



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:00 AM UTC

PDB ID : 7SPB / pdb_00007spb
EMDB ID : EMD-24769
Title : Models for C13 reconstruction of Outer Membrane Core Complex (OMCC) of Type IV Secretion System (T4SS) encoded by F-plasmid (pED208).
Authors : Liu, X.; Khara, P.; Baker, M.L.; Christie, P.J.; Hu, B.
Deposited on : 2021-11-02
Resolution : 3.31 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:

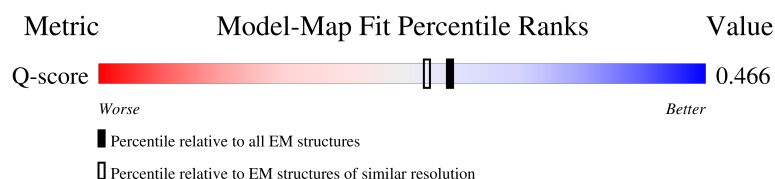
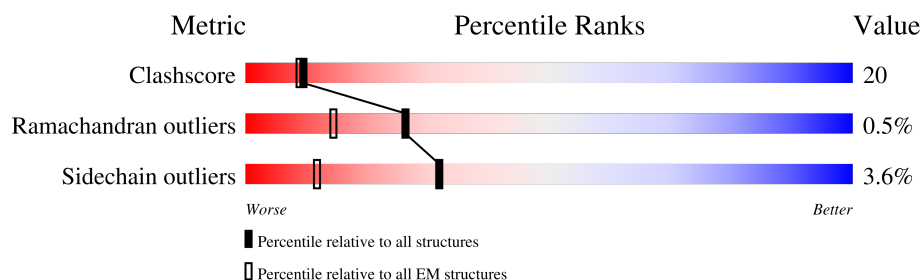
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.31 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.



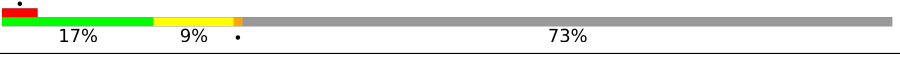
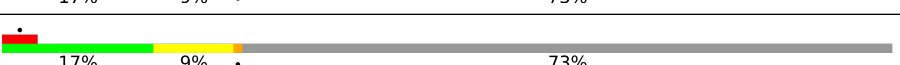
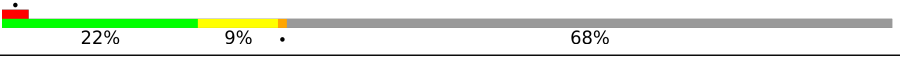
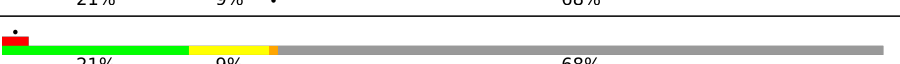
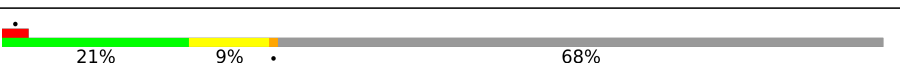
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14550 (2.81 - 3.81)

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	
1	A10	204	
1	A11	204	
1	A12	204	

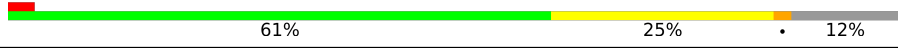
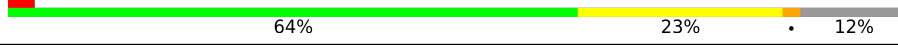
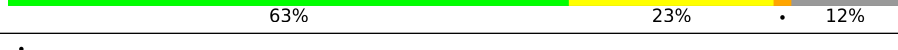
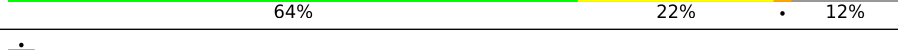
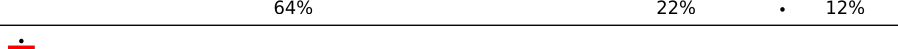
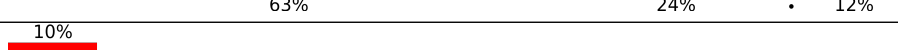
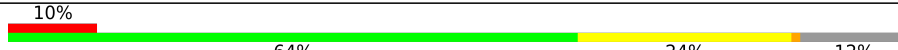
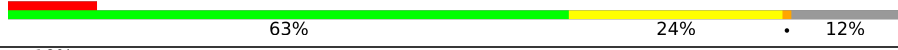
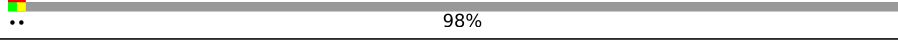
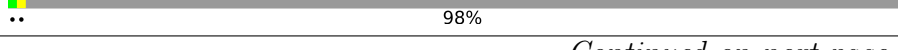
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Mol	Chain	Length	Quality of chain
1	A13	204	
1	A2	204	
1	A3	204	
1	A4	204	
1	A5	204	
1	A6	204	
1	A7	204	
1	A8	204	
1	A9	204	
1	B1	204	
1	B10	204	
1	B11	204	
1	B12	204	
1	B13	204	
1	B2	204	
1	B3	204	
1	B4	204	
1	B5	204	
1	B6	204	
1	B7	204	
1	B8	204	
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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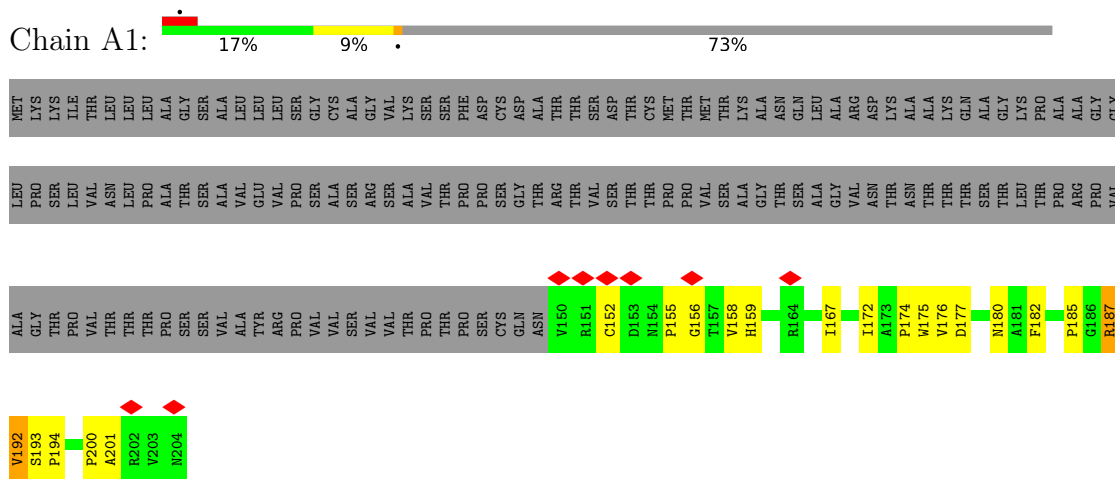
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F12	11	Total	C	N	O	S	0	0
			87	52	15	18	2		
3	F13	11	Total	C	N	O	S	0	0
			87	52	15	18	2		

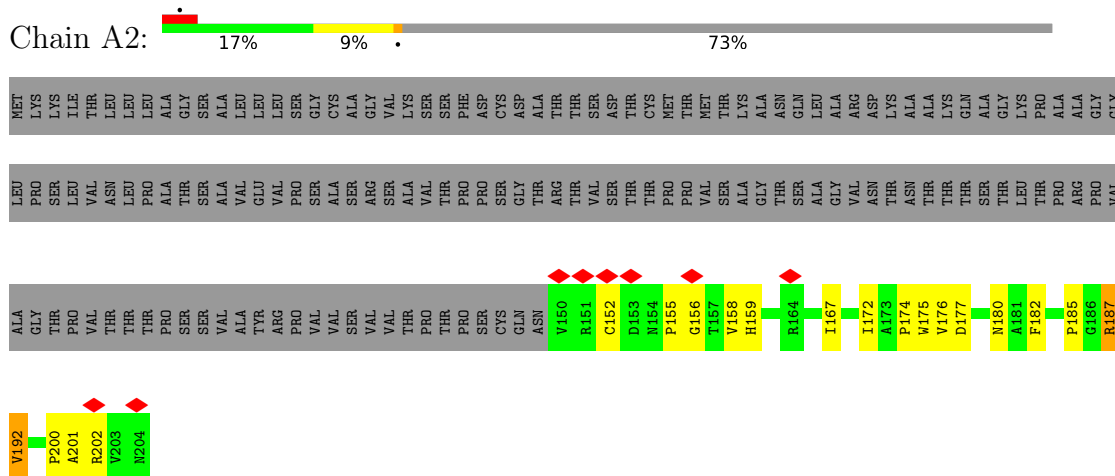
3 Residue-property plots

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.

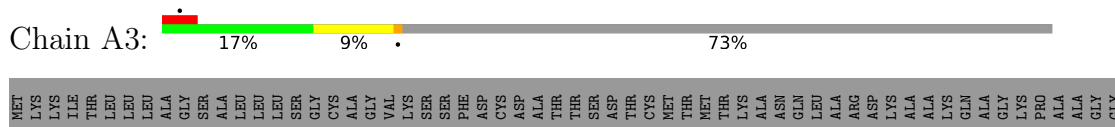
• Molecule 1: TraV

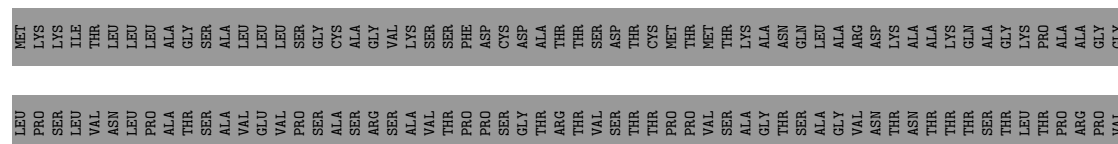


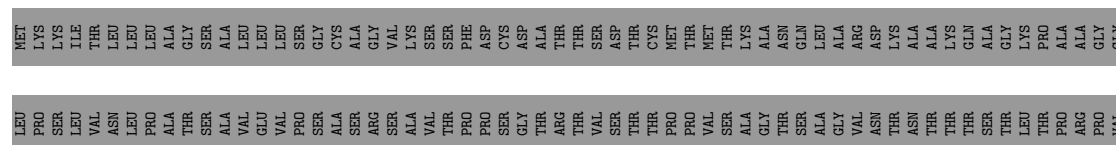
• Molecule 1: TraV

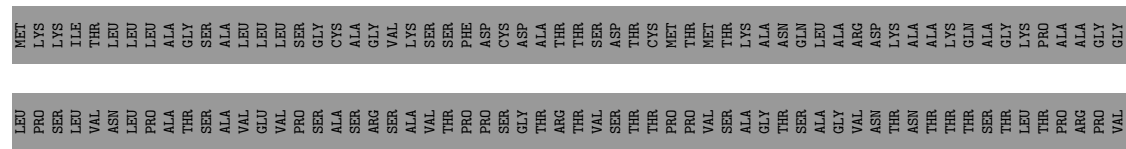


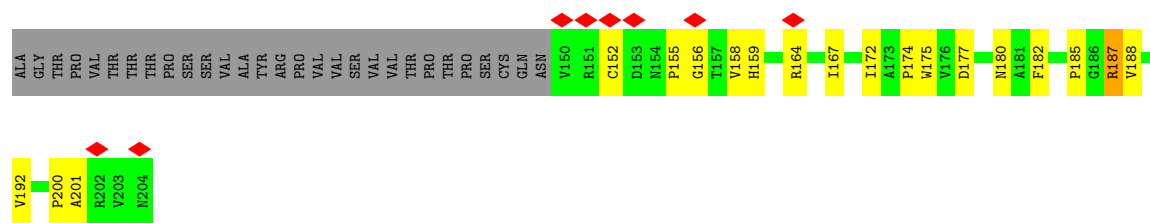
• Molecule 1: TraV





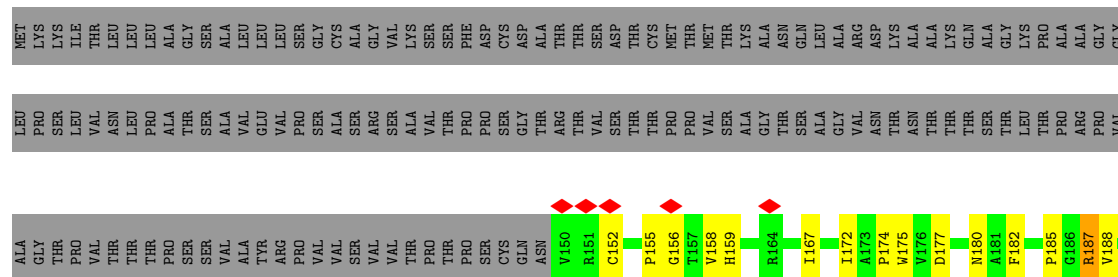






• Molecule 1: TraV

Chain A13: 17% 10% 73%



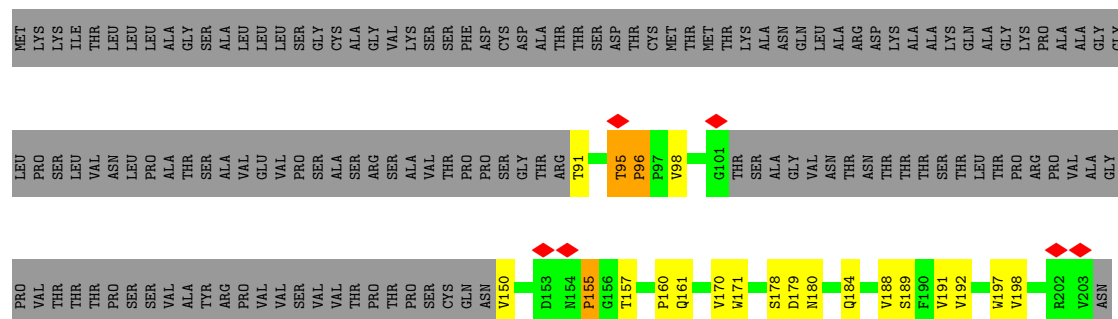
• Molecule 1: TraV

Chain B1: 21% 10% 68%



• Molecule 1: TraV

Chain B2: 22% 9% 68%



Chain B3:



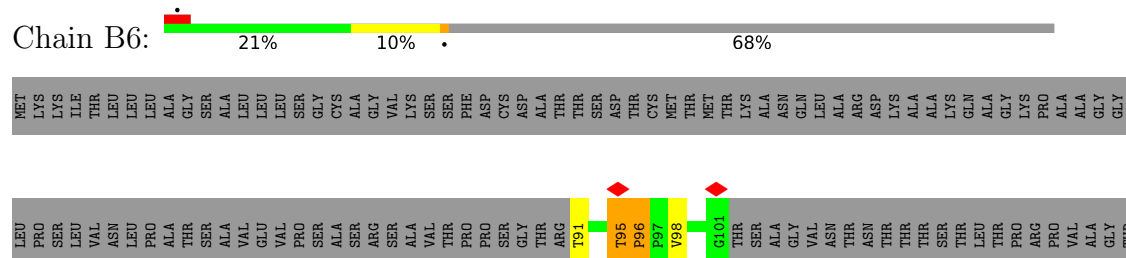
Chain B4:

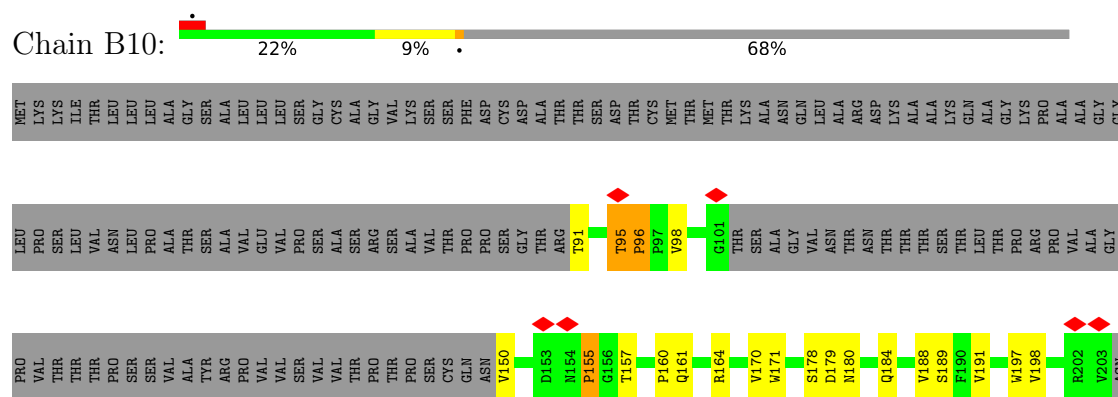


Chain B5:

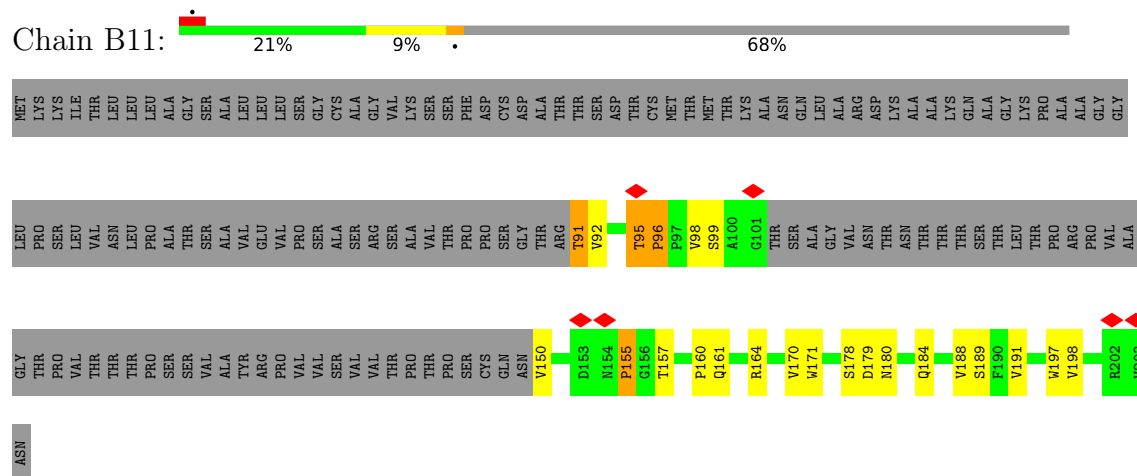


Chain B6:

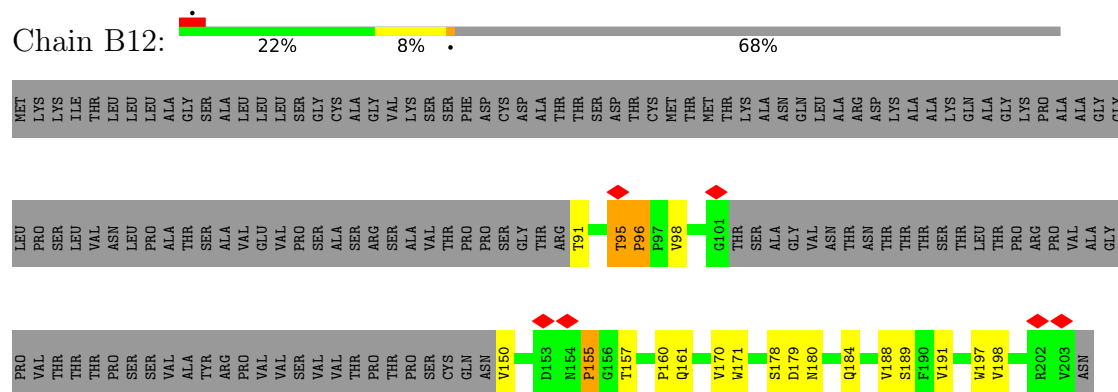




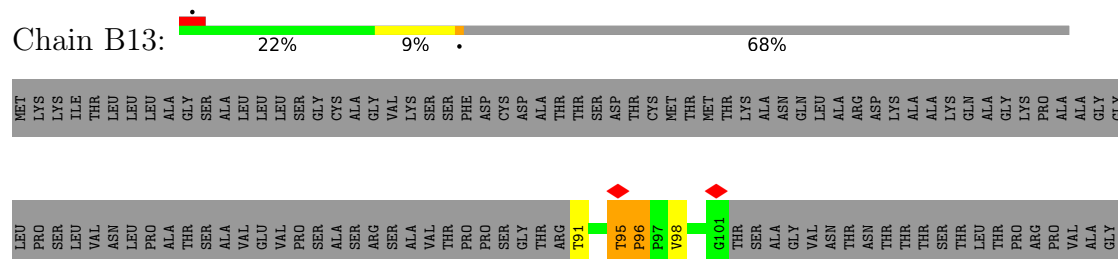
- Molecule 1: TraV

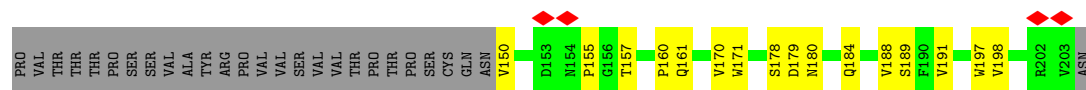


- Molecule 1: TraV

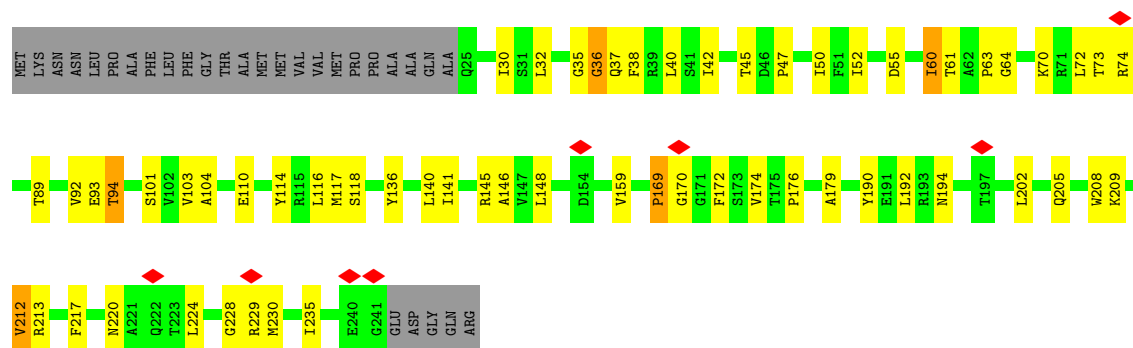


- Molecule 1: TraV

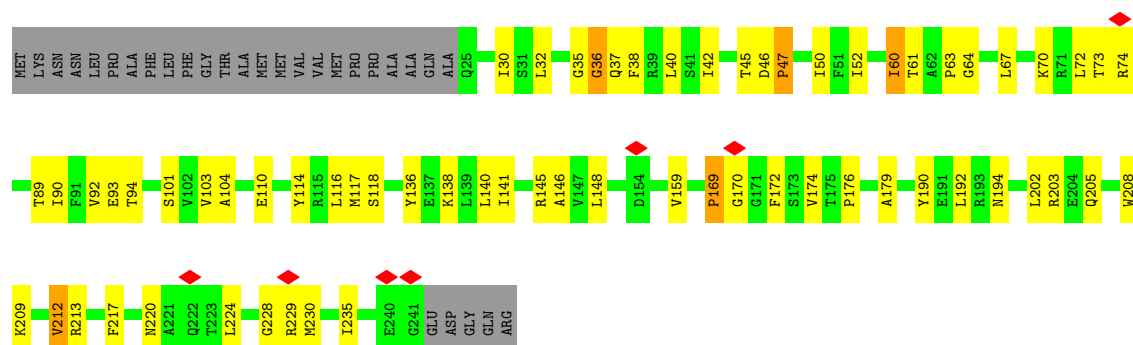




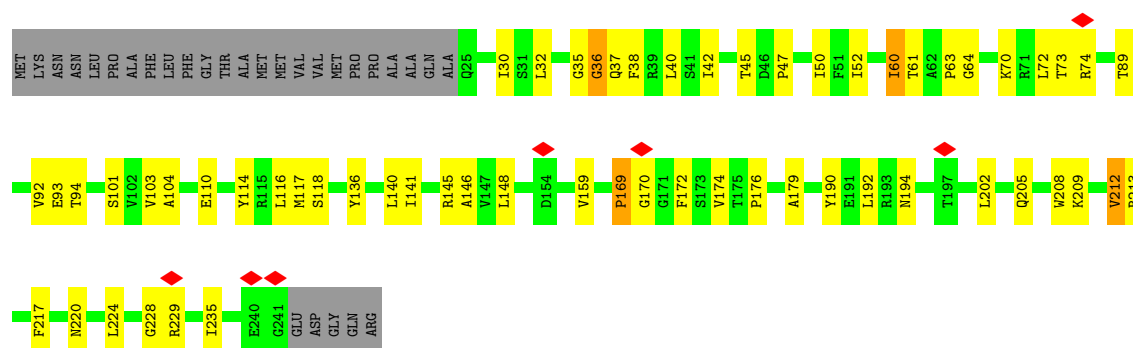
- Molecule 2: TraK



- Molecule 2: TraK

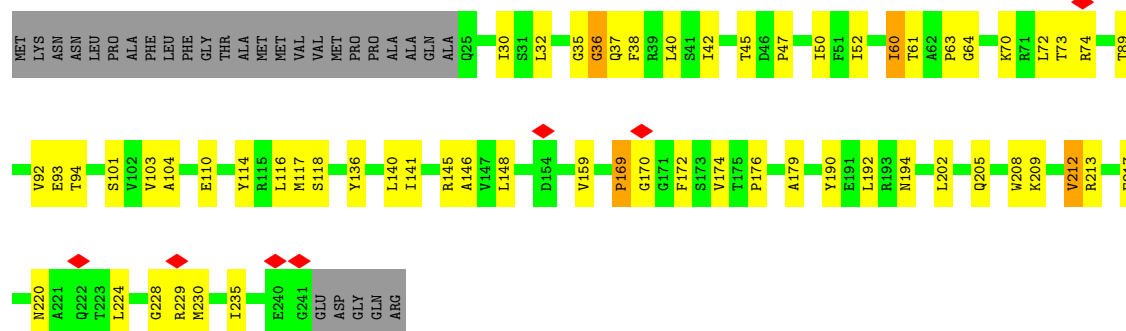


- Molecule 2: TraK



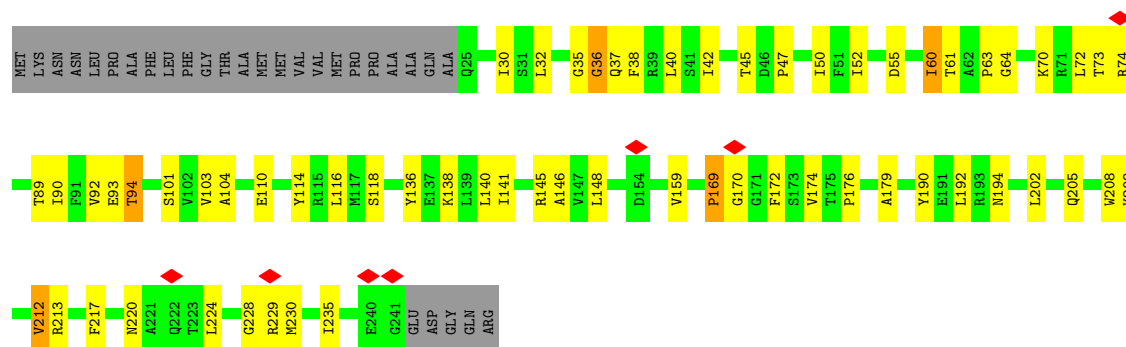
- Molecule 2: TraK

Chain C4: 



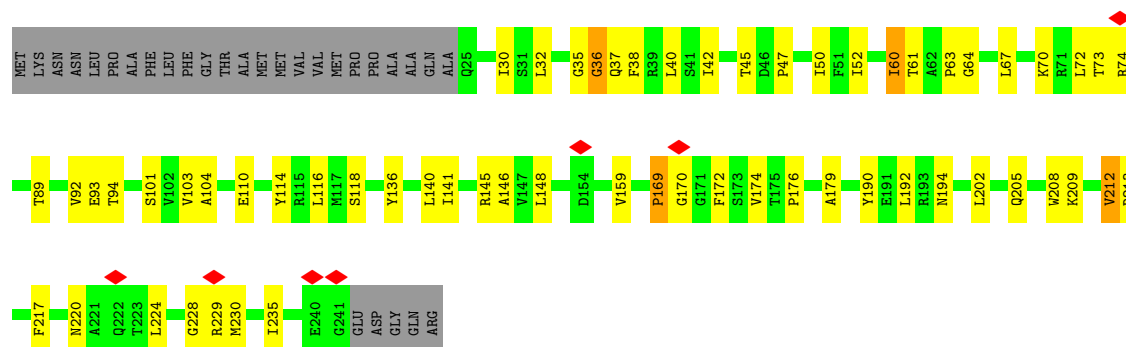
• Molecule 2: TraK

Chain C5: 



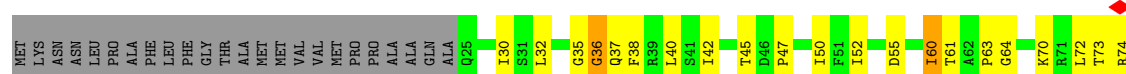
• Molecule 2: TraK

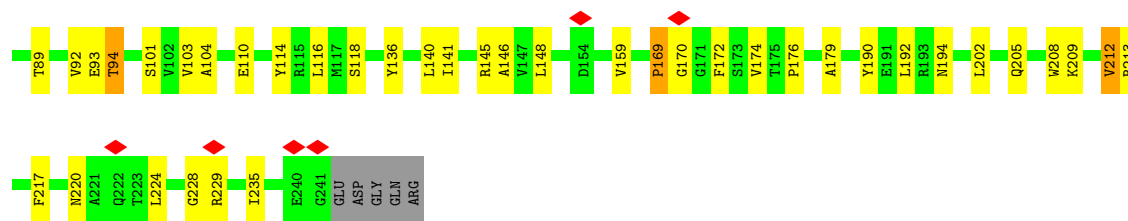
Chain C6: 



• Molecule 2: TraK

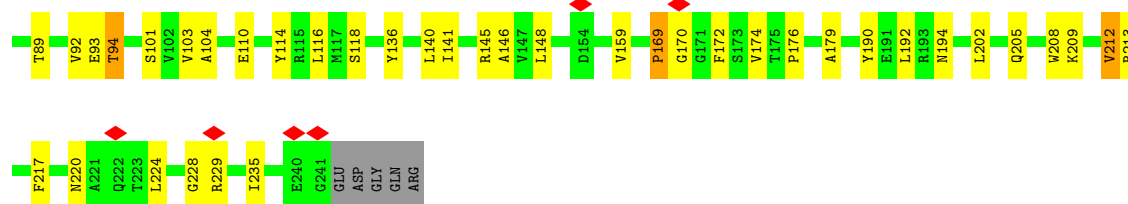
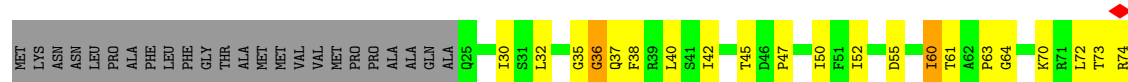
Chain C7: 





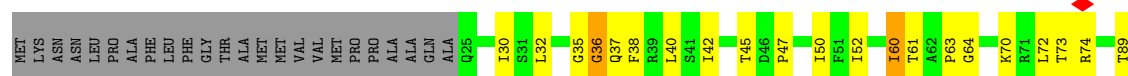
- Molecule 2: TraK

Chain C8: 64% 22% 12%



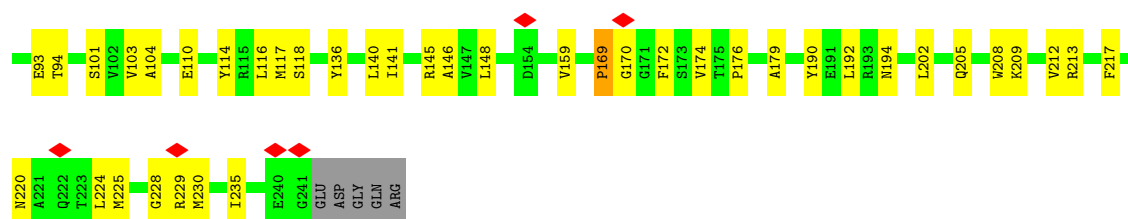
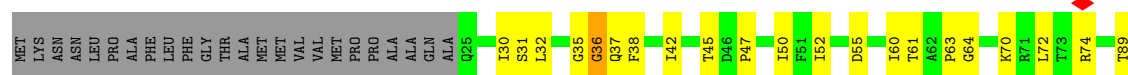
- Molecule 2: TraK

Chain C9: 63% 24% 12%



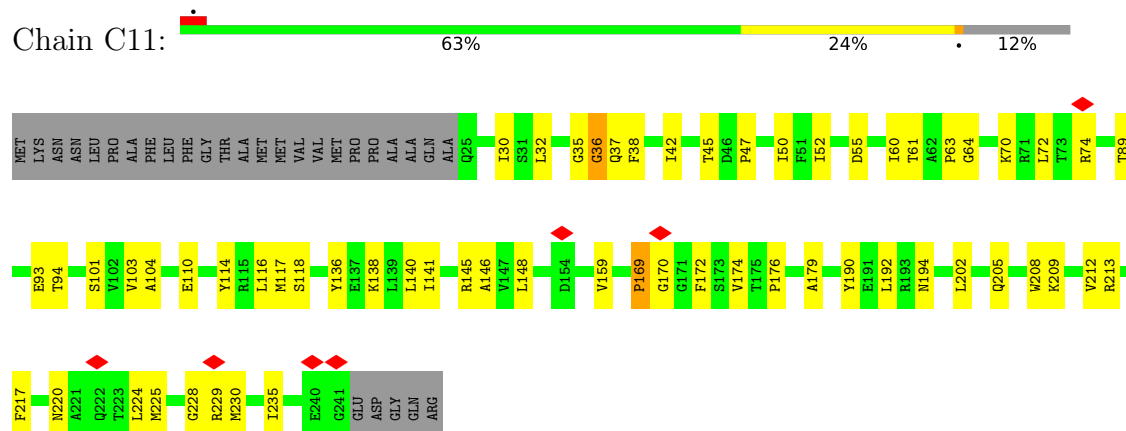
- Molecule 2: TraK

Chain C10: 63% 24% 12%



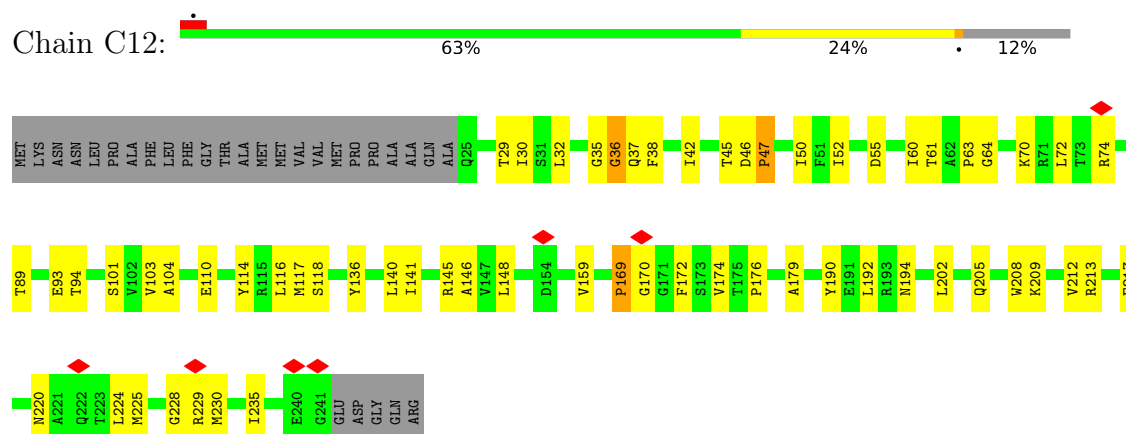
• Molecule 2: TraK

Chain C11:



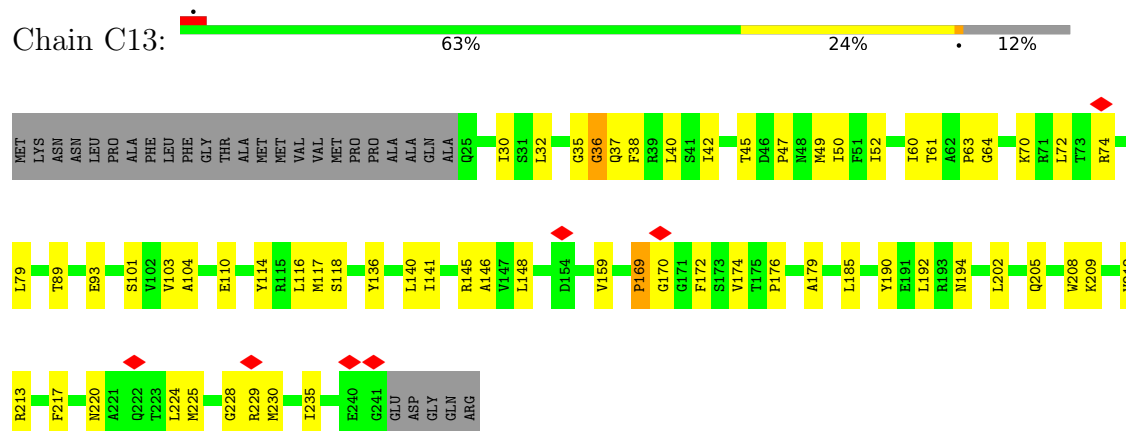
• Molecule 2: TraK

Chain C12:



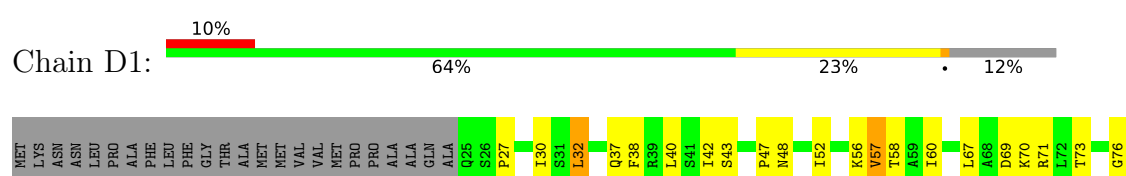
• Molecule 2: TraK

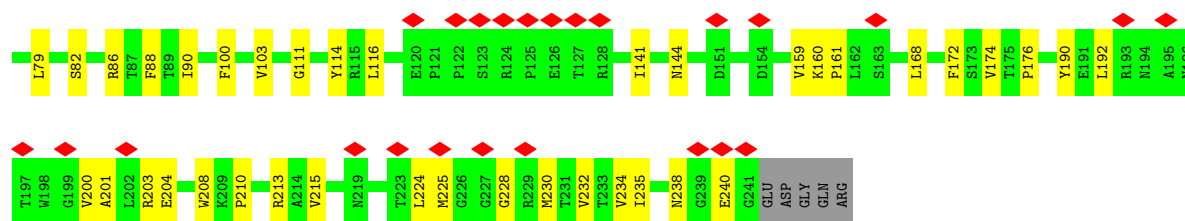
Chain C13:



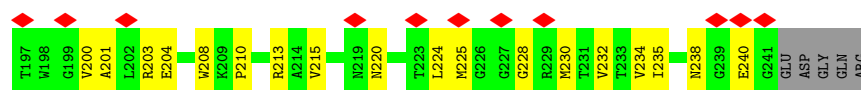
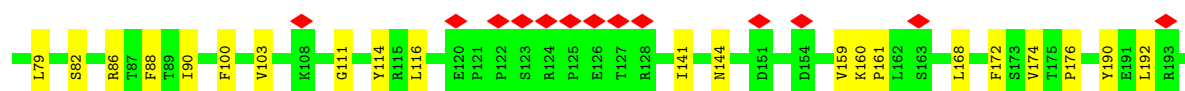
• Molecule 2: TraK

Chain D1:

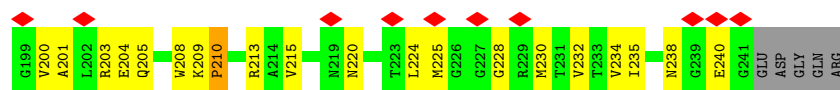
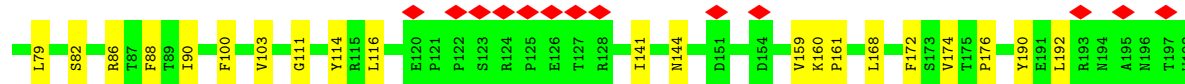




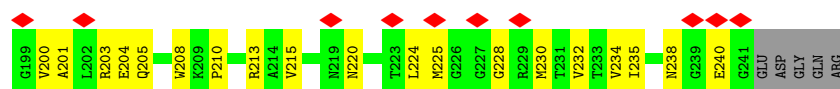
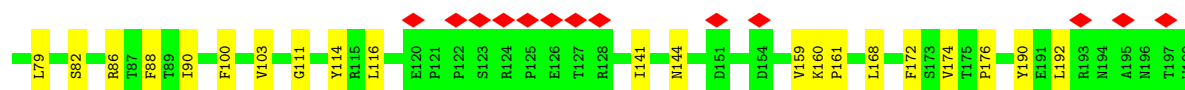
• Molecule 2: TraK



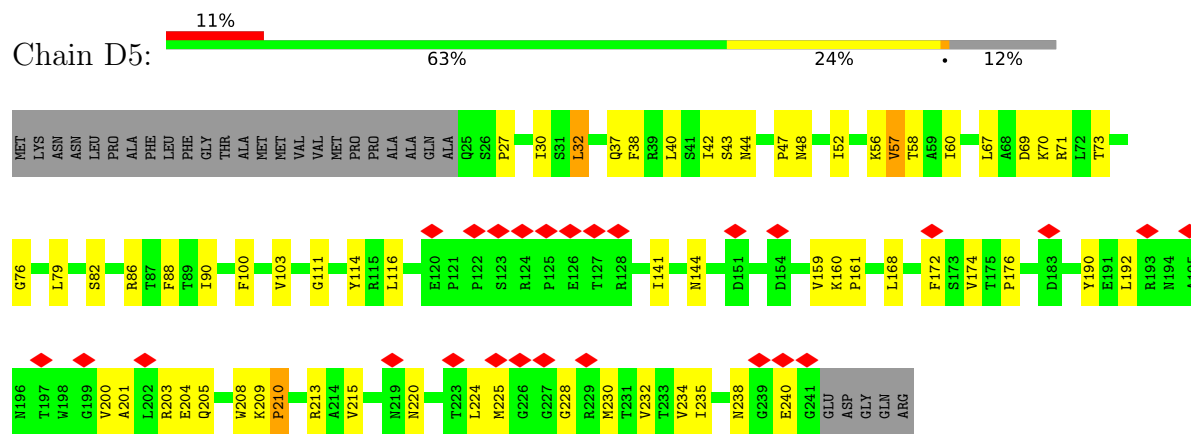
• Molecule 2: TraK



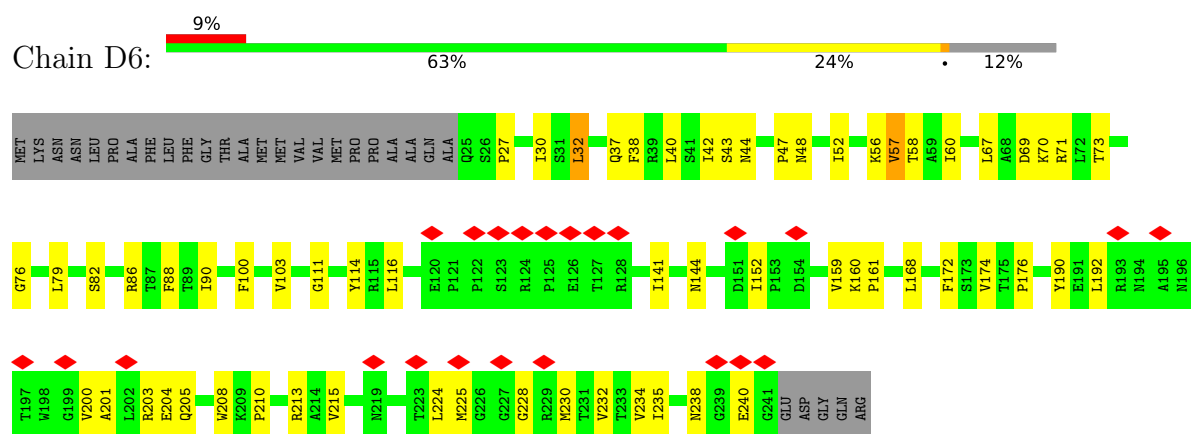
• Molecule 2: TraK



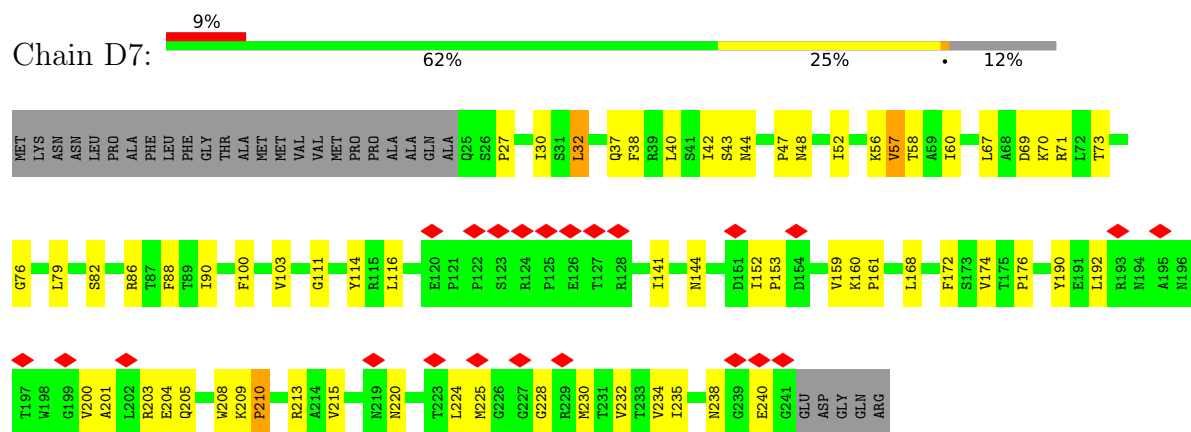
- Molecule 2: TraK



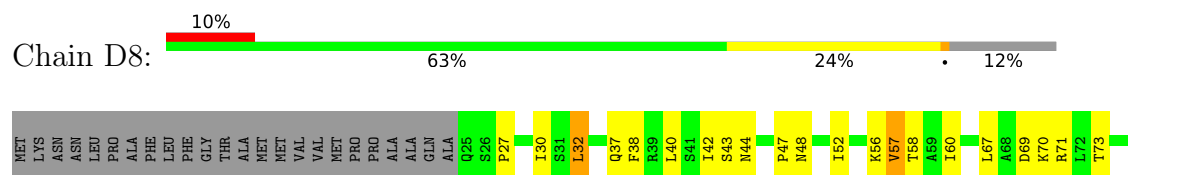
- Molecule 2: TraK

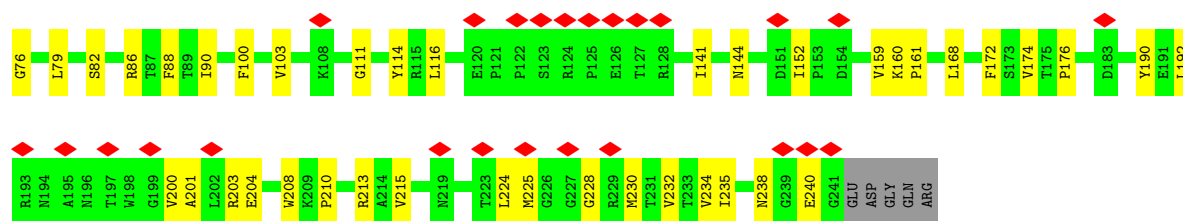


- Molecule 2: TraK

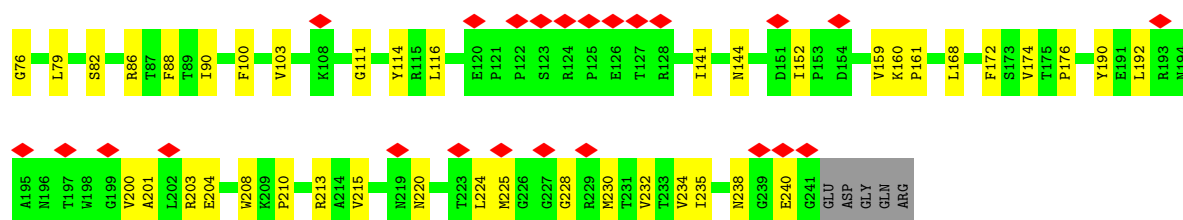


- Molecule 2: TraK

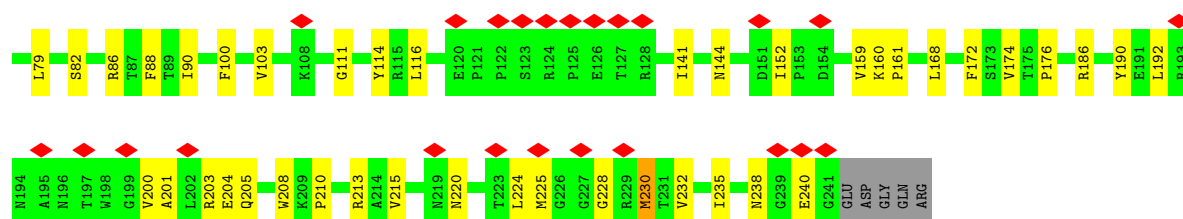




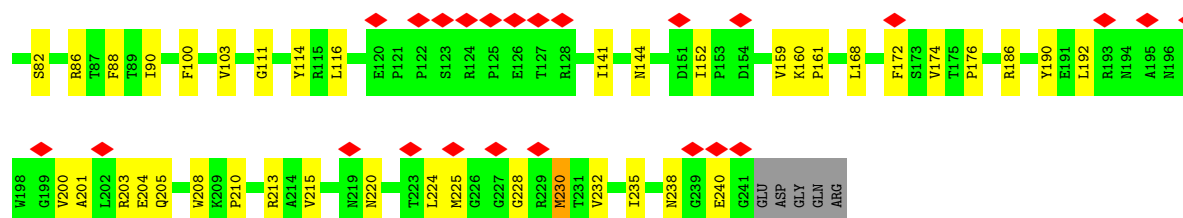
• Molecule 2: TraK



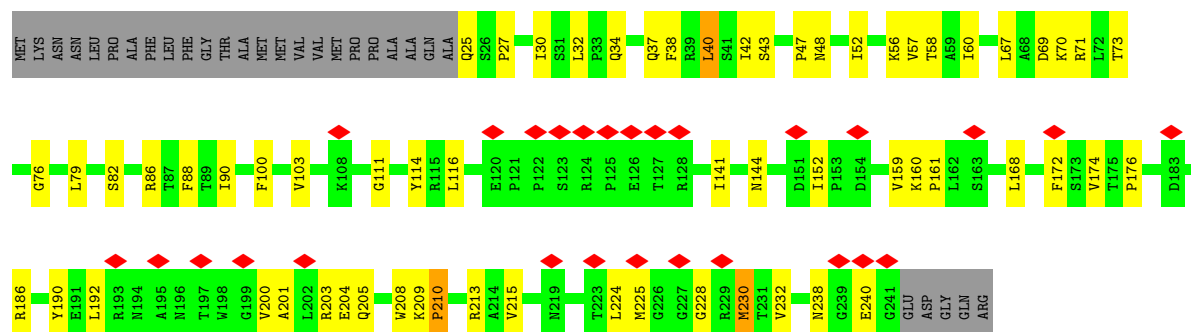
• Molecule 2: TraK



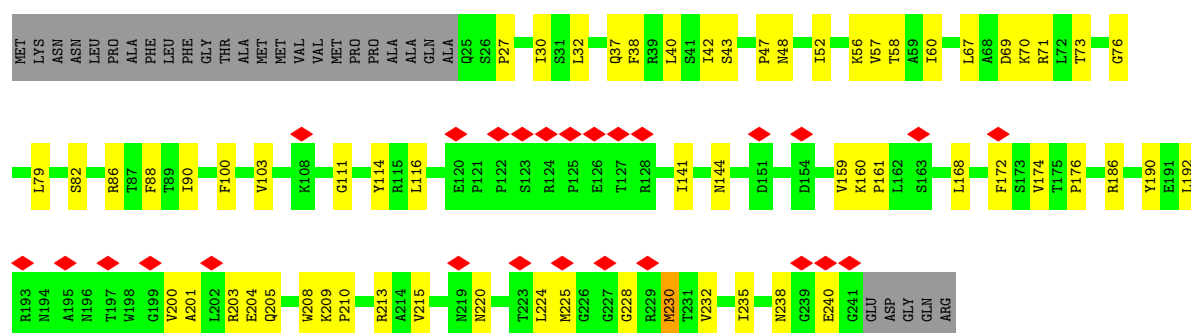
• Molecule 2: TraK



Chain D12: 11% 63% 24% 12%



Chain D13: 11% 63% 25% 12%



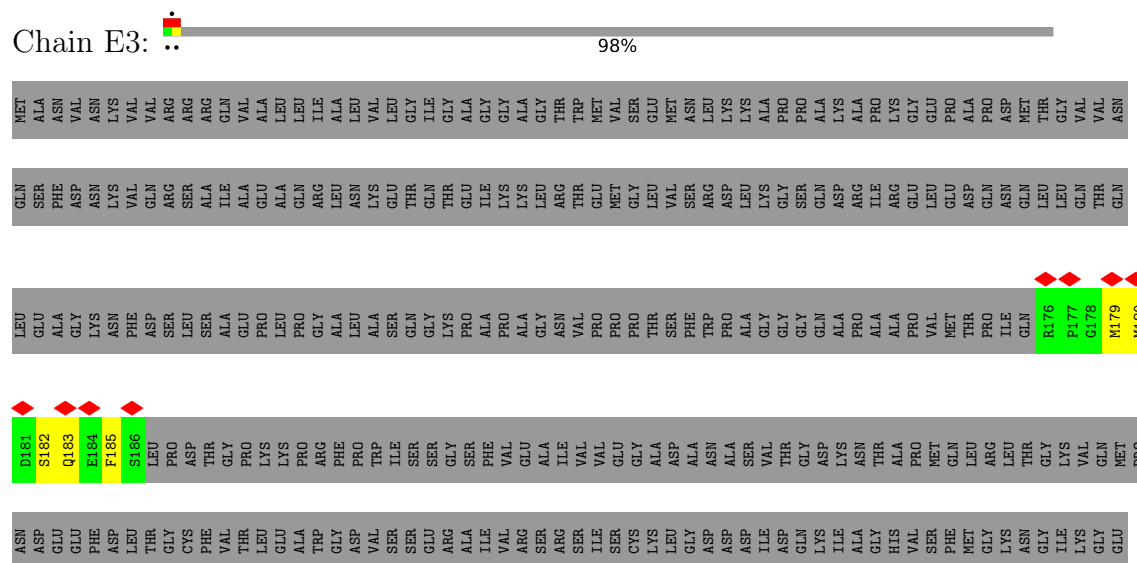
Chain E1: 98%



- Molecule 3: TraB



- Molecule 3: TraB



ALA	ALA	THR	VAL	ASN
ALA	MET	SER	VAL	ASP
PRO	PRO	ASP	ARG	GLU
ASN	GLY	TVR	ASN	PHE
THR	ASN	TVR	GLN	LEU
PRO	THR	ILE	GLN	THR
ASP	LYS	LYS	ILE	GLY
ASP	ARG	ARG	LEU	CYS
MET	ALA	ALA	LEU	PHE
LEU	GLU	GLU	TYR	VAL
LYS	GLN	GLN	ALA	THR
GLN	TVR	TVR	GLY	GLU
LEU	HIS	HIS	GLY	LEU
GLN	PRO	PRO	ALA	GLU
ASP	VAL	VAL	PHE	ALA
PHE	ILE	ILE	GLY	TRP
ARG	PRO	PRO	LEU	GLY
VAL	ILE	ILE	ASP	ASP
GLY	GLY	GLY	GLY	VAL
ASP	ALA	ALA	ILE	SER
PRO	THR	THR	LYS	GLU
ALA	VAL	ASN	ILE	ARG
ALA	THR	GLU	GLY	ALA
GLY	VAL	VAL	GLU	ILE
GLN	GLN	PHE	ALA	ARG
VAL	GLN	GLN	SER	SER
VAL	VAL	GLN	SER	ARG
THR	THR	GLY	THR	SER
GLN	GLN	PHE	VAL	ILE
		GLN	GLY	SER
		LEU	VAL	CYS
		GLU	VAL	LYS
		GLU	GLY	LEU
		THR	ALA	GLY
		LEU	THR	GLY
		GLU	ALA	ASP
		GLU	SER	ASP
		ALA	MET	ILE
		ARG	SER	ASP
		ALA	ALA	GLN
		LYS	ALA	LYS
		ALA	ILE	ILE
		ALA	GLY	GLY
		ARG	GLN	HIS
		LYS	ALA	VAL
		GLN	GLY	SER
		GLN	LEU	PHE
		ASN	GLY	MET
		GLN	GLY	GLY
		PRO	GLY	LYS
		SER	VAL	ASN
		ALA	SER	GLY
		SER	SER	ILE
		SER	ALA	LYS
		THR	LYS	GLY
		PRO	VAL	THR

- Molecule 3: TraB

Chain E6: 98%

[illegible]

- Molecule 3: TraB

Chain E7: 98%

[illegible]

LEU	GLU	ALA	GLY	LYS	ASN	PHE	ASP	LEU	SER	ALA	GLU	PRO	PRO	GLY	ALA	LEU	ALA	ALA	PRO	PRO	GLY	GLN	R176	P177	G178	M179	M180
D181	S182	Q183	E184	F185	S186	LEU	PRO	ASP	THR	GLY	PRO	GLY	LYS	LYS	TRP	ASP	PHE	ALA	PRO	THR	GLY	GLN	LYS	LYS	VAL	GLN	PRO
ASN	ASP	GLU	GLY	PHE	ASP	LEU	THR	GLY	ARG	PHE	VAL	THR	LEU	GLU	ALA	TRP	GLY	ARG	ILE	ASP	VAL	ILE	SER	ILE	GLY	LEU	PRO
VAL	VAL	MET	ARG	ASN	GLY	GLN	ILE	LEU	TYR	ALA	GLY	GLY	ALA	GLY	ALA	GLY	ILE	GLY	LYS	GLY	ILE	GLY	GLY	GLY	GLY	GLY	LYS
THR	LEU	SER	ASP	TYR	THR	ILE	LYS	ARG	ALA	GLN	THR	HIS	PRO	ILE	PHE	LEU	ASP	GLY	ILE	GLY	THR	PHE	GLY	ILE	GLY	ALA	PRO
ALA	ALA	MET	PRO	GLY	ASN	THR	PRO	ASP	MET	LEU	LYS	LEU	GLN	ASP	PHE	VAL	GLY	ASP	THR	GLY	THR	GLN	ALA	THR	THR	THR	GLN

● Molecule 3: TraB

Chain E10:  98%

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

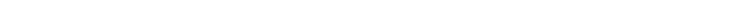
Chain E11:  98%

MET	ALA	ASN	VAL	ASN	LYS	VAL	VAL	VAL	ARG	ARG	GLN	VAL	ALA	LEU	ILE	ALA	LEU	VAL	VAL	ALA	LEU	VAL	GLY	VAL	VAL	VAL	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



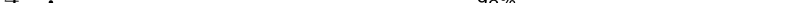
[illegible]

- Molecule 3: TraB

Chain F3:  98%

[illegible]

- Molecule 3: TraB

Chain F4: 

[illegible]

- Molecule 3: TraB

Chain F5: 98%

[illegible]

- Molecule 3: TraB

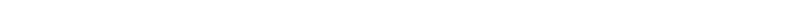
Chain F6: 98%



WORLD WIDE
PDB
PROTEIN DATA BANK

[illegible]

- Molecule 3: TraB

Chain F9:  98%

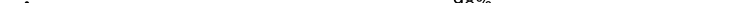
[illegible]

- Molecule 3: TraB

Chain F10: 98%

[illegible]

- Molecule 3: TraB

Chain F11:  98%

[illegible]

- Molecule 3: TraB

Chain F12: 98%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C13	Depositor
Number of particles used	70700	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	2.074	Depositor
Minimum map value	-1.310	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.35	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	0.62	0/451	1.02	3/622 (0.5%)
1	A10	0.62	0/451	1.02	3/622 (0.5%)
1	A11	0.63	0/451	1.02	3/622 (0.5%)
1	A12	0.63	0/451	1.02	3/622 (0.5%)
1	A13	0.63	0/451	1.02	3/622 (0.5%)
1	A2	0.63	0/451	1.02	3/622 (0.5%)
1	A3	0.63	0/451	1.02	3/622 (0.5%)
1	A4	0.63	0/451	1.02	3/622 (0.5%)
1	A5	0.63	0/451	1.02	3/622 (0.5%)
1	A6	0.63	0/451	1.02	3/622 (0.5%)
1	A7	0.63	0/451	1.02	3/622 (0.5%)
1	A8	0.63	0/451	1.02	3/622 (0.5%)
1	A9	0.63	0/451	1.02	3/622 (0.5%)
1	B1	0.60	0/514	1.22	5/710 (0.7%)
1	B10	0.60	0/514	1.22	5/710 (0.7%)
1	B11	0.60	0/514	1.22	5/710 (0.7%)
1	B12	0.60	0/514	1.22	5/710 (0.7%)
1	B13	0.60	0/514	1.22	5/710 (0.7%)
1	B2	0.60	0/514	1.22	5/710 (0.7%)
1	B3	0.60	0/514	1.22	5/710 (0.7%)
1	B4	0.60	0/514	1.22	5/710 (0.7%)
1	B5	0.60	0/514	1.22	5/710 (0.7%)
1	B6	0.60	0/514	1.22	5/710 (0.7%)
1	B7	0.60	0/514	1.22	5/710 (0.7%)
1	B8	0.60	0/514	1.22	5/710 (0.7%)
1	B9	0.60	0/514	1.22	5/710 (0.7%)
2	C1	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C10	0.73	2/1688 (0.1%)	0.97	7/2290 (0.3%)
2	C11	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C12	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C13	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C2	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C3	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C4	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	C5	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C6	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C7	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C8	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	C9	0.73	2/1688 (0.1%)	0.97	6/2290 (0.3%)
2	D1	0.70	0/1688	0.98	3/2290 (0.1%)
2	D10	0.70	0/1688	0.98	3/2290 (0.1%)
2	D11	0.70	0/1688	0.98	3/2290 (0.1%)
2	D12	0.70	0/1688	0.98	3/2290 (0.1%)
2	D13	0.70	0/1688	0.98	3/2290 (0.1%)
2	D2	0.70	0/1688	0.98	3/2290 (0.1%)
2	D3	0.70	0/1688	0.98	3/2290 (0.1%)
2	D4	0.70	0/1688	0.98	3/2290 (0.1%)
2	D5	0.70	0/1688	0.98	3/2290 (0.1%)
2	D6	0.70	0/1688	0.98	3/2290 (0.1%)
2	D7	0.70	0/1688	0.98	3/2290 (0.1%)
2	D8	0.70	0/1688	0.98	3/2290 (0.1%)
2	D9	0.70	0/1688	0.98	3/2290 (0.1%)
3	E1	0.30	0/88	0.92	0/115
3	E10	0.30	0/88	0.92	0/115
3	E11	0.30	0/88	0.92	0/115
3	E12	0.30	0/88	0.91	0/115
3	E13	0.30	0/88	0.92	0/115
3	E2	0.30	0/88	0.91	0/115
3	E3	0.30	0/88	0.91	0/115
3	E4	0.30	0/88	0.92	0/115
3	E5	0.30	0/88	0.92	0/115
3	E6	0.30	0/88	0.92	0/115
3	E7	0.29	0/88	0.92	0/115
3	E8	0.30	0/88	0.91	0/115
3	E9	0.30	0/88	0.91	0/115
3	F1	0.53	0/88	1.25	2/115 (1.7%)
3	F10	0.53	0/88	1.25	2/115 (1.7%)
3	F11	0.53	0/88	1.25	2/115 (1.7%)
3	F12	0.53	0/88	1.25	2/115 (1.7%)
3	F13	0.54	0/88	1.25	2/115 (1.7%)
3	F2	0.54	0/88	1.25	2/115 (1.7%)
3	F3	0.53	0/88	1.25	2/115 (1.7%)
3	F4	0.53	0/88	1.25	2/115 (1.7%)
3	F5	0.53	0/88	1.25	2/115 (1.7%)
3	F6	0.54	0/88	1.25	2/115 (1.7%)
3	F7	0.54	0/88	1.25	2/115 (1.7%)
3	F8	0.53	0/88	1.25	2/115 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	F9	0.53	0/88	1.25	2/115 (1.7%)
All	All	0.68	26/58721 (0.0%)	1.02	248/79846 (0.3%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C7	146	ALA	C-O	-5.15	1.18	1.24
2	C4	146	ALA	C-O	-5.14	1.18	1.24
2	C8	146	ALA	C-O	-5.13	1.18	1.24
2	C12	146	ALA	C-O	-5.13	1.18	1.24
2	C4	145	ARG	CA-C	-5.13	1.46	1.52
2	C5	145	ARG	CA-C	-5.13	1.46	1.52
2	C7	145	ARG	CA-C	-5.13	1.46	1.52
2	C2	145	ARG	CA-C	-5.12	1.46	1.52
2	C1	145	ARG	CA-C	-5.12	1.46	1.52
2	C8	145	ARG	CA-C	-5.12	1.46	1.52
2	C10	145	ARG	CA-C	-5.12	1.46	1.52
2	C3	145	ARG	CA-C	-5.12	1.46	1.52
2	C9	145	ARG	CA-C	-5.12	1.46	1.52
2	C9	146	ALA	C-O	-5.12	1.18	1.24
2	C6	145	ARG	CA-C	-5.12	1.46	1.52
2	C1	146	ALA	C-O	-5.12	1.18	1.24
2	C11	145	ARG	CA-C	-5.12	1.46	1.52
2	C12	145	ARG	CA-C	-5.12	1.46	1.52
2	C6	146	ALA	C-O	-5.11	1.18	1.24
2	C13	145	ARG	CA-C	-5.11	1.46	1.52
2	C11	146	ALA	C-O	-5.09	1.18	1.24
2	C3	146	ALA	C-O	-5.09	1.18	1.24
2	C2	146	ALA	C-O	-5.08	1.18	1.24
2	C10	146	ALA	C-O	-5.08	1.18	1.24
2	C5	146	ALA	C-O	-5.07	1.18	1.24
2	C13	146	ALA	C-O	-5.06	1.18	1.24

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B10	179	ASP	N-CA-C	-8.68	103.21	112.93
1	B12	179	ASP	N-CA-C	-8.68	103.21	112.93
1	B9	179	ASP	N-CA-C	-8.68	103.21	112.93
1	B3	179	ASP	N-CA-C	-8.68	103.21	112.93
1	B4	179	ASP	N-CA-C	-8.68	103.21	112.93
1	B1	179	ASP	N-CA-C	-8.67	103.22	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B7	179	ASP	N-CA-C	-8.67	103.22	112.93
1	B5	179	ASP	N-CA-C	-8.67	103.22	112.93
1	B13	179	ASP	N-CA-C	-8.67	103.22	112.93
1	B11	179	ASP	N-CA-C	-8.66	103.23	112.93
1	B8	179	ASP	N-CA-C	-8.65	103.25	112.93
1	B6	179	ASP	N-CA-C	-8.64	103.25	112.93
1	B2	179	ASP	N-CA-C	-8.64	103.25	112.93
2	C3	118	SER	N-CA-C	8.36	120.08	110.97
2	C12	118	SER	N-CA-C	8.36	120.08	110.97
2	C13	118	SER	N-CA-C	8.35	120.08	110.97
2	C11	118	SER	N-CA-C	8.34	120.06	110.97
2	C4	118	SER	N-CA-C	8.33	120.05	110.97
2	C10	118	SER	N-CA-C	8.33	120.05	110.97
2	C1	118	SER	N-CA-C	8.32	120.04	110.97
2	C8	118	SER	N-CA-C	8.32	120.04	110.97
2	C9	118	SER	N-CA-C	8.32	120.04	110.97
2	C5	118	SER	N-CA-C	8.32	120.04	110.97
2	C6	118	SER	N-CA-C	8.32	120.04	110.97
2	C7	118	SER	N-CA-C	8.31	120.03	110.97
2	C2	118	SER	N-CA-C	8.31	120.02	110.97
1	B5	95	THR	N-CA-C	7.22	123.42	113.16
1	B7	95	THR	N-CA-C	7.22	123.42	113.16
1	B8	95	THR	N-CA-C	7.22	123.41	113.16
1	B4	95	THR	N-CA-C	7.21	123.40	113.16
1	B1	95	THR	N-CA-C	7.21	123.39	113.16
1	B9	95	THR	N-CA-C	7.21	123.39	113.16
1	B12	95	THR	N-CA-C	7.21	123.39	113.16
1	B10	95	THR	N-CA-C	7.20	123.39	113.16
1	B6	95	THR	N-CA-C	7.20	123.39	113.16
1	B13	95	THR	N-CA-C	7.20	123.38	113.16
1	B11	95	THR	N-CA-C	7.19	123.37	113.16
1	B3	95	THR	N-CA-C	7.19	123.37	113.16
1	B2	95	THR	N-CA-C	7.18	123.35	113.16
2	D7	238	ASN	N-CA-C	-6.58	101.22	110.50
2	D6	238	ASN	N-CA-C	-6.57	101.23	110.50
2	D8	238	ASN	N-CA-C	-6.57	101.23	110.50
1	B5	96	PRO	N-CA-C	6.57	118.71	110.70
1	B7	96	PRO	N-CA-C	6.56	118.71	110.70
2	D11	238	ASN	N-CA-C	-6.56	101.25	110.50
2	D1	238	ASN	N-CA-C	-6.56	101.25	110.50
2	D2	238	ASN	N-CA-C	-6.55	101.26	110.50
2	D3	238	ASN	N-CA-C	-6.55	101.27	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D12	238	ASN	N-CA-C	-6.55	101.27	110.50
2	D9	238	ASN	N-CA-C	-6.54	101.27	110.50
2	D13	238	ASN	N-CA-C	-6.54	101.27	110.50
1	B11	96	PRO	N-CA-C	6.54	118.68	110.70
2	D10	238	ASN	N-CA-C	-6.54	101.28	110.50
1	B10	96	PRO	N-CA-C	6.54	118.68	110.70
2	D4	238	ASN	N-CA-C	-6.54	101.28	110.50
1	B1	96	PRO	N-CA-C	6.54	118.67	110.70
1	B6	96	PRO	N-CA-C	6.54	118.67	110.70
2	D5	238	ASN	N-CA-C	-6.53	101.29	110.50
1	B4	96	PRO	N-CA-C	6.53	118.67	110.70
1	B9	96	PRO	N-CA-C	6.53	118.67	110.70
1	B12	96	PRO	N-CA-C	6.53	118.67	110.70
1	B3	96	PRO	N-CA-C	6.53	118.66	110.70
1	B13	96	PRO	N-CA-C	6.53	118.66	110.70
1	B2	96	PRO	N-CA-C	6.52	118.66	110.70
1	B8	96	PRO	N-CA-C	6.51	118.65	110.70
2	C7	36	GLY	N-CA-C	6.10	119.83	111.54
2	C8	36	GLY	N-CA-C	6.10	119.83	111.54
2	C12	36	GLY	N-CA-C	6.09	119.83	111.54
2	C5	36	GLY	N-CA-C	6.09	119.82	111.54
2	C6	36	GLY	N-CA-C	6.09	119.82	111.54
2	C11	36	GLY	N-CA-C	6.08	119.81	111.54
2	C1	36	GLY	N-CA-C	6.08	119.80	111.54
2	C9	36	GLY	N-CA-C	6.07	119.80	111.54
2	C13	36	GLY	N-CA-C	6.07	119.80	111.54
2	C3	36	GLY	N-CA-C	6.07	119.79	111.54
2	C2	36	GLY	N-CA-C	6.07	119.79	111.54
2	C10	36	GLY	N-CA-C	6.06	119.78	111.54
2	C4	36	GLY	N-CA-C	6.05	119.77	111.54
3	F4	176	ARG	CA-C-N	-5.77	114.37	120.66
3	F4	176	ARG	C-N-CA	-5.77	114.37	120.66
3	F13	176	ARG	CA-C-N	-5.76	114.38	120.66
3	F13	176	ARG	C-N-CA	-5.76	114.38	120.66
3	F9	176	ARG	CA-C-N	-5.75	114.39	120.66
3	F9	176	ARG	C-N-CA	-5.75	114.39	120.66
3	F10	176	ARG	CA-C-N	-5.75	114.39	120.66
3	F10	176	ARG	C-N-CA	-5.75	114.39	120.66
3	F3	176	ARG	CA-C-N	-5.75	114.39	120.66
3	F3	176	ARG	C-N-CA	-5.75	114.39	120.66
3	F5	176	ARG	CA-C-N	-5.75	114.39	120.66
3	F5	176	ARG	C-N-CA	-5.75	114.39	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F7	176	ARG	CA-C-N	-5.75	114.39	120.66
3	F7	176	ARG	C-N-CA	-5.75	114.39	120.66
3	F1	176	ARG	CA-C-N	-5.75	114.40	120.66
3	F1	176	ARG	C-N-CA	-5.75	114.40	120.66
3	F11	176	ARG	CA-C-N	-5.75	114.40	120.66
3	F11	176	ARG	C-N-CA	-5.75	114.40	120.66
3	F8	176	ARG	CA-C-N	-5.75	114.40	120.66
3	F8	176	ARG	C-N-CA	-5.75	114.40	120.66
3	F2	176	ARG	CA-C-N	-5.72	114.42	120.66
3	F2	176	ARG	C-N-CA	-5.72	114.42	120.66
3	F6	176	ARG	CA-C-N	-5.72	114.43	120.66
3	F6	176	ARG	C-N-CA	-5.72	114.43	120.66
3	F12	176	ARG	CA-C-N	-5.71	114.43	120.66
3	F12	176	ARG	C-N-CA	-5.71	114.43	120.66
2	C6	176	PRO	CA-C-O	-5.69	115.03	122.19
2	C9	176	PRO	CA-C-O	-5.69	115.03	122.19
2	C11	176	PRO	CA-C-O	-5.68	115.04	122.19
2	D6	203	ARG	N-CA-C	-5.67	98.84	108.26
2	D13	203	ARG	N-CA-C	-5.67	98.84	108.26
2	C2	176	PRO	CA-C-O	-5.67	115.04	122.19
2	D10	203	ARG	N-CA-C	-5.67	98.84	108.26
2	D4	203	ARG	N-CA-C	-5.67	98.85	108.26
2	C12	176	PRO	CA-C-O	-5.67	115.05	122.19
2	D12	203	ARG	N-CA-C	-5.67	98.85	108.26
2	C5	176	PRO	CA-C-O	-5.67	115.05	122.19
2	D1	203	ARG	N-CA-C	-5.67	98.86	108.26
2	D9	203	ARG	N-CA-C	-5.67	98.85	108.26
2	D11	203	ARG	N-CA-C	-5.67	98.85	108.26
2	D2	203	ARG	N-CA-C	-5.66	98.86	108.26
2	C10	176	PRO	CA-C-O	-5.66	115.06	122.19
2	C1	176	PRO	CA-C-O	-5.66	115.06	122.19
2	D5	203	ARG	N-CA-C	-5.66	98.86	108.26
2	D8	203	ARG	N-CA-C	-5.66	98.87	108.26
2	D3	203	ARG	N-CA-C	-5.65	98.88	108.26
2	D7	203	ARG	N-CA-C	-5.65	98.88	108.26
2	C4	176	PRO	CA-C-O	-5.64	115.08	122.19
1	A8	177	ASP	N-CA-C	5.64	118.14	110.35
2	C7	176	PRO	CA-C-O	-5.64	115.08	122.19
2	C3	176	PRO	CA-C-O	-5.64	115.08	122.19
2	C13	176	PRO	CA-C-O	-5.64	115.08	122.19
1	A5	177	ASP	N-CA-C	5.63	118.12	110.35
1	A9	177	ASP	N-CA-C	5.63	118.13	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A4	177	ASP	N-CA-C	5.62	118.11	110.35
1	A6	177	ASP	N-CA-C	5.62	118.11	110.35
1	A1	177	ASP	N-CA-C	5.62	118.11	110.35
1	A3	177	ASP	N-CA-C	5.62	118.10	110.35
1	A13	177	ASP	N-CA-C	5.62	118.10	110.35
1	A12	177	ASP	N-CA-C	5.62	118.10	110.35
2	C8	176	PRO	CA-C-O	-5.62	115.11	122.19
1	A11	177	ASP	N-CA-C	5.61	118.09	110.35
1	A10	177	ASP	N-CA-C	5.60	118.08	110.35
1	A7	177	ASP	N-CA-C	5.59	118.07	110.35
1	A2	177	ASP	N-CA-C	5.59	118.07	110.35
1	A3	187	ARG	N-CA-C	5.59	117.77	108.99
1	A11	187	ARG	N-CA-C	5.59	117.77	108.99
1	A8	187	ARG	N-CA-C	5.58	117.76	108.99
1	A12	187	ARG	N-CA-C	5.58	117.75	108.99
1	A4	187	ARG	N-CA-C	5.58	117.75	108.99
1	A1	187	ARG	N-CA-C	5.58	117.75	108.99
1	A13	187	ARG	N-CA-C	5.58	117.75	108.99
1	A6	187	ARG	N-CA-C	5.58	117.74	108.99
1	A5	187	ARG	N-CA-C	5.57	117.74	108.99
1	A2	187	ARG	N-CA-C	5.57	117.73	108.99
1	A7	187	ARG	N-CA-C	5.57	117.73	108.99
1	A9	187	ARG	N-CA-C	5.56	117.72	108.99
1	A10	187	ARG	N-CA-C	5.56	117.72	108.99
1	B6	198	VAL	N-CA-C	5.50	115.81	108.27
1	B11	198	VAL	N-CA-C	5.50	115.81	108.27
1	B3	198	VAL	N-CA-C	5.50	115.81	108.27
1	B5	198	VAL	N-CA-C	5.49	115.79	108.27
1	B4	198	VAL	N-CA-C	5.49	115.79	108.27
1	B1	198	VAL	N-CA-C	5.49	115.79	108.27
1	B8	198	VAL	N-CA-C	5.48	115.78	108.27
1	B13	198	VAL	N-CA-C	5.48	115.78	108.27
1	B10	198	VAL	N-CA-C	5.48	115.78	108.27
1	B2	198	VAL	N-CA-C	5.48	115.78	108.27
1	B7	198	VAL	N-CA-C	5.48	115.78	108.27
1	B9	198	VAL	N-CA-C	5.47	115.77	108.27
1	B12	198	VAL	N-CA-C	5.47	115.77	108.27
1	A11	180	ASN	N-CA-C	5.44	119.34	111.56
1	A12	180	ASN	N-CA-C	5.43	119.33	111.56
1	A10	180	ASN	N-CA-C	5.43	119.32	111.56
1	A5	180	ASN	N-CA-C	5.43	119.32	111.56
1	A6	180	ASN	N-CA-C	5.43	119.32	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A4	180	ASN	N-CA-C	5.43	119.32	111.56
1	A7	180	ASN	N-CA-C	5.43	119.32	111.56
1	A1	180	ASN	N-CA-C	5.42	119.31	111.56
1	A8	180	ASN	N-CA-C	5.42	119.31	111.56
2	C11	209	LYS	N-CA-C	-5.42	101.81	110.10
1	A13	180	ASN	N-CA-C	5.42	119.31	111.56
1	A2	180	ASN	N-CA-C	5.41	119.30	111.56
1	A3	180	ASN	N-CA-C	5.41	119.30	111.56
2	C4	209	LYS	N-CA-C	-5.41	101.82	110.10
2	C13	209	LYS	N-CA-C	-5.41	101.83	110.10
2	C2	209	LYS	N-CA-C	-5.41	101.83	110.10
2	C10	209	LYS	N-CA-C	-5.41	101.83	110.10
2	C1	209	LYS	N-CA-C	-5.40	101.83	110.10
2	C9	209	LYS	N-CA-C	-5.40	101.84	110.10
1	A9	180	ASN	N-CA-C	5.40	119.28	111.56
2	C3	209	LYS	N-CA-C	-5.40	101.84	110.10
2	C7	209	LYS	N-CA-C	-5.39	101.86	110.10
2	C12	209	LYS	N-CA-C	-5.39	101.86	110.10
2	C5	209	LYS	N-CA-C	-5.39	101.86	110.10
2	C6	209	LYS	N-CA-C	-5.38	101.86	110.10
2	C8	209	LYS	N-CA-C	-5.38	101.87	110.10
2	C6	47	PRO	N-CA-C	5.33	119.60	111.34
2	C2	47	PRO	N-CA-C	5.33	119.59	111.34
2	C8	47	PRO	N-CA-C	5.33	119.59	111.34
2	C13	170	GLY	N-CA-C	5.32	123.33	113.76
2	C11	47	PRO	N-CA-C	5.32	119.58	111.34
2	C8	170	GLY	N-CA-C	5.31	123.33	113.76
2	C10	47	PRO	N-CA-C	5.31	119.58	111.34
2	C1	47	PRO	N-CA-C	5.31	119.57	111.34
2	C13	47	PRO	N-CA-C	5.31	119.57	111.34
2	C5	170	GLY	N-CA-C	5.31	123.31	113.76
2	C12	47	PRO	N-CA-C	5.31	119.57	111.34
2	C9	170	GLY	N-CA-C	5.31	123.31	113.76
2	C5	47	PRO	N-CA-C	5.30	119.56	111.34
2	C6	170	GLY	N-CA-C	5.30	123.31	113.76
2	C10	170	GLY	N-CA-C	5.30	123.31	113.76
2	C1	170	GLY	N-CA-C	5.30	123.30	113.76
2	C12	170	GLY	N-CA-C	5.30	123.30	113.76
2	C3	47	PRO	N-CA-C	5.30	119.55	111.34
2	C3	170	GLY	N-CA-C	5.30	123.29	113.76
2	C4	47	PRO	N-CA-C	5.29	119.55	111.34
2	C11	170	GLY	N-CA-C	5.29	123.29	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C4	170	GLY	N-CA-C	5.29	123.28	113.76
2	C2	170	GLY	N-CA-C	5.29	123.28	113.76
2	C7	170	GLY	N-CA-C	5.29	123.28	113.76
2	C9	47	PRO	N-CA-C	5.29	119.53	111.34
2	C7	47	PRO	N-CA-C	5.28	119.53	111.34
1	B10	155	PRO	N-CA-C	-5.15	106.69	113.65
1	B8	155	PRO	N-CA-C	-5.14	106.70	113.65
1	B11	155	PRO	N-CA-C	-5.13	106.72	113.65
2	D10	228	GLY	N-CA-C	-5.13	101.02	113.18
1	B1	155	PRO	N-CA-C	-5.13	106.73	113.65
1	B4	155	PRO	N-CA-C	-5.13	106.73	113.65
1	B7	155	PRO	N-CA-C	-5.13	106.73	113.65
2	D3	228	GLY	N-CA-C	-5.13	101.03	113.18
1	B2	155	PRO	N-CA-C	-5.12	106.73	113.65
1	B5	155	PRO	N-CA-C	-5.12	106.73	113.65
2	D13	228	GLY	N-CA-C	-5.12	101.04	113.18
1	B9	155	PRO	N-CA-C	-5.12	106.73	113.65
2	D6	228	GLY	N-CA-C	-5.12	101.04	113.18
1	B6	155	PRO	N-CA-C	-5.12	106.74	113.65
1	B13	155	PRO	N-CA-C	-5.12	106.74	113.65
2	D8	228	GLY	N-CA-C	-5.12	101.05	113.18
2	D4	228	GLY	N-CA-C	-5.12	101.05	113.18
2	D5	228	GLY	N-CA-C	-5.12	101.05	113.18
2	D7	228	GLY	N-CA-C	-5.12	101.05	113.18
2	D1	228	GLY	N-CA-C	-5.12	101.06	113.18
2	D9	228	GLY	N-CA-C	-5.12	101.06	113.18
1	B12	155	PRO	N-CA-C	-5.11	106.75	113.65
2	D2	228	GLY	N-CA-C	-5.11	101.07	113.18
2	D11	228	GLY	N-CA-C	-5.11	101.07	113.18
2	D12	228	GLY	N-CA-C	-5.11	101.07	113.18
1	B3	155	PRO	N-CA-C	-5.10	106.77	113.65
2	C10	31	SER	N-CA-C	5.00	118.04	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	436	0	414	50	0
1	A10	436	0	414	48	0
1	A11	436	0	414	52	0
1	A12	436	0	414	49	0
1	A13	436	0	414	49	0
1	A2	436	0	414	48	0
1	A3	436	0	414	49	0
1	A4	436	0	414	48	0
1	A5	436	0	414	48	0
1	A6	436	0	414	50	0
1	A7	436	0	414	48	0
1	A8	436	0	414	49	0
1	A9	436	0	414	51	0
1	B1	498	0	478	56	0
1	B10	498	0	478	59	0
1	B11	498	0	478	57	0
1	B12	498	0	478	56	0
1	B13	498	0	478	56	0
1	B2	498	0	478	56	0
1	B3	498	0	478	56	0
1	B4	498	0	478	56	0
1	B5	498	0	478	58	0
1	B6	498	0	478	58	0
1	B7	498	0	478	57	0
1	B8	498	0	478	56	0
1	B9	498	0	478	55	0
2	C1	1654	0	1664	69	0
2	C10	1654	0	1664	68	0
2	C11	1654	0	1664	73	0
2	C12	1654	0	1664	69	0
2	C13	1654	0	1664	71	0
2	C2	1654	0	1664	74	0
2	C3	1654	0	1664	69	0
2	C4	1654	0	1664	66	0
2	C5	1654	0	1664	70	0
2	C6	1654	0	1664	68	0
2	C7	1654	0	1664	68	0
2	C8	1654	0	1664	67	0
2	C9	1654	0	1664	70	0
2	D1	1654	0	1664	87	0
2	D10	1654	0	1664	88	0
2	D11	1654	0	1664	90	0
2	D12	1654	0	1664	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D13	1654	0	1664	89	0
2	D2	1654	0	1664	84	0
2	D3	1654	0	1664	86	0
2	D4	1654	0	1664	85	0
2	D5	1654	0	1664	90	0
2	D6	1654	0	1664	86	0
2	D7	1654	0	1664	92	0
2	D8	1654	0	1664	86	0
2	D9	1654	0	1664	86	0
3	E1	87	0	77	8	0
3	E10	87	0	77	7	0
3	E11	87	0	77	9	0
3	E12	87	0	77	8	0
3	E13	87	0	77	9	0
3	E2	87	0	77	7	0
3	E3	87	0	77	9	0
3	E4	87	0	77	9	0
3	E5	87	0	77	8	0
3	E6	87	0	77	9	0
3	E7	87	0	77	8	0
3	E8	87	0	77	8	0
3	E9	87	0	77	8	0
3	F1	87	0	77	3	0
3	F10	87	0	77	3	0
3	F11	87	0	77	3	0
3	F12	87	0	77	3	0
3	F13	87	0	77	3	0
3	F2	87	0	77	3	0
3	F3	87	0	77	3	0
3	F4	87	0	77	3	0
3	F5	87	0	77	3	0
3	F6	87	0	77	3	0
3	F7	87	0	77	3	0
3	F8	87	0	77	3	0
3	F9	87	0	77	3	0
All	All	57408	0	56862	2290	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 20.

All (2290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B6:98:VAL:HG22	2:D7:208:TRP:CD1	1.71	1.26
1:B10:98:VAL:HG22	2:D11:208:TRP:CD1	1.71	1.26
1:B11:98:VAL:HG22	2:D12:208:TRP:CD1	1.71	1.26
1:B7:98:VAL:HG22	2:D8:208:TRP:CD1	1.71	1.26
1:B2:98:VAL:HG22	2:D3:208:TRP:CD1	1.71	1.26
1:B1:98:VAL:HG22	2:D2:208:TRP:CD1	1.71	1.25
1:B5:98:VAL:HG22	2:D6:208:TRP:CD1	1.71	1.25
1:B3:98:VAL:HG22	2:D4:208:TRP:CD1	1.71	1.25
1:B9:98:VAL:HG22	2:D10:208:TRP:CD1	1.71	1.25
1:B12:98:VAL:HG22	2:D13:208:TRP:CD1	1.71	1.25
1:B13:98:VAL:HG22	2:D1:208:TRP:CD1	1.71	1.25
1:B8:98:VAL:HG22	2:D9:208:TRP:CD1	1.71	1.24
1:B4:98:VAL:HG22	2:D5:208:TRP:CD1	1.71	1.24
1:B7:98:VAL:CG2	2:D8:208:TRP:CD1	2.24	1.21
1:B6:98:VAL:CG2	2:D7:208:TRP:CD1	2.24	1.21
1:B1:98:VAL:CG2	2:D2:208:TRP:CD1	2.24	1.20
1:B5:98:VAL:CG2	2:D6:208:TRP:CD1	2.24	1.20
1:B8:98:VAL:CG2	2:D9:208:TRP:CD1	2.24	1.20
1:B2:98:VAL:CG2	2:D3:208:TRP:CD1	2.24	1.20
1:B13:98:VAL:CG2	2:D1:208:TRP:CD1	2.24	1.20
1:B9:98:VAL:CG2	2:D10:208:TRP:CD1	2.24	1.20
1:B10:98:VAL:CG2	2:D11:208:TRP:CD1	2.24	1.20
1:B3:98:VAL:CG2	2:D4:208:TRP:CD1	2.24	1.19
1:B4:98:VAL:CG2	2:D5:208:TRP:CD1	2.24	1.19
1:B12:98:VAL:CG2	2:D13:208:TRP:CD1	2.24	1.19
1:B11:98:VAL:CG2	2:D12:208:TRP:CD1	2.24	1.19
1:A12:155:PRO:HD3	1:B10:157:THR:HB	1.20	1.15
1:A1:155:PRO:HD3	1:B12:157:THR:HB	1.20	1.15
1:A2:155:PRO:HD3	1:B13:157:THR:HB	1.20	1.15
1:A11:155:PRO:HD3	1:B9:157:THR:HB	1.20	1.15
2:D5:159:VAL:HG12	2:D5:160:LYS:H	1.01	1.14
1:A13:155:PRO:HD3	1:B11:157:THR:HB	1.20	1.13
2:D3:159:VAL:HG12	2:D3:160:LYS:H	1.01	1.13
1:A3:155:PRO:HD3	1:B1:157:THR:HB	1.20	1.12
1:A10:155:PRO:HD3	1:B8:157:THR:HB	1.20	1.12
2:D11:159:VAL:HG12	2:D11:160:LYS:H	1.02	1.11
1:B13:98:VAL:CG2	2:D1:208:TRP:HD1	1.63	1.11
2:D7:159:VAL:HG12	2:D7:160:LYS:H	1.01	1.11
1:B12:98:VAL:CG2	2:D13:208:TRP:HD1	1.63	1.11
2:D12:159:VAL:HG12	2:D12:160:LYS:H	1.01	1.11
1:A5:155:PRO:HD3	1:B3:157:THR:HB	1.20	1.10
1:A8:155:PRO:HD3	1:B6:157:THR:HB	1.20	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:98:VAL:CG2	2:D2:208:TRP:HD1	1.63	1.10
1:B4:98:VAL:CG2	2:D5:208:TRP:HD1	1.63	1.10
2:D6:159:VAL:HG12	2:D6:160:LYS:H	1.01	1.10
1:B3:188:VAL:HG11	2:D3:141:ILE:HD11	1.34	1.10
1:B1:188:VAL:HG11	2:D1:141:ILE:HD11	1.34	1.09
1:B5:98:VAL:CG2	2:D6:208:TRP:HD1	1.63	1.09
1:B6:188:VAL:HG11	2:D6:141:ILE:HD11	1.34	1.09
1:B11:98:VAL:CG2	2:D12:208:TRP:HD1	1.63	1.09
2:D8:159:VAL:HG12	2:D8:160:LYS:H	1.01	1.09
1:A4:155:PRO:HD3	1:B2:157:THR:HB	1.20	1.09
1:A9:155:PRO:HD3	1:B7:157:THR:HB	1.20	1.09
1:B13:188:VAL:HG11	2:D13:141:ILE:HD11	1.34	1.09
2:D9:159:VAL:HG12	2:D9:160:LYS:H	1.01	1.09
1:B11:188:VAL:HG11	2:D11:141:ILE:HD11	1.34	1.09
1:B2:98:VAL:CG2	2:D3:208:TRP:HD1	1.63	1.09
1:B4:188:VAL:HG11	2:D4:141:ILE:HD11	1.34	1.09
1:B6:98:VAL:CG2	2:D7:208:TRP:HD1	1.63	1.08
2:D1:159:VAL:HG12	2:D1:160:LYS:H	1.01	1.08
1:A7:155:PRO:HD3	1:B5:157:THR:HB	1.20	1.08
1:B7:188:VAL:HG11	2:D7:141:ILE:HD11	1.34	1.08
1:B10:188:VAL:HG11	2:D10:141:ILE:HD11	1.34	1.08
1:A6:155:PRO:HD3	1:B4:157:THR:HB	1.20	1.08
1:B10:98:VAL:CG2	2:D11:208:TRP:HD1	1.63	1.08
2:D2:159:VAL:HG12	2:D2:160:LYS:H	1.01	1.08
2:D4:159:VAL:HG12	2:D4:160:LYS:H	1.01	1.08
1:B7:98:VAL:CG2	2:D8:208:TRP:HD1	1.63	1.08
1:B8:98:VAL:CG2	2:D9:208:TRP:HD1	1.63	1.07
2:D13:159:VAL:HG12	2:D13:160:LYS:H	1.02	1.07
1:B3:98:VAL:CG2	2:D4:208:TRP:HD1	1.63	1.07
1:B9:98:VAL:CG2	2:D10:208:TRP:HD1	1.63	1.07
2:D10:159:VAL:HG12	2:D10:160:LYS:H	1.01	1.07
1:B5:188:VAL:HG11	2:D5:141:ILE:HD11	1.34	1.06
1:B9:188:VAL:HG11	2:D9:141:ILE:HD11	1.34	1.05
1:B12:188:VAL:HG11	2:D12:141:ILE:HD11	1.34	1.05
1:B8:188:VAL:HG11	2:D8:141:ILE:HD11	1.34	1.05
1:B2:188:VAL:HG11	2:D2:141:ILE:HD11	1.34	1.04
1:B11:188:VAL:CG1	2:D11:141:ILE:HD11	1.88	1.03
2:D7:159:VAL:HG12	2:D7:160:LYS:N	1.72	1.03
1:B9:188:VAL:CG1	2:D9:141:ILE:HD11	1.88	1.03
1:B10:188:VAL:CG1	2:D10:141:ILE:HD11	1.88	1.03
1:B12:188:VAL:CG1	2:D12:141:ILE:HD11	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B13:188:VAL:CG1	2:D13:141:ILE:HD11	1.88	1.03
1:B1:188:VAL:CG1	2:D1:141:ILE:HD11	1.88	1.03
1:B2:188:VAL:CG1	2:D2:141:ILE:HD11	1.88	1.03
1:B8:188:VAL:CG1	2:D8:141:ILE:HD11	1.88	1.03
1:B3:188:VAL:CG1	2:D3:141:ILE:HD11	1.88	1.02
1:B4:188:VAL:CG1	2:D4:141:ILE:HD11	1.88	1.02
1:B7:188:VAL:CG1	2:D7:141:ILE:HD11	1.88	1.02
1:B5:188:VAL:CG1	2:D5:141:ILE:HD11	1.88	1.02
1:B6:188:VAL:CG1	2:D6:141:ILE:HD11	1.88	1.02
2:D8:159:VAL:HG12	2:D8:160:LYS:N	1.72	1.02
2:D1:159:VAL:HG12	2:D1:160:LYS:N	1.72	1.01
2:D11:159:VAL:HG12	2:D11:160:LYS:N	1.72	1.01
2:D12:159:VAL:HG12	2:D12:160:LYS:N	1.72	1.01
2:D10:159:VAL:HG12	2:D10:160:LYS:N	1.72	1.01
2:C1:202:LEU:HD13	2:C1:217:PHE:CZ	1.96	1.00
2:C2:202:LEU:HD13	2:C2:217:PHE:CZ	1.96	1.00
2:C7:202:LEU:HD13	2:C7:217:PHE:CZ	1.96	1.00
2:C8:202:LEU:HD13	2:C8:217:PHE:CZ	1.96	1.00
2:D13:159:VAL:HG12	2:D13:160:LYS:N	1.72	1.00
2:C9:202:LEU:HD13	2:C9:217:PHE:CZ	1.96	1.00
2:C3:202:LEU:HD13	2:C3:217:PHE:CZ	1.96	1.00
2:C13:202:LEU:HD13	2:C13:217:PHE:CZ	1.96	1.00
2:C6:202:LEU:HD13	2:C6:217:PHE:CZ	1.96	1.00
2:D9:159:VAL:HG12	2:D9:160:LYS:N	1.72	1.00
2:C12:202:LEU:HD13	2:C12:217:PHE:CZ	1.96	0.99
2:C4:202:LEU:HD13	2:C4:217:PHE:CZ	1.96	0.99
2:C10:202:LEU:HD13	2:C10:217:PHE:CZ	1.96	0.99
2:D2:159:VAL:HG12	2:D2:160:LYS:N	1.72	0.99
2:C5:202:LEU:HD13	2:C5:217:PHE:CZ	1.96	0.99
2:C11:202:LEU:HD13	2:C11:217:PHE:CZ	1.96	0.98
2:D3:159:VAL:HG12	2:D3:160:LYS:N	1.72	0.97
2:D3:159:VAL:CG1	2:D3:160:LYS:H	1.78	0.97
2:D8:159:VAL:CG1	2:D8:160:LYS:H	1.78	0.97
2:D1:159:VAL:CG1	2:D1:160:LYS:H	1.78	0.97
2:D11:159:VAL:CG1	2:D11:160:LYS:H	1.78	0.97
2:D6:159:VAL:CG1	2:D6:160:LYS:H	1.78	0.97
2:D10:159:VAL:CG1	2:D10:160:LYS:H	1.78	0.97
2:D13:159:VAL:CG1	2:D13:160:LYS:H	1.78	0.96
2:D4:159:VAL:CG1	2:D4:160:LYS:H	1.78	0.96
1:A3:172:ILE:HD12	2:C3:140:LEU:HD12	1.48	0.96
1:A12:172:ILE:HD12	2:C12:140:LEU:HD12	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D5:159:VAL:CG1	2:D5:160:LYS:H	1.78	0.96
2:D9:159:VAL:CG1	2:D9:160:LYS:H	1.78	0.96
1:A6:172:ILE:HD12	2:C6:140:LEU:HD12	1.48	0.96
1:A11:172:ILE:HD12	2:C11:140:LEU:HD12	1.48	0.96
1:A2:172:ILE:HD12	2:C2:140:LEU:HD12	1.48	0.96
1:A9:155:PRO:CD	1:B7:157:THR:HB	1.96	0.96
1:A9:172:ILE:HD12	2:C9:140:LEU:HD12	1.48	0.96
1:A10:155:PRO:CD	1:B8:157:THR:HB	1.96	0.96
1:A8:155:PRO:CD	1:B6:157:THR:HB	1.96	0.95
2:D7:159:VAL:CG1	2:D7:160:LYS:H	1.78	0.95
2:D12:159:VAL:CG1	2:D12:160:LYS:H	1.78	0.95
1:A11:155:PRO:CD	1:B9:157:THR:HB	1.96	0.95
2:D2:159:VAL:CG1	2:D2:160:LYS:H	1.78	0.95
1:A7:155:PRO:CD	1:B5:157:THR:HB	1.96	0.95
1:A3:155:PRO:CD	1:B1:157:THR:HB	1.96	0.95
1:A4:155:PRO:CD	1:B2:157:THR:HB	1.96	0.95
1:A8:172:ILE:HD12	2:C8:140:LEU:HD12	1.48	0.95
2:D4:159:VAL:HG12	2:D4:160:LYS:N	1.72	0.95
1:A2:155:PRO:CD	1:B13:157:THR:HB	1.96	0.95
1:A5:155:PRO:CD	1:B3:157:THR:HB	1.96	0.95
1:A5:172:ILE:HD12	2:C5:140:LEU:HD12	1.48	0.95
1:A6:155:PRO:CD	1:B4:157:THR:HB	1.96	0.95
1:A12:155:PRO:CD	1:B10:157:THR:HB	1.96	0.95
1:A4:172:ILE:HD12	2:C4:140:LEU:HD12	1.48	0.94
2:D6:159:VAL:HG12	2:D6:160:LYS:N	1.72	0.94
1:A13:172:ILE:HD12	2:C13:140:LEU:HD12	1.48	0.94
1:A1:155:PRO:CD	1:B12:157:THR:HB	1.96	0.94
1:A13:155:PRO:CD	1:B11:157:THR:HB	1.96	0.94
2:D3:43:SER:H	2:D3:48:ASN:HD21	1.16	0.94
2:D1:43:SER:H	2:D1:48:ASN:HD21	1.16	0.94
2:D12:43:SER:H	2:D12:48:ASN:HD21	1.16	0.94
1:A1:172:ILE:HD12	2:C1:140:LEU:HD12	1.48	0.94
2:D5:43:SER:H	2:D5:48:ASN:HD21	1.16	0.94
1:A7:172:ILE:HD12	2:C7:140:LEU:HD12	1.48	0.93
1:A5:192:VAL:HG13	2:C5:148:LEU:HD23	1.50	0.93
2:D5:159:VAL:HG12	2:D5:160:LYS:N	1.72	0.93
2:D11:43:SER:H	2:D11:48:ASN:HD21	1.16	0.93
2:D13:43:SER:H	2:D13:48:ASN:HD21	1.16	0.93
1:A6:192:VAL:HG13	2:C6:148:LEU:HD23	1.50	0.93
1:A10:172:ILE:HD12	2:C10:140:LEU:HD12	1.48	0.93
2:D2:43:SER:H	2:D2:48:ASN:HD21	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:43:SER:H	2:D4:48:ASN:HD21	1.16	0.93
1:A4:192:VAL:HG13	2:C4:148:LEU:HD23	1.50	0.93
1:A7:192:VAL:HG13	2:C7:148:LEU:HD23	1.50	0.93
1:A13:192:VAL:HG13	2:C13:148:LEU:HD23	1.50	0.93
2:D10:43:SER:H	2:D10:48:ASN:HD21	1.16	0.93
1:A1:192:VAL:HG13	2:C1:148:LEU:HD23	1.50	0.92
2:D9:43:SER:H	2:D9:48:ASN:HD21	1.16	0.92
1:B7:98:VAL:HG21	2:D8:208:TRP:HD1	1.33	0.92
1:B8:98:VAL:HG21	2:D9:208:TRP:HD1	1.33	0.92
1:B13:98:VAL:HG21	2:D1:208:TRP:HD1	1.33	0.92
2:D6:43:SER:H	2:D6:48:ASN:HD21	1.16	0.92
1:A12:192:VAL:HG13	2:C12:148:LEU:HD23	1.50	0.92
1:A8:192:VAL:HG13	2:C8:148:LEU:HD23	1.50	0.92
1:B1:98:VAL:HG21	2:D2:208:TRP:HD1	1.33	0.92
1:A3:192:VAL:HG13	2:C3:148:LEU:HD23	1.50	0.92
1:B9:98:VAL:HG21	2:D10:208:TRP:HD1	1.33	0.92
1:B12:98:VAL:HG21	2:D13:208:TRP:HD1	1.33	0.92
2:D8:43:SER:H	2:D8:48:ASN:HD21	1.16	0.92
1:A2:192:VAL:HG13	2:C2:148:LEU:HD23	1.50	0.91
1:B6:98:VAL:HG21	2:D7:208:TRP:HD1	1.33	0.91
2:D7:43:SER:H	2:D7:48:ASN:HD21	1.16	0.91
1:B2:98:VAL:HG21	2:D3:208:TRP:HD1	1.33	0.91
1:A11:192:VAL:HG13	2:C11:148:LEU:HD23	1.50	0.91
1:B11:98:VAL:HG21	2:D12:208:TRP:HD1	1.33	0.91
1:A9:192:VAL:HG13	2:C9:148:LEU:HD23	1.50	0.90
1:B3:98:VAL:HG21	2:D4:208:TRP:HD1	1.33	0.90
1:B4:98:VAL:HG21	2:D5:208:TRP:HD1	1.33	0.90
1:B10:98:VAL:HG21	2:D11:208:TRP:HD1	1.33	0.90
1:A5:155:PRO:HD3	1:B3:157:THR:CB	2.02	0.90
1:A7:155:PRO:HD3	1:B5:157:THR:CB	2.02	0.90
1:A10:155:PRO:HD3	1:B8:157:THR:CB	2.02	0.90
1:A8:155:PRO:HD3	1:B6:157:THR:CB	2.02	0.90
2:D8:168:LEU:HD21	2:D8:174:VAL:CG2	2.02	0.90
1:A4:155:PRO:HD3	1:B2:157:THR:CB	2.02	0.89
1:B5:98:VAL:HG21	2:D6:208:TRP:HD1	1.33	0.89
2:D12:168:LEU:HD21	2:D12:174:VAL:CG2	2.02	0.89
1:A10:192:VAL:HG13	2:C10:148:LEU:HD23	1.50	0.89
1:A11:155:PRO:HD3	1:B9:157:THR:CB	2.02	0.89
2:D9:168:LEU:HD21	2:D9:174:VAL:CG2	2.02	0.89
1:A1:155:PRO:HD3	1:B12:157:THR:CB	2.02	0.89
1:A2:155:PRO:HD3	1:B13:157:THR:CB	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D7:168:LEU:HD21	2:D7:174:VAL:CG2	2.02	0.89
2:D11:168:LEU:HD21	2:D11:174:VAL:CG2	2.02	0.89
1:A13:192:VAL:CG1	2:C13:148:LEU:HD23	2.03	0.89
1:A1:192:VAL:CG1	2:C1:148:LEU:HD23	2.03	0.89
1:A12:192:VAL:CG1	2:C12:148:LEU:HD23	2.03	0.89
2:D13:168:LEU:HD21	2:D13:174:VAL:CG2	2.02	0.89
1:A6:192:VAL:CG1	2:C6:148:LEU:HD23	2.03	0.89
1:A9:155:PRO:HD3	1:B7:157:THR:CB	2.02	0.89
1:A6:155:PRO:HD3	1:B4:157:THR:CB	2.02	0.89
1:A5:192:VAL:CG1	2:C5:148:LEU:HD23	2.03	0.88
1:A7:192:VAL:CG1	2:C7:148:LEU:HD23	2.03	0.88
1:A11:192:VAL:CG1	2:C11:148:LEU:HD23	2.03	0.88
1:A13:155:PRO:HD3	1:B11:157:THR:CB	2.02	0.88
2:C6:74:ARG:NH1	2:D5:58:THR:HG21	1.88	0.88
2:C11:74:ARG:NH1	2:D10:58:THR:HG21	1.88	0.88
2:C5:74:ARG:NH1	2:D4:58:THR:HG21	1.88	0.88
2:C10:74:ARG:NH1	2:D9:58:THR:HG21	1.88	0.88
1:A2:192:VAL:CG1	2:C2:148:LEU:HD23	2.03	0.88
1:A8:192:VAL:CG1	2:C8:148:LEU:HD23	2.03	0.88
2:D10:168:LEU:HD21	2:D10:174:VAL:CG2	2.02	0.88
1:A10:192:VAL:CG1	2:C10:148:LEU:HD23	2.03	0.88
2:C9:74:ARG:NH1	2:D8:58:THR:HG21	1.88	0.88
2:D1:168:LEU:HD21	2:D1:174:VAL:CG2	2.02	0.88
2:D4:168:LEU:HD21	2:D4:174:VAL:CG2	2.02	0.88
1:A3:155:PRO:HD3	1:B1:157:THR:CB	2.02	0.88
2:D3:168:LEU:HD21	2:D3:174:VAL:CG2	2.02	0.88
1:A4:192:VAL:CG1	2:C4:148:LEU:HD23	2.03	0.88
2:D6:168:LEU:HD21	2:D6:174:VAL:CG2	2.02	0.88
1:A12:155:PRO:HD3	1:B10:157:THR:CB	2.02	0.88
2:C2:74:ARG:NH1	2:D1:58:THR:HG21	1.88	0.88
2:D5:168:LEU:HD21	2:D5:174:VAL:CG2	2.02	0.88
2:C1:74:ARG:NH1	2:D13:58:THR:HG21	1.88	0.87
2:C1:202:LEU:CD1	2:C1:217:PHE:CE2	2.57	0.87
2:C2:202:LEU:CD1	2:C2:217:PHE:CE2	2.57	0.87
2:D2:168:LEU:HD21	2:D2:174:VAL:CG2	2.02	0.87
1:A9:192:VAL:CG1	2:C9:148:LEU:HD23	2.03	0.87
2:C3:202:LEU:CD1	2:C3:217:PHE:CE2	2.58	0.87
2:C8:74:ARG:NH1	2:D7:58:THR:HG21	1.88	0.87
1:A3:192:VAL:CG1	2:C3:148:LEU:HD23	2.03	0.87
2:C4:74:ARG:NH1	2:D3:58:THR:HG21	1.88	0.87
2:C7:74:ARG:NH1	2:D6:58:THR:HG21	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C12:74:ARG:NH1	2:D11:58:THR:HG21	1.88	0.87
2:C4:202:LEU:CD1	2:C4:217:PHE:CE2	2.57	0.87
2:C13:202:LEU:CD1	2:C13:217:PHE:CE2	2.57	0.87
2:C9:202:LEU:CD1	2:C9:217:PHE:CE2	2.57	0.87
2:C11:202:LEU:CD1	2:C11:217:PHE:CE2	2.57	0.87
2:C3:74:ARG:NH1	2:D2:58:THR:HG21	1.88	0.86
2:C12:202:LEU:CD1	2:C12:217:PHE:CE2	2.57	0.86
2:D9:42:ILE:HB	2:D9:48:ASN:ND2	1.90	0.86
2:D10:42:ILE:HB	2:D10:48:ASN:ND2	1.90	0.86
2:D3:42:ILE:HB	2:D3:48:ASN:ND2	1.90	0.86
2:D4:42:ILE:HB	2:D4:48:ASN:ND2	1.90	0.86
2:D11:42:ILE:HB	2:D11:48:ASN:ND2	1.90	0.86
2:D12:42:ILE:HB	2:D12:48:ASN:ND2	1.90	0.86
2:C6:202:LEU:CD1	2:C6:217:PHE:CE2	2.57	0.86
2:C7:202:LEU:CD1	2:C7:217:PHE:CE2	2.57	0.86
2:C8:202:LEU:CD1	2:C8:217:PHE:CE2	2.58	0.86
2:C10:202:LEU:CD1	2:C10:217:PHE:CE2	2.57	0.86
2:C5:202:LEU:CD1	2:C5:217:PHE:CE2	2.57	0.86
2:C13:74:ARG:NH1	2:D12:58:THR:HG21	1.88	0.86
2:D5:42:ILE:HB	2:D5:48:ASN:ND2	1.90	0.86
2:D8:42:ILE:HB	2:D8:48:ASN:ND2	1.90	0.86
2:D2:42:ILE:HB	2:D2:48:ASN:ND2	1.90	0.86
2:D13:42:ILE:HB	2:D13:48:ASN:ND2	1.90	0.86
2:D6:42:ILE:HB	2:D6:48:ASN:ND2	1.90	0.85
2:D7:42:ILE:HB	2:D7:48:ASN:ND2	1.90	0.85
2:C6:35:GLY:HA3	2:D6:27:PRO:HG3	1.59	0.85
2:D1:42:ILE:HB	2:D1:48:ASN:ND2	1.90	0.85
2:C2:35:GLY:HA3	2:D2:27:PRO:HG3	1.59	0.85
2:C5:35:GLY:HA3	2:D5:27:PRO:HG3	1.59	0.85
2:C7:35:GLY:HA3	2:D7:27:PRO:HG3	1.59	0.85
2:C3:35:GLY:HA3	2:D3:27:PRO:HG3	1.59	0.85
2:C8:202:LEU:HD13	2:C8:217:PHE:CE2	2.12	0.85
2:C9:202:LEU:HD13	2:C9:217:PHE:CE2	2.12	0.85
2:C1:35:GLY:HA3	2:D1:27:PRO:HG3	1.59	0.84
2:C5:35:GLY:HA3	2:D5:27:PRO:CG	2.07	0.84
2:C4:35:GLY:HA3	2:D4:27:PRO:HG3	1.59	0.84
2:C8:35:GLY:HA3	2:D8:27:PRO:HG3	1.59	0.84
2:C10:35:GLY:HA3	2:D10:27:PRO:CG	2.08	0.84
2:C11:35:GLY:HA3	2:D11:27:PRO:CG	2.08	0.84
2:C4:35:GLY:HA3	2:D4:27:PRO:CG	2.07	0.84
2:C7:202:LEU:HD13	2:C7:217:PHE:CE2	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C10:202:LEU:HD13	2:C10:217:PHE:CE2	2.12	0.84
2:C4:202:LEU:HD13	2:C4:217:PHE:CE2	2.12	0.84
2:C6:35:GLY:HA3	2:D6:27:PRO:CG	2.07	0.84
2:C12:35:GLY:HA3	2:D12:27:PRO:CG	2.07	0.84
2:C13:35:GLY:HA3	2:D13:27:PRO:HG3	1.59	0.84
2:C1:202:LEU:HD13	2:C1:217:PHE:CE2	2.12	0.84
2:C5:202:LEU:HD13	2:C5:217:PHE:CE2	2.12	0.84
2:C9:35:GLY:HA3	2:D9:27:PRO:CG	2.07	0.84
2:C13:202:LEU:HD13	2:C13:217:PHE:CE2	2.12	0.84
2:C3:202:LEU:HD13	2:C3:217:PHE:CE2	2.12	0.84
2:C9:35:GLY:HA3	2:D9:27:PRO:HG3	1.59	0.83
2:C13:35:GLY:HA3	2:D13:27:PRO:CG	2.07	0.83
2:C1:35:GLY:HA3	2:D1:27:PRO:CG	2.08	0.83
2:C8:35:GLY:HA3	2:D8:27:PRO:CG	2.07	0.83
2:C12:35:GLY:HA3	2:D12:27:PRO:HG3	1.59	0.83
2:C2:202:LEU:HD13	2:C2:217:PHE:CE2	2.12	0.83
2:C10:35:GLY:HA3	2:D10:27:PRO:HG3	1.59	0.83
2:C6:202:LEU:HD13	2:C6:217:PHE:CE2	2.12	0.83
2:D7:42:ILE:HB	2:D7:48:ASN:HD22	1.44	0.83
2:D8:42:ILE:HB	2:D8:48:ASN:HD22	1.44	0.83
2:C2:35:GLY:HA3	2:D2:27:PRO:CG	2.08	0.83
2:C3:35:GLY:HA3	2:D3:27:PRO:CG	2.08	0.83
2:C11:35:GLY:HA3	2:D11:27:PRO:HG3	1.59	0.83
2:D3:42:ILE:HB	2:D3:48:ASN:HD22	1.44	0.83
2:C11:202:LEU:HD13	2:C11:217:PHE:CE2	2.12	0.83
2:D2:42:ILE:HB	2:D2:48:ASN:HD22	1.44	0.83
2:D6:42:ILE:HB	2:D6:48:ASN:HD22	1.44	0.83
2:C7:35:GLY:HA3	2:D7:27:PRO:CG	2.08	0.83
2:C12:202:LEU:HD13	2:C12:217:PHE:CE2	2.12	0.83
2:D4:42:ILE:HB	2:D4:48:ASN:HD22	1.44	0.83
2:D5:42:ILE:HB	2:D5:48:ASN:HD22	1.44	0.83
2:D9:42:ILE:HB	2:D9:48:ASN:HD22	1.44	0.82
2:D1:42:ILE:HB	2:D1:48:ASN:HD22	1.44	0.82
2:D5:168:LEU:CD2	2:D5:174:VAL:HG23	2.11	0.81
2:D6:168:LEU:CD2	2:D6:174:VAL:HG23	2.11	0.81
2:D10:42:ILE:HB	2:D10:48:ASN:HD22	1.44	0.81
2:D11:168:LEU:CD2	2:D11:174:VAL:HG23	2.11	0.81
2:D12:168:LEU:CD2	2:D12:174:VAL:HG23	2.11	0.81
2:D7:168:LEU:CD2	2:D7:174:VAL:HG23	2.11	0.81
2:D4:168:LEU:CD2	2:D4:174:VAL:HG23	2.11	0.81
2:D13:42:ILE:HB	2:D13:48:ASN:HD22	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D13:168:LEU:CD2	2:D13:174:VAL:HG23	2.11	0.81
2:D12:42:ILE:HB	2:D12:48:ASN:HD22	1.44	0.81
2:D9:168:LEU:CD2	2:D9:174:VAL:HG23	2.11	0.81
2:D10:168:LEU:CD2	2:D10:174:VAL:HG23	2.11	0.81
2:D3:168:LEU:CD2	2:D3:174:VAL:HG23	2.11	0.81
2:D8:168:LEU:CD2	2:D8:174:VAL:HG23	2.11	0.81
2:D8:174:VAL:HG13	2:D8:190:TYR:HB3	1.63	0.80
1:B9:98:VAL:CG1	2:D10:208:TRP:CD1	2.65	0.80
2:D9:174:VAL:HG13	2:D9:190:TYR:HB3	1.63	0.80
2:D1:168:LEU:CD2	2:D1:174:VAL:HG23	2.11	0.80
1:B3:98:VAL:CG1	2:D4:208:TRP:CD1	2.65	0.80
2:C5:60:ILE:HG22	3:E5:185:PHE:HE2	1.47	0.80
1:B5:98:VAL:CG1	2:D6:208:TRP:CD1	2.65	0.80
2:D2:168:LEU:CD2	2:D2:174:VAL:HG23	2.11	0.80
1:B2:98:VAL:CG1	2:D3:208:TRP:CD1	2.65	0.80
1:B7:98:VAL:CG1	2:D8:208:TRP:CD1	2.65	0.80
1:B9:98:VAL:HG21	2:D10:208:TRP:CD1	2.12	0.80
2:D7:174:VAL:HG13	2:D7:190:TYR:HB3	1.63	0.80
1:B12:98:VAL:CG1	2:D13:208:TRP:CD1	2.65	0.80
2:D10:174:VAL:HG13	2:D10:190:TYR:HB3	1.63	0.80
1:B10:98:VAL:CG1	2:D11:208:TRP:CD1	2.65	0.80
1:B13:98:VAL:CG1	2:D1:208:TRP:CD1	2.65	0.79
2:C6:60:ILE:HG22	3:E6:185:PHE:HE2	1.47	0.79
2:C4:60:ILE:HG22	3:E4:185:PHE:HE2	1.47	0.79
2:C7:60:ILE:HG22	3:E7:185:PHE:HE2	1.47	0.79
2:D11:42:ILE:HB	2:D11:48:ASN:HD22	1.44	0.79
1:B4:98:VAL:CG1	2:D5:208:TRP:CD1	2.65	0.79
1:B8:98:VAL:CG1	2:D9:208:TRP:CD1	2.65	0.79
2:C12:60:ILE:HG22	3:E12:185:PHE:HE2	1.47	0.79
1:B4:98:VAL:HG21	2:D5:208:TRP:CD1	2.12	0.79
1:B11:98:VAL:CG1	2:D12:208:TRP:CD1	2.65	0.79
2:D1:174:VAL:HG13	2:D1:190:TYR:HB3	1.63	0.79
1:B6:98:VAL:CG1	2:D7:208:TRP:CD1	2.65	0.79
2:C13:60:ILE:HG22	3:E13:185:PHE:HE2	1.47	0.79
2:D6:174:VAL:HG13	2:D6:190:TYR:HB3	1.63	0.79
2:C11:60:ILE:HG22	3:E11:185:PHE:HE2	1.47	0.79
2:D2:174:VAL:HG13	2:D2:190:TYR:HB3	1.63	0.79
1:B10:98:VAL:HG21	2:D11:208:TRP:CD1	2.12	0.79
2:C8:60:ILE:HG22	3:E8:185:PHE:HE2	1.47	0.79
2:D13:174:VAL:HG13	2:D13:190:TYR:HB3	1.63	0.79
1:B1:98:VAL:CG1	2:D2:208:TRP:CD1	2.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D11:174:VAL:HG13	2:D11:190:TYR:HB3	1.63	0.78
1:B1:98:VAL:HG22	2:D2:208:TRP:NE1	1.99	0.78
1:B13:98:VAL:HG22	2:D1:208:TRP:NE1	1.99	0.78
2:C1:60:ILE:HG22	3:E1:185:PHE:HE2	1.47	0.78
2:D3:174:VAL:HG13	2:D3:190:TYR:HB3	1.63	0.78
1:A10:187:ARG:HD2	1:B10:184:GLN:OE1	1.84	0.78
1:B4:98:VAL:HG22	2:D5:208:TRP:NE1	1.98	0.78
1:B9:98:VAL:HG22	2:D10:208:TRP:NE1	1.99	0.78
1:B10:98:VAL:HG22	2:D11:208:TRP:NE1	1.99	0.78
1:A4:187:ARG:HD2	1:B4:184:GLN:OE1	1.84	0.78
1:B5:98:VAL:HG22	2:D6:208:TRP:NE1	1.99	0.78
1:A5:187:ARG:HD2	1:B5:184:GLN:OE1	1.84	0.78
2:C3:194:ASN:OD1	2:C3:224:LEU:HD23	1.84	0.78
2:C8:194:ASN:OD1	2:C8:224:LEU:HD23	1.84	0.78
2:C10:60:ILE:HG22	3:E10:185:PHE:HE2	1.47	0.78
1:A11:187:ARG:CG	1:B11:184:GLN:OE1	2.32	0.78
1:A11:187:ARG:HD2	1:B11:184:GLN:OE1	1.84	0.78
2:D12:174:VAL:HG13	2:D12:190:TYR:HB3	1.63	0.78
2:D4:174:VAL:HG13	2:D4:190:TYR:HB3	1.63	0.78
1:A1:187:ARG:HD2	1:B1:184:GLN:OE1	1.84	0.78
1:A9:187:ARG:HD2	1:B9:184:GLN:OE1	1.84	0.78
1:B12:98:VAL:HG22	2:D13:208:TRP:NE1	1.99	0.78
2:C3:60:ILE:HG22	3:E3:185:PHE:HE2	1.47	0.78
2:C6:194:ASN:OD1	2:C6:224:LEU:HD23	1.84	0.78
1:A2:187:ARG:HD2	1:B2:184:GLN:OE1	1.84	0.78
1:B8:98:VAL:HG22	2:D9:208:TRP:NE1	1.99	0.78
2:C9:60:ILE:HG22	3:E9:185:PHE:HE2	1.47	0.78
2:C9:194:ASN:OD1	2:C9:224:LEU:HD23	1.84	0.78
1:A7:187:ARG:CG	1:B7:184:GLN:OE1	2.32	0.77
1:A8:187:ARG:CG	1:B8:184:GLN:OE1	2.32	0.77
1:A12:187:ARG:HD2	1:B12:184:GLN:OE1	1.84	0.77
1:B3:98:VAL:HG22	2:D4:208:TRP:NE1	1.98	0.77
2:C2:194:ASN:OD1	2:C2:224:LEU:HD23	1.84	0.77
2:C5:194:ASN:OD1	2:C5:224:LEU:HD23	1.84	0.77
2:C12:194:ASN:OD1	2:C12:224:LEU:HD23	1.84	0.77
2:D5:174:VAL:HG13	2:D5:190:TYR:HB3	1.63	0.77
1:A10:187:ARG:CG	1:B10:184:GLN:OE1	2.32	0.77
1:B2:98:VAL:HG22	2:D3:208:TRP:NE1	1.99	0.77
2:C2:60:ILE:HG22	3:E2:185:PHE:HE2	1.47	0.77
2:C11:194:ASN:OD1	2:C11:224:LEU:HD23	1.84	0.77
1:A4:187:ARG:CG	1:B4:184:GLN:OE1	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:187:ARG:CG	1:B5:184:GLN:OE1	2.32	0.77
1:B6:98:VAL:HG22	2:D7:208:TRP:NE1	1.98	0.77
2:C7:194:ASN:OD1	2:C7:224:LEU:HD23	1.84	0.77
1:A2:187:ARG:CG	1:B2:184:GLN:OE1	2.32	0.77
1:A3:187:ARG:CG	1:B3:184:GLN:OE1	2.32	0.77
1:A12:187:ARG:CG	1:B12:184:GLN:OE1	2.32	0.77
1:A1:187:ARG:CG	1:B1:184:GLN:OE1	2.32	0.77
1:A6:187:ARG:HD2	1:B6:184:GLN:OE1	1.84	0.77
1:A13:187:ARG:CG	1:B13:184:GLN:OE1	2.32	0.77
1:B11:98:VAL:HG22	2:D12:208:TRP:NE1	1.99	0.77
1:A6:187:ARG:CG	1:B6:184:GLN:OE1	2.32	0.77
1:A13:187:ARG:HD2	1:B13:184:GLN:OE1	1.84	0.77
1:A7:187:ARG:HD2	1:B7:184:GLN:OE1	1.84	0.77
1:A8:187:ARG:HD2	1:B8:184:GLN:OE1	1.84	0.77
2:C13:194:ASN:OD1	2:C13:224:LEU:HD23	1.84	0.77
2:C4:194:ASN:OD1	2:C4:224:LEU:HD23	1.84	0.77
2:C1:194:ASN:OD1	2:C1:224:LEU:HD23	1.84	0.77
1:A3:187:ARG:HD2	1:B3:184:GLN:OE1	1.84	0.76
1:A1:155:PRO:CD	1:B12:157:THR:CB	2.63	0.76
1:A13:155:PRO:CD	1:B11:157:THR:CB	2.63	0.76
1:A2:155:PRO:CD	1:B13:157:THR:CB	2.63	0.76
1:A9:187:ARG:CG	1:B9:184:GLN:OE1	2.32	0.76
1:B7:98:VAL:HG22	2:D8:208:TRP:NE1	1.99	0.76
2:C10:194:ASN:OD1	2:C10:224:LEU:HD23	1.84	0.76
1:A7:152:CYS:SG	1:B5:150:VAL:HG13	2.26	0.76
1:A9:152:CYS:SG	1:B7:150:VAL:HG13	2.26	0.76
1:A1:152:CYS:SG	1:B12:150:VAL:HG13	2.26	0.76
1:A5:152:CYS:SG	1:B3:150:VAL:HG13	2.26	0.76
1:A7:155:PRO:CD	1:B5:157:THR:CB	2.63	0.76
1:A2:152:CYS:SG	1:B13:150:VAL:HG13	2.26	0.76
1:A3:155:PRO:CD	1:B1:157:THR:CB	2.63	0.76
1:A11:152:CYS:SG	1:B9:150:VAL:HG13	2.26	0.76
2:D8:168:LEU:HD21	2:D8:174:VAL:HG21	1.68	0.75
2:D9:168:LEU:HD21	2:D9:174:VAL:HG21	1.68	0.75
1:A4:152:CYS:SG	1:B2:150:VAL:HG13	2.26	0.75
2:D7:168:LEU:HD21	2:D7:174:VAL:HG21	1.68	0.75
1:A10:152:CYS:SG	1:B8:150:VAL:HG13	2.26	0.75
1:A13:152:CYS:SG	1:B11:150:VAL:HG13	2.26	0.75
1:B1:98:VAL:HG21	2:D2:208:TRP:CD1	2.12	0.75
2:D10:168:LEU:HD21	2:D10:174:VAL:HG21	1.68	0.75
1:B3:98:VAL:HG21	2:D4:208:TRP:CD1	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D2:168:LEU:HD21	2:D2:174:VAL:HG21	1.68	0.75
1:A6:152:CYS:SG	1:B4:150:VAL:HG13	2.26	0.75
1:A12:152:CYS:SG	1:B10:150:VAL:HG13	2.26	0.75
1:A3:152:CYS:SG	1:B1:150:VAL:HG13	2.26	0.75
1:A8:155:PRO:CD	1:B6:157:THR:CB	2.63	0.75
2:D1:168:LEU:HD21	2:D1:174:VAL:HG21	1.68	0.75
2:D3:168:LEU:HD21	2:D3:174:VAL:HG21	1.68	0.75
2:D6:168:LEU:HD21	2:D6:174:VAL:HG21	1.68	0.75
2:D11:168:LEU:HD21	2:D11:174:VAL:HG21	1.68	0.75
1:A4:155:PRO:CD	1:B2:157:THR:CB	2.63	0.74
2:D9:40:LEU:HD13	2:D9:114:TYR:CE2	2.23	0.74
2:D10:40:LEU:HD13	2:D10:114:TYR:CE2	2.23	0.74
2:D11:40:LEU:HD13	2:D11:114:TYR:CE2	2.23	0.74
1:A8:152:CYS:SG	1:B6:150:VAL:HG13	2.26	0.74
1:B2:98:VAL:HG13	2:D3:208:TRP:CD1	2.23	0.74
1:B12:98:VAL:HG13	2:D13:208:TRP:CD1	2.23	0.74
2:D8:40:LEU:HD13	2:D8:114:TYR:CE2	2.23	0.74
2:D13:168:LEU:HD21	2:D13:174:VAL:HG21	1.68	0.74
1:B6:98:VAL:HG21	2:D7:208:TRP:CD1	2.12	0.74
2:D4:168:LEU:HD21	2:D4:174:VAL:HG21	1.68	0.74
2:D12:40:LEU:HD13	2:D12:114:TYR:CE2	2.23	0.74
2:C10:30:ILE:HD11	2:C10:116:LEU:HD13	1.70	0.74
2:D7:40:LEU:HD13	2:D7:114:TYR:CE2	2.23	0.74
1:B10:98:VAL:HG13	2:D11:208:TRP:CD1	2.23	0.74
1:B13:98:VAL:HG21	2:D1:208:TRP:CD1	2.12	0.74
2:C6:30:ILE:HD11	2:C6:116:LEU:HD13	1.70	0.74
2:D2:168:LEU:CD2	2:D2:174:VAL:CG2	2.66	0.74
1:A11:155:PRO:CD	1:B9:157:THR:CB	2.63	0.73
1:B7:98:VAL:HG13	2:D8:208:TRP:CD1	2.23	0.73
1:B13:98:VAL:HG13	2:D1:208:TRP:CD1	2.23	0.73
2:C3:30:ILE:HD11	2:C3:116:LEU:HD13	1.70	0.73
2:D1:37:GLN:HE22	2:D1:103:VAL:HG23	1.54	0.73
2:D12:168:LEU:HD21	2:D12:174:VAL:HG21	1.68	0.73
1:B3:98:VAL:HG13	2:D4:208:TRP:CD1	2.23	0.73
2:D2:37:GLN:HE22	2:D2:103:VAL:HG23	1.53	0.73
2:D3:168:LEU:CD2	2:D3:174:VAL:CG2	2.66	0.73
2:D13:40:LEU:HD13	2:D13:114:TYR:CE2	2.23	0.73
1:B6:98:VAL:HG13	2:D7:208:TRP:CD1	2.23	0.73
2:D9:37:GLN:HE22	2:D9:103:VAL:HG23	1.54	0.73
2:D9:168:LEU:CD2	2:D9:174:VAL:CG2	2.66	0.73
1:A6:155:PRO:CD	1:B4:157:THR:CB	2.63	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A9:155:PRO:CD	1:B7:157:THR:CB	2.63	0.73
1:B5:98:VAL:HG13	2:D6:208:TRP:CD1	2.23	0.73
2:C13:30:ILE:HD11	2:C13:116:LEU:HD13	1.70	0.73
2:D6:40:LEU:HD13	2:D6:114:TYR:CE2	2.23	0.73
2:D10:168:LEU:CD2	2:D10:174:VAL:CG2	2.66	0.73
2:D13:37:GLN:HE22	2:D13:103:VAL:HG23	1.53	0.73
1:B1:98:VAL:HG13	2:D2:208:TRP:CD1	2.23	0.73
1:B4:98:VAL:HG13	2:D5:208:TRP:CD1	2.23	0.73
2:C5:30:ILE:HD11	2:C5:116:LEU:HD13	1.70	0.73
2:C7:30:ILE:HD11	2:C7:116:LEU:HD13	1.70	0.73
2:C9:30:ILE:HD11	2:C9:116:LEU:HD13	1.70	0.73
2:D5:168:LEU:HD21	2:D5:174:VAL:HG21	1.68	0.73
2:D11:37:GLN:HE22	2:D11:103:VAL:HG23	1.53	0.73
2:D11:168:LEU:CD2	2:D11:174:VAL:CG2	2.66	0.73
2:D12:37:GLN:HE22	2:D12:103:VAL:HG23	1.53	0.73
1:B9:170:VAL:HG11	2:D9:144:ASN:ND2	2.04	0.73
2:C11:30:ILE:HD11	2:C11:116:LEU:HD13	1.70	0.73
2:D4:168:LEU:CD2	2:D4:174:VAL:CG2	2.66	0.73
2:D6:37:GLN:HE22	2:D6:103:VAL:HG23	1.54	0.73
2:D8:168:LEU:CD2	2:D8:174:VAL:CG2	2.66	0.73
1:B11:98:VAL:HG13	2:D12:208:TRP:CD1	2.23	0.73
2:D3:40:LEU:HD13	2:D3:114:TYR:CE2	2.23	0.73
2:D8:37:GLN:HE22	2:D8:103:VAL:HG23	1.54	0.73
1:B6:170:VAL:HG11	2:D6:144:ASN:ND2	2.04	0.73
1:B7:170:VAL:HG11	2:D7:144:ASN:ND2	2.04	0.73
1:B10:170:VAL:HG11	2:D10:144:ASN:ND2	2.04	0.73
2:C2:30:ILE:HD11	2:C2:116:LEU:HD13	1.70	0.73
2:D3:37:GLN:HE22	2:D3:103:VAL:HG23	1.54	0.73
1:B5:170:VAL:HG11	2:D5:144:ASN:ND2	2.04	0.73
1:B11:170:VAL:HG11	2:D11:144:ASN:ND2	2.04	0.73
2:D1:40:LEU:HD13	2:D1:114:TYR:CE2	2.23	0.73
2:D5:40:LEU:HD13	2:D5:114:TYR:CE2	2.23	0.73
2:D4:40:LEU:HD13	2:D4:114:TYR:CE2	2.22	0.72
2:D7:168:LEU:CD2	2:D7:174:VAL:CG2	2.66	0.72
1:A5:155:PRO:CD	1:B3:157:THR:CB	2.63	0.72
1:B9:98:VAL:HG13	2:D10:208:TRP:CD1	2.23	0.72
2:C12:30:ILE:HD11	2:C12:116:LEU:HD13	1.70	0.72
2:D12:168:LEU:CD2	2:D12:174:VAL:CG2	2.66	0.72
1:B8:98:VAL:HG13	2:D9:208:TRP:CD1	2.23	0.72
2:C4:30:ILE:HD11	2:C4:116:LEU:HD13	1.70	0.72
1:B12:98:VAL:HG21	2:D13:208:TRP:CD1	2.12	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D2:40:LEU:HD13	2:D2:114:TYR:CE2	2.23	0.72
2:C1:30:ILE:HD11	2:C1:116:LEU:HD13	1.70	0.72
1:B2:170:VAL:HG11	2:D2:144:ASN:ND2	2.04	0.72
2:D4:37:GLN:HE22	2:D4:103:VAL:HG23	1.54	0.72
1:B12:170:VAL:HG11	2:D12:144:ASN:ND2	2.04	0.72
2:D5:168:LEU:CD2	2:D5:174:VAL:CG2	2.66	0.72
1:A10:155:PRO:CD	1:B8:157:THR:CB	2.63	0.72
2:C8:30:ILE:HD11	2:C8:116:LEU:HD13	1.70	0.72
2:C8:35:GLY:C	2:D8:27:PRO:HD3	2.15	0.72
2:C13:35:GLY:C	2:D13:27:PRO:HD3	2.15	0.72
2:D7:37:GLN:HE22	2:D7:103:VAL:HG23	1.54	0.72
1:B4:170:VAL:HG11	2:D4:144:ASN:ND2	2.04	0.71
2:C1:35:GLY:C	2:D1:27:PRO:HD3	2.15	0.71
2:D6:168:LEU:CD2	2:D6:174:VAL:CG2	2.66	0.71
2:D10:37:GLN:HE22	2:D10:103:VAL:HG23	1.54	0.71
1:B8:170:VAL:HG11	2:D8:144:ASN:ND2	2.04	0.71
1:B13:170:VAL:HG11	2:D13:144:ASN:ND2	2.04	0.71
2:D13:168:LEU:CD2	2:D13:174:VAL:CG2	2.66	0.71
1:B3:170:VAL:HG11	2:D3:144:ASN:ND2	2.04	0.71
2:C2:35:GLY:C	2:D2:27:PRO:HD3	2.15	0.71
2:C4:35:GLY:C	2:D4:27:PRO:HD3	2.15	0.71
2:C12:35:GLY:C	2:D12:27:PRO:HD3	2.15	0.71
2:D5:37:GLN:HE22	2:D5:103:VAL:HG23	1.54	0.71
2:C9:35:GLY:C	2:D9:27:PRO:HD3	2.15	0.71
1:B1:170:VAL:HG11	2:D1:144:ASN:ND2	2.04	0.71
2:C11:35:GLY:C	2:D11:27:PRO:HD3	2.15	0.71
1:A5:188:VAL:CG1	2:C5:141:ILE:HD11	2.21	0.71
2:C3:35:GLY:C	2:D3:27:PRO:HD3	2.15	0.71
2:C7:35:GLY:C	2:D7:27:PRO:HD3	2.15	0.71
2:D12:174:VAL:CG1	2:D12:190:TYR:HB3	2.21	0.71
2:D13:174:VAL:CG1	2:D13:190:TYR:HB3	2.21	0.71
1:A4:188:VAL:CG1	2:C4:141:ILE:HD11	2.21	0.71
1:A6:188:VAL:CG1	2:C6:141:ILE:HD11	2.21	0.71
1:B11:98:VAL:HG21	2:D12:208:TRP:CD1	2.12	0.71
2:D1:174:VAL:CG1	2:D1:190:TYR:HB3	2.21	0.71
2:D11:174:VAL:CG1	2:D11:190:TYR:HB3	2.21	0.71
2:C5:35:GLY:C	2:D5:27:PRO:HD3	2.15	0.71
2:D2:174:VAL:CG1	2:D2:190:TYR:HB3	2.21	0.71
2:D3:174:VAL:CG1	2:D3:190:TYR:HB3	2.21	0.71
1:A7:188:VAL:CG1	2:C7:141:ILE:HD11	2.21	0.71
2:C10:35:GLY:C	2:D10:27:PRO:HD3	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:188:VAL:CG1	2:C3:141:ILE:HD11	2.21	0.70
2:D7:67:LEU:HD23	2:D7:82:SER:HB3	1.73	0.70
2:D10:174:VAL:CG1	2:D10:190:TYR:HB3	2.21	0.70
2:D4:174:VAL:CG1	2:D4:190:TYR:HB3	2.21	0.70
2:C6:35:GLY:C	2:D6:27:PRO:HD3	2.15	0.70
2:D1:168:LEU:CD2	2:D1:174:VAL:CG2	2.66	0.70
2:D8:67:LEU:HD23	2:D8:82:SER:HB3	1.73	0.70
1:A8:188:VAL:CG1	2:C8:141:ILE:HD11	2.21	0.70
1:A10:188:VAL:CG1	2:C10:141:ILE:HD11	2.21	0.70
1:A13:188:VAL:CG1	2:C13:141:ILE:HD11	2.21	0.70
1:B2:98:VAL:HG21	2:D3:208:TRP:CD1	2.12	0.70
2:D9:174:VAL:CG1	2:D9:190:TYR:HB3	2.21	0.70
1:A2:188:VAL:CG1	2:C2:141:ILE:HD11	2.21	0.70
2:D5:174:VAL:CG1	2:D5:190:TYR:HB3	2.21	0.70
2:D11:67:LEU:HD23	2:D11:82:SER:HB3	1.73	0.70
2:C1:35:GLY:HA3	2:D1:27:PRO:HD3	1.74	0.70
1:A11:188:VAL:CG1	2:C11:141:ILE:HD11	2.21	0.70
1:A12:155:PRO:CD	1:B10:157:THR:CB	2.63	0.70
1:A1:188:VAL:CG1	2:C1:141:ILE:HD11	2.21	0.70
1:A9:188:VAL:CG1	2:C9:141:ILE:HD11	2.21	0.70
1:B13:171:TRP:HB2	2:D13:204:GLU:OE1	1.92	0.70
2:C3:35:GLY:HA3	2:D3:27:PRO:HD3	1.74	0.70
2:C12:35:GLY:HA3	2:D12:27:PRO:HD3	1.74	0.70
2:D8:174:VAL:CG1	2:D8:190:TYR:HB3	2.21	0.70
1:B9:171:TRP:HB2	2:D9:204:GLU:OE1	1.92	0.70
2:C2:35:GLY:HA3	2:D2:27:PRO:HD3	1.74	0.70
2:C13:35:GLY:HA3	2:D13:27:PRO:HD3	1.74	0.70
1:B2:171:TRP:HB2	2:D2:204:GLU:OE1	1.92	0.70
1:B7:171:TRP:HB2	2:D7:204:GLU:OE1	1.92	0.70
2:C11:35:GLY:HA3	2:D11:27:PRO:HD3	1.74	0.70
1:B3:171:TRP:HB2	2:D3:204:GLU:OE1	1.92	0.69
1:B11:171:TRP:HB2	2:D11:204:GLU:OE1	1.92	0.69
1:B5:98:VAL:HG21	2:D6:208:TRP:CD1	2.12	0.69
1:B6:171:TRP:HB2	2:D6:204:GLU:OE1	1.92	0.69
2:D10:67:LEU:HD23	2:D10:82:SER:HB3	1.73	0.69
2:D11:168:LEU:HD21	2:D11:174:VAL:HG23	1.73	0.69
1:A12:188:VAL:CG1	2:C12:141:ILE:HD11	2.21	0.69
1:B1:188:VAL:HG13	2:D1:141:ILE:HD11	1.75	0.69
2:D4:67:LEU:HD23	2:D4:82:SER:HB3	1.73	0.69
2:D6:67:LEU:HD23	2:D6:82:SER:HB3	1.73	0.69
2:D6:174:VAL:CG1	2:D6:190:TYR:HB3	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D7:174:VAL:CG1	2:D7:190:TYR:HB3	2.21	0.69
1:B4:171:TRP:HB2	2:D4:204:GLU:OE1	1.92	0.69
1:B8:171:TRP:HB2	2:D8:204:GLU:OE1	1.92	0.69
2:D12:67:LEU:HD23	2:D12:82:SER:HB3	1.73	0.69
2:C4:35:GLY:HA3	2:D4:27:PRO:HD3	1.74	0.69
2:D9:67:LEU:HD23	2:D9:82:SER:HB3	1.73	0.69
1:B10:188:VAL:HG13	2:D10:141:ILE:HD11	1.75	0.69
2:C5:35:GLY:HA3	2:D5:27:PRO:HD3	1.74	0.69
1:B13:188:VAL:HG13	2:D13:141:ILE:HD11	1.75	0.69
2:D5:67:LEU:HD23	2:D5:82:SER:HB3	1.73	0.69
1:B5:171:TRP:HB2	2:D5:204:GLU:OE1	1.92	0.69
1:B9:188:VAL:HG13	2:D9:141:ILE:HD11	1.75	0.69
2:C6:74:ARG:NH1	2:D5:58:THR:CG2	2.56	0.69
2:C9:74:ARG:NH1	2:D8:58:THR:CG2	2.56	0.69
2:C10:35:GLY:HA3	2:D10:27:PRO:HD3	1.74	0.69
2:C12:74:ARG:NH1	2:D11:58:THR:CG2	2.56	0.69
2:C13:202:LEU:CD1	2:C13:217:PHE:CZ	2.76	0.69
2:D1:67:LEU:HD23	2:D1:82:SER:HB3	1.73	0.69
1:A2:167:ILE:HG22	1:B1:197:TRP:HH2	1.58	0.69
1:A4:167:ILE:HG22	1:B3:197:TRP:HH2	1.58	0.69
1:B1:171:TRP:CB	2:D1:204:GLU:OE1	2.41	0.69
2:C5:35:GLY:HA3	2:D5:27:PRO:CD	2.23	0.69
2:C6:35:GLY:HA3	2:D6:27:PRO:CD	2.23	0.69
1:B2:171:TRP:CB	2:D2:204:GLU:OE1	2.41	0.69
1:B10:171:TRP:CB	2:D10:204:GLU:OE1	2.41	0.69
1:B12:171:TRP:CB	2:D12:204:GLU:OE1	2.41	0.69
2:C4:74:ARG:NH1	2:D3:58:THR:CG2	2.56	0.69
2:C7:74:ARG:NH1	2:D6:58:THR:CG2	2.56	0.69
1:B1:171:TRP:HB2	2:D1:204:GLU:OE1	1.92	0.68
1:B5:188:VAL:HG13	2:D5:141:ILE:HD11	1.75	0.68
1:B13:171:TRP:CB	2:D13:204:GLU:OE1	2.41	0.68
2:C4:35:GLY:HA3	2:D4:27:PRO:CD	2.23	0.68
2:C9:35:GLY:HA3	2:D9:27:PRO:HD3	1.74	0.68
2:C10:74:ARG:NH1	2:D9:58:THR:CG2	2.56	0.68
1:A7:167:ILE:HG22	1:B6:197:TRP:HH2	1.58	0.68
1:B3:171:TRP:CB	2:D3:204:GLU:OE1	2.41	0.68
1:A13:167:ILE:HG22	1:B12:197:TRP:HH2	1.58	0.68
1:B8:171:TRP:CB	2:D8:204:GLU:OE1	2.41	0.68
1:B10:171:TRP:HB2	2:D10:204:GLU:OE1	1.92	0.68
2:C6:35:GLY:HA3	2:D6:27:PRO:HD3	1.74	0.68
2:C9:35:GLY:HA3	2:D9:27:PRO:CD	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D1:60:ILE:HG22	3:F1:185:PHE:HE2	1.59	0.68
1:B7:171:TRP:CB	2:D7:204:GLU:OE1	2.41	0.68
1:B9:171:TRP:CB	2:D9:204:GLU:OE1	2.41	0.68
2:C1:74:ARG:NH1	2:D13:58:THR:CG2	2.56	0.68
2:C8:74:ARG:NH1	2:D7:58:THR:CG2	2.56	0.68
2:C10:35:GLY:HA3	2:D10:27:PRO:CD	2.23	0.68
2:C11:74:ARG:NH1	2:D10:58:THR:CG2	2.56	0.68
2:D2:67:LEU:HD23	2:D2:82:SER:HB3	1.73	0.68
2:D10:168:LEU:HD21	2:D10:174:VAL:HG23	1.73	0.68
2:D11:60:ILE:HG22	3:F11:185:PHE:HE2	1.59	0.68
1:B4:171:TRP:CB	2:D4:204:GLU:OE1	2.41	0.68
1:B6:171:TRP:CB	2:D6:204:GLU:OE1	2.41	0.68
2:C7:35:GLY:HA3	2:D7:27:PRO:HD3	1.74	0.68
1:A6:167:ILE:HG22	1:B5:197:TRP:HH2	1.58	0.68
1:A12:167:ILE:HG22	1:B11:197:TRP:HH2	1.58	0.68
1:B5:171:TRP:CB	2:D5:204:GLU:OE1	2.41	0.68
1:B6:188:VAL:HG13	2:D6:141:ILE:HD11	1.75	0.68
1:B12:171:TRP:HB2	2:D12:204:GLU:OE1	1.92	0.68
1:A5:167:ILE:HG22	1:B4:197:TRP:HH2	1.58	0.68
1:A10:167:ILE:HG22	1:B9:197:TRP:HH2	1.58	0.68
1:B4:188:VAL:HG13	2:D4:141:ILE:HD11	1.75	0.68
2:C2:74:ARG:NH1	2:D1:58:THR:CG2	2.56	0.68
2:D3:67:LEU:HD23	2:D3:82:SER:HB3	1.73	0.68
2:D6:60:ILE:HG22	3:F6:185:PHE:HE2	1.59	0.68
2:D8:60:ILE:HG22	3:F8:185:PHE:HE2	1.59	0.68
2:D13:67:LEU:HD23	2:D13:82:SER:HB3	1.73	0.68
2:C3:74:ARG:NH1	2:D2:58:THR:CG2	2.56	0.68
2:C7:35:GLY:HA3	2:D7:27:PRO:CD	2.23	0.68
2:C8:35:GLY:HA3	2:D8:27:PRO:HD3	1.74	0.68
2:C13:74:ARG:NH1	2:D12:58:THR:CG2	2.56	0.68
1:A11:167:ILE:HG22	1:B10:197:TRP:HH2	1.58	0.68
1:B12:188:VAL:HG13	2:D12:141:ILE:HD11	1.75	0.68
2:C2:35:GLY:HA3	2:D2:27:PRO:CD	2.23	0.68
2:C3:35:GLY:HA3	2:D3:27:PRO:CD	2.23	0.68
2:C1:35:GLY:HA3	2:D1:27:PRO:CD	2.23	0.68
2:C8:35:GLY:HA3	2:D8:27:PRO:CD	2.23	0.68
2:D3:60:ILE:HG22	3:F3:185:PHE:HE2	1.59	0.68
2:D9:60:ILE:HG22	3:F9:185:PHE:HE2	1.59	0.68
1:B11:171:TRP:CB	2:D11:204:GLU:OE1	2.41	0.67
2:C5:74:ARG:NH1	2:D4:58:THR:CG2	2.56	0.67
1:A3:167:ILE:HG22	1:B2:197:TRP:HH2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A9:167:ILE:HG22	1:B8:197:TRP:HH2	1.58	0.67
1:B8:188:VAL:HG13	2:D8:141:ILE:HD11	1.75	0.67
2:C11:35:GLY:HA3	2:D11:27:PRO:CD	2.23	0.67
2:D5:60:ILE:HG22	3:F5:185:PHE:HE2	1.59	0.67
2:D6:168:LEU:HD21	2:D6:174:VAL:HG23	1.73	0.67
1:A1:167:ILE:HG22	1:B13:197:TRP:HH2	1.58	0.67
2:C9:32:LEU:HD21	2:C9:38:PHE:HB2	1.77	0.67
2:C10:32:LEU:HD21	2:C10:38:PHE:HB2	1.77	0.67
2:D4:60:ILE:HG22	3:F4:185:PHE:HE2	1.59	0.67
2:C11:32:LEU:HD21	2:C11:38:PHE:HB2	1.77	0.67
2:C13:32:LEU:HD21	2:C13:38:PHE:HB2	1.77	0.67
2:D12:60:ILE:HG22	3:F12:185:PHE:HE2	1.59	0.67
2:C1:32:LEU:HD21	2:C1:38:PHE:HB2	1.77	0.67
2:C13:35:GLY:HA3	2:D13:27:PRO:CD	2.23	0.67
2:D13:60:ILE:HG22	3:F13:185:PHE:HE2	1.59	0.67
2:C7:32:LEU:HD21	2:C7:38:PHE:HB2	1.77	0.67
2:C8:32:LEU:HD21	2:C8:38:PHE:HB2	1.77	0.67
2:C12:32:LEU:HD21	2:C12:38:PHE:HB2	1.77	0.67
1:B7:188:VAL:HG13	2:D7:141:ILE:HD11	1.75	0.67
2:D2:60:ILE:HG22	3:F2:185:PHE:HE2	1.59	0.67
1:B3:188:VAL:HG13	2:D3:141:ILE:HD11	1.75	0.66
2:C2:32:LEU:HD21	2:C2:38:PHE:HB2	1.77	0.66
2:D5:168:LEU:HD21	2:D5:174:VAL:HG23	1.73	0.66
1:A8:167:ILE:HG22	1:B7:197:TRP:HH2	1.58	0.66
2:C3:32:LEU:HD21	2:C3:38:PHE:HB2	1.77	0.66
2:C12:35:GLY:HA3	2:D12:27:PRO:CD	2.23	0.66
1:A11:155:PRO:HG2	1:B9:157:THR:CG2	2.25	0.66
2:C5:32:LEU:HD21	2:C5:38:PHE:HB2	1.77	0.66
2:D10:60:ILE:HG22	3:F10:185:PHE:HE2	1.59	0.66
1:A10:155:PRO:HG2	1:B8:157:THR:CG2	2.25	0.66
2:D7:60:ILE:HG22	3:F7:185:PHE:HE2	1.59	0.66
1:A6:187:ARG:CD	1:B6:184:GLN:OE1	2.44	0.66
1:A7:187:ARG:CD	1:B7:184:GLN:OE1	2.44	0.66
2:C6:32:LEU:HD21	2:C6:38:PHE:HB2	1.77	0.66
1:A8:187:ARG:CD	1:B8:184:GLN:OE1	2.44	0.66
1:A3:155:PRO:HG2	1:B1:157:THR:CG2	2.25	0.66
1:A4:155:PRO:HG2	1:B2:157:THR:CG2	2.25	0.66
1:A9:187:ARG:CD	1:B9:184:GLN:OE1	2.44	0.66
2:D10:168:LEU:HD22	2:D10:174:VAL:HG23	1.77	0.66
1:A2:155:PRO:HG2	1:B13:157:THR:CG2	2.25	0.66
1:A5:187:ARG:CD	1:B5:184:GLN:OE1	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A12:155:PRO:HG2	1:B10:157:THR:CG2	2.25	0.66
2:C4:32:LEU:HD21	2:C4:38:PHE:HB2	1.77	0.66
2:D9:168:LEU:HD22	2:D9:174:VAL:HG23	1.77	0.66
1:A9:155:PRO:HG2	1:B7:157:THR:CG2	2.25	0.66
1:B11:188:VAL:HG13	2:D11:141:ILE:HD11	1.75	0.66
2:D4:168:LEU:HD21	2:D4:174:VAL:HG23	1.73	0.66
1:A5:155:PRO:HG2	1:B3:157:THR:CG2	2.25	0.65
1:A6:155:PRO:HG2	1:B4:157:THR:CG2	2.25	0.65
2:D1:168:LEU:HD22	2:D1:174:VAL:HG23	1.77	0.65
1:A4:187:ARG:CD	1:B4:184:GLN:OE1	2.44	0.65
1:A10:187:ARG:CD	1:B10:184:GLN:OE1	2.44	0.65
2:D11:168:LEU:HD22	2:D11:174:VAL:HG23	1.77	0.65
2:D13:168:LEU:HD22	2:D13:174:VAL:HG23	1.77	0.65
2:D4:168:LEU:HD22	2:D4:174:VAL:HG23	1.77	0.65
1:A8:155:PRO:HG2	1:B6:157:THR:CG2	2.25	0.65
2:D3:168:LEU:HD21	2:D3:174:VAL:HG23	1.73	0.65
1:A1:187:ARG:CD	1:B1:184:GLN:OE1	2.44	0.65
1:A13:187:ARG:CD	1:B13:184:GLN:OE1	2.44	0.65
1:A7:155:PRO:HG2	1:B5:157:THR:CG2	2.25	0.65
1:A13:155:PRO:HG2	1:B11:157:THR:CG2	2.25	0.65
2:D1:43:SER:N	2:D1:48:ASN:HD21	1.93	0.65
1:A1:155:PRO:HG2	1:B12:157:THR:CG2	2.25	0.65
1:A11:187:ARG:CD	1:B11:184:GLN:OE1	2.44	0.65
2:D2:168:LEU:HD22	2:D2:174:VAL:HG23	1.77	0.65
2:D5:168:LEU:HD22	2:D5:174:VAL:HG23	1.77	0.65
2:D6:168:LEU:HD22	2:D6:174:VAL:HG23	1.77	0.65
1:A3:187:ARG:CD	1:B3:184:GLN:OE1	2.44	0.65
1:A6:187:ARG:HG3	1:B6:184:GLN:OE1	1.97	0.65
1:A9:187:ARG:HG3	1:B9:184:GLN:OE1	1.97	0.65
1:A12:187:ARG:HG3	1:B12:184:GLN:OE1	1.97	0.65
2:D7:168:LEU:HD22	2:D7:174:VAL:HG23	1.77	0.65
1:A10:187:ARG:HG3	1:B10:184:GLN:OE1	1.97	0.64
1:B10:98:VAL:CG1	2:D11:208:TRP:CG	2.81	0.64
2:D5:43:SER:N	2:D5:48:ASN:HD21	1.93	0.64
2:D8:168:LEU:HD22	2:D8:174:VAL:HG23	1.77	0.64
1:B12:170:VAL:HG11	2:D12:144:ASN:HD22	1.63	0.64
2:C13:35:GLY:CA	2:D13:27:PRO:HD3	2.27	0.64
2:D2:168:LEU:HD21	2:D2:174:VAL:HG23	1.73	0.64
2:D3:168:LEU:HD22	2:D3:174:VAL:HG23	1.77	0.64
1:B6:98:VAL:CG1	2:D7:208:TRP:CG	2.81	0.64
1:B7:98:VAL:CG1	2:D8:208:TRP:CG	2.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B9:98:VAL:CG1	2:D10:208:TRP:CG	2.81	0.64
1:B11:98:VAL:CG1	2:D12:208:TRP:CG	2.81	0.64
1:B13:170:VAL:HG11	2:D13:144:ASN:HD22	1.63	0.64
2:C8:35:GLY:CA	2:D8:27:PRO:HD3	2.27	0.64
2:C12:35:GLY:CA	2:D12:27:PRO:HD3	2.27	0.64
1:B11:170:VAL:HG11	2:D11:144:ASN:HD22	1.63	0.64
2:C1:42:ILE:HB	2:C1:104:ALA:HB1	1.80	0.64
2:D12:168:LEU:HD22	2:D12:174:VAL:HG23	1.77	0.64
1:A2:187:ARG:CD	1:B2:184:GLN:OE1	2.44	0.64
1:B8:98:VAL:CG1	2:D9:208:TRP:CG	2.81	0.64
1:B8:170:VAL:HG11	2:D8:144:ASN:HD22	1.63	0.64
1:B12:98:VAL:CG1	2:D13:208:TRP:CG	2.81	0.64
2:C3:42:ILE:HB	2:C3:104:ALA:HB1	1.80	0.64
2:C7:42:ILE:HB	2:C7:104:ALA:HB1	1.80	0.64
2:D3:37:GLN:NE2	2:D3:103:VAL:HG23	2.13	0.64
2:D5:37:GLN:NE2	2:D5:103:VAL:HG23	2.13	0.64
2:D10:43:SER:N	2:D10:48:ASN:HD21	1.93	0.64
1:A3:187:ARG:HG3	1:B3:184:GLN:OE1	1.97	0.64
1:A4:187:ARG:HG3	1:B4:184:GLN:OE1	1.97	0.64
1:A12:187:ARG:CD	1:B12:184:GLN:OE1	2.44	0.64
1:B2:188:VAL:HG13	2:D2:141:ILE:HD11	1.75	0.64
1:B3:98:VAL:CG1	2:D4:208:TRP:CG	2.81	0.64
1:B10:170:VAL:HG11	2:D10:144:ASN:HD22	1.63	0.64
2:C4:35:GLY:CA	2:D4:27:PRO:HD3	2.27	0.64
2:C5:35:GLY:CA	2:D5:27:PRO:HD3	2.27	0.64
2:C5:42:ILE:HB	2:C5:104:ALA:HB1	1.80	0.64
2:C7:35:GLY:CA	2:D7:27:PRO:HD3	2.27	0.64
1:A5:187:ARG:HG3	1:B5:184:GLN:OE1	1.97	0.64
1:A7:187:ARG:HG3	1:B7:184:GLN:OE1	1.97	0.64
1:B4:98:VAL:CG1	2:D5:208:TRP:CG	2.81	0.64
2:C11:35:GLY:CA	2:D11:27:PRO:HD3	2.27	0.64
2:D2:37:GLN:NE2	2:D2:103:VAL:HG23	2.13	0.64
1:A1:187:ARG:HG3	1:B1:184:GLN:OE1	1.97	0.64
1:B1:170:VAL:HG11	2:D1:144:ASN:HD22	1.63	0.64
1:B2:98:VAL:CG1	2:D3:208:TRP:CG	2.81	0.64
1:B7:170:VAL:HG11	2:D7:144:ASN:HD22	1.63	0.64
1:B9:170:VAL:HG11	2:D9:144:ASN:HD22	1.63	0.64
1:B13:98:VAL:CG1	2:D1:208:TRP:CG	2.81	0.64
2:C1:35:GLY:CA	2:D1:27:PRO:HD3	2.27	0.64
2:C8:42:ILE:HB	2:C8:104:ALA:HB1	1.80	0.64
2:C8:202:LEU:CD1	2:C8:217:PHE:CZ	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C9:35:GLY:CA	2:D9:27:PRO:HD3	2.27	0.64
2:C12:42:ILE:HB	2:C12:104:ALA:HB1	1.80	0.64
2:C13:42:ILE:HB	2:C13:104:ALA:HB1	1.80	0.64
1:B1:98:VAL:CG1	2:D2:208:TRP:CG	2.81	0.64
1:B6:170:VAL:HG11	2:D6:144:ASN:HD22	1.63	0.64
2:C6:42:ILE:HB	2:C6:104:ALA:HB1	1.80	0.64
2:C7:202:LEU:CD1	2:C7:217:PHE:CZ	2.76	0.64
2:C9:42:ILE:HB	2:C9:104:ALA:HB1	1.80	0.64
2:D13:37:GLN:NE2	2:D13:103:VAL:HG23	2.13	0.64
1:B5:98:VAL:CG1	2:D6:208:TRP:CG	2.81	0.64
2:C2:42:ILE:HB	2:C2:104:ALA:HB1	1.80	0.64
2:C4:42:ILE:HB	2:C4:104:ALA:HB1	1.80	0.64
2:C9:202:LEU:CD1	2:C9:217:PHE:CZ	2.76	0.64
2:D6:37:GLN:NE2	2:D6:103:VAL:HG23	2.13	0.64
2:C10:42:ILE:HB	2:C10:104:ALA:HB1	1.80	0.63
2:D8:168:LEU:HD21	2:D8:174:VAL:HG23	1.73	0.63
2:C11:42:ILE:HB	2:C11:104:ALA:HB1	1.80	0.63
1:B5:170:VAL:HG11	2:D5:144:ASN:HD22	1.63	0.63
2:C3:35:GLY:CA	2:D3:27:PRO:HD3	2.27	0.63
2:C3:194:ASN:OD1	2:C3:224:LEU:CD2	2.47	0.63
1:A8:187:ARG:HG3	1:B8:184:GLN:OE1	1.97	0.63
1:A11:187:ARG:HG3	1:B11:184:GLN:OE1	1.97	0.63
2:C6:35:GLY:CA	2:D6:27:PRO:HD3	2.27	0.63
2:C6:202:LEU:CD1	2:C6:217:PHE:CZ	2.76	0.63
2:D12:43:SER:N	2:D12:48:ASN:HD21	1.93	0.63
1:A2:187:ARG:HG3	1:B2:184:GLN:OE1	1.97	0.63
1:B8:98:VAL:HG21	2:D9:208:TRP:CD1	2.12	0.63
2:C2:194:ASN:OD1	2:C2:224:LEU:CD2	2.47	0.63
2:D8:37:GLN:NE2	2:D8:103:VAL:HG23	2.13	0.63
2:D12:37:GLN:NE2	2:D12:103:VAL:HG23	2.13	0.63
1:A13:187:ARG:HG3	1:B13:184:GLN:OE1	1.97	0.63
2:C1:194:ASN:OD1	2:C1:224:LEU:CD2	2.47	0.63
2:C4:194:ASN:OD1	2:C4:224:LEU:CD2	2.47	0.63
2:D1:37:GLN:NE2	2:D1:103:VAL:HG23	2.13	0.63
2:D13:43:SER:N	2:D13:48:ASN:HD21	1.93	0.63
1:B2:170:VAL:HG11	2:D2:144:ASN:HD22	1.63	0.63
2:C2:35:GLY:CA	2:D2:27:PRO:HD3	2.27	0.63
2:C9:194:ASN:OD1	2:C9:224:LEU:CD2	2.47	0.63
2:C10:35:GLY:CA	2:D10:27:PRO:HD3	2.27	0.63
2:C10:194:ASN:OD1	2:C10:224:LEU:CD2	2.47	0.63
2:C10:202:LEU:CD1	2:C10:217:PHE:CZ	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C13:194:ASN:OD1	2:C13:224:LEU:CD2	2.47	0.63
2:D4:37:GLN:NE2	2:D4:103:VAL:HG23	2.13	0.63
2:D9:37:GLN:NE2	2:D9:103:VAL:HG23	2.13	0.63
2:C11:194:ASN:OD1	2:C11:224:LEU:CD2	2.47	0.63
2:C12:194:ASN:OD1	2:C12:224:LEU:CD2	2.47	0.63
2:D4:43:SER:N	2:D4:48:ASN:HD21	1.93	0.63
2:D10:37:GLN:NE2	2:D10:103:VAL:HG23	2.13	0.63
2:C8:194:ASN:OD1	2:C8:224:LEU:CD2	2.47	0.62
2:D7:43:SER:N	2:D7:48:ASN:HD21	1.93	0.62
2:C5:194:ASN:OD1	2:C5:224:LEU:CD2	2.47	0.62
2:C5:202:LEU:CD1	2:C5:217:PHE:CZ	2.76	0.62
2:D7:37:GLN:NE2	2:D7:103:VAL:HG23	2.13	0.62
2:D12:168:LEU:HD21	2:D12:174:VAL:HG23	1.73	0.62
1:B3:170:VAL:HG11	2:D3:144:ASN:HD22	1.63	0.62
2:D5:224:LEU:HD11	2:D5:230:MET:HG3	1.82	0.62
2:D3:224:LEU:HD11	2:D3:230:MET:HG3	1.82	0.62
2:D10:224:LEU:HD11	2:D10:230:MET:HG3	1.82	0.62
2:D11:224:LEU:HD11	2:D11:230:MET:HG3	1.82	0.62
2:D12:224:LEU:HD11	2:D12:230:MET:HG3	1.82	0.62
1:B4:170:VAL:HG11	2:D4:144:ASN:HD22	1.63	0.62
2:C6:194:ASN:OD1	2:C6:224:LEU:CD2	2.47	0.62
2:C7:194:ASN:OD1	2:C7:224:LEU:CD2	2.47	0.62
2:D1:224:LEU:HD11	2:D1:230:MET:HG3	1.82	0.62
2:D2:224:LEU:HD11	2:D2:230:MET:HG3	1.82	0.62
2:D9:224:LEU:HD11	2:D9:230:MET:HG3	1.82	0.62
2:D11:37:GLN:NE2	2:D11:103:VAL:HG23	2.13	0.62
2:D4:224:LEU:HD11	2:D4:230:MET:HG3	1.82	0.62
1:A10:167:ILE:CG2	1:B9:197:TRP:CH2	2.83	0.62
2:C4:202:LEU:CD1	2:C4:217:PHE:CZ	2.76	0.62
2:D7:224:LEU:HD11	2:D7:230:MET:HG3	1.82	0.62
1:A7:167:ILE:CG2	1:B6:197:TRP:CH2	2.83	0.62
1:A8:167:ILE:CG2	1:B7:197:TRP:CH2	2.83	0.62
1:A9:167:ILE:CG2	1:B8:197:TRP:CH2	2.83	0.62
2:D13:224:LEU:HD11	2:D13:230:MET:HG3	1.82	0.62
2:D6:224:LEU:HD11	2:D6:230:MET:HG3	1.82	0.61
2:D8:224:LEU:HD11	2:D8:230:MET:HG3	1.82	0.61
1:A11:167:ILE:CG2	1:B10:197:TRP:CH2	2.83	0.61
2:C11:202:LEU:CD1	2:C11:217:PHE:CZ	2.76	0.61
1:A9:192:VAL:HG11	2:C9:148:LEU:CD2	2.31	0.61
1:A10:192:VAL:HG11	2:C10:148:LEU:CD2	2.31	0.61
1:A11:167:ILE:HG22	1:B10:197:TRP:CH2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A11:192:VAL:HG11	2:C11:148:LEU:CD2	2.31	0.61
1:B7:98:VAL:HG21	2:D8:208:TRP:CD1	2.12	0.61
1:A4:158:VAL:HG21	1:A4:200:PRO:HB3	1.83	0.61
1:A4:192:VAL:HG11	2:C4:148:LEU:CD2	2.31	0.61
1:A9:167:ILE:HG22	1:B8:197:TRP:CH2	2.36	0.61
2:C3:202:LEU:CD1	2:C3:217:PHE:CZ	2.76	0.61
1:A1:192:VAL:CG1	2:C1:148:LEU:CD2	2.79	0.61
1:A5:158:VAL:HG21	1:A5:200:PRO:HB3	1.83	0.61
1:A5:192:VAL:HG11	2:C5:148:LEU:CD2	2.31	0.61
1:A6:167:ILE:HG22	1:B5:197:TRP:CH2	2.36	0.61
1:A12:167:ILE:CG2	1:B11:197:TRP:CH2	2.83	0.61
1:A12:192:VAL:HG11	2:C12:148:LEU:CD2	2.31	0.61
1:A13:192:VAL:HG11	2:C13:148:LEU:CD2	2.31	0.61
1:A2:167:ILE:HG21	1:B1:197:TRP:CZ3	2.36	0.61
1:A2:167:ILE:CG2	1:B1:197:TRP:CH2	2.83	0.61
1:A2:192:VAL:CG1	2:C2:148:LEU:CD2	2.79	0.61
1:A5:167:ILE:CG2	1:B4:197:TRP:CH2	2.83	0.61
1:A6:167:ILE:CG2	1:B5:197:TRP:CH2	2.83	0.61
1:A8:167:ILE:HG22	1:B7:197:TRP:CH2	2.36	0.61
1:A8:192:VAL:HG11	2:C8:148:LEU:CD2	2.31	0.61
1:A1:192:VAL:HG11	2:C1:148:LEU:CD2	2.31	0.61
1:A3:158:VAL:HG21	1:A3:200:PRO:HB3	1.83	0.61
1:A4:167:ILE:HG21	1:B3:197:TRP:CZ3	2.36	0.61
1:A8:167:ILE:HG21	1:B7:197:TRP:CZ3	2.36	0.61
1:A12:167:ILE:HG22	1:B11:197:TRP:CH2	2.36	0.61
1:A12:167:ILE:HG21	1:B11:197:TRP:CZ3	2.36	0.61
1:A13:167:ILE:CG2	1:B12:197:TRP:CH2	2.83	0.61
1:A13:192:VAL:CG1	2:C13:148:LEU:CD2	2.79	0.61
2:D9:43:SER:N	2:D9:48:ASN:HD21	1.93	0.61
1:A1:158:VAL:HG21	1:A1:200:PRO:HB3	1.83	0.61
1:A2:158:VAL:HG21	1:A2:200:PRO:HB3	1.83	0.61
1:A3:192:VAL:CG1	2:C3:148:LEU:CD2	2.79	0.61
1:A3:192:VAL:HG11	2:C3:148:LEU:CD2	2.31	0.61
1:A11:167:ILE:HG21	1:B10:197:TRP:CZ3	2.36	0.61
1:A1:167:ILE:CG2	1:B13:197:TRP:CH2	2.83	0.61
1:A5:167:ILE:HG21	1:B4:197:TRP:CZ3	2.36	0.61
1:A6:158:VAL:HG21	1:A6:200:PRO:HB3	1.83	0.61
1:A9:167:ILE:HG21	1:B8:197:TRP:CZ3	2.36	0.61
1:A12:192:VAL:CG1	2:C12:148:LEU:CD2	2.79	0.61
2:D2:43:SER:N	2:D2:48:ASN:HD21	1.93	0.61
1:A1:167:ILE:HG22	1:B13:197:TRP:CH2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:167:ILE:CG2	1:B2:197:TRP:CH2	2.83	0.60
1:A4:167:ILE:CG2	1:B3:197:TRP:CH2	2.83	0.60
1:A5:167:ILE:HG22	1:B4:197:TRP:CH2	2.36	0.60
1:A6:192:VAL:HG11	2:C6:148:LEU:CD2	2.31	0.60
1:A11:192:VAL:CG1	2:C11:148:LEU:CD2	2.79	0.60
1:A9:192:VAL:CG1	2:C9:148:LEU:CD2	2.79	0.60
1:A10:192:VAL:CG1	2:C10:148:LEU:CD2	2.79	0.60
1:A1:167:ILE:HG21	1:B13:197:TRP:CZ3	2.36	0.60
1:A2:167:ILE:HG22	1:B1:197:TRP:CH2	2.36	0.60
1:A4:192:VAL:CG1	2:C4:148:LEU:CD2	2.79	0.60
1:A7:192:VAL:HG11	2:C7:148:LEU:CD2	2.31	0.60
1:A7:158:VAL:HG21	1:A7:200:PRO:HB3	1.83	0.60
1:A7:167:ILE:HG22	1:B6:197:TRP:CH2	2.36	0.60
1:A8:192:VAL:CG1	2:C8:148:LEU:CD2	2.79	0.60
1:B2:95:THR:HG21	1:B2:197:TRP:HB2	1.83	0.60
1:A7:167:ILE:HG21	1:B6:197:TRP:CZ3	2.36	0.60
2:D3:43:SER:N	2:D3:48:ASN:HD21	1.93	0.60
1:A2:192:VAL:HG11	2:C2:148:LEU:CD2	2.31	0.60
1:A5:192:VAL:CG1	2:C5:148:LEU:CD2	2.79	0.60
1:A7:192:VAL:CG1	2:C7:148:LEU:CD2	2.79	0.60
1:B13:95:THR:HG21	1:B13:197:TRP:HB2	1.83	0.60
1:A6:167:ILE:HG21	1:B5:197:TRP:CZ3	2.36	0.60
2:D6:43:SER:N	2:D6:48:ASN:HD21	1.93	0.60
1:A3:167:ILE:HG22	1:B2:197:TRP:CH2	2.36	0.60
1:A3:167:ILE:HG21	1:B2:197:TRP:CZ3	2.36	0.60
1:A6:192:VAL:CG1	2:C6:148:LEU:CD2	2.79	0.60
1:A8:158:VAL:HG21	1:A8:200:PRO:HB3	1.83	0.60
1:A10:167:ILE:HG22	1:B9:197:TRP:CH2	2.36	0.60
1:A13:158:VAL:HG21	1:A13:200:PRO:HB3	1.83	0.60
1:A13:167:ILE:HG21	1:B12:197:TRP:CZ3	2.36	0.60
1:B12:95:THR:HG21	1:B12:197:TRP:HB2	1.83	0.60
1:A13:167:ILE:HG22	1:B12:197:TRP:CH2	2.36	0.60
1:B7:95:THR:HG21	1:B7:197:TRP:HB2	1.83	0.60
1:A12:158:VAL:HG21	1:A12:200:PRO:HB3	1.83	0.59
2:C12:202:LEU:CD1	2:C12:217:PHE:CZ	2.76	0.59
1:A9:158:VAL:HG21	1:A9:200:PRO:HB3	1.83	0.59
1:A10:158:VAL:HG21	1:A10:200:PRO:HB3	1.83	0.59
1:B8:95:THR:HG21	1:B8:197:TRP:HB2	1.83	0.59
2:D8:43:SER:N	2:D8:48:ASN:HD21	1.93	0.59
1:A4:167:ILE:HG22	1:B3:197:TRP:CH2	2.36	0.59
1:B3:95:THR:HG21	1:B3:197:TRP:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B6:95:THR:HG21	1:B6:197:TRP:HB2	1.83	0.59
1:A10:167:ILE:HG21	1:B9:197:TRP:CZ3	2.36	0.59
1:B1:95:THR:HG21	1:B1:197:TRP:HB2	1.83	0.59
2:C6:136:TYR:HE1	2:C6:213:ARG:HD3	1.68	0.59
1:A9:185:PRO:HG2	1:A10:156:GLY:O	2.03	0.59
1:A11:158:VAL:HG21	1:A11:200:PRO:HB3	1.83	0.59
1:B9:95:THR:HG21	1:B9:197:TRP:HB2	1.83	0.59
1:A5:185:PRO:HG2	1:A6:156:GLY:O	2.03	0.59
1:A7:185:PRO:HG2	1:A8:156:GLY:O	2.03	0.59
1:A12:185:PRO:HG2	1:A13:156:GLY:O	2.03	0.59
1:B4:95:THR:HG21	1:B4:197:TRP:HB2	1.83	0.59
2:C10:136:TYR:HE1	2:C10:213:ARG:HD3	1.68	0.59
1:A1:156:GLY:O	1:A13:185:PRO:HG2	2.03	0.59
1:B5:95:THR:HG21	1:B5:197:TRP:HB2	1.83	0.59
1:B10:95:THR:HG21	1:B10:197:TRP:HB2	1.83	0.59
2:C7:136:TYR:HE1	2:C7:213:ARG:HD3	1.68	0.59
2:C9:136:TYR:HE1	2:C9:213:ARG:HD3	1.68	0.59
1:A3:185:PRO:HG2	1:A4:156:GLY:O	2.03	0.58
1:A6:185:PRO:HG2	1:A7:156:GLY:O	2.03	0.58
1:A6:192:VAL:HG11	2:C6:148:LEU:HD23	1.85	0.58
1:A11:185:PRO:HG2	1:A12:156:GLY:O	2.03	0.58
2:C1:136:TYR:HE1	2:C1:213:ARG:HD3	1.68	0.58
2:C3:136:TYR:HE1	2:C3:213:ARG:HD3	1.68	0.58
2:C5:136:TYR:HE1	2:C5:213:ARG:HD3	1.68	0.58
2:C13:136:TYR:HE1	2:C13:213:ARG:HD3	1.68	0.58
1:A2:192:VAL:HG11	2:C2:148:LEU:HD23	1.86	0.58
1:A4:185:PRO:HG2	1:A5:156:GLY:O	2.03	0.58
2:C11:136:TYR:HE1	2:C11:213:ARG:HD3	1.68	0.58
1:A1:185:PRO:HG2	1:A2:156:GLY:O	2.03	0.58
1:A10:155:PRO:HG2	1:B8:157:THR:HG22	1.86	0.58
2:C7:169:PRO:HD2	2:C7:172:PHE:CD2	2.39	0.58
1:A1:192:VAL:HG11	2:C1:148:LEU:HD23	1.85	0.58
2:C5:202:LEU:O	2:C5:202:LEU:HD12	2.04	0.58
2:C13:202:LEU:HD12	2:C13:202:LEU:O	2.04	0.58
1:A1:155:PRO:HG2	1:B12:157:THR:HG22	1.86	0.58
1:A8:185:PRO:HG2	1:A9:156:GLY:O	2.03	0.58
2:C1:169:PRO:HD2	2:C1:172:PHE:CD2	2.39	0.58
2:C5:169:PRO:HD2	2:C5:172:PHE:CD2	2.39	0.58
2:C9:202:LEU:HD12	2:C9:202:LEU:O	2.04	0.58
2:C11:169:PRO:HD2	2:C11:172:PHE:CD2	2.39	0.58
2:C12:136:TYR:HE1	2:C12:213:ARG:HD3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:155:PRO:HG2	1:B2:157:THR:HG22	1.86	0.58
1:A7:155:PRO:HG2	1:B5:157:THR:HG22	1.86	0.58
2:C2:202:LEU:HD12	2:C2:202:LEU:O	2.04	0.58
2:C4:169:PRO:HD2	2:C4:172:PHE:CD2	2.39	0.58
2:C6:202:LEU:HD12	2:C6:202:LEU:O	2.04	0.58
2:C8:169:PRO:HD2	2:C8:172:PHE:CD2	2.39	0.58
2:C11:202:LEU:HD12	2:C11:202:LEU:O	2.04	0.58
2:C12:169:PRO:HD2	2:C12:172:PHE:CD2	2.39	0.58
2:C13:169:PRO:HD2	2:C13:172:PHE:CD2	2.39	0.58
1:A12:155:PRO:HG2	1:B10:157:THR:HG22	1.86	0.58
1:B11:95:THR:HG21	1:B11:197:TRP:HB2	1.83	0.58
2:C2:136:TYR:HE1	2:C2:213:ARG:HD3	1.68	0.58
2:C13:224:LEU:HD11	2:C13:228:GLY:HA3	1.86	0.58
1:A2:155:PRO:HG2	1:B13:157:THR:HG22	1.86	0.58
1:A5:192:VAL:HG11	2:C5:148:LEU:HD23	1.86	0.58
1:A10:185:PRO:HG2	1:A11:156:GLY:O	2.03	0.58
2:C12:224:LEU:HD11	2:C12:228:GLY:HA3	1.85	0.58
1:A9:172:ILE:HD12	2:C9:140:LEU:CD1	2.30	0.58
2:C6:169:PRO:HD2	2:C6:172:PHE:CD2	2.39	0.58
1:A2:185:PRO:HG2	1:A3:156:GLY:O	2.03	0.57
1:A5:155:PRO:HG2	1:B3:157:THR:HG22	1.86	0.57
1:A11:155:PRO:HG2	1:B9:157:THR:HG22	1.86	0.57
1:A13:155:PRO:HG2	1:B11:157:THR:HG22	1.86	0.57
2:C1:224:LEU:HD11	2:C1:228:GLY:HA3	1.86	0.57
2:C6:224:LEU:HD11	2:C6:228:GLY:HA3	1.85	0.57
2:C10:202:LEU:HD12	2:C10:202:LEU:O	2.04	0.57
1:B8:98:VAL:HG13	2:D9:208:TRP:CG	2.40	0.57
2:C2:72:LEU:HD22	3:E2:185:PHE:HB3	1.86	0.57
2:C4:202:LEU:HD12	2:C4:202:LEU:O	2.04	0.57
2:C11:224:LEU:HD11	2:C11:228:GLY:HA3	1.85	0.57
2:C12:202:LEU:HD12	2:C12:202:LEU:O	2.04	0.57
1:A2:172:ILE:HD12	2:C2:140:LEU:CD1	2.30	0.57
1:A9:155:PRO:HG2	1:B7:157:THR:HG22	1.86	0.57
1:B4:98:VAL:HG11	2:D5:208:TRP:CG	2.40	0.57
2:C2:169:PRO:HD2	2:C2:172:PHE:CD2	2.39	0.57
2:C3:169:PRO:HD2	2:C3:172:PHE:CD2	2.39	0.57
2:C5:224:LEU:HD11	2:C5:228:GLY:HA3	1.85	0.57
2:C7:224:LEU:HD11	2:C7:228:GLY:HA3	1.86	0.57
2:C8:202:LEU:O	2:C8:202:LEU:HD12	2.04	0.57
2:C10:169:PRO:HD2	2:C10:172:PHE:CD2	2.39	0.57
1:A1:172:ILE:HD12	2:C1:140:LEU:CD1	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:98:VAL:HG11	2:D6:208:TRP:CG	2.40	0.57
1:B8:98:VAL:HG11	2:D9:208:TRP:CG	2.40	0.57
2:C2:224:LEU:HD11	2:C2:228:GLY:HA3	1.86	0.57
2:C3:72:LEU:HD22	3:E3:185:PHE:HB3	1.86	0.57
1:A3:172:ILE:HD12	2:C3:140:LEU:CD1	2.30	0.57
1:B1:98:VAL:HG11	2:D2:208:TRP:CG	2.40	0.57
1:B9:98:VAL:HG11	2:D10:208:TRP:CG	2.40	0.57
2:C1:202:LEU:HD12	2:C1:202:LEU:O	2.04	0.57
2:C4:224:LEU:HD11	2:C4:228:GLY:HA3	1.85	0.57
2:C7:72:LEU:HD22	3:E7:185:PHE:HB3	1.86	0.57
2:C8:72:LEU:HD22	3:E8:185:PHE:HB3	1.86	0.57
2:C9:72:LEU:HD22	3:E9:185:PHE:HB3	1.86	0.57
2:C10:72:LEU:HD22	3:E10:185:PHE:HB3	1.86	0.57
1:A8:155:PRO:HG2	1:B6:157:THR:HG22	1.86	0.57
1:B10:98:VAL:HG13	2:D11:208:TRP:CG	2.40	0.57
1:B11:98:VAL:HG13	2:D12:208:TRP:CG	2.40	0.57
2:C4:136:TYR:HE1	2:C4:213:ARG:HD3	1.68	0.57
2:C8:136:TYR:HE1	2:C8:213:ARG:HD3	1.68	0.57
2:C8:224:LEU:HD11	2:C8:228:GLY:HA3	1.85	0.57
2:C9:169:PRO:HD2	2:C9:172:PHE:CD2	2.39	0.57
2:C10:224:LEU:HD11	2:C10:228:GLY:HA3	1.86	0.57
1:A9:192:VAL:HG11	2:C9:148:LEU:HD23	1.85	0.57
1:B11:98:VAL:HG11	2:D12:208:TRP:CG	2.40	0.57
2:C3:202:LEU:HD12	2:C3:202:LEU:O	2.04	0.57
2:C7:202:LEU:HD12	2:C7:202:LEU:O	2.04	0.57
2:C9:64:GLY:HA3	3:E9:179:MET:O	2.05	0.57
1:B5:98:VAL:HG13	2:D6:208:TRP:CG	2.40	0.57
1:B12:98:VAL:HG11	2:D13:208:TRP:CG	2.40	0.57
1:B13:98:VAL:HG11	2:D1:208:TRP:CG	2.40	0.57
2:C11:72:LEU:HD22	3:E11:185:PHE:HB3	1.86	0.57
2:D11:43:SER:N	2:D11:48:ASN:HD21	1.93	0.57
1:B3:98:VAL:HG11	2:D4:208:TRP:CG	2.40	0.57
1:B7:98:VAL:HG13	2:D8:208:TRP:CG	2.40	0.57
2:C7:64:GLY:HA3	3:E7:179:MET:O	2.05	0.57
1:B2:98:VAL:HG11	2:D3:208:TRP:CG	2.40	0.57
1:B7:98:VAL:HG11	2:D8:208:TRP:CG	2.40	0.57
1:B9:98:VAL:HG13	2:D10:208:TRP:CG	2.40	0.57
2:C8:64:GLY:HA3	3:E8:179:MET:O	2.05	0.57
1:A4:172:ILE:HD12	2:C4:140:LEU:CD1	2.30	0.56
2:C1:64:GLY:HA3	3:E1:179:MET:O	2.05	0.56
2:C1:72:LEU:HD22	3:E1:185:PHE:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C11:64:GLY:HA3	3:E11:179:MET:O	2.05	0.56
2:C12:64:GLY:HA3	3:E12:179:MET:O	2.05	0.56
2:C13:64:GLY:HA3	3:E13:179:MET:O	2.05	0.56
2:D12:159:VAL:CG1	2:D12:160:LYS:N	2.44	0.56
1:A6:155:PRO:HG2	1:B4:157:THR:HG22	1.86	0.56
1:A13:172:ILE:HD12	2:C13:140:LEU:CD1	2.30	0.56
2:C3:224:LEU:HD11	2:C3:228:GLY:HA3	1.86	0.56
2:C9:224:LEU:HD11	2:C9:228:GLY:HA3	1.85	0.56
1:A3:155:PRO:HG2	1:B1:157:THR:HG22	1.86	0.56
1:B1:98:VAL:HG13	2:D2:208:TRP:CG	2.40	0.56
1:B10:98:VAL:HG11	2:D11:208:TRP:CG	2.40	0.56
2:C5:72:LEU:HD22	3:E5:185:PHE:HB3	1.86	0.56
2:C6:72:LEU:HD22	3:E6:185:PHE:HB3	1.86	0.56
2:C12:72:LEU:HD22	3:E12:185:PHE:HB3	1.86	0.56
1:B4:98:VAL:HG13	2:D5:208:TRP:CG	2.40	0.56
1:B13:98:VAL:HG13	2:D1:208:TRP:CG	2.40	0.56
2:C5:64:GLY:HA3	3:E5:179:MET:O	2.05	0.56
1:B6:98:VAL:HG11	2:D7:208:TRP:CG	2.40	0.56
1:A2:167:ILE:O	2:C2:220:ASN:ND2	2.38	0.56
1:A5:172:ILE:HD12	2:C5:140:LEU:CD1	2.30	0.56
1:A8:155:PRO:CD	1:B6:157:THR:CG2	2.84	0.56
1:A9:155:PRO:CD	1:B7:157:THR:CG2	2.84	0.56
2:C4:72:LEU:HD22	3:E4:185:PHE:HB3	1.86	0.56
2:C13:72:LEU:HD22	3:E13:185:PHE:HB3	1.86	0.56
1:A10:156:GLY:N	2:C9:205:GLN:OE1	2.39	0.56
2:C3:64:GLY:HA3	3:E3:179:MET:O	2.05	0.56
2:C6:64:GLY:HA3	3:E6:179:MET:O	2.05	0.56
2:C10:64:GLY:HA3	3:E10:179:MET:O	2.05	0.56
2:D1:30:ILE:HG13	2:D1:116:LEU:HD23	1.88	0.56
2:D12:30:ILE:HG13	2:D12:116:LEU:HD23	1.88	0.56
1:A12:156:GLY:N	2:C11:205:GLN:OE1	2.39	0.56
1:A13:167:ILE:O	2:C13:220:ASN:ND2	2.38	0.56
1:B3:98:VAL:HG13	2:D4:208:TRP:CG	2.40	0.56
2:D3:30:ILE:HG13	2:D3:116:LEU:HD23	1.88	0.56
1:A5:155:PRO:CD	1:B3:157:THR:CG2	2.84	0.56
1:A8:156:GLY:N	2:C7:205:GLN:OE1	2.39	0.56
1:A10:167:ILE:O	2:C10:220:ASN:ND2	2.38	0.56
2:D2:30:ILE:HG13	2:D2:116:LEU:HD23	1.88	0.56
2:D13:30:ILE:HG13	2:D13:116:LEU:HD23	1.88	0.56
1:A3:156:GLY:N	2:C2:205:GLN:OE1	2.39	0.55
2:C2:64:GLY:HA3	3:E2:179:MET:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:155:PRO:CD	1:B2:157:THR:CG2	2.84	0.55
1:A4:156:GLY:N	2:C3:205:GLN:OE1	2.39	0.55
1:A7:155:PRO:CD	1:B5:157:THR:CG2	2.84	0.55
1:B6:98:VAL:HG13	2:D7:208:TRP:CG	2.40	0.55
1:A10:155:PRO:CD	1:B8:157:THR:CG2	2.84	0.55
1:A12:172:ILE:HD12	2:C12:140:LEU:CD1	2.30	0.55
2:D4:30:ILE:HG13	2:D4:116:LEU:HD23	1.88	0.55
1:A6:155:PRO:CD	1:B4:157:THR:CG2	2.84	0.55
1:A6:156:GLY:N	2:C5:205:GLN:OE1	2.39	0.55
1:A7:156:GLY:N	2:C6:205:GLN:OE1	2.39	0.55
1:B12:98:VAL:HG13	2:D13:208:TRP:CG	2.40	0.55
2:C1:202:LEU:CD1	2:C1:217:PHE:CZ	2.76	0.55
1:A1:156:GLY:N	2:C13:205:GLN:OE1	2.39	0.55
1:A10:172:ILE:HD12	2:C10:140:LEU:CD1	2.30	0.55
1:B10:91:THR:HG1	2:D11:213:ARG:HH22	1.53	0.55
2:C4:64:GLY:HA3	3:E4:179:MET:O	2.05	0.55
2:D9:56:LYS:HA	2:D9:76:GLY:HA3	1.89	0.55
1:A2:155:PRO:CD	1:B13:157:THR:CG2	2.84	0.55
1:A6:172:ILE:HD12	2:C6:140:LEU:CD1	2.30	0.55
2:D10:30:ILE:HG13	2:D10:116:LEU:HD23	1.88	0.55
2:D11:30:ILE:HG13	2:D11:116:LEU:HD23	1.88	0.55
1:A3:155:PRO:CD	1:B1:157:THR:CG2	2.84	0.55
1:B1:91:THR:CG2	2:D2:213:ARG:HH12	2.20	0.55
1:B8:91:THR:CG2	2:D9:213:ARG:HH12	2.20	0.55
1:B11:91:THR:CG2	2:D12:213:ARG:HH12	2.20	0.55
1:B12:91:THR:CG2	2:D13:213:ARG:HH12	2.20	0.55
1:B13:91:THR:CG2	2:D1:213:ARG:HH12	2.20	0.55
2:D5:30:ILE:HG13	2:D5:116:LEU:HD23	1.88	0.55
2:D7:56:LYS:HA	2:D7:76:GLY:HA3	1.89	0.55
2:D8:56:LYS:HA	2:D8:76:GLY:HA3	1.89	0.55
2:D9:168:LEU:HD21	2:D9:174:VAL:HG23	1.73	0.55
2:D10:56:LYS:HA	2:D10:76:GLY:HA3	1.89	0.55
1:A1:155:PRO:CD	1:B12:157:THR:CG2	2.84	0.55
1:A2:155:PRO:HD2	1:B13:157:THR:HG21	1.89	0.55
1:A9:156:GLY:N	2:C8:205:GLN:OE1	2.39	0.55
1:B7:91:THR:CG2	2:D8:213:ARG:HH12	2.20	0.55
1:A1:155:PRO:HD2	1:B12:157:THR:HG21	1.89	0.55
1:A13:156:GLY:N	2:C12:205:GLN:OE1	2.39	0.55
1:B10:91:THR:CG2	2:D11:213:ARG:HH12	2.20	0.55
2:D1:159:VAL:CG1	2:D1:160:LYS:N	2.44	0.55
2:D11:56:LYS:HA	2:D11:76:GLY:HA3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A9:167:ILE:HD12	1:B8:160:PRO:O	2.07	0.55
1:A11:192:VAL:HG11	2:C11:148:LEU:HD23	1.85	0.55
1:B2:91:THR:CG2	2:D3:213:ARG:HH12	2.20	0.55
1:A3:155:PRO:HD2	1:B1:157:THR:HG21	1.89	0.54
1:A5:156:GLY:N	2:C4:205:GLN:OE1	2.39	0.54
1:A7:172:ILE:HD12	2:C7:140:LEU:CD1	2.30	0.54
1:A12:167:ILE:HD12	1:B11:160:PRO:O	2.08	0.54
1:B2:98:VAL:HG13	2:D3:208:TRP:CG	2.40	0.54
1:B3:91:THR:CG2	2:D4:213:ARG:HH12	2.20	0.54
1:B9:91:THR:CG2	2:D10:213:ARG:HH12	2.20	0.54
2:D6:30:ILE:HG13	2:D6:116:LEU:HD23	1.88	0.54
1:A2:156:GLY:N	2:C1:205:GLN:OE1	2.39	0.54
1:A11:155:PRO:HD2	1:B9:157:THR:HG21	1.89	0.54
1:A12:155:PRO:CD	1:B10:157:THR:CG2	2.84	0.54
1:A12:155:PRO:HD2	1:B10:157:THR:HG21	1.89	0.54
2:D9:30:ILE:HG13	2:D9:116:LEU:HD23	1.88	0.54
2:D10:159:VAL:CG1	2:D10:160:LYS:N	2.44	0.54
1:A1:167:ILE:HD12	1:B13:160:PRO:O	2.07	0.54
1:A5:167:ILE:HD12	1:B4:160:PRO:O	2.07	0.54
1:A11:155:PRO:CD	1:B9:157:THR:CG2	2.84	0.54
1:A11:156:GLY:N	2:C10:205:GLN:OE1	2.39	0.54
1:A12:167:ILE:O	2:C12:220:ASN:ND2	2.38	0.54
1:A13:155:PRO:CD	1:B11:157:THR:CG2	2.84	0.54
1:A13:155:PRO:HD2	1:B11:157:THR:HG21	1.89	0.54
1:B6:91:THR:CG2	2:D7:213:ARG:HH12	2.20	0.54
2:D6:56:LYS:HA	2:D6:76:GLY:HA3	1.89	0.54
1:A11:167:ILE:HD12	1:B10:160:PRO:O	2.07	0.54
2:D8:30:ILE:HG13	2:D8:116:LEU:HD23	1.88	0.54
1:A2:167:ILE:HD12	1:B1:160:PRO:O	2.08	0.54
1:A3:167:ILE:CG2	1:B2:197:TRP:HH2	2.21	0.54
1:A8:172:ILE:HD12	2:C8:140:LEU:CD1	2.30	0.54
2:C8:110:GLU:H	2:C8:110:GLU:CD	2.16	0.54
1:A4:155:PRO:HD2	1:B2:157:THR:HG21	1.89	0.54
1:A10:155:PRO:HD2	1:B8:157:THR:HG21	1.89	0.54
2:C12:110:GLU:H	2:C12:110:GLU:CD	2.16	0.54
2:D12:56:LYS:HA	2:D12:76:GLY:HA3	1.89	0.54
1:A2:167:ILE:CG2	1:B1:197:TRP:HH2	2.21	0.54
1:A5:155:PRO:HD2	1:B3:157:THR:HG21	1.89	0.54
1:A6:167:ILE:HD12	1:B5:160:PRO:O	2.08	0.54
2:C5:110:GLU:H	2:C5:110:GLU:CD	2.16	0.54
2:C9:110:GLU:H	2:C9:110:GLU:CD	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D7:30:ILE:HG13	2:D7:116:LEU:HD23	1.88	0.54
1:A4:167:ILE:CG2	1:B3:197:TRP:HH2	2.21	0.54
1:B4:91:THR:CG2	2:D5:213:ARG:HH12	2.20	0.54
1:A3:167:ILE:HD12	1:B2:160:PRO:O	2.08	0.54
1:A6:155:PRO:HD2	1:B4:157:THR:HG21	1.89	0.54
1:A8:167:ILE:HD12	1:B7:160:PRO:O	2.08	0.54
1:B13:171:TRP:HB3	2:D13:204:GLU:OE1	2.08	0.54
2:C4:110:GLU:CD	2:C4:110:GLU:H	2.16	0.54
2:D2:56:LYS:HA	2:D2:76:GLY:HA3	1.89	0.54
1:A10:167:ILE:HD12	1:B9:160:PRO:O	2.08	0.54
1:A11:172:ILE:HD12	2:C11:140:LEU:CD1	2.30	0.54
1:B5:91:THR:CG2	2:D6:213:ARG:HH12	2.20	0.54
1:B11:171:TRP:HB3	2:D11:204:GLU:OE1	2.08	0.54
2:C7:110:GLU:H	2:C7:110:GLU:CD	2.16	0.54
2:C11:110:GLU:H	2:C11:110:GLU:CD	2.16	0.54
2:D7:60:ILE:HG22	3:F7:185:PHE:CE2	2.43	0.54
1:A9:155:PRO:HD2	1:B7:157:THR:HG21	1.89	0.53
1:B10:171:TRP:HB3	2:D10:204:GLU:OE1	2.08	0.53
2:C2:110:GLU:H	2:C2:110:GLU:CD	2.16	0.53
2:C8:74:ARG:HH11	2:D7:58:THR:HG21	1.73	0.53
2:D1:56:LYS:HA	2:D1:76:GLY:HA3	1.89	0.53
2:D5:56:LYS:HA	2:D5:76:GLY:HA3	1.89	0.53
1:A1:167:ILE:O	2:C1:220:ASN:ND2	2.38	0.53
1:A7:155:PRO:HD2	1:B5:157:THR:HG21	1.89	0.53
1:A8:155:PRO:HD2	1:B6:157:THR:HG21	1.89	0.53
1:A12:167:ILE:CG2	1:B11:197:TRP:HH2	2.21	0.53
1:A12:192:VAL:HG11	2:C12:148:LEU:HD23	1.86	0.53
2:C2:202:LEU:CD1	2:C2:217:PHE:CZ	2.76	0.53
2:D13:56:LYS:HA	2:D13:76:GLY:HA3	1.89	0.53
2:D3:56:LYS:HA	2:D3:76:GLY:HA3	1.89	0.53
2:D4:60:ILE:HG22	3:F4:185:PHE:CE2	2.43	0.53
2:D6:60:ILE:HG22	3:F6:185:PHE:CE2	2.43	0.53
1:A3:167:ILE:O	2:C3:220:ASN:ND2	2.38	0.53
1:A4:167:ILE:HD12	1:B3:160:PRO:O	2.07	0.53
1:A5:167:ILE:CG2	1:B4:197:TRP:HH2	2.21	0.53
1:B2:171:TRP:HB3	2:D2:204:GLU:OE1	2.08	0.53
2:C1:110:GLU:CD	2:C1:110:GLU:H	2.16	0.53
2:D5:60:ILE:HG22	3:F5:185:PHE:CE2	2.43	0.53
1:A5:167:ILE:O	2:C5:220:ASN:ND2	2.38	0.53
1:A7:167:ILE:HD12	1:B6:160:PRO:O	2.07	0.53
1:B8:171:TRP:HB3	2:D8:204:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C13:110:GLU:H	2:C13:110:GLU:CD	2.16	0.53
1:A7:167:ILE:O	2:C7:220:ASN:ND2	2.38	0.53
1:B12:171:TRP:HB3	2:D12:204:GLU:OE1	2.08	0.53
2:C6:110:GLU:H	2:C6:110:GLU:CD	2.16	0.53
2:C10:110:GLU:H	2:C10:110:GLU:CD	2.16	0.53
1:A13:167:ILE:HD12	1:B12:160:PRO:O	2.08	0.53
1:B9:171:TRP:HB3	2:D9:204:GLU:OE1	2.08	0.53
2:D4:56:LYS:HA	2:D4:76:GLY:HA3	1.89	0.53
1:B1:170:VAL:CG1	2:D1:144:ASN:ND2	2.72	0.53
1:B2:170:VAL:CG1	2:D2:144:ASN:ND2	2.72	0.53
2:C6:32:LEU:HB3	2:C6:36:GLY:HA3	1.91	0.53
1:A9:167:ILE:O	2:C9:220:ASN:ND2	2.38	0.53
1:B1:171:TRP:HB3	2:D1:204:GLU:OE1	2.08	0.53
2:C3:64:GLY:N	3:E3:180:MET:HA	2.24	0.53
1:A8:192:VAL:HG11	2:C8:148:LEU:HD23	1.86	0.52
1:A13:167:ILE:CG2	1:B12:197:TRP:HH2	2.21	0.52
1:B4:170:VAL:CG1	2:D4:144:ASN:ND2	2.72	0.52
1:B12:170:VAL:CG1	2:D12:144:ASN:ND2	2.72	0.52
2:C5:32:LEU:HB3	2:C5:36:GLY:HA3	1.91	0.52
2:C13:64:GLY:N	3:E13:180:MET:HA	2.25	0.52
2:D5:30:ILE:HG13	2:D5:30:ILE:O	2.10	0.52
1:A5:201:ALA:O	2:C4:208:TRP:HZ3	1.92	0.52
1:A6:167:ILE:CG2	1:B5:197:TRP:HH2	2.21	0.52
1:B11:170:VAL:CG1	2:D11:144:ASN:ND2	2.72	0.52
2:C3:110:GLU:H	2:C3:110:GLU:CD	2.16	0.52
2:D6:30:ILE:HG13	2:D6:30:ILE:O	2.10	0.52
1:A4:201:ALA:O	2:C3:208:TRP:HZ3	1.92	0.52
1:A7:192:VAL:HG11	2:C7:148:LEU:HD23	1.86	0.52
2:C1:32:LEU:HB3	2:C1:36:GLY:HA3	1.91	0.52
2:C2:32:LEU:HB3	2:C2:36:GLY:HA3	1.91	0.52
2:C7:32:LEU:HB3	2:C7:36:GLY:HA3	1.91	0.52
2:C7:74:ARG:HH11	2:D6:58:THR:HG21	1.73	0.52
2:D4:30:ILE:HG13	2:D4:30:ILE:O	2.10	0.52
1:A2:174:PRO:HG3	1:A2:185:PRO:HD3	1.92	0.52
1:A4:174:PRO:HG3	1:A4:185:PRO:HD3	1.92	0.52
1:A7:175:TRP:CE2	2:C7:136:TYR:CE2	2.98	0.52
1:B5:170:VAL:CG1	2:D5:144:ASN:ND2	2.72	0.52
1:B6:171:TRP:HB3	2:D6:204:GLU:OE1	2.08	0.52
2:C5:64:GLY:N	3:E5:180:MET:HA	2.25	0.52
2:C6:64:GLY:N	3:E6:180:MET:HA	2.25	0.52
2:C11:74:ARG:HH11	2:D10:58:THR:HG21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C12:74:ARG:HH11	2:D11:58:THR:HG21	1.73	0.52
2:D7:168:LEU:HD21	2:D7:174:VAL:HG23	1.73	0.52
1:A2:175:TRP:CE2	2:C2:136:TYR:CE2	2.98	0.52
1:A3:175:TRP:CE2	2:C3:136:TYR:CE2	2.98	0.52
1:A6:201:ALA:O	2:C5:208:TRP:HZ3	1.93	0.52
1:A8:175:TRP:CE2	2:C8:136:TYR:CE2	2.98	0.52
1:A11:201:ALA:O	2:C10:208:TRP:HZ3	1.93	0.52
2:C2:64:GLY:N	3:E2:180:MET:HA	2.25	0.52
1:A1:201:ALA:O	2:C13:208:TRP:HZ3	1.93	0.52
1:A3:201:ALA:O	2:C2:208:TRP:HZ3	1.92	0.52
2:C1:64:GLY:N	3:E1:180:MET:HA	2.25	0.52
2:D7:30:ILE:HG13	2:D7:30:ILE:O	2.10	0.52
1:B7:171:TRP:HB3	2:D7:204:GLU:OE1	2.08	0.52
2:C10:64:GLY:N	3:E10:180:MET:HA	2.25	0.52
2:C12:64:GLY:N	3:E12:180:MET:HA	2.24	0.52
1:A1:175:TRP:CE2	2:C1:136:TYR:CE2	2.98	0.52
1:A6:174:PRO:HG3	1:A6:185:PRO:HD3	1.92	0.52
1:A6:175:TRP:CE2	2:C6:136:TYR:CE2	2.98	0.52
1:A7:201:ALA:O	2:C6:208:TRP:HZ3	1.92	0.52
1:A12:201:ALA:O	2:C11:208:TRP:HZ3	1.93	0.52
1:A13:201:ALA:O	2:C12:208:TRP:HZ3	1.92	0.52
1:B4:171:TRP:HB3	2:D4:204:GLU:OE1	2.08	0.52
1:B9:170:VAL:CG1	2:D9:144:ASN:ND2	2.72	0.52
1:B13:170:VAL:CG1	2:D13:144:ASN:ND2	2.72	0.52
2:C3:32:LEU:HB3	2:C3:36:GLY:HA3	1.91	0.52
2:C13:32:LEU:HB3	2:C13:36:GLY:HA3	1.91	0.52
1:A9:175:TRP:CE2	2:C9:136:TYR:CE2	2.98	0.52
1:A13:174:PRO:HG3	1:A13:185:PRO:HD3	1.92	0.52
2:C4:32:LEU:HB3	2:C4:36:GLY:HA3	1.91	0.52
2:C9:64:GLY:N	3:E9:180:MET:HA	2.25	0.52
1:A4:175:TRP:CE2	2:C4:136:TYR:CE2	2.98	0.51
1:A9:201:ALA:O	2:C8:208:TRP:HZ3	1.92	0.51
1:B7:170:VAL:CG1	2:D7:144:ASN:ND2	2.72	0.51
2:C8:32:LEU:HB3	2:C8:36:GLY:HA3	1.91	0.51
2:C11:32:LEU:HB3	2:C11:36:GLY:HA3	1.91	0.51
2:C11:64:GLY:N	3:E11:180:MET:HA	2.25	0.51
1:B3:170:VAL:CG1	2:D3:144:ASN:ND2	2.72	0.51
1:B3:171:TRP:HB3	2:D3:204:GLU:OE1	2.08	0.51
1:B5:171:TRP:HB3	2:D5:204:GLU:OE1	2.08	0.51
2:C4:64:GLY:N	3:E4:180:MET:HA	2.25	0.51
2:C5:74:ARG:HH11	2:D4:58:THR:HG21	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D2:60:ILE:HG22	3:F2:185:PHE:CE2	2.43	0.51
2:D3:30:ILE:HG13	2:D3:30:ILE:O	2.10	0.51
1:A2:201:ALA:O	2:C1:208:TRP:HZ3	1.93	0.51
2:C7:64:GLY:N	3:E7:180:MET:HA	2.24	0.51
1:A4:155:PRO:CD	1:B2:157:THR:HG21	2.41	0.51
1:A4:167:ILE:HG21	1:B3:197:TRP:CH2	2.46	0.51
1:A5:155:PRO:CD	1:B3:157:THR:HG21	2.41	0.51
1:A5:167:ILE:HG21	1:B4:197:TRP:CH2	2.46	0.51
1:A8:167:ILE:HG21	1:B7:197:TRP:CH2	2.46	0.51
1:A11:167:ILE:HG21	1:B10:197:TRP:CH2	2.46	0.51
1:A11:167:ILE:O	2:C11:220:ASN:ND2	2.38	0.51
1:A13:175:TRP:CE2	2:C13:136:TYR:CE2	2.98	0.51
1:B6:170:VAL:CG1	2:D6:144:ASN:ND2	2.72	0.51
1:B10:170:VAL:CG1	2:D10:144:ASN:ND2	2.72	0.51
2:C8:64:GLY:N	3:E8:180:MET:HA	2.25	0.51
2:C10:32:LEU:HB3	2:C10:36:GLY:HA3	1.91	0.51
2:D8:30:ILE:HG13	2:D8:30:ILE:O	2.10	0.51
2:D12:30:ILE:HG13	2:D12:30:ILE:O	2.10	0.51
1:A1:167:ILE:CG2	1:B13:197:TRP:HH2	2.21	0.51
1:A3:167:ILE:HG21	1:B2:197:TRP:CH2	2.46	0.51
1:A4:155:PRO:CG	1:B2:157:THR:CG2	2.88	0.51
1:A5:155:PRO:CG	1:B3:157:THR:CG2	2.88	0.51
1:A7:167:ILE:HG21	1:B6:197:TRP:CH2	2.46	0.51
1:A10:175:TRP:CE2	2:C10:136:TYR:CE2	2.98	0.51
2:C9:32:LEU:HB3	2:C9:36:GLY:HA3	1.91	0.51
2:C12:32:LEU:HB3	2:C12:36:GLY:HA3	1.91	0.51
1:A3:155:PRO:CD	1:B1:157:THR:HG21	2.41	0.51
1:A11:155:PRO:CG	1:B9:157:THR:CG2	2.88	0.51
1:A12:155:PRO:CG	1:B10:157:THR:CG2	2.88	0.51
2:C2:61:THR:HG21	3:E2:180:MET:SD	2.51	0.51
2:C6:61:THR:HG21	3:E6:180:MET:SD	2.51	0.51
2:D1:30:ILE:HG13	2:D1:30:ILE:O	2.10	0.51
1:A5:175:TRP:CE2	2:C5:136:TYR:CE2	2.98	0.51
1:A6:155:PRO:CG	1:B4:157:THR:CG2	2.88	0.51
1:A6:167:ILE:HG21	1:B5:197:TRP:CH2	2.46	0.51
1:A8:174:PRO:HG3	1:A8:185:PRO:HD3	1.92	0.51
1:A8:201:ALA:O	2:C7:208:TRP:HZ3	1.93	0.51
1:A11:174:PRO:HG3	1:A11:185:PRO:HD3	1.92	0.51
1:A11:175:TRP:CE2	2:C11:136:TYR:CE2	2.98	0.51
1:A12:175:TRP:CE2	2:C12:136:TYR:CE2	2.98	0.51
1:A13:155:PRO:CG	1:B11:157:THR:CG2	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C13:61:THR:HG21	3:E13:180:MET:SD	2.51	0.51
2:D11:30:ILE:HG13	2:D11:30:ILE:O	2.10	0.51
1:A2:155:PRO:CD	1:B13:157:THR:HG21	2.41	0.51
1:A6:155:PRO:CD	1:B4:157:THR:HG21	2.41	0.51
1:A9:167:ILE:HG21	1:B8:197:TRP:CH2	2.46	0.51
1:A10:155:PRO:CG	1:B8:157:THR:CG2	2.88	0.51
2:D2:30:ILE:HG13	2:D2:30:ILE:O	2.10	0.51
2:D3:215:VAL:HG13	2:D3:232:VAL:HG21	1.93	0.51
2:D5:215:VAL:HG13	2:D5:232:VAL:HG21	1.93	0.51
2:D10:30:ILE:HG13	2:D10:30:ILE:O	2.10	0.51
1:A1:155:PRO:CD	1:B12:157:THR:HG21	2.41	0.51
1:A1:174:PRO:HG3	1:A1:185:PRO:HD3	1.92	0.51
1:A2:167:ILE:HG21	1:B1:197:TRP:CH2	2.46	0.51
1:A7:155:PRO:CG	1:B5:157:THR:CG2	2.88	0.51
1:A10:201:ALA:O	2:C9:208:TRP:HZ3	1.93	0.51
1:A12:167:ILE:HG21	1:B11:197:TRP:CH2	2.46	0.51
2:C3:61:THR:HG21	3:E3:180:MET:SD	2.51	0.51
2:C7:61:THR:HG21	3:E7:180:MET:SD	2.51	0.51
2:C8:61:THR:HG21	3:E8:180:MET:SD	2.51	0.51
2:C12:61:THR:HG21	3:E12:180:MET:SD	2.51	0.51
2:D7:215:VAL:HG13	2:D7:232:VAL:HG21	1.93	0.51
2:D13:30:ILE:HG13	2:D13:30:ILE:O	2.10	0.51
1:A3:155:PRO:CG	1:B1:157:THR:CG2	2.88	0.51
1:A7:155:PRO:CD	1:B5:157:THR:HG21	2.41	0.51
1:A8:155:PRO:CG	1:B6:157:THR:CG2	2.88	0.51
1:A9:155:PRO:CG	1:B7:157:THR:CG2	2.88	0.51
2:C9:61:THR:HG21	3:E9:180:MET:SD	2.51	0.51
2:D3:60:ILE:HG22	3:F3:185:PHE:CE2	2.43	0.51
2:D8:159:VAL:CG1	2:D8:160:LYS:N	2.44	0.51
1:A1:155:PRO:CG	1:B12:157:THR:CG2	2.88	0.50
1:A3:174:PRO:HG3	1:A3:185:PRO:HD3	1.92	0.50
1:A9:155:PRO:CD	1:B7:157:THR:HG21	2.41	0.50
1:A10:155:PRO:CD	1:B8:157:THR:HG21	2.41	0.50
1:A13:155:PRO:CD	1:B11:157:THR:HG21	2.41	0.50
2:C10:74:ARG:HH11	2:D9:58:THR:HG21	1.73	0.50
2:D4:215:VAL:HG13	2:D4:232:VAL:HG21	1.93	0.50
2:D6:215:VAL:HG13	2:D6:232:VAL:HG21	1.93	0.50
2:D7:44:ASN:OD1	2:D7:44:ASN:N	2.44	0.50
1:A10:167:ILE:HG21	1:B9:197:TRP:CH2	2.46	0.50
1:B8:170:VAL:CG1	2:D8:144:ASN:ND2	2.72	0.50
2:C1:61:THR:HG21	3:E1:180:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C5:61:THR:HG21	3:E5:180:MET:SD	2.51	0.50
2:D2:215:VAL:HG13	2:D2:232:VAL:HG21	1.93	0.50
2:D9:30:ILE:HG13	2:D9:30:ILE:O	2.10	0.50
1:A1:167:ILE:HG21	1:B13:197:TRP:CH2	2.46	0.50
2:D1:215:VAL:HG13	2:D1:232:VAL:HG21	1.93	0.50
1:A5:174:PRO:HG3	1:A5:185:PRO:HD3	1.92	0.50
1:A6:167:ILE:O	2:C6:220:ASN:ND2	2.38	0.50
1:A7:188:VAL:HG11	2:C7:141:ILE:HD11	1.93	0.50
1:A8:167:ILE:O	2:C8:220:ASN:ND2	2.38	0.50
1:A8:188:VAL:HG11	2:C8:141:ILE:HD11	1.93	0.50
2:C11:61:THR:HG21	3:E11:180:MET:SD	2.51	0.50
2:D13:168:LEU:HD21	2:D13:174:VAL:HG23	1.73	0.50
1:A2:155:PRO:CG	1:B13:157:THR:CG2	2.88	0.50
1:A6:188:VAL:HG11	2:C6:141:ILE:HD11	1.93	0.50
1:A9:174:PRO:HG3	1:A9:185:PRO:HD3	1.92	0.50
1:A9:188:VAL:HG11	2:C9:141:ILE:HD11	1.93	0.50
1:A10:188:VAL:HG11	2:C10:141:ILE:HD11	1.93	0.50
2:C6:194:ASN:CG	2:C6:224:LEU:HD23	2.37	0.50
2:C10:61:THR:HG21	3:E10:180:MET:SD	2.51	0.50
1:A11:155:PRO:CD	1:B9:157:THR:HG21	2.41	0.50
1:A13:167:ILE:HG21	1:B12:197:TRP:CH2	2.46	0.50
2:C4:74:ARG:HH11	2:D3:58:THR:HG21	1.73	0.50
2:C7:194:ASN:CG	2:C7:224:LEU:HD23	2.37	0.50
2:D8:215:VAL:HG13	2:D8:232:VAL:HG21	1.93	0.50
1:A12:155:PRO:CD	1:B10:157:THR:HG21	2.41	0.50
2:C4:61:THR:HG21	3:E4:180:MET:SD	2.51	0.50
2:C5:194:ASN:CG	2:C5:224:LEU:HD23	2.37	0.50
2:C8:194:ASN:CG	2:C8:224:LEU:HD23	2.37	0.50
2:C13:74:ARG:HH11	2:D12:58:THR:HG21	1.73	0.50
2:C2:74:ARG:HH11	2:D1:58:THR:HG21	1.73	0.50
2:D9:215:VAL:HG13	2:D9:232:VAL:HG21	1.93	0.50
2:D13:215:VAL:HG13	2:D13:232:VAL:HG21	1.93	0.50
1:A8:155:PRO:CD	1:B6:157:THR:HG21	2.41	0.50
2:C4:194:ASN:CG	2:C4:224:LEU:HD23	2.37	0.50
1:A10:174:PRO:HG3	1:A10:185:PRO:HD3	1.92	0.49
2:C9:89:THR:HG22	2:C9:103:VAL:HG22	1.94	0.49
2:C10:89:THR:HG22	2:C10:103:VAL:HG22	1.94	0.49
1:A7:174:PRO:HG3	1:A7:185:PRO:HD3	1.92	0.49
2:C1:74:ARG:HH11	2:D13:58:THR:HG21	1.73	0.49
2:C8:89:THR:HG22	2:C8:103:VAL:HG22	1.94	0.49
2:C9:194:ASN:CG	2:C9:224:LEU:HD23	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:98:VAL:CB	2:D2:208:TRP:CD1	2.95	0.49
1:A1:188:VAL:HG11	2:C1:141:ILE:HD11	1.93	0.49
1:A3:192:VAL:HG11	2:C3:148:LEU:HD23	1.86	0.49
1:A12:174:PRO:HG3	1:A12:185:PRO:HD3	1.92	0.49
2:D10:215:VAL:HG13	2:D10:232:VAL:HG21	1.93	0.49
1:A4:167:ILE:O	2:C4:220:ASN:ND2	2.38	0.49
1:A13:188:VAL:HG11	2:C13:141:ILE:HD11	1.93	0.49
2:C1:194:ASN:CG	2:C1:224:LEU:HD23	2.37	0.49
2:C2:194:ASN:CG	2:C2:224:LEU:HD23	2.37	0.49
2:C3:194:ASN:CG	2:C3:224:LEU:HD23	2.37	0.49
2:D11:215:VAL:HG13	2:D11:232:VAL:HG21	1.93	0.49
2:C6:74:ARG:HH11	2:D5:58:THR:HG21	1.73	0.49
2:C7:89:THR:HG22	2:C7:103:VAL:HG22	1.94	0.49
2:C11:89:THR:HG22	2:C11:103:VAL:HG22	1.94	0.49
2:D3:159:VAL:CG1	2:D3:160:LYS:N	2.44	0.49
2:D8:60:ILE:HG22	3:F8:185:PHE:CE2	2.43	0.49
2:D12:215:VAL:HG13	2:D12:232:VAL:HG21	1.93	0.49
2:C13:194:ASN:CG	2:C13:224:LEU:HD23	2.37	0.49
2:D11:60:ILE:HG22	3:F11:185:PHE:CE2	2.43	0.48
1:A2:188:VAL:HG11	2:C2:141:ILE:HD11	1.93	0.48
1:A5:167:ILE:CD1	1:B4:161:GLN:HA	2.44	0.48
2:D12:60:ILE:HG22	3:F12:185:PHE:CE2	2.43	0.48
1:A10:167:ILE:CD1	1:B9:161:GLN:HA	2.44	0.48
2:C6:89:THR:HG22	2:C6:103:VAL:HG22	1.94	0.48
1:A2:167:ILE:CD1	1:B1:161:GLN:HA	2.44	0.48
1:A4:167:ILE:CD1	1:B3:161:GLN:HA	2.44	0.48
1:A11:167:ILE:CD1	1:B10:161:GLN:HA	2.44	0.48
1:A13:167:ILE:CD1	1:B12:161:GLN:HA	2.44	0.48
2:C2:50:ILE:HG12	2:C2:114:TYR:HB2	1.96	0.48
2:C3:89:THR:HG22	2:C3:103:VAL:HG22	1.94	0.48
2:C12:194:ASN:CG	2:C12:224:LEU:HD23	2.37	0.48
2:D6:44:ASN:OD1	2:D6:44:ASN:N	2.44	0.48
2:D9:60:ILE:HG22	3:F9:185:PHE:CE2	2.43	0.48
2:D10:60:ILE:HG22	3:F10:185:PHE:CE2	2.43	0.48
1:A6:167:ILE:CD1	1:B5:161:GLN:HA	2.44	0.48
1:A12:188:VAL:HG11	2:C12:141:ILE:HD11	1.93	0.48
2:C1:50:ILE:HG12	2:C1:114:TYR:HB2	1.96	0.48
2:C4:89:THR:HG22	2:C4:103:VAL:HG22	1.94	0.48
2:C12:89:THR:HG22	2:C12:103:VAL:HG22	1.94	0.48
2:D8:168:LEU:CD2	2:D8:174:VAL:HG21	2.40	0.48
2:D8:200:VAL:HG12	2:D8:224:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D13:159:VAL:CG1	2:D13:160:LYS:N	2.44	0.48
1:A11:152:CYS:SG	1:B9:150:VAL:HA	2.54	0.48
2:C2:89:THR:HG22	2:C2:103:VAL:HG22	1.94	0.48
2:C3:50:ILE:HG12	2:C3:114:TYR:HB2	1.96	0.48
2:C7:93:GLU:OE2	2:D7:71:ARG:NH2	2.47	0.48
2:C8:93:GLU:OE2	2:D8:71:ARG:NH2	2.47	0.48
2:C10:93:GLU:OE2	2:D10:71:ARG:NH2	2.47	0.48
2:C10:194:ASN:CG	2:C10:224:LEU:HD23	2.37	0.48
2:C11:194:ASN:CG	2:C11:224:LEU:HD23	2.37	0.48
2:D3:215:VAL:HG13	2:D3:232:VAL:CG2	2.44	0.48
1:A9:167:ILE:CD1	1:B8:161:GLN:HA	2.44	0.48
1:A12:167:ILE:CD1	1:B11:161:GLN:HA	2.44	0.48
2:C11:93:GLU:OE2	2:D11:71:ARG:NH2	2.47	0.48
2:C13:93:GLU:OE2	2:D13:71:ARG:NH2	2.47	0.48
2:D1:200:VAL:HG12	2:D1:224:LEU:O	2.14	0.48
2:D8:44:ASN:OD1	2:D8:44:ASN:N	2.44	0.48
2:D9:200:VAL:HG12	2:D9:224:LEU:O	2.14	0.48
2:D9:215:VAL:HG13	2:D9:232:VAL:CG2	2.44	0.48
1:A3:167:ILE:CD1	1:B2:161:GLN:HA	2.44	0.48
1:A12:152:CYS:SG	1:B10:150:VAL:HA	2.54	0.48
1:B7:98:VAL:CB	2:D8:208:TRP:CD1	2.95	0.48
2:D7:200:VAL:HG12	2:D7:224:LEU:O	2.14	0.48
2:D8:215:VAL:HG13	2:D8:232:VAL:CG2	2.44	0.48
2:D11:159:VAL:CG1	2:D11:160:LYS:N	2.44	0.48
2:D11:200:VAL:HG12	2:D11:224:LEU:O	2.14	0.48
2:D13:200:VAL:HG12	2:D13:224:LEU:O	2.14	0.48
1:A4:188:VAL:HG11	2:C4:141:ILE:HD11	1.93	0.48
2:C1:89:THR:HG22	2:C1:103:VAL:HG22	1.94	0.48
2:C9:74:ARG:HH11	2:D8:58:THR:HG21	1.73	0.48
2:D5:215:VAL:HG13	2:D5:232:VAL:CG2	2.44	0.48
2:D6:215:VAL:HG13	2:D6:232:VAL:CG2	2.44	0.48
2:D12:215:VAL:HG13	2:D12:232:VAL:CG2	2.44	0.48
2:D13:60:ILE:HG22	3:F13:185:PHE:CE2	2.43	0.48
2:D13:215:VAL:HG13	2:D13:232:VAL:CG2	2.44	0.48
1:A3:188:VAL:HG11	2:C3:141:ILE:HD11	1.93	0.48
2:C5:89:THR:HG22	2:C5:103:VAL:HG22	1.94	0.48
2:C5:93:GLU:OE2	2:D5:71:ARG:NH2	2.47	0.48
2:C13:50:ILE:HG12	2:C13:114:TYR:HB2	1.96	0.48
2:D2:200:VAL:HG12	2:D2:224:LEU:O	2.14	0.48
2:D5:200:VAL:HG12	2:D5:224:LEU:O	2.14	0.48
2:C9:50:ILE:HG12	2:C9:114:TYR:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C10:50:ILE:HG12	2:C10:114:TYR:HB2	1.96	0.47
2:D9:168:LEU:CD2	2:D9:174:VAL:HG21	2.40	0.47
2:D12:32:LEU:HD22	2:D12:38:PHE:HB2	1.96	0.47
1:A1:152:CYS:SG	1:B12:150:VAL:HA	2.54	0.47
1:A4:152:CYS:SG	1:B2:150:VAL:HA	2.54	0.47
1:A7:167:ILE:CD1	1:B6:161:GLN:HA	2.44	0.47
1:A10:152:CYS:SG	1:B8:150:VAL:HA	2.54	0.47
1:A13:152:CYS:SG	1:B11:150:VAL:HA	2.54	0.47
2:C8:50:ILE:HG12	2:C8:114:TYR:HB2	1.96	0.47
2:D1:32:LEU:HD22	2:D1:38:PHE:HB2	1.96	0.47
2:D1:60:ILE:HG22	3:F1:185:PHE:CE2	2.43	0.47
2:D2:32:LEU:HD22	2:D2:38:PHE:HB2	1.96	0.47
2:D2:215:VAL:HG13	2:D2:232:VAL:CG2	2.44	0.47
2:D10:200:VAL:HG12	2:D10:224:LEU:O	2.14	0.47
2:D12:200:VAL:HG12	2:D12:224:LEU:O	2.14	0.47
1:B13:98:VAL:CB	2:D1:208:TRP:CD1	2.95	0.47
2:C4:230:MET:HB3	2:C4:230:MET:HE2	1.59	0.47
2:C7:50:ILE:HG12	2:C7:114:TYR:HB2	1.96	0.47
2:D3:200:VAL:HG12	2:D3:224:LEU:O	2.14	0.47
1:A1:167:ILE:CD1	1:B13:161:GLN:HA	2.44	0.47
1:A8:152:CYS:SG	1:B6:150:VAL:HA	2.54	0.47
2:C1:93:GLU:OE2	2:D1:71:ARG:NH2	2.47	0.47
2:C3:93:GLU:OE2	2:D3:71:ARG:NH2	2.47	0.47
2:C13:89:THR:HG22	2:C13:103:VAL:HG22	1.94	0.47
2:D1:215:VAL:HG13	2:D1:232:VAL:CG2	2.44	0.47
2:D6:200:VAL:HG12	2:D6:224:LEU:O	2.14	0.47
1:B6:98:VAL:CB	2:D7:208:TRP:CD1	2.95	0.47
2:C2:93:GLU:OE2	2:D2:71:ARG:NH2	2.47	0.47
2:C4:50:ILE:HG12	2:C4:114:TYR:HB2	1.96	0.47
2:C6:50:ILE:HG12	2:C6:114:TYR:HB2	1.96	0.47
2:C11:50:ILE:HG12	2:C11:114:TYR:HB2	1.96	0.47
2:C12:93:GLU:OE2	2:D12:71:ARG:NH2	2.47	0.47
2:D7:215:VAL:HG13	2:D7:232:VAL:CG2	2.44	0.47
2:D10:215:VAL:HG13	2:D10:232:VAL:CG2	2.44	0.47
2:D11:168:LEU:CD2	2:D11:174:VAL:HG21	2.40	0.47
1:A6:152:CYS:SG	1:B4:150:VAL:HA	2.54	0.47
1:A9:152:CYS:SG	1:B7:150:VAL:HA	2.54	0.47
1:B8:98:VAL:CB	2:D9:208:TRP:CD1	2.95	0.47
2:C9:93:GLU:OE2	2:D9:71:ARG:NH2	2.47	0.47
2:D11:215:VAL:HG13	2:D11:232:VAL:CG2	2.44	0.47
1:A5:152:CYS:SG	1:B3:150:VAL:HA	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:188:VAL:HG11	2:C5:141:ILE:HD11	1.93	0.47
1:A8:167:ILE:CD1	1:B7:161:GLN:HA	2.44	0.47
1:B2:98:VAL:CB	2:D3:208:TRP:CD1	2.95	0.47
2:C6:93:GLU:OE2	2:D6:71:ARG:NH2	2.47	0.47
2:D4:32:LEU:HD22	2:D4:38:PHE:HB2	1.96	0.47
2:D4:215:VAL:HG13	2:D4:232:VAL:CG2	2.44	0.47
1:A3:152:CYS:SG	1:B1:150:VAL:HA	2.54	0.47
1:A7:152:CYS:SG	1:B5:150:VAL:HA	2.54	0.47
2:C1:140:LEU:HD22	2:C1:235:ILE:HD11	1.97	0.47
2:C4:93:GLU:OE2	2:D4:71:ARG:NH2	2.47	0.47
2:C5:50:ILE:HG12	2:C5:114:TYR:HB2	1.96	0.47
2:C12:50:ILE:HG12	2:C12:114:TYR:HB2	1.96	0.47
2:D4:200:VAL:HG12	2:D4:224:LEU:O	2.14	0.47
1:A9:167:ILE:CG2	1:B8:197:TRP:HH2	2.21	0.47
1:A11:188:VAL:HG11	2:C11:141:ILE:HD11	1.93	0.47
2:C3:74:ARG:HH11	2:D2:58:THR:HG21	1.73	0.47
2:D13:32:LEU:HD22	2:D13:38:PHE:HB2	1.96	0.47
1:A2:152:CYS:SG	1:B13:150:VAL:HA	2.54	0.47
2:C2:140:LEU:HD22	2:C2:235:ILE:HD11	1.97	0.47
2:C4:140:LEU:HD22	2:C4:235:ILE:HD11	1.97	0.47
2:C13:140:LEU:HD22	2:C13:235:ILE:HD11	1.97	0.47
2:D8:32:LEU:HD22	2:D8:38:PHE:HB2	1.96	0.47
2:D11:32:LEU:HD22	2:D11:38:PHE:HB2	1.96	0.47
2:C5:140:LEU:HD22	2:C5:235:ILE:HD11	1.97	0.46
2:D7:32:LEU:HD22	2:D7:38:PHE:HB2	1.96	0.46
1:A6:188:VAL:HB	2:C6:141:ILE:HD11	1.97	0.46
1:A7:188:VAL:HB	2:C7:141:ILE:HD11	1.97	0.46
1:B9:98:VAL:CB	2:D10:208:TRP:CD1	2.95	0.46
2:C3:140:LEU:HD22	2:C3:235:ILE:HD11	1.97	0.46
2:C9:230:MET:HE2	2:C9:230:MET:HB3	1.59	0.46
2:C11:140:LEU:HD22	2:C11:235:ILE:HD11	1.97	0.46
2:C12:140:LEU:HD22	2:C12:235:ILE:HD11	1.97	0.46
2:D12:168:LEU:CD2	2:D12:174:VAL:HG21	2.40	0.46
2:C6:140:LEU:HD22	2:C6:235:ILE:HD11	1.97	0.46
2:C10:140:LEU:HD22	2:C10:235:ILE:HD11	1.97	0.46
2:D1:48:ASN:OD1	2:D1:111:GLY:HA2	2.16	0.46
2:D5:32:LEU:HD22	2:D5:38:PHE:HB2	1.96	0.46
2:D6:32:LEU:HD22	2:D6:38:PHE:HB2	1.96	0.46
2:D9:32:LEU:HD22	2:D9:38:PHE:HB2	1.96	0.46
1:A4:188:VAL:HB	2:C4:141:ILE:HD11	1.97	0.46
1:A12:188:VAL:HB	2:C12:141:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:98:VAL:CB	2:D6:208:TRP:CD1	2.95	0.46
1:B10:98:VAL:CB	2:D11:208:TRP:CD1	2.95	0.46
2:C9:140:LEU:HD22	2:C9:235:ILE:HD11	1.97	0.46
2:D10:32:LEU:HD22	2:D10:38:PHE:HB2	1.96	0.46
1:A5:188:VAL:HB	2:C5:141:ILE:HD11	1.97	0.46
2:D2:48:ASN:OD1	2:D2:111:GLY:HA2	2.16	0.46
2:D3:32:LEU:HD22	2:D3:38:PHE:HB2	1.96	0.46
2:D13:48:ASN:OD1	2:D13:111:GLY:HA2	2.16	0.46
2:C1:60:ILE:CG2	3:E1:185:PHE:HE2	2.25	0.46
2:C3:136:TYR:CE1	2:C3:213:ARG:HD3	2.50	0.46
2:C7:140:LEU:HD22	2:C7:235:ILE:HD11	1.97	0.46
2:C8:140:LEU:HD22	2:C8:235:ILE:HD11	1.97	0.46
2:C13:230:MET:HE2	2:C13:230:MET:HB3	1.59	0.46
1:A4:175:TRP:CE2	2:C4:136:TYR:HE2	2.34	0.46
1:A5:175:TRP:CE2	2:C5:136:TYR:HE2	2.34	0.46
1:A8:188:VAL:HB	2:C8:141:ILE:HD11	1.97	0.46
1:A9:172:ILE:CD1	2:C9:140:LEU:HD12	2.35	0.46
1:A11:188:VAL:HB	2:C11:141:ILE:HD11	1.97	0.46
1:B4:98:VAL:CB	2:D5:208:TRP:CD1	2.95	0.46
2:C2:70:LYS:HE2	3:E2:183:GLN:HB2	1.98	0.46
2:C7:110:GLU:OE1	2:C7:110:GLU:N	2.44	0.46
2:C13:136:TYR:CE1	2:C13:213:ARG:HD3	2.50	0.46
1:A3:188:VAL:HB	2:C3:141:ILE:HD11	1.97	0.46
1:A13:188:VAL:HB	2:C13:141:ILE:HD11	1.97	0.46
1:B13:91:THR:HG1	2:D1:213:ARG:HH22	1.62	0.46
2:C3:70:LYS:HE2	3:E3:183:GLN:HB2	1.98	0.46
2:D1:71:ARG:CD	3:E1:182:SER:OG	2.64	0.46
2:D2:52:ILE:HD12	2:D2:57:VAL:HG22	1.98	0.46
2:D3:48:ASN:OD1	2:D3:111:GLY:HA2	2.16	0.46
2:D3:52:ILE:HD12	2:D3:57:VAL:HG22	1.98	0.46
2:D10:52:ILE:HD12	2:D10:57:VAL:HG22	1.98	0.46
1:A3:175:TRP:CE2	2:C3:136:TYR:HE2	2.34	0.46
1:A7:175:TRP:CE2	2:C7:136:TYR:HE2	2.34	0.46
1:A11:167:ILE:CG2	1:B10:197:TRP:HH2	2.21	0.46
1:B8:178:SER:C	1:B8:180:ASN:H	2.24	0.46
1:B9:178:SER:C	1:B9:180:ASN:H	2.24	0.46
2:C1:136:TYR:CE1	2:C1:213:ARG:HD3	2.50	0.46
2:C1:159:VAL:O	2:C1:179:ALA:HB3	2.16	0.46
2:C2:159:VAL:O	2:C2:179:ALA:HB3	2.16	0.46
2:C3:159:VAL:O	2:C3:179:ALA:HB3	2.16	0.46
2:C5:110:GLU:OE1	2:C5:110:GLU:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C8:45:THR:HB	2:D7:86:ARG:HH22	1.81	0.46
2:C11:45:THR:HB	2:D10:86:ARG:HH22	1.81	0.46
2:C12:159:VAL:O	2:C12:179:ALA:HB3	2.16	0.46
2:C13:159:VAL:O	2:C13:179:ALA:HB3	2.16	0.46
2:D2:71:ARG:CD	3:E2:182:SER:OG	2.64	0.46
2:D4:88:PHE:CE2	2:D4:90:ILE:CG2	2.99	0.46
2:D9:52:ILE:HD12	2:D9:57:VAL:HG22	1.98	0.46
2:D9:71:ARG:CD	3:E9:182:SER:OG	2.64	0.46
2:D11:52:ILE:HD12	2:D11:57:VAL:HG22	1.98	0.46
2:D12:48:ASN:OD1	2:D12:111:GLY:HA2	2.16	0.46
1:B11:170:VAL:HG21	2:D11:144:ASN:HD22	1.82	0.45
1:B12:170:VAL:HG21	2:D12:144:ASN:HD22	1.82	0.45
2:C1:70:LYS:HE2	3:E1:183:GLN:HB2	1.98	0.45
2:C4:159:VAL:O	2:C4:179:ALA:HB3	2.16	0.45
2:C5:45:THR:HB	2:D4:86:ARG:HH22	1.81	0.45
2:C6:174:VAL:CG2	2:C6:190:TYR:HB3	2.46	0.45
2:C11:159:VAL:O	2:C11:179:ALA:HB3	2.16	0.45
2:C12:136:TYR:CE1	2:C12:213:ARG:HD3	2.50	0.45
2:D1:52:ILE:HD12	2:D1:57:VAL:HG22	1.98	0.45
2:D3:88:PHE:CE2	2:D3:90:ILE:CG2	2.99	0.45
2:D4:52:ILE:HD12	2:D4:57:VAL:HG22	1.98	0.45
2:D11:71:ARG:CD	3:E11:182:SER:OG	2.64	0.45
2:D13:52:ILE:HD12	2:D13:57:VAL:HG22	1.98	0.45
2:D13:71:ARG:CD	3:E13:182:SER:OG	2.64	0.45
1:A13:175:TRP:CE2	2:C13:136:TYR:HE2	2.34	0.45
2:C1:45:THR:HB	2:D13:86:ARG:HH22	1.81	0.45
2:C3:45:THR:HB	2:D2:86:ARG:HH22	1.81	0.45
2:C7:174:VAL:CG2	2:C7:190:TYR:HB3	2.47	0.45
2:C12:70:LYS:HE2	3:E12:183:GLN:HB2	1.98	0.45
2:C13:70:LYS:HE2	3:E13:183:GLN:HB2	1.98	0.45
2:D6:152:ILE:HD13	2:D6:152:ILE:HA	1.82	0.45
2:D7:71:ARG:CD	3:E7:182:SER:OG	2.64	0.45
2:D9:48:ASN:OD1	2:D9:111:GLY:HA2	2.16	0.45
2:D12:52:ILE:HD12	2:D12:57:VAL:HG22	1.98	0.45
2:D13:88:PHE:CE2	2:D13:90:ILE:CG2	2.99	0.45
1:A6:175:TRP:CE2	2:C6:136:TYR:HE2	2.34	0.45
1:A7:182:PHE:HB3	1:B7:189:SER:OG	2.17	0.45
2:C1:174:VAL:CG2	2:C1:190:TYR:HB3	2.46	0.45
2:C2:174:VAL:CG2	2:C2:190:TYR:HB3	2.46	0.45
2:C3:202:LEU:HD12	2:C3:202:LEU:C	2.42	0.45
2:C4:70:LYS:HE2	3:E4:183:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C5:174:VAL:CG2	2:C5:190:TYR:HB3	2.46	0.45
2:C8:174:VAL:CG2	2:C8:190:TYR:HB3	2.46	0.45
2:D3:71:ARG:CD	3:E3:182:SER:OG	2.64	0.45
2:D4:48:ASN:OD1	2:D4:111:GLY:HA2	2.16	0.45
2:D5:161:PRO:HB2	2:D5:176:PRO:HB3	1.99	0.45
2:D6:48:ASN:OD1	2:D6:111:GLY:HA2	2.16	0.45
2:D7:48:ASN:OD1	2:D7:111:GLY:HA2	2.16	0.45
2:D7:161:PRO:HB2	2:D7:176:PRO:HB3	1.99	0.45
2:D8:52:ILE:HD12	2:D8:57:VAL:HG22	1.98	0.45
2:D12:71:ARG:CD	3:E12:182:SER:OG	2.64	0.45
1:A2:188:VAL:HB	2:C2:141:ILE:HD11	1.97	0.45
1:A10:175:TRP:CE2	2:C10:136:TYR:HE2	2.34	0.45
1:B7:178:SER:C	1:B7:180:ASN:H	2.24	0.45
2:C5:159:VAL:O	2:C5:179:ALA:HB3	2.16	0.45
2:C6:45:THR:HB	2:D5:86:ARG:HH22	1.81	0.45
2:C13:45:THR:HB	2:D12:86:ARG:HH22	1.81	0.45
2:D1:88:PHE:CE2	2:D1:90:ILE:CG2	2.99	0.45
2:D8:48:ASN:OD1	2:D8:111:GLY:HA2	2.16	0.45
1:A2:182:PHE:HB3	1:B2:189:SER:OG	2.17	0.45
1:A3:182:PHE:HB3	1:B3:189:SER:OG	2.17	0.45
1:A6:182:PHE:HB3	1:B6:189:SER:OG	2.17	0.45
1:A9:188:VAL:HB	2:C9:141:ILE:HD11	1.97	0.45
1:A10:182:PHE:HB3	1:B10:189:SER:OG	2.17	0.45
1:A13:172:ILE:CD1	2:C13:140:LEU:HD12	2.35	0.45
2:C3:174:VAL:CG2	2:C3:190:TYR:HB3	2.46	0.45
2:C4:174:VAL:CG2	2:C4:190:TYR:HB3	2.46	0.45
2:C10:202:LEU:HD12	2:C10:202:LEU:C	2.42	0.45
2:C11:174:VAL:CG2	2:C11:190:TYR:HB3	2.46	0.45
2:C12:174:VAL:CG2	2:C12:190:TYR:HB3	2.46	0.45
2:C13:174:VAL:CG2	2:C13:190:TYR:HB3	2.46	0.45
2:D4:71:ARG:CD	3:E4:182:SER:OG	2.64	0.45
2:D5:52:ILE:HD12	2:D5:57:VAL:HG22	1.98	0.45
2:D5:71:ARG:CD	3:E5:182:SER:OG	2.64	0.45
2:D6:71:ARG:CD	3:E6:182:SER:OG	2.64	0.45
2:D6:161:PRO:HB2	2:D6:176:PRO:HB3	1.99	0.45
1:A8:182:PHE:HB3	1:B8:189:SER:OG	2.17	0.45
1:B1:178:SER:C	1:B1:180:ASN:H	2.24	0.45
1:B10:178:SER:C	1:B10:180:ASN:H	2.24	0.45
1:B13:170:VAL:HG21	2:D13:144:ASN:HD22	1.82	0.45
2:C2:202:LEU:HD12	2:C2:202:LEU:C	2.42	0.45
2:C3:60:ILE:CG2	3:E3:185:PHE:HE2	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D4:161:PRO:HB2	2:D4:176:PRO:HB3	1.99	0.45
2:D10:71:ARG:CD	3:E10:182:SER:OG	2.64	0.45
1:A12:182:PHE:HB3	1:B12:189:SER:OG	2.17	0.45
1:B10:170:VAL:HG21	2:D10:144:ASN:HD22	1.81	0.45
1:B11:98:VAL:CB	2:D12:208:TRP:CD1	2.95	0.45
1:B13:178:SER:C	1:B13:180:ASN:H	2.24	0.45
2:C7:159:VAL:O	2:C7:179:ALA:HB3	2.16	0.45
2:C7:202:LEU:HD12	2:C7:202:LEU:C	2.42	0.45
2:C10:159:VAL:O	2:C10:179:ALA:HB3	2.17	0.45
2:C11:70:LYS:HE2	3:E11:183:GLN:HB2	1.98	0.45
2:C11:117:MET:HE3	2:C11:117:MET:HB3	1.82	0.45
2:C11:136:TYR:CE1	2:C11:213:ARG:HD3	2.50	0.45
2:D2:88:PHE:CE2	2:D2:90:ILE:CG2	2.99	0.45
2:D4:168:LEU:CD2	2:D4:174:VAL:HG21	2.40	0.45
2:D5:48:ASN:OD1	2:D5:111:GLY:HA2	2.16	0.45
2:D5:88:PHE:CE2	2:D5:90:ILE:CG2	2.99	0.45
2:D5:168:LEU:CD2	2:D5:174:VAL:HG21	2.40	0.45
2:D7:52:ILE:HD12	2:D7:57:VAL:HG22	1.98	0.45
2:D8:161:PRO:HB2	2:D8:176:PRO:HB3	1.99	0.45
1:A13:182:PHE:HB3	1:B13:189:SER:OG	2.17	0.45
1:B10:188:VAL:HG13	2:D10:141:ILE:CD1	2.47	0.45
2:C2:136:TYR:CE1	2:C2:213:ARG:HD3	2.50	0.45
2:C5:70:LYS:HE2	3:E5:183:GLN:HB2	1.98	0.45
2:C9:202:LEU:HD12	2:C9:202:LEU:C	2.42	0.45
2:D6:52:ILE:HD12	2:D6:57:VAL:HG22	1.98	0.45
2:D6:88:PHE:CE2	2:D6:90:ILE:CG2	2.99	0.45
2:D7:172:PHE:HB3	2:D7:192:LEU:HD12	1.99	0.45
2:D8:58:THR:O	3:F8:185:PHE:HD2	2.00	0.45
2:D9:88:PHE:CE2	2:D9:90:ILE:CG2	2.99	0.45
2:D9:159:VAL:CG1	2:D9:160:LYS:N	2.44	0.45
2:D9:161:PRO:HB2	2:D9:176:PRO:HB3	1.99	0.45
2:D10:88:PHE:CE2	2:D10:90:ILE:CG2	2.99	0.45
2:D10:172:PHE:HB3	2:D10:192:LEU:HD12	1.99	0.45
1:A2:175:TRP:CE2	2:C2:136:TYR:HE2	2.34	0.45
2:C7:45:THR:HB	2:D6:86:ARG:HH22	1.81	0.45
2:C8:159:VAL:O	2:C8:179:ALA:HB3	2.16	0.45
2:C9:45:THR:HB	2:D8:86:ARG:HH22	1.81	0.45
2:C10:174:VAL:CG2	2:C10:190:TYR:HB3	2.46	0.45
2:C10:202:LEU:HD11	2:C10:217:PHE:CE2	2.51	0.45
2:D8:71:ARG:CD	3:E8:182:SER:OG	2.64	0.45
2:D9:58:THR:O	3:F9:185:PHE:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D9:172:PHE:HB3	2:D9:192:LEU:HD12	1.99	0.45
2:D11:48:ASN:OD1	2:D11:111:GLY:HA2	2.16	0.45
2:D13:168:LEU:CD2	2:D13:174:VAL:HG21	2.40	0.45
1:A9:182:PHE:HB3	1:B9:189:SER:OG	2.17	0.45
1:A11:182:PHE:HB3	1:B11:189:SER:OG	2.17	0.45
1:B2:178:SER:C	1:B2:180:ASN:H	2.24	0.45
1:B5:188:VAL:HG13	2:D5:141:ILE:CD1	2.46	0.45
2:C2:230:MET:HB3	2:C2:230:MET:HE2	1.59	0.45
2:C6:159:VAL:O	2:C6:179:ALA:HB3	2.16	0.45
2:C6:202:LEU:HD12	2:C6:202:LEU:C	2.42	0.45
2:C8:70:LYS:HE2	3:E8:183:GLN:HB2	1.98	0.45
2:C10:45:THR:HB	2:D9:86:ARG:HH22	1.82	0.45
2:C11:202:LEU:HD12	2:C11:202:LEU:C	2.42	0.45
2:D3:161:PRO:HB2	2:D3:176:PRO:HB3	1.99	0.45
2:D6:172:PHE:HB3	2:D6:192:LEU:HD12	1.99	0.45
2:D7:88:PHE:CE2	2:D7:90:ILE:CG2	2.99	0.45
2:D8:88:PHE:CE2	2:D8:90:ILE:CG2	2.99	0.45
2:D11:37:GLN:HE21	2:D11:37:GLN:HB3	1.59	0.45
2:D11:172:PHE:HB3	2:D11:192:LEU:HD12	1.99	0.45
1:A1:188:VAL:HB	2:C1:141:ILE:HD11	1.97	0.44
1:A10:188:VAL:HB	2:C10:141:ILE:HD11	1.97	0.44
1:B7:170:VAL:HG21	2:D7:144:ASN:HD22	1.82	0.44
2:C4:45:THR:HB	2:D3:86:ARG:HH22	1.81	0.44
2:C4:202:LEU:HD12	2:C4:202:LEU:C	2.42	0.44
2:C6:70:LYS:HE2	3:E6:183:GLN:HB2	1.98	0.44
2:C8:202:LEU:HD12	2:C8:202:LEU:C	2.42	0.44
2:C9:174:VAL:CG2	2:C9:190:TYR:HB3	2.46	0.44
2:C12:45:THR:HB	2:D11:86:ARG:HH22	1.81	0.44
2:C12:202:LEU:HD12	2:C12:202:LEU:C	2.42	0.44
2:D3:168:LEU:CD2	2:D3:174:VAL:HG21	2.40	0.44
2:D7:58:THR:O	3:F7:185:PHE:HD2	2.00	0.44
2:D8:172:PHE:HB3	2:D8:192:LEU:HD12	1.99	0.44
2:D9:37:GLN:HE22	2:D9:103:VAL:CG2	2.28	0.44
2:D11:88:PHE:CE2	2:D11:90:ILE:CG2	2.99	0.44
1:A4:182:PHE:HB3	1:B4:189:SER:OG	2.17	0.44
1:A8:175:TRP:CE2	2:C8:136:TYR:HE2	2.34	0.44
1:A11:175:TRP:CE2	2:C11:136:TYR:HE2	2.34	0.44
2:C6:230:MET:HB3	2:C6:230:MET:HE2	1.59	0.44
2:C13:202:LEU:HD12	2:C13:202:LEU:C	2.42	0.44
2:D5:172:PHE:HB3	2:D5:192:LEU:HD12	1.99	0.44
2:D10:161:PRO:HB2	2:D10:176:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D12:88:PHE:CE2	2:D12:90:ILE:CG2	2.99	0.44
1:A13:155:PRO:HG2	1:B11:157:THR:HG21	2.00	0.44
1:B3:170:VAL:HG21	2:D3:144:ASN:HD22	1.82	0.44
1:B4:170:VAL:HG21	2:D4:144:ASN:HD22	1.82	0.44
1:B5:170:VAL:HG21	2:D5:144:ASN:HD22	1.82	0.44
1:B6:170:VAL:HG21	2:D6:144:ASN:HD22	1.82	0.44
1:B6:178:SER:C	1:B6:180:ASN:H	2.24	0.44
2:C5:136:TYR:CE1	2:C5:213:ARG:HD3	2.50	0.44
2:C9:159:VAL:O	2:C9:179:ALA:HB3	2.16	0.44
2:D2:161:PRO:HB2	2:D2:176:PRO:HB3	1.99	0.44
2:D8:37:GLN:HE22	2:D8:103:VAL:CG2	2.28	0.44
2:D10:37:GLN:HE22	2:D10:103:VAL:CG2	2.28	0.44
2:D10:48:ASN:OD1	2:D10:111:GLY:HA2	2.16	0.44
2:D10:58:THR:O	3:F10:185:PHE:HD2	2.00	0.44
2:D12:172:PHE:HB3	2:D12:192:LEU:HD12	1.99	0.44
1:A1:182:PHE:HB3	1:B1:189:SER:OG	2.17	0.44
1:B4:178:SER:C	1:B4:180:ASN:H	2.24	0.44
1:B12:178:SER:C	1:B12:180:ASN:H	2.24	0.44
2:C3:110:GLU:OE1	2:C3:110:GLU:N	2.44	0.44
2:C10:55:ASP:OD2	2:C10:94:THR:OG1	2.33	0.44
2:C10:70:LYS:HE2	3:E10:183:GLN:HB2	1.98	0.44
2:D2:159:VAL:CG1	2:D2:160:LYS:N	2.44	0.44
2:D6:58:THR:O	3:F6:185:PHE:HD2	2.00	0.44
2:D12:58:THR:O	3:F12:185:PHE:HD2	2.00	0.44
1:B5:178:SER:C	1:B5:180:ASN:H	2.24	0.44
1:B8:170:VAL:HG21	2:D8:144:ASN:HD22	1.82	0.44
2:C2:45:THR:HB	2:D1:86:ARG:HH22	1.81	0.44
2:C7:70:LYS:HE2	3:E7:183:GLN:HB2	1.98	0.44
2:D10:71:ARG:HH21	2:D10:79:LEU:HD22	1.83	0.44
1:A10:172:ILE:CD1	2:C10:140:LEU:HD12	2.35	0.44
1:A12:175:TRP:CE2	2:C12:136:TYR:HE2	2.34	0.44
1:B1:170:VAL:HG21	2:D1:144:ASN:HD22	1.82	0.44
1:B11:188:VAL:HG13	2:D11:141:ILE:CD1	2.47	0.44
2:C1:202:LEU:HD12	2:C1:202:LEU:C	2.42	0.44
2:C6:202:LEU:HD11	2:C6:217:PHE:CE2	2.51	0.44
2:C9:70:LYS:HE2	3:E9:183:GLN:HB2	1.98	0.44
2:D2:71:ARG:HH21	2:D2:79:LEU:HD22	1.83	0.44
2:D2:168:LEU:CD2	2:D2:174:VAL:HG21	2.40	0.44
2:D4:71:ARG:HH21	2:D4:79:LEU:HD22	1.83	0.44
2:D5:44:ASN:OD1	2:D5:44:ASN:N	2.44	0.44
1:A1:175:TRP:CE2	2:C1:136:TYR:HE2	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:202:ARG:HA	1:A4:202:ARG:HD2	1.87	0.44
1:A5:182:PHE:HB3	1:B5:189:SER:OG	2.17	0.44
1:B2:170:VAL:HG21	2:D2:144:ASN:HD22	1.82	0.44
2:C5:202:LEU:HD12	2:C5:202:LEU:C	2.42	0.44
2:D4:172:PHE:HB3	2:D4:192:LEU:HD12	1.99	0.44
2:D11:161:PRO:HB2	2:D11:176:PRO:HB3	1.99	0.44
1:B3:178:SER:C	1:B3:180:ASN:H	2.24	0.44
1:B11:178:SER:C	1:B11:180:ASN:H	2.24	0.44
2:D7:71:ARG:HH21	2:D7:79:LEU:HD22	1.83	0.44
2:D11:37:GLN:HE22	2:D11:103:VAL:CG2	2.28	0.44
2:D13:172:PHE:HB3	2:D13:192:LEU:HD12	1.99	0.44
2:C11:60:ILE:CG2	3:E11:185:PHE:HE2	2.25	0.44
2:D4:159:VAL:CG1	2:D4:160:LYS:N	2.44	0.44
2:D5:71:ARG:HH21	2:D5:79:LEU:HD22	1.83	0.44
2:D5:159:VAL:CG1	2:D5:160:LYS:N	2.44	0.44
2:D7:37:GLN:HE22	2:D7:103:VAL:CG2	2.28	0.44
2:D13:58:THR:O	3:F13:185:PHE:HD2	2.00	0.44
1:B9:170:VAL:HG21	2:D9:144:ASN:HD22	1.82	0.43
2:C2:202:LEU:HD11	2:C2:217:PHE:CE2	2.51	0.43
2:D1:71:ARG:HH21	2:D1:79:LEU:HD22	1.83	0.43
2:D1:161:PRO:HB2	2:D1:176:PRO:HB3	1.99	0.43
2:D2:32:LEU:HD11	2:D2:100:PHE:HB3	2.01	0.43
2:D8:71:ARG:HH21	2:D8:79:LEU:HD22	1.83	0.43
2:D12:71:ARG:HH21	2:D12:79:LEU:HD22	1.83	0.43
1:A9:175:TRP:CE2	2:C9:136:TYR:HE2	2.34	0.43
1:B6:188:VAL:HG13	2:D6:141:ILE:CD1	2.47	0.43
1:B12:98:VAL:CB	2:D13:208:TRP:CD1	2.95	0.43
2:D1:172:PHE:HB3	2:D1:192:LEU:HD12	1.99	0.43
2:D2:172:PHE:HB3	2:D2:192:LEU:HD12	1.99	0.43
2:D3:172:PHE:HB3	2:D3:192:LEU:HD12	1.99	0.43
2:D7:152:ILE:HD13	2:D7:152:ILE:HA	1.82	0.43
2:D10:32:LEU:HD11	2:D10:100:PHE:HB3	2.00	0.43
2:D13:161:PRO:HB2	2:D13:176:PRO:HB3	1.99	0.43
2:C7:55:ASP:OD2	2:C7:94:THR:OG1	2.33	0.43
2:D1:32:LEU:HD11	2:D1:100:PHE:HB3	2.00	0.43
2:D1:200:VAL:HG22	2:D1:201:ALA:N	2.34	0.43
2:D3:58:THR:O	3:F3:185:PHE:HD2	2.00	0.43
2:D9:200:VAL:HG22	2:D9:201:ALA:N	2.34	0.43
2:D11:58:THR:O	3:F11:185:PHE:HD2	2.00	0.43
2:D11:200:VAL:HG22	2:D11:201:ALA:N	2.34	0.43
2:D13:71:ARG:HH21	2:D13:79:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:167:ILE:CG2	1:B6:197:TRP:HH2	2.21	0.43
2:D1:37:GLN:HE21	2:D1:37:GLN:HB3	1.58	0.43
2:D3:32:LEU:HD11	2:D3:100:PHE:HB3	2.01	0.43
2:D4:58:THR:O	3:F4:185:PHE:HD2	2.00	0.43
2:D4:200:VAL:HG22	2:D4:201:ALA:N	2.34	0.43
2:D12:161:PRO:HB2	2:D12:176:PRO:HB3	1.99	0.43
2:C1:117:MET:HE3	2:C1:117:MET:HB3	1.82	0.43
2:C11:89:THR:HG21	2:D11:111:GLY:H	1.84	0.43
2:D3:71:ARG:HH21	2:D3:79:LEU:HD22	1.83	0.43
2:D6:200:VAL:HG22	2:D6:201:ALA:N	2.34	0.43
2:D7:200:VAL:HG22	2:D7:201:ALA:N	2.34	0.43
2:D9:32:LEU:HD11	2:D9:100:PHE:HB3	2.01	0.43
1:A1:172:ILE:CD1	2:C1:140:LEU:HD12	2.35	0.43
2:D10:200:VAL:HG22	2:D10:201:ALA:N	2.34	0.43
2:D11:32:LEU:HD11	2:D11:100:PHE:HB3	2.00	0.43
2:D12:37:GLN:HE22	2:D12:103:VAL:CG2	2.28	0.43
2:D13:200:VAL:HG22	2:D13:201:ALA:N	2.34	0.43
1:A3:155:PRO:HG2	1:B1:157:THR:HG21	2.00	0.43
1:B4:188:VAL:CG1	2:D4:141:ILE:CD1	2.79	0.43
1:B12:188:VAL:HG13	2:D12:141:ILE:CD1	2.46	0.43
2:C8:60:ILE:CG2	3:E8:185:PHE:HE2	2.25	0.43
2:C10:230:MET:HE2	2:C10:230:MET:HB3	1.59	0.43
2:C12:55:ASP:OD2	2:C12:94:THR:OG1	2.33	0.43
2:C12:89:THR:HG21	2:D12:111:GLY:H	1.84	0.43
2:D3:200:VAL:HG22	2:D3:201:ALA:N	2.34	0.43
2:D8:32:LEU:HD11	2:D8:100:PHE:HB3	2.00	0.43
1:B7:188:VAL:CG1	2:D7:141:ILE:CD1	2.79	0.43
2:C2:117:MET:HE3	2:C2:117:MET:HB3	1.82	0.43
2:C7:89:THR:HG21	2:D7:111:GLY:H	1.84	0.43
2:C10:117:MET:HE3	2:C10:117:MET:HB3	1.82	0.43
2:D2:58:THR:O	3:F2:185:PHE:HD2	2.00	0.43
2:D2:200:VAL:HG22	2:D2:201:ALA:N	2.34	0.43
2:D9:71:ARG:HH21	2:D9:79:LEU:HD22	1.83	0.43
2:D11:71:ARG:HH21	2:D11:79:LEU:HD22	1.83	0.43
1:A1:155:PRO:HG2	1:B12:157:THR:HG21	2.00	0.43
1:A6:202:ARG:HD2	1:A6:202:ARG:HA	1.87	0.43
1:B3:188:VAL:CG1	2:D3:141:ILE:CD1	2.79	0.43
2:C4:89:THR:HG21	2:D4:111:GLY:H	1.84	0.43
2:C5:230:MET:HE2	2:C5:230:MET:HB3	1.59	0.43
2:C6:89:THR:HG21	2:D6:111:GLY:H	1.84	0.43
2:C8:89:THR:HG21	2:D8:111:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C11:202:LEU:HD11	2:C11:217:PHE:CE2	2.51	0.43
2:C13:117:MET:HE3	2:C13:117:MET:HB3	1.82	0.43
2:D1:58:THR:O	3:F1:185:PHE:HD2	2.00	0.43
2:D1:168:LEU:CD2	2:D1:174:VAL:HG21	2.40	0.43
2:D3:69:ASP:OD1	2:D3:70:LYS:N	2.52	0.43
2:D5:58:THR:O	3:F5:185:PHE:HD2	2.00	0.43
2:D5:69:ASP:OD1	2:D5:70:LYS:N	2.52	0.43
2:D8:200:VAL:HG22	2:D8:201:ALA:N	2.34	0.43
2:D13:32:LEU:HD11	2:D13:100:PHE:HB3	2.00	0.43
1:A5:202:ARG:HD2	1:A5:202:ARG:HA	1.87	0.43
1:A8:167:ILE:CG2	1:B7:197:TRP:HH2	2.21	0.43
2:C2:89:THR:HG21	2:D2:111:GLY:H	1.84	0.43
2:C3:89:THR:HG21	2:D3:111:GLY:H	1.84	0.43
2:C5:89:THR:HG21	2:D5:111:GLY:H	1.84	0.43
2:C9:89:THR:HG21	2:D9:111:GLY:H	1.84	0.43
2:D4:32:LEU:HD11	2:D4:100:PHE:HB3	2.01	0.43
2:D6:37:GLN:HE22	2:D6:103:VAL:CG2	2.28	0.43
2:D7:69:ASP:OD1	2:D7:70:LYS:N	2.52	0.43
1:A9:202:ARG:HA	1:A9:202:ARG:HD2	1.87	0.42
1:A10:167:ILE:CG2	1:B9:197:TRP:HH2	2.21	0.42
1:B9:91:THR:HG21	2:D10:213:ARG:HH12	1.83	0.42
2:C5:60:ILE:CG2	3:E5:185:PHE:HE2	2.25	0.42
2:C10:89:THR:HG21	2:D10:111:GLY:H	1.84	0.42
2:D1:69:ASP:OD1	2:D1:70:LYS:N	2.52	0.42
2:D4:69:ASP:OD1	2:D4:70:LYS:N	2.52	0.42
1:A7:188:VAL:CB	2:C7:141:ILE:HD11	2.50	0.42
1:B1:91:THR:HG23	2:D2:213:ARG:HH12	1.85	0.42
1:B4:91:THR:HG21	2:D5:213:ARG:HH12	1.83	0.42
1:B5:91:THR:HG21	2:D6:213:ARG:HH12	1.83	0.42
1:B5:188:VAL:CG1	2:D5:141:ILE:CD1	2.79	0.42
2:C1:89:THR:HG21	2:D1:111:GLY:H	1.84	0.42
2:C7:202:LEU:HD11	2:C7:217:PHE:CE2	2.51	0.42
2:C12:208:TRP:CD1	2:C12:212:VAL:HG22	2.54	0.42
2:D6:71:ARG:HH21	2:D6:79:LEU:HD22	1.83	0.42
2:D9:44:ASN:OD1	2:D9:44:ASN:N	2.44	0.42
2:D12:200:VAL:HG22	2:D12:201:ALA:N	2.34	0.42
1:A2:175:TRP:CD2	2:C2:136:TYR:CE2	3.08	0.42
1:A3:188:VAL:CB	2:C3:141:ILE:HD11	2.50	0.42
1:A7:175:TRP:CD2	2:C7:136:TYR:CE2	3.08	0.42
1:A8:188:VAL:CB	2:C8:141:ILE:HD11	2.50	0.42
1:A11:202:ARG:HD2	1:A11:202:ARG:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:110:GLU:OE1	2:C1:110:GLU:N	2.44	0.42
2:C7:136:TYR:CE1	2:C7:213:ARG:HD3	2.50	0.42
2:C10:136:TYR:CE1	2:C10:213:ARG:HD3	2.50	0.42
2:D7:32:LEU:HD11	2:D7:100:PHE:HB3	2.00	0.42
1:A1:175:TRP:CD2	2:C1:136:TYR:CE2	3.08	0.42
1:A4:188:VAL:CB	2:C4:141:ILE:HD11	2.50	0.42
1:A6:175:TRP:CD2	2:C6:136:TYR:CE2	3.08	0.42
1:B10:91:THR:HG21	2:D11:213:ARG:HH12	1.83	0.42
2:C5:208:TRP:CD1	2:C5:212:VAL:HG22	2.54	0.42
2:C10:208:TRP:CD1	2:C10:212:VAL:HG22	2.54	0.42
2:C12:37:GLN:HA	2:C12:101:SER:O	2.20	0.42
2:D7:159:VAL:CG1	2:D7:160:LYS:N	2.44	0.42
2:D9:69:ASP:OD1	2:D9:70:LYS:N	2.52	0.42
1:A4:175:TRP:CD2	2:C4:136:TYR:CE2	3.08	0.42
1:A5:175:TRP:CD2	2:C5:136:TYR:CE2	3.08	0.42
1:B2:91:THR:HG23	2:D3:213:ARG:HH12	1.85	0.42
1:B2:188:VAL:CG1	2:D2:141:ILE:CD1	2.79	0.42
1:B3:91:THR:HG21	2:D4:213:ARG:HH12	1.83	0.42
1:B7:91:THR:HG21	2:D8:213:ARG:HH12	1.83	0.42
1:B7:188:VAL:HG13	2:D7:141:ILE:CD1	2.47	0.42
1:B8:91:THR:HG21	2:D9:213:ARG:HH12	1.83	0.42
2:C6:60:ILE:CG2	3:E6:185:PHE:HE2	2.25	0.42
2:C6:208:TRP:CD1	2:C6:212:VAL:HG22	2.54	0.42
2:C7:208:TRP:CD1	2:C7:212:VAL:HG22	2.54	0.42
2:C8:55:ASP:OD2	2:C8:94:THR:OG1	2.33	0.42
2:C9:138:LYS:HB3	2:C9:138:LYS:HE2	1.75	0.42
2:C11:110:GLU:OE1	2:C11:110:GLU:N	2.44	0.42
2:C11:208:TRP:CD1	2:C11:212:VAL:HG22	2.54	0.42
2:C13:89:THR:HG21	2:D13:111:GLY:H	1.84	0.42
2:C13:208:TRP:CD1	2:C13:212:VAL:HG22	2.54	0.42
2:D3:37:GLN:HE21	2:D3:37:GLN:HB3	1.58	0.42
2:D5:200:VAL:HG22	2:D5:201:ALA:N	2.34	0.42
2:D10:37:GLN:HE21	2:D10:37:GLN:HB3	1.58	0.42
2:D12:32:LEU:HD11	2:D12:100:PHE:HB3	2.01	0.42
1:A3:175:TRP:CD2	2:C3:136:TYR:CE2	3.08	0.42
1:A8:175:TRP:CD2	2:C8:136:TYR:CE2	3.08	0.42
1:A11:193:SER:HA	1:A11:194:PRO:HD3	1.93	0.42
1:A12:155:PRO:HG2	1:B10:157:THR:HG21	2.00	0.42
1:A13:175:TRP:CD2	2:C13:136:TYR:CE2	3.08	0.42
1:B6:91:THR:HG21	2:D7:213:ARG:HH12	1.83	0.42
1:B13:91:THR:HG23	2:D1:213:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:230:MET:HB3	2:C1:230:MET:HE2	1.59	0.42
2:C3:52:ILE:HD13	2:C3:116:LEU:HB3	2.02	0.42
2:C4:208:TRP:CD1	2:C4:212:VAL:HG22	2.54	0.42
2:C5:55:ASP:OD2	2:C5:94:THR:OG1	2.33	0.42
2:C7:60:ILE:CG2	3:E7:185:PHE:HE2	2.25	0.42
2:C10:37:GLN:HA	2:C10:101:SER:O	2.20	0.42
1:A9:175:TRP:CD2	2:C9:136:TYR:CE2	3.08	0.42
2:C2:37:GLN:HA	2:C2:101:SER:O	2.20	0.42
2:C3:117:MET:HE3	2:C3:117:MET:HB3	1.82	0.42
2:C10:172:PHE:HB3	2:C10:192:LEU:HD12	2.02	0.42
2:C11:37:GLN:HA	2:C11:101:SER:O	2.20	0.42
2:C11:55:ASP:OD2	2:C11:94:THR:OG1	2.33	0.42
2:C13:37:GLN:HA	2:C13:101:SER:O	2.20	0.42
2:C13:110:GLU:OE1	2:C13:110:GLU:N	2.44	0.42
2:D5:37:GLN:HE21	2:D5:37:GLN:HB3	1.58	0.42
2:D8:69:ASP:OD1	2:D8:70:LYS:N	2.52	0.42
2:D8:152:ILE:HD13	2:D8:152:ILE:HA	1.82	0.42
2:D11:69:ASP:OD1	2:D11:70:LYS:N	2.52	0.42
2:D13:37:GLN:HE22	2:D13:103:VAL:CG2	2.28	0.42
1:A3:202:ARG:HD2	1:A3:202:ARG:HA	1.87	0.42
1:A4:201:ALA:O	2:C3:208:TRP:CZ3	2.73	0.42
1:A6:188:VAL:CB	2:C6:141:ILE:HD11	2.50	0.42
1:A9:201:ALA:O	2:C8:208:TRP:CZ3	2.73	0.42
1:A11:175:TRP:CD2	2:C11:136:TYR:CE2	3.08	0.42
1:A12:175:TRP:CD2	2:C12:136:TYR:CE2	3.08	0.42
1:A13:193:SER:HA	1:A13:194:PRO:HD3	1.93	0.42
1:B5:98:VAL:H	2:D6:208:TRP:NE1	2.18	0.42
1:B7:91:THR:HG23	2:D8:213:ARG:HH12	1.85	0.42
1:B8:91:THR:HG23	2:D9:213:ARG:HH12	1.85	0.42
1:B9:98:VAL:H	2:D10:208:TRP:NE1	2.18	0.42
1:B13:91:THR:HG21	2:D1:213:ARG:HH12	1.83	0.42
2:C1:208:TRP:CD1	2:C1:212:VAL:HG22	2.54	0.42
2:C2:52:ILE:HD13	2:C2:116:LEU:HB3	2.02	0.42
2:C3:208:TRP:CD1	2:C3:212:VAL:HG22	2.54	0.42
2:C4:52:ILE:HD13	2:C4:116:LEU:HB3	2.02	0.42
2:D5:32:LEU:HD11	2:D5:100:PHE:HB3	2.00	0.42
2:D12:69:ASP:OD1	2:D12:70:LYS:N	2.52	0.42
1:A10:155:PRO:HG2	1:B8:157:THR:HG21	2.00	0.42
1:A10:175:TRP:CD2	2:C10:136:TYR:CE2	3.08	0.42
1:A13:202:ARG:HA	1:A13:202:ARG:HD2	1.87	0.42
1:B6:98:VAL:H	2:D7:208:TRP:NE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B12:91:THR:HG21	2:D13:213:ARG:HH12	1.83	0.42
1:B13:188:VAL:HG13	2:D13:141:ILE:CD1	2.47	0.42
2:C3:37:GLN:HA	2:C3:101:SER:O	2.20	0.42
2:C3:172:PHE:HB3	2:C3:192:LEU:HD12	2.02	0.42
2:C4:172:PHE:HB3	2:C4:192:LEU:HD12	2.02	0.42
2:C5:138:LYS:HB3	2:C5:138:LYS:HE2	1.75	0.42
2:C8:37:GLN:HA	2:C8:101:SER:O	2.20	0.42
2:C9:172:PHE:HB3	2:C9:192:LEU:HD12	2.02	0.42
2:C11:52:ILE:HD13	2:C11:116:LEU:HB3	2.02	0.42
2:D6:69:ASP:OD1	2:D6:70:LYS:N	2.52	0.42
1:A6:155:PRO:HG2	1:B4:157:THR:HG21	2.00	0.42
1:A10:188:VAL:CB	2:C10:141:ILE:HD11	2.49	0.42
1:A11:188:VAL:CB	2:C11:141:ILE:HD11	2.50	0.42
1:B9:91:THR:HG23	2:D10:213:ARG:HH12	1.85	0.42
1:B11:91:THR:HG21	2:D12:213:ARG:HH12	1.83	0.42
1:B12:91:THR:HG23	2:D13:213:ARG:HH12	1.85	0.42
1:B12:98:VAL:H	2:D13:208:TRP:NE1	2.18	0.42
2:C10:52:ILE:HD13	2:C10:116:LEU:HB3	2.02	0.42
2:C11:172:PHE:HB3	2:C11:192:LEU:HD12	2.02	0.42
2:C12:117:MET:HE3	2:C12:117:MET:HB3	1.82	0.42
2:D5:70:LYS:HE3	2:D5:70:LYS:HB2	1.86	0.42
2:D6:32:LEU:HD11	2:D6:100:PHE:HB3	2.01	0.42
1:A13:188:VAL:CB	2:C13:141:ILE:HD11	2.50	0.41
1:B7:98:VAL:H	2:D8:208:TRP:NE1	2.18	0.41
1:B11:91:THR:HG23	2:D12:213:ARG:HH12	1.85	0.41
2:C2:208:TRP:CD1	2:C2:212:VAL:HG22	2.54	0.41
2:C5:172:PHE:HB3	2:C5:192:LEU:HD12	2.02	0.41
2:C6:67:LEU:HD23	2:C6:67:LEU:HA	1.91	0.41
2:C11:230:MET:HE2	2:C11:230:MET:HB3	1.59	0.41
2:C12:52:ILE:HD13	2:C12:116:LEU:HB3	2.02	0.41
2:D2:69:ASP:OD1	2:D2:70:LYS:N	2.52	0.41
2:D5:37:GLN:HE22	2:D5:103:VAL:CG2	2.28	0.41
2:D10:69:ASP:OD1	2:D10:70:LYS:N	2.52	0.41
1:A1:188:VAL:CB	2:C1:141:ILE:HD11	2.50	0.41
1:A2:188:VAL:CB	2:C2:141:ILE:HD11	2.50	0.41
1:A5:188:VAL:CB	2:C5:141:ILE:HD11	2.50	0.41
1:A7:155:PRO:HG2	1:B5:157:THR:HG21	2.00	0.41
1:A9:155:PRO:HG2	1:B7:157:THR:HG21	2.00	0.41
1:A11:172:ILE:CD1	2:C11:140:LEU:HD12	2.35	0.41
1:B3:91:THR:HG23	2:D4:213:ARG:HH12	1.85	0.41
1:B10:98:VAL:H	2:D11:208:TRP:NE1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C1:55:ASP:OD2	2:C1:94:THR:OG1	2.33	0.41
2:C7:37:GLN:HA	2:C7:101:SER:O	2.20	0.41
2:D2:220:ASN:CG	2:D2:220:ASN:O	2.63	0.41
1:A6:201:ALA:O	2:C5:208:TRP:CZ3	2.73	0.41
1:A9:188:VAL:CB	2:C9:141:ILE:HD11	2.49	0.41
1:B4:98:VAL:H	2:D5:208:TRP:NE1	2.18	0.41
2:C3:202:LEU:HD11	2:C3:217:PHE:CE2	2.51	0.41
2:C5:37:GLN:HA	2:C5:101:SER:O	2.20	0.41
2:C6:63:PRO:HG3	2:D6:47:PRO:HD3	2.03	0.41
2:C9:37:GLN:HA	2:C9:101:SER:O	2.20	0.41
2:C9:117:MET:HE3	2:C9:117:MET:HB3	1.82	0.41
2:C9:208:TRP:CD1	2:C9:212:VAL:HG22	2.54	0.41
2:C13:63:PRO:HG3	2:D13:47:PRO:HD3	2.03	0.41
2:D13:69:ASP:OD1	2:D13:70:LYS:N	2.52	0.41
1:A2:172:ILE:CD1	2:C2:140:LEU:HD12	2.35	0.41
1:A12:201:ALA:O	2:C11:208:TRP:CZ3	2.73	0.41
1:B1:188:VAL:CG1	2:D1:141:ILE:CD1	2.79	0.41
1:B6:91:THR:HG23	2:D7:213:ARG:HH12	1.85	0.41
1:B6:188:VAL:CG1	2:D6:141:ILE:CD1	2.79	0.41
2:C1:52:ILE:HD13	2:C1:116:LEU:HB3	2.02	0.41
2:C2:172:PHE:HB3	2:C2:192:LEU:HD12	2.02	0.41
2:C3:63:PRO:HG3	2:D3:47:PRO:HD3	2.03	0.41
2:C4:37:GLN:HA	2:C4:101:SER:O	2.20	0.41
2:C8:172:PHE:HB3	2:C8:192:LEU:HD12	2.02	0.41
2:C8:208:TRP:CD1	2:C8:212:VAL:HG22	2.54	0.41
2:C13:60:ILE:CG2	3:E13:185:PHE:HE2	2.25	0.41
2:D1:192:LEU:HD13	2:D1:192:LEU:HA	1.93	0.41
1:A5:155:PRO:HG2	1:B3:157:THR:HG21	2.00	0.41
1:A8:155:PRO:HG2	1:B6:157:THR:HG21	2.00	0.41
1:B2:91:THR:HG21	2:D3:213:ARG:HH12	1.83	0.41
2:C1:63:PRO:HG3	2:D1:47:PRO:HD3	2.03	0.41
2:C5:52:ILE:HD13	2:C5:116:LEU:HB3	2.02	0.41
2:C9:52:ILE:HD13	2:C9:116:LEU:HB3	2.02	0.41
2:D1:37:GLN:HE22	2:D1:103:VAL:CG2	2.28	0.41
1:A1:201:ALA:O	2:C13:208:TRP:CZ3	2.73	0.41
1:B1:98:VAL:H	2:D2:208:TRP:NE1	2.18	0.41
1:B2:98:VAL:H	2:D3:208:TRP:NE1	2.18	0.41
1:B10:91:THR:HG23	2:D11:213:ARG:HH12	1.85	0.41
2:C4:72:LEU:HD22	3:E4:185:PHE:CB	2.50	0.41
2:C4:136:TYR:CE1	2:C4:213:ARG:HD3	2.50	0.41
2:C12:172:PHE:HB3	2:C12:192:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D7:37:GLN:HE21	2:D7:37:GLN:HB3	1.59	0.41
2:D9:220:ASN:CG	2:D9:220:ASN:O	2.63	0.41
2:D11:70:LYS:HE3	2:D11:70:LYS:HB2	1.86	0.41
2:C6:136:TYR:CE1	2:C6:213:ARG:HD3	2.51	0.41
2:C9:63:PRO:HG3	2:D9:47:PRO:HD3	2.03	0.41
2:C9:110:GLU:OE1	2:C9:110:GLU:N	2.44	0.41
2:C12:110:GLU:OE1	2:C12:110:GLU:N	2.44	0.41
2:C13:52:ILE:HD13	2:C13:116:LEU:HB3	2.02	0.41
2:D7:152:ILE:HA	2:D7:153:PRO:HD3	1.97	0.41
2:D8:70:LYS:HB2	2:D8:70:LYS:HE3	1.86	0.41
2:D9:152:ILE:HD13	2:D9:152:ILE:HA	1.82	0.41
1:B11:98:VAL:H	2:D12:208:TRP:NE1	2.18	0.41
2:C4:63:PRO:HG3	2:D4:47:PRO:HD3	2.03	0.41
2:C8:136:TYR:CE1	2:C8:213:ARG:HD3	2.50	0.41
2:C10:63:PRO:HG3	2:D10:47:PRO:HD3	2.03	0.41
2:D4:220:ASN:O	2:D4:220:ASN:CG	2.63	0.41
2:D7:192:LEU:HD13	2:D7:192:LEU:HA	1.93	0.41
2:D7:220:ASN:O	2:D7:220:ASN:CG	2.63	0.41
2:D13:220:ASN:CG	2:D13:220:ASN:O	2.63	0.41
1:A2:202:ARG:HD2	1:A2:202:ARG:HA	1.87	0.41
1:A3:201:ALA:O	2:C2:208:TRP:CZ3	2.73	0.41
1:A9:193:SER:HA	1:A9:194:PRO:HD3	1.93	0.41
1:A10:158:VAL:HG21	1:A10:200:PRO:CB	2.51	0.41
1:A11:201:ALA:O	2:C10:208:TRP:CZ3	2.73	0.41
1:B1:188:VAL:HG13	2:D1:141:ILE:CD1	2.46	0.41
1:B3:98:VAL:H	2:D4:208:TRP:NE1	2.18	0.41
1:B3:155:PRO:CD	2:D4:205:GLN:HG3	2.51	0.41
1:B4:155:PRO:CD	2:D5:205:GLN:HG3	2.51	0.41
1:B5:155:PRO:CD	2:D6:205:GLN:HG3	2.51	0.41
1:B8:98:VAL:H	2:D9:208:TRP:NE1	2.18	0.41
2:C1:37:GLN:HA	2:C1:101:SER:O	2.20	0.41
2:C2:67:LEU:HD23	2:C2:67:LEU:HA	1.91	0.41
2:C2:203:ARG:H	2:C2:203:ARG:HG2	1.77	0.41
2:C4:60:ILE:CG2	3:E4:185:PHE:HE2	2.25	0.41
2:C6:37:GLN:HA	2:C6:101:SER:O	2.20	0.41
2:C6:172:PHE:HB3	2:C6:192:LEU:HD12	2.02	0.41
2:C7:63:PRO:HG3	2:D7:47:PRO:HD3	2.03	0.41
2:C11:138:LYS:HE2	2:C11:138:LYS:HB3	1.75	0.41
2:D1:70:LYS:HE3	2:D1:70:LYS:HB2	1.86	0.41
1:A8:201:ALA:O	2:C7:208:TRP:CZ3	2.73	0.41
1:A12:164:ARG:HB3	1:B11:164:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A12:188:VAL:CB	2:C12:141:ILE:HD11	2.50	0.41
1:B8:188:VAL:HG13	2:D8:141:ILE:CD1	2.46	0.41
1:B11:155:PRO:CD	2:D12:205:GLN:HG3	2.51	0.41
2:C4:117:MET:HE3	2:C4:117:MET:HB3	1.82	0.41
2:C5:63:PRO:HG3	2:D5:47:PRO:HD3	2.03	0.41
2:C7:52:ILE:HD13	2:C7:116:LEU:HB3	2.02	0.41
2:D3:220:ASN:CG	2:D3:220:ASN:O	2.63	0.41
2:D7:209:LYS:HE3	2:D7:209:LYS:HB2	1.95	0.41
2:D10:152:ILE:HD13	2:D10:152:ILE:HA	1.82	0.41
2:D12:209:LYS:HE3	2:D12:209:LYS:HB2	1.95	0.41
2:D12:209:LYS:O	2:D12:210:PRO:C	2.64	0.41
2:D13:209:LYS:HE3	2:D13:209:LYS:HB2	1.95	0.41
1:A6:158:VAL:HG21	1:A6:200:PRO:CB	2.51	0.40
1:B5:91:THR:HG23	2:D6:213:ARG:HH12	1.85	0.40
1:B10:155:PRO:CD	2:D11:205:GLN:HG3	2.51	0.40
2:C1:172:PHE:HB3	2:C1:192:LEU:HD12	2.02	0.40
2:C2:46:ASP:HA	2:C2:47:PRO:HD3	1.98	0.40
2:C3:72:LEU:HD22	3:E3:185:PHE:CB	2.51	0.40
2:C6:52:ILE:HD13	2:C6:116:LEU:HB3	2.02	0.40
2:C8:63:PRO:HG3	2:D8:47:PRO:HD3	2.03	0.40
2:C13:172:PHE:HB3	2:C13:192:LEU:HD12	2.02	0.40
2:C13:185:LEU:HD23	2:C13:185:LEU:HA	1.89	0.40
2:D5:209:LYS:O	2:D5:210:PRO:C	2.64	0.40
2:D5:220:ASN:O	2:D5:220:ASN:CG	2.63	0.40
1:A1:193:SER:HA	1:A1:194:PRO:HD3	1.93	0.40
1:A8:164:ARG:HB3	1:B7:164:ARG:HH11	1.87	0.40
1:B6:155:PRO:CD	2:D7:205:GLN:HG3	2.51	0.40
1:B13:98:VAL:H	2:D1:208:TRP:NE1	2.18	0.40
2:C2:90:ILE:HD13	2:C2:90:ILE:HG21	1.81	0.40
2:C2:110:GLU:OE1	2:C2:110:GLU:N	2.44	0.40
2:C8:52:ILE:HD13	2:C8:116:LEU:HB3	2.02	0.40
2:C9:60:ILE:CG2	3:E9:185:PHE:HE2	2.25	0.40
2:C11:72:LEU:HD22	3:E11:185:PHE:CB	2.50	0.40
2:C12:63:PRO:HG3	2:D12:47:PRO:HD3	2.03	0.40
2:C12:72:LEU:HD22	3:E12:185:PHE:CB	2.51	0.40
1:A4:155:PRO:HG2	1:B2:157:THR:HG21	2.00	0.40
1:B2:155:PRO:CD	2:D3:205:GLN:HG3	2.51	0.40
1:B4:91:THR:HG23	2:D5:213:ARG:HH12	1.85	0.40
1:B10:170:VAL:CG1	2:D10:144:ASN:HD22	2.33	0.40
2:C2:138:LYS:HE2	2:C2:138:LYS:HB3	1.75	0.40
2:C9:136:TYR:CE1	2:C9:213:ARG:HD3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C12:46:ASP:HA	2:C12:47:PRO:HD3	1.98	0.40
2:D4:37:GLN:HE22	2:D4:103:VAL:CG2	2.28	0.40
2:D10:220:ASN:CG	2:D10:220:ASN:O	2.63	0.40
2:D11:144:ASN:OD1	2:D11:235:ILE:HD13	2.22	0.40
2:D11:152:ILE:HD13	2:D11:152:ILE:HA	1.82	0.40
1:A7:164:ARG:HB3	1:B6:164:ARG:HH11	1.87	0.40
1:A11:155:PRO:HG2	1:B9:157:THR:HG21	2.00	0.40
1:A11:164:ARG:HB3	1:B10:164:ARG:HH11	1.87	0.40
1:B8:98:VAL:HG13	2:D9:208:TRP:NE1	2.37	0.40
1:B9:155:PRO:CD	2:D10:205:GLN:HG3	2.51	0.40
1:B12:155:PRO:CD	2:D13:205:GLN:HG3	2.51	0.40
1:B13:188:VAL:CG1	2:D13:141:ILE:CD1	2.79	0.40
2:C5:90:ILE:HD13	2:C5:90:ILE:HG21	1.81	0.40
2:C7:172:PHE:HB3	2:C7:192:LEU:HD12	2.02	0.40
2:C8:202:LEU:HD11	2:C8:217:PHE:CE2	2.51	0.40
2:C13:72:LEU:HD22	3:E13:185:PHE:CB	2.51	0.40
2:D10:144:ASN:OD1	2:D10:235:ILE:HD13	2.22	0.40
2:D12:70:LYS:HE3	2:D12:70:LYS:HB2	1.86	0.40
2:D12:152:ILE:HD13	2:D12:152:ILE:HA	1.82	0.40
1:B1:91:THR:HG21	2:D2:213:ARG:HH12	1.83	0.40
1:B3:98:VAL:HG13	2:D4:208:TRP:NE1	2.37	0.40
1:B5:98:VAL:HG13	2:D6:208:TRP:NE1	2.37	0.40
2:C2:63:PRO:HG3	2:D2:47:PRO:HD3	2.03	0.40
2:C6:72:LEU:HD22	3:E6:185:PHE:CB	2.51	0.40
2:C9:148:LEU:HD12	2:C9:148:LEU:HA	1.96	0.40
2:C11:63:PRO:HG3	2:D11:47:PRO:HD3	2.03	0.40
2:C12:230:MET:HE2	2:C12:230:MET:HB3	1.59	0.40
2:C13:49:MET:HB2	2:C13:79:LEU:HD23	2.04	0.40
2:D2:37:GLN:HE22	2:D2:103:VAL:CG2	2.28	0.40
2:D3:209:LYS:O	2:D3:210:PRO:C	2.64	0.40
2:D7:209:LYS:O	2:D7:210:PRO:C	2.64	0.40
2:D11:220:ASN:O	2:D11:220:ASN:CG	2.63	0.40
2:D13:144:ASN:OD1	2:D13:235:ILE:HD13	2.22	0.40
2:D13:192:LEU:HD13	2:D13:192:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A10	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A11	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A12	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A13	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A2	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A3	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A4	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A5	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A6	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A7	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A8	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	A9	53/204 (26%)	47 (89%)	6 (11%)	0	100	100
1	B1	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B10	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B11	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B12	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B13	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B2	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B3	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B4	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B5	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B6	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B7	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
1	B8	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B9	61/204 (30%)	56 (92%)	4 (7%)	1 (2%)	7	32
2	C1	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C10	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C11	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C12	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C13	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C2	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C3	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C4	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C5	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C6	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C7	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C8	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	C9	215/246 (87%)	208 (97%)	6 (3%)	1 (0%)	24	56
2	D1	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D10	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D11	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D12	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D13	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D2	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D3	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D4	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D5	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D6	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D7	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D8	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
2	D9	215/246 (87%)	205 (95%)	9 (4%)	1 (0%)	24	56
3	E1	9/453 (2%)	9 (100%)	0	0	100	100
3	E10	9/453 (2%)	9 (100%)	0	0	100	100
3	E11	9/453 (2%)	9 (100%)	0	0	100	100
3	E12	9/453 (2%)	9 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E13	9/453 (2%)	9 (100%)	0	0	100	100
3	E2	9/453 (2%)	9 (100%)	0	0	100	100
3	E3	9/453 (2%)	9 (100%)	0	0	100	100
3	E4	9/453 (2%)	9 (100%)	0	0	100	100
3	E5	9/453 (2%)	9 (100%)	0	0	100	100
3	E6	9/453 (2%)	9 (100%)	0	0	100	100
3	E7	9/453 (2%)	9 (100%)	0	0	100	100
3	E8	9/453 (2%)	9 (100%)	0	0	100	100
3	E9	9/453 (2%)	9 (100%)	0	0	100	100
3	F1	9/453 (2%)	9 (100%)	0	0	100	100
3	F10	9/453 (2%)	9 (100%)	0	0	100	100
3	F11	9/453 (2%)	9 (100%)	0	0	100	100
3	F12	9/453 (2%)	9 (100%)	0	0	100	100
3	F13	9/453 (2%)	9 (100%)	0	0	100	100
3	F2	9/453 (2%)	9 (100%)	0	0	100	100
3	F3	9/453 (2%)	9 (100%)	0	0	100	100
3	F4	9/453 (2%)	9 (100%)	0	0	100	100
3	F5	9/453 (2%)	9 (100%)	0	0	100	100
3	F6	9/453 (2%)	9 (100%)	0	0	100	100
3	F7	9/453 (2%)	9 (100%)	0	0	100	100
3	F8	9/453 (2%)	9 (100%)	0	0	100	100
3	F9	9/453 (2%)	9 (100%)	0	0	100	100
All	All	7306/23478 (31%)	6942 (95%)	325 (4%)	39 (0%)	26	56

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C1	169	PRO
2	C2	169	PRO
2	C3	169	PRO
2	C4	169	PRO
2	C5	169	PRO
2	C6	169	PRO
2	C7	169	PRO

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Mol	Chain	Res	Type
2	C8	169	PRO
2	C9	169	PRO
2	C10	169	PRO
2	C11	169	PRO
2	C12	169	PRO
2	C13	169	PRO
1	B1	96	PRO
1	B2	96	PRO
1	B3	96	PRO
1	B6	96	PRO
1	B7	96	PRO
1	B8	96	PRO
1	B9	96	PRO
1	B10	96	PRO
1	B12	96	PRO
1	B13	96	PRO
1	B4	96	PRO
1	B5	96	PRO
1	B11	96	PRO
2	D1	210	PRO
2	D2	210	PRO
2	D3	210	PRO
2	D4	210	PRO
2	D5	210	PRO
2	D6	210	PRO
2	D7	210	PRO
2	D8	210	PRO
2	D9	210	PRO
2	D10	210	PRO
2	D11	210	PRO
2	D12	210	PRO
2	D13	210	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	A10	48/168 (29%)	47 (98%)	1 (2%)	47	66
1	A11	48/168 (29%)	47 (98%)	1 (2%)	47	66
1	A12	48/168 (29%)	47 (98%)	1 (2%)	47	66
1	A13	48/168 (29%)	47 (98%)	1 (2%)	47	66
1	A2	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	A3	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	A4	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	A5	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	A6	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	A7	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	A8	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	A9	48/168 (29%)	45 (94%)	3 (6%)	16	44
1	B1	56/168 (33%)	53 (95%)	3 (5%)	20	48
1	B10	56/168 (33%)	55 (98%)	1 (2%)	51	69
1	B11	56/168 (33%)	52 (93%)	4 (7%)	13	40
1	B12	56/168 (33%)	55 (98%)	1 (2%)	51	69
1	B13	56/168 (33%)	55 (98%)	1 (2%)	51	69
1	B2	56/168 (33%)	54 (96%)	2 (4%)	31	58
1	B3	56/168 (33%)	53 (95%)	3 (5%)	20	48
1	B4	56/168 (33%)	53 (95%)	3 (5%)	20	48
1	B5	56/168 (33%)	53 (95%)	3 (5%)	20	48
1	B6	56/168 (33%)	53 (95%)	3 (5%)	20	48
1	B7	56/168 (33%)	53 (95%)	3 (5%)	20	48
1	B8	56/168 (33%)	53 (95%)	3 (5%)	20	48
1	B9	56/168 (33%)	54 (96%)	2 (4%)	31	58
2	C1	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	C10	173/195 (89%)	171 (99%)	2 (1%)	63	74
2	C11	173/195 (89%)	171 (99%)	2 (1%)	63	74
2	C12	173/195 (89%)	170 (98%)	3 (2%)	53	70
2	C13	173/195 (89%)	170 (98%)	3 (2%)	53	70
2	C2	173/195 (89%)	166 (96%)	7 (4%)	28	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C3	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	C4	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	C5	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	C6	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	C7	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	C8	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	C9	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D1	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D10	173/195 (89%)	168 (97%)	5 (3%)	37	62
2	D11	173/195 (89%)	169 (98%)	4 (2%)	44	66
2	D12	173/195 (89%)	165 (95%)	8 (5%)	24	53
2	D13	173/195 (89%)	168 (97%)	5 (3%)	37	62
2	D2	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D3	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D4	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D5	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D6	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D7	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D8	173/195 (89%)	166 (96%)	7 (4%)	28	56
2	D9	173/195 (89%)	166 (96%)	7 (4%)	28	56
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E8	10/353 (3%)	10 (100%)	0	100	100
3	E9	10/353 (3%)	10 (100%)	0	100	100
3	F1	10/353 (3%)	10 (100%)	0	100	100
3	F10	10/353 (3%)	10 (100%)	0	100	100
3	F11	10/353 (3%)	10 (100%)	0	100	100
3	F12	10/353 (3%)	10 (100%)	0	100	100
3	F13	10/353 (3%)	10 (100%)	0	100	100
3	F2	10/353 (3%)	10 (100%)	0	100	100
3	F3	10/353 (3%)	10 (100%)	0	100	100
3	F4	10/353 (3%)	10 (100%)	0	100	100
3	F5	10/353 (3%)	10 (100%)	0	100	100
3	F6	10/353 (3%)	10 (100%)	0	100	100
3	F7	10/353 (3%)	10 (100%)	0	100	100
3	F8	10/353 (3%)	10 (100%)	0	100	100
3	F9	10/353 (3%)	10 (100%)	0	100	100
All	All	6110/18616 (33%)	5889 (96%)	221 (4%)	32	58

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	159	HIS
1	A1	176	VAL
1	A1	192	VAL
1	A2	159	HIS
1	A2	176	VAL
1	A2	192	VAL
1	A3	159	HIS
1	A3	176	VAL
1	A3	192	VAL
1	A4	159	HIS
1	A4	176	VAL
1	A4	192	VAL
1	A5	159	HIS
1	A5	176	VAL
1	A5	192	VAL
1	A6	159	HIS
1	A6	176	VAL

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Mol	Chain	Res	Type
1	A6	192	VAL
1	A7	159	HIS
1	A7	176	VAL
1	A7	192	VAL
1	A8	159	HIS
1	A8	176	VAL
1	A8	192	VAL
1	A9	159	HIS
1	A9	176	VAL
1	A9	192	VAL
1	A10	159	HIS
1	A11	159	HIS
1	A12	159	HIS
1	A13	159	HIS
1	B1	191	VAL
1	B1	192	VAL
1	B1	199	LEU
1	B2	191	VAL
1	B2	192	VAL
1	B3	191	VAL
1	B3	192	VAL
1	B3	199	LEU
1	B4	191	VAL
1	B4	192	VAL
1	B4	199	LEU
1	B5	191	VAL
1	B5	192	VAL
1	B5	199	LEU
1	B6	191	VAL
1	B6	192	VAL
1	B6	199	LEU
1	B7	191	VAL
1	B7	192	VAL
1	B7	199	LEU
1	B8	191	VAL
1	B8	192	VAL
1	B8	199	LEU
1	B9	191	VAL
1	B9	192	VAL
1	B10	191	VAL
1	B11	91	THR
1	B11	92	VAL

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Mol	Chain	Res	Type
1	B11	99	SER
1	B11	191	VAL
1	B12	191	VAL
1	B13	191	VAL
2	C1	40	LEU
2	C1	60	ILE
2	C1	73	THR
2	C1	92	VAL
2	C1	94	THR
2	C1	212	VAL
2	C1	229	ARG
2	C2	40	LEU
2	C2	60	ILE
2	C2	73	THR
2	C2	92	VAL
2	C2	94	THR
2	C2	212	VAL
2	C2	229	ARG
2	C3	40	LEU
2	C3	60	ILE
2	C3	73	THR
2	C3	92	VAL
2	C3	94	THR
2	C3	212	VAL
2	C3	229	ARG
2	C4	40	LEU
2	C4	60	ILE
2	C4	73	THR
2	C4	92	VAL
2	C4	94	THR
2	C4	212	VAL
2	C4	229	ARG
2	C5	40	LEU
2	C5	60	ILE
2	C5	73	THR
2	C5	92	VAL
2	C5	94	THR
2	C5	212	VAL
2	C5	229	ARG
2	C6	40	LEU
2	C6	60	ILE
2	C6	73	THR

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Mol	Chain	Res	Type
2	C6	92	VAL
2	C6	94	THR
2	C6	212	VAL
2	C6	229	ARG
2	C7	40	LEU
2	C7	60	ILE
2	C7	73	THR
2	C7	92	VAL
2	C7	94	THR
2	C7	212	VAL
2	C7	229	ARG
2	C8	40	LEU
2	C8	60	ILE
2	C8	73	THR
2	C8	92	VAL
2	C8	94	THR
2	C8	212	VAL
2	C8	229	ARG
2	C9	40	LEU
2	C9	60	ILE
2	C9	73	THR
2	C9	92	VAL
2	C9	94	THR
2	C9	212	VAL
2	C9	229	ARG
2	C10	225	MET
2	C10	229	ARG
2	C11	225	MET
2	C11	229	ARG
2	C12	29	THR
2	C12	225	MET
2	C12	229	ARG
2	C13	40	LEU
2	C13	225	MET
2	C13	229	ARG
2	D1	32	LEU
2	D1	57	VAL
2	D1	73	THR
2	D1	225	MET
2	D1	234	VAL
2	D1	235	ILE
2	D1	240	GLU

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Mol	Chain	Res	Type
2	D2	32	LEU
2	D2	57	VAL
2	D2	73	THR
2	D2	225	MET
2	D2	234	VAL
2	D2	235	ILE
2	D2	240	GLU
2	D3	32	LEU
2	D3	57	VAL
2	D3	73	THR
2	D3	225	MET
2	D3	234	VAL
2	D3	235	ILE
2	D3	240	GLU
2	D4	32	LEU
2	D4	57	VAL
2	D4	73	THR
2	D4	225	MET
2	D4	234	VAL
2	D4	235	ILE
2	D4	240	GLU
2	D5	32	LEU
2	D5	57	VAL
2	D5	73	THR
2	D5	225	MET
2	D5	234	VAL
2	D5	235	ILE
2	D5	240	GLU
2	D6	32	LEU
2	D6	57	VAL
2	D6	73	THR
2	D6	225	MET
2	D6	234	VAL
2	D6	235	ILE
2	D6	240	GLU
2	D7	32	LEU
2	D7	57	VAL
2	D7	73	THR
2	D7	225	MET
2	D7	234	VAL
2	D7	235	ILE
2	D7	240	GLU

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Mol	Chain	Res	Type
2	D8	32	LEU
2	D8	57	VAL
2	D8	73	THR
2	D8	225	MET
2	D8	234	VAL
2	D8	235	ILE
2	D8	240	GLU
2	D9	32	LEU
2	D9	57	VAL
2	D9	73	THR
2	D9	225	MET
2	D9	234	VAL
2	D9	235	ILE
2	D9	240	GLU
2	D10	73	THR
2	D10	186	ARG
2	D10	225	MET
2	D10	230	MET
2	D10	240	GLU
2	D11	186	ARG
2	D11	225	MET
2	D11	230	MET
2	D11	240	GLU
2	D12	25	GLN
2	D12	34	GLN
2	D12	40	LEU
2	D12	73	THR
2	D12	186	ARG
2	D12	225	MET
2	D12	230	MET
2	D12	240	GLU
2	D13	73	THR
2	D13	186	ARG
2	D13	225	MET
2	D13	230	MET
2	D13	240	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	B1	159	HIS
1	B1	161	GLN

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Mol	Chain	Res	Type
1	B2	159	HIS
1	B2	161	GLN
1	B3	159	HIS
1	B3	161	GLN
1	B4	159	HIS
1	B4	161	GLN
1	B5	159	HIS
1	B5	161	GLN
1	B6	159	HIS
1	B6	161	GLN
1	B7	159	HIS
1	B7	161	GLN
1	B8	159	HIS
1	B8	161	GLN
1	B9	159	HIS
1	B9	161	GLN
2	C1	37	GLN
2	C2	37	GLN
2	C2	134	GLN
2	C3	37	GLN
2	C3	134	GLN
2	C3	222	GLN
2	C4	37	GLN
2	C5	37	GLN
2	C5	98	GLN
2	C6	37	GLN
2	C6	98	GLN
2	C7	37	GLN
2	C8	37	GLN
2	C9	37	GLN
2	D1	37	GLN
2	D1	48	ASN
2	D1	144	ASN
2	D2	37	GLN
2	D2	48	ASN
2	D2	98	GLN
2	D2	144	ASN
2	D3	37	GLN
2	D3	98	GLN
2	D3	144	ASN
2	D4	37	GLN
2	D4	48	ASN

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Mol	Chain	Res	Type
2	D4	144	ASN
2	D5	37	GLN
2	D5	48	ASN
2	D5	144	ASN
2	D6	37	GLN
2	D6	144	ASN
2	D7	37	GLN
2	D7	48	ASN
2	D7	144	ASN
2	D8	37	GLN
2	D8	144	ASN
2	D9	37	GLN
2	D9	144	ASN

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.

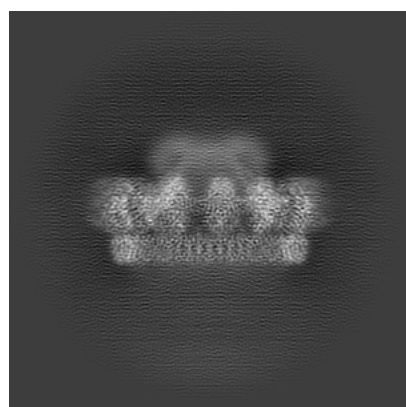
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24769. These allow visual inspection of the internal detail of the map and identification of artifacts.

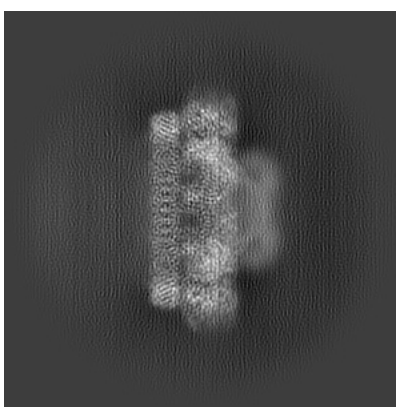
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

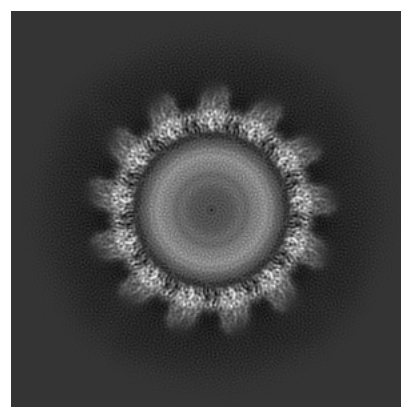
6.1.1 Primary map



X



Y

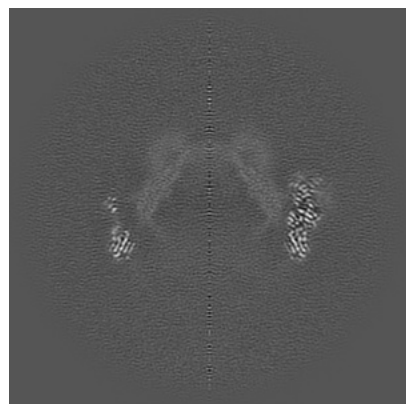


Z

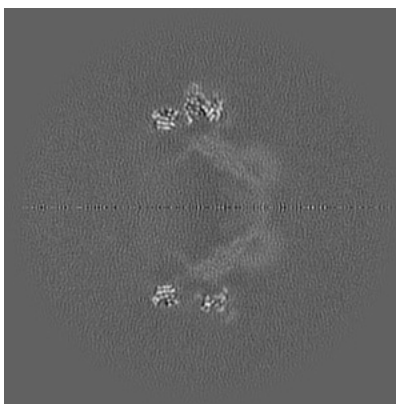
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

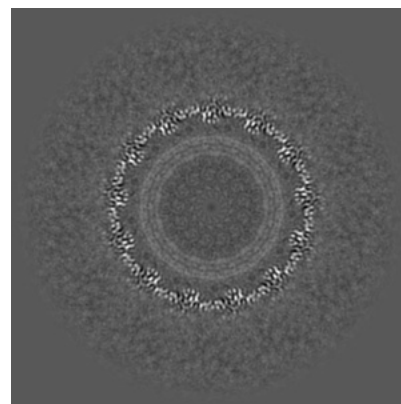
6.2.1 Primary map



X Index: 200



Y Index: 200

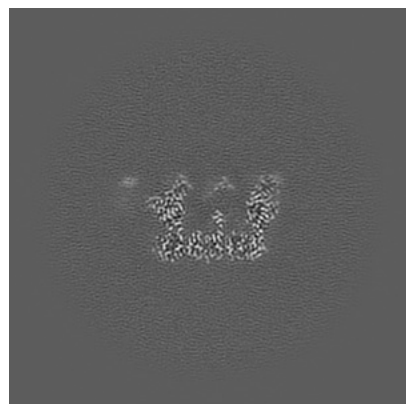


Z Index: 200

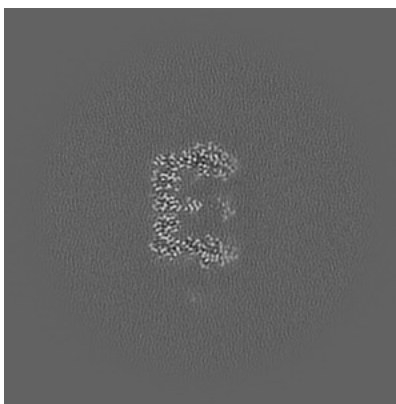
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

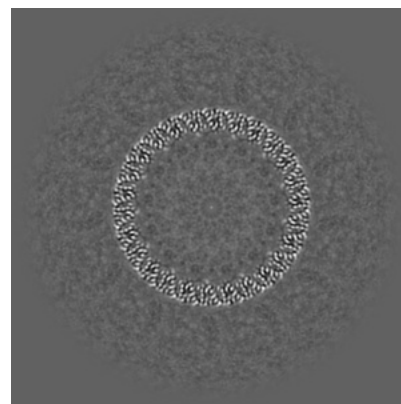
6.3.1 Primary map



X Index: 282



Y Index: 283

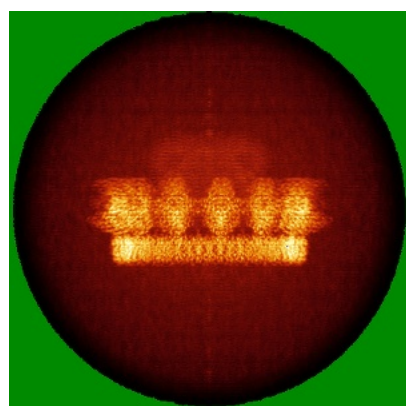


Z Index: 167

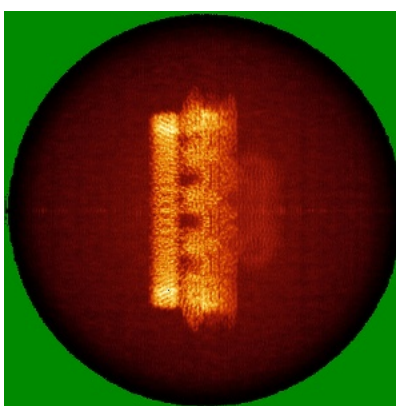
The images above show the largest variance slices of the map in three orthogonal directions.

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

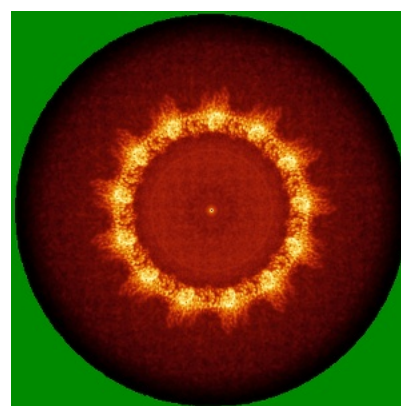
6.4.1 Primary map



X



Y

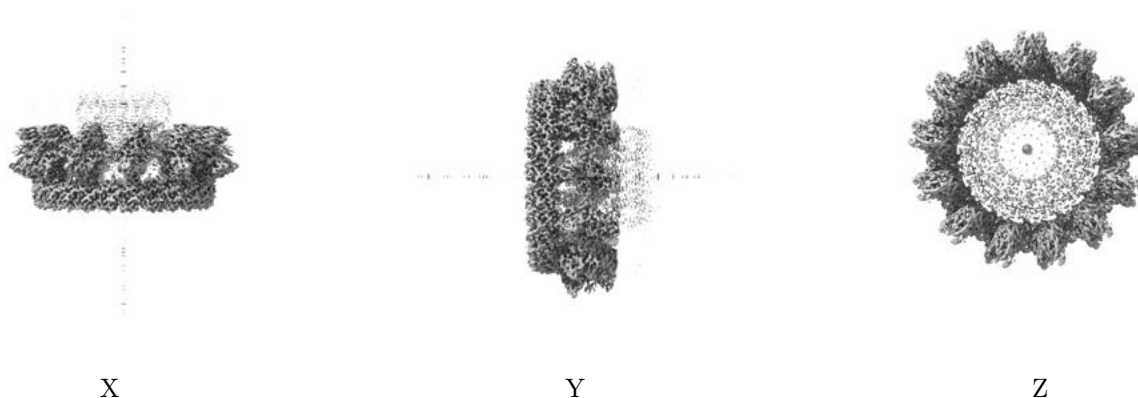


Z

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 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

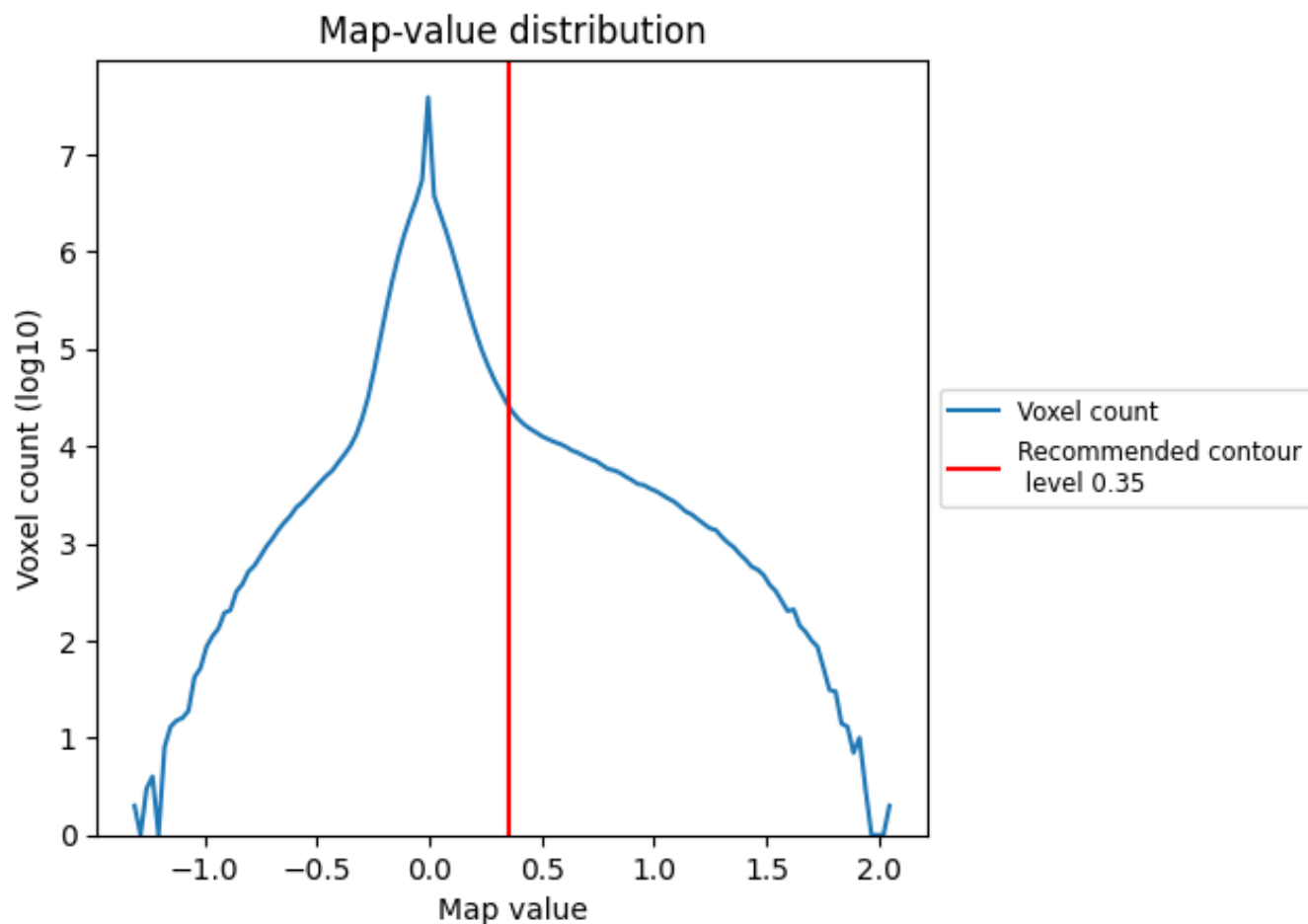
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

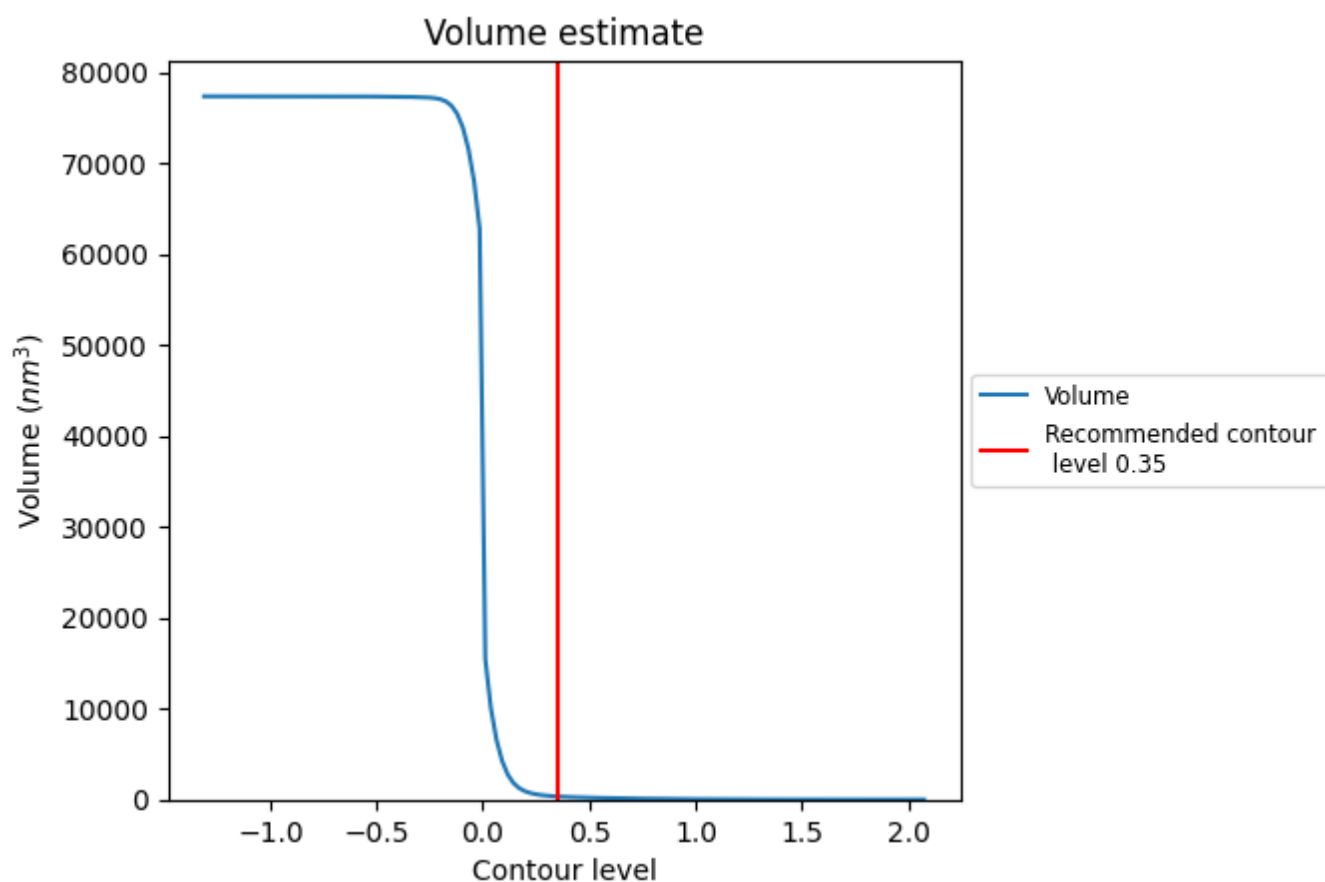
This section contains the results of statistical analysis of the map.

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.

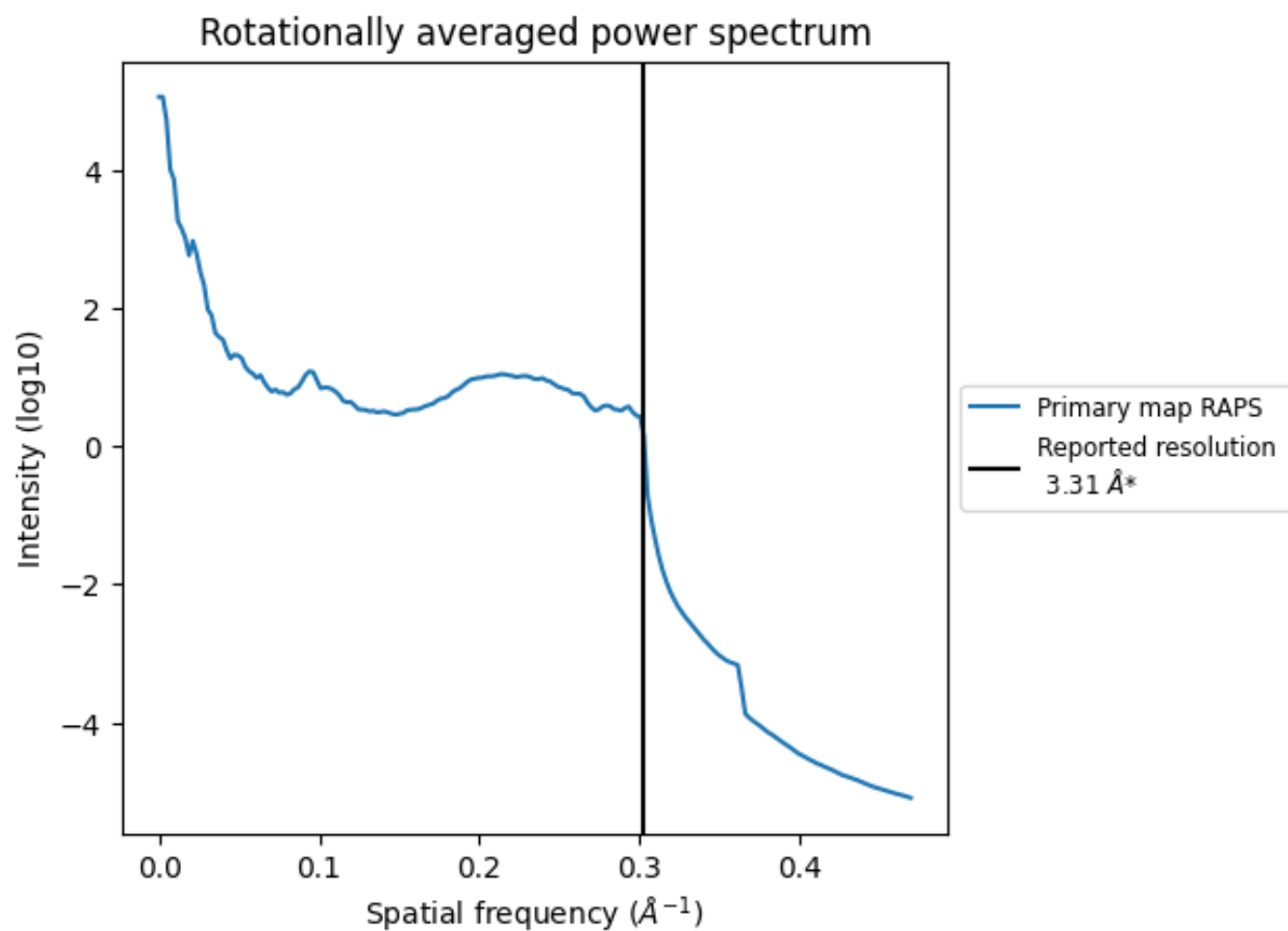
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 306 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 0.302 Å⁻¹

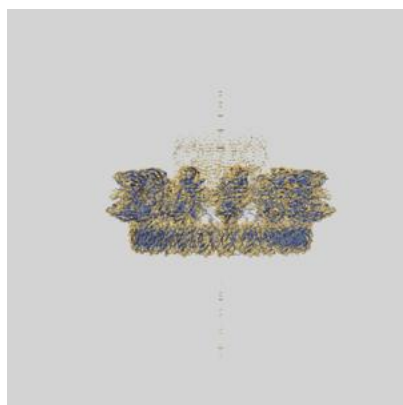
8 Fourier-Shell correlation

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

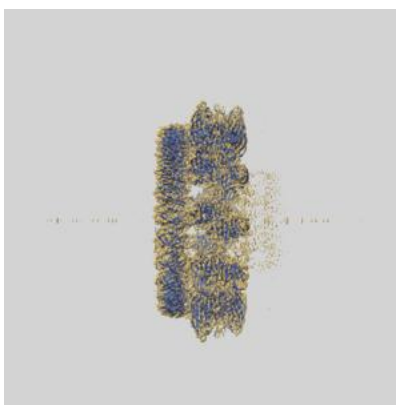
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24769 and PDB model 7SPB. Per-residue inclusion information can be found in section [3](#) on page [11](#).

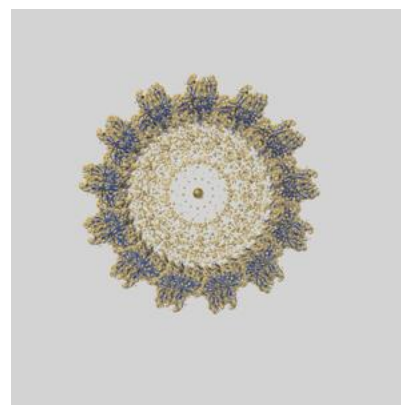
9.1 Map-model overlay [i](#)



X



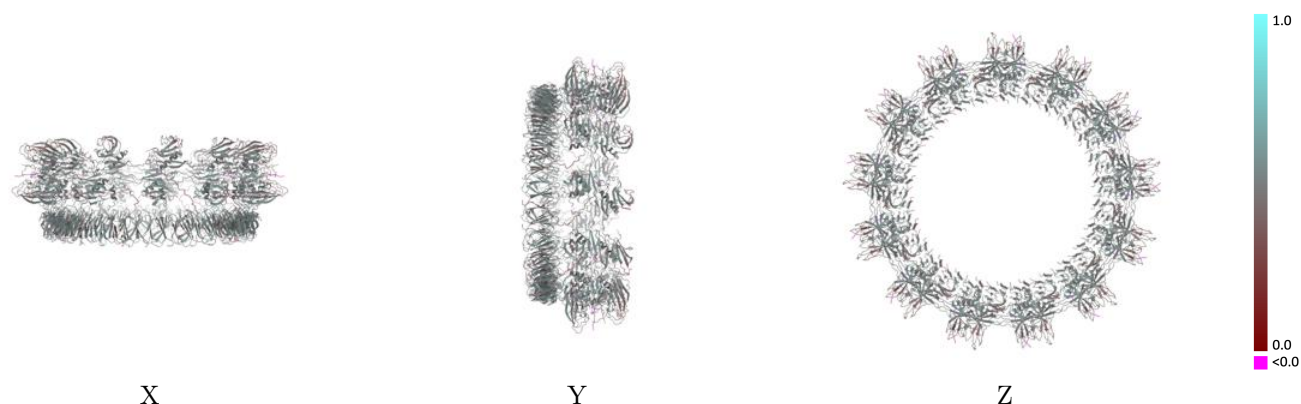
Y



Z

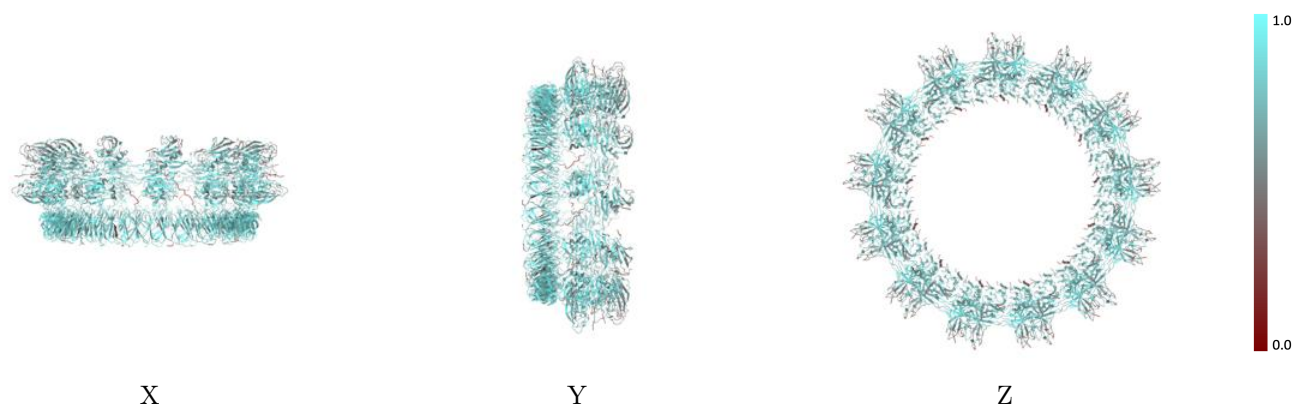
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



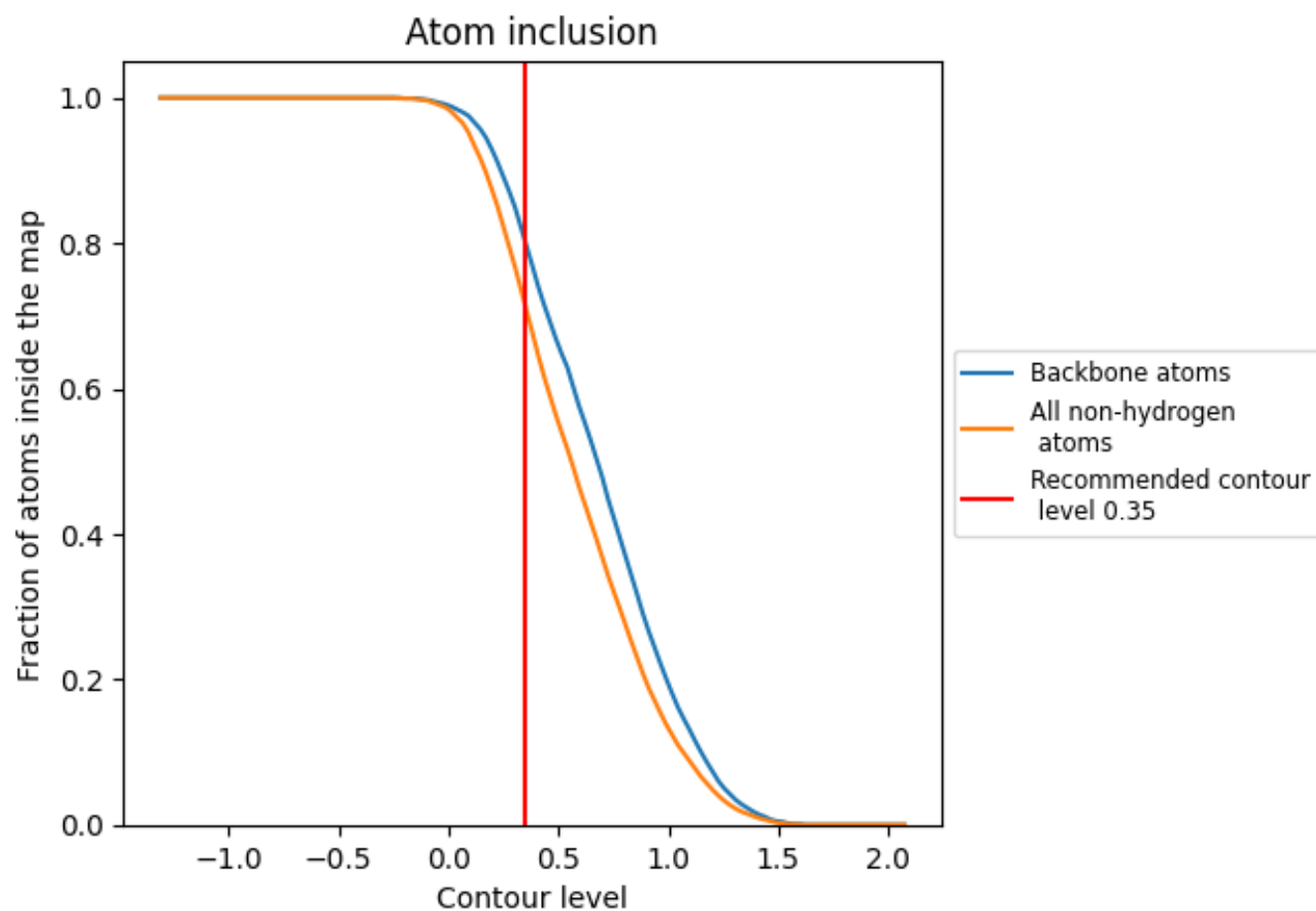
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.4660
A1	 0.7050	 0.4430
A10	 0.7020	 0.4410
A11	 0.7070	 0.4400
A12	 0.7120	 0.4440
A13	 0.7070	 0.4400
A2	 0.7070	 0.4440
A3	 0.7070	 0.4430
A4	 0.7070	 0.4430
A5	 0.7020	 0.4480
A6	 0.7000	 0.4450
A7	 0.7120	 0.4430
A8	 0.7090	 0.4440
A9	 0.7120	 0.4450
B1	 0.7010	 0.4710
B10	 0.7090	 0.4680
B11	 0.7130	 0.4680
B12	 0.7090	 0.4680
B13	 0.7160	 0.4640
B2	 0.7110	 0.4690
B3	 0.7090	 0.4640
B4	 0.7070	 0.4660
B5	 0.7050	 0.4630
B6	 0.7110	 0.4670
B7	 0.7110	 0.4640
B8	 0.7090	 0.4660
B9	 0.7030	 0.4650
C1	 0.7790	 0.4970
C10	 0.7810	 0.4940
C11	 0.7810	 0.4960
C12	 0.7800	 0.4950
C13	 0.7780	 0.4930
C2	 0.7790	 0.4960
C3	 0.7780	 0.4940
C4	 0.7790	 0.4940



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Chain	Atom inclusion	Q-score
C5	 0.7830	 0.4970
C6	 0.7790	 0.4960
C7	 0.7790	 0.4940
C8	 0.7760	 0.4950
C9	 0.7780	 0.4940
D1	 0.6730	 0.4540
D10	 0.6750	 0.4540
D11	 0.6790	 0.4560
D12	 0.6700	 0.4540
D13	 0.6770	 0.4530
D2	 0.6810	 0.4540
D3	 0.6790	 0.4550
D4	 0.6770	 0.4550
D5	 0.6760	 0.4550
D6	 0.6830	 0.4530
D7	 0.6810	 0.4560
D8	 0.6780	 0.4540
D9	 0.6780	 0.4550
E1	 0.2240	 0.2950
E10	 0.2350	 0.2910
E11	 0.2120	 0.2890
E12	 0.2120	 0.2910
E13	 0.2470	 0.3010
E2	 0.2350	 0.3020
E3	 0.2240	 0.2940
E4	 0.2350	 0.2860
E5	 0.2240	 0.2870
E6	 0.2240	 0.2910
E7	 0.2350	 0.2900
E8	 0.2350	 0.2890
E9	 0.2240	 0.2980
F1	 0.6350	 0.4230
F10	 0.6470	 0.4170
F11	 0.6470	 0.4130
F12	 0.6350	 0.4170
F13	 0.6470	 0.4120
F2	 0.6470	 0.4180
F3	 0.6470	 0.4080
F4	 0.6470	 0.4140
F5	 0.6590	 0.4120
F6	 0.6470	 0.4060
F7	 0.6350	 0.4090

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Chain	Atom inclusion	Q-score
F8	 0.6350	 0.4120
F9	 0.6470	 0.4160