



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:04 AM UTC

PDB ID : 7SPI / pdb_00007spi
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

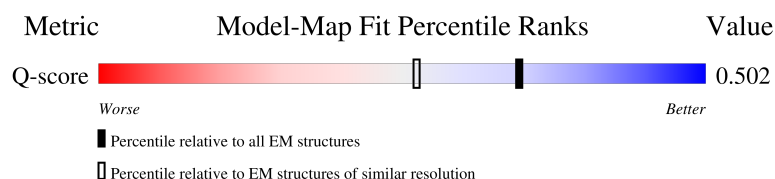
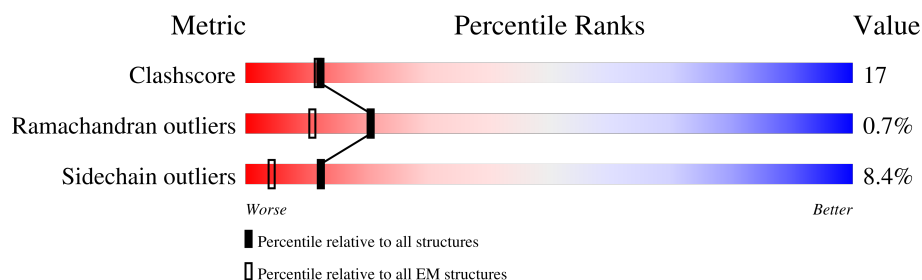
1 Overall quality at a glance i

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.



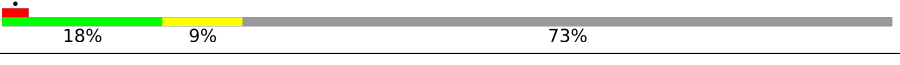
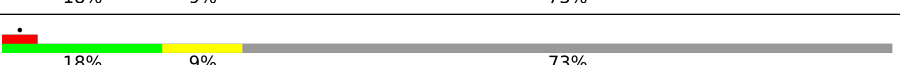
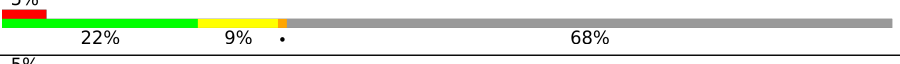
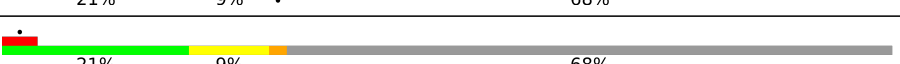
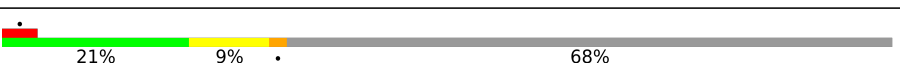
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13205 (2.47 - 3.47)

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

Mol	Chain	Length	Quality of chain
1	A1	204	 18% 9% 73%
1	A10	204	 18% 9% 73%
1	A11	204	 18% 9% 73%
1	A12	204	 18% 9% 73%

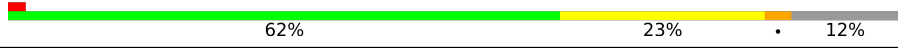
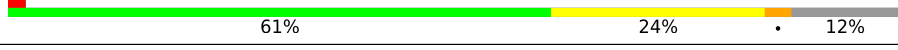
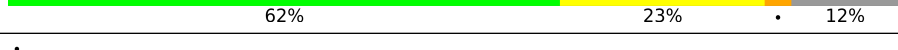
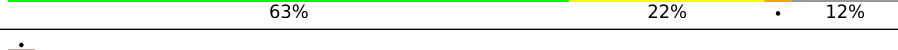
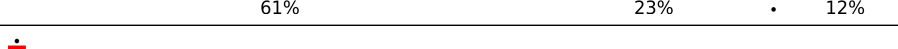
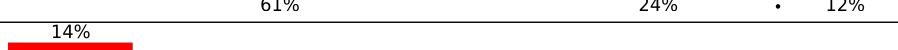
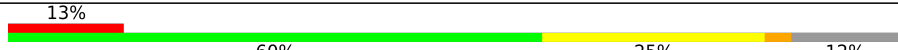
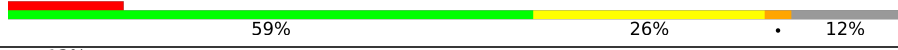
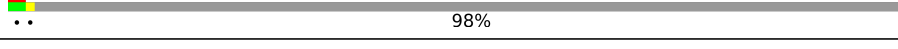
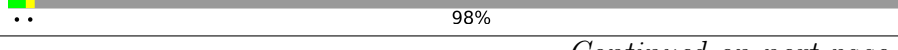
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Mol	Chain	Length	Quality of chain
1	A13	204	
1	A2	204	
1	A3	204	
1	A4	204	
1	A5	204	
1	A6	204	
1	A7	204	
1	A8	204	
1	A9	204	
1	B1	204	
1	B10	204	
1	B11	204	
1	B12	204	
1	B13	204	
1	B2	204	
1	B3	204	
1	B4	204	
1	B5	204	
1	B6	204	
1	B7	204	
1	B8	204	
1	B9	204	
2	C1	246	
2	C10	246	
2	C11	246	

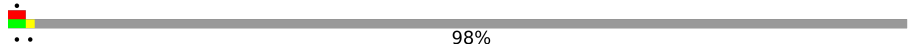
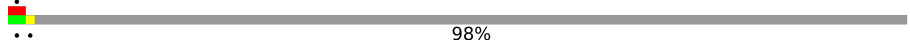
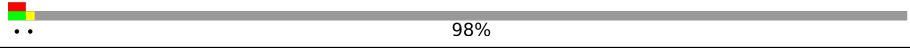
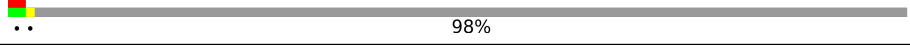
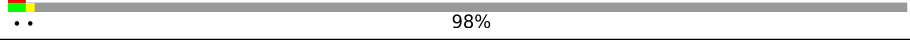
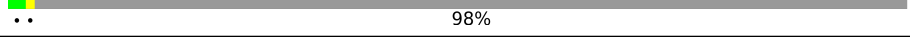
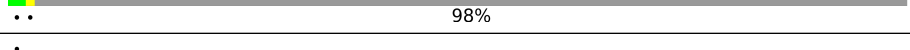
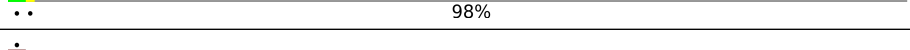
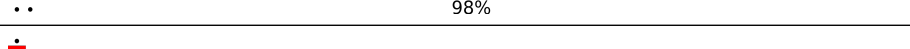
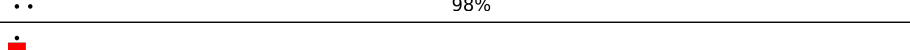
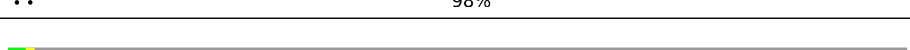
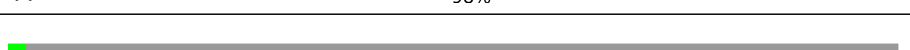
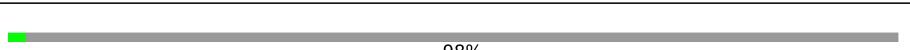
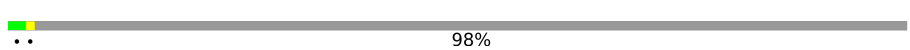
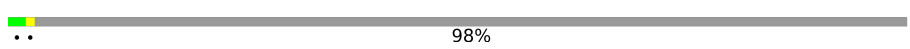
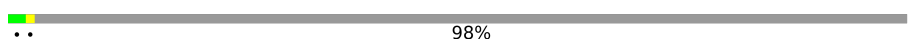
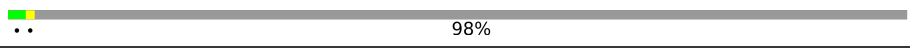
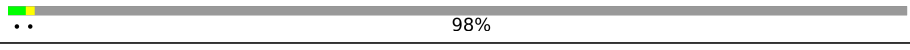
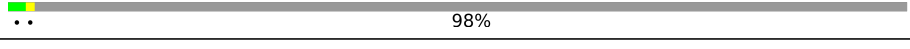
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Mol	Chain	Length	Quality of chain
2	C12	246	
2	C13	246	
2	C2	246	
2	C3	246	
2	C4	246	
2	C5	246	
2	C6	246	
2	C7	246	
2	C8	246	
2	C9	246	
2	D1	246	
2	D10	246	
2	D11	246	
2	D12	246	
2	D13	246	
2	D2	246	
2	D3	246	
2	D4	246	
2	D5	246	
2	D6	246	
2	D7	246	
2	D8	246	
2	D9	246	
3	E1	453	
3	E10	453	

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Mol	Chain	Length	Quality of chain
3	E11	453	 98%
3	E12	453	 98%
3	E13	453	 98%
3	E2	453	 98%
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 498	C 314	N 92	O 91	S 1	0	0
1	B6	65	Total 498	C 314	N 92	O 91	S 1	0	0
1	B7	65	Total 498	C 314	N 92	O 91	S 1	0	0
1	B8	65	Total 498	C 314	N 92	O 91	S 1	0	0
1	B9	65	Total 498	C 314	N 92	O 91	S 1	0	0
1	B10	65	Total 498	C 314	N 92	O 91	S 1	0	0
1	B11	65	Total 498	C 314	N 92	O 91	S 1	0	0
1	B12	65	Total 498	C 314	N 92	O 91	S 1	0	0
1	B13	65	Total 498	C 314	N 92	O 91	S 1	0	0

- Molecule 2 is a protein called TraK.

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

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

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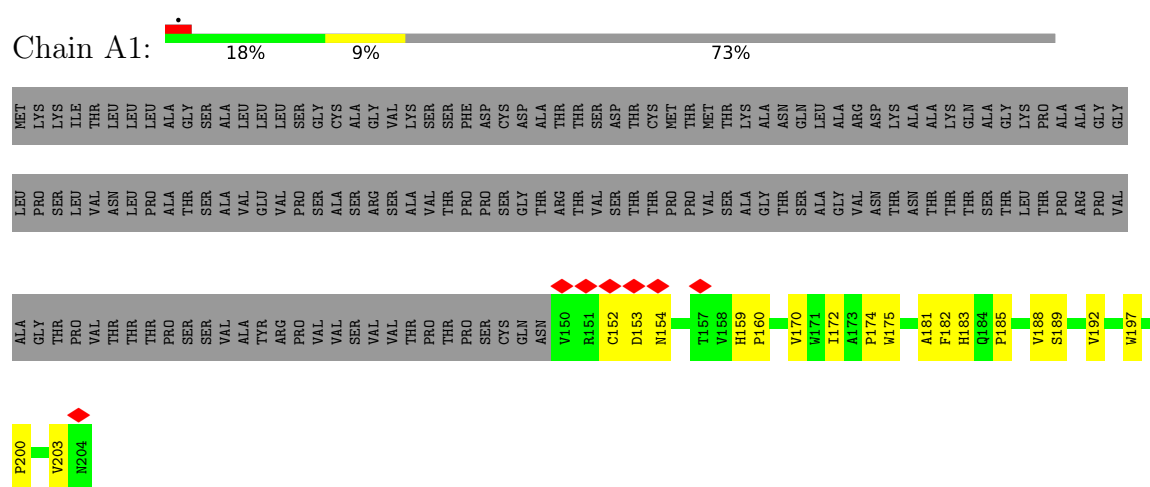
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F12	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F13	11	Total	C	N	O	S	0	0
			87	52	15	18	2		

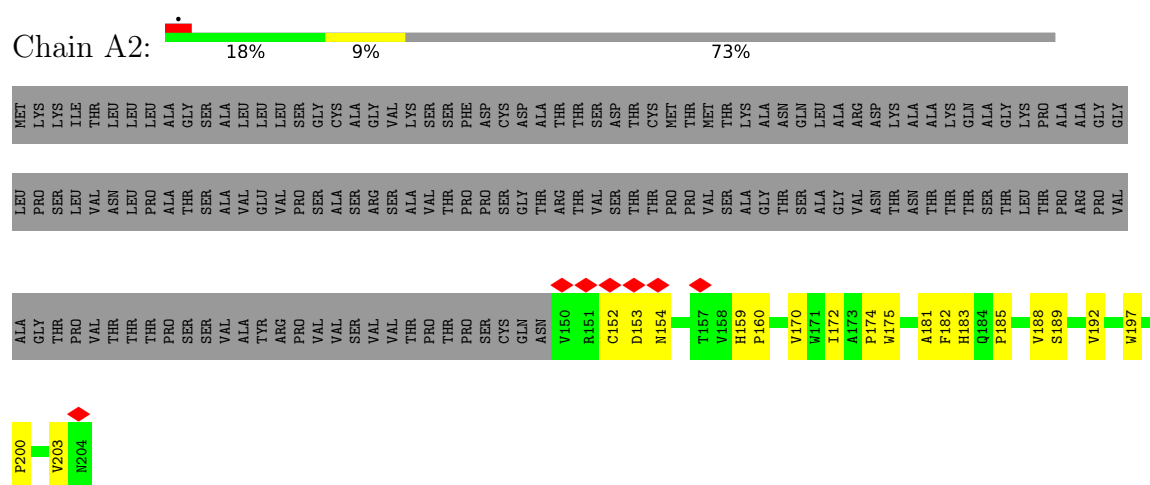
3 Residue-property plots

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.

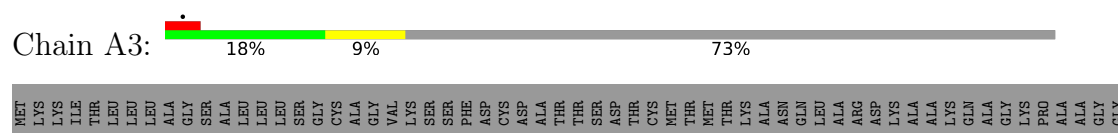
• Molecule 1: TraV

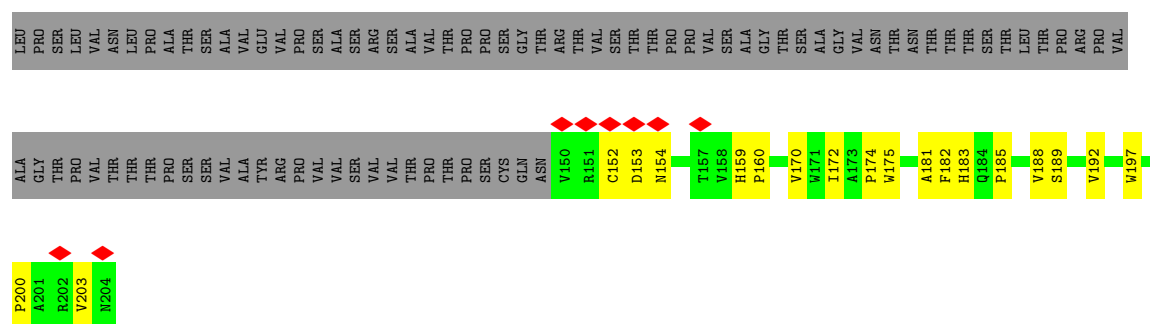


• Molecule 1: TraV

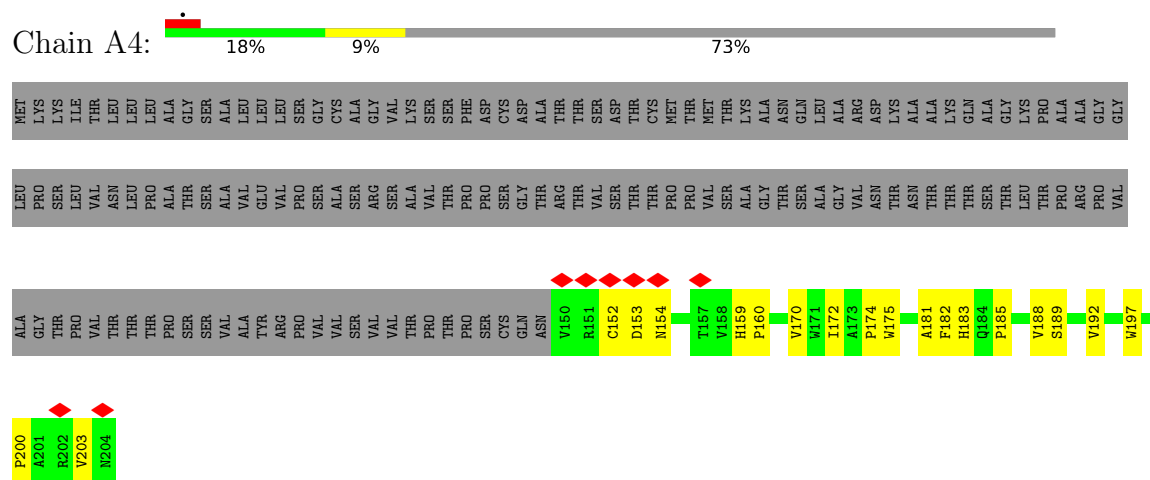


• Molecule 1: TraV

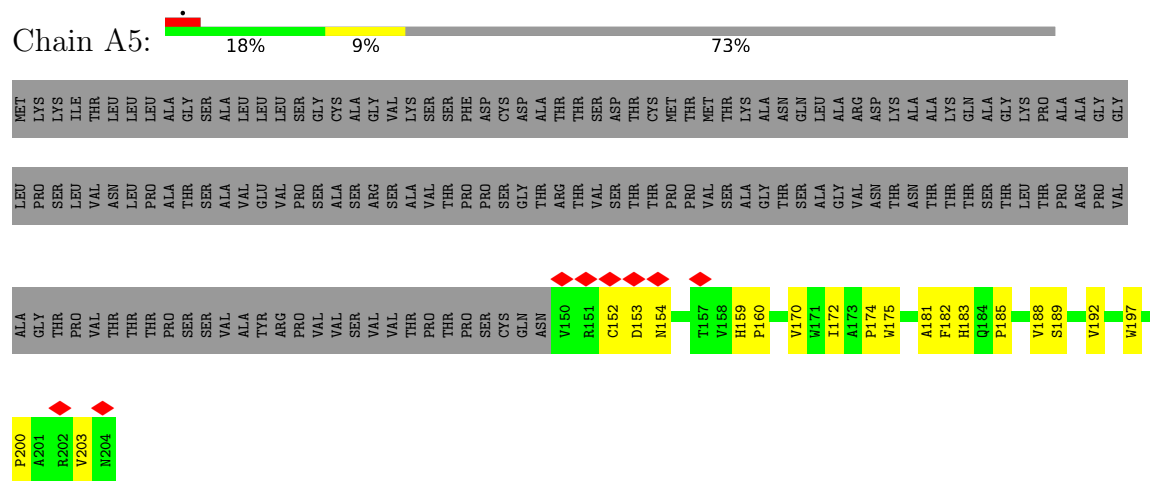




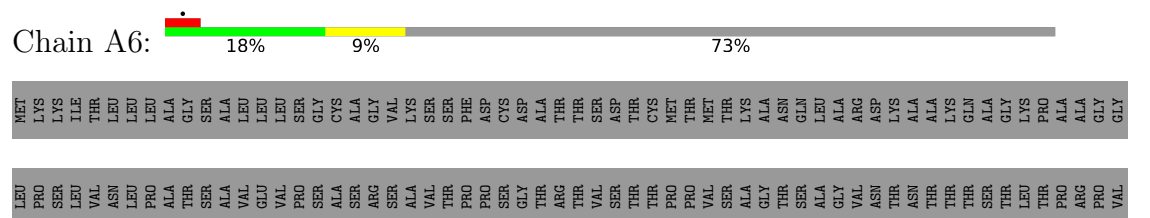
- Molecule 1: TraV

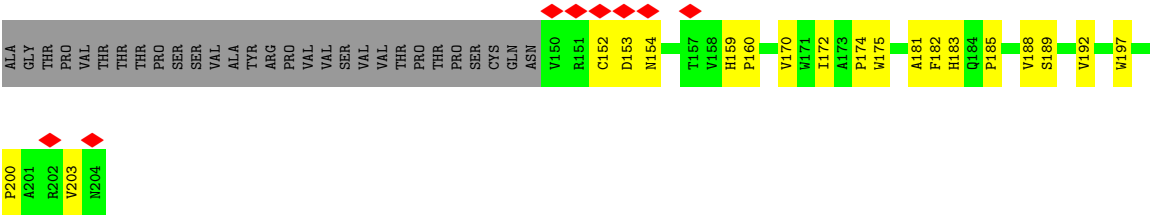


- Molecule 1: TraV

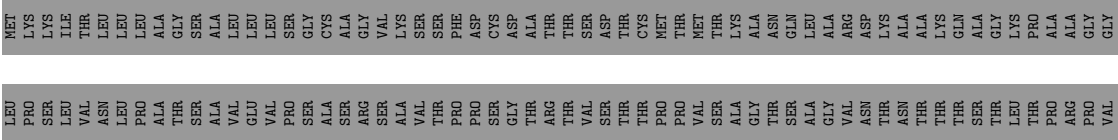


- Molecule 1: TraV

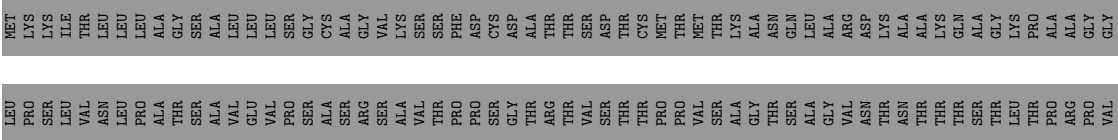




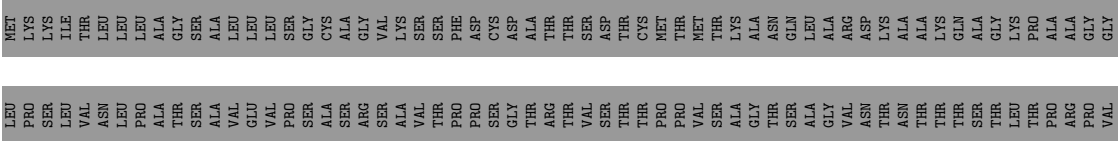
• Molecule 1: TraV

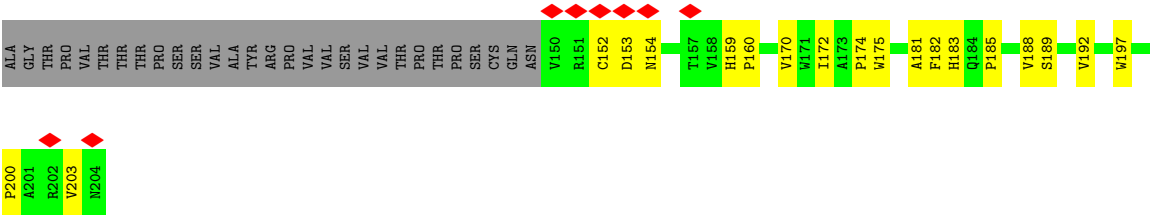


• Molecule 1: TraV

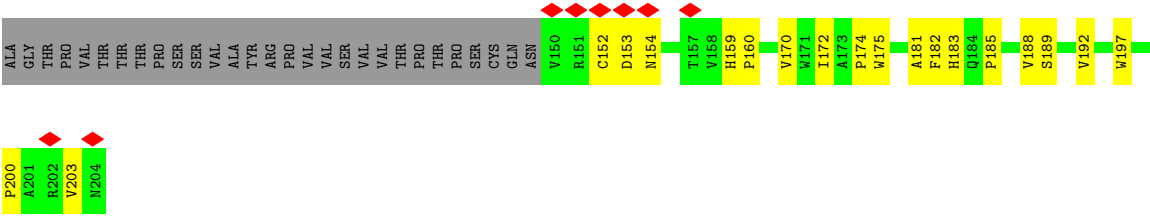
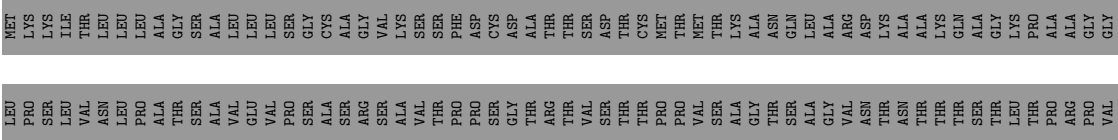


• Molecule 1: TraV

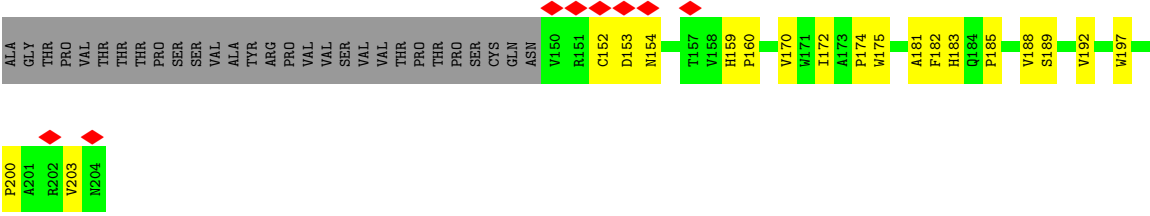
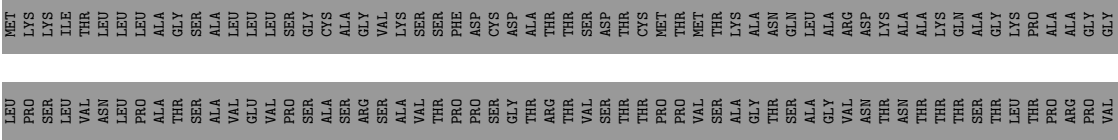




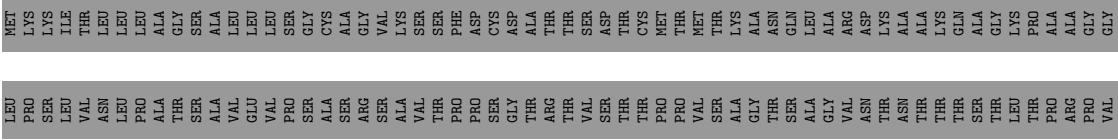
• Molecule 1: TraV

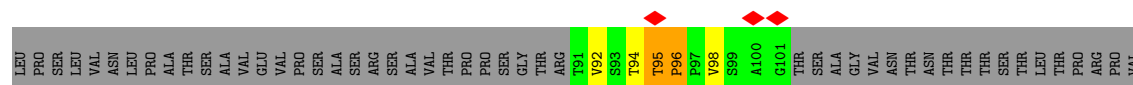


• Molecule 1: TraV

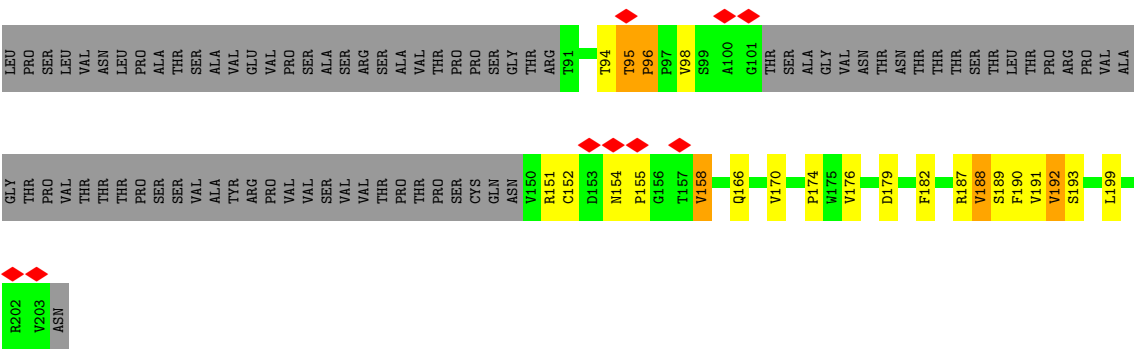


• Molecule 1: TraV

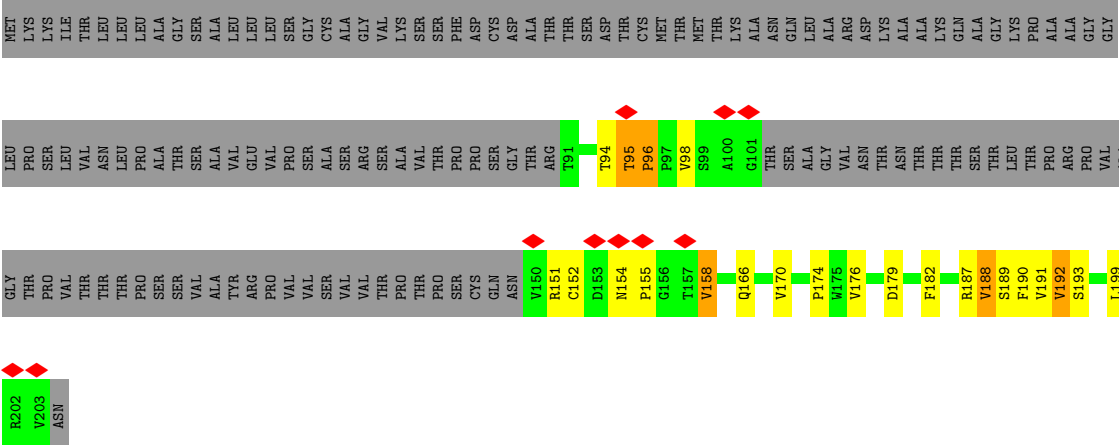




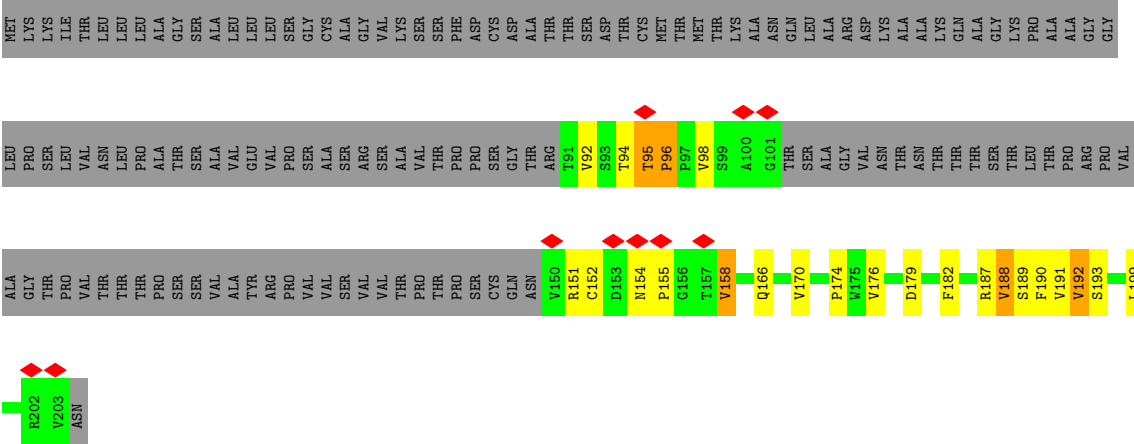




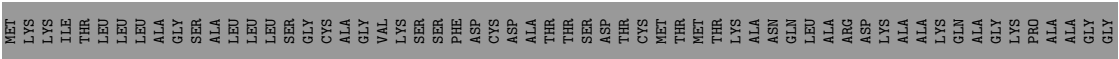
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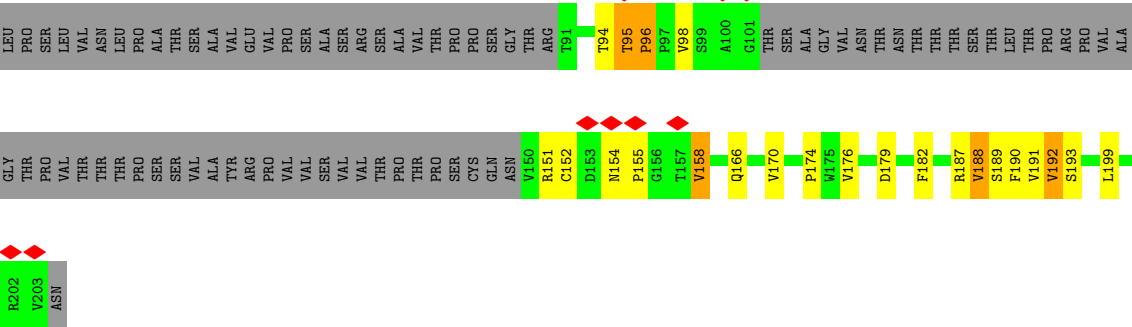


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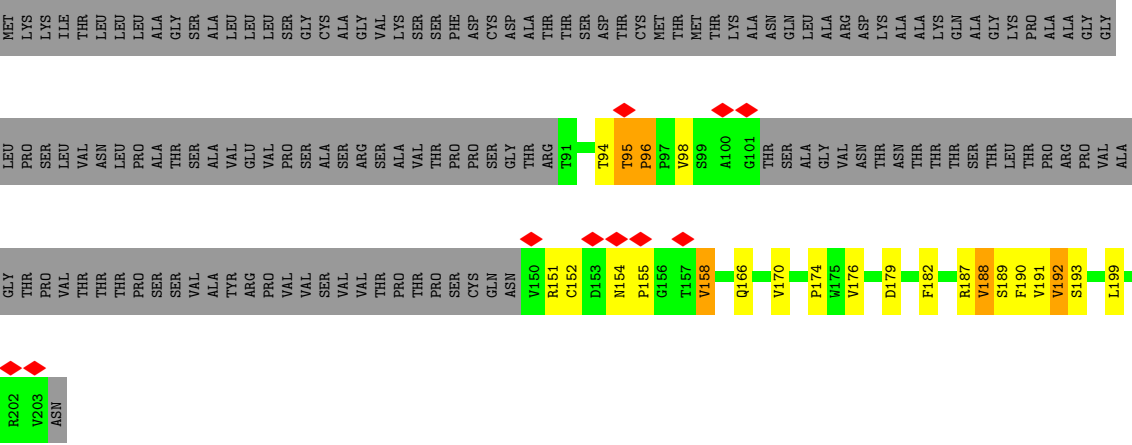


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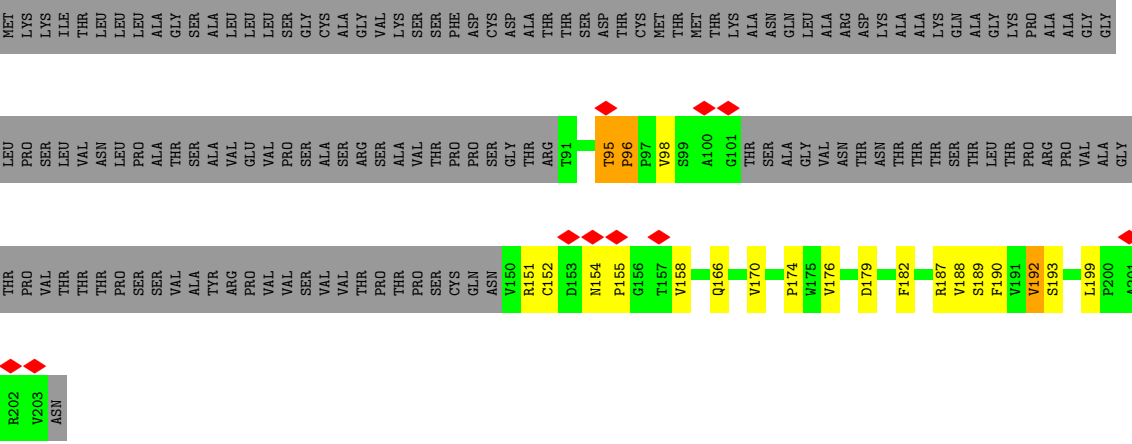




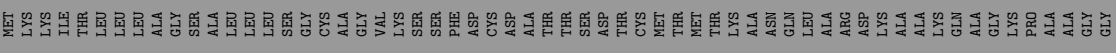
• Molecule 1: TraV

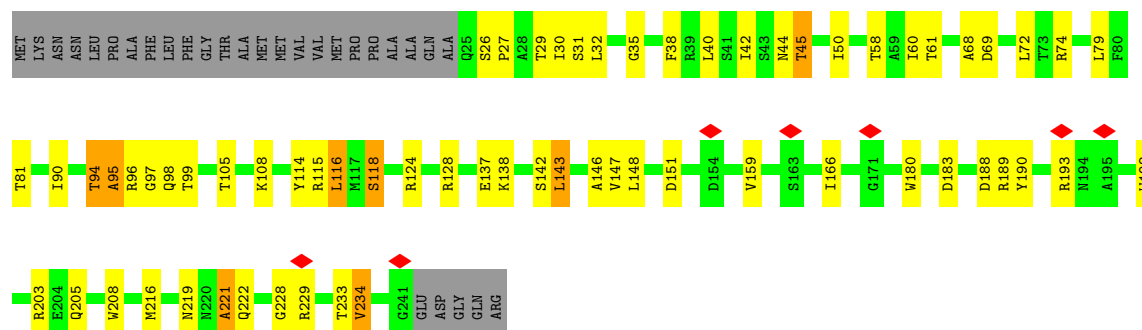


• Molecule 1: TraV

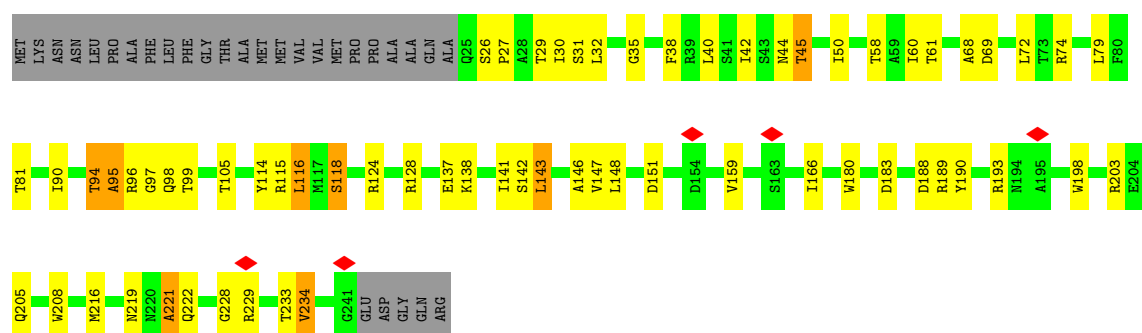


• Molecule 1: TraV

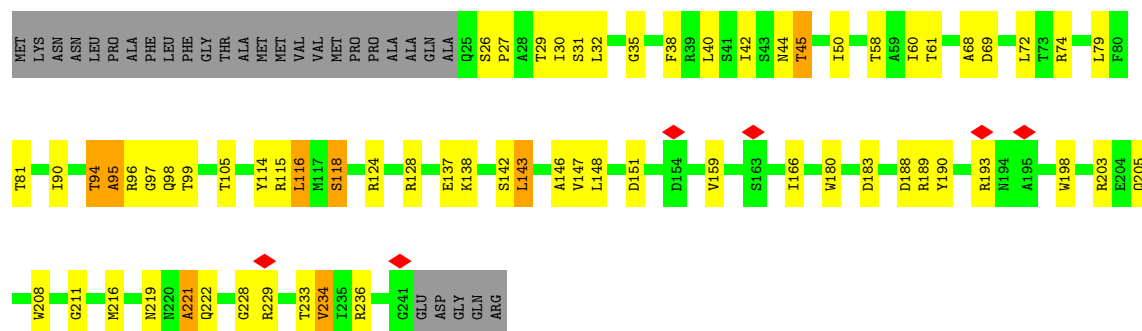




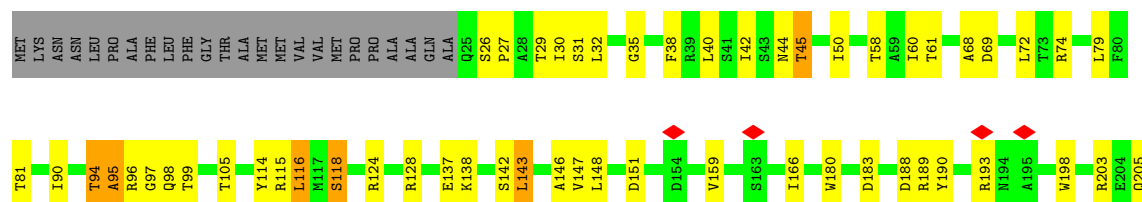
• Molecule 2: TraK

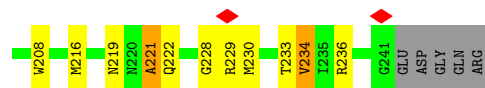


• Molecule 2: TraK

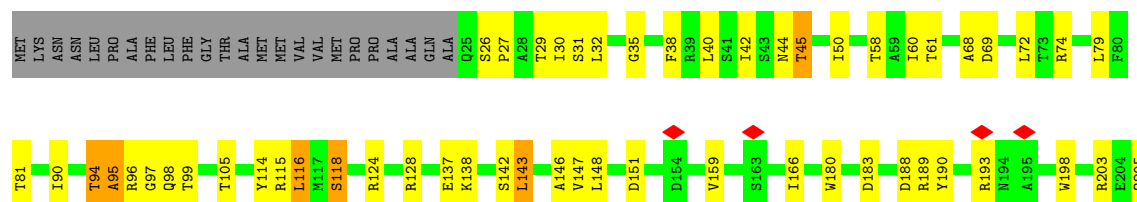


• Molecule 2: TraK

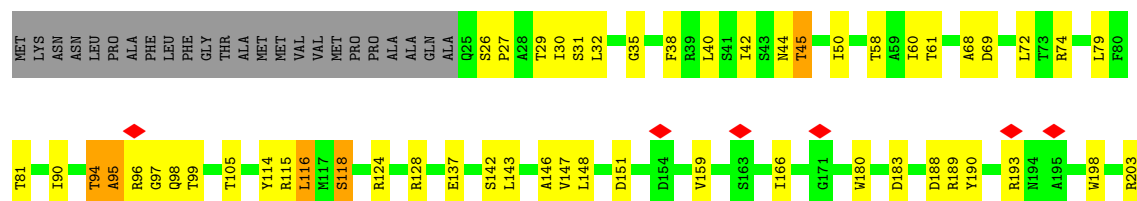




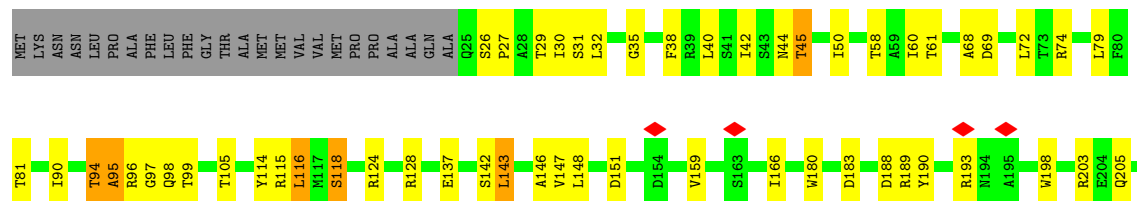
• Molecule 2: TraK



• Molecule 2: TraK

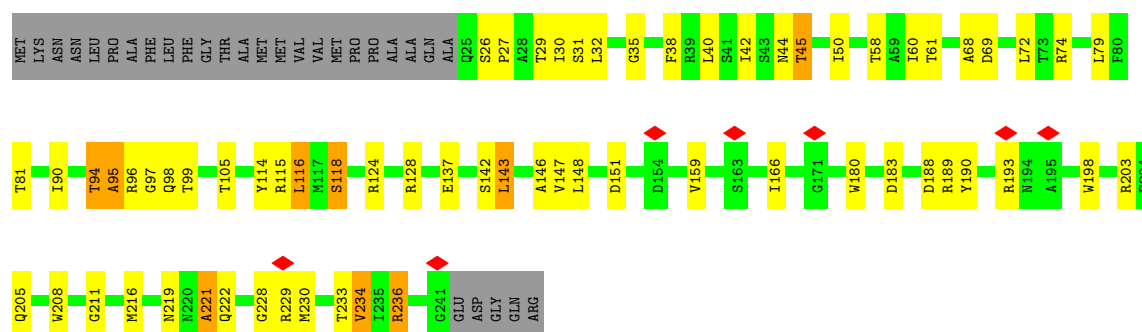


• Molecule 2: TraK



• Molecule 2: TraK





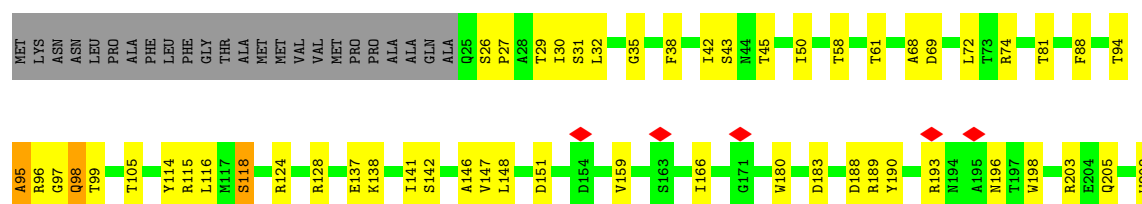
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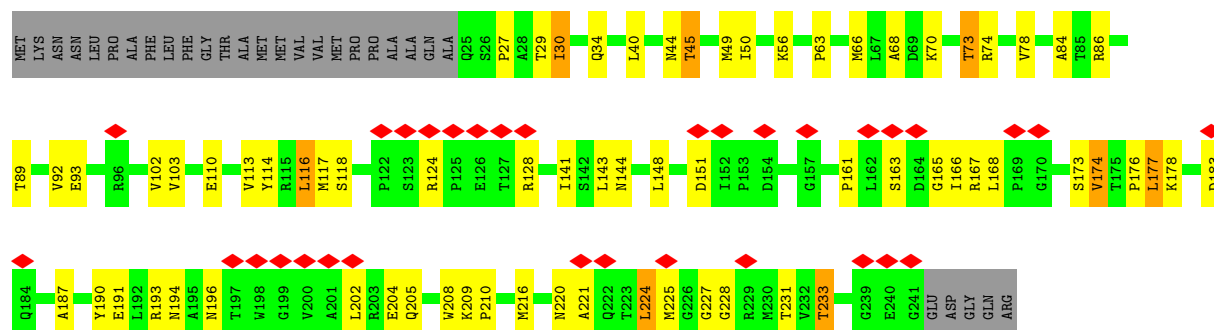
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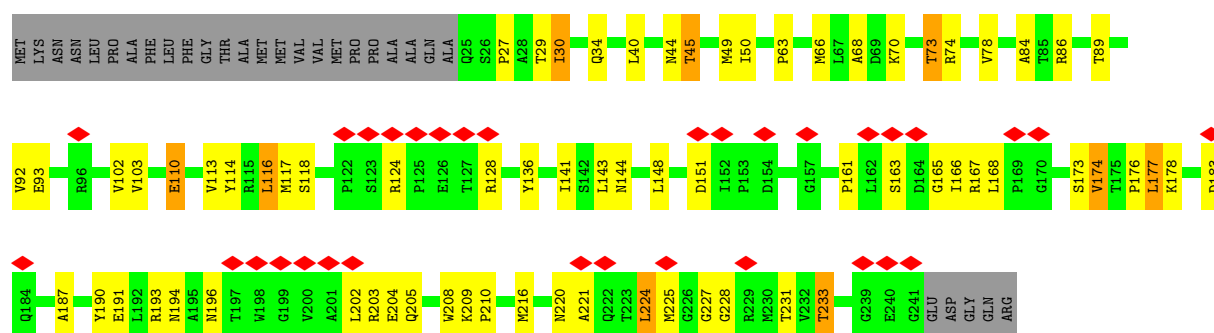
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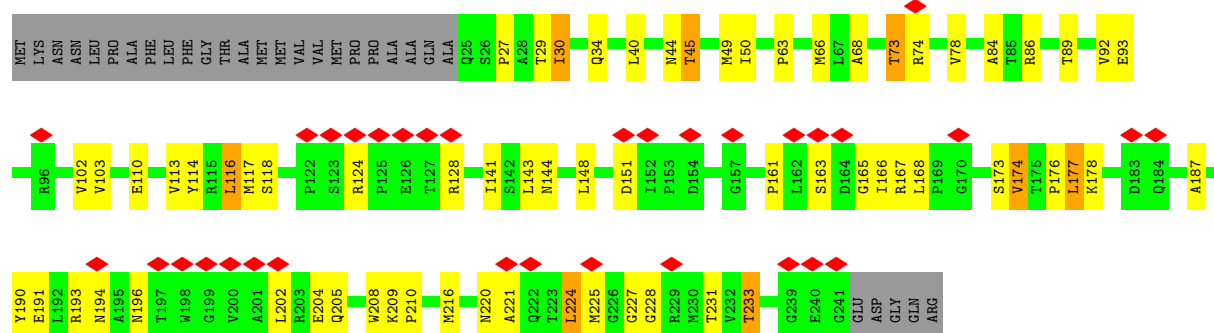




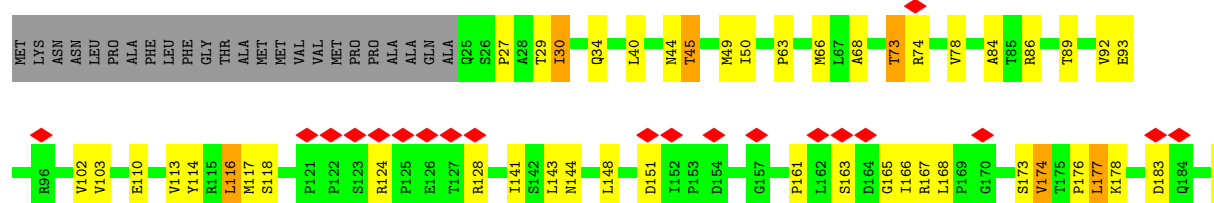
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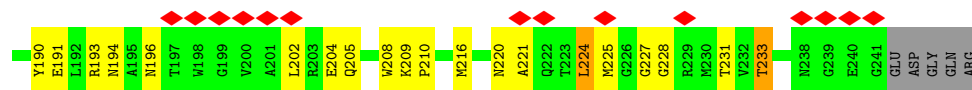


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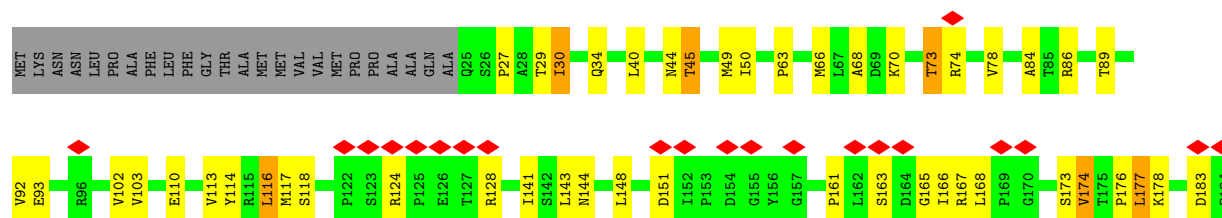


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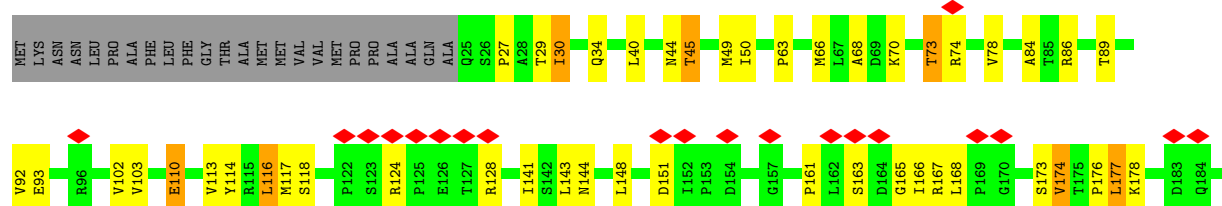




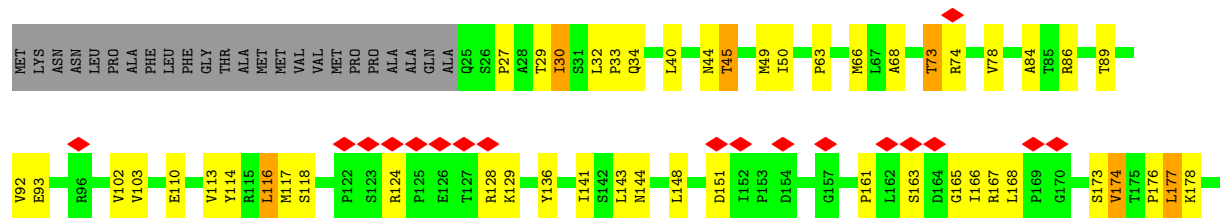
- Molecule 2: TraK



- Molecule 2: TraK

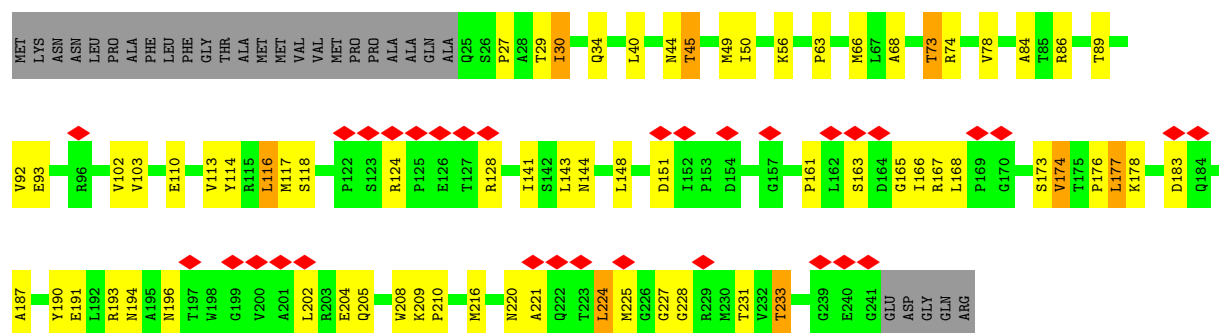


- Molecule 2: TraK



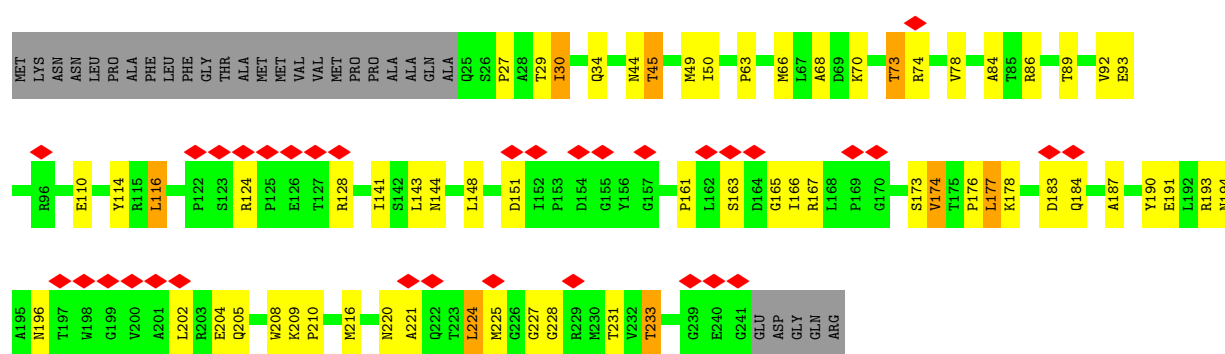
- Molecule 2: TraK

Chain D9: 



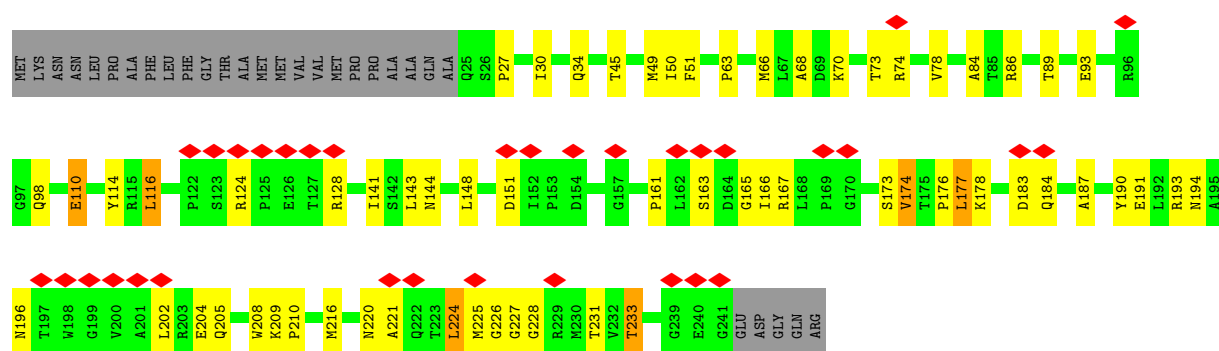
• Molecule 2: TraK

Chain D10: 



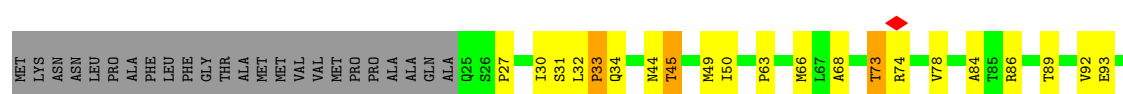
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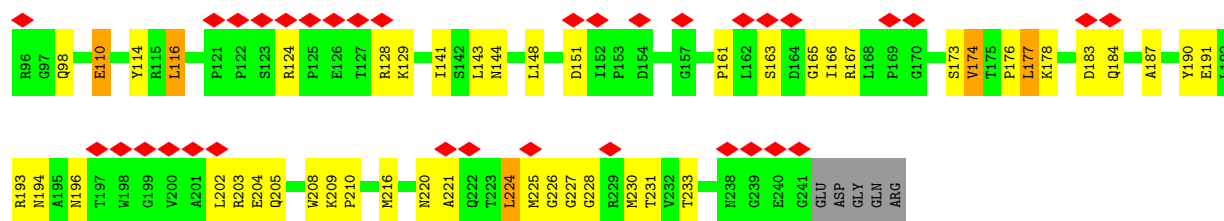
Chain D11: 



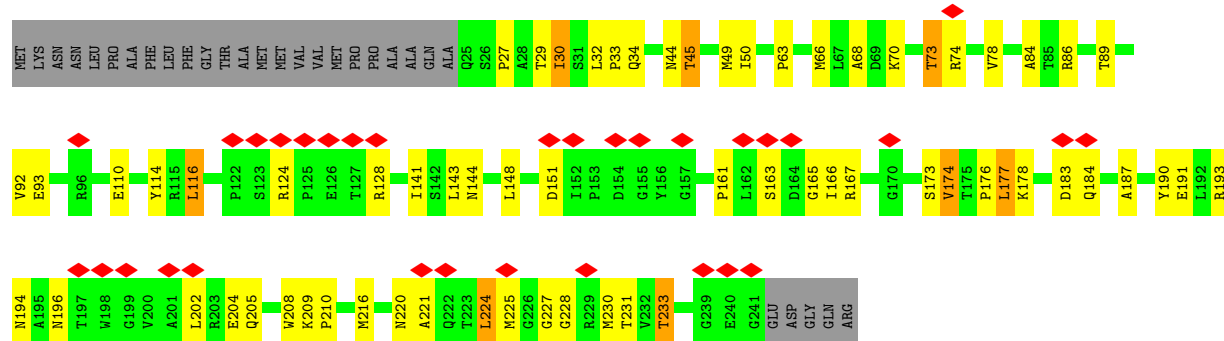
• Molecule 2: TraK

Chain D12: 

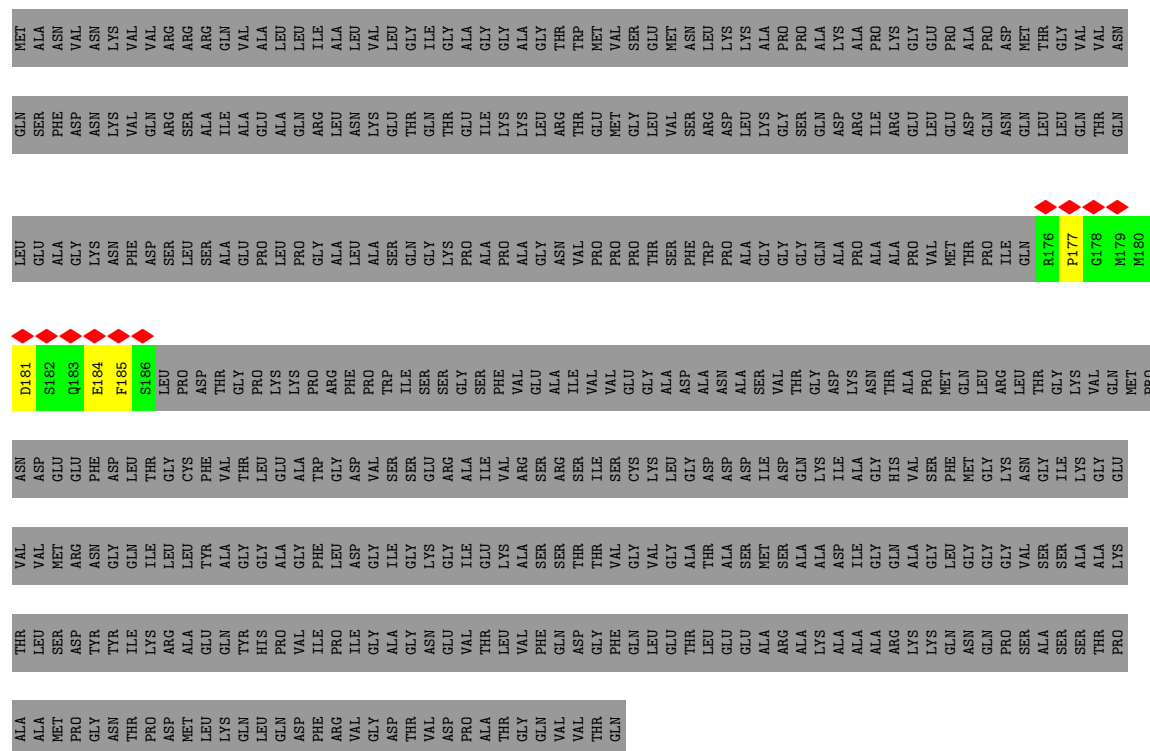




• Molecule 2: TraK



• Molecule 3: TraB



• Molecule 3: TraB

98%

D181	S182	Q183	E184	F185	S186	LEU	PRO	PRO	THR	GLY	PRO	LYS	LYS	PRO	ARG	PHE	PRO	TRP	ILE	SER	GLY	SER	PHE	VAL	GLU	ALA	ILE	VAL	VAL	GLU	GLY	ASP	ALA	ASN	ALA	SER	VAL	THR	GLY	ASP	LYS	ASN	THR	ALA	PRO	MET	GLN	LEU	ARG	LEU	THR	GLY	LYS	VAL	GLN	MET	PRO
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- Molecule 3: TraB

98%

D181	S182	Q183	E184	F185	S186	LEU	PRO	ASP	THR	GLY	PRO	LYS	LYS	PRO	ARG	PHE	PRO	TRP	ILE	SER	SER	GLY	GLY	PHE	VAL	GLU	ALA	ILE	VAL	VAL	GLU	GLY	ALA	ASP	ALA	ASN	ALA	ALA	SER	SER	VAL	THR	VAL	GLY	ASP	LYS	ASN	THR	THR	ALA	PRO	MET	GLN	LEU	ARG	LEU	THR	GLY	LYS	VAL	GLN	MET	PRO
------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain E4: 98%

ALA	ALA	THR	VAL	ASN	D181
ALA	MET	LEU	VAL	ASP	S182
PRO	PRO	SER	MET	GLU	Q183
GLY	GLY	ASP	ARG	GLU	E184
ASN	ASN	TYR	ASN	PHE	F185
THR	THR	ILE	GLN	ASP	S186
PRO	PRO	LYS	ILE	LEU	LEU
ASP	ASP	ARG	LEU	GLY	PRO
MET	MET	ALA	LEU	PHE	ASP
LEU	LEU	GLN	VAL	THR	THR
LYS	LYS	GLY	ALA	VAL	GLY
GLN	GLN	TYR	GLY	THR	PRO
LEU	LEU	HIS	GLY	LEU	LYS
GLN	GLN	PRO	ALA	GLU	LYS
ASP	ASP	VAL	GLY	ALA	PRO
PHE	PHE	ILE	PHE	TRP	ARG
ARG	ARG	PRO	LEU	GLY	PHE
VAL	VAL	ILE	ASP	ASP	PRO
GLY	GLY	GLY	GLY	VAL	TRP
ASP	ASP	ALA	ILE	SER	ILE
THR	THR	ASN	GLY	SER	SER
VAL	VAL	VAL	LYS	GLU	SER
ASP	ASP	GLY	GLY	ARG	GLY
PRO	PRO	VAL	ILE	ALA	SER
ALA	ALA	THR	LEU	ILE	SER
THR	THR	LEU	GLY	VAL	PHE
ALA	ALA	VAL	LYS	VAL	VAL
GLN	GLN	PHE	ALA	ARG	GLU
GLY	GLY	ASN	ALA	SER	ALA
VAL	VAL	GLN	SER	ARG	ILE
VAL	VAL	ASP	THR	SER	VAL
THR	THR	GLY	THR	ILE	VAL
GLN	GLN	PHE	GLY	CYS	GLU
		LEU	GLY	LYS	GLY
		GLY	GLY	LEU	ALA
		THR	ALA	GLY	ASP
		LEU	THR	ASP	ALA
		GLU	ALA	ASP	ASN
		GLY	GLY	ASP	ALA
		ALA	MET	ILE	SER
		ARG	SER	ASP	SER
		ALA	VAL	ASP	THR
		LYS	ALA	GLN	GLY
		LYS	ALA	LYS	ASP
		ALA	ASP	ILE	LYS
		ALA	ILE	ALA	ASN
		ARG	GLY	GLY	THR
		LYS	GLN	HIS	ALA
		VAL	ALA	VAL	VAL
		SER	GLY	SER	PRO
		ALA	LEU	PHE	MET
		GLN	GLY	MET	GLN
		PRO	GLY	GLY	LEU
		SER	GLY	LYS	ARG
		ALA	VAL	ASN	LEU
		THR	SER	GLY	THR
		SER	SER	ILE	GLY
		SER	ALA	LYS	LYS
		THR	ALA	GLY	VAL
		PRO	LYS	GLU	GLN
					MET
					PRO

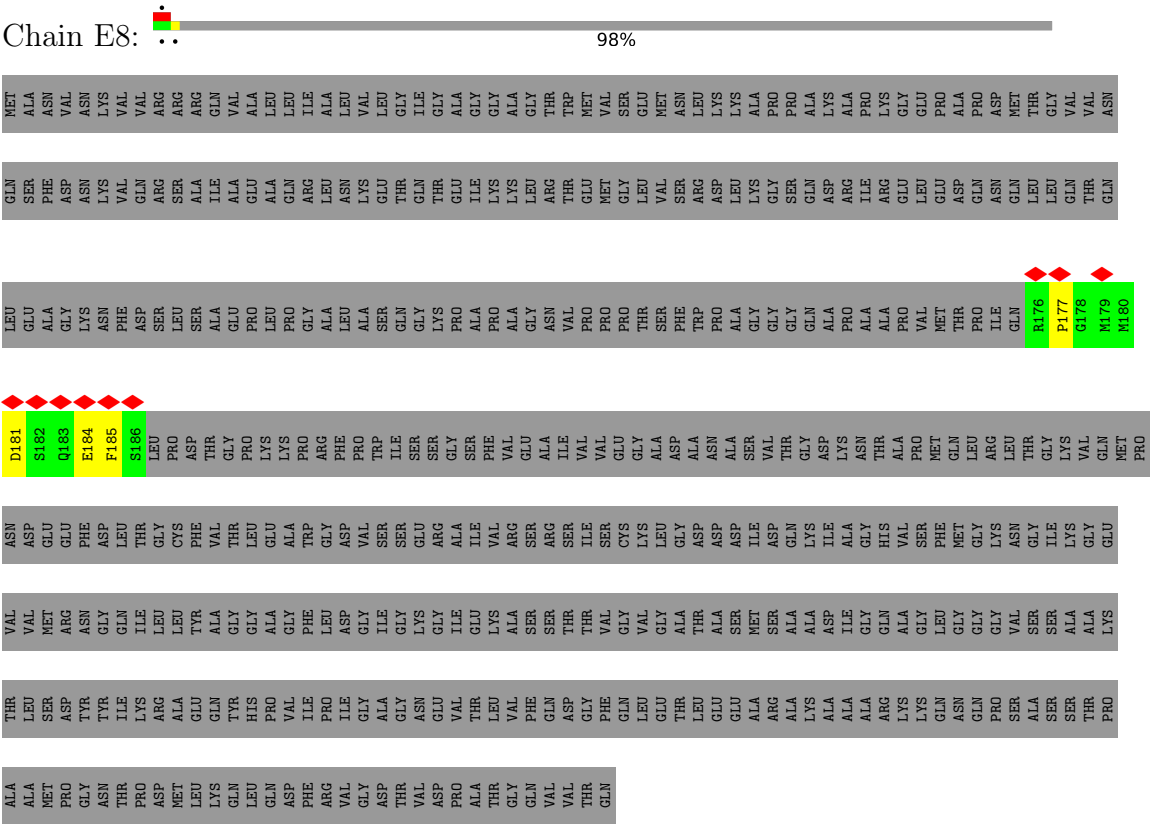
Chain E5: 98%

ALA	ALA	THR	VAL	ASN	D181
ALA	ALA	THR	VAL	ASP	S182
MET	MET	SER	MET	GLU	Q183
PRO	PRO	ARG	ASN	PHE	E184
GLY	GLY	TYR	GLY	ASP	F185
ASN	ASN	TYR	GLN	LEU	S186
THR	THR	ILE	ILE	THR	LEU
PRO	PRO	LYS	ARG	GLY	PRO
ASP	ASP	ALA	LEU	PHE	ASP
MET	MET	ALA	LEU	THR	THR
LEU	LEU	GLN	TYR	VAL	PRO
LYS	LYS	GLY	ALA	THR	GLY
GLN	GLN	TYR	GLY	LEU	PRO
LEU	LEU	HIS	GLY	GLU	LYS
GLN	GLN	PRO	ALA	ALA	PRO
ASP	ASP	VAL	GLY	GLY	LYS
PHE	PHE	ILE	PHE	TRP	ALA
ARG	ARG	PRO	LEU	GLY	ARG
VAL	VAL	ILE	ASP	ASP	PHE
GLY	GLY	GLY	GLY	VAL	PRO
ASP	ASP	ALA	ILE	SER	TRP
THR	THR	ALA	GLY	SER	ILE
VAL	VAL	ASN	LYS	GLU	SER
ASP	ASP	GLU	GLY	ARG	SER
PRO	PRO	VAL	ILE	ALA	GLY
ALA	ALA	THR	GLU	ILE	SER
THR	THR	LEU	LYS	VAL	PHE
GLY	GLY	PHE	ALA	ARG	VAL
GLN	GLN	VAL	SER	SER	GLU
VAL	VAL	GLN	SER	ARG	ALA
THR	THR	ASP	THR	SER	ILE
GLN	GLN	PHE	VAL	ILE	VAL
		LEU	GLY	CYS	GLU
		GLU	VAL	LYS	GLY
		THR	GLY	LEU	ALA
		LEU	ALA	GLY	ASP
		LEU	THR	ASP	ALA
		GLU	ALA	ASP	ASN
		GLU	SER	ASP	ALA
		ALA	MET	ILE	SER
		ARG	SER	ASP	VAL
		LYS	ALA	GLN	THR
		ALA	ALA	LYS	GLY
		ALA	ASP	ILE	ASP
		ALA	ILE	GLY	ASN
		ALA	GLY	HIS	THR
		ARG	GLN	VAL	ALA
		LYS	ALA	VAL	PRO
		LYS	GLY	SER	MET
		GLN	LEU	PHE	GLN
		ASN	GLY	MET	LEU
		GLN	GLY	GLY	ARG
		PRO	GLY	LYS	LEU
		SER	VAL	ASN	THR
		ALA	SER	GLY	GLY
		SER	SER	ILE	LYS
		SER	ALA	LYS	VAL
		THR	ALA	GLY	GLN
		PRO	LYS	GLU	MET
					PRO

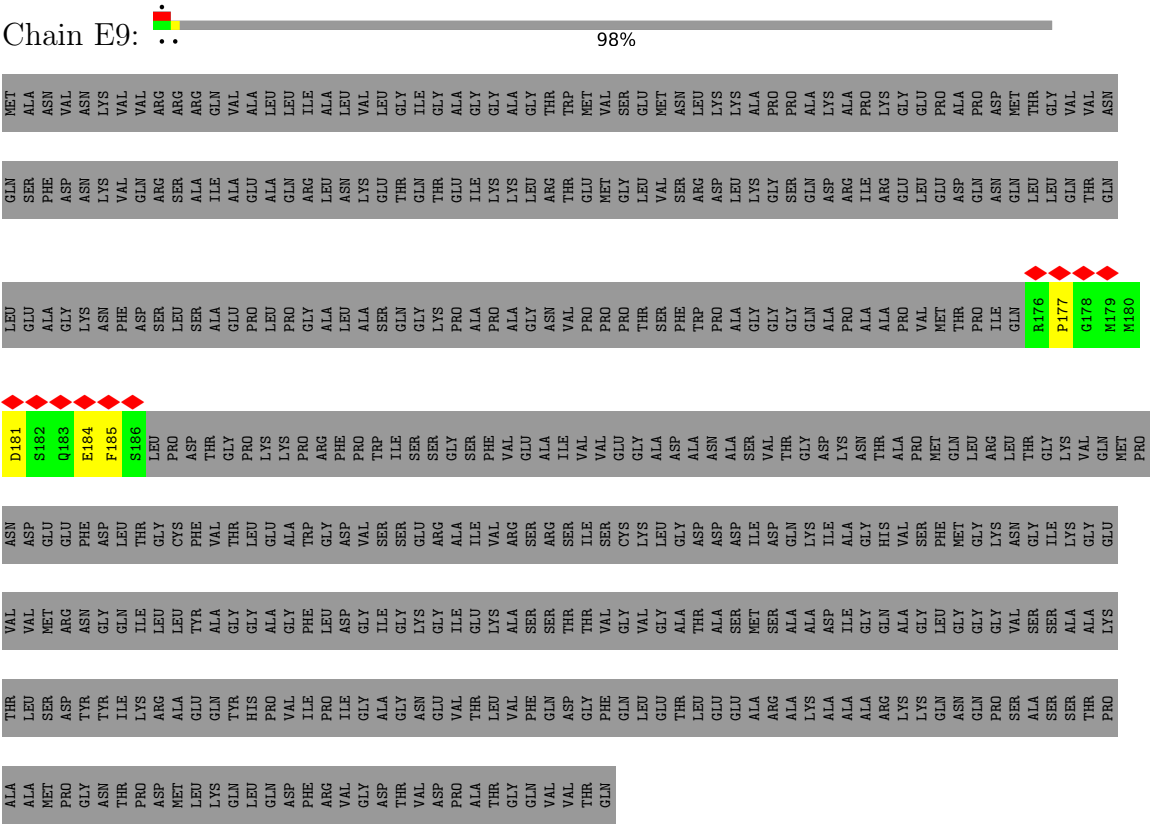
Chain E6: 98%



● Molecule 3: TraB



● Molecule 3: TraB



Chain E10: 98%



Chain E12: 98%

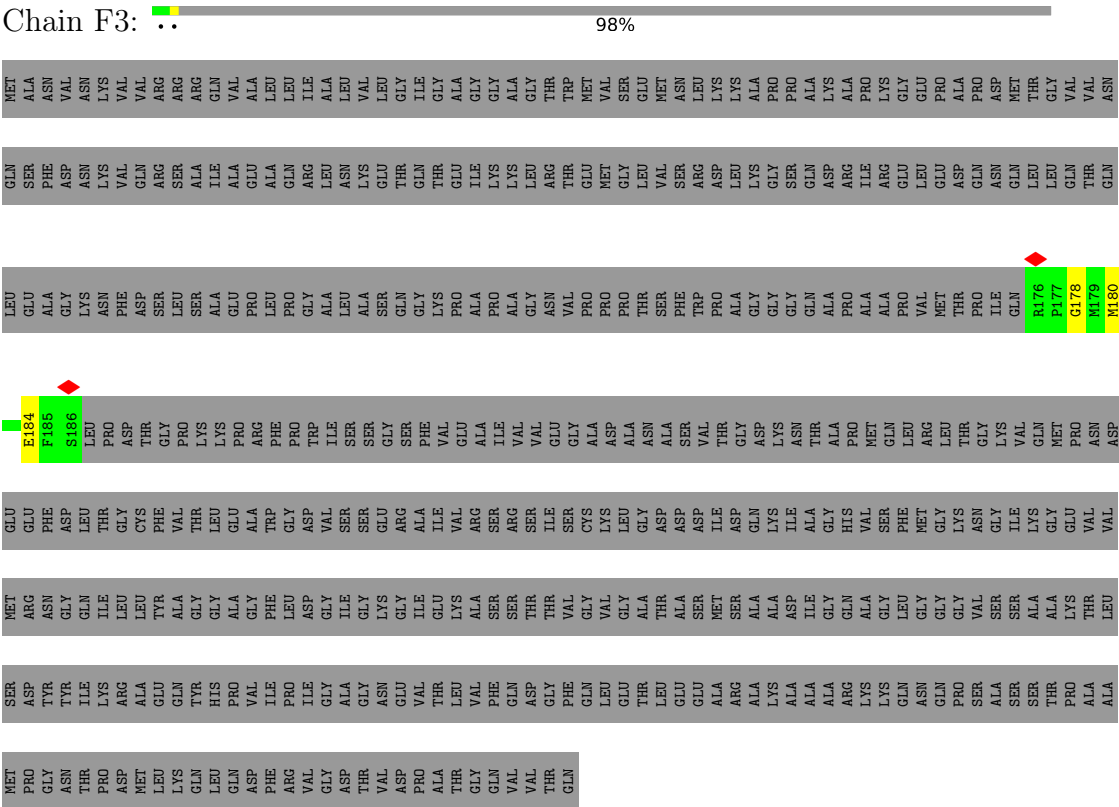


Chain F1: 98%

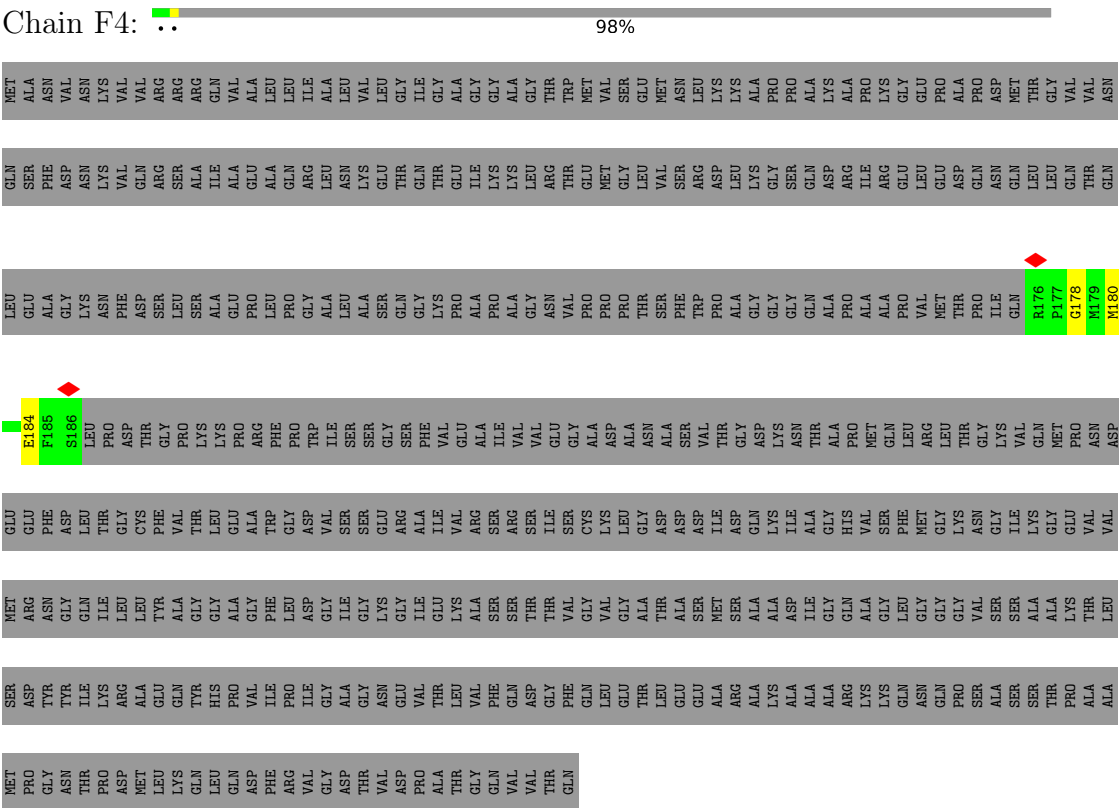
Chain F2: .. 98%



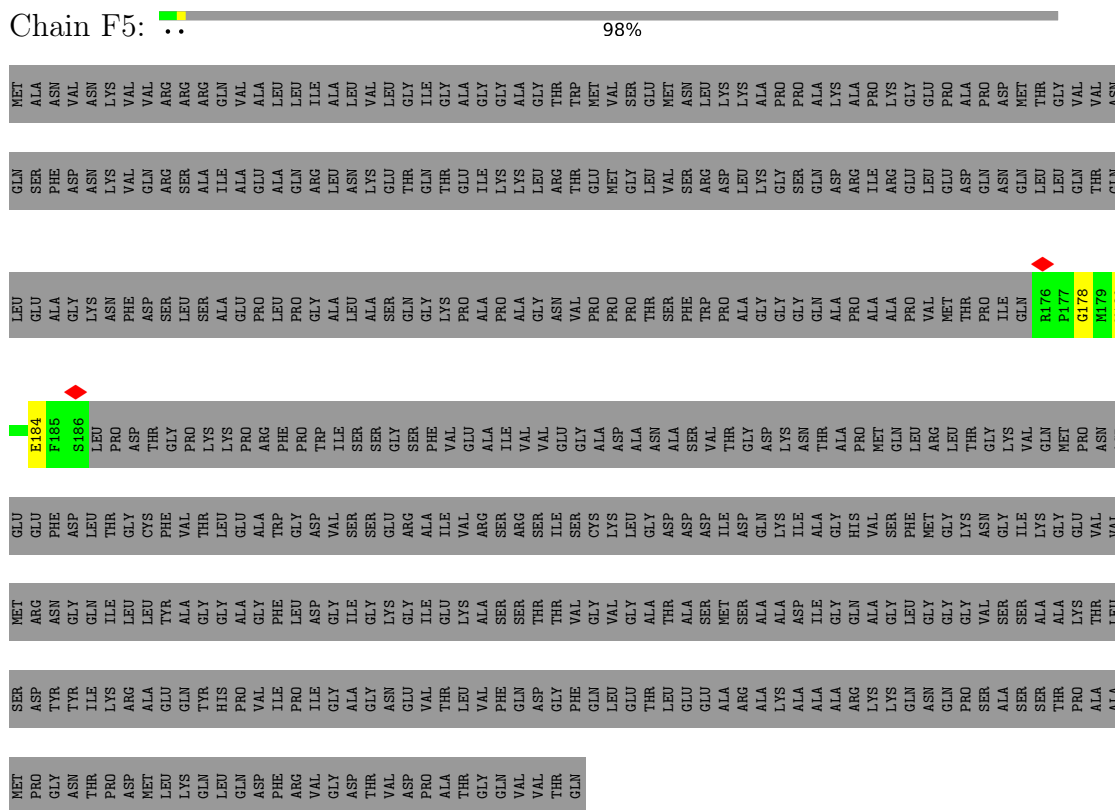
● Molecule 3: TraB



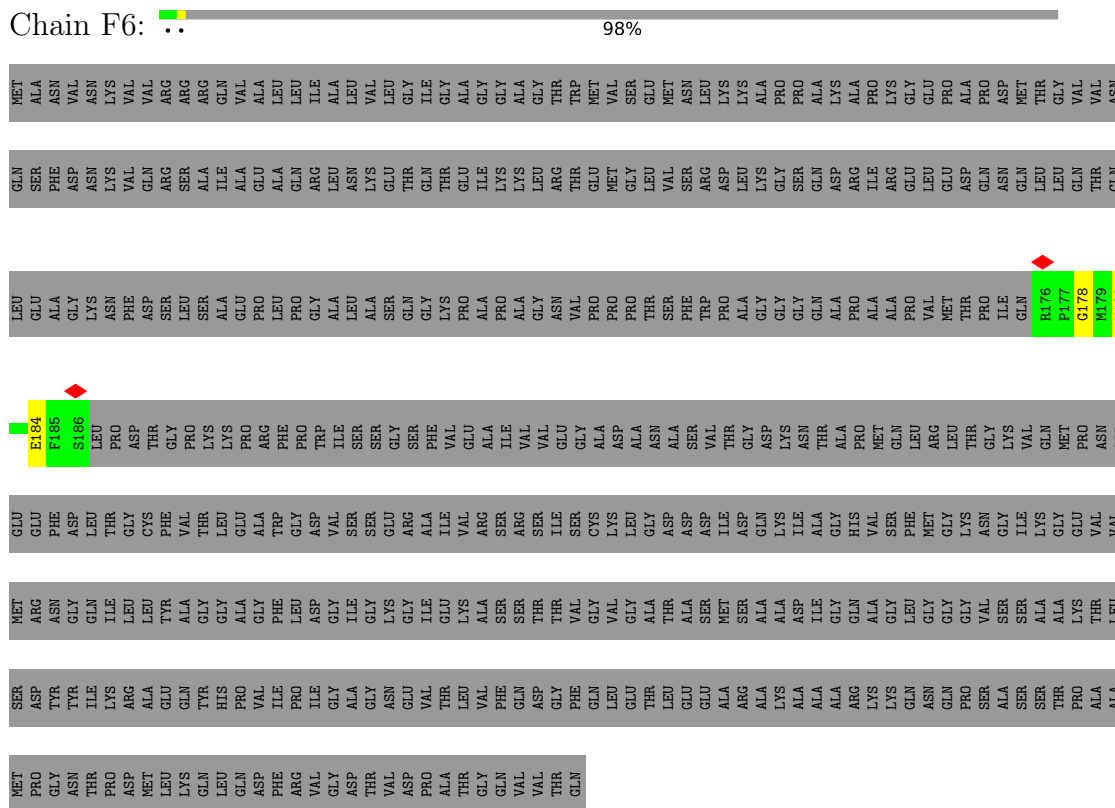
● Molecule 3: TraB



- Molecule 3: TraB



- Molecule 3: TraB

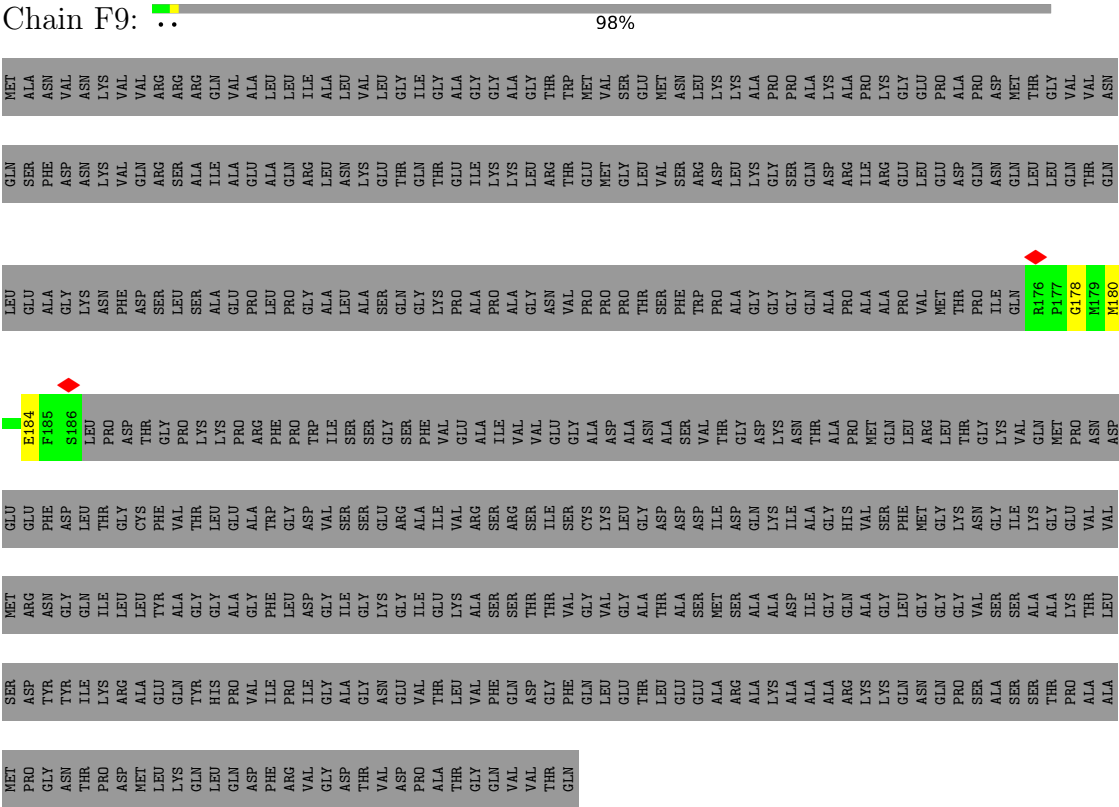


Chain F7: 98%

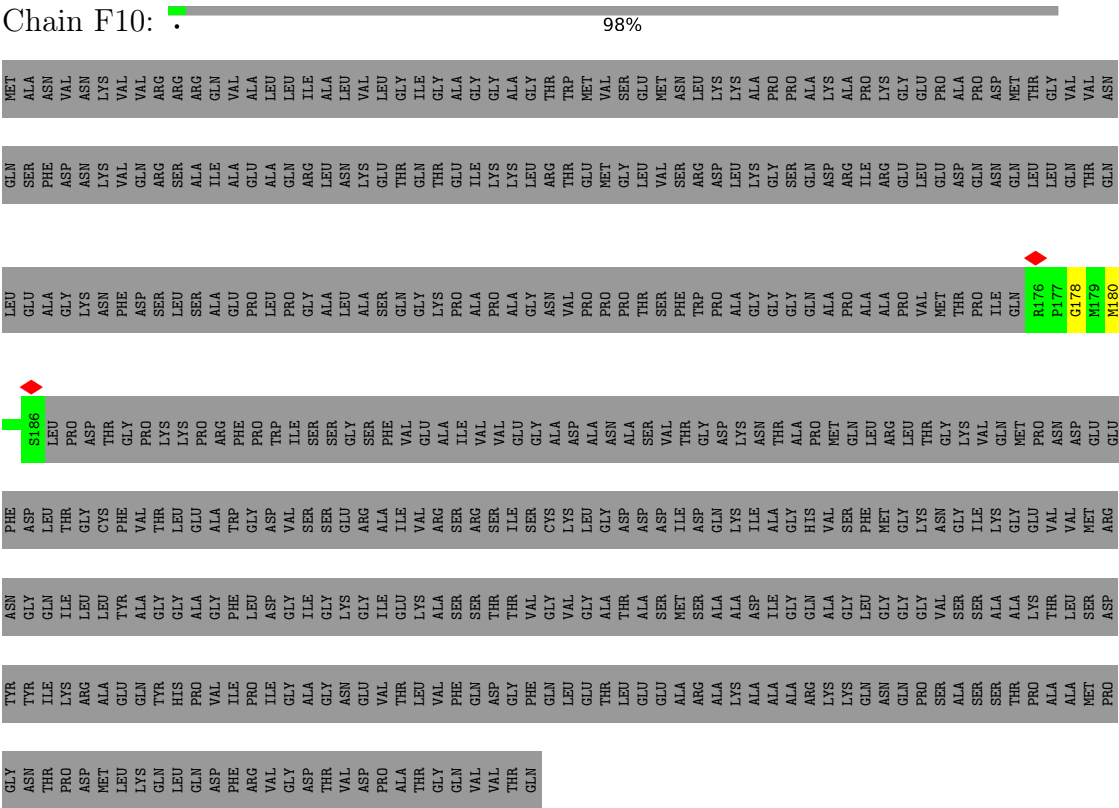
Chain F8: 98%



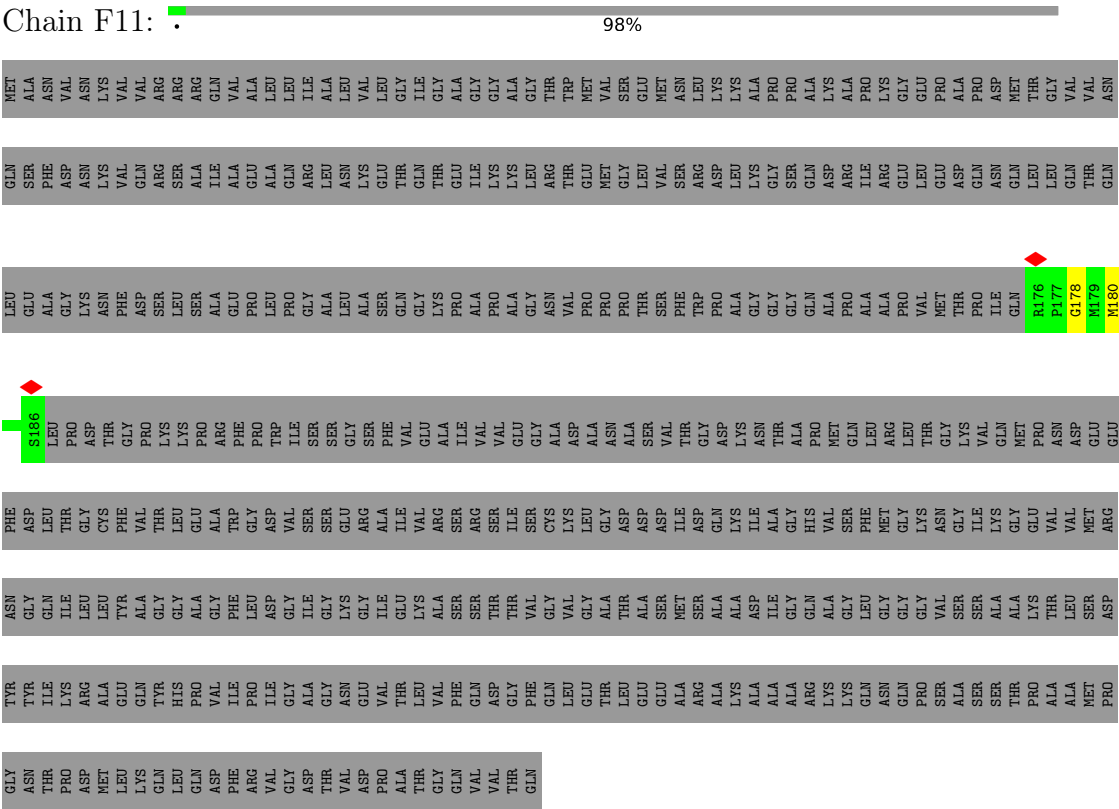
● Molecule 3: TraB



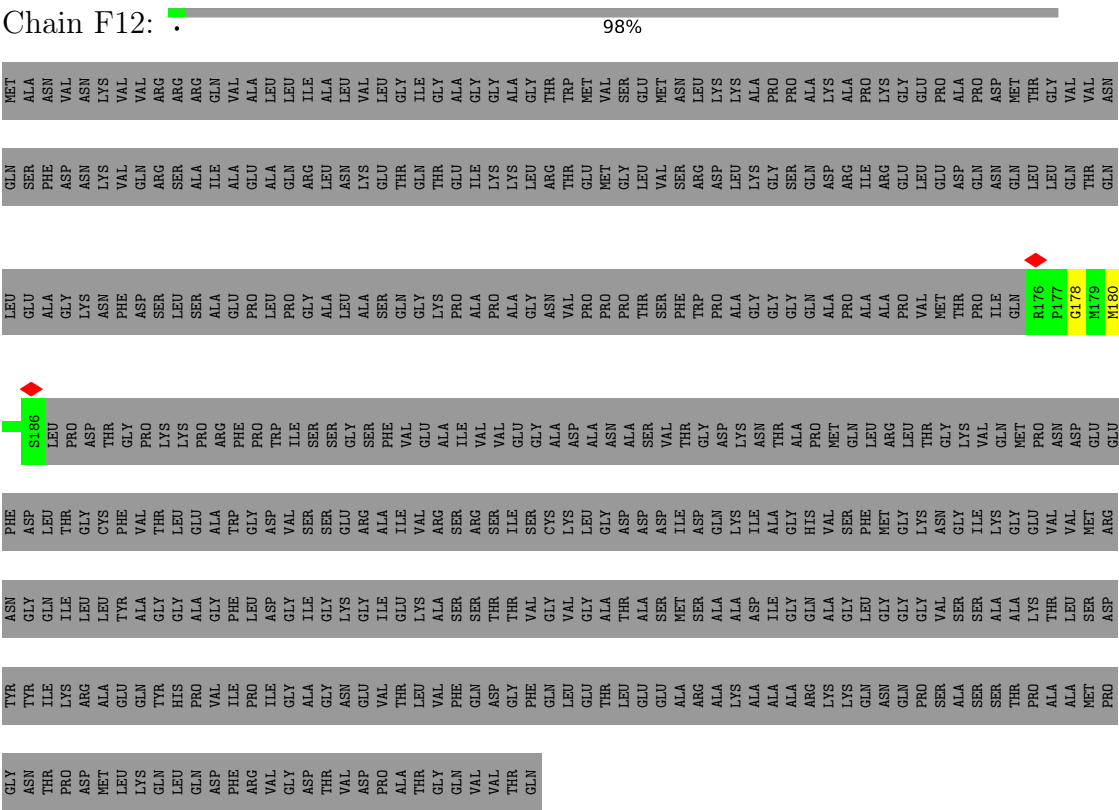
● Molecule 3: TraB



● Molecule 3: TraB



● Molecule 3: TraB



Chain F13: 98%

[illegible]

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.52	0/451	1.05	3/622 (0.5%)
1	A10	0.52	0/451	1.05	3/622 (0.5%)
1	A11	0.52	0/451	1.05	3/622 (0.5%)
1	A12	0.52	0/451	1.05	3/622 (0.5%)
1	A13	0.52	0/451	1.05	3/622 (0.5%)
1	A2	0.52	0/451	1.05	3/622 (0.5%)
1	A3	0.52	0/451	1.05	3/622 (0.5%)
1	A4	0.52	0/451	1.05	3/622 (0.5%)
1	A5	0.52	0/451	1.04	3/622 (0.5%)
1	A6	0.52	0/451	1.04	3/622 (0.5%)
1	A7	0.52	0/451	1.05	3/622 (0.5%)
1	A8	0.52	0/451	1.05	3/622 (0.5%)
1	A9	0.52	0/451	1.05	3/622 (0.5%)
1	B1	0.59	0/514	1.06	6/710 (0.8%)
1	B10	0.59	0/514	1.06	6/710 (0.8%)
1	B11	0.59	0/514	1.06	6/710 (0.8%)
1	B12	0.59	0/514	1.06	6/710 (0.8%)
1	B13	0.59	0/514	1.06	6/710 (0.8%)
1	B2	0.59	0/514	1.06	6/710 (0.8%)
1	B3	0.59	0/514	1.06	6/710 (0.8%)
1	B4	0.59	0/514	1.06	6/710 (0.8%)
1	B5	0.59	0/514	1.06	6/710 (0.8%)
1	B6	0.59	0/514	1.06	6/710 (0.8%)
1	B7	0.59	0/514	1.06	6/710 (0.8%)
1	B8	0.59	0/514	1.06	6/710 (0.8%)
1	B9	0.59	0/514	1.06	6/710 (0.8%)
2	C1	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C10	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C11	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C12	0.83	2/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C13	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C2	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C3	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C4	0.83	2/1688 (0.1%)	1.03	8/2290 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	C5	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C6	0.83	2/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C7	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C8	0.83	2/1688 (0.1%)	1.03	8/2290 (0.3%)
2	C9	0.83	1/1688 (0.1%)	1.03	8/2290 (0.3%)
2	D1	0.61	0/1688	1.07	11/2290 (0.5%)
2	D10	0.62	0/1688	1.07	11/2290 (0.5%)
2	D11	0.61	0/1688	1.07	11/2290 (0.5%)
2	D12	0.61	0/1688	1.07	11/2290 (0.5%)
2	D13	0.62	0/1688	1.07	11/2290 (0.5%)
2	D2	0.62	0/1688	1.07	11/2290 (0.5%)
2	D3	0.62	0/1688	1.07	11/2290 (0.5%)
2	D4	0.62	0/1688	1.07	11/2290 (0.5%)
2	D5	0.61	0/1688	1.07	11/2290 (0.5%)
2	D6	0.61	0/1688	1.07	11/2290 (0.5%)
2	D7	0.62	0/1688	1.07	11/2290 (0.5%)
2	D8	0.62	0/1688	1.07	11/2290 (0.5%)
2	D9	0.62	0/1688	1.07	11/2290 (0.5%)
3	E1	0.66	0/88	0.83	0/115
3	E10	0.66	0/88	0.83	0/115
3	E11	0.67	0/88	0.83	0/115
3	E12	0.66	0/88	0.84	0/115
3	E13	0.66	0/88	0.83	0/115
3	E2	0.67	0/88	0.84	0/115
3	E3	0.66	0/88	0.83	0/115
3	E4	0.67	0/88	0.83	0/115
3	E5	0.67	0/88	0.83	0/115
3	E6	0.67	0/88	0.83	0/115
3	E7	0.67	0/88	0.83	0/115
3	E8	0.67	0/88	0.84	0/115
3	E9	0.66	0/88	0.84	0/115
3	F1	0.68	0/88	1.21	0/115
3	F10	0.68	0/88	1.20	0/115
3	F11	0.68	0/88	1.21	0/115
3	F12	0.68	0/88	1.20	0/115
3	F13	0.68	0/88	1.21	0/115
3	F2	0.68	0/88	1.20	0/115
3	F3	0.68	0/88	1.21	0/115
3	F4	0.68	0/88	1.20	0/115
3	F5	0.69	0/88	1.21	0/115
3	F6	0.68	0/88	1.21	0/115
3	F7	0.67	0/88	1.21	0/115
3	F8	0.68	0/88	1.21	0/115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	F9	0.68	0/88	1.20	0/115
All	All	0.69	17/58721 (0.0%)	1.05	364/79846 (0.5%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C11	180	TRP	CA-C	-5.12	1.46	1.52
2	C7	180	TRP	CA-C	-5.09	1.46	1.52
2	C4	180	TRP	CA-C	-5.09	1.46	1.52
2	C5	180	TRP	CA-C	-5.09	1.46	1.52
2	C8	180	TRP	CA-C	-5.09	1.46	1.52
2	C10	180	TRP	CA-C	-5.09	1.46	1.52
2	C1	180	TRP	CA-C	-5.07	1.46	1.52
2	C12	180	TRP	CA-C	-5.07	1.46	1.52
2	C2	180	TRP	CA-C	-5.06	1.46	1.52
2	C13	180	TRP	CA-C	-5.04	1.46	1.52
2	C3	180	TRP	CA-C	-5.04	1.46	1.52
2	C6	180	TRP	CA-C	-5.04	1.46	1.52
2	C6	236	ARG	CA-C	-5.04	1.47	1.53
2	C8	236	ARG	CA-C	-5.04	1.47	1.53
2	C4	236	ARG	CA-C	-5.04	1.47	1.53
2	C12	236	ARG	CA-C	-5.03	1.47	1.53
2	C9	180	TRP	CA-C	-5.00	1.46	1.52

All (364) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D5	165	GLY	N-CA-C	9.81	124.51	112.73
2	D2	165	GLY	N-CA-C	9.80	124.50	112.73
2	D7	165	GLY	N-CA-C	9.80	124.49	112.73
2	D10	165	GLY	N-CA-C	9.80	124.49	112.73
2	D4	165	GLY	N-CA-C	9.79	124.48	112.73
2	D1	165	GLY	N-CA-C	9.79	124.48	112.73
2	D6	165	GLY	N-CA-C	9.79	124.48	112.73
2	D9	165	GLY	N-CA-C	9.79	124.48	112.73
2	D8	165	GLY	N-CA-C	9.79	124.47	112.73
2	D13	165	GLY	N-CA-C	9.78	124.47	112.73
2	D12	165	GLY	N-CA-C	9.77	124.46	112.73
2	D11	165	GLY	N-CA-C	9.77	124.45	112.73
2	D3	165	GLY	N-CA-C	9.76	124.45	112.73
2	D6	166	ILE	N-CA-C	9.36	121.27	108.17
2	D8	166	ILE	N-CA-C	9.36	121.27	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D4	166	ILE	N-CA-C	9.35	121.25	108.17
2	D9	166	ILE	N-CA-C	9.35	121.25	108.17
2	D12	166	ILE	N-CA-C	9.34	121.25	108.17
2	D10	166	ILE	N-CA-C	9.34	121.25	108.17
2	D2	166	ILE	N-CA-C	9.33	121.23	108.17
2	D5	166	ILE	N-CA-C	9.33	121.23	108.17
2	D1	166	ILE	N-CA-C	9.33	121.23	108.17
2	D7	166	ILE	N-CA-C	9.32	121.22	108.17
2	D13	166	ILE	N-CA-C	9.31	121.21	108.17
2	D11	166	ILE	N-CA-C	9.31	121.20	108.17
2	D3	166	ILE	N-CA-C	9.31	121.20	108.17
2	D8	163	SER	N-CA-C	-7.94	102.88	114.39
2	D12	163	SER	N-CA-C	-7.94	102.88	114.39
2	D6	163	SER	N-CA-C	-7.93	102.89	114.39
2	D5	163	SER	N-CA-C	-7.92	102.90	114.39
2	D7	163	SER	N-CA-C	-7.92	102.90	114.39
2	D1	163	SER	N-CA-C	-7.92	102.90	114.39
2	D3	163	SER	N-CA-C	-7.92	102.90	114.39
2	D11	163	SER	N-CA-C	-7.92	102.90	114.39
2	D4	163	SER	N-CA-C	-7.92	102.90	114.39
2	D13	163	SER	N-CA-C	-7.92	102.90	114.39
2	D9	163	SER	N-CA-C	-7.92	102.91	114.39
2	D10	163	SER	N-CA-C	-7.92	102.91	114.39
2	D2	163	SER	N-CA-C	-7.92	102.91	114.39
2	D9	220	ASN	N-CA-C	7.89	122.67	112.41
2	D10	220	ASN	N-CA-C	7.89	122.67	112.41
2	D6	220	ASN	N-CA-C	7.89	122.66	112.41
2	D4	220	ASN	N-CA-C	7.88	122.66	112.41
2	D1	220	ASN	N-CA-C	7.88	122.65	112.41
2	D5	220	ASN	N-CA-C	7.88	122.65	112.41
2	D3	220	ASN	N-CA-C	7.88	122.65	112.41
2	D8	220	ASN	N-CA-C	7.88	122.65	112.41
2	D7	220	ASN	N-CA-C	7.87	122.64	112.41
2	D12	220	ASN	N-CA-C	7.87	122.65	112.41
2	D13	220	ASN	N-CA-C	7.87	122.64	112.41
2	D2	220	ASN	N-CA-C	7.87	122.64	112.41
2	D11	220	ASN	N-CA-C	7.87	122.64	112.41
2	D6	45	THR	N-CA-C	7.71	119.76	111.36
2	D2	45	THR	N-CA-C	7.70	119.75	111.36
2	D4	45	THR	N-CA-C	7.69	119.75	111.36
2	D5	45	THR	N-CA-C	7.69	119.75	111.36
2	D1	45	THR	N-CA-C	7.69	119.74	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D12	45	THR	N-CA-C	7.69	119.74	111.36
2	D8	45	THR	N-CA-C	7.68	119.73	111.36
2	D11	45	THR	N-CA-C	7.68	119.73	111.36
2	D13	45	THR	N-CA-C	7.68	119.73	111.36
2	D7	45	THR	N-CA-C	7.68	119.73	111.36
2	D9	45	THR	N-CA-C	7.68	119.73	111.36
2	D3	45	THR	N-CA-C	7.67	119.72	111.36
2	D10	45	THR	N-CA-C	7.67	119.72	111.36
2	C6	118	SER	N-CA-C	7.61	120.46	111.71
2	C7	118	SER	N-CA-C	7.61	120.46	111.71
2	C3	118	SER	N-CA-C	7.61	120.46	111.71
2	C13	118	SER	N-CA-C	7.61	120.46	111.71
2	C2	118	SER	N-CA-C	7.60	120.45	111.71
2	C5	118	SER	N-CA-C	7.60	120.45	111.71
2	C1	118	SER	N-CA-C	7.58	120.43	111.71
2	C12	118	SER	N-CA-C	7.58	120.43	111.71
2	C8	118	SER	N-CA-C	7.58	120.42	111.71
2	C9	118	SER	N-CA-C	7.57	120.42	111.71
2	C11	118	SER	N-CA-C	7.55	120.40	111.71
2	C10	118	SER	N-CA-C	7.54	120.39	111.71
2	C4	118	SER	N-CA-C	7.54	120.38	111.71
2	D11	224	LEU	N-CA-C	-7.29	99.49	110.28
2	D10	224	LEU	N-CA-C	-7.29	99.50	110.28
2	D6	224	LEU	N-CA-C	-7.27	99.52	110.28
2	D3	224	LEU	N-CA-C	-7.27	99.52	110.28
2	D7	224	LEU	N-CA-C	-6.81	99.44	110.20
2	D5	224	LEU	N-CA-C	-6.80	99.46	110.20
2	D8	224	LEU	N-CA-C	-6.79	99.48	110.20
2	D1	224	LEU	N-CA-C	-6.78	99.49	110.20
2	D4	224	LEU	N-CA-C	-6.78	99.49	110.20
2	D13	224	LEU	N-CA-C	-6.78	99.49	110.20
2	D9	224	LEU	N-CA-C	-6.77	99.50	110.20
2	D2	224	LEU	N-CA-C	-6.77	99.51	110.20
2	D12	224	LEU	N-CA-C	-6.76	99.52	110.20
2	C7	45	THR	N-CA-C	6.62	119.48	111.40
2	C9	45	THR	N-CA-C	6.62	119.47	111.40
2	C3	45	THR	N-CA-C	6.61	119.46	111.40
2	C10	45	THR	N-CA-C	6.60	119.46	111.40
2	C13	45	THR	N-CA-C	6.60	119.45	111.40
2	C1	45	THR	N-CA-C	6.60	119.45	111.40
2	C8	45	THR	N-CA-C	6.60	119.45	111.40
2	C12	45	THR	N-CA-C	6.60	119.45	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C5	45	THR	N-CA-C	6.60	119.45	111.40
2	C4	45	THR	N-CA-C	6.59	119.44	111.40
2	C2	45	THR	N-CA-C	6.58	119.43	111.40
2	C11	45	THR	N-CA-C	6.58	119.43	111.40
1	A4	200	PRO	N-CA-C	6.57	121.51	111.19
1	A6	200	PRO	N-CA-C	6.57	121.50	111.19
2	C6	45	THR	N-CA-C	6.57	119.42	111.40
1	A7	200	PRO	N-CA-C	6.56	121.50	111.19
1	A13	200	PRO	N-CA-C	6.56	121.50	111.19
1	A10	200	PRO	N-CA-C	6.56	121.49	111.19
1	A1	200	PRO	N-CA-C	6.56	121.49	111.19
1	A9	200	PRO	N-CA-C	6.56	121.49	111.19
1	A8	200	PRO	N-CA-C	6.56	121.49	111.19
1	A11	200	PRO	N-CA-C	6.55	121.48	111.19
1	A2	200	PRO	N-CA-C	6.55	121.48	111.19
1	A3	200	PRO	N-CA-C	6.55	121.47	111.19
1	A12	200	PRO	N-CA-C	6.55	121.47	111.19
1	A5	200	PRO	N-CA-C	6.54	121.46	111.19
2	C4	95	ALA	N-CA-C	6.34	118.19	111.28
2	C6	95	ALA	N-CA-C	6.34	118.19	111.28
2	C3	95	ALA	N-CA-C	6.34	118.19	111.28
2	C2	95	ALA	N-CA-C	6.33	118.18	111.28
2	C8	95	ALA	N-CA-C	6.33	118.17	111.28
2	C9	95	ALA	N-CA-C	6.32	118.17	111.28
2	C13	95	ALA	N-CA-C	6.31	118.16	111.28
2	C7	95	ALA	N-CA-C	6.31	118.16	111.28
2	C1	95	ALA	N-CA-C	6.31	118.16	111.28
2	C11	95	ALA	N-CA-C	6.31	118.16	111.28
2	C12	95	ALA	N-CA-C	6.30	118.15	111.28
1	B7	95	THR	CA-C-N	-6.30	113.89	120.38
1	B7	95	THR	C-N-CA	-6.30	113.89	120.38
2	C5	95	ALA	N-CA-C	6.30	118.14	111.28
1	B6	95	THR	CA-C-N	-6.29	113.90	120.38
1	B6	95	THR	C-N-CA	-6.29	113.90	120.38
1	B5	95	THR	CA-C-N	-6.28	113.91	120.38
1	B5	95	THR	C-N-CA	-6.28	113.91	120.38
1	B4	95	THR	CA-C-N	-6.28	113.91	120.38
1	B4	95	THR	C-N-CA	-6.28	113.91	120.38
1	B10	95	THR	CA-C-N	-6.28	113.91	120.38
1	B10	95	THR	C-N-CA	-6.28	113.91	120.38
2	C12	26	SER	N-CA-C	-6.28	100.49	110.10
1	B11	95	THR	CA-C-N	-6.27	113.92	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B11	95	THR	C-N-CA	-6.27	113.92	120.38
1	B13	95	THR	CA-C-N	-6.27	113.92	120.38
1	B13	95	THR	C-N-CA	-6.27	113.92	120.38
1	B12	95	THR	CA-C-N	-6.27	113.92	120.38
1	B12	95	THR	C-N-CA	-6.27	113.92	120.38
2	C7	26	SER	N-CA-C	-6.27	100.51	110.10
2	C4	26	SER	N-CA-C	-6.27	100.51	110.10
2	C8	26	SER	N-CA-C	-6.27	100.51	110.10
2	C10	95	ALA	N-CA-C	6.27	118.11	111.28
2	C2	26	SER	N-CA-C	-6.26	100.52	110.10
2	C10	26	SER	N-CA-C	-6.26	100.52	110.10
2	C11	26	SER	N-CA-C	-6.26	100.52	110.10
1	B3	95	THR	CA-C-N	-6.26	113.93	120.38
1	B3	95	THR	C-N-CA	-6.26	113.93	120.38
1	B1	95	THR	CA-C-N	-6.26	113.93	120.38
1	B1	95	THR	C-N-CA	-6.26	113.93	120.38
1	B8	95	THR	CA-C-N	-6.26	113.93	120.38
1	B8	95	THR	C-N-CA	-6.26	113.93	120.38
2	C1	26	SER	N-CA-C	-6.26	100.52	110.10
2	C9	26	SER	N-CA-C	-6.26	100.52	110.10
2	C5	26	SER	N-CA-C	-6.26	100.52	110.10
2	C6	26	SER	N-CA-C	-6.26	100.52	110.10
2	C3	26	SER	N-CA-C	-6.25	100.53	110.10
1	B9	95	THR	CA-C-N	-6.25	113.94	120.38
1	B9	95	THR	C-N-CA	-6.25	113.94	120.38
2	C13	26	SER	N-CA-C	-6.25	100.53	110.10
1	B2	95	THR	CA-C-N	-6.22	113.97	120.38
1	B2	95	THR	C-N-CA	-6.22	113.97	120.38
1	A5	159	HIS	CA-C-N	-5.86	113.50	119.83
1	A5	159	HIS	C-N-CA	-5.86	113.50	119.83
1	A11	159	HIS	CA-C-N	-5.85	113.51	119.83
1	A11	159	HIS	C-N-CA	-5.85	113.51	119.83
1	A4	159	HIS	CA-C-N	-5.85	113.52	119.83
1	A4	159	HIS	C-N-CA	-5.85	113.52	119.83
1	A12	159	HIS	CA-C-N	-5.85	113.52	119.83
1	A12	159	HIS	C-N-CA	-5.85	113.52	119.83
1	A13	159	HIS	CA-C-N	-5.84	113.52	119.83
1	A13	159	HIS	C-N-CA	-5.84	113.52	119.83
1	A2	159	HIS	CA-C-N	-5.84	113.52	119.83
1	A2	159	HIS	C-N-CA	-5.84	113.52	119.83
1	A8	159	HIS	CA-C-N	-5.84	113.53	119.83
1	A8	159	HIS	C-N-CA	-5.84	113.53	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	159	HIS	CA-C-N	-5.84	113.53	119.83
1	A1	159	HIS	C-N-CA	-5.84	113.53	119.83
1	A10	159	HIS	CA-C-N	-5.84	113.53	119.83
1	A10	159	HIS	C-N-CA	-5.84	113.53	119.83
1	A3	159	HIS	CA-C-N	-5.83	113.53	119.83
1	A3	159	HIS	C-N-CA	-5.83	113.53	119.83
1	A7	159	HIS	CA-C-N	-5.83	113.53	119.83
1	A7	159	HIS	C-N-CA	-5.83	113.53	119.83
1	A6	159	HIS	CA-C-N	-5.82	113.55	119.83
1	A6	159	HIS	C-N-CA	-5.82	113.55	119.83
1	A9	159	HIS	CA-C-N	-5.81	113.56	119.83
1	A9	159	HIS	C-N-CA	-5.81	113.56	119.83
2	D4	174	VAL	N-CA-C	5.79	116.27	108.17
2	D2	174	VAL	N-CA-C	5.78	116.27	108.17
2	D9	174	VAL	N-CA-C	5.78	116.27	108.17
2	D3	174	VAL	N-CA-C	5.78	116.27	108.17
2	D6	174	VAL	N-CA-C	5.78	116.26	108.17
2	D1	174	VAL	N-CA-C	5.78	116.25	108.17
2	D7	174	VAL	N-CA-C	5.78	116.25	108.17
2	D8	174	VAL	N-CA-C	5.78	116.26	108.17
2	D12	174	VAL	N-CA-C	5.77	116.25	108.17
2	D10	174	VAL	N-CA-C	5.77	116.25	108.17
2	C3	68	ALA	N-CA-C	5.77	117.57	111.28
2	C12	68	ALA	N-CA-C	5.77	117.57	111.28
2	D5	174	VAL	N-CA-C	5.77	116.25	108.17
2	D11	174	VAL	N-CA-C	5.77	116.24	108.17
2	D13	174	VAL	N-CA-C	5.77	116.25	108.17
2	C2	68	ALA	N-CA-C	5.76	117.56	111.28
2	C4	68	ALA	N-CA-C	5.76	117.56	111.28
2	C9	68	ALA	N-CA-C	5.76	117.56	111.28
2	C6	68	ALA	N-CA-C	5.76	117.56	111.28
2	C13	68	ALA	N-CA-C	5.76	117.55	111.28
2	C1	68	ALA	N-CA-C	5.75	117.55	111.28
2	C11	68	ALA	N-CA-C	5.75	117.54	111.28
2	C7	68	ALA	N-CA-C	5.74	117.54	111.28
2	C10	68	ALA	N-CA-C	5.74	117.54	111.28
2	C8	68	ALA	N-CA-C	5.74	117.54	111.28
2	C5	68	ALA	N-CA-C	5.73	117.53	111.28
2	D3	124	ARG	CA-C-N	-5.70	114.06	119.76
2	D3	124	ARG	C-N-CA	-5.70	114.06	119.76
2	D6	124	ARG	CA-C-N	-5.70	114.06	119.76
2	D6	124	ARG	C-N-CA	-5.70	114.06	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D13	124	ARG	CA-C-N	-5.69	114.07	119.76
2	D13	124	ARG	C-N-CA	-5.69	114.07	119.76
2	D5	124	ARG	CA-C-N	-5.69	114.07	119.76
2	D5	124	ARG	C-N-CA	-5.69	114.07	119.76
2	D10	124	ARG	CA-C-N	-5.69	114.07	119.76
2	D10	124	ARG	C-N-CA	-5.69	114.07	119.76
2	D7	124	ARG	CA-C-N	-5.68	114.08	119.76
2	D7	124	ARG	C-N-CA	-5.68	114.08	119.76
2	D9	124	ARG	CA-C-N	-5.68	114.08	119.76
2	D9	124	ARG	C-N-CA	-5.68	114.08	119.76
2	D12	124	ARG	CA-C-N	-5.67	114.09	119.76
2	D12	124	ARG	C-N-CA	-5.67	114.09	119.76
2	D1	124	ARG	CA-C-N	-5.67	114.09	119.76
2	D1	124	ARG	C-N-CA	-5.67	114.09	119.76
2	D2	124	ARG	CA-C-N	-5.67	114.09	119.76
2	D2	124	ARG	C-N-CA	-5.67	114.09	119.76
2	D4	124	ARG	CA-C-N	-5.67	114.09	119.76
2	D4	124	ARG	C-N-CA	-5.67	114.09	119.76
2	D11	124	ARG	CA-C-N	-5.67	114.09	119.76
2	D11	124	ARG	C-N-CA	-5.67	114.09	119.76
2	D8	124	ARG	CA-C-N	-5.64	114.11	119.76
2	D8	124	ARG	C-N-CA	-5.64	114.11	119.76
1	B7	95	THR	N-CA-C	5.62	120.40	112.75
1	B11	192	VAL	N-CA-C	-5.62	106.20	111.48
1	B9	192	VAL	N-CA-C	-5.61	106.21	111.48
1	B5	95	THR	N-CA-C	5.61	120.37	112.75
1	B4	192	VAL	N-CA-C	-5.60	106.22	111.48
1	B2	95	THR	N-CA-C	5.60	120.36	112.75
1	B5	192	VAL	N-CA-C	-5.59	106.22	111.48
1	B4	95	THR	N-CA-C	5.59	120.36	112.75
1	B13	95	THR	N-CA-C	5.59	120.35	112.75
1	B13	192	VAL	N-CA-C	-5.59	106.23	111.48
1	B1	192	VAL	N-CA-C	-5.59	106.23	111.48
1	B8	192	VAL	N-CA-C	-5.59	106.23	111.48
1	B2	192	VAL	N-CA-C	-5.58	106.23	111.48
1	B3	192	VAL	N-CA-C	-5.58	106.23	111.48
1	B7	192	VAL	N-CA-C	-5.58	106.23	111.48
1	B10	95	THR	N-CA-C	5.58	120.34	112.75
1	B1	95	THR	N-CA-C	5.58	120.34	112.75
1	B10	192	VAL	N-CA-C	-5.58	106.24	111.48
1	B8	95	THR	N-CA-C	5.58	120.33	112.75
1	B6	192	VAL	N-CA-C	-5.57	106.24	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B12	192	VAL	N-CA-C	-5.57	106.24	111.48
1	B9	95	THR	N-CA-C	5.57	120.32	112.75
1	B6	95	THR	N-CA-C	5.56	120.31	112.75
1	B11	95	THR	N-CA-C	5.56	120.31	112.75
1	B3	95	THR	N-CA-C	5.54	120.28	112.75
1	B12	95	THR	N-CA-C	5.53	120.27	112.75
1	B13	158	VAL	N-CA-C	-5.52	104.03	110.05
1	B4	158	VAL	N-CA-C	-5.51	104.04	110.05
1	B11	158	VAL	N-CA-C	-5.50	104.05	110.05
1	B12	158	VAL	N-CA-C	-5.49	104.06	110.05
1	B8	158	VAL	N-CA-C	-5.49	104.06	110.05
2	D9	84	ALA	N-CA-C	5.49	117.78	110.53
1	B2	158	VAL	N-CA-C	-5.49	104.07	110.05
1	B1	158	VAL	N-CA-C	-5.48	104.07	110.05
1	B5	158	VAL	N-CA-C	-5.48	104.08	110.05
1	B3	158	VAL	N-CA-C	-5.48	104.08	110.05
1	B6	158	VAL	N-CA-C	-5.47	104.09	110.05
2	D4	84	ALA	N-CA-C	5.47	117.75	110.53
2	D11	84	ALA	N-CA-C	5.47	117.75	110.53
1	B9	158	VAL	N-CA-C	-5.47	104.09	110.05
1	B10	158	VAL	N-CA-C	-5.46	104.10	110.05
2	D2	84	ALA	N-CA-C	5.46	117.74	110.53
2	D5	84	ALA	N-CA-C	5.46	117.74	110.53
2	D6	84	ALA	N-CA-C	5.46	117.74	110.53
2	D3	84	ALA	N-CA-C	5.46	117.74	110.53
1	B7	158	VAL	N-CA-C	-5.46	104.10	110.05
2	D13	84	ALA	N-CA-C	5.46	117.73	110.53
2	D1	84	ALA	N-CA-C	5.46	117.73	110.53
2	D7	84	ALA	N-CA-C	5.46	117.73	110.53
2	D8	84	ALA	N-CA-C	5.44	117.72	110.53
2	D12	84	ALA	N-CA-C	5.44	117.71	110.53
2	D10	84	ALA	N-CA-C	5.43	117.70	110.53
1	B12	96	PRO	N-CA-C	5.25	117.10	110.70
1	B2	96	PRO	N-CA-C	5.24	117.09	110.70
1	B10	96	PRO	N-CA-C	5.24	117.09	110.70
1	B8	96	PRO	N-CA-C	5.23	117.08	110.70
1	B1	96	PRO	N-CA-C	5.22	117.08	110.70
1	B5	96	PRO	N-CA-C	5.22	117.06	110.70
1	B9	96	PRO	N-CA-C	5.21	117.06	110.70
1	B11	96	PRO	N-CA-C	5.21	117.06	110.70
1	B3	96	PRO	N-CA-C	5.21	117.06	110.70
1	B7	96	PRO	N-CA-C	5.21	117.06	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B6	96	PRO	N-CA-C	5.21	117.05	110.70
1	B4	96	PRO	N-CA-C	5.20	117.05	110.70
1	B13	96	PRO	N-CA-C	5.20	117.05	110.70
2	C3	221	ALA	N-CA-C	5.17	117.31	108.67
2	C12	221	ALA	N-CA-C	5.16	117.29	108.67
2	C1	221	ALA	N-CA-C	5.16	117.28	108.67
2	C5	221	ALA	N-CA-C	5.16	117.28	108.67
2	C6	221	ALA	N-CA-C	5.16	117.28	108.67
2	C7	221	ALA	N-CA-C	5.16	117.28	108.67
2	C11	221	ALA	N-CA-C	5.15	117.28	108.67
2	C8	221	ALA	N-CA-C	5.15	117.27	108.67
2	C13	221	ALA	N-CA-C	5.15	117.27	108.67
2	C2	221	ALA	N-CA-C	5.15	117.27	108.67
2	C4	221	ALA	N-CA-C	5.15	117.27	108.67
2	C9	221	ALA	N-CA-C	5.15	117.27	108.67
2	C10	221	ALA	N-CA-C	5.15	117.27	108.67
2	D10	68	ALA	N-CA-C	5.12	116.67	111.14
2	D4	68	ALA	N-CA-C	5.12	116.67	111.14
2	D5	68	ALA	N-CA-C	5.11	116.66	111.14
2	D6	68	ALA	N-CA-C	5.11	116.66	111.14
2	D7	68	ALA	N-CA-C	5.11	116.66	111.14
2	D12	68	ALA	N-CA-C	5.11	116.66	111.14
2	D1	68	ALA	N-CA-C	5.11	116.66	111.14
2	D13	68	ALA	N-CA-C	5.11	116.66	111.14
2	C5	221	ALA	CB-CA-C	-5.11	110.29	117.23
2	D3	68	ALA	N-CA-C	5.11	116.65	111.14
2	D11	68	ALA	N-CA-C	5.11	116.65	111.14
2	D2	68	ALA	N-CA-C	5.10	116.65	111.14
2	D8	68	ALA	N-CA-C	5.10	116.65	111.14
2	C2	221	ALA	CB-CA-C	-5.09	110.31	117.23
2	C9	221	ALA	CB-CA-C	-5.09	110.31	117.23
2	D9	68	ALA	N-CA-C	5.09	116.64	111.14
2	C10	219	ASN	N-CA-C	-5.08	102.24	110.32
2	C11	219	ASN	N-CA-C	-5.08	102.24	110.32
2	C11	221	ALA	CB-CA-C	-5.08	110.32	117.23
2	C3	221	ALA	CB-CA-C	-5.08	110.32	117.23
2	C12	221	ALA	CB-CA-C	-5.08	110.32	117.23
2	C8	221	ALA	CB-CA-C	-5.08	110.33	117.23
2	C12	219	ASN	N-CA-C	-5.07	102.25	110.32
2	C6	221	ALA	CB-CA-C	-5.07	110.33	117.23
2	C4	219	ASN	N-CA-C	-5.07	102.26	110.32
2	C4	221	ALA	CB-CA-C	-5.07	110.34	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C1	221	ALA	CB-CA-C	-5.07	110.34	117.23
2	C7	221	ALA	CB-CA-C	-5.07	110.34	117.23
2	C13	221	ALA	CB-CA-C	-5.06	110.34	117.23
2	C5	219	ASN	N-CA-C	-5.06	102.27	110.32
2	C1	219	ASN	N-CA-C	-5.06	102.28	110.32
2	C3	219	ASN	N-CA-C	-5.06	102.28	110.32
2	C13	219	ASN	N-CA-C	-5.06	102.28	110.32
2	C6	219	ASN	N-CA-C	-5.06	102.28	110.32
2	C10	221	ALA	CB-CA-C	-5.05	110.36	117.23
2	C9	219	ASN	N-CA-C	-5.05	102.30	110.32
2	C8	219	ASN	N-CA-C	-5.04	102.30	110.32
2	C7	219	ASN	N-CA-C	-5.04	102.31	110.32
2	C2	219	ASN	N-CA-C	-5.03	102.32	110.32

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	26	0
1	A11	436	0	414	26	0
1	A12	436	0	414	26	0
1	A13	436	0	414	26	0
1	A2	436	0	414	26	0
1	A3	436	0	414	25	0
1	A4	436	0	414	26	0
1	A5	436	0	414	26	0
1	A6	436	0	414	26	0
1	A7	436	0	414	26	0
1	A8	436	0	414	26	0
1	A9	436	0	414	26	0
1	B1	498	0	478	67	0
1	B10	498	0	478	69	0
1	B11	498	0	478	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	69	0
1	B4	498	0	478	69	0
1	B5	498	0	478	68	0
1	B6	498	0	478	67	0
1	B7	498	0	478	69	0
1	B8	498	0	478	69	0
1	B9	498	0	478	69	0
2	C1	1654	0	1664	65	0
2	C10	1654	0	1664	64	0
2	C11	1654	0	1664	65	0
2	C12	1654	0	1664	64	0
2	C13	1654	0	1664	66	0
2	C2	1654	0	1664	65	0
2	C3	1654	0	1664	63	0
2	C4	1654	0	1664	65	0
2	C5	1654	0	1664	65	0
2	C6	1654	0	1664	64	0
2	C7	1654	0	1664	62	0
2	C8	1654	0	1664	63	0
2	C9	1654	0	1664	64	0
2	D1	1654	0	1664	61	0
2	D10	1654	0	1664	56	0
2	D11	1654	0	1664	59	0
2	D12	1654	0	1664	63	0
2	D13	1654	0	1664	59	0
2	D2	1654	0	1664	58	0
2	D3	1654	0	1664	59	0
2	D4	1654	0	1664	52	0
2	D5	1654	0	1664	54	0
2	D6	1654	0	1664	56	0
2	D7	1654	0	1664	57	0
2	D8	1654	0	1664	57	0
2	D9	1654	0	1664	55	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1945	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 (1945) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B12:187:ARG:HH11	2:D12:204:GLU:CD	1.80	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
1:B13:187:ARG:HH11	2:D13:204:GLU:CD	1.80	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:B2:187:ARG:HH11	2:D2:204:GLU:CD	1.80	0.89
1:B7:170:VAL:HG11	2:D7:144:ASN:ND2	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B11:187:ARG:HH11	2:D11:204:GLU:CD	1.80	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:B10:187:ARG:HH11	2:D10:204:GLU:CD	1.80	0.89
1:B3:187:ARG:HH11	2:D3:204:GLU:CD	1.80	0.89
1:B5:95:THR:HG22	1:B6:176:VAL:CG2	2.02	0.89
1:B9:187:ARG:HH11	2:D9:204:GLU:CD	1.80	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
1:B2:170:VAL:HG11	2:D2:144:ASN:ND2	1.87	0.89
1:B8:187:ARG:HH11	2:D8:204:GLU:CD	1.80	0.88
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:B1:187:ARG:HH11	2:D1:204:GLU:CD	1.80	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:B6:187:ARG:HH11	2:D6:204:GLU:CD	1.80	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:B5:187:ARG:HH11	2:D5:204:GLU:CD	1.80	0.88
1:B7:187:ARG:HH11	2:D7:204:GLU:CD	1.80	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:B4:187:ARG:HH11	2:D4:204:GLU:CD	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
2:C1:35:GLY:HA3	2:D1:27:PRO:HD3	1.58	0.85
1:A10:152:CYS:SG	1:B8:151:ARG:N	2.50	0.84
2:C11:35:GLY:HA3	2:D11:27:PRO:HD3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:152:CYS:SG	1:B13:151:ARG:N	2.50	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
2:C3:35:GLY:HA3	2:D3:27:PRO:HD3	1.59	0.83
1:B10:155:PRO:HD2	2:D11:205:GLN:HG2	1.58	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D11:66:MET:HE3	2:D11:86:ARG:HH21	1.64	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:D7:225:MET:C	2:D7:227:GLY:H	2.07	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
2:D11:225:MET:C	2:D11:227:GLY:H	2.07	0.62
2:D12:225:MET:C	2:D12:227:GLY:H	2.07	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:D8:225:MET:C	2:D8:227:GLY:H	2.08	0.62
2:D10:66:MET:HE3	2:D10:86:ARG:HH21	1.64	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
2:D2:66:MET:HE3	2:D2:86:ARG:HH21	1.64	0.62
2:D9:66:MET:HE3	2:D9:86:ARG:HH21	1.64	0.62
2:D12:66:MET:HE3	2:D12:86:ARG:HH21	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D6:225:MET:C	2:D6:227:GLY:H	2.07	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
2:D8:66:MET:HE3	2:D8:86:ARG:HH21	1.64	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
2:D1:66:MET:HE3	2:D1:86:ARG:HH21	1.64	0.61
2:D13:225:MET:C	2:D13:227:GLY:H	2.07	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
2:D7:66:MET:HE3	2:D7:86:ARG:HH21	1.64	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
2:D1:225:MET:C	2:D1:227:GLY:N	2.57	0.61
2:D10:225:MET:C	2:D10:227:GLY:H	2.07	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
2:D2:225:MET:C	2:D2:227:GLY:N	2.57	0.61
2:D3:66:MET:HE3	2:D3:86:ARG:HH21	1.64	0.61
1:B1:95:THR:HG21	1:B2:176:VAL:CG2	2.30	0.61
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
2:D9:225:MET:C	2:D9:227:GLY:H	2.07	0.61
2:D13:66:MET:HE3	2:D13:86:ARG:HH21	1.64	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
2:D6:66:MET:HE3	2:D6:86:ARG:HH21	1.64	0.61
1:B5:95:THR:HG21	1:B6:176:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:72:LEU:CD1	3:E1:185:PHE:CG	2.79	0.61
2:D4:225:MET:C	2:D4:227:GLY:N	2.57	0.61
1:B8:95:THR:HG21	1:B9:176:VAL:CG2	2.30	0.61
2:D6:225:MET:C	2:D6:227:GLY:N	2.57	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
2:D5:66:MET:HE3	2:D5:86:ARG:HH21	1.64	0.60
2:D1:225:MET:C	2:D1:227:GLY:H	2.07	0.60
2:D4:66:MET:HE3	2:D4:86:ARG:HH21	1.64	0.60
2:D5:225:MET:C	2:D5:227:GLY:H	2.07	0.60
2:D13:225:MET:C	2:D13:227:GLY:N	2.57	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
2:D3:225:MET:C	2:D3:227:GLY:N	2.57	0.60
1:B9:95:THR:HG21	1:B10:176:VAL:CG2	2.30	0.60
2:D2:225:MET:C	2:D2:227:GLY:H	2.08	0.60
2:D5:225:MET:C	2:D5:227:GLY:N	2.57	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:B13:187:ARG:NH1	2:D13:204:GLU:CD	2.58	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
1:B11:187:ARG:NH1	2:D11:204:GLU:CD	2.58	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:B12:187:ARG:NH1	2:D12:204:GLU:CD	2.58	0.59
2:D3:225:MET:C	2:D3:227:GLY:H	2.07	0.59
1:B1:170:VAL:HG11	2:D1:144:ASN:HD21	1.63	0.59
2:D4:225:MET:C	2:D4:227:GLY:H	2.07	0.59
1:B10:187:ARG:NH1	2:D10:204:GLU:CD	2.58	0.59
1:B11:95:THR:HG21	1:B12:176:VAL:CG2	2.30	0.59
2:D12:225:MET:C	2:D12:227:GLY:N	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B2:187:ARG:NH1	2:D2:204:GLU:CD	2.58	0.58
2:D11:225:MET:C	2:D11:227:GLY:N	2.57	0.58
1:B1:176:VAL:HG23	1:B13:95:THR:CG2	2.24	0.58
1:B1:187:ARG:NH1	2:D1:204:GLU:CD	2.58	0.58
2:D7:225:MET:C	2:D7:227:GLY:N	2.57	0.58
2:D9:225:MET:C	2:D9:227:GLY:N	2.57	0.58
1:A1:182:PHE:O	1:B1:188:VAL:HG23	2.03	0.58
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
1:B9:187:ARG:NH1	2:D9:204:GLU:CD	2.58	0.58
1:B9:166:GLN:HB2	1:B9:193:SER:HB3	1.86	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
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
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:D10:225:MET:C	2:D10:227:GLY:N	2.57	0.57
1:B5:166:GLN:HB2	1:B5:193:SER:HB3	1.86	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
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:D8:225:MET:C	2:D8:227:GLY:N	2.57	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:C2:30:ILE:HG22	2:C2:32:LEU:HG	1.86	0.56
2:C11:72:LEU:HD11	3:E11:185:PHE:CE2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B8:187:ARG:NH1	2:D8:204:GLU:CD	2.58	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:D5:183:ASP:OD1	2:D5:183:ASP:N	2.34	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:B3:187:ARG:NH1	2:D3:204:GLU:CD	2.58	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
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
1:A4:160:PRO:CG	1:B3:189:SER:OG	2.52	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
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:B4:187:ARG:NH1	2:D4:204:GLU:CD	2.58	0.56
1:B7:154:ASN:HA	2:D8:205:GLN:HE21	1.71	0.56
1:B7:187:ARG:NH1	2:D7:204:GLU:CD	2.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C8:72:LEU:HD21	3:E8:185:PHE:CB	2.27	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
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:B5:187:ARG:NH1	2:D5:204:GLU:CD	2.58	0.55
1:B5:199:LEU:HD21	1:B6:182:PHE:HE2	1.72	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B6:187:ARG:NH1	2:D6:204: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
1:A4:203:VAL:HG23	2:C3:208:TRP:CD2	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:C4:72:LEU:HD22	3:E4:185:PHE:CD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:175:TRP:CZ2	2:C7:137:GLU:OE1	2.62	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D11:209:LYS:O	2:D11:210:PRO:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D1:209:LYS:O	2:D1:210:PRO:C	2.58	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
2:D9:209:LYS:O	2:D9:210:PRO:C	2.58	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: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
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
2:D13:209:LYS:O	2:D13:210:PRO:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D3:209:LYS:O	2:D3:210:PRO:C	2.58	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
2:D8:209:LYS:O	2:D8:210:PRO:C	2.58	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
2:D6:209:LYS:O	2:D6:210:PRO:C	2.58	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
2:D12:128:ARG:HG3	2:D12:128:ARG:O	2.15	0.46
1:B5:96:PRO:HG2	1:B6:174:PRO:HB2	1.93	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
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
2:D1:128:ARG:HG3	2:D1:128:ARG:O	2.15	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
2:D10:209:LYS:O	2:D10:210:PRO:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D2:209:LYS:O	2:D2:210:PRO:C	2.58	0.45
2:D4:209:LYS:O	2:D4:210:PRO:C	2.58	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:D5:209:LYS:O	2:D5:210:PRO:C	2.58	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
2:D2:49:MET:HE3	2:D2:73:THR:HG21	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D7:209:LYS:O	2:D7:210:PRO:C	2.58	0.45
2:D12:49:MET:HE3	2:D12:73:THR:HG21	1.99	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
2:D11:49:MET:HE3	2:D11:73:THR:HG21	1.99	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:D1:49:MET:HE3	2:D1:73:THR:HG21	1.99	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
2:D12:209:LYS:O	2:D12:210:PRO:C	2.58	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:D3:49:MET:HE3	2:D3:73:THR:HG21	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D5:49:MET:HE3	2:D5:73:THR:HG21	1.99	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:C4:230:MET:HE3	2:C4:230:MET:HB2	1.88	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:D13:49:MET:HE3	2:D13:73:THR:HG21	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D3:50:ILE:HG23	2:D3:116:LEU:HD23	2.00	0.43
2:D6:30:ILE:HG13	2:D6:116:LEU:HD13	2.00	0.43
2:D7:49:MET:HE3	2:D7:73:THR:HG21	1.99	0.43
2:D7:167:ARG:HB2	2:D7:209:LYS:NZ	2.33	0.43
2:D8:49:MET:HE3	2:D8:73:THR:HG21	1.99	0.43
2:D8:50:ILE:HG23	2:D8:116:LEU:HD23	2.00	0.43
2:D10:49:MET:HE3	2:D10:73:THR:HG21	1.99	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:C10:230:MET:HE3	2:C10:230:MET:HB2	1.88	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:D9:49:MET:HE3	2:D9:73:THR:HG21	1.99	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
2:C5:29:THR:HG22	2:C5:115:ARG:HE	1.84	0.43
2:C7:95:ALA:C	2:C7:97:GLY:H	2.27	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:C13:230:MET:HE3	2:C13:230:MET:HB2	1.88	0.43
2:D2:50:ILE:HG23	2:D2:116:LEU:HD23	2.00	0.43
2:D4:49:MET:HE3	2:D4:73:THR:HG21	1.99	0.43
2:D5:167:ARG:HB2	2:D5:209:LYS:NZ	2.33	0.43
2:D6:49:MET:HE3	2:D6:73:THR:HG21	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C3:95:ALA:C	2:C3:97:GLY:H	2.27	0.43
2:C4:95:ALA:C	2:C4:97:GLY:H	2.27	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:C8:95:ALA:C	2:C8:97:GLY:H	2.27	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
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:C2:95:ALA:C	2:C2:97:GLY:H	2.27	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: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
2:C1:95:ALA:C	2:C1:97:GLY:H	2.27	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:C5:95:ALA:C	2:C5:97:GLY:H	2.27	0.43
2:C6:95:ALA:C	2:C6:97:GLY:H	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C8:30:ILE:HB	2:C8:116:LEU:HD13	2.01	0.43
2:C9:95:ALA:C	2:C9:97:GLY:H	2.27	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
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:C13:95:ALA:C	2:C13:97:GLY:H	2.27	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D7:230:MET:HE2	2:D7:230:MET:HB3	1.95	0.42
2:D13:230:MET:HE2	2:D13:230:MET:HB3	1.95	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
2:C3:190:TYR:HE2	2:C3:234:VAL:HG22	1.84	0.42
2:C5:230:MET:HE3	2:C5:230:MET:HB2	1.88	0.42
2:C6:118:SER:OG	2:C6:159:VAL:HG12	2.20	0.42
2:C10:95:ALA:C	2:C10:97:GLY:H	2.27	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
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:C12:95:ALA:C	2:C12:97:GLY:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:C11:95:ALA:C	2:C11:97:GLY:H	2.27	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: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
2:D12:230:MET:HE2	2:D12:230:MET:HB3	1.95	0.42
1:A2:197:TRP:HZ2	1:B1:190:PHE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D7:161:PRO:HG2	2:D7:176:PRO:HB2	2.01	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
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:D7:216:MET:HE3	2:D7:216:MET:HB2	2.00	0.41
2:D11:224:LEU:HD23	2:D11:224:LEU:HA	1.92	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
2:D13:216:MET:HE3	2:D13:216:MET:HB2	2.00	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:D1:216:MET:HE3	2:D1:216:MET:HB2	2.00	0.41
2:D3:216:MET:HG3	2:D3:233:THR:HG23	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D1:230:MET:HE2	2:D1:230:MET:HB3	1.95	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
2:D12:216:MET:HE3	2:D12:216:MET:HB2	2.00	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:D6:224:LEU:HD23	2:D6:224:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D2:216:MET:HE3	2:D2:216:MET:HB2	2.00	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
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:C8:230:MET:HE3	2:C8:230:MET:HB2	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C2:128:ARG:HB2	2:C2:183:ASP:OD2	2.20	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	21/204 (10%)	21 (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	A3	38/204 (19%)	38 (100%)	0	0	100	100
1	A4	53/204 (26%)	53 (100%)	0	0	100	100
1	A5	31/204 (15%)	31 (100%)	0	0	100	100
1	A6	50/204 (24%)	50 (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%)	7	31
1	B10	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B11	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B12	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B13	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B2	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B3	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B4	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B5	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B6	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B7	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B8	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
1	B9	61/204 (30%)	58 (95%)	2 (3%)	1 (2%)	7	31
2	C1	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	24	58
2	C10	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	24	58
2	C11	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	24	58
2	C12	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	24	58
2	C13	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	24	58
2	C2	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	24	58
2	C3	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	24	58
2	C4	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	24	58
2	C5	215/246 (87%)	196 (91%)	18 (8%)	1 (0%)	24	58
2	C6	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	24	58
2	C7	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	24	58
2	C8	215/246 (87%)	197 (92%)	17 (8%)	1 (0%)	24	58
2	C9	215/246 (87%)	198 (92%)	16 (7%)	1 (0%)	24	58
2	D1	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D10	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D11	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D12	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D13	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D2	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D3	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D4	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D5	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D6	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D7	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D8	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
2	D9	215/246 (87%)	202 (94%)	12 (6%)	1 (0%)	24	58
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
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	7181/23274 (31%)	6732 (94%)	397 (6%)	52 (1%)	20	50

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
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

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Mol	Chain	Res	Type
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
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%)	47	74
1	A10	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A11	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A12	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A13	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A2	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A3	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A4	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A5	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A6	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A7	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A8	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	A9	48/168 (29%)	47 (98%)	1 (2%)	47	74
1	B1	56/168 (33%)	51 (91%)	5 (9%)	9	32
1	B10	56/168 (33%)	55 (98%)	1 (2%)	51	76
1	B11	56/168 (33%)	54 (96%)	2 (4%)	31	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B12	56/168 (33%)	55 (98%)	1 (2%)	51	76
1	B13	56/168 (33%)	55 (98%)	1 (2%)	51	76
1	B2	56/168 (33%)	51 (91%)	5 (9%)	9	32
1	B3	56/168 (33%)	51 (91%)	5 (9%)	9	32
1	B4	56/168 (33%)	51 (91%)	5 (9%)	9	32
1	B5	56/168 (33%)	51 (91%)	5 (9%)	9	32
1	B6	56/168 (33%)	51 (91%)	5 (9%)	9	32
1	B7	56/168 (33%)	51 (91%)	5 (9%)	9	32
1	B8	56/168 (33%)	51 (91%)	5 (9%)	9	32
1	B9	56/168 (33%)	51 (91%)	5 (9%)	9	32
2	C1	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	C10	173/195 (89%)	164 (95%)	9 (5%)	21	53
2	C11	173/195 (89%)	163 (94%)	10 (6%)	18	49
2	C12	173/195 (89%)	162 (94%)	11 (6%)	16	45
2	C13	173/195 (89%)	164 (95%)	9 (5%)	21	53
2	C2	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	C3	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	C4	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	C5	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	C6	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	C7	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	C8	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	C9	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	D1	173/195 (89%)	151 (87%)	22 (13%)	4	18
2	D10	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	D11	173/195 (89%)	162 (94%)	11 (6%)	16	45
2	D12	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	D13	173/195 (89%)	157 (91%)	16 (9%)	8	31
2	D2	173/195 (89%)	151 (87%)	22 (13%)	4	18
2	D3	173/195 (89%)	151 (87%)	22 (13%)	4	18
2	D4	173/195 (89%)	151 (87%)	22 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D5	173/195 (89%)	151 (87%)	22 (13%)	4	18
2	D6	173/195 (89%)	151 (87%)	22 (13%)	4	18
2	D7	173/195 (89%)	151 (87%)	22 (13%)	4	18
2	D8	173/195 (89%)	151 (87%)	22 (13%)	4	18
2	D9	173/195 (89%)	151 (87%)	22 (13%)	4	18
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%)	9 (90%)	1 (10%)	7	27
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%)	9 (90%)	1 (10%)	7	27
3	F3	10/353 (3%)	9 (90%)	1 (10%)	7	27
3	F4	10/353 (3%)	9 (90%)	1 (10%)	7	27
3	F5	10/353 (3%)	9 (90%)	1 (10%)	7	27
3	F6	10/353 (3%)	9 (90%)	1 (10%)	7	27
3	F7	10/353 (3%)	9 (90%)	1 (10%)	7	27
3	F8	10/353 (3%)	9 (90%)	1 (10%)	7	27
3	F9	10/353 (3%)	9 (90%)	1 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6110/18616 (33%)	5598 (92%)	512 (8%)	12	35

All (512) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	153	ASP
1	A2	153	ASP
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	94	THR
1	B1	158	VAL
1	B1	179	ASP
1	B1	188	VAL
1	B1	191	VAL
1	B2	94	THR
1	B2	158	VAL
1	B2	179	ASP
1	B2	188	VAL
1	B2	191	VAL
1	B3	94	THR
1	B3	158	VAL
1	B3	179	ASP
1	B3	188	VAL
1	B3	191	VAL
1	B4	94	THR
1	B4	158	VAL
1	B4	179	ASP
1	B4	188	VAL
1	B4	191	VAL
1	B5	94	THR
1	B5	158	VAL
1	B5	179	ASP
1	B5	188	VAL

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Mol	Chain	Res	Type
1	B5	191	VAL
1	B6	94	THR
1	B6	158	VAL
1	B6	179	ASP
1	B6	188	VAL
1	B6	191	VAL
1	B7	94	THR
1	B7	158	VAL
1	B7	179	ASP
1	B7	188	VAL
1	B7	191	VAL
1	B8	94	THR
1	B8	158	VAL
1	B8	179	ASP
1	B8	188	VAL
1	B8	191	VAL
1	B9	94	THR
1	B9	158	VAL
1	B9	179	ASP
1	B9	188	VAL
1	B9	191	VAL
1	B10	179	ASP
1	B11	91	THR
1	B11	179	ASP
1	B12	179	ASP
1	B13	179	ASP
2	C1	40	LEU
2	C1	42	ILE
2	C1	44	ASN
2	C1	45	THR
2	C1	60	ILE
2	C1	79	LEU
2	C1	90	ILE
2	C1	94	THR
2	C1	105	THR
2	C1	116	LEU
2	C1	142	SER
2	C1	143	LEU
2	C1	188	ASP
2	C1	198	TRP
2	C1	229	ARG
2	C1	234	VAL

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Mol	Chain	Res	Type
2	C2	40	LEU
2	C2	42	ILE
2	C2	44	ASN
2	C2	45	THR
2	C2	60	ILE
2	C2	79	LEU
2	C2	90	ILE
2	C2	94	THR
2	C2	105	THR
2	C2	116	LEU
2	C2	142	SER
2	C2	143	LEU
2	C2	188	ASP
2	C2	198	TRP
2	C2	229	ARG
2	C2	234	VAL
2	C3	40	LEU
2	C3	42	ILE
2	C3	44	ASN
2	C3	45	THR
2	C3	60	ILE
2	C3	79	LEU
2	C3	90	ILE
2	C3	94	THR
2	C3	105	THR
2	C3	116	LEU
2	C3	142	SER
2	C3	143	LEU
2	C3	188	ASP
2	C3	198	TRP
2	C3	229	ARG
2	C3	234	VAL
2	C4	40	LEU
2	C4	42	ILE
2	C4	44	ASN
2	C4	45	THR
2	C4	60	ILE
2	C4	79	LEU
2	C4	90	ILE
2	C4	94	THR
2	C4	105	THR
2	C4	116	LEU

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Mol	Chain	Res	Type
2	C4	142	SER
2	C4	143	LEU
2	C4	188	ASP
2	C4	198	TRP
2	C4	229	ARG
2	C4	234	VAL
2	C5	40	LEU
2	C5	42	ILE
2	C5	44	ASN
2	C5	45	THR
2	C5	60	ILE
2	C5	79	LEU
2	C5	90	ILE
2	C5	94	THR
2	C5	105	THR
2	C5	116	LEU
2	C5	142	SER
2	C5	143	LEU
2	C5	188	ASP
2	C5	198	TRP
2	C5	229	ARG
2	C5	234	VAL
2	C6	40	LEU
2	C6	42	ILE
2	C6	44	ASN
2	C6	45	THR
2	C6	60	ILE
2	C6	79	LEU
2	C6	90	ILE
2	C6	94	THR
2	C6	105	THR
2	C6	116	LEU
2	C6	142	SER
2	C6	143	LEU
2	C6	188	ASP
2	C6	198	TRP
2	C6	229	ARG
2	C6	234	VAL
2	C7	40	LEU
2	C7	42	ILE
2	C7	44	ASN
2	C7	45	THR

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Mol	Chain	Res	Type
2	C7	60	ILE
2	C7	79	LEU
2	C7	90	ILE
2	C7	94	THR
2	C7	105	THR
2	C7	116	LEU
2	C7	142	SER
2	C7	143	LEU
2	C7	188	ASP
2	C7	198	TRP
2	C7	229	ARG
2	C7	234	VAL
2	C8	40	LEU
2	C8	42	ILE
2	C8	44	ASN
2	C8	45	THR
2	C8	60	ILE
2	C8	79	LEU
2	C8	90	ILE
2	C8	94	THR
2	C8	105	THR
2	C8	116	LEU
2	C8	142	SER
2	C8	143	LEU
2	C8	188	ASP
2	C8	198	TRP
2	C8	229	ARG
2	C8	234	VAL
2	C9	40	LEU
2	C9	42	ILE
2	C9	44	ASN
2	C9	45	THR
2	C9	60	ILE
2	C9	79	LEU
2	C9	90	ILE
2	C9	94	THR
2	C9	105	THR
2	C9	116	LEU
2	C9	142	SER
2	C9	143	LEU
2	C9	188	ASP
2	C9	198	TRP

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Mol	Chain	Res	Type
2	C9	229	ARG
2	C9	234	VAL
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	42	ILE
2	C11	43	SER
2	C11	88	PHE
2	C11	98	GLN
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	29	THR
2	C12	34	GLN
2	C12	44	ASN
2	C12	60	ILE
2	C12	90	ILE
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

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Mol	Chain	Res	Type
2	D1	30	ILE
2	D1	40	LEU
2	D1	44	ASN
2	D1	45	THR
2	D1	73	THR
2	D1	78	VAL
2	D1	92	VAL
2	D1	102	VAL
2	D1	103	VAL
2	D1	110	GLU
2	D1	113	VAL
2	D1	116	LEU
2	D1	117	MET
2	D1	118	SER
2	D1	151	ASP
2	D1	168	LEU
2	D1	177	LEU
2	D1	178	LYS
2	D1	208	TRP
2	D1	231	THR
2	D1	233	THR
2	D2	29	THR
2	D2	30	ILE
2	D2	40	LEU
2	D2	44	ASN
2	D2	45	THR
2	D2	73	THR
2	D2	78	VAL
2	D2	92	VAL
2	D2	102	VAL
2	D2	103	VAL
2	D2	110	GLU
2	D2	113	VAL
2	D2	116	LEU
2	D2	117	MET
2	D2	118	SER
2	D2	151	ASP
2	D2	168	LEU
2	D2	177	LEU
2	D2	178	LYS
2	D2	208	TRP
2	D2	231	THR

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Mol	Chain	Res	Type
2	D2	233	THR
2	D3	29	THR
2	D3	30	ILE
2	D3	40	LEU
2	D3	44	ASN
2	D3	45	THR
2	D3	73	THR
2	D3	78	VAL
2	D3	92	VAL
2	D3	102	VAL
2	D3	103	VAL
2	D3	110	GLU
2	D3	113	VAL
2	D3	116	LEU
2	D3	117	MET
2	D3	118	SER
2	D3	151	ASP
2	D3	168	LEU
2	D3	177	LEU
2	D3	178	LYS
2	D3	208	TRP
2	D3	231	THR
2	D3	233	THR
2	D4	29	THR
2	D4	30	ILE
2	D4	40	LEU
2	D4	44	ASN
2	D4	45	THR
2	D4	73	THR
2	D4	78	VAL
2	D4	92	VAL
2	D4	102	VAL
2	D4	103	VAL
2	D4	110	GLU
2	D4	113	VAL
2	D4	116	LEU
2	D4	117	MET
2	D4	118	SER
2	D4	151	ASP
2	D4	168	LEU
2	D4	177	LEU
2	D4	178	LYS

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Mol	Chain	Res	Type
2	D4	208	TRP
2	D4	231	THR
2	D4	233	THR
2	D5	29	THR
2	D5	30	ILE
2	D5	40	LEU
2	D5	44	ASN
2	D5	45	THR
2	D5	73	THR
2	D5	78	VAL
2	D5	92	VAL
2	D5	102	VAL
2	D5	103	VAL
2	D5	110	GLU
2	D5	113	VAL
2	D5	116	LEU
2	D5	117	MET
2	D5	118	SER
2	D5	151	ASP
2	D5	168	LEU
2	D5	177	LEU
2	D5	178	LYS
2	D5	208	TRP
2	D5	231	THR
2	D5	233	THR
2	D6	29	THR
2	D6	30	ILE
2	D6	40	LEU
2	D6	44	ASN
2	D6	45	THR
2	D6	73	THR
2	D6	78	VAL
2	D6	92	VAL
2	D6	102	VAL
2	D6	103	VAL
2	D6	110	GLU
2	D6	113	VAL
2	D6	116	LEU
2	D6	117	MET
2	D6	118	SER
2	D6	151	ASP
2	D6	168	LEU

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Mol	Chain	Res	Type
2	D6	177	LEU
2	D6	178	LYS
2	D6	208	TRP
2	D6	231	THR
2	D6	233	THR
2	D7	29	THR
2	D7	30	ILE
2	D7	40	LEU
2	D7	44	ASN
2	D7	45	THR
2	D7	73	THR
2	D7	78	VAL
2	D7	92	VAL
2	D7	102	VAL
2	D7	103	VAL
2	D7	110	GLU
2	D7	113	VAL
2	D7	116	LEU
2	D7	117	MET
2	D7	118	SER
2	D7	151	ASP
2	D7	168	LEU
2	D7	177	LEU
2	D7	178	LYS
2	D7	208	TRP
2	D7	231	THR
2	D7	233	THR
2	D8	29	THR
2	D8	30	ILE
2	D8	40	LEU
2	D8	44	ASN
2	D8	45	THR
2	D8	73	THR
2	D8	78	VAL
2	D8	92	VAL
2	D8	102	VAL
2	D8	103	VAL
2	D8	110	GLU
2	D8	113	VAL
2	D8	116	LEU
2	D8	117	MET
2	D8	118	SER

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Mol	Chain	Res	Type
2	D8	151	ASP
2	D8	168	LEU
2	D8	177	LEU
2	D8	178	LYS
2	D8	208	TRP
2	D8	231	THR
2	D8	233	THR
2	D9	29	THR
2	D9	30	ILE
2	D9	40	LEU
2	D9	44	ASN
2	D9	45	THR
2	D9	73	THR
2	D9	78	VAL
2	D9	92	VAL
2	D9	102	VAL
2	D9	103	VAL
2	D9	110	GLU
2	D9	113	VAL
2	D9	116	LEU
2	D9	117	MET
2	D9	118	SER
2	D9	151	ASP
2	D9	168	LEU
2	D9	177	LEU
2	D9	178	LYS
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
2	D10	151	ASP
2	D10	177	LEU
2	D10	178	LYS
2	D10	184	GLN

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Mol	Chain	Res	Type
2	D10	208	TRP
2	D10	231	THR
2	D10	233	THR
2	D11	51	PHE
2	D11	78	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	31	SER
2	D12	33	PRO
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
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

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Mol	Chain	Res	Type
2	D13	184	GLN
2	D13	208	TRP
2	D13	231	THR
2	D13	233	THR
3	F1	184	GLU
3	F2	184	GLU
3	F3	184	GLU
3	F4	184	GLU
3	F5	184	GLU
3	F6	184	GLU
3	F7	184	GLU
3	F8	184	GLU
3	F9	184	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
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	34	GLN
2	C1	37	GLN
2	C1	184	GLN
2	C1	194	ASN
2	C1	222	GLN
2	C2	37	GLN
2	C2	184	GLN
2	C2	194	ASN
2	C2	222	GLN
2	C3	37	GLN
2	C3	184	GLN
2	C3	194	ASN
2	C3	222	GLN
2	C4	37	GLN
2	C4	184	GLN
2	C4	194	ASN

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Mol	Chain	Res	Type
2	C4	222	GLN
2	C5	34	GLN
2	C5	37	GLN
2	C5	184	GLN
2	C5	194	ASN
2	C5	222	GLN
2	C6	34	GLN
2	C6	37	GLN
2	C6	184	GLN
2	C6	194	ASN
2	C6	222	GLN
2	C7	34	GLN
2	C7	37	GLN
2	C7	184	GLN
2	C7	194	ASN
2	C7	222	GLN
2	C8	34	GLN
2	C8	37	GLN
2	C8	184	GLN
2	C8	194	ASN
2	C8	222	GLN
2	C9	34	GLN
2	C9	37	GLN
2	C9	184	GLN
2	C9	194	ASN
2	C9	222	GLN
2	D1	144	ASN
2	D1	219	ASN
2	D1	222	GLN
2	D2	144	ASN
2	D2	219	ASN
2	D2	222	GLN
2	D3	144	ASN
2	D3	219	ASN
2	D3	222	GLN
2	D4	144	ASN
2	D4	219	ASN
2	D4	222	GLN
2	D5	144	ASN
2	D5	219	ASN
2	D5	222	GLN
2	D6	144	ASN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

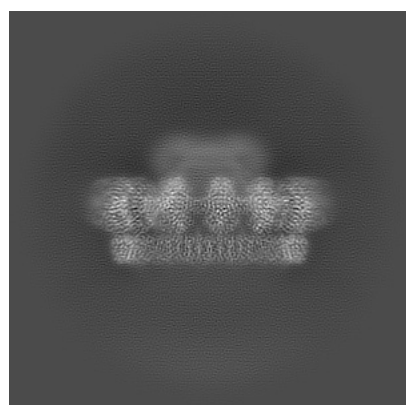
6 Map visualisation [i](#)

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

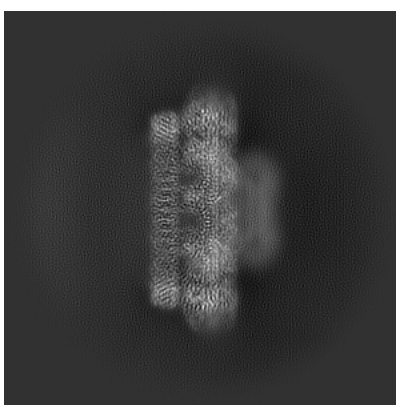
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

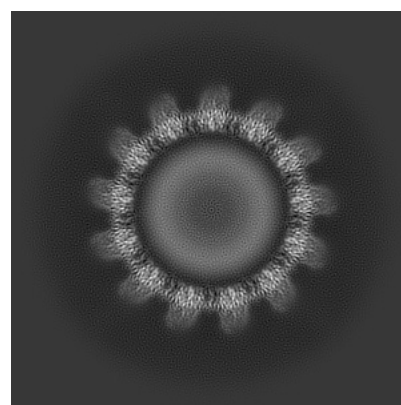
6.1.1 Primary map



X



Y

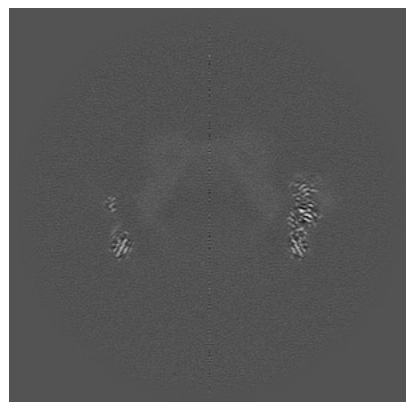


Z

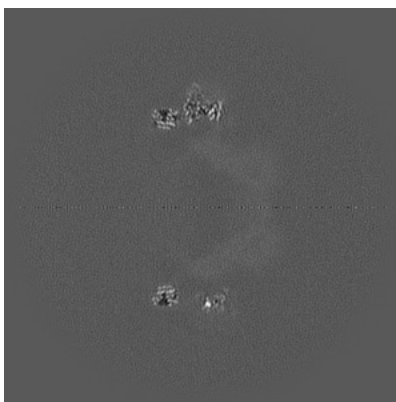
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

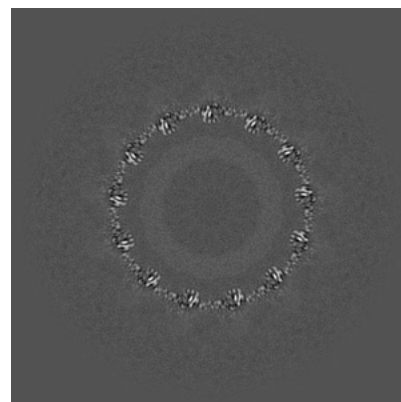
6.2.1 Primary map



X Index: 200



Y Index: 200

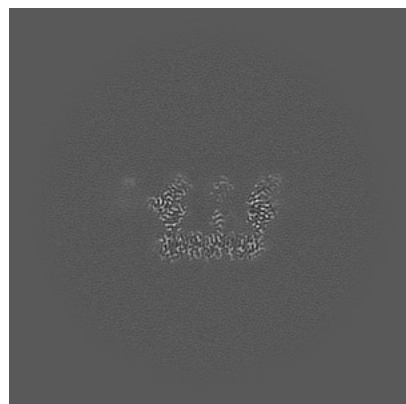


Z Index: 200

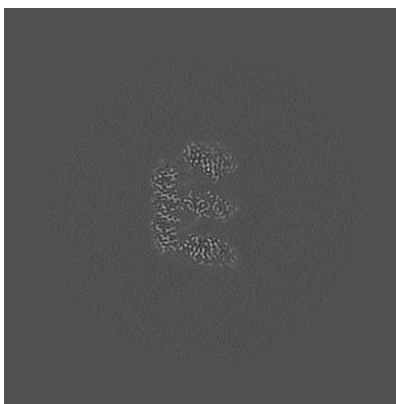
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

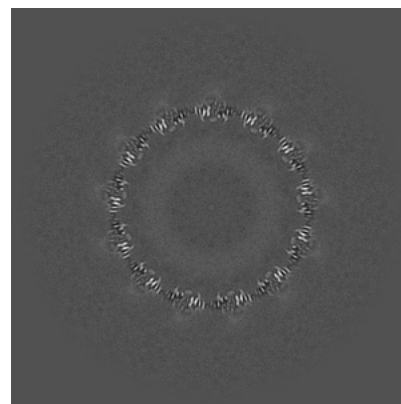
6.3.1 Primary map



X Index: 283



Y Index: 288

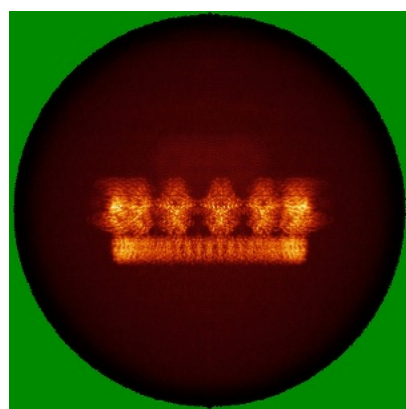


Z Index: 204

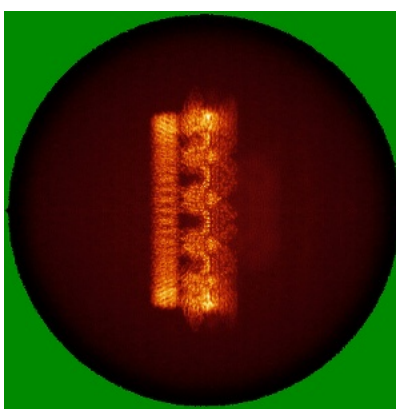
The images above show the largest variance slices of the map in three orthogonal directions.

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

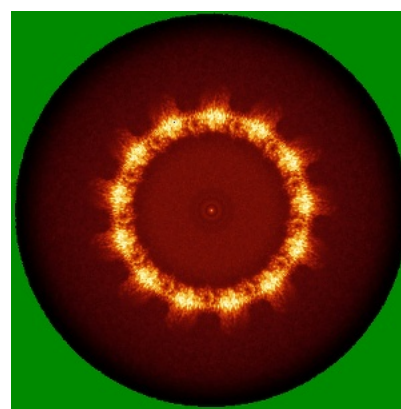
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

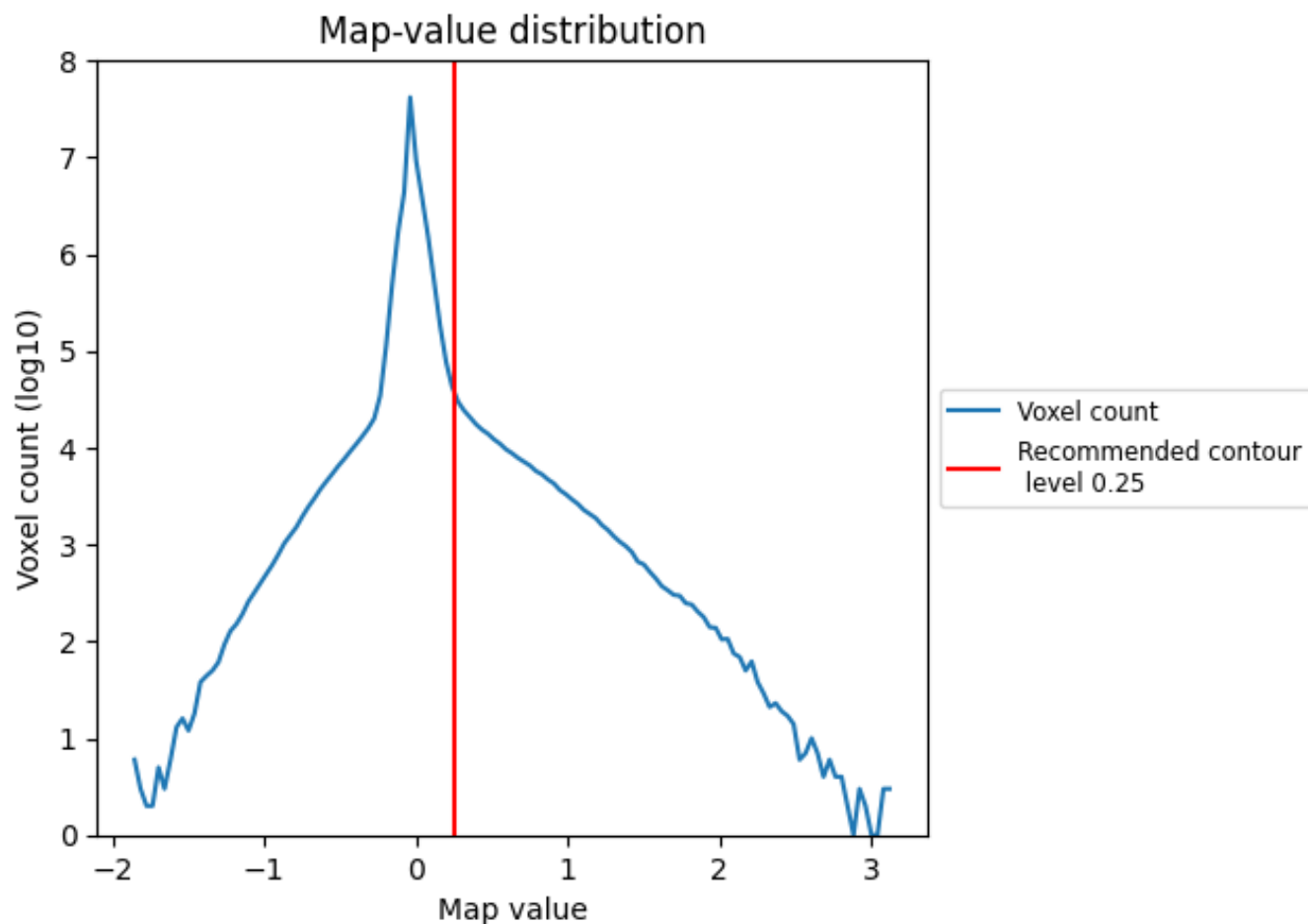
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

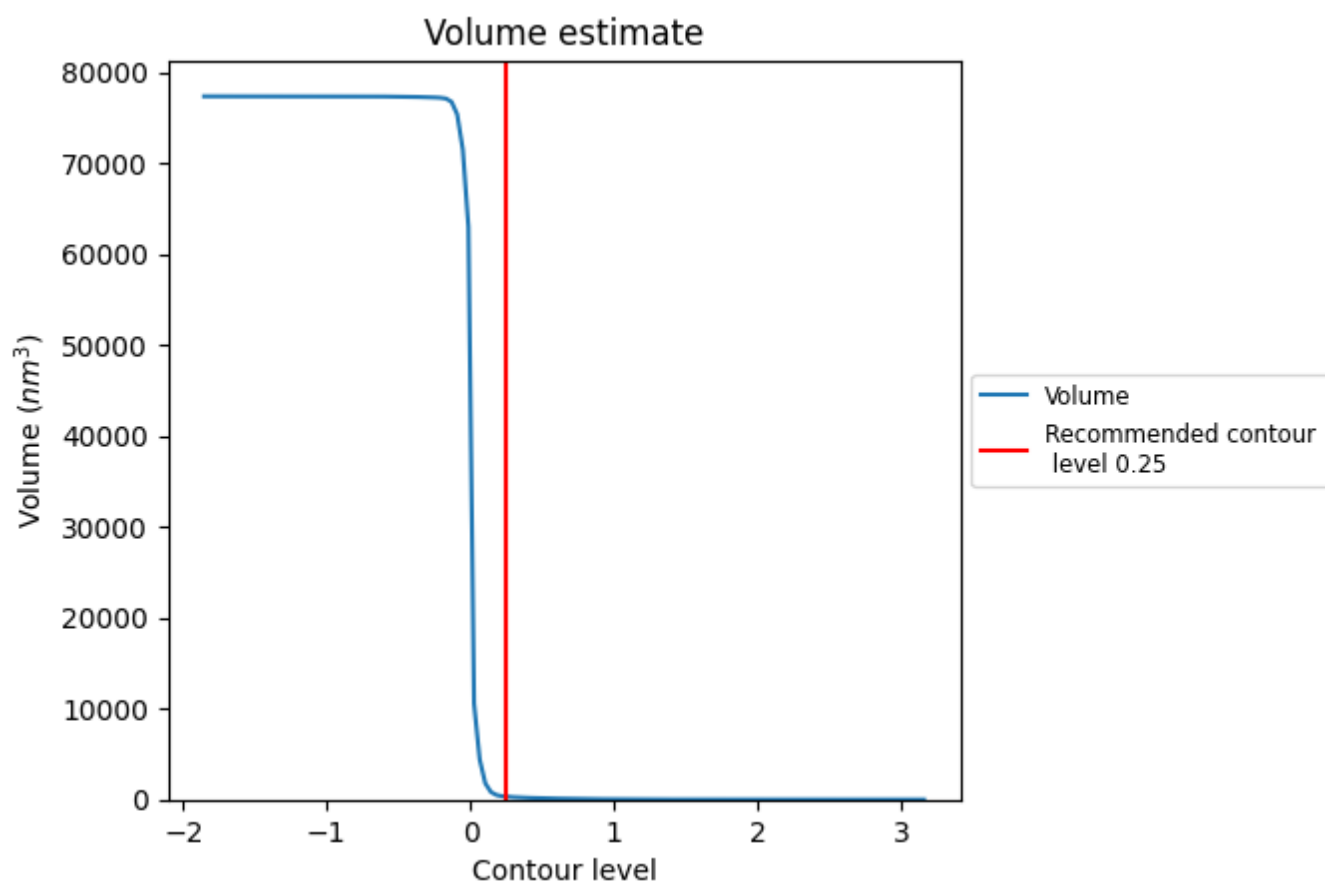
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

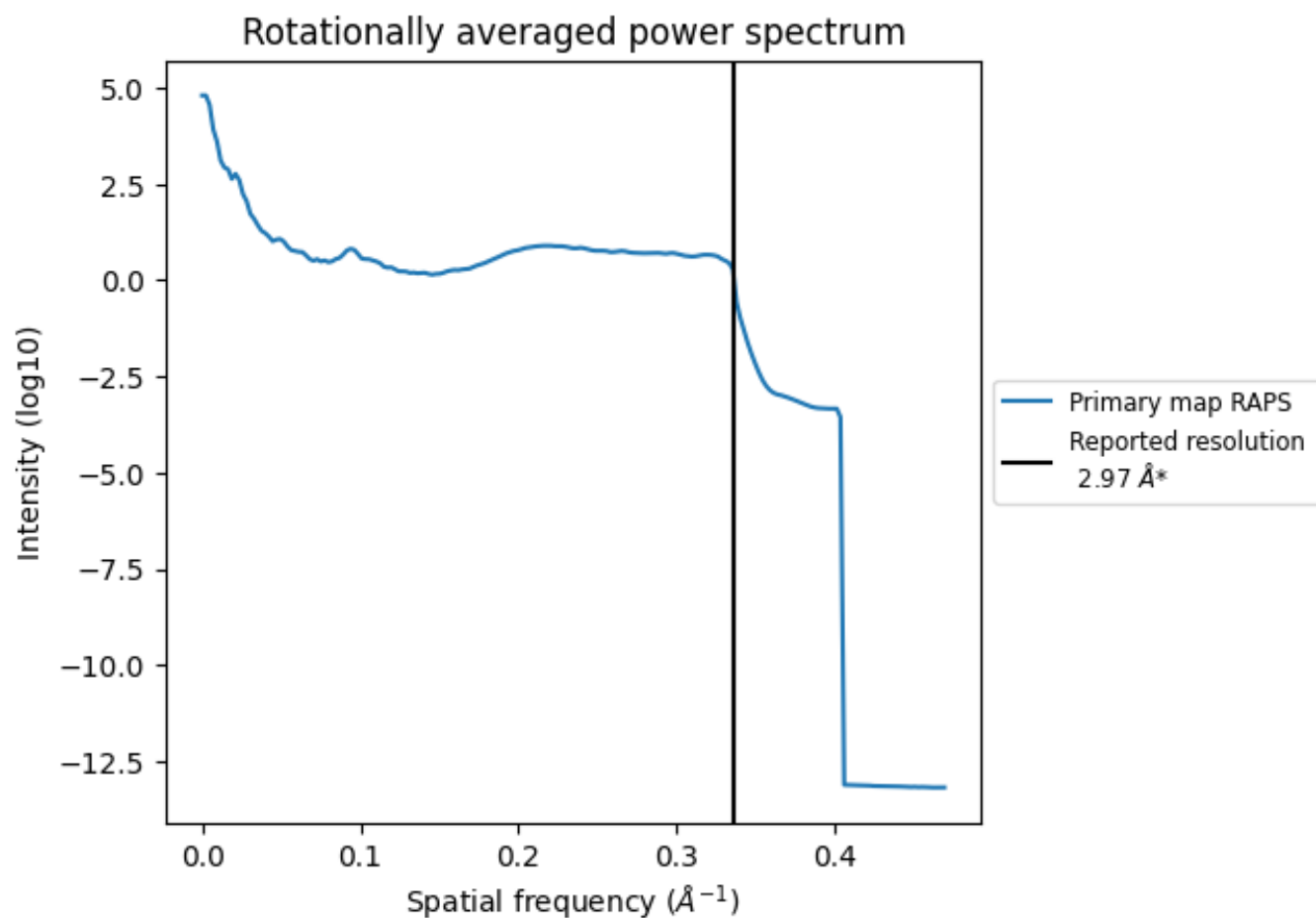
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 322 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

8 Fourier-Shell correlation

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

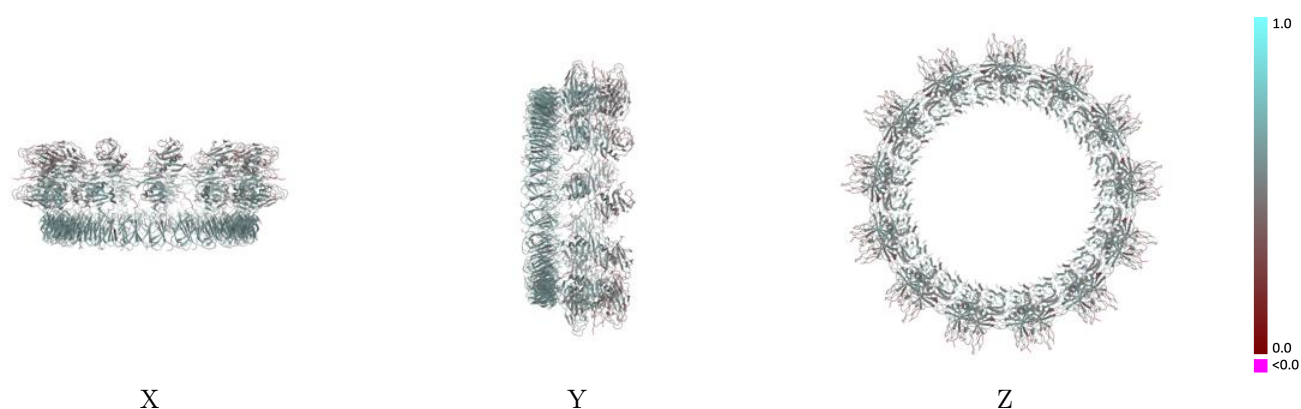
9 Map-model fit [i](#)

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 [i](#)

This section was not generated.

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

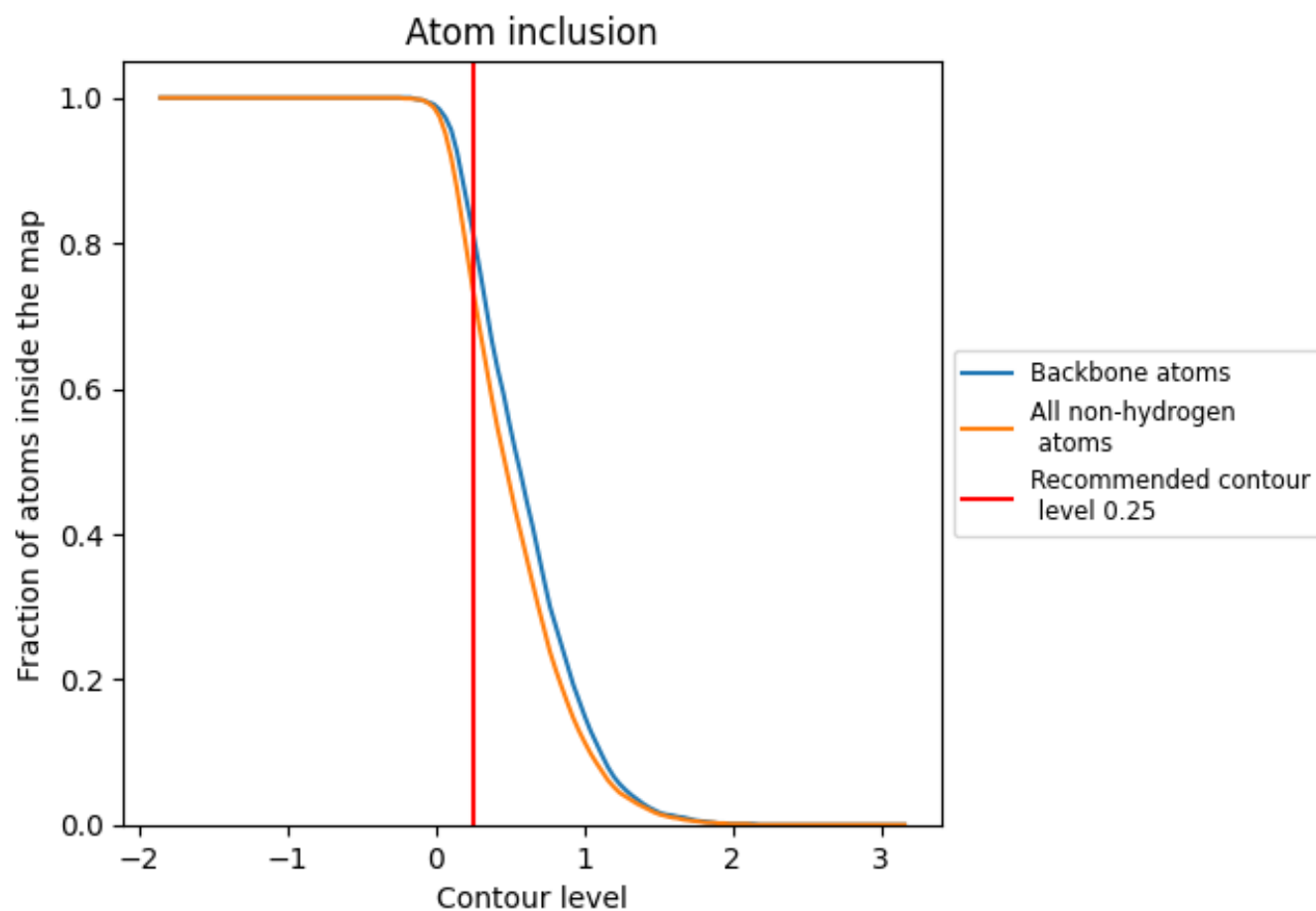


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

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	Q-score
All	 0.7370	 0.5020
A1	 0.7450	 0.4910
A10	 0.7330	 0.4930
A11	 0.7280	 0.4860
A12	 0.7420	 0.4900
A13	 0.7450	 0.4910
A2	 0.7520	 0.4910
A3	 0.7350	 0.4910
A4	 0.7400	 0.4910
A5	 0.7400	 0.4910
A6	 0.7400	 0.4920
A7	 0.7420	 0.4940
A8	 0.7400	 0.4900
A9	 0.7400	 0.4900
B1	 0.6950	 0.4650
B10	 0.6970	 0.4650
B11	 0.6930	 0.4630
B12	 0.7010	 0.4640
B13	 0.6950	 0.4640
B2	 0.7010	 0.4630
B3	 0.6990	 0.4620
B4	 0.7010	 0.4650
B5	 0.7010	 0.4640
B6	 0.6930	 0.4660
B7	 0.6970	 0.4650
B8	 0.7030	 0.4660
B9	 0.6990	 0.4670
C1	 0.8210	 0.5400
C10	 0.8190	 0.5370
C11	 0.8200	 0.5380
C12	 0.8180	 0.5380
C13	 0.8230	 0.5390
C2	 0.8220	 0.5380
C3	 0.8220	 0.5390
C4	 0.8170	 0.5390



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Chain	Atom inclusion	Q-score
C5	 0.8200	 0.5380
C6	 0.8210	 0.5380
C7	 0.8180	 0.5370
C8	 0.8220	 0.5370
C9	 0.8160	 0.5370
D1	 0.7060	 0.4890
D10	 0.7030	 0.4840
D11	 0.7030	 0.4860
D12	 0.7030	 0.4870
D13	 0.7060	 0.4850
D2	 0.7010	 0.4880
D3	 0.7070	 0.4860
D4	 0.7060	 0.4890
D5	 0.7040	 0.4880
D6	 0.7050	 0.4880
D7	 0.7030	 0.4860
D8	 0.7040	 0.4860
D9	 0.7080	 0.4860
E1	 0.1060	 0.3830
E10	 0.1180	 0.3690
E11	 0.1180	 0.3860
E12	 0.1180	 0.3770
E13	 0.1180	 0.3820
E2	 0.1060	 0.3820
E3	 0.1180	 0.3860
E4	 0.1180	 0.3830
E5	 0.1290	 0.3780
E6	 0.1180	 0.3810
E7	 0.1060	 0.3770
E8	 0.1290	 0.3760
E9	 0.0820	 0.3710
F1	 0.6240	 0.5220
F10	 0.6000	 0.5090
F11	 0.6350	 0.5170
F12	 0.6240	 0.5100
F13	 0.6240	 0.5220
F2	 0.6120	 0.5080
F3	 0.6350	 0.5110
F4	 0.6120	 0.5080
F5	 0.6240	 0.5160
F6	 0.6350	 0.5150
F7	 0.6350	 0.5120

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Chain	Atom inclusion	Q-score
F8	 0.6470	 0.5070
F9	 0.6350	 0.5190