:180:MET:HG2	1.91	0.71
2:C13:69:ASP:OD2	3:F12:180:MET:HG2	1.91	0.71
2:C1:69:ASP:OD2	3:F13:180:MET:HG2	1.91	0.71
1:A3:189:SER:OG	1:B3:182:PHE:HB3	1.91	0.71
1:A8:170:VAL:HG22	2:C8:216:MET:CB	2.18	0.71
1:A12:170:VAL:HG22	2:C12:216:MET:CB	2.18	0.71
2:C6:72:LEU:HD13	3:E6:185:PHE:CD1	2.26	0.70
2:C10:69:ASP:OD2	3:F9:180:MET:HG2	1.91	0.70
1:A11:189:SER:OG	1:B11:182:PHE:HB3	1.91	0.70
2:C3:72:LEU:HD13	3:E3:185:PHE:CD1	2.26	0.70
2:C4:72:LEU:HD13	3:E4:185:PHE:CD1	2.26	0.70
2:C7:72:LEU:HD13	3:E7:185:PHE:CD1	2.26	0.70
2:C8:72:LEU:HD13	3:E8:185:PHE:CD1	2.26	0.70
2:C12:72:LEU:HD13	3:E12:185:PHE:CD1	2.26	0.70
1:A9:189:SER:OG	1:B9:182:PHE:HB3	1.90	0.70
2:C8:69:ASP:OD2	3:F7:180:MET:HG2	1.91	0.70
2:C9:72:LEU:HD13	3:E9:185:PHE:CD1	2.27	0.70
2:C10:72:LEU:HD13	3:E10:185:PHE:CD1	2.26	0.70
2:C11:72:LEU:HD13	3:E11:185:PHE:CD1	2.26	0.70
2:C13:72:LEU:HD13	3:E13:185:PHE:CD1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C13:72:LEU:HD11	3:E13:185:PHE:CE2	2.23	0.70
2:C5:72:LEU:HD13	3:E5:185:PHE:CD1	2.26	0.70
1:A2:189:SER:OG	1:B2:182:PHE:HB3	1.91	0.70
1:B2:188:VAL:CG1	2:D2:141:ILE:HD11	2.22	0.70
1:B8:188:VAL:CG1	2:D8:141:ILE:HD11	2.22	0.70
2:C2:72:LEU:HD13	3:E2:185:PHE:CD1	2.26	0.70
2:C4:72:LEU:HD11	3:E4:185:PHE:CE2	2.23	0.70
1:A6:189:SER:OG	1:B6:182:PHE:HB3	1.91	0.69
2:C9:69:ASP:OD2	3:F8:180:MET:HG2	1.90	0.69
1:B1:188:VAL:CG1	2:D1:141:ILE:HD11	2.22	0.69
1:B6:188:VAL:CG1	2:D6:141:ILE:HD11	2.22	0.69
1:A12:189:SER:OG	1:B12:182:PHE:HB3	1.91	0.69
1:B3:188:VAL:CG1	2:D3:141:ILE:HD11	2.22	0.69
2:C1:72:LEU:HD13	3:E1:185:PHE:CD1	2.26	0.69
1:A4:170:VAL:HG22	2:C4:216:MET:CB	2.18	0.69
2:C3:72:LEU:HD11	3:E3:185:PHE:CE2	2.23	0.69
1:B7:188:VAL:CG1	2:D7:141:ILE:HD11	2.22	0.69
1:B13:188:VAL:CG1	2:D13:141:ILE:HD11	2.22	0.69
1:B10:188:VAL:CG1	2:D10:141:ILE:HD11	2.22	0.69
2:C1:72:LEU:HD11	3:E1:185:PHE:CE2	2.23	0.69
1:B4:188:VAL:CG1	2:D4:141:ILE:HD11	2.22	0.69
1:B8:170:VAL:HA	2:D8:216:MET:HB3	1.75	0.69
2:C2:72:LEU:HD11	3:E2:185:PHE:CE2	2.23	0.69
1:B5:188:VAL:CG1	2:D5:141:ILE:HD11	2.22	0.69
1:B6:170:VAL:HA	2:D6:216:MET:HB3	1.75	0.69
1:B10:170:VAL:HA	2:D10:216:MET:HB3	1.75	0.68
1:B12:188:VAL:CG1	2:D12:141:ILE:HD11	2.22	0.68
1:B9:188:VAL:CG1	2:D9:141:ILE:HD11	2.22	0.68
1:A7:170:VAL:HG22	2:C7:216:MET:CB	2.18	0.68
1:B4:95:THR:HG23	1:B4:96:PRO:HD3	1.76	0.68
1:B5:95:THR:HG23	1:B5:96:PRO:HD3	1.76	0.68
1:B2:95:THR:HG23	1:B2:96:PRO:HD3	1.76	0.68
1:B3:95:THR:HG23	1:B3:96:PRO:HD3	1.76	0.68
1:B11:188:VAL:CG1	2:D11:141:ILE:HD11	2.22	0.68
1:B4:170:VAL:HA	2:D4:216:MET:HB3	1.75	0.68
1:B5:170:VAL:HA	2:D5:216:MET:HB3	1.75	0.68
1:B7:170:VAL:HA	2:D7:216:MET:HB3	1.75	0.68
2:C4:72:LEU:HD21	3:E4:185:PHE:HB2	1.76	0.68
1:B1:95:THR:HG23	1:B1:96:PRO:HD3	1.76	0.68
2:C3:72:LEU:HD21	3:E3:185:PHE:HB2	1.76	0.68
1:B11:95:THR:CG2	1:B11:96:PRO:HD3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B2:170:VAL:HA	2:D2:216:MET:HB3	1.75	0.67
1:B6:95:THR:HG23	1:B6:96:PRO:HD3	1.76	0.67
1:B10:95:THR:CG2	1:B10:96:PRO:HD3	2.25	0.67
1:B12:95:THR:CG2	1:B12:96:PRO:HD3	2.25	0.67
1:B13:95:THR:HG23	1:B13:96:PRO:HD3	1.76	0.67
1:B7:95:THR:CG2	1:B7:96:PRO:HD3	2.25	0.67
1:B7:95:THR:HG23	1:B7:96:PRO:HD3	1.76	0.67
2:C5:72:LEU:HD21	3:E5:185:PHE:HB2	1.76	0.67
2:C12:72:LEU:HD21	3:E12:185:PHE:HB2	1.76	0.67
2:C13:35:GLY:CA	2:D13:27:PRO:HD3	2.25	0.67
1:B13:95:THR:CG2	1:B13:96:PRO:HD3	2.25	0.67
2:C1:35:GLY:CA	2:D1:27:PRO:HD3	2.25	0.67
1:B1:170:VAL:HG21	2:D1:144:ASN:HD22	1.60	0.67
1:B2:95:THR:CG2	1:B2:96:PRO:HD3	2.25	0.67
1:B3:170:VAL:HG21	2:D3:144:ASN:HD22	1.60	0.67
1:B9:170:VAL:HG21	2:D9:144:ASN:HD22	1.60	0.67
1:B9:170:VAL:HA	2:D9:216:MET:HB3	1.75	0.67
2:C2:72:LEU:HD21	3:E2:185:PHE:HB2	1.76	0.67
2:C13:72:LEU:HD21	3:E13:185:PHE:HB2	1.76	0.67
1:B1:95:THR:CG2	1:B1:96:PRO:HD3	2.25	0.67
1:B4:170:VAL:HG21	2:D4:144:ASN:HD22	1.60	0.67
1:B6:170:VAL:HG21	2:D6:144:ASN:HD22	1.60	0.67
1:B7:170:VAL:HG21	2:D7:144:ASN:HD22	1.60	0.67
1:B12:170:VAL:HA	2:D12:216:MET:HB3	1.75	0.67
1:B6:95:THR:CG2	1:B6:96:PRO:HD3	2.25	0.67
1:B13:170:VAL:HA	2:D13:216:MET:HB3	1.75	0.67
1:B5:95:THR:CG2	1:B5:96:PRO:HD3	2.24	0.67
1:B11:170:VAL:HA	2:D11:216:MET:HB3	1.75	0.67
2:C11:72:LEU:HD21	3:E11:185:PHE:HB2	1.76	0.67
1:B4:190:PHE:CE1	2:D4:141:ILE:HD12	2.30	0.67
1:B8:95:THR:CG2	1:B8:96:PRO:HD3	2.25	0.67
1:B9:95:THR:HG23	1:B9:96:PRO:HD3	1.76	0.67
1:B10:190:PHE:CE1	2:D10:141:ILE:HD12	2.30	0.67
2:C12:35:GLY:CA	2:D12:27:PRO:HD3	2.25	0.67
2:D6:74:ARG:HH22	3:E6:184:GLU:HG3	1.60	0.67
1:B1:170:VAL:HA	2:D1:216:MET:HB3	1.75	0.66
1:B5:190:PHE:CE1	2:D5:141:ILE:HD12	2.30	0.66
1:B9:95:THR:CG2	1:B9:96:PRO:HD3	2.25	0.66
1:B11:190:PHE:CE1	2:D11:141:ILE:HD12	2.30	0.66
2:C2:35:GLY:CA	2:D2:27:PRO:HD3	2.25	0.66
2:C9:72:LEU:HD21	3:E9:185:PHE:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B3:190:PHE:CE1	2:D3:141:ILE:HD12	2.30	0.66
1:B9:190:PHE:CE1	2:D9:141:ILE:HD12	2.30	0.66
1:B12:95:THR:HG23	1:B12:96:PRO:HD3	1.76	0.66
1:B3:95:THR:CG2	1:B3:96:PRO:HD3	2.25	0.66
1:B11:95:THR:HG23	1:B11:96:PRO:HD3	1.76	0.66
1:B11:170:VAL:HG21	2:D11:144:ASN:HD22	1.60	0.66
1:B2:190:PHE:CE1	2:D2:141:ILE:HD12	2.30	0.66
1:B4:95:THR:CG2	1:B4:96:PRO:HD3	2.25	0.66
1:B6:190:PHE:CE1	2:D6:141:ILE:HD12	2.30	0.66
2:C1:72:LEU:HD21	3:E1:185:PHE:HB2	1.76	0.66
2:C9:35:GLY:CA	2:D9:27:PRO:HD3	2.25	0.66
2:D2:74:ARG:HH22	3:E2:184:GLU:HG3	1.61	0.66
1:B8:95:THR:HG23	1:B8:96:PRO:HD3	1.76	0.66
1:B8:170:VAL:HG21	2:D8:144:ASN:HD22	1.60	0.66
1:B10:95:THR:HG23	1:B10:96:PRO:HD3	1.76	0.66
2:C2:72:LEU:CD1	3:E2:185:PHE:CG	2.79	0.66
2:C7:72:LEU:HD21	3:E7:185:PHE:HB2	1.76	0.66
1:B10:170:VAL:HG21	2:D10:144:ASN:HD22	1.60	0.66
2:C6:72:LEU:HD21	3:E6:185:PHE:HB2	1.76	0.66
2:C8:72:LEU:HD21	3:E8:185:PHE:HB2	1.76	0.66
2:D5:74:ARG:HH22	3:E5:184:GLU:HG3	1.60	0.66
2:D10:74:ARG:HH22	3:E10:184:GLU:HG3	1.60	0.66
1:B1:190:PHE:CE1	2:D1:141:ILE:HD12	2.30	0.66
1:B3:170:VAL:HA	2:D3:216:MET:HB3	1.75	0.66
1:B12:170:VAL:HG21	2:D12:144:ASN:HD22	1.60	0.66
1:B12:190:PHE:CE1	2:D12:141:ILE:HD12	2.31	0.66
2:C7:72:LEU:HD11	3:E7:185:PHE:CE2	2.23	0.66
2:C8:35:GLY:CA	2:D8:27:PRO:HD3	2.25	0.66
2:C10:72:LEU:HD21	3:E10:185:PHE:HB2	1.76	0.66
1:B2:170:VAL:HG21	2:D2:144:ASN:HD22	1.60	0.66
1:B5:95:THR:CG2	1:B6:176:VAL:HG23	2.24	0.66
1:B13:170:VAL:HG21	2:D13:144:ASN:HD22	1.60	0.66
2:C3:72:LEU:CD1	3:E3:185:PHE:CG	2.79	0.66
2:D7:74:ARG:HH22	3:E7:184:GLU:HG3	1.61	0.66
1:A13:175:TRP:HZ2	2:C13:137:GLU:OE1	1.79	0.66
1:B8:190:PHE:CE1	2:D8:141:ILE:HD12	2.30	0.66
2:C5:35:GLY:CA	2:D5:27:PRO:HD3	2.25	0.66
1:A6:175:TRP:HZ2	2:C6:137:GLU:OE1	1.79	0.66
1:B1:170:VAL:CG1	2:D1:144:ASN:ND2	2.59	0.66
1:B3:170:VAL:CG1	2:D3:144:ASN:ND2	2.59	0.66
2:C4:35:GLY:CA	2:D4:27:PRO:HD3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C7:35:GLY:CA	2:D7:27:PRO:HD3	2.25	0.66
2:C11:35:GLY:CA	2:D11:27:PRO:HD3	2.25	0.66
2:D1:74:ARG:HH22	3:E1:184:GLU:HG3	1.61	0.66
1:A5:175:TRP:HZ2	2:C5:137:GLU:OE1	1.79	0.65
1:A7:175:TRP:HZ2	2:C7:137:GLU:OE1	1.79	0.65
1:A8:175:TRP:HZ2	2:C8:137:GLU:OE1	1.79	0.65
2:C9:72:LEU:CD2	3:E9:185:PHE:HB2	2.26	0.65
2:D3:74:ARG:HH22	3:E3:184:GLU:HG3	1.60	0.65
2:D9:74:ARG:HH22	3:E9:184:GLU:HG3	1.60	0.65
2:D11:74:ARG:HH22	3:E11:184:GLU:HG3	1.60	0.65
1:B7:190:PHE:CE1	2:D7:141:ILE:HD12	2.30	0.65
2:C4:72:LEU:CD2	3:E4:185:PHE:HB2	2.26	0.65
2:C8:72:LEU:CD2	3:E8:185:PHE:HB2	2.26	0.65
2:C9:72:LEU:HD21	3:E9:185:PHE:CB	2.27	0.65
1:A11:175:TRP:HZ2	2:C11:137:GLU:OE1	1.79	0.65
1:B11:170:VAL:CG1	2:D11:144:ASN:ND2	2.59	0.65
1:B12:170:VAL:CG1	2:D12:144:ASN:ND2	2.59	0.65
1:B13:190:PHE:CE1	2:D13:141:ILE:HD12	2.30	0.65
2:C6:35:GLY:CA	2:D6:27:PRO:HD3	2.25	0.65
2:C7:50:ILE:HD13	2:C7:114:TYR:HB2	1.79	0.65
2:C10:72:LEU:CD2	3:E10:185:PHE:HB2	2.26	0.65
2:C10:72:LEU:HD21	3:E10:185:PHE:CB	2.26	0.65
2:D2:202:LEU:HD11	2:D2:224:LEU:HG	1.79	0.65
1:A3:175:TRP:HZ2	2:C3:137:GLU:OE1	1.79	0.65
1:A4:175:TRP:HZ2	2:C4:137:GLU:OE1	1.79	0.65
2:C4:72:LEU:CD1	3:E4:185:PHE:CG	2.79	0.65
2:C9:50:ILE:HD13	2:C9:114:TYR:HB2	1.79	0.65
2:D8:202:LEU:HD11	2:D8:224:LEU:HG	1.79	0.65
1:B4:170:VAL:HG11	2:D4:144:ASN:HD22	1.61	0.65
1:B5:170:VAL:HG11	2:D5:144:ASN:HD22	1.61	0.65
1:B5:170:VAL:HG21	2:D5:144:ASN:HD22	1.60	0.65
2:C8:72:LEU:CD1	3:E8:185:PHE:CG	2.79	0.65
2:D5:202:LEU:HD11	2:D5:224:LEU:HG	1.79	0.65
1:A9:175:TRP:HZ2	2:C9:137:GLU:OE1	1.79	0.65
2:C3:35:GLY:CA	2:D3:27:PRO:HD3	2.25	0.65
2:C5:50:ILE:HD13	2:C5:114:TYR:HB2	1.79	0.65
2:C5:72:LEU:CD2	3:E5:185:PHE:HB2	2.26	0.65
2:C7:72:LEU:CD1	3:E7:185:PHE:CG	2.79	0.65
2:D12:202:LEU:HD11	2:D12:224:LEU:HG	1.79	0.65
1:B5:170:VAL:CG1	2:D5:144:ASN:ND2	2.59	0.65
2:C7:72:LEU:CD2	3:E7:185:PHE:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C8:50:ILE:HD13	2:C8:114:TYR:HB2	1.79	0.65
2:C10:50:ILE:HD13	2:C10:114:TYR:HB2	1.79	0.65
1:A10:175:TRP:HZ2	2:C10:137:GLU:OE1	1.79	0.65
1:B3:170:VAL:HG11	2:D3:144:ASN:HD22	1.61	0.65
1:B4:170:VAL:CG1	2:D4:144:ASN:ND2	2.59	0.65
2:C1:72:LEU:HD21	3:E1:185:PHE:CB	2.26	0.65
2:C9:72:LEU:CD1	3:E9:185:PHE:CG	2.79	0.65
2:C11:50:ILE:HD13	2:C11:114:TYR:HB2	1.79	0.65
2:D7:202:LEU:HD11	2:D7:224:LEU:HG	1.79	0.65
1:A1:175:TRP:HZ2	2:C1:137:GLU:OE1	1.79	0.65
1:B1:187:ARG:NH1	2:D1:204:GLU:OE2	2.31	0.65
1:B6:170:VAL:CG1	2:D6:144:ASN:ND2	2.59	0.65
1:B7:187:ARG:NH1	2:D7:204:GLU:OE2	2.30	0.65
1:B8:187:ARG:NH1	2:D8:204:GLU:OE2	2.31	0.65
2:C4:50:ILE:HD13	2:C4:114:TYR:HB2	1.79	0.65
2:C6:50:ILE:HD13	2:C6:114:TYR:HB2	1.79	0.65
2:C11:72:LEU:HD21	3:E11:185:PHE:CB	2.26	0.65
1:A2:175:TRP:HZ2	2:C2:137:GLU:OE1	1.79	0.64
2:C2:72:LEU:HD21	3:E2:185:PHE:CB	2.27	0.64
2:C12:50:ILE:HD13	2:C12:114:TYR:HB2	1.79	0.64
2:D11:202:LEU:HD11	2:D11:224:LEU:HG	1.79	0.64
1:B9:170:VAL:CG1	2:D9:144:ASN:ND2	2.59	0.64
1:B11:187:ARG:NH1	2:D11:204:GLU:OE2	2.30	0.64
2:C3:50:ILE:HD13	2:C3:114:TYR:HB2	1.79	0.64
1:B9:187:ARG:NH1	2:D9:204:GLU:OE2	2.31	0.64
2:D3:202:LEU:HD11	2:D3:224:LEU:HG	1.79	0.64
1:A12:175:TRP:HZ2	2:C12:137:GLU:OE1	1.79	0.64
1:B2:170:VAL:CG1	2:D2:144:ASN:ND2	2.59	0.64
1:B6:187:ARG:NH1	2:D6:204:GLU:OE2	2.31	0.64
2:C10:35:GLY:CA	2:D10:27:PRO:HD3	2.25	0.64
2:D4:74:ARG:HH22	3:E4:184:GLU:HG3	1.60	0.64
2:D13:202:LEU:HD11	2:D13:224:LEU:HG	1.79	0.64
1:B4:187:ARG:NH1	2:D4:204:GLU:OE2	2.31	0.64
1:B10:187:ARG:NH1	2:D10:204:GLU:OE2	2.30	0.64
2:C8:72:LEU:HD11	3:E8:185:PHE:CE2	2.23	0.64
2:C9:72:LEU:HD11	3:E9:185:PHE:CE2	2.23	0.64
2:C13:50:ILE:HD13	2:C13:114:TYR:HB2	1.79	0.64
2:D1:202:LEU:HD11	2:D1:224:LEU:HG	1.79	0.64
2:D4:202:LEU:HD11	2:D4:224:LEU:HG	1.79	0.64
2:D9:202:LEU:HD11	2:D9:224:LEU:HG	1.79	0.64
1:B2:187:ARG:NH1	2:D2:204:GLU:OE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B6:170:VAL:HG11	2:D6:144:ASN:HD22	1.61	0.64
1:B8:170:VAL:CG1	2:D8:144:ASN:ND2	2.59	0.64
1:B13:187:ARG:NH1	2:D13:204:GLU:OE2	2.31	0.64
2:C6:72:LEU:CD1	3:E6:185:PHE:CG	2.79	0.64
1:B2:170:VAL:HG11	2:D2:144:ASN:HD22	1.61	0.64
1:B5:187:ARG:NH1	2:D5:204:GLU:OE2	2.30	0.64
2:D8:74:ARG:HH22	3:E8:184:GLU:HG3	1.60	0.64
2:D13:74:ARG:HH22	3:E13:184:GLU:HG3	1.60	0.64
1:B10:170:VAL:CG1	2:D10:144:ASN:ND2	2.59	0.64
2:C1:50:ILE:HD13	2:C1:114:TYR:HB2	1.79	0.64
2:C2:50:ILE:HD13	2:C2:114:TYR:HB2	1.79	0.64
2:C6:72:LEU:CD2	3:E6:185:PHE:HB2	2.26	0.64
2:C10:72:LEU:CD1	3:E10:185:PHE:CG	2.79	0.64
1:B3:187:ARG:NH1	2:D3:204:GLU:OE2	2.31	0.64
1:B12:187:ARG:NH1	2:D12:204:GLU:OE2	2.30	0.64
2:C9:35:GLY:HA3	2:D9:27:PRO:CD	2.28	0.64
2:D6:202:LEU:HD11	2:D6:224:LEU:HG	1.79	0.64
2:C8:35:GLY:HA3	2:D8:27:PRO:CD	2.28	0.64
2:D10:202:LEU:HD11	2:D10:224:LEU:HG	1.79	0.63
1:B12:170:VAL:HG11	2:D12:144:ASN:HD22	1.61	0.63
1:B13:170:VAL:HG11	2:D13:144:ASN:HD22	1.61	0.63
2:C2:35:GLY:HA3	2:D2:27:PRO:CD	2.29	0.63
2:C13:72:LEU:CD2	3:E13:185:PHE:HB2	2.26	0.63
2:D12:74:ARG:HH22	3:E12:184:GLU:HG3	1.61	0.63
1:B13:170:VAL:CG1	2:D13:144:ASN:ND2	2.59	0.63
2:C1:35:GLY:HA3	2:D1:27:PRO:CD	2.28	0.63
2:C13:193:ARG:HA	2:C13:228:GLY:O	1.99	0.63
1:B7:170:VAL:CG1	2:D7:144:ASN:ND2	2.59	0.63
2:C7:35:GLY:HA3	2:D7:27:PRO:CD	2.28	0.63
2:C12:193:ARG:HA	2:C12:228:GLY:O	1.99	0.63
1:B11:170:VAL:HG11	2:D11:144:ASN:HD22	1.61	0.63
2:C5:193:ARG:HA	2:C5:228:GLY:O	1.99	0.63
2:C6:193:ARG:HA	2:C6:228:GLY:O	1.99	0.63
2:C11:193:ARG:HA	2:C11:228:GLY:O	1.99	0.63
2:C13:35:GLY:HA3	2:D13:27:PRO:CD	2.28	0.63
2:C1:193:ARG:HA	2:C1:228:GLY:O	1.99	0.63
2:C6:35:GLY:HA3	2:D6:27:PRO:CD	2.28	0.63
1:B1:170:VAL:HG11	2:D1:144:ASN:HD22	1.61	0.63
1:B9:95:THR:CG2	1:B10:176:VAL:HG21	2.29	0.63
2:C1:72:LEU:CD2	3:E1:185:PHE:HB2	2.26	0.63
2:C8:193:ARG:HA	2:C8:228:GLY:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C9:193:ARG:HA	2:C9:228:GLY:O	1.99	0.63
2:C10:193:ARG:HA	2:C10:228:GLY:O	1.99	0.63
1:B7:170:VAL:HG11	2:D7:144:ASN:HD21	1.64	0.62
2:C5:72:LEU:CD1	3:E5:185:PHE:CG	2.79	0.62
2:C7:193:ARG:HA	2:C7:228:GLY:O	1.99	0.62
2:C11:72:LEU:CD1	3:E11:185:PHE:CG	2.79	0.62
1:B4:95:THR:CG2	1:B5:176:VAL:HG21	2.29	0.62
1:B7:170:VAL:HG11	2:D7:144:ASN:HD22	1.61	0.62
2:C4:193:ARG:HA	2:C4:228:GLY:O	1.99	0.62
1:B2:95:THR:CG2	1:B3:176:VAL:HG21	2.29	0.62
1:B11:95:THR:CG2	1:B12:176:VAL:HG21	2.29	0.62
2:C5:35:GLY:HA3	2:D5:27:PRO:CD	2.28	0.62
2:C12:35:GLY:HA3	2:D12:27:PRO:CD	2.28	0.62
2:C12:72:LEU:CD1	3:E12:185:PHE:CG	2.79	0.62
1:B1:176:VAL:HG21	1:B13:95:THR:CG2	2.29	0.62
1:B2:170:VAL:HG11	2:D2:144:ASN:HD21	1.64	0.62
1:B5:170:VAL:HG11	2:D5:144:ASN:HD21	1.64	0.62
1:B6:95:THR:CG2	1:B7:176:VAL:HG21	2.29	0.62
1:B10:170:VAL:HG11	2:D10:144:ASN:HD22	1.61	0.62
2:C2:193:ARG:HA	2:C2:228:GLY:O	1.99	0.62
1:B1:95:THR:CG2	1:B2:176:VAL:HG21	2.29	0.62
1:B7:95:THR:CG2	1:B8:176:VAL:HG21	2.29	0.62
1:B13:170:VAL:HG11	2:D13:144:ASN:HD21	1.64	0.62
2:C2:72:LEU:CD2	3:E2:185:PHE:HB2	2.26	0.62
1:B3:95:THR:CG2	1:B4:176:VAL:HG21	2.29	0.62
1:B6:95:THR:HG21	1:B7:176:VAL:HG21	1.82	0.62
1:B2:95:THR:HG21	1:B3:176:VAL:CG2	2.30	0.62
1:B5:95:THR:HG21	1:B6:176:VAL:HG21	1.82	0.62
1:B8:95:THR:CG2	1:B9:176:VAL:HG21	2.29	0.62
2:C3:193:ARG:HA	2:C3:228:GLY:O	1.99	0.62
1:B1:176:VAL:HG21	1:B13:95:THR:HG21	1.82	0.61
1:B7:95:THR:HG21	1:B8:176:VAL:HG21	1.82	0.61
1:B9:170:VAL:HG11	2:D9:144:ASN:HD22	1.61	0.61
1:B12:95:THR:HG21	1:B13:176:VAL:HG21	1.82	0.61
1:B3:95:THR:HG21	1:B4:176:VAL:CG2	2.30	0.61
2:C13:72:LEU:CD1	3:E13:185:PHE:CG	2.79	0.61
1:B1:95:THR:HG21	1:B2:176:VAL:HG21	1.82	0.61
1:B10:95:THR:CG2	1:B11:176:VAL:HG21	2.29	0.61
1:B10:170:VAL:HG11	2:D10:144:ASN:HD21	1.64	0.61
2:C4:35:GLY:HA3	2:D4:27:PRO:CD	2.28	0.61
1:B1:95:THR:HG21	1:B2:176:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B12:95:THR:CG2	1:B13:176:VAL:HG21	2.29	0.61
1:B4:170:VAL:HG11	2:D4:144:ASN:HD21	1.64	0.61
1:B6:95:THR:HG21	1:B7:176:VAL:CG2	2.30	0.61
1:B11:95:THR:HG21	1:B12:176:VAL:HG21	1.82	0.61
1:B4:95:THR:HG21	1:B5:176:VAL:HG21	1.82	0.61
1:B7:95:THR:HG21	1:B8:176:VAL:CG2	2.30	0.61
1:B8:95:THR:HG21	1:B9:176:VAL:HG21	1.82	0.61
1:B8:170:VAL:HG11	2:D8:144:ASN:HD22	1.61	0.61
2:C6:72:LEU:HD11	3:E6:185:PHE:CE2	2.23	0.61
2:C6:72:LEU:HD21	3:E6:185:PHE:CB	2.26	0.61
2:C11:35:GLY:HA3	2:D11:27:PRO:CD	2.29	0.61
1:B5:95:THR:HG21	1:B6:176:VAL:CG2	2.30	0.61
2:C1:72:LEU:CD1	3:E1:185:PHE:CG	2.79	0.61
1:B8:95:THR:HG21	1:B9:176:VAL:CG2	2.30	0.61
1:B2:95:THR:HG21	1:B3:176:VAL:HG21	1.82	0.60
1:B10:95:THR:HG21	1:B11:176:VAL:HG21	1.82	0.60
1:B3:170:VAL:HG11	2:D3:144:ASN:HD21	1.64	0.60
1:B9:170:VAL:HG11	2:D9:144:ASN:HD21	1.64	0.60
2:C3:35:GLY:HA3	2:D3:27:PRO:CD	2.28	0.60
1:B9:95:THR:HG21	1:B10:176:VAL:CG2	2.30	0.60
1:B4:95:THR:HG21	1:B5:176:VAL:CG2	2.30	0.60
1:B1:176:VAL:CG2	1:B13:95:THR:HG21	2.30	0.60
1:B3:95:THR:HG21	1:B4:176:VAL:HG21	1.82	0.60
1:B10:95:THR:HG21	1:B11:176:VAL:CG2	2.30	0.60
1:B6:170:VAL:HG11	2:D6:144:ASN:HD21	1.64	0.60
1:B9:95:THR:HG21	1:B10:176:VAL:HG21	1.82	0.60
2:C11:72:LEU:CD2	3:E11:185:PHE:HB2	2.26	0.60
2:C10:35:GLY:HA3	2:D10:27:PRO:CD	2.28	0.60
1:B11:170:VAL:HG11	2:D11:144:ASN:HD21	1.64	0.59
1:B1:170:VAL:HG11	2:D1:144:ASN:HD21	1.63	0.59
1:B11:95:THR:HG21	1:B12:176:VAL:CG2	2.30	0.59
1:A4:182:PHE:O	1:B4:188:VAL:HG23	2.03	0.59
1:A5:182:PHE:O	1:B5:188:VAL:HG23	2.03	0.59
1:A9:182:PHE:O	1:B9:188:VAL:HG23	2.03	0.58
1:B5:95:THR:CG2	1:B6:176:VAL:HG21	2.29	0.58
1:A3:182:PHE:O	1:B3:188:VAL:HG23	2.03	0.58
1:A6:182:PHE:O	1:B6:188:VAL:HG23	2.03	0.58
1:A8:182:PHE:O	1:B8:188:VAL:HG23	2.03	0.58
1:A2:182:PHE:O	1:B2:188:VAL:HG23	2.03	0.58
1:B1:176:VAL:HG23	1:B13:95:THR:CG2	2.24	0.58
1:A1:182:PHE:O	1:B1:188:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:182:PHE:O	1:B7:188:VAL:HG23	2.03	0.58
1:A11:182:PHE:O	1:B11:188:VAL:HG23	2.03	0.58
1:A12:182:PHE:O	1:B12:188:VAL:HG23	2.03	0.58
1:A13:182:PHE:O	1:B13:188:VAL:HG23	2.03	0.58
2:D9:225:MET:C	2:D9:227:GLY:N	2.57	0.58
2:D7:225:MET:C	2:D7:227:GLY:N	2.57	0.58
1:B9:166:GLN:HB2	1:B9:193:SER:HB3	1.86	0.58
2:D7:225:MET:C	2:D7:227:GLY:H	2.07	0.58
1:B12:95:THR:HG21	1:B13:176:VAL:CG2	2.30	0.58
1:B7:166:GLN:HB2	1:B7:193:SER:HB3	1.86	0.58
2:D11:225:MET:C	2:D11:227:GLY:H	2.07	0.58
2:D12:225:MET:C	2:D12:227:GLY:H	2.07	0.58
1:B11:166:GLN:HB2	1:B11:193:SER:HB3	1.86	0.57
1:A10:182:PHE:O	1:B10:188:VAL:HG23	2.03	0.57
2:D8:225:MET:C	2:D8:227:GLY:H	2.08	0.57
1:A2:160:PRO:CG	1:B1:189:SER:OG	2.52	0.57
1:B8:166:GLN:HB2	1:B8:193:SER:HB3	1.86	0.57
1:B10:166:GLN:HB2	1:B10:193:SER:HB3	1.86	0.57
2:D6:225:MET:C	2:D6:227:GLY:H	2.07	0.57
2:D6:225:MET:C	2:D6:227:GLY:N	2.57	0.57
1:B5:166:GLN:HB2	1:B5:193:SER:HB3	1.86	0.57
2:D8:225:MET:C	2:D8:227:GLY:N	2.57	0.57
2:D10:225:MET:C	2:D10:227:GLY:N	2.57	0.57
1:B6:166:GLN:HB2	1:B6:193:SER:HB3	1.86	0.57
2:C10:72:LEU:HD11	3:E10:185:PHE:CE2	2.23	0.57
1:A6:160:PRO:CG	1:B5:189:SER:OG	2.52	0.57
1:A7:160:PRO:CG	1:B6:189:SER:OG	2.52	0.57
1:B12:166:GLN:HB2	1:B12:193:SER:HB3	1.86	0.57
2:D13:225:MET:C	2:D13:227:GLY:H	2.07	0.57
1:A9:160:PRO:CG	1:B8:189:SER:OG	2.52	0.57
2:C9:30:ILE:HG22	2:C9:32:LEU:HG	1.86	0.57
2:C10:30:ILE:HG22	2:C10:32:LEU:HG	1.86	0.57
2:C11:30:ILE:HG22	2:C11:32:LEU:HG	1.86	0.57
2:D10:225:MET:C	2:D10:227:GLY:H	2.07	0.57
2:C1:30:ILE:HG22	2:C1:32:LEU:HG	1.86	0.57
2:C8:30:ILE:HG22	2:C8:32:LEU:HG	1.86	0.57
2:C12:30:ILE:HG22	2:C12:32:LEU:HG	1.86	0.57
2:D1:183:ASP:OD1	2:D1:183:ASP:N	2.34	0.57
2:D1:225:MET:C	2:D1:227:GLY:N	2.57	0.57
2:D3:225:MET:C	2:D3:227:GLY:N	2.57	0.57
2:C2:30:ILE:HG22	2:C2:32:LEU:HG	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C11:72:LEU:HD11	3:E11:185:PHE:CE2	2.23	0.56
1:B13:166:GLN:HB2	1:B13:193:SER:HB3	1.86	0.56
2:C5:30:ILE:HG22	2:C5:32:LEU:HG	1.86	0.56
2:C6:30:ILE:HG22	2:C6:32:LEU:HG	1.86	0.56
1:A13:160:PRO:CG	1:B12:189:SER:OG	2.52	0.56
1:B3:95:THR:CG2	1:B4:176:VAL:HG23	2.24	0.56
1:B3:166:GLN:HB2	1:B3:193:SER:HB3	1.86	0.56
1:B4:166:GLN:HB2	1:B4:193:SER:HB3	1.86	0.56
1:B8:170:VAL:HG11	2:D8:144:ASN:HD21	1.63	0.56
1:B12:95:THR:CG2	1:B13:176:VAL:HG23	2.24	0.56
1:B12:170:VAL:HG11	2:D12:144:ASN:HD21	1.64	0.56
2:C7:30:ILE:HG22	2:C7:32:LEU:HG	1.86	0.56
2:D4:225:MET:C	2:D4:227:GLY:N	2.57	0.56
2:D5:183:ASP:OD1	2:D5:183:ASP:N	2.34	0.56
2:D9:225:MET:C	2:D9:227:GLY:H	2.07	0.56
1:B1:166:GLN:HB2	1:B1:193:SER:HB3	1.86	0.56
2:C13:30:ILE:HG22	2:C13:32:LEU:HG	1.86	0.56
1:B10:154:ASN:HA	2:D11:205:GLN:HE21	1.71	0.56
2:C4:30:ILE:HG22	2:C4:32:LEU:HG	1.86	0.56
2:D13:225:MET:C	2:D13:227:GLY:N	2.57	0.56
1:B2:166:GLN:HB2	1:B2:193:SER:HB3	1.86	0.56
1:B11:154:ASN:HA	2:D12:205:GLN:HE21	1.71	0.56
2:C3:30:ILE:HG22	2:C3:32:LEU:HG	1.86	0.56
2:D1:225:MET:C	2:D1:227:GLY:H	2.07	0.56
2:D5:225:MET:C	2:D5:227:GLY:H	2.07	0.56
1:A4:160:PRO:CG	1:B3:189:SER:OG	2.52	0.56
2:D2:225:MET:C	2:D2:227:GLY:N	2.57	0.56
1:A8:203:VAL:CG2	2:C7:208:TRP:CD2	2.89	0.56
1:B9:154:ASN:HA	2:D10:205:GLN:HE21	1.71	0.56
1:B12:154:ASN:HA	2:D13:205:GLN:HE21	1.71	0.56
2:D6:183:ASP:OD1	2:D6:183:ASP:N	2.34	0.56
2:D12:225:MET:C	2:D12:227:GLY:N	2.57	0.56
1:A1:203:VAL:CG2	2:C13:208:TRP:CD2	2.89	0.56
1:A5:203:VAL:CG2	2:C4:208:TRP:CD2	2.89	0.56
1:B2:95:THR:CG2	1:B3:176:VAL:HG23	2.24	0.56
1:B7:154:ASN:HA	2:D8:205:GLN:HE21	1.71	0.56
1:A4:203:VAL:CG2	2:C3:208:TRP:CD2	2.89	0.56
1:A5:160:PRO:CG	1:B4:189:SER:OG	2.52	0.56
1:A9:203:VAL:CG2	2:C8:208:TRP:CD2	2.89	0.56
1:A10:160:PRO:CG	1:B9:189:SER:OG	2.52	0.56
1:A12:203:VAL:CG2	2:C11:208:TRP:CD2	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B8:154:ASN:HA	2:D9:205:GLN:HE21	1.71	0.56
2:D13:183:ASP:OD1	2:D13:183:ASP:N	2.34	0.56
1:B4:95:THR:CG2	1:B5:176:VAL:HG23	2.24	0.55
1:B6:154:ASN:HA	2:D7:205:GLN:HE21	1.71	0.55
1:B12:187:ARG:NH1	2:D12:204:GLU:CD	2.58	0.55
2:C8:72:LEU:HD21	3:E8:185:PHE:CB	2.27	0.55
2:D2:225:MET:C	2:D2:227:GLY:H	2.08	0.55
1:A6:203:VAL:HG23	2:C5:208:TRP:CD2	2.42	0.55
1:A7:203:VAL:CG2	2:C6:208:TRP:CD2	2.89	0.55
1:A8:160:PRO:CG	1:B7:189:SER:OG	2.52	0.55
1:A11:160:PRO:CG	1:B10:189:SER:OG	2.52	0.55
1:A3:160:PRO:CG	1:B2:189:SER:OG	2.52	0.55
1:A6:203:VAL:CG2	2:C5:208:TRP:CD2	2.89	0.55
1:B5:154:ASN:HA	2:D6:205:GLN:HE21	1.71	0.55
1:B13:154:ASN:HA	2:D1:205:GLN:HE21	1.71	0.55
1:A3:203:VAL:CG2	2:C2:208:TRP:CD2	2.89	0.55
1:A7:203:VAL:HG23	2:C6:208:TRP:CD2	2.42	0.55
2:C7:72:LEU:HD21	3:E7:185:PHE:CB	2.27	0.55
1:A5:203:VAL:HG23	2:C4:208:TRP:CD2	2.42	0.55
1:A10:203:VAL:CG2	2:C9:208:TRP:CD2	2.89	0.55
2:D3:225:MET:C	2:D3:227:GLY:H	2.07	0.55
1:B10:199:LEU:HD21	1:B11:182:PHE:HE2	1.72	0.55
1:A3:154:ASN:ND2	1:B1:152:CYS:O	2.40	0.55
1:A10:203:VAL:HG23	2:C9:208:TRP:CD2	2.42	0.55
1:B5:199:LEU:HD21	1:B6:182:PHE:HE2	1.72	0.55
2:D4:225:MET:C	2:D4:227:GLY:H	2.07	0.55
1:A5:154:ASN:ND2	1:B3:152:CYS:O	2.40	0.55
1:A9:203:VAL:HG23	2:C8:208:TRP:CD2	2.42	0.55
1:A12:160:PRO:CG	1:B11:189:SER:OG	2.52	0.55
1:B2:199:LEU:HD21	1:B3:182:PHE:HE2	1.72	0.55
1:B3:199:LEU:HD21	1:B4:182:PHE:HE2	1.72	0.55
1:B10:187:ARG:NH1	2:D10:204:GLU:CD	2.58	0.55
2:D5:225:MET:C	2:D5:227:GLY:N	2.57	0.55
1:A2:154:ASN:ND2	1:B13:152:CYS:O	2.40	0.55
1:A6:154:ASN:ND2	1:B4:152:CYS:O	2.40	0.55
1:A8:154:ASN:ND2	1:B6:152:CYS:O	2.40	0.55
1:A13:154:ASN:ND2	1:B11:152:CYS:O	2.40	0.55
1:A13:203:VAL:CG2	2:C12:208:TRP:CD2	2.89	0.55
1:B1:154:ASN:HA	2:D2:205:GLN:HE21	1.71	0.55
1:B1:182:PHE:HE2	1:B13:199:LEU:HD21	1.72	0.55
1:B10:95:THR:CG2	1:B11:176:VAL:HG23	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:203:VAL:HG23	2:C2:208:TRP:CD2	2.42	0.54
1:A13:203:VAL:HG23	2:C12:208:TRP:CD2	2.42	0.54
1:B6:199:LEU:HD21	1:B7:182:PHE:HE2	1.72	0.54
1:B7:199:LEU:HD21	1:B8:182:PHE:HE2	1.72	0.54
1:B12:199:LEU:HD21	1:B13:182:PHE:HE2	1.72	0.54
1:A1:203:VAL:HG23	2:C13:208:TRP:CD2	2.42	0.54
1:A2:203:VAL:CG2	2:C1:208:TRP:CD2	2.89	0.54
1:A11:203:VAL:CG2	2:C10:208:TRP:CD2	2.89	0.54
1:A12:203:VAL:HG23	2:C11:208:TRP:CD2	2.42	0.54
1:B3:154:ASN:HA	2:D4:205:GLN:HE21	1.71	0.54
1:B4:154:ASN:HA	2:D5:205:GLN:HE21	1.71	0.54
1:B9:199:LEU:HD21	1:B10:182:PHE:HE2	1.72	0.54
2:C7:72:LEU:HD22	3:E7:185:PHE:CD1	2.42	0.54
1:A2:203:VAL:HG23	2:C1:208:TRP:CD2	2.42	0.54
1:A8:203:VAL:HG23	2:C7:208:TRP:CD2	2.42	0.54
1:B2:154:ASN:HA	2:D3:205:GLN:HE21	1.71	0.54
1:B1:187:ARG:NH1	2:D1:204:GLU:CD	2.58	0.54
1:A1:154:ASN:ND2	1:B12:152:CYS:O	2.40	0.54
1:A1:160:PRO:CG	1:B13:189:SER:OG	2.52	0.54
1:A7:154:ASN:ND2	1:B5:152:CYS:O	2.40	0.54
1:A11:203:VAL:HG23	2:C10:208:TRP:CD2	2.42	0.54
1:B8:199:LEU:HD21	1:B9:182:PHE:HE2	1.72	0.54
2:C1:72:LEU:HD22	3:E1:185:PHE:CD1	2.42	0.54
2:D11:225:MET:C	2:D11:227:GLY:N	2.57	0.54
1:A4:203:VAL:HG23	2:C3:208:TRP:CD2	2.42	0.54
1:B2:187:ARG:NH1	2:D2:204:GLU:CD	2.58	0.54
1:A11:154:ASN:ND2	1:B9:152:CYS:O	2.40	0.54
1:B4:199:LEU:HD21	1:B5:182:PHE:HE2	1.72	0.54
2:C8:72:LEU:HD22	3:E8:185:PHE:CD1	2.42	0.54
2:C13:96:ARG:HD3	2:C13:124:ARG:HG2	1.90	0.54
2:D12:183:ASP:OD1	2:D12:183:ASP:N	2.34	0.54
1:A10:154:ASN:ND2	1:B8:152:CYS:O	2.40	0.54
2:C2:99:THR:HG21	2:D2:49:MET:SD	2.48	0.54
1:B1:95:THR:CG2	1:B2:176:VAL:HG23	2.24	0.54
2:C6:99:THR:HG21	2:D6:49:MET:SD	2.48	0.54
2:C12:96:ARG:HD3	2:C12:124:ARG:HG2	1.90	0.54
2:D12:174:VAL:HG13	2:D12:190:TYR:HB3	1.91	0.54
1:A4:154:ASN:ND2	1:B2:152:CYS:O	2.40	0.53
1:A9:154:ASN:ND2	1:B7:152:CYS:O	2.40	0.53
1:A13:172:ILE:HD11	1:A13:188:VAL:HG23	1.91	0.53
2:C5:99:THR:HG21	2:D5:49:MET:SD	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:50:ILE:HD13	2:D4:114:TYR:HB2	1.91	0.53
2:D6:174:VAL:HG13	2:D6:190:TYR:HB3	1.90	0.53
2:D10:50:ILE:HD13	2:D10:114:TYR:HB2	1.90	0.53
1:A8:172:ILE:HD11	1:A8:188:VAL:HG23	1.91	0.53
1:B1:95:THR:HG23	1:B1:96:PRO:CD	2.39	0.53
2:C1:99:THR:HG21	2:D1:49:MET:SD	2.48	0.53
2:C3:96:ARG:HD3	2:C3:124:ARG:HG2	1.90	0.53
2:C7:99:THR:HG21	2:D7:49:MET:SD	2.48	0.53
2:D3:174:VAL:HG13	2:D3:190:TYR:HB3	1.90	0.53
2:D6:50:ILE:HD13	2:D6:114:TYR:HB2	1.90	0.53
2:D12:50:ILE:HD13	2:D12:114:TYR:HB2	1.91	0.53
2:D13:50:ILE:HD13	2:D13:114:TYR:HB2	1.91	0.53
1:A12:154:ASN:ND2	1:B10:152:CYS:O	2.40	0.53
1:B2:95:THR:HG23	1:B2:96:PRO:CD	2.39	0.53
2:C1:96:ARG:HD3	2:C1:124:ARG:HG2	1.90	0.53
2:C8:99:THR:HG21	2:D8:49:MET:SD	2.48	0.53
2:C12:72:LEU:HD22	3:E12:185:PHE:CD1	2.42	0.53
2:D2:50:ILE:HD13	2:D2:114:TYR:HB2	1.91	0.53
2:D9:174:VAL:HG13	2:D9:190:TYR:HB3	1.90	0.53
2:D11:50:ILE:HD13	2:D11:114:TYR:HB2	1.91	0.53
1:A7:172:ILE:HD11	1:A7:188:VAL:HG23	1.91	0.53
1:A10:172:ILE:HD11	1:A10:188:VAL:HG23	1.91	0.53
1:B8:95:THR:HG23	1:B8:96:PRO:CD	2.39	0.53
1:B11:199:LEU:HD21	1:B12:182:PHE:HE2	1.72	0.53
2:C3:99:THR:HG21	2:D3:49:MET:SD	2.48	0.53
2:C13:99:THR:HG21	2:D13:49:MET:SD	2.48	0.53
2:D1:50:ILE:HD13	2:D1:114:TYR:HB2	1.91	0.53
2:D3:50:ILE:HD13	2:D3:114:TYR:HB2	1.91	0.53
2:D5:50:ILE:HD13	2:D5:114:TYR:HB2	1.91	0.53
1:A11:172:ILE:HD11	1:A11:188:VAL:HG23	1.91	0.53
1:B7:95:THR:HG23	1:B7:96:PRO:CD	2.39	0.53
1:B9:95:THR:HG23	1:B9:96:PRO:CD	2.39	0.53
1:B13:95:THR:HG23	1:B13:96:PRO:CD	2.39	0.53
2:D4:174:VAL:HG13	2:D4:190:TYR:HB3	1.90	0.53
2:D7:174:VAL:HG13	2:D7:190:TYR:HB3	1.91	0.53
2:D8:50:ILE:HD13	2:D8:114:TYR:HB2	1.91	0.53
2:D13:174:VAL:HG13	2:D13:190:TYR:HB3	1.90	0.53
1:B3:95:THR:HG23	1:B3:96:PRO:CD	2.39	0.53
1:B10:170:VAL:CG2	2:D10:144:ASN:HD22	2.22	0.53
2:C4:96:ARG:HD3	2:C4:124:ARG:HG2	1.90	0.53
2:D2:174:VAL:HG13	2:D2:190:TYR:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D9:50:ILE:HD13	2:D9:114:TYR:HB2	1.91	0.53
1:A1:172:ILE:HD11	1:A1:188:VAL:HG23	1.91	0.53
1:B1:199:LEU:HD21	1:B2:182:PHE:HE2	1.72	0.53
2:C9:72:LEU:HD22	3:E9:185:PHE:CD1	2.42	0.53
2:C12:99:THR:HG21	2:D12:49:MET:SD	2.48	0.53
2:D10:174:VAL:HG13	2:D10:190:TYR:HB3	1.90	0.53
1:A4:172:ILE:HD11	1:A4:188:VAL:HG23	1.91	0.53
1:B2:170:VAL:CG2	2:D2:144:ASN:HD22	2.22	0.53
1:B11:95:THR:CG2	1:B12:176:VAL:HG23	2.24	0.53
2:C9:99:THR:HG21	2:D9:49:MET:SD	2.48	0.53
2:C10:96:ARG:HD3	2:C10:124:ARG:HG2	1.90	0.53
2:D7:50:ILE:HD13	2:D7:114:TYR:HB2	1.90	0.53
2:D11:174:VAL:HG13	2:D11:190:TYR:HB3	1.90	0.53
1:A3:172:ILE:HD11	1:A3:188:VAL:HG23	1.91	0.53
1:B4:95:THR:HG23	1:B4:96:PRO:CD	2.39	0.53
1:B9:170:VAL:CG2	2:D9:144:ASN:HD22	2.22	0.53
1:B10:95:THR:HG23	1:B10:96:PRO:CD	2.39	0.53
1:B11:170:VAL:CG2	2:D11:144:ASN:HD22	2.22	0.53
2:C4:99:THR:HG21	2:D4:49:MET:SD	2.48	0.53
2:C9:96:ARG:HD3	2:C9:124:ARG:HG2	1.90	0.53
2:C10:72:LEU:HD22	3:E10:185:PHE:CD1	2.42	0.53
1:B1:170:VAL:CG2	2:D1:144:ASN:HD22	2.22	0.53
1:B3:170:VAL:CG2	2:D3:144:ASN:HD22	2.22	0.53
2:C3:146:ALA:HB1	2:C3:151:ASP:O	2.09	0.53
2:C8:146:ALA:HB1	2:C8:151:ASP:O	2.09	0.53
2:D6:177:LEU:HD21	2:D6:191:GLU:HB2	1.91	0.53
2:D8:177:LEU:HD21	2:D8:191:GLU:HB2	1.91	0.53
1:A8:175:TRP:CZ2	2:C8:137:GLU:OE1	2.62	0.52
1:B12:95:THR:HG23	1:B12:96:PRO:CD	2.39	0.52
2:C6:146:ALA:HB1	2:C6:151:ASP:O	2.09	0.52
2:C9:146:ALA:HB1	2:C9:151:ASP:O	2.09	0.52
2:C13:146:ALA:HB1	2:C13:151:ASP:O	2.09	0.52
1:A12:175:TRP:CZ2	2:C12:137:GLU:OE1	2.62	0.52
1:B6:95:THR:HG23	1:B6:96:PRO:CD	2.39	0.52
1:B8:187:ARG:NH1	2:D8:204:GLU:CD	2.58	0.52
1:B9:95:THR:CG2	1:B10:176:VAL:HG23	2.24	0.52
2:C2:146:ALA:HB1	2:C2:151:ASP:O	2.09	0.52
2:C5:146:ALA:HB1	2:C5:151:ASP:O	2.09	0.52
2:C7:96:ARG:HD3	2:C7:124:ARG:HG2	1.90	0.52
2:C12:146:ALA:HB1	2:C12:151:ASP:O	2.09	0.52
2:D5:177:LEU:HD21	2:D5:191:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D7:177:LEU:HD21	2:D7:191:GLU:HB2	1.91	0.52
2:D9:177:LEU:HD21	2:D9:191:GLU:HB2	1.91	0.52
1:A10:175:TRP:CZ2	2:C10:137:GLU:OE1	2.62	0.52
2:C2:96:ARG:HD3	2:C2:124:ARG:HG2	1.90	0.52
2:C11:146:ALA:HB1	2:C11:151:ASP:O	2.09	0.52
2:D4:177:LEU:HD21	2:D4:191:GLU:HB2	1.91	0.52
1:A12:172:ILE:HD11	1:A12:188:VAL:HG23	1.91	0.52
1:B5:95:THR:HG23	1:B5:96:PRO:CD	2.39	0.52
2:C8:96:ARG:HD3	2:C8:124:ARG:HG2	1.90	0.52
1:A5:172:ILE:HD11	1:A5:188:VAL:HG23	1.91	0.52
1:B4:170:VAL:CG2	2:D4:144:ASN:HD22	2.22	0.52
1:B7:95:THR:CG2	1:B8:176:VAL:HG23	2.24	0.52
1:B8:170:VAL:CG2	2:D8:144:ASN:HD22	2.22	0.52
1:B11:170:VAL:CG1	2:D11:144:ASN:HD22	2.22	0.52
2:C8:166:ILE:HG21	2:C8:234:VAL:HG11	1.92	0.52
2:D2:143:LEU:HD21	2:D2:187:ALA:HB2	1.92	0.52
2:D5:174:VAL:HG13	2:D5:190:TYR:HB3	1.90	0.52
2:D13:143:LEU:HD21	2:D13:187:ALA:HB2	1.92	0.52
1:A2:172:ILE:HD11	1:A2:188:VAL:HG23	1.91	0.52
2:C7:166:ILE:HG21	2:C7:234:VAL:HG11	1.92	0.52
2:C11:99:THR:HG21	2:D11:49:MET:SD	2.48	0.52
2:D8:174:VAL:HG13	2:D8:190:TYR:HB3	1.90	0.52
2:D10:177:LEU:HD21	2:D10:191:GLU:HB2	1.91	0.52
2:D11:143:LEU:HD21	2:D11:187:ALA:HB2	1.92	0.52
1:A9:172:ILE:HD11	1:A9:188:VAL:HG23	1.91	0.52
1:A9:175:TRP:CZ2	2:C9:137:GLU:OE1	2.62	0.52
1:B11:95:THR:HG23	1:B11:96:PRO:CD	2.39	0.52
2:C2:166:ILE:HG21	2:C2:234:VAL:HG11	1.92	0.52
2:C3:166:ILE:HG21	2:C3:234:VAL:HG11	1.92	0.52
2:C10:146:ALA:HB1	2:C10:151:ASP:O	2.09	0.52
2:C11:96:ARG:HD3	2:C11:124:ARG:HG2	1.90	0.52
2:D4:143:LEU:HD21	2:D4:187:ALA:HB2	1.92	0.52
1:A6:172:ILE:HD11	1:A6:188:VAL:HG23	1.91	0.52
1:B5:170:VAL:CG1	2:D5:144:ASN:HD22	2.22	0.52
1:B6:95:THR:CG2	1:B7:176:VAL:HG23	2.24	0.52
1:B13:170:VAL:CG2	2:D13:144:ASN:HD22	2.22	0.52
2:C1:166:ILE:HG21	2:C1:234:VAL:HG11	1.92	0.52
2:C6:96:ARG:HD3	2:C6:124:ARG:HG2	1.90	0.52
2:C9:166:ILE:HG21	2:C9:234:VAL:HG11	1.92	0.52
2:D1:174:VAL:HG13	2:D1:190:TYR:HB3	1.90	0.52
1:B9:187:ARG:NH1	2:D9:204:GLU:CD	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C5:96:ARG:HD3	2:C5:124:ARG:HG2	1.90	0.52
2:C10:99:THR:HG21	2:D10:49:MET:SD	2.48	0.52
2:C12:72:LEU:CD2	3:E12:185:PHE:HB2	2.26	0.52
2:D2:194:ASN:HB3	2:D2:228:GLY:H	1.75	0.52
2:D8:194:ASN:HB3	2:D8:228:GLY:H	1.75	0.52
2:D11:177:LEU:HD21	2:D11:191:GLU:HB2	1.91	0.52
1:B3:187:ARG:NH1	2:D3:204:GLU:CD	2.58	0.52
1:B5:170:VAL:CG2	2:D5:144:ASN:HD22	2.22	0.52
1:B6:170:VAL:CG1	2:D6:144:ASN:HD22	2.22	0.52
1:B12:170:VAL:CG1	2:D12:144:ASN:HD22	2.22	0.52
2:C1:146:ALA:HB1	2:C1:151:ASP:O	2.09	0.52
2:C10:72:LEU:CD1	3:E10:185:PHE:CZ	2.79	0.52
2:D5:194:ASN:HB3	2:D5:228:GLY:H	1.75	0.52
1:B4:187:ARG:NH1	2:D4:204:GLU:CD	2.58	0.51
2:C4:72:LEU:HD22	3:E4:185:PHE:CD1	2.42	0.51
2:C6:166:ILE:HG21	2:C6:234:VAL:HG11	1.92	0.51
1:B4:170:VAL:CG1	2:D4:144:ASN:HD22	2.22	0.51
1:B7:170:VAL:CG2	2:D7:144:ASN:HD22	2.22	0.51
2:C3:72:LEU:HD22	3:E3:185:PHE:CD1	2.42	0.51
2:C5:72:LEU:HD21	3:E5:185:PHE:CB	2.27	0.51
2:C7:146:ALA:HB1	2:C7:151:ASP:O	2.09	0.51
2:C13:166:ILE:HG21	2:C13:234:VAL:HG11	1.92	0.51
2:D3:177:LEU:HD21	2:D3:191:GLU:HB2	1.91	0.51
2:D6:143:LEU:HD21	2:D6:187:ALA:HB2	1.92	0.51
2:D11:183:ASP:OD1	2:D11:183:ASP:N	2.34	0.51
2:D7:194:ASN:HB3	2:D7:228:GLY:H	1.75	0.51
2:D9:143:LEU:HD21	2:D9:187:ALA:HB2	1.92	0.51
2:D10:194:ASN:HB3	2:D10:228:GLY:H	1.75	0.51
2:D13:177:LEU:HD21	2:D13:191:GLU:HB2	1.91	0.51
2:C4:146:ALA:HB1	2:C4:151:ASP:O	2.09	0.51
2:C4:166:ILE:HG21	2:C4:234:VAL:HG11	1.92	0.51
2:C5:72:LEU:HD22	3:E5:185:PHE:CD1	2.42	0.51
2:D2:177:LEU:HD21	2:D2:191:GLU:HB2	1.91	0.51
2:D3:143:LEU:HD21	2:D3:187:ALA:HB2	1.92	0.51
2:D12:194:ASN:HB3	2:D12:228:GLY:H	1.75	0.51
2:D9:194:ASN:HB3	2:D9:228:GLY:H	1.75	0.51
2:D11:194:ASN:HB3	2:D11:228:GLY:H	1.75	0.51
2:D13:194:ASN:HB3	2:D13:228:GLY:H	1.75	0.51
1:B3:170:VAL:CG1	2:D3:144:ASN:HD22	2.22	0.51
1:B7:170:VAL:CG1	2:D7:144:ASN:HD22	2.22	0.51
1:B9:170:VAL:HG22	2:D9:216:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B10:170:VAL:HG22	2:D10:216:MET:SD	2.51	0.51
1:B11:170:VAL:HG22	2:D11:216:MET:SD	2.51	0.51
2:D1:143:LEU:HD21	2:D1:187:ALA:HB2	1.92	0.51
1:B6:170:VAL:CG2	2:D6:144:ASN:HD22	2.22	0.51
1:B8:170:VAL:HG22	2:D8:216:MET:SD	2.51	0.51
1:B10:96:PRO:HG2	1:B11:174:PRO:HB2	1.93	0.51
1:B11:96:PRO:HG2	1:B12:174:PRO:HB2	1.93	0.51
1:B12:170:VAL:HG22	2:D12:216:MET:SD	2.51	0.51
2:C10:166:ILE:HG21	2:C10:234:VAL:HG11	1.92	0.51
2:C11:72:LEU:HD22	3:E11:185:PHE:CD1	2.42	0.51
2:C12:166:ILE:HG21	2:C12:234:VAL:HG11	1.92	0.51
2:D3:194:ASN:HB3	2:D3:228:GLY:H	1.75	0.51
2:D12:177:LEU:HD21	2:D12:191:GLU:HB2	1.91	0.51
1:B3:170:VAL:HG22	2:D3:216:MET:SD	2.51	0.51
2:C2:72:LEU:HD22	3:E2:185:PHE:CD1	2.42	0.51
1:A7:175:TRP:CZ2	2:C7:137:GLU:OE1	2.62	0.51
1:B6:187:ARG:NH1	2:D6:204:GLU:CD	2.58	0.51
1:B12:170:VAL:CG2	2:D12:144:ASN:HD22	2.22	0.51
1:B13:170:VAL:CG1	2:D13:144:ASN:HD22	2.22	0.51
2:D1:177:LEU:HD21	2:D1:191:GLU:HB2	1.91	0.51
2:D1:194:ASN:HB3	2:D1:228:GLY:H	1.75	0.51
2:D8:143:LEU:HD21	2:D8:187:ALA:HB2	1.92	0.51
1:B7:170:VAL:HG22	2:D7:216:MET:SD	2.51	0.51
2:C5:166:ILE:HG21	2:C5:234:VAL:HG11	1.92	0.51
2:D4:194:ASN:HB3	2:D4:228:GLY:H	1.75	0.51
1:B13:170:VAL:HG22	2:D13:216:MET:SD	2.51	0.50
1:B4:170:VAL:HG22	2:D4:216:MET:SD	2.51	0.50
1:B8:170:VAL:CG1	2:D8:144:ASN:HD22	2.22	0.50
2:C11:166:ILE:HG21	2:C11:234:VAL:HG11	1.92	0.50
2:D12:143:LEU:HD21	2:D12:187:ALA:HB2	1.92	0.50
1:A7:170:VAL:CG2	2:C7:216:MET:HB2	2.26	0.50
1:A11:175:TRP:CZ2	2:C11:137:GLU:OE1	2.62	0.50
2:D10:143:LEU:HD21	2:D10:187:ALA:HB2	1.92	0.50
1:A13:175:TRP:CZ2	2:C13:137:GLU:OE1	2.62	0.50
1:B6:170:VAL:HG22	2:D6:216:MET:SD	2.51	0.50
1:B12:96:PRO:HG2	1:B13:174:PRO:HB2	1.93	0.50
1:B5:170:VAL:HG22	2:D5:216:MET:SD	2.51	0.50
1:B9:96:PRO:HG2	1:B10:174:PRO:HB2	1.93	0.50
2:C6:72:LEU:HD22	3:E6:185:PHE:CD1	2.42	0.50
2:C12:72:LEU:HD21	3:E12:185:PHE:CB	2.26	0.50
2:C13:72:LEU:HD22	3:E13:185:PHE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D7:143:LEU:HD21	2:D7:187:ALA:HB2	1.92	0.50
1:A8:160:PRO:HG3	1:B7:189:SER:HB3	1.93	0.50
1:B1:170:VAL:HG22	2:D1:216:MET:SD	2.51	0.50
1:B2:170:VAL:CG1	2:D2:144:ASN:HD22	2.22	0.50
1:B2:170:VAL:HG22	2:D2:216:MET:SD	2.51	0.50
2:D5:143:LEU:HD21	2:D5:187:ALA:HB2	1.92	0.50
2:D6:194:ASN:HB3	2:D6:228:GLY:H	1.75	0.50
1:A3:175:TRP:CZ2	2:C3:137:GLU:OE1	2.62	0.50
1:B8:96:PRO:HG2	1:B9:174:PRO:HB2	1.93	0.50
1:B10:170:VAL:CG1	2:D10:144:ASN:HD22	2.22	0.50
1:A6:160:PRO:HG3	1:B5:189:SER:HG	1.76	0.49
1:A13:160:PRO:HG3	1:B12:189:SER:HB3	1.93	0.49
1:A5:160:PRO:HG3	1:B4:189:SER:HB3	1.93	0.49
1:A13:170:VAL:CG2	2:C13:216:MET:HB2	2.26	0.49
1:B1:170:VAL:CG1	2:D1:144:ASN:HD22	2.22	0.49
1:B2:154:ASN:CB	2:D3:205:GLN:NE2	2.76	0.49
1:B5:154:ASN:CB	2:D6:205:GLN:NE2	2.76	0.49
1:B5:187:ARG:NH1	2:D5:204:GLU:CD	2.58	0.49
1:B7:187:ARG:NH1	2:D7:204:GLU:CD	2.58	0.49
1:B10:154:ASN:CB	2:D11:205:GLN:NE2	2.75	0.49
2:C12:94:THR:OG1	2:C12:98:GLN:HB2	2.12	0.49
1:A7:160:PRO:HG3	1:B6:189:SER:HB3	1.93	0.49
1:B8:95:THR:CG2	1:B9:176:VAL:HG23	2.24	0.49
1:B8:154:ASN:CB	2:D9:205:GLN:NE2	2.76	0.49
1:B9:170:VAL:CG1	2:D9:144:ASN:HD22	2.22	0.49
1:B12:154:ASN:CB	2:D13:205:GLN:NE2	2.76	0.49
1:A2:175:TRP:CZ2	2:C2:137:GLU:OE1	2.62	0.49
1:A5:175:TRP:CZ2	2:C5:137:GLU:OE1	2.62	0.49
1:B6:154:ASN:CB	2:D7:205:GLN:NE2	2.76	0.49
1:B3:154:ASN:CB	2:D4:205:GLN:NE2	2.76	0.49
1:B13:154:ASN:CB	2:D1:205:GLN:NE2	2.76	0.49
2:C13:94:THR:OG1	2:C13:98:GLN:HB2	2.13	0.49
2:D10:183:ASP:OD1	2:D10:183:ASP:N	2.34	0.49
1:A4:175:TRP:CZ2	2:C4:137:GLU:OE1	2.62	0.49
1:B1:154:ASN:CB	2:D2:205:GLN:NE2	2.75	0.49
1:B4:154:ASN:CB	2:D5:205:GLN:NE2	2.76	0.49
1:B11:154:ASN:CB	2:D12:205:GLN:NE2	2.76	0.49
2:C1:94:THR:OG1	2:C1:98:GLN:HB2	2.12	0.49
2:C10:94:THR:OG1	2:C10:98:GLN:HB2	2.13	0.49
2:C11:72:LEU:CD1	3:E11:185:PHE:CZ	2.79	0.49
2:D2:183:ASP:OD1	2:D2:183:ASP:N	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B13:155:PRO:CD	2:D1:205:GLN:HG2	2.39	0.49
2:C5:94:THR:OG1	2:C5:98:GLN:HB2	2.12	0.49
1:B12:95:THR:CG2	1:B12:96:PRO:CD	2.91	0.49
2:C11:94:THR:OG1	2:C11:98:GLN:HB2	2.12	0.49
1:A1:175:TRP:CZ2	2:C1:137:GLU:OE1	2.62	0.48
1:B9:154:ASN:CB	2:D10:205:GLN:NE2	2.76	0.48
1:B13:95:THR:CG2	1:B13:96:PRO:CD	2.91	0.48
2:C4:72:LEU:HD21	3:E4:185:PHE:CB	2.26	0.48
2:C9:94:THR:OG1	2:C9:98:GLN:HB2	2.13	0.48
2:D3:183:ASP:OD1	2:D3:183:ASP:N	2.34	0.48
1:B7:154:ASN:CB	2:D8:205:GLN:NE2	2.76	0.48
1:B11:95:THR:CG2	1:B11:96:PRO:CD	2.91	0.48
2:C4:94:THR:OG1	2:C4:98:GLN:HB2	2.12	0.48
1:B1:95:THR:CG2	1:B1:96:PRO:CD	2.91	0.48
1:B10:95:THR:CG2	1:B10:96:PRO:CD	2.91	0.48
1:A3:160:PRO:HG3	1:B2:189:SER:HB3	1.93	0.48
1:A10:160:PRO:HG3	1:B9:189:SER:HB3	1.93	0.48
2:C1:221:ALA:O	2:C1:222:GLN:HB2	2.14	0.48
2:C4:221:ALA:O	2:C4:222:GLN:HB2	2.14	0.48
2:C7:94:THR:OG1	2:C7:98:GLN:HB2	2.13	0.48
2:C8:221:ALA:O	2:C8:222:GLN:HB2	2.14	0.48
2:C13:221:ALA:O	2:C13:222:GLN:HB2	2.14	0.48
1:A6:175:TRP:CZ2	2:C6:137:GLU:OE1	2.62	0.48
1:B9:95:THR:CG2	1:B9:96:PRO:CD	2.91	0.48
2:C2:94:THR:OG1	2:C2:98:GLN:HB2	2.12	0.48
2:C6:94:THR:OG1	2:C6:98:GLN:HB2	2.13	0.48
1:A11:160:PRO:HG3	1:B10:189:SER:HB3	1.93	0.48
2:C5:58:THR:CG2	2:C5:95:ALA:HB2	2.44	0.48
2:C6:221:ALA:O	2:C6:222:GLN:HB2	2.14	0.48
2:C7:221:ALA:O	2:C7:222:GLN:HB2	2.14	0.48
2:C12:221:ALA:O	2:C12:222:GLN:HB2	2.14	0.48
2:D1:194:ASN:HB2	2:D1:227:GLY:HA2	1.96	0.48
1:B2:95:THR:CG2	1:B2:96:PRO:CD	2.91	0.48
1:B8:95:THR:CG2	1:B8:96:PRO:CD	2.91	0.48
2:C1:58:THR:CG2	2:C1:95:ALA:HB2	2.44	0.48
2:C1:147:VAL:HG22	2:C1:189:ARG:HH11	1.79	0.48
2:C3:58:THR:CG2	2:C3:95:ALA:HB2	2.44	0.48
2:C12:58:THR:CG2	2:C12:95:ALA:HB2	2.44	0.48
2:C13:147:VAL:HG22	2:C13:189:ARG:HH11	1.79	0.48
2:D3:194:ASN:HB2	2:D3:227:GLY:HA2	1.96	0.48
2:D12:194:ASN:HB2	2:D12:227:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B7:95:THR:CG2	1:B7:96:PRO:CD	2.91	0.48
2:C9:221:ALA:O	2:C9:222:GLN:HB2	2.14	0.48
1:A4:160:PRO:HG3	1:B3:189:SER:HB3	1.93	0.48
2:C2:147:VAL:HG22	2:C2:189:ARG:HH11	1.79	0.48
2:C3:147:VAL:HG22	2:C3:189:ARG:HH11	1.79	0.48
2:C7:58:THR:CG2	2:C7:95:ALA:HB2	2.44	0.48
2:C7:72:LEU:CD1	3:E7:185:PHE:CZ	2.79	0.48
2:C8:94:THR:OG1	2:C8:98:GLN:HB2	2.12	0.48
2:C10:58:THR:CG2	2:C10:95:ALA:HB2	2.44	0.48
2:D10:194:ASN:HB2	2:D10:227:GLY:HA2	1.96	0.48
2:D13:194:ASN:HB2	2:D13:227:GLY:HA2	1.96	0.48
2:C4:147:VAL:HG22	2:C4:189:ARG:HH11	1.79	0.47
2:C6:72:LEU:CD1	3:E6:185:PHE:CZ	2.79	0.47
2:C12:147:VAL:HG22	2:C12:189:ARG:HH11	1.79	0.47
2:D2:194:ASN:HB2	2:D2:227:GLY:HA2	1.96	0.47
2:D4:194:ASN:HB2	2:D4:227:GLY:HA2	1.96	0.47
2:D11:194:ASN:HB2	2:D11:227:GLY:HA2	1.96	0.47
1:A10:170:VAL:CG2	2:C10:216:MET:HB2	2.26	0.47
1:B3:95:THR:CG2	1:B3:96:PRO:CD	2.91	0.47
2:C2:221:ALA:O	2:C2:222:GLN:HB2	2.14	0.47
2:C3:221:ALA:O	2:C3:222:GLN:HB2	2.14	0.47
2:C11:221:ALA:O	2:C11:222:GLN:HB2	2.14	0.47
1:B6:95:THR:CG2	1:B6:96:PRO:CD	2.91	0.47
1:B12:155:PRO:CD	2:D13:205:GLN:HG2	2.39	0.47
2:C4:35:GLY:HA3	2:D4:27:PRO:CG	2.45	0.47
2:C5:35:GLY:HA3	2:D5:27:PRO:CG	2.45	0.47
2:C8:58:THR:CG2	2:C8:95:ALA:HB2	2.44	0.47
2:C13:58:THR:CG2	2:C13:95:ALA:HB2	2.44	0.47
2:D9:194:ASN:HB2	2:D9:227:GLY:HA2	1.96	0.47
1:A9:174:PRO:HD3	1:A9:185:PRO:HD3	1.97	0.47
1:B4:95:THR:CG2	1:B4:96:PRO:CD	2.91	0.47
1:B4:155:PRO:CD	2:D5:205:GLN:HG2	2.39	0.47
1:B5:95:THR:CG2	1:B5:96:PRO:CD	2.91	0.47
2:C5:221:ALA:O	2:C5:222:GLN:HB2	2.14	0.47
2:C6:35:GLY:HA3	2:D6:27:PRO:CG	2.45	0.47
2:C11:147:VAL:HG22	2:C11:189:ARG:HH11	1.79	0.47
2:D5:128:ARG:HG3	2:D5:128:ARG:O	2.15	0.47
1:A1:197:TRP:CZ2	1:B13:190:PHE:HA	2.50	0.47
1:A2:160:PRO:HG3	1:B1:189:SER:HB3	1.93	0.47
1:A4:174:PRO:HD3	1:A4:185:PRO:HD3	1.97	0.47
1:B3:96:PRO:HG2	1:B4:174:PRO:HB2	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C3:35:GLY:HA3	2:D3:27:PRO:CG	2.45	0.47
2:C3:94:THR:OG1	2:C3:98:GLN:HB2	2.12	0.47
2:C5:72:LEU:CD1	3:E5:185:PHE:CZ	2.79	0.47
2:C10:221:ALA:O	2:C10:222:GLN:HB2	2.14	0.47
2:D5:194:ASN:HB2	2:D5:227:GLY:HA2	1.96	0.47
2:D6:194:ASN:HB2	2:D6:227:GLY:HA2	1.96	0.47
2:D8:128:ARG:HG3	2:D8:128:ARG:O	2.15	0.47
1:A1:174:PRO:HD3	1:A1:185:PRO:HD3	1.97	0.47
1:A2:174:PRO:HD3	1:A2:185:PRO:HD3	1.97	0.47
1:A2:197:TRP:CZ2	1:B1:190:PHE:HA	2.50	0.47
1:A7:174:PRO:HD3	1:A7:185:PRO:HD3	1.97	0.47
1:A8:197:TRP:CZ2	1:B7:190:PHE:HA	2.50	0.47
1:A11:174:PRO:HD3	1:A11:185:PRO:HD3	1.97	0.47
1:A12:197:TRP:CZ2	1:B11:190:PHE:HA	2.50	0.47
1:A13:197:TRP:CZ2	1:B12:190:PHE:HA	2.50	0.47
1:B3:155:PRO:CD	2:D4:205:GLN:HG2	2.39	0.47
2:C2:58:THR:CG2	2:C2:95:ALA:HB2	2.44	0.47
2:C4:58:THR:CG2	2:C4:95:ALA:HB2	2.44	0.47
2:C6:58:THR:CG2	2:C6:95:ALA:HB2	2.44	0.47
2:C7:35:GLY:HA3	2:D7:27:PRO:CG	2.45	0.47
2:C9:58:THR:CG2	2:C9:95:ALA:HB2	2.44	0.47
2:C11:58:THR:CG2	2:C11:95:ALA:HB2	2.44	0.47
2:C12:35:GLY:HA3	2:D12:27:PRO:CG	2.45	0.47
2:C13:35:GLY:HA3	2:D13:27:PRO:CG	2.45	0.47
2:D2:128:ARG:HG3	2:D2:128:ARG:O	2.15	0.47
2:D7:194:ASN:HB2	2:D7:227:GLY:HA2	1.96	0.47
2:D8:194:ASN:HB2	2:D8:227:GLY:HA2	1.96	0.47
2:D9:128:ARG:HG3	2:D9:128:ARG:O	2.15	0.47
1:A6:174:PRO:HD3	1:A6:185:PRO:HD3	1.97	0.47
1:A6:197:TRP:CZ2	1:B5:190:PHE:HA	2.50	0.47
1:A9:197:TRP:CZ2	1:B8:190:PHE:HA	2.50	0.47
1:B2:96:PRO:HG2	1:B3:174:PRO:HB2	1.93	0.47
1:B4:96:PRO:HG2	1:B5:174:PRO:HB2	1.93	0.47
2:C11:35:GLY:HA3	2:D11:27:PRO:CG	2.45	0.47
2:D12:128:ARG:HG3	2:D12:128:ARG:O	2.15	0.47
2:D13:128:ARG:HG3	2:D13:128:ARG:O	2.15	0.47
1:A5:197:TRP:CZ2	1:B4:190:PHE:HA	2.50	0.47
1:A13:174:PRO:HD3	1:A13:185:PRO:HD3	1.97	0.47
1:B5:155:PRO:CD	2:D6:205:GLN:HG2	2.39	0.47
2:D6:128:ARG:HG3	2:D6:128:ARG:O	2.15	0.47
1:A4:170:VAL:CG2	2:C4:216:MET:HB2	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:170:VAL:CG2	2:C5:216:MET:HB2	2.26	0.47
1:A8:170:VAL:CG2	2:C8:216:MET:HB2	2.26	0.47
1:A9:160:PRO:HG3	1:B8:189:SER:HB3	1.93	0.47
2:C1:35:GLY:HA3	2:D1:27:PRO:CG	2.45	0.47
2:C4:72:LEU:CD1	3:E4:185:PHE:CZ	2.79	0.47
2:C10:147:VAL:HG22	2:C10:189:ARG:HH11	1.79	0.47
1:A3:170:VAL:CG2	2:C3:216:MET:HB2	2.26	0.46
1:A4:197:TRP:CZ2	1:B3:190:PHE:HA	2.50	0.46
1:A11:197:TRP:CZ2	1:B10:190:PHE:HA	2.50	0.46
2:C2:35:GLY:HA3	2:D2:27:PRO:CG	2.45	0.46
2:C5:147:VAL:HG22	2:C5:189:ARG:HH11	1.79	0.46
2:C10:35:GLY:HA3	2:D10:27:PRO:CG	2.45	0.46
2:C13:72:LEU:CD1	3:E13:185:PHE:CZ	2.79	0.46
2:D6:70:LYS:HE3	2:D6:70:LYS:HB2	1.73	0.46
2:D9:183:ASP:OD1	2:D9:183:ASP:N	2.34	0.46
1:A1:160:PRO:HG3	1:B13:189:SER:HB3	1.93	0.46
1:A10:197:TRP:CZ2	1:B9:190:PHE:HA	2.50	0.46
1:A12:160:PRO:HG3	1:B11:189:SER:HB3	1.93	0.46
1:A12:174:PRO:HD3	1:A12:185:PRO:HD3	1.97	0.46
2:D4:128:ARG:HG3	2:D4:128:ARG:O	2.15	0.46
1:A3:174:PRO:HD3	1:A3:185:PRO:HD3	1.97	0.46
2:C8:35:GLY:HA3	2:D8:27:PRO:CG	2.45	0.46
2:C8:147:VAL:HG22	2:C8:189:ARG:HH11	1.79	0.46
1:A8:174:PRO:HD3	1:A8:185:PRO:HD3	1.97	0.46
2:C9:35:GLY:HA3	2:D9:27:PRO:CG	2.45	0.46
2:C9:147:VAL:HG22	2:C9:189:ARG:HH11	1.79	0.46
2:D3:128:ARG:HG3	2:D3:128:ARG:O	2.15	0.46
2:D10:128:ARG:HG3	2:D10:128:ARG:O	2.15	0.46
1:A3:197:TRP:CZ2	1:B2:190:PHE:HA	2.50	0.46
1:A6:160:PRO:HG3	1:B5:189:SER:HB3	1.93	0.46
1:A7:197:TRP:CZ2	1:B6:190:PHE:HA	2.50	0.46
1:A10:174:PRO:HD3	1:A10:185:PRO:HD3	1.97	0.46
1:B1:96:PRO:HG2	1:B2:174:PRO:HB2	1.93	0.46
1:B2:155:PRO:CD	2:D3:205:GLN:HG2	2.39	0.46
1:B10:155:PRO:CD	2:D11:205:GLN:HG2	2.39	0.46
2:C7:147:VAL:HG22	2:C7:189:ARG:HH11	1.79	0.46
2:D7:128:ARG:O	2:D7:128:ARG:HG3	2.15	0.46
1:B5:96:PRO:HG2	1:B6:174:PRO:HB2	1.93	0.46
2:D1:128:ARG:HG3	2:D1:128:ARG:O	2.15	0.46
2:D11:128:ARG:HG3	2:D11:128:ARG:O	2.15	0.46
1:A12:170:VAL:CG2	2:C12:216:MET:HB2	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C5:143:LEU:HD13	2:C5:143:LEU:HA	1.79	0.46
2:C10:203:ARG:HB3	2:C10:205:GLN:HG2	1.98	0.46
1:B6:155:PRO:CD	2:D7:205:GLN:HG2	2.39	0.46
1:B11:95:THR:HG22	1:B11:96:PRO:HD3	1.98	0.46
1:B12:95:THR:HG22	1:B12:96:PRO:HD3	1.98	0.46
2:C3:72:LEU:HD21	3:E3:185:PHE:CB	2.27	0.46
2:C8:203:ARG:HB3	2:C8:205:GLN:HG2	1.98	0.46
1:A5:174:PRO:HD3	1:A5:185:PRO:HD3	1.97	0.46
2:C1:143:LEU:HD13	2:C1:143:LEU:HA	1.79	0.46
1:B1:96:PRO:HG3	1:B2:182:PHE:CZ	2.51	0.45
1:B6:96:PRO:HG3	1:B7:182:PHE:CZ	2.52	0.45
1:B7:96:PRO:HG2	1:B8:174:PRO:HB2	1.93	0.45
2:C9:203:ARG:HB3	2:C9:205:GLN:HG2	1.98	0.45
2:C12:203:ARG:HB3	2:C12:205:GLN:HG2	1.98	0.45
1:A3:160:PRO:CB	1:B2:189:SER:OG	2.65	0.45
1:A7:160:PRO:CB	1:B6:189:SER:OG	2.65	0.45
1:B8:96:PRO:HG3	1:B9:182:PHE:CZ	2.51	0.45
2:C11:203:ARG:HB3	2:C11:205:GLN:HG2	1.98	0.45
2:C12:72:LEU:CD1	3:E12:185:PHE:CZ	2.79	0.45
1:B4:96:PRO:HG3	1:B5:182:PHE:CZ	2.52	0.45
1:B11:96:PRO:HG3	1:B12:182:PHE:CZ	2.51	0.45
1:B12:96:PRO:HG3	1:B13:182:PHE:CZ	2.52	0.45
2:C6:147:VAL:HG22	2:C6:189:ARG:HH11	1.79	0.45
2:C6:203:ARG:HB3	2:C6:205:GLN:HG2	1.98	0.45
2:D7:70:LYS:HB2	2:D7:70:LYS:HE3	1.73	0.45
1:A6:160:PRO:CB	1:B5:189:SER:OG	2.65	0.45
1:A8:160:PRO:CB	1:B7:189:SER:OG	2.65	0.45
1:A10:160:PRO:CB	1:B9:189:SER:OG	2.65	0.45
1:A13:160:PRO:CB	1:B12:189:SER:OG	2.65	0.45
1:B3:96:PRO:HG3	1:B4:182:PHE:CZ	2.51	0.45
1:B9:155:PRO:CD	2:D10:205:GLN:HG2	2.39	0.45
1:B11:155:PRO:CD	2:D12:205:GLN:HG2	2.39	0.45
2:C7:203:ARG:HB3	2:C7:205:GLN:HG2	1.98	0.45
2:C12:81:THR:HB	3:F11:178:GLY:O	2.17	0.45
2:C13:81:THR:HB	3:F12:178:GLY:O	2.17	0.45
1:A10:160:PRO:HG3	1:B9:189:SER:HG	1.77	0.45
1:B10:96:PRO:HG3	1:B11:182:PHE:CZ	2.51	0.45
2:C1:81:THR:HB	3:F13:178:GLY:O	2.17	0.45
2:C13:203:ARG:HB3	2:C13:205:GLN:HG2	1.98	0.45
2:D1:63:PRO:HD3	2:D1:89:THR:O	2.17	0.45
2:D2:70:LYS:HE3	2:D2:70:LYS:HB2	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D12:63:PRO:HD3	2:D12:89:THR:O	2.17	0.45
2:D13:63:PRO:HD3	2:D13:89:THR:O	2.17	0.45
1:A11:160:PRO:CB	1:B10:189:SER:OG	2.65	0.45
1:B9:96:PRO:HG3	1:B10:182:PHE:CZ	2.52	0.45
1:B13:95:THR:HG22	1:B13:96:PRO:HD3	1.98	0.45
2:D11:63:PRO:HD3	2:D11:89:THR:O	2.17	0.45
1:A1:160:PRO:CB	1:B13:189:SER:OG	2.65	0.45
2:C1:203:ARG:HB3	2:C1:205:GLN:HG2	1.98	0.45
2:C11:81:THR:HB	3:F10:178:GLY:O	2.17	0.45
2:D2:63:PRO:HD3	2:D2:89:THR:O	2.17	0.45
2:D7:63:PRO:HD3	2:D7:89:THR:O	2.17	0.45
1:A5:160:PRO:CB	1:B4:189:SER:OG	2.65	0.45
1:B1:174:PRO:HB2	1:B13:96:PRO:HG2	1.93	0.45
1:B1:182:PHE:CZ	1:B13:96:PRO:HG3	2.52	0.45
1:B5:96:PRO:HG3	1:B6:182:PHE:CZ	2.51	0.45
2:C2:81:THR:HB	3:F1:178:GLY:O	2.17	0.45
1:A2:170:VAL:CG2	2:C2:216:MET:HB2	2.26	0.45
1:B2:96:PRO:HG3	1:B3:182:PHE:CZ	2.51	0.45
1:B6:96:PRO:HG2	1:B7:174:PRO:HB2	1.93	0.45
2:D6:63:PRO:HD3	2:D6:89:THR:O	2.17	0.45
2:D10:63:PRO:HD3	2:D10:89:THR:O	2.17	0.45
1:A2:160:PRO:CB	1:B1:189:SER:OG	2.65	0.45
1:A4:160:PRO:CB	1:B3:189:SER:OG	2.65	0.45
1:B7:95:THR:HG22	1:B7:96:PRO:HD3	1.98	0.45
1:B7:96:PRO:HG3	1:B8:182:PHE:CZ	2.52	0.45
2:C4:203:ARG:HB3	2:C4:205:GLN:HG2	1.98	0.45
2:C5:203:ARG:HB3	2:C5:205:GLN:HG2	1.98	0.45
2:C9:143:LEU:HA	2:C9:143:LEU:HD13	1.79	0.45
2:D3:63:PRO:HD3	2:D3:89:THR:O	2.17	0.45
2:D9:167:ARG:HB2	2:D9:209:LYS:NZ	2.33	0.45
2:D12:110:GLU:H	2:D12:110:GLU:HG3	1.62	0.45
1:A9:160:PRO:CB	1:B8:189:SER:OG	2.65	0.44
1:A12:160:PRO:CB	1:B11:189:SER:OG	2.65	0.44
2:C10:81:THR:HB	3:F9:178:GLY:O	2.17	0.44
2:C10:27:PRO:HG3	2:D9:34:GLN:O	2.18	0.44
2:D2:167:ARG:HB2	2:D2:209:LYS:NZ	2.33	0.44
2:D8:183:ASP:OD1	2:D8:183:ASP:N	2.34	0.44
2:D11:70:LYS:HB2	2:D11:70:LYS:HE3	1.73	0.44
2:D11:167:ARG:HB2	2:D11:209:LYS:NZ	2.33	0.44
2:C2:203:ARG:HB3	2:C2:205:GLN:HG2	1.98	0.44
2:C3:81:THR:HB	3:F2:178:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C3:203:ARG:HB3	2:C3:205:GLN:HG2	1.98	0.44
2:D4:63:PRO:HD3	2:D4:89:THR:O	2.17	0.44
2:D12:167:ARG:HB2	2:D12:209:LYS:NZ	2.33	0.44
1:B1:155:PRO:CD	2:D2:205:GLN:HG2	2.39	0.44
1:B7:155:PRO:CD	2:D8:205:GLN:HG2	2.39	0.44
2:C1:27:PRO:HG3	2:D13:34:GLN:O	2.18	0.44
2:C9:81:THR:HB	3:F8:178:GLY:O	2.17	0.44
2:C12:27:PRO:HG3	2:D11:34:GLN:O	2.18	0.44
2:D9:63:PRO:HD3	2:D9:89:THR:O	2.17	0.44
2:D9:224:LEU:HD23	2:D9:224:LEU:HA	1.92	0.44
2:D10:167:ARG:HB2	2:D10:209:LYS:NZ	2.33	0.44
1:B8:155:PRO:CD	2:D9:205:GLN:HG2	2.39	0.44
2:D8:30:ILE:HG13	2:D8:116:LEU:HD13	2.00	0.44
1:B3:95:THR:HG22	1:B3:96:PRO:HD3	1.98	0.44
2:C4:81:THR:HB	3:F3:178:GLY:O	2.17	0.44
2:C5:27:PRO:HG3	2:D4:34:GLN:O	2.18	0.44
2:C7:81:THR:HB	3:F6:178:GLY:O	2.17	0.44
2:C8:27:PRO:HG3	2:D7:34:GLN:O	2.18	0.44
2:C11:27:PRO:HG3	2:D10:34:GLN:O	2.18	0.44
2:D8:63:PRO:HD3	2:D8:89:THR:O	2.17	0.44
2:D13:167:ARG:HB2	2:D13:209:LYS:NZ	2.33	0.44
1:B1:95:THR:HG22	1:B1:96:PRO:HD3	1.98	0.44
2:C1:72:LEU:CD1	3:E1:185:PHE:CZ	2.79	0.44
2:C4:27:PRO:HG3	2:D3:34:GLN:O	2.18	0.44
2:C6:27:PRO:HG3	2:D5:34:GLN:O	2.18	0.44
2:C6:81:THR:HB	3:F5:178:GLY:O	2.17	0.44
2:C8:81:THR:HB	3:F7:178:GLY:O	2.17	0.44
2:D7:30:ILE:HG13	2:D7:116:LEU:HD13	2.00	0.44
2:D9:30:ILE:HG13	2:D9:116:LEU:HD13	2.00	0.44
2:C6:74:ARG:CB	2:D5:93:GLU:OE2	2.53	0.44
2:C13:27:PRO:HG3	2:D12:34:GLN:O	2.18	0.44
2:D1:167:ARG:HB2	2:D1:209:LYS:NZ	2.33	0.44
2:D4:167:ARG:HB2	2:D4:209:LYS:NZ	2.33	0.44
2:D10:30:ILE:HG13	2:D10:116:LEU:HD13	2.00	0.44
2:C5:81:THR:HB	3:F4:178:GLY:O	2.17	0.44
2:D4:50:ILE:HG23	2:D4:116:LEU:HD23	2.00	0.44
2:D6:50:ILE:HG23	2:D6:116:LEU:HD23	2.00	0.44
2:D7:50:ILE:HG23	2:D7:116:LEU:HD23	2.00	0.44
2:C9:27:PRO:HG3	2:D8:34:GLN:O	2.18	0.43
2:C9:138:LYS:HE3	2:C9:138:LYS:HB3	1.85	0.43
2:D3:50:ILE:HG23	2:D3:116:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D6:30:ILE:HG13	2:D6:116:LEU:HD13	2.00	0.43
2:D7:167:ARG:HB2	2:D7:209:LYS:NZ	2.33	0.43
2:D8:50:ILE:HG23	2:D8:116:LEU:HD23	2.00	0.43
2:C3:27:PRO:HG3	2:D2:34:GLN:O	2.18	0.43
2:C9:74:ARG:CB	2:D8:93:GLU:OE2	2.53	0.43
2:D8:167:ARG:HB2	2:D8:209:LYS:NZ	2.33	0.43
2:D10:70:LYS:HE3	2:D10:70:LYS:HB2	1.73	0.43
2:D12:225:MET:HB3	2:D12:226:GLY:H	1.66	0.43
1:A10:181:ALA:HB1	1:B10:188:VAL:CG2	2.49	0.43
1:B4:95:THR:HG22	1:B4:96:PRO:HD3	1.98	0.43
1:B5:95:THR:HG22	1:B5:96:PRO:HD3	1.98	0.43
1:B6:95:THR:HG22	1:B6:96:PRO:HD3	1.98	0.43
2:C7:27:PRO:HG3	2:D6:34:GLN:O	2.18	0.43
2:D5:50:ILE:HG23	2:D5:116:LEU:HD23	2.00	0.43
2:D6:167:ARG:HB2	2:D6:209:LYS:NZ	2.33	0.43
2:D13:70:LYS:HE3	2:D13:70:LYS:HB2	1.73	0.43
1:A11:181:ALA:HB1	1:B11:188:VAL:CG2	2.49	0.43
1:B8:95:THR:HG22	1:B8:96:PRO:HD3	1.98	0.43
2:C2:74:ARG:CB	2:D1:93:GLU:OE2	2.53	0.43
2:C11:138:LYS:HE3	2:C11:138:LYS:HB3	1.85	0.43
2:D5:63:PRO:HD3	2:D5:89:THR:O	2.17	0.43
2:D11:30:ILE:HG13	2:D11:116:LEU:HD13	2.00	0.43
2:D13:30:ILE:HG13	2:D13:116:LEU:HD13	2.00	0.43
1:A9:181:ALA:HB1	1:B9:188:VAL:CG2	2.49	0.43
1:B11:187:ARG:NH1	2:D11:204:GLU:CD	2.58	0.43
2:C5:29:THR:HG22	2:C5:115:ARG:HE	1.84	0.43
2:C10:143:LEU:HD13	2:C10:143:LEU:HA	1.79	0.43
2:C10:190:TYR:HE2	2:C10:234:VAL:HG22	1.84	0.43
2:D2:50:ILE:HG23	2:D2:116:LEU:HD23	2.00	0.43
2:D5:167:ARG:HB2	2:D5:209:LYS:NZ	2.33	0.43
1:A3:174:PRO:HA	1:A3:183:HIS:O	2.19	0.43
1:A4:181:ALA:HB1	1:B4:188:VAL:CG2	2.49	0.43
1:A12:181:ALA:HB1	1:B12:188:VAL:CG2	2.49	0.43
1:A13:174:PRO:HA	1:A13:183:HIS:O	2.19	0.43
2:C4:190:TYR:HE2	2:C4:234:VAL:HG22	1.84	0.43
2:C6:29:THR:HG22	2:C6:115:ARG:HE	1.84	0.43
2:D1:30:ILE:HG13	2:D1:116:LEU:HD13	2.00	0.43
2:D1:161:PRO:HG2	2:D1:176:PRO:HB2	2.01	0.43
2:D5:30:ILE:HG13	2:D5:116:LEU:HD13	1.99	0.43
2:D10:224:LEU:HD23	2:D10:224:LEU:HA	1.92	0.43
2:D12:30:ILE:HG13	2:D12:116:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D13:161:PRO:HG2	2:D13:176:PRO:HB2	2.01	0.43
1:A12:174:PRO:HA	1:A12:183:HIS:O	2.19	0.43
2:C13:29:THR:HG22	2:C13:115:ARG:HE	1.84	0.43
2:C13:190:TYR:HE2	2:C13:234:VAL:HG22	1.84	0.43
2:D3:167:ARG:HB2	2:D3:209:LYS:NZ	2.33	0.43
2:D6:66:MET:HE3	2:D6:86:ARG:HH21	1.84	0.43
2:D9:50:ILE:HG23	2:D9:116:LEU:HD23	2.00	0.43
2:D12:161:PRO:HG2	2:D12:176:PRO:HB2	2.01	0.43
1:A3:181:ALA:HB1	1:B3:188:VAL:CG2	2.49	0.43
1:A4:197:TRP:HZ2	1:B3:190:PHE:HA	1.84	0.43
1:A5:181:ALA:HB1	1:B5:188:VAL:CG2	2.49	0.43
1:A10:192:VAL:HG21	2:C10:148:LEU:HD23	2.01	0.43
1:A12:160:PRO:HG3	1:B11:189:SER:HG	1.81	0.43
2:C1:190:TYR:HE2	2:C1:234:VAL:HG22	1.84	0.43
2:C2:27:PRO:HG3	2:D1:34:GLN:O	2.18	0.43
2:C7:190:TYR:HE2	2:C7:234:VAL:HG22	1.84	0.43
2:C9:29:THR:HG22	2:C9:115:ARG:HE	1.84	0.43
2:C9:30:ILE:HB	2:C9:116:LEU:HD13	2.01	0.43
2:C10:30:ILE:HB	2:C10:116:LEU:HD13	2.01	0.43
2:D2:161:PRO:HG2	2:D2:176:PRO:HB2	2.01	0.43
1:A2:174:PRO:HA	1:A2:183:HIS:O	2.19	0.43
1:A4:160:PRO:HG3	1:B3:189:SER:HG	1.79	0.43
1:A8:181:ALA:HB1	1:B8:188:VAL:CG2	2.49	0.43
1:A11:170:VAL:CG2	2:C11:216:MET:HB2	2.26	0.43
1:B9:95:THR:HG22	1:B9:96:PRO:HD3	1.98	0.43
2:C2:29:THR:HG22	2:C2:115:ARG:HE	1.84	0.43
2:C5:190:TYR:HE2	2:C5:234:VAL:HG22	1.84	0.43
2:C7:30:ILE:HB	2:C7:116:LEU:HD13	2.01	0.43
2:C8:30:ILE:HB	2:C8:116:LEU:HD13	2.01	0.43
2:C10:29:THR:HG22	2:C10:115:ARG:HE	1.84	0.43
1:A7:197:TRP:HZ2	1:B6:190:PHE:HA	1.84	0.43
1:A10:203:VAL:HG21	2:C9:208:TRP:CD2	2.54	0.43
1:A13:203:VAL:HG21	2:C12:208:TRP:CD2	2.54	0.43
2:C11:30:ILE:HB	2:C11:116:LEU:HD13	2.01	0.43
2:C12:29:THR:HG22	2:C12:115:ARG:HE	1.84	0.43
2:D1:70:LYS:HE3	2:D1:70:LYS:HB2	1.73	0.43
2:D11:161:PRO:HG2	2:D11:176:PRO:HB2	2.01	0.43
1:A1:181:ALA:HB1	1:B1:188:VAL:CG2	2.49	0.42
1:A1:197:TRP:HZ2	1:B13:190:PHE:HA	1.84	0.42
1:A2:203:VAL:HG21	2:C1:208:TRP:CD2	2.54	0.42
1:A10:197:TRP:HZ2	1:B9:190:PHE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A11:192:VAL:HG21	2:C11:148:LEU:HD23	2.01	0.42
1:A12:192:VAL:HG21	2:C12:148:LEU:HD23	2.01	0.42
2:C2:138:LYS:HE3	2:C2:138:LYS:HB3	1.85	0.42
2:C6:30:ILE:HB	2:C6:116:LEU:HD13	2.01	0.42
2:C8:143:LEU:HD13	2:C8:143:LEU:HA	1.79	0.42
2:D1:50:ILE:HG23	2:D1:116:LEU:HD23	2.00	0.42
2:D2:30:ILE:HG13	2:D2:116:LEU:HD13	2.00	0.42
1:A2:181:ALA:HB1	1:B2:188:VAL:CG2	2.49	0.42
1:A6:181:ALA:HB1	1:B6:188:VAL:CG2	2.49	0.42
1:A7:160:PRO:HG3	1:B6:189:SER:HG	1.83	0.42
1:A8:192:VAL:HG21	2:C8:148:LEU:HD23	2.01	0.42
1:A9:192:VAL:HG21	2:C9:148:LEU:HD23	2.01	0.42
1:A12:197:TRP:HZ2	1:B11:190:PHE:HA	1.84	0.42
1:A13:181:ALA:HB1	1:B13:188:VAL:CG2	2.49	0.42
2:C1:74:ARG:CB	2:D13:93:GLU:OE2	2.53	0.42
2:C6:190:TYR:HE2	2:C6:234:VAL:HG22	1.84	0.42
2:D4:30:ILE:HG13	2:D4:116:LEU:HD13	2.00	0.42
1:A7:181:ALA:HB1	1:B7:188:VAL:CG2	2.49	0.42
1:B13:187:ARG:NH1	2:D13:204:GLU:CD	2.58	0.42
2:C4:118:SER:OG	2:C4:159:VAL:HG12	2.20	0.42
2:C8:29:THR:HG22	2:C8:115:ARG:HE	1.84	0.42
2:C9:190:TYR:HE2	2:C9:234:VAL:HG22	1.84	0.42
2:C11:29:THR:HG22	2:C11:115:ARG:HE	1.84	0.42
2:C11:190:TYR:HE2	2:C11:234:VAL:HG22	1.84	0.42
2:D3:161:PRO:HG2	2:D3:176:PRO:HB2	2.01	0.42
2:D10:50:ILE:HG23	2:D10:116:LEU:HD23	2.00	0.42
2:D11:209:LYS:O	2:D11:210:PRO:C	2.58	0.42
1:A4:192:VAL:HG21	2:C4:148:LEU:HD23	2.01	0.42
1:A7:203:VAL:HG21	2:C6:208:TRP:CD2	2.54	0.42
1:A8:203:VAL:HG21	2:C7:208:TRP:CD2	2.54	0.42
1:B12:96:PRO:HG3	1:B13:182:PHE:HZ	1.85	0.42
2:C3:118:SER:OG	2:C3:159:VAL:HG12	2.20	0.42
2:C4:29:THR:HG22	2:C4:115:ARG:HE	1.84	0.42
2:C5:30:ILE:HB	2:C5:116:LEU:HD13	2.01	0.42
2:C5:118:SER:OG	2:C5:159:VAL:HG12	2.20	0.42
2:C8:190:TYR:HE2	2:C8:234:VAL:HG22	1.84	0.42
2:D1:209:LYS:O	2:D1:210:PRO:C	2.58	0.42
1:A10:174:PRO:HA	1:A10:183:HIS:O	2.19	0.42
1:A12:203:VAL:HG21	2:C11:208:TRP:CD2	2.54	0.42
1:B1:182:PHE:HZ	1:B13:96:PRO:HG3	1.85	0.42
1:B2:95:THR:HG22	1:B2:96:PRO:HD3	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C3:190:TYR:HE2	2:C3:234:VAL:HG22	1.84	0.42
2:C6:118:SER:OG	2:C6:159:VAL:HG12	2.20	0.42
2:C11:118:SER:OG	2:C11:159:VAL:HG12	2.20	0.42
2:D1:110:GLU:H	2:D1:110:GLU:HG3	1.62	0.42
2:D9:209:LYS:O	2:D9:210:PRO:C	2.58	0.42
1:A1:174:PRO:HA	1:A1:183:HIS:O	2.19	0.42
1:A3:192:VAL:HG21	2:C3:148:LEU:HD23	2.01	0.42
1:A5:192:VAL:HG21	2:C5:148:LEU:HD23	2.01	0.42
1:A13:192:VAL:HG21	2:C13:148:LEU:HD23	2.01	0.42
1:B4:199:LEU:HD21	1:B5:182:PHE:CE2	2.55	0.42
2:C2:118:SER:OG	2:C2:159:VAL:HG12	2.20	0.42
2:C2:190:TYR:HE2	2:C2:234:VAL:HG22	1.84	0.42
2:C4:30:ILE:HB	2:C4:116:LEU:HD13	2.01	0.42
2:C10:118:SER:OG	2:C10:159:VAL:HG12	2.20	0.42
2:C12:138:LYS:HE3	2:C12:138:LYS:HB3	1.85	0.42
2:C12:190:TYR:HE2	2:C12:234:VAL:HG22	1.84	0.42
2:D3:30:ILE:HG13	2:D3:116:LEU:HD13	2.00	0.42
2:D6:225:MET:HB3	2:D6:226:GLY:H	1.66	0.42
2:D10:161:PRO:HG2	2:D10:176:PRO:HB2	2.01	0.42
2:D11:50:ILE:HG23	2:D11:116:LEU:HD23	2.00	0.42
2:D13:50:ILE:HG23	2:D13:116:LEU:HD23	2.00	0.42
1:A4:174:PRO:HA	1:A4:183:HIS:O	2.19	0.42
1:A5:174:PRO:HA	1:A5:183:HIS:O	2.19	0.42
1:A5:203:VAL:HG21	2:C4:208:TRP:CD2	2.54	0.42
1:A9:203:VAL:HG21	2:C8:208:TRP:CD2	2.54	0.42
2:C12:30:ILE:HB	2:C12:116:LEU:HD13	2.01	0.42
2:D1:32:LEU:HA	2:D1:33:PRO:HD3	1.93	0.42
2:D3:70:LYS:HB2	2:D3:70:LYS:HE3	1.73	0.42
2:D3:209:LYS:HE2	2:D3:209:LYS:HB2	1.87	0.42
2:D7:110:GLU:H	2:D7:110:GLU:HG3	1.62	0.42
2:D8:161:PRO:HG2	2:D8:176:PRO:HB2	2.01	0.42
2:D8:209:LYS:O	2:D8:210:PRO:C	2.58	0.42
1:A2:192:VAL:HG21	2:C2:148:LEU:HD23	2.01	0.42
1:A4:203:VAL:HG21	2:C3:208:TRP:CD2	2.54	0.42
1:A5:197:TRP:HZ2	1:B4:190:PHE:HA	1.84	0.42
1:A6:170:VAL:CG2	2:C6:216:MET:HB2	2.26	0.42
1:A7:174:PRO:HA	1:A7:183:HIS:O	2.19	0.42
1:A8:174:PRO:HA	1:A8:183:HIS:O	2.19	0.42
2:C1:29:THR:HG22	2:C1:115:ARG:HE	1.84	0.42
2:C1:118:SER:OG	2:C1:159:VAL:HG12	2.20	0.42
2:D3:209:LYS:O	2:D3:210:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:161:PRO:HG2	2:D4:176:PRO:HB2	2.01	0.42
2:D5:202:LEU:HD12	2:D5:221:ALA:HA	2.02	0.42
2:D8:129:LYS:HD3	2:D8:129:LYS:HA	1.88	0.42
2:D9:161:PRO:HG2	2:D9:176:PRO:HB2	2.01	0.42
2:D12:32:LEU:HA	2:D12:33:PRO:HD3	1.93	0.42
2:D12:50:ILE:HG23	2:D12:116:LEU:HD23	2.00	0.42
2:D13:202:LEU:HD12	2:D13:221:ALA:HA	2.02	0.42
2:D13:209:LYS:O	2:D13:210:PRO:C	2.58	0.42
1:A2:160:PRO:HG3	1:B1:189:SER:HG	1.81	0.42
1:A3:203:VAL:HG21	2:C2:208:TRP:CD2	2.54	0.42
1:A6:192:VAL:HG21	2:C6:148:LEU:HD23	2.01	0.42
1:A6:203:VAL:HG21	2:C5:208:TRP:CD2	2.54	0.42
1:A9:174:PRO:HA	1:A9:183:HIS:O	2.19	0.42
1:A9:197:TRP:HZ2	1:B8:190:PHE:HA	1.84	0.42
2:C3:128:ARG:HB2	2:C3:183:ASP:OD2	2.20	0.42
2:C3:138:LYS:HE3	2:C3:138:LYS:HB3	1.85	0.42
2:C4:138:LYS:HE3	2:C4:138:LYS:HB3	1.85	0.42
2:C6:128:ARG:HB2	2:C6:183:ASP:OD2	2.20	0.42
2:C7:118:SER:OG	2:C7:159:VAL:HG12	2.20	0.42
2:C8:128:ARG:HB2	2:C8:183:ASP:OD2	2.20	0.42
2:C13:143:LEU:HD13	2:C13:143:LEU:HA	1.79	0.42
2:D1:202:LEU:HD12	2:D1:221:ALA:HA	2.02	0.42
2:D2:209:LYS:O	2:D2:210:PRO:C	2.58	0.42
2:D4:202:LEU:HD12	2:D4:221:ALA:HA	2.02	0.42
2:D7:209:LYS:HB2	2:D7:209:LYS:HE2	1.87	0.42
2:D8:202:LEU:HD12	2:D8:221:ALA:HA	2.02	0.42
2:D10:202:LEU:HD12	2:D10:221:ALA:HA	2.02	0.42
2:D12:129:LYS:HD3	2:D12:129:LYS:HA	1.88	0.42
1:A2:197:TRP:HZ2	1:B1:190:PHE:HA	1.84	0.42
1:A6:154:ASN:HD21	1:B4:152:CYS:H	1.68	0.42
1:A6:174:PRO:HA	1:A6:183:HIS:O	2.19	0.42
1:A7:192:VAL:HG21	2:C7:148:LEU:HD23	2.01	0.42
1:A11:174:PRO:HA	1:A11:183:HIS:O	2.19	0.42
1:B1:96:PRO:HG3	1:B2:182:PHE:HZ	1.85	0.42
1:B3:199:LEU:HD21	1:B4:182:PHE:CE2	2.54	0.42
1:B11:96:PRO:HG3	1:B12:182:PHE:HZ	1.85	0.42
2:C2:72:LEU:CD1	3:E2:185:PHE:CZ	2.79	0.42
2:C3:74:ARG:CB	2:D2:93:GLU:OE2	2.53	0.42
2:C7:128:ARG:HB2	2:C7:183:ASP:OD2	2.20	0.42
2:C11:74:ARG:CB	2:D10:93:GLU:OE2	2.53	0.42
2:C13:74:ARG:CB	2:D12:93:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D8:32:LEU:HA	2:D8:33:PRO:HD3	1.93	0.42
2:D11:202:LEU:HD12	2:D11:221:ALA:HA	2.02	0.42
2:D11:225:MET:HB3	2:D11:226:GLY:H	1.66	0.42
1:A1:170:VAL:CG2	2:C1:216:MET:HB2	2.26	0.41
1:A1:192:VAL:HG21	2:C1:148:LEU:HD23	2.01	0.41
1:A11:197:TRP:HZ2	1:B10:190:PHE:HA	1.84	0.41
1:B10:95:THR:HG22	1:B10:96:PRO:HD3	1.98	0.41
2:C3:30:ILE:HB	2:C3:116:LEU:HD13	2.01	0.41
2:C11:128:ARG:HB2	2:C11:183:ASP:OD2	2.20	0.41
2:C13:30:ILE:HB	2:C13:116:LEU:HD13	2.01	0.41
2:D5:161:PRO:HG2	2:D5:176:PRO:HB2	2.01	0.41
2:D7:202:LEU:HD12	2:D7:221:ALA:HA	2.02	0.41
1:A11:203:VAL:HG21	2:C10:208:TRP:CD2	2.54	0.41
1:B9:199:LEU:HD21	1:B10:182:PHE:CE2	2.54	0.41
2:C1:108:LYS:HD3	2:C1:108:LYS:HA	1.93	0.41
2:C1:128:ARG:HB2	2:C1:183:ASP:OD2	2.20	0.41
2:C2:30:ILE:HB	2:C2:116:LEU:HD13	2.01	0.41
2:C3:29:THR:HG22	2:C3:115:ARG:HE	1.84	0.41
2:C5:128:ARG:HB2	2:C5:183:ASP:OD2	2.20	0.41
2:C6:61:THR:HA	3:E6:181:ASP:O	2.20	0.41
2:C7:29:THR:HG22	2:C7:115:ARG:HE	1.84	0.41
2:C8:118:SER:OG	2:C8:159:VAL:HG12	2.20	0.41
2:D12:224:LEU:HD23	2:D12:224:LEU:HA	1.92	0.41
1:A1:203:VAL:HG21	2:C13:208:TRP:CD2	2.54	0.41
1:B10:199:LEU:HD21	1:B11:182:PHE:CE2	2.55	0.41
2:C1:30:ILE:HB	2:C1:116:LEU:HD13	2.01	0.41
2:C4:74:ARG:CB	2:D3:93:GLU:OE2	2.53	0.41
2:C4:128:ARG:HB2	2:C4:183:ASP:OD2	2.20	0.41
2:C9:61:THR:HA	3:E9:181:ASP:O	2.21	0.41
2:C9:128:ARG:HB2	2:C9:183:ASP:OD2	2.20	0.41
2:C10:128:ARG:HB2	2:C10:183:ASP:OD2	2.20	0.41
2:C13:118:SER:OG	2:C13:159:VAL:HG12	2.20	0.41
2:D6:209:LYS:O	2:D6:210:PRO:C	2.58	0.41
2:D7:161:PRO:HG2	2:D7:176:PRO:HB2	2.01	0.41
2:D10:209:LYS:O	2:D10:210:PRO:C	2.58	0.41
2:C13:138:LYS:HE3	2:C13:138:LYS:HB3	1.85	0.41
1:A5:154:ASN:HD21	1:B3:152:CYS:H	1.69	0.41
1:A7:154:ASN:HD21	1:B5:152:CYS:H	1.69	0.41
2:C1:138:LYS:HE3	2:C1:138:LYS:HB3	1.85	0.41
2:C6:32:LEU:HD21	2:C6:38:PHE:HB2	2.02	0.41
2:C6:137:GLU:H	2:C6:137:GLU:HG2	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C10:61:THR:HA	3:E10:181:ASP:O	2.21	0.41
2:C12:118:SER:OG	2:C12:159:VAL:HG12	2.20	0.41
2:C13:128:ARG:HB2	2:C13:183:ASP:OD2	2.20	0.41
2:D2:209:LYS:HE2	2:D2:209:LYS:HB2	1.87	0.41
2:D6:161:PRO:HG2	2:D6:176:PRO:HB2	2.01	0.41
2:D11:224:LEU:HD23	2:D11:224:LEU:HA	1.92	0.41
2:D12:66:MET:HE3	2:D12:86:ARG:HH21	1.85	0.41
1:B11:199:LEU:HD21	1:B12:182:PHE:CE2	2.54	0.41
2:C1:61:THR:HA	3:E1:181:ASP:O	2.21	0.41
2:C2:61:THR:HA	3:E2:181:ASP:O	2.21	0.41
2:C3:143:LEU:HA	2:C3:143:LEU:HD13	1.79	0.41
2:C5:32:LEU:HD21	2:C5:38:PHE:HB2	2.02	0.41
2:C5:61:THR:HA	3:E5:181:ASP:O	2.21	0.41
2:C7:32:LEU:HD21	2:C7:38:PHE:HB2	2.02	0.41
2:C12:143:LEU:HA	2:C12:143:LEU:HD13	1.79	0.41
2:C13:61:THR:HA	3:E13:181:ASP:O	2.20	0.41
1:A6:197:TRP:HZ2	1:B5:190:PHE:HA	1.84	0.41
1:A8:197:TRP:HZ2	1:B7:190:PHE:HA	1.84	0.41
1:B2:199:LEU:HD21	1:B3:182:PHE:CE2	2.54	0.41
1:B6:96:PRO:HG3	1:B7:182:PHE:HZ	1.85	0.41
1:B8:199:LEU:HD21	1:B9:182:PHE:CE2	2.55	0.41
1:B10:96:PRO:HG3	1:B11:182:PHE:HZ	1.85	0.41
2:C3:61:THR:HA	3:E3:181:ASP:O	2.20	0.41
2:C4:32:LEU:HD21	2:C4:38:PHE:HB2	2.02	0.41
2:C8:61:THR:HA	3:E8:181:ASP:O	2.21	0.41
2:D3:216:MET:HG3	2:D3:233:THR:HG23	2.02	0.41
2:D12:209:LYS:O	2:D12:210:PRO:C	2.58	0.41
1:A11:154:ASN:HD21	1:B9:152:CYS:H	1.69	0.41
1:A13:197:TRP:HZ2	1:B12:190:PHE:HA	1.84	0.41
1:B2:96:PRO:HG3	1:B3:182:PHE:HZ	1.85	0.41
2:C5:138:LYS:HE3	2:C5:138:LYS:HB3	1.85	0.41
2:C8:32:LEU:HD21	2:C8:38:PHE:HB2	2.02	0.41
2:C11:141:ILE:HD13	2:C11:141:ILE:HA	1.93	0.41
2:C13:72:LEU:HD21	3:E13:185:PHE:CB	2.26	0.41
2:D2:56:LYS:HE2	2:D2:56:LYS:HB3	1.94	0.41
2:D2:202:LEU:HD12	2:D2:221:ALA:HA	2.02	0.41
2:D2:216:MET:HG3	2:D2:233:THR:HG23	2.02	0.41
2:D3:202:LEU:HD12	2:D3:221:ALA:HA	2.02	0.41
2:D6:202:LEU:HD12	2:D6:221:ALA:HA	2.02	0.41
2:D11:98:GLN:HE21	2:D11:98:GLN:HB3	1.75	0.41
2:D12:202:LEU:HD12	2:D12:221:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:197:TRP:HZ2	1:B2:190:PHE:HA	1.84	0.41
1:A4:154:ASN:HD21	1:B2:152:CYS:H	1.68	0.41
1:A9:170:VAL:CG2	2:C9:216:MET:HB2	2.26	0.41
1:A10:154:ASN:HD21	1:B8:152:CYS:H	1.69	0.41
1:B8:96:PRO:HG3	1:B9:182:PHE:HZ	1.85	0.41
1:B12:199:LEU:HD21	1:B13:182:PHE:CE2	2.54	0.41
2:C2:141:ILE:HD13	2:C2:141:ILE:HA	1.93	0.41
2:C3:32:LEU:HD21	2:C3:38:PHE:HB2	2.02	0.41
2:C3:211:GLY:HA3	2:C3:236:ARG:HH21	1.86	0.41
2:C7:61:THR:HA	3:E7:181:ASP:O	2.21	0.41
2:C8:211:GLY:HA3	2:C8:236:ARG:HH21	1.86	0.41
2:C9:118:SER:OG	2:C9:159:VAL:HG12	2.20	0.41
2:C11:32:LEU:HD21	2:C11:38:PHE:HB2	2.02	0.41
2:C12:32:LEU:HD21	2:C12:38:PHE:HB2	2.02	0.41
2:C12:61:THR:HA	3:E12:181:ASP:O	2.20	0.41
2:C13:32:LEU:HD21	2:C13:38:PHE:HB2	2.02	0.41
2:D4:209:LYS:O	2:D4:210:PRO:C	2.58	0.41
2:D7:66:MET:HE3	2:D7:86:ARG:HH21	1.86	0.41
2:D8:216:MET:HG3	2:D8:233:THR:HG23	2.02	0.41
2:D9:216:MET:HG3	2:D9:233:THR:HG23	2.02	0.41
2:D10:216:MET:HG3	2:D10:233:THR:HG23	2.02	0.41
1:A12:154:ASN:HD21	1:B10:152:CYS:H	1.69	0.41
2:C9:32:LEU:HD21	2:C9:38:PHE:HB2	2.02	0.41
2:C10:32:LEU:HD21	2:C10:38:PHE:HB2	2.02	0.41
2:C11:211:GLY:HA3	2:C11:236:ARG:HH21	1.86	0.41
2:C13:211:GLY:HA3	2:C13:236:ARG:HH21	1.86	0.41
2:D1:98:GLN:HE21	2:D1:98:GLN:HB3	1.75	0.41
2:D1:209:LYS:HE2	2:D1:209:LYS:HB2	1.87	0.41
2:D4:216:MET:HG3	2:D4:233:THR:HG23	2.03	0.41
2:D5:209:LYS:O	2:D5:210:PRO:C	2.58	0.41
2:D6:224:LEU:HD23	2:D6:224:LEU:HA	1.92	0.41
2:D11:110:GLU:H	2:D11:110:GLU:HG3	1.62	0.41
2:D13:209:LYS:HE2	2:D13:209:LYS:HB2	1.87	0.41
1:A13:154:ASN:HD21	1:B11:152:CYS:H	1.69	0.40
1:B4:96:PRO:HG3	1:B5:182:PHE:HZ	1.85	0.40
1:B7:96:PRO:HG3	1:B8:182:PHE:HZ	1.85	0.40
1:B7:199:LEU:HD21	1:B8:182:PHE:CE2	2.55	0.40
2:C2:32:LEU:HD21	2:C2:38:PHE:HB2	2.02	0.40
2:C2:143:LEU:HD13	2:C2:143:LEU:HA	1.79	0.40
2:C4:143:LEU:HD13	2:C4:143:LEU:HA	1.79	0.40
2:D1:216:MET:HG3	2:D1:233:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:63:PRO:HB2	2:D4:66:MET:HE3	2.03	0.40
2:D5:216:MET:HG3	2:D5:233:THR:HG23	2.03	0.40
1:A1:154:ASN:HD21	1:B12:152:CYS:H	1.68	0.40
1:A8:154:ASN:HD21	1:B6:152:CYS:H	1.68	0.40
2:C1:32:LEU:HD21	2:C1:38:PHE:HB2	2.02	0.40
2:C6:211:GLY:HA3	2:C6:236:ARG:HH21	1.86	0.40
2:C10:138:LYS:HE3	2:C10:138:LYS:HB3	1.85	0.40
2:C12:128:ARG:HB2	2:C12:183:ASP:OD2	2.20	0.40
2:D3:110:GLU:H	2:D3:110:GLU:HG3	1.62	0.40
2:D8:66:MET:HE3	2:D8:86:ARG:HH21	1.87	0.40
1:B3:96:PRO:HG3	1:B4:182:PHE:HZ	1.85	0.40
1:B7:92:VAL:HG22	2:D8:136:TYR:CE1	2.57	0.40
1:B9:96:PRO:HG3	1:B10:182:PHE:HZ	1.85	0.40
2:C5:211:GLY:HA3	2:C5:236:ARG:HH21	1.86	0.40
2:D6:209:LYS:HB2	2:D6:209:LYS:HE2	1.87	0.40
2:D7:216:MET:HG3	2:D7:233:THR:HG23	2.03	0.40
2:D9:56:LYS:HE2	2:D9:56:LYS:HB3	1.94	0.40
2:D11:216:MET:HG3	2:D11:233:THR:HG23	2.02	0.40
2:D12:209:LYS:HE2	2:D12:209:LYS:HB2	1.87	0.40
2:D13:32:LEU:HA	2:D13:33:PRO:HD3	1.93	0.40
2:D13:216:MET:HG3	2:D13:233:THR:HG23	2.02	0.40
1:B2:92:VAL:HG22	2:D3:136:TYR:CE1	2.57	0.40
1:B5:96:PRO:HG3	1:B6:182:PHE:HZ	1.85	0.40
2:C4:61:THR:HA	3:E4:181:ASP:O	2.20	0.40
2:C7:143:LEU:HD13	2:C7:143:LEU:HA	1.79	0.40
2:C9:211:GLY:HA3	2:C9:236:ARG:HH21	1.86	0.40
2:C11:61:THR:HA	3:E11:181:ASP:O	2.21	0.40
2:C12:74:ARG:CB	2:D11:93:GLU:OE2	2.53	0.40
2:D7:209:LYS:O	2:D7:210:PRO:C	2.58	0.40
1:A2:154:ASN:HD21	1:B13:152:CYS:H	1.68	0.40
1:A9:154:ASN:HD21	1:B7:152:CYS:H	1.69	0.40
1:B1:182:PHE:CE2	1:B13:199:LEU:HD21	2.54	0.40
2:C2:128:ARG:HB2	2:C2:183:ASP:OD2	2.20	0.40
2:D2:66:MET:HE3	2:D2:86:ARG:HH21	1.86	0.40
2:D3:203:ARG:HA	2:D3:203:ARG:HD3	1.94	0.40
2:D9:202:LEU:HD12	2:D9:221:ALA:HA	2.02	0.40
2:D12:98:GLN:HE21	2:D12:98:GLN:HB3	1.75	0.40
2:D12:203:ARG:HD3	2:D12:203:ARG:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	53/204 (26%)	53 (100%)	0	0	100	100
1	A10	53/204 (26%)	53 (100%)	0	0	100	100
1	A11	53/204 (26%)	53 (100%)	0	0	100	100
1	A12	53/204 (26%)	53 (100%)	0	0	100	100
1	A13	53/204 (26%)	53 (100%)	0	0	100	100
1	A2	53/204 (26%)	53 (100%)	0	0	100	100
1	A3	53/204 (26%)	53 (100%)	0	0	100	100
1	A4	53/204 (26%)	53 (100%)	0	0	100	100
1	A5	53/204 (26%)	53 (100%)	0	0	100	100
1	A6	53/204 (26%)	53 (100%)	0	0	100	100
1	A7	53/204 (26%)	53 (100%)	0	0	100	100
1	A8	53/204 (26%)	53 (100%)	0	0	100	100
1	A9	53/204 (26%)	53 (100%)	0	0	100	100
1	B1	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B10	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B11	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B12	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B13	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B2	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B3	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B4	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B5	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B6	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B7	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38
1	B8	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B9	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	9 38
2	C1	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	29 66
2	C10	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	29 66
2	C11	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	29 66
2	C12	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	29 66
2	C13	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	29 66
2	C2	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	29 66
2	C3	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	29 66
2	C4	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	29 66
2	C5	215/246 (87%)	196 (91%)	18 (8%)	1 (0%)	29 66
2	C6	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	29 66
2	C7	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	29 66
2	C8	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	29 66
2	C9	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	29 66
2	D1	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D10	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D11	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D12	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D13	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D2	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D3	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D4	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D5	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D6	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D7	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D8	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
2	D9	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	29 66
3	E1	9/453 (2%)	8 (89%)	0	1 (11%)	0 1
3	E10	9/453 (2%)	8 (89%)	0	1 (11%)	0 1
3	E11	9/453 (2%)	8 (89%)	0	1 (11%)	0 1
3	E12	9/453 (2%)	8 (89%)	0	1 (11%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E13	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	E2	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	E3	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	E4	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	E5	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	E6	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	E7	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	E8	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	E9	9/453 (2%)	8 (89%)	0	1 (11%)	0	1
3	F1	9/453 (2%)	9 (100%)	0	0	100	100
3	F10	9/453 (2%)	9 (100%)	0	0	100	100
3	F11	9/453 (2%)	9 (100%)	0	0	100	100
3	F12	9/453 (2%)	9 (100%)	0	0	100	100
3	F13	9/453 (2%)	9 (100%)	0	0	100	100
3	F2	9/453 (2%)	9 (100%)	0	0	100	100
3	F3	9/453 (2%)	9 (100%)	0	0	100	100
3	F4	9/453 (2%)	9 (100%)	0	0	100	100
3	F5	9/453 (2%)	9 (100%)	0	0	100	100
3	F6	9/453 (2%)	9 (100%)	0	0	100	100
3	F7	9/453 (2%)	9 (100%)	0	0	100	100
3	F8	9/453 (2%)	9 (100%)	0	0	100	100
3	F9	9/453 (2%)	9 (100%)	0	0	100	100
All	All	7306/23478 (31%)	6857 (94%)	397 (5%)	52 (1%)	26	58

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D1	196	ASN
2	D2	196	ASN
2	D3	196	ASN
2	D4	196	ASN
2	D5	196	ASN
2	D6	196	ASN
2	D7	196	ASN

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Mol	Chain	Res	Type
2	D8	196	ASN
2	D9	196	ASN
2	D10	196	ASN
2	D11	196	ASN
2	D12	196	ASN
2	D13	196	ASN
1	B1	98	VAL
1	B2	98	VAL
1	B3	98	VAL
1	B4	98	VAL
1	B5	98	VAL
1	B6	98	VAL
1	B7	98	VAL
1	B8	98	VAL
1	B9	98	VAL
1	B10	98	VAL
1	B11	98	VAL
1	B12	98	VAL
1	B13	98	VAL
2	C1	31	SER
2	C2	31	SER
2	C3	31	SER
2	C4	31	SER
2	C5	31	SER
2	C6	31	SER
2	C7	31	SER
2	C8	31	SER
2	C9	31	SER
2	C10	31	SER
2	C11	31	SER
2	C12	31	SER
2	C13	31	SER
3	E1	177	PRO
3	E2	177	PRO
3	E3	177	PRO
3	E4	177	PRO
3	E5	177	PRO
3	E6	177	PRO
3	E7	177	PRO
3	E8	177	PRO
3	E9	177	PRO
3	E10	177	PRO

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Mol	Chain	Res	Type
3	E11	177	PRO
3	E12	177	PRO
3	E13	177	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A10	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A11	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A12	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A13	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A2	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A3	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A4	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A5	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A6	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A7	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A8	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	A9	48/168 (29%)	47 (98%)	1 (2%)	53	80
1	B1	56/168 (33%)	55 (98%)	1 (2%)	59	83
1	B10	56/168 (33%)	55 (98%)	1 (2%)	59	83
1	B11	56/168 (33%)	55 (98%)	1 (2%)	59	83
1	B12	56/168 (33%)	55 (98%)	1 (2%)	59	83
1	B13	56/168 (33%)	55 (98%)	1 (2%)	59	83
1	B2	56/168 (33%)	55 (98%)	1 (2%)	59	83
1	B3	56/168 (33%)	55 (98%)	1 (2%)	59	83
1	B4	56/168 (33%)	55 (98%)	1 (2%)	59	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B5	56/168 (33%)	55 (98%)	1 (2%)	59 83
1	B6	56/168 (33%)	55 (98%)	1 (2%)	59 83
1	B7	56/168 (33%)	55 (98%)	1 (2%)	59 83
1	B8	56/168 (33%)	55 (98%)	1 (2%)	59 83
1	B9	56/168 (33%)	55 (98%)	1 (2%)	59 83
2	C1	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C10	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C11	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C12	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C13	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C2	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C3	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C4	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C5	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C6	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C7	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C8	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	C9	173/195 (89%)	164 (95%)	9 (5%)	23 57
2	D1	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D10	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D11	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D12	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D13	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D2	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D3	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D4	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D5	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D6	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D7	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D8	173/195 (89%)	157 (91%)	16 (9%)	9 32
2	D9	173/195 (89%)	157 (91%)	16 (9%)	9 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E1	10/353 (3%)	10 (100%)	0	100	100
3	E10	10/353 (3%)	10 (100%)	0	100	100
3	E11	10/353 (3%)	10 (100%)	0	100	100
3	E12	10/353 (3%)	10 (100%)	0	100	100
3	E13	10/353 (3%)	10 (100%)	0	100	100
3	E2	10/353 (3%)	10 (100%)	0	100	100
3	E3	10/353 (3%)	10 (100%)	0	100	100
3	E4	10/353 (3%)	10 (100%)	0	100	100
3	E5	10/353 (3%)	10 (100%)	0	100	100
3	E6	10/353 (3%)	10 (100%)	0	100	100
3	E7	10/353 (3%)	10 (100%)	0	100	100
3	E8	10/353 (3%)	10 (100%)	0	100	100
3	E9	10/353 (3%)	10 (100%)	0	100	100
3	F1	10/353 (3%)	10 (100%)	0	100	100
3	F10	10/353 (3%)	10 (100%)	0	100	100
3	F11	10/353 (3%)	10 (100%)	0	100	100
3	F12	10/353 (3%)	10 (100%)	0	100	100
3	F13	10/353 (3%)	10 (100%)	0	100	100
3	F2	10/353 (3%)	10 (100%)	0	100	100
3	F3	10/353 (3%)	10 (100%)	0	100	100
3	F4	10/353 (3%)	10 (100%)	0	100	100
3	F5	10/353 (3%)	10 (100%)	0	100	100
3	F6	10/353 (3%)	10 (100%)	0	100	100
3	F7	10/353 (3%)	10 (100%)	0	100	100
3	F8	10/353 (3%)	10 (100%)	0	100	100
3	F9	10/353 (3%)	10 (100%)	0	100	100
All	All	6110/18616 (33%)	5759 (94%)	351 (6%)	24	54

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	153	ASP
1	A2	153	ASP

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Mol	Chain	Res	Type
1	A3	153	ASP
1	A4	153	ASP
1	A5	153	ASP
1	A6	153	ASP
1	A7	153	ASP
1	A8	153	ASP
1	A9	153	ASP
1	A10	153	ASP
1	A11	153	ASP
1	A12	153	ASP
1	A13	153	ASP
1	B1	179	ASP
1	B2	179	ASP
1	B3	179	ASP
1	B4	179	ASP
1	B5	179	ASP
1	B6	179	ASP
1	B7	179	ASP
1	B8	179	ASP
1	B9	179	ASP
1	B10	179	ASP
1	B11	179	ASP
1	B12	179	ASP
1	B13	179	ASP
2	C1	44	ASN
2	C1	60	ILE
2	C1	90	ILE
2	C1	105	THR
2	C1	142	SER
2	C1	188	ASP
2	C1	196	ASN
2	C1	198	TRP
2	C1	229	ARG
2	C2	44	ASN
2	C2	60	ILE
2	C2	90	ILE
2	C2	105	THR
2	C2	142	SER
2	C2	188	ASP
2	C2	196	ASN
2	C2	198	TRP
2	C2	229	ARG

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Mol	Chain	Res	Type
2	C3	44	ASN
2	C3	60	ILE
2	C3	90	ILE
2	C3	105	THR
2	C3	142	SER
2	C3	188	ASP
2	C3	196	ASN
2	C3	198	TRP
2	C3	229	ARG
2	C4	44	ASN
2	C4	60	ILE
2	C4	90	ILE
2	C4	105	THR
2	C4	142	SER
2	C4	188	ASP
2	C4	196	ASN
2	C4	198	TRP
2	C4	229	ARG
2	C5	44	ASN
2	C5	60	ILE
2	C5	90	ILE
2	C5	105	THR
2	C5	142	SER
2	C5	188	ASP
2	C5	196	ASN
2	C5	198	TRP
2	C5	229	ARG
2	C6	44	ASN
2	C6	60	ILE
2	C6	90	ILE
2	C6	105	THR
2	C6	142	SER
2	C6	188	ASP
2	C6	196	ASN
2	C6	198	TRP
2	C6	229	ARG
2	C7	44	ASN
2	C7	60	ILE
2	C7	90	ILE
2	C7	105	THR
2	C7	142	SER
2	C7	188	ASP

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Mol	Chain	Res	Type
2	C7	196	ASN
2	C7	198	TRP
2	C7	229	ARG
2	C8	44	ASN
2	C8	60	ILE
2	C8	90	ILE
2	C8	105	THR
2	C8	142	SER
2	C8	188	ASP
2	C8	196	ASN
2	C8	198	TRP
2	C8	229	ARG
2	C9	44	ASN
2	C9	60	ILE
2	C9	90	ILE
2	C9	105	THR
2	C9	142	SER
2	C9	188	ASP
2	C9	196	ASN
2	C9	198	TRP
2	C9	229	ARG
2	C10	44	ASN
2	C10	60	ILE
2	C10	90	ILE
2	C10	105	THR
2	C10	142	SER
2	C10	188	ASP
2	C10	196	ASN
2	C10	198	TRP
2	C10	229	ARG
2	C11	44	ASN
2	C11	60	ILE
2	C11	90	ILE
2	C11	105	THR
2	C11	142	SER
2	C11	188	ASP
2	C11	196	ASN
2	C11	198	TRP
2	C11	229	ARG
2	C12	44	ASN
2	C12	60	ILE
2	C12	90	ILE

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Mol	Chain	Res	Type
2	C12	105	THR
2	C12	142	SER
2	C12	188	ASP
2	C12	196	ASN
2	C12	198	TRP
2	C12	229	ARG
2	C13	44	ASN
2	C13	60	ILE
2	C13	90	ILE
2	C13	105	THR
2	C13	142	SER
2	C13	188	ASP
2	C13	196	ASN
2	C13	198	TRP
2	C13	229	ARG
2	D1	29	THR
2	D1	30	ILE
2	D1	44	ASN
2	D1	45	THR
2	D1	73	THR
2	D1	78	VAL
2	D1	92	VAL
2	D1	110	GLU
2	D1	116	LEU
2	D1	151	ASP
2	D1	177	LEU
2	D1	178	LYS
2	D1	184	GLN
2	D1	208	TRP
2	D1	231	THR
2	D1	233	THR
2	D2	29	THR
2	D2	30	ILE
2	D2	44	ASN
2	D2	45	THR
2	D2	73	THR
2	D2	78	VAL
2	D2	92	VAL
2	D2	110	GLU
2	D2	116	LEU
2	D2	151	ASP
2	D2	177	LEU

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Mol	Chain	Res	Type
2	D2	178	LYS
2	D2	184	GLN
2	D2	208	TRP
2	D2	231	THR
2	D2	233	THR
2	D3	29	THR
2	D3	30	ILE
2	D3	44	ASN
2	D3	45	THR
2	D3	73	THR
2	D3	78	VAL
2	D3	92	VAL
2	D3	110	GLU
2	D3	116	LEU
2	D3	151	ASP
2	D3	177	LEU
2	D3	178	LYS
2	D3	184	GLN
2	D3	208	TRP
2	D3	231	THR
2	D3	233	THR
2	D4	29	THR
2	D4	30	ILE
2	D4	44	ASN
2	D4	45	THR
2	D4	73	THR
2	D4	78	VAL
2	D4	92	VAL
2	D4	110	GLU
2	D4	116	LEU
2	D4	151	ASP
2	D4	177	LEU
2	D4	178	LYS
2	D4	184	GLN
2	D4	208	TRP
2	D4	231	THR
2	D4	233	THR
2	D5	29	THR
2	D5	30	ILE
2	D5	44	ASN
2	D5	45	THR
2	D5	73	THR

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Mol	Chain	Res	Type
2	D5	78	VAL
2	D5	92	VAL
2	D5	110	GLU
2	D5	116	LEU
2	D5	151	ASP
2	D5	177	LEU
2	D5	178	LYS
2	D5	184	GLN
2	D5	208	TRP
2	D5	231	THR
2	D5	233	THR
2	D6	29	THR
2	D6	30	ILE
2	D6	44	ASN
2	D6	45	THR
2	D6	73	THR
2	D6	78	VAL
2	D6	92	VAL
2	D6	110	GLU
2	D6	116	LEU
2	D6	151	ASP
2	D6	177	LEU
2	D6	178	LYS
2	D6	184	GLN
2	D6	208	TRP
2	D6	231	THR
2	D6	233	THR
2	D7	29	THR
2	D7	30	ILE
2	D7	44	ASN
2	D7	45	THR
2	D7	73	THR
2	D7	78	VAL
2	D7	92	VAL
2	D7	110	GLU
2	D7	116	LEU
2	D7	151	ASP
2	D7	177	LEU
2	D7	178	LYS
2	D7	184	GLN
2	D7	208	TRP
2	D7	231	THR

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Mol	Chain	Res	Type
2	D7	233	THR
2	D8	29	THR
2	D8	30	ILE
2	D8	44	ASN
2	D8	45	THR
2	D8	73	THR
2	D8	78	VAL
2	D8	92	VAL
2	D8	110	GLU
2	D8	116	LEU
2	D8	151	ASP
2	D8	177	LEU
2	D8	178	LYS
2	D8	184	GLN
2	D8	208	TRP
2	D8	231	THR
2	D8	233	THR
2	D9	29	THR
2	D9	30	ILE
2	D9	44	ASN
2	D9	45	THR
2	D9	73	THR
2	D9	78	VAL
2	D9	92	VAL
2	D9	110	GLU
2	D9	116	LEU
2	D9	151	ASP
2	D9	177	LEU
2	D9	178	LYS
2	D9	184	GLN
2	D9	208	TRP
2	D9	231	THR
2	D9	233	THR
2	D10	29	THR
2	D10	30	ILE
2	D10	44	ASN
2	D10	45	THR
2	D10	73	THR
2	D10	78	VAL
2	D10	92	VAL
2	D10	110	GLU
2	D10	116	LEU

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Mol	Chain	Res	Type
2	D10	151	ASP
2	D10	177	LEU
2	D10	178	LYS
2	D10	184	GLN
2	D10	208	TRP
2	D10	231	THR
2	D10	233	THR
2	D11	29	THR
2	D11	30	ILE
2	D11	44	ASN
2	D11	45	THR
2	D11	73	THR
2	D11	78	VAL
2	D11	92	VAL
2	D11	110	GLU
2	D11	116	LEU
2	D11	151	ASP
2	D11	177	LEU
2	D11	178	LYS
2	D11	184	GLN
2	D11	208	TRP
2	D11	231	THR
2	D11	233	THR
2	D12	29	THR
2	D12	30	ILE
2	D12	44	ASN
2	D12	45	THR
2	D12	73	THR
2	D12	78	VAL
2	D12	92	VAL
2	D12	110	GLU
2	D12	116	LEU
2	D12	151	ASP
2	D12	177	LEU
2	D12	178	LYS
2	D12	184	GLN
2	D12	208	TRP
2	D12	231	THR
2	D12	233	THR
2	D13	29	THR
2	D13	30	ILE
2	D13	44	ASN

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Mol	Chain	Res	Type
2	D13	45	THR
2	D13	73	THR
2	D13	78	VAL
2	D13	92	VAL
2	D13	110	GLU
2	D13	116	LEU
2	D13	151	ASP
2	D13	177	LEU
2	D13	178	LYS
2	D13	184	GLN
2	D13	208	TRP
2	D13	231	THR
2	D13	233	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	154	ASN
1	A2	154	ASN
1	A3	154	ASN
1	A4	154	ASN
1	A5	154	ASN
1	A6	154	ASN
1	A7	154	ASN
1	A8	154	ASN
1	A9	154	ASN
1	B1	161	GLN
1	B2	161	GLN
1	B3	161	GLN
1	B4	161	GLN
1	B5	161	GLN
1	B6	161	GLN
1	B7	161	GLN
1	B8	161	GLN
1	B9	161	GLN
2	C1	184	GLN
2	C1	194	ASN
2	C1	196	ASN
2	C1	222	GLN
2	C2	184	GLN
2	C2	194	ASN
2	C2	196	ASN

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Mol	Chain	Res	Type
2	C2	222	GLN
2	C3	184	GLN
2	C3	194	ASN
2	C3	196	ASN
2	C3	222	GLN
2	C4	184	GLN
2	C4	194	ASN
2	C4	196	ASN
2	C4	222	GLN
2	C5	184	GLN
2	C5	194	ASN
2	C5	196	ASN
2	C5	222	GLN
2	C6	184	GLN
2	C6	194	ASN
2	C6	196	ASN
2	C6	222	GLN
2	C7	184	GLN
2	C7	194	ASN
2	C7	196	ASN
2	C7	222	GLN
2	C8	184	GLN
2	C8	194	ASN
2	C8	196	ASN
2	C8	222	GLN
2	C9	184	GLN
2	C9	194	ASN
2	C9	196	ASN
2	C9	222	GLN
2	D1	98	GLN
2	D1	144	ASN
2	D1	219	ASN
2	D1	222	GLN
2	D2	98	GLN
2	D2	144	ASN
2	D2	219	ASN
2	D2	222	GLN
2	D3	98	GLN
2	D3	144	ASN
2	D3	219	ASN
2	D3	222	GLN
2	D4	98	GLN

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Mol	Chain	Res	Type
2	D4	144	ASN
2	D4	219	ASN
2	D4	222	GLN
2	D5	98	GLN
2	D5	144	ASN
2	D5	219	ASN
2	D5	222	GLN
2	D6	98	GLN
2	D6	144	ASN
2	D6	219	ASN
2	D6	222	GLN
2	D7	98	GLN
2	D7	144	ASN
2	D7	219	ASN
2	D7	222	GLN
2	D8	98	GLN
2	D8	144	ASN
2	D8	219	ASN
2	D8	222	GLN
2	D9	98	GLN
2	D9	144	ASN
2	D9	219	ASN
2	D9	222	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

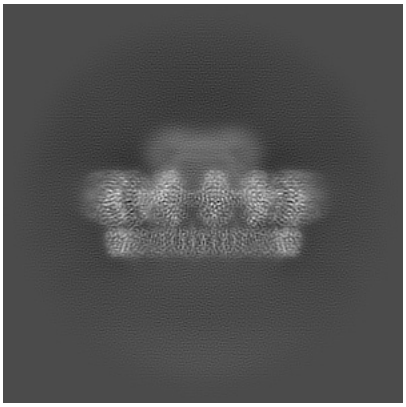
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24771. These allow visual inspection of the internal detail of the map and identification of artifacts.

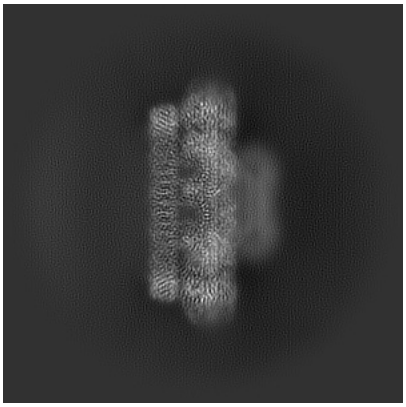
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

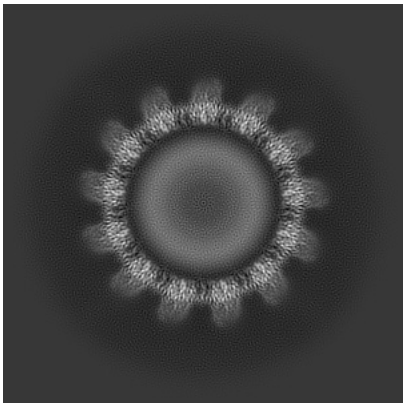
6.1.1 Primary map



X



Y

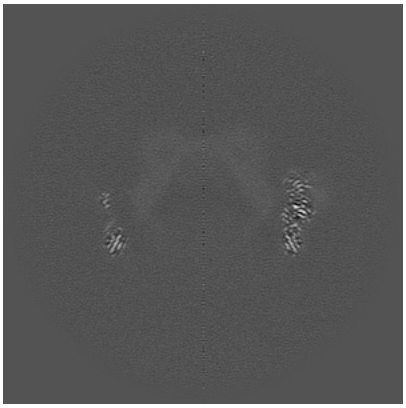


Z

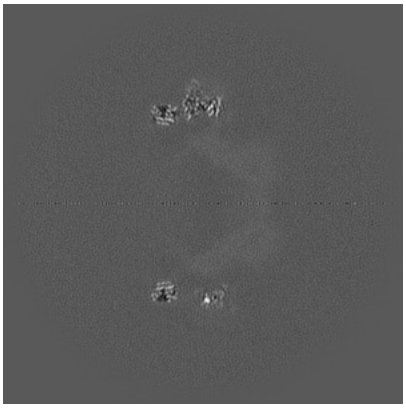
The images above show the map projected in three orthogonal directions.

6.2 Central slices

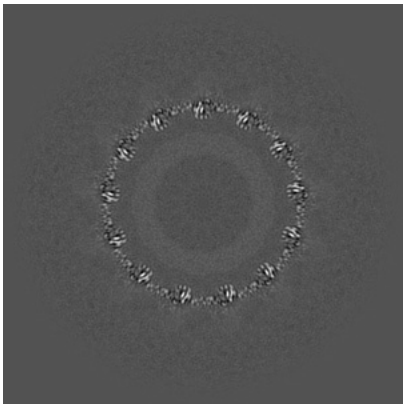
6.2.1 Primary map



X Index: 200



Y Index: 200

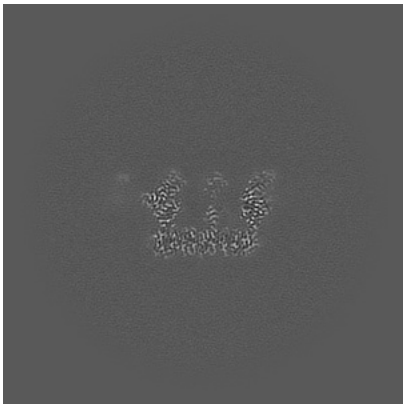


Z Index: 200

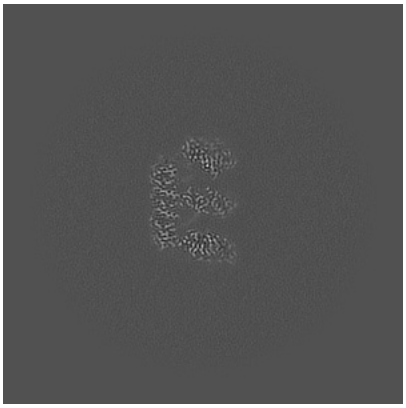
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

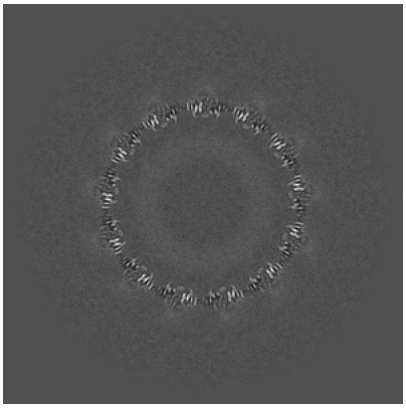
6.3.1 Primary map



X Index: 283



Y Index: 288

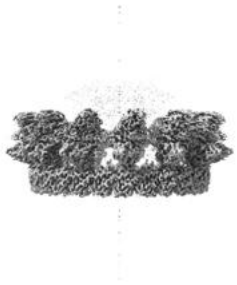


Z Index: 204

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

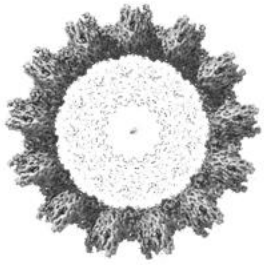
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

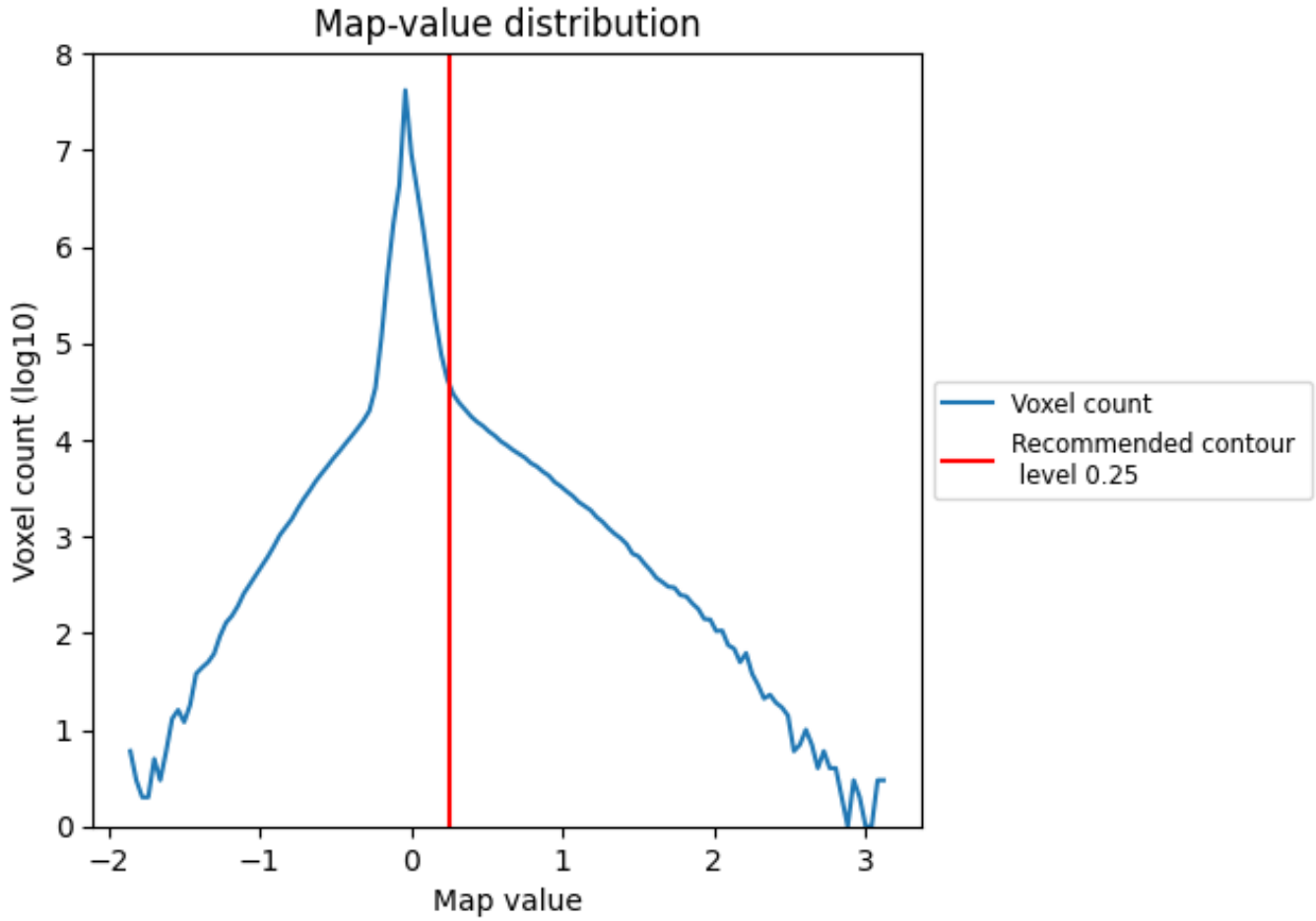
6.5 Mask visualisation (i)

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

7 Map analysis

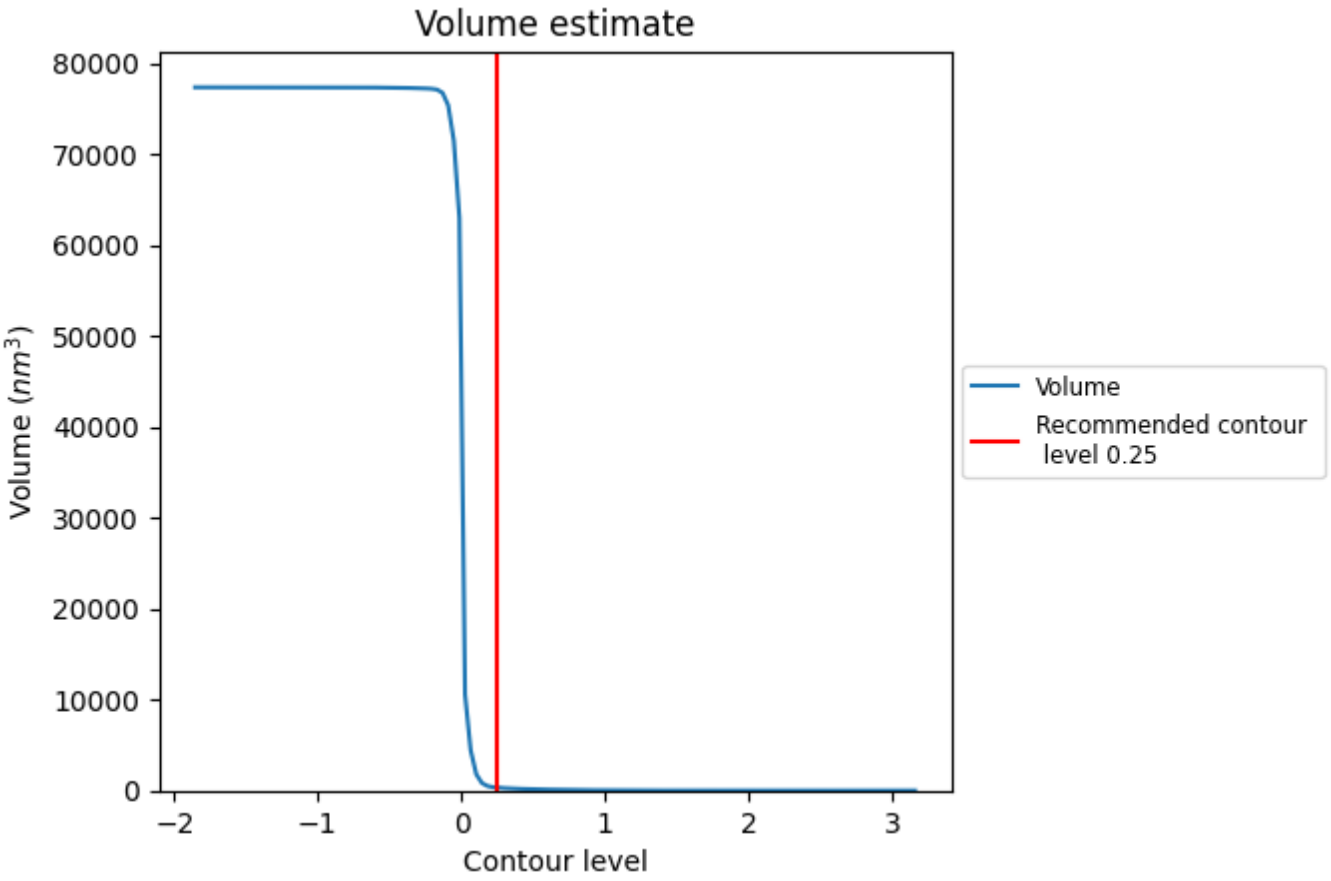
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

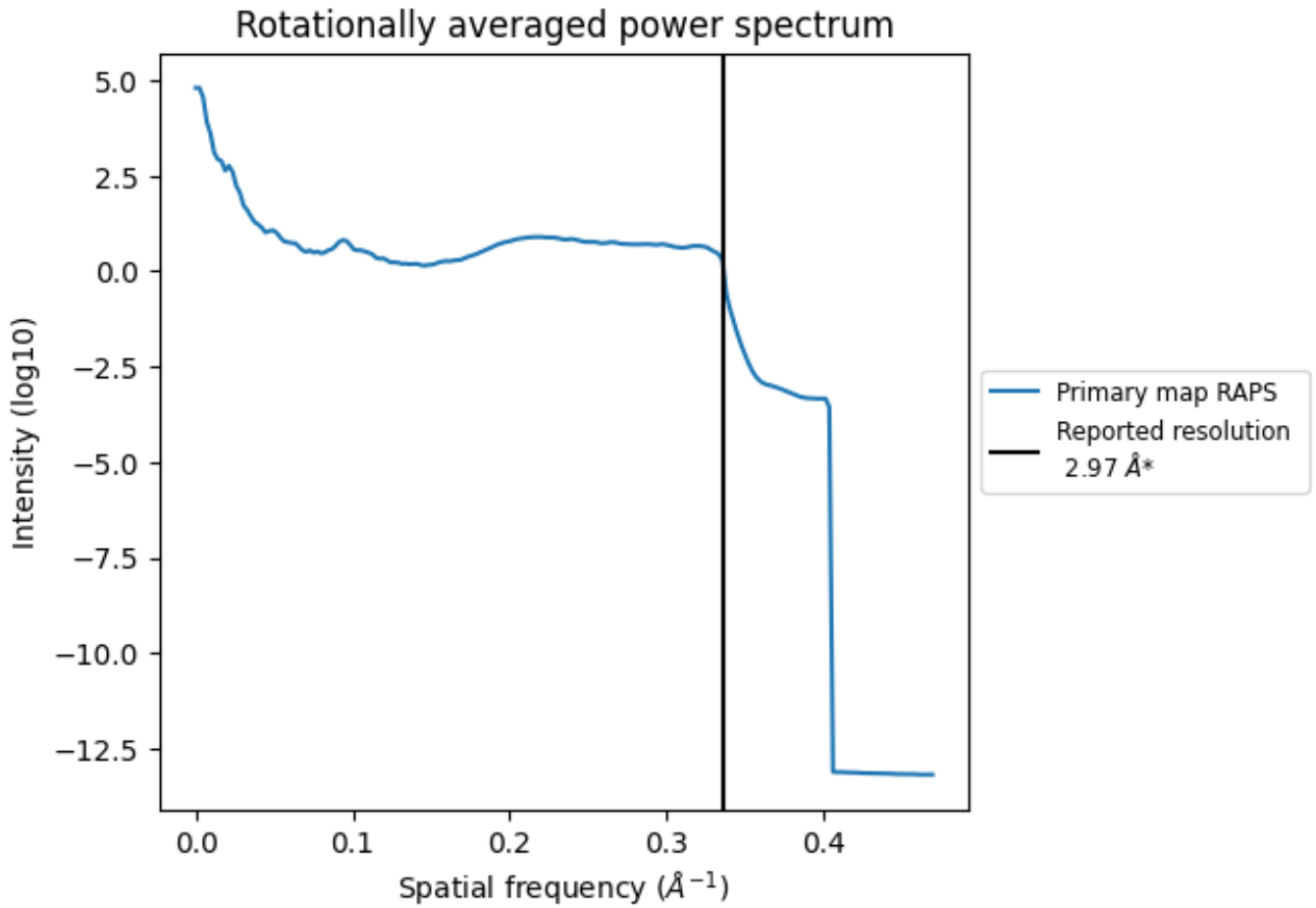
7.2 Volume estimate



The volume at the recommended contour level is 322 nm^3; this corresponds to an approximate mass of 291 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

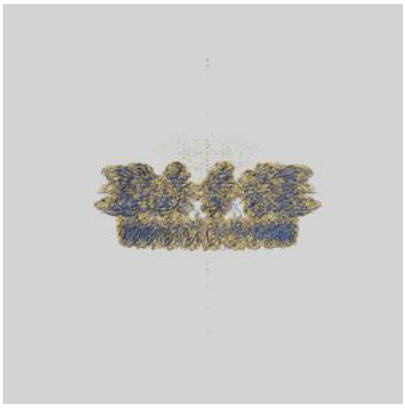
8 Fourier-Shell correlation (i)

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

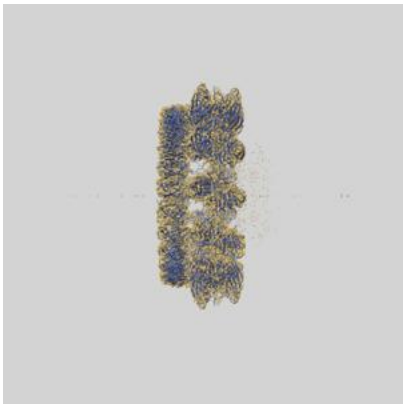
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24771 and PDB model 7SPI. Per-residue inclusion information can be found in section 3 on page 11.

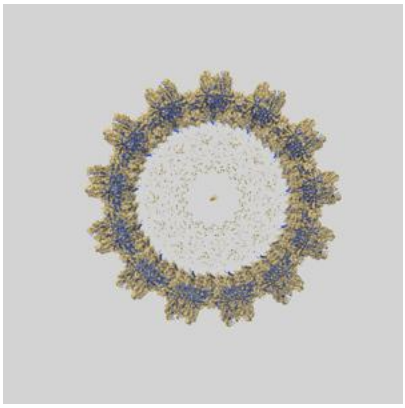
9.1 Map-model overlay



X



Y



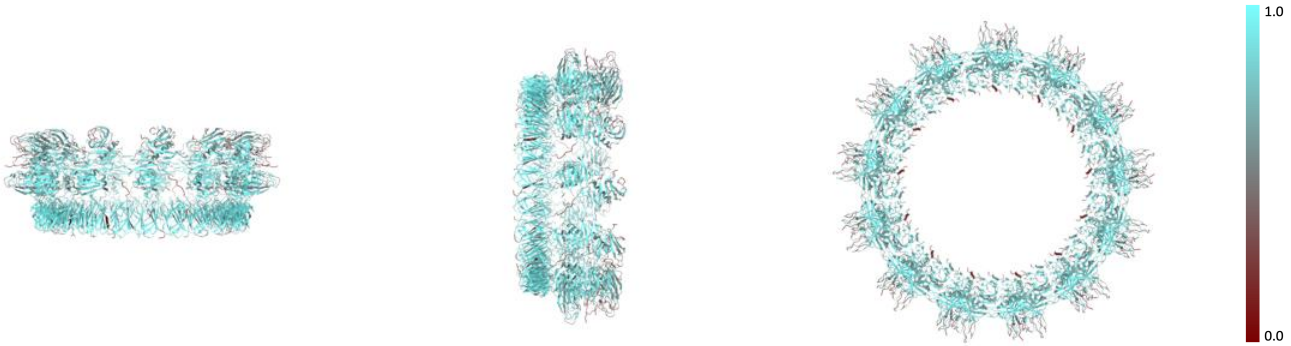
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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

This section was not generated.

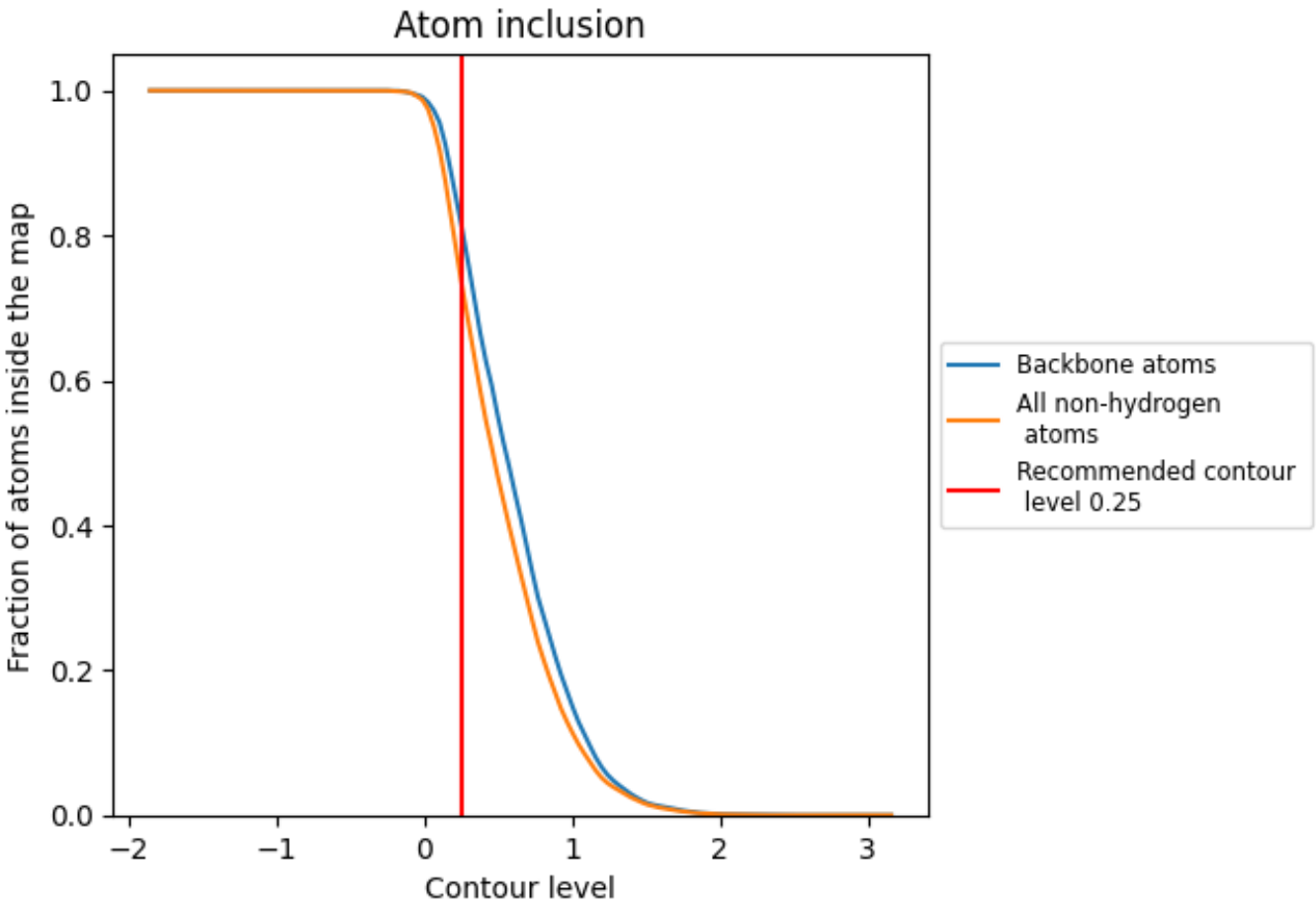
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.7372
A1	0.7447
A10	0.7329
A11	0.7281
A12	0.7423
A13	0.7447
A2	0.7518
A3	0.7352
A4	0.7400
A5	0.7400
A6	0.7400
A7	0.7423
A8	0.7400
A9	0.7400
B1	0.6948
B10	0.6969
B11	0.6928
B12	0.7010
B13	0.6948
B2	0.7010
B3	0.6990
B4	0.7010
B5	0.7010
B6	0.6928
B7	0.6969
B8	0.7031
B9	0.6990
C1	0.8211
C10	0.8186
C11	0.8199
C12	0.8180
C13	0.8230
C2	0.8217
C3	0.8224
C4	0.8174

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Chain	Atom inclusion
C5	0.8199
C6	0.8205
C7	0.8180
C8	0.8224
C9	0.8155
D1	0.7056
D10	0.7031
D11	0.7031
D12	0.7031
D13	0.7062
D2	0.7006
D3	0.7068
D4	0.7056
D5	0.7043
D6	0.7050
D7	0.7025
D8	0.7037
D9	0.7075
E1	0.1059
E10	0.1176
E11	0.1176
E12	0.1176
E13	0.1176
E2	0.1059
E3	0.1176
E4	0.1176
E5	0.1294
E6	0.1176
E7	0.1059
E8	0.1294
E9	0.0824
F1	0.6235
F10	0.6000
F11	0.6353
F12	0.6235
F13	0.6235
F2	0.6118
F3	0.6353
F4	0.6118
F5	0.6235
F6	0.6353
F7	0.6353

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Chain	Atom inclusion
F8	0.6471
F9	0.6353