



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:21 PM UTC

PDB ID : 3JC8 / pdb_00003jc8
EMDB ID : EMD-3247
Title : Architectural model of the type IVa pilus machine in a piliated state
Authors : Chang, Y.-W.; Rettberg, L.A.; Jensen, G.J.
Deposited on : 2015-11-24
Resolution : Not provided

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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

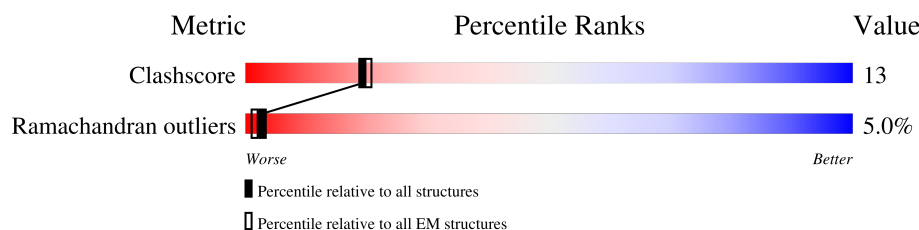
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A1	158	 84% 13% .
1	A2	158	 86% 10% .
1	A3	158	 85% 11% .
1	A4	158	 84% 12% .
1	A5	158	 85% 11% .
1	A6	158	 86% 11% .
1	A7	158	 85% 11% .
1	A8	158	 87% 10% .
1	A9	158	 86% 10% .
1	Aa	158	 82% 14% .

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Mol	Chain	Length	Quality of chain
1	Ab	158	 85% 11% .
1	Ac	158	 85% 11% .
1	Ad	158	 85% 11% .
1	Ae	158	 85% 11% .
1	Af	158	 85% 11% .
1	Ag	158	 85% 11% .
1	Ah	158	 84% 13% .
1	Ai	158	 85% 11% .
1	Aj	158	 85% 11% .
1	Ak	158	 85% 11% .
1	Al	158	 85% 11% .
1	Am	158	 85% 11% .
1	An	158	 83% 12% 5% .
1	Ao	158	 84% 12% .
1	Ap	158	 85% 11% .
1	Aq	158	 86% 10% .
1	Ar	158	 85% 11% .
1	As	158	 86% 11% .
1	At	158	 84% 12% .
1	Au	158	 84% 13% .
1	Av	158	 84% 13% .
1	Aw	158	 85% 11% .
1	Ax	158	 85% 11% .
1	Ay	158	 86% 11% .
1	Az	158	 84% 12% .

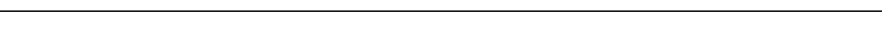
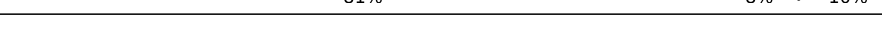
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Mol	Chain	Length	Quality of chain
2	Ba	566	
2	Bb	566	
2	Bc	566	
2	Bd	566	
2	Be	566	
2	Bf	566	
3	Ca	417	
3	Cb	417	
4	Na	225	
4	Nb	225	
4	Nc	225	
4	Nd	225	
4	Ne	225	
4	Nf	225	
4	Ng	225	
4	Nh	225	
4	Ni	225	
4	Nj	225	
4	Nk	225	
4	Nl	225	
5	Oa	205	
5	Ob	205	
5	Oc	205	
5	Od	205	
5	Oe	205	

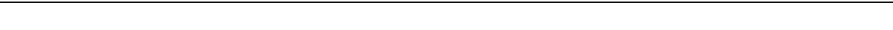
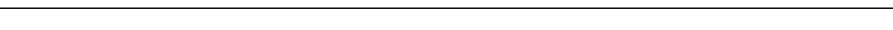
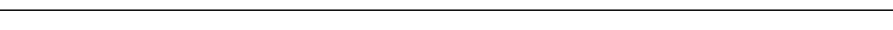
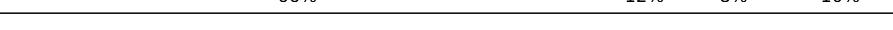
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Mol	Chain	Length	Quality of chain
5	Of	205	 89% 8%
5	Og	205	 89% 8%
5	Oh	205	 89% 8%
5	Oi	205	 87% 8%
5	Oj	205	 88% 8%
5	Ok	205	 87% 8%
5	Ol	205	 88% 8%
6	Ma	395	 84% 5% 10%
6	Mb	395	 81% 9% 10%
6	Mc	395	 84% 5% 10%
6	Md	395	 81% 9% 10%
6	Me	395	 83% 6% 10%
6	Mf	395	 82% 8% 10%
6	Mg	395	 84% 6% 10%
6	Mh	395	 81% 8% 10%
6	Mi	395	 83% 6% 10%
6	Mj	395	 81% 9% 10%
6	Mk	395	 84% 6% 10%
6	Ml	395	 82% 8% 10%
7	Qa	901	 40% 5% 54%
7	Qb	901	 40% 5% 54%
7	Qc	901	 40% 5% 54%
7	Qd	901	 40% 5% 54%
7	Qe	901	 40% 5% 54%
7	Qf	901	 40% 5% 54%

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Mol	Chain	Length	Quality of chain
7	Qg	901	
7	Qh	901	
7	Qi	901	
7	Qj	901	
7	Qk	901	
7	Ql	901	
8	Pa	172	
8	Pb	172	
8	Pc	172	
8	Pd	172	
8	Pe	172	
8	Pf	172	
8	Pg	172	
8	Ph	172	
8	Pi	172	
8	Pj	172	
8	Pk	172	
8	Pl	172	
9	Ta	411	
9	Tb	411	
9	Tc	411	
9	Td	411	
9	Te	411	
9	Tf	411	
9	Tg	411	

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Mol	Chain	Length	Quality of chain
9	Th	411	 32% 8% 60%
9	Ti	411	 31% 9% 60%
9	Tj	411	 31% 8% 60%
9	Tk	411	 31% 8% 60%
9	Tl	411	 31% 8% 60%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 107640 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 PilA.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Aa	158	Total 632	C 316	N 158	O 158	0	0
1	Ab	158	Total 632	C 316	N 158	O 158	0	0
1	Ac	158	Total 632	C 316	N 158	O 158	0	0
1	Ad	158	Total 632	C 316	N 158	O 158	0	0
1	Ae	158	Total 632	C 316	N 158	O 158	0	0
1	Af	158	Total 632	C 316	N 158	O 158	0	0
1	Ag	158	Total 632	C 316	N 158	O 158	0	0
1	Ah	158	Total 632	C 316	N 158	O 158	0	0
1	Ai	158	Total 632	C 316	N 158	O 158	0	0
1	Aj	158	Total 632	C 316	N 158	O 158	0	0
1	Ak	158	Total 632	C 316	N 158	O 158	0	0
1	Al	158	Total 632	C 316	N 158	O 158	0	0
1	Am	158	Total 632	C 316	N 158	O 158	0	0
1	An	158	Total 632	C 316	N 158	O 158	0	0
1	Ao	158	Total 632	C 316	N 158	O 158	0	0
1	Ap	158	Total 632	C 316	N 158	O 158	0	0
1	Aq	158	Total 632	C 316	N 158	O 158	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	Ar	158	Total 632	C 316	N 158	O 158	0	0
1	As	158	Total 632	C 316	N 158	O 158	0	0
1	At	158	Total 632	C 316	N 158	O 158	0	0
1	Au	158	Total 632	C 316	N 158	O 158	0	0
1	Av	158	Total 632	C 316	N 158	O 158	0	0
1	Aw	158	Total 632	C 316	N 158	O 158	0	0
1	Ax	158	Total 632	C 316	N 158	O 158	0	0
1	Ay	158	Total 632	C 316	N 158	O 158	0	0
1	Az	158	Total 632	C 316	N 158	O 158	0	0
1	A1	158	Total 632	C 316	N 158	O 158	0	0
1	A2	158	Total 632	C 316	N 158	O 158	0	0
1	A3	158	Total 632	C 316	N 158	O 158	0	0
1	A4	158	Total 632	C 316	N 158	O 158	0	0
1	A5	158	Total 632	C 316	N 158	O 158	0	0
1	A6	158	Total 632	C 316	N 158	O 158	0	0
1	A7	158	Total 632	C 316	N 158	O 158	0	0
1	A8	158	Total 632	C 316	N 158	O 158	0	0
1	A9	158	Total 632	C 316	N 158	O 158	0	0

- Molecule 2 is a protein called Type IV-A pilus assembly ATPase PilB.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Ba	452	Total 1808	C 904	N 452	O 452	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	Bb	452	Total	C	N	O	0	0
			1808	904	452	452		
2	Bc	452	Total	C	N	O	0	0
			1808	904	452	452		
2	Bd	452	Total	C	N	O	0	0
			1808	904	452	452		
2	Be	452	Total	C	N	O	0	0
			1808	904	452	452		
2	Bf	452	Total	C	N	O	0	0
			1808	904	452	452		

- Molecule 3 is a protein called Type 4 fimbrial assembly protein PilC.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Ca	316	Total	C	N	O	0	0
			1264	632	316	316		
3	Cb	316	Total	C	N	O	0	0
			1264	632	316	316		

- Molecule 4 is a protein called PilN.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Na	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nb	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nc	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nd	223	Total	C	N	O	0	0
			892	446	223	223		
4	Ne	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nf	223	Total	C	N	O	0	0
			892	446	223	223		
4	Ng	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nh	223	Total	C	N	O	0	0
			892	446	223	223		
4	Ni	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nj	223	Total	C	N	O	0	0
			892	446	223	223		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	Nk	223	Total	C	N	O	0	0
			892	446	223	223		
4	Nl	223	Total	C	N	O	0	0
			892	446	223	223		

- Molecule 5 is a protein called PilO.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Oa	189	Total	C	N	O	0	0
			756	378	189	189		
5	Ob	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oc	189	Total	C	N	O	0	0
			756	378	189	189		
5	Od	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oe	189	Total	C	N	O	0	0
			756	378	189	189		
5	Of	189	Total	C	N	O	0	0
			756	378	189	189		
5	Og	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oh	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oi	189	Total	C	N	O	0	0
			756	378	189	189		
5	Oj	189	Total	C	N	O	0	0
			756	378	189	189		
5	Ok	189	Total	C	N	O	0	0
			756	378	189	189		
5	Ol	189	Total	C	N	O	0	0
			756	378	189	189		

- Molecule 6 is a protein called Type IV pilus biogenesis protein PilM.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	Ma	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mb	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mc	355	Total	C	N	O	0	0
			1420	710	355	355		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	Md	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Me	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mf	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mg	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mh	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mi	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mj	355	Total	C	N	O	0	0
			1420	710	355	355		
6	Mk	355	Total	C	N	O	0	0
			1420	710	355	355		
6	ML	355	Total	C	N	O	0	0
			1420	710	355	355		

- Molecule 7 is a protein called PilQ.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Qa	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qb	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qc	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qd	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qe	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qf	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qg	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qh	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qi	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Qj	418	Total	C	N	O	0	0
			1672	836	418	418		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	Qk	418	Total	C	N	O	0	0
			1672	836	418	418		
7	Ql	418	Total	C	N	O	0	0
			1672	836	418	418		

- Molecule 8 is a protein called PilP.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Pa	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pb	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pc	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pd	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pe	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pf	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pg	155	Total	C	N	O	0	0
			620	310	155	155		
8	Ph	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pi	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pj	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pk	155	Total	C	N	O	0	0
			620	310	155	155		
8	Pl	155	Total	C	N	O	0	0
			620	310	155	155		

- Molecule 9 is a protein called LysM domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Ta	163	Total	C	N	O	0	0
			652	326	163	163		
9	Tb	163	Total	C	N	O	0	0
			652	326	163	163		
9	Tc	163	Total	C	N	O	0	0
			652	326	163	163		

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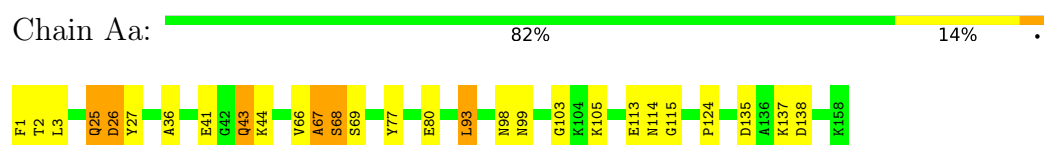
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Mol	Chain	Residues	Atoms				AltConf	Trace
9	Td	163	Total 652	C 326	N 163	O 163	0	0
9	Te	163	Total 652	C 326	N 163	O 163	0	0
9	Tf	163	Total 652	C 326	N 163	O 163	0	0
9	Tg	163	Total 652	C 326	N 163	O 163	0	0
9	Th	163	Total 652	C 326	N 163	O 163	0	0
9	Ti	163	Total 652	C 326	N 163	O 163	0	0
9	Tj	163	Total 652	C 326	N 163	O 163	0	0
9	Tk	163	Total 652	C 326	N 163	O 163	0	0
9	Tl	163	Total 652	C 326	N 163	O 163	0	0

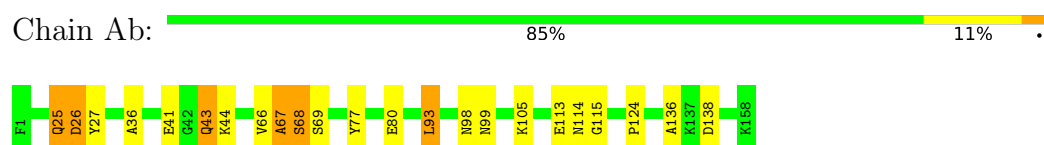
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

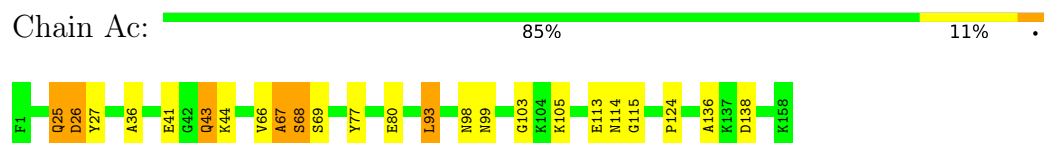
- Molecule 1: PilA



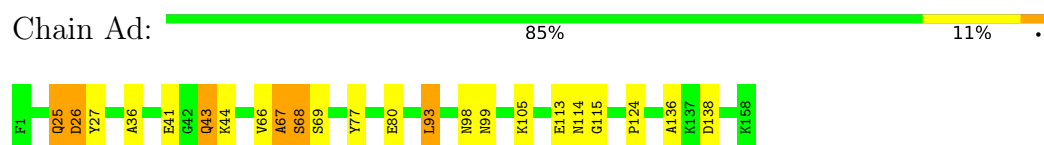
- Molecule 1: PilA



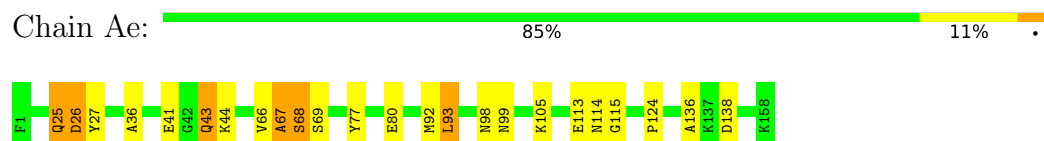
- Molecule 1: PilA



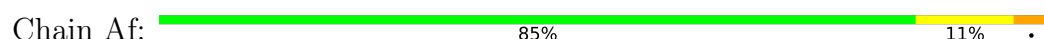
- Molecule 1: PilA



- Molecule 1: PilA

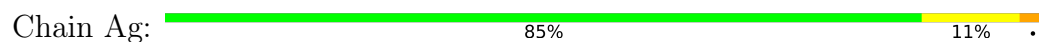


- Molecule 1: PilA

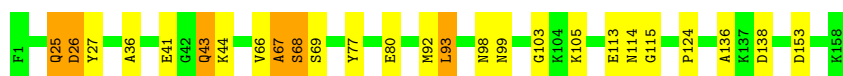
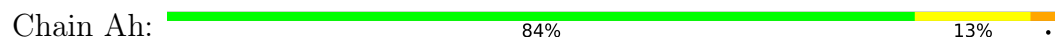




- Molecule 1: PilA



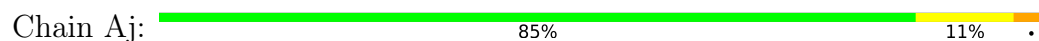
- Molecule 1: PilA



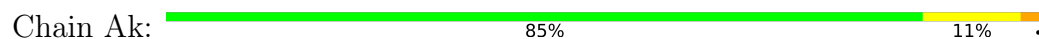
- Molecule 1: PilA



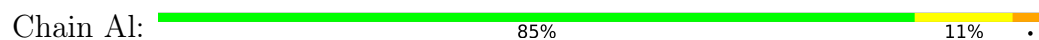
- Molecule 1: PilA



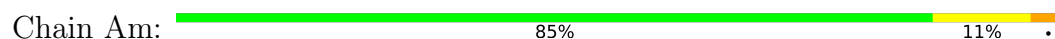
- Molecule 1: PilA



- Molecule 1: PilA



- Molecule 1: PilA





- Molecule 1: PilA

Chain An: 83% 12% 5%



- Molecule 1: PilA

Chain Ao: 84% 12% .



- Molecule 1: PilA

Chain Ap: 85% 11% .



- Molecule 1: PilA

Chain Aq: 86% 10% .



- Molecule 1: PilA

Chain Ar: 85% 11% .



- Molecule 1: PilA

Chain As: 86% 11% .

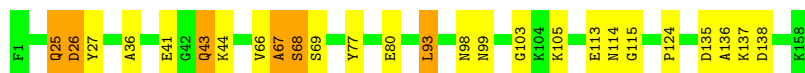
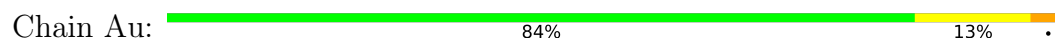


- Molecule 1: PilA

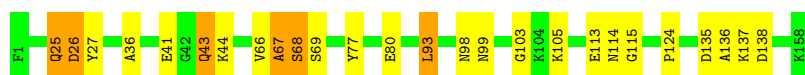
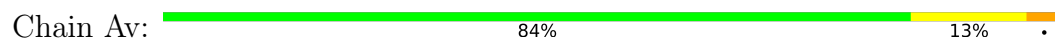
Chain At: 84% 12% .



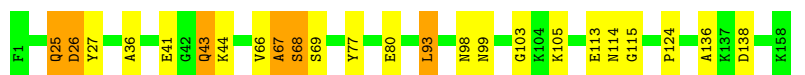
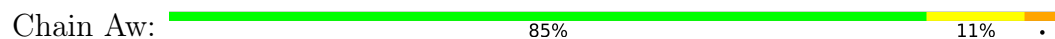
- Molecule 1: PilA



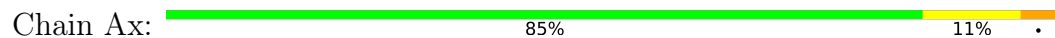
- Molecule 1: PilA



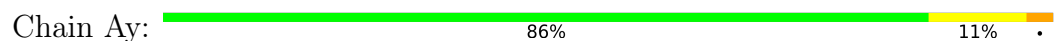
- Molecule 1: PilA



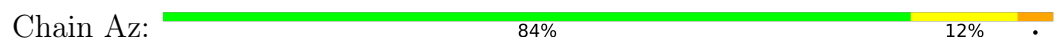
- Molecule 1: PilA



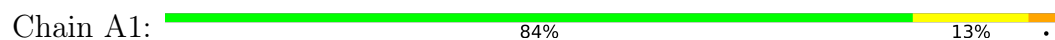
- Molecule 1: PilA



- Molecule 1: PilA



- Molecule 1: PilA





- Molecule 1: PilA

Chain A2: 86% 10% .



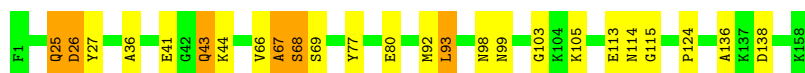
- Molecule 1: PilA

Chain A3: 85% 11% .



- Molecule 1: PilA

Chain A4: 84% 12% .



- Molecule 1: PilA

Chain A5: 85% 11% .



- Molecule 1: PilA

Chain A6: 86% 11% .



- Molecule 1: PilA

Chain A7: 85% 11% .



- Molecule 1: PilA

Chain A8: 87% 10% .



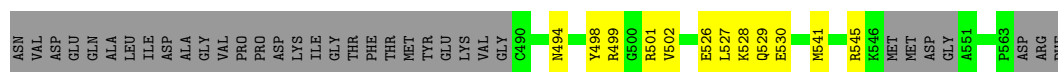
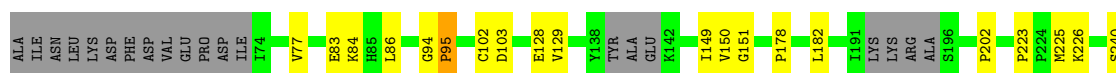
- Molecule 1: PilA

Chain A9: 86% 10%



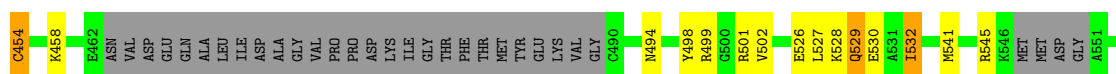
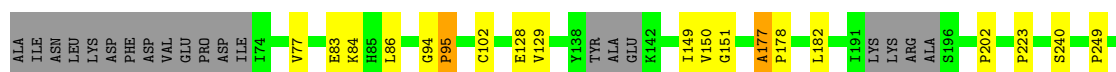
- Molecule 2: Type IV-A pilus assembly ATPase PilB

Chain Ba: 69% 10% 20%



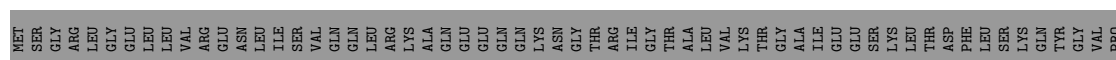
- Molecule 2: Type IV-A pilus assembly ATPase PilB

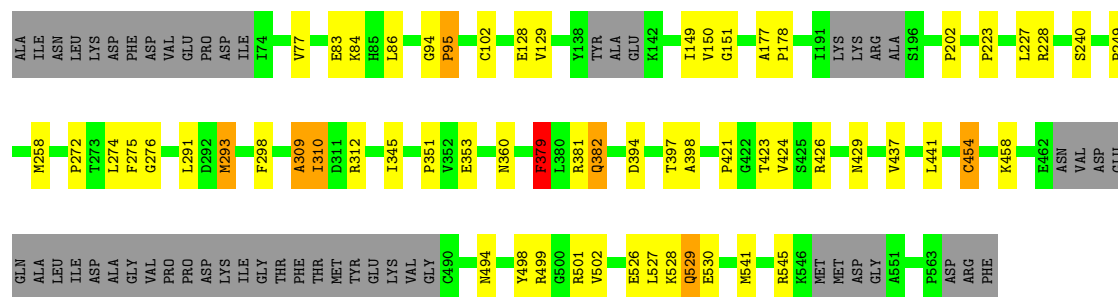
Chain Bb: 67% 10% 20%



- Molecule 2: Type IV-A pilus assembly ATPase PilB

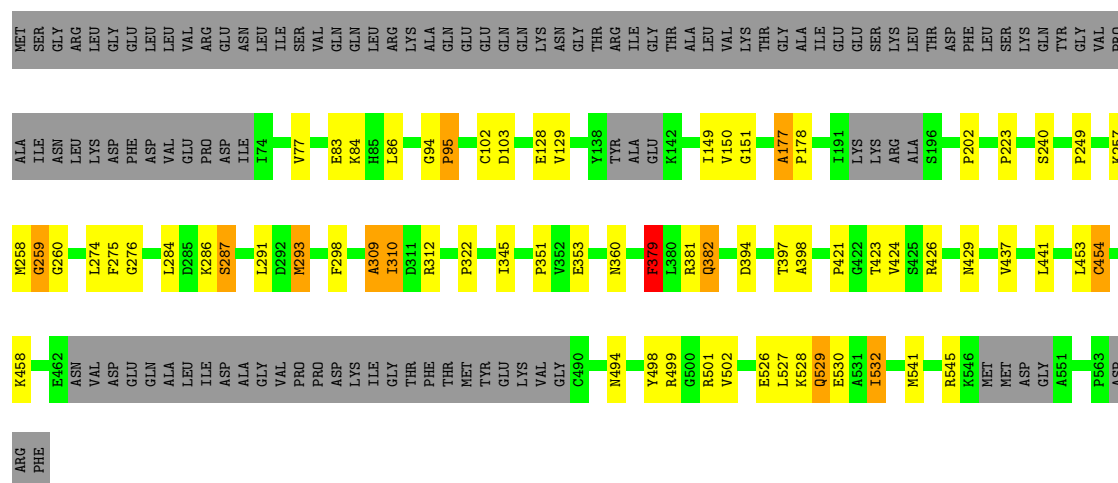
Chain Bc: 69% 10% 20%





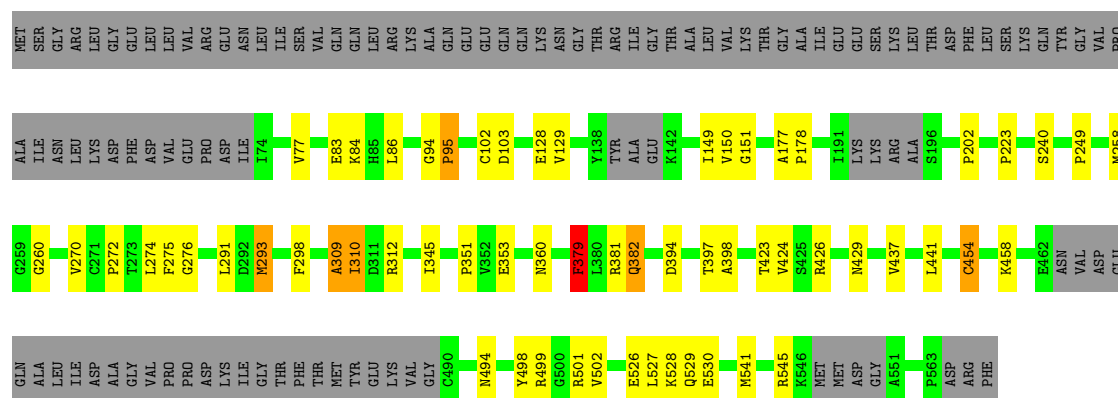
• Molecule 2: Type IV-A pilus assembly ATPase PilB

Chain Bd: 68% 10% 20%



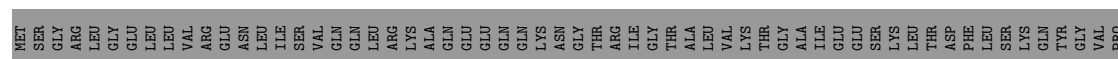
• Molecule 2: Type IV-A pilus assembly ATPase PilB

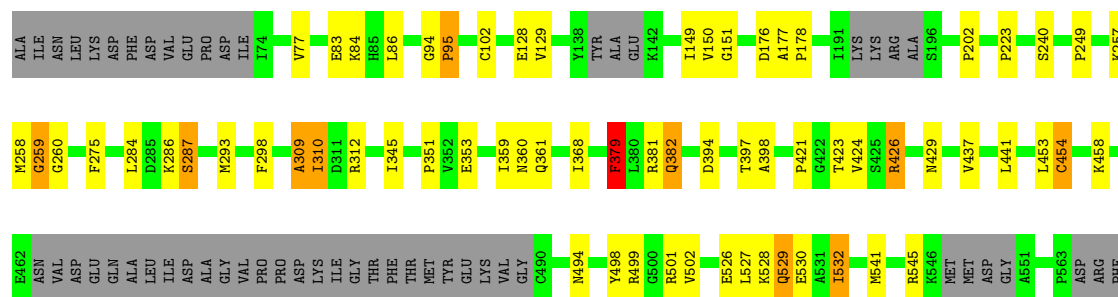
Chain Be: 69% 10% 20%



• Molecule 2: Type IV-A pilus assembly ATPase PilB

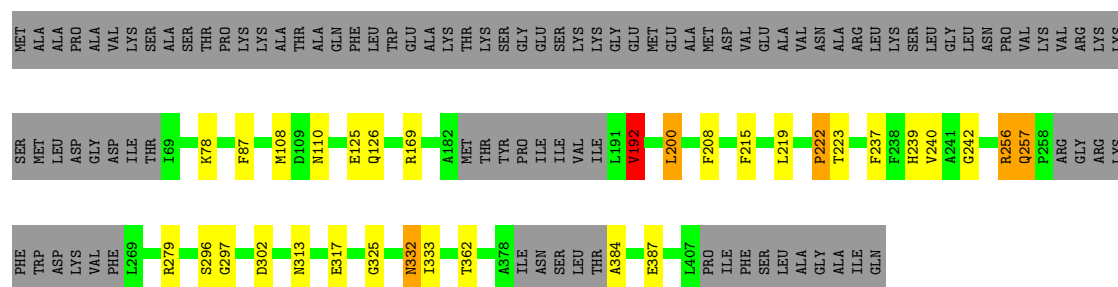
Chain Bf: 68% 10% 20%





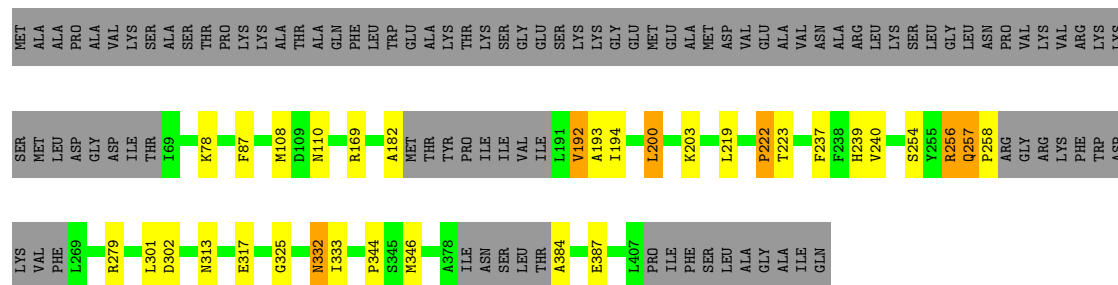
• Molecule 3: Type 4 fimbrial assembly protein PilC

Chain Ca: 68% 6% 24%



• Molecule 3: Type 4 fimbrial assembly protein PilC

Chain Cb: 68% 6% 24%



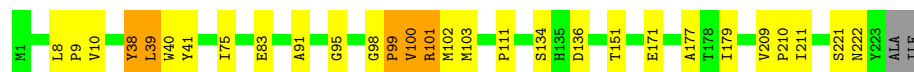
• Molecule 4: PilN

Chain Na: 85% 11% ..



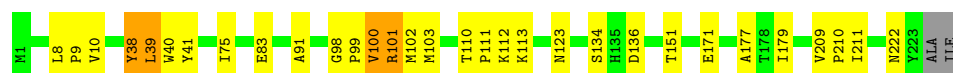
• Molecule 4: PilN

Chain Nb: 86% 11% ..



• Molecule 4: PilN

Chain Nc:  85% 12% ..



• Molecule 4: PiIN

Chain Nd:  87% 10% ..



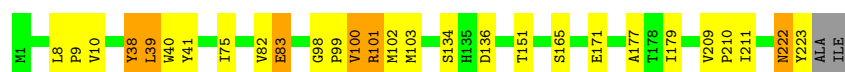
• Molecule 4: PiIN

Chain Ne:  87% 10% ..



• Molecule 4: PiIN

Chain Nf:  87% 10% ..



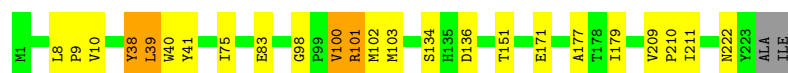
• Molecule 4: PiIN

Chain Ng:  88% 9% ..



• Molecule 4: PiIN

Chain Nh:  88% 9% ..



• Molecule 4: PiIN

Chain Ni:  88% 9% ..



• Molecule 4: PiIN

Chain Nj:  87% 10% ..



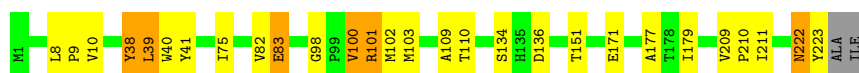
- Molecule 4: PilN

Chain Nk: 88% 9% ..



- Molecule 4: PilN

Chain Nl: 87% 10% ..



- Molecule 5: PilO

Chain Oa: 86% 5% 8%



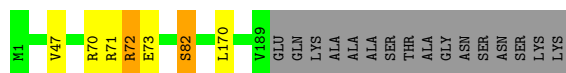
- Molecule 5: PilO

Chain Ob: 87% 5% 8%



- Molecule 5: PilO

Chain Oc: 89% .. 8%



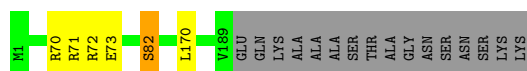
- Molecule 5: PilO

Chain Od: 88% . 8%



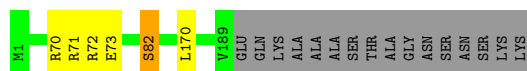
- Molecule 5: PilO

Chain Oe: 89% . 8%



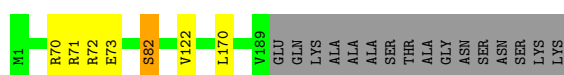
- Molecule 5: PiLO

Chain Of: 89% 8%



- Molecule 5: PiLO

Chain Og: 89% 8%



- Molecule 5: PiLO

Chain Oh: 89% 8%



- Molecule 5: PiLO

Chain Oi: 87% 8%



- Molecule 5: PiLO

Chain Oj: 88% 8%



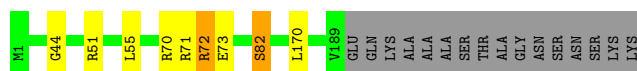
- Molecule 5: PiLO

Chain Ok: 87% 8%



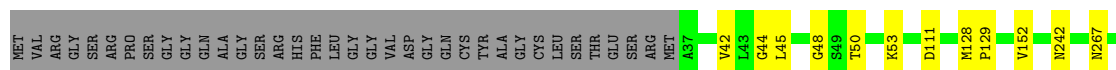
- Molecule 5: PiLO

Chain Ol: 88% 8%



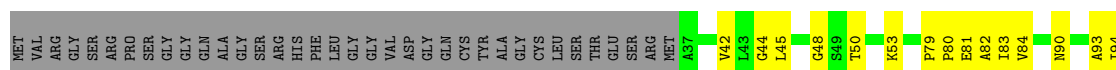
• Molecule 6: Type IV pilus biogenesis protein PilM

Chain Ma: 84% 5% 10%



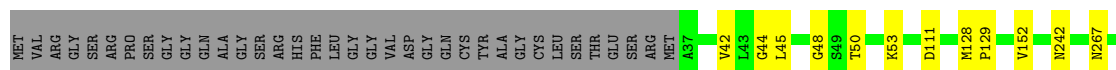
• Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mb: 81% 9% 10%



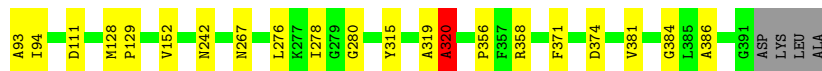
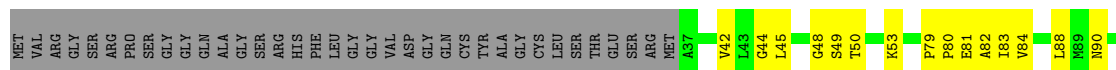
• Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mc: 84% 5% 10%



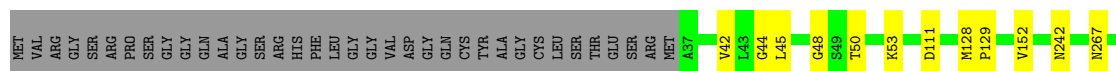
• Molecule 6: Type IV pilus biogenesis protein PilM

Chain Md: 81% 9% 10%



• Molecule 6: Type IV pilus biogenesis protein PilM

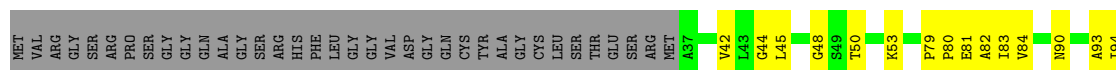
Chain Me: 83% 6% 10%





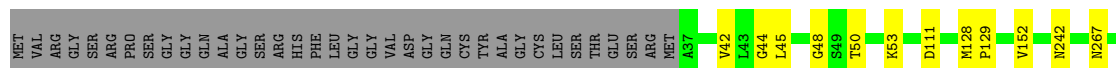
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mf: 82% 8% 10%



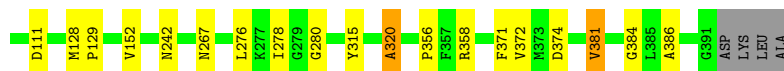
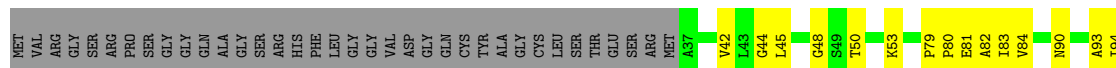
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mg: 84% 6% 10%



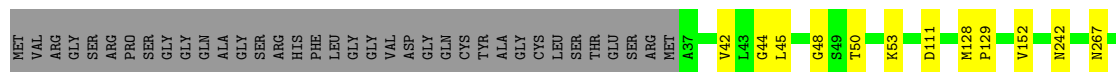
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mh: 81% 8% 10%



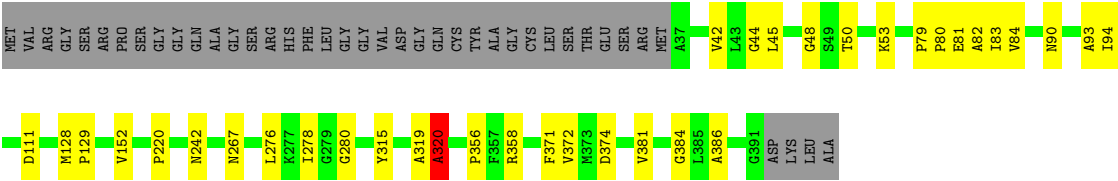
- Molecule 6: Type IV pilus biogenesis protein PilM

Chain Mi: 83% 6% 10%

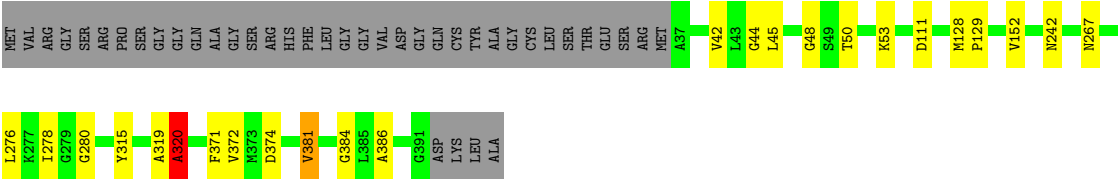
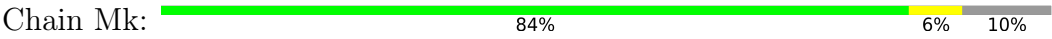


- Molecule 6: Type IV pilus biogenesis protein PilM

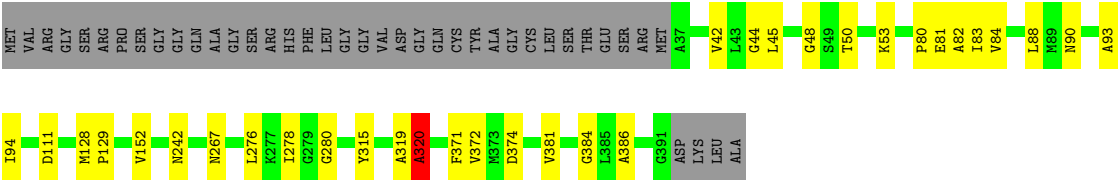
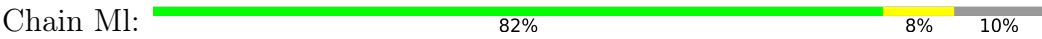
Chain Mj: 81% 9% 10%



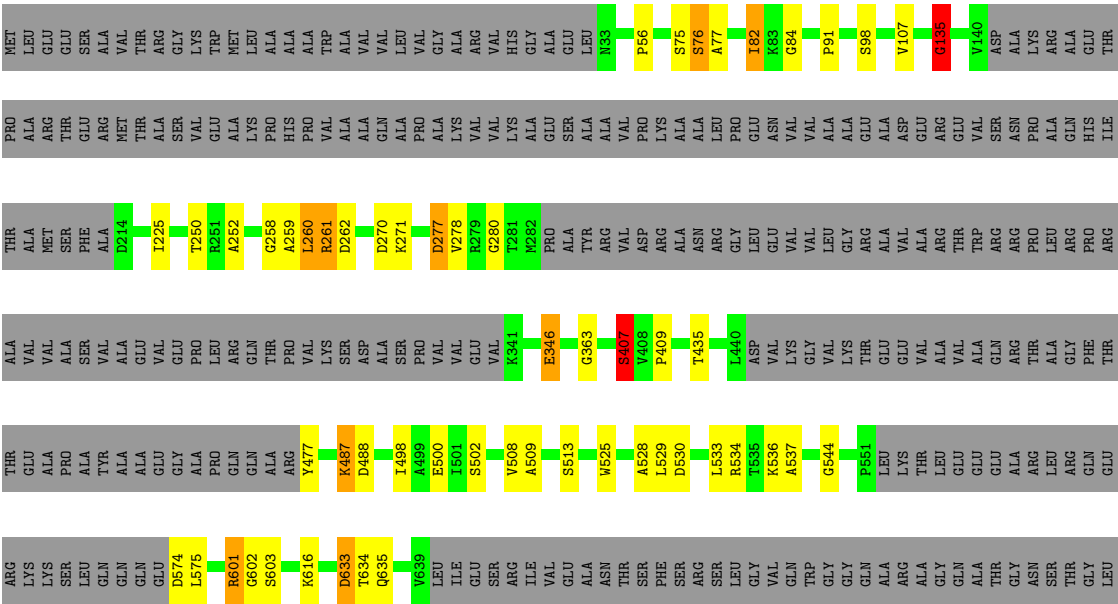
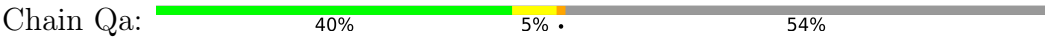
• Molecule 6: Type IV pilus biogenesis protein PilM



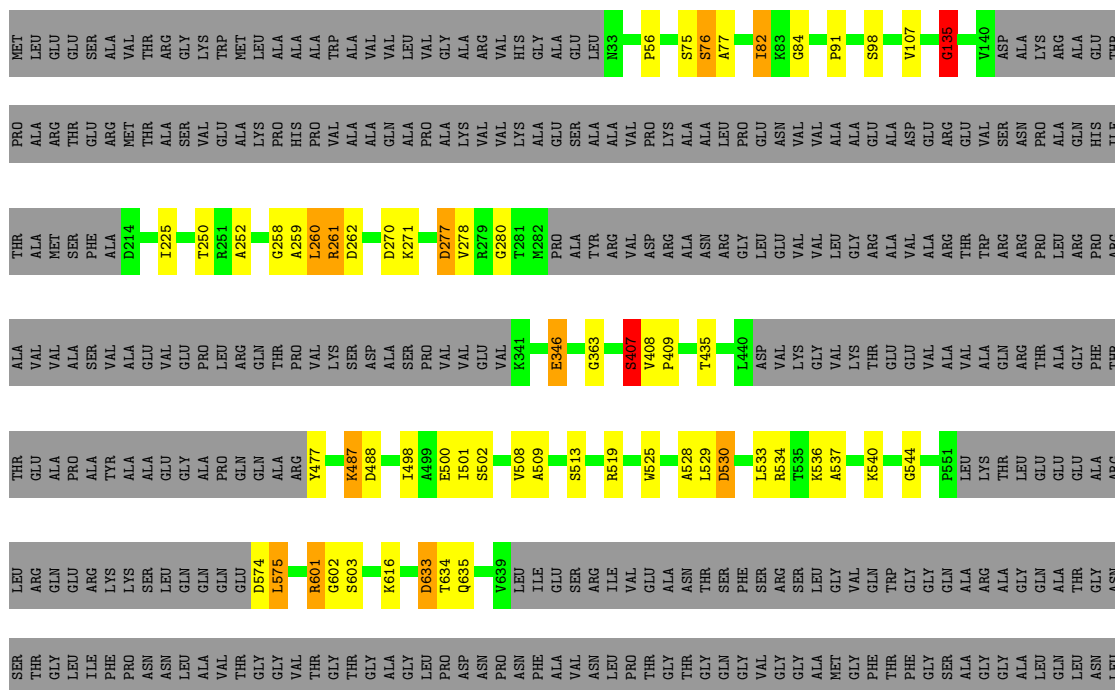
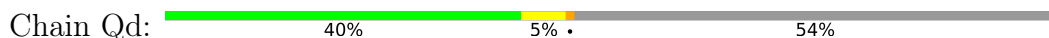
• Molecule 6: Type IV pilus biogenesis protein PilM

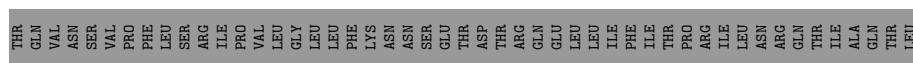


• Molecule 7: PilQ

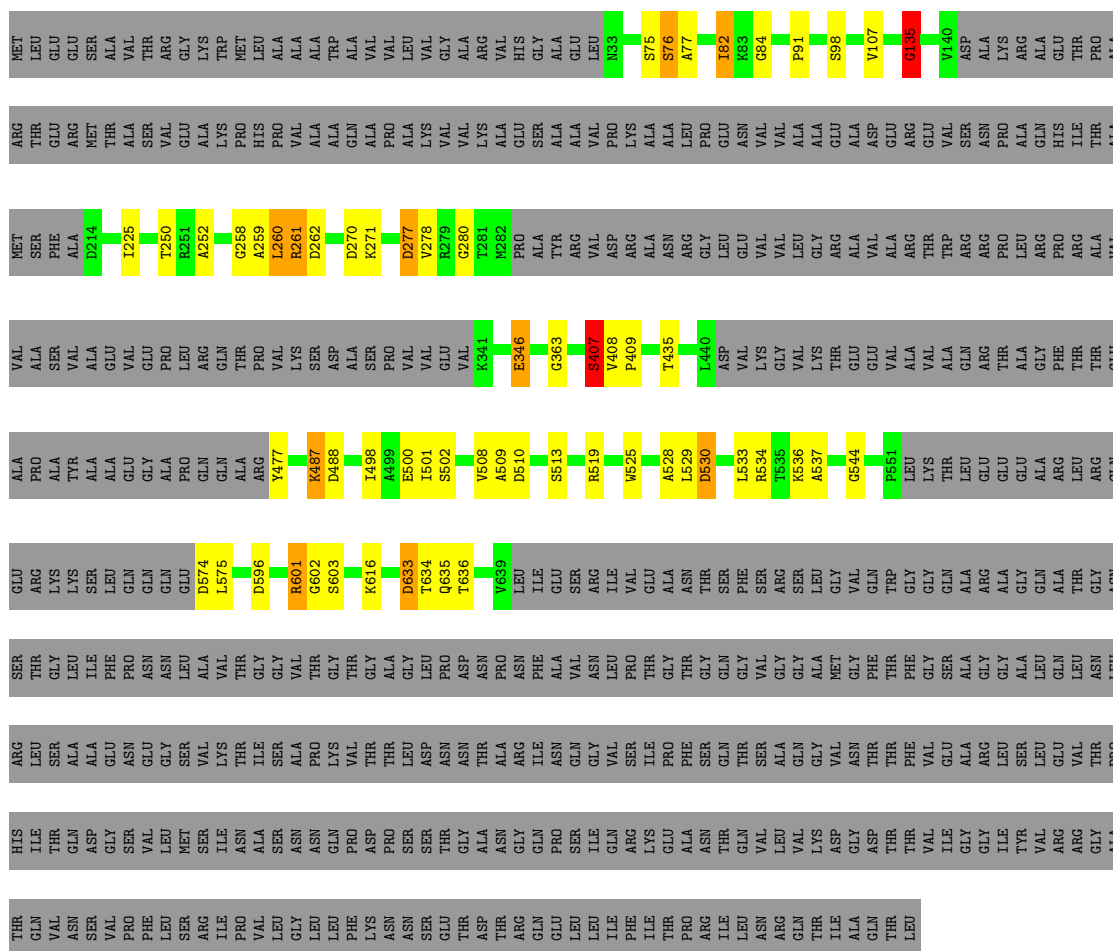


- Molecule 7: PilQ

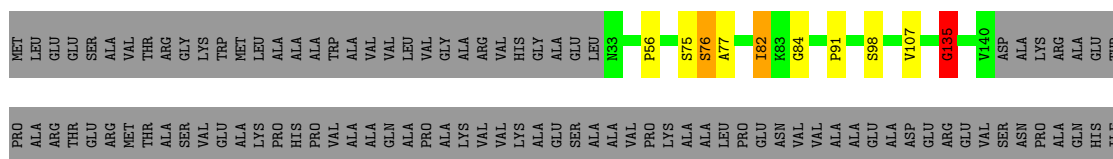




Chain Qe:



Chain Qf: 40% 5% 54%



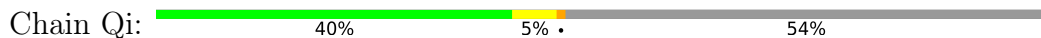


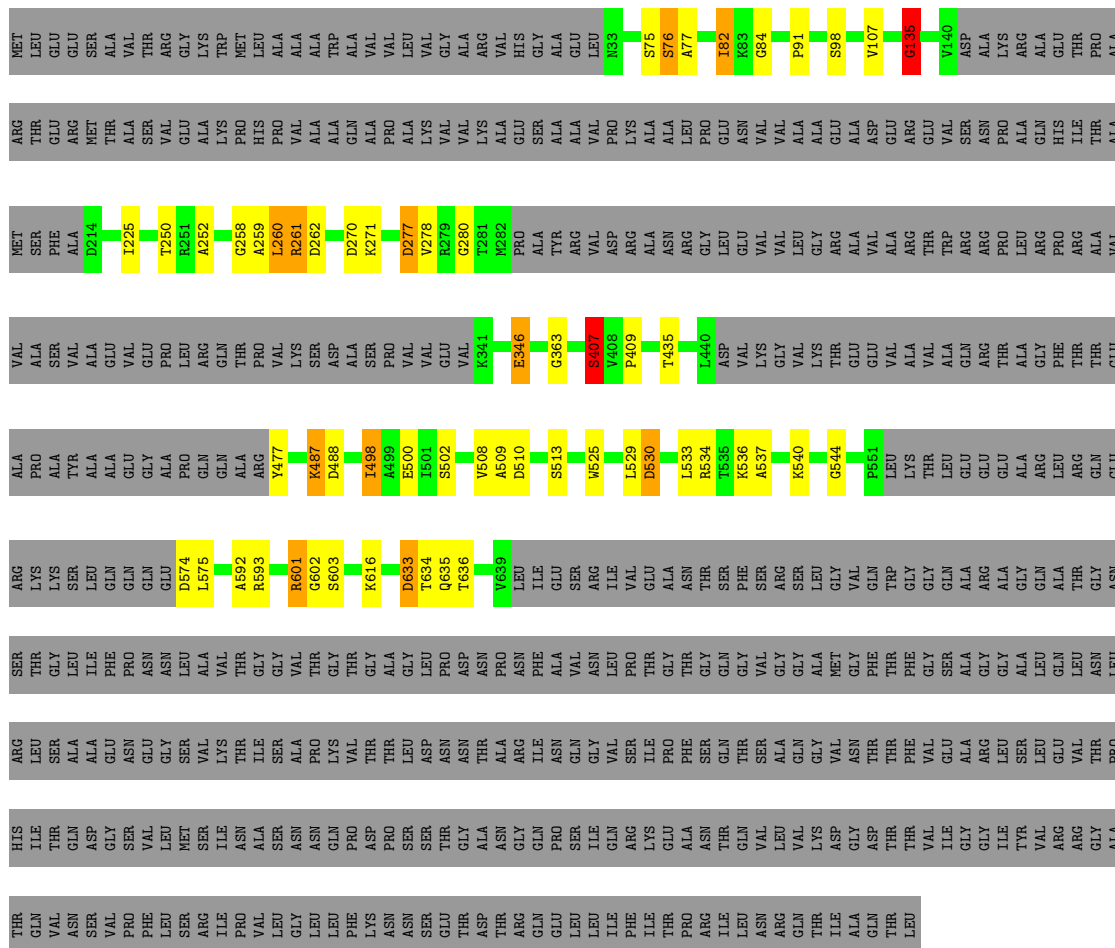
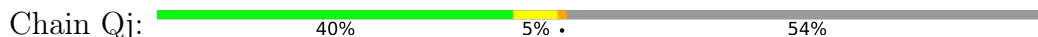
- Molecule 7: PilQ



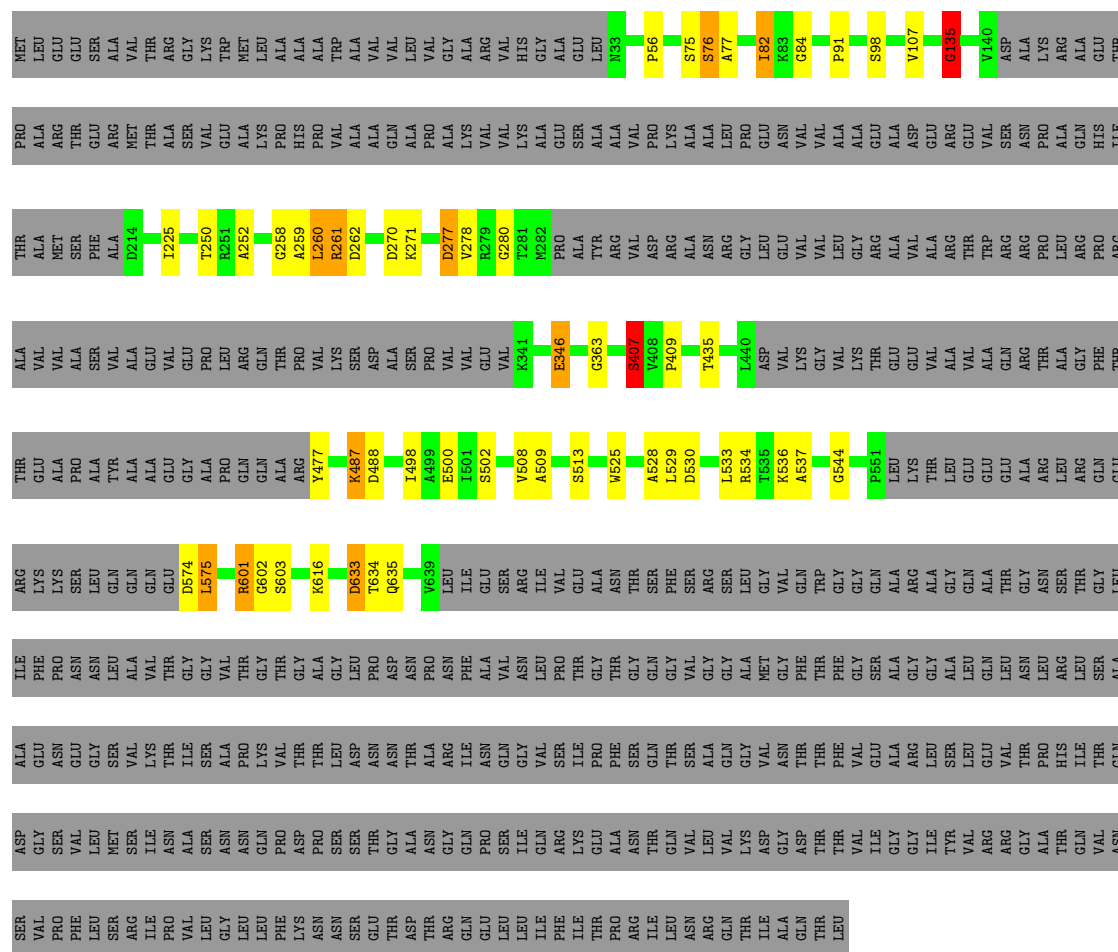
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PRO	PRO	ASN	PRO	ASN	GLY	SER	ALA	SER	PHE	GLU	LEU
PHE	VAL	SER	ASN	GLY	ASN	LEU	ALA	VAL	ALA	ARG	GLU
LEU	LEU	GLN	ASN	LEU	GLN	GLN	ALA	ALA	D214	MET	SER
MET	SER	GLN	ALA	GLU	GLN	ALA	GLU	VAL		THR	ALA
SER	ARG	ALA	ALA	VAL	ALA	GLN	GLY	VAL	I225	ALA	VAL
ILE	ILE	LYS	VAL	LYS	THR	GLN	GLY	GLU		SER	THR
PRO	PRO	THR	THR	THR	GLY	GLY	PRO	PRO	T250	VAL	GLY
VAL	VAL	ILE	GLY	ILE	D574	D574	PRO	LEU	R251	GLU	ARG
SER	SER	ALA	GLY	SER	L575	L575	GLN	ARG	A252	ALA	LYS
ASN	ASN	PRO	THR	PRO	R601	R601	ALA	THR	G258	PRO	MET
LEU	LEU	GLN	GLY	GLY	G602	G602	ARG	PRO	A259	HIS	LEU
PHE	PHE	VAL	THR	THR	S603	S603	VAL	VAL	L260	PRO	ALA
LYS	LYS	THR	GLY	THR	K616	K616	LYS	LYS	R261	VAL	ALA
ASN	ASN	THR	ALA	THR			SER	SER	D262	ALA	ALA
ASN	ASN	LEU	GLY	ASP	D488	D488	ASP	ASP		ALA	TRP
SER	SER	LEU	LEU	ASP			ALA	ALA	D270	GLN	ALA
GLU	GLU	ASN	PRO	ASN	D633	D633	SER	SER	K271	VAL	ALA
THR	THR	ASN	PRO	THR	T634	T634	ALA	ALA		ALA	VAL
GLY	GLY	ASP	ASP	ASN	Q635	Q635	PRO	PRO		PRO	VAL
THR	THR	ALA	ASN	THR	E500	E500	VAL	VAL	D277	ALA	LEU
ASN	ASN	ALA	PRO	ALA	I501	I501	VAL	VAL	R278	LYS	VAL
ARG	ARG	ILE	ASN	ARG	V639	V639	GLU	GLU	V279	VAL	GLY
GLN	GLN	ILE	PHE	ILE	LEU	LEU	VAL	VAL	G280	VAL	ALA
PRO	PRO	ASN	ALA	ASN	GLU	GLU	R341	R341	T281	LYS	ARG
LEU	LEU	GLN	VAL	GLN	SER	SER	A509	A509	M282	ALA	VAL
ILE	ILE	GLY	ASN	GLY	ARG	ARG	S513	S513	PRO	GLU	HIS
ILE	ILE	VAL	LEU	VAL	ILE	ILE			ALA	SER	GLY
PHE	PHE	SER	SER	SER	VAL	VAL	W513	W513	ALA	ALA	ALA
THR	THR	ILE	THR	ILE	GLU	GLU	W525	W525	ARG	VAL	LEU
PRO	PRO	PHE	THR	GLY	ALA	ALA			ARG	VAL	VAL
ASN	ASN	SER	THR	GLY	ASN	ASN	A528	A528	ASP	PRO	PRO
ILE	ILE	THR	GLN	THR	SER	SER	L529	L529	ARG	LYS	ALA
GLN	GLN	THR	GLY	THR	PHE	PHE	D530	D530	ALA	ALA	ALA
VAL	VAL	THR	GLY	SER	VAL	VAL	L533	L533	ASN	ALA	ALA
ASN	ASN	SER	VAL	SER	VAL	VAL	R534	R534	ARG	ARG	LEU
GLN	GLN	ARG	ALA	GLN	GLY	GLY	T535	T535	GLY	PRO	GLU
VAL	VAL	THR	ALA	GLN	SER	SER	K536	K536	LEU	ASN	ASN
ILE	ILE	THR	THR	VAL	GLY	GLY	A537	A537	GLU	VAL	VAL
ALA	ALA	ASN	GLY	VAL	VAL	VAL			VAL	VAL	VAL
GLN	GLN	THR	PHE	THR	PHE	PHE	K540	K540	LEU	ALA	ALA
THR	THR	THR	THR	THR	TRP	TRP	G544	G544	GLY	ALA	ALA
VAL	VAL	VAL	VAL	VAL	GLY	GLY			ARG	GLU	GLU
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GLY	GLY	GLY	ALA	ALA	ALA	ALA	LEU	LEU	ALA	GLU	GLU
GLY	GLY	ILE	SER	ARG	LYS	LYS	LYS	LYS	ALA	ARG	ARG
ILE	ILE	THR	THR	THR	GLY	GLY	VAL	VAL	TRP	VAL	VAL
VAL	VAL	VAL	LEU	LEU	LEU	LEU	GLN	GLN	ARG	SER	SER
ARG	ARG	VAL	GLU	GLU	GLU	ALA	GLU	ARG	PRO	ASN	ALA
GLY	GLY	THR	THR	THR	GLY	GLY	ALA	ALA	LEU	PRO	LYS
ALA	ALA	PRO	PRO	PRO	ASN	ASN	ALA	ALA	GLN	ALA	ARG
HIS	HIS	THR	THR	THR	SER	SER	LEU	PHE	GLN	HIS	THR
ILE	ILE	THR	THR	THR	LEU	LEU	THR	THR	THR	ILE	THR
THR	THR	GLN	GLN	THR	GLY	GLY	THR	THR	THR	THR	THR
VAL	VAL	ASN	ALA	GLN	THR	THR	GLN	THR	VAL	VAL	ALA

- Molecule 7: PilQ

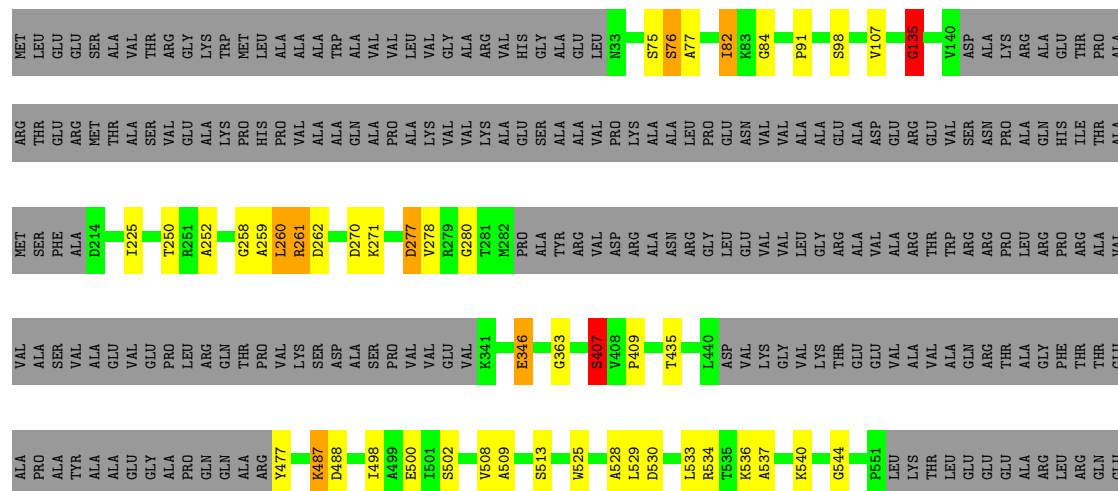
[illegible]

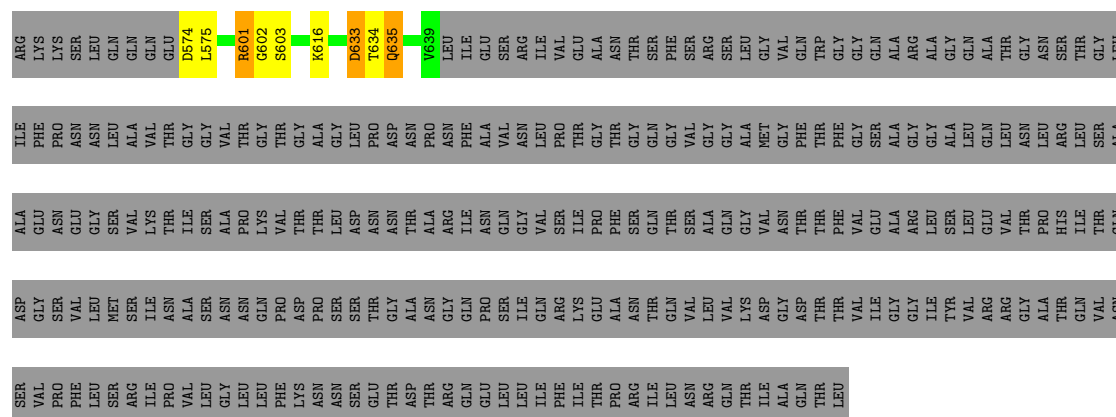


Chain Qk:



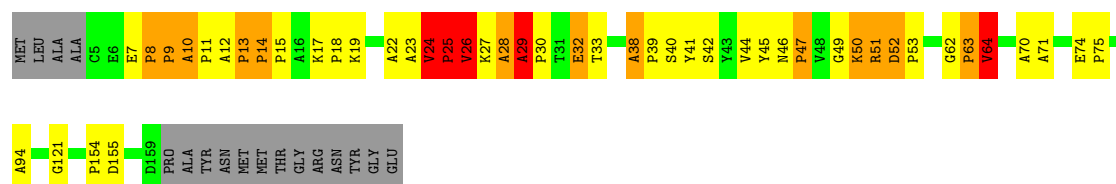
Chain Q1: 40% 5% 54%





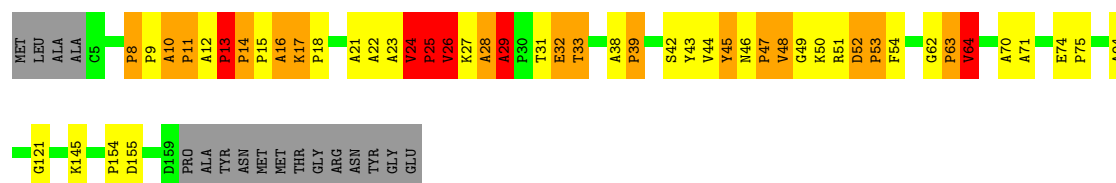
• Molecule 8: PilP

Chain Pa: 62% 17% 8% 10%



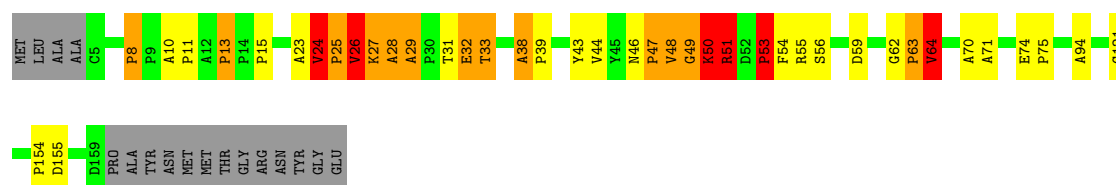
• Molecule 8: PilP

Chain Pb: 61% 16% 9% 10%



• Molecule 8: PilP

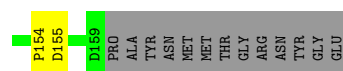
Chain Pc: 66% 13% 8% 10%



• Molecule 8: PilP

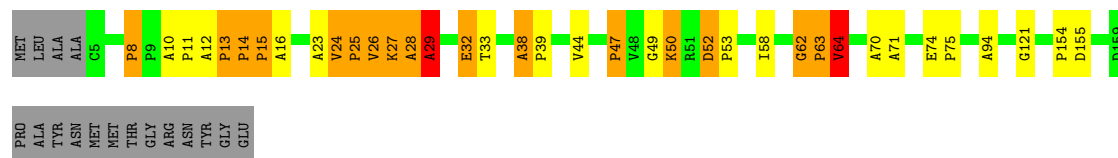
Chain Pd: 66% 13% 9% 10%





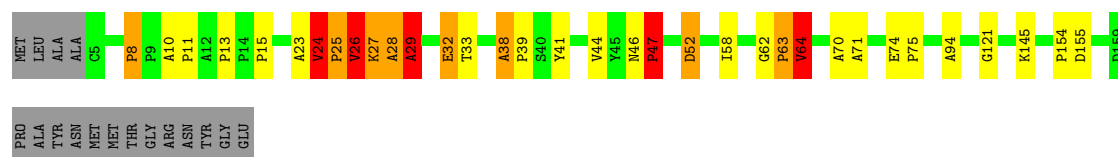
• Molecule 8: PiIP

Chain Pe: 69% 11% 9% • 10%



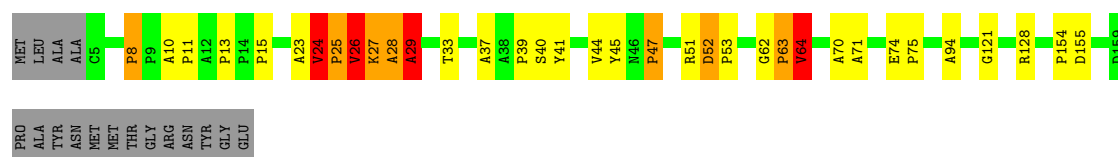
• Molecule 8: PiIP

Chain Pf: 70% 12% 5% • 10%



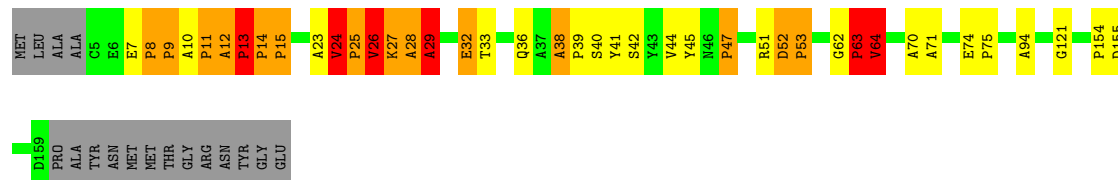
• Molecule 8: PiIP

Chain Pg: 70% 14% • • 10%



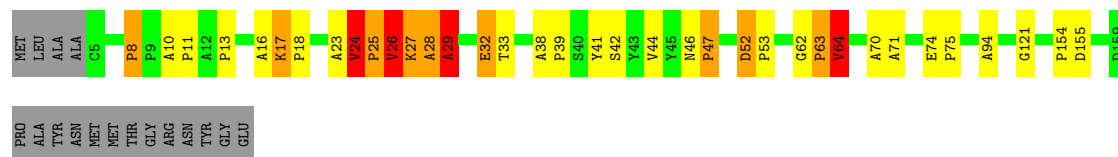
• Molecule 8: PiIP

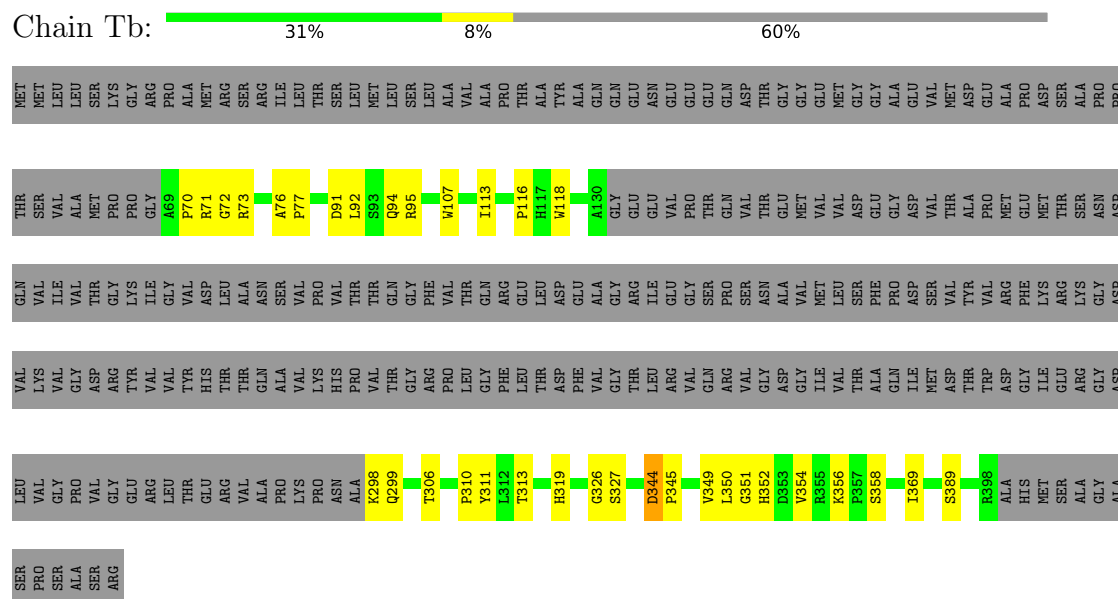
Chain Ph: 66% 12% 8% • 10%



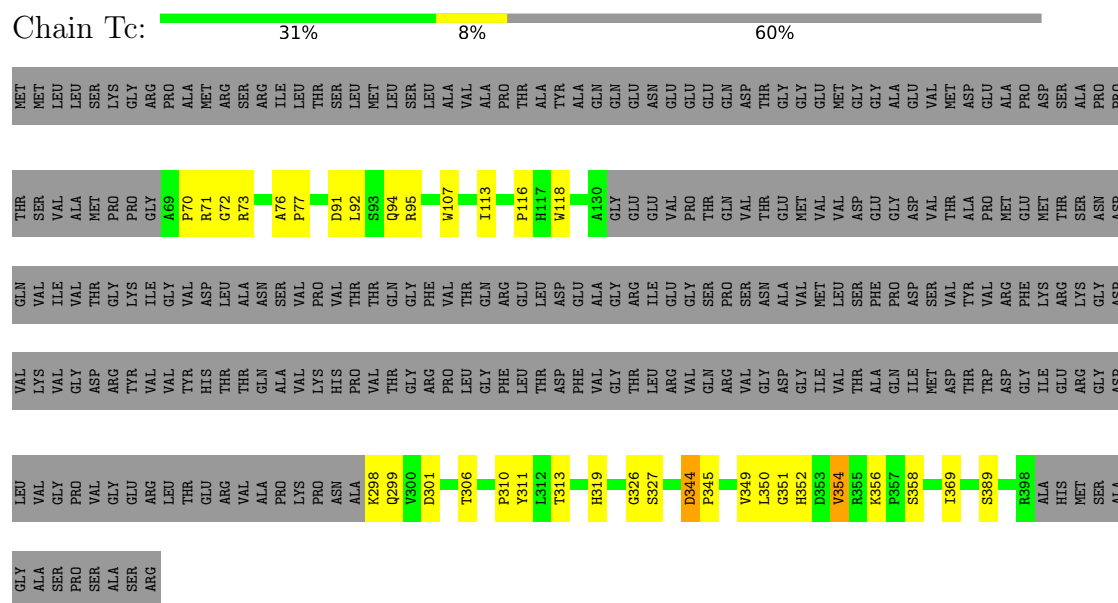
• Molecule 8: PiIP

Chain Pi: 69% 13% 5% • 10%

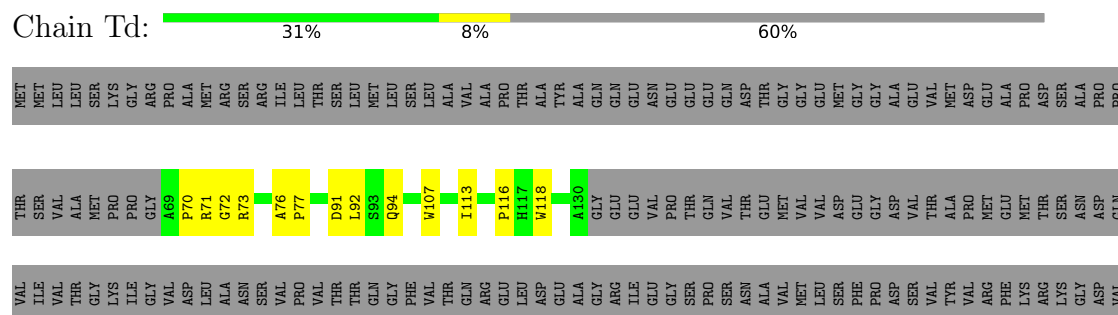




- Molecule 9: LysM domain protein



- Molecule 9: LysM domain protein



PRO	VAL	LYS	VAL	THR	VAL	THR	MET
SER	GLY	VAL	GLY	ILE	SER	SER	LEU
ALA	PRO	GLY	ASP	THR	ALA	VAL	LEU
SER	VAL	ARG	TYR	GLY	GLY	MET	SER
ARG	GLU	TYR	VAL	LYS	PRO	LYS	LYS
	ARG	VAL	VAL	ILE	PRO	GLY	GLY
	THR	THR	THR	VAL	ASP	A69	PRO
	GLU	HIS	HIS	LEU	R71	R71	ALA
	ARG	THR	THR	ALA	G72	G72	MET
	VAL	THR	THR	ASN	R73	R73	ARG
	ALA	GLN	GLN	SER			SER
	PRO	VAL	VAL	VAL	A76	A76	ILE
	LYS	VAL	VAL	PRO	P77	P77	LEU
	ASN	HIS	VAL	THR	D91	D91	THR
	ALA	PRO	THR	THR			SER
	K298	VAL	THR	THR			LEU
	Q299	GLY	GLY	GLN	Q94	Q94	MET
		ARG	ARG	PHE	R95	R95	LEU
	T306	PRO	PRO	VAL	W107	W107	SER
	P310	LEU	LEU	THR			LEU
	Y311	GLY	GLY	GLN	I113	I113	ALA
	I312	PHE	ARG	ARG			VAL
	T313	LEU	LEU	GLU	P116	P116	ALA
		THR	THR	LEU	W117	W117	THR
	H319	ASP	ASP	GLU	W118	W118	ALA
		PHE	PHE	GLU			TYR
	G326	VAL	VAL	ALA	A130	A130	ALA
	S327	GLY	GLY	GLY			GLN
		THR	THR	ARG	GLU	GLU	GLN
	D344	LEU	LEU	ILE	GLU	GLU	GLU
	P345	ARG	ARG	GLU	VAL	VAL	ASN
		VAL	VAL	GLY	PRO	PRO	GLU
	V349	GLN	GLN	SER	THR	THR	GLU
	I350	ARG	ARG	PRO	GLN	GLN	GLU
	G351	VAL	VAL	SER	VAL	VAL	GLN
	H352	GLY	GLY	ASN	THR	THR	THR
	P353	ASP	ASP	ALA	GLU	GLU	ASP
	V354	GLY	GLY	VAL	MET	MET	GLY
	R355	ILE	ILE	LEU	VAL	VAL	GLY
	K356	THR	THR	SER	ASP	ASP	MET
	P357	ALA	ALA	PHE	GLU	GLU	GLY
	S358	GLN	GLN	PRO	GLY	GLY	ALA
		ILE	ILE	ASP	ASP	ASP	ALA
	I369	MET	MET	SER	VAL	VAL	GLU
		ASP	ASP	THR	THR	THR	GLU
	S389	THR	THR	VAL	ALA	ALA	VAL
		TRP	TRP	ARG	PRO	PRO	ASP
	R398	ASP	ASP	VAL	MET	MET	ASP
	ALA	GLY	GLY	PHE	GLU	GLU	ALA
	HIS	ILE	ILE	LYS	THR	THR	PRO
	MET	GLU	GLU	ARG	MET	MET	ASP
	SER	ALA	ALA	LYS	ASN	ASN	SER
	GLY	GLY	GLY	GLY	ASP	ASP	ALA
	ALA	ASP	ASP	VAL	GLN	GLN	PRO
	SER	LEU	LEU	VAL	THR	THR	PRO

PRO	VAL	LYS	VAL	MET	THR	ALA	THR	MET
SER	GLY	VAL	ILE	SER	SER	GLY	VAL	LEU
ALA	PRO	GLY	VAL	ALA	ALA	GLY	VAL	ALA
SER	VAL	ASP	THR	GLY	PRO	GLY	MET	SER
ARG	GLY	ARG	GLY	THR	LYS	PRO	GLY	LYS
	GLU	TYR	ILE	ILE	ILE	PRO	GLY	ARG
	ARG	VAL	VAL	VAL	VAL	PRO	GLY	PRO
	LEU	VAL	VAL	VAL	VAL	PRO	GLY	ALA
	THR	TYR	ASP	P70	A69	ALA	THR	ALA
	GLU	HIS	ASP	LEU	R71	MET	THR	ARG
	ARG	THR	THR	ALA	G72	SER	THR	ARG
	VAL	THR	ASN	ASN	R73	ARG	THR	ARG
	ALA	GLN	VAL	VAL	A76	ILE	THR	LEU
	PRO	ALA	VAL	VAL	P77	THR	THR	THR
	PRO	LYS	VAL	VAL			SER	SER
	ASN	HIS	THR	THR	D91	THR	THR	THR
	ALA	PRO	THR	THR	L92	THR	THR	SER
	K298	VAL	GLN	GLN	S93	GLN	GLN	MET
	Q299	THR	GLY	GLY	Q94	GLY	GLY	MET
		ARG	ARG	PHE				SER
	T306	PRO	VAL	VAL	W107	LEU	LEU	LEU
		LEU	THR	THR		ALA	ALA	ALA
	P310	GLY	GLN	GLN	I113	VAL	VAL	VAL
	V311	PHE	ARG	ARG		ALA	ALA	ALA
	L312	LEU	GLU	GLU	P116	PRO	PRO	PRO
	T313	THR	LEU	LEU	H117	THR	THR	THR
		ASP	ASP	ASP	W118	ALA	ALA	ALA
	H319	PHE	GLU	GLU		TYR	TYR	TYR
		VAL	ALA	ALA	A130	ALA	ALA	ALA
	G326	VAL	GLY	GLY	GLY	GLN	GLN	GLN
	S327	THR	THR	THR	GLU	GLU	GLU	GLU
	D344	LEU	ILE	ILE	GLU	GLU	GLU	GLU
	P345	ARG	GLY	GLY	VAL	ASN	ASN	ASN
		VAL	GLY	GLY	PRO	GLU	GLU	GLU
	V349	GLN	SER	SER	THR	THR	THR	THR
	L350	ARG	PRO	PRO	GLN	GLN	GLN	GLN
	G351	VAL	SER	SER	VAL	VAL	VAL	VAL
	H352	GLY	ASN	ASN	THR	THR	THR	THR
	P353	ASP	ALA	ALA	GLU	GLU	GLU	GLU
	V354	GLY	VAL	VAL	MET	MET	MET	MET
	R355	ILE	MET	MET	VAL	VAL	VAL	VAL
	K356	THR	SER	SER	ASP	ASP	ASP	ASP
	P357	ALA	PHE	PHE	GLU	GLU	GLU	GLU
	S358	GLN	PRO	PRO	GLY	GLY	GLY	GLY
		ILE	ASP	ASP	ASP	ALA	ALA	ALA
	T369	MET	SER	SER	VAL	VAL	VAL	VAL
		THR	THR	THR	THR	THR	THR	THR
	S389	ASP	VAL	VAL	ALA	ALA	ALA	ALA
		TRP	VAL	VAL	PRO	PRO	PRO	PRO
	R398	ASP	ARG	ARG	MET	MET	MET	MET
	ALA	GLY	PHE	PHE	GLU	GLU	GLU	GLU
	HIS	GLY	THR	THR	GLU	GLU	GLU	GLU
	VAL	ILE	LYS	LYS	MET	MET	MET	MET
	MET	GLU	ARG	ARG	THR	THR	THR	THR
	SER	GLY	LYS	LYS	ASN	ASN	ASN	ASN
	ALA	ASP	ASP	ASP	GLN	GLN	GLN	GLN
	SER	THR	VAL	VAL	THR	THR	THR	THR

[illegible]

Response	Percentage
Used	31%
Not used	8%
Don't know	60%



4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	150	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MEA

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	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
1	A2	1.14	1/627 (0.2%)	1.43	9/782 (1.2%)
1	A3	1.14	1/627 (0.2%)	1.44	11/782 (1.4%)
1	A4	1.14	1/627 (0.2%)	1.44	11/782 (1.4%)
1	A5	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	A6	1.11	1/627 (0.2%)	1.45	11/782 (1.4%)
1	A7	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
1	A8	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	A9	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Aa	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Ab	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Ac	1.13	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Ad	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Ae	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Af	1.13	1/627 (0.2%)	1.42	9/782 (1.2%)
1	Ag	1.14	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Ah	1.13	1/627 (0.2%)	1.43	12/782 (1.5%)
1	Ai	1.12	1/627 (0.2%)	1.44	11/782 (1.4%)
1	Aj	1.14	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Ak	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Al	1.13	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Am	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
1	An	1.11	1/627 (0.2%)	1.42	9/782 (1.2%)
1	Ao	1.13	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Ap	1.13	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Aq	1.14	1/627 (0.2%)	1.42	9/782 (1.2%)
1	Ar	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
1	As	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	At	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Au	1.14	1/627 (0.2%)	1.43	11/782 (1.4%)
1	Av	1.14	1/627 (0.2%)	1.44	11/782 (1.4%)
1	Aw	1.14	1/627 (0.2%)	1.43	11/782 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ax	1.14	1/627 (0.2%)	1.44	10/782 (1.3%)
1	Ay	1.14	1/627 (0.2%)	1.43	10/782 (1.3%)
1	Az	1.13	1/627 (0.2%)	1.44	11/782 (1.4%)
2	Ba	0.61	0/1803	1.13	17/2245 (0.8%)
2	Bb	0.79	2/1803 (0.1%)	1.16	19/2245 (0.8%)
2	Bc	0.61	0/1803	1.14	17/2245 (0.8%)
2	Bd	0.66	1/1803 (0.1%)	1.18	22/2245 (1.0%)
2	Be	0.61	0/1803	1.13	17/2245 (0.8%)
2	Bf	0.65	2/1803 (0.1%)	1.19	22/2245 (1.0%)
3	Ca	1.09	1/1260 (0.1%)	1.71	10/1568 (0.6%)
3	Cb	1.10	1/1260 (0.1%)	1.71	10/1568 (0.6%)
4	Na	0.37	0/891	0.89	1/1112 (0.1%)
4	Nb	0.38	0/891	0.90	1/1112 (0.1%)
4	Nc	0.38	0/891	0.90	1/1112 (0.1%)
4	Nd	0.38	0/891	0.90	1/1112 (0.1%)
4	Ne	0.39	0/891	0.90	1/1112 (0.1%)
4	Nf	0.38	0/891	0.90	1/1112 (0.1%)
4	Ng	0.38	0/891	0.90	1/1112 (0.1%)
4	Nh	0.39	0/891	0.90	1/1112 (0.1%)
4	Ni	0.38	0/891	0.90	1/1112 (0.1%)
4	Nj	0.39	0/891	0.90	1/1112 (0.1%)
4	Nk	0.37	0/891	0.90	1/1112 (0.1%)
4	Nl	0.37	0/891	0.90	1/1112 (0.1%)
5	Oa	0.32	0/755	0.69	0/942
5	Ob	0.33	0/755	0.68	0/942
5	Oc	0.32	0/755	0.69	2/942 (0.2%)
5	Od	0.33	0/755	0.68	0/942
5	Oe	0.33	0/755	0.68	0/942
5	Of	0.32	0/755	0.69	0/942
5	Og	0.32	0/755	0.69	0/942
5	Oh	0.32	0/755	0.69	2/942 (0.2%)
5	Oi	0.34	0/755	0.69	2/942 (0.2%)
5	Oj	0.32	0/755	0.69	0/942
5	Ok	0.32	0/755	0.68	0/942
5	Ol	0.33	0/755	0.69	2/942 (0.2%)
6	Ma	0.39	0/1419	0.81	4/1772 (0.2%)
6	Mb	0.40	0/1419	0.81	2/1772 (0.1%)
6	Mc	0.39	0/1419	0.81	4/1772 (0.2%)
6	Md	0.39	0/1419	0.82	2/1772 (0.1%)
6	Me	0.38	0/1419	0.81	2/1772 (0.1%)
6	Mf	0.38	0/1419	0.83	4/1772 (0.2%)
6	Mg	0.38	0/1419	0.80	4/1772 (0.2%)
6	Mh	0.39	0/1419	0.82	4/1772 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Mi	0.38	0/1419	0.82	2/1772 (0.1%)
6	Mj	0.39	0/1419	0.82	2/1772 (0.1%)
6	Mk	0.38	0/1419	0.80	4/1772 (0.2%)
6	Ml	0.39	0/1419	0.82	2/1772 (0.1%)
7	Qa	1.05	6/1667 (0.4%)	2.32	28/2075 (1.3%)
7	Qb	1.06	7/1667 (0.4%)	2.31	29/2075 (1.4%)
7	Qc	1.06	7/1667 (0.4%)	2.32	28/2075 (1.3%)
7	Qd	1.06	8/1667 (0.5%)	2.32	29/2075 (1.4%)
7	Qe	1.06	6/1667 (0.4%)	2.32	32/2075 (1.5%)
7	Qf	1.06	7/1667 (0.4%)	2.32	32/2075 (1.5%)
7	Qg	1.06	7/1667 (0.4%)	2.32	29/2075 (1.4%)
7	Qh	1.06	6/1667 (0.4%)	2.32	29/2075 (1.4%)
7	Qi	1.05	6/1667 (0.4%)	2.31	30/2075 (1.4%)
7	Qj	1.05	5/1667 (0.3%)	2.32	28/2075 (1.3%)
7	Qk	1.06	7/1667 (0.4%)	2.32	28/2075 (1.3%)
7	Ql	1.06	5/1667 (0.3%)	2.32	29/2075 (1.4%)
8	Pa	1.35	1/619 (0.2%)	1.81	12/772 (1.6%)
8	Pb	1.34	1/619 (0.2%)	1.76	9/772 (1.2%)
8	Pc	1.38	2/619 (0.3%)	1.79	11/772 (1.4%)
8	Pd	1.39	1/619 (0.2%)	1.80	10/772 (1.3%)
8	Pe	1.38	1/619 (0.2%)	1.85	12/772 (1.6%)
8	Pf	1.42	2/619 (0.3%)	1.91	12/772 (1.6%)
8	Pg	1.38	2/619 (0.3%)	1.81	12/772 (1.6%)
8	Ph	1.30	1/619 (0.2%)	1.76	10/772 (1.3%)
8	Pi	1.42	2/619 (0.3%)	1.92	13/772 (1.7%)
8	Pj	1.39	1/619 (0.2%)	1.91	13/772 (1.7%)
8	Pk	1.44	2/619 (0.3%)	1.90	14/772 (1.8%)
8	Pl	1.39	1/619 (0.2%)	1.86	13/772 (1.7%)
9	Ta	1.13	1/650 (0.2%)	1.45	4/809 (0.5%)
9	Tb	1.14	0/650	1.46	4/809 (0.5%)
9	Tc	1.14	1/650 (0.2%)	1.46	4/809 (0.5%)
9	Td	1.14	2/650 (0.3%)	1.46	4/809 (0.5%)
9	Te	1.15	1/650 (0.2%)	1.46	4/809 (0.5%)
9	Tf	1.15	0/650	1.47	4/809 (0.5%)
9	Tg	1.13	0/650	1.46	4/809 (0.5%)
9	Th	1.14	0/650	1.47	4/809 (0.5%)
9	Ti	1.15	2/650 (0.3%)	1.47	6/809 (0.7%)
9	Tj	1.14	0/650	1.46	4/809 (0.5%)
9	Tk	1.13	0/650	1.45	4/809 (0.5%)
9	Tl	1.15	0/650	1.47	6/809 (0.7%)
All	All	0.90	143/107295 (0.1%)	1.50	1097/133760 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Ba	0	3
2	Bb	0	7
2	Bc	0	4
2	Bd	0	7
2	Be	0	4
2	Bf	0	7
3	Ca	0	18
3	Cb	0	18
4	Na	0	6
4	Nb	0	6
4	Nc	0	5
4	Nd	0	5
4	Ne	0	5
4	Nf	0	5
4	Ng	0	5
4	Nh	0	5
4	Ni	0	5
4	Nj	0	5
4	Nk	0	5
4	Nl	0	5
5	Oa	0	1
5	Ob	0	1
5	Oc	0	1
5	Od	0	1
5	Oe	0	1
5	Of	0	1
5	Og	0	1
5	Oh	0	1
5	Oi	0	1
5	Oj	0	1
5	Ok	0	1
5	Ol	0	1
6	Ma	0	2
6	Mb	0	2
6	Mc	0	2
6	Md	0	2
6	Me	0	2
6	Mf	0	2
6	Mg	0	2
6	Mh	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	Mi	0	2
6	Mj	0	2
6	Mk	0	2
6	Ml	0	2
7	Qa	0	20
7	Qb	0	23
7	Qc	0	21
7	Qd	0	21
7	Qe	0	21
7	Qf	0	20
7	Qg	0	21
7	Qh	0	20
7	Qi	0	22
7	Qj	0	23
7	Qk	0	21
7	Ql	0	21
8	Pa	0	25
8	Pb	0	28
8	Pc	0	20
8	Pd	0	24
8	Pe	0	22
8	Pf	0	21
8	Pg	0	21
8	Ph	0	26
8	Pi	0	21
8	Pj	0	19
8	Pk	0	19
8	Pl	0	21
9	Ta	0	6
9	Tb	0	6
9	Tc	0	7
9	Td	0	6
9	Te	0	6
9	Tf	0	6
9	Tg	0	6
9	Th	0	6
9	Ti	0	7
9	Tj	0	7
9	Tk	0	6
9	Tl	0	6
All	All	0	762

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Pc	63	PRO	C-N	24.45	1.66	1.33
8	Pk	63	PRO	C-N	24.28	1.66	1.33
8	Pi	63	PRO	C-N	24.26	1.66	1.33
1	Ay	26	ASP	N-CA	24.21	1.76	1.46
1	Ae	26	ASP	N-CA	24.12	1.76	1.46
1	Ad	26	ASP	N-CA	24.12	1.76	1.46
1	Aa	26	ASP	N-CA	24.05	1.76	1.46
8	Pb	63	PRO	C-N	24.05	1.66	1.33
1	Ag	26	ASP	N-CA	24.03	1.76	1.46
1	Ak	26	ASP	N-CA	24.02	1.76	1.46
1	Av	26	ASP	N-CA	24.00	1.76	1.46
1	As	26	ASP	N-CA	23.98	1.76	1.46
1	Aw	26	ASP	N-CA	23.98	1.76	1.46
1	Aq	26	ASP	N-CA	23.97	1.76	1.46
1	Aj	26	ASP	N-CA	23.96	1.76	1.46
1	Au	26	ASP	N-CA	23.93	1.76	1.46
1	Ah	26	ASP	N-CA	23.93	1.76	1.46
1	A7	26	ASP	N-CA	23.93	1.76	1.46
1	Ab	26	ASP	N-CA	23.93	1.76	1.46
1	A9	26	ASP	N-CA	23.93	1.76	1.46
1	A8	26	ASP	N-CA	23.91	1.76	1.46
8	Pd	63	PRO	C-N	23.91	1.66	1.33
1	A5	26	ASP	N-CA	23.90	1.76	1.46
1	At	26	ASP	N-CA	23.89	1.76	1.46
1	Ax	26	ASP	N-CA	23.89	1.76	1.46
1	A2	26	ASP	N-CA	23.89	1.76	1.46
1	A3	26	ASP	N-CA	23.86	1.76	1.46
1	Af	26	ASP	N-CA	23.86	1.76	1.46
1	Ao	26	ASP	N-CA	23.85	1.76	1.46
1	A1	26	ASP	N-CA	23.84	1.76	1.46
1	Ac	26	ASP	N-CA	23.82	1.76	1.46
1	Ap	26	ASP	N-CA	23.82	1.76	1.46
1	Az	26	ASP	N-CA	23.81	1.76	1.46
1	A4	26	ASP	N-CA	23.80	1.76	1.46
1	Ar	26	ASP	N-CA	23.79	1.76	1.46
1	Al	26	ASP	N-CA	23.77	1.76	1.46
1	Am	26	ASP	N-CA	23.75	1.76	1.46
1	An	26	ASP	N-CA	23.68	1.76	1.46
1	A6	26	ASP	N-CA	23.68	1.76	1.46
8	Pl	63	PRO	C-N	23.64	1.65	1.33
8	Pf	63	PRO	C-N	23.64	1.65	1.33
1	Ai	26	ASP	N-CA	23.58	1.76	1.46
8	Pg	63	PRO	C-N	23.45	1.65	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Pe	63	PRO	C-N	23.39	1.65	1.33
8	Pj	63	PRO	C-N	23.38	1.65	1.33
8	Ph	63	PRO	C-N	23.36	1.65	1.33
8	Pa	63	PRO	C-N	23.21	1.65	1.33
2	Bb	177	ALA	CA-C	-18.89	1.39	1.53
2	Bd	177	ALA	CA-C	-10.02	1.46	1.53
7	Qk	107	VAL	C-N	9.91	1.44	1.33
7	Qe	107	VAL	C-N	9.89	1.44	1.33
7	Qb	107	VAL	C-N	9.88	1.44	1.33
7	Qf	107	VAL	C-N	9.88	1.44	1.33
7	Qi	107	VAL	C-N	9.87	1.44	1.33
7	Qh	107	VAL	C-N	9.87	1.44	1.33
7	Qc	107	VAL	C-N	9.86	1.44	1.33
7	Qa	107	VAL	C-N	9.84	1.44	1.33
7	Qd	107	VAL	C-N	9.82	1.44	1.33
7	Qg	107	VAL	C-N	9.82	1.44	1.33
7	Ql	107	VAL	C-N	9.82	1.44	1.33
7	Qj	107	VAL	C-N	9.80	1.44	1.33
2	Bb	177	ALA	N-CA	8.61	1.52	1.46
7	Qj	82	ILE	C-N	-6.54	1.25	1.33
7	Ql	82	ILE	C-N	-6.50	1.25	1.33
7	Qc	82	ILE	C-N	-6.50	1.25	1.33
7	Qb	82	ILE	C-N	-6.49	1.25	1.33
7	Qk	82	ILE	C-N	-6.48	1.25	1.33
7	Qg	82	ILE	C-N	-6.47	1.25	1.33
7	Qh	82	ILE	C-N	-6.45	1.25	1.33
7	Qd	82	ILE	C-N	-6.45	1.25	1.33
7	Qe	82	ILE	C-N	-6.45	1.25	1.33
7	Qi	82	ILE	C-N	-6.45	1.25	1.33
7	Qf	82	ILE	C-N	-6.44	1.25	1.33
7	Qa	82	ILE	C-N	-6.43	1.25	1.33
2	Bf	176	ASP	C-O	-6.32	1.15	1.24
7	Qd	346	GLU	C-N	-6.21	1.25	1.33
7	Qf	346	GLU	C-N	-6.18	1.25	1.33
7	Qe	346	GLU	C-N	-6.18	1.25	1.33
7	Qj	346	GLU	C-N	-6.18	1.25	1.33
7	Ql	346	GLU	C-N	-6.17	1.25	1.33
7	Qd	252	ALA	C-O	-6.17	1.18	1.24
7	Qg	346	GLU	C-N	-6.17	1.25	1.33
7	Qb	346	GLU	C-N	-6.17	1.25	1.33
7	Ql	252	ALA	C-O	-6.17	1.18	1.24
7	Qc	346	GLU	C-N	-6.16	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Qc	252	ALA	C-O	-6.15	1.18	1.24
7	Qi	346	GLU	C-N	-6.15	1.25	1.33
7	Qk	252	ALA	C-O	-6.14	1.18	1.24
7	Qh	346	GLU	C-N	-6.14	1.25	1.33
7	Qe	252	ALA	C-O	-6.14	1.18	1.24
7	Qa	346	GLU	C-N	-6.13	1.25	1.33
7	Qb	252	ALA	C-O	-6.13	1.18	1.24
7	Qj	252	ALA	C-O	-6.13	1.18	1.24
7	Qg	252	ALA	C-O	-6.11	1.18	1.24
7	Qi	252	ALA	C-O	-6.10	1.18	1.24
7	Qk	346	GLU	C-N	-6.10	1.25	1.33
7	Qa	252	ALA	C-O	-6.09	1.18	1.24
7	Qh	252	ALA	C-O	-6.06	1.18	1.24
7	Qf	252	ALA	C-O	-6.04	1.18	1.24
7	Qg	501	ILE	CA-C	5.84	1.60	1.53
7	Qc	501	ILE	CA-C	5.83	1.59	1.53
8	Pk	13	PRO	CA-C	5.82	1.57	1.52
8	Pc	13	PRO	CA-C	5.74	1.57	1.52
7	Qe	501	ILE	CA-C	5.72	1.59	1.53
3	Cb	256	ARG	CA-C	-5.72	1.45	1.52
8	Pf	13	PRO	CA-C	5.70	1.57	1.52
8	Pi	13	PRO	CA-C	5.51	1.57	1.52
9	Td	394	VAL	CA-C	5.47	1.58	1.52
8	Pg	13	PRO	CA-C	5.43	1.57	1.52
3	Ca	362	THR	N-CA	-5.39	1.39	1.46
7	Qf	501	ILE	CA-C	5.38	1.59	1.53
7	Qk	575	LEU	CA-C	-5.35	1.45	1.52
9	Td	354	VAL	N-CA	5.34	1.53	1.46
7	Qc	277	ASP	C-O	-5.29	1.17	1.23
7	Qh	277	ASP	C-O	-5.29	1.17	1.23
7	Qg	277	ASP	C-O	-5.27	1.17	1.23
7	Qd	575	LEU	CA-C	-5.26	1.45	1.52
7	Qk	277	ASP	C-O	-5.25	1.17	1.23
7	Qj	277	ASP	C-O	-5.25	1.17	1.23
7	Qd	277	ASP	C-O	-5.24	1.17	1.23
7	Qe	277	ASP	C-O	-5.24	1.17	1.23
7	Qa	277	ASP	C-O	-5.23	1.17	1.23
7	Qb	277	ASP	C-O	-5.22	1.17	1.23
7	Qi	277	ASP	C-O	-5.22	1.17	1.23
7	Ql	277	ASP	C-O	-5.21	1.17	1.23
7	Qd	501	ILE	CA-C	5.21	1.59	1.53
7	Qh	575	LEU	CA-C	-5.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Bf	426	ARG	C-O	-5.20	1.18	1.24
7	Qf	277	ASP	C-O	-5.20	1.17	1.23
9	Tc	354	VAL	N-CA	5.14	1.52	1.46
9	Ti	354	VAL	N-CA	5.12	1.52	1.46
7	Qb	575	LEU	CA-C	-5.12	1.46	1.52
9	Ta	354	VAL	N-CA	5.11	1.52	1.46
7	Qi	56	PRO	CA-C	5.08	1.56	1.52
7	Qa	56	PRO	CA-C	5.06	1.56	1.52
7	Qb	56	PRO	CA-C	5.04	1.56	1.52
9	Te	354	VAL	N-CA	5.02	1.52	1.46
7	Qg	56	PRO	CA-C	5.02	1.56	1.52
7	Qd	56	PRO	CA-C	5.01	1.56	1.52
7	Qc	56	PRO	CA-C	5.01	1.56	1.52
7	Qf	56	PRO	CA-C	5.01	1.56	1.52
9	Ti	394	VAL	CA-C	5.01	1.58	1.52
7	Qk	56	PRO	CA-C	5.00	1.56	1.52

All (1097) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qi	407	SER	O-C-N	-64.94	36.22	122.59
7	Qj	407	SER	O-C-N	-64.94	36.22	122.59
7	Qb	407	SER	O-C-N	-64.93	36.23	122.59
7	Qk	407	SER	O-C-N	-64.93	36.23	122.59
7	Qe	407	SER	O-C-N	-64.93	36.23	122.59
7	Qd	407	SER	O-C-N	-64.92	36.24	122.59
7	Qg	407	SER	O-C-N	-64.92	36.24	122.59
7	Qc	407	SER	O-C-N	-64.92	36.25	122.59
7	Qh	407	SER	O-C-N	-64.92	36.25	122.59
7	Ql	407	SER	O-C-N	-64.91	36.26	122.59
7	Qa	407	SER	O-C-N	-64.91	36.26	122.59
7	Qf	407	SER	O-C-N	-64.90	36.28	122.59
7	Qk	135	GLY	O-C-N	-38.91	72.11	122.70
7	Qc	135	GLY	O-C-N	-38.91	72.11	122.70
7	Qh	135	GLY	O-C-N	-38.91	72.12	122.70
7	Ql	135	GLY	O-C-N	-38.90	72.13	122.70
7	Qg	135	GLY	O-C-N	-38.89	72.14	122.70
7	Qa	135	GLY	O-C-N	-38.88	72.15	122.70
7	Qe	135	GLY	O-C-N	-38.88	72.16	122.70
7	Qi	135	GLY	O-C-N	-38.88	72.16	122.70
7	Qd	135	GLY	O-C-N	-38.87	72.17	122.70
7	Qj	135	GLY	O-C-N	-38.87	72.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qb	135	GLY	O-C-N	-38.86	72.18	122.70
7	Qf	135	GLY	O-C-N	-38.86	72.18	122.70
7	Qa	76	SER	O-C-N	-16.08	101.20	122.59
7	Qh	76	SER	O-C-N	-16.07	101.21	122.59
7	Qf	76	SER	O-C-N	-16.07	101.21	122.59
7	Qd	76	SER	O-C-N	-16.05	101.24	122.59
7	Qj	76	SER	O-C-N	-16.05	101.24	122.59
7	Qk	76	SER	O-C-N	-16.05	101.24	122.59
7	Ql	76	SER	O-C-N	-16.05	101.24	122.59
7	Qc	76	SER	O-C-N	-16.05	101.24	122.59
7	Qg	76	SER	O-C-N	-16.04	101.26	122.59
7	Qb	76	SER	O-C-N	-16.04	101.26	122.59
7	Qi	76	SER	O-C-N	-16.04	101.26	122.59
7	Qe	76	SER	O-C-N	-16.02	101.28	122.59
8	Pi	64	VAL	O-C-N	-12.25	107.26	122.57
8	Pg	64	VAL	O-C-N	-12.21	107.31	122.57
4	Nk	10	VAL	N-CA-C	12.11	122.04	110.42
8	Pd	64	VAL	O-C-N	-12.08	107.47	122.57
8	Pk	64	VAL	O-C-N	-12.04	107.52	122.57
8	Pc	64	VAL	O-C-N	-12.00	107.58	122.57
8	Pf	64	VAL	O-C-N	-11.95	107.63	122.57
8	Ph	64	VAL	O-C-N	-11.92	107.67	122.57
8	Pj	64	VAL	O-C-N	-11.91	107.69	122.57
4	Nc	10	VAL	N-CA-C	11.85	121.80	110.42
8	Pl	64	VAL	O-C-N	-11.85	107.75	122.57
8	Pa	64	VAL	O-C-N	-11.84	107.77	122.57
8	Pe	64	VAL	O-C-N	-11.82	107.79	122.57
4	Nl	10	VAL	N-CA-C	11.80	121.75	110.42
4	Nb	10	VAL	N-CA-C	11.74	121.69	110.42
4	Nh	10	VAL	N-CA-C	11.71	121.66	110.42
4	Ni	10	VAL	N-CA-C	11.69	121.64	110.42
4	Na	10	VAL	N-CA-C	11.66	121.61	110.42
4	Ne	10	VAL	N-CA-C	11.66	121.61	110.42
7	Qg	346	GLU	O-C-N	-11.57	109.41	122.72
4	Ng	10	VAL	N-CA-C	11.57	121.52	110.42
4	Nf	10	VAL	N-CA-C	11.56	121.52	110.42
7	Qa	346	GLU	O-C-N	-11.55	109.43	122.72
7	Qf	346	GLU	O-C-N	-11.56	109.43	122.72
4	Nd	10	VAL	N-CA-C	11.55	121.51	110.42
7	Qb	346	GLU	O-C-N	-11.55	109.44	122.72
7	Qc	346	GLU	O-C-N	-11.55	109.44	122.72
8	Pc	70	ALA	CA-C-N	11.54	143.59	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Pc	70	ALA	C-N-CA	11.54	143.59	121.54
7	Qk	346	GLU	O-C-N	-11.54	109.45	122.72
7	Qe	346	GLU	O-C-N	-11.54	109.45	122.72
7	Qi	346	GLU	O-C-N	-11.53	109.46	122.72
7	Qh	346	GLU	O-C-N	-11.53	109.46	122.72
7	Qj	346	GLU	O-C-N	-11.53	109.47	122.72
8	Pb	64	VAL	O-C-N	-11.52	108.17	122.57
7	Ql	346	GLU	O-C-N	-11.51	109.48	122.72
7	Qd	346	GLU	O-C-N	-11.49	109.50	122.72
8	Pb	70	ALA	CA-C-N	11.40	143.32	121.54
8	Pb	70	ALA	C-N-CA	11.40	143.32	121.54
8	Pj	70	ALA	CA-C-N	11.24	143.01	121.54
8	Pj	70	ALA	C-N-CA	11.24	143.01	121.54
4	Nj	10	VAL	N-CA-C	11.21	121.18	110.42
8	Pk	70	ALA	CA-C-N	11.16	142.85	121.54
8	Pk	70	ALA	C-N-CA	11.16	142.85	121.54
3	Ca	110	ASN	CA-C-O	-11.15	110.82	120.19
8	Pa	70	ALA	CA-C-N	11.11	142.77	121.54
8	Pa	70	ALA	C-N-CA	11.11	142.77	121.54
8	Pe	70	ALA	CA-C-N	11.10	142.74	121.54
8	Pe	70	ALA	C-N-CA	11.10	142.74	121.54
8	Pl	70	ALA	CA-C-N	11.09	142.72	121.54
8	Pl	70	ALA	C-N-CA	11.09	142.72	121.54
8	Pg	70	ALA	CA-C-N	11.07	142.69	121.54
8	Pg	70	ALA	C-N-CA	11.07	142.69	121.54
8	Pi	70	ALA	CA-C-N	11.00	142.55	121.54
8	Pi	70	ALA	C-N-CA	11.00	142.55	121.54
8	Ph	70	ALA	CA-C-N	10.96	142.47	121.54
8	Ph	70	ALA	C-N-CA	10.96	142.47	121.54
3	Cb	110	ASN	CA-C-O	-10.95	110.99	120.19
1	A6	25	GLN	CA-C-N	-10.91	102.56	122.09
1	A6	25	GLN	C-N-CA	-10.91	102.56	122.09
8	Pd	70	ALA	CA-C-N	10.90	142.35	121.54
8	Pd	70	ALA	C-N-CA	10.90	142.35	121.54
1	An	25	GLN	CA-C-N	-10.87	102.63	122.09
1	An	25	GLN	C-N-CA	-10.87	102.63	122.09
1	Az	25	GLN	CA-C-N	-10.86	102.65	122.09
1	Az	25	GLN	C-N-CA	-10.86	102.65	122.09
1	A9	25	GLN	CA-C-N	-10.85	102.67	122.09
1	A9	25	GLN	C-N-CA	-10.85	102.67	122.09
1	A5	25	GLN	CA-C-N	-10.84	102.68	122.09
1	A5	25	GLN	C-N-CA	-10.84	102.68	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A4	25	GLN	CA-C-N	-10.84	102.69	122.09
1	A4	25	GLN	C-N-CA	-10.84	102.69	122.09
1	A1	25	GLN	CA-C-N	-10.83	102.70	122.09
1	A1	25	GLN	C-N-CA	-10.83	102.70	122.09
1	A1	25	GLN	CA-C-N	-10.83	102.71	122.09
1	A1	25	GLN	C-N-CA	-10.83	102.71	122.09
1	Ao	25	GLN	CA-C-N	-10.83	102.71	122.09
1	Ao	25	GLN	C-N-CA	-10.83	102.71	122.09
1	A7	25	GLN	CA-C-N	-10.83	102.71	122.09
1	A7	25	GLN	C-N-CA	-10.83	102.71	122.09
1	A8	25	GLN	CA-C-N	-10.81	102.73	122.09
1	A8	25	GLN	C-N-CA	-10.81	102.73	122.09
1	Ai	25	GLN	CA-C-N	-10.79	102.77	122.09
1	Ai	25	GLN	C-N-CA	-10.79	102.77	122.09
1	A2	25	GLN	CA-C-N	-10.79	102.77	122.09
1	A2	25	GLN	C-N-CA	-10.79	102.77	122.09
9	Tc	356	LYS	CA-C-O	-10.79	109.56	120.02
1	Ad	25	GLN	CA-C-N	-10.78	102.79	122.09
1	Ad	25	GLN	C-N-CA	-10.78	102.79	122.09
1	Ac	25	GLN	CA-C-N	-10.78	102.80	122.09
1	Ac	25	GLN	C-N-CA	-10.78	102.80	122.09
1	At	25	GLN	CA-C-N	-10.77	102.81	122.09
1	At	25	GLN	C-N-CA	-10.77	102.81	122.09
1	Ax	25	GLN	CA-C-N	-10.77	102.82	122.09
1	Ax	25	GLN	C-N-CA	-10.77	102.82	122.09
1	Ah	25	GLN	CA-C-N	-10.77	102.82	122.09
1	Ah	25	GLN	C-N-CA	-10.77	102.82	122.09
1	Av	25	GLN	CA-C-N	-10.77	102.82	122.09
1	Av	25	GLN	C-N-CA	-10.77	102.82	122.09
1	A3	25	GLN	CA-C-N	-10.77	102.82	122.09
1	A3	25	GLN	C-N-CA	-10.77	102.82	122.09
8	Pf	70	ALA	CA-C-N	10.76	142.10	121.54
8	Pf	70	ALA	C-N-CA	10.76	142.10	121.54
1	Ar	25	GLN	CA-C-N	-10.76	102.83	122.09
1	Ar	25	GLN	C-N-CA	-10.76	102.83	122.09
1	Au	25	GLN	CA-C-N	-10.76	102.83	122.09
1	Au	25	GLN	C-N-CA	-10.76	102.83	122.09
1	Am	25	GLN	CA-C-N	-10.76	102.83	122.09
1	Am	25	GLN	C-N-CA	-10.76	102.83	122.09
1	Ay	25	GLN	CA-C-N	-10.76	102.84	122.09
1	Ay	25	GLN	C-N-CA	-10.76	102.84	122.09
1	Ap	25	GLN	CA-C-N	-10.75	102.84	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ap	25	GLN	C-N-CA	-10.75	102.84	122.09
1	Ag	25	GLN	CA-C-N	-10.75	102.85	122.09
1	Ag	25	GLN	C-N-CA	-10.75	102.85	122.09
1	Ak	25	GLN	CA-C-N	-10.72	102.89	122.09
1	Ak	25	GLN	C-N-CA	-10.72	102.89	122.09
1	Ab	25	GLN	CA-C-N	-10.72	102.90	122.09
1	Ab	25	GLN	C-N-CA	-10.72	102.90	122.09
1	Aw	25	GLN	CA-C-N	-10.72	102.90	122.09
1	Aw	25	GLN	C-N-CA	-10.72	102.90	122.09
1	Aa	25	GLN	CA-C-N	-10.70	102.93	122.09
1	Aa	25	GLN	C-N-CA	-10.70	102.93	122.09
1	Aj	25	GLN	CA-C-N	-10.68	102.97	122.09
1	Aj	25	GLN	C-N-CA	-10.68	102.97	122.09
1	Ae	25	GLN	CA-C-N	-10.67	103.00	122.09
1	Ae	25	GLN	C-N-CA	-10.67	103.00	122.09
1	Af	25	GLN	CA-C-N	-10.63	103.06	122.09
1	Af	25	GLN	C-N-CA	-10.63	103.06	122.09
1	Aq	25	GLN	CA-C-N	-10.63	103.06	122.09
1	Aq	25	GLN	C-N-CA	-10.63	103.06	122.09
9	Tl	356	LYS	CA-C-O	-10.62	109.72	120.02
9	Th	356	LYS	CA-C-O	-10.58	109.76	120.02
1	As	25	GLN	CA-C-N	-10.57	103.17	122.09
1	As	25	GLN	C-N-CA	-10.57	103.17	122.09
9	Tk	356	LYS	CA-C-O	-10.19	109.57	120.17
9	Tf	356	LYS	CA-C-O	-10.06	110.26	120.02
8	Ph	63	PRO	O-C-N	-10.01	109.12	122.64
8	Pj	63	PRO	O-C-N	-10.00	109.14	122.64
8	Pk	63	PRO	O-C-N	-10.00	109.15	122.64
9	Td	356	LYS	CA-C-O	-9.97	109.80	120.17
9	Tj	356	LYS	CA-C-O	-9.92	109.85	120.17
8	Pb	63	PRO	O-C-N	-9.91	109.25	122.64
8	Pl	63	PRO	O-C-N	-9.91	109.27	122.64
7	Qf	258	GLY	CA-C-O	-9.90	103.35	120.57
7	Qj	258	GLY	CA-C-O	-9.89	103.37	120.57
7	Qg	258	GLY	CA-C-O	-9.88	103.38	120.57
7	Qb	258	GLY	CA-C-O	-9.88	103.38	120.57
7	Qi	258	GLY	CA-C-O	-9.88	103.38	120.57
7	Qh	258	GLY	CA-C-O	-9.87	103.39	120.57
7	Qe	258	GLY	CA-C-O	-9.87	103.39	120.57
8	Pc	63	PRO	O-C-N	-9.87	109.31	122.64
7	Qc	258	GLY	CA-C-O	-9.87	103.40	120.57
7	Qa	258	GLY	CA-C-O	-9.87	103.40	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qk	258	GLY	CA-C-O	-9.87	103.40	120.57
7	Qd	258	GLY	CA-C-O	-9.87	103.40	120.57
7	Ql	258	GLY	CA-C-O	-9.87	103.41	120.57
9	Tb	356	LYS	CA-C-O	-9.85	109.93	120.17
7	Qb	277	ASP	O-C-N	-9.84	110.89	122.89
8	Pa	63	PRO	O-C-N	-9.83	109.37	122.64
7	Qi	277	ASP	O-C-N	-9.82	110.91	122.89
7	Qa	277	ASP	O-C-N	-9.81	110.92	122.89
9	Ta	356	LYS	CA-C-O	-9.79	109.98	120.17
7	Qf	277	ASP	O-C-N	-9.79	110.95	122.89
9	Tg	356	LYS	CA-C-O	-9.79	109.99	120.17
7	Qe	277	ASP	O-C-N	-9.77	110.97	122.89
8	Pg	13	PRO	N-CA-C	9.77	122.62	110.70
8	Pg	63	PRO	O-C-N	-9.77	109.45	122.64
7	Ql	277	ASP	O-C-N	-9.77	110.97	122.89
7	Qd	277	ASP	O-C-N	-9.77	110.98	122.89
7	Qh	277	ASP	O-C-N	-9.76	110.98	122.89
7	Qj	277	ASP	O-C-N	-9.75	110.99	122.89
7	Qc	277	ASP	O-C-N	-9.75	111.00	122.89
7	Qg	277	ASP	O-C-N	-9.75	111.00	122.89
8	Pc	13	PRO	N-CA-C	9.73	122.57	110.70
7	Qk	277	ASP	O-C-N	-9.73	111.02	122.89
8	Pe	63	PRO	O-C-N	-9.69	109.56	122.64
8	Pi	63	PRO	O-C-N	-9.64	109.62	122.64
8	Pd	63	PRO	O-C-N	-9.63	109.64	122.64
9	Ti	356	LYS	CA-C-O	-9.62	110.16	120.17
8	Pf	63	PRO	O-C-N	-9.61	109.67	122.64
9	Te	356	LYS	CA-C-O	-9.58	110.20	120.17
8	Pk	13	PRO	N-CA-C	9.43	122.20	110.70
8	Pf	13	PRO	N-CA-C	9.33	122.09	110.70
8	Pj	13	PRO	N-CA-C	9.25	121.98	110.70
8	Pd	13	PRO	N-CA-C	9.20	121.92	110.70
8	Pi	13	PRO	N-CA-C	9.09	121.79	110.70
7	Qf	270	ASP	CA-C-N	9.04	137.97	121.70
7	Qf	270	ASP	C-N-CA	9.04	137.97	121.70
7	Qc	270	ASP	CA-C-N	9.02	137.94	121.70
7	Qc	270	ASP	C-N-CA	9.02	137.94	121.70
7	Qk	270	ASP	CA-C-N	9.02	137.94	121.70
7	Qk	270	ASP	C-N-CA	9.02	137.94	121.70
7	Qa	270	ASP	CA-C-N	9.01	137.93	121.70
7	Qa	270	ASP	C-N-CA	9.01	137.93	121.70
7	Qe	270	ASP	CA-C-N	9.01	137.91	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qe	270	ASP	C-N-CA	9.01	137.91	121.70
7	Qh	270	ASP	CA-C-N	9.01	137.91	121.70
7	Qh	270	ASP	C-N-CA	9.01	137.91	121.70
7	Qj	270	ASP	CA-C-N	9.00	137.91	121.70
7	Qj	270	ASP	C-N-CA	9.00	137.91	121.70
7	Qd	270	ASP	CA-C-N	8.99	137.89	121.70
7	Qd	270	ASP	C-N-CA	8.99	137.89	121.70
7	Ql	270	ASP	CA-C-N	8.99	137.89	121.70
7	Ql	270	ASP	C-N-CA	8.99	137.89	121.70
7	Qg	270	ASP	CA-C-N	8.99	137.88	121.70
7	Qg	270	ASP	C-N-CA	8.99	137.88	121.70
7	Qi	270	ASP	CA-C-N	8.99	137.88	121.70
7	Qi	270	ASP	C-N-CA	8.99	137.88	121.70
7	Qb	270	ASP	CA-C-N	8.98	137.87	121.70
7	Qb	270	ASP	C-N-CA	8.98	137.87	121.70
7	Qa	601	ARG	CA-C-N	8.07	130.57	122.66
7	Qa	601	ARG	C-N-CA	8.07	130.57	122.66
2	Bf	499	ARG	N-CA-C	7.97	119.22	108.23
2	Bd	499	ARG	N-CA-C	7.92	119.16	108.23
8	Pb	62	GLY	CA-C-N	7.91	129.73	119.84
8	Pb	62	GLY	C-N-CA	7.91	129.73	119.84
2	Be	458	LYS	CA-C-N	-7.88	108.84	123.65
2	Be	458	LYS	C-N-CA	-7.88	108.84	123.65
7	Qj	258	GLY	O-C-N	7.80	132.85	122.70
7	Qb	258	GLY	O-C-N	7.80	132.84	122.70
7	Qk	258	GLY	O-C-N	7.78	132.82	122.70
7	Qd	258	GLY	O-C-N	7.78	132.81	122.70
7	Ql	258	GLY	O-C-N	7.78	132.81	122.70
7	Qa	258	GLY	O-C-N	7.78	132.81	122.70
7	Qe	258	GLY	O-C-N	7.77	132.80	122.70
2	Be	499	ARG	N-CA-C	7.76	118.94	108.23
2	Ba	499	ARG	N-CA-C	7.76	118.94	108.23
7	Qh	258	GLY	O-C-N	7.76	132.79	122.70
7	Qf	258	GLY	O-C-N	7.76	132.79	122.70
7	Qc	258	GLY	O-C-N	7.76	132.79	122.70
7	Qg	258	GLY	O-C-N	7.75	132.78	122.70
7	Qi	258	GLY	O-C-N	7.74	132.76	122.70
2	Bb	499	ARG	N-CA-C	7.70	118.86	108.23
7	Qg	601	ARG	CA-C-N	7.70	130.21	122.66
7	Qg	601	ARG	C-N-CA	7.70	130.21	122.66
8	Ph	62	GLY	CA-C-N	7.69	129.45	119.84
8	Ph	62	GLY	C-N-CA	7.69	129.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Pl	62	GLY	CA-C-N	7.67	129.43	119.84
8	Pl	62	GLY	C-N-CA	7.67	129.43	119.84
7	Qi	633	ASP	CA-C-O	-7.67	112.77	120.82
2	Bb	458	LYS	CA-C-N	-7.67	108.38	123.56
2	Bb	458	LYS	C-N-CA	-7.67	108.38	123.56
7	Qj	633	ASP	CA-C-O	-7.65	112.97	121.00
7	Qj	601	ARG	CA-C-N	7.65	130.16	122.66
7	Qj	601	ARG	C-N-CA	7.65	130.16	122.66
2	Bd	458	LYS	CA-C-N	-7.64	108.44	123.56
2	Bd	458	LYS	C-N-CA	-7.64	108.44	123.56
7	Qf	633	ASP	CA-C-O	-7.63	112.99	121.00
3	Ca	208	PHE	CA-C-O	7.59	129.02	120.90
8	Pe	62	GLY	CA-C-N	7.56	129.29	119.84
8	Pe	62	GLY	C-N-CA	7.56	129.29	119.84
7	Qk	601	ARG	CA-C-N	7.56	130.07	122.66
7	Qk	601	ARG	C-N-CA	7.56	130.07	122.66
2	Bc	499	ARG	N-CA-C	7.53	118.63	108.23
2	Ba	458	LYS	CA-C-N	-7.51	108.69	123.56
2	Ba	458	LYS	C-N-CA	-7.51	108.69	123.56
7	Qh	633	ASP	CA-C-O	-7.50	113.12	121.00
2	Bf	458	LYS	CA-C-N	-7.49	108.73	123.56
2	Bf	458	LYS	C-N-CA	-7.49	108.73	123.56
7	Qe	633	ASP	N-CA-C	-7.47	102.82	110.97
7	Qe	633	ASP	CA-C-O	-7.46	113.16	121.00
8	Pg	62	GLY	CA-C-N	7.46	129.17	119.84
8	Pg	62	GLY	C-N-CA	7.46	129.17	119.84
7	Ql	633	ASP	CA-C-O	-7.45	113.17	121.00
7	Qh	601	ARG	CA-C-N	7.44	129.95	122.66
7	Qh	601	ARG	C-N-CA	7.44	129.95	122.66
7	Qa	633	ASP	CA-C-O	-7.42	113.22	121.00
7	Qf	633	ASP	N-CA-C	-7.40	102.90	110.97
7	Qc	601	ARG	CA-C-N	7.40	129.91	122.66
7	Qc	601	ARG	C-N-CA	7.40	129.91	122.66
8	Pa	62	GLY	CA-C-N	7.38	129.07	119.84
8	Pa	62	GLY	C-N-CA	7.38	129.07	119.84
7	Qk	633	ASP	CA-C-O	-7.38	113.25	121.00
7	Ql	601	ARG	CA-C-N	7.38	129.89	122.66
7	Ql	601	ARG	C-N-CA	7.38	129.89	122.66
7	Qb	601	ARG	CA-C-N	7.36	129.88	122.66
7	Qb	601	ARG	C-N-CA	7.36	129.88	122.66
7	Qh	252	ALA	CA-C-N	7.33	127.35	119.28
7	Qh	252	ALA	C-N-CA	7.33	127.35	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qd	252	ALA	CA-C-N	7.33	127.34	119.28
7	Qd	252	ALA	C-N-CA	7.33	127.34	119.28
8	Pf	62	GLY	CA-C-N	7.33	129.00	119.84
8	Pf	62	GLY	C-N-CA	7.33	129.00	119.84
7	Qg	633	ASP	CA-C-O	-7.33	113.30	121.00
7	Qd	601	ARG	CA-C-N	7.31	129.82	122.66
7	Qd	601	ARG	C-N-CA	7.31	129.82	122.66
7	Qe	252	ALA	CA-C-N	7.31	127.32	119.28
7	Qe	252	ALA	C-N-CA	7.31	127.32	119.28
7	Qc	252	ALA	CA-C-N	7.30	127.31	119.28
7	Qc	252	ALA	C-N-CA	7.30	127.31	119.28
7	Qk	252	ALA	CA-C-N	7.30	127.31	119.28
7	Qk	252	ALA	C-N-CA	7.30	127.31	119.28
7	Qb	252	ALA	CA-C-N	7.30	127.31	119.28
7	Qb	252	ALA	C-N-CA	7.30	127.31	119.28
8	Pd	62	GLY	CA-C-N	7.29	128.95	119.84
8	Pd	62	GLY	C-N-CA	7.29	128.95	119.84
7	Qg	252	ALA	CA-C-N	7.29	127.30	119.28
7	Qg	252	ALA	C-N-CA	7.29	127.30	119.28
7	Qa	252	ALA	CA-C-N	7.28	127.29	119.28
7	Qa	252	ALA	C-N-CA	7.28	127.29	119.28
7	Qe	601	ARG	CA-C-N	7.28	129.79	122.66
7	Qe	601	ARG	C-N-CA	7.28	129.79	122.66
8	Pk	62	GLY	CA-C-N	7.28	128.93	119.84
8	Pk	62	GLY	C-N-CA	7.28	128.93	119.84
7	Ql	252	ALA	CA-C-N	7.26	127.27	119.28
7	Ql	252	ALA	C-N-CA	7.26	127.27	119.28
8	Pi	62	GLY	CA-C-N	7.22	128.87	119.84
8	Pi	62	GLY	C-N-CA	7.22	128.87	119.84
7	Qf	601	ARG	CA-C-N	7.20	129.71	122.66
7	Qf	601	ARG	C-N-CA	7.20	129.71	122.66
7	Qk	633	ASP	N-CA-C	-7.17	103.15	110.97
7	Qa	633	ASP	N-CA-C	-7.15	103.17	110.97
7	Qb	633	ASP	N-CA-C	-7.14	103.19	110.97
7	Qi	601	ARG	CA-C-N	7.12	129.63	122.66
7	Qi	601	ARG	C-N-CA	7.12	129.63	122.66
7	Qi	633	ASP	N-CA-C	-7.11	103.46	111.07
3	Ca	256	ARG	N-CA-C	-7.09	100.50	110.50
7	Qh	633	ASP	N-CA-C	-7.09	103.24	110.97
2	Bc	458	LYS	CA-C-N	-7.08	109.54	123.56
2	Bc	458	LYS	C-N-CA	-7.08	109.54	123.56
7	Qc	633	ASP	CA-C-O	-7.08	113.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qb	633	ASP	CA-C-O	-7.05	113.60	121.00
1	A7	43	GLN	N-CA-C	-7.04	103.05	113.61
1	Al	43	GLN	N-CA-C	-7.04	103.05	113.61
7	Qj	633	ASP	N-CA-C	-7.03	103.31	110.97
1	At	43	GLN	N-CA-C	-7.02	103.08	113.61
1	A4	43	GLN	N-CA-C	-7.01	103.09	113.61
1	As	43	GLN	N-CA-C	-6.99	103.12	113.61
8	Pb	8	PRO	N-CA-C	6.99	119.23	110.70
1	Aa	43	GLN	N-CA-C	-6.95	103.18	113.61
1	A6	43	GLN	N-CA-C	-6.93	103.21	113.61
8	Pj	62	GLY	CA-C-N	6.93	128.50	119.84
8	Pj	62	GLY	C-N-CA	6.93	128.50	119.84
1	Ad	43	GLN	N-CA-C	-6.93	103.22	113.61
1	Ap	43	GLN	N-CA-C	-6.92	103.23	113.61
1	Ab	43	GLN	N-CA-C	-6.90	103.26	113.61
1	A9	43	GLN	N-CA-C	-6.90	103.26	113.61
3	Ca	200	LEU	CA-C-O	-6.90	113.24	120.55
1	A8	43	GLN	N-CA-C	-6.90	103.26	113.61
7	Qg	633	ASP	N-CA-C	-6.90	103.45	110.97
1	Av	43	GLN	N-CA-C	-6.89	103.27	113.61
8	Ph	8	PRO	N-CA-C	6.88	119.10	110.70
7	Ql	633	ASP	N-CA-C	-6.88	103.47	110.97
1	Aj	43	GLN	N-CA-C	-6.87	103.31	113.61
1	A1	43	GLN	N-CA-C	-6.86	103.32	113.61
1	Ak	43	GLN	N-CA-C	-6.86	103.32	113.61
7	Qd	633	ASP	CA-C-O	-6.86	113.80	121.00
7	Qd	633	ASP	N-CA-C	-6.86	103.49	110.97
1	Ax	27	TYR	N-CA-C	-6.86	103.81	111.28
1	Ag	43	GLN	N-CA-C	-6.85	103.33	113.61
1	A2	43	GLN	N-CA-C	-6.84	103.35	113.61
8	Pi	8	PRO	N-CA-C	6.83	119.03	110.70
1	Ax	44	LYS	N-CA-C	-6.82	103.92	111.36
1	A5	27	TYR	N-CA-C	-6.82	103.84	111.28
1	Au	43	GLN	N-CA-C	-6.82	103.38	113.61
1	Ax	43	GLN	N-CA-C	-6.81	103.39	113.61
1	Ar	43	GLN	N-CA-C	-6.81	103.39	113.61
7	Qf	252	ALA	CA-C-N	6.81	127.37	119.47
7	Qf	252	ALA	C-N-CA	6.81	127.37	119.47
1	Af	43	GLN	N-CA-C	-6.80	103.41	113.61
1	A6	27	TYR	N-CA-C	-6.78	103.89	111.28
1	Am	44	LYS	N-CA-C	-6.78	103.97	111.36
1	Av	44	LYS	N-CA-C	-6.78	103.97	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ar	27	TYR	N-CA-C	-6.78	103.89	111.28
7	Qi	252	ALA	CA-C-N	6.78	127.33	119.47
7	Qi	252	ALA	C-N-CA	6.78	127.33	119.47
1	Ah	43	GLN	N-CA-C	-6.77	103.45	113.61
1	An	43	GLN	N-CA-C	-6.77	103.45	113.61
1	A3	27	TYR	N-CA-C	-6.77	103.90	111.28
1	A5	43	GLN	N-CA-C	-6.77	103.46	113.61
1	Ao	43	GLN	N-CA-C	-6.77	103.46	113.61
8	Pl	8	PRO	N-CA-C	6.76	118.95	110.70
1	Am	43	GLN	N-CA-C	-6.75	103.48	113.61
1	Ay	43	GLN	N-CA-C	-6.75	103.49	113.61
1	Am	36	ALA	N-CA-C	-6.74	103.96	111.71
7	Qj	252	ALA	CA-C-N	6.73	127.27	119.47
7	Qj	252	ALA	C-N-CA	6.73	127.27	119.47
1	Ap	27	TYR	N-CA-C	-6.72	103.95	111.28
3	Cb	256	ARG	N-CA-C	-6.72	101.03	110.50
8	Pc	8	PRO	N-CA-C	6.71	118.89	110.70
1	Ai	43	GLN	N-CA-C	-6.71	103.54	113.61
1	A7	27	TYR	N-CA-C	-6.71	103.97	111.28
3	Cb	200	LEU	CA-C-O	-6.71	113.44	120.55
1	A3	36	ALA	N-CA-C	-6.69	104.02	111.71
1	A3	43	GLN	N-CA-C	-6.69	103.58	113.61
1	A4	105	LYS	N-CA-C	6.68	119.09	109.14
1	Ae	27	TYR	N-CA-C	-6.67	104.01	111.28
1	Az	43	GLN	N-CA-C	-6.67	103.60	113.61
1	Ar	105	LYS	N-CA-C	6.67	119.08	109.14
1	A1	27	TYR	N-CA-C	-6.66	104.02	111.28
8	Pk	8	PRO	N-CA-C	6.66	118.83	110.70
1	Au	27	TYR	N-CA-C	-6.66	104.02	111.28
1	Aw	43	GLN	N-CA-C	-6.66	103.62	113.61
1	Aj	27	TYR	N-CA-C	-6.66	104.03	111.28
1	As	36	ALA	N-CA-C	-6.66	104.06	111.71
1	Al	27	TYR	N-CA-C	-6.65	104.03	111.28
1	A8	27	TYR	N-CA-C	-6.65	104.03	111.28
8	Pd	8	PRO	N-CA-C	6.65	118.81	110.70
7	Qj	270	ASP	CA-C-O	-6.65	111.00	120.51
1	Ag	27	TYR	N-CA-C	-6.64	104.04	111.28
1	Aq	43	GLN	N-CA-C	-6.64	103.65	113.61
7	Qh	270	ASP	CA-C-O	-6.63	111.03	120.51
7	Qb	270	ASP	CA-C-O	-6.62	111.04	120.51
1	Ae	43	GLN	N-CA-C	-6.62	103.67	113.61
7	Qd	270	ASP	CA-C-O	-6.62	111.05	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ao	36	ALA	N-CA-C	-6.62	104.10	111.71
7	Qf	270	ASP	CA-C-O	-6.61	111.05	120.51
1	Aa	27	TYR	N-CA-C	-6.61	104.07	111.28
1	Ad	105	LYS	N-CA-C	6.61	118.99	109.14
1	A9	27	TYR	N-CA-C	-6.61	104.08	111.28
1	A6	105	LYS	N-CA-C	6.61	118.99	109.14
1	Ai	105	LYS	N-CA-C	6.61	118.98	109.14
1	Az	27	TYR	N-CA-C	-6.60	104.08	111.28
1	Aw	27	TYR	N-CA-C	-6.60	104.08	111.28
7	Ql	270	ASP	CA-C-O	-6.60	111.07	120.51
1	An	36	ALA	N-CA-C	-6.60	104.12	111.71
7	Qe	270	ASP	CA-C-O	-6.60	111.07	120.51
1	As	27	TYR	N-CA-C	-6.60	104.09	111.28
7	Qa	270	ASP	CA-C-O	-6.60	111.08	120.51
1	A9	36	ALA	N-CA-C	-6.59	104.13	111.71
1	Al	105	LYS	N-CA-C	6.59	118.96	109.14
1	Ac	43	GLN	N-CA-C	-6.59	103.73	113.61
7	Qk	270	ASP	CA-C-O	-6.59	111.09	120.51
7	Qg	270	ASP	CA-C-O	-6.58	111.09	120.51
1	A2	27	TYR	N-CA-C	-6.58	104.11	111.28
1	An	27	TYR	N-CA-C	-6.58	104.11	111.28
1	Ao	27	TYR	N-CA-C	-6.58	104.11	111.28
7	Qc	270	ASP	CA-C-O	-6.58	111.11	120.51
1	Ai	36	ALA	N-CA-C	-6.57	104.16	111.71
1	Aj	36	ALA	N-CA-C	-6.56	104.16	111.71
8	Pf	8	PRO	N-CA-C	6.56	118.70	110.70
7	Qi	270	ASP	CA-C-O	-6.56	111.13	120.51
1	A4	27	TYR	N-CA-C	-6.56	104.13	111.28
1	Ai	27	TYR	N-CA-C	-6.55	104.14	111.28
1	Ab	44	LYS	N-CA-C	-6.55	104.22	111.36
1	Ac	27	TYR	N-CA-C	-6.55	104.14	111.28
1	Ab	27	TYR	N-CA-C	-6.54	104.15	111.28
1	Af	36	ALA	N-CA-C	-6.54	104.18	111.71
1	Aq	27	TYR	N-CA-C	-6.54	104.15	111.28
1	Ab	105	LYS	N-CA-C	6.54	118.88	109.14
7	Qj	634	THR	N-CA-C	6.54	120.12	111.75
1	At	27	TYR	N-CA-C	-6.53	104.16	111.28
7	Qk	498	ILE	O-C-N	-6.53	115.53	121.87
7	Qc	633	ASP	N-CA-C	-6.52	103.86	110.97
1	Av	105	LYS	N-CA-C	6.52	118.85	109.14
1	An	105	LYS	N-CA-C	6.52	118.85	109.14
1	A6	44	LYS	N-CA-C	-6.51	103.68	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ac	105	LYS	N-CA-C	6.51	118.84	109.14
1	At	36	ALA	N-CA-C	-6.51	104.22	111.71
1	Ad	27	TYR	N-CA-C	-6.50	104.19	111.28
1	Ak	27	TYR	N-CA-C	-6.50	104.19	111.28
8	Pj	8	PRO	N-CA-C	6.50	118.63	110.70
1	Af	105	LYS	N-CA-C	6.50	118.82	109.14
1	Aa	36	ALA	N-CA-C	-6.50	104.24	111.71
1	A1	44	LYS	N-CA-C	-6.49	103.70	111.69
1	A3	105	LYS	N-CA-C	6.49	118.82	109.14
1	Am	105	LYS	N-CA-C	6.49	118.81	109.14
1	A9	105	LYS	N-CA-C	6.49	118.81	109.14
1	Ay	27	TYR	N-CA-C	-6.49	104.21	111.28
1	A8	36	ALA	N-CA-C	-6.48	104.26	111.71
1	Ad	44	LYS	N-CA-C	-6.48	103.72	111.69
1	Af	27	TYR	N-CA-C	-6.48	104.22	111.28
1	Ak	36	ALA	N-CA-C	-6.47	104.27	111.71
1	Ap	36	ALA	N-CA-C	-6.47	104.27	111.71
1	Ap	44	LYS	N-CA-C	-6.47	103.73	111.69
1	Av	27	TYR	N-CA-C	-6.47	104.23	111.28
1	Ag	44	LYS	N-CA-C	-6.47	103.74	111.69
1	Ap	105	LYS	N-CA-C	6.46	118.77	109.14
1	Ao	44	LYS	N-CA-C	-6.46	103.74	111.69
1	A2	44	LYS	N-CA-C	-6.46	103.74	111.69
1	A2	105	LYS	N-CA-C	6.46	118.77	109.14
1	Ar	36	ALA	N-CA-C	-6.46	104.28	111.71
1	A7	36	ALA	N-CA-C	-6.46	104.28	111.71
1	A7	44	LYS	N-CA-C	-6.46	103.75	111.69
7	Qe	634	THR	N-CA-C	6.45	120.01	111.75
1	A1	105	LYS	N-CA-C	6.45	118.75	109.14
1	A6	36	ALA	N-CA-C	-6.45	104.29	111.71
1	Ah	36	ALA	N-CA-C	-6.45	104.30	111.71
8	Pe	8	PRO	N-CA-C	6.44	118.56	110.70
1	A5	105	LYS	N-CA-C	6.44	118.74	109.14
1	Ak	44	LYS	N-CA-C	-6.44	103.77	111.69
1	Aq	105	LYS	N-CA-C	6.44	118.73	109.14
1	An	44	LYS	N-CA-C	-6.43	103.78	111.69
1	A1	36	ALA	N-CA-C	-6.43	104.31	111.71
1	Ao	105	LYS	N-CA-C	6.43	118.72	109.14
1	A5	36	ALA	N-CA-C	-6.43	104.32	111.71
1	Aw	44	LYS	N-CA-C	-6.42	103.79	111.69
8	Pa	8	PRO	N-CA-C	6.42	118.53	110.70
1	Ax	105	LYS	N-CA-C	6.42	118.70	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ah	105	LYS	N-CA-C	6.42	118.70	109.14
1	Al	36	ALA	N-CA-C	-6.41	104.34	111.71
1	Am	27	TYR	N-CA-C	-6.41	104.29	111.28
1	A9	44	LYS	N-CA-C	-6.41	103.81	111.69
1	Ae	44	LYS	N-CA-C	-6.41	103.81	111.69
1	Aq	44	LYS	N-CA-C	-6.41	103.81	111.69
1	A4	36	ALA	N-CA-C	-6.41	104.34	111.71
7	Qg	634	THR	N-CA-C	6.41	119.95	111.75
1	Au	105	LYS	N-CA-C	6.40	118.68	109.14
1	Af	44	LYS	N-CA-C	-6.40	103.82	111.69
1	Ay	36	ALA	N-CA-C	-6.40	104.35	111.71
1	Ak	105	LYS	N-CA-C	6.39	118.67	109.14
1	A7	105	LYS	N-CA-C	6.39	118.67	109.14
1	A8	105	LYS	N-CA-C	6.39	118.66	109.14
1	Aa	105	LYS	N-CA-C	6.39	118.66	109.14
1	Az	105	LYS	N-CA-C	6.38	118.65	109.14
1	A5	44	LYS	N-CA-C	-6.38	103.84	111.69
1	A4	44	LYS	N-CA-C	-6.38	103.85	111.69
1	Ae	36	ALA	N-CA-C	-6.38	104.38	111.71
1	Ae	105	LYS	N-CA-C	6.37	118.64	109.14
7	Qd	259	ALA	CA-C-N	6.37	133.17	121.70
7	Qd	259	ALA	C-N-CA	6.37	133.17	121.70
1	Ah	44	LYS	N-CA-C	-6.37	103.86	111.69
7	Qh	259	ALA	CA-C-N	6.37	133.16	121.70
7	Qh	259	ALA	C-N-CA	6.37	133.16	121.70
1	Ay	105	LYS	N-CA-C	6.36	118.62	109.14
7	Qj	259	ALA	CA-C-N	6.36	133.15	121.70
7	Qj	259	ALA	C-N-CA	6.36	133.15	121.70
1	Aj	105	LYS	N-CA-C	6.36	118.62	109.14
1	Aj	44	LYS	N-CA-C	-6.36	103.86	111.69
2	Bf	260	GLY	CA-C-N	-6.36	116.81	122.47
2	Bf	260	GLY	C-N-CA	-6.36	116.81	122.47
7	Ql	259	ALA	CA-C-N	6.36	133.15	121.70
7	Ql	259	ALA	C-N-CA	6.36	133.15	121.70
1	Aq	36	ALA	N-CA-C	-6.36	104.40	111.71
8	Pl	44	VAL	CA-C-N	6.36	133.14	121.70
8	Pl	44	VAL	C-N-CA	6.36	133.14	121.70
1	Ai	44	LYS	N-CA-C	-6.36	103.87	111.69
8	Pi	44	VAL	CA-C-N	6.35	133.13	121.70
8	Pi	44	VAL	C-N-CA	6.35	133.13	121.70
7	Qc	259	ALA	CA-C-N	6.35	133.13	121.70
7	Qc	259	ALA	C-N-CA	6.35	133.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qa	259	ALA	CA-C-N	6.35	133.12	121.70
7	Qa	259	ALA	C-N-CA	6.35	133.12	121.70
7	Qi	259	ALA	CA-C-N	6.35	133.13	121.70
7	Qi	259	ALA	C-N-CA	6.35	133.13	121.70
7	Qk	259	ALA	CA-C-N	6.35	133.12	121.70
7	Qk	259	ALA	C-N-CA	6.35	133.12	121.70
1	Az	44	LYS	N-CA-C	-6.35	103.89	111.69
7	Qb	259	ALA	CA-C-N	6.35	133.12	121.70
7	Qb	259	ALA	C-N-CA	6.35	133.12	121.70
1	At	44	LYS	N-CA-C	-6.34	103.89	111.69
1	A8	44	LYS	N-CA-C	-6.34	103.89	111.69
7	Qf	259	ALA	CA-C-N	6.34	133.11	121.70
7	Qf	259	ALA	C-N-CA	6.34	133.11	121.70
7	Qh	498	ILE	O-C-N	-6.34	115.72	121.87
7	Qe	259	ALA	CA-C-N	6.33	133.10	121.70
7	Qe	259	ALA	C-N-CA	6.33	133.10	121.70
7	Qg	259	ALA	CA-C-N	6.33	133.10	121.70
7	Qg	259	ALA	C-N-CA	6.33	133.10	121.70
1	Aa	44	LYS	N-CA-C	-6.32	103.92	111.69
2	Bb	532	ILE	N-CA-C	6.32	122.49	109.34
1	Ab	36	ALA	N-CA-C	-6.32	104.44	111.71
7	Qk	529	LEU	CA-C-O	-6.32	114.37	121.00
1	A2	36	ALA	N-CA-C	-6.31	104.45	111.71
1	Ad	36	ALA	N-CA-C	-6.31	104.45	111.71
1	Av	36	ALA	N-CA-C	-6.31	104.46	111.71
1	At	105	LYS	N-CA-C	6.31	118.53	109.14
1	Au	36	ALA	N-CA-C	-6.29	104.48	111.71
1	Aw	105	LYS	N-CA-C	6.28	118.50	109.14
7	Qb	634	THR	N-CA-C	6.27	119.78	111.75
1	Ac	44	LYS	N-CA-C	-6.27	103.97	111.69
1	As	105	LYS	N-CA-C	6.27	118.48	109.14
1	Az	36	ALA	N-CA-C	-6.27	104.50	111.71
1	As	44	LYS	N-CA-C	-6.27	103.98	111.69
7	Qd	634	THR	N-CA-C	6.26	119.77	111.75
1	Al	44	LYS	N-CA-C	-6.26	103.99	111.69
1	A3	44	LYS	N-CA-C	-6.26	103.99	111.69
8	Pf	44	VAL	CA-C-N	6.23	132.92	121.70
8	Pf	44	VAL	C-N-CA	6.23	132.92	121.70
7	Qc	634	THR	N-CA-C	6.23	119.73	111.75
1	Aw	36	ALA	N-CA-C	-6.22	104.55	111.71
2	Ba	454	CYS	CA-C-N	-6.22	113.27	119.99
2	Ba	454	CYS	C-N-CA	-6.22	113.27	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ag	36	ALA	N-CA-C	-6.22	104.56	111.71
1	Ag	105	LYS	N-CA-C	6.22	118.41	109.14
7	Qb	498	ILE	O-C-N	-6.19	115.87	121.87
7	Qa	498	ILE	O-C-N	-6.19	115.87	121.87
1	Au	44	LYS	N-CA-C	-6.18	104.09	111.69
1	Ah	27	TYR	N-CA-C	-6.17	104.56	111.28
2	Bf	532	ILE	N-CA-C	6.16	122.15	109.34
2	Bc	454	CYS	CA-C-N	-6.15	113.34	119.99
2	Bc	454	CYS	C-N-CA	-6.15	113.34	119.99
8	Pg	8	PRO	N-CA-C	6.15	118.20	110.70
7	Ql	634	THR	N-CA-C	6.13	119.60	111.75
7	Qh	634	THR	N-CA-C	6.13	119.60	111.75
1	Ax	36	ALA	N-CA-C	-6.12	104.68	111.71
1	Ay	44	LYS	N-CA-C	-6.12	104.17	111.69
7	Qj	498	ILE	O-C-N	-6.11	115.94	121.87
1	Ar	44	LYS	N-CA-C	-6.10	104.18	111.69
8	Pe	44	VAL	CA-C-N	6.10	132.68	121.70
8	Pe	44	VAL	C-N-CA	6.10	132.68	121.70
7	Qd	498	ILE	O-C-N	-6.08	115.97	121.87
7	Qa	634	THR	N-CA-C	6.07	119.52	111.75
7	Qf	634	THR	N-CA-C	6.07	119.51	111.75
1	Ac	36	ALA	N-CA-C	-6.06	104.74	111.71
2	Bf	176	ASP	CA-C-N	6.05	129.36	122.83
2	Bf	176	ASP	C-N-CA	6.05	129.36	122.83
8	Pa	44	VAL	CA-C-N	6.05	132.58	121.70
8	Pa	44	VAL	C-N-CA	6.05	132.58	121.70
7	Qh	529	LEU	CA-C-O	-6.04	114.66	121.00
7	Qd	525	TRP	N-CA-C	6.03	117.85	111.28
2	Bc	429	ASN	N-CA-C	6.03	120.49	113.20
2	Bd	532	ILE	N-CA-C	6.02	121.86	109.34
7	Ql	498	ILE	O-C-N	-6.00	116.05	121.87
2	Bd	429	ASN	N-CA-C	6.00	120.46	113.20
8	Pj	63	PRO	CA-C-N	6.00	132.76	121.97
8	Pj	63	PRO	C-N-CA	6.00	132.76	121.97
2	Ba	394	ASP	CA-C-N	-5.97	109.94	121.58
2	Ba	394	ASP	C-N-CA	-5.97	109.94	121.58
3	Cb	332	ASN	CA-C-O	-5.96	113.90	120.69
8	Pa	63	PRO	CA-C-N	5.95	132.68	121.97
8	Pa	63	PRO	C-N-CA	5.95	132.68	121.97
7	Ql	529	LEU	CA-C-O	-5.95	114.76	121.00
2	Bb	429	ASN	N-CA-C	5.94	120.39	113.20
7	Qc	498	ILE	O-C-N	-5.93	116.12	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Be	454	CYS	CA-C-N	-5.93	113.58	119.99
2	Be	454	CYS	C-N-CA	-5.93	113.58	119.99
2	Bb	394	ASP	CA-C-N	-5.93	110.02	121.58
2	Bb	394	ASP	C-N-CA	-5.93	110.02	121.58
2	Bc	95	PRO	N-CA-C	5.92	124.66	112.47
3	Ca	192	VAL	CA-C-N	5.91	128.13	120.44
3	Ca	192	VAL	C-N-CA	5.91	128.13	120.44
8	Pc	44	VAL	CA-C-N	5.90	132.31	121.70
8	Pc	44	VAL	C-N-CA	5.90	132.31	121.70
2	Bf	95	PRO	N-CA-C	5.89	124.59	112.47
7	Qk	634	THR	N-CA-C	5.88	119.28	111.75
2	Bf	382	GLN	CA-C-N	-5.88	115.52	123.46
2	Bf	382	GLN	C-N-CA	-5.88	115.52	123.46
8	Pe	63	PRO	CA-C-N	5.88	132.55	121.97
8	Pe	63	PRO	C-N-CA	5.88	132.55	121.97
7	Qf	529	LEU	CA-C-O	-5.88	114.83	121.00
2	Be	95	PRO	N-CA-C	5.86	124.53	112.47
2	Bd	394	ASP	CA-C-N	-5.85	110.17	121.58
2	Bd	394	ASP	C-N-CA	-5.85	110.17	121.58
2	Be	394	ASP	CA-C-N	-5.85	110.17	121.58
2	Be	394	ASP	C-N-CA	-5.85	110.17	121.58
2	Bf	394	ASP	CA-C-N	-5.85	110.17	121.58
2	Bf	394	ASP	C-N-CA	-5.85	110.17	121.58
2	Bb	95	PRO	N-CA-C	5.85	124.52	112.47
2	Bd	95	PRO	N-CA-C	5.84	124.51	112.47
7	Qg	525	TRP	N-CA-C	5.84	117.64	111.28
3	Ca	332	ASN	CA-C-O	-5.83	114.04	120.69
2	Bd	529	GLN	CA-C-N	-5.82	113.67	122.81
2	Bd	529	GLN	C-N-CA	-5.82	113.67	122.81
7	Qk	525	TRP	N-CA-C	5.82	117.62	111.28
8	Pg	63	PRO	CA-C-N	5.81	132.43	121.97
8	Pg	63	PRO	C-N-CA	5.81	132.43	121.97
8	Ph	63	PRO	CA-C-N	5.81	132.42	121.97
8	Ph	63	PRO	C-N-CA	5.81	132.42	121.97
2	Ba	353	GLU	N-CA-C	-5.80	107.44	114.75
8	Pj	44	VAL	CA-C-N	5.79	132.13	121.70
8	Pj	44	VAL	C-N-CA	5.79	132.13	121.70
2	Bc	394	ASP	CA-C-N	-5.79	110.29	121.58
2	Bc	394	ASP	C-N-CA	-5.79	110.29	121.58
7	Qe	525	TRP	N-CA-C	5.79	117.59	111.28
2	Bf	298	PHE	CA-C-N	-5.78	114.55	122.93
2	Bf	298	PHE	C-N-CA	-5.78	114.55	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Be	298	PHE	CA-C-N	-5.75	114.59	122.93
2	Be	298	PHE	C-N-CA	-5.75	114.59	122.93
2	Bc	353	GLU	N-CA-C	-5.74	107.52	114.75
7	Qi	634	THR	N-CA-C	5.74	119.09	111.75
8	Pl	63	PRO	CA-C-N	5.74	132.30	121.97
8	Pl	63	PRO	C-N-CA	5.74	132.30	121.97
2	Be	429	ASN	N-CA-C	5.72	120.12	113.20
2	Ba	95	PRO	N-CA-C	5.71	124.24	112.47
2	Ba	382	GLN	CA-C-N	-5.70	115.76	123.46
2	Ba	382	GLN	C-N-CA	-5.70	115.76	123.46
9	Ti	369	ILE	CA-C-N	5.68	126.09	120.98
9	Ti	369	ILE	C-N-CA	5.68	126.09	120.98
7	Qa	525	TRP	N-CA-C	5.67	117.46	111.28
8	Pk	44	VAL	CA-C-N	5.67	131.91	121.70
8	Pk	44	VAL	C-N-CA	5.67	131.91	121.70
7	Qe	261	ARG	CA-C-N	5.67	135.22	122.19
7	Qe	261	ARG	C-N-CA	5.67	135.22	122.19
7	Qg	261	ARG	CA-C-N	5.66	135.22	122.19
7	Qg	261	ARG	C-N-CA	5.66	135.22	122.19
9	Th	369	ILE	CA-C-N	5.66	126.08	120.98
9	Th	369	ILE	C-N-CA	5.66	126.08	120.98
2	Bd	298	PHE	CA-C-N	-5.66	114.72	122.93
2	Bd	298	PHE	C-N-CA	-5.66	114.72	122.93
7	Qj	261	ARG	CA-C-N	5.66	135.21	122.19
7	Qj	261	ARG	C-N-CA	5.66	135.21	122.19
7	Qd	261	ARG	CA-C-N	5.66	135.21	122.19
7	Qd	261	ARG	C-N-CA	5.66	135.21	122.19
7	Ql	261	ARG	CA-C-N	5.66	135.21	122.19
7	Ql	261	ARG	C-N-CA	5.66	135.21	122.19
2	Ba	429	ASN	N-CA-C	5.66	120.05	113.20
7	Qa	261	ARG	CA-C-N	5.66	135.20	122.19
7	Qa	261	ARG	C-N-CA	5.66	135.20	122.19
7	Qb	261	ARG	CA-C-N	5.66	135.20	122.19
7	Qb	261	ARG	C-N-CA	5.66	135.20	122.19
8	Pf	63	PRO	CA-C-N	5.66	132.15	121.97
8	Pf	63	PRO	C-N-CA	5.66	132.15	121.97
7	Qk	261	ARG	CA-C-N	5.66	135.20	122.19
7	Qk	261	ARG	C-N-CA	5.66	135.20	122.19
7	Qc	261	ARG	CA-C-N	5.65	135.19	122.19
7	Qc	261	ARG	C-N-CA	5.65	135.19	122.19
7	Qf	261	ARG	CA-C-N	5.65	135.18	122.19
7	Qf	261	ARG	C-N-CA	5.65	135.18	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qi	261	ARG	CA-C-N	5.64	135.17	122.19
7	Qi	261	ARG	C-N-CA	5.64	135.17	122.19
7	Qf	498	ILE	O-C-N	-5.64	116.40	121.87
7	Qi	528	ALA	CA-C-N	5.64	128.09	120.65
7	Qi	528	ALA	C-N-CA	5.64	128.09	120.65
9	Tj	311	TYR	N-CA-C	5.64	119.64	112.87
7	Qg	498	ILE	O-C-N	-5.63	116.41	121.87
7	Qh	261	ARG	CA-C-N	5.63	135.14	122.19
7	Qh	261	ARG	C-N-CA	5.63	135.14	122.19
9	Tl	369	ILE	CA-C-N	5.63	126.05	120.98
9	Tl	369	ILE	C-N-CA	5.63	126.05	120.98
2	Bf	353	GLU	N-CA-C	-5.61	107.68	114.75
7	Qg	528	ALA	CA-C-N	5.60	128.04	120.65
7	Qg	528	ALA	C-N-CA	5.60	128.04	120.65
2	Bd	260	GLY	CA-C-N	-5.60	116.64	122.69
2	Bd	260	GLY	C-N-CA	-5.60	116.64	122.69
2	Bb	529	GLN	CA-C-N	-5.60	114.02	122.81
2	Bb	529	GLN	C-N-CA	-5.60	114.02	122.81
7	Qj	525	TRP	N-CA-C	5.60	117.46	111.36
8	Pk	63	PRO	CA-C-N	5.60	132.04	121.97
8	Pk	63	PRO	C-N-CA	5.60	132.04	121.97
1	Aq	113	GLU	N-CA-C	-5.59	106.50	113.38
7	Qf	525	TRP	N-CA-C	5.59	117.45	111.36
1	As	113	GLU	N-CA-C	-5.58	106.52	113.38
2	Be	353	GLU	N-CA-C	-5.58	107.72	114.75
9	Td	369	ILE	CA-C-N	5.57	126.00	120.98
9	Td	369	ILE	C-N-CA	5.57	126.00	120.98
9	Te	311	TYR	N-CA-C	5.57	119.55	112.87
2	Bb	353	GLU	N-CA-C	-5.56	107.74	114.75
8	Pd	63	PRO	CA-C-N	5.56	131.98	121.97
8	Pd	63	PRO	C-N-CA	5.56	131.98	121.97
1	Ag	113	GLU	N-CA-C	-5.56	106.55	113.38
2	Bf	529	GLN	CA-C-N	-5.55	114.10	122.81
2	Bf	529	GLN	C-N-CA	-5.55	114.10	122.81
7	Qa	529	LEU	CA-C-O	-5.54	115.18	121.00
7	Qg	529	LEU	CA-C-O	-5.54	115.18	121.00
9	Tk	369	ILE	CA-C-N	5.54	125.97	120.98
9	Tk	369	ILE	C-N-CA	5.54	125.97	120.98
1	Aa	113	GLU	N-CA-C	-5.54	106.57	113.38
2	Bd	382	GLN	CA-C-N	-5.53	115.99	123.46
2	Bd	382	GLN	C-N-CA	-5.53	115.99	123.46
8	Pb	63	PRO	CA-C-N	5.53	131.93	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Pb	63	PRO	C-N-CA	5.53	131.93	121.97
1	Am	113	GLU	N-CA-C	-5.52	106.59	113.38
9	Ti	311	TYR	N-CA-C	5.51	119.49	112.87
9	Th	311	TYR	N-CA-C	5.51	119.48	112.87
2	Bd	421	PRO	N-CA-C	-5.51	106.36	113.57
1	Ah	113	GLU	N-CA-C	-5.50	106.61	113.38
1	Ay	26	ASP	N-CA-C	-5.50	106.70	113.41
1	A1	113	GLU	N-CA-C	-5.50	106.62	113.38
9	Tb	311	TYR	N-CA-C	5.50	119.47	112.87
7	Qe	528	ALA	CA-C-N	5.50	127.90	120.65
7	Qe	528	ALA	C-N-CA	5.50	127.90	120.65
8	Pi	63	PRO	CA-C-N	5.50	131.86	121.97
8	Pi	63	PRO	C-N-CA	5.50	131.86	121.97
2	Bc	529	GLN	CA-C-N	-5.49	113.59	122.81
2	Bc	529	GLN	C-N-CA	-5.49	113.59	122.81
8	Pk	44	VAL	O-C-N	-5.48	116.75	123.00
1	A8	26	ASP	N-CA-C	-5.47	106.73	113.41
7	Qc	529	LEU	CA-C-O	-5.47	115.25	121.00
7	Qh	528	ALA	CA-C-N	5.47	127.87	120.65
7	Qh	528	ALA	C-N-CA	5.47	127.87	120.65
1	Au	113	GLU	N-CA-C	-5.47	106.65	113.38
1	Ak	113	GLU	N-CA-C	-5.47	106.65	113.38
1	A5	113	GLU	N-CA-C	-5.47	106.66	113.38
9	Td	311	TYR	N-CA-C	5.47	119.43	112.87
7	Qi	498	ILE	O-C-N	-5.46	116.57	121.87
1	Az	113	GLU	N-CA-C	-5.46	106.66	113.38
1	A4	136	ALA	N-CA-C	-5.46	102.24	110.70
1	A7	113	GLU	N-CA-C	-5.46	106.66	113.38
2	Ba	298	PHE	CA-C-N	-5.46	115.01	122.93
2	Ba	298	PHE	C-N-CA	-5.46	115.01	122.93
2	Bd	454	CYS	CA-C-N	-5.46	112.88	120.25
2	Bd	454	CYS	C-N-CA	-5.46	112.88	120.25
9	Tk	311	TYR	N-CA-C	5.46	119.42	112.87
7	Qi	525	TRP	N-CA-C	5.46	117.23	111.28
9	Tc	311	TYR	N-CA-C	5.46	119.42	112.87
1	Ao	113	GLU	N-CA-C	-5.45	106.68	113.38
1	A2	113	GLU	N-CA-C	-5.45	106.68	113.38
7	Ql	528	ALA	CA-C-N	5.45	127.84	120.65
7	Ql	528	ALA	C-N-CA	5.45	127.84	120.65
1	Ah	136	ALA	N-CA-C	-5.44	102.26	110.70
1	A9	26	ASP	N-CA-C	-5.44	106.77	113.41
1	Ar	113	GLU	N-CA-C	-5.44	106.69	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ai	113	GLU	N-CA-C	-5.44	106.69	113.38
1	At	113	GLU	N-CA-C	-5.44	106.69	113.38
7	Ql	525	TRP	N-CA-C	5.44	117.29	111.36
3	Cb	192	VAL	CA-C-N	5.43	127.50	120.44
3	Cb	192	VAL	C-N-CA	5.43	127.50	120.44
1	Az	136	ALA	N-CA-C	-5.43	102.28	110.70
1	Av	113	GLU	N-CA-C	-5.43	106.71	113.38
9	Tg	311	TYR	N-CA-C	5.43	119.38	112.87
1	Ag	136	ALA	N-CA-C	-5.42	102.30	110.70
1	Ad	26	ASP	N-CA-C	-5.42	106.80	113.41
7	Qf	530	ASP	CA-C-O	5.42	126.48	120.63
7	Qh	525	TRP	N-CA-C	5.42	117.18	111.28
1	Ax	136	ALA	N-CA-C	-5.42	102.31	110.70
9	Ta	311	TYR	N-CA-C	5.42	119.37	112.87
1	Ay	113	GLU	N-CA-C	-5.41	106.72	113.38
6	Mk	152	VAL	CA-C-N	5.41	131.44	121.70
6	Mk	152	VAL	C-N-CA	5.41	131.44	121.70
1	Aj	113	GLU	N-CA-C	-5.41	106.72	113.38
2	Bb	298	PHE	CA-C-N	-5.41	115.08	122.93
2	Bb	298	PHE	C-N-CA	-5.41	115.08	122.93
2	Bf	421	PRO	N-CA-C	-5.41	106.48	113.57
1	Ad	113	GLU	N-CA-C	-5.41	106.73	113.38
1	A3	113	GLU	N-CA-C	-5.41	106.73	113.38
1	Ae	26	ASP	N-CA-C	-5.41	106.81	113.41
1	Av	26	ASP	N-CA-C	-5.41	106.81	113.41
3	Ca	87	PHE	N-CA-C	5.41	117.25	111.36
1	Aw	26	ASP	N-CA-C	-5.41	106.81	113.41
1	Aj	136	ALA	N-CA-C	-5.40	102.32	110.70
9	Tl	311	TYR	N-CA-C	5.40	119.35	112.87
6	Ml	152	VAL	CA-C-N	5.40	131.42	121.70
6	Ml	152	VAL	C-N-CA	5.40	131.42	121.70
9	Tj	369	ILE	CA-C-N	5.40	125.84	120.98
9	Tj	369	ILE	C-N-CA	5.40	125.84	120.98
1	A8	113	GLU	N-CA-C	-5.40	106.74	113.38
1	Ax	113	GLU	N-CA-C	-5.40	106.74	113.38
1	A5	136	ALA	N-CA-C	-5.40	102.33	110.70
1	A9	136	ALA	N-CA-C	-5.39	102.34	110.70
6	Mh	152	VAL	CA-C-N	5.39	131.41	121.70
6	Mh	152	VAL	C-N-CA	5.39	131.41	121.70
1	Ap	113	GLU	N-CA-C	-5.39	106.75	113.38
6	Mj	152	VAL	CA-C-N	5.39	131.40	121.70
6	Mj	152	VAL	C-N-CA	5.39	131.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Bc	421	PRO	N-CA-C	-5.39	106.51	113.57
2	Bf	429	ASN	N-CA-C	5.39	119.72	113.20
9	Ta	369	ILE	CA-C-N	5.38	125.82	120.98
9	Ta	369	ILE	C-N-CA	5.38	125.82	120.98
1	A6	113	GLU	N-CA-C	-5.38	106.77	113.38
1	Av	136	ALA	N-CA-C	-5.37	102.37	110.70
9	Tf	311	TYR	N-CA-C	5.37	119.32	112.87
1	Ac	136	ALA	N-CA-C	-5.37	102.38	110.70
1	Az	26	ASP	N-CA-C	-5.37	106.86	113.41
6	Mi	152	VAL	CA-C-N	5.37	131.36	121.70
6	Mi	152	VAL	C-N-CA	5.37	131.36	121.70
7	Qe	530	ASP	CA-C-O	5.37	126.43	120.63
1	Ac	113	GLU	N-CA-C	-5.36	106.78	113.38
1	Ah	26	ASP	N-CA-C	-5.36	106.87	113.41
1	At	26	ASP	N-CA-C	-5.36	106.87	113.41
1	Aw	113	GLU	N-CA-C	-5.36	106.79	113.38
7	Qj	280	GLY	O-C-N	-5.36	118.78	123.76
8	Pc	63	PRO	CA-C-N	5.35	131.61	121.97
8	Pc	63	PRO	C-N-CA	5.35	131.61	121.97
6	Ma	152	VAL	CA-C-N	5.35	131.34	121.70
6	Ma	152	VAL	C-N-CA	5.35	131.34	121.70
6	Mb	152	VAL	CA-C-N	5.35	131.33	121.70
6	Mb	152	VAL	C-N-CA	5.35	131.33	121.70
7	Qb	528	ALA	CA-C-N	5.35	127.71	120.65
7	Qb	528	ALA	C-N-CA	5.35	127.71	120.65
1	Ar	26	ASP	N-CA-C	-5.35	106.89	113.41
1	Al	113	GLU	N-CA-C	-5.34	106.81	113.38
7	Qc	280	GLY	O-C-N	-5.34	118.79	123.76
9	Tf	369	ILE	CA-C-N	5.34	125.79	120.98
9	Tf	369	ILE	C-N-CA	5.34	125.79	120.98
6	Mc	152	VAL	CA-C-N	5.34	131.31	121.70
6	Mc	152	VAL	C-N-CA	5.34	131.31	121.70
1	A9	113	GLU	N-CA-C	-5.34	106.81	113.38
7	Ql	280	GLY	O-C-N	-5.34	118.80	123.76
1	Ab	113	GLU	N-CA-C	-5.34	106.81	113.38
1	Ak	136	ALA	N-CA-C	-5.34	102.43	110.70
2	Bc	382	GLN	CA-C-N	-5.34	116.26	123.46
2	Bc	382	GLN	C-N-CA	-5.34	116.26	123.46
1	Ab	136	ALA	N-CA-C	-5.33	102.43	110.70
7	Qb	280	GLY	O-C-N	-5.33	118.80	123.76
3	Cb	87	PHE	N-CA-C	5.33	117.17	111.36
1	Ag	26	ASP	N-CA-C	-5.33	106.91	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qj	529	LEU	CA-C-O	-5.33	115.41	121.00
1	Ak	26	ASP	N-CA-C	-5.33	106.91	113.41
7	Qg	280	GLY	O-C-N	-5.32	118.81	123.76
1	Aw	136	ALA	N-CA-C	-5.32	102.46	110.70
1	A5	26	ASP	N-CA-C	-5.32	106.92	113.41
1	Ad	136	ALA	N-CA-C	-5.31	102.46	110.70
7	Qf	528	ALA	CA-C-N	5.31	127.66	120.65
7	Qf	528	ALA	C-N-CA	5.31	127.66	120.65
1	Au	103	GLY	N-CA-C	-5.31	107.65	115.30
7	Qe	529	LEU	CA-C-O	-5.31	115.42	121.00
7	Qk	280	GLY	O-C-N	-5.31	118.82	123.76
1	Ao	26	ASP	N-CA-C	-5.31	106.94	113.41
1	Ax	26	ASP	N-CA-C	-5.31	106.94	113.41
9	Tg	369	ILE	CA-C-N	5.31	125.75	120.98
9	Tg	369	ILE	C-N-CA	5.31	125.75	120.98
1	Ai	136	ALA	N-CA-C	-5.30	102.48	110.70
1	An	113	GLU	N-CA-C	-5.30	106.86	113.38
7	Qf	280	GLY	O-C-N	-5.30	118.83	123.76
1	Ae	113	GLU	N-CA-C	-5.30	106.86	113.38
1	A6	136	ALA	N-CA-C	-5.30	102.48	110.70
6	Mf	152	VAL	CA-C-N	5.30	131.24	121.70
6	Mf	152	VAL	C-N-CA	5.30	131.24	121.70
7	Qb	529	LEU	CA-C-O	-5.30	115.43	121.00
1	A7	26	ASP	N-CA-C	-5.30	106.94	113.41
6	Me	152	VAL	CA-C-N	5.30	131.24	121.70
6	Me	152	VAL	C-N-CA	5.30	131.24	121.70
7	Qb	534	ARG	N-CA-C	5.30	117.80	111.71
7	Qi	280	GLY	O-C-N	-5.30	118.83	123.76
7	Qa	280	GLY	O-C-N	-5.29	118.84	123.76
7	Qe	280	GLY	O-C-N	-5.29	118.83	123.76
1	Am	136	ALA	N-CA-C	-5.29	102.50	110.70
6	Md	152	VAL	CA-C-N	5.29	131.22	121.70
6	Md	152	VAL	C-N-CA	5.29	131.22	121.70
1	A7	136	ALA	N-CA-C	-5.28	102.51	110.70
7	Qg	534	ARG	N-CA-C	5.28	117.79	111.71
1	Ap	26	ASP	N-CA-C	-5.28	106.97	113.41
1	A1	136	ALA	N-CA-C	-5.28	102.52	110.70
1	A4	26	ASP	N-CA-C	-5.28	106.97	113.41
7	Qh	280	GLY	O-C-N	-5.28	118.85	123.76
1	A4	113	GLU	N-CA-C	-5.28	106.89	113.38
1	A7	103	GLY	N-CA-C	-5.27	107.71	115.30
1	Af	113	GLU	N-CA-C	-5.26	106.91	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Mg	152	VAL	CA-C-N	5.26	131.17	121.70
6	Mg	152	VAL	C-N-CA	5.26	131.17	121.70
7	Qd	280	GLY	O-C-N	-5.26	118.87	123.76
1	Au	136	ALA	N-CA-C	-5.26	102.55	110.70
1	A3	136	ALA	N-CA-C	-5.26	102.55	110.70
1	Ac	26	ASP	N-CA-C	-5.25	107.00	113.41
8	Pi	53	PRO	O-C-N	-5.25	115.55	122.64
1	A6	26	ASP	N-CA-C	-5.25	107.00	113.41
1	A1	26	ASP	N-CA-C	-5.25	107.01	113.41
2	Bc	298	PHE	CA-C-N	-5.25	115.32	122.93
2	Bc	298	PHE	C-N-CA	-5.25	115.32	122.93
1	Ae	136	ALA	N-CA-C	-5.25	102.57	110.70
1	Aa	103	GLY	N-CA-C	-5.25	107.75	115.30
9	Te	369	ILE	CA-C-N	5.24	125.70	120.98
9	Te	369	ILE	C-N-CA	5.24	125.70	120.98
1	Aj	103	GLY	N-CA-C	-5.24	107.75	115.30
1	As	103	GLY	N-CA-C	-5.24	107.75	115.30
1	Ab	26	ASP	N-CA-C	-5.24	107.02	113.41
7	Qi	529	LEU	CA-C-O	-5.24	115.50	121.00
2	Be	382	GLN	CA-C-N	-5.24	116.39	123.46
2	Be	382	GLN	C-N-CA	-5.24	116.39	123.46
7	Qa	528	ALA	CA-C-N	5.24	127.56	120.65
7	Qa	528	ALA	C-N-CA	5.24	127.56	120.65
3	Cb	333	ILE	CA-C-N	5.23	127.28	120.28
3	Cb	333	ILE	C-N-CA	5.23	127.28	120.28
2	Bd	353	GLU	N-CA-C	-5.23	108.17	114.75
1	Al	26	ASP	N-CA-C	-5.22	107.03	113.41
1	Ap	136	ALA	N-CA-C	-5.22	102.61	110.70
8	Pl	53	PRO	O-C-N	-5.22	115.59	122.64
1	Ar	136	ALA	N-CA-C	-5.22	102.61	110.70
9	Tc	369	ILE	CA-C-N	5.22	125.68	120.98
9	Tc	369	ILE	C-N-CA	5.22	125.68	120.98
1	A2	26	ASP	N-CA-C	-5.22	107.05	113.41
1	Aj	26	ASP	N-CA-C	-5.21	107.05	113.41
1	Au	26	ASP	N-CA-C	-5.21	107.05	113.41
1	A8	136	ALA	N-CA-C	-5.21	102.62	110.70
1	Am	26	ASP	N-CA-C	-5.21	107.06	113.41
2	Bd	322	PRO	CA-C-N	-5.21	113.66	120.95
2	Bd	322	PRO	C-N-CA	-5.21	113.66	120.95
8	Pg	128	ARG	CA-C-N	5.20	130.52	122.26
8	Pg	128	ARG	C-N-CA	5.20	130.52	122.26
1	An	26	ASP	N-CA-C	-5.20	107.07	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	26	ASP	N-CA-C	-5.19	107.07	113.41
1	Ay	136	ALA	N-CA-C	-5.19	102.66	110.70
3	Ca	333	ILE	CA-C-N	5.19	127.23	120.28
3	Ca	333	ILE	C-N-CA	5.19	127.23	120.28
8	Ph	53	PRO	O-C-N	-5.19	115.64	122.64
1	Av	103	GLY	N-CA-C	-5.18	107.84	115.30
1	Ao	103	GLY	N-CA-C	-5.18	107.84	115.30
2	Bb	454	CYS	CA-C-N	-5.18	113.26	120.25
2	Bb	454	CYS	C-N-CA	-5.18	113.26	120.25
7	Qf	635	GLN	CA-C-N	5.18	126.56	120.09
7	Qf	635	GLN	C-N-CA	5.18	126.56	120.09
8	Pc	44	VAL	O-C-N	-5.18	117.10	123.00
2	Bb	322	PRO	CA-C-N	-5.18	113.70	120.95
2	Bb	322	PRO	C-N-CA	-5.18	113.70	120.95
2	Be	260	GLY	CA-C-N	-5.17	117.10	122.69
2	Be	260	GLY	C-N-CA	-5.17	117.10	122.69
9	Tb	369	ILE	CA-C-N	5.17	125.63	120.98
9	Tb	369	ILE	C-N-CA	5.17	125.63	120.98
7	Qg	530	ASP	CA-C-O	5.16	126.21	120.63
8	Pa	29	ALA	CA-C-O	-5.16	113.09	120.16
7	Qd	528	ALA	CA-C-N	5.15	127.45	120.65
7	Qd	528	ALA	C-N-CA	5.15	127.45	120.65
1	A3	26	ASP	N-CA-C	-5.15	107.13	113.41
1	Am	103	GLY	N-CA-C	-5.15	107.89	115.30
2	Bf	454	CYS	CA-C-N	-5.15	113.30	120.25
2	Bf	454	CYS	C-N-CA	-5.15	113.30	120.25
7	Qe	636	THR	CA-C-N	5.14	124.94	119.28
7	Qe	636	THR	C-N-CA	5.14	124.94	119.28
6	Mg	381	VAL	CA-C-N	5.14	127.89	120.38
6	Mg	381	VAL	C-N-CA	5.14	127.89	120.38
1	Aq	26	ASP	N-CA-C	-5.14	107.14	113.41
1	At	103	GLY	N-CA-C	-5.13	107.91	115.30
1	As	26	ASP	N-CA-C	-5.13	107.16	113.41
7	Qj	636	THR	CA-C-N	5.13	124.92	119.28
7	Qj	636	THR	C-N-CA	5.13	124.92	119.28
7	Qb	525	TRP	N-CA-C	5.12	116.95	111.36
1	A6	103	GLY	N-CA-C	-5.12	107.92	115.30
8	Pj	44	VAL	O-C-N	-5.12	117.16	123.00
1	Ah	103	GLY	N-CA-C	-5.12	107.93	115.30
6	Mc	381	VAL	CA-C-N	5.12	127.85	120.38
6	Mc	381	VAL	C-N-CA	5.12	127.85	120.38
7	Qc	528	ALA	CA-C-N	5.12	127.40	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Qc	528	ALA	C-N-CA	5.12	127.40	120.65
8	Pk	53	PRO	O-C-N	-5.12	115.73	122.64
6	Mk	381	VAL	CA-C-N	5.11	127.84	120.38
6	Mk	381	VAL	C-N-CA	5.11	127.84	120.38
3	Cb	346	MET	N-CA-C	5.11	117.98	111.69
2	Ba	270	VAL	N-CA-C	-5.11	108.30	113.20
7	Qi	534	ARG	N-CA-C	5.11	117.59	111.71
7	Ql	635	GLN	CA-C-N	5.11	126.48	120.09
7	Ql	635	GLN	C-N-CA	5.11	126.48	120.09
9	Ti	361	GLU	CA-C-N	5.11	129.81	122.35
9	Ti	361	GLU	C-N-CA	5.11	129.81	122.35
1	A4	103	GLY	N-CA-C	-5.11	107.95	115.30
7	Qd	529	LEU	CA-C-O	-5.11	115.64	121.00
7	Qd	519	ARG	N-CA-C	5.10	116.49	107.61
1	Ag	103	GLY	N-CA-C	-5.10	107.95	115.30
7	Qb	530	ASP	CA-C-O	5.10	126.14	120.63
1	Al	103	GLY	N-CA-C	-5.09	107.96	115.30
6	Mf	381	VAL	CA-C-N	5.09	127.81	120.38
6	Mf	381	VAL	C-N-CA	5.09	127.81	120.38
1	Ac	103	GLY	N-CA-C	-5.09	107.97	115.30
7	Qi	530	ASP	CA-C-O	5.09	126.12	120.63
1	A3	103	GLY	N-CA-C	-5.08	107.98	115.30
7	Qj	530	ASP	CA-C-O	5.08	126.11	120.63
1	A1	103	GLY	N-CA-C	-5.08	107.99	115.30
7	Qe	498	ILE	O-C-N	-5.08	116.95	121.87
2	Be	270	VAL	N-CA-C	-5.07	108.34	113.20
1	Ar	103	GLY	N-CA-C	-5.06	108.01	115.30
6	Mh	381	VAL	CA-C-N	5.06	127.77	120.38
6	Mh	381	VAL	C-N-CA	5.06	127.77	120.38
5	Oc	72	ARG	CA-C-N	-5.06	113.17	121.92
5	Oc	72	ARG	C-N-CA	-5.06	113.17	121.92
7	Qf	252	ALA	O-C-N	-5.05	115.70	120.70
7	Qf	519	ARG	N-CA-C	5.05	116.39	107.61
9	Tl	359	LYS	CA-C-N	5.05	127.31	120.44
9	Tl	359	LYS	C-N-CA	5.05	127.31	120.44
1	Ai	26	ASP	N-CA-C	-5.04	107.26	113.41
2	Ba	182	LEU	CA-C-N	-5.04	113.11	121.63
2	Ba	182	LEU	C-N-CA	-5.04	113.11	121.63
6	Ma	381	VAL	CA-C-N	5.04	127.54	120.28
6	Ma	381	VAL	C-N-CA	5.04	127.54	120.28
7	Qe	252	ALA	O-C-N	-5.04	115.71	120.70
7	Qe	519	ARG	N-CA-C	5.04	116.38	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Bb	182	LEU	CA-C-N	-5.04	113.12	121.63
2	Bb	182	LEU	C-N-CA	-5.04	113.12	121.63
8	Pl	62	GLY	O-C-N	5.04	122.88	121.07
1	Ah	153	ASP	N-CA-C	5.03	117.73	110.28
5	Oi	72	ARG	CA-C-N	-5.03	113.21	121.92
5	Oi	72	ARG	C-N-CA	-5.03	113.21	121.92
8	Pe	53	PRO	O-C-N	-5.03	115.85	122.64
7	Qa	252	ALA	O-C-N	-5.02	115.73	120.70
7	Qc	519	ARG	N-CA-C	5.02	116.34	107.61
7	Qk	252	ALA	O-C-N	-5.02	115.73	120.70
1	Af	103	GLY	N-CA-C	-5.02	108.08	115.30
7	Qh	252	ALA	O-C-N	-5.02	115.73	120.70
7	Qd	530	ASP	CA-C-O	5.01	126.05	120.63
7	Qi	252	ALA	O-C-N	-5.01	115.74	120.70
1	Ai	103	GLY	N-CA-C	-5.01	108.08	115.30
1	Aw	103	GLY	N-CA-C	-5.01	108.09	115.30
5	Oh	72	ARG	CA-C-N	-5.01	113.25	121.92
5	Oh	72	ARG	C-N-CA	-5.01	113.25	121.92
5	Ol	72	ARG	CA-C-N	-5.01	113.26	121.92
5	Ol	72	ARG	C-N-CA	-5.01	113.26	121.92
7	Qc	252	ALA	O-C-N	-5.01	115.74	120.70
1	Az	103	GLY	N-CA-C	-5.00	108.10	115.30
7	Qh	534	ARG	N-CA-C	5.00	117.46	111.71
7	Qk	528	ALA	CA-C-N	5.00	127.25	120.65
7	Qk	528	ALA	C-N-CA	5.00	127.25	120.65

There are no chirality outliers.

All (762) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Ba	293	MET	Peptide
2	Ba	345	ILE	Peptide
2	Ba	379	PHE	Peptide
2	Bb	177	ALA	Peptide
2	Bb	284	LEU	Peptide
2	Bb	286	LYS	Peptide
2	Bb	287	SER	Peptide
2	Bb	293	MET	Peptide
2	Bb	345	ILE	Peptide
2	Bb	379	PHE	Peptide
2	Bc	177	ALA	Peptide
2	Bc	293	MET	Peptide

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Mol	Chain	Res	Type	Group
2	Bc	345	ILE	Peptide
2	Bc	379	PHE	Peptide
2	Bd	177	ALA	Peptide
2	Bd	284	LEU	Peptide
2	Bd	286	LYS	Peptide
2	Bd	287	SER	Peptide
2	Bd	293	MET	Peptide
2	Bd	345	ILE	Peptide
2	Bd	379	PHE	Peptide
2	Be	177	ALA	Peptide
2	Be	293	MET	Peptide
2	Be	345	ILE	Peptide
2	Be	379	PHE	Peptide
2	Bf	177	ALA	Peptide
2	Bf	284	LEU	Peptide
2	Bf	286	LYS	Peptide
2	Bf	287	SER	Peptide
2	Bf	293	MET	Peptide
2	Bf	345	ILE	Peptide
2	Bf	379	PHE	Peptide
3	Ca	108	MET	Mainchain
3	Ca	169	ARG	Mainchain
3	Ca	192	VAL	Mainchain
3	Ca	200	LEU	Mainchain
3	Ca	222	PRO	Peptide,Mainchain
3	Ca	223	THR	Peptide
3	Ca	242	GLY	Mainchain
3	Ca	256	ARG	Mainchain
3	Ca	257	GLN	Mainchain
3	Ca	279	ARG	Mainchain
3	Ca	302	ASP	Mainchain
3	Ca	313	ASN	Mainchain
3	Ca	317	GLU	Mainchain
3	Ca	325	GLY	Mainchain
3	Ca	332	ASN	Mainchain
3	Ca	384	ALA	Mainchain
3	Ca	78	LYS	Mainchain
3	Cb	108	MET	Mainchain
3	Cb	169	ARG	Mainchain
3	Cb	200	LEU	Mainchain
3	Cb	203	LYS	Mainchain
3	Cb	222	PRO	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
3	Cb	223	THR	Peptide
3	Cb	256	ARG	Mainchain
3	Cb	257	GLN	Mainchain
3	Cb	279	ARG	Mainchain
3	Cb	302	ASP	Mainchain
3	Cb	313	ASN	Mainchain
3	Cb	317	GLU	Mainchain
3	Cb	325	GLY	Mainchain
3	Cb	332	ASN	Mainchain
3	Cb	344	PRO	Mainchain
3	Cb	384	ALA	Mainchain
3	Cb	78	LYS	Mainchain
6	Ma	315	TYR	Peptide
6	Ma	320	ALA	Peptide
6	Mb	315	TYR	Peptide
6	Mb	320	ALA	Peptide
6	Mc	315	TYR	Peptide
6	Mc	320	ALA	Peptide
6	Md	315	TYR	Peptide
6	Md	320	ALA	Peptide
6	Me	315	TYR	Peptide
6	Me	320	ALA	Peptide
6	Mf	315	TYR	Peptide
6	Mf	320	ALA	Peptide
6	Mg	315	TYR	Peptide
6	Mg	320	ALA	Peptide
6	Mh	315	TYR	Peptide
6	Mh	320	ALA	Peptide
6	Mi	315	TYR	Peptide
6	Mi	320	ALA	Peptide
6	Mj	315	TYR	Peptide
6	Mj	320	ALA	Peptide
6	Mk	315	TYR	Peptide
6	Mk	320	ALA	Peptide
6	Ml	315	TYR	Peptide
6	Ml	320	ALA	Peptide
4	Na	100	VAL	Peptide
4	Na	101	ARG	Peptide
4	Na	171	GLU	Peptide
4	Na	209	VAL	Peptide
4	Na	221	SER	Peptide
4	Na	222	ASN	Peptide

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Mol	Chain	Res	Type	Group
4	Nb	100	VAL	Peptide
4	Nb	101	ARG	Peptide
4	Nb	171	GLU	Peptide
4	Nb	209	VAL	Peptide
4	Nb	221	SER	Peptide
4	Nb	222	ASN	Peptide
4	Nc	100	VAL	Peptide
4	Nc	101	ARG	Peptide
4	Nc	171	GLU	Peptide
4	Nc	209	VAL	Peptide
4	Nc	222	ASN	Peptide
4	Nd	100	VAL	Peptide
4	Nd	101	ARG	Peptide
4	Nd	171	GLU	Peptide
4	Nd	209	VAL	Peptide
4	Nd	222	ASN	Peptide
4	Ne	100	VAL	Peptide
4	Ne	101	ARG	Peptide
4	Ne	171	GLU	Peptide
4	Ne	209	VAL	Peptide
4	Ne	222	ASN	Peptide
4	Nf	100	VAL	Peptide
4	Nf	101	ARG	Peptide
4	Nf	171	GLU	Peptide
4	Nf	209	VAL	Peptide
4	Nf	222	ASN	Peptide
4	Ng	100	VAL	Peptide
4	Ng	101	ARG	Peptide
4	Ng	171	GLU	Peptide
4	Ng	209	VAL	Peptide
4	Ng	222	ASN	Peptide
4	Nh	100	VAL	Peptide
4	Nh	101	ARG	Peptide
4	Nh	171	GLU	Peptide
4	Nh	209	VAL	Peptide
4	Nh	222	ASN	Peptide
4	Ni	100	VAL	Peptide
4	Ni	101	ARG	Peptide
4	Ni	171	GLU	Peptide
4	Ni	209	VAL	Peptide
4	Ni	222	ASN	Peptide
4	Nj	100	VAL	Peptide

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Mol	Chain	Res	Type	Group
4	Nj	101	ARG	Peptide
4	Nj	171	GLU	Peptide
4	Nj	209	VAL	Peptide
4	Nj	222	ASN	Peptide
4	Nk	100	VAL	Peptide
4	Nk	101	ARG	Peptide
4	Nk	171	GLU	Peptide
4	Nk	209	VAL	Peptide
4	Nk	222	ASN	Peptide
4	Nl	100	VAL	Peptide
4	Nl	101	ARG	Peptide
4	Nl	171	GLU	Peptide
4	Nl	209	VAL	Peptide
4	Nl	222	ASN	Peptide
5	Oa	82	SER	Peptide
5	Ob	82	SER	Peptide
5	Oc	82	SER	Peptide
5	Od	82	SER	Peptide
5	Oe	82	SER	Peptide
5	Of	82	SER	Peptide
5	Og	82	SER	Peptide
5	Oh	82	SER	Peptide
5	Oi	82	SER	Peptide
5	Oj	82	SER	Peptide
5	Ok	82	SER	Peptide
5	Ol	82	SER	Peptide
8	Pa	10	ALA	Peptide
8	Pa	12	ALA	Peptide
8	Pa	13	PRO	Peptide
8	Pa	14	PRO	Peptide
8	Pa	23	ALA	Peptide
8	Pa	24	VAL	Peptide
8	Pa	25	PRO	Peptide
8	Pa	26	VAL	Peptide
8	Pa	28	ALA	Peptide
8	Pa	29	ALA	Peptide,Mainchain
8	Pa	30	PRO	Mainchain
8	Pa	32	GLU	Peptide
8	Pa	33	THR	Peptide
8	Pa	38	ALA	Peptide
8	Pa	46	ASN	Peptide
8	Pa	47	PRO	Peptide

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Mol	Chain	Res	Type	Group
8	Pa	49	GLY	Peptide
8	Pa	50	LYS	Peptide
8	Pa	51	ARG	Peptide
8	Pa	52	ASP	Peptide
8	Pa	53	PRO	Peptide
8	Pa	64	VAL	Mainchain
8	Pa	74	GLU	Peptide
8	Pa	8	PRO	Peptide
8	Pb	11	PRO	Peptide
8	Pb	13	PRO	Peptide
8	Pb	14	PRO	Peptide
8	Pb	145	LYS	Mainchain
8	Pb	15	PRO	Peptide
8	Pb	23	ALA	Peptide
8	Pb	24	VAL	Peptide
8	Pb	25	PRO	Peptide
8	Pb	26	VAL	Peptide
8	Pb	28	ALA	Peptide
8	Pb	29	ALA	Peptide
8	Pb	32	GLU	Peptide
8	Pb	33	THR	Peptide
8	Pb	38	ALA	Peptide
8	Pb	39	PRO	Peptide
8	Pb	44	VAL	Peptide
8	Pb	45	TYR	Peptide
8	Pb	47	PRO	Peptide
8	Pb	48	VAL	Peptide
8	Pb	49	GLY	Peptide
8	Pb	52	ASP	Peptide
8	Pb	53	PRO	Peptide
8	Pb	54	PHE	Peptide
8	Pb	64	VAL	Mainchain
8	Pb	74	GLU	Peptide,Mainchain
8	Pb	8	PRO	Peptide,Mainchain
8	Pc	15	PRO	Peptide
8	Pc	23	ALA	Peptide
8	Pc	24	VAL	Peptide
8	Pc	25	PRO	Peptide
8	Pc	26	VAL	Peptide
8	Pc	27	LYS	Peptide
8	Pc	28	ALA	Peptide
8	Pc	32	GLU	Peptide

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Mol	Chain	Res	Type	Group
8	Pc	33	THR	Peptide
8	Pc	38	ALA	Peptide
8	Pc	47	PRO	Peptide
8	Pc	49	GLY	Peptide
8	Pc	50	LYS	Peptide
8	Pc	51	ARG	Peptide
8	Pc	53	PRO	Peptide
8	Pc	54	PHE	Peptide
8	Pc	64	VAL	Mainchain
8	Pc	74	GLU	Peptide
8	Pc	8	PRO	Peptide,Mainchain
8	Pd	145	LYS	Mainchain
8	Pd	15	PRO	Peptide
8	Pd	23	ALA	Peptide
8	Pd	24	VAL	Peptide
8	Pd	25	PRO	Peptide
8	Pd	26	VAL	Peptide
8	Pd	27	LYS	Peptide
8	Pd	28	ALA	Peptide
8	Pd	29	ALA	Peptide
8	Pd	32	GLU	Peptide
8	Pd	33	THR	Peptide
8	Pd	38	ALA	Peptide
8	Pd	44	VAL	Peptide
8	Pd	45	TYR	Peptide
8	Pd	47	PRO	Peptide
8	Pd	48	VAL	Peptide
8	Pd	49	GLY	Peptide
8	Pd	51	ARG	Peptide
8	Pd	52	ASP	Peptide
8	Pd	53	PRO	Peptide
8	Pd	64	VAL	Mainchain
8	Pd	74	GLU	Peptide
8	Pd	8	PRO	Peptide,Mainchain
8	Pe	13	PRO	Peptide
8	Pe	14	PRO	Peptide
8	Pe	15	PRO	Peptide
8	Pe	23	ALA	Peptide
8	Pe	24	VAL	Peptide
8	Pe	25	PRO	Peptide
8	Pe	26	VAL	Peptide
8	Pe	27	LYS	Peptide

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Mol	Chain	Res	Type	Group
8	Pe	28	ALA	Peptide
8	Pe	29	ALA	Peptide
8	Pe	32	GLU	Peptide
8	Pe	33	THR	Peptide
8	Pe	38	ALA	Peptide
8	Pe	47	PRO	Peptide
8	Pe	49	GLY	Peptide
8	Pe	50	LYS	Peptide
8	Pe	52	ASP	Peptide
8	Pe	64	VAL	Mainchain
8	Pe	74	GLU	Peptide,Mainchain
8	Pe	8	PRO	Peptide,Mainchain
8	Pf	145	LYS	Mainchain
8	Pf	15	PRO	Peptide
8	Pf	23	ALA	Peptide
8	Pf	24	VAL	Peptide
8	Pf	25	PRO	Peptide
8	Pf	26	VAL	Peptide
8	Pf	27	LYS	Peptide
8	Pf	28	ALA	Peptide
8	Pf	29	ALA	Peptide
8	Pf	32	GLU	Peptide
8	Pf	33	THR	Peptide
8	Pf	38	ALA	Peptide
8	Pf	46	ASN	Peptide
8	Pf	47	PRO	Peptide,Mainchain
8	Pf	52	ASP	Peptide,Mainchain
8	Pf	64	VAL	Mainchain
8	Pf	74	GLU	Peptide
8	Pf	8	PRO	Peptide,Mainchain
8	Pg	15	PRO	Peptide
8	Pg	23	ALA	Peptide
8	Pg	24	VAL	Peptide
8	Pg	25	PRO	Peptide
8	Pg	26	VAL	Peptide
8	Pg	27	LYS	Peptide
8	Pg	28	ALA	Peptide
8	Pg	29	ALA	Peptide
8	Pg	33	THR	Peptide
8	Pg	37	ALA	Peptide
8	Pg	40	SER	Peptide
8	Pg	44	VAL	Peptide

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Mol	Chain	Res	Type	Group
8	Pg	45	TYR	Peptide
8	Pg	47	PRO	Peptide
8	Pg	51	ARG	Peptide
8	Pg	52	ASP	Peptide
8	Pg	53	PRO	Peptide
8	Pg	64	VAL	Mainchain
8	Pg	74	GLU	Peptide
8	Pg	8	PRO	Peptide,Mainchain
8	Ph	11	PRO	Peptide
8	Ph	13	PRO	Peptide
8	Ph	14	PRO	Peptide
8	Ph	15	PRO	Peptide
8	Ph	23	ALA	Peptide
8	Ph	24	VAL	Peptide
8	Ph	25	PRO	Peptide
8	Ph	26	VAL	Peptide
8	Ph	27	LYS	Peptide
8	Ph	28	ALA	Peptide
8	Ph	29	ALA	Peptide
8	Ph	32	GLU	Peptide
8	Ph	33	THR	Peptide
8	Ph	36	GLN	Peptide
8	Ph	38	ALA	Peptide
8	Ph	40	SER	Peptide
8	Ph	44	VAL	Peptide
8	Ph	45	TYR	Peptide
8	Ph	47	PRO	Peptide
8	Ph	51	ARG	Peptide
8	Ph	52	ASP	Peptide
8	Ph	63	PRO	Mainchain
8	Ph	64	VAL	Mainchain
8	Ph	74	GLU	Peptide,Mainchain
8	Ph	8	PRO	Peptide
8	Pi	16	ALA	Mainchain
8	Pi	17	LYS	Mainchain
8	Pi	23	ALA	Peptide
8	Pi	24	VAL	Peptide
8	Pi	25	PRO	Peptide
8	Pi	26	VAL	Peptide
8	Pi	27	LYS	Peptide
8	Pi	28	ALA	Peptide
8	Pi	29	ALA	Peptide

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Mol	Chain	Res	Type	Group
8	Pi	32	GLU	Peptide
8	Pi	33	THR	Peptide
8	Pi	38	ALA	Peptide
8	Pi	46	ASN	Peptide
8	Pi	47	PRO	Peptide,Mainchain
8	Pi	52	ASP	Peptide,Mainchain
8	Pi	64	VAL	Mainchain
8	Pi	74	GLU	Peptide
8	Pi	8	PRO	Peptide,Mainchain
8	Pj	15	PRO	Peptide
8	Pj	24	VAL	Peptide
8	Pj	25	PRO	Peptide
8	Pj	26	VAL	Peptide
8	Pj	27	LYS	Peptide
8	Pj	28	ALA	Peptide
8	Pj	29	ALA	Peptide
8	Pj	33	THR	Peptide
8	Pj	38	ALA	Peptide
8	Pj	46	ASN	Peptide
8	Pj	47	PRO	Peptide,Mainchain
8	Pj	52	ASP	Peptide,Mainchain
8	Pj	64	VAL	Mainchain
8	Pj	74	GLU	Peptide,Mainchain
8	Pj	8	PRO	Peptide,Mainchain
8	Pk	17	LYS	Peptide
8	Pk	23	ALA	Peptide
8	Pk	24	VAL	Peptide
8	Pk	25	PRO	Peptide
8	Pk	26	VAL	Peptide
8	Pk	27	LYS	Peptide
8	Pk	28	ALA	Peptide
8	Pk	29	ALA	Peptide
8	Pk	33	THR	Peptide
8	Pk	38	ALA	Peptide
8	Pk	46	ASN	Peptide
8	Pk	47	PRO	Peptide,Mainchain
8	Pk	52	ASP	Peptide,Mainchain
8	Pk	64	VAL	Mainchain
8	Pk	74	GLU	Peptide
8	Pk	8	PRO	Peptide,Mainchain
8	Pl	13	PRO	Peptide
8	Pl	14	PRO	Peptide

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Mol	Chain	Res	Type	Group
8	Pl	145	LYS	Mainchain
8	Pl	15	PRO	Peptide
8	Pl	24	VAL	Peptide
8	Pl	25	PRO	Peptide
8	Pl	26	VAL	Peptide
8	Pl	27	LYS	Peptide
8	Pl	28	ALA	Peptide
8	Pl	29	ALA	Peptide
8	Pl	33	THR	Peptide
8	Pl	38	ALA	Peptide
8	Pl	46	ASN	Peptide
8	Pl	47	PRO	Peptide,Mainchain
8	Pl	52	ASP	Peptide,Mainchain
8	Pl	64	VAL	Mainchain
8	Pl	74	GLU	Peptide
8	Pl	8	PRO	Peptide,Mainchain
7	Qa	135	GLY	Mainchain
7	Qa	250	THR	Mainchain
7	Qa	278	VAL	Mainchain
7	Qa	346	GLU	Mainchain
7	Qa	407	SER	Mainchain
7	Qa	487	LYS	Mainchain
7	Qa	508	VAL	Peptide
7	Qa	530	ASP	Mainchain
7	Qa	533	LEU	Mainchain
7	Qa	534	ARG	Mainchain
7	Qa	536	LYS	Mainchain
7	Qa	537	ALA	Mainchain
7	Qa	575	LEU	Mainchain
7	Qa	601	ARG	Mainchain
7	Qa	602	GLY	Peptide
7	Qa	616	LYS	Mainchain
7	Qa	633	ASP	Mainchain
7	Qa	635	GLN	Mainchain
7	Qa	76	SER	Mainchain
7	Qa	98	SER	Mainchain
7	Qb	135	GLY	Mainchain
7	Qb	250	THR	Mainchain
7	Qb	278	VAL	Mainchain
7	Qb	346	GLU	Mainchain
7	Qb	407	SER	Mainchain
7	Qb	487	LYS	Mainchain

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Mol	Chain	Res	Type	Group
7	Qb	498	ILE	Mainchain
7	Qb	508	VAL	Peptide
7	Qb	510	ASP	Mainchain
7	Qb	530	ASP	Mainchain
7	Qb	533	LEU	Mainchain
7	Qb	534	ARG	Mainchain
7	Qb	536	LYS	Mainchain
7	Qb	537	ALA	Mainchain
7	Qb	575	LEU	Mainchain
7	Qb	601	ARG	Mainchain
7	Qb	602	GLY	Peptide,Mainchain
7	Qb	616	LYS	Mainchain
7	Qb	633	ASP	Mainchain
7	Qb	635	GLN	Mainchain
7	Qb	76	SER	Mainchain
7	Qb	98	SER	Mainchain
7	Qc	135	GLY	Mainchain
7	Qc	250	THR	Mainchain
7	Qc	278	VAL	Mainchain
7	Qc	346	GLU	Mainchain
7	Qc	407	SER	Mainchain
7	Qc	498	ILE	Mainchain
7	Qc	508	VAL	Peptide
7	Qc	530	ASP	Mainchain
7	Qc	533	LEU	Mainchain
7	Qc	534	ARG	Mainchain
7	Qc	536	LYS	Mainchain
7	Qc	537	ALA	Mainchain
7	Qc	575	LEU	Mainchain
7	Qc	601	ARG	Mainchain
7	Qc	602	GLY	Peptide,Mainchain
7	Qc	616	LYS	Mainchain
7	Qc	633	ASP	Mainchain
7	Qc	635	GLN	Mainchain
7	Qc	76	SER	Mainchain
7	Qc	98	SER	Mainchain
7	Qd	135	GLY	Mainchain
7	Qd	250	THR	Mainchain
7	Qd	278	VAL	Mainchain
7	Qd	346	GLU	Mainchain
7	Qd	407	SER	Mainchain
7	Qd	487	LYS	Mainchain

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Mol	Chain	Res	Type	Group
7	Qd	508	VAL	Peptide
7	Qd	530	ASP	Mainchain
7	Qd	533	LEU	Mainchain
7	Qd	534	ARG	Mainchain
7	Qd	536	LYS	Mainchain
7	Qd	537	ALA	Mainchain
7	Qd	540	LYS	Mainchain
7	Qd	575	LEU	Mainchain
7	Qd	601	ARG	Mainchain
7	Qd	602	GLY	Peptide
7	Qd	616	LYS	Mainchain
7	Qd	633	ASP	Mainchain
7	Qd	635	GLN	Mainchain
7	Qd	76	SER	Mainchain
7	Qd	98	SER	Mainchain
7	Qe	135	GLY	Mainchain
7	Qe	250	THR	Mainchain
7	Qe	278	VAL	Mainchain
7	Qe	346	GLU	Mainchain
7	Qe	407	SER	Mainchain
7	Qe	487	LYS	Mainchain
7	Qe	508	VAL	Peptide
7	Qe	510	ASP	Mainchain
7	Qe	530	ASP	Mainchain
7	Qe	533	LEU	Mainchain
7	Qe	534	ARG	Mainchain
7	Qe	536	LYS	Mainchain
7	Qe	537	ALA	Mainchain
7	Qe	575	LEU	Mainchain
7	Qe	601	ARG	Mainchain
7	Qe	602	GLY	Peptide
7	Qe	616	LYS	Mainchain
7	Qe	633	ASP	Mainchain
7	Qe	635	GLN	Mainchain
7	Qe	76	SER	Mainchain
7	Qe	98	SER	Mainchain
7	Qf	135	GLY	Mainchain
7	Qf	250	THR	Mainchain
7	Qf	278	VAL	Mainchain
7	Qf	346	GLU	Mainchain
7	Qf	407	SER	Mainchain
7	Qf	487	LYS	Mainchain

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Mol	Chain	Res	Type	Group
7	Qf	508	VAL	Peptide
7	Qf	530	ASP	Mainchain
7	Qf	533	LEU	Mainchain
7	Qf	534	ARG	Mainchain
7	Qf	536	LYS	Mainchain
7	Qf	537	ALA	Mainchain
7	Qf	575	LEU	Mainchain
7	Qf	601	ARG	Mainchain
7	Qf	602	GLY	Peptide
7	Qf	616	LYS	Mainchain
7	Qf	633	ASP	Mainchain
7	Qf	635	GLN	Mainchain
7	Qf	76	SER	Mainchain
7	Qf	98	SER	Mainchain
7	Qg	135	GLY	Mainchain
7	Qg	250	THR	Mainchain
7	Qg	278	VAL	Mainchain
7	Qg	346	GLU	Mainchain
7	Qg	407	SER	Mainchain
7	Qg	487	LYS	Mainchain
7	Qg	508	VAL	Peptide
7	Qg	530	ASP	Mainchain
7	Qg	533	LEU	Mainchain
7	Qg	534	ARG	Mainchain
7	Qg	536	LYS	Mainchain
7	Qg	537	ALA	Mainchain
7	Qg	575	LEU	Mainchain
7	Qg	582	VAL	Mainchain
7	Qg	601	ARG	Mainchain
7	Qg	602	GLY	Peptide
7	Qg	616	LYS	Mainchain
7	Qg	633	ASP	Mainchain
7	Qg	635	GLN	Mainchain
7	Qg	76	SER	Mainchain
7	Qg	98	SER	Mainchain
7	Qh	135	GLY	Mainchain
7	Qh	250	THR	Mainchain
7	Qh	278	VAL	Mainchain
7	Qh	346	GLU	Mainchain
7	Qh	407	SER	Mainchain
7	Qh	508	VAL	Peptide
7	Qh	530	ASP	Mainchain

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Mol	Chain	Res	Type	Group
7	Qh	533	LEU	Mainchain
7	Qh	534	ARG	Mainchain
7	Qh	536	LYS	Mainchain
7	Qh	537	ALA	Mainchain
7	Qh	540	LYS	Mainchain
7	Qh	575	LEU	Mainchain
7	Qh	601	ARG	Mainchain
7	Qh	602	GLY	Peptide
7	Qh	616	LYS	Mainchain
7	Qh	633	ASP	Mainchain
7	Qh	635	GLN	Mainchain
7	Qh	76	SER	Mainchain
7	Qh	98	SER	Mainchain
7	Qi	135	GLY	Mainchain
7	Qi	250	THR	Mainchain
7	Qi	278	VAL	Mainchain
7	Qi	346	GLU	Mainchain
7	Qi	407	SER	Mainchain
7	Qi	487	LYS	Mainchain
7	Qi	498	ILE	Mainchain
7	Qi	508	VAL	Peptide
7	Qi	530	ASP	Mainchain
7	Qi	533	LEU	Mainchain
7	Qi	534	ARG	Mainchain
7	Qi	536	LYS	Mainchain
7	Qi	537	ALA	Mainchain
7	Qi	540	LYS	Mainchain
7	Qi	575	LEU	Mainchain
7	Qi	601	ARG	Mainchain
7	Qi	602	GLY	Peptide
7	Qi	616	LYS	Mainchain
7	Qi	633	ASP	Mainchain
7	Qi	635	GLN	Mainchain
7	Qi	76	SER	Mainchain
7	Qi	98	SER	Mainchain
7	Qj	135	GLY	Mainchain
7	Qj	250	THR	Mainchain
7	Qj	278	VAL	Mainchain
7	Qj	346	GLU	Mainchain
7	Qj	407	SER	Mainchain
7	Qj	487	LYS	Mainchain
7	Qj	498	ILE	Mainchain

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Mol	Chain	Res	Type	Group
7	Qj	508	VAL	Peptide
7	Qj	510	ASP	Mainchain
7	Qj	530	ASP	Mainchain
7	Qj	533	LEU	Mainchain
7	Qj	534	ARG	Mainchain
7	Qj	536	LYS	Mainchain
7	Qj	537	ALA	Mainchain
7	Qj	540	LYS	Mainchain
7	Qj	575	LEU	Mainchain
7	Qj	601	ARG	Mainchain
7	Qj	602	GLY	Peptide
7	Qj	616	LYS	Mainchain
7	Qj	633	ASP	Mainchain
7	Qj	635	GLN	Mainchain
7	Qj	76	SER	Mainchain
7	Qj	98	SER	Mainchain
7	Qk	135	GLY	Mainchain
7	Qk	250	THR	Mainchain
7	Qk	278	VAL	Mainchain
7	Qk	346	GLU	Mainchain
7	Qk	407	SER	Mainchain
7	Qk	487	LYS	Mainchain
7	Qk	508	VAL	Peptide
7	Qk	530	ASP	Mainchain
7	Qk	533	LEU	Mainchain
7	Qk	534	ARG	Mainchain
7	Qk	536	LYS	Mainchain
7	Qk	537	ALA	Mainchain
7	Qk	575	LEU	Mainchain
7	Qk	601	ARG	Mainchain
7	Qk	602	GLY	Peptide,Mainchain
7	Qk	616	LYS	Mainchain
7	Qk	633	ASP	Mainchain
7	Qk	635	GLN	Mainchain
7	Qk	76	SER	Mainchain
7	Qk	98	SER	Mainchain
7	Ql	135	GLY	Mainchain
7	Ql	250	THR	Mainchain
7	Ql	278	VAL	Mainchain
7	Ql	346	GLU	Mainchain
7	Ql	407	SER	Mainchain
7	Ql	487	LYS	Mainchain

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Mol	Chain	Res	Type	Group
7	Ql	508	VAL	Peptide
7	Ql	530	ASP	Mainchain
7	Ql	533	LEU	Mainchain
7	Ql	534	ARG	Mainchain
7	Ql	536	LYS	Mainchain
7	Ql	537	ALA	Mainchain
7	Ql	540	LYS	Mainchain
7	Ql	575	LEU	Mainchain
7	Ql	601	ARG	Mainchain
7	Ql	602	GLY	Peptide
7	Ql	616	LYS	Mainchain
7	Ql	633	ASP	Mainchain
7	Ql	635	GLN	Mainchain
7	Ql	76	SER	Mainchain
7	Ql	98	SER	Mainchain
9	Ta	306	THR	Peptide
9	Ta	319	HIS	Mainchain
9	Ta	344	ASP	Peptide
9	Ta	345	PRO	Peptide,Mainchain
9	Ta	352	HIS	Mainchain
9	Tb	306	THR	Peptide
9	Tb	319	HIS	Mainchain
9	Tb	344	ASP	Peptide
9	Tb	345	PRO	Peptide,Mainchain
9	Tb	352	HIS	Mainchain
9	Tc	301	ASP	Mainchain
9	Tc	306	THR	Peptide
9	Tc	319	HIS	Mainchain
9	Tc	344	ASP	Peptide
9	Tc	345	PRO	Peptide,Mainchain
9	Tc	352	HIS	Mainchain
9	Td	306	THR	Peptide
9	Td	319	HIS	Mainchain
9	Td	344	ASP	Peptide
9	Td	345	PRO	Peptide,Mainchain
9	Td	352	HIS	Mainchain
9	Te	306	THR	Peptide
9	Te	319	HIS	Mainchain
9	Te	344	ASP	Peptide
9	Te	345	PRO	Peptide,Mainchain
9	Te	352	HIS	Mainchain
9	Tf	306	THR	Peptide

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Mol	Chain	Res	Type	Group
9	Tf	319	HIS	Mainchain
9	Tf	344	ASP	Peptide
9	Tf	345	PRO	Peptide,Mainchain
9	Tf	352	HIS	Mainchain
9	Tg	306	THR	Peptide
9	Tg	319	HIS	Mainchain
9	Tg	344	ASP	Peptide
9	Tg	345	PRO	Peptide,Mainchain
9	Tg	352	HIS	Mainchain
9	Th	306	THR	Peptide
9	Th	319	HIS	Mainchain
9	Th	344	ASP	Peptide
9	Th	345	PRO	Peptide,Mainchain
9	Th	352	HIS	Mainchain
9	Ti	127	PHE	Peptide
9	Ti	306	THR	Peptide
9	Ti	319	HIS	Mainchain
9	Ti	344	ASP	Peptide
9	Ti	345	PRO	Peptide,Mainchain
9	Ti	352	HIS	Mainchain
9	Tj	301	ASP	Mainchain
9	Tj	306	THR	Peptide
9	Tj	319	HIS	Mainchain
9	Tj	344	ASP	Peptide
9	Tj	345	PRO	Peptide,Mainchain
9	Tj	352	HIS	Mainchain
9	Tk	306	THR	Peptide
9	Tk	319	HIS	Mainchain
9	Tk	344	ASP	Peptide
9	Tk	345	PRO	Peptide,Mainchain
9	Tk	352	HIS	Mainchain
9	Tl	306	THR	Peptide
9	Tl	319	HIS	Mainchain
9	Tl	344	ASP	Peptide
9	Tl	345	PRO	Peptide,Mainchain
9	Tl	352	HIS	Mainchain

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	632	0	174	17	0
1	A2	632	0	174	13	0
1	A3	632	0	174	14	0
1	A4	632	0	174	17	0
1	A5	632	0	174	15	0
1	A6	632	0	174	11	0
1	A7	632	0	174	13	0
1	A8	632	0	174	13	0
1	A9	632	0	174	13	0
1	Aa	632	0	174	26	0
1	Ab	632	0	174	13	0
1	Ac	632	0	174	12	0
1	Ad	632	0	174	12	0
1	Ae	632	0	174	17	0
1	Af	632	0	174	15	0
1	Ag	632	0	174	14	0
1	Ah	632	0	174	16	0
1	Ai	632	0	174	14	0
1	Aj	632	0	174	15	0
1	Ak	632	0	174	16	0
1	Al	632	0	174	18	0
1	Am	632	0	174	14	0
1	An	632	0	174	28	0
1	Ao	632	0	174	16	0
1	Ap	632	0	174	15	0
1	Aq	632	0	174	15	0
1	Ar	632	0	174	14	0
1	As	632	0	174	14	0
1	At	632	0	174	16	0
1	Au	632	0	174	17	0
1	Av	632	0	174	15	0
1	Aw	632	0	174	14	0
1	Ax	632	0	174	16	0
1	Ay	632	0	174	14	0
1	Az	632	0	174	14	0
2	Ba	1808	0	487	43	0
2	Bb	1808	0	487	37	0
2	Bc	1808	0	487	31	0
2	Bd	1808	0	487	39	0
2	Be	1808	0	487	34	0
2	Bf	1808	0	487	33	0
3	Ca	1264	0	354	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Cb	1264	0	354	21	0
4	Na	892	0	248	23	0
4	Nb	892	0	248	16	0
4	Nc	892	0	248	31	0
4	Nd	892	0	248	13	0
4	Ne	892	0	248	9	0
4	Nf	892	0	248	11	0
4	Ng	892	0	248	8	0
4	Nh	892	0	248	5	0
4	Ni	892	0	248	6	0
4	Nj	892	0	248	8	0
4	Nk	892	0	248	8	0
4	Nl	892	0	248	14	0
5	Oa	756	0	207	14	0
5	Ob	756	0	207	14	0
5	Oc	756	0	207	3	0
5	Od	756	0	207	6	0
5	Oe	756	0	207	2	0
5	Of	756	0	207	2	0
5	Og	756	0	207	3	0
5	Oh	756	0	207	4	0
5	Oi	756	0	207	9	0
5	Oj	756	0	207	5	0
5	Ok	756	0	207	15	0
5	Ol	756	0	207	6	0
6	Ma	1420	0	396	11	0
6	Mb	1420	0	396	32	0
6	Mc	1420	0	396	10	0
6	Md	1420	0	396	29	0
6	Me	1420	0	396	13	0
6	Mf	1420	0	396	34	0
6	Mg	1420	0	396	12	0
6	Mh	1420	0	396	33	0
6	Mi	1420	0	396	13	0
6	Mj	1420	0	396	31	0
6	Mk	1420	0	396	12	0
6	Ml	1420	0	396	38	0
7	Qa	1672	0	462	33	0
7	Qb	1672	0	462	36	0
7	Qc	1672	0	462	35	0
7	Qd	1672	0	462	36	0
7	Qe	1672	0	462	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Qf	1672	0	462	34	0
7	Qg	1672	0	462	35	0
7	Qh	1672	0	462	34	0
7	Qi	1672	0	462	36	0
7	Qj	1672	0	462	44	0
7	Qk	1672	0	462	35	0
7	Ql	1672	0	462	35	0
8	Pa	620	0	155	37	0
8	Pb	620	0	155	36	0
8	Pc	620	0	155	38	0
8	Pd	620	0	155	18	0
8	Pe	620	0	155	12	0
8	Pf	620	0	155	11	0
8	Pg	620	0	155	8	0
8	Ph	620	0	155	15	0
8	Pi	620	0	155	9	0
8	Pj	620	0	155	10	0
8	Pk	620	0	155	24	0
8	Pl	620	0	155	18	0
9	Ta	652	0	177	51	0
9	Tb	652	0	177	51	0
9	Tc	652	0	177	51	0
9	Td	652	0	177	51	0
9	Te	652	0	177	51	0
9	Tf	652	0	177	51	0
9	Tg	652	0	177	51	0
9	Th	652	0	177	51	0
9	Ti	652	0	177	51	0
9	Tj	652	0	177	51	0
9	Tk	652	0	177	51	0
9	Tl	652	0	177	51	0
All	All	107640	0	29460	1744	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 13.

All (1744) 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:Ac:26:ASP:N	1:Ac:26:ASP:CA	1.76	1.49
1:A2:26:ASP:N	1:A2:26:ASP:CA	1.76	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Af:26:ASP:N	1:Af:26:ASP:CA	1.76	1.49
1:An:26:ASP:N	1:An:26:ASP:CA	1.76	1.49
1:Aw:26:ASP:N	1:Aw:26:ASP:CA	1.76	1.49
1:A5:26:ASP:N	1:A5:26:ASP:CA	1.76	1.49
1:A4:26:ASP:N	1:A4:26:ASP:CA	1.76	1.48
1:Az:26:ASP:N	1:Az:26:ASP:CA	1.76	1.48
1:Ae:26:ASP:N	1:Ae:26:ASP:CA	1.76	1.48
1:Ak:26:ASP:N	1:Ak:26:ASP:CA	1.76	1.48
1:Aa:26:ASP:N	1:Aa:26:ASP:CA	1.76	1.48
1:Ao:26:ASP:CA	1:Ao:26:ASP:N	1.76	1.48
1:Ad:26:ASP:N	1:Ad:26:ASP:CA	1.76	1.47
1:A3:26:ASP:N	1:A3:26:ASP:CA	1.76	1.47
1:Ag:26:ASP:N	1:Ag:26:ASP:CA	1.76	1.47
1:A6:26:ASP:N	1:A6:26:ASP:CA	1.76	1.47
1:As:26:ASP:CA	1:As:26:ASP:N	1.76	1.47
1:At:26:ASP:N	1:At:26:ASP:CA	1.76	1.47
1:A1:26:ASP:N	1:A1:26:ASP:CA	1.76	1.46
1:Ab:26:ASP:N	1:Ab:26:ASP:CA	1.76	1.46
1:Aq:26:ASP:N	1:Aq:26:ASP:CA	1.76	1.46
1:Ar:26:ASP:N	1:Ar:26:ASP:CA	1.76	1.46
1:Ap:26:ASP:N	1:Ap:26:ASP:CA	1.76	1.46
1:Ay:26:ASP:N	1:Ay:26:ASP:CA	1.76	1.46
9:Tc:298:LYS:C	9:Td:350:LEU:CA	1.88	1.46
1:Ax:26:ASP:N	1:Ax:26:ASP:CA	1.76	1.46
5:Oi:123:GLY:CA	8:Ph:42:SER:O	1.63	1.46
1:Al:26:ASP:N	1:Al:26:ASP:CA	1.76	1.46
1:A9:26:ASP:N	1:A9:26:ASP:CA	1.76	1.46
9:Th:298:LYS:C	9:Ti:350:LEU:CA	1.89	1.46
9:Tj:298:LYS:C	9:Tk:350:LEU:CA	1.89	1.46
1:Aj:26:ASP:N	1:Aj:26:ASP:CA	1.76	1.45
1:Av:26:ASP:N	1:Av:26:ASP:CA	1.76	1.45
9:Ta:298:LYS:C	9:Tb:350:LEU:CA	1.89	1.45
9:Tk:298:LYS:C	9:Tl:350:LEU:CA	1.89	1.45
9:Ta:350:LEU:CA	9:Tl:298:LYS:C	1.89	1.45
1:Ah:26:ASP:N	1:Ah:26:ASP:CA	1.76	1.45
1:A7:26:ASP:N	1:A7:26:ASP:CA	1.76	1.45
9:Tb:298:LYS:C	9:Tc:350:LEU:CA	1.89	1.45
9:Te:298:LYS:C	9:Tf:350:LEU:CA	1.89	1.45
9:Tg:298:LYS:C	9:Th:350:LEU:CA	1.89	1.45
9:Ti:298:LYS:C	9:Tj:350:LEU:CA	1.90	1.45
1:Au:26:ASP:N	1:Au:26:ASP:CA	1.76	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Tf:298:LYS:C	9:Tg:350:LEU:CA	1.89	1.45
9:Td:298:LYS:C	9:Te:350:LEU:CA	1.89	1.44
1:Ai:26:ASP:N	1:Ai:26:ASP:CA	1.76	1.44
1:Am:26:ASP:N	1:Am:26:ASP:CA	1.76	1.43
1:A8:26:ASP:N	1:A8:26:ASP:CA	1.76	1.43
2:Ba:226:LYS:CA	3:Ca:125:GLU:O	1.67	1.42
1:An:137:LYS:C	7:Qj:592:ALA:CA	1.94	1.41
7:Qc:544:GLY:CA	7:Qd:487:LYS:O	1.71	1.38
7:Qh:544:GLY:CA	7:Qi:487:LYS:O	1.71	1.38
7:Qe:544:GLY:CA	7:Qf:487:LYS:O	1.72	1.38
7:Qb:544:GLY:CA	7:Qc:487:LYS:O	1.72	1.37
4:Nc:99:PRO:CA	8:Pc:46:ASN:O	1.71	1.37
7:Qi:544:GLY:CA	7:Qj:487:LYS:O	1.71	1.36
7:Qa:487:LYS:O	7:Ql:544:GLY:CA	1.71	1.36
7:Qg:544:GLY:CA	7:Qh:487:LYS:O	1.71	1.35
7:Qd:544:GLY:CA	7:Qe:487:LYS:O	1.71	1.35
7:Qj:544:GLY:CA	7:Qk:487:LYS:O	1.72	1.35
7:Qk:544:GLY:CA	7:Ql:487:LYS:O	1.72	1.35
7:Qf:544:GLY:CA	7:Qg:487:LYS:O	1.72	1.35
7:Qa:544:GLY:CA	7:Qb:487:LYS:O	1.71	1.34
5:Ob:44:GLY:O	8:Pb:13:PRO:CA	1.77	1.31
1:An:137:LYS:O	7:Qj:592:ALA:CA	1.73	1.31
2:Be:83:GLU:C	6:Mh:90:ASN:CA	2.08	1.27
1:Ad:115:GLY:O	1:Ah:25:GLN:CA	1.83	1.27
1:A3:115:GLY:O	1:A7:25:GLN:CA	1.83	1.27
1:As:115:GLY:O	1:Aw:25:GLN:CA	1.83	1.26
1:Ak:115:GLY:O	1:Ao:25:GLN:CA	1.84	1.26
1:Aq:115:GLY:O	1:Au:25:GLN:CA	1.83	1.26
1:Ab:115:GLY:O	1:Af:25:GLN:CA	1.83	1.26
1:Ah:115:GLY:O	1:Al:25:GLN:CA	1.84	1.26
1:A1:115:GLY:O	1:A5:25:GLN:CA	1.83	1.26
1:Ac:115:GLY:O	1:Ag:25:GLN:CA	1.83	1.26
1:A2:115:GLY:O	1:A6:25:GLN:CA	1.83	1.26
1:Aa:1:MEA:N	3:Cb:258:PRO:C	1.91	1.25
1:An:115:GLY:O	1:Ar:25:GLN:CA	1.83	1.25
1:At:115:GLY:O	1:Ax:25:GLN:CA	1.83	1.25
1:Aa:115:GLY:O	1:Ae:25:GLN:CA	1.83	1.25
1:Al:115:GLY:O	1:Ap:25:GLN:CA	1.84	1.25
1:Av:115:GLY:O	1:Az:25:GLN:CA	1.84	1.25
1:Az:115:GLY:O	1:A4:25:GLN:CA	1.83	1.25
1:Ao:115:GLY:O	1:As:25:GLN:CA	1.83	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ax:115:GLY:O	1:A2:25:GLN:CA	1.83	1.25
1:Ay:115:GLY:O	1:A3:25:GLN:CA	1.83	1.25
1:A5:115:GLY:O	1:A9:25:GLN:CA	1.83	1.25
1:Ag:115:GLY:O	1:Ak:25:GLN:CA	1.83	1.25
1:Ar:115:GLY:O	1:Av:25:GLN:CA	1.84	1.25
1:Ae:115:GLY:O	1:Ai:25:GLN:CA	1.83	1.25
1:Ai:115:GLY:O	1:Am:25:GLN:CA	1.83	1.25
1:Au:115:GLY:O	1:Ay:25:GLN:CA	1.83	1.25
1:A4:115:GLY:O	1:A8:25:GLN:CA	1.83	1.25
4:Nl:109:ALA:CA	8:Pl:50:LYS:C	2.09	1.25
9:Tc:299:GLN:N	9:Td:350:LEU:CA	2.00	1.25
1:Af:115:GLY:O	1:Aj:25:GLN:CA	1.83	1.24
1:Aj:115:GLY:O	1:An:25:GLN:CA	1.83	1.24
1:Am:115:GLY:O	1:Aq:25:GLN:CA	1.83	1.24
1:Ap:115:GLY:O	1:At:25:GLN:CA	1.83	1.24
9:Th:299:GLN:N	9:Ti:350:LEU:CA	2.00	1.24
4:Na:88:VAL:O	8:Pa:42:SER:CA	1.85	1.24
9:Td:299:GLN:N	9:Te:350:LEU:CA	2.00	1.24
1:Aw:115:GLY:O	1:A1:25:GLN:CA	1.83	1.24
9:Tg:299:GLN:N	9:Th:350:LEU:CA	2.02	1.23
9:Tj:298:LYS:CA	9:Tk:350:LEU:C	2.12	1.23
9:Tk:298:LYS:CA	9:Tl:350:LEU:C	2.12	1.23
9:Ta:298:LYS:CA	9:Tb:350:LEU:C	2.11	1.23
9:Ti:298:LYS:CA	9:Tj:350:LEU:C	2.12	1.23
9:Ti:299:GLN:N	9:Tj:350:LEU:CA	2.01	1.23
9:Tj:299:GLN:N	9:Tk:350:LEU:CA	2.01	1.23
9:Tb:298:LYS:CA	9:Tc:350:LEU:C	2.12	1.23
9:Ta:299:GLN:N	9:Tb:350:LEU:CA	2.01	1.23
9:Ta:350:LEU:CA	9:Tl:299:GLN:N	2.01	1.23
9:Ta:350:LEU:C	9:Tl:298:LYS:CA	2.12	1.23
9:Th:298:LYS:CA	9:Ti:350:LEU:C	2.12	1.23
1:Aa:1:MEA:CA	3:Cb:258:PRO:C	2.13	1.22
9:Tb:299:GLN:N	9:Tc:350:LEU:CA	2.01	1.22
9:Tc:298:LYS:CA	9:Td:350:LEU:C	2.12	1.22
9:Tf:299:GLN:N	9:Tg:350:LEU:CA	2.00	1.22
9:Tg:298:LYS:CA	9:Th:350:LEU:C	2.12	1.22
9:Te:299:GLN:N	9:Tf:350:LEU:CA	2.01	1.22
7:Qb:544:GLY:HA3	7:Qc:487:LYS:O	1.04	1.21
9:Td:298:LYS:CA	9:Te:350:LEU:C	2.12	1.21
7:Qf:544:GLY:HA3	7:Qg:487:LYS:O	1.04	1.21
9:Tf:298:LYS:CA	9:Tg:350:LEU:C	2.12	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Tk:299:GLN:N	9:Tl:350:LEU:CA	2.01	1.21
9:Te:298:LYS:CA	9:Tf:350:LEU:C	2.12	1.21
7:Qg:544:GLY:HA3	7:Qh:487:LYS:O	1.04	1.20
4:Na:88:VAL:CA	8:Pa:41:TYR:C	2.14	1.20
7:Qi:544:GLY:HA3	7:Qj:487:LYS:O	1.03	1.19
7:Qc:544:GLY:HA3	7:Qd:487:LYS:O	1.03	1.19
7:Qj:544:GLY:HA3	7:Qk:487:LYS:O	1.04	1.19
7:Qa:487:LYS:O	7:Ql:544:GLY:HA3	1.03	1.19
7:Qk:544:GLY:HA3	7:Ql:487:LYS:O	1.03	1.18
4:Nc:110:THR:O	8:Pc:50:LYS:CA	1.92	1.18
7:Qh:544:GLY:HA3	7:Qi:487:LYS:O	1.03	1.18
7:Qd:544:GLY:HA3	7:Qe:487:LYS:O	1.03	1.17
5:Oh:122:VAL:CA	8:Pg:41:TYR:CA	2.22	1.17
7:Qa:544:GLY:HA3	7:Qb:487:LYS:O	1.03	1.17
3:Cb:182:ALA:O	3:Cb:194:ILE:N	1.78	1.16
7:Qe:544:GLY:HA3	7:Qf:487:LYS:O	1.03	1.16
2:Be:84:LYS:CA	6:Mh:93:ALA:H	1.58	1.15
2:Bf:84:LYS:CA	6:Mj:93:ALA:H	1.59	1.15
5:Ob:44:GLY:C	8:Pb:13:PRO:CA	2.19	1.15
1:Al:128:THR:C	7:Qe:596:ASP:O	1.69	1.14
2:Ba:246:ARG:CA	3:Ca:296:SER:O	1.96	1.14
1:Aa:2:THR:CA	3:Cb:254:SER:CA	2.27	1.12
7:Qj:477:TYR:N	7:Qk:574:ASP:N	1.98	1.11
2:Bc:84:LYS:CA	6:Md:93:ALA:H	1.61	1.11
7:Qa:477:TYR:N	7:Qb:574:ASP:N	1.98	1.11
2:Bd:84:LYS:CA	6:Mf:93:ALA:H	1.62	1.11
7:Qb:477:TYR:N	7:Qc:574:ASP:N	1.98	1.11
2:Ba:84:LYS:CA	6:Mi:93:ALA:H	1.62	1.10
3:Cb:182:ALA:C	3:Cb:194:ILE:CA	2.24	1.10
2:Bb:84:LYS:CA	6:Mb:93:ALA:H	1.63	1.10
7:Qg:477:TYR:N	7:Qh:574:ASP:N	1.98	1.10
7:Qd:477:TYR:N	7:Qe:574:ASP:N	1.99	1.10
7:Qk:477:TYR:N	7:Ql:574:ASP:N	1.98	1.09
7:Qf:477:TYR:N	7:Qg:574:ASP:N	1.99	1.09
7:Qa:574:ASP:N	7:Ql:477:TYR:N	1.98	1.09
7:Qh:477:TYR:N	7:Qi:574:ASP:N	1.99	1.09
1:Aa:1:MEA:N	3:Cb:258:PRO:O	1.84	1.08
7:Qi:477:TYR:N	7:Qj:574:ASP:N	1.99	1.08
7:Qc:477:TYR:N	7:Qd:574:ASP:N	1.99	1.08
7:Qe:477:TYR:N	7:Qf:574:ASP:N	1.99	1.08
5:Ol:55:LEU:CA	8:Pl:22:ALA:O	2.02	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:102:CYS:CA	6:Mf:80:PRO:CA	2.33	1.07
2:Be:129:VAL:CA	6:Mh:84:VAL:CA	2.33	1.06
5:Ok:51:ARG:C	8:Pk:18:PRO:O	1.97	1.06
1:Aa:2:THR:N	3:Cb:254:SER:O	1.89	1.06
2:Ba:129:VAL:CA	6:Mi:84:VAL:CA	2.34	1.06
4:Nc:110:THR:O	8:Pc:50:LYS:N	1.89	1.06
2:Bd:129:VAL:CA	6:Mf:84:VAL:CA	2.35	1.05
2:Bf:129:VAL:CA	6:Mj:84:VAL:CA	2.33	1.05
2:Ba:86:LEU:CA	6:Mi:81:GLU:C	2.30	1.05
2:Bf:86:LEU:CA	6:Mj:81:GLU:C	2.30	1.04
5:Ob:44:GLY:CA	8:Pb:13:PRO:N	2.19	1.04
4:Nb:91:ALA:O	8:Pb:43:TYR:O	1.73	1.03
2:Bc:129:VAL:CA	6:Md:84:VAL:CA	2.36	1.03
2:Bb:129:VAL:CA	6:Mb:84:VAL:CA	2.36	1.02
4:Na:88:VAL:CA	8:Pa:41:TYR:O	2.06	1.02
3:Cb:182:ALA:C	3:Cb:194:ILE:N	2.17	1.02
5:Ob:44:GLY:CA	8:Pb:13:PRO:CA	2.38	1.02
2:Be:84:LYS:CA	6:Mh:93:ALA:N	2.22	1.02
2:Be:86:LEU:CA	6:Mh:81:GLU:C	2.32	1.02
2:Bb:86:LEU:CA	6:Mb:81:GLU:C	2.33	1.01
2:Ba:84:LYS:CA	6:Mi:93:ALA:N	2.24	1.01
2:Bd:83:GLU:C	6:Mf:90:ASN:CA	2.33	1.01
2:Bf:84:LYS:CA	6:Mj:93:ALA:N	2.22	1.01
9:Td:299:GLN:O	9:Te:350:LEU:N	1.93	1.01
9:Tf:299:GLN:O	9:Tg:350:LEU:N	1.94	1.01
2:Bd:84:LYS:CA	6:Mf:93:ALA:N	2.23	1.01
7:Qh:544:GLY:CA	7:Qi:487:LYS:C	2.34	1.01
8:Pk:15:PRO:O	8:Pk:17:LYS:N	1.93	1.01
2:Bb:83:GLU:C	6:Mb:90:ASN:CA	2.34	1.00
7:Qb:544:GLY:CA	7:Qc:487:LYS:C	2.34	1.00
9:Tg:299:GLN:O	9:Th:350:LEU:N	1.94	1.00
7:Qf:544:GLY:CA	7:Qg:487:LYS:C	2.35	1.00
9:Ti:299:GLN:O	9:Tj:350:LEU:N	1.94	1.00
7:Qc:544:GLY:CA	7:Qd:487:LYS:C	2.34	1.00
7:Qg:544:GLY:CA	7:Qh:487:LYS:C	2.34	1.00
9:Tk:299:GLN:O	9:Ti:350:LEU:N	1.94	1.00
9:Ta:299:GLN:O	9:Tb:350:LEU:N	1.94	1.00
2:Bd:86:LEU:CA	6:Mf:81:GLU:C	2.35	1.00
7:Qi:544:GLY:CA	7:Qj:487:LYS:C	2.35	1.00
7:Qj:544:GLY:CA	7:Qk:487:LYS:C	2.35	1.00
7:Qe:544:GLY:CA	7:Qf:487:LYS:C	2.35	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Te:299:GLN:O	9:Tf:350:LEU:N	1.94	0.99
9:Tj:299:GLN:O	9:Tk:350:LEU:N	1.94	0.99
5:Ok:48:ALA:O	8:Pk:18:PRO:CA	2.10	0.99
9:Ta:350:LEU:N	9:Tl:299:GLN:O	1.94	0.99
2:Bc:84:LYS:CA	6:Md:93:ALA:N	2.24	0.99
7:Qd:544:GLY:CA	7:Qe:487:LYS:C	2.34	0.99
2:Bc:86:LEU:CA	6:Md:81:GLU:C	2.35	0.99
9:Tc:299:GLN:O	9:Td:350:LEU:N	1.94	0.99
9:Th:299:GLN:O	9:Ti:350:LEU:N	1.94	0.99
7:Qa:544:GLY:CA	7:Qb:487:LYS:C	2.34	0.99
9:Tb:299:GLN:O	9:Tc:350:LEU:N	1.94	0.99
1:An:138:ASP:N	7:Qj:592:ALA:CA	2.25	0.99
7:Qa:487:LYS:C	7:Ql:544:GLY:CA	2.34	0.99
5:Oa:55:LEU:O	8:Pa:25:PRO:O	1.79	0.99
2:Bb:84:LYS:CA	6:Mb:93:ALA:N	2.25	0.98
8:Pb:16:ALA:O	8:Pb:18:PRO:N	1.95	0.98
9:Te:298:LYS:CA	9:Tf:350:LEU:CA	2.41	0.98
2:Ba:83:GLU:C	6:Mi:90:ASN:CA	2.36	0.98
2:Be:102:CYS:CA	6:Mh:80:PRO:CA	2.42	0.98
7:Qk:544:GLY:CA	7:Ql:487:LYS:C	2.35	0.98
4:Nc:123:ASN:CA	8:Pc:62:GLY:HA2	1.93	0.97
9:Th:298:LYS:CA	9:Ti:350:LEU:CA	2.41	0.97
9:Ta:298:LYS:CA	9:Tb:350:LEU:CA	2.41	0.97
9:Tb:298:LYS:CA	9:Tc:350:LEU:CA	2.41	0.97
5:Ok:55:LEU:CA	8:Pk:22:ALA:O	2.12	0.97
9:Tf:298:LYS:CA	9:Tg:350:LEU:CA	2.42	0.97
2:Ba:86:LEU:O	6:Mi:80:PRO:O	1.83	0.96
2:Ba:102:CYS:CA	6:Mi:80:PRO:CA	2.44	0.96
9:Tj:298:LYS:CA	9:Tk:350:LEU:CA	2.41	0.96
3:Cb:182:ALA:O	3:Cb:193:ALA:C	2.07	0.96
9:Ti:299:GLN:O	9:Tj:350:LEU:CA	2.14	0.95
9:Tk:299:GLN:O	9:Tl:350:LEU:CA	2.14	0.95
1:An:138:ASP:CA	7:Qj:592:ALA:CA	2.44	0.95
9:Tj:299:GLN:O	9:Tk:350:LEU:CA	2.14	0.95
9:Th:299:GLN:O	9:Ti:350:LEU:CA	2.14	0.95
9:Tk:298:LYS:CA	9:Tl:350:LEU:CA	2.42	0.95
4:Nc:110:THR:C	8:Pc:50:LYS:CA	2.38	0.95
7:Qe:544:GLY:HA3	7:Qf:487:LYS:C	1.92	0.95
9:Ta:350:LEU:CA	9:Tl:299:GLN:O	2.15	0.95
9:Ta:299:GLN:O	9:Tb:350:LEU:CA	2.15	0.95
9:Ta:350:LEU:CA	9:Tl:298:LYS:CA	2.42	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Te:299:GLN:O	9:Tf:350:LEU:CA	2.14	0.95
2:Bd:86:LEU:O	6:Mf:80:PRO:O	1.84	0.95
5:Oi:123:GLY:HA3	8:Ph:42:SER:C	1.92	0.95
7:Qd:544:GLY:HA3	7:Qe:487:LYS:C	1.92	0.95
9:Tg:299:GLN:O	9:Th:350:LEU:CA	2.14	0.95
7:Qh:544:GLY:HA3	7:Qi:487:LYS:C	1.92	0.94
9:Td:299:GLN:O	9:Te:350:LEU:CA	2.14	0.94
9:Tg:298:LYS:CA	9:Th:350:LEU:CA	2.41	0.94
2:Bd:83:GLU:CA	6:Mf:90:ASN:CA	2.45	0.94
4:Nl:109:ALA:CA	8:Pl:50:LYS:O	2.14	0.94
9:Tb:299:GLN:O	9:Tc:350:LEU:CA	2.14	0.94
9:Ti:298:LYS:CA	9:Tj:350:LEU:CA	2.42	0.94
7:Qb:544:GLY:HA2	7:Qc:487:LYS:C	1.93	0.94
4:Ng:206:GLN:N	8:Pf:47:PRO:O	2.00	0.94
9:Tc:299:GLN:O	9:Td:350:LEU:CA	2.14	0.94
7:Qg:544:GLY:HA3	7:Qh:487:LYS:C	1.92	0.94
7:Qc:544:GLY:HA3	7:Qd:487:LYS:C	1.91	0.93
7:Qa:544:GLY:HA3	7:Qb:487:LYS:C	1.92	0.93
9:Tf:299:GLN:O	9:Tg:350:LEU:CA	2.14	0.93
5:Ok:51:ARG:O	8:Pk:18:PRO:O	1.87	0.93
9:Tk:299:GLN:C	9:Tl:350:LEU:N	2.27	0.93
1:An:137:LYS:C	7:Qj:592:ALA:C	2.35	0.93
7:Qj:544:GLY:HA2	7:Qk:487:LYS:C	1.94	0.93
9:Ta:299:GLN:C	9:Tb:350:LEU:N	2.27	0.93
9:Tc:298:LYS:CA	9:Td:350:LEU:CA	2.41	0.93
9:Td:299:GLN:C	9:Te:350:LEU:N	2.27	0.93
2:Be:86:LEU:O	6:Mh:80:PRO:O	1.85	0.93
9:Tb:299:GLN:C	9:Tc:350:LEU:N	2.27	0.93
2:Be:83:GLU:O	6:Mh:90:ASN:CA	2.16	0.92
7:Qh:544:GLY:HA2	7:Qi:487:LYS:C	1.94	0.92
9:Te:299:GLN:C	9:Tf:350:LEU:N	2.27	0.92
9:Ta:350:LEU:N	9:Tl:299:GLN:C	2.27	0.92
9:Td:298:LYS:CA	9:Te:350:LEU:CA	2.42	0.92
9:Tg:299:GLN:C	9:Th:350:LEU:N	2.27	0.92
1:A6:25:GLN:C	1:A6:26:ASP:CA	2.43	0.92
5:Ob:44:GLY:HA3	8:Pb:13:PRO:N	1.85	0.92
7:Qa:487:LYS:C	7:Ql:544:GLY:HA2	1.94	0.92
1:A4:25:GLN:C	1:A4:26:ASP:CA	2.43	0.92
2:Bf:102:CYS:CA	6:Mj:80:PRO:CA	2.48	0.92
9:Tf:299:GLN:C	9:Tg:350:LEU:N	2.27	0.92
1:Ae:25:GLN:C	1:Ae:26:ASP:CA	2.43	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:25:GLN:C	1:Az:26:ASP:CA	2.43	0.92
7:Qc:544:GLY:HA2	7:Qd:487:LYS:C	1.93	0.92
9:Th:299:GLN:C	9:Ti:350:LEU:N	2.27	0.92
7:Qf:544:GLY:HA2	7:Qg:487:LYS:C	1.93	0.92
9:Tc:299:GLN:C	9:Td:350:LEU:N	2.27	0.92
1:Ar:25:GLN:C	1:Ar:26:ASP:CA	2.43	0.92
1:A2:25:GLN:C	1:A2:26:ASP:CA	2.43	0.92
7:Qa:487:LYS:C	7:Ql:544:GLY:HA3	1.92	0.92
7:Qg:544:GLY:HA2	7:Qh:487:LYS:C	1.93	0.92
9:Ti:299:GLN:C	9:Tj:350:LEU:N	2.27	0.92
9:Tj:299:GLN:C	9:Tk:350:LEU:N	2.27	0.92
1:At:25:GLN:C	1:At:26:ASP:CA	2.43	0.92
1:Av:25:GLN:C	1:Av:26:ASP:CA	2.43	0.92
1:Ax:25:GLN:C	1:Ax:26:ASP:CA	2.43	0.92
1:A3:25:GLN:C	1:A3:26:ASP:CA	2.43	0.92
7:Qi:544:GLY:HA3	7:Qj:487:LYS:C	1.92	0.92
7:Qj:544:GLY:HA3	7:Qk:487:LYS:C	1.93	0.92
7:Qk:544:GLY:HA2	7:Ql:487:LYS:C	1.95	0.92
1:Ah:25:GLN:C	1:Ah:26:ASP:CA	2.43	0.91
1:Ak:25:GLN:C	1:Ak:26:ASP:CA	2.43	0.91
1:As:25:GLN:C	1:As:26:ASP:CA	2.43	0.91
7:Qb:544:GLY:HA3	7:Qc:487:LYS:C	1.92	0.91
1:Aa:25:GLN:C	1:Aa:26:ASP:CA	2.44	0.91
1:Ag:25:GLN:C	1:Ag:26:ASP:CA	2.43	0.91
1:A8:25:GLN:C	1:A8:26:ASP:CA	2.43	0.91
1:Ad:25:GLN:C	1:Ad:26:ASP:CA	2.43	0.91
1:Ai:25:GLN:C	1:Ai:26:ASP:CA	2.43	0.91
1:Aq:25:GLN:C	1:Aq:26:ASP:CA	2.43	0.91
1:A7:25:GLN:C	1:A7:26:ASP:CA	2.43	0.91
7:Qf:544:GLY:HA3	7:Qg:487:LYS:C	1.94	0.91
1:A9:25:GLN:C	1:A9:26:ASP:CA	2.43	0.91
1:Ac:25:GLN:C	1:Ac:26:ASP:CA	2.44	0.91
1:Aw:25:GLN:C	1:Aw:26:ASP:CA	2.44	0.91
7:Qi:544:GLY:HA2	7:Qj:487:LYS:C	1.94	0.91
7:Qk:544:GLY:HA3	7:Ql:487:LYS:C	1.92	0.91
1:Au:25:GLN:C	1:Au:26:ASP:CA	2.43	0.91
1:A1:25:GLN:C	1:A1:26:ASP:CA	2.43	0.91
5:Od:154:MET:O	8:Pd:39:PRO:CA	2.19	0.91
1:Aj:25:GLN:C	1:Aj:26:ASP:CA	2.43	0.91
1:Ao:25:GLN:C	1:Ao:26:ASP:CA	2.43	0.91
1:Ap:25:GLN:C	1:Ap:26:ASP:CA	2.43	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:25:GLN:C	1:Ay:26:ASP:CA	2.43	0.91
4:Nd:111:PRO:O	8:Pd:50:LYS:N	2.03	0.91
1:Al:25:GLN:C	1:Al:26:ASP:CA	2.43	0.90
1:Am:25:GLN:C	1:Am:26:ASP:CA	2.43	0.90
1:An:25:GLN:C	1:An:26:ASP:CA	2.43	0.90
7:Qd:544:GLY:HA2	7:Qe:487:LYS:C	1.94	0.90
1:A5:25:GLN:C	1:A5:26:ASP:CA	2.43	0.90
1:Ab:25:GLN:C	1:Ab:26:ASP:CA	2.43	0.90
1:Af:25:GLN:C	1:Af:26:ASP:CA	2.43	0.90
7:Qa:544:GLY:HA2	7:Qb:487:LYS:C	1.93	0.90
5:Ob:44:GLY:HA2	8:Pb:13:PRO:N	1.87	0.89
7:Qg:502:SER:CA	8:Ph:155:ASP:CA	2.51	0.89
7:Qe:544:GLY:HA2	7:Qf:487:LYS:C	1.95	0.89
2:Bf:86:LEU:O	6:Mj:80:PRO:O	1.89	0.88
7:Ql:500:GLU:O	8:Pl:94:ALA:O	1.92	0.88
7:Qe:500:GLU:O	8:Pe:94:ALA:O	1.92	0.88
7:Qi:502:SER:CA	8:Pj:155:ASP:CA	2.51	0.88
7:Qe:502:SER:CA	8:Pf:155:ASP:CA	2.51	0.88
7:Qd:502:SER:CA	8:Pe:155:ASP:CA	2.52	0.88
7:Qb:500:GLU:O	8:Pb:94:ALA:O	1.92	0.88
7:Qi:500:GLU:O	8:Pi:94:ALA:O	1.92	0.88
7:Qc:500:GLU:O	8:Pc:94:ALA:O	1.92	0.88
7:Qh:500:GLU:O	8:Ph:94:ALA:O	1.92	0.88
7:Qk:500:GLU:O	8:Pk:94:ALA:O	1.92	0.88
2:Bb:86:LEU:O	6:Mb:80:PRO:O	1.92	0.88
7:Qc:502:SER:CA	8:Pd:155:ASP:CA	2.52	0.88
7:Qd:500:GLU:O	8:Pd:94:ALA:O	1.92	0.88
2:Be:83:GLU:CA	6:Mh:90:ASN:CA	2.52	0.88
5:Ob:58:ALA:CA	8:Pb:25:PRO:O	2.22	0.88
7:Qa:502:SER:CA	8:Pb:155:ASP:CA	2.52	0.88
4:Nc:99:PRO:CA	8:Pc:46:ASN:C	2.46	0.88
7:Qa:500:GLU:O	8:Pa:94:ALA:O	1.92	0.88
7:Qf:500:GLU:O	8:Pf:94:ALA:O	1.92	0.88
7:Qk:502:SER:CA	8:Pl:155:ASP:CA	2.51	0.88
2:Bc:102:CYS:CA	6:Md:80:PRO:CA	2.53	0.87
8:Pa:155:ASP:CA	7:Ql:502:SER:CA	2.52	0.87
7:Qh:502:SER:CA	8:Pi:155:ASP:CA	2.51	0.87
7:Qj:502:SER:CA	8:Pk:155:ASP:CA	2.52	0.87
7:Qf:502:SER:CA	8:Pg:155:ASP:CA	2.52	0.87
7:Qb:502:SER:CA	8:Pc:155:ASP:CA	2.53	0.87
1:Aa:3:LEU:N	3:Cb:254:SER:CA	2.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Qg:500:GLU:O	8:Pg:94:ALA:O	1.92	0.86
7:Qj:500:GLU:O	8:Pj:94:ALA:O	1.91	0.85
2:Bc:86:LEU:O	6:Md:80:PRO:O	1.95	0.85
5:Oa:51:ARG:N	8:Pa:18:PRO:CA	2.38	0.85
2:Bb:102:CYS:CA	6:Mb:80:PRO:CA	2.54	0.85
5:Oi:123:GLY:HA3	8:Ph:42:SER:O	0.71	0.85
2:Bd:84:LYS:CA	6:Mf:93:ALA:CA	2.55	0.85
4:Ne:223:TYR:O	8:Pe:58:ILE:O	1.95	0.84
2:Bf:84:LYS:CA	6:Mj:93:ALA:CA	2.55	0.84
4:Nd:123:ASN:O	8:Pd:62:GLY:HA2	1.76	0.84
2:Be:84:LYS:CA	6:Mh:93:ALA:CA	2.54	0.84
5:Oa:51:ARG:CA	8:Pa:18:PRO:CA	2.55	0.84
5:Oa:54:ASP:C	8:Pa:22:ALA:O	2.21	0.84
2:Ba:84:LYS:CA	6:Mi:93:ALA:CA	2.55	0.83
2:Bb:83:GLU:CA	6:Mb:90:ASN:CA	2.56	0.83
4:Nb:91:ALA:CA	8:Pb:42:SER:CA	2.56	0.83
2:Bb:84:LYS:CA	6:Mb:93:ALA:CA	2.56	0.83
4:Nc:99:PRO:N	8:Pc:46:ASN:CA	2.42	0.83
2:Bc:83:GLU:C	6:Md:90:ASN:CA	2.51	0.82
2:Bc:84:LYS:CA	6:Md:93:ALA:CA	2.56	0.82
4:Nc:113:LYS:CA	8:Pc:48:VAL:CA	2.57	0.82
2:Bf:83:GLU:C	6:Mj:90:ASN:CA	2.53	0.82
2:Ba:226:LYS:CA	3:Ca:125:GLU:C	2.52	0.81
9:Ta:298:LYS:CA	9:Tb:351:GLY:N	2.44	0.81
5:Ob:44:GLY:HA2	8:Pb:13:PRO:CA	2.08	0.81
9:Tc:298:LYS:CA	9:Td:351:GLY:N	2.44	0.81
7:Qi:544:GLY:HA2	7:Qj:487:LYS:O	1.80	0.80
9:Tk:298:LYS:CA	9:Tl:351:GLY:N	2.44	0.80
9:Te:298:LYS:CA	9:Tf:351:GLY:N	2.44	0.80
9:Ti:298:LYS:CA	9:Tj:351:GLY:N	2.43	0.80
9:Th:298:LYS:CA	9:Ti:351:GLY:N	2.44	0.80
9:Tg:298:LYS:CA	9:Th:351:GLY:N	2.45	0.80
9:Tj:298:LYS:CA	9:Tk:351:GLY:N	2.44	0.80
4:Nf:38:TYR:O	4:Nf:41:TYR:N	2.15	0.80
4:Nj:38:TYR:O	4:Nj:41:TYR:N	2.15	0.80
4:Ni:38:TYR:O	4:Ni:41:TYR:N	2.15	0.80
4:Nc:113:LYS:O	8:Pc:48:VAL:N	2.14	0.79
2:Be:84:LYS:C	6:Mh:93:ALA:CA	2.55	0.79
1:Aa:3:LEU:H	3:Cb:254:SER:C	1.91	0.79
4:Nk:38:TYR:O	4:Nk:41:TYR:N	2.15	0.79
9:Td:298:LYS:CA	9:Te:351:GLY:N	2.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ta:351:GLY:N	9:Tl:298:LYS:CA	2.45	0.79
4:Ng:38:TYR:O	4:Ng:41:TYR:N	2.15	0.79
9:Tb:298:LYS:CA	9:Tc:351:GLY:N	2.45	0.79
4:Ne:38:TYR:O	4:Ne:41:TYR:N	2.15	0.79
9:Tf:298:LYS:CA	9:Tg:351:GLY:N	2.45	0.79
2:Bd:84:LYS:C	6:Mf:93:ALA:CA	2.55	0.79
2:Bf:84:LYS:C	6:Mj:93:ALA:CA	2.55	0.79
4:Na:38:TYR:O	4:Na:41:TYR:N	2.15	0.79
9:Tc:299:GLN:C	9:Td:350:LEU:CA	2.56	0.79
7:Qd:544:GLY:HA2	7:Qe:487:LYS:O	1.80	0.79
2:Ba:84:LYS:C	6:Mi:93:ALA:CA	2.56	0.79
4:Nh:38:TYR:O	4:Nh:41:TYR:N	2.16	0.79
9:Tb:299:GLN:C	9:Tc:350:LEU:CA	2.56	0.79
9:Ti:299:GLN:C	9:Tj:350:LEU:CA	2.56	0.79
2:Ba:226:LYS:CA	3:Ca:126:GLN:CA	2.61	0.78
9:Ta:299:GLN:C	9:Tb:350:LEU:CA	2.56	0.78
4:Nb:38:TYR:O	4:Nb:41:TYR:N	2.15	0.78
4:Nc:110:THR:O	8:Pc:49:GLY:CA	2.30	0.78
4:Nd:38:TYR:O	4:Nd:41:TYR:N	2.16	0.78
9:Ta:350:LEU:CA	9:Tl:299:GLN:C	2.57	0.78
9:Tg:299:GLN:C	9:Th:350:LEU:CA	2.57	0.78
9:Tk:299:GLN:C	9:Tl:350:LEU:CA	2.56	0.78
4:Nl:38:TYR:O	4:Nl:41:TYR:N	2.15	0.78
9:Td:299:GLN:C	9:Te:350:LEU:CA	2.56	0.78
2:Bc:84:LYS:C	6:Md:93:ALA:CA	2.57	0.78
9:Tj:299:GLN:C	9:Tk:350:LEU:CA	2.56	0.78
4:Nl:109:ALA:CA	8:Pl:51:ARG:N	2.47	0.77
2:Bf:83:GLU:CA	6:Mj:90:ASN:CA	2.61	0.77
4:Nc:38:TYR:O	4:Nc:41:TYR:N	2.15	0.77
9:Te:299:GLN:C	9:Tf:350:LEU:CA	2.56	0.77
2:Bb:84:LYS:C	6:Mb:93:ALA:CA	2.57	0.77
9:Tf:299:GLN:C	9:Tg:350:LEU:CA	2.56	0.77
4:Nd:123:ASN:CA	8:Pd:61:LEU:C	2.57	0.77
4:Na:88:VAL:CA	8:Pa:42:SER:N	2.47	0.77
9:Th:299:GLN:C	9:Ti:350:LEU:CA	2.56	0.77
4:Nb:91:ALA:C	8:Pb:43:TYR:H	1.92	0.76
7:Qh:544:GLY:CA	7:Qi:488:ASP:CA	2.64	0.76
7:Qi:544:GLY:CA	7:Qj:488:ASP:CA	2.64	0.76
4:Nc:98:GLY:HA3	8:Pc:46:ASN:H	1.50	0.76
7:Qb:544:GLY:CA	7:Qc:488:ASP:CA	2.64	0.76
7:Qe:544:GLY:CA	7:Qf:488:ASP:CA	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Qa:488:ASP:CA	7:Ql:544:GLY:CA	2.64	0.76
7:Qa:544:GLY:CA	7:Qb:488:ASP:CA	2.64	0.75
6:Ma:371:PHE:O	6:Ma:374:ASP:N	2.19	0.75
7:Qc:544:GLY:CA	7:Qd:488:ASP:CA	2.64	0.75
5:Oh:122:VAL:CA	8:Pg:41:TYR:C	2.59	0.75
6:Md:371:PHE:O	6:Md:374:ASP:N	2.20	0.75
6:Mf:371:PHE:O	6:Mf:374:ASP:N	2.20	0.75
7:Qj:544:GLY:CA	7:Qk:488:ASP:CA	2.64	0.75
7:Qd:544:GLY:CA	7:Qe:488:ASP:CA	2.64	0.74
7:Qf:544:GLY:CA	7:Qg:488:ASP:CA	2.64	0.74
6:Mh:371:PHE:O	6:Mh:374:ASP:N	2.21	0.74
2:Ba:226:LYS:N	3:Ca:125:GLU:O	2.21	0.74
2:Bc:83:GLU:CA	6:Md:90:ASN:CA	2.65	0.74
6:Mb:371:PHE:O	6:Mb:374:ASP:N	2.21	0.74
7:Qg:544:GLY:CA	7:Qh:488:ASP:CA	2.65	0.74
7:Qf:544:GLY:HA2	7:Qg:487:LYS:O	1.79	0.74
8:Pb:16:ALA:C	8:Pb:18:PRO:N	2.43	0.74
8:Pc:53:PRO:CA	8:Pc:56:SER:H	2.00	0.74
6:Mk:371:PHE:O	6:Mk:374:ASP:N	2.21	0.74
5:Oa:54:ASP:O	8:Pa:22:ALA:O	2.06	0.74
5:Oi:122:VAL:O	8:Ph:41:TYR:CA	2.36	0.74
6:Mi:371:PHE:O	6:Mi:374:ASP:N	2.21	0.73
6:Mj:371:PHE:O	6:Mj:374:ASP:N	2.20	0.73
5:Oa:59:ASP:CA	8:Pa:27:LYS:O	2.36	0.73
6:Mc:371:PHE:O	6:Mc:374:ASP:N	2.20	0.73
7:Qk:544:GLY:CA	7:Ql:488:ASP:CA	2.64	0.73
1:Aa:1:MEA:CA	3:Cb:258:PRO:CA	2.66	0.73
9:Ta:344:ASP:H	9:Tl:326:GLY:HA3	1.53	0.73
9:Ti:326:GLY:HA3	9:Tj:344:ASP:H	1.53	0.73
7:Qb:544:GLY:HA2	7:Qc:487:LYS:O	1.80	0.73
6:Mi:371:PHE:O	6:Mi:374:ASP:N	2.21	0.73
6:Mg:371:PHE:O	6:Mg:374:ASP:N	2.20	0.73
9:Te:91:ASP:O	9:Te:94:GLN:N	2.19	0.73
6:Me:371:PHE:O	6:Me:374:ASP:N	2.21	0.73
9:Tj:326:GLY:HA3	9:Tk:344:ASP:H	1.54	0.72
4:Nl:109:ALA:O	8:Pl:53:PRO:O	2.07	0.72
9:Tc:326:GLY:HA3	9:Td:344:ASP:H	1.54	0.72
9:Tf:326:GLY:HA3	9:Tg:344:ASP:H	1.53	0.72
2:Ba:83:GLU:CA	6:Mi:90:ASN:CA	2.68	0.72
9:Tb:326:GLY:HA3	9:Tc:344:ASP:H	1.54	0.72
7:Qc:260:LEU:C	7:Qc:262:ASP:H	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Th:326:GLY:HA3	9:Ti:344:ASP:H	1.54	0.72
7:Qd:260:LEU:C	7:Qd:262:ASP:H	1.98	0.72
7:Qe:260:LEU:C	7:Qe:262:ASP:H	1.98	0.72
7:Qj:260:LEU:C	7:Qj:262:ASP:H	1.98	0.72
9:Td:91:ASP:O	9:Td:94:GLN:N	2.19	0.72
5:Ol:44:GLY:O	8:Pl:13:PRO:O	2.08	0.71
9:Tk:326:GLY:HA3	9:Tl:344:ASP:H	1.54	0.71
7:Qa:260:LEU:C	7:Qa:262:ASP:H	1.98	0.71
7:Qb:260:LEU:C	7:Qb:262:ASP:H	1.98	0.71
9:Td:326:GLY:HA3	9:Te:344:ASP:H	1.54	0.71
9:Tf:91:ASP:O	9:Tf:94:GLN:N	2.19	0.71
9:Tf:326:GLY:HA3	9:Tg:344:ASP:C	2.16	0.71
4:Nd:123:ASN:CA	8:Pd:61:LEU:CA	2.68	0.71
7:Qf:260:LEU:C	7:Qf:262:ASP:H	1.98	0.71
9:Th:326:GLY:HA3	9:Ti:344:ASP:C	2.16	0.71
6:Mg:45:LEU:N	6:Mg:53:LYS:O	2.24	0.71
9:Td:326:GLY:HA3	9:Te:344:ASP:C	2.16	0.71
9:Tg:326:GLY:HA3	9:Th:344:ASP:H	1.54	0.71
9:Ta:326:GLY:HA3	9:Tb:344:ASP:H	1.54	0.71
9:Tb:91:ASP:O	9:Tb:94:GLN:N	2.19	0.71
9:Te:326:GLY:HA3	9:Tf:344:ASP:H	1.54	0.71
9:Ti:326:GLY:HA3	9:Tj:344:ASP:C	2.16	0.71
4:Nc:111:PRO:CA	8:Pc:51:ARG:N	2.53	0.71
7:Qg:260:LEU:C	7:Qg:262:ASP:H	1.98	0.71
9:Tl:91:ASP:O	9:Tl:94:GLN:N	2.19	0.70
5:Oj:122:VAL:O	8:Pi:41:TYR:CA	2.39	0.70
7:Qi:260:LEU:C	7:Qi:262:ASP:H	1.98	0.70
9:Tg:326:GLY:HA3	9:Th:344:ASP:C	2.16	0.70
7:Qh:260:LEU:C	7:Qh:262:ASP:H	1.98	0.70
9:Te:326:GLY:HA3	9:Tf:344:ASP:C	2.16	0.70
9:Th:91:ASP:O	9:Th:94:GLN:N	2.19	0.70
7:Ql:260:LEU:C	7:Ql:262:ASP:H	1.98	0.70
9:Ta:344:ASP:C	9:Tl:326:GLY:HA3	2.16	0.70
9:Tk:326:GLY:HA3	9:Tl:344:ASP:C	2.17	0.70
6:Mb:45:LEU:N	6:Mb:53:LYS:O	2.24	0.70
9:Ti:91:ASP:O	9:Ti:94:GLN:N	2.19	0.70
9:Tb:326:GLY:HA3	9:Tc:344:ASP:C	2.16	0.70
8:Pk:15:PRO:C	8:Pk:17:LYS:H	1.99	0.70
6:Mh:45:LEU:N	6:Mh:53:LYS:O	2.24	0.70
6:Mi:45:LEU:N	6:Mi:53:LYS:O	2.23	0.70
7:Qk:260:LEU:C	7:Qk:262:ASP:H	1.98	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ta:326:GLY:HA3	9:Tb:344:ASP:C	2.17	0.69
5:Ok:48:ALA:CA	8:Pk:16:ALA:CA	2.71	0.69
9:Tj:326:GLY:HA3	9:Tk:344:ASP:C	2.16	0.69
6:Mk:45:LEU:N	6:Mk:53:LYS:O	2.23	0.69
9:Tc:91:ASP:O	9:Tc:94:GLN:N	2.19	0.69
9:Tc:326:GLY:HA3	9:Td:344:ASP:C	2.17	0.69
9:Tg:91:ASP:O	9:Tg:94:GLN:N	2.19	0.69
9:Ta:91:ASP:O	9:Ta:94:GLN:N	2.19	0.69
6:Mf:45:LEU:N	6:Mf:53:LYS:O	2.23	0.69
5:Ok:51:ARG:C	8:Pk:18:PRO:C	2.59	0.69
1:Aa:3:LEU:H	3:Cb:254:SER:CA	2.03	0.69
6:Ma:45:LEU:N	6:Ma:53:LYS:O	2.24	0.69
4:Ng:206:GLN:CA	8:Pf:47:PRO:O	2.41	0.68
8:Pl:24:VAL:O	8:Pl:26:VAL:N	2.26	0.68
4:Nc:110:THR:O	8:Pc:49:GLY:HA3	1.93	0.68
6:Mc:45:LEU:N	6:Mc:53:LYS:O	2.24	0.68
4:Nl:222:ASN:O	4:Nl:223:TYR:O	2.12	0.68
6:Md:45:LEU:N	6:Md:53:LYS:O	2.24	0.67
7:Qk:544:GLY:HA2	7:Ql:487:LYS:O	1.81	0.67
7:Qa:487:LYS:O	7:Ql:544:GLY:HA2	1.80	0.67
2:Ba:86:LEU:CA	6:Mi:82:ALA:N	2.58	0.67
4:Nc:110:THR:O	8:Pc:49:GLY:C	2.37	0.67
1:Aa:2:THR:C	3:Cb:254:SER:CA	2.68	0.67
9:Tj:91:ASP:O	9:Tj:94:GLN:N	2.19	0.67
4:Na:84:LYS:O	8:Pa:40:SER:CA	2.43	0.67
6:Me:45:LEU:N	6:Me:53:LYS:O	2.24	0.67
1:An:137:LYS:O	7:Qj:592:ALA:N	2.28	0.67
2:Ba:86:LEU:C	6:Mi:80:PRO:O	2.38	0.67
2:Bf:86:LEU:CA	6:Mj:82:ALA:N	2.58	0.67
9:Tc:299:GLN:C	9:Td:350:LEU:H	2.03	0.67
4:Na:88:VAL:C	8:Pa:42:SER:CA	2.68	0.66
5:Ok:47:VAL:C	8:Pk:16:ALA:CA	2.69	0.66
9:Tb:299:GLN:CA	9:Tc:350:LEU:CA	2.74	0.66
2:Bd:102:CYS:C	6:Mf:80:PRO:N	2.54	0.66
2:Ba:86:LEU:CA	6:Mi:81:GLU:CA	2.72	0.66
6:Mj:45:LEU:N	6:Mj:53:LYS:O	2.24	0.66
8:Pb:27:LYS:O	8:Pb:29:ALA:N	2.29	0.66
9:Ta:350:LEU:H	9:Ti:299:GLN:C	2.03	0.66
4:Na:109:ALA:CA	8:Pa:51:ARG:N	2.59	0.66
2:Bf:84:LYS:O	6:Mj:94:ILE:N	2.29	0.65
9:Ti:299:GLN:C	9:Tj:350:LEU:H	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ok:51:ARG:CA	8:Pk:18:PRO:C	2.70	0.65
9:Tb:299:GLN:C	9:Tc:350:LEU:H	2.03	0.65
9:Td:299:GLN:CA	9:Te:350:LEU:CA	2.75	0.65
2:Bb:86:LEU:CA	6:Mb:82:ALA:N	2.58	0.65
9:Tc:299:GLN:CA	9:Td:350:LEU:CA	2.74	0.65
9:Tf:299:GLN:CA	9:Tg:350:LEU:CA	2.75	0.65
1:Al:128:THR:CA	7:Qe:596:ASP:O	2.45	0.65
2:Be:84:LYS:O	6:Mh:94:ILE:N	2.30	0.65
9:Tj:299:GLN:CA	9:Tk:350:LEU:CA	2.75	0.65
5:Oc:47:VAL:CA	8:Pc:13:PRO:O	2.45	0.65
6:Mi:45:LEU:N	6:Mi:53:LYS:O	2.24	0.65
9:Ta:350:LEU:CA	9:Tl:299:GLN:CA	2.75	0.65
9:Te:299:GLN:CA	9:Tf:350:LEU:CA	2.74	0.65
9:Tk:91:ASP:O	9:Tk:94:GLN:N	2.19	0.65
9:Tk:299:GLN:C	9:Tl:350:LEU:H	2.03	0.65
4:Nc:99:PRO:CA	8:Pc:46:ASN:CA	2.74	0.65
7:Qd:544:GLY:N	7:Qe:488:ASP:CA	2.41	0.65
9:Tf:299:GLN:C	9:Tg:350:LEU:H	2.04	0.65
9:Th:299:GLN:CA	9:Ti:350:LEU:CA	2.74	0.65
9:Ti:299:GLN:CA	9:Tj:350:LEU:CA	2.75	0.65
2:Be:86:LEU:CA	6:Mh:82:ALA:N	2.59	0.64
9:Tg:299:GLN:CA	9:Th:350:LEU:CA	2.75	0.64
5:Ob:54:ASP:CA	8:Pb:22:ALA:CA	2.76	0.64
5:Ok:48:ALA:N	8:Pk:16:ALA:CA	2.60	0.64
2:Bc:86:LEU:CA	6:Md:82:ALA:N	2.60	0.64
9:Tk:299:GLN:CA	9:Tl:350:LEU:CA	2.75	0.64
9:Ta:299:GLN:C	9:Tb:350:LEU:H	2.04	0.64
9:Tg:299:GLN:C	9:Th:350:LEU:H	2.03	0.64
2:Bb:528:LYS:O	2:Bb:530:GLU:N	2.31	0.64
2:Bd:528:LYS:O	2:Bd:530:GLU:N	2.30	0.64
2:Bf:528:LYS:O	2:Bf:530:GLU:N	2.30	0.64
9:Td:327:SER:H	9:Te:344:ASP:N	1.96	0.64
9:Ta:299:GLN:CA	9:Tb:350:LEU:CA	2.75	0.63
9:Tc:327:SER:H	9:Td:344:ASP:N	1.97	0.63
2:Ba:84:LYS:O	6:Mi:94:ILE:N	2.31	0.63
2:Bd:86:LEU:CA	6:Mf:82:ALA:N	2.60	0.63
2:Bd:84:LYS:O	6:Mf:94:ILE:N	2.31	0.63
7:Qi:502:SER:O	8:Pj:155:ASP:N	2.30	0.63
9:Ta:344:ASP:N	9:Tl:327:SER:H	1.96	0.63
9:Tg:327:SER:H	9:Th:344:ASP:N	1.97	0.63
9:Tf:327:SER:H	9:Tg:344:ASP:N	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bc:84:LYS:O	6:Md:94:ILE:N	2.32	0.63
9:Ta:327:SER:H	9:Tb:344:ASP:N	1.96	0.63
2:Bf:86:LEU:CA	6:Mj:81:GLU:CA	2.77	0.63
4:Nc:99:PRO:N	8:Pc:46:ASN:O	2.32	0.63
7:Qh:544:GLY:N	7:Qi:488:ASP:CA	2.41	0.63
9:Te:299:GLN:C	9:Tf:350:LEU:H	2.03	0.63
9:Te:327:SER:H	9:Tf:344:ASP:N	1.97	0.63
9:Ti:327:SER:H	9:Tj:344:ASP:N	1.97	0.63
9:Tj:299:GLN:C	9:Tk:350:LEU:H	2.04	0.63
2:Bc:128:GLU:CA	6:Md:81:GLU:H	2.12	0.62
9:Th:327:SER:H	9:Ti:344:ASP:N	1.97	0.62
7:Qj:502:SER:O	8:Pk:155:ASP:N	2.31	0.62
9:Tj:327:SER:H	9:Tk:344:ASP:N	1.96	0.62
9:Tl:107:TRP:O	9:Tl:113:ILE:N	2.29	0.62
1:An:137:LYS:CA	7:Qj:592:ALA:C	2.72	0.62
9:Th:299:GLN:C	9:Ti:350:LEU:H	2.04	0.62
7:Qh:502:SER:O	8:Pi:155:ASP:N	2.31	0.62
2:Bb:84:LYS:O	6:Mb:94:ILE:N	2.32	0.62
6:Ma:276:LEU:O	6:Ma:280:GLY:HA3	2.00	0.62
4:Nc:111:PRO:CA	8:Pc:51:ARG:CA	2.77	0.62
9:Tc:326:GLY:CA	9:Td:344:ASP:H	2.13	0.62
9:Ti:107:TRP:O	9:Ti:113:ILE:N	2.28	0.62
9:Te:326:GLY:CA	9:Tf:344:ASP:H	2.13	0.62
9:Ti:326:GLY:CA	9:Tj:344:ASP:H	2.13	0.62
2:Bc:528:LYS:O	2:Bc:530:GLU:N	2.33	0.62
9:Tb:327:SER:H	9:Tc:344:ASP:N	1.96	0.62
9:Tk:326:GLY:CA	9:Tl:344:ASP:H	2.13	0.62
2:Be:86:LEU:CA	6:Mh:81:GLU:CA	2.78	0.61
3:Cb:182:ALA:O	3:Cb:194:ILE:CA	2.35	0.61
6:Mc:276:LEU:O	6:Mc:280:GLY:HA3	2.00	0.61
9:Tf:326:GLY:HA3	9:Tg:344:ASP:N	2.15	0.61
9:Tj:107:TRP:O	9:Tj:113:ILE:N	2.29	0.61
9:Tj:326:GLY:CA	9:Tk:344:ASP:H	2.13	0.61
2:Ba:528:LYS:O	2:Ba:530:GLU:N	2.34	0.61
7:Qb:502:SER:O	8:Pc:155:ASP:N	2.32	0.61
9:Ta:326:GLY:CA	9:Tb:344:ASP:H	2.13	0.61
9:Th:107:TRP:O	9:Th:113:ILE:N	2.29	0.61
2:Be:528:LYS:O	2:Be:530:GLU:N	2.33	0.61
9:Td:299:GLN:C	9:Te:350:LEU:H	2.03	0.61
9:Tk:107:TRP:O	9:Tk:113:ILE:N	2.28	0.61
1:An:135:ASP:C	1:An:137:LYS:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bb:368:ILE:O	3:Ca:297:GLY:O	2.18	0.61
7:Qd:260:LEU:O	7:Qd:277:ASP:O	2.19	0.61
9:Tf:326:GLY:CA	9:Tg:344:ASP:H	2.13	0.61
9:Tk:326:GLY:HA3	9:Tl:344:ASP:N	2.16	0.61
7:Qa:260:LEU:O	7:Qa:277:ASP:O	2.19	0.61
7:Qe:260:LEU:O	7:Qe:277:ASP:O	2.19	0.61
7:Qj:260:LEU:O	7:Qj:277:ASP:O	2.19	0.61
7:Qk:502:SER:O	8:Pl:155:ASP:N	2.31	0.61
6:Me:276:LEU:O	6:Me:280:GLY:HA3	2.01	0.61
7:Qg:260:LEU:O	7:Qg:277:ASP:O	2.19	0.61
7:Qk:260:LEU:O	7:Qk:277:ASP:O	2.19	0.61
1:A9:25:GLN:O	1:A9:26:ASP:CA	2.49	0.61
9:Ta:344:ASP:N	9:Tl:326:GLY:HA3	2.15	0.61
9:Tg:326:GLY:HA3	9:Th:344:ASP:N	2.16	0.61
1:Aj:25:GLN:O	1:Aj:26:ASP:CA	2.49	0.61
1:Am:25:GLN:O	1:Am:26:ASP:CA	2.49	0.61
1:An:25:GLN:O	1:An:26:ASP:CA	2.49	0.61
6:Mi:276:LEU:O	6:Mi:280:GLY:HA3	2.01	0.61
9:Tg:326:GLY:CA	9:Th:344:ASP:H	2.13	0.61
9:Ti:326:GLY:HA3	9:Tj:344:ASP:N	2.15	0.61
5:Oa:54:ASP:CA	8:Pa:22:ALA:O	2.49	0.61
6:Mb:276:LEU:O	6:Mb:280:GLY:HA3	2.01	0.61
6:Mg:48:GLY:O	6:Mg:50:THR:N	2.34	0.61
6:Mj:276:LEU:O	6:Mj:280:GLY:HA3	2.01	0.61
8:Pj:24:VAL:O	8:Pj:26:VAL:N	2.34	0.61
9:Ta:344:ASP:H	9:Tl:326:GLY:CA	2.13	0.61
9:Tb:326:GLY:CA	9:Tc:344:ASP:H	2.13	0.61
9:Tc:326:GLY:HA3	9:Td:344:ASP:N	2.16	0.61
6:Mh:276:LEU:O	6:Mh:280:GLY:HA3	2.00	0.60
9:Td:326:GLY:HA3	9:Te:344:ASP:N	2.16	0.60
9:Tk:327:SER:H	9:Tl:344:ASP:N	1.97	0.60
6:Md:48:GLY:O	6:Md:50:THR:N	2.34	0.60
7:Qc:260:LEU:O	7:Qc:277:ASP:O	2.19	0.60
7:Qi:260:LEU:O	7:Qi:277:ASP:O	2.19	0.60
9:Te:326:GLY:HA3	9:Tf:344:ASP:N	2.16	0.60
9:Tg:107:TRP:O	9:Tg:113:ILE:N	2.29	0.60
9:Th:326:GLY:CA	9:Ti:344:ASP:H	2.14	0.60
1:Aa:25:GLN:O	1:Aa:26:ASP:CA	2.50	0.60
1:Au:25:GLN:O	1:Au:26:ASP:CA	2.49	0.60
1:Av:25:GLN:O	1:Av:26:ASP:CA	2.50	0.60
1:Az:25:GLN:O	1:Az:26:ASP:CA	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Qf:544:GLY:CA	7:Qg:488:ASP:N	2.64	0.60
1:Ah:25:GLN:O	1:Ah:26:ASP:CA	2.49	0.60
1:Ak:25:GLN:O	1:Ak:26:ASP:CA	2.49	0.60
1:Ar:25:GLN:O	1:Ar:26:ASP:CA	2.49	0.60
2:Bb:86:LEU:CA	6:Mb:81:GLU:CA	2.79	0.60
9:Ta:107:TRP:O	9:Ta:113:ILE:N	2.28	0.60
9:Tb:326:GLY:HA3	9:Tc:344:ASP:N	2.16	0.60
9:Tj:326:GLY:HA3	9:Tk:344:ASP:N	2.16	0.60
1:Ay:25:GLN:O	1:Ay:26:ASP:CA	2.50	0.60
6:Mj:48:GLY:O	6:Mj:50:THR:N	2.35	0.60
9:Tb:107:TRP:O	9:Tb:113:ILE:N	2.29	0.60
1:Ao:25:GLN:O	1:Ao:26:ASP:CA	2.49	0.60
1:A1:25:GLN:O	1:A1:26:ASP:CA	2.49	0.60
4:Na:109:ALA:O	8:Pa:51:ARG:C	2.44	0.60
5:Ob:55:LEU:O	8:Pb:25:PRO:O	2.20	0.60
4:Nd:123:ASN:O	8:Pd:62:GLY:CA	2.49	0.60
7:Qc:544:GLY:HA2	7:Qd:488:ASP:N	2.17	0.60
7:Qh:544:GLY:CA	7:Qi:488:ASP:N	2.64	0.60
9:Td:107:TRP:O	9:Td:113:ILE:N	2.29	0.60
9:Ti:298:LYS:O	9:Tj:350:LEU:CA	2.48	0.60
1:Ab:25:GLN:O	1:Ab:26:ASP:CA	2.50	0.60
1:Ad:25:GLN:O	1:Ad:26:ASP:CA	2.49	0.60
1:A3:25:GLN:O	1:A3:26:ASP:CA	2.49	0.60
6:Mc:48:GLY:O	6:Mc:50:THR:N	2.34	0.60
7:Qe:544:GLY:CA	7:Qf:488:ASP:N	2.64	0.60
7:Qh:260:LEU:O	7:Qh:277:ASP:O	2.19	0.60
1:Ae:25:GLN:O	1:Ae:26:ASP:CA	2.49	0.60
1:A4:25:GLN:O	1:A4:26:ASP:CA	2.49	0.60
1:A6:25:GLN:O	1:A6:26:ASP:CA	2.49	0.60
6:Mk:276:LEU:O	6:Mk:280:GLY:HA3	2.01	0.60
1:Ai:66:VAL:O	1:Ai:67:ALA:C	2.45	0.60
1:At:25:GLN:O	1:At:26:ASP:CA	2.49	0.60
1:A8:66:VAL:O	1:A8:67:ALA:C	2.45	0.60
6:Mg:276:LEU:O	6:Mg:280:GLY:HA3	2.02	0.60
6:Mi:48:GLY:O	6:Mi:50:THR:N	2.34	0.60
8:Pb:16:ALA:O	8:Pb:17:LYS:C	2.44	0.60
1:Al:25:GLN:O	1:Al:26:ASP:CA	2.50	0.60
1:A7:25:GLN:O	1:A7:26:ASP:CA	2.50	0.60
6:Mb:48:GLY:O	6:Mb:50:THR:N	2.34	0.60
5:Od:155:ARG:CA	8:Pd:39:PRO:N	2.65	0.60
7:Qf:260:LEU:O	7:Qf:277:ASP:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Qg:544:GLY:CA	7:Qh:488:ASP:N	2.65	0.60
7:Ql:260:LEU:O	7:Ql:277:ASP:O	2.19	0.60
1:Ac:25:GLN:O	1:Ac:26:ASP:CA	2.49	0.59
1:Ai:25:GLN:O	1:Ai:26:ASP:CA	2.49	0.59
1:A2:25:GLN:O	1:A2:26:ASP:CA	2.49	0.59
6:Mf:276:LEU:O	6:Mf:280:GLY:HA3	2.02	0.59
1:Aq:66:VAL:O	1:Aq:67:ALA:C	2.45	0.59
1:Ax:25:GLN:O	1:Ax:26:ASP:CA	2.49	0.59
1:Ay:66:VAL:O	1:Ay:67:ALA:C	2.45	0.59
6:Ma:48:GLY:O	6:Ma:50:THR:N	2.34	0.59
7:Qd:544:GLY:CA	7:Qe:488:ASP:N	2.65	0.59
1:Ae:66:VAL:O	1:Ae:67:ALA:C	2.45	0.59
1:Av:66:VAL:O	1:Av:67:ALA:C	2.45	0.59
1:A5:66:VAL:O	1:A5:67:ALA:C	2.45	0.59
6:Mi:48:GLY:O	6:Mi:50:THR:N	2.34	0.59
8:Pa:155:ASP:N	7:Ql:502:SER:O	2.30	0.59
7:Qb:260:LEU:O	7:Qb:277:ASP:O	2.19	0.59
9:Tc:298:LYS:O	9:Td:350:LEU:CA	2.48	0.59
1:Aa:66:VAL:O	1:Aa:67:ALA:C	2.45	0.59
1:Ac:66:VAL:O	1:Ac:67:ALA:C	2.45	0.59
1:Al:66:VAL:O	1:Al:67:ALA:C	2.45	0.59
1:Au:66:VAL:O	1:Au:67:ALA:C	2.46	0.59
1:A4:66:VAL:O	1:A4:67:ALA:C	2.45	0.59
5:Oa:47:VAL:O	8:Pa:18:PRO:N	2.35	0.59
7:Qc:502:SER:O	8:Pd:155:ASP:N	2.32	0.59
7:Qc:544:GLY:CA	7:Qd:488:ASP:N	2.64	0.59
7:Qf:544:GLY:HA2	7:Qg:488:ASP:N	2.17	0.59
7:Qi:544:GLY:CA	7:Qj:488:ASP:N	2.65	0.59
7:Qj:544:GLY:CA	7:Qk:488:ASP:N	2.64	0.59
9:Ta:326:GLY:HA3	9:Tb:344:ASP:N	2.16	0.59
1:Ar:66:VAL:O	1:Ar:67:ALA:C	2.45	0.59
1:A5:25:GLN:O	1:A5:26:ASP:CA	2.49	0.59
1:A8:25:GLN:O	1:A8:26:ASP:CA	2.49	0.59
7:Qa:544:GLY:CA	7:Qb:488:ASP:N	2.65	0.59
7:Qh:544:GLY:HA2	7:Qi:488:ASP:N	2.17	0.59
1:Af:25:GLN:O	1:Af:26:ASP:CA	2.49	0.59
1:Af:66:VAL:O	1:Af:67:ALA:C	2.45	0.59
1:Ag:25:GLN:O	1:Ag:26:ASP:CA	2.49	0.59
1:Ak:66:VAL:O	1:Ak:67:ALA:C	2.45	0.59
1:Ap:25:GLN:O	1:Ap:26:ASP:CA	2.50	0.59
1:Ax:66:VAL:O	1:Ax:67:ALA:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:66:VAL:O	1:A7:67:ALA:C	2.45	0.59
6:Md:276:LEU:O	6:Md:280:GLY:HA3	2.01	0.59
9:Ta:350:LEU:CA	9:Tl:298:LYS:O	2.47	0.59
9:Td:326:GLY:CA	9:Te:344:ASP:H	2.13	0.59
1:Ah:66:VAL:O	1:Ah:67:ALA:C	2.45	0.59
1:Aq:25:GLN:O	1:Aq:26:ASP:CA	2.49	0.59
1:As:25:GLN:O	1:As:26:ASP:CA	2.50	0.59
1:Az:66:VAL:O	1:Az:67:ALA:C	2.45	0.59
7:Qa:488:ASP:N	7:Ql:544:GLY:CA	2.65	0.59
7:Qb:544:GLY:CA	7:Qc:488:ASP:N	2.65	0.59
7:Qe:544:GLY:HA2	7:Qf:488:ASP:N	2.18	0.59
1:An:66:VAL:O	1:An:67:ALA:C	2.46	0.59
2:Ba:86:LEU:O	6:Ml:80:PRO:C	2.46	0.59
6:Ml:276:LEU:O	6:Ml:280:GLY:HA3	2.02	0.59
7:Qa:544:GLY:HA2	7:Qb:488:ASP:N	2.17	0.59
1:Aw:66:VAL:O	1:Aw:67:ALA:C	2.46	0.59
1:A2:66:VAL:O	1:A2:67:ALA:C	2.46	0.59
2:Bd:379:PHE:H	2:Bd:381:ARG:H	1.51	0.59
6:Mh:48:GLY:O	6:Mh:50:THR:N	2.34	0.59
2:Be:379:PHE:H	2:Be:381:ARG:H	1.50	0.59
7:Qj:544:GLY:HA2	7:Qk:488:ASP:N	2.17	0.59
7:Qk:544:GLY:CA	7:Ql:488:ASP:N	2.65	0.58
1:A6:66:VAL:O	1:A6:67:ALA:C	2.45	0.58
2:Bb:257:LYS:C	2:Bb:259:GLY:H	2.11	0.58
9:Td:298:LYS:O	9:Te:350:LEU:CA	2.48	0.58
1:As:66:VAL:O	1:As:67:ALA:C	2.45	0.58
6:Mk:48:GLY:O	6:Mk:50:THR:N	2.34	0.58
7:Qa:488:ASP:N	7:Ql:544:GLY:HA2	2.17	0.58
7:Qi:544:GLY:HA2	7:Qj:488:ASP:N	2.18	0.58
9:Tf:107:TRP:O	9:Tf:113:ILE:N	2.29	0.58
1:Ao:66:VAL:O	1:Ao:67:ALA:C	2.45	0.58
4:Nc:123:ASN:CA	8:Pe:62:GLY:CA	2.75	0.58
5:Oi:122:VAL:C	8:Ph:41:TYR:CA	2.76	0.58
7:Qb:544:GLY:N	7:Qc:488:ASP:CA	2.41	0.58
7:Qd:502:SER:O	8:Pe:155:ASP:N	2.31	0.58
7:Qg:544:GLY:HA2	7:Qh:488:ASP:N	2.18	0.58
1:Ad:66:VAL:O	1:Ad:67:ALA:C	2.45	0.58
1:A3:66:VAL:O	1:A3:67:ALA:C	2.45	0.58
2:Bd:86:LEU:CA	6:Mf:81:GLU:CA	2.81	0.58
6:Mf:48:GLY:O	6:Mf:50:THR:N	2.34	0.58
7:Qb:544:GLY:HA2	7:Qc:488:ASP:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Tb:326:GLY:HA3	9:Tc:344:ASP:CA	2.34	0.58
9:Tj:326:GLY:HA3	9:Tk:344:ASP:CA	2.34	0.58
1:Ap:66:VAL:O	1:Ap:67:ALA:C	2.45	0.58
1:A1:66:VAL:O	1:A1:67:ALA:C	2.45	0.58
4:Nf:222:ASN:O	8:Pf:58:ILE:CA	2.50	0.58
9:Td:326:GLY:HA3	9:Te:344:ASP:CA	2.34	0.58
1:Ab:66:VAL:O	1:Ab:67:ALA:C	2.45	0.58
1:Am:66:VAL:O	1:Am:67:ALA:C	2.45	0.58
2:Bb:379:PHE:H	2:Bb:381:ARG:H	1.52	0.58
2:Bc:379:PHE:H	2:Bc:381:ARG:H	1.51	0.58
4:Ne:223:TYR:O	8:Pe:58:ILE:C	2.47	0.58
6:Mk:381:VAL:O	6:Mk:384:GLY:N	2.37	0.58
9:Tf:298:LYS:O	9:Tg:350:LEU:CA	2.47	0.58
9:Th:326:GLY:HA3	9:Ti:344:ASP:N	2.16	0.58
6:Mi:381:VAL:O	6:Mi:384:GLY:N	2.37	0.58
9:Tg:326:GLY:HA3	9:Th:344:ASP:CA	2.34	0.58
9:Ti:326:GLY:HA3	9:Tj:344:ASP:CA	2.34	0.58
9:Tk:326:GLY:HA3	9:Tl:344:ASP:CA	2.34	0.58
1:Ag:66:VAL:O	1:Ag:67:ALA:C	2.46	0.58
1:Aw:25:GLN:O	1:Aw:26:ASP:CA	2.50	0.58
7:Qa:502:SER:O	8:Pb:155:ASP:N	2.31	0.58
7:Qc:544:GLY:HA2	7:Qd:487:LYS:O	1.81	0.58
7:Qk:544:GLY:HA2	7:Ql:488:ASP:N	2.18	0.58
9:Tf:326:GLY:HA3	9:Tg:344:ASP:CA	2.34	0.58
9:Th:326:GLY:HA3	9:Ti:344:ASP:CA	2.34	0.58
1:Aj:66:VAL:O	1:Aj:67:ALA:C	2.45	0.58
1:At:66:VAL:O	1:At:67:ALA:C	2.45	0.58
2:Bd:128:GLU:CA	6:Mf:81:GLU:H	2.17	0.58
9:Tc:326:GLY:HA3	9:Td:344:ASP:CA	2.34	0.58
1:A9:66:VAL:O	1:A9:67:ALA:C	2.45	0.57
6:Mg:381:VAL:O	6:Mg:384:GLY:N	2.37	0.57
7:Qd:544:GLY:HA2	7:Qe:488:ASP:N	2.18	0.57
2:Ba:86:LEU:CA	6:Mi:80:PRO:O	2.52	0.57
7:Qi:544:GLY:N	7:Qj:488:ASP:CA	2.42	0.57
9:Ta:344:ASP:CA	9:Tl:326:GLY:HA3	2.34	0.57
2:Ba:379:PHE:H	2:Ba:381:ARG:H	1.50	0.57
4:Na:190:PHE:O	4:Na:222:ASN:N	2.38	0.57
9:Ta:326:GLY:HA3	9:Tb:344:ASP:CA	2.34	0.57
9:Tb:298:LYS:O	9:Tc:350:LEU:CA	2.47	0.57
9:Tc:107:TRP:O	9:Tc:113:ILE:N	2.28	0.57
6:Mb:381:VAL:O	6:Mb:384:GLY:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Th:298:LYS:O	9:Ti:350:LEU:CA	2.48	0.57
4:Nc:112:LYS:O	8:Pc:49:GLY:HA3	2.04	0.57
6:Mh:381:VAL:O	6:Mh:384:GLY:N	2.37	0.57
2:Bf:379:PHE:H	2:Bf:381:ARG:H	1.52	0.57
7:Qe:502:SER:O	8:Pf:155:ASP:N	2.31	0.57
6:Mc:381:VAL:O	6:Mc:384:GLY:N	2.37	0.57
4:Nk:38:TYR:O	4:Nk:40:TRP:N	2.38	0.57
6:Md:381:VAL:O	6:Md:384:GLY:N	2.37	0.57
6:Mj:381:VAL:O	6:Mj:384:GLY:N	2.37	0.57
5:Od:152:ALA:O	8:Pd:40:SER:O	2.22	0.57
9:Te:107:TRP:O	9:Te:113:ILE:N	2.29	0.57
4:Na:109:ALA:CA	8:Pa:51:ARG:H	2.18	0.56
6:Mi:381:VAL:O	6:Mi:384:GLY:N	2.37	0.56
4:Na:109:ALA:CA	8:Pa:50:LYS:CA	2.83	0.56
5:Ob:44:GLY:O	8:Pb:13:PRO:C	2.47	0.56
6:Me:381:VAL:O	6:Me:384:GLY:N	2.37	0.56
8:Pe:12:ALA:C	8:Pe:14:PRO:CA	2.78	0.56
9:Te:326:GLY:HA3	9:Tf:344:ASP:CA	2.34	0.56
4:Nc:38:TYR:O	4:Nc:40:TRP:N	2.39	0.56
6:Me:48:GLY:O	6:Me:50:THR:N	2.34	0.56
4:Nf:222:ASN:O	4:Nf:223:TYR:O	2.21	0.56
8:Pc:55:ARG:O	8:Pc:59:ASP:N	2.36	0.56
4:Ne:38:TYR:O	4:Ne:40:TRP:N	2.38	0.56
2:Bf:257:LYS:C	2:Bf:259:GLY:H	2.13	0.56
4:Na:38:TYR:O	4:Na:40:TRP:N	2.38	0.56
4:Ni:38:TYR:O	4:Ni:39:LEU:C	2.49	0.56
4:Na:38:TYR:O	4:Na:39:LEU:C	2.49	0.56
7:Qc:544:GLY:N	7:Qd:488:ASP:CA	2.43	0.56
2:Bc:86:LEU:CA	6:Md:81:GLU:CA	2.83	0.56
4:Nh:38:TYR:O	4:Nh:40:TRP:N	2.39	0.56
4:Nj:38:TYR:O	4:Nj:40:TRP:N	2.39	0.56
8:Pj:26:VAL:CA	8:Pj:28:ALA:H	2.18	0.56
4:Nf:38:TYR:O	4:Nf:39:LEU:C	2.49	0.56
4:Nl:38:TYR:O	4:Nl:39:LEU:C	2.49	0.56
9:Tj:298:LYS:C	9:Tk:350:LEU:N	2.63	0.56
4:Ne:38:TYR:O	4:Ne:39:LEU:C	2.49	0.55
4:Ng:38:TYR:O	4:Ng:40:TRP:N	2.39	0.55
4:Ni:38:TYR:O	4:Ni:40:TRP:N	2.39	0.55
5:Ol:51:ARG:CA	8:Pl:18:PRO:CA	2.84	0.55
7:Qh:260:LEU:C	7:Qh:262:ASP:N	2.64	0.55
9:Td:299:GLN:O	9:Te:349:VAL:C	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bb:128:GLU:CA	6:Mb:81:GLU:H	2.19	0.55
2:Be:102:CYS:C	6:Mh:80:PRO:N	2.64	0.55
4:Nb:38:TYR:O	4:Nb:40:TRP:N	2.39	0.55
6:Mf:381:VAL:O	6:Mf:384:GLY:N	2.37	0.55
9:Te:298:LYS:C	9:Tf:350:LEU:N	2.63	0.55
4:Nf:38:TYR:O	4:Nf:40:TRP:N	2.39	0.55
4:Nl:109:ALA:CA	8:Pl:51:ARG:CA	2.84	0.55
6:Mi:88:LEU:C	6:Mi:90:ASN:H	2.15	0.55
7:Qf:502:SER:O	8:Pg:155:ASP:N	2.31	0.55
7:Qg:502:SER:O	8:Ph:155:ASP:N	2.30	0.55
2:Bd:257:LYS:C	2:Bd:259:GLY:H	2.13	0.55
4:Na:95:GLY:O	8:Pa:45:TYR:CA	2.54	0.55
4:Nl:38:TYR:O	4:Nl:40:TRP:N	2.39	0.55
1:Aa:2:THR:CA	3:Cb:254:SER:C	2.79	0.55
6:Ma:381:VAL:O	6:Ma:384:GLY:N	2.39	0.55
4:Nj:38:TYR:O	4:Nj:39:LEU:C	2.50	0.55
4:Nj:222:ASN:O	4:Nj:223:TYR:O	2.25	0.55
4:Nk:38:TYR:O	4:Nk:39:LEU:C	2.49	0.55
8:Pc:27:LYS:O	8:Pc:29:ALA:N	2.39	0.55
9:Tb:298:LYS:C	9:Tc:350:LEU:N	2.63	0.55
4:Nd:38:TYR:O	4:Nd:40:TRP:N	2.39	0.55
5:Og:122:VAL:N	8:Pf:41:TYR:CA	2.61	0.55
4:Nd:38:TYR:O	4:Nd:39:LEU:C	2.49	0.55
8:Ph:27:LYS:O	8:Ph:29:ALA:N	2.40	0.55
4:Nh:38:TYR:O	4:Nh:39:LEU:C	2.49	0.54
9:Tf:299:GLN:O	9:Tg:349:VAL:C	2.51	0.54
8:Pf:27:LYS:O	8:Pf:29:ALA:N	2.40	0.54
8:Pd:27:LYS:O	8:Pd:29:ALA:N	2.40	0.54
9:Tj:299:GLN:O	9:Tk:349:VAL:C	2.50	0.54
2:Bd:84:LYS:CA	6:Mf:90:ASN:O	2.55	0.54
4:Nc:38:TYR:O	4:Nc:39:LEU:C	2.49	0.54
8:Pi:27:LYS:O	8:Pi:29:ALA:N	2.41	0.54
8:Pl:26:VAL:CA	8:Pl:28:ALA:H	2.19	0.54
2:Bd:541:MET:O	2:Bd:545:ARG:N	2.40	0.54
2:Be:86:LEU:C	6:Mh:80:PRO:O	2.50	0.54
8:Pg:27:LYS:O	8:Pg:29:ALA:N	2.40	0.54
9:Ta:298:LYS:C	9:Tb:350:LEU:N	2.63	0.54
9:Ta:299:GLN:O	9:Tb:349:VAL:C	2.50	0.54
9:Tc:299:GLN:O	9:Td:349:VAL:C	2.51	0.54
9:Tf:298:LYS:C	9:Tg:350:LEU:N	2.63	0.54
2:Bd:102:CYS:C	6:Mf:80:PRO:CA	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Nb:111:PRO:CA	8:Pb:51:ARG:CA	2.85	0.54
8:Pj:27:LYS:O	8:Pj:29:ALA:N	2.40	0.54
4:Ng:38:TYR:O	4:Ng:39:LEU:C	2.49	0.54
9:Ta:349:VAL:C	9:Tl:299:GLN:O	2.51	0.54
9:Tc:298:LYS:C	9:Td:350:LEU:N	2.63	0.54
8:Pk:15:PRO:O	8:Pk:16:ALA:C	2.50	0.54
9:Ti:299:GLN:O	9:Tj:349:VAL:C	2.51	0.54
9:Th:298:LYS:C	9:Ti:350:LEU:N	2.62	0.54
9:Tk:298:LYS:O	9:Tl:350:LEU:CA	2.49	0.54
1:Aa:2:THR:N	3:Cb:254:SER:C	2.64	0.53
2:Bb:83:GLU:O	6:Mb:90:ASN:CA	2.56	0.53
4:Nb:38:TYR:O	4:Nb:39:LEU:C	2.49	0.53
7:Qh:260:LEU:O	7:Qh:262:ASP:N	2.33	0.53
2:Ba:83:GLU:O	6:Mi:90:ASN:CA	2.55	0.53
5:Ol:55:LEU:CA	8:Pl:22:ALA:C	2.79	0.53
7:Qf:260:LEU:O	7:Qf:262:ASP:N	2.33	0.53
9:Te:299:GLN:O	9:Tf:349:VAL:C	2.50	0.53
9:Tk:298:LYS:C	9:Tl:350:LEU:N	2.63	0.53
2:Ba:437:VAL:O	2:Ba:441:LEU:N	2.36	0.53
9:Tb:299:GLN:O	9:Tc:349:VAL:C	2.51	0.53
9:Ti:298:LYS:C	9:Tj:350:LEU:N	2.64	0.53
8:Pa:7:GLU:O	8:Pa:9:PRO:CA	2.56	0.53
8:Pa:24:VAL:O	8:Pa:26:VAL:N	2.42	0.53
7:Qg:260:LEU:O	7:Qg:262:ASP:N	2.33	0.53
7:Qk:477:TYR:CA	7:Ql:574:ASP:N	2.72	0.53
2:Bb:541:MET:O	2:Bb:545:ARG:N	2.40	0.53
2:Bf:309:ALA:O	2:Bf:312:ARG:N	2.41	0.53
1:Ai:26:ASP:N	1:Ai:26:ASP:C	2.63	0.53
1:A8:26:ASP:N	1:A8:26:ASP:C	2.63	0.53
5:Oa:54:ASP:CA	8:Pa:22:ALA:CA	2.86	0.53
7:Qe:544:GLY:N	7:Qf:488:ASP:CA	2.41	0.53
9:Ta:298:LYS:O	9:Tb:350:LEU:CA	2.48	0.53
8:Ph:7:GLU:O	8:Ph:9:PRO:CA	2.58	0.52
2:Be:541:MET:O	2:Be:545:ARG:N	2.40	0.52
7:Qj:502:SER:C	8:Pk:155:ASP:CA	2.82	0.52
7:Qk:502:SER:C	8:Pl:155:ASP:CA	2.82	0.52
9:Tg:299:GLN:O	9:Th:349:VAL:C	2.50	0.52
1:Aa:26:ASP:N	1:Aa:26:ASP:C	2.63	0.52
1:Az:26:ASP:N	1:Az:26:ASP:C	2.63	0.52
2:Ba:103:ASP:N	6:Mi:80:PRO:N	2.58	0.52
2:Bf:128:GLU:CA	6:Mj:81:GLU:H	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Pc:31:THR:O	8:Pc:33:THR:N	2.41	0.52
9:Te:298:LYS:O	9:Tf:350:LEU:CA	2.48	0.52
9:Tg:298:LYS:O	9:Th:350:LEU:CA	2.47	0.52
1:Ak:26:ASP:N	1:Ak:26:ASP:C	2.63	0.52
2:Bc:541:MET:O	2:Bc:545:ARG:N	2.40	0.52
4:Nc:98:GLY:CA	8:Pc:46:ASN:H	2.21	0.52
7:Qa:477:TYR:CA	7:Qb:574:ASP:N	2.73	0.52
7:Ql:260:LEU:O	7:Ql:262:ASP:N	2.33	0.52
2:Bc:309:ALA:O	2:Bc:312:ARG:N	2.41	0.52
9:Tg:298:LYS:C	9:Th:350:LEU:N	2.63	0.52
5:Od:154:MET:O	8:Pd:39:PRO:N	2.43	0.52
2:Bf:102:CYS:C	6:Mj:80:PRO:N	2.67	0.52
8:Pj:15:PRO:O	8:Pj:17:LYS:N	2.43	0.52
9:Th:299:GLN:O	9:Ti:349:VAL:C	2.51	0.52
7:Qf:477:TYR:CA	7:Qg:574:ASP:N	2.73	0.52
7:Qk:260:LEU:C	7:Qk:262:ASP:N	2.64	0.52
2:Ba:102:CYS:C	6:Mi:80:PRO:CA	2.83	0.52
2:Be:128:GLU:CA	6:Mh:81:GLU:H	2.23	0.52
7:Qa:544:GLY:N	7:Qb:488:ASP:CA	2.41	0.52
7:Qh:502:SER:C	8:Pi:155:ASP:CA	2.82	0.52
1:Ao:26:ASP:N	1:Ao:26:ASP:C	2.63	0.52
2:Ba:541:MET:O	2:Ba:545:ARG:N	2.40	0.52
2:Be:128:GLU:C	6:Mh:83:ILE:O	2.53	0.52
4:Nl:109:ALA:C	8:Pl:50:LYS:O	2.53	0.52
8:Pb:31:THR:O	8:Pb:33:THR:N	2.42	0.52
7:Qe:502:SER:C	8:Pf:155:ASP:CA	2.83	0.52
2:Be:437:VAL:O	2:Be:441:LEU:N	2.36	0.51
7:Qc:502:SER:C	8:Pd:155:ASP:CA	2.83	0.51
7:Qh:477:TYR:CA	7:Qi:574:ASP:N	2.73	0.51
9:Tk:299:GLN:O	9:Tl:349:VAL:C	2.51	0.51
2:Bf:128:GLU:C	6:Mj:83:ILE:O	2.53	0.51
4:Nc:111:PRO:N	8:Pc:51:ARG:N	2.58	0.51
7:Qi:502:SER:C	8:Pj:155:ASP:CA	2.83	0.51
2:Bd:437:VAL:O	2:Bd:441:LEU:N	2.36	0.51
7:Qa:502:SER:C	8:Pb:155:ASP:CA	2.83	0.51
7:Qa:574:ASP:N	7:Ql:477:TYR:CA	2.73	0.51
7:Qi:477:TYR:CA	7:Qj:574:ASP:N	2.73	0.51
8:Pc:53:PRO:CA	8:Pc:55:ARG:N	2.74	0.51
1:An:137:LYS:O	7:Qj:592:ALA:C	2.45	0.51
1:Au:26:ASP:N	1:Au:26:ASP:C	2.64	0.51
2:Bc:437:VAL:O	2:Bc:441:LEU:N	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Qb:477:TYR:CA	7:Qc:574:ASP:N	2.72	0.51
7:Qb:502:SER:C	8:Pc:155:ASP:CA	2.84	0.51
7:Qe:260:LEU:O	7:Qe:262:ASP:N	2.33	0.51
7:Qf:502:SER:C	8:Pg:155:ASP:CA	2.84	0.51
7:Qc:82:ILE:C	7:Qc:84:GLY:H	2.19	0.51
7:Qh:82:ILE:C	7:Qh:84:GLY:H	2.19	0.51
7:Ql:75:SER:C	7:Ql:77:ALA:H	2.19	0.51
2:Bf:437:VAL:O	2:Bf:441:LEU:N	2.36	0.51
4:Na:109:ALA:C	8:Pa:51:ARG:N	2.69	0.51
8:Pa:155:ASP:CA	7:Ql:502:SER:C	2.83	0.51
7:Qd:82:ILE:C	7:Qd:84:GLY:H	2.19	0.51
7:Qi:75:SER:C	7:Qi:77:ALA:H	2.18	0.51
2:Bd:309:ALA:O	2:Bd:312:ARG:N	2.41	0.51
7:Qb:75:SER:C	7:Qb:77:ALA:H	2.19	0.51
7:Qd:477:TYR:CA	7:Qe:574:ASP:N	2.73	0.51
7:Qg:502:SER:C	8:Ph:155:ASP:CA	2.83	0.51
1:A9:26:ASP:N	1:A9:26:ASP:C	2.63	0.50
2:Ba:128:GLU:C	6:Ml:83:ILE:O	2.54	0.50
2:Bf:541:MET:O	2:Bf:545:ARG:N	2.40	0.50
4:Nf:222:ASN:C	4:Nf:223:TYR:O	2.55	0.50
7:Qc:477:TYR:CA	7:Qd:574:ASP:N	2.73	0.50
7:Qd:75:SER:C	7:Qd:77:ALA:H	2.19	0.50
7:Qk:75:SER:C	7:Qk:77:ALA:H	2.19	0.50
2:Bd:423:THR:O	2:Bd:424:VAL:C	2.54	0.50
4:Nb:99:PRO:N	8:Pb:46:ASN:H	2.08	0.50
7:Qe:260:LEU:C	7:Qe:277:ASP:O	2.55	0.50
7:Qf:82:ILE:C	7:Qf:84:GLY:H	2.19	0.50
7:Qg:82:ILE:C	7:Qg:84:GLY:H	2.19	0.50
7:Qg:477:TYR:CA	7:Qh:574:ASP:N	2.72	0.50
7:Qg:544:GLY:N	7:Qh:488:ASP:CA	2.42	0.50
9:Ta:350:LEU:N	9:Tl:298:LYS:C	2.63	0.50
1:Ad:26:ASP:N	1:Ad:26:ASP:C	2.63	0.50
2:Bd:128:GLU:C	6:Mf:83:ILE:O	2.55	0.50
7:Qc:75:SER:C	7:Qc:77:ALA:H	2.19	0.50
7:Qe:75:SER:C	7:Qe:77:ALA:H	2.18	0.50
7:Qk:82:ILE:C	7:Qk:84:GLY:H	2.19	0.50
1:Aj:41:GLU:C	1:Aj:43:GLN:H	2.20	0.50
5:Ol:70:ARG:O	5:Ol:73:GLU:N	2.45	0.50
7:Qa:75:SER:C	7:Qa:77:ALA:H	2.18	0.50
7:Qe:477:TYR:CA	7:Qf:574:ASP:N	2.74	0.50
7:Qh:260:LEU:C	7:Qh:277:ASP:O	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Qj:75:SER:C	7:Qj:77:ALA:H	2.19	0.50
8:Pk:24:VAL:O	8:Pk:26:VAL:N	2.44	0.50
9:Td:327:SER:H	9:Te:344:ASP:H	1.58	0.50
1:Az:41:GLU:C	1:Az:43:GLN:H	2.20	0.50
1:A3:26:ASP:N	1:A3:26:ASP:C	2.63	0.50
1:A9:41:GLU:C	1:A9:43:GLN:H	2.20	0.50
2:Bc:102:CYS:C	6:Md:80:PRO:N	2.70	0.50
5:Oa:70:ARG:O	5:Oa:73:GLU:N	2.45	0.50
9:Tj:327:SER:H	9:Tk:344:ASP:H	1.59	0.50
1:Aj:26:ASP:N	1:Aj:26:ASP:C	2.64	0.50
1:Am:41:GLU:C	1:Am:43:GLN:H	2.20	0.50
1:Aw:26:ASP:N	1:Aw:26:ASP:C	2.63	0.50
2:Be:423:THR:O	2:Be:424:VAL:C	2.54	0.50
7:Qa:260:LEU:C	7:Qa:277:ASP:O	2.55	0.50
7:Qd:502:SER:C	8:Pe:155:ASP:CA	2.83	0.50
7:Qk:260:LEU:C	7:Qk:277:ASP:O	2.55	0.50
9:Tj:298:LYS:O	9:Tk:350:LEU:CA	2.48	0.50
1:An:26:ASP:N	1:An:26:ASP:C	2.63	0.50
2:Bc:149:ILE:C	2:Bc:151:GLY:H	2.20	0.50
4:Nb:91:ALA:C	8:Pb:43:TYR:N	2.66	0.50
6:Mc:384:GLY:C	6:Mc:386:ALA:H	2.20	0.50
6:Mj:384:GLY:C	6:Mj:386:ALA:H	2.19	0.50
7:Qc:260:LEU:C	7:Qc:277:ASP:O	2.55	0.50
8:Pd:31:THR:O	8:Pd:33:THR:N	2.42	0.50
7:Qf:75:SER:C	7:Qf:77:ALA:H	2.18	0.50
7:Qi:260:LEU:C	7:Qi:277:ASP:O	2.55	0.50
7:Qj:82:ILE:C	7:Qj:84:GLY:H	2.19	0.50
9:Tf:327:SER:H	9:Tg:344:ASP:H	1.60	0.50
1:Av:41:GLU:C	1:Av:43:GLN:H	2.20	0.50
1:A6:26:ASP:N	1:A6:26:ASP:C	2.63	0.50
7:Qa:82:ILE:C	7:Qa:84:GLY:H	2.19	0.50
7:Qb:260:LEU:C	7:Qb:277:ASP:O	2.55	0.50
7:Qd:260:LEU:C	7:Qd:277:ASP:O	2.55	0.50
1:Af:41:GLU:C	1:Af:43:GLN:H	2.20	0.50
1:Ag:26:ASP:N	1:Ag:26:ASP:C	2.63	0.50
1:As:41:GLU:C	1:As:43:GLN:H	2.20	0.50
1:A3:41:GLU:C	1:A3:43:GLN:H	2.20	0.50
2:Bb:102:CYS:C	6:Mb:80:PRO:N	2.70	0.50
7:Qb:82:ILE:C	7:Qb:84:GLY:H	2.19	0.50
7:Qg:75:SER:C	7:Qg:77:ALA:H	2.19	0.50
7:Qh:75:SER:C	7:Qh:77:ALA:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Ql:260:LEU:C	7:Ql:277:ASP:O	2.55	0.50
1:Aa:41:GLU:C	1:Aa:43:GLN:H	2.20	0.49
1:Ad:41:GLU:C	1:Ad:43:GLN:H	2.20	0.49
2:Bb:128:GLU:C	6:Mb:83:ILE:O	2.55	0.49
7:Ql:82:ILE:C	7:Ql:84:GLY:H	2.19	0.49
1:Ar:41:GLU:C	1:Ar:43:GLN:H	2.20	0.49
1:Ay:41:GLU:C	1:Ay:43:GLN:H	2.20	0.49
1:A2:41:GLU:C	1:A2:43:GLN:H	2.20	0.49
2:Bb:309:ALA:O	2:Bb:312:ARG:N	2.42	0.49
2:Be:102:CYS:C	6:Mh:80:PRO:CA	2.85	0.49
5:Ob:70:ARG:O	5:Ob:73:GLU:N	2.45	0.49
6:Mb:384:GLY:C	6:Mb:386:ALA:H	2.20	0.49
4:Nk:222:ASN:O	4:Nk:223:TYR:O	2.29	0.49
7:Qj:477:TYR:CA	7:Qk:574:ASP:N	2.72	0.49
7:Qk:260:LEU:O	7:Qk:262:ASP:N	2.33	0.49
9:Tk:327:SER:H	9:Tl:344:ASP:H	1.60	0.49
1:Ac:41:GLU:C	1:Ac:43:GLN:H	2.20	0.49
1:Ax:26:ASP:N	1:Ax:26:ASP:C	2.63	0.49
6:Mc:384:GLY:C	6:Mc:386:ALA:N	2.70	0.49
6:Mg:384:GLY:C	6:Mg:386:ALA:N	2.70	0.49
5:Oj:70:ARG:O	5:Oj:73:GLU:N	2.45	0.49
7:Qf:260:LEU:C	7:Qf:277:ASP:O	2.55	0.49
7:Qf:544:GLY:N	7:Qg:488:ASP:CA	2.42	0.49
7:Qg:260:LEU:C	7:Qg:277:ASP:O	2.55	0.49
7:Qi:82:ILE:C	7:Qi:84:GLY:H	2.19	0.49
9:Te:327:SER:H	9:Tf:344:ASP:H	1.60	0.49
1:Aq:26:ASP:N	1:Aq:26:ASP:C	2.63	0.49
1:Ay:26:ASP:N	1:Ay:26:ASP:C	2.63	0.49
5:Od:70:ARG:O	5:Od:73:GLU:N	2.45	0.49
5:Oe:70:ARG:O	5:Oe:73:GLU:N	2.45	0.49
9:Ti:327:SER:H	9:Tj:344:ASP:H	1.60	0.49
1:Ao:41:GLU:C	1:Ao:43:GLN:H	2.20	0.49
1:At:26:ASP:N	1:At:26:ASP:C	2.64	0.49
1:A5:41:GLU:C	1:A5:43:GLN:H	2.20	0.49
5:Oh:70:ARG:O	5:Oh:73:GLU:N	2.45	0.49
6:Mi:384:GLY:C	6:Mi:386:ALA:N	2.70	0.49
5:Oj:123:GLY:CA	8:Pi:42:SER:O	2.61	0.49
5:Ok:70:ARG:O	5:Ok:73:GLU:N	2.45	0.49
8:Pe:13:PRO:N	8:Pe:14:PRO:CA	2.75	0.49
1:Ab:115:GLY:C	1:Af:25:GLN:CA	2.79	0.49
1:Ae:26:ASP:N	1:Ae:26:ASP:C	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:26:ASP:N	1:A4:26:ASP:C	2.63	0.49
2:Ba:309:ALA:O	2:Ba:312:ARG:N	2.42	0.49
2:Bd:149:ILE:C	2:Bd:151:GLY:H	2.20	0.49
7:Qj:260:LEU:C	7:Qj:277:ASP:O	2.55	0.49
1:Ah:41:GLU:C	1:Ah:43:GLN:H	2.20	0.49
1:An:41:GLU:C	1:An:43:GLN:H	2.20	0.49
1:A1:115:GLY:C	1:A5:25:GLN:CA	2.79	0.49
2:Bb:149:ILE:C	2:Bb:151:GLY:H	2.20	0.49
2:Bf:149:ILE:C	2:Bf:151:GLY:H	2.21	0.49
5:Oc:70:ARG:O	5:Oc:73:GLU:N	2.45	0.49
6:Md:42:VAL:N	6:Md:111:ASP:O	2.46	0.49
6:Md:384:GLY:C	6:Md:386:ALA:H	2.21	0.49
5:Oi:70:ARG:O	5:Oi:73:GLU:N	2.45	0.49
6:Mj:384:GLY:C	6:Mj:386:ALA:N	2.70	0.49
9:Tc:327:SER:H	9:Td:344:ASP:H	1.59	0.49
1:Ai:41:GLU:C	1:Ai:43:GLN:H	2.20	0.49
1:Aw:41:GLU:C	1:Aw:43:GLN:H	2.20	0.49
2:Be:149:ILE:C	2:Be:151:GLY:H	2.20	0.49
6:Ma:384:GLY:C	6:Ma:386:ALA:H	2.20	0.49
6:Ma:384:GLY:C	6:Ma:386:ALA:N	2.71	0.49
6:Me:384:GLY:C	6:Me:386:ALA:H	2.20	0.49
5:Of:70:ARG:O	5:Of:73:GLU:N	2.45	0.49
6:Mi:42:VAL:N	6:Mi:111:ASP:O	2.46	0.49
7:Qe:82:ILE:C	7:Qe:84:GLY:H	2.19	0.49
1:Ag:41:GLU:C	1:Ag:43:GLN:H	2.20	0.49
1:A7:41:GLU:C	1:A7:43:GLN:H	2.20	0.49
2:Bc:423:THR:O	2:Bc:424:VAL:C	2.54	0.49
6:Mb:42:VAL:N	6:Mb:111:ASP:O	2.46	0.49
6:Me:42:VAL:N	6:Me:111:ASP:O	2.46	0.49
5:Og:70:ARG:O	5:Og:73:GLU:N	2.46	0.49
6:Mi:384:GLY:C	6:Mi:386:ALA:H	2.20	0.49
6:Mk:384:GLY:C	6:Mk:386:ALA:N	2.70	0.49
9:Ta:298:LYS:CA	9:Tb:350:LEU:O	2.57	0.49
9:Tg:327:SER:H	9:Th:344:ASP:H	1.60	0.49
2:Ba:84:LYS:CA	6:Mi:90:ASN:O	2.61	0.49
2:Bc:128:GLU:C	6:Md:83:ILE:O	2.56	0.49
9:Tb:327:SER:H	9:Tc:344:ASP:H	1.59	0.49
2:Bf:423:THR:O	2:Bf:424:VAL:C	2.55	0.48
4:Nc:98:GLY:C	8:Pc:46:ASN:O	2.56	0.48
6:Mh:384:GLY:C	6:Mh:386:ALA:N	2.70	0.48
8:Pg:24:VAL:O	8:Pg:26:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A8:41:GLU:C	1:A8:43:GLN:H	2.20	0.48
2:Bf:86:LEU:C	6:Mj:80:PRO:O	2.55	0.48
9:Th:327:SER:H	9:Ti:344:ASP:H	1.60	0.48
1:Ab:41:GLU:C	1:Ab:43:GLN:H	2.20	0.48
1:Ak:77:TYR:O	1:Ak:93:LEU:N	2.36	0.48
1:A1:41:GLU:C	1:A1:43:GLN:H	2.20	0.48
1:A5:26:ASP:N	1:A5:26:ASP:C	2.63	0.48
7:Qa:260:LEU:C	7:Qa:262:ASP:N	2.65	0.48
7:Qg:260:LEU:C	7:Qg:262:ASP:N	2.65	0.48
8:Pk:27:LYS:O	8:Pk:29:ALA:N	2.46	0.48
9:Td:298:LYS:C	9:Te:350:LEU:N	2.63	0.48
1:Ae:41:GLU:C	1:Ae:43:GLN:H	2.20	0.48
1:Af:26:ASP:N	1:Af:26:ASP:C	2.64	0.48
1:Ak:41:GLU:C	1:Ak:43:GLN:H	2.20	0.48
1:An:115:GLY:C	1:Ar:25:GLN:CA	2.80	0.48
1:An:138:ASP:C	1:An:140:LYS:H	2.19	0.48
1:Ap:41:GLU:C	1:Ap:43:GLN:H	2.20	0.48
1:As:26:ASP:N	1:As:26:ASP:C	2.63	0.48
1:At:41:GLU:C	1:At:43:GLN:H	2.20	0.48
1:A6:41:GLU:C	1:A6:43:GLN:H	2.20	0.48
4:Nb:91:ALA:CA	8:Pb:43:TYR:N	2.76	0.48
6:Mh:42:VAL:N	6:Mh:111:ASP:O	2.46	0.48
6:Mh:384:GLY:C	6:Mh:386:ALA:H	2.20	0.48
7:Qf:260:LEU:C	7:Qf:262:ASP:N	2.65	0.48
8:Pk:15:PRO:C	8:Pk:17:LYS:N	2.56	0.48
1:Al:41:GLU:C	1:Al:43:GLN:H	2.20	0.48
1:Ap:77:TYR:O	1:Ap:93:LEU:N	2.36	0.48
1:Aq:41:GLU:C	1:Aq:43:GLN:H	2.20	0.48
6:Mk:42:VAL:N	6:Mk:111:ASP:O	2.46	0.48
6:Mi:384:GLY:C	6:Mi:386:ALA:H	2.20	0.48
7:Qd:260:LEU:O	7:Qd:262:ASP:N	2.33	0.48
7:Qi:260:LEU:C	7:Qi:262:ASP:N	2.64	0.48
1:Au:41:GLU:C	1:Au:43:GLN:H	2.20	0.48
2:Ba:149:ILE:C	2:Ba:151:GLY:H	2.21	0.48
6:Mf:384:GLY:C	6:Mf:386:ALA:H	2.20	0.48
7:Qk:544:GLY:N	7:Ql:488:ASP:CA	2.41	0.48
1:Ax:77:TYR:O	1:Ax:93:LEU:N	2.36	0.48
1:A1:26:ASP:N	1:A1:26:ASP:C	2.63	0.48
6:Mf:384:GLY:C	6:Mf:386:ALA:N	2.70	0.48
6:Mi:42:VAL:N	6:Mi:111:ASP:O	2.46	0.48
1:Ab:26:ASP:N	1:Ab:26:ASP:C	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:77:TYR:O	1:Am:93:LEU:N	2.36	0.48
1:Ao:115:GLY:C	1:As:25:GLN:CA	2.80	0.48
1:A4:41:GLU:C	1:A4:43:GLN:H	2.20	0.48
2:Bb:86:LEU:C	6:Mb:80:PRO:O	2.57	0.48
6:Ma:42:VAL:N	6:Ma:111:ASP:O	2.46	0.48
9:Te:298:LYS:CA	9:Tf:350:LEU:O	2.58	0.48
2:Be:309:ALA:O	2:Be:312:ARG:N	2.42	0.48
3:Cb:182:ALA:C	3:Cb:194:ILE:H	2.17	0.48
6:Mc:42:VAL:N	6:Mc:111:ASP:O	2.46	0.48
6:Mj:42:VAL:N	6:Mj:111:ASP:O	2.46	0.48
6:Mk:384:GLY:C	6:Mk:386:ALA:H	2.20	0.48
7:Qe:260:LEU:C	7:Qe:262:ASP:N	2.64	0.48
6:Mf:42:VAL:N	6:Mf:111:ASP:O	2.46	0.47
6:Mg:42:VAL:N	6:Mg:111:ASP:O	2.46	0.47
8:Ph:24:VAL:O	8:Ph:26:VAL:N	2.47	0.47
9:Ta:327:SER:H	9:Tb:344:ASP:H	1.59	0.47
2:Ba:423:THR:O	2:Ba:424:VAL:C	2.54	0.47
4:Nf:165:SER:O	8:Pe:62:GLY:O	2.33	0.47
7:Ql:260:LEU:C	7:Ql:262:ASP:N	2.64	0.47
1:Ax:41:GLU:C	1:Ax:43:GLN:H	2.20	0.47
2:Bb:257:LYS:C	2:Bb:259:GLY:N	2.73	0.47
2:Bd:86:LEU:C	6:Mf:80:PRO:O	2.56	0.47
6:Mg:384:GLY:C	6:Mg:386:ALA:H	2.20	0.47
9:Tc:70:PRO:O	9:Tc:72:GLY:N	2.47	0.47
9:Td:298:LYS:CA	9:Te:350:LEU:O	2.58	0.47
9:Tj:298:LYS:CA	9:Tk:350:LEU:O	2.58	0.47
9:Tk:70:PRO:O	9:Tk:72:GLY:N	2.47	0.47
5:Ok:55:LEU:CA	8:Pk:22:ALA:C	2.86	0.47
8:Pf:24:VAL:O	8:Pf:26:VAL:N	2.48	0.47
9:Te:70:PRO:O	9:Te:72:GLY:N	2.48	0.47
1:An:137:LYS:CA	7:Qj:593:ARG:N	2.78	0.47
1:Aw:77:TYR:O	1:Aw:93:LEU:N	2.36	0.47
9:Ta:70:PRO:O	9:Ta:72:GLY:N	2.48	0.47
1:Ap:115:GLY:C	1:At:25:GLN:CA	2.80	0.47
5:Ok:48:ALA:N	8:Pk:16:ALA:H	2.12	0.47
5:Ok:51:ARG:CA	8:Pk:18:PRO:O	2.60	0.47
4:Nl:110:THR:N	8:Pl:50:LYS:O	2.47	0.47
9:Ta:344:ASP:H	9:Tl:327:SER:H	1.59	0.47
9:Tb:70:PRO:O	9:Tb:72:GLY:N	2.47	0.47
9:Tg:70:PRO:O	9:Tg:72:GLY:N	2.47	0.47
9:Tl:70:PRO:O	9:Tl:72:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Oj:70:ARG:O	5:Oj:71:ARG:C	2.58	0.47
9:Td:70:PRO:O	9:Td:72:GLY:N	2.48	0.47
1:Av:26:ASP:N	1:Av:26:ASP:C	2.63	0.47
2:Bb:423:THR:O	2:Bb:424:VAL:C	2.54	0.47
6:Md:384:GLY:C	6:Md:386:ALA:N	2.70	0.47
5:Oi:51:ARG:O	8:Pi:18:PRO:O	2.32	0.47
5:Oi:189:VAL:O	8:Ph:38:ALA:CA	2.63	0.47
8:Pd:24:VAL:O	8:Pd:26:VAL:N	2.48	0.47
9:Tf:70:PRO:O	9:Tf:72:GLY:N	2.48	0.47
1:At:77:TYR:O	1:At:93:LEU:N	2.36	0.47
2:Bd:103:ASP:N	6:Mf:80:PRO:N	2.62	0.47
1:Am:138:ASP:CA	7:Qb:600:GLU:H	2.28	0.46
1:At:115:GLY:C	1:Ax:25:GLN:CA	2.80	0.46
2:Bf:257:LYS:C	2:Bf:259:GLY:N	2.73	0.46
5:Oh:70:ARG:O	5:Oh:71:ARG:C	2.58	0.46
5:Ok:48:ALA:N	8:Pk:16:ALA:N	2.62	0.46
9:Ta:350:LEU:O	9:Tl:298:LYS:CA	2.58	0.46
1:Am:26:ASP:N	1:Am:26:ASP:C	2.63	0.46
1:An:125:VAL:CA	1:An:136:ALA:H	2.29	0.46
2:Ba:526:GLU:C	2:Ba:528:LYS:H	2.23	0.46
2:Bb:526:GLU:C	2:Bb:528:LYS:H	2.23	0.46
5:Od:70:ARG:O	5:Od:71:ARG:C	2.59	0.46
5:Of:70:ARG:O	5:Of:71:ARG:C	2.58	0.46
7:Qj:260:LEU:O	7:Qj:262:ASP:N	2.33	0.46
9:Th:70:PRO:O	9:Th:72:GLY:N	2.47	0.46
9:Tk:298:LYS:CA	9:Tl:350:LEU:O	2.58	0.46
1:Au:77:TYR:O	1:Au:93:LEU:N	2.37	0.46
5:Ob:70:ARG:O	5:Ob:71:ARG:C	2.59	0.46
4:Nf:223:TYR:C	8:Pf:58:ILE:O	2.57	0.46
9:Tj:70:PRO:O	9:Tj:72:GLY:N	2.48	0.46
8:Ph:12:ALA:C	8:Ph:14:PRO:CA	2.89	0.46
2:Bc:526:GLU:C	2:Bc:528:LYS:H	2.24	0.46
5:Ol:70:ARG:O	5:Ol:71:ARG:C	2.58	0.46
1:Ap:26:ASP:N	1:Ap:26:ASP:C	2.63	0.46
5:Oe:70:ARG:O	5:Oe:71:ARG:C	2.58	0.46
5:Ok:70:ARG:O	5:Ok:71:ARG:C	2.58	0.46
6:Mi:384:GLY:C	6:Mi:386:ALA:N	2.70	0.46
9:Ti:70:PRO:O	9:Ti:72:GLY:N	2.48	0.46
1:Ay:115:GLY:C	1:A3:25:GLN:CA	2.80	0.46
2:Bd:257:LYS:C	2:Bd:259:GLY:N	2.73	0.46
7:Qb:260:LEU:O	7:Qb:262:ASP:N	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:77:TYR:O	1:Aa:93:LEU:N	2.36	0.46
1:Ar:26:ASP:N	1:Ar:26:ASP:C	2.63	0.46
2:Be:103:ASP:N	6:Mh:80:PRO:N	2.63	0.46
5:Og:70:ARG:O	5:Og:71:ARG:C	2.58	0.46
1:An:135:ASP:C	1:An:137:LYS:N	2.73	0.46
6:Mb:384:GLY:C	6:Mb:386:ALA:N	2.70	0.46
4:Nc:113:LYS:C	8:Pc:48:VAL:N	2.73	0.46
5:Oi:70:ARG:O	5:Oi:71:ARG:C	2.59	0.46
6:Mk:381:VAL:C	6:Mk:384:GLY:H	2.24	0.46
8:Pb:27:LYS:C	8:Pb:29:ALA:H	2.22	0.46
8:Pc:24:VAL:O	8:Pc:26:VAL:N	2.48	0.46
9:Tc:298:LYS:CA	9:Td:350:LEU:O	2.58	0.46
9:Ti:298:LYS:CA	9:Tj:350:LEU:O	2.58	0.46
1:Ah:26:ASP:N	1:Ah:26:ASP:C	2.63	0.45
1:Aq:77:TYR:O	1:Aq:93:LEU:N	2.36	0.45
1:A5:115:GLY:C	1:A9:25:GLN:CA	2.79	0.45
6:Me:384:GLY:C	6:Me:386:ALA:N	2.70	0.45
5:Oc:70:ARG:O	5:Oc:71:ARG:C	2.58	0.45
6:Ml:381:VAL:C	6:Ml:384:GLY:H	2.24	0.45
1:A7:26:ASP:N	1:A7:26:ASP:C	2.63	0.45
4:Na:88:VAL:CA	8:Pa:42:SER:CA	2.95	0.45
9:Tf:298:LYS:O	9:Tg:350:LEU:N	2.50	0.45
9:Tg:298:LYS:O	9:Th:350:LEU:N	2.50	0.45
6:Mc:381:VAL:C	6:Mc:384:GLY:H	2.24	0.45
7:Qh:544:GLY:HA2	7:Qi:487:LYS:O	1.80	0.45
1:Ar:77:TYR:O	1:Ar:93:LEU:N	2.36	0.45
8:Pi:24:VAL:O	8:Pi:26:VAL:N	2.50	0.45
7:Qj:260:LEU:C	7:Qj:262:ASP:N	2.64	0.45
5:Oa:70:ARG:O	5:Oa:71:ARG:C	2.58	0.45
9:Tg:298:LYS:CA	9:Th:350:LEU:O	2.58	0.45
8:Ph:13:PRO:N	8:Ph:14:PRO:CA	2.79	0.45
8:Pj:15:PRO:C	8:Pj:17:LYS:H	2.24	0.45
1:Af:115:GLY:C	1:Aj:25:GLN:CA	2.80	0.45
1:Ak:115:GLY:C	1:Ao:25:GLN:CA	2.80	0.45
1:Az:77:TYR:O	1:Az:93:LEU:N	2.37	0.45
2:Ba:86:LEU:C	6:Mi:81:GLU:CA	2.90	0.45
7:Qc:260:LEU:O	7:Qc:262:ASP:N	2.33	0.45
9:Tc:298:LYS:O	9:Td:350:LEU:N	2.50	0.45
1:Ae:67:ALA:C	1:Ae:69:SER:N	2.75	0.45
1:Af:67:ALA:C	1:Af:69:SER:N	2.75	0.45
1:Ah:67:ALA:C	1:Ah:69:SER:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ax:67:ALA:C	1:Ax:69:SER:N	2.75	0.45
1:A5:67:ALA:C	1:A5:69:SER:N	2.75	0.45
2:Bb:437:VAL:O	2:Bb:441:LEU:N	2.35	0.45
2:Bd:83:GLU:C	6:Mf:90:ASN:C	2.85	0.45
2:Be:86:LEU:O	6:Mh:80:PRO:C	2.59	0.45
7:Qd:260:LEU:C	7:Qd:262:ASP:N	2.65	0.45
5:Oa:58:ALA:C	8:Pa:27:LYS:CA	2.90	0.45
9:Te:298:LYS:O	9:Tf:350:LEU:N	2.50	0.45
9:Th:298:LYS:O	9:Ti:350:LEU:N	2.50	0.45
1:Ag:67:ALA:C	1:Ag:69:SER:N	2.75	0.44
1:Ar:67:ALA:C	1:Ar:69:SER:N	2.75	0.44
1:A9:67:ALA:C	1:A9:69:SER:N	2.75	0.44
6:Md:381:VAL:C	6:Md:384:GLY:H	2.25	0.44
6:Mh:381:VAL:C	6:Mh:384:GLY:H	2.24	0.44
6:Mi:381:VAL:C	6:Mi:384:GLY:H	2.25	0.44
9:Ta:350:LEU:N	9:Tl:298:LYS:O	2.50	0.44
1:Aa:3:LEU:N	3:Cb:254:SER:C	2.64	0.44
1:Ac:26:ASP:N	1:Ac:26:ASP:C	2.63	0.44
1:Ae:115:GLY:C	1:Ai:25:GLN:CA	2.80	0.44
1:Ay:67:ALA:C	1:Ay:69:SER:N	2.75	0.44
1:A6:67:ALA:C	1:A6:69:SER:N	2.75	0.44
6:Me:381:VAL:C	6:Me:384:GLY:H	2.25	0.44
6:Ml:88:LEU:C	6:Ml:90:ASN:N	2.73	0.44
7:Qb:260:LEU:C	7:Qb:262:ASP:N	2.64	0.44
9:Td:327:SER:N	9:Te:344:ASP:H	2.15	0.44
9:Th:298:LYS:CA	9:Ti:350:LEU:O	2.58	0.44
1:Aa:67:ALA:C	1:Aa:69:SER:N	2.75	0.44
1:Ao:67:ALA:C	1:Ao:69:SER:N	2.75	0.44
1:A2:77:TYR:O	1:A2:93:LEU:N	2.36	0.44
2:Ba:102:CYS:C	6:Mi:80:PRO:N	2.75	0.44
6:Mb:381:VAL:C	6:Mb:384:GLY:H	2.24	0.44
6:Mg:381:VAL:C	6:Mg:384:GLY:H	2.25	0.44
1:Ac:77:TYR:O	1:Ac:93:LEU:N	2.36	0.44
1:Ai:67:ALA:C	1:Ai:69:SER:N	2.75	0.44
1:Al:115:GLY:C	1:Ap:25:GLN:CA	2.80	0.44
1:Au:67:ALA:C	1:Au:69:SER:N	2.75	0.44
1:Au:115:GLY:C	1:Ay:25:GLN:CA	2.80	0.44
1:A4:67:ALA:C	1:A4:69:SER:N	2.75	0.44
1:A4:115:GLY:C	1:A8:25:GLN:CA	2.80	0.44
4:Nb:95:GLY:HA2	8:Pb:45:TYR:CA	2.47	0.44
7:Qi:260:LEU:O	7:Qi:262:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Tb:298:LYS:O	9:Tc:350:LEU:N	2.50	0.44
1:Ak:67:ALA:C	1:Ak:69:SER:N	2.75	0.44
1:An:67:ALA:C	1:An:69:SER:N	2.75	0.44
6:Mf:381:VAL:C	6:Mf:384:GLY:H	2.25	0.44
1:Ac:67:ALA:C	1:Ac:69:SER:N	2.75	0.44
1:A2:26:ASP:N	1:A2:26:ASP:C	2.64	0.44
1:A2:67:ALA:C	1:A2:69:SER:N	2.75	0.44
9:Tj:327:SER:N	9:Tk:344:ASP:H	2.15	0.44
1:Av:77:TYR:O	1:Av:93:LEU:N	2.37	0.44
1:A8:67:ALA:C	1:A8:69:SER:N	2.75	0.44
2:Bf:102:CYS:C	6:Mj:80:PRO:CA	2.91	0.44
4:Nd:111:PRO:CA	8:Pd:50:LYS:CA	2.96	0.44
9:Tj:298:LYS:O	9:Tk:350:LEU:N	2.50	0.44
1:An:77:TYR:O	1:An:93:LEU:N	2.36	0.44
1:Aq:67:ALA:C	1:Aq:69:SER:N	2.75	0.44
4:Nb:91:ALA:CA	8:Pb:42:SER:C	2.91	0.44
9:Td:298:LYS:O	9:Te:350:LEU:N	2.50	0.44
1:Aa:115:GLY:C	1:Ae:25:GLN:CA	2.80	0.44
1:Ae:77:TYR:O	1:Ae:93:LEU:N	2.36	0.44
1:Al:67:ALA:C	1:Al:69:SER:N	2.76	0.44
1:Av:115:GLY:C	1:Az:25:GLN:CA	2.80	0.44
1:Aw:67:ALA:C	1:Aw:69:SER:N	2.75	0.44
1:A7:67:ALA:C	1:A7:69:SER:N	2.76	0.44
5:Oa:55:LEU:CA	8:Pa:25:PRO:N	2.81	0.44
9:Tc:327:SER:N	9:Td:344:ASP:H	2.16	0.44
1:Aj:67:ALA:C	1:Aj:69:SER:N	2.75	0.43
4:Nb:91:ALA:CA	8:Pb:43:TYR:H	2.31	0.43
9:Ta:327:SER:N	9:Tb:344:ASP:H	2.16	0.43
9:Ta:344:ASP:H	9:Tl:327:SER:N	2.16	0.43
9:Tg:327:SER:N	9:Th:344:ASP:H	2.16	0.43
9:Ti:298:LYS:O	9:Tj:350:LEU:N	2.50	0.43
1:Az:67:ALA:C	1:Az:69:SER:N	2.76	0.43
1:Az:115:GLY:C	1:A4:25:GLN:CA	2.80	0.43
2:Be:397:THR:O	2:Be:398:ALA:C	2.61	0.43
2:Bf:397:THR:O	2:Bf:398:ALA:C	2.61	0.43
8:Pa:17:LYS:C	8:Pa:19:LYS:N	2.76	0.43
9:Ta:298:LYS:O	9:Tb:350:LEU:N	2.51	0.43
9:Tb:327:SER:N	9:Tc:344:ASP:H	2.16	0.43
4:Ni:134:SER:C	4:Ni:136:ASP:H	2.27	0.43
9:Te:327:SER:N	9:Tf:344:ASP:H	2.16	0.43
9:Tk:298:LYS:O	9:Tl:350:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:67:ALA:C	1:Am:69:SER:N	2.75	0.43
1:Aq:66:VAL:O	1:Aq:68:SER:N	2.52	0.43
1:Av:67:ALA:C	1:Av:69:SER:N	2.76	0.43
1:Ax:66:VAL:O	1:Ax:68:SER:N	2.52	0.43
8:Pb:27:LYS:C	8:Pb:29:ALA:N	2.76	0.43
9:Tf:327:SER:N	9:Tg:344:ASP:H	2.16	0.43
9:Tk:327:SER:N	9:Tl:344:ASP:H	2.16	0.43
4:Nc:98:GLY:O	8:Pc:46:ASN:O	2.35	0.43
6:Me:44:GLY:HA2	6:Me:53:LYS:O	2.19	0.43
6:Mj:381:VAL:C	6:Mj:384:GLY:H	2.25	0.43
1:A3:67:ALA:C	1:A3:69:SER:N	2.75	0.43
2:Ba:274:LEU:C	2:Ba:276:GLY:H	2.27	0.43
2:Bb:257:LYS:O	2:Bb:259:GLY:N	2.46	0.43
2:Be:526:GLU:C	2:Be:528:LYS:H	2.27	0.43
9:Tf:298:LYS:CA	9:Tg:350:LEU:O	2.58	0.43
9:Ti:327:SER:N	9:Tj:344:ASP:H	2.16	0.43
1:Ah:66:VAL:O	1:Ah:68:SER:N	2.52	0.43
1:Al:66:VAL:O	1:Al:68:SER:N	2.52	0.43
1:Aw:66:VAL:O	1:Aw:68:SER:N	2.52	0.43
1:A4:77:TYR:O	1:A4:93:LEU:N	2.37	0.43
1:A6:66:VAL:O	1:A6:68:SER:N	2.51	0.43
2:Bd:83:GLU:O	6:Mf:90:ASN:CA	2.63	0.43
2:Bf:526:GLU:C	2:Bf:528:LYS:H	2.27	0.43
4:Nb:111:PRO:N	8:Pb:51:ARG:CA	2.82	0.43
6:Mh:44:GLY:HA2	6:Mh:53:LYS:O	2.19	0.43
7:Qa:488:ASP:CA	7:Ql:544:GLY:N	2.41	0.43
2:Bf:368:ILE:C	3:Cb:301:LEU:H	2.27	0.43
6:Ma:44:GLY:HA2	6:Ma:53:LYS:O	2.19	0.43
6:Mc:44:GLY:HA2	6:Mc:53:LYS:O	2.19	0.43
4:Ne:134:SER:C	4:Ne:136:ASP:H	2.27	0.43
6:Mf:44:GLY:HA2	6:Mf:53:LYS:O	2.19	0.43
8:Pa:17:LYS:C	8:Pa:19:LYS:H	2.26	0.43
1:Ah:77:TYR:O	1:Ah:93:LEU:N	2.36	0.43
1:Am:66:VAL:O	1:Am:68:SER:N	2.52	0.43
1:Aq:115:GLY:C	1:Au:25:GLN:CA	2.80	0.43
1:As:67:ALA:C	1:As:69:SER:N	2.76	0.43
1:A1:67:ALA:C	1:A1:69:SER:N	2.75	0.43
1:A9:77:TYR:O	1:A9:93:LEU:N	2.36	0.43
2:Bf:309:ALA:O	2:Bf:310:ILE:C	2.61	0.43
9:Tb:298:LYS:CA	9:Tc:350:LEU:O	2.58	0.43
1:Ab:67:ALA:C	1:Ab:69:SER:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Mg:44:GLY:HA2	6:Mg:53:LYS:O	2.19	0.43
4:Nj:134:SER:C	4:Nj:136:ASP:H	2.27	0.43
8:Pc:53:PRO:CA	8:Pc:56:SER:N	2.76	0.43
1:Ap:66:VAL:O	1:Ap:68:SER:N	2.52	0.42
1:Av:66:VAL:O	1:Av:68:SER:N	2.52	0.42
1:A5:66:VAL:O	1:A5:68:SER:N	2.52	0.42
2:Bd:526:GLU:C	2:Bd:528:LYS:H	2.27	0.42
6:Ma:381:VAL:C	6:Ma:384:GLY:H	2.26	0.42
5:Ob:51:ARG:O	8:Pb:21:ALA:O	2.36	0.42
6:Mi:44:GLY:HA2	6:Mi:53:LYS:O	2.19	0.42
6:Ml:80:PRO:C	6:Ml:82:ALA:H	2.26	0.42
1:Ad:67:ALA:C	1:Ad:69:SER:N	2.76	0.42
1:Af:66:VAL:O	1:Af:68:SER:N	2.52	0.42
1:Ao:66:VAL:O	1:Ao:68:SER:N	2.52	0.42
1:As:115:GLY:C	1:Aw:25:GLN:CA	2.80	0.42
1:At:66:VAL:O	1:At:68:SER:N	2.52	0.42
1:Aw:115:GLY:C	1:A1:25:GLN:CA	2.80	0.42
2:Bb:309:ALA:O	2:Bb:310:ILE:C	2.61	0.42
4:Nd:98:GLY:C	4:Nd:100:VAL:H	2.27	0.42
4:Nd:134:SER:C	4:Nd:136:ASP:H	2.27	0.42
4:Nf:134:SER:C	4:Nf:136:ASP:H	2.27	0.42
1:Ah:67:ALA:O	1:Ah:69:SER:N	2.52	0.42
1:Aj:115:GLY:C	1:An:25:GLN:CA	2.80	0.42
1:A3:66:VAL:O	1:A3:68:SER:N	2.52	0.42
1:A9:67:ALA:O	1:A9:69:SER:N	2.52	0.42
2:Bc:397:THR:O	2:Bc:398:ALA:C	2.62	0.42
2:Be:309:ALA:O	2:Be:310:ILE:C	2.63	0.42
4:Ne:111:PRO:O	8:Pe:50:LYS:N	2.36	0.42
6:Ml:44:GLY:HA2	6:Ml:53:LYS:O	2.19	0.42
1:Ai:66:VAL:O	1:Ai:68:SER:N	2.52	0.42
1:Al:77:TYR:O	1:Al:93:LEU:N	2.36	0.42
1:Ar:66:VAL:O	1:Ar:68:SER:N	2.52	0.42
1:A7:66:VAL:O	1:A7:68:SER:N	2.53	0.42
2:Ba:291:LEU:C	2:Ba:293:MET:N	2.78	0.42
4:Na:134:SER:C	4:Na:136:ASP:H	2.27	0.42
4:Nf:98:GLY:C	4:Nf:100:VAL:H	2.28	0.42
6:Mj:44:GLY:HA2	6:Mj:53:LYS:O	2.19	0.42
7:Qb:407:SER:O	7:Qb:408:VAL:O	2.33	0.42
7:Qj:544:GLY:N	7:Qk:488:ASP:CA	2.42	0.42
1:Ad:66:VAL:O	1:Ad:68:SER:N	2.52	0.42
1:Ag:66:VAL:O	1:Ag:68:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:66:VAL:O	1:Aj:68:SER:N	2.52	0.42
1:As:66:VAL:O	1:As:68:SER:N	2.52	0.42
1:A1:66:VAL:O	1:A1:68:SER:N	2.52	0.42
1:A5:67:ALA:O	1:A5:69:SER:N	2.53	0.42
1:A8:66:VAL:O	1:A8:68:SER:N	2.52	0.42
1:A9:66:VAL:O	1:A9:68:SER:N	2.52	0.42
2:Bd:291:LEU:C	2:Bd:293:MET:N	2.78	0.42
2:Be:423:THR:O	2:Be:426:ARG:N	2.53	0.42
4:Nj:98:GLY:C	4:Nj:100:VAL:H	2.28	0.42
6:Mk:44:GLY:HA2	6:Mk:53:LYS:O	2.19	0.42
9:Th:327:SER:N	9:Ti:344:ASP:H	2.17	0.42
1:Ak:66:VAL:O	1:Ak:68:SER:N	2.52	0.42
1:An:66:VAL:O	1:An:68:SER:N	2.53	0.42
1:Ap:67:ALA:O	1:Ap:69:SER:N	2.53	0.42
1:Av:67:ALA:O	1:Av:69:SER:N	2.53	0.42
1:A9:67:ALA:C	1:A9:69:SER:H	2.28	0.42
2:Bc:309:ALA:O	2:Bc:310:ILE:C	2.62	0.42
4:Na:98:GLY:C	4:Na:100:VAL:H	2.28	0.42
4:Nh:134:SER:C	4:Nh:136:ASP:H	2.27	0.42
4:Nl:134:SER:C	4:Nl:136:ASP:H	2.26	0.42
8:Pe:27:LYS:O	8:Pe:29:ALA:N	2.49	0.42
8:Pl:16:ALA:C	8:Pl:18:PRO:N	2.77	0.42
1:Ac:66:VAL:O	1:Ac:68:SER:N	2.52	0.42
1:Au:66:VAL:O	1:Au:68:SER:N	2.53	0.42
1:Ay:66:VAL:O	1:Ay:68:SER:N	2.52	0.42
2:Bb:423:THR:O	2:Bb:426:ARG:N	2.53	0.42
2:Be:274:LEU:C	2:Be:276:GLY:H	2.27	0.42
2:Bf:423:THR:O	2:Bf:426:ARG:N	2.53	0.42
4:Nb:134:SER:C	4:Nb:136:ASP:H	2.27	0.42
4:Nc:91:ALA:CA	8:Pc:43:TYR:H	2.32	0.42
6:Mj:371:PHE:O	6:Mj:372:VAL:C	2.63	0.42
4:Nk:98:GLY:C	4:Nk:100:VAL:H	2.28	0.42
1:Ah:67:ALA:C	1:Ah:69:SER:H	2.28	0.42
1:At:67:ALA:O	1:At:69:SER:N	2.53	0.42
1:Ax:115:GLY:C	1:A2:25:GLN:CA	2.79	0.42
2:Ba:246:ARG:CA	3:Ca:296:SER:C	2.84	0.42
2:Bb:397:THR:O	2:Bb:398:ALA:C	2.62	0.42
2:Bd:397:THR:O	2:Bd:398:ALA:C	2.62	0.42
4:Ng:134:SER:C	4:Ng:136:ASP:H	2.27	0.42
5:Oj:48:ALA:O	8:Pj:18:PRO:CA	2.67	0.42
1:Ab:66:VAL:O	1:Ab:68:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:66:VAL:O	1:Ae:68:SER:N	2.52	0.42
1:Am:67:ALA:O	1:Am:69:SER:N	2.53	0.42
1:Aw:67:ALA:O	1:Aw:69:SER:N	2.53	0.42
1:A7:77:TYR:O	1:A7:93:LEU:N	2.37	0.42
2:Ba:423:THR:O	2:Ba:426:ARG:N	2.53	0.42
4:Na:84:LYS:CA	8:Pa:40:SER:N	2.83	0.42
4:Na:109:ALA:C	8:Pa:51:ARG:CA	2.93	0.42
4:Nc:134:SER:C	4:Nc:136:ASP:H	2.27	0.42
6:Md:44:GLY:HA2	6:Md:53:LYS:O	2.19	0.42
4:Nl:98:GLY:C	4:Nl:100:VAL:H	2.28	0.42
8:Pe:13:PRO:C	8:Pe:15:PRO:CA	2.93	0.42
1:Ad:77:TYR:O	1:Ad:93:LEU:N	2.36	0.42
1:Aj:77:TYR:O	1:Aj:93:LEU:N	2.37	0.42
1:An:138:ASP:C	1:An:140:LYS:N	2.77	0.42
1:Au:67:ALA:O	1:Au:69:SER:N	2.53	0.42
1:A3:77:TYR:O	1:A3:93:LEU:N	2.36	0.42
1:A4:66:VAL:O	1:A4:68:SER:N	2.52	0.42
2:Bc:274:LEU:C	2:Bc:276:GLY:H	2.27	0.42
4:Nb:98:GLY:C	4:Nb:100:VAL:H	2.28	0.42
1:Aa:66:VAL:O	1:Aa:68:SER:N	2.52	0.41
1:Af:67:ALA:O	1:Af:69:SER:N	2.53	0.41
1:At:67:ALA:C	1:At:69:SER:N	2.75	0.41
2:Bc:291:LEU:C	2:Bc:293:MET:N	2.78	0.41
2:Bd:309:ALA:O	2:Bd:310:ILE:C	2.62	0.41
2:Bd:423:THR:O	2:Bd:426:ARG:N	2.53	0.41
4:Nc:99:PRO:N	8:Pc:46:ASN:C	2.73	0.41
4:Ne:98:GLY:C	4:Ne:100:VAL:H	2.27	0.41
4:Nk:134:SER:C	4:Nk:136:ASP:H	2.28	0.41
7:Qc:260:LEU:C	7:Qc:262:ASP:N	2.64	0.41
1:A7:67:ALA:O	1:A7:69:SER:N	2.53	0.41
2:Ba:397:THR:O	2:Ba:398:ALA:C	2.62	0.41
1:Ae:67:ALA:C	1:Ae:69:SER:H	2.28	0.41
1:Ag:67:ALA:C	1:Ag:69:SER:H	2.28	0.41
1:Aj:67:ALA:O	1:Aj:69:SER:N	2.53	0.41
1:Al:67:ALA:O	1:Al:69:SER:N	2.53	0.41
1:An:67:ALA:O	1:An:69:SER:N	2.53	0.41
1:Ao:67:ALA:O	1:Ao:69:SER:N	2.53	0.41
1:Ar:67:ALA:C	1:Ar:69:SER:H	2.29	0.41
1:At:67:ALA:C	1:At:69:SER:H	2.28	0.41
2:Bd:379:PHE:C	2:Bd:381:ARG:N	2.76	0.41
6:Mb:371:PHE:O	6:Mb:372:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Me:319:ALA:O	6:Me:320:ALA:C	2.64	0.41
6:Mf:371:PHE:O	6:Mf:372:VAL:C	2.64	0.41
6:Mh:371:PHE:O	6:Mh:372:VAL:C	2.63	0.41
8:Pb:9:PRO:C	8:Pb:10:ALA:O	2.63	0.41
1:Ac:67:ALA:O	1:Ac:69:SER:N	2.53	0.41
1:Ai:67:ALA:O	1:Ai:69:SER:N	2.53	0.41
1:Ar:67:ALA:O	1:Ar:69:SER:N	2.53	0.41
1:As:67:ALA:O	1:As:69:SER:N	2.53	0.41
1:Ax:67:ALA:C	1:Ax:69:SER:H	2.28	0.41
1:Ax:67:ALA:O	1:Ax:69:SER:N	2.53	0.41
1:A2:67:ALA:O	1:A2:69:SER:N	2.53	0.41
1:A5:67:ALA:C	1:A5:69:SER:H	2.28	0.41
1:A6:67:ALA:O	1:A6:69:SER:N	2.53	0.41
1:A8:67:ALA:O	1:A8:69:SER:N	2.53	0.41
2:Bd:257:LYS:O	2:Bd:259:GLY:N	2.47	0.41
4:Ng:98:GLY:C	4:Ng:100:VAL:H	2.28	0.41
4:Nh:98:GLY:C	4:Nh:100:VAL:H	2.28	0.41
1:Af:67:ALA:C	1:Af:69:SER:H	2.28	0.41
1:Af:77:TYR:O	1:Af:93:LEU:N	2.36	0.41
1:Ag:67:ALA:O	1:Ag:69:SER:N	2.53	0.41
1:Ap:67:ALA:C	1:Ap:69:SER:H	2.28	0.41
2:Bc:86:LEU:C	6:Md:80:PRO:O	2.63	0.41
3:Cb:239:HIS:O	3:Cb:240:VAL:C	2.63	0.41
6:Me:371:PHE:O	6:Me:372:VAL:C	2.63	0.41
6:Mi:371:PHE:O	6:Mi:372:VAL:C	2.63	0.41
7:Qj:544:GLY:HA3	7:Qk:488:ASP:CA	2.48	0.41
1:Ab:67:ALA:O	1:Ab:69:SER:N	2.53	0.41
1:Ak:67:ALA:O	1:Ak:69:SER:N	2.53	0.41
1:Al:26:ASP:N	1:Al:26:ASP:C	2.64	0.41
1:Ap:67:ALA:C	1:Ap:69:SER:N	2.75	0.41
1:Aq:67:ALA:O	1:Aq:69:SER:N	2.54	0.41
1:Ay:67:ALA:C	1:Ay:69:SER:H	2.28	0.41
1:Ay:67:ALA:O	1:Ay:69:SER:N	2.53	0.41
1:A1:67:ALA:O	1:A1:69:SER:N	2.53	0.41
1:A2:66:VAL:O	1:A2:68:SER:N	2.53	0.41
5:Oa:54:ASP:C	8:Pa:22:ALA:C	2.87	0.41
4:Ni:98:GLY:C	4:Ni:100:VAL:H	2.28	0.41
4:Nj:160:ASP:O	4:Nj:164:ASP:N	2.52	0.41
1:Az:66:VAL:O	1:Az:68:SER:N	2.53	0.41
1:A4:67:ALA:O	1:A4:69:SER:N	2.53	0.41
2:Ba:309:ALA:O	2:Ba:310:ILE:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bb:291:LEU:C	2:Bb:293:MET:N	2.77	0.41
4:Nd:111:PRO:O	8:Pd:50:LYS:CA	2.67	0.41
4:Ne:82:VAL:O	4:Ne:83:GLU:C	2.64	0.41
4:Nf:82:VAL:O	4:Nf:83:GLU:C	2.64	0.41
6:Mg:319:ALA:O	6:Mg:320:ALA:C	2.64	0.41
6:Mi:319:ALA:O	6:Mi:320:ALA:C	2.63	0.41
8:Pb:24:VAL:O	8:Pb:26:VAL:N	2.54	0.41
1:Ac:67:ALA:C	1:Ac:69:SER:H	2.29	0.41
1:Ae:67:ALA:O	1:Ae:69:SER:N	2.53	0.41
1:Ah:115:GLY:C	1:Al:25:GLN:CA	2.80	0.41
1:Aj:67:ALA:C	1:Aj:69:SER:H	2.29	0.41
1:Ak:67:ALA:C	1:Ak:69:SER:H	2.29	0.41
2:Bc:423:THR:O	2:Bc:426:ARG:N	2.53	0.41
6:Mb:44:GLY:HA2	6:Mb:53:LYS:O	2.19	0.41
6:Mj:319:ALA:O	6:Mj:320:ALA:C	2.64	0.41
1:Aa:67:ALA:O	1:Aa:69:SER:N	2.53	0.41
1:Ag:115:GLY:C	1:Ak:25:GLN:CA	2.80	0.41
1:Ai:67:ALA:C	1:Ai:69:SER:H	2.29	0.41
1:Al:41:GLU:C	1:Al:43:GLN:N	2.79	0.41
1:Am:67:ALA:C	1:Am:69:SER:H	2.28	0.41
1:Aq:41:GLU:C	1:Aq:43:GLN:N	2.79	0.41
1:Au:67:ALA:C	1:Au:69:SER:H	2.28	0.41
1:A1:77:TYR:O	1:A1:93:LEU:N	2.36	0.41
1:A7:67:ALA:C	1:A7:69:SER:H	2.29	0.41
1:A8:67:ALA:C	1:A8:69:SER:H	2.28	0.41
2:Bb:274:LEU:C	2:Bb:276:GLY:H	2.29	0.41
6:Ma:371:PHE:O	6:Ma:372:VAL:C	2.64	0.41
6:Mb:319:ALA:O	6:Mb:320:ALA:C	2.64	0.41
4:Nc:98:GLY:C	4:Nc:100:VAL:H	2.28	0.41
4:Ng:82:VAL:O	4:Ng:83:GLU:C	2.64	0.41
7:Qd:407:SER:O	7:Qd:408:VAL:O	2.33	0.41
1:Aq:67:ALA:C	1:Aq:69:SER:H	2.29	0.41
1:A4:67:ALA:C	1:A4:69:SER:H	2.29	0.41
2:Bf:359:ILE:O	2:Bf:361:GLN:N	2.54	0.41
6:Md:319:ALA:O	6:Md:320:ALA:C	2.64	0.41
6:Me:356:PRO:O	6:Me:358:ARG:N	2.54	0.41
6:Mj:356:PRO:O	6:Mj:358:ARG:N	2.54	0.41
4:Nl:82:VAL:O	4:Nl:83:GLU:C	2.64	0.41
1:Ab:77:TYR:O	1:Ab:93:LEU:N	2.37	0.40
1:Ad:67:ALA:O	1:Ad:69:SER:N	2.53	0.40
1:Ai:41:GLU:C	1:Ai:43:GLN:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:67:ALA:C	1:Al:69:SER:H	2.29	0.40
1:Ao:67:ALA:C	1:Ao:69:SER:H	2.28	0.40
1:Ax:41:GLU:C	1:Ax:43:GLN:N	2.80	0.40
1:A3:67:ALA:O	1:A3:69:SER:N	2.53	0.40
4:Nd:82:VAL:O	4:Nd:83:GLU:C	2.64	0.40
4:Ni:82:VAL:O	4:Ni:83:GLU:C	2.63	0.40
1:Aa:135:ASP:C	1:Aa:137:LYS:H	2.29	0.40
1:Ad:67:ALA:C	1:Ad:69:SER:H	2.29	0.40
1:Ag:41:GLU:C	1:Ag:43:GLN:N	2.79	0.40
1:A3:67:ALA:C	1:A3:69:SER:H	2.29	0.40
1:A6:67:ALA:C	1:A6:69:SER:H	2.29	0.40
2:Ba:225:MET:C	3:Ca:125:GLU:O	2.64	0.40
4:Nj:82:VAL:O	4:Nj:83:GLU:C	2.64	0.40
6:Ml:371:PHE:O	6:Ml:372:VAL:C	2.63	0.40
1:Ab:41:GLU:C	1:Ab:43:GLN:N	2.79	0.40
1:Au:41:GLU:C	1:Au:43:GLN:N	2.80	0.40
1:A5:77:TYR:O	1:A5:93:LEU:N	2.37	0.40
1:A8:41:GLU:C	1:A8:43:GLN:N	2.80	0.40
2:Bc:227:LEU:O	2:Bc:228:ARG:C	2.65	0.40
2:Be:291:LEU:C	2:Be:293:MET:N	2.78	0.40
4:Na:84:LYS:CA	8:Pa:40:SER:CA	3.00	0.40
6:Mg:356:PRO:O	6:Mg:358:ARG:N	2.55	0.40
6:Mh:356:PRO:O	6:Mh:358:ARG:N	2.55	0.40
6:Mi:356:PRO:O	6:Mi:358:ARG:N	2.54	0.40
4:Nk:82:VAL:O	4:Nk:83:GLU:C	2.64	0.40
4:Nk:222:ASN:C	4:Nk:223:TYR:O	2.64	0.40
6:Mk:319:ALA:O	6:Mk:320:ALA:C	2.63	0.40
6:Ml:319:ALA:O	6:Ml:320:ALA:C	2.64	0.40
8:Pa:24:VAL:C	8:Pa:26:VAL:N	2.79	0.40
1:Ae:41:GLU:C	1:Ae:43:GLN:N	2.80	0.40
1:Ah:92:MET:O	1:Ah:93:LEU:O	2.40	0.40
1:As:41:GLU:C	1:As:43:GLN:N	2.79	0.40
1:Av:41:GLU:C	1:Av:43:GLN:N	2.80	0.40
1:A1:41:GLU:C	1:A1:43:GLN:N	2.79	0.40
1:A4:92:MET:O	1:A4:93:LEU:O	2.40	0.40
1:A7:92:MET:O	1:A7:93:LEU:O	2.40	0.40
2:Bb:359:ILE:O	2:Bb:361:GLN:N	2.54	0.40
3:Ca:239:HIS:O	3:Ca:240:VAL:C	2.63	0.40
4:Na:82:VAL:O	4:Na:83:GLU:C	2.64	0.40
6:Mb:356:PRO:O	6:Mb:358:ARG:N	2.54	0.40
7:Qe:407:SER:O	7:Qe:408:VAL:O	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Qg:407:SER:O	7:Qg:408:VAL:O	2.33	0.40
1:Ae:92:MET:O	1:Ae:93:LEU:O	2.40	0.40
1:Ah:41:GLU:C	1:Ah:43:GLN:N	2.79	0.40
1:Ak:41:GLU:C	1:Ak:43:GLN:N	2.80	0.40
1:Ao:92:MET:O	1:Ao:93:LEU:O	2.40	0.40
1:Ao:135:ASP:C	1:Ao:137:LYS:H	2.30	0.40
1:At:135:ASP:C	1:At:137:LYS:H	2.30	0.40
1:Au:135:ASP:C	1:Au:137:LYS:H	2.30	0.40
1:Av:135:ASP:C	1:Av:137:LYS:H	2.30	0.40
1:Az:92:MET:O	1:Az:93:LEU:O	2.40	0.40
1:A1:67:ALA:C	1:A1:69:SER:H	2.29	0.40
1:A1:135:ASP:C	1:A1:137:LYS:H	2.30	0.40
1:A4:41:GLU:C	1:A4:43:GLN:N	2.80	0.40
2:Bb:84:LYS:CA	6:Mb:90:ASN:O	2.70	0.40
2:Bd:274:LEU:C	2:Bd:276:GLY:H	2.30	0.40
6:Md:356:PRO:O	6:Md:358:ARG:N	2.55	0.40
6:Mf:319:ALA:O	6:Mf:320:ALA:C	2.63	0.40
6:Mk:371:PHE:O	6:Mk:372:VAL:C	2.64	0.40
7:Qi:407:SER:O	7:Qi:408:VAL:O	2.33	0.40
8:Pk:24:VAL:C	8:Pk:26:VAL:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A2	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A3	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A4	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A5	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A6	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A7	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A8	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	A9	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Aa	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ab	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ac	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ad	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ae	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Af	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ag	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ah	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ai	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Aj	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ak	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Al	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Am	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	An	156/158 (99%)	135 (86%)	11 (7%)	10 (6%)	1	1
1	Ao	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ap	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Aq	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ar	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	As	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	At	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Au	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Av	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Aw	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ax	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Ay	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1
1	Az	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ba	442/566 (78%)	362 (82%)	55 (12%)	25 (6%)	1	1
2	Bb	442/566 (78%)	365 (83%)	49 (11%)	28 (6%)	1	1
2	Bc	442/566 (78%)	363 (82%)	54 (12%)	25 (6%)	1	1
2	Bd	442/566 (78%)	363 (82%)	51 (12%)	28 (6%)	1	1
2	Be	442/566 (78%)	362 (82%)	55 (12%)	25 (6%)	1	1
2	Bf	442/566 (78%)	362 (82%)	52 (12%)	28 (6%)	1	1
3	Ca	308/417 (74%)	292 (95%)	9 (3%)	7 (2%)	5	5
3	Cb	308/417 (74%)	292 (95%)	10 (3%)	6 (2%)	6	6
4	Na	221/225 (98%)	180 (81%)	27 (12%)	14 (6%)	1	1
4	Nb	221/225 (98%)	181 (82%)	25 (11%)	15 (7%)	1	1
4	Nc	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
4	Nd	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
4	Ne	221/225 (98%)	181 (82%)	25 (11%)	15 (7%)	1	1
4	Nf	221/225 (98%)	181 (82%)	25 (11%)	15 (7%)	1	1
4	Ng	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
4	Nh	221/225 (98%)	182 (82%)	25 (11%)	14 (6%)	1	1
4	Ni	221/225 (98%)	182 (82%)	24 (11%)	15 (7%)	1	1
4	Nj	221/225 (98%)	183 (83%)	24 (11%)	14 (6%)	1	1
4	Nk	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
4	Nl	221/225 (98%)	181 (82%)	26 (12%)	14 (6%)	1	1
5	Oa	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Ob	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oc	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Od	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oe	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Of	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Og	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oh	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oi	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Oj	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7
5	Ok	187/205 (91%)	169 (90%)	15 (8%)	3 (2%)	7	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ol	187/205 (91%)	170 (91%)	14 (8%)	3 (2%)	7	7
6	Ma	353/395 (89%)	320 (91%)	27 (8%)	6 (2%)	7	7
6	Mb	353/395 (89%)	320 (91%)	26 (7%)	7 (2%)	6	6
6	Mc	353/395 (89%)	321 (91%)	26 (7%)	6 (2%)	7	7
6	Md	353/395 (89%)	320 (91%)	24 (7%)	9 (2%)	4	4
6	Me	353/395 (89%)	321 (91%)	26 (7%)	6 (2%)	7	7
6	Mf	353/395 (89%)	318 (90%)	28 (8%)	7 (2%)	6	6
6	Mg	353/395 (89%)	320 (91%)	27 (8%)	6 (2%)	7	7
6	Mh	353/395 (89%)	317 (90%)	29 (8%)	7 (2%)	6	6
6	Mi	353/395 (89%)	321 (91%)	26 (7%)	6 (2%)	7	7
6	Mj	353/395 (89%)	319 (90%)	26 (7%)	8 (2%)	5	5
6	Mk	353/395 (89%)	319 (90%)	28 (8%)	6 (2%)	7	7
6	Ml	353/395 (89%)	319 (90%)	28 (8%)	6 (2%)	7	7
7	Qa	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qb	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qc	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qd	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qe	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qf	408/901 (45%)	359 (88%)	36 (9%)	13 (3%)	3	3
7	Qg	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qh	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qi	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qj	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Qk	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
7	Ql	408/901 (45%)	360 (88%)	35 (9%)	13 (3%)	3	3
8	Pa	153/172 (89%)	110 (72%)	21 (14%)	22 (14%)	0	0
8	Pb	153/172 (89%)	106 (69%)	22 (14%)	25 (16%)	0	0
8	Pc	153/172 (89%)	108 (71%)	24 (16%)	21 (14%)	0	0
8	Pd	153/172 (89%)	109 (71%)	22 (14%)	22 (14%)	0	0
8	Pe	153/172 (89%)	111 (72%)	23 (15%)	19 (12%)	0	0
8	Pf	153/172 (89%)	115 (75%)	20 (13%)	18 (12%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Pg	153/172 (89%)	112 (73%)	25 (16%)	16 (10%)	0	0
8	Ph	153/172 (89%)	110 (72%)	21 (14%)	22 (14%)	0	0
8	Pi	153/172 (89%)	116 (76%)	19 (12%)	18 (12%)	0	0
8	Pj	153/172 (89%)	116 (76%)	20 (13%)	17 (11%)	0	0
8	Pk	153/172 (89%)	115 (75%)	20 (13%)	18 (12%)	0	0
8	Pl	153/172 (89%)	115 (75%)	16 (10%)	22 (14%)	0	0
9	Ta	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Tb	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Tc	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Td	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Te	159/411 (39%)	114 (72%)	34 (21%)	11 (7%)	1	1
9	Tf	159/411 (39%)	114 (72%)	34 (21%)	11 (7%)	1	1
9	Tg	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Th	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Ti	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Tj	159/411 (39%)	114 (72%)	33 (21%)	12 (8%)	1	1
9	Tk	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
9	Tl	159/411 (39%)	114 (72%)	32 (20%)	13 (8%)	0	0
All	All	26500/37468 (71%)	22659 (86%)	2521 (10%)	1320 (5%)	3	1

All (1320) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Aa	93	LEU
1	Aa	98	ASN
1	Ab	93	LEU
1	Ab	98	ASN
1	Ac	93	LEU
1	Ac	98	ASN
1	Ad	93	LEU
1	Ad	98	ASN
1	Ae	93	LEU
1	Ae	98	ASN
1	Af	93	LEU
1	Af	98	ASN
1	Ag	93	LEU

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Mol	Chain	Res	Type
1	Ag	98	ASN
1	Ah	93	LEU
1	Ah	98	ASN
1	Ai	93	LEU
1	Ai	98	ASN
1	Aj	93	LEU
1	Aj	98	ASN
1	Ak	93	LEU
1	Ak	98	ASN
1	Al	93	LEU
1	Al	98	ASN
1	Am	93	LEU
1	Am	98	ASN
1	An	93	LEU
1	An	98	ASN
1	Ao	93	LEU
1	Ao	98	ASN
1	Ap	93	LEU
1	Ap	98	ASN
1	Aq	93	LEU
1	Aq	98	ASN
1	Ar	93	LEU
1	Ar	98	ASN
1	As	93	LEU
1	As	98	ASN
1	At	93	LEU
1	At	98	ASN
1	Au	93	LEU
1	Au	98	ASN
1	Av	93	LEU
1	Av	98	ASN
1	Aw	93	LEU
1	Aw	98	ASN
1	Ax	93	LEU
1	Ax	98	ASN
1	Ay	93	LEU
1	Ay	98	ASN
1	Az	93	LEU
1	Az	98	ASN
1	A1	93	LEU
1	A1	98	ASN
1	A2	93	LEU

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Mol	Chain	Res	Type
1	A2	98	ASN
1	A3	93	LEU
1	A3	98	ASN
1	A4	93	LEU
1	A4	98	ASN
1	A5	93	LEU
1	A5	98	ASN
1	A6	93	LEU
1	A6	98	ASN
1	A7	93	LEU
1	A7	98	ASN
1	A8	93	LEU
1	A8	98	ASN
1	A9	93	LEU
1	A9	98	ASN
2	Ba	77	VAL
2	Ba	95	PRO
2	Ba	202	PRO
2	Ba	223	PRO
2	Ba	379	PHE
2	Ba	494	ASN
2	Ba	501	ARG
2	Ba	529	GLN
2	Bb	77	VAL
2	Bb	95	PRO
2	Bb	178	PRO
2	Bb	202	PRO
2	Bb	223	PRO
2	Bb	379	PHE
2	Bb	494	ASN
2	Bb	501	ARG
2	Bb	529	GLN
2	Bc	77	VAL
2	Bc	95	PRO
2	Bc	178	PRO
2	Bc	202	PRO
2	Bc	223	PRO
2	Bc	379	PHE
2	Bc	494	ASN
2	Bc	501	ARG
2	Bc	529	GLN
2	Bd	77	VAL

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Mol	Chain	Res	Type
2	Bd	95	PRO
2	Bd	178	PRO
2	Bd	202	PRO
2	Bd	223	PRO
2	Bd	379	PHE
2	Bd	494	ASN
2	Bd	501	ARG
2	Bd	529	GLN
2	Be	77	VAL
2	Be	95	PRO
2	Be	178	PRO
2	Be	202	PRO
2	Be	223	PRO
2	Be	379	PHE
2	Be	494	ASN
2	Be	501	ARG
2	Be	529	GLN
2	Bf	77	VAL
2	Bf	95	PRO
2	Bf	178	PRO
2	Bf	202	PRO
2	Bf	223	PRO
2	Bf	351	PRO
2	Bf	379	PHE
2	Bf	494	ASN
2	Bf	501	ARG
2	Bf	529	GLN
3	Ca	219	LEU
3	Ca	257	GLN
3	Cb	257	GLN
4	Na	9	PRO
4	Na	38	TYR
4	Na	83	GLU
4	Na	101	ARG
4	Na	103	MET
4	Na	151	THR
4	Na	177	ALA
4	Na	179	ILE
4	Na	210	PRO
4	Na	211	ILE
6	Ma	278	ILE
4	Nb	9	PRO

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Mol	Chain	Res	Type
4	Nb	38	TYR
4	Nb	83	GLU
4	Nb	101	ARG
4	Nb	103	MET
4	Nb	151	THR
4	Nb	177	ALA
4	Nb	179	ILE
4	Nb	210	PRO
4	Nb	211	ILE
6	Mb	278	ILE
4	Nc	9	PRO
4	Nc	38	TYR
4	Nc	83	GLU
4	Nc	101	ARG
4	Nc	103	MET
4	Nc	151	THR
4	Nc	177	ALA
4	Nc	179	ILE
4	Nc	210	PRO
4	Nc	211	ILE
6	Mc	278	ILE
4	Nd	9	PRO
4	Nd	38	TYR
4	Nd	83	GLU
4	Nd	101	ARG
4	Nd	103	MET
4	Nd	151	THR
4	Nd	177	ALA
4	Nd	179	ILE
4	Nd	210	PRO
4	Nd	211	ILE
6	Md	278	ILE
4	Ne	9	PRO
4	Ne	38	TYR
4	Ne	83	GLU
4	Ne	101	ARG
4	Ne	103	MET
4	Ne	151	THR
4	Ne	177	ALA
4	Ne	179	ILE
4	Ne	210	PRO
4	Ne	211	ILE

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Mol	Chain	Res	Type
6	Me	278	ILE
4	Nf	9	PRO
4	Nf	38	TYR
4	Nf	83	GLU
4	Nf	101	ARG
4	Nf	103	MET
4	Nf	151	THR
4	Nf	177	ALA
4	Nf	179	ILE
4	Nf	210	PRO
4	Nf	211	ILE
6	Mf	278	ILE
4	Ng	9	PRO
4	Ng	38	TYR
4	Ng	83	GLU
4	Ng	101	ARG
4	Ng	103	MET
4	Ng	151	THR
4	Ng	177	ALA
4	Ng	179	ILE
4	Ng	210	PRO
4	Ng	211	ILE
6	Mg	278	ILE
4	Nh	9	PRO
4	Nh	38	TYR
4	Nh	83	GLU
4	Nh	101	ARG
4	Nh	103	MET
4	Nh	151	THR
4	Nh	177	ALA
4	Nh	179	ILE
4	Nh	210	PRO
4	Nh	211	ILE
6	Mh	278	ILE
4	Ni	9	PRO
4	Ni	38	TYR
4	Ni	83	GLU
4	Ni	101	ARG
4	Ni	103	MET
4	Ni	151	THR
4	Ni	177	ALA
4	Ni	179	ILE

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Mol	Chain	Res	Type
4	Ni	210	PRO
4	Ni	211	ILE
6	Mi	278	ILE
4	Nj	9	PRO
4	Nj	38	TYR
4	Nj	83	GLU
4	Nj	101	ARG
4	Nj	103	MET
4	Nj	151	THR
4	Nj	177	ALA
4	Nj	179	ILE
4	Nj	210	PRO
4	Nj	211	ILE
6	Mj	278	ILE
4	Nk	9	PRO
4	Nk	38	TYR
4	Nk	83	GLU
4	Nk	101	ARG
4	Nk	103	MET
4	Nk	151	THR
4	Nk	177	ALA
4	Nk	179	ILE
4	Nk	210	PRO
4	Nk	211	ILE
6	Mk	278	ILE
4	Nl	9	PRO
4	Nl	38	TYR
4	Nl	83	GLU
4	Nl	101	ARG
4	Nl	103	MET
4	Nl	151	THR
4	Nl	177	ALA
4	Nl	179	ILE
4	Nl	210	PRO
4	Nl	211	ILE
6	Ml	278	ILE
7	Qa	225	ILE
7	Qa	260	LEU
7	Qa	271	LYS
7	Qa	409	PRO
7	Qa	603	SER
8	Pa	10	ALA

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Mol	Chain	Res	Type
8	Pa	11	PRO
8	Pa	14	PRO
8	Pa	24	VAL
8	Pa	25	PRO
8	Pa	26	VAL
8	Pa	28	ALA
8	Pa	29	ALA
8	Pa	32	GLU
8	Pa	39	PRO
8	Pa	47	PRO
8	Pa	52	ASP
7	Qb	225	ILE
7	Qb	260	LEU
7	Qb	271	LYS
7	Qb	409	PRO
7	Qb	603	SER
8	Pb	10	ALA
8	Pb	11	PRO
8	Pb	17	LYS
8	Pb	24	VAL
8	Pb	25	PRO
8	Pb	26	VAL
8	Pb	28	ALA
8	Pb	29	ALA
8	Pb	32	GLU
8	Pb	39	PRO
8	Pb	47	PRO
8	Pb	48	VAL
8	Pb	52	ASP
7	Qc	225	ILE
7	Qc	260	LEU
7	Qc	271	LYS
7	Qc	409	PRO
7	Qc	603	SER
8	Pc	11	PRO
8	Pc	24	VAL
8	Pc	25	PRO
8	Pc	26	VAL
8	Pc	28	ALA
8	Pc	29	ALA
8	Pc	32	GLU
8	Pc	39	PRO

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Mol	Chain	Res	Type
8	Pc	48	VAL
8	Pc	53	PRO
7	Qd	225	ILE
7	Qd	260	LEU
7	Qd	271	LYS
7	Qd	409	PRO
7	Qd	603	SER
8	Pd	11	PRO
8	Pd	24	VAL
8	Pd	25	PRO
8	Pd	26	VAL
8	Pd	28	ALA
8	Pd	29	ALA
8	Pd	32	GLU
8	Pd	39	PRO
8	Pd	47	PRO
8	Pd	52	ASP
8	Pd	55	ARG
7	Qe	225	ILE
7	Qe	260	LEU
7	Qe	271	LYS
7	Qe	409	PRO
7	Qe	603	SER
8	Pe	11	PRO
8	Pe	24	VAL
8	Pe	26	VAL
8	Pe	28	ALA
8	Pe	29	ALA
8	Pe	32	GLU
8	Pe	39	PRO
8	Pe	47	PRO
8	Pe	52	ASP
7	Qf	225	ILE
7	Qf	260	LEU
7	Qf	271	LYS
7	Qf	409	PRO
7	Qf	603	SER
8	Pf	11	PRO
8	Pf	24	VAL
8	Pf	25	PRO
8	Pf	26	VAL
8	Pf	28	ALA

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Mol	Chain	Res	Type
8	Pf	29	ALA
8	Pf	32	GLU
8	Pf	39	PRO
8	Pf	47	PRO
8	Pf	52	ASP
7	Qg	225	ILE
7	Qg	260	LEU
7	Qg	271	LYS
7	Qg	409	PRO
7	Qg	513	SER
7	Qg	603	SER
8	Pg	11	PRO
8	Pg	24	VAL
8	Pg	25	PRO
8	Pg	26	VAL
8	Pg	28	ALA
8	Pg	29	ALA
8	Pg	39	PRO
8	Pg	47	PRO
7	Qh	225	ILE
7	Qh	260	LEU
7	Qh	271	LYS
7	Qh	409	PRO
7	Qh	603	SER
8	Ph	9	PRO
8	Ph	10	ALA
8	Ph	11	PRO
8	Ph	24	VAL
8	Ph	25	PRO
8	Ph	26	VAL
8	Ph	28	ALA
8	Ph	29	ALA
8	Ph	32	GLU
8	Ph	39	PRO
8	Ph	47	PRO
8	Ph	52	ASP
7	Qi	225	ILE
7	Qi	260	LEU
7	Qi	271	LYS
7	Qi	409	PRO
7	Qi	603	SER
8	Pi	11	PRO

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Mol	Chain	Res	Type
8	Pi	24	VAL
8	Pi	25	PRO
8	Pi	26	VAL
8	Pi	28	ALA
8	Pi	29	ALA
8	Pi	32	GLU
8	Pi	39	PRO
8	Pi	47	PRO
8	Pi	52	ASP
7	Qj	225	ILE
7	Qj	260	LEU
7	Qj	271	LYS
7	Qj	409	PRO
7	Qj	603	SER
8	Pj	11	PRO
8	Pj	24	VAL
8	Pj	25	PRO
8	Pj	26	VAL
8	Pj	28	ALA
8	Pj	29	ALA
8	Pj	39	PRO
8	Pj	47	PRO
8	Pj	52	ASP
7	Qk	225	ILE
7	Qk	260	LEU
7	Qk	271	LYS
7	Qk	409	PRO
7	Qk	603	SER
8	Pk	11	PRO
8	Pk	16	ALA
8	Pk	24	VAL
8	Pk	26	VAL
8	Pk	28	ALA
8	Pk	29	ALA
8	Pk	39	PRO
8	Pk	47	PRO
8	Pk	52	ASP
7	Ql	225	ILE
7	Ql	260	LEU
7	Ql	271	LYS
7	Ql	409	PRO
7	Ql	603	SER

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Mol	Chain	Res	Type
8	Pl	11	PRO
8	Pl	24	VAL
8	Pl	26	VAL
8	Pl	29	ALA
8	Pl	39	PRO
8	Pl	47	PRO
8	Pl	52	ASP
9	Ta	76	ALA
9	Ta	77	PRO
9	Ta	313	THR
9	Tb	76	ALA
9	Tb	77	PRO
9	Tb	313	THR
9	Tc	76	ALA
9	Tc	77	PRO
9	Tc	313	THR
9	Td	76	ALA
9	Td	77	PRO
9	Td	313	THR
9	Te	76	ALA
9	Te	77	PRO
9	Te	313	THR
9	Tf	76	ALA
9	Tf	77	PRO
9	Tf	313	THR
9	Tg	76	ALA
9	Tg	77	PRO
9	Tg	313	THR
9	Th	76	ALA
9	Th	77	PRO
9	Th	313	THR
9	Ti	76	ALA
9	Ti	77	PRO
9	Ti	313	THR
9	Tj	76	ALA
9	Tj	77	PRO
9	Tj	313	THR
9	Tk	76	ALA
9	Tk	77	PRO
9	Tk	313	THR
9	Tl	76	ALA
9	Tl	77	PRO

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Mol	Chain	Res	Type
9	Tl	313	THR
1	Aa	99	ASN
1	Ab	99	ASN
1	Ac	99	ASN
1	Ad	99	ASN
1	Ae	99	ASN
1	Af	99	ASN
1	Ag	99	ASN
1	Ah	99	ASN
1	Ai	99	ASN
1	Aj	99	ASN
1	Ak	99	ASN
1	Al	99	ASN
1	Am	99	ASN
1	An	99	ASN
1	An	136	ALA
1	Ao	99	ASN
1	Ap	99	ASN
1	Aq	99	ASN
1	Ar	99	ASN
1	As	99	ASN
1	At	99	ASN
1	Au	99	ASN
1	Av	99	ASN
1	Aw	99	ASN
1	Ax	99	ASN
1	Ay	99	ASN
1	Az	99	ASN
1	A1	99	ASN
1	A2	99	ASN
1	A3	99	ASN
1	A4	99	ASN
1	A5	99	ASN
1	A6	99	ASN
1	A7	99	ASN
1	A8	99	ASN
1	A9	99	ASN
2	Ba	150	VAL
2	Ba	178	PRO
2	Ba	240	SER
2	Ba	309	ALA
2	Ba	351	PRO

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Mol	Chain	Res	Type
2	Ba	360	ASN
2	Ba	502	VAL
2	Bb	150	VAL
2	Bb	240	SER
2	Bb	258	MET
2	Bb	259	GLY
2	Bb	309	ALA
2	Bb	351	PRO
2	Bb	360	ASN
2	Bb	502	VAL
2	Bb	532	ILE
2	Bc	150	VAL
2	Bc	240	SER
2	Bc	309	ALA
2	Bc	351	PRO
2	Bc	360	ASN
2	Bc	502	VAL
2	Bd	150	VAL
2	Bd	240	SER
2	Bd	258	MET
2	Bd	259	GLY
2	Bd	309	ALA
2	Bd	351	PRO
2	Bd	360	ASN
2	Bd	502	VAL
2	Bd	527	LEU
2	Bd	532	ILE
2	Be	150	VAL
2	Be	240	SER
2	Be	309	ALA
2	Be	351	PRO
2	Be	360	ASN
2	Be	502	VAL
2	Be	527	LEU
2	Bf	150	VAL
2	Bf	240	SER
2	Bf	258	MET
2	Bf	259	GLY
2	Bf	287	SER
2	Bf	309	ALA
2	Bf	360	ASN
2	Bf	502	VAL

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Mol	Chain	Res	Type
2	Bf	527	LEU
2	Bf	532	ILE
3	Ca	237	PHE
3	Cb	219	LEU
3	Cb	237	PHE
4	Na	39	LEU
4	Na	102	MET
5	Oa	82	SER
4	Nb	102	MET
5	Ob	82	SER
4	Nc	102	MET
5	Oc	82	SER
4	Nd	102	MET
5	Od	82	SER
4	Ne	39	LEU
4	Ne	102	MET
5	Oe	82	SER
4	Nf	102	MET
5	Of	82	SER
6	Mf	320	ALA
4	Ng	102	MET
5	Og	82	SER
6	Mg	320	ALA
4	Nh	39	LEU
4	Nh	102	MET
5	Oh	82	SER
4	Ni	102	MET
5	Oi	82	SER
6	Mi	320	ALA
4	Nj	39	LEU
4	Nj	102	MET
5	Oj	82	SER
6	Mj	320	ALA
4	Nk	39	LEU
4	Nk	102	MET
5	Ok	82	SER
4	Nl	39	LEU
4	Nl	102	MET
5	Ol	82	SER
6	Mr	320	ALA
7	Qa	91	PRO
7	Qa	135	GLY

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Mol	Chain	Res	Type
7	Qa	261	ARG
7	Qa	435	THR
7	Qa	509	ALA
7	Qa	513	SER
8	Pa	9	PRO
8	Pa	13	PRO
8	Pa	63	PRO
8	Pa	71	ALA
7	Qb	91	PRO
7	Qb	135	GLY
7	Qb	261	ARG
7	Qb	435	THR
7	Qb	509	ALA
7	Qb	513	SER
8	Pb	13	PRO
8	Pb	63	PRO
8	Pb	71	ALA
7	Qc	91	PRO
7	Qc	135	GLY
7	Qc	261	ARG
7	Qc	435	THR
7	Qc	509	ALA
7	Qc	513	SER
8	Pc	51	ARG
8	Pc	63	PRO
8	Pc	71	ALA
7	Qd	91	PRO
7	Qd	135	GLY
7	Qd	261	ARG
7	Qd	435	THR
7	Qd	509	ALA
7	Qd	513	SER
8	Pd	48	VAL
8	Pd	63	PRO
8	Pd	71	ALA
7	Qe	91	PRO
7	Qe	135	GLY
7	Qe	261	ARG
7	Qe	435	THR
7	Qe	509	ALA
7	Qe	513	SER
8	Pe	25	PRO

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Mol	Chain	Res	Type
8	Pe	63	PRO
8	Pe	71	ALA
7	Qf	91	PRO
7	Qf	135	GLY
7	Qf	261	ARG
7	Qf	435	THR
7	Qf	509	ALA
7	Qf	513	SER
8	Pf	63	PRO
8	Pf	71	ALA
7	Qg	91	PRO
7	Qg	135	GLY
7	Qg	261	ARG
7	Qg	435	THR
7	Qg	509	ALA
8	Pg	52	ASP
8	Pg	63	PRO
8	Pg	71	ALA
7	Qh	91	PRO
7	Qh	135	GLY
7	Qh	261	ARG
7	Qh	435	THR
7	Qh	509	ALA
7	Qh	513	SER
8	Ph	63	PRO
8	Ph	71	ALA
7	Qi	91	PRO
7	Qi	135	GLY
7	Qi	261	ARG
7	Qi	435	THR
7	Qi	509	ALA
7	Qi	513	SER
8	Pi	63	PRO
8	Pi	71	ALA
7	Qj	91	PRO
7	Qj	135	GLY
7	Qj	261	ARG
7	Qj	435	THR
7	Qj	509	ALA
7	Qj	513	SER
8	Pj	63	PRO
8	Pj	71	ALA

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Mol	Chain	Res	Type
7	Qk	91	PRO
7	Qk	135	GLY
7	Qk	261	ARG
7	Qk	435	THR
7	Qk	509	ALA
7	Qk	513	SER
8	Pk	25	PRO
8	Pk	63	PRO
8	Pk	71	ALA
7	Ql	91	PRO
7	Ql	135	GLY
7	Ql	261	ARG
7	Ql	435	THR
7	Ql	509	ALA
7	Ql	513	SER
8	Pl	13	PRO
8	Pl	63	PRO
8	Pl	71	ALA
9	Ta	71	ARG
9	Ta	116	PRO
9	Ta	118	TRP
9	Ta	358	SER
9	Tb	71	ARG
9	Tb	116	PRO
9	Tb	118	TRP
9	Tb	358	SER
9	Tc	71	ARG
9	Tc	116	PRO
9	Tc	118	TRP
9	Tc	358	SER
9	Td	71	ARG
9	Td	116	PRO
9	Td	118	TRP
9	Td	358	SER
9	Te	71	ARG
9	Te	116	PRO
9	Te	118	TRP
9	Te	358	SER
9	Tf	71	ARG
9	Tf	116	PRO
9	Tf	118	TRP
9	Tf	358	SER

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Mol	Chain	Res	Type
9	Tg	71	ARG
9	Tg	116	PRO
9	Tg	118	TRP
9	Tg	358	SER
9	Th	71	ARG
9	Th	116	PRO
9	Th	118	TRP
9	Th	358	SER
9	Ti	71	ARG
9	Ti	116	PRO
9	Ti	118	TRP
9	Ti	358	SER
9	Tj	71	ARG
9	Tj	116	PRO
9	Tj	118	TRP
9	Tj	358	SER
9	Tk	71	ARG
9	Tk	116	PRO
9	Tk	118	TRP
9	Tk	358	SER
9	Tl	71	ARG
9	Tl	116	PRO
9	Tl	118	TRP
9	Tl	358	SER
1	Aa	67	ALA
1	Aa	68	SER
1	Aa	114	ASN
1	Aa	124	PRO
1	Ab	67	ALA
1	Ab	68	SER
1	Ab	114	ASN
1	Ab	124	PRO
1	Ac	67	ALA
1	Ac	68	SER
1	Ac	114	ASN
1	Ac	124	PRO
1	Ad	67	ALA
1	Ad	68	SER
1	Ad	114	ASN
1	Ad	124	PRO
1	Ae	67	ALA
1	Ae	68	SER

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Mol	Chain	Res	Type
1	Ae	114	ASN
1	Ae	124	PRO
1	Af	67	ALA
1	Af	68	SER
1	Af	114	ASN
1	Af	124	PRO
1	Ag	67	ALA
1	Ag	68	SER
1	Ag	114	ASN
1	Ag	124	PRO
1	Ah	67	ALA
1	Ah	68	SER
1	Ah	114	ASN
1	Ah	124	PRO
1	Ai	67	ALA
1	Ai	68	SER
1	Ai	114	ASN
1	Ai	124	PRO
1	Aj	67	ALA
1	Aj	68	SER
1	Aj	114	ASN
1	Aj	124	PRO
1	Ak	67	ALA
1	Ak	68	SER
1	Ak	114	ASN
1	Ak	124	PRO
1	Al	67	ALA
1	Al	68	SER
1	Al	114	ASN
1	Al	124	PRO
1	Am	67	ALA
1	Am	68	SER
1	Am	114	ASN
1	Am	124	PRO
1	An	67	ALA
1	An	68	SER
1	An	114	ASN
1	An	124	PRO
1	Ao	67	ALA
1	Ao	68	SER
1	Ao	114	ASN
1	Ao	124	PRO

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Mol	Chain	Res	Type
1	Ap	67	ALA
1	Ap	68	SER
1	Ap	114	ASN
1	Ap	124	PRO
1	Aq	67	ALA
1	Aq	68	SER
1	Aq	114	ASN
1	Aq	124	PRO
1	Ar	67	ALA
1	Ar	68	SER
1	Ar	124	PRO
1	As	67	ALA
1	As	68	SER
1	As	114	ASN
1	As	124	PRO
1	At	67	ALA
1	At	68	SER
1	At	114	ASN
1	At	124	PRO
1	Au	67	ALA
1	Au	68	SER
1	Au	114	ASN
1	Au	124	PRO
1	Av	67	ALA
1	Av	68	SER
1	Av	124	PRO
1	Aw	67	ALA
1	Aw	68	SER
1	Aw	114	ASN
1	Aw	124	PRO
1	Ax	67	ALA
1	Ax	68	SER
1	Ax	114	ASN
1	Ax	124	PRO
1	Ay	67	ALA
1	Ay	68	SER
1	Ay	114	ASN
1	Ay	124	PRO
1	Az	67	ALA
1	Az	68	SER
1	Az	114	ASN
1	Az	124	PRO

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Mol	Chain	Res	Type
1	A1	67	ALA
1	A1	68	SER
1	A1	114	ASN
1	A1	124	PRO
1	A2	67	ALA
1	A2	68	SER
1	A2	114	ASN
1	A2	124	PRO
1	A3	67	ALA
1	A3	68	SER
1	A3	114	ASN
1	A3	124	PRO
1	A4	67	ALA
1	A4	68	SER
1	A4	124	PRO
1	A5	67	ALA
1	A5	68	SER
1	A5	114	ASN
1	A5	124	PRO
1	A6	67	ALA
1	A6	68	SER
1	A6	114	ASN
1	A6	124	PRO
1	A7	67	ALA
1	A7	68	SER
1	A7	114	ASN
1	A7	124	PRO
1	A8	67	ALA
1	A8	68	SER
1	A8	124	PRO
1	A9	67	ALA
1	A9	68	SER
1	A9	114	ASN
1	A9	124	PRO
2	Ba	498	TYR
2	Ba	527	LEU
2	Bb	287	SER
2	Bb	498	TYR
2	Bb	527	LEU
2	Bc	498	TYR
2	Bc	527	LEU
2	Bd	287	SER

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Mol	Chain	Res	Type
2	Bd	498	TYR
2	Be	498	TYR
2	Bf	498	TYR
3	Ca	222	PRO
3	Cb	222	PRO
6	Ma	129	PRO
6	Ma	267	ASN
6	Ma	320	ALA
4	Nb	39	LEU
6	Mb	129	PRO
6	Mb	320	ALA
4	Nc	39	LEU
6	Mc	129	PRO
6	Mc	267	ASN
6	Mc	320	ALA
4	Nd	39	LEU
6	Md	88	LEU
6	Md	129	PRO
6	Md	267	ASN
6	Md	320	ALA
6	Me	129	PRO
6	Me	320	ALA
4	Nf	39	LEU
6	Mf	129	PRO
6	Mf	267	ASN
4	Ng	39	LEU
6	Mg	129	PRO
6	Mg	267	ASN
6	Mh	129	PRO
6	Mh	267	ASN
6	Mh	320	ALA
4	Ni	39	LEU
6	Mi	129	PRO
6	Mi	267	ASN
6	Mj	129	PRO
6	Mj	267	ASN
6	Mk	129	PRO
6	Mk	267	ASN
6	Mk	320	ALA
6	MI	129	PRO
6	MI	267	ASN
8	Pa	75	PRO

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Mol	Chain	Res	Type
8	Pb	14	PRO
8	Pb	16	ALA
8	Pb	50	LYS
8	Pb	75	PRO
8	Pc	75	PRO
8	Pd	45	TYR
8	Pd	75	PRO
8	Pe	75	PRO
8	Pf	75	PRO
8	Pg	75	PRO
8	Ph	75	PRO
8	Pi	75	PRO
8	Pj	75	PRO
8	Pk	75	PRO
8	Pl	14	PRO
8	Pl	16	ALA
8	Pl	75	PRO
9	Td	389	SER
9	Th	389	SER
9	Tk	389	SER
1	Aa	80	GLU
1	Ab	80	GLU
1	Ac	80	GLU
1	Ad	80	GLU
1	Ae	80	GLU
1	Af	80	GLU
1	Ag	80	GLU
1	Ah	80	GLU
1	Aj	80	GLU
1	Ak	80	GLU
1	Al	80	GLU
1	An	80	GLU
1	Ao	80	GLU
1	Ap	80	GLU
1	Aq	80	GLU
1	Ar	80	GLU
1	Ar	114	ASN
1	As	80	GLU
1	Au	80	GLU
1	Av	114	ASN
1	Aw	80	GLU
1	Ax	80	GLU

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Mol	Chain	Res	Type
1	A1	80	GLU
1	A2	80	GLU
1	A4	80	GLU
1	A4	114	ASN
1	A5	80	GLU
1	A6	80	GLU
1	A7	80	GLU
1	A8	80	GLU
1	A8	114	ASN
1	A9	80	GLU
2	Ba	275	PHE
2	Ba	382	GLN
2	Bb	275	PHE
2	Bb	382	GLN
2	Bc	275	PHE
2	Bd	275	PHE
2	Bd	382	GLN
2	Be	275	PHE
2	Bf	275	PHE
2	Bf	382	GLN
5	Oa	72	ARG
5	Ob	72	ARG
5	Ob	170	LEU
6	Mb	79	PRO
6	Mb	267	ASN
5	Oc	72	ARG
5	Od	72	ARG
5	Od	170	LEU
6	Md	79	PRO
5	Oe	72	ARG
5	Oe	170	LEU
6	Me	267	ASN
5	Of	72	ARG
5	Of	170	LEU
5	Og	72	ARG
5	Oh	72	ARG
5	Oi	72	ARG
5	Oi	170	LEU
5	Oj	72	ARG
5	Oj	170	LEU
6	Mj	79	PRO
5	Ok	72	ARG

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Mol	Chain	Res	Type
4	Nl	75	ILE
5	Ol	72	ARG
5	Ol	170	LEU
7	Qa	407	SER
8	Pa	15	PRO
8	Pa	38	ALA
8	Pa	121	GLY
7	Qb	407	SER
7	Qc	407	SER
8	Pc	38	ALA
8	Pc	50	LYS
7	Qd	407	SER
8	Pd	38	ALA
8	Pd	50	LYS
7	Qe	407	SER
8	Pe	16	ALA
8	Pe	38	ALA
7	Qf	407	SER
8	Pf	38	ALA
7	Qg	407	SER
7	Qh	407	SER
8	Ph	53	PRO
7	Qi	407	SER
7	Qj	407	SER
8	Pj	38	ALA
7	Qk	407	SER
8	Pk	38	ALA
7	Ql	407	SER
8	Pl	10	ALA
8	Pl	38	ALA
9	Ta	73	ARG
9	Ta	389	SER
9	Tb	73	ARG
9	Tb	389	SER
9	Tc	73	ARG
9	Tc	389	SER
9	Td	73	ARG
9	Te	73	ARG
9	Te	389	SER
9	Tf	73	ARG
9	Tf	389	SER
9	Tg	73	ARG

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Mol	Chain	Res	Type
9	Tg	389	SER
9	Th	73	ARG
9	Ti	73	ARG
9	Tj	73	ARG
9	Tj	389	SER
9	Tk	73	ARG
9	Tl	73	ARG
9	Tl	389	SER
1	Aa	138	ASP
1	Ab	138	ASP
1	Ac	138	ASP
1	Ad	138	ASP
1	Ae	138	ASP
1	Af	138	ASP
1	Ag	138	ASP
1	Ah	138	ASP
1	Ai	80	GLU
1	Ai	138	ASP
1	Aj	138	ASP
1	Ak	138	ASP
1	Al	138	ASP
1	Am	80	GLU
1	Am	138	ASP
1	An	135	ASP
1	Ao	138	ASP
1	Ap	138	ASP
1	Aq	138	ASP
1	Ar	138	ASP
1	As	138	ASP
1	At	80	GLU
1	At	138	ASP
1	Au	138	ASP
1	Av	80	GLU
1	Av	138	ASP
1	Aw	138	ASP
1	Ax	138	ASP
1	Ay	80	GLU
1	Ay	138	ASP
1	Az	80	GLU
1	Az	138	ASP
1	A1	138	ASP
1	A2	138	ASP

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Mol	Chain	Res	Type
1	A3	80	GLU
1	A3	138	ASP
1	A4	138	ASP
1	A5	138	ASP
1	A6	138	ASP
1	A7	138	ASP
1	A8	138	ASP
1	A9	138	ASP
2	Ba	249	PRO
2	Ba	258	MET
2	Bb	249	PRO
2	Bc	249	PRO
2	Bc	258	MET
2	Bc	382	GLN
2	Bd	249	PRO
2	Bd	453	LEU
2	Be	249	PRO
2	Be	258	MET
2	Be	382	GLN
2	Be	454	CYS
2	Bf	249	PRO
2	Bf	453	LEU
3	Ca	215	PHE
4	Na	8	LEU
4	Na	75	ILE
5	Oa	170	LEU
6	Ma	242	ASN
4	Nb	8	LEU
4	Nb	75	ILE
6	Mb	242	ASN
4	Nc	8	LEU
4	Nc	75	ILE
5	Oc	170	LEU
6	Mc	242	ASN
4	Nd	8	LEU
4	Nd	75	ILE
6	Md	242	ASN
4	Ne	8	LEU
4	Ne	75	ILE
6	Me	242	ASN
4	Nf	8	LEU
4	Nf	75	ILE

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Mol	Chain	Res	Type
6	Mf	79	PRO
6	Mf	242	ASN
4	Ng	8	LEU
4	Ng	75	ILE
5	Og	170	LEU
6	Mg	242	ASN
4	Nh	8	LEU
4	Nh	75	ILE
5	Oh	170	LEU
6	Mh	79	PRO
6	Mh	242	ASN
4	Ni	8	LEU
4	Ni	75	ILE
6	Mi	242	ASN
4	Nj	8	LEU
4	Nj	75	ILE
6	Mj	242	ASN
4	Nk	8	LEU
4	Nk	75	ILE
5	Ok	170	LEU
4	Nl	8	LEU
6	Ml	242	ASN
8	Pb	53	PRO
8	Pb	121	GLY
8	Pc	10	ALA
8	Pc	121	GLY
8	Pd	10	ALA
8	Pd	121	GLY
8	Pe	10	ALA
8	Pe	121	GLY
8	Pf	10	ALA
8	Pf	121	GLY
8	Pg	10	ALA
8	Pg	121	GLY
8	Ph	121	GLY
8	Pi	10	ALA
8	Pi	121	GLY
8	Pj	10	ALA
8	Pj	121	GLY
8	Pk	10	ALA
8	Pk	121	GLY
8	Pl	28	ALA

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Mol	Chain	Res	Type
8	Pl	121	GLY
9	Ti	389	SER
9	Tj	92	LEU
9	Tk	92	LEU
2	Ba	454	CYS
2	Bb	453	LEU
2	Bb	454	CYS
2	Bc	454	CYS
2	Bd	454	CYS
2	Bf	94	GLY
2	Bf	454	CYS
3	Ca	192	VAL
3	Cb	192	VAL
6	Md	49	SER
6	Mk	242	ASN
8	Pa	154	PRO
8	Pb	154	PRO
8	Pc	154	PRO
8	Pe	154	PRO
8	Pf	154	PRO
8	Pg	154	PRO
8	Pi	17	LYS
8	Pi	154	PRO
8	Pj	154	PRO
8	Pk	154	PRO
8	Pl	154	PRO
9	Ta	92	LEU
9	Ta	95	ARG
9	Tb	92	LEU
9	Tb	95	ARG
9	Tc	92	LEU
9	Tc	95	ARG
9	Td	92	LEU
9	Tg	95	ARG
9	Th	92	LEU
9	Ti	92	LEU
9	Ti	95	ARG
9	Tk	95	ARG
9	Tl	92	LEU
9	Tl	95	ARG
9	Tl	310	PRO
2	Ba	94	GLY

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Mol	Chain	Res	Type
2	Bb	94	GLY
2	Bc	94	GLY
2	Bd	94	GLY
2	Be	94	GLY
3	Cb	387	GLU
6	Mg	128	MET
8	Pb	12	ALA
8	Pd	154	PRO
8	Ph	154	PRO
8	Pl	15	PRO
9	Ta	310	PRO
9	Tb	310	PRO
9	Tc	310	PRO
9	Td	310	PRO
9	Te	310	PRO
9	Tf	310	PRO
9	Th	310	PRO
9	Ti	310	PRO
9	Tj	310	PRO
2	Bb	310	ILE
2	Bc	310	ILE
2	Be	310	ILE
2	Bf	310	ILE
3	Ca	387	GLU
6	Ma	128	MET
6	Mb	128	MET
6	Me	128	MET
6	Mh	128	MET
6	Mi	128	MET
6	Mj	128	MET
8	Pc	64	VAL
8	Pd	64	VAL
8	Pf	64	VAL
8	Pg	64	VAL
8	Ph	64	VAL
8	Pi	64	VAL
8	Pj	64	VAL
8	Pk	64	VAL
8	Pl	17	LYS
8	Pl	64	VAL
9	Tg	310	PRO
9	Tk	310	PRO

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Mol	Chain	Res	Type
2	Ba	272	PRO
2	Ba	310	ILE
2	Bd	310	ILE
2	Be	272	PRO
6	Mc	128	MET
6	Md	128	MET
6	Mf	128	MET
6	Mk	128	MET
6	Ml	128	MET
7	Qa	363	GLY
8	Pa	64	VAL
7	Qb	363	GLY
8	Pb	64	VAL
7	Qc	363	GLY
8	Pc	47	PRO
7	Qd	363	GLY
7	Qe	363	GLY
8	Pe	64	VAL
7	Qf	363	GLY
7	Qg	363	GLY
7	Qh	363	GLY
8	Ph	13	PRO
7	Qi	363	GLY
7	Qj	363	GLY
7	Qk	363	GLY
7	Ql	363	GLY
9	Ta	354	VAL
9	Tb	354	VAL
9	Tc	354	VAL
9	Td	354	VAL
9	Te	354	VAL
9	Tf	354	VAL
9	Tg	354	VAL
9	Th	354	VAL
9	Ti	354	VAL
9	Tj	354	VAL
9	Tk	354	VAL
9	Tl	354	VAL
2	Bc	272	PRO
4	Ne	99	PRO
8	Ph	12	ALA
8	Ph	15	PRO

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Mol	Chain	Res	Type
8	Pl	25	PRO
4	Nb	99	PRO
4	Nf	99	PRO
4	Ni	99	PRO
6	Mj	220	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

35 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MEA	An	1	1	3,3,13	0.97	0	1,2,16	0.34	0
1	MEA	Aq	1	1	3,3,13	1.01	0	1,2,16	0.32	0
1	MEA	Aj	1	1	3,3,13	0.96	0	1,2,16	0.35	0
1	MEA	Av	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	A5	1	1	3,3,13	0.96	0	1,2,16	0.33	0
1	MEA	At	1	1	3,3,13	0.95	0	1,2,16	0.35	0
1	MEA	Ay	1	1	3,3,13	0.98	0	1,2,16	0.32	0
1	MEA	Al	1	1	3,3,13	0.97	0	1,2,16	0.33	0
1	MEA	Ao	1	1	3,3,13	0.91	0	1,2,16	0.35	0
1	MEA	Ad	1	1	3,3,13	1.01	0	1,2,16	0.33	0
1	MEA	Ag	1	1	3,3,13	0.97	0	1,2,16	0.33	0
1	MEA	Ai	1	1	3,3,13	0.99	0	1,2,16	0.32	0
1	MEA	A3	1	1	3,3,13	0.92	0	1,2,16	0.34	0
1	MEA	Aa	1	1	3,3,13	0.94	0	1,2,16	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MEA	Ah	1	1	3,3,13	0.95	0	1,2,16	0.33	0
1	MEA	A6	1	1	3,3,13	0.96	0	1,2,16	0.33	0
1	MEA	A1	1	1	3,3,13	1.01	0	1,2,16	0.32	0
1	MEA	Aw	1	1	3,3,13	0.97	0	1,2,16	0.34	0
1	MEA	A2	1	1	3,3,13	0.97	0	1,2,16	0.35	0
1	MEA	Ac	1	1	3,3,13	0.98	0	1,2,16	0.32	0
1	MEA	Ae	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	A7	1	1	3,3,13	1.01	0	1,2,16	0.34	0
1	MEA	Ap	1	1	3,3,13	0.98	0	1,2,16	0.33	0
1	MEA	As	1	1	3,3,13	0.97	0	1,2,16	0.34	0
1	MEA	Ab	1	1	3,3,13	0.97	0	1,2,16	0.35	0
1	MEA	Au	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	Ax	1	1	3,3,13	0.98	0	1,2,16	0.33	0
1	MEA	Az	1	1	3,3,13	1.00	0	1,2,16	0.32	0
1	MEA	A9	1	1	3,3,13	0.97	0	1,2,16	0.33	0
1	MEA	Af	1	1	3,3,13	0.96	0	1,2,16	0.33	0
1	MEA	Ar	1	1	3,3,13	0.99	0	1,2,16	0.33	0
1	MEA	Am	1	1	3,3,13	0.90	0	1,2,16	0.36	0
1	MEA	Ak	1	1	3,3,13	0.93	0	1,2,16	0.34	0
1	MEA	A8	1	1	3,3,13	0.98	0	1,2,16	0.34	0
1	MEA	A4	1	1	3,3,13	0.96	0	1,2,16	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEA	An	1	1	-	0/0/1/10	-
1	MEA	Aq	1	1	-	0/0/1/10	-
1	MEA	Aj	1	1	-	0/0/1/10	-
1	MEA	Av	1	1	-	0/0/1/10	-
1	MEA	A5	1	1	-	0/0/1/10	-
1	MEA	At	1	1	-	0/0/1/10	-
1	MEA	Ay	1	1	-	0/0/1/10	-
1	MEA	Al	1	1	-	0/0/1/10	-
1	MEA	Ao	1	1	-	0/0/1/10	-
1	MEA	Ad	1	1	-	0/0/1/10	-
1	MEA	Ag	1	1	-	0/0/1/10	-
1	MEA	Ai	1	1	-	0/0/1/10	-
1	MEA	A3	1	1	-	0/0/1/10	-
1	MEA	Aa	1	1	-	0/0/1/10	-
1	MEA	Ah	1	1	-	0/0/1/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEA	A6	1	1	-	0/0/1/10	-
1	MEA	A1	1	1	-	0/0/1/10	-
1	MEA	Aw	1	1	-	0/0/1/10	-
1	MEA	A2	1	1	-	0/0/1/10	-
1	MEA	Ac	1	1	-	0/0/1/10	-
1	MEA	Ae	1	1	-	0/0/1/10	-
1	MEA	A7	1	1	-	0/0/1/10	-
1	MEA	Ap	1	1	-	0/0/1/10	-
1	MEA	As	1	1	-	0/0/1/10	-
1	MEA	Ab	1	1	-	0/0/1/10	-
1	MEA	Au	1	1	-	0/0/1/10	-
1	MEA	Ax	1	1	-	0/0/1/10	-
1	MEA	Az	1	1	-	0/0/1/10	-
1	MEA	A9	1	1	-	0/0/1/10	-
1	MEA	Af	1	1	-	0/0/1/10	-
1	MEA	Ar	1	1	-	0/0/1/10	-
1	MEA	Am	1	1	-	0/0/1/10	-
1	MEA	Ak	1	1	-	0/0/1/10	-
1	MEA	A8	1	1	-	0/0/1/10	-
1	MEA	A4	1	1	-	0/0/1/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Aa	1	MEA	4	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	Pb	1
8	Pc	1
8	Pd	1
8	Pi	1
8	Pk	1
8	Pa	1
8	Pe	1
8	Pf	1
8	Pg	1
8	Ph	1
8	Pj	1
8	Pl	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Pb	63:PRO	C	64:VAL	N	1.66
1	Pc	63:PRO	C	64:VAL	N	1.66
1	Pd	63:PRO	C	64:VAL	N	1.66
1	Pi	63:PRO	C	64:VAL	N	1.66
1	Pk	63:PRO	C	64:VAL	N	1.66
1	Pa	63:PRO	C	64:VAL	N	1.65
1	Pe	63:PRO	C	64:VAL	N	1.65
1	Pf	63:PRO	C	64:VAL	N	1.65
1	Pg	63:PRO	C	64:VAL	N	1.65
1	Ph	63:PRO	C	64:VAL	N	1.65
1	Pj	63:PRO	C	64:VAL	N	1.65
1	Pl	63:PRO	C	64:VAL	N	1.65

6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-3247. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Mask visualisation

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

7 Tomogram analysis

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

7.1 Map-value distribution

This section was not generated.

8 Map-model fit

This section was not generated.