



## Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 03:46 PM EDT

PDB ID : 9YDT / pdb\_00009ydt  
EMDB ID : EMD-72834  
Title : LPHT-ring in Vibrio cholerae at disassembled, closed state  
Authors : Guo, W.; Yue, J.  
Deposited on : 2025-09-23  
Resolution : 2.75 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

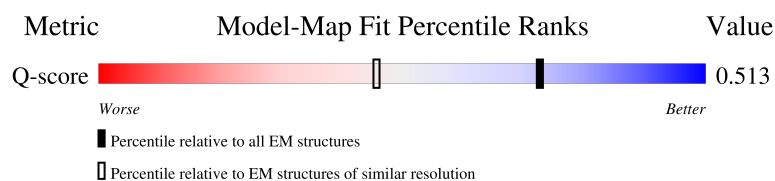
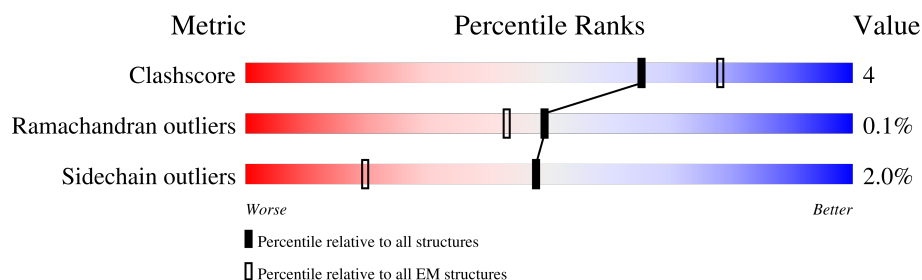
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 ( 2.25 - 3.25 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Aa	227	<div> <div>9%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	Ab	227	<div> <div>9%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	Ac	227	<div> <div>8%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	Ad	227	<div> <div>7%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>







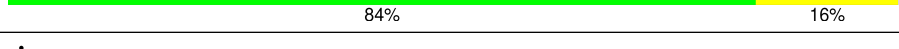
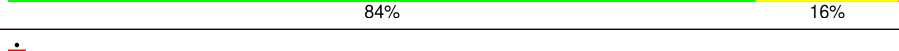
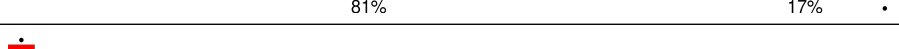
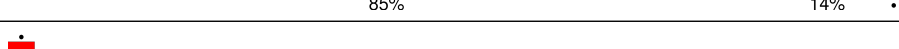
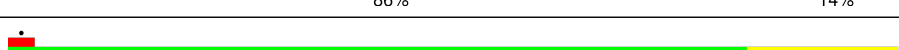

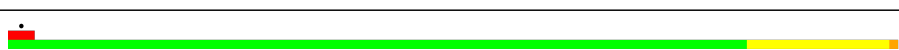

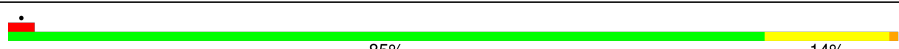





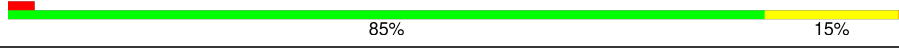
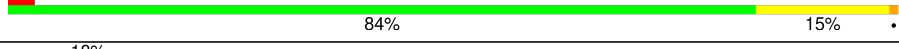



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Mol	Chain	Length	Quality of chain
1	Ae	227	
1	Af	227	
1	Ag	227	
1	Ah	227	
1	Ai	227	
1	Aj	227	
1	Ak	227	
1	Al	227	
1	Am	227	
1	An	227	
1	Ao	227	
1	Ap	227	
1	Aq	227	
1	Ar	227	
1	As	227	
1	At	227	
1	Au	227	
1	Av	227	
1	Aw	227	
1	Ax	227	
1	Ay	227	
1	Az	227	
2	Ba	343	
2	Bb	343	
2	Bc	343	

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Mol	Chain	Length	Quality of chain
2	Bd	343	
2	Be	343	
2	Bf	343	
2	Bg	343	
2	Bh	343	
2	Bi	343	
2	Bj	343	
2	Bk	343	
2	Bl	343	
2	Bm	343	
2	Bn	343	
2	Bo	343	
2	Bp	343	
2	Bq	343	
2	Br	343	
2	Bs	343	
2	Bt	343	
2	Bu	343	
2	Bv	343	
2	Bw	343	
2	Bx	343	
2	By	343	
2	Bz	343	
3	Ca	352	
3	Cb	352	

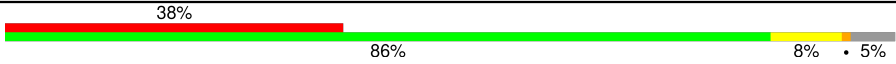
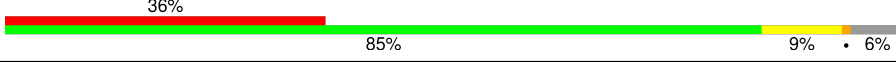
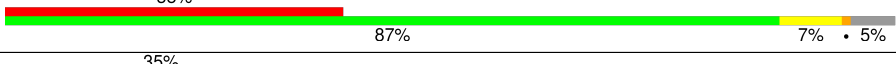


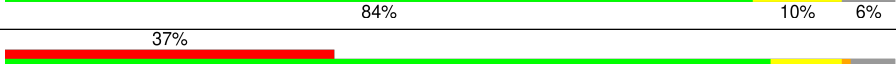
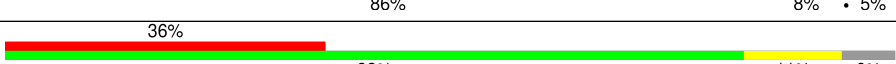
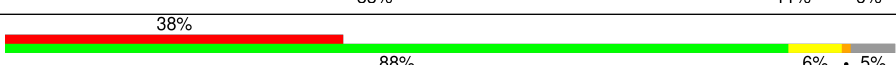
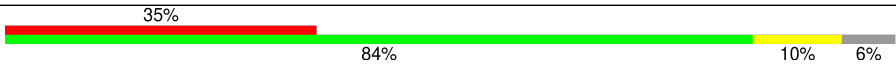


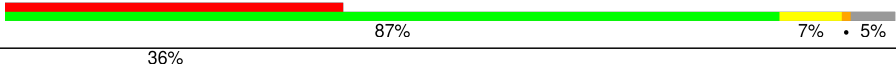
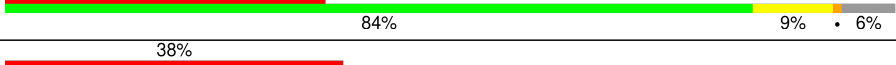

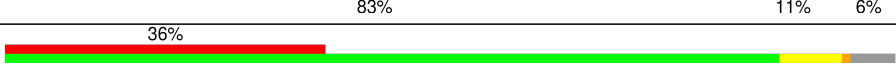










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Mol	Chain	Length	Quality of chain
3	Cc	352	
3	Cd	352	
3	Ce	352	
3	Cf	352	
3	Cg	352	
3	Ch	352	
3	Ci	352	
3	Cj	352	
3	Ck	352	
3	Cl	352	
3	Cm	352	
3	Cn	352	
3	Co	352	
3	Cp	352	
3	Cq	352	
3	Cr	352	
3	Cs	352	
3	Ct	352	
3	Cu	352	
3	Cv	352	
3	Cw	352	
3	Cx	352	
3	Cy	352	
3	Cz	352	
4	Da	272	

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Mol	Chain	Length	Quality of chain
4	Db	272	
4	Dc	272	
4	Dd	272	
4	De	272	
4	Df	272	
4	Dg	272	
4	Dh	272	
4	Di	272	
4	Dj	272	
4	Dk	272	
4	Dl	272	
4	Dm	272	
4	Dn	272	
4	Do	272	
4	Dp	272	
4	Dq	272	
4	Dr	272	
4	Ds	272	
4	Dt	272	
4	Du	272	
4	Dv	272	
4	Dw	272	
4	Dx	272	
4	Dy	272	
4	Dz	272	

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Mol	Chain	Length	Quality of chain
5	Fa	15	67% 100%
5	Fb	15	73% 93% 7%
5	Fc	15	60% 100%
5	Fd	15	73% 93% 7%
5	Fe	15	67% 100%
5	Ff	15	73% 87% 13%
5	Fg	15	60% 100%
5	Fh	15	60% 93% 7%
5	Fi	15	60% 100%
5	Fj	15	60% 100%
5	Fk	15	67% 100%
5	Fl	15	60% 93% 7%
5	Fm	15	67% 93% 7%
5	Fn	15	73% 100%
5	Fo	15	60% 93% 7%
5	Fp	15	60% 100%
5	Fq	15	60% 93% 7%
5	Fr	15	67% 100%
5	Fs	15	60% 100%
5	Ft	15	67% 100%
5	Fu	15	60% 100%
5	Fv	15	60% 93% 7%
5	Fw	15	67% 93% 7%
5	Fx	15	67% 100%
5	Fy	15	67% 100%

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Mol	Chain	Length	Quality of chain
5	Fz	15	
5	Ga	15	
5	Gb	15	
5	Gc	15	
5	Gd	15	
5	Ge	15	
5	Gf	15	
5	Gg	15	
5	Gh	15	
5	Gi	15	
5	Gj	15	
5	Gk	15	
5	Gl	15	
5	Gm	15	
5	Gn	15	
5	Go	15	
5	Gp	15	
5	Gq	15	
5	Gr	15	
5	Gs	15	
5	Gt	15	
5	Gu	15	
5	Gv	15	
5	Gw	15	
5	Gx	15	

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Mol	Chain	Length	Quality of chain
5	Gy	15	<div><div></div><div>60%</div><div></div><div>80%</div><div></div><div>7%</div><div>13%</div></div>
5	Gz	15	<div><div></div><div>67%</div><div></div><div>80%</div><div></div><div>7%</div><div>13%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 240877 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 Flagellar L-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ab	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ac	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ad	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ae	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Af	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ag	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ah	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ai	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Aj	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ak	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Al	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Am	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	An	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ao	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ap	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Aq	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	As	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	At	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Au	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Av	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Aw	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ax	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Ay	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		
1	Az	223	Total	C	N	O	S	0	0
			1674	1027	290	353	4		

- Molecule 2 is a protein called Flagellar P-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ba	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bb	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bc	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bd	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Be	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bf	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bg	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bh	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bi	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bj	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bk	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bl	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bm	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bn	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bo	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bp	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bq	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Br	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bs	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bt	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bu	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bv	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bw	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bx	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	By	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		
2	Bz	343	Total	C	N	O	S	0	0
			2501	1570	436	488	7		

- Molecule 3 is a protein called Flagellar protein FlgT.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ca	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cb	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cc	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Cd	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Ce	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cf	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cg	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Ch	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Ci	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cj	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Ck	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cl	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cm	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cn	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Co	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cp	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cq	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cr	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cs	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Ct	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cu	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cv	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cw	352	Total 2770	C 1741	N 477	O 535	S 17	0	0
3	Cx	352	Total 2770	C 1741	N 477	O 535	S 17	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Cy	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cz	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		

- Molecule 4 is a protein called Sodium-type flagellar protein MotY.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Da	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Db	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Dc	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dd	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	De	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Df	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Dg	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dh	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Di	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dj	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Dk	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dl	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Dm	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dn	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Do	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dp	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Dq	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Dr	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Ds	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dt	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Du	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dv	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Dw	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dx	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		
4	Dy	257	Total	C	N	O	S	0	0
			2085	1312	362	404	7		
4	Dz	258	Total	C	N	O	S	0	0
			2080	1310	358	405	7		

- Molecule 5 is a protein called Flagellar assembly lipoprotein FlgP.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Fa	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Fb	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Fc	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Fd	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Fe	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Ff	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Fg	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Fh	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Fi	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
5	Fj	15	Total	C	N	O	S	0	0
			125	78	22	24	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Fk	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fl	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fm	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fn	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fo	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fp	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fq	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fr	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fs	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Ft	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fu	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fv	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fw	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fx	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fy	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Fz	15	Total 125	C 78	N 22	O 24	S 1	0	0
5	Ga	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gb	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gc	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gd	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Ge	13	Total 112	C 71	N 20	O 20	S 1	0	0

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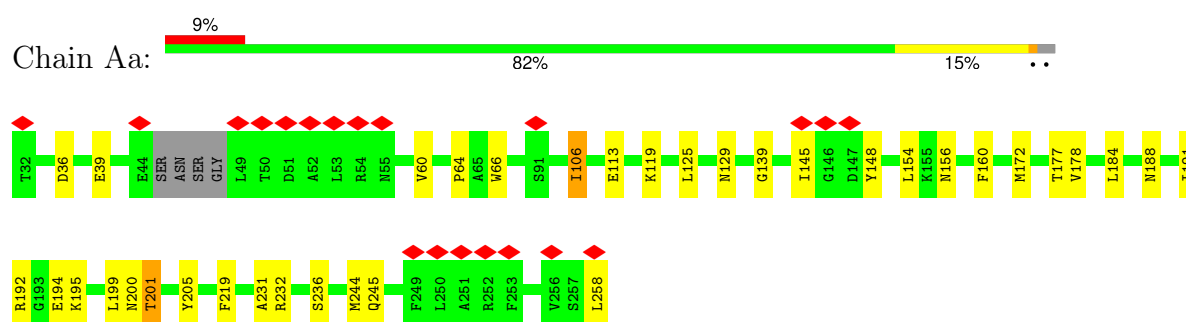
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Mol	Chain	Residues	Atoms					AltConf	Trace
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5	Gh	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gi	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gj	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gk	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gl	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gm	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gn	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Go	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gp	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gq	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gr	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gs	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gt	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gu	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gv	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gw	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gx	13	Total 112	C 71	N 20	O 20	S 1	0	0
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5	Gz	13	Total 112	C 71	N 20	O 20	S 1	0	0

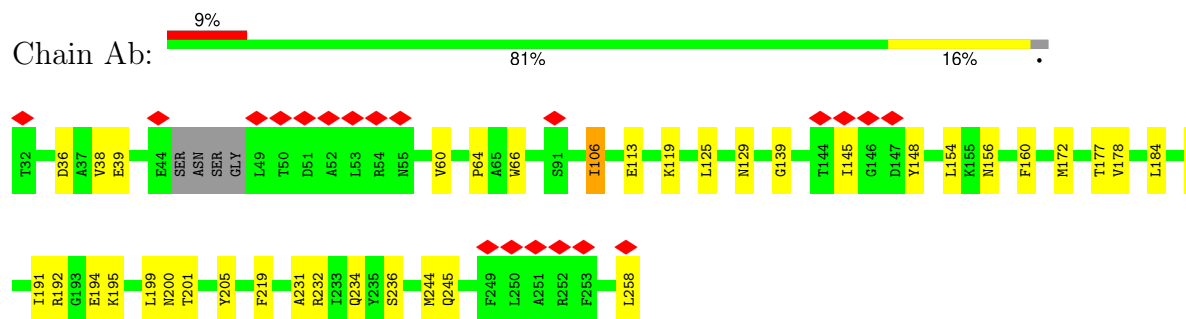
### 3 Residue-property plots [i](#)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

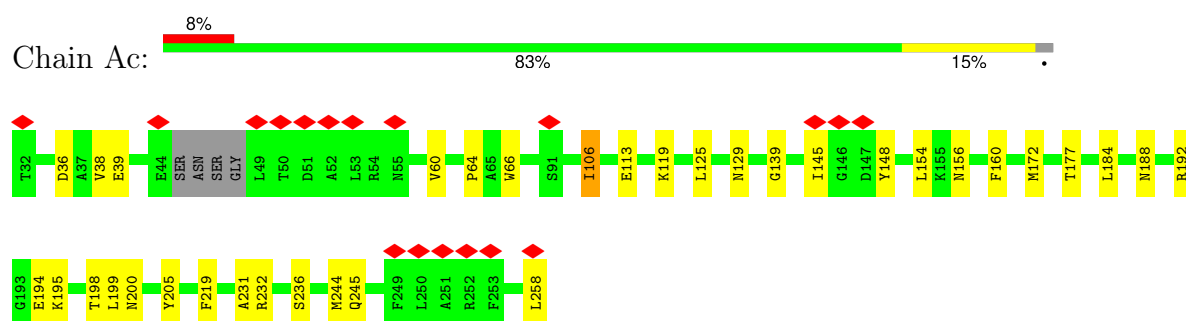
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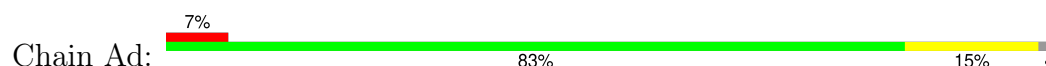
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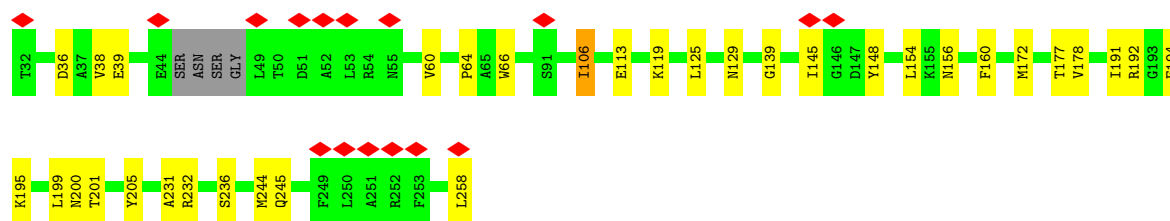


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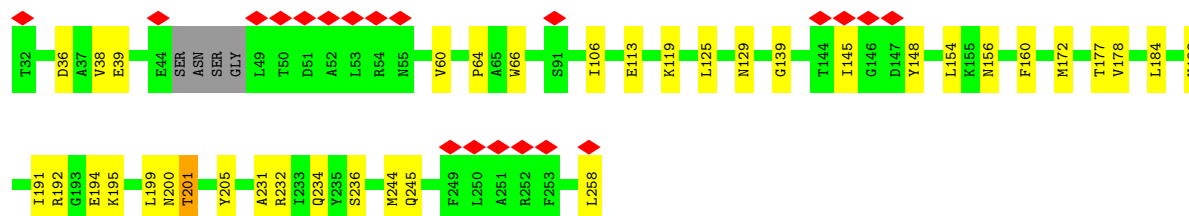
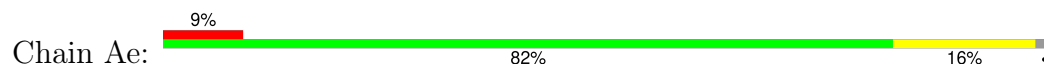


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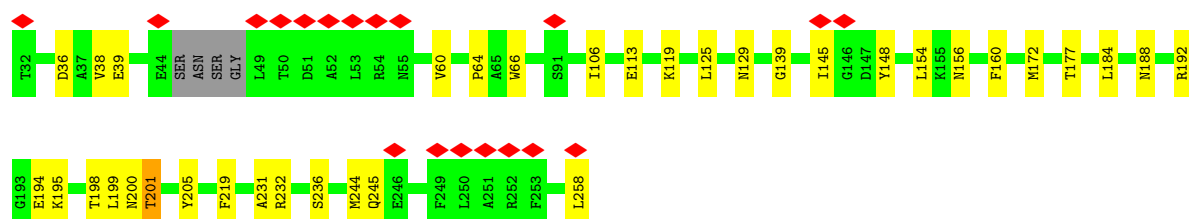
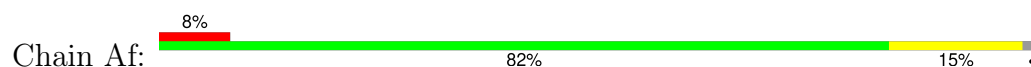




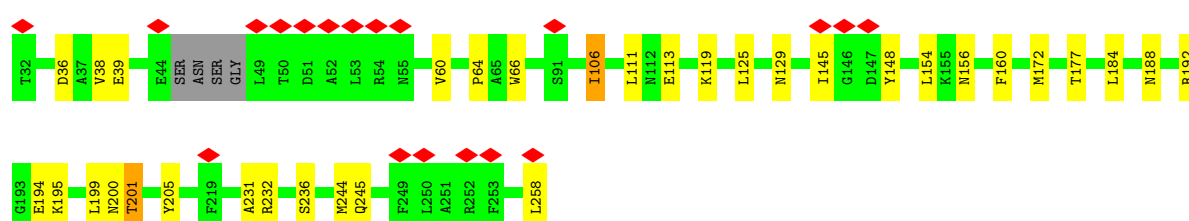
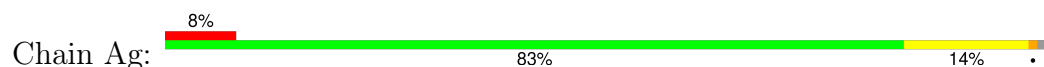
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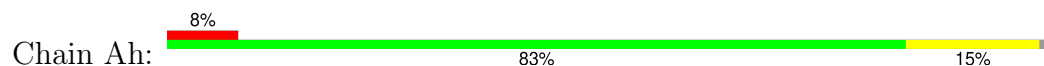
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

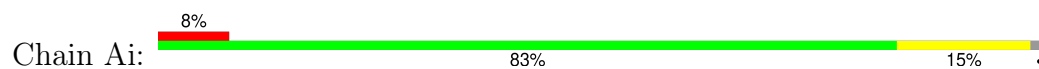


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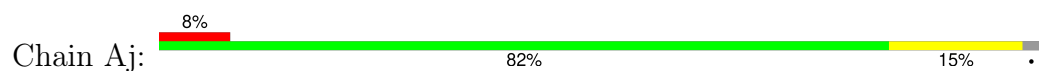




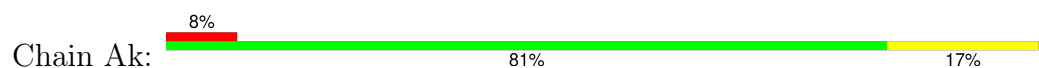
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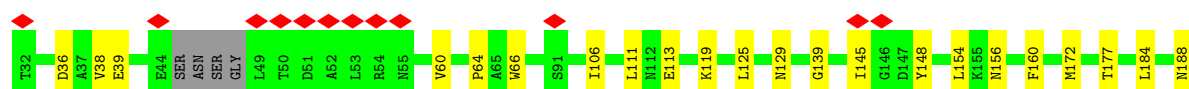
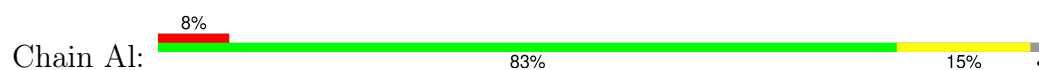
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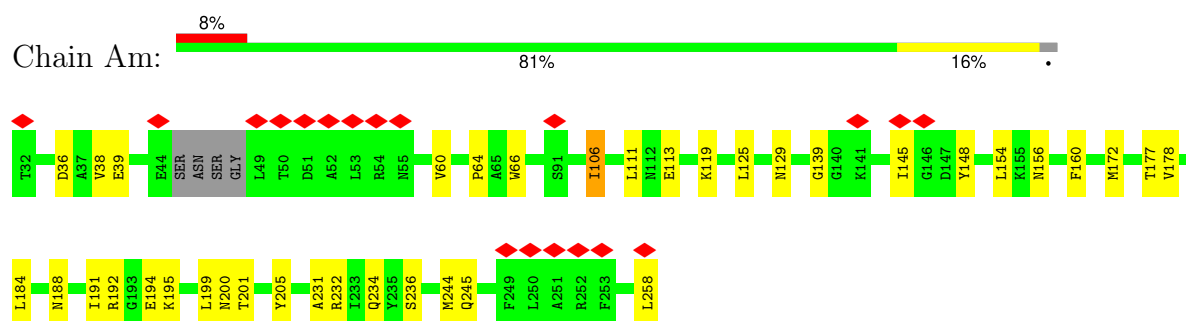
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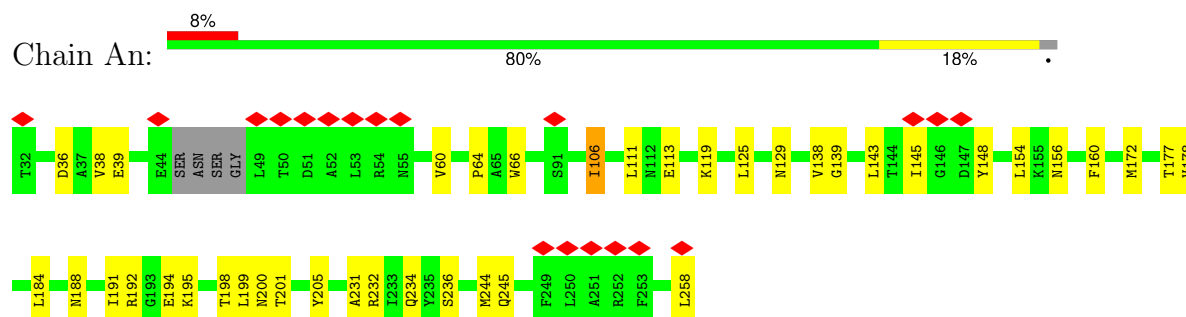
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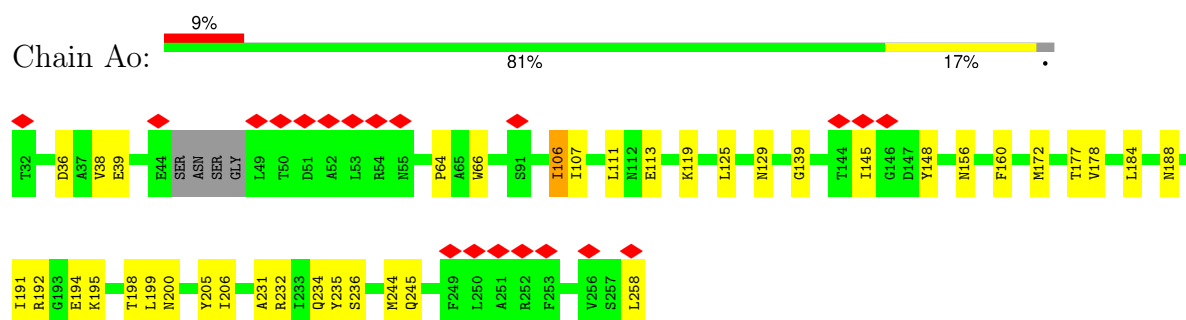
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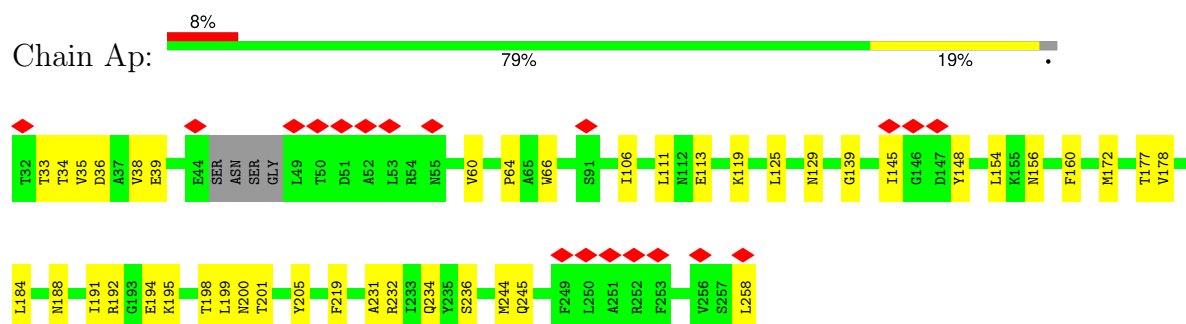
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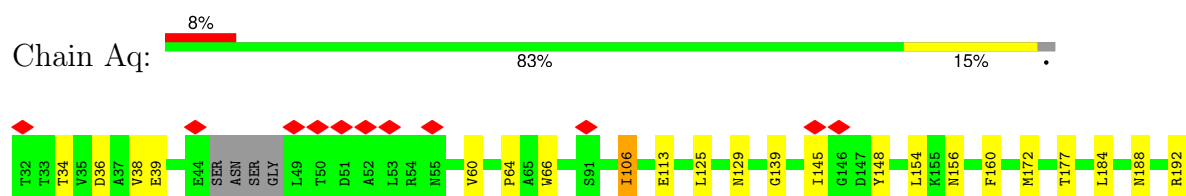
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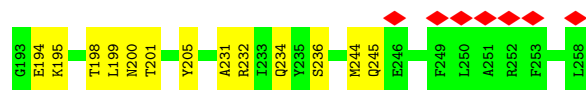


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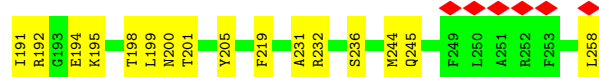
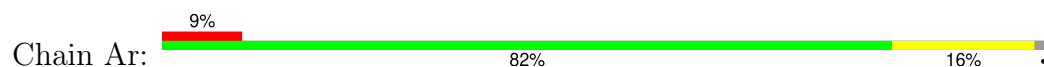


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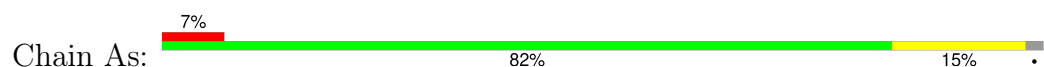




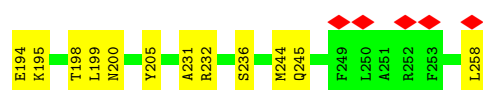
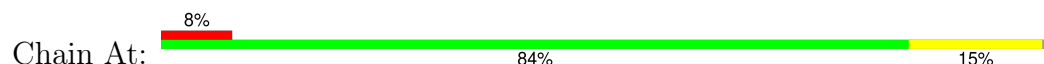
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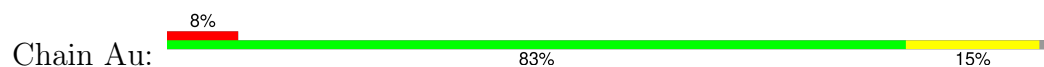
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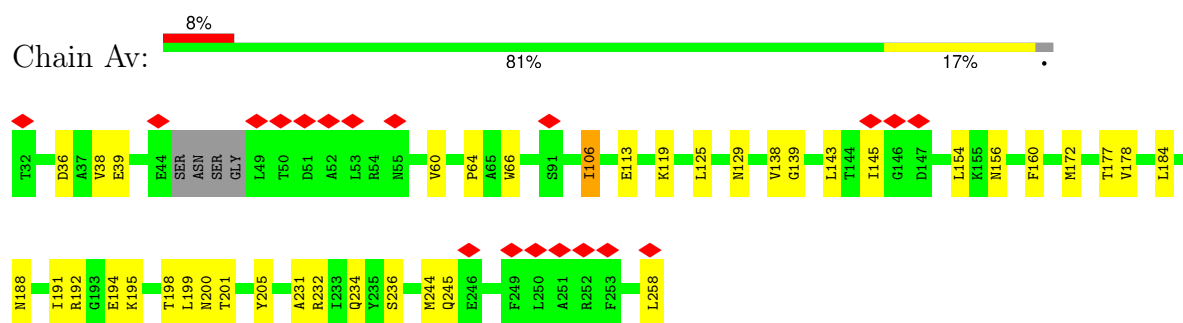
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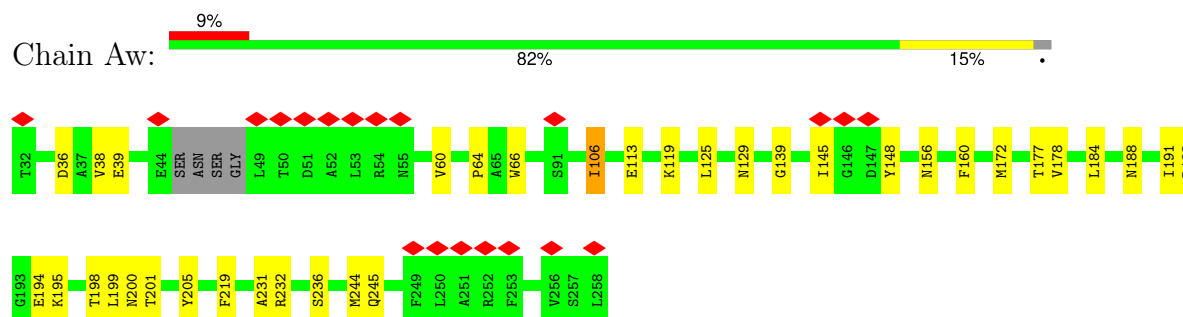
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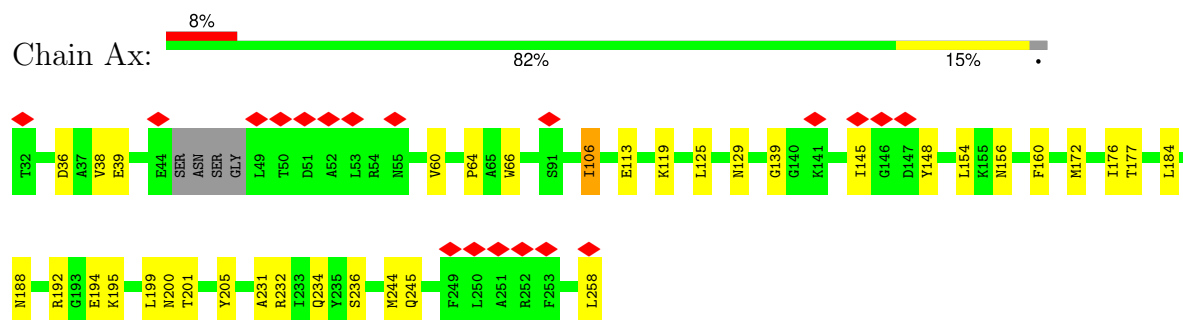
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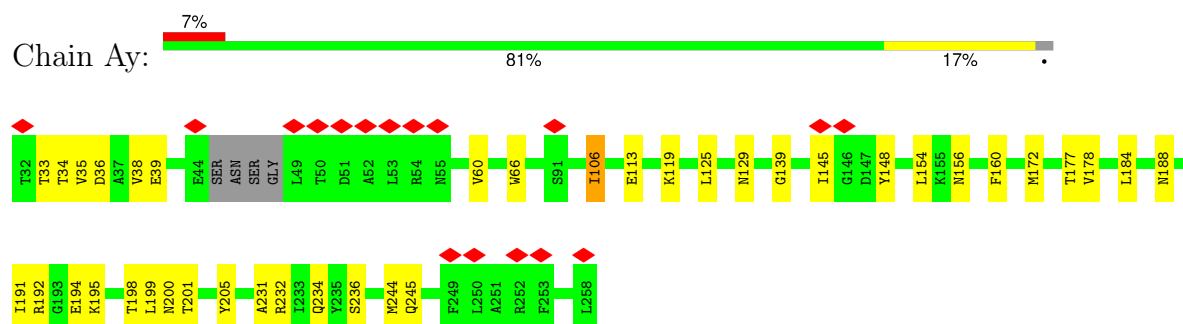
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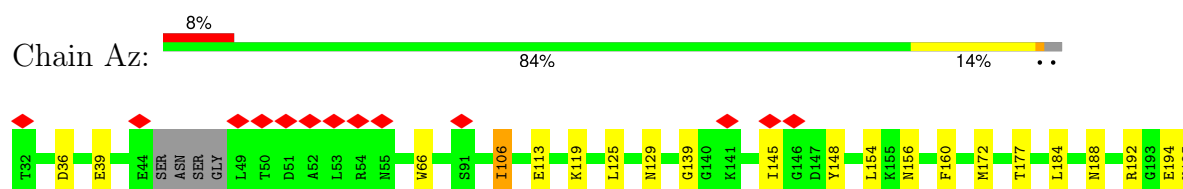
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

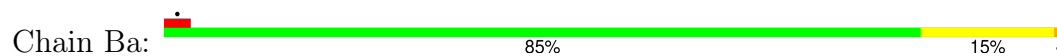


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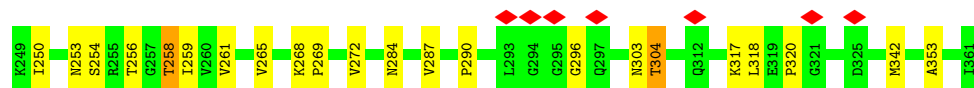
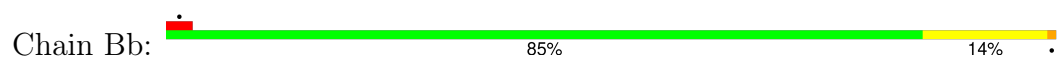




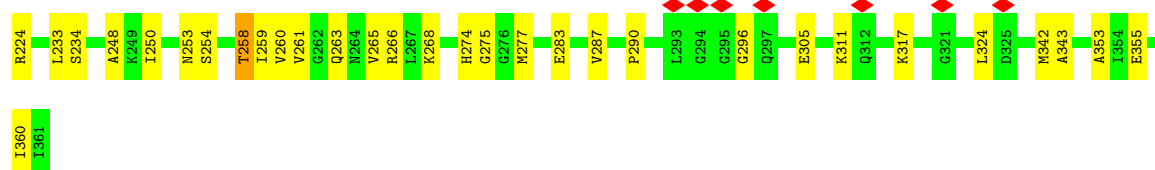
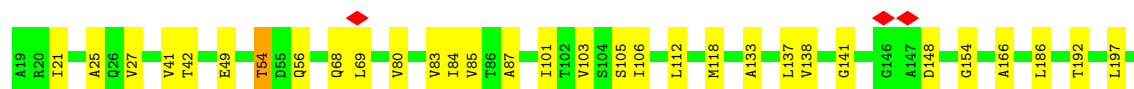
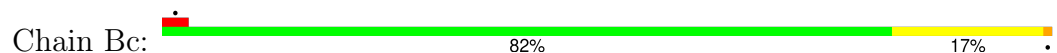
• Molecule 2: Flagellar P-ring protein



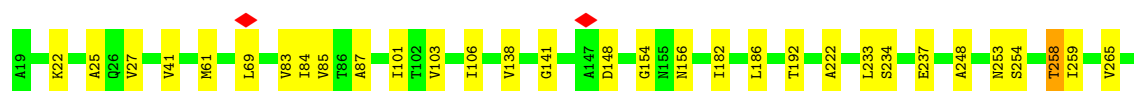
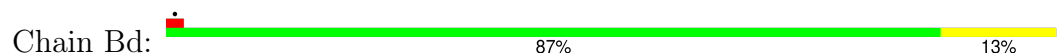
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• Molecule 2: Flagellar P-ring protein

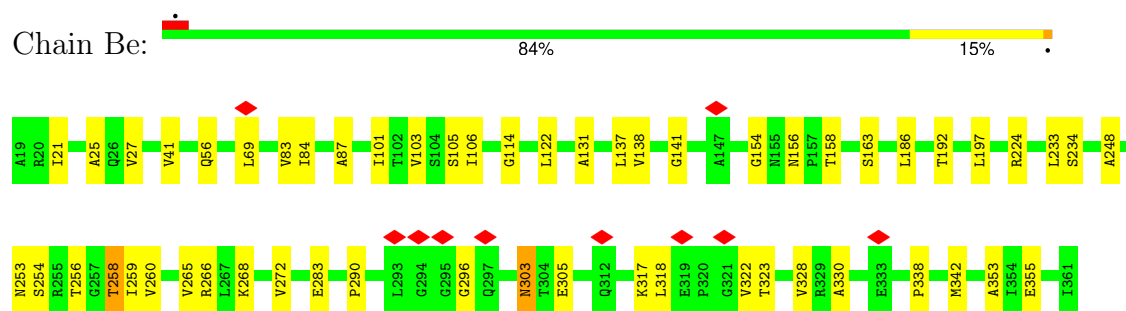


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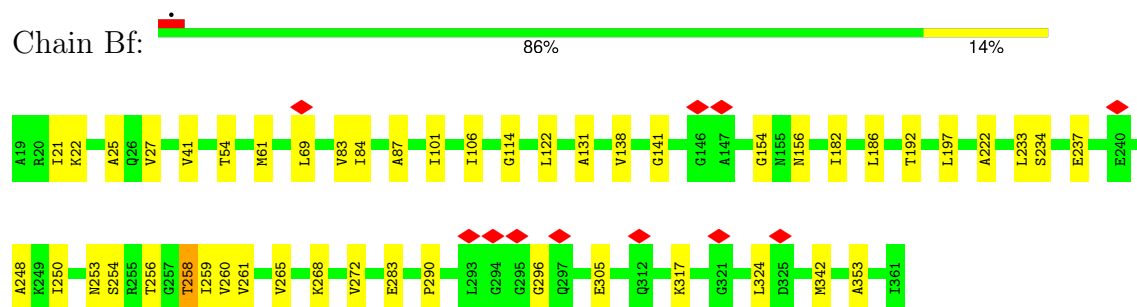




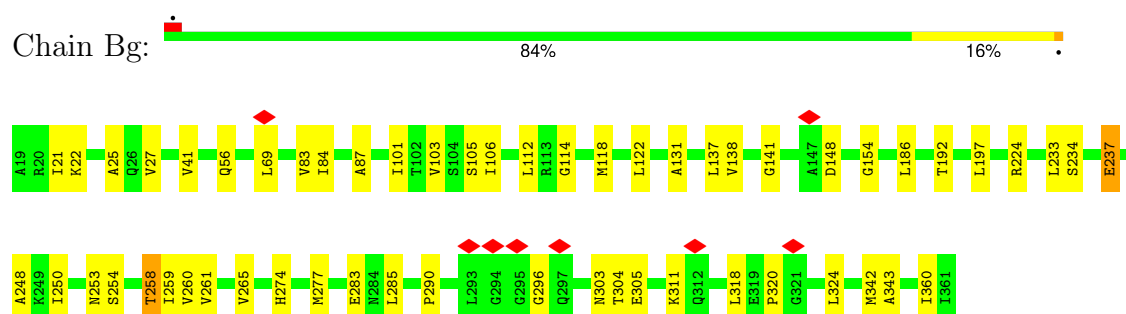
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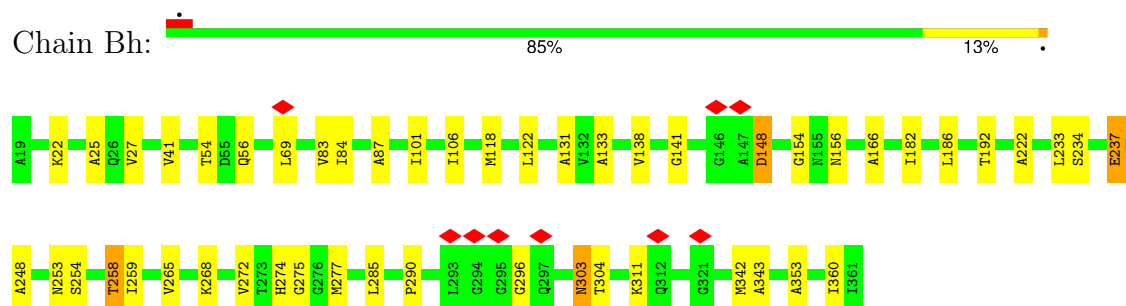
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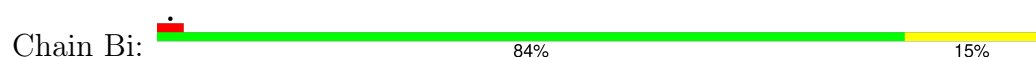
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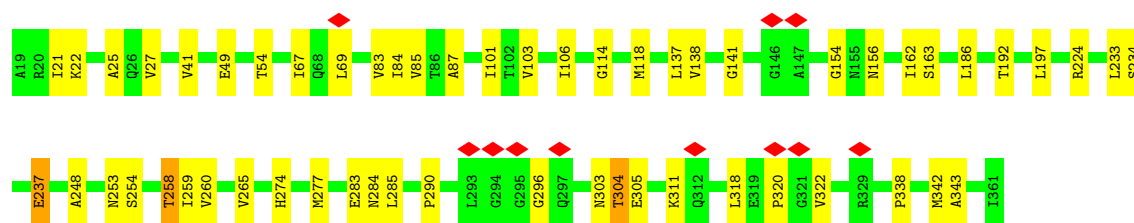


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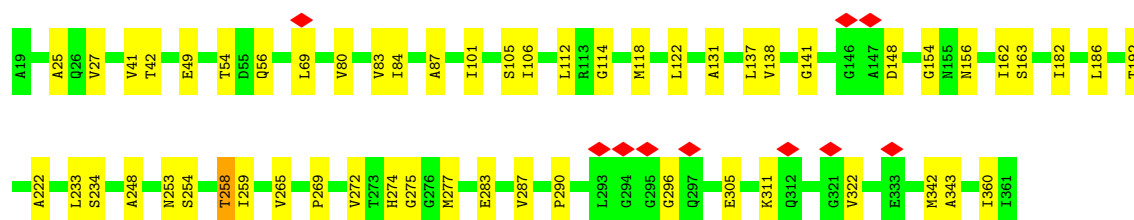
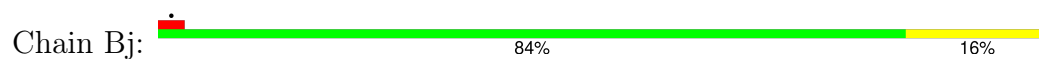


- Molecule 2: Flagellar P-ring protein

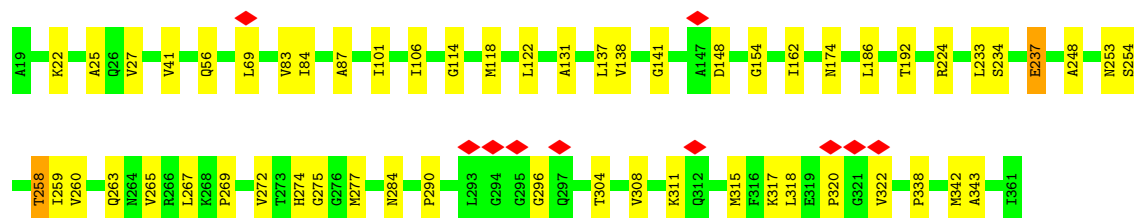
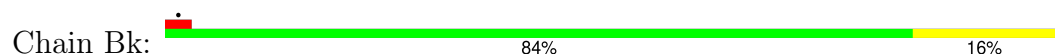




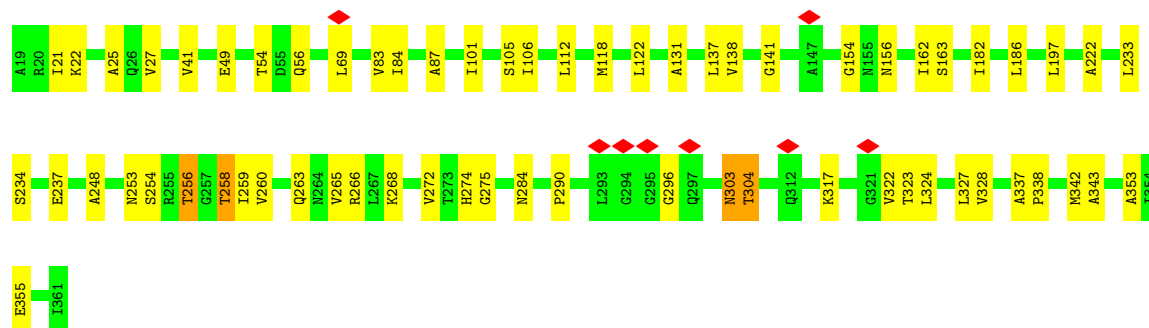
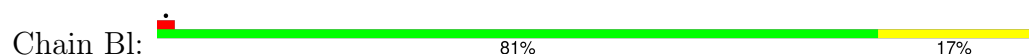
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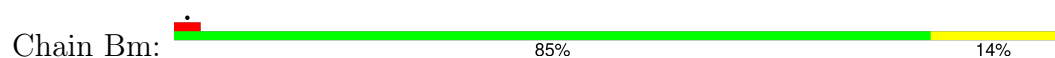
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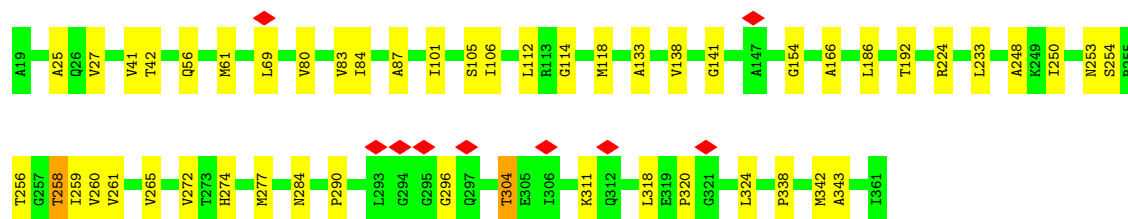


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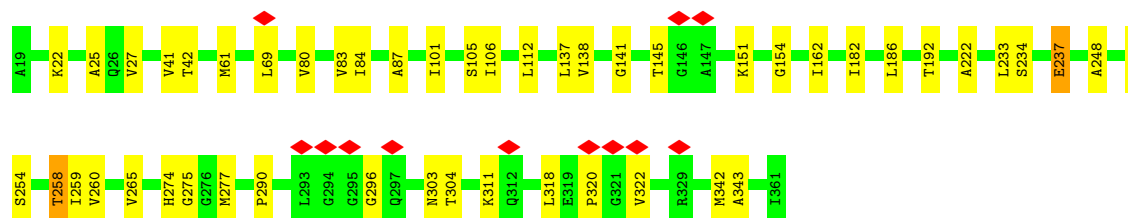
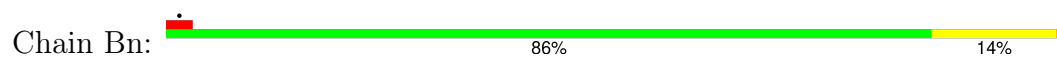


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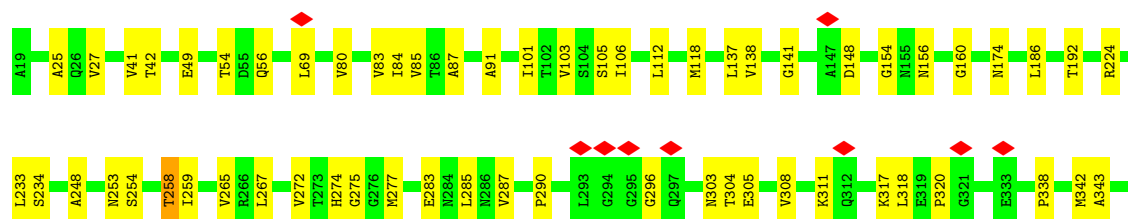
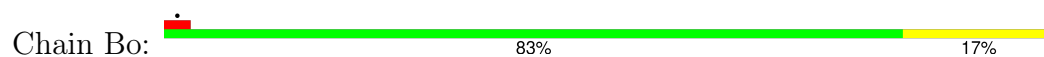




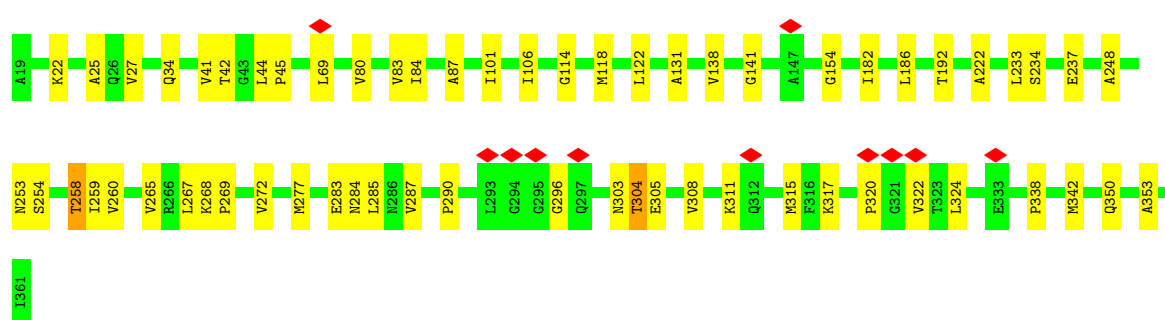
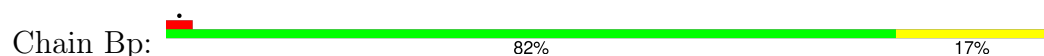
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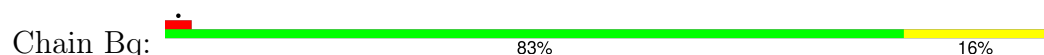
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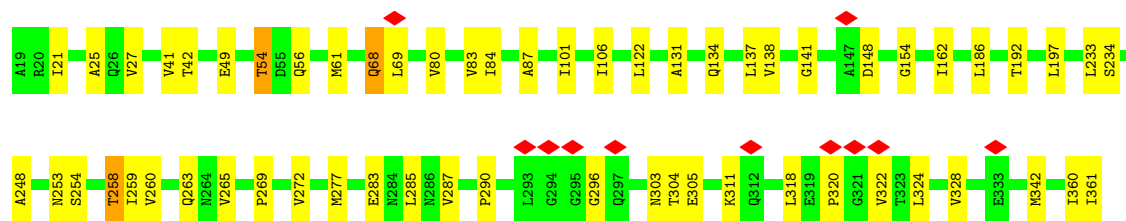


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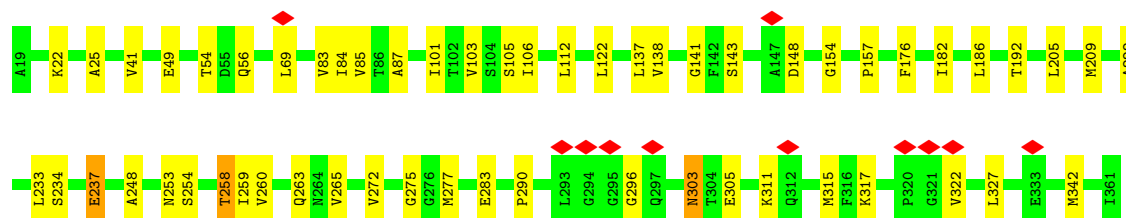
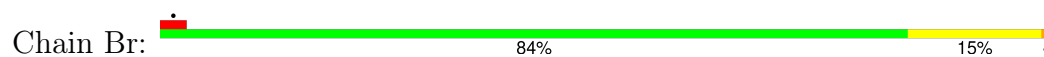


• Molecule 2: Flagellar P-ring protein

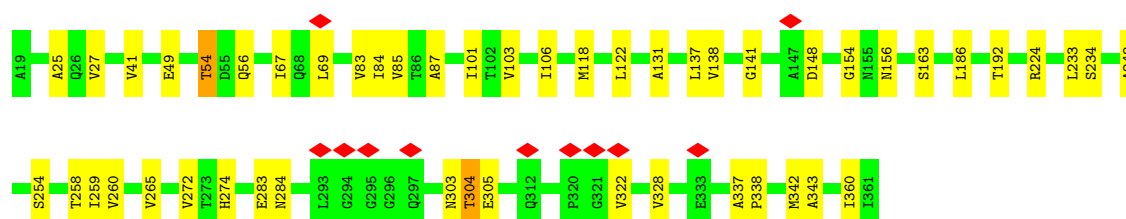
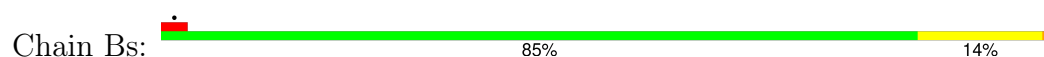




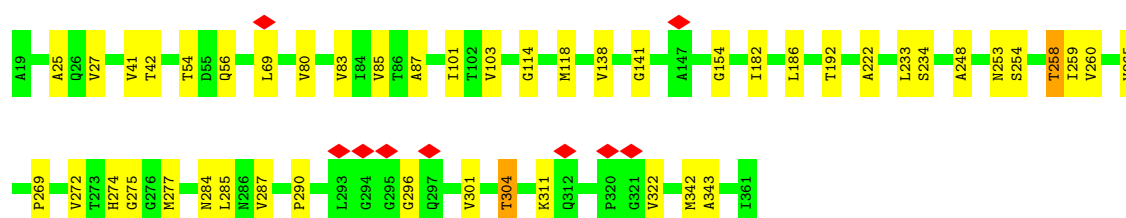
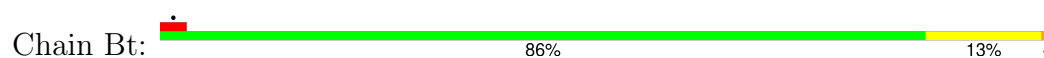
• Molecule 2: Flagellar P-ring protein



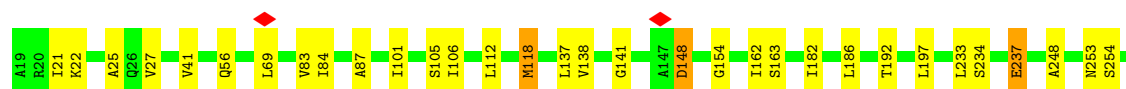
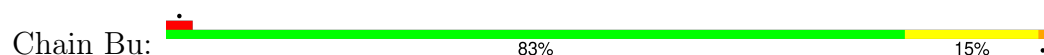
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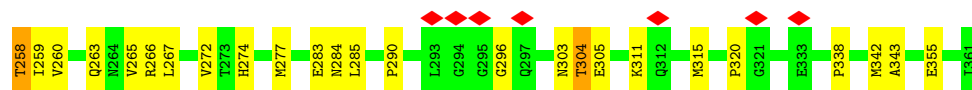


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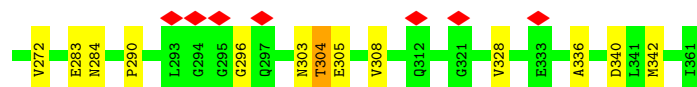


• Molecule 2: Flagellar P-ring protein

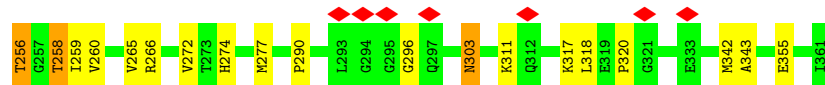
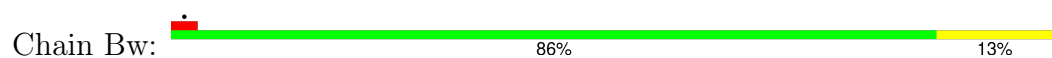




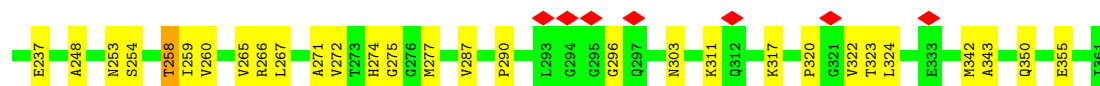
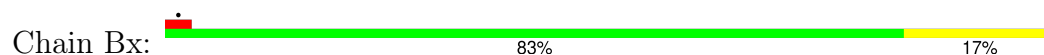
- Molecule 2: Flagellar P-ring protein



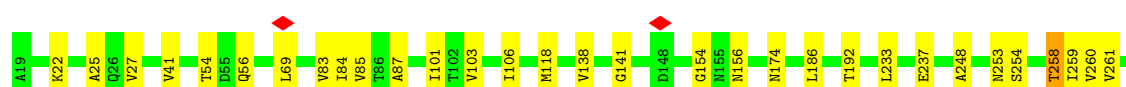
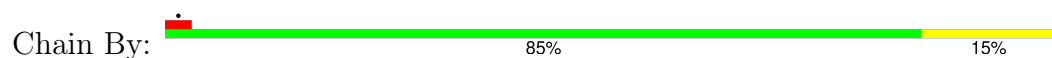
- Molecule 2: Flagellar P-ring protein




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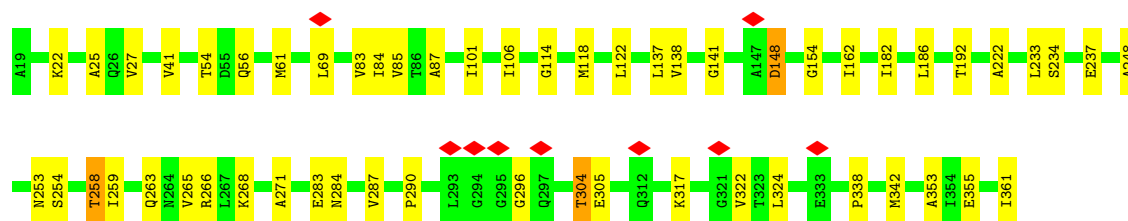


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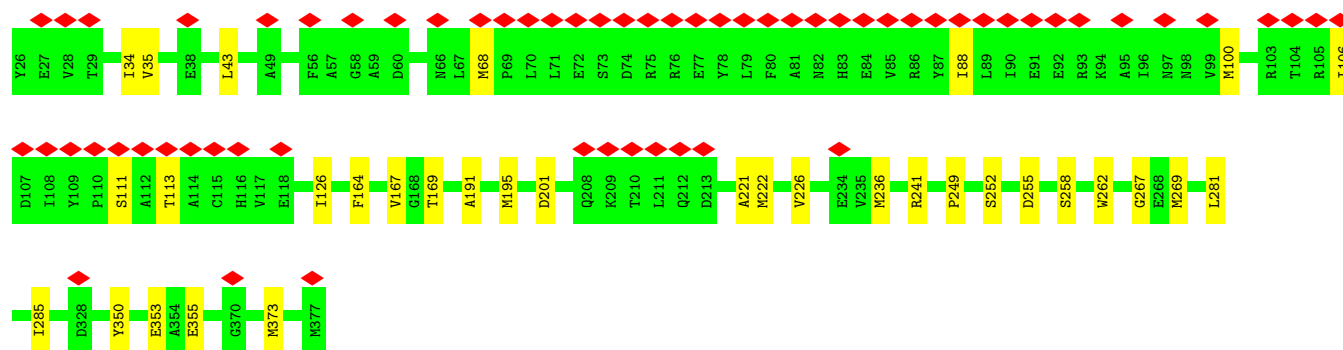
- Molecule 2: Flagellar P-ring protein

Chain Bz:  84% 15%




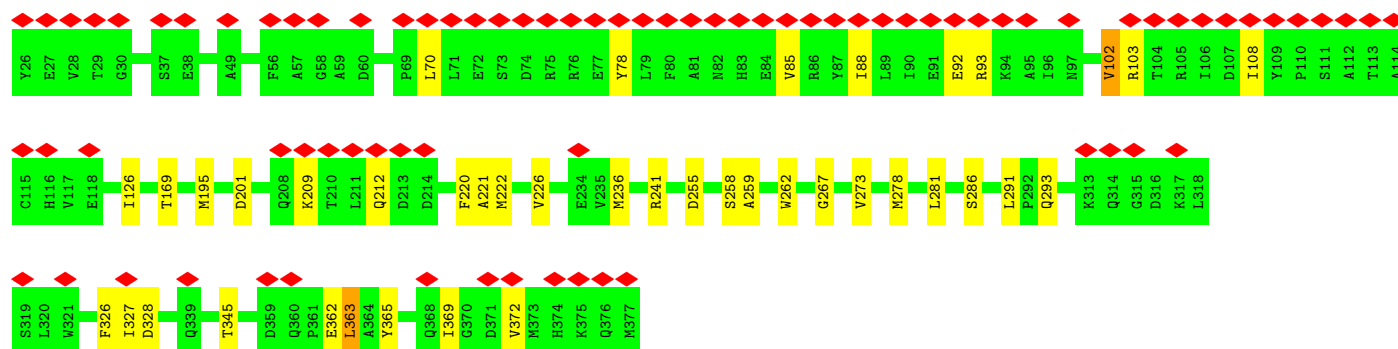
• Molecule 3: Flagellar protein FlgT

Chain Ca:  18% 90% 10%



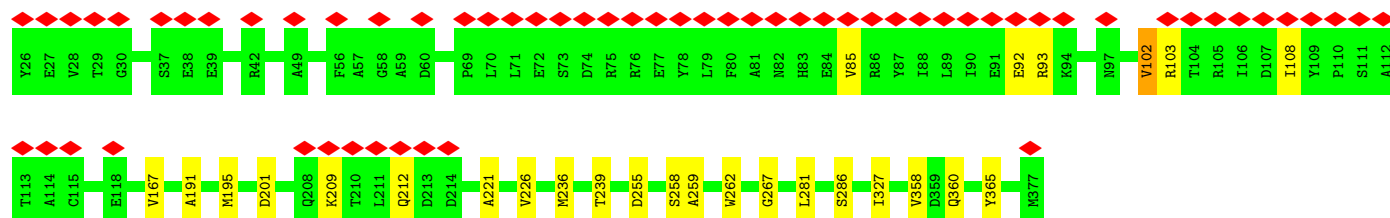
• Molecule 3: Flagellar protein FlgT

Chain Cb:  23% 88% 11%

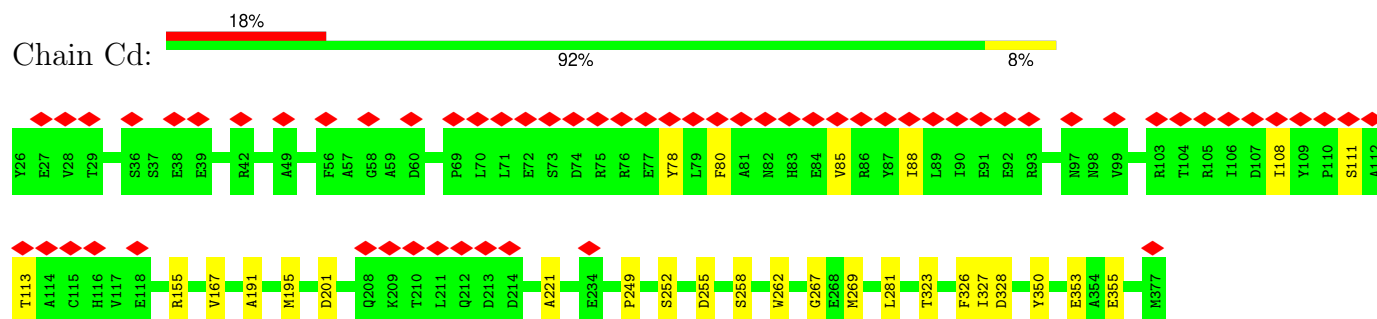


• Molecule 3: Flagellar protein FlgT

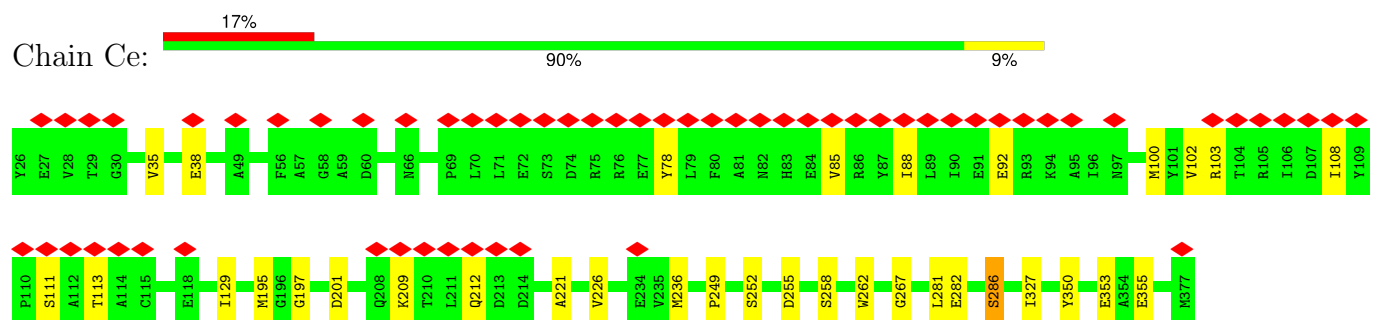
Chain Cc:  18% 92% 7%



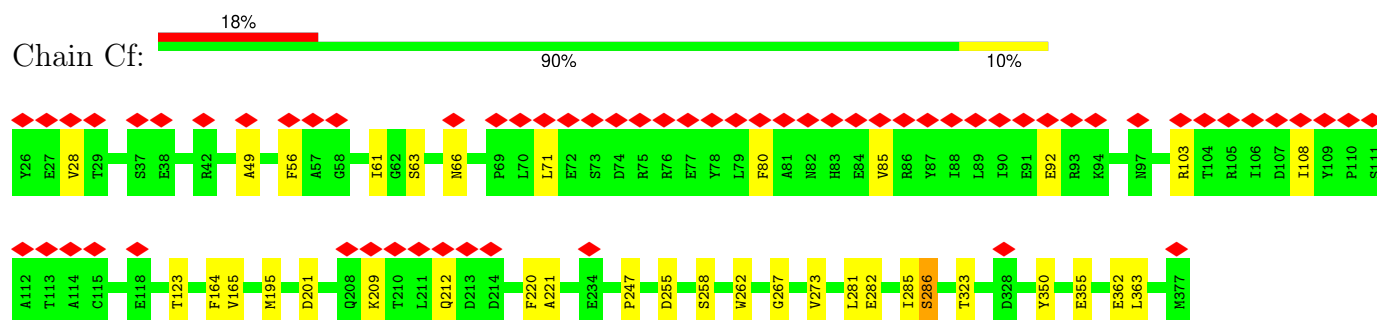
- Molecule 3: Flagellar protein FlgT



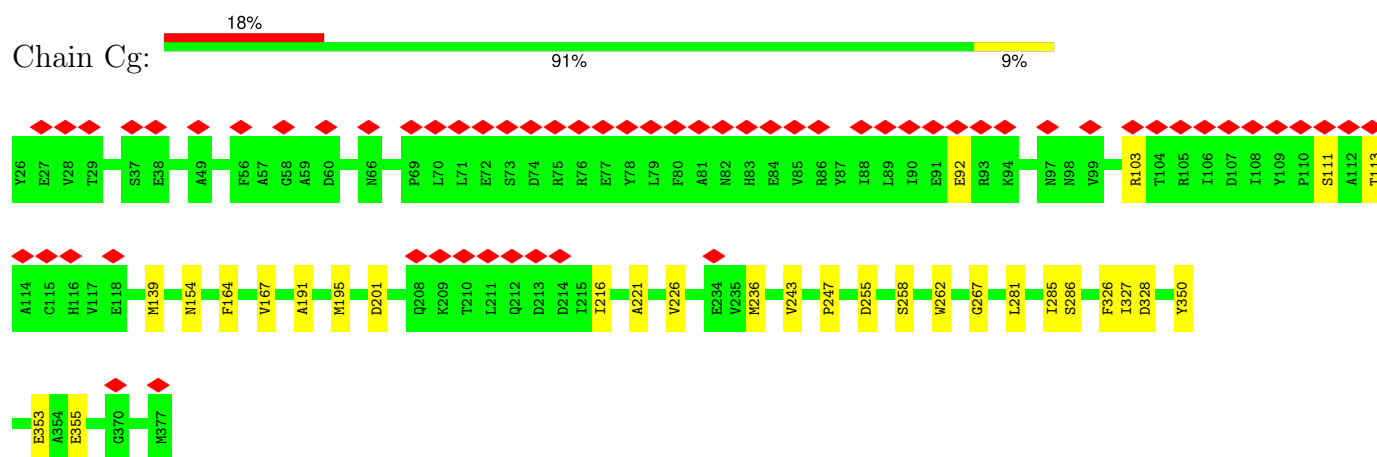
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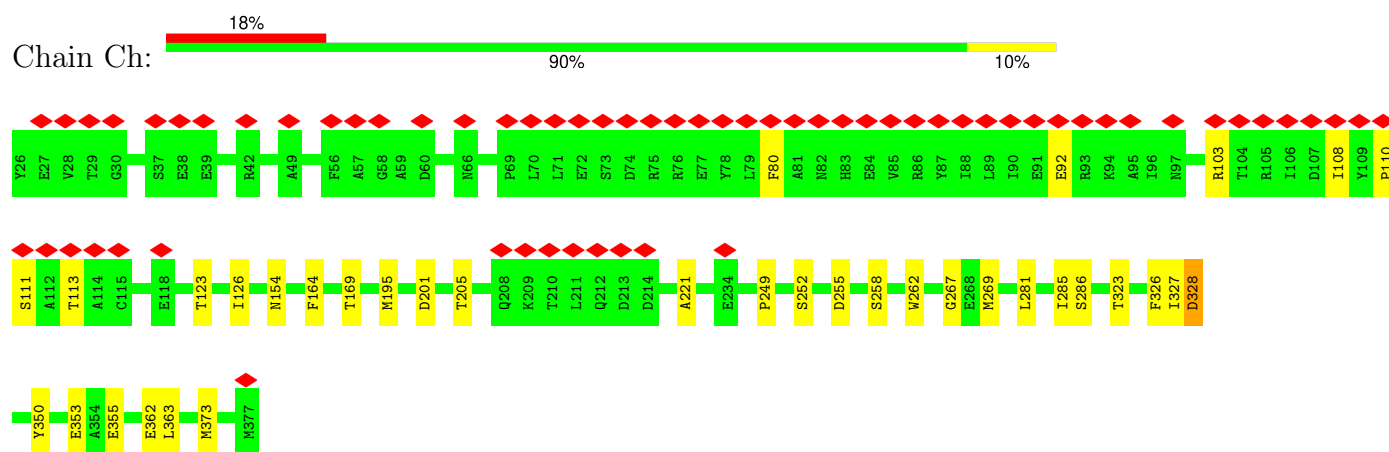
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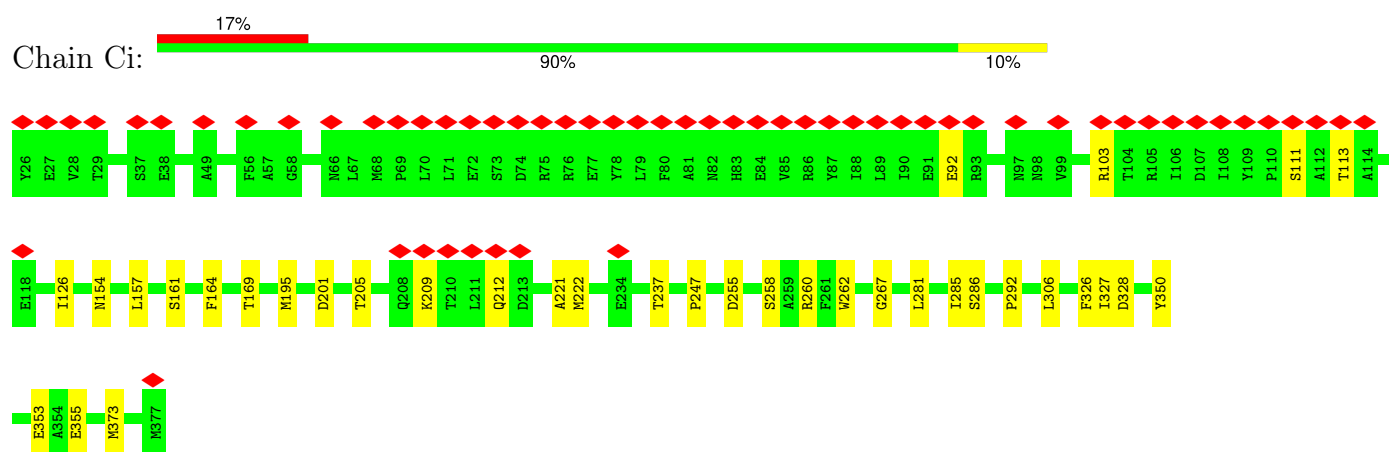
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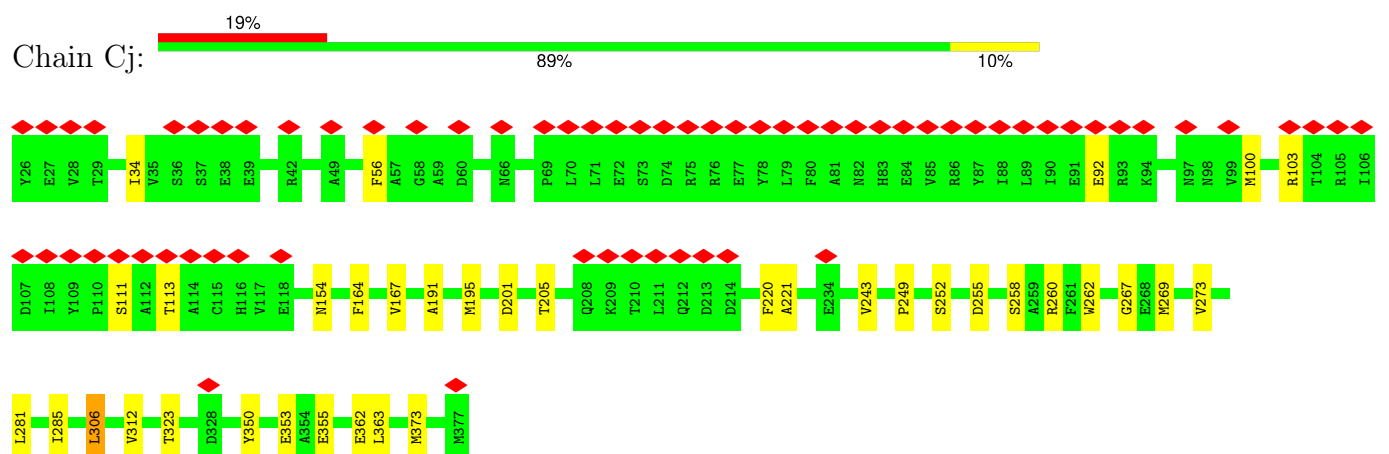
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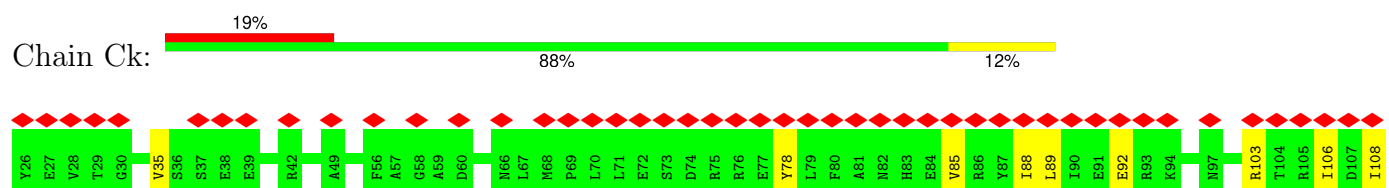
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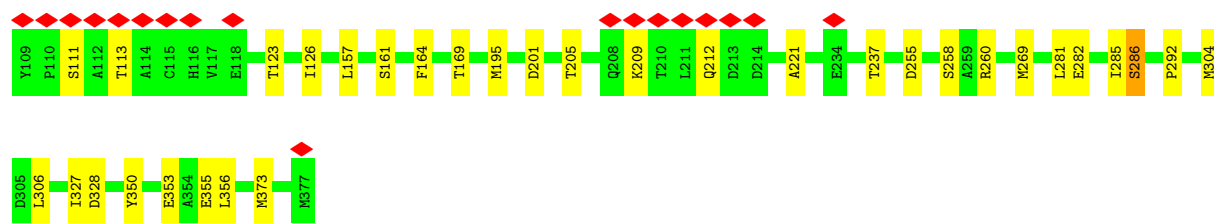
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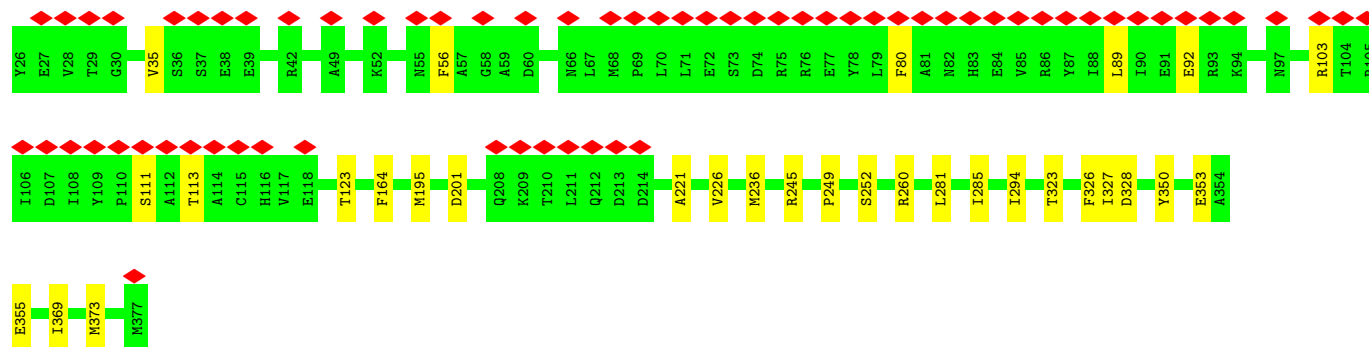
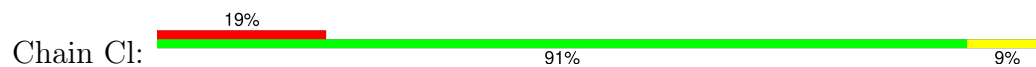
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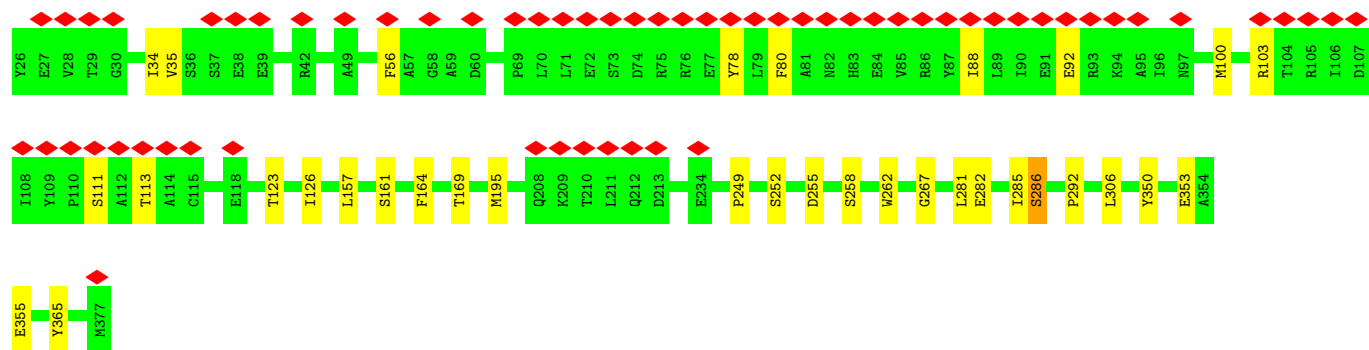




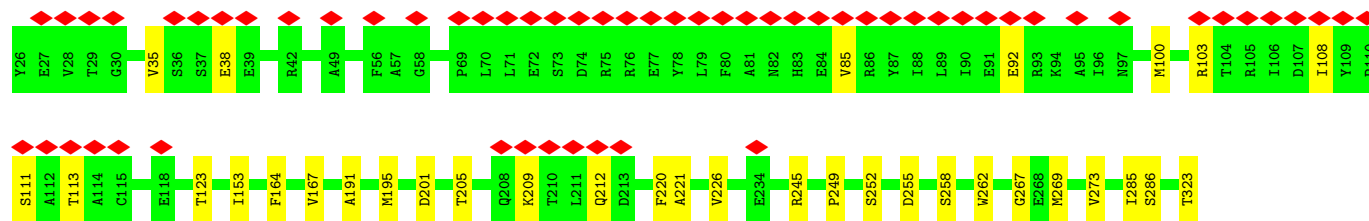
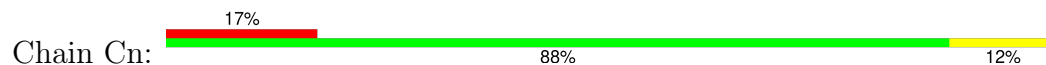
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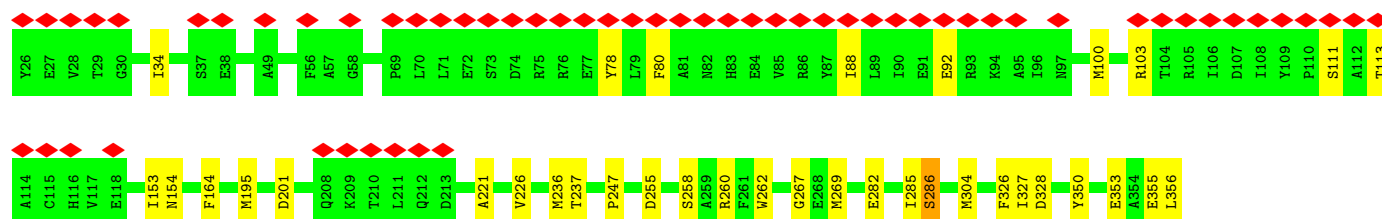
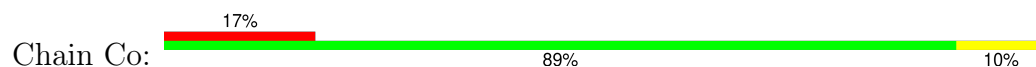


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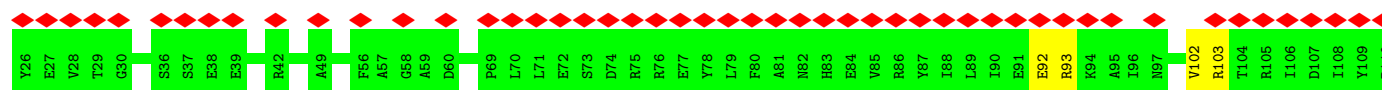
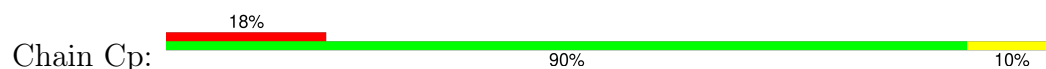




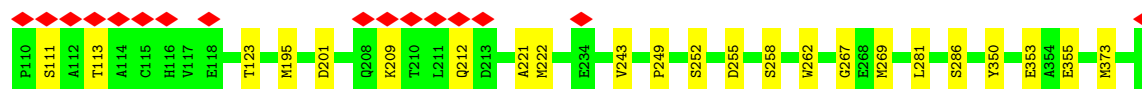
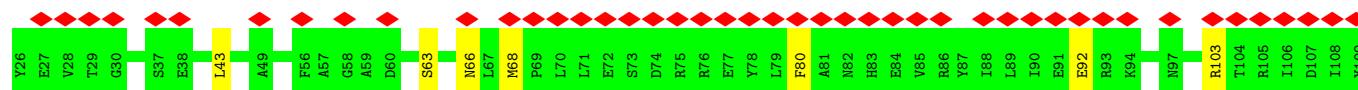
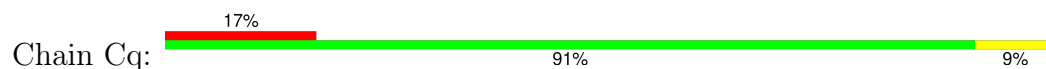
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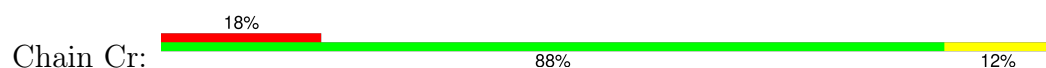
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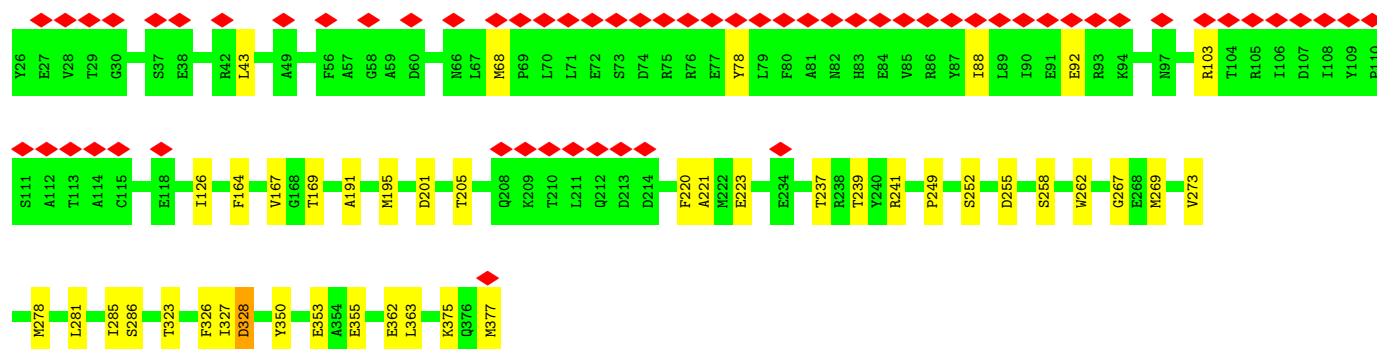


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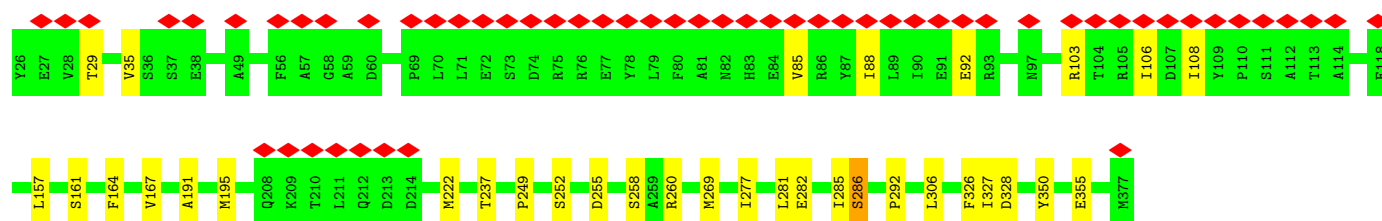
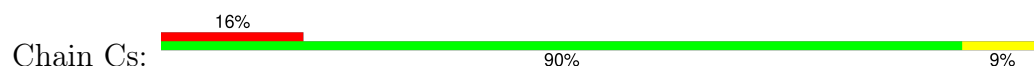


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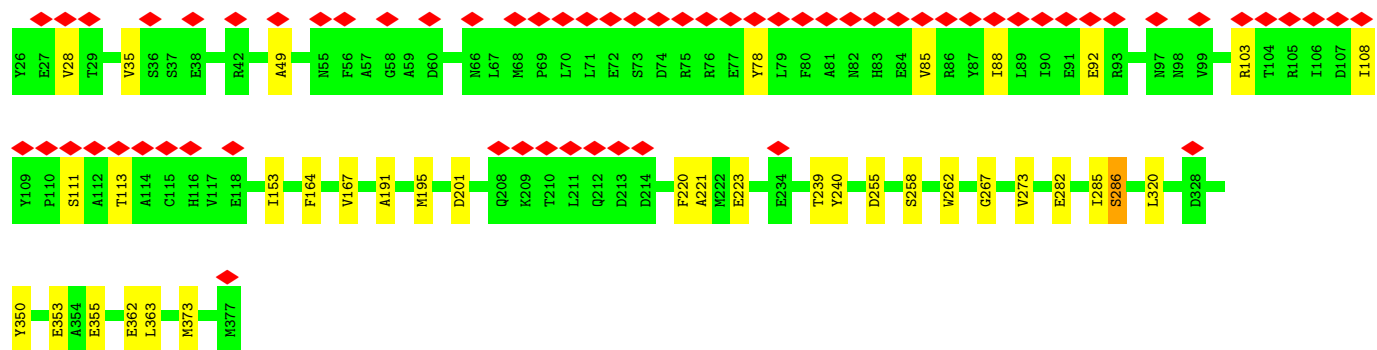
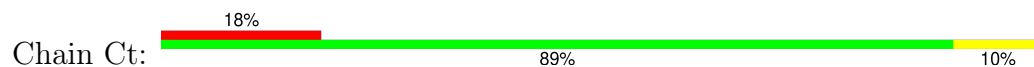




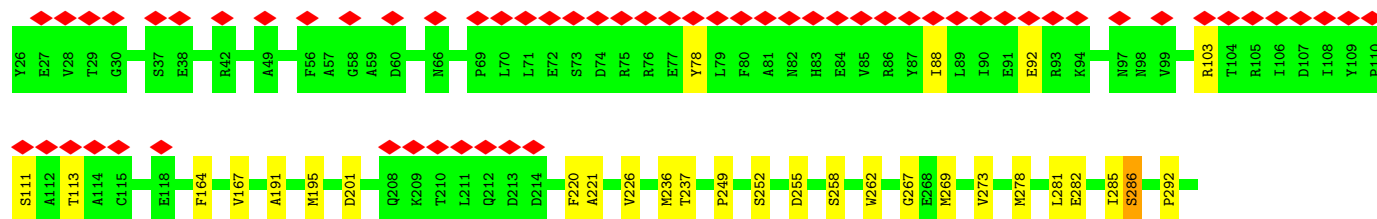
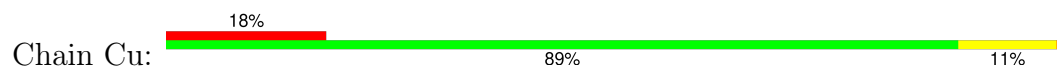
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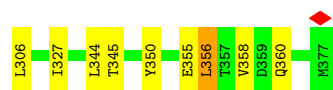


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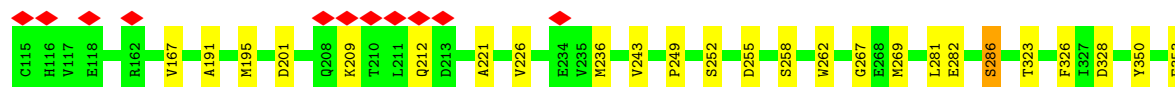
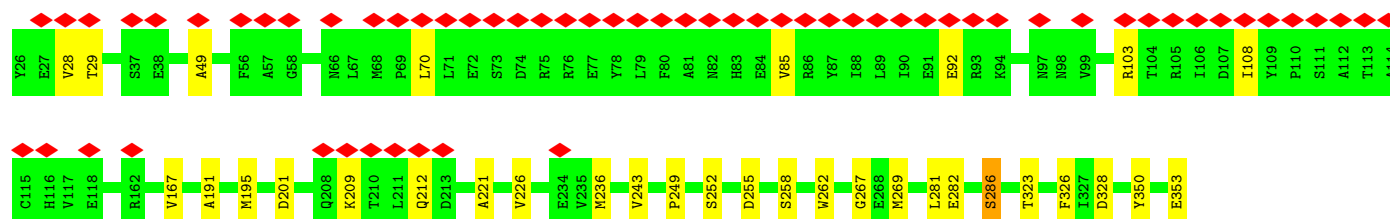
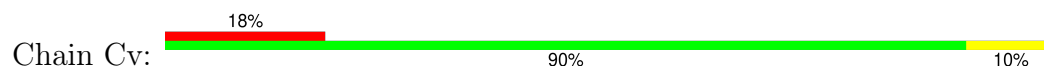


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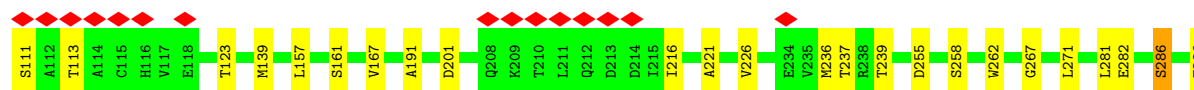




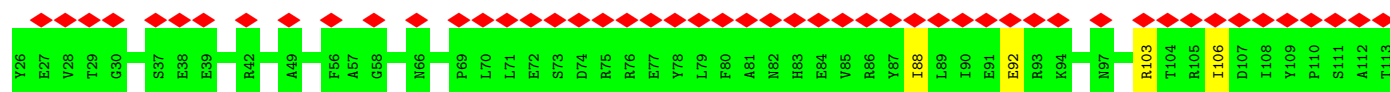
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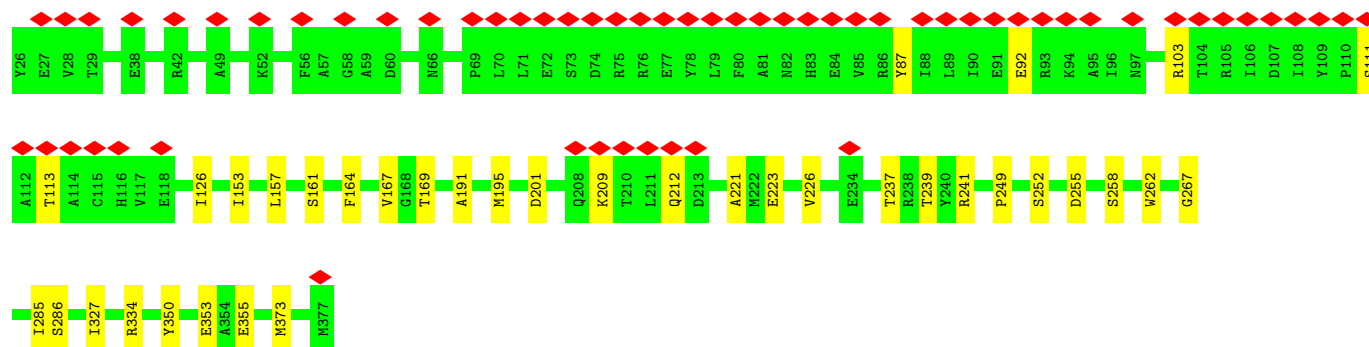
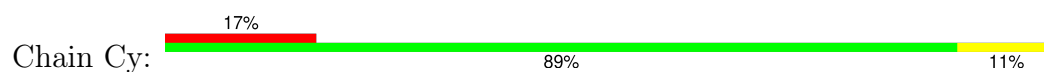
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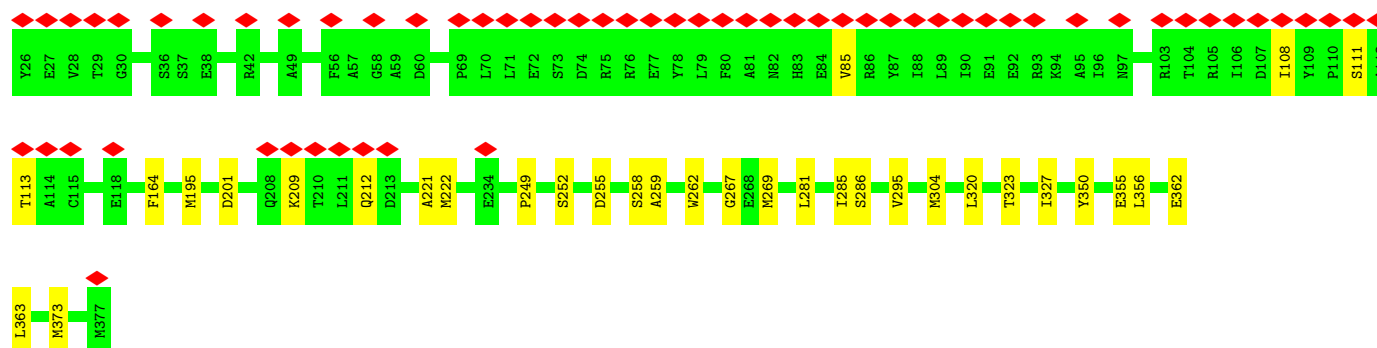
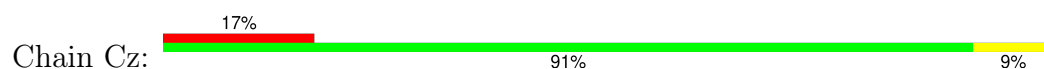
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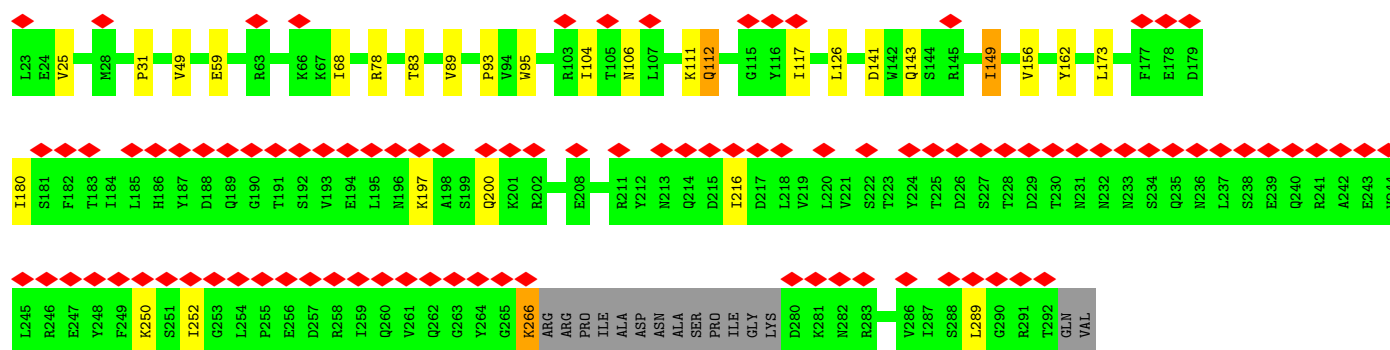
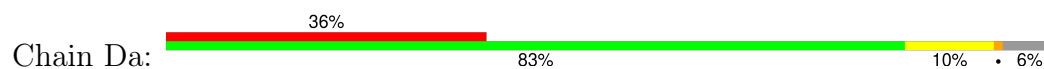
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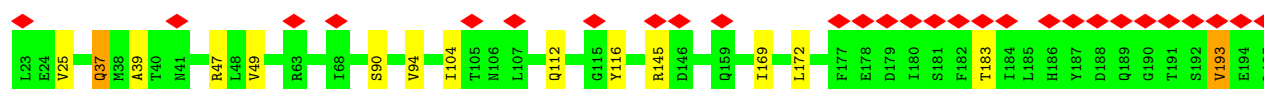
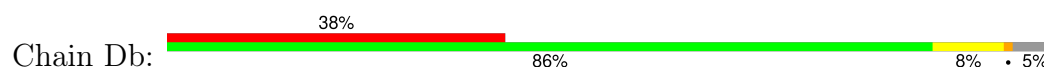
• Molecule 3: Flagellar protein FlgT

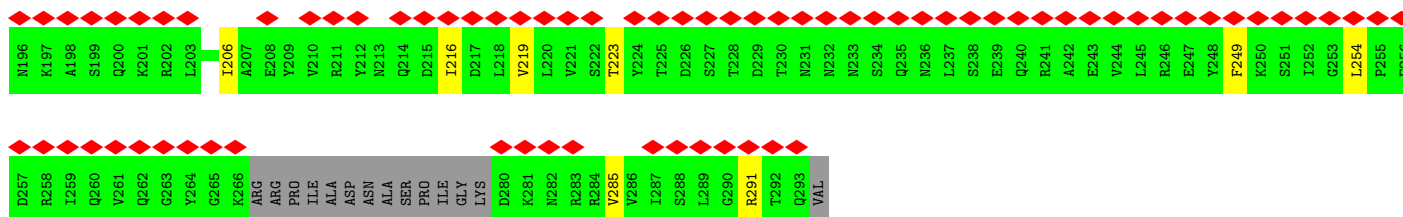


• Molecule 4: Sodium-type flagellar protein MotY

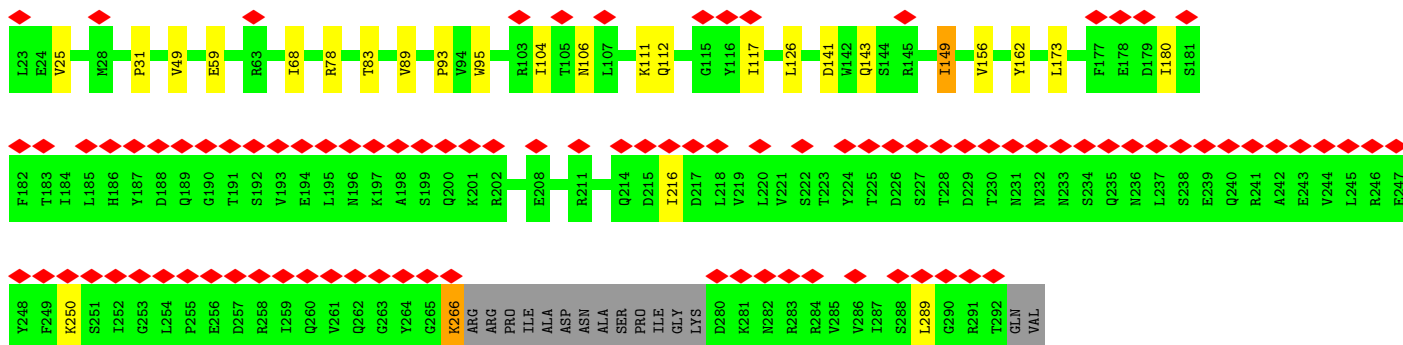
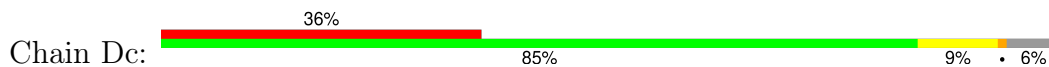


• Molecule 4: Sodium-type flagellar protein MotY

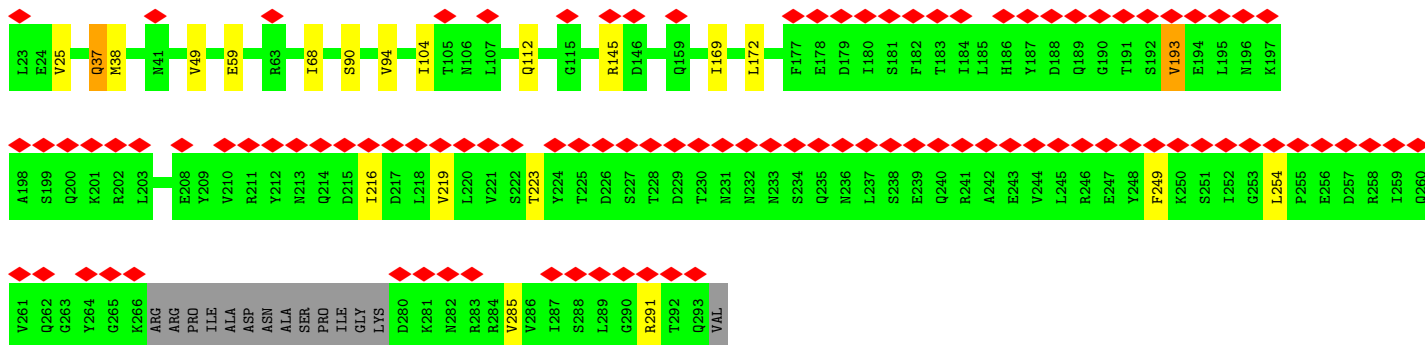
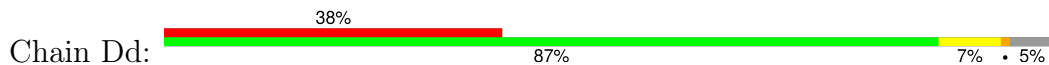




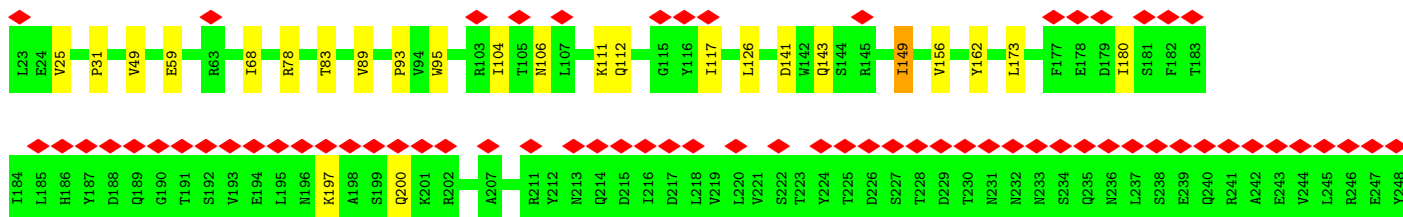
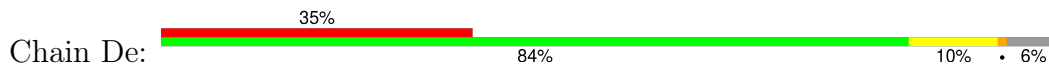
• Molecule 4: Sodium-type flagellar protein MotY

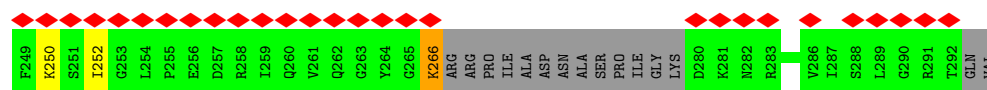


• Molecule 4: Sodium-type flagellar protein MotY

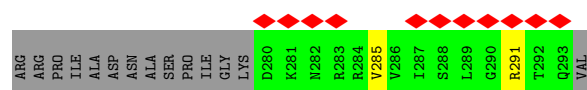
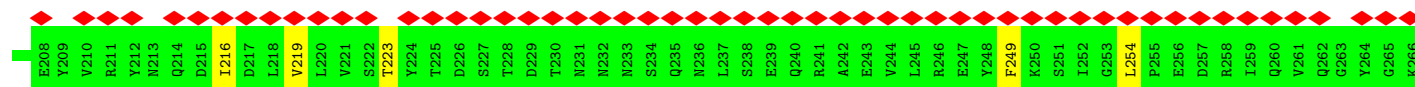
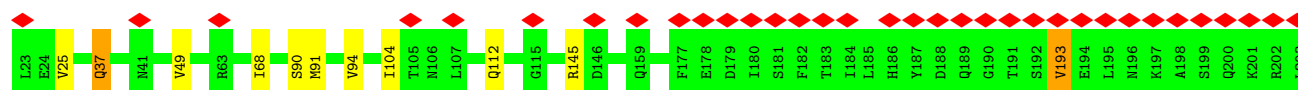
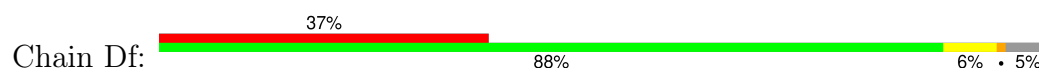


• Molecule 4: Sodium-type flagellar protein MotY

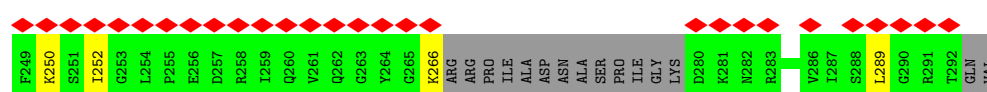
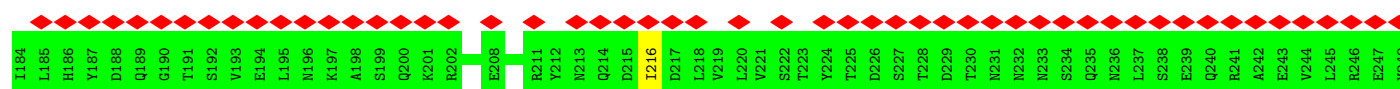
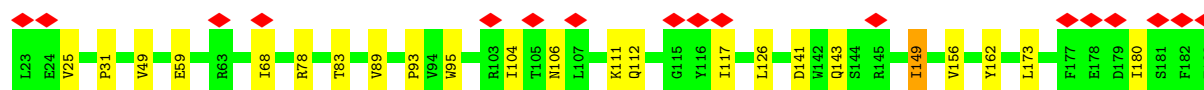
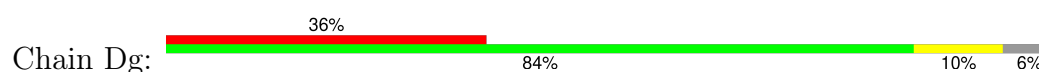




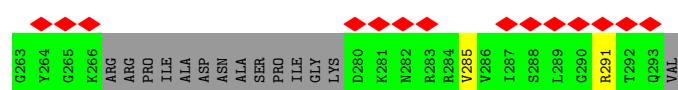
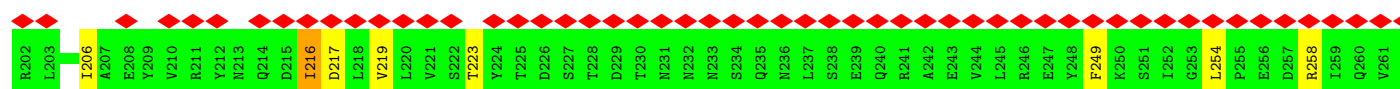
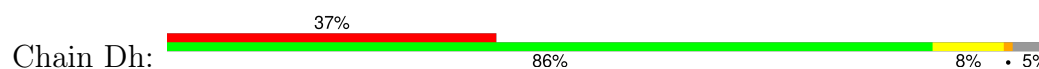
• Molecule 4: Sodium-type flagellar protein MotY



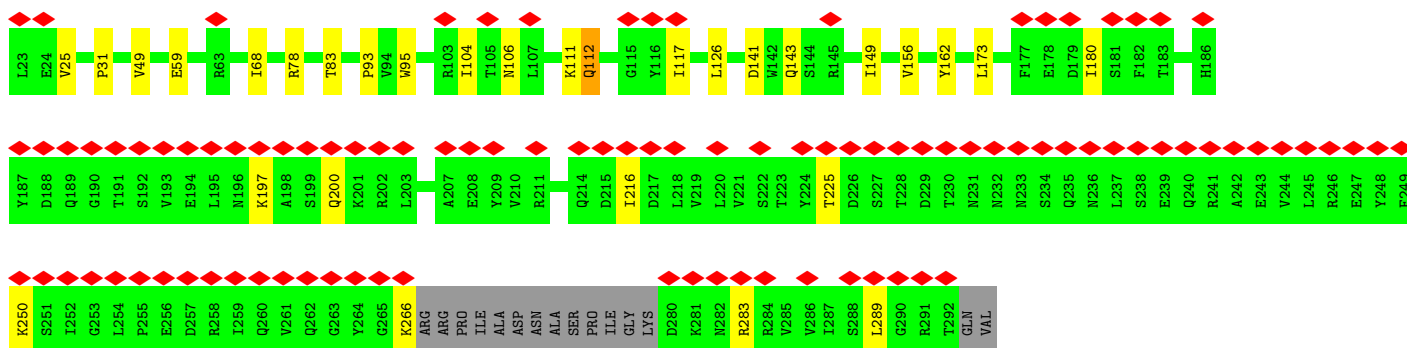
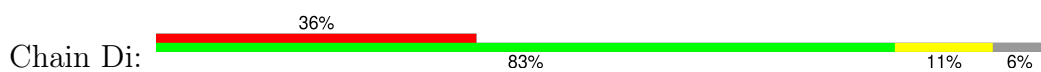
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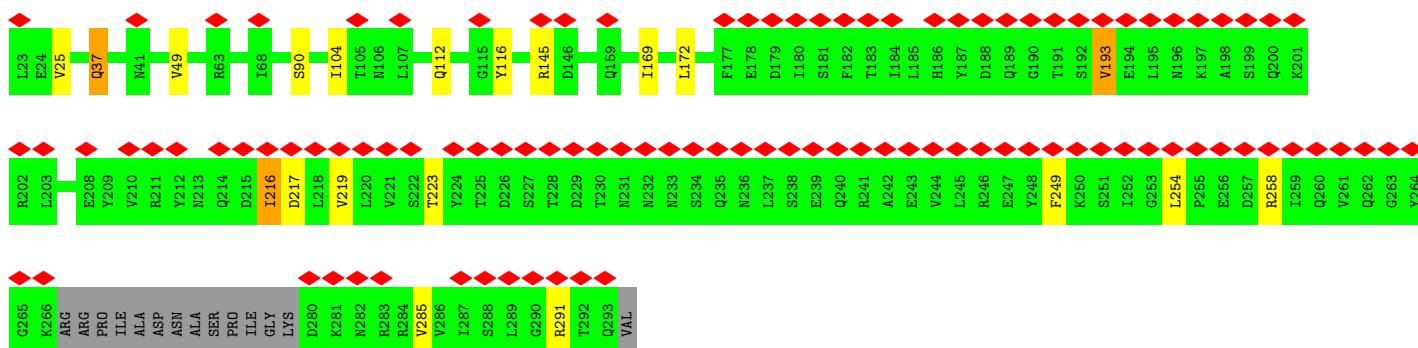
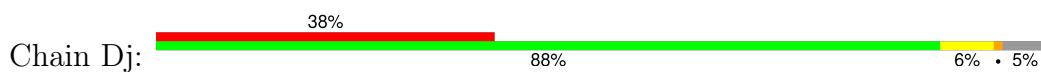
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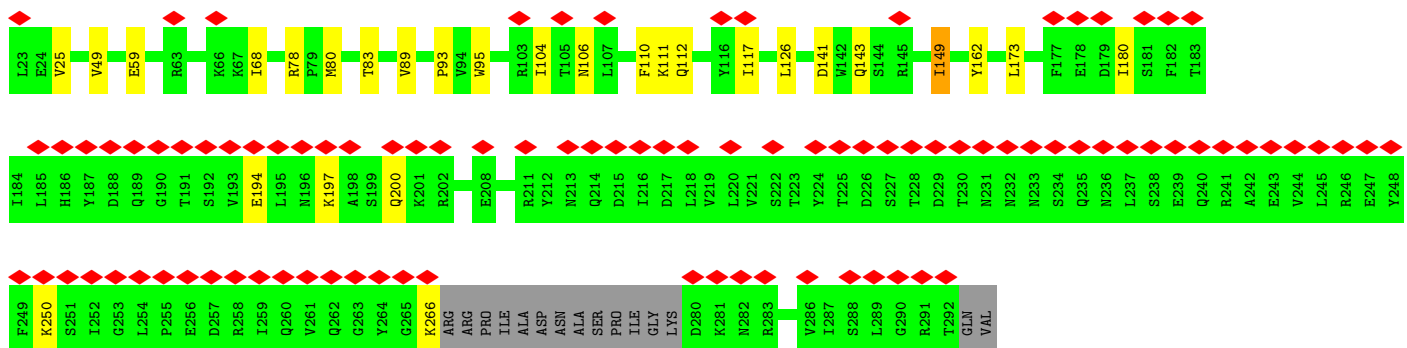
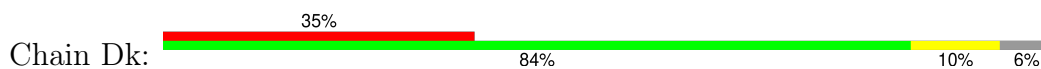
• Molecule 4: Sodium-type flagellar protein MotY



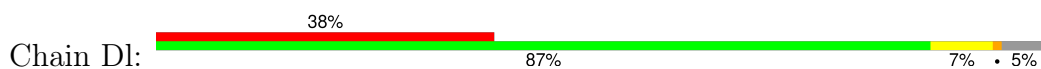
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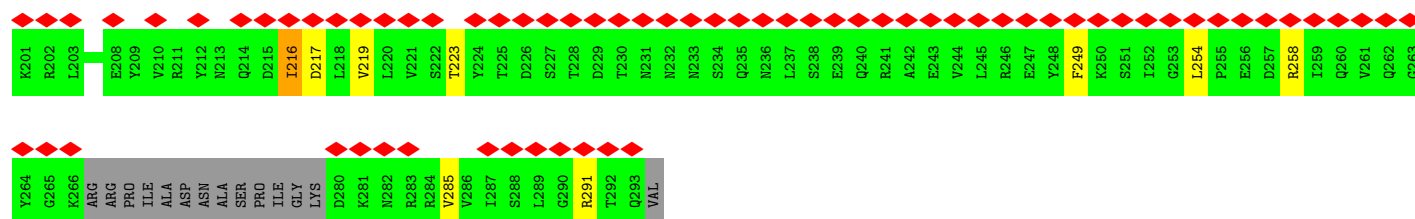
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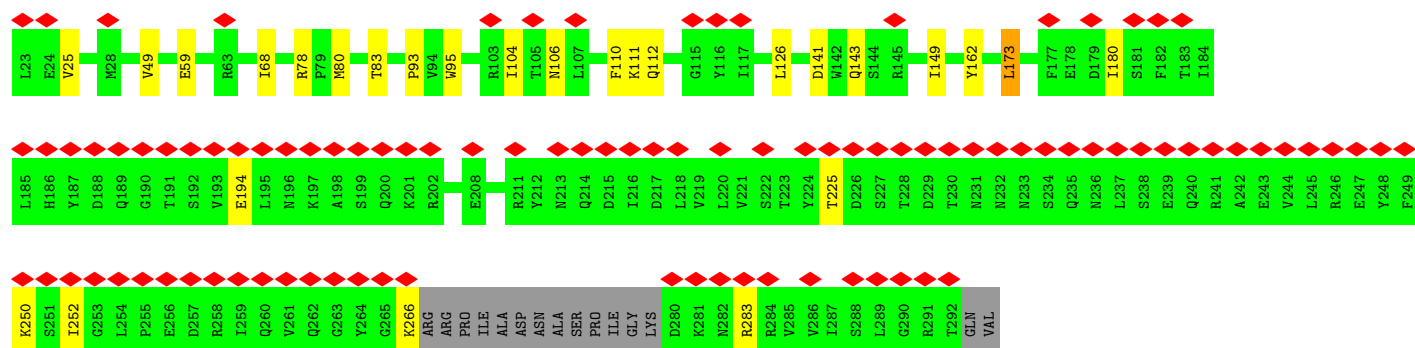
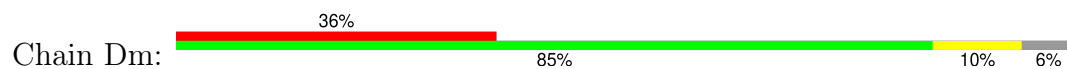
• Molecule 4: Sodium-type flagellar protein MotY



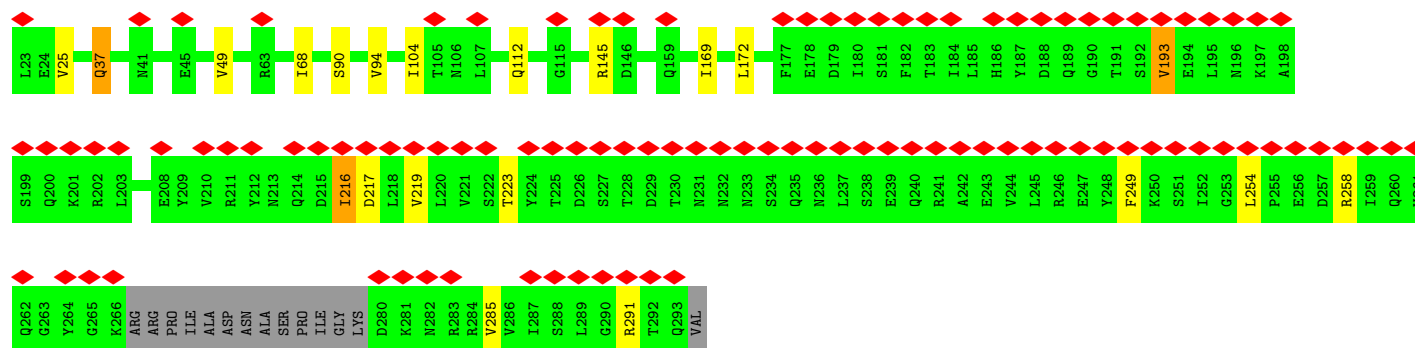
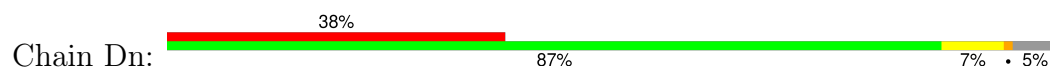




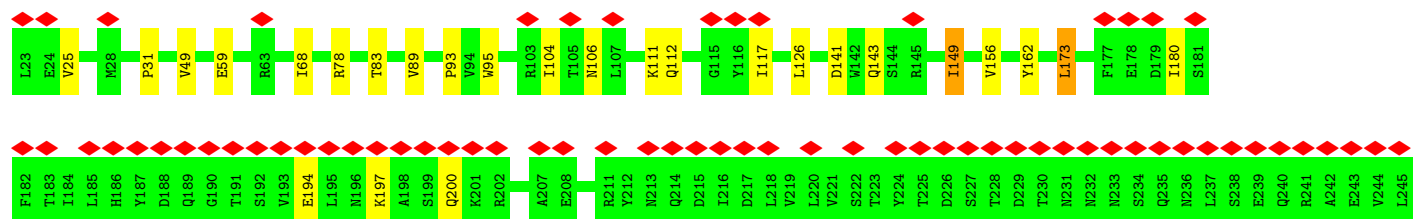
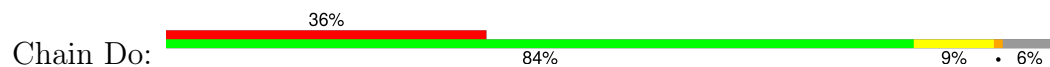
• Molecule 4: Sodium-type flagellar protein MotY

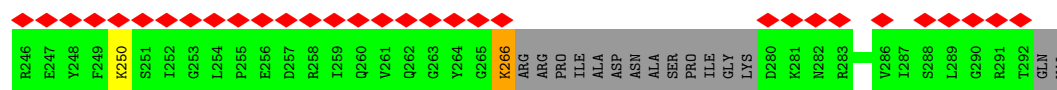


• Molecule 4: Sodium-type flagellar protein MotY



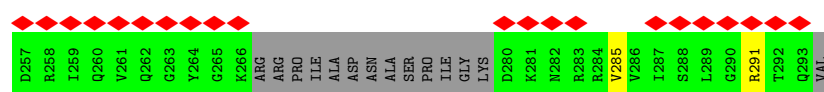
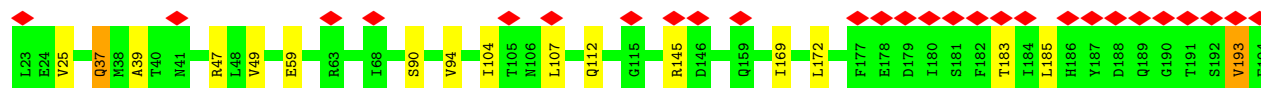
• Molecule 4: Sodium-type flagellar protein MotY





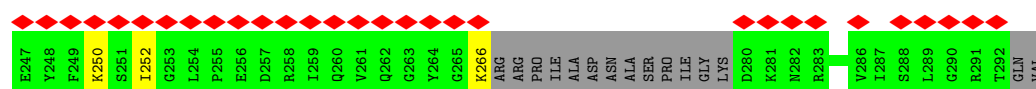
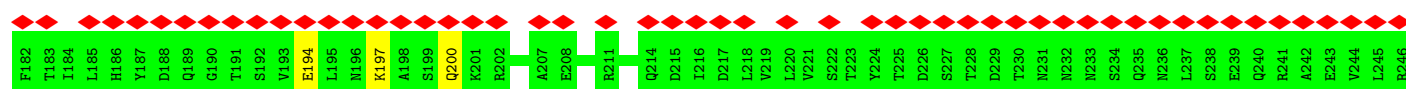
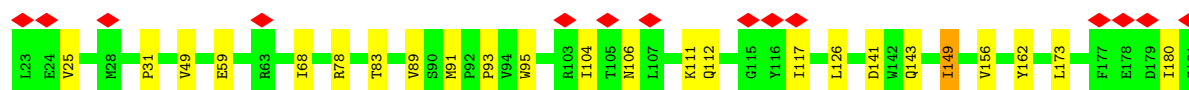
• Molecule 4: Sodium-type flagellar protein MotY

Chain Dp: 38% 85% 9% • 5%



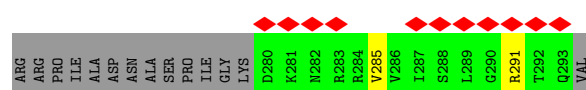
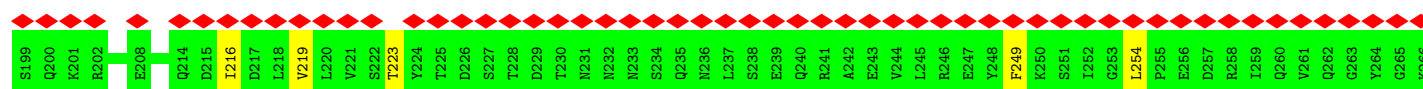
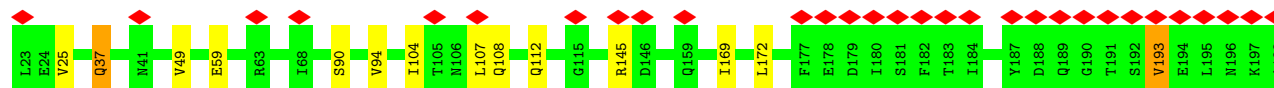
• Molecule 4: Sodium-type flagellar protein MotY

Chain Dq: 36% 83% 11% 6%




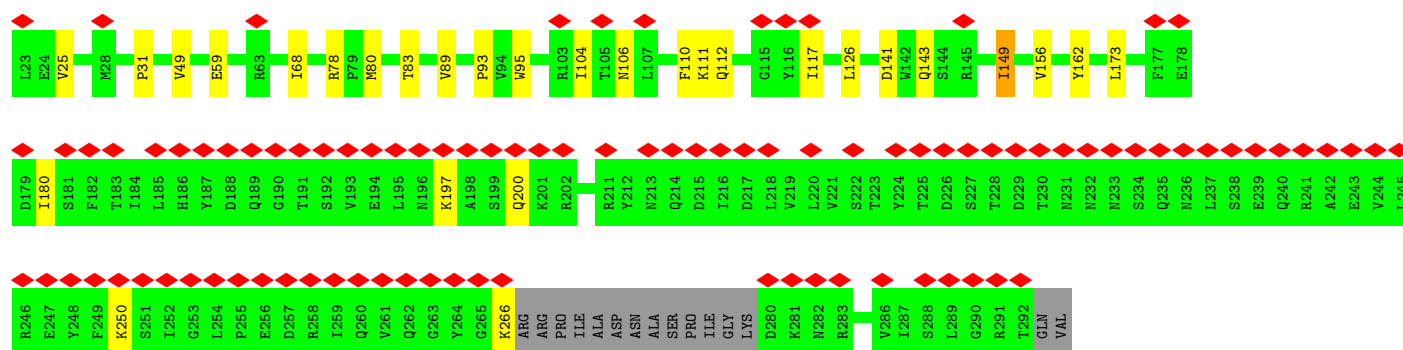
• Molecule 4: Sodium-type flagellar protein MotY

Chain Dr: 36% 87% 7% • 5%




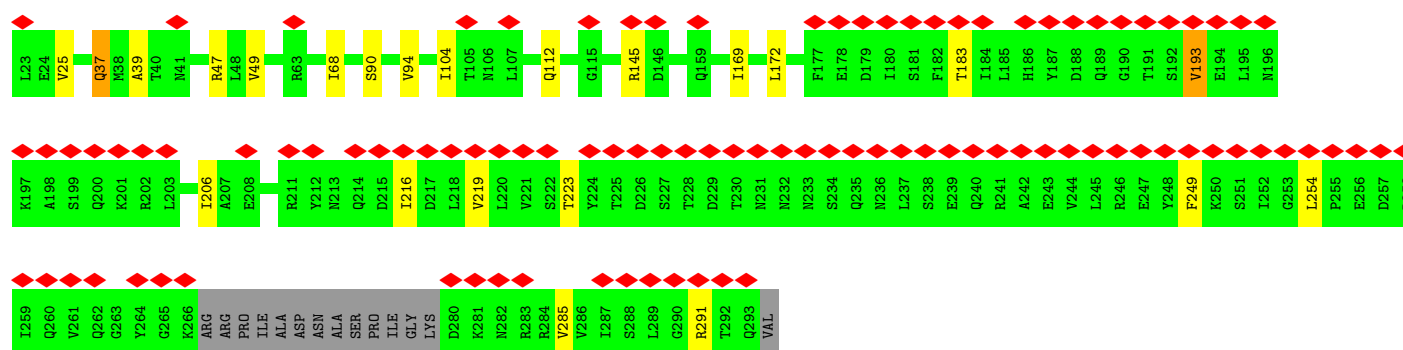
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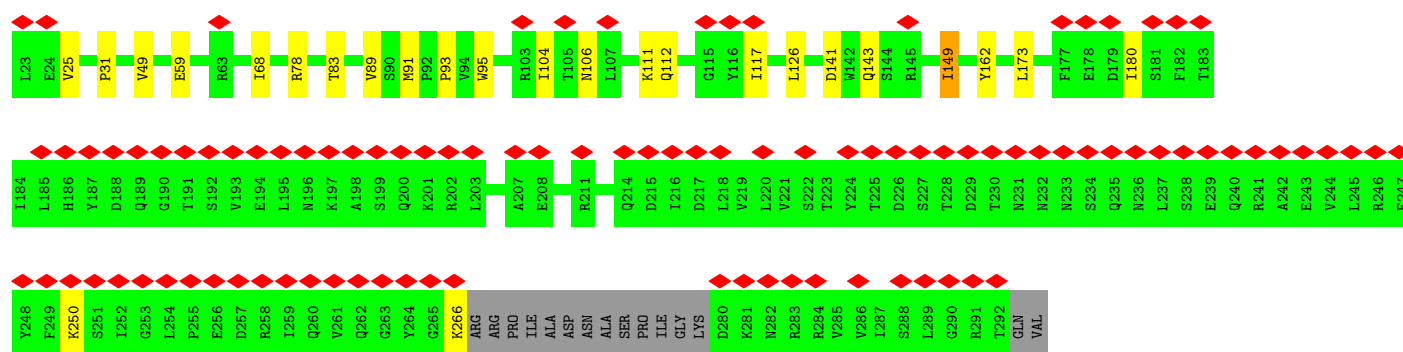
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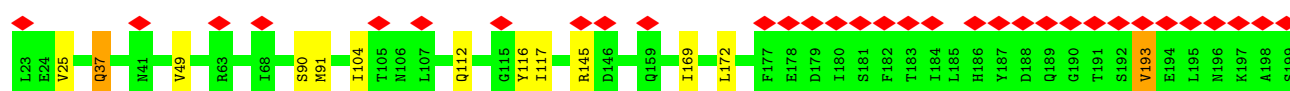
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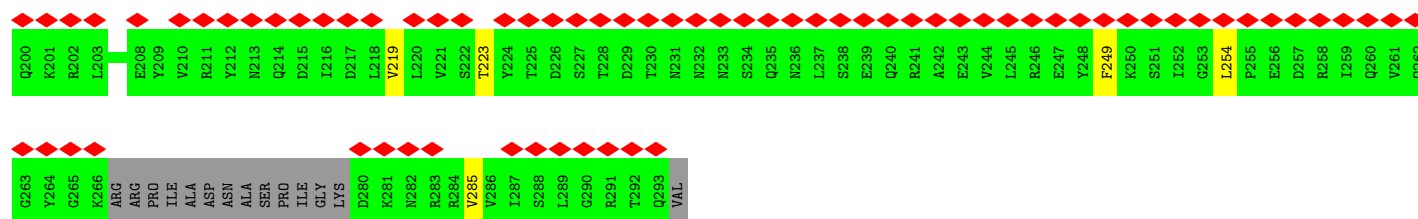
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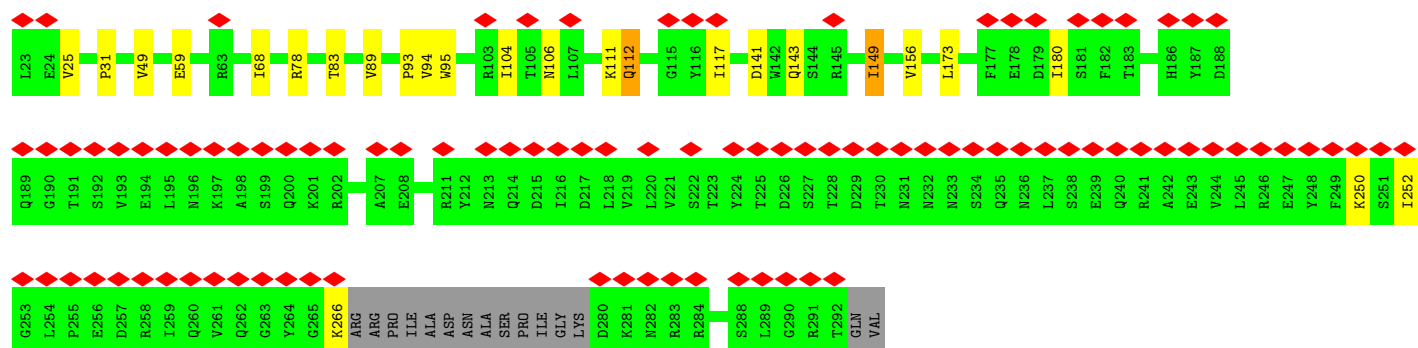
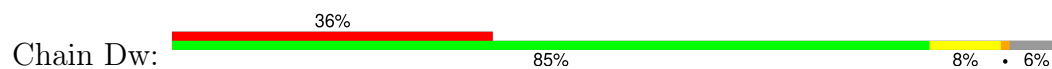
• Molecule 4: Sodium-type flagellar protein MotY

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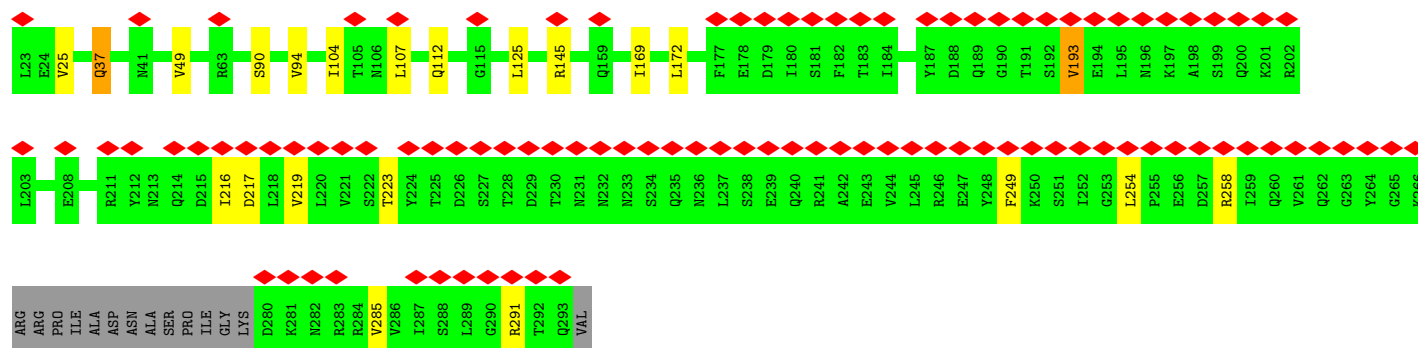
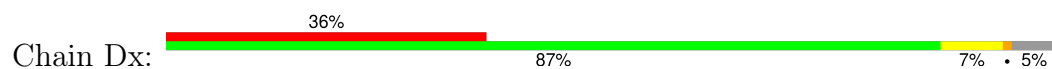




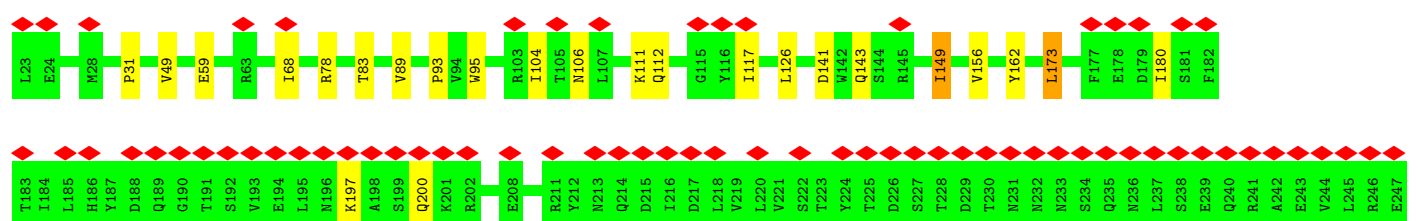
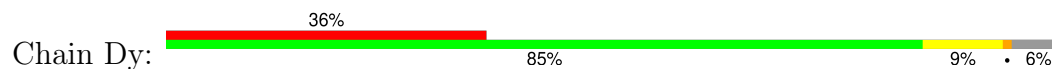
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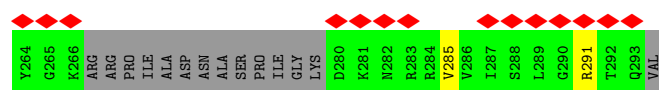
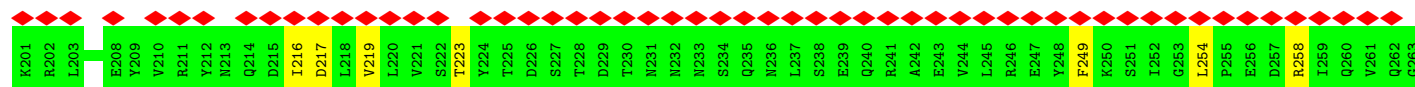
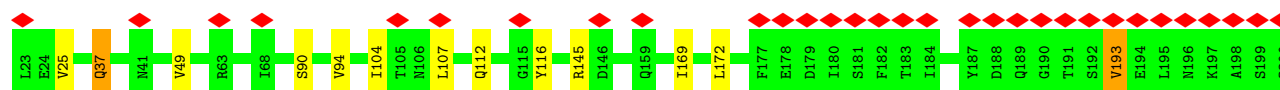
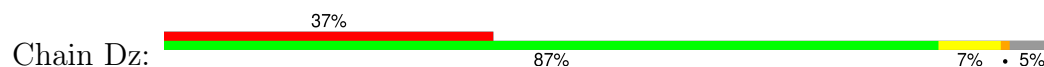


• Molecule 4: Sodium-type flagellar protein MotY

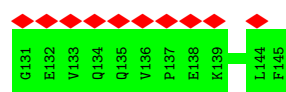




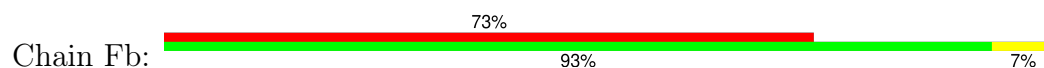
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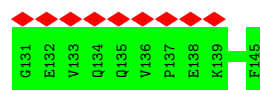
• Molecule 5: Flagellar assembly lipoprotein FlgP



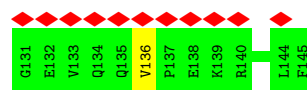
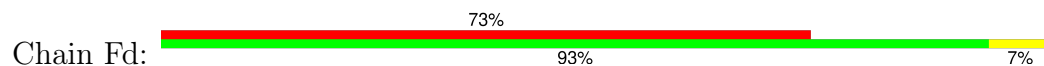
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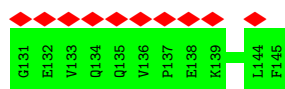
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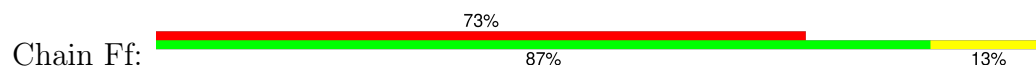
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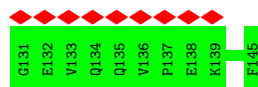
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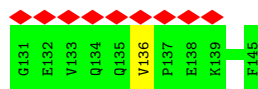
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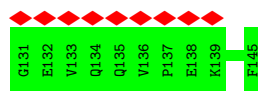
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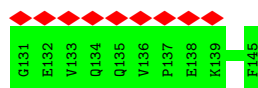
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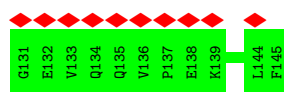


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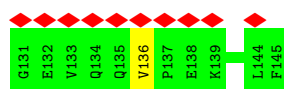




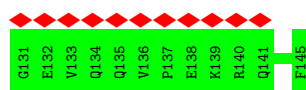
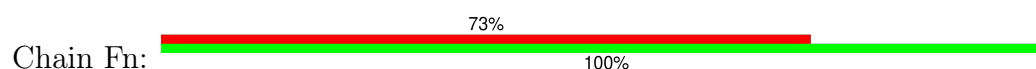
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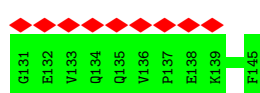
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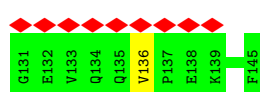
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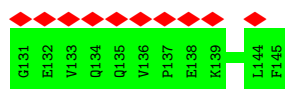
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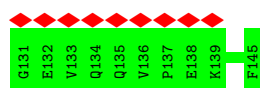
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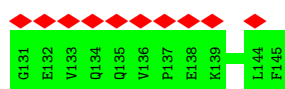
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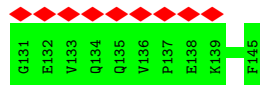
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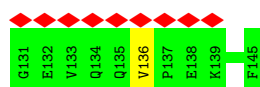
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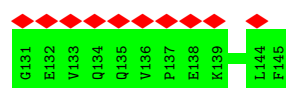


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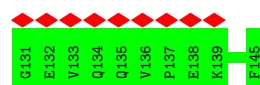




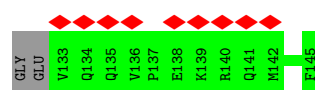
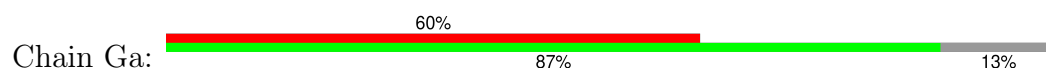
## • Molecule 5: Flagellar assembly lipoprotein FlgP



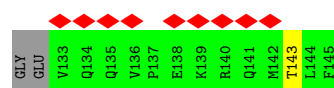
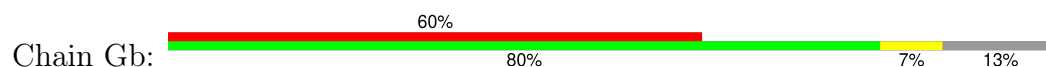
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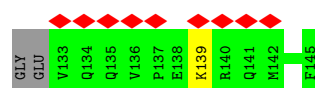
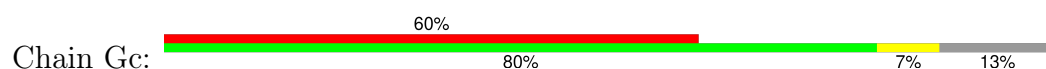
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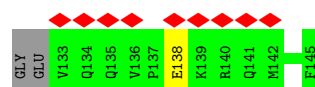
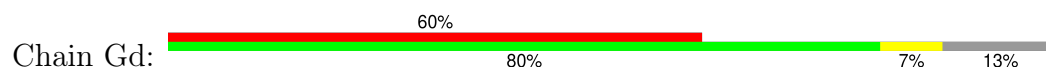
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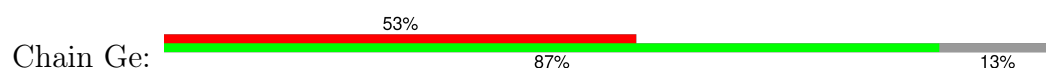
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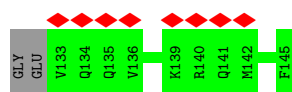


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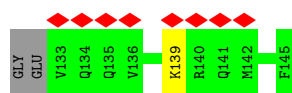
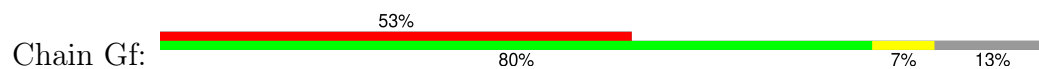


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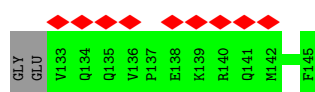
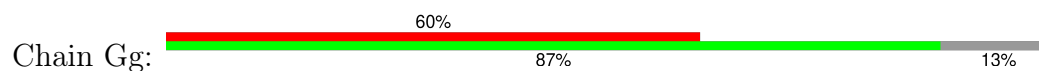




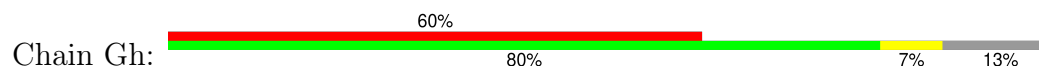
- Molecule 5: Flagellar assembly lipoprotein FlgP



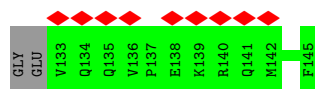
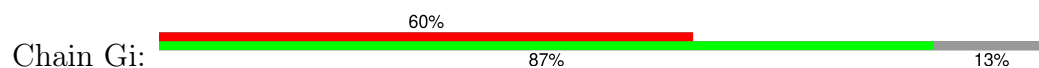
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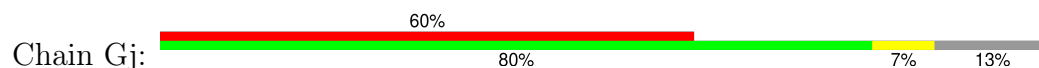
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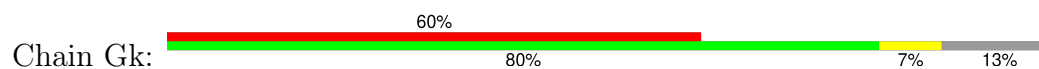
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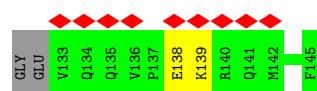
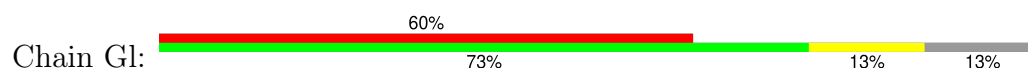
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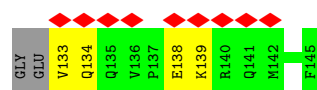
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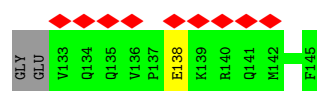
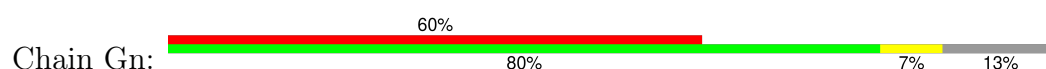
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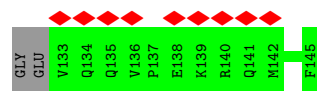
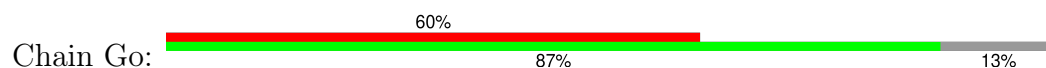
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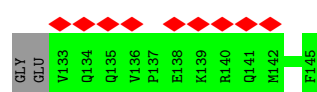
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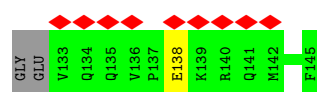
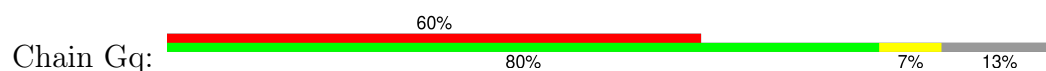
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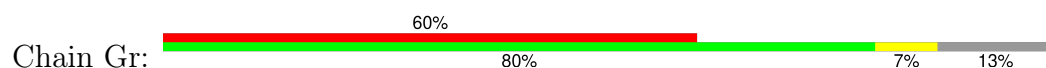
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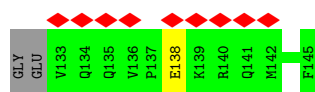


• Molecule 5: Flagellar assembly lipoprotein FlgP

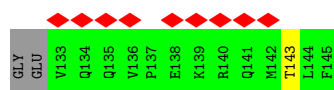
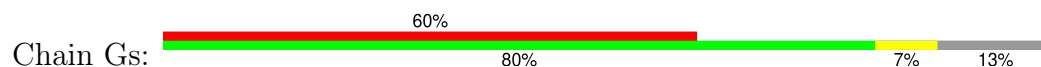


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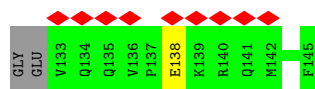
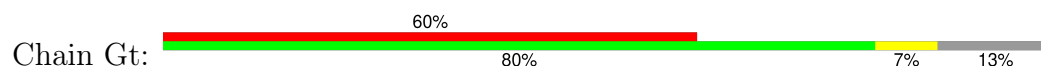




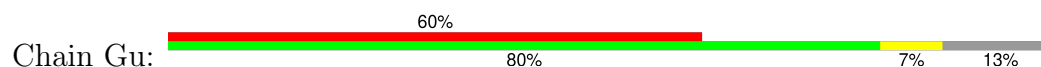
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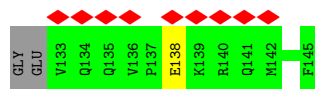
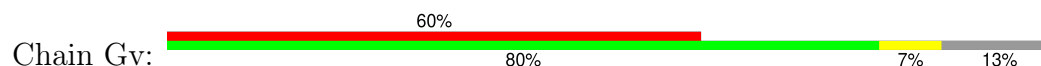
- Molecule 5: Flagellar assembly lipoprotein FlgP



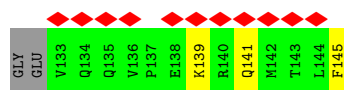
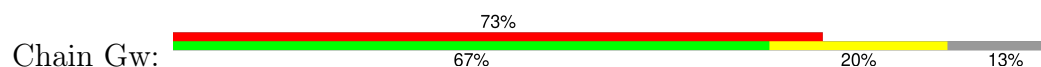
- Molecule 5: Flagellar assembly lipoprotein FlgP



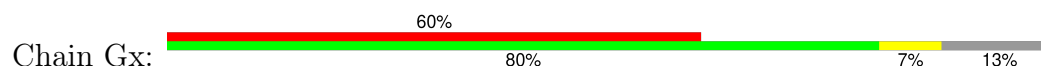
- Molecule 5: Flagellar assembly lipoprotein FlgP



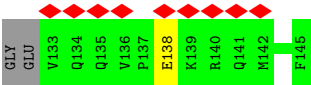
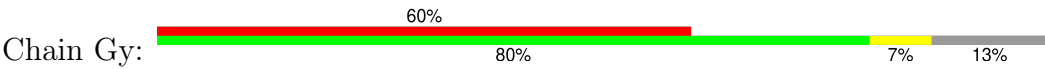
- Molecule 5: Flagellar assembly lipoprotein FlgP



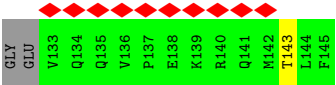
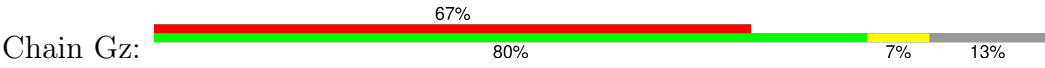
- Molecule 5: Flagellar assembly lipoprotein FlgP



- Molecule 5: Flagellar assembly lipoprotein FlgP



• Molecule 5: Flagellar assembly lipoprotein FlgP



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C26	Depositor
Number of particles used	31668	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.252	Depositor
Minimum map value	-0.664	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.188	Depositor
Map size (Å)	478.464, 478.464, 478.464	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	Aa	0.11	0/1699	0.30	0/2303
1	Ab	0.12	0/1699	0.31	0/2303
1	Ac	0.12	0/1699	0.31	0/2303
1	Ad	0.12	0/1699	0.31	0/2303
1	Ae	0.12	0/1699	0.30	0/2303
1	Af	0.11	0/1699	0.31	0/2303
1	Ag	0.12	0/1699	0.31	0/2303
1	Ah	0.11	0/1699	0.30	0/2303
1	Ai	0.11	0/1699	0.30	0/2303
1	Aj	0.12	0/1699	0.30	0/2303
1	Ak	0.12	0/1699	0.30	0/2303
1	Al	0.11	0/1699	0.30	0/2303
1	Am	0.12	0/1699	0.30	0/2303
1	An	0.11	0/1699	0.30	0/2303
1	Ao	0.12	0/1699	0.30	0/2303
1	Ap	0.12	0/1699	0.30	0/2303
1	Aq	0.12	0/1699	0.31	0/2303
1	Ar	0.12	0/1699	0.30	0/2303
1	As	0.12	0/1699	0.31	0/2303
1	At	0.12	0/1699	0.30	0/2303
1	Au	0.12	0/1699	0.31	0/2303
1	Av	0.12	0/1699	0.30	0/2303
1	Aw	0.12	0/1699	0.30	0/2303
1	Ax	0.11	0/1699	0.30	0/2303
1	Ay	0.12	0/1699	0.30	0/2303
1	Az	0.12	0/1699	0.30	0/2303
2	Ba	0.13	0/2535	0.32	0/3442
2	Bb	0.13	0/2535	0.32	0/3442
2	Bc	0.12	0/2535	0.31	0/3442
2	Bd	0.13	0/2535	0.31	0/3442
2	Be	0.13	0/2535	0.31	0/3442
2	Bf	0.13	0/2535	0.32	0/3442
2	Bg	0.13	0/2535	0.32	0/3442
2	Bh	0.13	0/2535	0.32	0/3442

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Bi	0.13	0/2535	0.32	0/3442
2	Bj	0.12	0/2535	0.31	0/3442
2	Bk	0.13	0/2535	0.32	0/3442
2	Bl	0.13	0/2535	0.32	0/3442
2	Bm	0.13	0/2535	0.32	0/3442
2	Bn	0.13	0/2535	0.32	0/3442
2	Bo	0.13	0/2535	0.32	0/3442
2	Bp	0.13	0/2535	0.32	0/3442
2	Bq	0.13	0/2535	0.33	0/3442
2	Br	0.13	0/2535	0.32	0/3442
2	Bs	0.13	0/2535	0.32	0/3442
2	Bt	0.13	0/2535	0.32	0/3442
2	Bu	0.12	0/2535	0.31	0/3442
2	Bv	0.13	0/2535	0.33	0/3442
2	Bw	0.13	0/2535	0.32	0/3442
2	Bx	0.13	0/2535	0.33	0/3442
2	By	0.13	0/2535	0.33	0/3442
2	Bz	0.13	0/2535	0.32	0/3442
3	Ca	0.12	0/2816	0.31	0/3809
3	Cb	0.12	0/2816	0.32	0/3809
3	Cc	0.12	0/2816	0.31	0/3809
3	Cd	0.13	0/2816	0.31	0/3809
3	Ce	0.12	0/2816	0.31	0/3809
3	Cf	0.12	0/2816	0.31	0/3809
3	Cg	0.12	0/2816	0.32	0/3809
3	Ch	0.12	0/2816	0.30	0/3809
3	Ci	0.12	0/2816	0.31	0/3809
3	Cj	0.12	0/2816	0.31	0/3809
3	Ck	0.11	0/2816	0.30	0/3809
3	Cl	0.12	0/2816	0.33	0/3809
3	Cm	0.12	0/2816	0.32	0/3809
3	Cn	0.12	0/2816	0.31	0/3809
3	Co	0.12	0/2816	0.31	0/3809
3	Cp	0.12	0/2816	0.31	0/3809
3	Cq	0.12	0/2816	0.31	0/3809
3	Cr	0.11	0/2816	0.29	0/3809
3	Cs	0.12	0/2816	0.31	0/3809
3	Ct	0.12	0/2816	0.31	0/3809
3	Cu	0.12	0/2816	0.32	0/3809
3	Cv	0.12	0/2816	0.30	0/3809
3	Cw	0.12	0/2816	0.30	0/3809
3	Cx	0.12	0/2816	0.31	0/3809
3	Cy	0.12	0/2816	0.31	0/3809



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	Cz	0.12	0/2816	0.30	0/3809
4	Da	0.13	0/2129	0.35	0/2882
4	Db	0.13	0/2124	0.34	0/2877
4	Dc	0.13	0/2129	0.34	0/2882
4	Dd	0.14	0/2124	0.35	0/2877
4	De	0.13	0/2129	0.34	0/2882
4	Df	0.13	0/2124	0.35	0/2877
4	Dg	0.14	0/2129	0.34	0/2882
4	Dh	0.13	0/2124	0.34	0/2877
4	Di	0.13	0/2129	0.34	0/2882
4	Dj	0.13	0/2124	0.35	0/2877
4	Dk	0.13	0/2129	0.35	0/2882
4	Dl	0.13	0/2124	0.34	0/2877
4	Dm	0.13	0/2129	0.34	0/2882
4	Dn	0.14	0/2124	0.35	0/2877
4	Do	0.13	0/2129	0.33	0/2882
4	Dp	0.14	0/2124	0.35	0/2877
4	Dq	0.13	0/2129	0.34	0/2882
4	Dr	0.14	0/2124	0.35	0/2877
4	Ds	0.13	0/2129	0.33	0/2882
4	Dt	0.13	0/2124	0.34	0/2877
4	Du	0.14	0/2129	0.34	0/2882
4	Dv	0.14	0/2124	0.34	0/2877
4	Dw	0.13	0/2129	0.34	0/2882
4	Dx	0.14	0/2124	0.35	0/2877
4	Dy	0.13	0/2129	0.34	0/2882
4	Dz	0.13	0/2124	0.34	0/2877
5	Fa	0.15	0/126	0.41	0/166
5	Fb	0.13	0/126	0.33	0/166
5	Fc	0.14	0/126	0.37	0/166
5	Fd	0.16	0/126	0.39	0/166
5	Fe	0.15	0/126	0.37	0/166
5	Ff	0.14	0/126	0.39	0/166
5	Fg	0.15	0/126	0.39	0/166
5	Fh	0.15	0/126	0.40	0/166
5	Fi	0.14	0/126	0.39	0/166
5	Fj	0.15	0/126	0.40	0/166
5	Fk	0.15	0/126	0.39	0/166
5	Fl	0.16	0/126	0.41	0/166
5	Fm	0.15	0/126	0.40	0/166
5	Fn	0.16	0/126	0.41	0/166
5	Fo	0.17	0/126	0.44	0/166
5	Fp	0.15	0/126	0.40	0/166

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	Fq	0.15	0/126	0.40	0/166
5	Fr	0.16	0/126	0.40	0/166
5	Fs	0.15	0/126	0.39	0/166
5	Ft	0.16	0/126	0.39	0/166
5	Fu	0.18	0/126	0.41	0/166
5	Fv	0.14	0/126	0.39	0/166
5	Fw	0.15	0/126	0.37	0/166
5	Fx	0.15	0/126	0.43	0/166
5	Fy	0.15	0/126	0.38	0/166
5	Fz	0.16	0/126	0.43	0/166
5	Ga	0.15	0/113	0.45	0/149
5	Gb	0.16	0/113	0.42	0/149
5	Gc	0.16	0/113	0.47	0/149
5	Gd	0.13	0/113	0.41	0/149
5	Ge	0.19	0/113	0.49	0/149
5	Gf	0.15	0/113	0.41	0/149
5	Gg	0.15	0/113	0.42	0/149
5	Gh	0.15	0/113	0.44	0/149
5	Gi	0.19	0/113	0.52	0/149
5	Gj	0.14	0/113	0.43	0/149
5	Gk	0.13	0/113	0.42	0/149
5	Gl	0.16	0/113	0.47	0/149
5	Gm	0.15	0/113	0.42	0/149
5	Gn	0.15	0/113	0.42	0/149
5	Go	0.14	0/113	0.41	0/149
5	Gp	0.15	0/113	0.43	0/149
5	Gq	0.14	0/113	0.45	0/149
5	Gr	0.15	0/113	0.44	0/149
5	Gs	0.12	0/113	0.41	0/149
5	Gt	0.17	0/113	0.45	0/149
5	Gu	0.12	0/113	0.41	0/149
5	Gv	0.18	0/113	0.50	0/149
5	Gw	0.20	0/113	0.59	0/149
5	Gx	0.15	0/113	0.41	0/149
5	Gy	0.19	0/113	0.50	0/149
5	Gz	0.16	0/113	0.43	0/149
All	All	0.13	0/244803	0.32	0/331461

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	1674	0	1609	26	0
1	Ab	1674	0	1609	27	0
1	Ac	1674	0	1609	27	0
1	Ad	1674	0	1609	25	0
1	Ae	1674	0	1609	28	0
1	Af	1674	0	1609	28	0
1	Ag	1674	0	1609	26	0
1	Ah	1674	0	1609	26	0
1	Ai	1674	0	1609	25	0
1	Aj	1674	0	1609	27	0
1	Ak	1674	0	1609	27	0
1	Al	1674	0	1609	25	0
1	Am	1674	0	1609	27	0
1	An	1674	0	1609	29	0
1	Ao	1674	0	1609	28	0
1	Ap	1674	0	1609	31	0
1	Aq	1674	0	1609	25	0
1	Ar	1674	0	1609	27	0
1	As	1674	0	1609	26	0
1	At	1674	0	1609	23	0
1	Au	1674	0	1609	27	0
1	Av	1674	0	1609	27	0
1	Aw	1674	0	1609	25	0
1	Ax	1674	0	1609	27	0
1	Ay	1674	0	1609	27	0
1	Az	1674	0	1609	26	0
2	Ba	2501	0	2549	34	0
2	Bb	2501	0	2549	31	0
2	Bc	2501	0	2549	39	0
2	Bd	2501	0	2549	31	0
2	Be	2501	0	2549	35	0
2	Bf	2501	0	2549	30	0
2	Bg	2501	0	2549	35	0
2	Bh	2501	0	2549	30	0
2	Bi	2501	0	2549	33	0
2	Bj	2501	0	2549	33	0
2	Bk	2501	0	2549	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bl	2501	0	2549	43	0
2	Bm	2501	0	2549	32	0
2	Bn	2501	0	2549	28	0
2	Bo	2501	0	2549	39	0
2	Bp	2501	0	2549	39	0
2	Bq	2501	0	2549	38	0
2	Br	2501	0	2549	38	0
2	Bs	2501	0	2549	35	0
2	Bt	2501	0	2549	30	0
2	Bu	2501	0	2549	38	0
2	Bv	2501	0	2549	27	0
2	Bw	2501	0	2549	31	0
2	Bx	2501	0	2549	37	0
2	By	2501	0	2549	34	0
2	Bz	2501	0	2549	36	0
3	Ca	2770	0	2749	19	0
3	Cb	2770	0	2749	22	0
3	Cc	2770	0	2749	14	0
3	Cd	2770	0	2749	15	0
3	Ce	2770	0	2749	15	0
3	Cf	2770	0	2749	20	0
3	Cg	2770	0	2749	13	0
3	Ch	2770	0	2749	18	0
3	Ci	2770	0	2749	18	0
3	Cj	2770	0	2749	20	0
3	Ck	2770	0	2749	20	0
3	Cl	2770	0	2749	16	0
3	Cm	2770	0	2749	18	0
3	Cn	2770	0	2749	22	0
3	Co	2770	0	2749	19	0
3	Cp	2770	0	2749	16	0
3	Cq	2770	0	2749	15	0
3	Cr	2770	0	2749	23	0
3	Cs	2770	0	2749	18	0
3	Ct	2770	0	2749	18	0
3	Cu	2770	0	2749	19	0
3	Cv	2770	0	2749	19	0
3	Cw	2770	0	2749	16	0
3	Cx	2770	0	2749	14	0
3	Cy	2770	0	2749	20	0
3	Cz	2770	0	2749	18	0
4	Da	2085	0	2022	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Db	2080	0	2003	11	0
4	Dc	2085	0	2022	12	0
4	Dd	2080	0	2003	11	0
4	De	2085	0	2022	12	0
4	Df	2080	0	2003	9	0
4	Dg	2085	0	2022	11	0
4	Dh	2080	0	2003	12	0
4	Di	2085	0	2022	14	0
4	Dj	2080	0	2003	10	0
4	Dk	2085	0	2022	11	0
4	Dl	2080	0	2003	11	0
4	Dm	2085	0	2022	12	0
4	Dn	2080	0	2003	10	0
4	Do	2085	0	2022	14	0
4	Dp	2080	0	2003	14	0
4	Dq	2085	0	2022	13	0
4	Dr	2080	0	2003	11	0
4	Ds	2085	0	2022	11	0
4	Dt	2080	0	2003	11	0
4	Du	2085	0	2022	11	0
4	Dv	2080	0	2003	10	0
4	Dw	2085	0	2022	10	0
4	Dx	2080	0	2003	11	0
4	Dy	2085	0	2022	12	0
4	Dz	2080	0	2003	11	0
5	Fa	125	0	125	0	0
5	Fb	125	0	125	1	0
5	Fc	125	0	125	0	0
5	Fd	125	0	125	1	0
5	Fe	125	0	125	0	0
5	Ff	125	0	125	1	0
5	Fg	125	0	125	0	0
5	Fh	125	0	125	1	0
5	Fi	125	0	125	0	0
5	Fj	125	0	125	0	0
5	Fk	125	0	125	0	0
5	Fl	125	0	125	1	0
5	Fm	125	0	125	1	0
5	Fn	125	0	125	0	0
5	Fo	125	0	125	1	0
5	Fp	125	0	125	0	0
5	Fq	125	0	125	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Fr	125	0	125	0	0
5	Fs	125	0	125	0	0
5	Ft	125	0	125	0	0
5	Fu	125	0	125	0	0
5	Fv	125	0	125	1	0
5	Fw	125	0	125	1	0
5	Fx	125	0	125	0	0
5	Fy	125	0	125	0	0
5	Fz	125	0	125	0	0
5	Ga	112	0	116	0	0
5	Gb	112	0	116	1	0
5	Gc	112	0	116	1	0
5	Gd	112	0	116	0	0
5	Ge	112	0	116	0	0
5	Gf	112	0	116	1	0
5	Gg	112	0	116	0	0
5	Gh	112	0	116	0	0
5	Gi	112	0	116	0	0
5	Gj	112	0	116	1	0
5	Gk	112	0	116	0	0
5	Gl	112	0	116	1	0
5	Gm	112	0	116	2	0
5	Gn	112	0	116	0	0
5	Go	112	0	116	0	0
5	Gp	112	0	116	0	0
5	Gq	112	0	116	0	0
5	Gr	112	0	116	0	0
5	Gs	112	0	116	1	0
5	Gt	112	0	116	0	0
5	Gu	112	0	116	0	0
5	Gv	112	0	116	0	0
5	Gw	112	0	116	2	0
5	Gx	112	0	116	0	0
5	Gy	112	0	116	0	0
5	Gz	112	0	116	1	0
All	All	240877	0	238173	1907	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 4.

All (1907) 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:Ap:125:LEU:HB3	1:As:244:MET:HE3	1.70	0.72
1:Aa:244:MET:HE3	1:Ax:125:LEU:HB3	1.74	0.68
1:Ae:125:LEU:HB3	1:Ah:244:MET:HE3	1.76	0.68
1:Am:125:LEU:HB3	1:Ap:244:MET:HE3	1.76	0.67
1:Av:125:LEU:HB3	1:Ay:244:MET:HE3	1.76	0.67
1:Ar:125:LEU:HB3	1:Au:244:MET:HE3	1.76	0.66
1:Ab:244:MET:HE3	1:Ay:125:LEU:HB3	1.78	0.66
1:At:125:LEU:HB3	1:Aw:244:MET:HE3	1.76	0.66
1:Ao:125:LEU:HB3	1:Ar:244:MET:HE3	1.78	0.66
1:Ai:125:LEU:HB3	1:Al:244:MET:HE3	1.79	0.65
1:Ac:244:MET:HE3	1:Az:125:LEU:HB3	1.79	0.65
1:Ah:125:LEU:HB3	1:Ak:244:MET:HE3	1.79	0.65
4:Dy:78:ARG:HB3	4:Dy:143:GLN:HE22	1.60	0.65
1:Ad:125:LEU:HB3	1:Ag:244:MET:HE3	1.80	0.64
1:As:125:LEU:HB3	1:Av:244:MET:HE3	1.80	0.64
4:Dc:78:ARG:HB3	4:Dc:143:GLN:HE22	1.62	0.64
1:Az:219:PHE:HA	2:Bo:69:LEU:HD13	1.81	0.63
1:Aw:125:LEU:HB3	1:Az:244:MET:HE3	1.81	0.63
2:Bj:269:PRO:HB2	2:Bk:263:GLN:HE21	1.64	0.63
1:Ag:125:LEU:HB3	1:Aj:244:MET:HE3	1.81	0.63
1:Ab:125:LEU:HB3	1:Ae:244:MET:HE3	1.81	0.63
1:Au:125:LEU:HB3	1:Ax:244:MET:HE3	1.81	0.63
2:Bi:318:LEU:HG	2:Bi:320:PRO:HG3	1.80	0.62
4:Dm:78:ARG:HB3	4:Dm:143:GLN:HE22	1.64	0.62
1:Aa:125:LEU:HB3	1:Ad:244:MET:HE3	1.82	0.62
1:Ab:219:PHE:HA	2:Bq:69:LEU:HD13	1.82	0.62
3:Cb:85:VAL:HG22	3:Cb:108:ILE:HG12	1.81	0.62
2:Br:303:ASN:HB2	2:Bu:148:ASP:HB2	1.81	0.62
2:By:269:PRO:HB2	2:Bz:263:GLN:HE21	1.65	0.62
2:Bb:269:PRO:HB2	2:Bc:263:GLN:HE21	1.65	0.62
4:De:78:ARG:HB3	4:De:143:GLN:HE22	1.65	0.62
1:An:125:LEU:HB3	1:Aq:244:MET:HE3	1.82	0.62
4:Du:78:ARG:HB3	4:Du:143:GLN:HE22	1.64	0.62
2:Bi:253:ASN:HB3	2:Bi:258:THR:HG23	1.83	0.61
2:Bt:56:GLN:HE22	2:Bu:69:LEU:H	1.49	0.61
2:Bg:283:GLU:HG2	2:Bg:305:GLU:HG2	1.81	0.61
1:Aq:125:LEU:HB3	1:At:244:MET:HE3	1.82	0.61
4:Di:78:ARG:HB3	4:Di:143:GLN:HE22	1.65	0.61
1:Ad:113:GLU:HB2	1:Ad:172:MET:HB3	1.83	0.61
4:Do:78:ARG:HB3	4:Do:143:GLN:HE22	1.65	0.61
1:Ak:125:LEU:HB3	1:An:244:MET:HE3	1.83	0.61
1:Au:219:PHE:HA	2:Bj:69:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cb:92:GLU:HB2	3:Cb:103:ARG:HB3	1.83	0.61
3:Cw:271:LEU:HD21	5:Gw:145:PHE:HB3	1.82	0.61
1:Ag:113:GLU:HB2	1:Ag:172:MET:HB3	1.83	0.61
4:Dg:78:ARG:HB3	4:Dg:143:GLN:HE22	1.64	0.61
4:Da:78:ARG:HB3	4:Da:143:GLN:HE22	1.63	0.61
3:Ca:226:VAL:HB	3:Ca:236:MET:HB3	1.82	0.60
2:Ba:148:ASP:HB2	2:Bx:303:ASN:HB2	1.83	0.60
2:Be:303:ASN:HB2	2:Bh:148:ASP:HB2	1.81	0.60
2:Br:283:GLU:HG2	2:Br:305:GLU:HG2	1.82	0.60
2:Ba:283:GLU:HG2	2:Ba:305:GLU:HG2	1.82	0.60
3:Cy:92:GLU:HB2	3:Cy:103:ARG:HB3	1.83	0.60
4:Dj:219:VAL:HG21	4:Dj:254:LEU:HD21	1.83	0.60
1:Ac:113:GLU:HB2	1:Ac:172:MET:HB3	1.84	0.60
1:Ac:125:LEU:HB3	1:Af:244:MET:HE3	1.83	0.60
1:Ak:66:TRP:HA	1:Ak:192:ARG:HD3	1.84	0.60
2:By:56:GLN:HE22	2:Bz:69:LEU:H	1.50	0.60
1:Al:125:LEU:HB3	1:Ao:244:MET:HE3	1.84	0.60
1:Ap:113:GLU:HB2	1:Ap:172:MET:HB3	1.83	0.60
2:Bp:283:GLU:HG2	2:Bp:305:GLU:HG2	1.83	0.60
4:Dw:78:ARG:HB3	4:Dw:143:GLN:HE22	1.66	0.60
2:Bk:56:GLN:HE22	2:Bl:69:LEU:H	1.49	0.59
4:Ds:78:ARG:HB3	4:Ds:143:GLN:HE22	1.66	0.59
1:Ai:66:TRP:HA	1:Ai:192:ARG:HD3	1.84	0.59
1:Ax:125:LEU:HB2	1:Ax:160:PHE:HB3	1.83	0.59
2:Ba:253:ASN:HB3	2:Ba:258:THR:HG23	1.84	0.59
4:Dq:78:ARG:HB3	4:Dq:143:GLN:HE22	1.67	0.59
1:Ae:113:GLU:HB2	1:Ae:172:MET:HB3	1.85	0.59
2:Bd:253:ASN:HB3	2:Bd:258:THR:HG23	1.84	0.59
2:Bt:269:PRO:HB2	2:Bu:263:GLN:HE21	1.66	0.59
1:Av:125:LEU:HB2	1:Av:160:PHE:HB3	1.84	0.59
2:Bn:253:ASN:HB3	2:Bn:258:THR:HG23	1.83	0.59
4:Dl:219:VAL:HG21	4:Dl:254:LEU:HD21	1.85	0.59
4:Dx:219:VAL:HG21	4:Dx:254:LEU:HD21	1.84	0.59
1:As:66:TRP:HA	1:As:192:ARG:HD3	1.84	0.59
1:Aj:66:TRP:HA	1:Aj:192:ARG:HD3	1.84	0.59
1:Ak:113:GLU:HB2	1:Ak:172:MET:HB3	1.85	0.59
1:Ao:66:TRP:HA	1:Ao:192:ARG:HD3	1.85	0.59
2:Br:56:GLN:HE22	2:Bs:69:LEU:H	1.50	0.59
1:Am:113:GLU:HB2	1:Am:172:MET:HB3	1.84	0.59
3:Cw:92:GLU:HB2	3:Cw:103:ARG:HB3	1.85	0.59
3:Cz:85:VAL:HG22	3:Cz:108:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:125:LEU:HB2	1:Ay:160:PHE:HB3	1.83	0.59
2:Bj:253:ASN:HB3	2:Bj:258:THR:HG23	1.84	0.59
2:Br:317:LYS:HB2	2:Bs:328:VAL:HG21	1.84	0.59
2:Ba:56:GLN:HE22	2:Bb:69:LEU:H	1.51	0.59
1:Al:66:TRP:HA	1:Al:192:ARG:HD3	1.85	0.59
3:Cn:92:GLU:HB2	3:Cn:103:ARG:HB3	1.85	0.59
4:Dn:219:VAL:HG21	4:Dn:254:LEU:HD21	1.85	0.59
1:Al:113:GLU:HB2	1:Al:172:MET:HB3	1.85	0.58
1:Av:113:GLU:HB2	1:Av:172:MET:HB3	1.84	0.58
1:Ay:113:GLU:HB2	1:Ay:172:MET:HB3	1.84	0.58
1:Az:66:TRP:HA	1:Az:192:ARG:HD3	1.85	0.58
1:Az:113:GLU:HB2	1:Az:172:MET:HB3	1.85	0.58
3:Cx:92:GLU:HB2	3:Cx:103:ARG:HB3	1.84	0.58
1:Aa:113:GLU:HB2	1:Aa:172:MET:HB3	1.86	0.58
1:Ab:113:GLU:HB2	1:Ab:172:MET:HB3	1.86	0.58
2:Bj:283:GLU:HG2	2:Bj:305:GLU:HG2	1.86	0.58
2:Bq:56:GLN:HE22	2:Br:69:LEU:H	1.51	0.58
1:Aj:113:GLU:HB2	1:Aj:172:MET:HB3	1.85	0.58
1:Af:113:GLU:HB2	1:Af:172:MET:HB3	1.86	0.58
2:Be:283:GLU:HG2	2:Be:305:GLU:HG2	1.84	0.58
3:Ck:85:VAL:HG22	3:Ck:108:ILE:HG12	1.83	0.58
1:Am:66:TRP:HA	1:Am:192:ARG:HD3	1.85	0.58
1:Aq:66:TRP:HA	1:Aq:192:ARG:HD3	1.85	0.58
3:Ch:126:ILE:HB	3:Ch:169:THR:HG22	1.86	0.58
1:Ap:66:TRP:HA	1:Ap:192:ARG:HD3	1.86	0.58
1:Ar:125:LEU:HB2	1:Ar:160:PHE:HB3	1.84	0.58
3:Cg:255:ASP:HB3	3:Cg:258:SER:HB3	1.84	0.58
1:Ah:125:LEU:HB2	1:Ah:160:PHE:HB3	1.85	0.58
1:Aj:125:LEU:HB2	1:Aj:160:PHE:HB3	1.86	0.58
3:Ca:126:ILE:HB	3:Ca:169:THR:HG22	1.86	0.58
4:Dz:219:VAL:HG21	4:Dz:254:LEU:HD21	1.84	0.58
2:Bf:22:LYS:HZ1	2:Bf:237:GLU:HB3	1.68	0.58
1:Ax:113:GLU:HB2	1:Ax:172:MET:HB3	1.85	0.58
2:Bq:269:PRO:HB2	2:Br:263:GLN:HE21	1.67	0.58
3:Cg:92:GLU:HB2	3:Cg:103:ARG:HB3	1.84	0.58
4:Dk:78:ARG:HB3	4:Dk:143:GLN:HE22	1.68	0.58
1:Ae:66:TRP:HA	1:Ae:192:ARG:HD3	1.86	0.57
1:Au:125:LEU:HB2	1:Au:160:PHE:HB3	1.85	0.57
2:Ba:25:ALA:HB2	2:Ba:186:LEU:HD23	1.86	0.57
2:Ba:87:ALA:HB2	2:Ba:101:ILE:HG22	1.84	0.57
2:Bi:87:ALA:HB2	2:Bi:101:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ct:92:GLU:HB2	3:Ct:103:ARG:HB3	1.86	0.57
4:Dx:37:GLN:HG3	4:Dx:49:VAL:HG23	1.86	0.57
1:Ah:113:GLU:HB2	1:Ah:172:MET:HB3	1.86	0.57
1:Av:66:TRP:HA	1:Av:192:ARG:HD3	1.86	0.57
1:Av:129:ASN:HB2	1:Av:156:ASN:HB3	1.85	0.57
1:Ay:66:TRP:HA	1:Ay:192:ARG:HD3	1.86	0.57
2:Bo:56:GLN:HE22	2:Bp:69:LEU:H	1.52	0.57
2:Bq:253:ASN:HB3	2:Bq:258:THR:HG23	1.85	0.57
3:Cm:92:GLU:HB2	3:Cm:103:ARG:HB3	1.86	0.57
4:Dh:219:VAL:HG21	4:Dh:254:LEU:HD21	1.85	0.57
1:Ar:113:GLU:HB2	1:Ar:172:MET:HB3	1.84	0.57
1:Au:113:GLU:HB2	1:Au:172:MET:HB3	1.85	0.57
2:Bm:56:GLN:HE22	2:Bn:69:LEU:H	1.52	0.57
2:Bs:87:ALA:HB2	2:Bs:101:ILE:HG22	1.86	0.57
4:Dd:219:VAL:HG21	4:Dd:254:LEU:HD21	1.86	0.57
2:Be:87:ALA:HB2	2:Be:101:ILE:HG22	1.87	0.57
2:Bw:303:ASN:HB2	2:Bz:148:ASP:HB2	1.87	0.57
2:Bx:87:ALA:HB2	2:Bx:101:ILE:HG22	1.86	0.57
1:Ah:219:PHE:HA	2:Bw:69:LEU:HD13	1.86	0.57
1:Ap:231:ALA:HB3	1:Aq:195:LYS:HG3	1.85	0.57
3:Ca:255:ASP:HB3	3:Ca:258:SER:HB3	1.87	0.57
4:Dv:219:VAL:HG21	4:Dv:254:LEU:HD21	1.86	0.57
1:At:66:TRP:HA	1:At:192:ARG:HD3	1.85	0.57
2:Bg:87:ALA:HB2	2:Bg:101:ILE:HG22	1.87	0.57
2:Bw:56:GLN:HE22	2:Bx:69:LEU:H	1.53	0.57
1:Aa:66:TRP:HA	1:Aa:192:ARG:HD3	1.86	0.57
1:Aw:125:LEU:HB2	1:Aw:160:PHE:HB3	1.85	0.57
2:Bb:87:ALA:HB2	2:Bb:101:ILE:HG22	1.87	0.57
1:Ad:66:TRP:HA	1:Ad:192:ARG:HD3	1.87	0.57
1:Ad:119:LYS:HB3	1:Af:199:LEU:HD12	1.87	0.57
1:Ad:125:LEU:HB2	1:Ad:160:PHE:HB3	1.87	0.57
1:Ap:129:ASN:HB2	1:Ap:156:ASN:HB3	1.87	0.57
2:Bh:253:ASN:HB3	2:Bh:258:THR:HG23	1.87	0.57
2:Bj:87:ALA:HB2	2:Bj:101:ILE:HG22	1.86	0.57
2:Bm:87:ALA:HB2	2:Bm:101:ILE:HG22	1.87	0.57
2:Bn:87:ALA:HB2	2:Bn:101:ILE:HG22	1.87	0.57
3:Ck:126:ILE:HB	3:Ck:169:THR:HG22	1.87	0.57
2:Bc:25:ALA:HB2	2:Bc:186:LEU:HD23	1.87	0.57
2:Bd:87:ALA:HB2	2:Bd:101:ILE:HG22	1.87	0.57
2:Bh:56:GLN:HE22	2:Bi:69:LEU:H	1.53	0.57
2:Bs:56:GLN:HE22	2:Bt:69:LEU:H	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cb:362:GLU:HG2	3:Cb:363:LEU:HD23	1.86	0.57
2:Bi:25:ALA:HB2	2:Bi:186:LEU:HD23	1.87	0.57
3:Cq:255:ASP:HB3	3:Cq:258:SER:HB3	1.86	0.57
1:Aq:113:GLU:HB2	1:Aq:172:MET:HB3	1.86	0.56
1:Aq:125:LEU:HB2	1:Aq:160:PHE:HB3	1.86	0.56
2:Bo:87:ALA:HB2	2:Bo:101:ILE:HG22	1.87	0.56
3:Cc:92:GLU:HB2	3:Cc:103:ARG:HB3	1.86	0.56
3:Cd:255:ASP:HB3	3:Cd:258:SER:HB3	1.87	0.56
3:Cl:80:PHE:HA	5:Fl:136:VAL:HG21	1.87	0.56
3:Cr:92:GLU:HB2	3:Cr:103:ARG:HB3	1.87	0.56
4:Du:93:PRO:HB2	4:Du:95:TRP:HE3	1.70	0.56
1:Aa:232:ARG:HH22	1:Ab:194:GLU:HG3	1.69	0.56
1:Ag:125:LEU:HB2	1:Ag:160:PHE:HB3	1.86	0.56
1:Ai:113:GLU:HB2	1:Ai:172:MET:HB3	1.88	0.56
2:Bl:87:ALA:HB2	2:Bl:101:ILE:HG22	1.87	0.56
2:Bp:269:PRO:HB2	2:Bq:263:GLN:HE21	1.71	0.56
3:Co:92:GLU:HB2	3:Co:103:ARG:HB3	1.87	0.56
1:Ac:125:LEU:HB2	1:Ac:160:PHE:HB3	1.87	0.56
1:Ag:66:TRP:HA	1:Ag:192:ARG:HD3	1.87	0.56
1:Au:66:TRP:HA	1:Au:192:ARG:HD3	1.87	0.56
1:Ay:232:ARG:HH22	1:Az:194:GLU:HG3	1.70	0.56
2:Bc:283:GLU:HG2	2:Bc:305:GLU:HG2	1.86	0.56
2:Bf:283:GLU:HG2	2:Bf:305:GLU:HG2	1.87	0.56
2:Bp:87:ALA:HB2	2:Bp:101:ILE:HG22	1.85	0.56
2:By:87:ALA:HB2	2:By:101:ILE:HG22	1.86	0.56
3:Cl:92:GLU:HB2	3:Cl:103:ARG:HB3	1.85	0.56
3:Cm:126:ILE:HB	3:Cm:169:THR:HG22	1.86	0.56
3:Cm:255:ASP:HB3	3:Cm:258:SER:HB3	1.86	0.56
3:Cs:85:VAL:HG22	3:Cs:108:ILE:HG12	1.87	0.56
1:Ar:231:ALA:HB3	1:As:195:LYS:HG3	1.87	0.56
2:Bz:253:ASN:HB3	2:Bz:258:THR:HG23	1.87	0.56
4:Du:104:ILE:HG23	4:Dv:145:ARG:HD3	1.88	0.56
1:Ah:66:TRP:HA	1:Ah:192:ARG:HD3	1.87	0.56
2:Bk:253:ASN:HB3	2:Bk:258:THR:HG23	1.87	0.56
2:Bq:87:ALA:HB2	2:Bq:101:ILE:HG22	1.87	0.56
2:Bz:283:GLU:HG2	2:Bz:305:GLU:HG2	1.86	0.56
3:Ci:126:ILE:HB	3:Ci:169:THR:HG22	1.88	0.56
3:Cq:92:GLU:HB2	3:Cq:103:ARG:HB3	1.87	0.56
1:Ao:113:GLU:HB2	1:Ao:172:MET:HB3	1.86	0.56
1:As:113:GLU:HB2	1:As:172:MET:HB3	1.86	0.56
1:Au:232:ARG:HH22	1:Av:194:GLU:HG3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bc:56:GLN:HE22	2:Bd:69:LEU:H	1.53	0.56
2:Be:56:GLN:HE22	2:Bf:69:LEU:H	1.53	0.56
2:Br:87:ALA:HB2	2:Br:101:ILE:HG22	1.86	0.56
2:Bx:290:PRO:HB3	2:Bx:296:GLY:HA3	1.87	0.56
2:By:25:ALA:HB2	2:By:186:LEU:HD23	1.88	0.56
3:Cf:255:ASP:HB3	3:Cf:258:SER:HB3	1.88	0.56
1:As:125:LEU:HB2	1:As:160:PHE:HB3	1.86	0.56
1:Aw:66:TRP:HA	1:Aw:192:ARG:HD3	1.87	0.56
2:Bh:87:ALA:HB2	2:Bh:101:ILE:HG22	1.87	0.56
2:Bw:87:ALA:HB2	2:Bw:101:ILE:HG22	1.87	0.56
3:Cc:255:ASP:HB3	3:Cc:258:SER:HB3	1.86	0.56
3:Co:255:ASP:HB3	3:Co:258:SER:HB3	1.88	0.56
1:Ab:125:LEU:HB2	1:Ab:160:PHE:HB3	1.88	0.56
1:An:66:TRP:HA	1:An:192:ARG:HD3	1.88	0.56
1:At:113:GLU:HB2	1:At:172:MET:HB3	1.87	0.56
2:Bl:253:ASN:HB3	2:Bl:258:THR:HG23	1.88	0.56
4:Dc:68:ILE:HD11	4:Dd:112:GLN:HE21	1.71	0.56
4:Dw:68:ILE:HD11	4:Dx:112:GLN:HE21	1.71	0.56
1:Ae:125:LEU:HB2	1:Ae:160:PHE:HB3	1.88	0.56
2:Be:317:LYS:HE3	2:Bf:324:LEU:HD23	1.88	0.56
2:Bk:87:ALA:HB2	2:Bk:101:ILE:HG22	1.88	0.56
2:Bs:25:ALA:HB2	2:Bs:186:LEU:HD23	1.86	0.56
3:Ck:92:GLU:HB2	3:Ck:103:ARG:HB3	1.86	0.56
1:Ap:125:LEU:HB2	1:Ap:160:PHE:HB3	1.88	0.56
2:Bo:253:ASN:HB3	2:Bo:258:THR:HG23	1.86	0.56
2:Bt:87:ALA:HB2	2:Bt:101:ILE:HG22	1.87	0.56
2:Bz:25:ALA:HB2	2:Bz:186:LEU:HD23	1.88	0.56
3:Cp:92:GLU:HB2	3:Cp:103:ARG:HB3	1.85	0.56
2:Bu:25:ALA:HB2	2:Bu:186:LEU:HD23	1.88	0.55
2:Bu:87:ALA:HB2	2:Bu:101:ILE:HG22	1.86	0.55
3:Cp:255:ASP:HB3	3:Cp:258:SER:HB3	1.88	0.55
3:Cw:255:ASP:HB3	3:Cw:258:SER:HB3	1.88	0.55
4:Db:219:VAL:HG21	4:Db:254:LEU:HD21	1.88	0.55
1:Ac:232:ARG:HH22	1:Ad:194:GLU:HG3	1.70	0.55
1:Ag:36:ASP:HB3	1:Ag:39:GLU:HG2	1.88	0.55
2:Bq:25:ALA:HB2	2:Bq:186:LEU:HD23	1.87	0.55
3:Ci:255:ASP:HB3	3:Ci:258:SER:HB3	1.88	0.55
1:Ad:231:ALA:HB3	1:Ae:195:LYS:HG3	1.88	0.55
1:Ag:119:LYS:HB3	1:Ai:199:LEU:HD12	1.88	0.55
1:An:113:GLU:HB2	1:An:172:MET:HB3	1.87	0.55
2:Bc:87:ALA:HB2	2:Bc:101:ILE:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bp:285:LEU:HD23	2:Bp:303:ASN:HB3	1.87	0.55
2:Bv:87:ALA:HB2	2:Bv:101:ILE:HG22	1.87	0.55
2:Bz:87:ALA:HB2	2:Bz:101:ILE:HG22	1.88	0.55
1:Ab:129:ASN:HB2	1:Ab:156:ASN:HB3	1.88	0.55
1:Ah:119:LYS:HB3	1:Aj:199:LEU:HD12	1.89	0.55
1:Am:125:LEU:HB2	1:Am:160:PHE:HB3	1.88	0.55
1:At:125:LEU:HB2	1:At:160:PHE:HB3	1.87	0.55
1:Aw:231:ALA:HB3	1:Ax:195:LYS:HG3	1.87	0.55
1:Az:36:ASP:HB3	1:Az:39:GLU:HG2	1.88	0.55
2:By:253:ASN:HB3	2:By:258:THR:HG23	1.88	0.55
3:Cv:85:VAL:HG22	3:Cv:108:ILE:HG12	1.89	0.55
1:Af:66:TRP:HA	1:Af:192:ARG:HD3	1.88	0.55
1:Ak:125:LEU:HB2	1:Ak:160:PHE:HB3	1.88	0.55
1:An:36:ASP:HB3	1:An:39:GLU:HG2	1.89	0.55
1:An:231:ALA:HB3	1:Ao:195:LYS:HG3	1.87	0.55
3:Ch:92:GLU:HB2	3:Ch:103:ARG:HB3	1.86	0.55
3:Cr:126:ILE:HB	3:Cr:169:THR:HG22	1.88	0.55
1:Aa:125:LEU:HB2	1:Aa:160:PHE:HB3	1.88	0.55
1:Ac:66:TRP:HA	1:Ac:192:ARG:HD3	1.89	0.55
1:Ao:231:ALA:HB3	1:Ap:195:LYS:HG3	1.88	0.55
2:Bj:25:ALA:HB2	2:Bj:186:LEU:HD23	1.89	0.55
2:Br:253:ASN:HB3	2:Br:258:THR:HG23	1.87	0.55
3:Ci:92:GLU:HB2	3:Ci:103:ARG:HB3	1.88	0.55
1:Ai:231:ALA:HB3	1:Aj:195:LYS:HG3	1.87	0.55
1:Ax:231:ALA:HB3	1:Ay:195:LYS:HG3	1.87	0.55
2:Bd:25:ALA:HB2	2:Bd:186:LEU:HD23	1.89	0.55
2:Be:25:ALA:HB2	2:Be:186:LEU:HD23	1.89	0.55
2:Bg:25:ALA:HB2	2:Bg:186:LEU:HD23	1.89	0.55
2:Bn:277:MET:HE2	2:Bn:311:LYS:HD2	1.89	0.55
3:Cc:262:TRP:HA	3:Cc:267:GLY:HA3	1.89	0.55
1:As:231:ALA:HB3	1:At:195:LYS:HG3	1.89	0.55
1:Am:232:ARG:HH22	1:An:194:GLU:HG3	1.71	0.55
2:Bb:284:ASN:HB2	2:Bb:304:THR:HG23	1.89	0.55
2:Bf:87:ALA:HB2	2:Bf:101:ILE:HG22	1.89	0.55
2:Bk:224:ARG:HH22	3:Cn:323:THR:HB	1.72	0.55
1:Ad:232:ARG:HH22	1:Ae:194:GLU:HG3	1.72	0.55
1:Am:119:LYS:HB3	1:Ao:199:LEU:HD12	1.89	0.55
1:Ar:36:ASP:HB3	1:Ar:39:GLU:HG2	1.89	0.55
1:Ax:232:ARG:HH22	1:Ay:194:GLU:HG3	1.72	0.55
2:Bk:290:PRO:HB3	2:Bk:296:GLY:HA3	1.89	0.55
2:Bl:290:PRO:HB3	2:Bl:296:GLY:HA3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bv:25:ALA:HB2	2:Bv:186:LEU:HD23	1.89	0.55
4:Df:219:VAL:HG21	4:Df:254:LEU:HD21	1.89	0.55
1:Ab:232:ARG:HH22	1:Ac:194:GLU:HG3	1.72	0.54
1:Af:129:ASN:HB2	1:Af:156:ASN:HB3	1.88	0.54
2:Ba:324:LEU:HD23	2:Bz:317:LYS:HE3	1.89	0.54
2:Bt:275:GLY:HA3	2:Bu:338:PRO:HG2	1.89	0.54
2:Bx:25:ALA:HB2	2:Bx:186:LEU:HD23	1.89	0.54
1:Ae:129:ASN:HB2	1:Ae:156:ASN:HB3	1.88	0.54
1:Au:231:ALA:HB3	1:Av:195:LYS:HG3	1.88	0.54
1:Aw:113:GLU:HB2	1:Aw:172:MET:HB3	1.88	0.54
2:Bl:25:ALA:HB2	2:Bl:186:LEU:HD23	1.90	0.54
3:Cp:145:VAL:HA	3:Cp:256:THR:HG21	1.90	0.54
4:Do:141:ASP:HB2	4:Do:149:ILE:HG12	1.89	0.54
1:Ax:129:ASN:HB2	1:Ax:156:ASN:HB3	1.88	0.54
2:Br:25:ALA:HB2	2:Br:186:LEU:HD23	1.89	0.54
3:Cf:85:VAL:HG22	3:Cf:108:ILE:HG12	1.89	0.54
4:Dk:104:ILE:HG23	4:Dl:145:ARG:HD3	1.90	0.54
1:At:232:ARG:HH22	1:Au:194:GLU:HG3	1.73	0.54
1:Au:129:ASN:HB2	1:Au:156:ASN:HB3	1.90	0.54
1:Av:231:ALA:HB3	1:Aw:195:LYS:HG3	1.88	0.54
2:Bb:25:ALA:HB2	2:Bb:186:LEU:HD23	1.90	0.54
2:Bj:254:SER:HB2	2:Bl:138:VAL:HG22	1.88	0.54
2:Bp:267:LEU:HB2	2:Bp:320:PRO:HB2	1.89	0.54
2:Bt:25:ALA:HB2	2:Bt:186:LEU:HD23	1.89	0.54
3:Cf:92:GLU:HB2	3:Cf:103:ARG:HB3	1.88	0.54
3:Cg:262:TRP:HA	3:Cg:267:GLY:HA3	1.90	0.54
1:Af:232:ARG:HH22	1:Ag:194:GLU:HG3	1.72	0.54
1:Az:125:LEU:HB2	1:Az:160:PHE:HB3	1.89	0.54
2:Bv:253:ASN:HB3	2:Bv:258:THR:HG23	1.88	0.54
3:Cv:255:ASP:HB3	3:Cv:258:SER:HB3	1.89	0.54
4:Dk:141:ASP:HB2	4:Dk:149:ILE:HG12	1.90	0.54
4:Dn:37:GLN:HG3	4:Dn:49:VAL:HG23	1.89	0.54
1:Ae:231:ALA:HB3	1:Af:195:LYS:HG3	1.89	0.54
1:Ak:231:ALA:HB3	1:Al:195:LYS:HG3	1.89	0.54
1:Am:231:ALA:HB3	1:An:195:LYS:HG3	1.89	0.54
1:Aq:231:ALA:HB3	1:Ar:195:LYS:HG3	1.89	0.54
1:Av:232:ARG:HH22	1:Aw:194:GLU:HG3	1.72	0.54
1:Aw:129:ASN:HB2	1:Aw:156:ASN:HB3	1.89	0.54
2:Bz:290:PRO:HB3	2:Bz:296:GLY:HA3	1.89	0.54
4:Dv:37:GLN:HG3	4:Dv:49:VAL:HG23	1.90	0.54
4:Dw:104:ILE:HG23	4:Dx:145:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Af:125:LEU:HB2	1:Af:160:PHE:HB3	1.89	0.54
1:An:125:LEU:HB2	1:An:160:PHE:HB3	1.88	0.54
1:As:232:ARG:HH22	1:At:194:GLU:HG3	1.73	0.54
2:Bx:317:LYS:HE3	2:By:324:LEU:HD23	1.89	0.54
3:Cj:92:GLU:HB2	3:Cj:103:ARG:HB3	1.89	0.54
3:Cs:255:ASP:HB3	3:Cs:258:SER:HB3	1.89	0.54
1:Ag:232:ARG:HH22	1:Ah:194:GLU:HG3	1.72	0.54
1:Ak:232:ARG:HH22	1:Al:194:GLU:HG3	1.72	0.54
1:Aq:129:ASN:HB2	1:Aq:156:ASN:HB3	1.90	0.54
1:At:129:ASN:HB2	1:At:156:ASN:HB3	1.90	0.54
1:At:231:ALA:HB3	1:Au:195:LYS:HG3	1.88	0.54
1:Aw:232:ARG:HH22	1:Ax:194:GLU:HG3	1.72	0.54
2:Bl:317:LYS:HE3	2:Bm:324:LEU:HD23	1.88	0.54
4:Dg:93:PRO:HB2	4:Dg:95:TRP:HE3	1.73	0.54
4:Dg:104:ILE:HG23	4:Dh:145:ARG:HD3	1.90	0.54
4:Dy:93:PRO:HB2	4:Dy:95:TRP:HE3	1.73	0.54
1:Ae:232:ARG:HH22	1:Af:194:GLU:HG3	1.72	0.54
1:Ag:129:ASN:HB2	1:Ag:156:ASN:HB3	1.90	0.54
1:Ai:119:LYS:HB3	1:Ak:199:LEU:HD12	1.90	0.54
3:Cy:126:ILE:HB	3:Cy:169:THR:HG22	1.90	0.54
4:De:93:PRO:HB2	4:De:95:TRP:HE3	1.72	0.54
1:Aa:194:GLU:HG3	1:Az:232:ARG:HH22	1.73	0.54
1:Aj:232:ARG:HH22	1:Ak:194:GLU:HG3	1.71	0.54
1:Ao:232:ARG:HH22	1:Ap:194:GLU:HG3	1.72	0.54
1:Ar:232:ARG:HH22	1:As:194:GLU:HG3	1.72	0.54
2:Bf:27:VAL:HG21	2:Bf:233:LEU:HD21	1.89	0.54
2:Bn:25:ALA:HB2	2:Bn:186:LEU:HD23	1.90	0.54
3:Cc:85:VAL:HG22	3:Cc:108:ILE:HG12	1.88	0.54
4:Dd:37:GLN:HG3	4:Dd:49:VAL:HG23	1.90	0.54
4:Dy:104:ILE:HG23	4:Dz:145:ARG:HD3	1.89	0.54
1:An:119:LYS:HB3	1:Ap:199:LEU:HD12	1.90	0.53
1:Aq:232:ARG:HH22	1:Ar:194:GLU:HG3	1.71	0.53
2:Bk:269:PRO:HB2	2:Bl:263:GLN:HE21	1.72	0.53
2:Bp:25:ALA:HB2	2:Bp:186:LEU:HD23	1.90	0.53
3:Ct:223:GLU:HG2	3:Ct:239:THR:HG22	1.90	0.53
4:Db:37:GLN:HG3	4:Db:49:VAL:HG23	1.90	0.53
4:Di:68:ILE:HD11	4:Dj:112:GLN:HE21	1.73	0.53
1:Ai:125:LEU:HB2	1:Ai:160:PHE:HB3	1.90	0.53
1:An:129:ASN:HB2	1:An:156:ASN:HB3	1.90	0.53
1:Ap:36:ASP:HB3	1:Ap:39:GLU:HG2	1.91	0.53
2:Bn:254:SER:HB2	2:Bp:138:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bv:254:SER:HB2	2:Bx:138:VAL:HG22	1.90	0.53
3:Cn:255:ASP:HB3	3:Cn:258:SER:HB3	1.90	0.53
4:Dm:104:ILE:HG23	4:Dn:145:ARG:HD3	1.89	0.53
1:Aj:36:ASP:HB3	1:Aj:39:GLU:HG2	1.90	0.53
2:Bl:303:ASN:HB2	2:Bo:148:ASP:HB3	1.90	0.53
2:Br:290:PRO:HB3	2:Br:296:GLY:HA3	1.91	0.53
2:Bs:254:SER:HB2	2:Bu:138:VAL:HG22	1.90	0.53
2:Bw:25:ALA:HB2	2:Bw:186:LEU:HD23	1.90	0.53
2:Bw:277:MET:HE2	2:Bw:311:LYS:HD2	1.90	0.53
3:Cr:255:ASP:HB3	3:Cr:258:SER:HB3	1.90	0.53
4:Dg:68:ILE:HD11	4:Dh:112:GLN:HE21	1.72	0.53
4:Di:104:ILE:HG23	4:Dj:145:ARG:HD3	1.90	0.53
4:Do:104:ILE:HG23	4:Dp:145:ARG:HD3	1.90	0.53
4:Dq:93:PRO:HB2	4:Dq:95:TRP:HE3	1.74	0.53
4:Ds:141:ASP:HB2	4:Ds:149:ILE:HG12	1.89	0.53
4:Dt:37:GLN:HG3	4:Dt:49:VAL:HG23	1.90	0.53
2:Bh:25:ALA:HB2	2:Bh:186:LEU:HD23	1.90	0.53
1:Aa:129:ASN:HB2	1:Aa:156:ASN:HB3	1.91	0.53
1:Aj:231:ALA:HB3	1:Ak:195:LYS:HG3	1.90	0.53
1:As:36:ASP:HB3	1:As:39:GLU:HG2	1.91	0.53
2:Ba:303:ASN:HB2	2:Bd:148:ASP:HB2	1.89	0.53
2:Be:253:ASN:HB3	2:Be:258:THR:HG23	1.89	0.53
2:Bz:22:LYS:HB3	2:Bz:237:GLU:HG2	1.89	0.53
3:Cn:85:VAL:HG22	3:Cn:108:ILE:HG12	1.91	0.53
4:Da:104:ILE:HG23	4:Db:145:ARG:HD3	1.90	0.53
1:Ac:219:PHE:HD1	2:Br:69:LEU:HD13	1.73	0.53
1:Al:232:ARG:HH22	1:Am:194:GLU:HG3	1.72	0.53
2:Bj:56:GLN:HE22	2:Bk:69:LEU:H	1.57	0.53
4:Dk:93:PRO:HB2	4:Dk:95:TRP:HE3	1.73	0.53
2:Ba:41:VAL:HG23	2:Ba:83:VAL:HG21	1.90	0.53
2:Bf:317:LYS:HE3	2:Bg:324:LEU:HD23	1.89	0.53
2:Bi:85:VAL:HG22	2:Bi:103:VAL:HG13	1.89	0.53
4:De:104:ILE:HG23	4:Df:145:ARG:HD3	1.90	0.53
1:Ag:231:ALA:HB3	1:Ah:195:LYS:HG3	1.89	0.53
1:Ah:129:ASN:HB2	1:Ah:156:ASN:HB3	1.90	0.53
1:Ar:66:TRP:HA	1:Ar:192:ARG:HD3	1.91	0.53
2:Bb:138:VAL:HG22	2:Bz:254:SER:HB2	1.91	0.53
2:Bk:25:ALA:HB2	2:Bk:186:LEU:HD23	1.91	0.53
2:Bv:290:PRO:HB3	2:Bv:296:GLY:HA3	1.91	0.53
4:Ds:93:PRO:HB2	4:Ds:95:TRP:HE3	1.74	0.53
4:Ds:104:ILE:HG23	4:Dt:145:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Du:141:ASP:HB2	4:Du:149:ILE:HG12	1.90	0.53
1:Am:129:ASN:HB2	1:Am:156:ASN:HB3	1.91	0.53
2:Ba:138:VAL:HG22	2:By:254:SER:HB2	1.91	0.53
2:Be:254:SER:HB2	2:Bg:138:VAL:HG22	1.90	0.53
2:Bh:254:SER:HB2	2:Bj:138:VAL:HG22	1.90	0.53
4:Dy:68:ILE:HD11	4:Dz:112:GLN:HE21	1.74	0.53
1:Ai:232:ARG:HH22	1:Aj:194:GLU:HG3	1.73	0.53
1:Ao:125:LEU:HB2	1:Ao:160:PHE:HB3	1.90	0.53
2:Bd:41:VAL:HG23	2:Bd:83:VAL:HG21	1.90	0.53
2:Bo:285:LEU:HD23	2:Bo:303:ASN:HB3	1.91	0.53
2:Bu:272:VAL:HG22	2:Bv:260:VAL:HG22	1.90	0.53
2:Bu:315:MET:HG3	2:Bv:328:VAL:HG13	1.91	0.53
4:Dm:93:PRO:HB2	4:Dm:95:TRP:HE3	1.72	0.53
1:Ap:34:THR:HG21	3:Cf:247:PRO:HB2	1.91	0.52
2:Bg:254:SER:HB2	2:Bi:138:VAL:HG22	1.90	0.52
2:Bh:27:VAL:HG21	2:Bh:233:LEU:HD21	1.89	0.52
2:Bj:27:VAL:HG21	2:Bj:233:LEU:HD21	1.90	0.52
2:Bk:272:VAL:HG22	2:Bl:260:VAL:HG22	1.90	0.52
3:Ce:262:TRP:HA	3:Ce:267:GLY:HA3	1.92	0.52
1:Ab:66:TRP:HA	1:Ab:192:ARG:HD3	1.91	0.52
1:Ao:36:ASP:HB3	1:Ao:39:GLU:HG2	1.92	0.52
2:Bx:277:MET:HE2	2:Bx:311:LYS:HD2	1.91	0.52
4:Du:68:ILE:HD11	4:Dv:112:GLN:HE21	1.75	0.52
2:Bm:284:ASN:HB2	2:Bm:304:THR:HG23	1.91	0.52
3:Ch:255:ASP:HB3	3:Ch:258:SER:HB3	1.90	0.52
1:Aa:245:GLN:HG3	1:Ab:200:ASN:HD21	1.74	0.52
1:Ah:232:ARG:HH22	1:Ai:194:GLU:HG3	1.73	0.52
1:Ap:232:ARG:HH22	1:Aq:194:GLU:HG3	1.72	0.52
2:Bl:275:GLY:HA3	2:Bm:338:PRO:HG2	1.92	0.52
4:Dm:68:ILE:HD11	4:Dn:112:GLN:HE21	1.74	0.52
1:Ad:129:ASN:HB2	1:Ad:156:ASN:HB3	1.92	0.52
1:Al:231:ALA:HB3	1:Am:195:LYS:HG3	1.90	0.52
1:Ao:245:GLN:HG3	1:Ap:200:ASN:HD21	1.75	0.52
1:Ar:219:PHE:HA	2:Bg:69:LEU:HD13	1.91	0.52
2:Bm:25:ALA:HB2	2:Bm:186:LEU:HD23	1.92	0.52
2:Bo:25:ALA:HB2	2:Bo:186:LEU:HD23	1.92	0.52
2:Bo:254:SER:HB2	2:Bq:138:VAL:HG22	1.91	0.52
2:Bq:283:GLU:HG2	2:Bq:305:GLU:HB3	1.91	0.52
3:Cu:78:TYR:HD2	3:Cu:88:ILE:HB	1.74	0.52
4:De:141:ASP:HB2	4:De:149:ILE:HG12	1.90	0.52
1:Ab:36:ASP:HB3	1:Ab:39:GLU:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:129:ASN:HB2	1:Al:156:ASN:HB3	1.91	0.52
1:An:232:ARG:HH22	1:Ao:194:GLU:HG3	1.73	0.52
1:Ax:66:TRP:HA	1:Ax:192:ARG:HD3	1.92	0.52
2:Bd:315:MET:HG3	2:Be:328:VAL:HG13	1.92	0.52
2:Bs:283:GLU:HG2	2:Bs:305:GLU:HG3	1.92	0.52
2:Bt:27:VAL:HG21	2:Bt:233:LEU:HD21	1.91	0.52
4:Dw:93:PRO:HB2	4:Dw:95:TRP:HE3	1.75	0.52
1:Ab:231:ALA:HB3	1:Ac:195:LYS:HG3	1.90	0.52
2:Bf:253:ASN:HB3	2:Bf:258:THR:HG23	1.92	0.52
3:Cy:262:TRP:HA	3:Cy:267:GLY:HA3	1.91	0.52
4:Dp:219:VAL:HG21	4:Dp:254:LEU:HD21	1.90	0.52
4:Dq:68:ILE:HD11	4:Dr:112:GLN:HE21	1.75	0.52
1:Ac:231:ALA:HB3	1:Ad:195:LYS:HG3	1.91	0.52
1:Ad:245:GLN:HG3	1:Ae:200:ASN:HD21	1.73	0.52
2:Bc:290:PRO:HB3	2:Bc:296:GLY:HA3	1.92	0.52
3:Co:262:TRP:HA	3:Co:267:GLY:HA3	1.91	0.52
3:Cv:195:MET:HE2	3:Cv:281:LEU:HD11	1.92	0.52
4:Do:93:PRO:HB2	4:Do:95:TRP:HE3	1.75	0.52
1:Aa:231:ALA:HB3	1:Ab:195:LYS:HG3	1.91	0.52
3:Cf:56:PHE:HD1	5:Gf:139:LYS:HE2	1.74	0.52
1:Aa:195:LYS:HG3	1:Az:231:ALA:HB3	1.91	0.52
1:Av:64:PRO:HB2	1:Aw:38:VAL:HG13	1.91	0.52
2:Bp:317:LYS:HE3	2:Bq:324:LEU:HD23	1.91	0.52
2:Br:254:SER:HB2	2:Bt:138:VAL:HG22	1.92	0.52
2:Bs:224:ARG:HH22	3:Cv:323:THR:HB	1.75	0.52
2:Bv:41:VAL:HG23	2:Bv:83:VAL:HG21	1.91	0.52
3:Cr:223:GLU:HG2	3:Cr:239:THR:HG22	1.92	0.52
3:Cy:223:GLU:HG2	3:Cy:239:THR:HG22	1.91	0.52
4:Dc:93:PRO:HB2	4:Dc:95:TRP:HE3	1.75	0.52
4:Dc:141:ASP:HB2	4:Dc:149:ILE:HG12	1.91	0.52
1:Ak:245:GLN:HG3	1:Al:200:ASN:HD21	1.74	0.51
1:Ar:245:GLN:HG3	1:As:200:ASN:HD21	1.74	0.51
1:As:245:GLN:HG3	1:At:200:ASN:HD21	1.75	0.51
2:Bg:253:ASN:HB3	2:Bg:258:THR:HG23	1.92	0.51
2:Bm:41:VAL:HG23	2:Bm:83:VAL:HG21	1.92	0.51
1:Av:245:GLN:HG3	1:Aw:200:ASN:HD21	1.76	0.51
3:Ci:262:TRP:HA	3:Ci:267:GLY:HA3	1.92	0.51
4:Da:68:ILE:HD11	4:Db:112:GLN:HE21	1.75	0.51
4:Dc:104:ILE:HG23	4:Dd:145:ARG:HD3	1.90	0.51
4:Dq:104:ILE:HG23	4:Dr:145:ARG:HD3	1.91	0.51
4:Dz:37:GLN:HG3	4:Dz:49:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ah:231:ALA:HB3	1:Ai:195:LYS:HG3	1.91	0.51
1:Ak:129:ASN:HB2	1:Ak:156:ASN:HB3	1.91	0.51
1:Ay:129:ASN:HB2	1:Ay:156:ASN:HB3	1.92	0.51
1:Ay:231:ALA:HB3	1:Az:195:LYS:HG3	1.91	0.51
2:Bf:25:ALA:HB2	2:Bf:186:LEU:HD23	1.92	0.51
2:Bl:254:SER:HB2	2:Bn:138:VAL:HG22	1.92	0.51
2:Br:315:MET:HG3	2:Bs:328:VAL:HG13	1.91	0.51
3:Cu:92:GLU:HB2	3:Cu:103:ARG:HB3	1.92	0.51
3:Cz:262:TRP:HA	3:Cz:267:GLY:HA3	1.91	0.51
4:Dy:141:ASP:HB2	4:Dy:149:ILE:HG12	1.92	0.51
1:Al:36:ASP:HB3	1:Al:39:GLU:HG2	1.93	0.51
1:Ax:36:ASP:HB3	1:Ax:39:GLU:HG2	1.92	0.51
1:Ay:245:GLN:HG3	1:Az:200:ASN:HD21	1.75	0.51
2:Br:41:VAL:HG23	2:Br:83:VAL:HG21	1.92	0.51
2:Bv:27:VAL:HG21	2:Bv:233:LEU:HD21	1.92	0.51
3:Cj:255:ASP:HB3	3:Cj:258:SER:HB3	1.91	0.51
3:Cz:255:ASP:HB3	3:Cz:258:SER:HB3	1.92	0.51
4:Da:93:PRO:HB2	4:Da:95:TRP:HE3	1.75	0.51
4:Dr:219:VAL:HG21	4:Dr:254:LEU:HD21	1.91	0.51
2:Bl:41:VAL:HG23	2:Bl:83:VAL:HG21	1.92	0.51
3:Ct:255:ASP:HB3	3:Ct:258:SER:HB3	1.92	0.51
4:Dk:68:ILE:HD11	4:Dl:112:GLN:HE21	1.75	0.51
4:Dt:219:VAL:HG21	4:Dt:254:LEU:HD21	1.91	0.51
2:Bb:248:ALA:HB1	2:Bb:265:VAL:HG22	1.93	0.51
2:Bb:250:ILE:HG12	2:Bb:261:VAL:HG13	1.92	0.51
2:Bb:253:ASN:HB3	2:Bb:258:THR:HG23	1.93	0.51
2:Bk:318:LEU:HG	2:Bk:320:PRO:HG3	1.92	0.51
3:Ca:195:MET:HE2	3:Ca:281:LEU:HD11	1.93	0.51
4:Df:37:GLN:HG3	4:Df:49:VAL:HG23	1.93	0.51
4:Di:93:PRO:HB2	4:Di:95:TRP:HE3	1.74	0.51
1:Az:129:ASN:HB2	1:Az:156:ASN:HB3	1.93	0.51
2:Bb:22:LYS:HB3	2:Bb:237:GLU:HG2	1.93	0.51
2:Bk:254:SER:HB2	2:Bm:138:VAL:HG22	1.92	0.51
2:Bl:27:VAL:HG21	2:Bl:233:LEU:HD21	1.91	0.51
2:Bm:27:VAL:HG21	2:Bm:233:LEU:HD21	1.92	0.51
2:Bw:253:ASN:HB3	2:Bw:258:THR:HG23	1.91	0.51
3:Cv:262:TRP:HA	3:Cv:267:GLY:HA3	1.93	0.51
1:Aa:119:LYS:HB3	1:Ac:199:LEU:HD12	1.92	0.51
1:Af:125:LEU:HB3	1:Ai:244:MET:HE3	1.92	0.51
1:Aj:129:ASN:HB2	1:Aj:156:ASN:HB3	1.92	0.51
2:Bc:141:GLY:CA	2:Bc:154:GLY:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:141:GLY:CA	2:Bd:154:GLY:O	2.59	0.51
2:Bp:272:VAL:HG22	2:Bq:260:VAL:HG22	1.92	0.51
3:Cb:262:TRP:HA	3:Cb:267:GLY:HA3	1.93	0.51
1:Aa:36:ASP:HB3	1:Aa:39:GLU:HG2	1.92	0.51
1:Af:36:ASP:HB3	1:Af:39:GLU:HG2	1.92	0.51
1:Af:119:LYS:HB3	1:Ah:199:LEU:HD12	1.93	0.51
1:Ap:245:GLN:HG3	1:Aq:200:ASN:HD21	1.75	0.51
1:Au:36:ASP:HB3	1:Au:39:GLU:HG2	1.93	0.51
2:Bd:254:SER:HB2	2:Bf:138:VAL:HG22	1.92	0.51
2:Bp:22:LYS:HB3	2:Bp:237:GLU:HG2	1.92	0.51
4:Do:68:ILE:HD11	4:Dp:112:GLN:HE21	1.76	0.51
1:Al:245:GLN:HG3	1:Am:200:ASN:HD21	1.74	0.51
1:Ax:245:GLN:HG3	1:Ay:200:ASN:HD21	1.76	0.51
2:Bg:290:PRO:HB3	2:Bg:296:GLY:HA3	1.93	0.51
2:Bh:41:VAL:HG23	2:Bh:83:VAL:HG21	1.91	0.51
2:Bm:290:PRO:HB3	2:Bm:296:GLY:HA3	1.93	0.51
2:Bq:290:PRO:HB3	2:Bq:296:GLY:HA3	1.93	0.51
3:Ch:80:PHE:HA	5:Fh:136:VAL:HG21	1.93	0.51
1:Aq:36:ASP:HB3	1:Aq:39:GLU:HG2	1.93	0.50
1:As:119:LYS:HB3	1:Au:199:LEU:HD12	1.93	0.50
1:Ay:36:ASP:HB3	1:Ay:39:GLU:HG2	1.92	0.50
2:Bc:317:LYS:HE3	2:Bd:324:LEU:HD23	1.93	0.50
2:Bg:285:LEU:HD23	2:Bg:303:ASN:HB3	1.93	0.50
2:Bi:254:SER:HB2	2:Bk:138:VAL:HG22	1.93	0.50
2:Bm:254:SER:HB2	2:Bo:138:VAL:HG22	1.93	0.50
2:Bp:315:MET:HG3	2:Bq:328:VAL:HG13	1.92	0.50
3:Cj:201:ASP:HB3	3:Cj:221:ALA:HB3	1.93	0.50
3:Cl:56:PHE:HD1	5:Gl:139:LYS:HE2	1.76	0.50
4:De:68:ILE:HD11	4:Df:112:GLN:HE21	1.76	0.50
1:Ad:36:ASP:HB3	1:Ad:39:GLU:HG2	1.93	0.50
1:Ak:36:ASP:HB3	1:Ak:39:GLU:HG2	1.93	0.50
2:Bs:27:VAL:HG21	2:Bs:233:LEU:HD21	1.93	0.50
2:Bt:254:SER:HB2	2:Bv:138:VAL:HG22	1.93	0.50
3:Cj:262:TRP:HA	3:Cj:267:GLY:HA3	1.93	0.50
4:Dl:37:GLN:HG3	4:Dl:49:VAL:HG23	1.92	0.50
1:Av:36:ASP:HB3	1:Av:39:GLU:HG2	1.93	0.50
2:Bn:27:VAL:HG21	2:Bn:233:LEU:HD21	1.92	0.50
2:Bo:41:VAL:HG23	2:Bo:83:VAL:HG21	1.92	0.50
2:Bp:192:THR:HA	2:Bq:234:SER:HB2	1.94	0.50
2:Bx:41:VAL:HG23	2:Bx:83:VAL:HG21	1.94	0.50
3:Ce:255:ASP:HB3	3:Ce:258:SER:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cj:195:MET:HE2	3:Cj:281:LEU:HD11	1.93	0.50
3:Cs:88:ILE:HG12	3:Cs:106:ILE:HG23	1.94	0.50
4:Dz:169:ILE:HG13	4:Dz:172:LEU:HD12	1.94	0.50
1:Ai:245:GLN:HG3	1:Aj:200:ASN:HD21	1.77	0.50
1:Aj:64:PRO:HB2	1:Ak:38:VAL:HG13	1.94	0.50
1:Am:245:GLN:HG3	1:An:200:ASN:HD21	1.76	0.50
1:Ao:119:LYS:HB3	1:Aq:199:LEU:HD12	1.93	0.50
1:As:129:ASN:HB2	1:As:156:ASN:HB3	1.93	0.50
1:At:245:GLN:HG3	1:Au:200:ASN:HD21	1.76	0.50
2:Ba:69:LEU:H	2:Bz:56:GLN:HE22	1.60	0.50
2:Bb:56:GLN:HE22	2:Bc:69:LEU:H	1.59	0.50
2:Bg:248:ALA:HB1	2:Bg:265:VAL:HG22	1.94	0.50
1:Ak:219:PHE:HD1	2:Bz:69:LEU:HD13	1.77	0.50
1:Au:245:GLN:HG3	1:Av:200:ASN:HD21	1.75	0.50
2:Bq:27:VAL:HG21	2:Bq:233:LEU:HD21	1.93	0.50
2:Br:85:VAL:HG22	2:Br:103:VAL:HG13	1.94	0.50
3:Cm:56:PHE:HD1	5:Gm:139:LYS:HE2	1.76	0.50
4:Dz:217:ASP:HA	4:Dz:258:ARG:HD3	1.93	0.50
2:Ba:141:GLY:CA	2:Ba:154:GLY:O	2.60	0.50
2:Bb:41:VAL:HG23	2:Bb:83:VAL:HG21	1.93	0.50
2:Bp:27:VAL:HG21	2:Bp:233:LEU:HD21	1.93	0.50
3:Cf:195:MET:HE2	3:Cf:281:LEU:HD11	1.93	0.50
3:Cm:249:PRO:HG2	3:Cm:252:SER:HB3	1.94	0.50
3:Ct:85:VAL:HG22	3:Ct:108:ILE:HG12	1.93	0.50
3:Cw:262:TRP:HA	3:Cw:267:GLY:HA3	1.93	0.50
1:Ai:129:ASN:HB2	1:Ai:156:ASN:HB3	1.94	0.50
1:Aj:245:GLN:HG3	1:Ak:200:ASN:HD21	1.76	0.50
2:Bb:317:LYS:HE3	2:Bc:324:LEU:HD23	1.92	0.50
2:Bv:141:GLY:CA	2:Bv:154:GLY:O	2.59	0.50
3:Ch:262:TRP:HA	3:Ch:267:GLY:HA3	1.94	0.50
4:Dg:141:ASP:HB2	4:Dg:149:ILE:HG12	1.94	0.50
4:Dl:223:THR:HG22	4:Dl:285:VAL:HG22	1.94	0.50
1:Aa:200:ASN:HD21	1:Az:245:GLN:HG3	1.77	0.50
1:Ah:36:ASP:HB3	1:Ah:39:GLU:HG2	1.94	0.50
1:Am:64:PRO:HB2	1:An:38:VAL:HG13	1.94	0.50
1:Aw:245:GLN:HG3	1:Ax:200:ASN:HD21	1.75	0.50
2:Ba:110:LYS:HD2	2:Ba:151:LYS:HZ1	1.77	0.50
2:Bq:285:LEU:HD23	2:Bq:303:ASN:HB3	1.94	0.50
2:Bw:317:LYS:HE3	2:Bx:324:LEU:HD23	1.92	0.50
2:Bx:91:ALA:HB1	2:Bx:174:ASN:HD21	1.77	0.50
4:Dj:90:SER:HB2	4:Dj:104:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Af:231:ALA:HB3	1:Ag:195:LYS:HG3	1.92	0.50
2:Bb:141:GLY:CA	2:Bb:154:GLY:O	2.59	0.50
2:Bc:41:VAL:HG23	2:Bc:83:VAL:HG21	1.93	0.50
2:Bd:272:VAL:HG22	2:Be:260:VAL:HG22	1.93	0.50
2:Bg:27:VAL:HG21	2:Bg:233:LEU:HD21	1.93	0.50
2:Bg:41:VAL:HG23	2:Bg:83:VAL:HG21	1.93	0.50
2:Br:277:MET:HE2	2:Br:311:LYS:HD2	1.94	0.50
2:Bt:141:GLY:CA	2:Bt:154:GLY:O	2.60	0.50
2:Bx:56:GLN:HE22	2:By:69:LEU:H	1.59	0.50
3:Cb:293:GLN:HB2	3:Cb:369:ILE:HG23	1.94	0.50
3:Cx:255:ASP:HB3	3:Cx:258:SER:HB3	1.93	0.50
4:Dq:141:ASP:HB2	4:Dq:149:ILE:HG12	1.94	0.50
1:Ac:129:ASN:HB2	1:Ac:156:ASN:HB3	1.94	0.49
1:At:119:LYS:HB3	1:Av:199:LEU:HD12	1.94	0.49
2:Bx:248:ALA:HB1	2:Bx:265:VAL:HG22	1.95	0.49
2:By:290:PRO:HB3	2:By:296:GLY:HA3	1.94	0.49
3:Cd:262:TRP:HA	3:Cd:267:GLY:HA3	1.93	0.49
3:Cr:262:TRP:HA	3:Cr:267:GLY:HA3	1.94	0.49
1:Ac:245:GLN:HG3	1:Ad:200:ASN:HD21	1.77	0.49
1:Al:64:PRO:HB2	1:Am:38:VAL:HG13	1.93	0.49
2:Bc:27:VAL:HG21	2:Bc:233:LEU:HD21	1.93	0.49
2:Bk:315:MET:HG3	2:Bl:328:VAL:HG13	1.93	0.49
2:Bp:254:SER:HB2	2:Br:138:VAL:HG22	1.93	0.49
2:Bt:287:VAL:HG22	2:Bt:301:VAL:HG13	1.94	0.49
2:By:41:VAL:HG23	2:By:83:VAL:HG21	1.93	0.49
4:Di:49:VAL:HG12	4:Di:59:GLU:HG2	1.94	0.49
1:Ag:245:GLN:HG3	1:Ah:200:ASN:HD21	1.76	0.49
1:An:245:GLN:HG3	1:Ao:200:ASN:HD21	1.75	0.49
2:Ba:27:VAL:HG21	2:Ba:233:LEU:HD21	1.94	0.49
2:Bp:41:VAL:HG23	2:Bp:83:VAL:HG21	1.93	0.49
2:Bp:290:PRO:HB3	2:Bp:296:GLY:HA3	1.93	0.49
2:Bu:253:ASN:HB3	2:Bu:258:THR:HG23	1.94	0.49
3:Cl:294:ILE:HG22	3:Cl:369:ILE:HG22	1.94	0.49
3:Cx:262:TRP:HA	3:Cx:267:GLY:HA3	1.93	0.49
4:Dh:37:GLN:HG3	4:Dh:49:VAL:HG23	1.94	0.49
1:Al:119:LYS:HB3	1:An:199:LEU:HD12	1.94	0.49
1:Au:119:LYS:HB3	1:Aw:199:LEU:HD12	1.95	0.49
2:Bc:21:ILE:HG23	2:Bc:197:LEU:HD11	1.94	0.49
2:Be:224:ARG:HH22	3:Ch:323:THR:HB	1.78	0.49
2:Bo:290:PRO:HB3	2:Bo:296:GLY:HA3	1.94	0.49
2:Bx:275:GLY:HA3	2:By:338:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cf:262:TRP:HA	3:Cf:267:GLY:HA3	1.94	0.49
3:Cl:195:MET:HE2	3:Cl:281:LEU:HD11	1.94	0.49
1:Ab:119:LYS:HB3	1:Ad:199:LEU:HD12	1.94	0.49
1:Ax:64:PRO:HB2	1:Ay:38:VAL:HG13	1.94	0.49
2:Bc:254:SER:HB2	2:Be:138:VAL:HG22	1.95	0.49
2:Bs:41:VAL:HG23	2:Bs:83:VAL:HG21	1.93	0.49
2:Bu:56:GLN:HE22	2:Bv:69:LEU:H	1.60	0.49
3:Cb:255:ASP:HB3	3:Cb:258:SER:HB3	1.93	0.49
1:Aq:245:GLN:HG3	1:Ar:200:ASN:HD21	1.77	0.49
2:Bx:22:LYS:HB3	2:Bx:237:GLU:HG2	1.94	0.49
2:Bx:182:ILE:HG12	2:Bx:222:ALA:HB2	1.95	0.49
3:Cz:195:MET:HE2	3:Cz:281:LEU:HD11	1.95	0.49
1:Ap:219:PHE:HA	2:Be:69:LEU:HD13	1.95	0.49
2:Bj:42:THR:HG22	2:Bj:80:VAL:HG22	1.94	0.49
2:Bo:27:VAL:HG21	2:Bo:233:LEU:HD21	1.94	0.49
2:Bo:85:VAL:HG22	2:Bo:103:VAL:HG13	1.93	0.49
2:Bw:224:ARG:HH22	3:Cz:323:THR:HB	1.78	0.49
3:Ch:326:PHE:HD1	3:Ch:328:ASP:H	1.61	0.49
4:Dx:249:PHE:HB3	4:Dx:254:LEU:HD23	1.95	0.49
2:Ba:254:SER:HB2	2:Bc:138:VAL:HG22	1.95	0.49
2:Bf:41:VAL:HG23	2:Bf:83:VAL:HG21	1.94	0.49
2:Bn:22:LYS:HB3	2:Bn:237:GLU:HG2	1.94	0.49
2:Bq:141:GLY:CA	2:Bq:154:GLY:O	2.60	0.49
2:Bw:41:VAL:HG23	2:Bw:83:VAL:HG21	1.95	0.49
2:By:22:LYS:HB3	2:By:237:GLU:HG2	1.95	0.49
3:Cd:326:PHE:HD1	3:Cd:328:ASP:H	1.60	0.49
3:Cy:255:ASP:HB3	3:Cy:258:SER:HB3	1.93	0.49
4:Dm:49:VAL:HG12	4:Dm:59:GLU:HG2	1.95	0.49
1:Ao:64:PRO:HB2	1:Ap:38:VAL:HG13	1.95	0.49
1:At:36:ASP:HB3	1:At:39:GLU:HG2	1.95	0.49
2:Bf:272:VAL:HG22	2:Bg:260:VAL:HG22	1.95	0.49
2:Bi:290:PRO:HB3	2:Bi:296:GLY:HA3	1.95	0.49
2:Bl:284:ASN:HB2	2:Bl:304:THR:HG23	1.95	0.49
2:Bv:248:ALA:HB1	2:Bv:265:VAL:HG22	1.94	0.49
3:Cn:262:TRP:HA	3:Cn:267:GLY:HA3	1.93	0.49
3:Cv:201:ASP:HB3	3:Cv:221:ALA:HB3	1.95	0.49
1:Ab:245:GLN:HG3	1:Ac:200:ASN:HD21	1.77	0.49
2:Bg:56:GLN:HE22	2:Bh:69:LEU:H	1.59	0.49
2:Bg:360:ILE:HD12	2:Bi:163:SER:H	1.77	0.49
2:Bq:254:SER:HB2	2:Bs:138:VAL:HG22	1.94	0.49
2:Bx:254:SER:HB2	2:Bz:138:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ca:249:PRO:HG2	3:Ca:252:SER:HB3	1.94	0.49
4:Dg:49:VAL:HG12	4:Dg:59:GLU:HG2	1.95	0.49
4:Dl:169:ILE:HG13	4:Dl:172:LEU:HD12	1.94	0.49
4:Do:49:VAL:HG12	4:Do:59:GLU:HG2	1.95	0.49
1:Aq:34:THR:HG21	3:Cg:247:PRO:HB2	1.95	0.48
1:Ar:129:ASN:HB2	1:Ar:156:ASN:HB3	1.94	0.48
2:Ba:261:VAL:HB	2:Bz:271:ALA:HB3	1.95	0.48
2:Bd:85:VAL:HG22	2:Bd:103:VAL:HG13	1.95	0.48
2:Bs:272:VAL:HG22	2:Bt:260:VAL:HG22	1.94	0.48
2:Bw:22:LYS:HB3	2:Bw:237:GLU:HG2	1.94	0.48
2:Bx:27:VAL:HG21	2:Bx:233:LEU:HD21	1.94	0.48
3:Cr:78:TYR:HD2	3:Cr:88:ILE:HB	1.77	0.48
4:Dh:223:THR:HG22	4:Dh:285:VAL:HG22	1.95	0.48
4:Dj:249:PHE:HB3	4:Dj:254:LEU:HD23	1.95	0.48
4:Ds:68:ILE:HD11	4:Dt:112:GLN:HE21	1.77	0.48
1:Ae:245:GLN:HG3	1:Af:200:ASN:HD21	1.78	0.48
2:Bd:22:LYS:HB3	2:Bd:237:GLU:HG2	1.95	0.48
2:Bd:275:GLY:HA3	2:Be:338:PRO:HG2	1.95	0.48
2:Be:27:VAL:HG21	2:Be:233:LEU:HD21	1.95	0.48
2:Bk:27:VAL:HG21	2:Bk:233:LEU:HD21	1.94	0.48
2:Bz:27:VAL:HG21	2:Bz:233:LEU:HD21	1.94	0.48
4:Dj:37:GLN:HG3	4:Dj:49:VAL:HG23	1.95	0.48
4:Dm:141:ASP:HB2	4:Dm:149:ILE:HG12	1.95	0.48
4:Dp:249:PHE:HB3	4:Dp:254:LEU:HD23	1.95	0.48
1:Ai:36:ASP:HB3	1:Ai:39:GLU:HG2	1.95	0.48
2:Bb:27:VAL:HG21	2:Bb:233:LEU:HD21	1.94	0.48
2:Bq:122:LEU:HB2	2:Bq:131:ALA:HB3	1.96	0.48
2:Bt:41:VAL:HG23	2:Bt:83:VAL:HG21	1.95	0.48
2:Bw:274:HIS:HE1	2:Bw:343:ALA:HB3	1.79	0.48
3:Cm:78:TYR:HD2	3:Cm:88:ILE:HB	1.77	0.48
3:Cu:255:ASP:HB3	3:Cu:258:SER:HB3	1.94	0.48
4:Db:223:THR:HG22	4:Db:285:VAL:HG22	1.95	0.48
2:Ba:85:VAL:HG22	2:Ba:103:VAL:HG13	1.95	0.48
2:Bf:254:SER:HB2	2:Bh:138:VAL:HG22	1.94	0.48
2:Bw:141:GLY:CA	2:Bw:154:GLY:O	2.61	0.48
4:Dj:169:ILE:HG13	4:Dj:172:LEU:HD12	1.94	0.48
4:Dj:217:ASP:HA	4:Dj:258:ARG:HD3	1.95	0.48
4:Du:49:VAL:HG12	4:Du:59:GLU:HG2	1.95	0.48
4:Dw:141:ASP:HB2	4:Dw:149:ILE:HG12	1.95	0.48
2:Bb:192:THR:HA	2:Bc:234:SER:HB2	1.96	0.48
2:Bz:141:GLY:CA	2:Bz:154:GLY:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dd:249:PHE:HB3	4:Dd:254:LEU:HD23	1.95	0.48
4:Dh:216:ILE:HA	4:Dh:291:ARG:HA	1.95	0.48
2:Bb:254:SER:HB2	2:Bd:138:VAL:HG22	1.95	0.48
2:Bi:137:LEU:HA	2:Bi:162:ILE:HG12	1.95	0.48
2:Bj:141:GLY:CA	2:Bj:154:GLY:O	2.61	0.48
2:Bo:91:ALA:HB1	2:Bo:174:ASN:HD21	1.78	0.48
2:Bo:141:GLY:CA	2:Bo:154:GLY:O	2.61	0.48
2:Br:85:VAL:HG13	2:Br:103:VAL:HG22	1.94	0.48
2:Bs:360:ILE:HD12	2:Bu:163:SER:H	1.79	0.48
2:Bu:248:ALA:HB1	2:Bu:265:VAL:HG22	1.95	0.48
3:Cd:195:MET:HE2	3:Cd:281:LEU:HD11	1.94	0.48
3:Cl:35:VAL:HG23	3:Cl:245:ARG:HG3	1.95	0.48
3:Cm:262:TRP:HA	3:Cm:267:GLY:HA3	1.94	0.48
4:Dl:249:PHE:HB3	4:Dl:254:LEU:HD23	1.95	0.48
1:Ah:184:LEU:HD12	1:Ah:188:ASN:HB2	1.96	0.48
1:Al:125:LEU:HB2	1:Al:160:PHE:HB3	1.94	0.48
2:Bi:284:ASN:HB2	2:Bi:304:THR:HG23	1.96	0.48
2:Bm:253:ASN:HB3	2:Bm:258:THR:HG23	1.93	0.48
2:By:141:GLY:CA	2:By:154:GLY:O	2.61	0.48
3:Ch:195:MET:HE2	3:Ch:281:LEU:HD11	1.96	0.48
4:Df:223:THR:HG22	4:Df:285:VAL:HG22	1.95	0.48
4:Dh:249:PHE:HB3	4:Dh:254:LEU:HD23	1.96	0.48
4:Dn:249:PHE:HB3	4:Dn:254:LEU:HD23	1.95	0.48
1:Ag:64:PRO:HB2	1:Ah:38:VAL:HG13	1.96	0.48
1:Ap:184:LEU:HD12	1:Ap:188:ASN:HB2	1.94	0.48
2:Bd:27:VAL:HG21	2:Bd:233:LEU:HD21	1.96	0.48
2:Bg:122:LEU:HB2	2:Bg:131:ALA:HB3	1.96	0.48
2:Bw:266:ARG:HB3	2:Bw:355:GLU:HG3	1.96	0.48
2:Bw:272:VAL:HG22	2:Bx:260:VAL:HG22	1.95	0.48
3:Ck:201:ASP:HB3	3:Ck:221:ALA:HB3	1.96	0.48
3:Cl:164:PHE:HZ	3:Cl:285:ILE:HB	1.78	0.48
4:Dz:223:THR:HG22	4:Dz:285:VAL:HG22	1.96	0.48
1:Aw:64:PRO:HB2	1:Ax:38:VAL:HG13	1.96	0.48
2:Bn:84:ILE:HG13	2:Bn:106:ILE:HD13	1.95	0.48
2:Bo:248:ALA:HB1	2:Bo:265:VAL:HG22	1.95	0.48
2:Bx:272:VAL:HG22	2:By:260:VAL:HG22	1.96	0.48
3:Ci:209:LYS:HD3	3:Ci:212:GLN:HE21	1.79	0.48
4:Dj:223:THR:HG22	4:Dj:285:VAL:HG22	1.96	0.48
1:Ah:245:GLN:HG3	1:Ai:200:ASN:HD21	1.77	0.48
1:Aw:36:ASP:HB3	1:Aw:39:GLU:HG2	1.95	0.48
1:Ax:119:LYS:HB3	1:Az:199:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ba:234:SER:HB2	2:Bz:192:THR:HA	1.95	0.48
2:Be:41:VAL:HG23	2:Be:83:VAL:HG21	1.95	0.48
2:Be:141:GLY:CA	2:Be:154:GLY:O	2.62	0.48
2:Bm:248:ALA:HB1	2:Bm:265:VAL:HG22	1.96	0.48
2:Bp:317:LYS:HB2	2:Bq:328:VAL:HG21	1.95	0.48
2:Bu:254:SER:HB2	2:Bw:138:VAL:HG22	1.95	0.48
3:Ca:164:PHE:HZ	3:Ca:285:ILE:HB	1.79	0.48
3:Cp:167:VAL:HG21	3:Cp:191:ALA:HB2	1.96	0.48
3:Cs:249:PRO:HG2	3:Cs:252:SER:HB3	1.96	0.48
3:Cw:80:PHE:HA	5:Fw:136:VAL:HG21	1.95	0.48
4:Dc:49:VAL:HG12	4:Dc:59:GLU:HG2	1.96	0.48
4:Dx:223:THR:HG22	4:Dx:285:VAL:HG22	1.96	0.48
2:Bb:182:ILE:HG12	2:Bb:222:ALA:HB2	1.96	0.47
2:Bd:277:MET:HE2	2:Bd:311:LYS:HD2	1.96	0.47
2:Bh:360:ILE:HD12	2:Bj:163:SER:H	1.79	0.47
2:Bi:41:VAL:HG23	2:Bi:83:VAL:HG21	1.96	0.47
2:Bq:137:LEU:HA	2:Bq:162:ILE:HG12	1.96	0.47
2:Bu:41:VAL:HG23	2:Bu:83:VAL:HG21	1.96	0.47
2:Bw:118:MET:HE2	2:Bw:118:MET:HB3	1.79	0.47
2:By:277:MET:HE2	2:By:311:LYS:HD2	1.96	0.47
3:Cq:262:TRP:HA	3:Cq:267:GLY:HA3	1.95	0.47
3:Cr:249:PRO:HG2	3:Cr:252:SER:HB3	1.96	0.47
4:Db:216:ILE:HA	4:Db:291:ARG:HA	1.95	0.47
4:Dr:249:PHE:HB3	4:Dr:254:LEU:HD23	1.96	0.47
4:Dv:90:SER:HB2	4:Dv:104:ILE:HD11	1.95	0.47
1:Af:245:GLN:HG3	1:Ag:200:ASN:HD21	1.79	0.47
2:Bb:122:LEU:HB2	2:Bb:131:ALA:HB3	1.96	0.47
2:Bf:248:ALA:HB1	2:Bf:265:VAL:HG22	1.97	0.47
2:Bg:141:GLY:CA	2:Bg:154:GLY:O	2.62	0.47
2:Bn:259:ILE:HD11	2:Bn:342:MET:HG3	1.96	0.47
2:Bn:318:LEU:HG	2:Bn:320:PRO:HG3	1.95	0.47
2:Bu:141:GLY:CA	2:Bu:154:GLY:O	2.61	0.47
3:Cb:209:LYS:HD2	3:Cb:212:GLN:HB2	1.96	0.47
3:Cd:78:TYR:HD2	3:Cd:88:ILE:HB	1.79	0.47
3:Cn:35:VAL:HG23	3:Cn:245:ARG:HG3	1.96	0.47
4:Dn:223:THR:HG22	4:Dn:285:VAL:HG22	1.96	0.47
1:Aa:199:LEU:HD12	1:Ay:119:LYS:HB3	1.96	0.47
1:Ac:36:ASP:HB3	1:Ac:39:GLU:HG2	1.95	0.47
2:Bl:137:LEU:HA	2:Bl:162:ILE:HG12	1.95	0.47
2:Bn:141:GLY:CA	2:Bn:154:GLY:O	2.62	0.47
2:Bz:233:LEU:O	2:Bz:237:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cm:195:MET:HE2	3:Cm:281:LEU:HD11	1.96	0.47
4:Dr:37:GLN:HG3	4:Dr:49:VAL:HG23	1.96	0.47
4:Dv:249:PHE:HB3	4:Dv:254:LEU:HD23	1.95	0.47
1:Ab:64:PRO:HB2	1:Ac:38:VAL:HG13	1.96	0.47
1:Ac:154:LEU:HD21	1:Ae:258:LEU:HD11	1.95	0.47
2:Be:272:VAL:HG22	2:Bf:260:VAL:HG22	1.96	0.47
2:Bn:41:VAL:HG23	2:Bn:83:VAL:HG21	1.95	0.47
4:Dp:216:ILE:HA	4:Dp:291:ARG:HA	1.95	0.47
4:Dz:216:ILE:HA	4:Dz:291:ARG:HA	1.97	0.47
1:Ab:139:GLY:HA3	1:Ac:148:TYR:HD1	1.80	0.47
1:Ao:129:ASN:HB2	1:Ao:156:ASN:HB3	1.96	0.47
1:Ap:64:PRO:HB2	1:Aq:38:VAL:HG13	1.96	0.47
1:Aw:119:LYS:HB3	1:Ay:199:LEU:HD12	1.97	0.47
2:Be:122:LEU:HB2	2:Be:131:ALA:HB3	1.96	0.47
2:Be:141:GLY:HA2	2:Be:154:GLY:O	2.14	0.47
2:Bh:272:VAL:HG22	2:Bi:260:VAL:HG22	1.94	0.47
2:Bl:322:VAL:HG12	2:Bl:323:THR:HG23	1.95	0.47
2:Bt:277:MET:HE2	2:Bt:311:LYS:HD2	1.96	0.47
3:Cc:93:ARG:HG2	3:Cc:102:VAL:HG23	1.96	0.47
3:Cs:222:MET:HE1	3:Cs:277:ILE:HD11	1.96	0.47
3:Cx:201:ASP:HB3	3:Cx:221:ALA:HB3	1.97	0.47
4:Dp:90:SER:HB2	4:Dp:104:ILE:HD11	1.95	0.47
4:Dz:249:PHE:HB3	4:Dz:254:LEU:HD23	1.95	0.47
5:Gm:133:VAL:HG12	5:Gm:134:GLN:HG2	1.95	0.47
1:Ap:119:LYS:HB3	1:Ar:199:LEU:HD12	1.97	0.47
1:Ar:64:PRO:HB2	1:As:38:VAL:HG13	1.96	0.47
2:Bb:290:PRO:HB3	2:Bb:296:GLY:HA3	1.97	0.47
2:Bc:248:ALA:HB1	2:Bc:265:VAL:HG22	1.96	0.47
2:Bj:41:VAL:HG23	2:Bj:83:VAL:HG21	1.96	0.47
2:Bl:21:ILE:HG23	2:Bl:197:LEU:HD11	1.97	0.47
2:Bl:141:GLY:CA	2:Bl:154:GLY:O	2.62	0.47
2:Br:182:ILE:HG12	2:Br:222:ALA:HB2	1.95	0.47
3:Cc:209:LYS:HD2	3:Cc:212:GLN:HB2	1.96	0.47
3:Cf:80:PHE:HD1	5:Ff:136:VAL:HG11	1.80	0.47
3:Ch:108:ILE:HG23	3:Ch:110:PRO:HD3	1.97	0.47
4:Dt:216:ILE:HA	4:Dt:291:ARG:HA	1.96	0.47
1:Aa:184:LEU:HD12	1:Aa:188:ASN:HB2	1.97	0.47
1:Ac:119:LYS:HB3	1:Ae:199:LEU:HD12	1.97	0.47
1:As:178:VAL:HG21	1:As:191:ILE:HD12	1.97	0.47
2:Bl:122:LEU:HB2	2:Bl:131:ALA:HB3	1.97	0.47
2:Bo:267:LEU:HB2	2:Bo:320:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Br:141:GLY:CA	2:Br:154:GLY:O	2.63	0.47
2:Bt:182:ILE:HG12	2:Bt:222:ALA:HB2	1.97	0.47
2:Bu:27:VAL:HG21	2:Bu:233:LEU:HD21	1.95	0.47
2:By:27:VAL:HG21	2:By:233:LEU:HD21	1.96	0.47
3:Cc:226:VAL:HB	3:Cc:236:MET:HB3	1.97	0.47
3:Ct:262:TRP:HA	3:Ct:267:GLY:HA3	1.97	0.47
3:Cu:201:ASP:HB3	3:Cu:221:ALA:HB3	1.97	0.47
3:Cu:262:TRP:HA	3:Cu:267:GLY:HA3	1.97	0.47
3:Cx:167:VAL:HG21	3:Cx:191:ALA:HB2	1.97	0.47
4:Dh:169:ILE:HG13	4:Dh:172:LEU:HD12	1.96	0.47
4:Dj:216:ILE:HA	4:Dj:291:ARG:HA	1.96	0.47
1:Aa:64:PRO:HB2	1:Ab:38:VAL:HG13	1.97	0.47
2:Bx:49:GLU:HG3	2:Bx:54:THR:HG21	1.97	0.47
3:Ce:78:TYR:HD2	3:Ce:88:ILE:HB	1.79	0.47
3:Ci:164:PHE:HZ	3:Ci:285:ILE:HB	1.79	0.47
4:Da:49:VAL:HG12	4:Da:59:GLU:HG2	1.97	0.47
4:Dw:49:VAL:HG12	4:Dw:59:GLU:HG2	1.97	0.47
4:Dx:90:SER:HB2	4:Dx:104:ILE:HD11	1.96	0.47
1:Aq:64:PRO:HB2	1:Ar:38:VAL:HG13	1.97	0.47
2:Ba:21:ILE:HG23	2:Ba:197:LEU:HD11	1.97	0.47
2:Bm:84:ILE:HG13	2:Bm:106:ILE:HD13	1.97	0.47
2:Bw:248:ALA:HB1	2:Bw:265:VAL:HG22	1.97	0.47
3:Cb:291:LEU:HD22	3:Cb:372:VAL:HA	1.97	0.47
3:Co:78:TYR:HD2	3:Co:88:ILE:HB	1.79	0.47
3:Cv:362:GLU:HG2	3:Cv:363:LEU:HG	1.97	0.47
1:Aj:154:LEU:HD21	1:Al:258:LEU:HD11	1.97	0.47
1:Ao:184:LEU:HD12	1:Ao:188:ASN:HB2	1.97	0.47
1:Aq:184:LEU:HD12	1:Aq:188:ASN:HB2	1.96	0.47
2:Bd:305:GLU:HG3	2:Bg:148:ASP:HB2	1.97	0.47
2:Bh:182:ILE:HG12	2:Bh:222:ALA:HB2	1.97	0.47
2:Bk:277:MET:HE2	2:Bk:311:LYS:HD2	1.97	0.47
2:Bx:253:ASN:HB3	2:Bx:258:THR:HG23	1.96	0.47
4:Df:249:PHE:HB3	4:Df:254:LEU:HD23	1.95	0.47
4:Dl:216:ILE:HA	4:Dl:291:ARG:HA	1.96	0.47
4:Dr:90:SER:HB2	4:Dr:104:ILE:HD11	1.96	0.47
1:Ae:139:GLY:HA3	1:Af:148:TYR:HD1	1.80	0.46
1:At:184:LEU:HD12	1:At:188:ASN:HB2	1.97	0.46
2:Bc:253:ASN:HB3	2:Bc:258:THR:HG23	1.97	0.46
2:Bg:21:ILE:HG23	2:Bg:197:LEU:HD11	1.97	0.46
2:Bk:122:LEU:HB2	2:Bk:131:ALA:HB3	1.97	0.46
2:Bs:85:VAL:HG22	2:Bs:103:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bt:284:ASN:HB2	2:Bt:304:THR:HG23	1.96	0.46
2:By:85:VAL:HG22	2:By:103:VAL:HG13	1.97	0.46
3:Ca:262:TRP:HA	3:Ca:267:GLY:HA3	1.96	0.46
3:Cd:167:VAL:HG21	3:Cd:191:ALA:HB2	1.96	0.46
3:Ci:195:MET:HE2	3:Ci:281:LEU:HD11	1.97	0.46
3:Ck:195:MET:HE2	3:Ck:281:LEU:HD11	1.97	0.46
3:Co:80:PHE:HA	5:Fo:136:VAL:HG21	1.97	0.46
3:Cx:226:VAL:HB	3:Cx:236:MET:HB3	1.97	0.46
4:Da:141:ASP:HB2	4:Da:149:ILE:HG12	1.98	0.46
4:Dy:49:VAL:HG12	4:Dy:59:GLU:HG2	1.97	0.46
1:Ae:119:LYS:HD2	1:Ag:199:LEU:HB2	1.97	0.46
2:Bc:84:ILE:HG13	2:Bc:106:ILE:HD13	1.97	0.46
2:Bg:103:VAL:HB	2:Bg:137:LEU:HD21	1.97	0.46
2:Bg:250:ILE:HG12	2:Bg:261:VAL:HG13	1.96	0.46
2:Bu:277:MET:HE2	2:Bu:311:LYS:HD2	1.96	0.46
2:Bx:141:GLY:CA	2:Bx:154:GLY:O	2.63	0.46
2:Bz:268:LYS:HD2	2:Bz:353:ALA:HA	1.97	0.46
3:Ck:269:MET:HE3	3:Ck:269:MET:HB3	1.81	0.46
3:Cl:201:ASP:HB3	3:Cl:221:ALA:HB3	1.98	0.46
4:Dr:216:ILE:HA	4:Dr:291:ARG:HA	1.96	0.46
4:Ds:83:THR:HG22	4:Ds:111:LYS:HA	1.97	0.46
4:Dv:223:THR:HG22	4:Dv:285:VAL:HG22	1.98	0.46
4:Dx:216:ILE:HA	4:Dx:291:ARG:HA	1.96	0.46
1:Af:139:GLY:HA3	1:Ag:148:TYR:HD1	1.80	0.46
1:Au:64:PRO:HB2	1:Av:38:VAL:HG13	1.97	0.46
2:Bb:118:MET:HE2	2:Bb:118:MET:HB3	1.76	0.46
2:Bp:141:GLY:CA	2:Bp:154:GLY:O	2.64	0.46
2:Bp:253:ASN:HB3	2:Bp:258:THR:HG23	1.95	0.46
3:Cf:63:SER:HA	3:Cf:66:ASN:HD21	1.80	0.46
4:Dd:90:SER:HB2	4:Dd:104:ILE:HD11	1.97	0.46
4:Dn:90:SER:HB2	4:Dn:104:ILE:HD11	1.98	0.46
4:Du:91:MET:HE2	4:Du:91:MET:HB3	1.86	0.46
1:Ad:139:GLY:HA3	1:Ae:148:TYR:HD1	1.81	0.46
1:Ai:64:PRO:HB2	1:Aj:38:VAL:HG13	1.98	0.46
1:An:64:PRO:HB2	1:Ao:38:VAL:HG13	1.97	0.46
1:Ar:119:LYS:HB3	1:At:199:LEU:HD12	1.98	0.46
1:Aw:184:LEU:HD12	1:Aw:188:ASN:HB2	1.97	0.46
1:Ay:34:THR:HG21	3:Co:247:PRO:HB2	1.97	0.46
2:Bg:224:ARG:HH22	3:Cj:323:THR:HB	1.79	0.46
2:Bo:274:HIS:HE1	2:Bo:343:ALA:HB3	1.81	0.46
3:Cc:167:VAL:HG21	3:Cc:191:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cq:195:MET:HE2	3:Cq:281:LEU:HD11	1.97	0.46
1:Av:139:GLY:HA3	1:Aw:148:TYR:HD1	1.80	0.46
2:Bd:84:ILE:HG13	2:Bd:106:ILE:HD13	1.96	0.46
2:Bf:84:ILE:HG13	2:Bf:106:ILE:HD13	1.97	0.46
2:Bg:84:ILE:HG13	2:Bg:106:ILE:HD13	1.97	0.46
2:Bi:259:ILE:HD11	2:Bi:342:MET:HG3	1.98	0.46
2:Bm:141:GLY:CA	2:Bm:154:GLY:O	2.63	0.46
2:Bn:248:ALA:HB1	2:Bn:265:VAL:HG22	1.98	0.46
2:Bp:182:ILE:HG12	2:Bp:222:ALA:HB2	1.96	0.46
2:Br:259:ILE:HD11	2:Br:342:MET:HG3	1.98	0.46
2:Bs:141:GLY:CA	2:Bs:154:GLY:O	2.63	0.46
3:Cn:195:MET:HG3	3:Cn:226:VAL:HG22	1.97	0.46
3:Cq:269:MET:HE3	3:Cq:269:MET:HB3	1.83	0.46
3:Cs:326:PHE:HD1	3:Cs:328:ASP:H	1.63	0.46
4:Df:216:ILE:HA	4:Df:291:ARG:HA	1.97	0.46
4:Dn:217:ASP:HA	4:Dn:258:ARG:HD3	1.97	0.46
1:Ai:184:LEU:HD12	1:Ai:188:ASN:HB2	1.98	0.46
1:Ak:184:LEU:HD12	1:Ak:188:ASN:HB2	1.96	0.46
2:Bj:84:ILE:HG13	2:Bj:106:ILE:HD13	1.97	0.46
3:Co:269:MET:HE3	3:Co:269:MET:HB3	1.82	0.46
3:Cr:43:LEU:HD21	3:Cr:68:MET:HE1	1.97	0.46
3:Cr:269:MET:HE3	3:Cr:269:MET:HB3	1.85	0.46
3:Ct:164:PHE:HZ	3:Ct:285:ILE:HB	1.81	0.46
3:Cx:269:MET:HE3	3:Cx:269:MET:HB3	1.80	0.46
3:Cy:126:ILE:O	3:Cy:169:THR:HA	2.15	0.46
2:Bf:141:GLY:CA	2:Bf:154:GLY:O	2.64	0.46
2:Bk:41:VAL:HG23	2:Bk:83:VAL:HG21	1.97	0.46
2:Bn:182:ILE:HG12	2:Bn:222:ALA:HB2	1.97	0.46
2:Bw:21:ILE:HG23	2:Bw:197:LEU:HD11	1.97	0.46
3:Cj:164:PHE:HZ	3:Cj:285:ILE:HB	1.80	0.46
3:Cn:326:PHE:HD1	3:Cn:328:ASP:H	1.63	0.46
4:Db:249:PHE:HB3	4:Db:254:LEU:HD23	1.97	0.46
4:De:49:VAL:HG12	4:De:59:GLU:HG2	1.98	0.46
1:Aa:148:TYR:HD1	1:Az:139:GLY:HA3	1.80	0.46
1:Ac:184:LEU:HD12	1:Ac:188:ASN:HB2	1.98	0.46
1:Aj:139:GLY:HA3	1:Ak:148:TYR:HD1	1.81	0.46
1:An:184:LEU:HD12	1:An:188:ASN:HB2	1.98	0.46
1:Aw:139:GLY:HA3	1:Ax:148:TYR:HD1	1.81	0.46
2:Bd:290:PRO:HB3	2:Bd:296:GLY:HA3	1.98	0.46
2:Bj:192:THR:HA	2:Bk:234:SER:HB2	1.97	0.46
2:Bm:259:ILE:HD11	2:Bm:342:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Br:49:GLU:HG3	2:Br:54:THR:HG21	1.98	0.46
2:Bv:182:ILE:HG12	2:Bv:222:ALA:HB2	1.98	0.46
4:Dp:49:VAL:HG12	4:Dp:59:GLU:HG2	1.98	0.46
1:Al:154:LEU:HD21	1:An:258:LEU:HD11	1.98	0.46
2:Bj:277:MET:HE2	2:Bj:311:LYS:HD2	1.97	0.46
2:Bn:275:GLY:HA3	2:Bo:338:PRO:HG2	1.97	0.46
2:Bo:317:LYS:HE3	2:Bp:324:LEU:HD23	1.97	0.46
2:Bq:248:ALA:HB1	2:Bq:265:VAL:HG22	1.98	0.46
2:Bs:274:HIS:HE1	2:Bs:343:ALA:HB3	1.81	0.46
3:Cd:249:PRO:HG2	3:Cd:252:SER:HB3	1.97	0.46
4:Dt:249:PHE:HB3	4:Dt:254:LEU:HD23	1.97	0.46
1:Ac:139:GLY:HA3	1:Ad:148:TYR:HD1	1.80	0.46
1:Ar:139:GLY:HA3	1:As:148:TYR:HD1	1.81	0.46
1:Av:184:LEU:HD12	1:Av:188:ASN:HB2	1.98	0.46
2:Ba:34:GLN:HG2	2:Bb:134:GLN:HB3	1.98	0.46
2:Bi:277:MET:HE2	2:Bi:311:LYS:HD2	1.97	0.46
2:Bq:318:LEU:HG	2:Bq:320:PRO:HG3	1.96	0.46
2:Bs:103:VAL:HB	2:Bs:137:LEU:HD21	1.98	0.46
2:Bu:267:LEU:HB2	2:Bu:320:PRO:HG2	1.98	0.46
3:Cj:111:SER:HB3	3:Cj:113:THR:HG22	1.98	0.46
3:Cp:93:ARG:HG2	3:Cp:102:VAL:HG23	1.98	0.46
4:Dt:39:ALA:HB3	4:Dt:47:ARG:HB2	1.98	0.46
2:Ba:224:ARG:HH22	3:Cd:323:THR:HB	1.81	0.45
2:Bc:268:LYS:HD2	2:Bc:353:ALA:HA	1.98	0.45
2:Bk:84:ILE:HG13	2:Bk:106:ILE:HD13	1.98	0.45
2:Bl:248:ALA:HB1	2:Bl:265:VAL:HG22	1.98	0.45
2:Bn:290:PRO:HB3	2:Bn:296:GLY:HA3	1.98	0.45
2:Bo:224:ARG:HH22	3:Cr:323:THR:HB	1.81	0.45
2:Bq:192:THR:HA	2:Br:234:SER:HB2	1.98	0.45
2:Bv:250:ILE:HG12	2:Bv:261:VAL:HG13	1.98	0.45
3:Cd:80:PHE:HA	5:Fd:136:VAL:HG21	1.97	0.45
3:Cj:34:ILE:HD11	3:Cj:100:MET:HB2	1.98	0.45
3:Cp:227:PHE:HD1	3:Cp:234:GLU:HA	1.81	0.45
5:Gw:139:LYS:HB3	5:Gw:141:GLN:HE22	1.81	0.45
2:Bc:274:HIS:HE1	2:Bc:343:ALA:HB3	1.81	0.45
2:Bj:182:ILE:HG12	2:Bj:222:ALA:HB2	1.98	0.45
2:Bl:182:ILE:HG12	2:Bl:222:ALA:HB2	1.98	0.45
2:Bn:192:THR:HA	2:Bo:234:SER:HB2	1.99	0.45
2:Bo:118:MET:HE2	2:Bo:118:MET:HB3	1.76	0.45
2:Bu:192:THR:HA	2:Bv:234:SER:HB2	1.98	0.45
2:Bv:259:ILE:HD11	2:Bv:342:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Co:326:PHE:HD1	3:Co:328:ASP:H	1.62	0.45
3:Cs:92:GLU:HB2	3:Cs:103:ARG:HB2	1.98	0.45
1:Ad:64:PRO:HB2	1:Ae:38:VAL:HG13	1.98	0.45
1:Ah:139:GLY:HA3	1:Ai:148:TYR:HD1	1.81	0.45
1:Ai:139:GLY:HA3	1:Aj:148:TYR:HD1	1.81	0.45
2:Bg:274:HIS:HE1	2:Bg:343:ALA:HB3	1.82	0.45
2:Bk:118:MET:HE2	2:Bk:118:MET:HB3	1.77	0.45
2:Bm:42:THR:HG22	2:Bm:80:VAL:HG22	1.99	0.45
2:Bm:274:HIS:HE1	2:Bm:343:ALA:HB3	1.82	0.45
2:Bv:284:ASN:HB2	2:Bv:304:THR:HG23	1.98	0.45
2:By:84:ILE:HG13	2:By:106:ILE:HD13	1.98	0.45
3:Ch:362:GLU:HG2	3:Ch:363:LEU:HG	1.98	0.45
3:Ci:201:ASP:HB3	3:Ci:221:ALA:HB3	1.99	0.45
3:Cq:209:LYS:HD2	3:Cq:212:GLN:HB2	1.98	0.45
3:Cu:344:LEU:HB3	3:Cu:356:LEU:HB3	1.98	0.45
4:Da:126:LEU:HD13	4:Da:162:TYR:HE1	1.81	0.45
1:Ar:184:LEU:HD12	1:Ar:188:ASN:HB2	1.99	0.45
1:Av:178:VAL:HG21	1:Av:191:ILE:HD12	1.99	0.45
2:Ba:248:ALA:HB1	2:Ba:265:VAL:HG22	1.97	0.45
2:Bf:182:ILE:HG12	2:Bf:222:ALA:HB2	1.99	0.45
2:Bi:22:LYS:HB3	2:Bi:237:GLU:HG2	1.98	0.45
2:Bk:141:GLY:CA	2:Bk:154:GLY:O	2.64	0.45
2:Bo:272:VAL:HG22	2:Bp:260:VAL:HG22	1.98	0.45
3:Cd:111:SER:HB3	3:Cd:113:THR:HG22	1.99	0.45
3:Ci:326:PHE:HD1	3:Ci:328:ASP:H	1.65	0.45
3:Cj:269:MET:HE3	3:Cj:269:MET:HB3	1.83	0.45
3:Ck:205:THR:HG22	3:Cl:260:ARG:HD3	1.99	0.45
3:Cn:350:TYR:HE2	3:Cn:355:GLU:HG3	1.82	0.45
3:Cq:63:SER:HA	3:Cq:66:ASN:HD21	1.80	0.45
3:Cr:126:ILE:O	3:Cr:169:THR:HA	2.16	0.45
4:Dq:91:MET:HE2	4:Dq:91:MET:HB3	1.77	0.45
1:Ae:36:ASP:HB3	1:Ae:39:GLU:HG2	1.97	0.45
1:Aj:119:LYS:HB3	1:Al:199:LEU:HD12	1.99	0.45
2:Bd:156:ASN:HD22	2:Be:114:GLY:HA3	1.81	0.45
2:Bf:290:PRO:HB3	2:Bf:296:GLY:HA3	1.99	0.45
2:Bi:141:GLY:CA	2:Bi:154:GLY:O	2.64	0.45
2:Bi:248:ALA:HB1	2:Bi:265:VAL:HG22	1.99	0.45
2:Bj:137:LEU:HA	2:Bj:162:ILE:HG12	1.98	0.45
2:Bk:137:LEU:HA	2:Bk:162:ILE:HG12	1.99	0.45
2:Bs:248:ALA:HB1	2:Bs:265:VAL:HG22	1.99	0.45
2:Bu:259:ILE:HD11	2:Bu:342:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bx:266:ARG:HB3	2:Bx:355:GLU:HG3	1.97	0.45
2:Bz:137:LEU:HA	2:Bz:162:ILE:HG12	1.98	0.45
3:Cm:164:PHE:HZ	3:Cm:285:ILE:HB	1.80	0.45
3:Cv:282:GLU:HA	3:Cv:286:SER:HB3	1.98	0.45
1:Au:184:LEU:HD12	1:Au:188:ASN:HB2	1.99	0.45
2:Bb:268:LYS:HD2	2:Bb:353:ALA:HA	1.98	0.45
2:Bf:250:ILE:HG12	2:Bf:261:VAL:HG13	1.98	0.45
2:Bl:22:LYS:HZ1	2:Bl:237:GLU:HB3	1.80	0.45
2:Bo:85:VAL:HG13	2:Bo:103:VAL:HG22	1.99	0.45
3:Cg:111:SER:HB3	3:Cg:113:THR:HG22	1.99	0.45
3:Ct:201:ASP:HB3	3:Ct:221:ALA:HB3	1.99	0.45
4:Ds:49:VAL:HG12	4:Ds:59:GLU:HG2	1.99	0.45
1:Ab:184:LEU:HD12	1:Ab:188:ASN:HB2	1.99	0.45
1:Am:36:ASP:HB3	1:Am:39:GLU:HG2	1.98	0.45
1:Ay:139:GLY:HA3	1:Az:148:TYR:HD1	1.82	0.45
2:Be:268:LYS:HD2	2:Be:353:ALA:HA	1.99	0.45
2:Bi:21:ILE:HG23	2:Bi:197:LEU:HD11	1.99	0.45
2:Bq:272:VAL:HG22	2:Br:260:VAL:HG22	1.98	0.45
2:By:156:ASN:HD22	2:Bz:114:GLY:HA3	1.81	0.45
3:Ca:34:ILE:HD11	3:Ca:100:MET:HB2	1.98	0.45
3:Ca:241:ARG:HB3	5:Gb:143:THR:HG21	1.98	0.45
3:Cb:70:LEU:HG	5:Fb:136:VAL:HG13	1.97	0.45
3:Cd:201:ASP:HB3	3:Cd:221:ALA:HB3	1.98	0.45
3:Ce:201:ASP:HB3	3:Ce:221:ALA:HB3	1.98	0.45
4:Df:90:SER:HB2	4:Df:104:ILE:HD11	1.99	0.45
4:Dx:169:ILE:HG13	4:Dx:172:LEU:HD12	1.98	0.45
1:Ah:154:LEU:HD21	1:Aj:258:LEU:HD11	1.99	0.45
1:Aj:111:LEU:HB3	1:Aj:172:MET:HG3	1.99	0.45
1:Ak:64:PRO:HB2	1:Al:38:VAL:HG13	1.98	0.45
1:At:139:GLY:HA3	1:Au:148:TYR:HD1	1.82	0.45
2:Bh:122:LEU:HB2	2:Bh:131:ALA:HB3	1.99	0.45
2:Bm:318:LEU:HG	2:Bm:320:PRO:HG3	1.99	0.45
2:Bp:122:LEU:HB2	2:Bp:131:ALA:HB3	1.99	0.45
2:Bp:277:MET:HE2	2:Bp:311:LYS:HD2	1.98	0.45
2:Bu:118:MET:HE2	2:Bu:118:MET:HB3	1.67	0.45
3:Ce:92:GLU:HB2	3:Ce:103:ARG:HB3	1.97	0.45
3:Ci:373:MET:HE3	3:Ci:373:MET:HB2	1.79	0.45
3:Cm:80:PHE:HA	5:Fm:136:VAL:HG21	1.99	0.45
3:Cq:373:MET:HE3	3:Cq:373:MET:HB2	1.91	0.45
3:Ct:153:ILE:HG21	3:Ct:195:MET:HE1	1.99	0.45
3:Cu:282:GLU:HA	3:Cu:286:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cz:111:SER:HB3	3:Cz:113:THR:HG22	1.99	0.45
4:Dg:216:ILE:HD12	4:Dg:289:LEU:HB3	1.98	0.45
4:Dz:90:SER:HB2	4:Dz:104:ILE:HD11	1.99	0.45
1:Aa:139:GLY:HA3	1:Ab:148:TYR:HD1	1.82	0.45
1:Ag:184:LEU:HD12	1:Ag:188:ASN:HB2	1.99	0.45
1:An:139:GLY:HA3	1:Ao:148:TYR:HD1	1.81	0.45
2:Be:192:THR:HA	2:Bf:234:SER:HB2	1.99	0.45
3:Cg:201:ASP:HB3	3:Cg:221:ALA:HB3	1.99	0.45
4:Dd:169:ILE:HG13	4:Dd:172:LEU:HD12	1.99	0.45
4:Dl:90:SER:HB2	4:Dl:104:ILE:HD11	1.99	0.45
4:Dr:223:THR:HG22	4:Dr:285:VAL:HG22	1.99	0.45
4:Dt:223:THR:HG22	4:Dt:285:VAL:HG22	1.99	0.45
1:Ak:139:GLY:HA3	1:Al:148:TYR:HD1	1.81	0.45
2:Bg:118:MET:HB3	2:Bg:118:MET:HE2	1.78	0.45
2:Bh:248:ALA:HB1	2:Bh:265:VAL:HG22	1.99	0.45
2:Bl:118:MET:HE3	2:Bl:118:MET:HB3	1.78	0.45
2:Bn:137:LEU:HA	2:Bn:162:ILE:HG12	1.98	0.45
2:Br:22:LYS:HB3	2:Br:237:GLU:HG2	1.99	0.45
2:Br:248:ALA:HB1	2:Br:265:VAL:HG22	1.99	0.45
2:Bv:49:GLU:HG3	2:Bv:54:THR:HG21	1.99	0.45
2:Bw:259:ILE:HD11	2:Bw:342:MET:HG3	1.99	0.45
3:Ce:282:GLU:HA	3:Ce:286:SER:HB3	1.98	0.45
3:Cj:205:THR:HG22	3:Ck:260:ARG:HD3	1.99	0.45
3:Ck:350:TYR:HE2	3:Ck:355:GLU:HG3	1.82	0.45
3:Cp:111:SER:HB3	3:Cp:113:THR:HG22	1.99	0.45
3:Ct:362:GLU:HG2	3:Ct:363:LEU:HG	1.99	0.45
4:Db:169:ILE:HG13	4:Db:172:LEU:HD12	1.98	0.45
4:Dv:126:LEU:HD13	4:Dv:162:TYR:HE1	1.82	0.45
1:Ap:234:GLN:HA	1:Aq:198:THR:HB	1.98	0.44
1:Ar:154:LEU:HD21	1:At:258:LEU:HD11	1.99	0.44
2:Bd:248:ALA:HB1	2:Bd:265:VAL:HG22	1.99	0.44
2:Bf:192:THR:HA	2:Bf:234:SER:HB2	1.99	0.44
2:Bo:84:ILE:HG13	2:Bo:106:ILE:HD13	1.98	0.44
2:Bt:272:VAL:HG22	2:Bu:260:VAL:HG22	1.99	0.44
2:Bu:22:LYS:HB3	2:Bu:237:GLU:HG2	1.98	0.44
2:Bu:137:LEU:HA	2:Bu:162:ILE:HG12	1.99	0.44
2:Bx:259:ILE:HD11	2:Bx:342:MET:HG3	1.98	0.44
3:Ch:205:THR:HG22	3:Ci:260:ARG:HD3	1.99	0.44
3:Cp:262:TRP:HA	3:Cp:267:GLY:HA3	1.98	0.44
3:Cu:220:PHE:HE2	3:Cu:273:VAL:HG11	1.82	0.44
4:Dt:90:SER:HB2	4:Dt:104:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Af:64:PRO:HB2	1:Ag:38:VAL:HG13	1.98	0.44
1:Ag:200:ASN:HB3	1:Ag:201:THR:H	1.66	0.44
1:As:184:LEU:HD12	1:As:188:ASN:HB2	1.99	0.44
1:Av:119:LYS:HB3	1:Ax:199:LEU:HD12	1.99	0.44
2:Bh:84:ILE:HG13	2:Bh:106:ILE:HD13	1.99	0.44
2:Bh:285:LEU:HD23	2:Bh:303:ASN:HB3	2.00	0.44
2:Bk:192:THR:HA	2:Bl:234:SER:HB2	1.98	0.44
2:Bo:259:ILE:HD11	2:Bo:342:MET:HG3	2.00	0.44
2:Bp:42:THR:HG22	2:Bp:80:VAL:HG22	2.00	0.44
2:Bq:277:MET:HE2	2:Bq:311:LYS:HD2	1.99	0.44
2:Br:103:VAL:HB	2:Br:137:LEU:HD21	1.99	0.44
2:By:275:GLY:HA3	2:Bz:338:PRO:HG2	1.99	0.44
3:Cs:282:GLU:HA	3:Cs:286:SER:HB3	1.98	0.44
3:Cu:195:MET:HE2	3:Cu:281:LEU:HD11	1.98	0.44
1:Ae:184:LEU:HD12	1:Ae:188:ASN:HB2	1.99	0.44
1:Am:139:GLY:HA3	1:An:148:TYR:HD1	1.83	0.44
1:Ao:139:GLY:HA3	1:Ap:148:TYR:HD1	1.82	0.44
2:Be:21:ILE:HG23	2:Be:197:LEU:HD11	2.00	0.44
2:Bh:141:GLY:CA	2:Bh:154:GLY:O	2.65	0.44
2:Bh:259:ILE:HD11	2:Bh:342:MET:HG3	1.99	0.44
2:Bh:274:HIS:HE1	2:Bh:343:ALA:HB3	1.82	0.44
2:Bm:272:VAL:HG22	2:Bn:260:VAL:HG22	1.98	0.44
2:Br:192:THR:HA	2:Bs:234:SER:HB2	1.99	0.44
2:Bx:103:VAL:HB	2:Bx:137:LEU:HD21	1.98	0.44
3:Cd:85:VAL:HG22	3:Cd:108:ILE:HG12	2.00	0.44
3:Ch:201:ASP:HB3	3:Ch:221:ALA:HB3	1.99	0.44
3:Ck:78:TYR:HD2	3:Ck:88:ILE:HB	1.82	0.44
3:Cl:111:SER:HB3	3:Cl:113:THR:HG22	1.98	0.44
3:Cq:201:ASP:HB3	3:Cq:221:ALA:HB3	1.99	0.44
4:Dm:83:THR:HG22	4:Dm:111:LYS:HA	2.00	0.44
2:Bb:137:LEU:HA	2:Bb:162:ILE:HG12	1.99	0.44
2:Bj:248:ALA:HB1	2:Bj:265:VAL:HG22	2.00	0.44
2:Bq:41:VAL:HG23	2:Bq:83:VAL:HG21	2.00	0.44
2:Br:84:ILE:HG13	2:Br:106:ILE:HD13	1.99	0.44
2:Br:272:VAL:HG22	2:Bs:260:VAL:HG22	1.99	0.44
3:Cp:222:MET:HE1	3:Cp:277:ILE:HD11	2.00	0.44
3:Cs:195:MET:HE2	3:Cs:281:LEU:HD11	1.99	0.44
3:Cx:326:PHE:HD1	3:Cx:328:ASP:H	1.65	0.44
4:Di:112:GLN:HE21	4:Di:112:GLN:HB3	1.61	0.44
1:Am:234:GLN:HA	1:An:198:THR:HB	1.99	0.44
2:Ba:284:ASN:HB2	2:Ba:304:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Be:266:ARG:HB3	2:Be:355:GLU:HG3	1.99	0.44
2:Bh:192:THR:HA	2:Bi:234:SER:HB2	1.99	0.44
2:Bi:27:VAL:HG21	2:Bi:233:LEU:HD21	1.98	0.44
2:Bo:277:MET:HE2	2:Bo:311:LYS:HD2	1.99	0.44
2:Bu:283:GLU:HG2	2:Bu:305:GLU:HG2	1.98	0.44
2:Bu:290:PRO:HB3	2:Bu:296:GLY:HA3	1.99	0.44
2:Bw:27:VAL:HG21	2:Bw:233:LEU:HD21	1.98	0.44
3:Ca:201:ASP:HB3	3:Ca:221:ALA:HB3	1.99	0.44
3:Cb:78:TYR:HD2	3:Cb:88:ILE:HB	1.83	0.44
3:Ce:350:TYR:HE2	3:Ce:355:GLU:HG3	1.83	0.44
3:Cf:350:TYR:HE2	3:Cf:355:GLU:HG3	1.83	0.44
3:Cg:164:PHE:HZ	3:Cg:285:ILE:HB	1.83	0.44
3:Cu:164:PHE:HZ	3:Cu:285:ILE:HB	1.83	0.44
3:Cv:28:VAL:HG13	3:Cv:49:ALA:HB1	2.00	0.44
4:Da:31:PRO:HB3	4:Da:156:VAL:HG21	2.00	0.44
4:Da:216:ILE:HD12	4:Da:289:LEU:HB3	1.98	0.44
4:Dq:83:THR:HG22	4:Dq:111:LYS:HA	1.99	0.44
4:Dv:169:ILE:HG13	4:Dv:172:LEU:HD12	2.00	0.44
2:Bc:250:ILE:HG12	2:Bc:261:VAL:HG13	1.98	0.44
2:Bm:277:MET:HE2	2:Bm:311:LYS:HD2	2.00	0.44
2:Bo:283:GLU:HG2	2:Bo:305:GLU:HB3	2.00	0.44
2:Bv:272:VAL:HG22	2:Bw:260:VAL:HG22	1.99	0.44
2:Bz:41:VAL:HG23	2:Bz:83:VAL:HG21	2.00	0.44
3:Ce:195:MET:HE2	3:Ce:281:LEU:HD11	1.99	0.44
3:Cp:350:TYR:HE2	3:Cp:355:GLU:HG3	1.82	0.44
3:Cr:195:MET:HE2	3:Cr:281:LEU:HD11	1.99	0.44
3:Ct:78:TYR:HD2	3:Ct:88:ILE:HB	1.83	0.44
3:Cv:226:VAL:HB	3:Cv:236:MET:HB3	2.00	0.44
4:Dg:31:PRO:HB3	4:Dg:156:VAL:HG21	2.00	0.44
1:Af:219:PHE:HD1	2:Bu:69:LEU:HD13	1.83	0.44
1:Am:178:VAL:HG21	1:Am:191:ILE:HD12	1.99	0.44
1:Ay:178:VAL:HG21	1:Ay:191:ILE:HD12	2.00	0.44
2:Bi:118:MET:HE3	2:Bi:118:MET:HB3	1.78	0.44
3:Cc:365:TYR:HB3	4:Dv:91:MET:HE2	1.98	0.44
3:Ce:85:VAL:HG22	3:Ce:108:ILE:HG12	1.99	0.44
3:Cj:373:MET:HE3	3:Cj:373:MET:HB2	1.80	0.44
3:Cn:373:MET:HE3	3:Cn:373:MET:HB2	1.81	0.44
3:Cy:350:TYR:HE2	3:Cy:355:GLU:HG3	1.83	0.44
4:Dc:83:THR:HG22	4:Dc:111:LYS:HA	1.99	0.44
1:An:111:LEU:HB3	1:An:172:MET:HG3	2.00	0.44
1:Ax:234:GLN:HA	1:Ay:198:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bc:275:GLY:HA3	2:Bd:338:PRO:HG2	1.99	0.44
2:Bm:256:THR:HB	2:Bm:258:THR:HG22	2.00	0.44
2:Bo:156:ASN:HD22	2:Bp:114:GLY:HA3	1.83	0.44
2:Bt:253:ASN:HB3	2:Bt:258:THR:HG23	1.99	0.44
2:Bx:84:ILE:HG13	2:Bx:106:ILE:HD13	2.00	0.44
3:Ce:111:SER:HB3	3:Ce:113:THR:HG22	2.00	0.44
3:Ci:350:TYR:HE2	3:Ci:355:GLU:HG3	1.83	0.44
3:Cm:126:ILE:O	3:Cm:169:THR:HA	2.18	0.44
3:Cn:153:ILE:HG21	3:Cn:195:MET:HE1	2.00	0.44
3:Cn:201:ASP:HB3	3:Cn:221:ALA:HB3	2.00	0.44
3:Cq:350:TYR:HE2	3:Cq:355:GLU:HG3	1.83	0.44
3:Cr:350:TYR:HE2	3:Cr:355:GLU:HG3	1.82	0.44
3:Cs:167:VAL:HG21	3:Cs:191:ALA:HB2	2.00	0.44
3:Cw:326:PHE:HD1	3:Cw:328:ASP:H	1.66	0.44
3:Cy:111:SER:HB3	3:Cy:113:THR:HG22	1.99	0.44
4:Db:183:THR:HG21	4:Db:206:ILE:HD11	2.00	0.44
4:Dn:216:ILE:HA	4:Dn:291:ARG:HA	1.99	0.44
1:Ak:205:TYR:CZ	1:Ak:236:SER:HB3	2.53	0.44
1:Ay:184:LEU:HD12	1:Ay:188:ASN:HB2	1.98	0.44
2:Bb:85:VAL:HG22	2:Bb:103:VAL:HG13	2.00	0.44
2:Bc:118:MET:HE3	2:Bc:118:MET:HB2	1.80	0.44
2:Bf:61:MET:HE2	2:Bf:61:MET:HB3	1.93	0.44
2:Bi:224:ARG:HH22	3:Cl:323:THR:HB	1.83	0.44
2:By:284:ASN:HB2	2:By:304:THR:HG23	2.00	0.44
2:By:318:LEU:HG	2:By:320:PRO:HD3	1.99	0.44
2:Bz:266:ARG:HB3	2:Bz:355:GLU:HG3	1.99	0.44
3:Cc:239:THR:HG21	3:Cd:155:ARG:HD3	1.99	0.44
3:Cf:362:GLU:HG2	3:Cf:363:LEU:HG	2.00	0.44
4:Di:197:LYS:HA	4:Di:200:GLN:HB2	2.00	0.44
4:Dq:49:VAL:HG12	4:Dq:59:GLU:HG2	2.00	0.44
4:Dy:31:PRO:HB3	4:Dy:156:VAL:HG21	2.00	0.44
1:Aa:200:ASN:HB3	1:Aa:201:THR:H	1.66	0.43
1:Au:178:VAL:HG21	1:Au:191:ILE:HD12	2.00	0.43
1:Au:234:GLN:HA	1:Av:198:THR:HB	2.00	0.43
2:Be:84:ILE:HG13	2:Be:106:ILE:HD13	1.99	0.43
2:Be:248:ALA:HB1	2:Be:265:VAL:HG22	2.00	0.43
2:Bj:290:PRO:HB3	2:Bj:296:GLY:HA3	1.99	0.43
2:Bt:248:ALA:HB1	2:Bt:265:VAL:HG22	2.00	0.43
3:Ch:350:TYR:HE2	3:Ch:355:GLU:HG3	1.83	0.43
3:Ck:255:ASP:HB3	3:Ck:258:SER:HB3	2.00	0.43
3:Cm:282:GLU:HA	3:Cm:286:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cs:164:PHE:HZ	3:Cs:285:ILE:HB	1.83	0.43
3:Cy:334:ARG:HE	3:Cz:295:VAL:HG21	1.83	0.43
4:Dc:126:LEU:HD13	4:Dc:162:TYR:HE1	1.83	0.43
1:Ap:178:VAL:HG21	1:Ap:191:ILE:HD12	2.00	0.43
2:Ba:259:ILE:HD11	2:Ba:342:MET:HG3	2.00	0.43
2:Bb:141:GLY:HA2	2:Bb:154:GLY:O	2.18	0.43
2:Bb:259:ILE:HD11	2:Bb:342:MET:HG3	1.99	0.43
2:Be:259:ILE:HD11	2:Be:342:MET:HG3	2.00	0.43
2:Bq:259:ILE:HD11	2:Bq:342:MET:HG3	2.00	0.43
2:Br:275:GLY:HA3	2:Bs:338:PRO:HG2	2.00	0.43
2:Bu:118:MET:H	2:Bu:118:MET:HG2	1.59	0.43
2:Bu:284:ASN:HB2	2:Bu:304:THR:HG23	1.99	0.43
3:Cb:201:ASP:HB3	3:Cb:221:ALA:HB3	2.00	0.43
3:Cb:226:VAL:HB	3:Cb:236:MET:HB3	2.00	0.43
3:Cc:201:ASP:HB3	3:Cc:221:ALA:HB3	2.00	0.43
3:Cg:326:PHE:HD1	3:Cg:328:ASP:H	1.65	0.43
3:Ck:88:ILE:HG12	3:Ck:106:ILE:HG23	2.01	0.43
3:Co:350:TYR:HE2	3:Co:355:GLU:HG3	1.83	0.43
3:Cr:220:PHE:HE2	3:Cr:273:VAL:HG11	1.83	0.43
4:Ds:197:LYS:HA	4:Ds:200:GLN:HB2	2.00	0.43
1:Af:184:LEU:HD12	1:Af:188:ASN:HB2	2.00	0.43
1:At:205:TYR:CZ	1:At:236:SER:HB3	2.53	0.43
1:Az:184:LEU:HD12	1:Az:188:ASN:HB2	2.00	0.43
2:Bv:122:LEU:HB2	2:Bv:131:ALA:HB3	2.00	0.43
2:By:118:MET:HE3	2:By:118:MET:HB3	1.78	0.43
3:Cd:350:TYR:HE2	3:Cd:355:GLU:HG3	1.84	0.43
3:Ci:111:SER:HB3	3:Ci:113:THR:HG22	2.00	0.43
3:Co:111:SER:HB3	3:Co:113:THR:HG22	2.00	0.43
3:Cz:201:ASP:HB3	3:Cz:221:ALA:HB3	2.00	0.43
4:Dx:217:ASP:HA	4:Dx:258:ARG:HD3	2.00	0.43
1:Ai:106:ILE:HD12	1:Ai:177:THR:HG21	2.00	0.43
1:Az:200:ASN:HB3	1:Az:201:THR:H	1.67	0.43
2:Bc:266:ARG:HB3	2:Bc:355:GLU:HG3	2.00	0.43
2:Bd:182:ILE:HG12	2:Bd:222:ALA:HB2	2.00	0.43
2:Bl:266:ARG:HB3	2:Bl:355:GLU:HG3	1.99	0.43
2:Bq:42:THR:HG22	2:Bq:80:VAL:HG22	2.01	0.43
2:Bu:105:SER:HB2	2:Bu:112:LEU:HD11	2.00	0.43
2:Bw:192:THR:HA	2:Bx:234:SER:HB2	1.99	0.43
3:Ck:111:SER:HB3	3:Ck:113:THR:HG22	1.99	0.43
3:Cl:350:TYR:HE2	3:Cl:355:GLU:HG3	1.82	0.43
3:Cu:226:VAL:HB	3:Cu:236:MET:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:154:LEU:HD21	1:Ai:258:LEU:HD11	2.00	0.43
1:Ai:154:LEU:HD21	1:Ak:258:LEU:HD11	2.01	0.43
1:Aj:125:LEU:HB3	1:Am:244:MET:HE3	2.01	0.43
1:Ak:178:VAL:HG21	1:Ak:191:ILE:HD12	2.00	0.43
1:Ao:234:GLN:HA	1:Ap:198:THR:HB	2.00	0.43
1:Ap:205:TYR:CZ	1:Ap:236:SER:HB3	2.54	0.43
1:Ay:234:GLN:HA	1:Az:198:THR:HB	2.00	0.43
2:Ba:49:GLU:HG3	2:Ba:54:THR:HG21	2.00	0.43
2:Ba:122:LEU:HB2	2:Ba:131:ALA:HB3	2.00	0.43
2:Bb:256:THR:HB	2:Bb:258:THR:HG22	2.01	0.43
2:Bc:360:ILE:HD12	2:Be:163:SER:H	1.83	0.43
2:Bm:250:ILE:HG12	2:Bm:261:VAL:HG13	2.00	0.43
2:Bz:182:ILE:HG12	2:Bz:222:ALA:HB2	2.01	0.43
2:Bz:259:ILE:HD11	2:Bz:342:MET:HG3	2.01	0.43
3:Ca:111:SER:HB3	3:Ca:113:THR:HG22	2.00	0.43
3:Cb:126:ILE:HB	3:Cb:169:THR:HG22	2.00	0.43
3:Cj:167:VAL:HG21	3:Cj:191:ALA:HB2	2.00	0.43
4:Dc:31:PRO:HB3	4:Dc:156:VAL:HG21	2.00	0.43
4:Do:31:PRO:HB3	4:Do:156:VAL:HG21	1.99	0.43
1:Aa:205:TYR:CZ	1:Aa:236:SER:HB3	2.54	0.43
1:Af:205:TYR:CZ	1:Af:236:SER:HB3	2.54	0.43
1:Al:184:LEU:HD12	1:Al:188:ASN:HB2	2.00	0.43
1:Ap:33:THR:HG23	1:Ap:35:VAL:H	1.84	0.43
1:Ap:111:LEU:HB3	1:Ap:172:MET:HG3	2.01	0.43
1:Aq:234:GLN:HA	1:Ar:198:THR:HB	2.00	0.43
1:Au:106:ILE:HD12	1:Au:177:THR:HG21	2.00	0.43
2:Bd:192:THR:HA	2:Be:234:SER:HB2	2.00	0.43
2:Bm:224:ARG:HH22	3:Cp:323:THR:HB	1.82	0.43
2:Bp:259:ILE:HD11	2:Bp:342:MET:HG3	2.01	0.43
2:Bq:360:ILE:HD12	2:Bs:163:SER:H	1.82	0.43
2:Bs:259:ILE:HD11	2:Bs:342:MET:HG3	2.01	0.43
2:Bu:84:ILE:HG13	2:Bu:106:ILE:HD13	2.00	0.43
2:Bw:254:SER:HB2	2:By:138:VAL:HG22	2.00	0.43
2:By:274:HIS:HE1	2:By:343:ALA:HB3	1.83	0.43
2:Bz:85:VAL:HB	2:Bz:122:LEU:HD21	1.99	0.43
3:Cd:269:MET:HE3	3:Cd:269:MET:HB3	1.79	0.43
3:Cf:201:ASP:HB3	3:Cf:221:ALA:HB3	2.01	0.43
3:Cj:350:TYR:HE2	3:Cj:355:GLU:HG3	1.83	0.43
3:Cl:326:PHE:HD1	3:Cl:328:ASP:H	1.66	0.43
3:Cm:350:TYR:HE2	3:Cm:355:GLU:HG3	1.83	0.43
3:Cn:209:LYS:HD2	3:Cn:212:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cr:201:ASP:HB3	3:Cr:221:ALA:HB3	2.01	0.43
3:Cr:205:THR:HG22	3:Cs:260:ARG:HD3	1.99	0.43
3:Cw:167:VAL:HG21	3:Cw:191:ALA:HB2	2.00	0.43
3:Cw:350:TYR:HE2	3:Cw:355:GLU:HG3	1.83	0.43
3:Cy:153:ILE:HG21	3:Cy:195:MET:HE1	2.00	0.43
4:Di:83:THR:HG22	4:Di:111:LYS:HA	2.00	0.43
4:Do:126:LEU:HD13	4:Do:162:TYR:HE1	1.84	0.43
1:Ac:205:TYR:CZ	1:Ac:236:SER:HB3	2.54	0.43
1:Ak:119:LYS:HB3	1:Am:199:LEU:HD12	2.01	0.43
1:Am:106:ILE:HD12	1:Am:177:THR:HG21	2.01	0.43
1:Am:205:TYR:CZ	1:Am:236:SER:HB3	2.54	0.43
1:Ao:106:ILE:HD12	1:Ao:177:THR:HG21	2.01	0.43
1:As:154:LEU:HD21	1:Au:258:LEU:HD11	2.01	0.43
1:Ax:139:GLY:HA3	1:Ay:148:TYR:HD1	1.84	0.43
2:Bh:22:LYS:HB3	2:Bh:237:GLU:HG2	1.99	0.43
2:Bk:22:LYS:HB3	2:Bk:237:GLU:HG2	2.01	0.43
2:Bq:61:MET:HE2	2:Bq:61:MET:HB3	1.92	0.43
3:Cg:195:MET:HE2	3:Cg:281:LEU:HD11	2.01	0.43
3:Cr:241:ARG:HB3	5:Gs:143:THR:HG21	2.01	0.43
3:Ct:111:SER:HB3	3:Ct:113:THR:HG22	2.01	0.43
3:Cv:209:LYS:HD2	3:Cv:212:GLN:HB2	2.01	0.43
3:Cw:139:MET:HE1	3:Cw:216:ILE:HD13	2.00	0.43
3:Cw:282:GLU:HA	3:Cw:286:SER:HB3	1.99	0.43
3:Cx:249:PRO:HG2	3:Cx:252:SER:HB3	2.01	0.43
3:Cy:157:LEU:HA	3:Cy:161:SER:HB2	2.00	0.43
4:Dg:31:PRO:HG3	4:Dg:95:TRP:HZ2	1.84	0.43
4:Dg:126:LEU:HD13	4:Dg:162:TYR:HE1	1.84	0.43
1:Ad:154:LEU:HD21	1:Af:258:LEU:HD11	2.00	0.43
1:Ae:106:ILE:HD12	1:Ae:177:THR:HG21	2.00	0.43
1:Ae:178:VAL:HG21	1:Ae:191:ILE:HD12	2.01	0.43
1:As:119:LYS:HD2	1:Au:199:LEU:HB2	2.00	0.43
1:Ax:184:LEU:HD12	1:Ax:188:ASN:HB2	2.00	0.43
2:Ba:84:ILE:HG13	2:Ba:106:ILE:HD13	2.01	0.43
2:Bi:192:THR:HA	2:Bj:234:SER:HB2	2.00	0.43
2:Bi:283:GLU:HG2	2:Bi:305:GLU:HG2	2.00	0.43
2:Bk:259:ILE:HD11	2:Bk:342:MET:HG3	2.01	0.43
2:Bx:271:ALA:HB3	2:By:261:VAL:HB	2.01	0.43
3:Cb:326:PHE:HD1	3:Cb:328:ASP:H	1.66	0.43
3:Cu:111:SER:HB3	3:Cu:113:THR:HG22	2.01	0.43
3:Cw:111:SER:HB3	3:Cw:113:THR:HG22	2.01	0.43
3:Cy:249:PRO:HG2	3:Cy:252:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cz:350:TYR:HE2	3:Cz:355:GLU:HG3	1.83	0.43
4:Dh:217:ASP:HA	4:Dh:258:ARG:HD3	2.00	0.43
4:Dt:169:ILE:HG13	4:Dt:172:LEU:HD12	2.00	0.43
1:Aa:219:PHE:HD1	2:Bp:69:LEU:HD13	1.83	0.43
1:Ae:119:LYS:HB3	1:Ag:199:LEU:HD12	2.01	0.43
1:Ae:200:ASN:HB3	1:Ae:201:THR:H	1.67	0.43
1:Af:200:ASN:HB3	1:Af:201:THR:H	1.66	0.43
1:Ag:205:TYR:CZ	1:Ag:236:SER:HB3	2.54	0.43
1:Ar:205:TYR:CZ	1:Ar:236:SER:HB3	2.54	0.43
2:Ba:318:LEU:HG	2:Ba:320:PRO:HG3	2.01	0.43
2:Bc:85:VAL:HG22	2:Bc:103:VAL:HG13	2.01	0.43
2:Bc:277:MET:HE2	2:Bc:311:LYS:HD2	1.99	0.43
2:Bf:259:ILE:HD11	2:Bf:342:MET:HG3	2.01	0.43
2:Bg:192:THR:HA	2:Bh:234:SER:HB2	2.01	0.43
2:Bl:274:HIS:HE1	2:Bl:343:ALA:HB3	1.84	0.43
2:By:248:ALA:HB1	2:By:265:VAL:HG22	2.00	0.43
2:By:259:ILE:HD11	2:By:342:MET:HG3	2.00	0.43
3:Cb:222:MET:HE3	3:Cb:222:MET:HB2	1.93	0.43
3:Ck:373:MET:HE3	3:Ck:373:MET:HB2	1.83	0.43
3:Cn:167:VAL:HG21	3:Cn:191:ALA:HB2	2.01	0.43
3:Cr:164:PHE:HZ	3:Cr:285:ILE:HB	1.84	0.43
3:Cr:326:PHE:HD1	3:Cr:328:ASP:H	1.67	0.43
3:Cr:362:GLU:HG2	3:Cr:363:LEU:HG	2.00	0.43
4:Di:126:LEU:HD13	4:Di:162:TYR:HE1	1.82	0.43
4:Dk:80:MET:HE1	4:Dk:110:PHE:HB3	2.01	0.43
4:Dk:83:THR:HG22	4:Dk:111:LYS:HA	2.00	0.43
4:Dq:31:PRO:HG3	4:Dq:95:TRP:HZ2	1.83	0.43
1:Ac:64:PRO:HB2	1:Ad:38:VAL:HG13	2.01	0.43
1:Ad:106:ILE:HD12	1:Ad:177:THR:HG21	2.01	0.43
1:Al:106:ILE:HD12	1:Al:177:THR:HG21	2.01	0.43
1:An:106:ILE:HD12	1:An:177:THR:HG21	2.01	0.43
1:Au:205:TYR:CZ	1:Au:236:SER:HB3	2.53	0.43
2:Be:103:VAL:HB	2:Be:137:LEU:HD21	2.00	0.43
2:Bi:84:ILE:HG13	2:Bi:106:ILE:HD13	2.00	0.43
2:Bs:85:VAL:HG13	2:Bs:103:VAL:HG22	2.01	0.43
2:Bt:85:VAL:HG13	2:Bt:103:VAL:HG22	2.01	0.43
2:Bu:21:ILE:HG23	2:Bu:197:LEU:HD11	2.01	0.43
2:Bz:248:ALA:HB1	2:Bz:265:VAL:HG22	2.00	0.43
3:Cf:28:VAL:HG13	3:Cf:49:ALA:HB1	2.01	0.43
3:Cq:43:LEU:HD21	3:Cq:68:MET:HE1	2.00	0.43
1:Ak:106:ILE:HD12	1:Ak:177:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:138:VAL:HB	1:An:143:LEU:HD21	2.01	0.42
1:Ap:106:ILE:HD12	1:Ap:177:THR:HG21	2.01	0.42
1:Aq:106:ILE:HD12	1:Aq:177:THR:HG21	2.01	0.42
1:As:106:ILE:HD12	1:As:177:THR:HG21	2.00	0.42
2:Bd:85:VAL:HG13	2:Bd:103:VAL:HG22	2.01	0.42
2:Bm:61:MET:HE2	2:Bm:61:MET:HB3	1.90	0.42
2:Bo:137:LEU:HD22	2:Bo:160:GLY:HA3	2.00	0.42
2:Bo:192:THR:HA	2:Bp:234:SER:HB2	2.00	0.42
2:Bt:259:ILE:HD11	2:Bt:342:MET:HG3	2.01	0.42
3:Ch:164:PHE:HZ	3:Ch:285:ILE:HB	1.83	0.42
3:Cl:249:PRO:HG2	3:Cl:252:SER:HB3	2.01	0.42
3:Co:201:ASP:HB3	3:Co:221:ALA:HB3	2.01	0.42
3:Cu:269:MET:HE3	3:Cu:269:MET:HB3	1.91	0.42
3:Cz:222:MET:HE3	3:Cz:222:MET:HB2	1.89	0.42
4:Di:216:ILE:HD12	4:Di:289:LEU:HB3	2.00	0.42
4:Dk:126:LEU:HD13	4:Dk:162:TYR:HE1	1.84	0.42
1:Ak:154:LEU:HD21	1:Am:258:LEU:HD11	2.02	0.42
1:Am:184:LEU:HD12	1:Am:188:ASN:HB2	2.01	0.42
2:Be:105:SER:HB3	2:Be:158:THR:HB	2.01	0.42
2:Bh:277:MET:HE2	2:Bh:311:LYS:HD2	2.01	0.42
2:Bj:360:ILE:HD12	2:Bl:163:SER:H	1.84	0.42
2:Bl:259:ILE:HD11	2:Bl:342:MET:HG3	2.01	0.42
2:Bl:324:LEU:HD12	2:Bl:327:LEU:HD23	2.01	0.42
2:Bp:268:LYS:HD2	2:Bp:353:ALA:HA	2.00	0.42
2:Bq:84:ILE:HG13	2:Bq:106:ILE:HD13	2.01	0.42
2:Bs:49:GLU:HG3	2:Bs:54:THR:HG21	2.01	0.42
2:Bs:192:THR:HA	2:Bt:234:SER:HB2	2.00	0.42
2:Bv:118:MET:HE2	2:Bv:118:MET:HB3	1.80	0.42
3:Ca:88:ILE:HG12	3:Ca:106:ILE:HG12	2.01	0.42
3:Ca:373:MET:HE3	3:Ca:373:MET:HB2	1.84	0.42
3:Co:164:PHE:HZ	3:Co:285:ILE:HB	1.84	0.42
3:Cu:278:MET:HE2	3:Cu:278:MET:HB3	1.97	0.42
3:Cy:241:ARG:HB3	5:Gz:143:THR:HG21	2.01	0.42
3:Cz:209:LYS:HD2	3:Cz:212:GLN:HB2	2.00	0.42
1:Ab:205:TYR:CZ	1:Ab:236:SER:HB3	2.55	0.42
1:Ad:178:VAL:HG21	1:Ad:191:ILE:HD12	2.01	0.42
1:Ag:106:ILE:HD12	1:Ag:177:THR:HG21	2.00	0.42
1:Ax:154:LEU:HD21	1:Az:258:LEU:HD11	2.01	0.42
1:Ay:106:ILE:HD12	1:Ay:177:THR:HG21	2.01	0.42
2:Bd:61:MET:HE2	2:Bd:61:MET:HB3	1.89	0.42
2:Be:290:PRO:HB3	2:Be:296:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bf:21:ILE:HG23	2:Bf:197:LEU:HD11	2.02	0.42
2:Bk:284:ASN:HB2	2:Bk:304:THR:HB	2.01	0.42
2:Bl:105:SER:HB2	2:Bl:112:LEU:HD11	2.01	0.42
2:Bn:105:SER:HB2	2:Bn:112:LEU:HD11	2.01	0.42
2:Bw:318:LEU:HG	2:Bw:320:PRO:HG3	2.00	0.42
3:Cm:111:SER:HB3	3:Cm:113:THR:HG22	1.99	0.42
3:Cn:111:SER:HB3	3:Cn:113:THR:HG22	1.99	0.42
3:Cn:205:THR:HG22	3:Co:260:ARG:HD3	2.01	0.42
3:Cn:220:PHE:HE2	3:Cn:273:VAL:HG11	1.84	0.42
3:Cn:269:MET:HE3	3:Cn:269:MET:HB3	1.86	0.42
3:Co:153:ILE:HG21	3:Co:195:MET:HE1	2.00	0.42
3:Cs:29:THR:HB	3:Cs:103:ARG:HG2	2.01	0.42
3:Ct:220:PHE:HE2	3:Ct:273:VAL:HG11	1.84	0.42
3:Cu:249:PRO:HG2	3:Cu:252:SER:HB3	2.00	0.42
3:Cw:226:VAL:HB	3:Cw:236:MET:HB3	2.02	0.42
3:Cx:88:ILE:HG12	3:Cx:106:ILE:HG12	2.01	0.42
3:Cy:209:LYS:HD2	3:Cy:212:GLN:HB2	2.00	0.42
4:Da:197:LYS:HA	4:Da:200:GLN:HB2	2.01	0.42
4:Dc:216:ILE:HD12	4:Dc:289:LEU:HB3	2.01	0.42
4:Do:83:THR:HG22	4:Do:111:LYS:HA	2.01	0.42
1:Af:106:ILE:HD12	1:Af:177:THR:HG21	2.00	0.42
1:Ao:206:ILE:HG12	1:Ao:235:TYR:HD1	1.85	0.42
1:Aq:205:TYR:CZ	1:Aq:236:SER:HB3	2.54	0.42
2:Bc:224:ARG:HH22	3:Cf:323:THR:HB	1.83	0.42
2:Bg:259:ILE:HD11	2:Bg:342:MET:HG3	2.02	0.42
2:Bh:290:PRO:HB3	2:Bh:296:GLY:HA3	2.01	0.42
2:Bu:285:LEU:HD23	2:Bu:303:ASN:HB3	2.00	0.42
2:Bw:290:PRO:HB3	2:Bw:296:GLY:HA3	2.02	0.42
3:Cg:167:VAL:HG21	3:Cg:191:ALA:HB2	2.02	0.42
3:Ck:209:LYS:HD2	3:Ck:212:GLN:HB2	2.02	0.42
3:Cn:249:PRO:HG2	3:Cn:252:SER:HB3	2.01	0.42
3:Cq:80:PHE:HA	5:Fq:136:VAL:HG21	2.01	0.42
3:Cv:326:PHE:HD1	3:Cv:328:ASP:H	1.67	0.42
4:De:31:PRO:HG3	4:De:95:TRP:HZ2	1.84	0.42
4:Dh:90:SER:HB2	4:Dh:104:ILE:HD11	2.01	0.42
4:Di:141:ASP:HB2	4:Di:149:ILE:HG12	2.00	0.42
4:Dp:223:THR:HG22	4:Dp:285:VAL:HG22	2.01	0.42
4:Dy:83:THR:HG22	4:Dy:111:LYS:HA	2.01	0.42
2:Bb:318:LEU:HG	2:Bb:320:PRO:HG3	2.02	0.42
2:Bd:141:GLY:HA2	2:Bd:154:GLY:O	2.19	0.42
2:Bg:22:LYS:HB3	2:Bg:237:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bj:118:MET:HE3	2:Bj:118:MET:HB2	1.81	0.42
2:Bx:267:LEU:HB2	2:Bx:320:PRO:HG2	2.00	0.42
3:Cl:226:VAL:HB	3:Cl:236:MET:HB3	2.00	0.42
3:Cl:373:MET:HE3	3:Cl:373:MET:HB2	1.82	0.42
3:Cm:34:ILE:HD11	3:Cm:100:MET:HB2	2.01	0.42
3:Cr:375:LYS:HE3	3:Cr:377:MET:HE2	2.02	0.42
3:Cs:157:LEU:HA	3:Cs:161:SER:HB2	2.01	0.42
3:Cx:350:TYR:HE2	3:Cx:355:GLU:HG3	1.85	0.42
3:Cy:195:MET:HG3	3:Cy:226:VAL:HG22	2.02	0.42
3:Cz:362:GLU:HG2	3:Cz:363:LEU:HG	2.02	0.42
4:Dd:49:VAL:HG12	4:Dd:59:GLU:HG2	2.02	0.42
1:Ad:205:TYR:CZ	1:Ad:236:SER:HB3	2.55	0.42
1:Ae:205:TYR:CZ	1:Ae:236:SER:HB3	2.55	0.42
1:Aj:106:ILE:HD12	1:Aj:177:THR:HG21	2.01	0.42
1:Aj:184:LEU:HD12	1:Aj:188:ASN:HB2	2.01	0.42
1:Al:139:GLY:HA3	1:Am:148:TYR:HD1	1.84	0.42
2:Bd:259:ILE:HD11	2:Bd:342:MET:HG3	2.01	0.42
2:Bk:317:LYS:HB2	2:Bl:328:VAL:HG21	2.02	0.42
2:Bn:61:MET:HE2	2:Bn:61:MET:HB3	1.88	0.42
2:Bo:42:THR:HG22	2:Bo:80:VAL:HG22	2.02	0.42
2:Bq:21:ILE:HG23	2:Bq:197:LEU:HD11	2.01	0.42
2:Br:105:SER:HB2	2:Br:112:LEU:HD11	2.02	0.42
2:Bx:303:ASN:H	2:By:285:LEU:HD12	1.83	0.42
2:By:350:GLN:HG3	2:Bz:361:ILE:HD13	2.02	0.42
3:Cp:326:PHE:HD1	3:Cp:328:ASP:H	1.67	0.42
3:Cq:222:MET:HE3	3:Cq:222:MET:HB2	1.90	0.42
3:Cv:70:LEU:HD22	5:Fv:136:VAL:HG13	2.01	0.42
4:Di:31:PRO:HG3	4:Di:95:TRP:HZ2	1.84	0.42
4:Dm:194:GLU:H	4:Dm:194:GLU:HG3	1.68	0.42
4:Ds:126:LEU:HD13	4:Ds:162:TYR:HE1	1.85	0.42
1:Al:205:TYR:CZ	1:Al:236:SER:HB3	2.54	0.42
1:An:154:LEU:HD21	1:Ap:258:LEU:HD11	2.02	0.42
1:Ao:205:TYR:CZ	1:Ao:236:SER:HB3	2.55	0.42
1:As:205:TYR:CZ	1:As:236:SER:HB3	2.54	0.42
2:Bl:49:GLU:HG3	2:Bl:54:THR:HG21	2.02	0.42
2:Bl:56:GLN:HE22	2:Bm:69:LEU:H	1.68	0.42
2:Bt:141:GLY:HA2	2:Bt:154:GLY:O	2.19	0.42
2:By:317:LYS:HE3	2:Bz:324:LEU:HD23	2.00	0.42
3:Ca:167:VAL:HG21	3:Ca:191:ALA:HB2	2.01	0.42
3:Ce:129:ILE:HA	3:Ce:197:GLY:O	2.19	0.42
3:Cf:164:PHE:HZ	3:Cf:285:ILE:HB	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cf:209:LYS:HD2	3:Cf:212:GLN:HB2	2.01	0.42
3:Cf:220:PHE:HE2	3:Cf:273:VAL:HG11	1.85	0.42
3:Cp:362:GLU:HG2	3:Cp:363:LEU:HG	2.01	0.42
3:Cx:358:VAL:HG12	3:Cx:360:GLN:H	1.85	0.42
4:Da:31:PRO:HG3	4:Da:95:TRP:HZ2	1.84	0.42
4:Dq:31:PRO:HB3	4:Dq:156:VAL:HG21	2.01	0.42
4:Dq:126:LEU:HD13	4:Dq:162:TYR:HE1	1.85	0.42
4:Dz:107:LEU:HD13	4:Dz:107:LEU:HA	1.97	0.42
1:Ah:111:LEU:HB3	1:Ah:172:MET:HG3	2.01	0.42
1:Aw:219:PHE:HD1	2:Bl:69:LEU:HD13	1.84	0.42
2:Be:318:LEU:HD22	2:Be:330:ALA:HB1	2.01	0.42
2:Bh:268:LYS:HD2	2:Bh:353:ALA:HA	2.01	0.42
2:Bj:156:ASN:HD22	2:Bk:114:GLY:HA3	1.85	0.42
2:Bl:272:VAL:HG22	2:Bm:260:VAL:HG22	2.01	0.42
2:Bq:49:GLU:HG3	2:Bq:54:THR:HG21	2.02	0.42
2:Br:85:VAL:HB	2:Br:122:LEU:HD21	2.02	0.42
2:Bt:290:PRO:HB3	2:Bt:296:GLY:HA3	2.02	0.42
3:Co:34:ILE:HD11	3:Co:100:MET:HB2	2.01	0.42
3:Ct:282:GLU:HA	3:Ct:286:SER:HB3	2.00	0.42
3:Cz:373:MET:HE3	3:Cz:373:MET:HB2	1.83	0.42
4:Db:90:SER:HB2	4:Db:104:ILE:HD11	2.02	0.42
4:Dp:37:GLN:HG3	4:Dp:49:VAL:HG23	2.00	0.42
1:Aa:106:ILE:HD12	1:Aa:177:THR:HG21	2.00	0.42
1:At:154:LEU:HD21	1:Av:258:LEU:HD11	2.01	0.42
1:Av:154:LEU:HD11	1:Ax:258:LEU:HD21	2.02	0.42
2:Ba:143:SER:HB2	2:Ba:157:PRO:HG3	2.01	0.42
2:Bf:256:THR:HB	2:Bf:258:THR:HG22	2.02	0.42
2:Bg:277:MET:HE2	2:Bg:311:LYS:HD2	2.00	0.42
2:Bo:49:GLU:HG3	2:Bo:54:THR:HG21	2.02	0.42
2:Bs:303:ASN:H	2:Bt:285:LEU:HD12	1.84	0.42
2:Bw:256:THR:HB	2:Bw:258:THR:HG22	2.02	0.42
3:Cg:350:TYR:HE2	3:Cg:355:GLU:HG3	1.85	0.42
3:Cm:365:TYR:HB3	4:Df:91:MET:HE2	2.02	0.42
3:Cn:362:GLU:HG2	3:Cn:363:LEU:HG	2.02	0.42
3:Cp:209:LYS:HD2	3:Cp:212:GLN:HB2	2.02	0.42
3:Cv:29:THR:HB	3:Cv:103:ARG:HG2	2.01	0.42
3:Cv:269:MET:HB3	3:Cv:269:MET:HE3	1.76	0.42
3:Cz:164:PHE:HZ	3:Cz:285:ILE:HB	1.85	0.42
3:Cz:269:MET:HE3	3:Cz:269:MET:HB3	1.91	0.42
4:Da:266:LYS:HE3	4:Da:266:LYS:HB3	1.93	0.42
4:Dh:117:ILE:HD12	4:Dh:117:ILE:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dh:183:THR:HG21	4:Dh:206:ILE:HD11	2.02	0.42
4:Di:31:PRO:HB3	4:Di:156:VAL:HG21	2.01	0.42
1:Aa:258:LEU:HD11	1:Ay:154:LEU:HD21	2.02	0.42
1:As:33:THR:HG23	1:As:35:VAL:H	1.85	0.42
1:Av:234:GLN:HA	1:Aw:198:THR:HB	2.01	0.42
1:Ax:205:TYR:CZ	1:Ax:236:SER:HB3	2.55	0.42
2:Bc:42:THR:HG22	2:Bc:80:VAL:HG22	2.02	0.42
2:Bp:350:GLN:HG3	2:Bq:361:ILE:HD13	2.01	0.42
2:Bt:118:MET:HB3	2:Bt:118:MET:HE3	1.80	0.42
2:Bv:283:GLU:HG2	2:Bv:305:GLU:HG3	2.01	0.42
2:Bw:84:ILE:HG13	2:Bw:106:ILE:HD13	2.01	0.42
2:Bw:105:SER:HB2	2:Bw:112:LEU:HD11	2.01	0.42
3:Cw:239:THR:HG21	3:Cx:155:ARG:HD3	2.02	0.42
3:Cz:249:PRO:HG2	3:Cz:252:SER:HB3	2.02	0.42
4:De:31:PRO:HB3	4:De:156:VAL:HG21	2.02	0.42
4:De:83:THR:HG22	4:De:111:LYS:HA	2.02	0.42
4:Dk:49:VAL:HG12	4:Dk:59:GLU:HG2	2.02	0.42
4:Dy:266:LYS:HE3	4:Dy:266:LYS:HB3	1.94	0.42
1:Ae:234:GLN:HA	1:Af:198:THR:HB	2.01	0.41
1:Ah:234:GLN:HA	1:Ai:198:THR:HB	2.01	0.41
1:At:64:PRO:HB2	1:Au:38:VAL:HG13	2.02	0.41
1:Aw:205:TYR:CZ	1:Aw:236:SER:HB3	2.55	0.41
2:Ba:103:VAL:HB	2:Ba:137:LEU:HD21	2.01	0.41
2:Bc:103:VAL:HB	2:Bc:137:LEU:HD21	2.01	0.41
2:Bm:118:MET:HE3	2:Bm:118:MET:HB2	1.80	0.41
2:Bx:122:LEU:HB2	2:Bx:131:ALA:HB3	2.02	0.41
2:Bz:84:ILE:HG13	2:Bz:106:ILE:HD13	2.02	0.41
3:Ce:38:GLU:HB2	3:Ce:100:MET:HE1	2.02	0.41
3:Ck:157:LEU:HA	3:Ck:161:SER:HB2	2.01	0.41
3:Cs:222:MET:HE2	3:Cs:222:MET:HB3	1.70	0.41
3:Cu:350:TYR:HE2	3:Cu:355:GLU:HG3	1.85	0.41
3:Cx:220:PHE:HE2	3:Cx:273:VAL:HG11	1.84	0.41
4:Da:112:GLN:HE21	4:Da:112:GLN:HB3	1.62	0.41
4:Db:39:ALA:HB3	4:Db:47:ARG:HB2	2.01	0.41
1:Ab:258:LEU:HD11	1:Az:154:LEU:HD21	2.01	0.41
1:Af:154:LEU:HD21	1:Ah:258:LEU:HD11	2.02	0.41
1:Ax:106:ILE:HD12	1:Ax:177:THR:HG21	2.02	0.41
1:Ax:119:LYS:HD2	1:Az:199:LEU:HB2	2.02	0.41
2:Ba:137:LEU:HD22	2:Ba:160:GLY:HA3	2.02	0.41
2:Bd:318:LEU:HG	2:Bd:320:PRO:HG3	2.02	0.41
2:Be:156:ASN:HD22	2:Bf:114:GLY:HA3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bi:285:LEU:HD23	2:Bi:303:ASN:HB3	2.02	0.41
2:Bj:272:VAL:HG22	2:Bk:260:VAL:HG22	2.01	0.41
2:Bl:256:THR:HB	2:Bl:258:THR:HG22	2.02	0.41
2:Bx:21:ILE:HG23	2:Bx:197:LEU:HD11	2.02	0.41
2:By:141:GLY:HA2	2:By:154:GLY:O	2.20	0.41
4:Da:83:THR:HG22	4:Da:111:LYS:HA	2.02	0.41
4:Dc:31:PRO:HG3	4:Dc:95:TRP:HZ2	1.84	0.41
4:Dd:223:THR:HG22	4:Dd:285:VAL:HG22	2.01	0.41
4:Dn:169:ILE:HG13	4:Dn:172:LEU:HD12	2.01	0.41
1:Aj:178:VAL:HG21	1:Aj:191:ILE:HD12	2.03	0.41
1:Aq:139:GLY:HA3	1:Ar:148:TYR:HD1	1.86	0.41
1:Ar:106:ILE:HD12	1:Ar:177:THR:HG21	2.01	0.41
2:Bb:272:VAL:HG22	2:Bc:260:VAL:HG22	2.03	0.41
2:Bc:105:SER:HB2	2:Bc:112:LEU:HD11	2.01	0.41
2:Bk:248:ALA:HB1	2:Bk:265:VAL:HG22	2.03	0.41
2:Bk:274:HIS:HE1	2:Bk:343:ALA:HB3	1.85	0.41
2:Bl:84:ILE:HG13	2:Bl:106:ILE:HD13	2.01	0.41
2:Bp:44:LEU:HA	2:Bp:45:PRO:HD3	1.92	0.41
2:Bp:284:ASN:HB2	2:Bp:304:THR:HG23	2.01	0.41
2:Br:205:LEU:HD13	2:Br:209:MET:HE2	2.01	0.41
3:Cc:195:MET:HE2	3:Cc:281:LEU:HD11	2.02	0.41
3:Ck:164:PHE:HZ	3:Ck:285:ILE:HB	1.84	0.41
3:Ct:350:TYR:HE2	3:Ct:355:GLU:HG3	1.85	0.41
3:Cv:167:VAL:HG21	3:Cv:191:ALA:HB2	2.02	0.41
4:Du:83:THR:HG22	4:Du:111:LYS:HA	2.01	0.41
1:Ab:106:ILE:HD12	1:Ab:177:THR:HG21	2.01	0.41
1:Am:111:LEU:HB3	1:Am:172:MET:HG3	2.02	0.41
1:An:205:TYR:CZ	1:An:236:SER:HB3	2.55	0.41
2:Bj:122:LEU:HB2	2:Bj:131:ALA:HB3	2.03	0.41
2:Bp:34:GLN:HG2	2:Bq:134:GLN:HB3	2.02	0.41
2:Bx:61:MET:HE2	2:Bx:61:MET:HB3	1.91	0.41
2:Bx:350:GLN:HG3	2:By:361:ILE:HD13	2.02	0.41
2:Bz:61:MET:HE2	2:Bz:61:MET:HB3	1.90	0.41
3:Ca:350:TYR:HE2	3:Ca:355:GLU:HG3	1.85	0.41
3:Cp:201:ASP:HB3	3:Cp:221:ALA:HB3	2.03	0.41
3:Cr:167:VAL:HG21	3:Cr:191:ALA:HB2	2.02	0.41
3:Cw:201:ASP:HB3	3:Cw:221:ALA:HB3	2.03	0.41
4:Dd:38:MET:HE2	4:Dd:38:MET:HB2	1.95	0.41
4:Dm:80:MET:HE1	4:Dm:110:PHE:HB3	2.03	0.41
4:Dp:169:ILE:HG13	4:Dp:172:LEU:HD12	2.01	0.41
1:Ab:199:LEU:HD12	1:Az:119:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:154:LEU:HD21	1:Ag:258:LEU:HD11	2.03	0.41
1:An:234:GLN:HA	1:Ao:198:THR:HB	2.01	0.41
2:Bg:105:SER:HB2	2:Bg:112:LEU:HD11	2.02	0.41
2:Bg:318:LEU:HG	2:Bg:320:PRO:HG3	2.02	0.41
2:Bq:141:GLY:HA2	2:Bq:154:GLY:O	2.20	0.41
2:Br:143:SER:HB2	2:Br:157:PRO:HG3	2.02	0.41
2:Bu:274:HIS:HE1	2:Bu:343:ALA:HB3	1.86	0.41
2:Bz:118:MET:HB3	2:Bz:118:MET:HE2	1.79	0.41
3:Cb:195:MET:HE2	3:Cb:281:LEU:HD11	2.01	0.41
3:Ch:249:PRO:HG2	3:Ch:252:SER:HB3	2.02	0.41
3:Ch:269:MET:HE3	3:Ch:269:MET:HB3	1.78	0.41
3:Cn:38:GLU:HB2	3:Cn:100:MET:HE1	2.03	0.41
4:Dq:197:LYS:HA	4:Dq:200:GLN:HB2	2.03	0.41
4:Dt:183:THR:HG21	4:Dt:206:ILE:HD11	2.03	0.41
4:Dv:117:ILE:HD12	4:Dv:117:ILE:HA	1.95	0.41
4:Dw:112:GLN:HE21	4:Dw:112:GLN:HB3	1.62	0.41
1:Ai:205:TYR:CZ	1:Ai:236:SER:HB3	2.56	0.41
2:Bf:268:LYS:HD2	2:Bf:353:ALA:HA	2.01	0.41
2:Bl:156:ASN:HD22	2:Bm:114:GLY:HA3	1.84	0.41
2:Bv:192:THR:HA	2:Bw:234:SER:HB2	2.02	0.41
3:Ci:157:LEU:HA	3:Ci:161:SER:HB2	2.02	0.41
3:Ck:282:GLU:HA	3:Ck:286:SER:HB3	2.02	0.41
3:Cm:157:LEU:HA	3:Cm:161:SER:HB2	2.02	0.41
3:Ct:221:ALA:HA	3:Ct:240:TYR:O	2.20	0.41
3:Cu:167:VAL:HG21	3:Cu:191:ALA:HB2	2.03	0.41
3:Cu:358:VAL:HG12	3:Cu:360:GLN:H	1.86	0.41
3:Cv:92:GLU:HB2	3:Cv:103:ARG:HB2	2.03	0.41
4:Dl:117:ILE:HD12	4:Dl:117:ILE:HA	1.92	0.41
4:Do:194:GLU:H	4:Do:194:GLU:HG3	1.69	0.41
4:Dp:107:LEU:HD13	4:Dp:107:LEU:HA	1.97	0.41
4:Dr:49:VAL:HG12	4:Dr:59:GLU:HG2	2.03	0.41
5:Ge:139:LYS:HD2	5:Ge:139:LYS:HA	1.81	0.41
1:Ak:249:PHE:HA	1:Ak:252:ARG:HE	1.86	0.41
1:As:234:GLN:HA	1:At:198:THR:HB	2.03	0.41
1:Av:138:VAL:HB	1:Av:143:LEU:HD21	2.02	0.41
1:Av:205:TYR:CZ	1:Av:236:SER:HB3	2.55	0.41
1:Az:205:TYR:CZ	1:Az:236:SER:HB3	2.56	0.41
2:Bn:145:THR:HB	2:Bn:151:LYS:HG3	2.01	0.41
2:Bo:105:SER:HB2	2:Bo:112:LEU:HD11	2.03	0.41
2:Bp:84:ILE:HG13	2:Bp:106:ILE:HD13	2.01	0.41
2:Bq:68:GLN:HE21	2:Bq:68:GLN:HB3	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Br:311:LYS:HE3	2:Bs:337:ALA:HB1	2.02	0.41
2:Bs:122:LEU:HB2	2:Bs:131:ALA:HB3	2.03	0.41
2:Bw:42:THR:HG22	2:Bw:80:VAL:HG22	2.03	0.41
3:Ca:222:MET:HE3	3:Ca:222:MET:HB2	1.93	0.41
3:Cs:350:TYR:HE2	3:Cs:355:GLU:HG3	1.85	0.41
3:Cw:226:VAL:HG21	3:Cw:281:LEU:HD21	2.03	0.41
3:Cy:373:MET:HE3	3:Cy:373:MET:HB2	1.85	0.41
4:De:197:LYS:HA	4:De:200:GLN:HB2	2.02	0.41
4:Ds:31:PRO:HB3	4:Ds:156:VAL:HG21	2.01	0.41
1:Aa:154:LEU:HD21	1:Ac:258:LEU:HD11	2.01	0.41
1:Ap:154:LEU:HD11	1:Ar:258:LEU:HD21	2.03	0.41
1:Ar:178:VAL:HG21	1:Ar:191:ILE:HD12	2.03	0.41
2:Ba:85:VAL:HG13	2:Ba:103:VAL:HG22	2.02	0.41
2:Bf:122:LEU:HB2	2:Bf:131:ALA:HB3	2.03	0.41
2:Bk:275:GLY:HA3	2:Bl:338:PRO:HG2	2.03	0.41
2:Bl:268:LYS:HD2	2:Bl:353:ALA:HA	2.02	0.41
2:Bo:318:LEU:HG	2:Bo:320:PRO:HG3	2.03	0.41
2:Bs:84:ILE:HG13	2:Bs:106:ILE:HD13	2.03	0.41
2:Bv:141:GLY:HA3	2:Bv:154:GLY:O	2.20	0.41
3:Ca:43:LEU:HD21	3:Ca:68:MET:HE1	2.01	0.41
3:Cc:358:VAL:HG12	3:Cc:360:GLN:H	1.86	0.41
3:Ce:226:VAL:HB	3:Ce:236:MET:HB3	2.03	0.41
3:Ce:249:PRO:HG2	3:Ce:252:SER:HB3	2.02	0.41
3:Ch:373:MET:HE3	3:Ch:373:MET:HB2	1.81	0.41
3:Cq:111:SER:HB3	3:Cq:113:THR:HG22	2.02	0.41
3:Cq:249:PRO:HG2	3:Cq:252:SER:HB3	2.02	0.41
3:Cr:278:MET:HE2	3:Cr:278:MET:HB3	2.00	0.41
3:Ct:167:VAL:HG21	3:Ct:191:ALA:HB2	2.03	0.41
3:Cv:350:TYR:HE2	3:Cv:355:GLU:HG3	1.85	0.41
1:Aa:178:VAL:HG21	1:Aa:191:ILE:HD12	2.03	0.41
1:Ac:106:ILE:HD12	1:Ac:177:THR:HG21	2.03	0.41
1:Ah:106:ILE:HD12	1:Ah:177:THR:HG21	2.02	0.41
1:Ao:178:VAL:HG21	1:Ao:191:ILE:HD12	2.03	0.41
1:Aq:154:LEU:HD11	1:As:258:LEU:HD21	2.03	0.41
2:Ba:268:LYS:HD2	2:Ba:353:ALA:HA	2.03	0.41
2:Bc:141:GLY:HA2	2:Bc:154:GLY:O	2.21	0.41
2:Bh:156:ASN:HD22	2:Bi:114:GLY:HA3	1.86	0.41
2:Bi:156:ASN:HD22	2:Bj:114:GLY:HA3	1.86	0.41
2:Bi:274:HIS:HE1	2:Bi:343:ALA:HB3	1.84	0.41
2:Bj:49:GLU:HG3	2:Bj:54:THR:HG21	2.03	0.41
2:Bm:105:SER:HB2	2:Bm:112:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bm:133:ALA:HA	2:Bm:166:ALA:HA	2.02	0.41
2:Bm:192:THR:HA	2:Bn:234:SER:HB2	2.02	0.41
2:Bn:274:HIS:HE1	2:Bn:343:ALA:HB3	1.86	0.41
2:Bo:103:VAL:HB	2:Bo:137:LEU:HD21	2.02	0.41
2:Bs:118:MET:HB3	2:Bs:118:MET:HE3	1.77	0.41
2:Bs:156:ASN:HD22	2:Bt:114:GLY:HA3	1.84	0.41
2:Bs:284:ASN:HB2	2:Bs:304:THR:HG23	2.02	0.41
2:Bv:61:MET:HE2	2:Bv:61:MET:HB3	1.89	0.41
2:Bx:274:HIS:HE1	2:Bx:343:ALA:HB3	1.86	0.41
3:Cb:93:ARG:HG2	3:Cb:102:VAL:HG23	2.02	0.41
3:Cb:220:PHE:HE2	3:Cb:273:VAL:HG11	1.85	0.41
3:Cb:365:TYR:HB3	4:Du:91:MET:HE1	2.02	0.41
3:Ci:222:MET:HE3	3:Ci:222:MET:HB2	1.91	0.41
3:Cj:249:PRO:HG2	3:Cj:252:SER:HB3	2.02	0.41
3:Cm:292:PRO:HB3	3:Cm:306:LEU:HD13	2.03	0.41
3:Cn:164:PHE:HZ	3:Cn:285:ILE:HB	1.86	0.41
3:Ct:28:VAL:HG13	3:Ct:49:ALA:HB1	2.02	0.41
3:Cv:249:PRO:HG2	3:Cv:252:SER:HB3	2.03	0.41
4:Dd:216:ILE:HA	4:Dd:291:ARG:HA	2.02	0.41
4:De:266:LYS:HE3	4:De:266:LYS:HB3	1.94	0.41
4:Dk:197:LYS:HA	4:Dk:200:GLN:HB2	2.03	0.41
4:Dl:217:ASP:HA	4:Dl:258:ARG:HD3	2.03	0.41
4:Dp:185:LEU:HD22	4:Dp:199:SER:HB3	2.02	0.41
4:Dw:83:THR:HG22	4:Dw:111:LYS:HA	2.02	0.41
1:Ab:178:VAL:HG21	1:Ab:191:ILE:HD12	2.03	0.41
1:Ah:205:TYR:CZ	1:Ah:236:SER:HB3	2.56	0.41
1:Al:111:LEU:HB3	1:Al:172:MET:HG3	2.03	0.41
1:An:178:VAL:HG21	1:An:191:ILE:HD12	2.03	0.41
1:Ao:111:LEU:HB3	1:Ao:172:MET:HG3	2.03	0.41
2:Bc:259:ILE:HD11	2:Bc:342:MET:HG3	2.03	0.41
2:Bi:49:GLU:HG3	2:Bi:54:THR:HG21	2.02	0.41
2:Bk:311:LYS:HE3	2:Bl:337:ALA:HB1	2.03	0.41
2:Bo:141:GLY:HA2	2:Bo:154:GLY:O	2.21	0.41
2:Bo:275:GLY:HA3	2:Bp:338:PRO:HG2	2.03	0.41
2:Bp:248:ALA:HB1	2:Bp:265:VAL:HG22	2.02	0.41
2:Br:176:PHE:HE1	2:Br:233:LEU:HD13	1.86	0.41
2:Bu:266:ARG:HB3	2:Bu:355:GLU:HG3	2.03	0.41
2:Bz:284:ASN:HB2	2:Bz:304:THR:HG23	2.03	0.41
3:Ch:111:SER:HB3	3:Ch:113:THR:HG22	2.02	0.41
3:Co:226:VAL:HB	3:Co:236:MET:HB3	2.02	0.41
3:Co:282:GLU:HA	3:Co:286:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cp:141:GLN:HG3	3:Cp:253:GLN:HG2	2.03	0.41
4:Dc:266:LYS:HE3	4:Dc:266:LYS:HB3	1.94	0.41
4:De:126:LEU:HD13	4:De:162:TYR:HE1	1.86	0.41
4:Dg:83:THR:HG22	4:Dg:111:LYS:HA	2.03	0.41
4:Dm:173:LEU:HD13	4:Dm:173:LEU:HA	1.97	0.41
4:Do:173:LEU:HD13	4:Do:173:LEU:HA	1.96	0.41
4:Dy:126:LEU:HD13	4:Dy:162:TYR:HE1	1.86	0.41
1:Ae:64:PRO:HB2	1:Af:38:VAL:HG13	2.03	0.40
1:Ap:139:GLY:HA3	1:Aq:148:TYR:HD1	1.86	0.40
1:Au:195:LYS:HE2	1:Au:195:LYS:HB3	1.94	0.40
1:Av:106:ILE:HD12	1:Av:177:THR:HG21	2.02	0.40
1:Ay:33:THR:HG23	1:Ay:35:VAL:H	1.86	0.40
1:Az:106:ILE:HD12	1:Az:177:THR:HG21	2.01	0.40
2:Bb:205:LEU:HD13	2:Bb:209:MET:HE2	2.03	0.40
2:Bj:259:ILE:HD11	2:Bj:342:MET:HG3	2.03	0.40
2:Bt:192:THR:HA	2:Bu:234:SER:HB2	2.02	0.40
2:Bt:274:HIS:HE1	2:Bt:343:ALA:HB3	1.86	0.40
2:Bu:305:GLU:HG3	2:Bx:148:ASP:HB2	2.03	0.40
2:Bv:336:ALA:HB1	2:Bv:340:ASP:HB2	2.03	0.40
2:By:192:THR:HA	2:Bz:234:SER:HB2	2.03	0.40
3:Ca:269:MET:HE3	3:Ca:269:MET:HB3	1.95	0.40
3:Cf:282:GLU:HA	3:Cf:286:SER:HB3	2.03	0.40
3:Cg:139:MET:HE1	3:Cg:216:ILE:HD13	2.04	0.40
3:Cj:220:PHE:HE2	3:Cj:273:VAL:HG11	1.86	0.40
4:Do:31:PRO:HG3	4:Do:95:TRP:HZ2	1.85	0.40
4:Dp:183:THR:HG21	4:Dp:206:ILE:HD11	2.03	0.40
4:Dq:194:GLU:H	4:Dq:194:GLU:HG3	1.69	0.40
4:Dr:107:LEU:HB3	4:Dr:108:GLN:H	1.81	0.40
4:Dr:169:ILE:HG13	4:Dr:172:LEU:HD12	2.03	0.40
4:Ds:80:MET:HE1	4:Ds:110:PHE:HB3	2.04	0.40
1:Ad:119:LYS:HD2	1:Af:199:LEU:HB2	2.02	0.40
1:Am:154:LEU:HD21	1:Ao:258:LEU:HD11	2.03	0.40
1:As:34:THR:HG21	3:Ci:247:PRO:HB2	2.02	0.40
2:Bf:156:ASN:HD22	2:Bg:114:GLY:HA3	1.86	0.40
2:Bg:141:GLY:HA2	2:Bg:154:GLY:O	2.21	0.40
2:Bh:118:MET:HE2	2:Bh:118:MET:HB3	1.82	0.40
2:Bh:133:ALA:HA	2:Bh:166:ALA:HA	2.02	0.40
3:Cb:241:ARG:NH1	3:Cc:259:ALA:HB2	2.36	0.40
3:Cb:278:MET:HE2	3:Cb:278:MET:HB3	2.00	0.40
3:Cg:226:VAL:HB	3:Cg:236:MET:HB3	2.03	0.40
3:Ck:304:MET:HE2	3:Ck:356:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cw:157:LEU:HA	3:Cw:161:SER:HB2	2.02	0.40
4:Dp:39:ALA:HB3	4:Dp:47:ARG:HB2	2.03	0.40
1:Ab:154:LEU:HD21	1:Ad:258:LEU:HD11	2.02	0.40
1:Ab:234:GLN:HA	1:Ac:198:THR:HB	2.03	0.40
1:Ai:234:GLN:HA	1:Aj:198:THR:HB	2.02	0.40
1:Ax:200:ASN:HB3	1:Ax:201:THR:H	1.66	0.40
1:Ay:205:TYR:CZ	1:Ay:236:SER:HB3	2.57	0.40
2:Bc:49:GLU:HG3	2:Bc:54:THR:HG21	2.02	0.40
2:Bc:141:GLY:HA3	2:Bc:154:GLY:O	2.21	0.40
2:Bk:141:GLY:HA2	2:Bk:154:GLY:O	2.21	0.40
2:Bn:42:THR:HG22	2:Bn:80:VAL:HG22	2.03	0.40
2:Bs:85:VAL:HB	2:Bs:122:LEU:HD21	2.03	0.40
3:Cf:123:THR:HA	3:Cf:165:VAL:O	2.21	0.40
3:Cj:362:GLU:HG2	3:Cj:363:LEU:HG	2.02	0.40
3:Cs:292:PRO:HB3	3:Cs:306:LEU:HD13	2.03	0.40
3:Cy:167:VAL:HG21	3:Cy:191:ALA:HB2	2.04	0.40
4:Du:31:PRO:HG3	4:Du:95:TRP:HZ2	1.86	0.40
1:Ac:219:PHE:HA	2:Br:69:LEU:HD22	2.02	0.40
1:Ag:111:LEU:HB3	1:Ag:172:MET:HG3	2.03	0.40
1:At:178:VAL:HG21	1:At:191:ILE:HD12	2.03	0.40
1:Aw:178:VAL:HG21	1:Aw:191:ILE:HD12	2.04	0.40
2:Bj:274:HIS:HE1	2:Bj:343:ALA:HB3	1.85	0.40
2:Bk:267:LEU:HB3	2:Bk:320:PRO:HG2	2.04	0.40
2:Bn:141:GLY:HA2	2:Bn:154:GLY:O	2.21	0.40
3:Ci:292:PRO:HB3	3:Ci:306:LEU:HD13	2.03	0.40
3:Cj:306:LEU:HB3	3:Cj:312:VAL:HG21	2.02	0.40
3:Ck:292:PRO:HB3	3:Ck:306:LEU:HD13	2.03	0.40
3:Co:304:MET:HE2	3:Co:356:LEU:HD21	2.03	0.40
3:Co:373:MET:HE3	3:Co:373:MET:HB2	1.84	0.40
3:Cs:269:MET:HE3	3:Cs:269:MET:HB3	1.93	0.40
3:Cu:292:PRO:HB3	3:Cu:306:LEU:HD13	2.03	0.40
3:Cy:201:ASP:HB3	3:Cy:221:ALA:HB3	2.03	0.40
4:Di:225:THR:HA	4:Di:283:ARG:HA	2.03	0.40
4:Dm:225:THR:HA	4:Dm:283:ARG:HA	2.03	0.40
4:Do:197:LYS:HA	4:Do:200:GLN:HB2	2.04	0.40
4:Dw:31:PRO:HB3	4:Dw:156:VAL:HG21	2.02	0.40
1:Ah:154:LEU:HD11	1:Aj:258:LEU:HD21	2.04	0.40
1:Aw:106:ILE:HD12	1:Aw:177:THR:HG21	2.02	0.40
2:Ba:223:PRO:HB3	4:Dw:94:VAL:HB	2.04	0.40
2:Bc:133:ALA:HA	2:Bc:166:ALA:HA	2.03	0.40
2:Bc:192:THR:HA	2:Bd:234:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bh:275:GLY:HA3	2:Bi:338:PRO:HG2	2.03	0.40
2:Bj:105:SER:HB2	2:Bj:112:LEU:HD11	2.03	0.40
2:Bj:275:GLY:HA3	2:Bk:338:PRO:HG2	2.03	0.40
2:Bp:118:MET:HE3	2:Bp:118:MET:HB2	1.80	0.40
2:Bt:42:THR:HG22	2:Bt:80:VAL:HG22	2.03	0.40
3:Ca:241:ARG:NH1	3:Cb:259:ALA:HB2	2.37	0.40
3:Ce:209:LYS:HD2	3:Ce:212:GLN:HB2	2.03	0.40
3:Cf:61:ILE:HD11	3:Cf:282:GLU:HG3	2.04	0.40
3:Ci:205:THR:HG22	3:Cj:260:ARG:HD3	2.04	0.40
3:Cj:56:PHE:HD1	5:Gj:139:LYS:HE2	1.85	0.40
3:Ct:373:MET:HE3	3:Ct:373:MET:HB2	1.93	0.40
3:Cy:164:PHE:HZ	3:Cy:285:ILE:HB	1.86	0.40
3:Cy:241:ARG:NH1	3:Cz:259:ALA:HB2	2.37	0.40
3:Cz:304:MET:HE2	3:Cz:356:LEU:HD21	2.02	0.40
4:Dk:194:GLU:H	4:Dk:194:GLU:HG3	1.69	0.40
4:Dm:126:LEU:HD13	4:Dm:162:TYR:HE1	1.87	0.40
4:Do:266:LYS:HE3	4:Do:266:LYS:HB3	1.94	0.40
4:Dx:107:LEU:HD13	4:Dx:107:LEU:HA	1.97	0.40
4:Dy:173:LEU:HD13	4:Dy:173:LEU:HA	1.95	0.40
4:Dy:197:LYS:HA	4:Dy:200:GLN:HB2	2.03	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	Aa	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ab	219/227 (96%)	216 (99%)	3 (1%)	0	100	100
1	Ac	219/227 (96%)	217 (99%)	2 (1%)	0	100	100
1	Ad	219/227 (96%)	215 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ae	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Af	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ag	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Ah	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ai	219/227 (96%)	216 (99%)	3 (1%)	0	100	100
1	Aj	219/227 (96%)	216 (99%)	3 (1%)	0	100	100
1	Ak	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Al	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Am	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	An	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ao	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ap	219/227 (96%)	216 (99%)	3 (1%)	0	100	100
1	Aq	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ar	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	As	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	At	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Au	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Av	219/227 (96%)	217 (99%)	2 (1%)	0	100	100
1	Aw	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Ax	219/227 (96%)	216 (99%)	3 (1%)	0	100	100
1	Ay	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Az	219/227 (96%)	216 (99%)	3 (1%)	0	100	100
2	Ba	341/343 (99%)	333 (98%)	8 (2%)	0	100	100
2	Bb	341/343 (99%)	333 (98%)	8 (2%)	0	100	100
2	Bc	341/343 (99%)	331 (97%)	10 (3%)	0	100	100
2	Bd	341/343 (99%)	328 (96%)	13 (4%)	0	100	100
2	Be	341/343 (99%)	333 (98%)	8 (2%)	0	100	100
2	Bf	341/343 (99%)	332 (97%)	9 (3%)	0	100	100
2	Bg	341/343 (99%)	332 (97%)	9 (3%)	0	100	100
2	Bh	341/343 (99%)	330 (97%)	11 (3%)	0	100	100
2	Bi	341/343 (99%)	329 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bj	341/343 (99%)	330 (97%)	11 (3%)	0	100	100
2	Bk	341/343 (99%)	327 (96%)	14 (4%)	0	100	100
2	Bl	341/343 (99%)	329 (96%)	12 (4%)	0	100	100
2	Bm	341/343 (99%)	328 (96%)	13 (4%)	0	100	100
2	Bn	341/343 (99%)	327 (96%)	14 (4%)	0	100	100
2	Bo	341/343 (99%)	332 (97%)	9 (3%)	0	100	100
2	Bp	341/343 (99%)	327 (96%)	14 (4%)	0	100	100
2	Bq	341/343 (99%)	329 (96%)	12 (4%)	0	100	100
2	Br	341/343 (99%)	327 (96%)	14 (4%)	0	100	100
2	Bs	341/343 (99%)	327 (96%)	14 (4%)	0	100	100
2	Bt	341/343 (99%)	329 (96%)	12 (4%)	0	100	100
2	Bu	341/343 (99%)	329 (96%)	12 (4%)	0	100	100
2	Bv	341/343 (99%)	328 (96%)	13 (4%)	0	100	100
2	Bw	341/343 (99%)	329 (96%)	12 (4%)	0	100	100
2	Bx	341/343 (99%)	329 (96%)	12 (4%)	0	100	100
2	By	341/343 (99%)	329 (96%)	12 (4%)	0	100	100
2	Bz	341/343 (99%)	329 (96%)	12 (4%)	0	100	100
3	Ca	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Cb	350/352 (99%)	332 (95%)	18 (5%)	0	100	100
3	Cc	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Cd	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Ce	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
3	Cf	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Cg	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Ch	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Ci	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Cj	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Ck	350/352 (99%)	339 (97%)	11 (3%)	0	100	100
3	Cl	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
3	Cm	350/352 (99%)	339 (97%)	11 (3%)	0	100	100
3	Cn	350/352 (99%)	339 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Co	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Cp	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Cq	350/352 (99%)	335 (96%)	15 (4%)	0	100	100
3	Cr	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Cs	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Ct	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
3	Cu	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
3	Cv	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Cw	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Cx	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Cy	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Cz	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
4	Da	253/272 (93%)	235 (93%)	18 (7%)	0	100	100
4	Db	254/272 (93%)	232 (91%)	20 (8%)	2 (1%)	16	30
4	Dc	253/272 (93%)	234 (92%)	19 (8%)	0	100	100
4	Dd	254/272 (93%)	230 (91%)	23 (9%)	1 (0%)	30	50
4	De	253/272 (93%)	237 (94%)	16 (6%)	0	100	100
4	Df	254/272 (93%)	231 (91%)	22 (9%)	1 (0%)	30	50
4	Dg	253/272 (93%)	235 (93%)	18 (7%)	0	100	100
4	Dh	254/272 (93%)	233 (92%)	19 (8%)	2 (1%)	16	30
4	Di	253/272 (93%)	235 (93%)	18 (7%)	0	100	100
4	Dj	254/272 (93%)	233 (92%)	19 (8%)	2 (1%)	16	30
4	Dk	253/272 (93%)	232 (92%)	21 (8%)	0	100	100
4	Dl	254/272 (93%)	231 (91%)	21 (8%)	2 (1%)	16	30
4	Dm	253/272 (93%)	237 (94%)	16 (6%)	0	100	100
4	Dn	254/272 (93%)	232 (91%)	21 (8%)	1 (0%)	30	50
4	Do	253/272 (93%)	236 (93%)	17 (7%)	0	100	100
4	Dp	254/272 (93%)	229 (90%)	24 (9%)	1 (0%)	30	50
4	Dq	253/272 (93%)	235 (93%)	18 (7%)	0	100	100
4	Dr	254/272 (93%)	232 (91%)	21 (8%)	1 (0%)	30	50
4	Ds	253/272 (93%)	237 (94%)	16 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Dt	254/272 (93%)	233 (92%)	20 (8%)	1 (0%)	30	50
4	Du	253/272 (93%)	234 (92%)	19 (8%)	0	100	100
4	Dv	254/272 (93%)	232 (91%)	20 (8%)	2 (1%)	16	30
4	Dw	253/272 (93%)	235 (93%)	18 (7%)	0	100	100
4	Dx	254/272 (93%)	231 (91%)	22 (9%)	1 (0%)	30	50
4	Dy	253/272 (93%)	236 (93%)	17 (7%)	0	100	100
4	Dz	254/272 (93%)	235 (92%)	17 (7%)	2 (1%)	16	30
5	Fa	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fb	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fc	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fd	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
5	Fe	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Ff	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fg	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fh	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fi	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fj	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fk	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fl	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fm	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fn	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
5	Fo	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fp	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fq	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fr	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fs	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Ft	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fu	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fv	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fw	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fx	13/15 (87%)	12 (92%)	1 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Fy	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Fz	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
5	Ga	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gb	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gc	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gd	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Ge	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gf	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gg	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gh	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gi	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gj	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gk	11/15 (73%)	7 (64%)	4 (36%)	0	100	100
5	Gl	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gm	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gn	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Go	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gp	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gq	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gr	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gs	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gt	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gu	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gv	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gw	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gx	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
5	Gy	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gz	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
All	All	30875/31824 (97%)	29558 (96%)	1298 (4%)	19 (0%)	49	71

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Db	193	VAL
4	Df	193	VAL
4	Dh	193	VAL
4	Di	193	VAL
4	Dj	193	VAL
4	Dn	193	VAL
4	Dr	193	VAL
4	Dt	193	VAL
4	Dx	193	VAL
4	Db	116	TYR
4	Dh	116	TYR
4	Dj	116	TYR
4	Di	116	TYR
4	Dv	116	TYR
4	Dz	116	TYR
4	Dd	193	VAL
4	Dp	193	VAL
4	Dv	193	VAL
4	Dz	193	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ab	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ac	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Ad	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ae	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Af	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Ag	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ah	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ai	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Aj	182/186 (98%)	178 (98%)	4 (2%)	45	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ak	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Al	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Am	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	An	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ao	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Ap	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Aq	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ar	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	As	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	At	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Au	182/186 (98%)	179 (98%)	3 (2%)	55	73
1	Av	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Aw	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ax	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Ay	182/186 (98%)	178 (98%)	4 (2%)	45	67
1	Az	182/186 (98%)	179 (98%)	3 (2%)	55	73
2	Ba	267/269 (99%)	263 (98%)	4 (2%)	57	74
2	Bb	267/269 (99%)	263 (98%)	4 (2%)	57	74
2	Bc	267/269 (99%)	262 (98%)	5 (2%)	50	70
2	Bd	267/269 (99%)	266 (100%)	1 (0%)	84	91
2	Be	267/269 (99%)	262 (98%)	5 (2%)	50	70
2	Bf	267/269 (99%)	265 (99%)	2 (1%)	76	86
2	Bg	267/269 (99%)	264 (99%)	3 (1%)	65	79
2	Bh	267/269 (99%)	261 (98%)	6 (2%)	45	67
2	Bi	267/269 (99%)	262 (98%)	5 (2%)	50	70
2	Bj	267/269 (99%)	263 (98%)	4 (2%)	57	74
2	Bk	267/269 (99%)	261 (98%)	6 (2%)	45	67
2	Bl	267/269 (99%)	263 (98%)	4 (2%)	57	74
2	Bm	267/269 (99%)	265 (99%)	2 (1%)	76	86
2	Bn	267/269 (99%)	262 (98%)	5 (2%)	50	70
2	Bo	267/269 (99%)	263 (98%)	4 (2%)	57	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bp	267/269 (99%)	262 (98%)	5 (2%)	50	70
2	Bq	267/269 (99%)	260 (97%)	7 (3%)	40	63
2	Br	267/269 (99%)	261 (98%)	6 (2%)	45	67
2	Bs	267/269 (99%)	261 (98%)	6 (2%)	45	67
2	Bt	267/269 (99%)	263 (98%)	4 (2%)	57	74
2	Bu	267/269 (99%)	261 (98%)	6 (2%)	45	67
2	Bv	267/269 (99%)	262 (98%)	5 (2%)	50	70
2	Bw	267/269 (99%)	263 (98%)	4 (2%)	57	74
2	Bx	267/269 (99%)	263 (98%)	4 (2%)	57	74
2	By	267/269 (99%)	262 (98%)	5 (2%)	50	70
2	Bz	267/269 (99%)	261 (98%)	6 (2%)	45	67
3	Ca	299/303 (99%)	297 (99%)	2 (1%)	76	86
3	Cb	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Cc	299/303 (99%)	296 (99%)	3 (1%)	68	81
3	Cd	299/303 (99%)	297 (99%)	2 (1%)	76	86
3	Ce	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Cf	299/303 (99%)	297 (99%)	2 (1%)	76	86
3	Cg	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Ch	299/303 (99%)	293 (98%)	6 (2%)	48	69
3	Ci	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Cj	299/303 (99%)	295 (99%)	4 (1%)	61	76
3	Ck	299/303 (99%)	291 (97%)	8 (3%)	39	62
3	Cl	299/303 (99%)	295 (99%)	4 (1%)	61	76
3	Cm	299/303 (99%)	295 (99%)	4 (1%)	61	76
3	Cn	299/303 (99%)	296 (99%)	3 (1%)	68	81
3	Co	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Cp	299/303 (99%)	295 (99%)	4 (1%)	61	76
3	Cq	299/303 (99%)	295 (99%)	4 (1%)	61	76
3	Cr	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Cs	299/303 (99%)	295 (99%)	4 (1%)	61	76
3	Ct	299/303 (99%)	295 (99%)	4 (1%)	61	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Cu	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Cv	299/303 (99%)	296 (99%)	3 (1%)	68	81
3	Cw	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Cx	299/303 (99%)	296 (99%)	3 (1%)	68	81
3	Cy	299/303 (99%)	294 (98%)	5 (2%)	53	71
3	Cz	299/303 (99%)	296 (99%)	3 (1%)	68	81
4	Da	231/244 (95%)	220 (95%)	11 (5%)	23	44
4	Db	229/244 (94%)	225 (98%)	4 (2%)	53	71
4	Dc	231/244 (95%)	221 (96%)	10 (4%)	26	47
4	Dd	229/244 (94%)	224 (98%)	5 (2%)	45	67
4	De	231/244 (95%)	220 (95%)	11 (5%)	23	44
4	Df	229/244 (94%)	224 (98%)	5 (2%)	45	67
4	Dg	231/244 (95%)	220 (95%)	11 (5%)	23	44
4	Dh	229/244 (94%)	224 (98%)	5 (2%)	45	67
4	Di	231/244 (95%)	223 (96%)	8 (4%)	32	56
4	Dj	229/244 (94%)	225 (98%)	4 (2%)	53	71
4	Dk	231/244 (95%)	221 (96%)	10 (4%)	26	47
4	Dl	229/244 (94%)	225 (98%)	4 (2%)	53	71
4	Dm	231/244 (95%)	223 (96%)	8 (4%)	32	56
4	Dn	229/244 (94%)	223 (97%)	6 (3%)	40	63
4	Do	231/244 (95%)	221 (96%)	10 (4%)	26	47
4	Dp	229/244 (94%)	225 (98%)	4 (2%)	53	71
4	Dq	231/244 (95%)	220 (95%)	11 (5%)	23	44
4	Dr	229/244 (94%)	225 (98%)	4 (2%)	53	71
4	Ds	231/244 (95%)	221 (96%)	10 (4%)	26	47
4	Dt	229/244 (94%)	224 (98%)	5 (2%)	45	67
4	Du	231/244 (95%)	221 (96%)	10 (4%)	26	47
4	Dv	229/244 (94%)	226 (99%)	3 (1%)	61	76
4	Dw	231/244 (95%)	220 (95%)	11 (5%)	23	44
4	Dx	229/244 (94%)	224 (98%)	5 (2%)	45	67
4	Dy	231/244 (95%)	221 (96%)	10 (4%)	26	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Dz	229/244 (94%)	225 (98%)	4 (2%)	53	71
5	Fa	14/14 (100%)	14 (100%)	0	100	100
5	Fb	14/14 (100%)	14 (100%)	0	100	100
5	Fc	14/14 (100%)	14 (100%)	0	100	100
5	Fd	14/14 (100%)	14 (100%)	0	100	100
5	Fe	14/14 (100%)	14 (100%)	0	100	100
5	Ff	14/14 (100%)	13 (93%)	1 (7%)	13	25
5	Fg	14/14 (100%)	14 (100%)	0	100	100
5	Fh	14/14 (100%)	14 (100%)	0	100	100
5	Fi	14/14 (100%)	14 (100%)	0	100	100
5	Fj	14/14 (100%)	14 (100%)	0	100	100
5	Fk	14/14 (100%)	14 (100%)	0	100	100
5	Fl	14/14 (100%)	14 (100%)	0	100	100
5	Fm	14/14 (100%)	14 (100%)	0	100	100
5	Fn	14/14 (100%)	14 (100%)	0	100	100
5	Fo	14/14 (100%)	14 (100%)	0	100	100
5	Fp	14/14 (100%)	14 (100%)	0	100	100
5	Fq	14/14 (100%)	14 (100%)	0	100	100
5	Fr	14/14 (100%)	14 (100%)	0	100	100
5	Fs	14/14 (100%)	14 (100%)	0	100	100
5	Ft	14/14 (100%)	14 (100%)	0	100	100
5	Fu	14/14 (100%)	14 (100%)	0	100	100
5	Fv	14/14 (100%)	14 (100%)	0	100	100
5	Fw	14/14 (100%)	14 (100%)	0	100	100
5	Fx	14/14 (100%)	14 (100%)	0	100	100
5	Fy	14/14 (100%)	14 (100%)	0	100	100
5	Fz	14/14 (100%)	14 (100%)	0	100	100
5	Ga	13/14 (93%)	13 (100%)	0	100	100
5	Gb	13/14 (93%)	13 (100%)	0	100	100
5	Gc	13/14 (93%)	13 (100%)	0	100	100
5	Gd	13/14 (93%)	12 (92%)	1 (8%)	12	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Ge	13/14 (93%)	13 (100%)	0	100	100
5	Gf	13/14 (93%)	13 (100%)	0	100	100
5	Gg	13/14 (93%)	13 (100%)	0	100	100
5	Gh	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gi	13/14 (93%)	13 (100%)	0	100	100
5	Gj	13/14 (93%)	13 (100%)	0	100	100
5	Gk	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gl	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gm	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gn	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Go	13/14 (93%)	13 (100%)	0	100	100
5	Gp	13/14 (93%)	13 (100%)	0	100	100
5	Gq	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gr	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gs	13/14 (93%)	13 (100%)	0	100	100
5	Gt	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gu	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gv	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gw	13/14 (93%)	13 (100%)	0	100	100
5	Gx	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gy	13/14 (93%)	12 (92%)	1 (8%)	12	22
5	Gz	13/14 (93%)	13 (100%)	0	100	100
All	All	26130/26780 (98%)	25609 (98%)	521 (2%)	48	69

All (521) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	60	VAL
1	Aa	106	ILE
1	Aa	145	ILE
1	Aa	201	THR
1	Ab	60	VAL
1	Ab	106	ILE
1	Ab	145	ILE

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Mol	Chain	Res	Type
1	Ab	201	THR
1	Ac	60	VAL
1	Ac	106	ILE
1	Ac	145	ILE
1	Ad	60	VAL
1	Ad	106	ILE
1	Ad	145	ILE
1	Ad	201	THR
1	Ae	60	VAL
1	Ae	145	ILE
1	Ae	201	THR
1	Af	60	VAL
1	Af	145	ILE
1	Af	201	THR
1	Ag	60	VAL
1	Ag	106	ILE
1	Ag	145	ILE
1	Ag	201	THR
1	Ah	60	VAL
1	Ah	106	ILE
1	Ah	145	ILE
1	Ah	201	THR
1	Ai	60	VAL
1	Ai	106	ILE
1	Ai	145	ILE
1	Aj	60	VAL
1	Aj	106	ILE
1	Aj	145	ILE
1	Aj	201	THR
1	Ak	60	VAL
1	Ak	106	ILE
1	Ak	145	ILE
1	Ak	201	THR
1	Al	60	VAL
1	Al	145	ILE
1	Al	201	THR
1	Am	60	VAL
1	Am	106	ILE
1	Am	145	ILE
1	Am	201	THR
1	An	60	VAL
1	An	106	ILE

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Mol	Chain	Res	Type
1	An	145	ILE
1	An	201	THR
1	Ao	106	ILE
1	Ao	107	ILE
1	Ao	145	ILE
1	Ap	60	VAL
1	Ap	145	ILE
1	Ap	201	THR
1	Aq	60	VAL
1	Aq	106	ILE
1	Aq	145	ILE
1	Aq	201	THR
1	Ar	106	ILE
1	Ar	145	ILE
1	Ar	201	THR
1	As	60	VAL
1	As	106	ILE
1	As	145	ILE
1	At	60	VAL
1	At	106	ILE
1	At	145	ILE
1	Au	60	VAL
1	Au	106	ILE
1	Au	145	ILE
1	Av	60	VAL
1	Av	106	ILE
1	Av	145	ILE
1	Av	201	THR
1	Aw	60	VAL
1	Aw	106	ILE
1	Aw	145	ILE
1	Aw	201	THR
1	Ax	60	VAL
1	Ax	106	ILE
1	Ax	145	ILE
1	Ax	176	ILE
1	Ay	60	VAL
1	Ay	106	ILE
1	Ay	145	ILE
1	Ay	201	THR
1	Az	106	ILE
1	Az	145	ILE

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Mol	Chain	Res	Type
1	Az	201	THR
2	Ba	258	THR
2	Ba	287	VAL
2	Ba	303	ASN
2	Ba	304	THR
2	Bb	258	THR
2	Bb	287	VAL
2	Bb	303	ASN
2	Bb	304	THR
2	Bc	54	THR
2	Bc	68	GLN
2	Bc	148	ASP
2	Bc	258	THR
2	Bc	287	VAL
2	Bd	258	THR
2	Be	256	THR
2	Be	258	THR
2	Be	303	ASN
2	Be	322	VAL
2	Be	323	THR
2	Bf	54	THR
2	Bf	258	THR
2	Bg	237	GLU
2	Bg	258	THR
2	Bg	304	THR
2	Bh	54	THR
2	Bh	148	ASP
2	Bh	237	GLU
2	Bh	258	THR
2	Bh	303	ASN
2	Bh	304	THR
2	Bi	67	ILE
2	Bi	237	GLU
2	Bi	258	THR
2	Bi	304	THR
2	Bi	322	VAL
2	Bj	148	ASP
2	Bj	258	THR
2	Bj	287	VAL
2	Bj	322	VAL
2	Bk	148	ASP
2	Bk	174	ASN

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Mol	Chain	Res	Type
2	Bk	237	GLU
2	Bk	258	THR
2	Bk	308	VAL
2	Bk	322	VAL
2	Bl	256	THR
2	Bl	258	THR
2	Bl	303	ASN
2	Bl	304	THR
2	Bm	258	THR
2	Bm	304	THR
2	Bn	237	GLU
2	Bn	258	THR
2	Bn	303	ASN
2	Bn	304	THR
2	Bn	322	VAL
2	Bo	258	THR
2	Bo	287	VAL
2	Bo	304	THR
2	Bo	308	VAL
2	Bp	258	THR
2	Bp	287	VAL
2	Bp	304	THR
2	Bp	308	VAL
2	Bp	322	VAL
2	Bq	54	THR
2	Bq	68	GLN
2	Bq	148	ASP
2	Bq	258	THR
2	Bq	287	VAL
2	Bq	304	THR
2	Bq	322	VAL
2	Br	148	ASP
2	Br	237	GLU
2	Br	258	THR
2	Br	303	ASN
2	Br	322	VAL
2	Br	327	LEU
2	Bs	54	THR
2	Bs	67	ILE
2	Bs	148	ASP
2	Bs	258	THR
2	Bs	304	THR

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Mol	Chain	Res	Type
2	Bs	322	VAL
2	Bt	54	THR
2	Bt	258	THR
2	Bt	304	THR
2	Bt	322	VAL
2	Bu	118	MET
2	Bu	148	ASP
2	Bu	182	ILE
2	Bu	237	GLU
2	Bu	258	THR
2	Bu	304	THR
2	Bv	237	GLU
2	Bv	258	THR
2	Bv	303	ASN
2	Bv	304	THR
2	Bv	308	VAL
2	Bw	237	GLU
2	Bw	256	THR
2	Bw	258	THR
2	Bw	303	ASN
2	Bx	258	THR
2	Bx	287	VAL
2	Bx	322	VAL
2	Bx	323	THR
2	By	54	THR
2	By	174	ASN
2	By	258	THR
2	By	304	THR
2	By	322	VAL
2	Bz	54	THR
2	Bz	148	ASP
2	Bz	258	THR
2	Bz	287	VAL
2	Bz	304	THR
2	Bz	322	VAL
3	Ca	35	VAL
3	Ca	353	GLU
3	Cb	102	VAL
3	Cb	286	SER
3	Cb	327	ILE
3	Cb	345	THR
3	Cb	363	LEU

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Mol	Chain	Res	Type
3	Cc	102	VAL
3	Cc	286	SER
3	Cc	327	ILE
3	Cd	327	ILE
3	Cd	353	GLU
3	Ce	35	VAL
3	Ce	102	VAL
3	Ce	286	SER
3	Ce	327	ILE
3	Ce	353	GLU
3	Cf	71	LEU
3	Cf	286	SER
3	Cg	154	ASN
3	Cg	243	VAL
3	Cg	286	SER
3	Cg	327	ILE
3	Cg	353	GLU
3	Ch	123	THR
3	Ch	154	ASN
3	Ch	286	SER
3	Ch	327	ILE
3	Ch	328	ASP
3	Ch	353	GLU
3	Ci	154	ASN
3	Ci	237	THR
3	Ci	286	SER
3	Ci	327	ILE
3	Ci	353	GLU
3	Cj	154	ASN
3	Cj	243	VAL
3	Cj	306	LEU
3	Cj	353	GLU
3	Ck	35	VAL
3	Ck	89	LEU
3	Ck	123	THR
3	Ck	237	THR
3	Ck	286	SER
3	Ck	327	ILE
3	Ck	328	ASP
3	Ck	353	GLU
3	Cl	89	LEU
3	Cl	123	THR

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Mol	Chain	Res	Type
3	Cl	327	ILE
3	Cl	353	GLU
3	Cm	35	VAL
3	Cm	123	THR
3	Cm	286	SER
3	Cm	353	GLU
3	Cn	123	THR
3	Cn	286	SER
3	Cn	327	ILE
3	Co	154	ASN
3	Co	237	THR
3	Co	286	SER
3	Co	327	ILE
3	Co	353	GLU
3	Cp	123	THR
3	Cp	286	SER
3	Cp	327	ILE
3	Cp	353	GLU
3	Cq	123	THR
3	Cq	243	VAL
3	Cq	286	SER
3	Cq	353	GLU
3	Cr	237	THR
3	Cr	286	SER
3	Cr	327	ILE
3	Cr	328	ASP
3	Cr	353	GLU
3	Cs	35	VAL
3	Cs	237	THR
3	Cs	286	SER
3	Cs	327	ILE
3	Ct	35	VAL
3	Ct	286	SER
3	Ct	320	LEU
3	Ct	353	GLU
3	Cu	237	THR
3	Cu	286	SER
3	Cu	327	ILE
3	Cu	345	THR
3	Cu	356	LEU
3	Cv	243	VAL
3	Cv	286	SER

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Mol	Chain	Res	Type
3	Cv	353	GLU
3	Cw	123	THR
3	Cw	237	THR
3	Cw	286	SER
3	Cw	327	ILE
3	Cw	353	GLU
3	Cx	327	ILE
3	Cx	353	GLU
3	Cx	363	LEU
3	Cy	87	TYR
3	Cy	237	THR
3	Cy	286	SER
3	Cy	327	ILE
3	Cy	353	GLU
3	Cz	286	SER
3	Cz	320	LEU
3	Cz	327	ILE
4	Da	25	VAL
4	Da	89	VAL
4	Da	106	ASN
4	Da	112	GLN
4	Da	117	ILE
4	Da	149	ILE
4	Da	173	LEU
4	Da	180	ILE
4	Da	250	LYS
4	Da	252	ILE
4	Da	266	LYS
4	Db	25	VAL
4	Db	37	GLN
4	Db	94	VAL
4	Db	193	VAL
4	Dc	25	VAL
4	Dc	89	VAL
4	Dc	106	ASN
4	Dc	112	GLN
4	Dc	117	ILE
4	Dc	149	ILE
4	Dc	173	LEU
4	Dc	180	ILE
4	Dc	250	LYS
4	Dc	266	LYS

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Mol	Chain	Res	Type
4	Dd	25	VAL
4	Dd	37	GLN
4	Dd	68	ILE
4	Dd	94	VAL
4	Dd	193	VAL
4	De	25	VAL
4	De	89	VAL
4	De	106	ASN
4	De	112	GLN
4	De	117	ILE
4	De	149	ILE
4	De	173	LEU
4	De	180	ILE
4	De	250	LYS
4	De	252	ILE
4	De	266	LYS
4	Df	25	VAL
4	Df	37	GLN
4	Df	68	ILE
4	Df	94	VAL
4	Df	193	VAL
4	Dg	25	VAL
4	Dg	89	VAL
4	Dg	106	ASN
4	Dg	112	GLN
4	Dg	117	ILE
4	Dg	149	ILE
4	Dg	173	LEU
4	Dg	180	ILE
4	Dg	250	LYS
4	Dg	252	ILE
4	Dg	266	LYS
4	Dh	25	VAL
4	Dh	37	GLN
4	Dh	94	VAL
4	Dh	193	VAL
4	Dh	216	ILE
4	Di	25	VAL
4	Di	106	ASN
4	Di	112	GLN
4	Di	117	ILE
4	Di	173	LEU

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Mol	Chain	Res	Type
4	Di	180	ILE
4	Di	250	LYS
4	Di	266	LYS
4	Dj	25	VAL
4	Dj	37	GLN
4	Dj	193	VAL
4	Dj	216	ILE
4	Dk	25	VAL
4	Dk	89	VAL
4	Dk	106	ASN
4	Dk	112	GLN
4	Dk	117	ILE
4	Dk	149	ILE
4	Dk	173	LEU
4	Dk	180	ILE
4	Dk	250	LYS
4	Dk	266	LYS
4	Dl	25	VAL
4	Dl	37	GLN
4	Dl	193	VAL
4	Dl	216	ILE
4	Dm	25	VAL
4	Dm	106	ASN
4	Dm	112	GLN
4	Dm	173	LEU
4	Dm	180	ILE
4	Dm	250	LYS
4	Dm	252	ILE
4	Dm	266	LYS
4	Dn	25	VAL
4	Dn	37	GLN
4	Dn	68	ILE
4	Dn	94	VAL
4	Dn	193	VAL
4	Dn	216	ILE
4	Do	25	VAL
4	Do	89	VAL
4	Do	106	ASN
4	Do	112	GLN
4	Do	117	ILE
4	Do	149	ILE
4	Do	173	LEU

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Mol	Chain	Res	Type
4	Do	180	ILE
4	Do	250	LYS
4	Do	266	LYS
4	Dp	25	VAL
4	Dp	37	GLN
4	Dp	94	VAL
4	Dp	193	VAL
4	Dq	25	VAL
4	Dq	89	VAL
4	Dq	106	ASN
4	Dq	112	GLN
4	Dq	117	ILE
4	Dq	149	ILE
4	Dq	173	LEU
4	Dq	180	ILE
4	Dq	250	LYS
4	Dq	252	ILE
4	Dq	266	LYS
4	Dr	25	VAL
4	Dr	37	GLN
4	Dr	94	VAL
4	Dr	193	VAL
4	Ds	25	VAL
4	Ds	89	VAL
4	Ds	106	ASN
4	Ds	112	GLN
4	Ds	117	ILE
4	Ds	149	ILE
4	Ds	173	LEU
4	Ds	180	ILE
4	Ds	250	LYS
4	Ds	266	LYS
4	Dt	25	VAL
4	Dt	37	GLN
4	Dt	68	ILE
4	Dt	94	VAL
4	Dt	193	VAL
4	Du	25	VAL
4	Du	89	VAL
4	Du	106	ASN
4	Du	112	GLN
4	Du	117	ILE

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Mol	Chain	Res	Type
4	Du	149	ILE
4	Du	173	LEU
4	Du	180	ILE
4	Du	250	LYS
4	Du	266	LYS
4	Dv	25	VAL
4	Dv	37	GLN
4	Dv	193	VAL
4	Dw	25	VAL
4	Dw	89	VAL
4	Dw	106	ASN
4	Dw	112	GLN
4	Dw	117	ILE
4	Dw	149	ILE
4	Dw	173	LEU
4	Dw	180	ILE
4	Dw	250	LYS
4	Dw	252	ILE
4	Dw	266	LYS
4	Dx	25	VAL
4	Dx	37	GLN
4	Dx	94	VAL
4	Dx	125	LEU
4	Dx	193	VAL
4	Dy	89	VAL
4	Dy	106	ASN
4	Dy	112	GLN
4	Dy	117	ILE
4	Dy	149	ILE
4	Dy	173	LEU
4	Dy	180	ILE
4	Dy	250	LYS
4	Dy	252	ILE
4	Dy	266	LYS
4	Dz	25	VAL
4	Dz	37	GLN
4	Dz	94	VAL
4	Dz	193	VAL
5	Ff	133	VAL
5	Gd	138	GLU
5	Gh	138	GLU
5	Gk	138	GLU

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Mol	Chain	Res	Type
5	Gl	138	GLU
5	Gm	138	GLU
5	Gn	138	GLU
5	Gq	138	GLU
5	Gr	138	GLU
5	Gt	138	GLU
5	Gu	138	GLU
5	Gv	138	GLU
5	Gx	138	GLU
5	Gy	138	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (592) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	112	ASN
1	Aa	129	ASN
1	Aa	149	ASN
1	Aa	156	ASN
1	Aa	158	ASN
1	Aa	167	ASN
1	Aa	200	ASN
1	Ab	112	ASN
1	Ab	129	ASN
1	Ab	149	ASN
1	Ab	156	ASN
1	Ab	158	ASN
1	Ab	167	ASN
1	Ab	200	ASN
1	Ac	77	HIS
1	Ac	112	ASN
1	Ac	129	ASN
1	Ac	149	ASN
1	Ac	156	ASN
1	Ac	158	ASN
1	Ac	167	ASN
1	Ac	200	ASN
1	Ac	255	ASN
1	Ad	112	ASN
1	Ad	158	ASN
1	Ad	167	ASN
1	Ad	200	ASN
1	Ae	77	HIS

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Mol	Chain	Res	Type
1	Ae	112	ASN
1	Ae	129	ASN
1	Ae	149	ASN
1	Ae	156	ASN
1	Ae	158	ASN
1	Ae	167	ASN
1	Ae	200	ASN
1	Ae	255	ASN
1	Af	112	ASN
1	Af	129	ASN
1	Af	149	ASN
1	Af	156	ASN
1	Af	158	ASN
1	Af	167	ASN
1	Af	200	ASN
1	Af	221	ASN
1	Ag	70	HIS
1	Ag	112	ASN
1	Ag	129	ASN
1	Ag	149	ASN
1	Ag	156	ASN
1	Ag	158	ASN
1	Ag	167	ASN
1	Ag	200	ASN
1	Ag	242	GLN
1	Ah	70	HIS
1	Ah	112	ASN
1	Ah	129	ASN
1	Ah	156	ASN
1	Ah	158	ASN
1	Ah	167	ASN
1	Ah	200	ASN
1	Ai	77	HIS
1	Ai	112	ASN
1	Ai	129	ASN
1	Ai	156	ASN
1	Ai	158	ASN
1	Ai	200	ASN
1	Ai	221	ASN
1	Ai	255	ASN
1	Aj	70	HIS
1	Aj	77	HIS

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Mol	Chain	Res	Type
1	Aj	112	ASN
1	Aj	129	ASN
1	Aj	156	ASN
1	Aj	158	ASN
1	Aj	167	ASN
1	Aj	200	ASN
1	Aj	221	ASN
1	Ak	112	ASN
1	Ak	129	ASN
1	Ak	156	ASN
1	Ak	158	ASN
1	Ak	167	ASN
1	Ak	200	ASN
1	Al	77	HIS
1	Al	112	ASN
1	Al	129	ASN
1	Al	156	ASN
1	Al	158	ASN
1	Al	167	ASN
1	Al	200	ASN
1	Am	70	HIS
1	Am	77	HIS
1	Am	112	ASN
1	Am	129	ASN
1	Am	156	ASN
1	Am	158	ASN
1	Am	167	ASN
1	Am	200	ASN
1	Am	255	ASN
1	An	77	HIS
1	An	112	ASN
1	An	129	ASN
1	An	149	ASN
1	An	156	ASN
1	An	158	ASN
1	An	167	ASN
1	An	200	ASN
1	An	221	ASN
1	Ao	112	ASN
1	Ao	129	ASN
1	Ao	149	ASN
1	Ao	158	ASN

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Mol	Chain	Res	Type
1	Ao	167	ASN
1	Ao	200	ASN
1	Ao	221	ASN
1	Ap	112	ASN
1	Ap	129	ASN
1	Ap	156	ASN
1	Ap	158	ASN
1	Ap	167	ASN
1	Ap	200	ASN
1	Aq	112	ASN
1	Aq	129	ASN
1	Aq	149	ASN
1	Aq	156	ASN
1	Aq	158	ASN
1	Aq	167	ASN
1	Aq	200	ASN
1	Ar	77	HIS
1	Ar	112	ASN
1	Ar	129	ASN
1	Ar	156	ASN
1	Ar	158	ASN
1	Ar	167	ASN
1	Ar	200	ASN
1	As	70	HIS
1	As	77	HIS
1	As	112	ASN
1	As	129	ASN
1	As	149	ASN
1	As	156	ASN
1	As	158	ASN
1	As	167	ASN
1	As	170	ASN
1	As	200	ASN
1	At	70	HIS
1	At	77	HIS
1	At	112	ASN
1	At	129	ASN
1	At	156	ASN
1	At	158	ASN
1	At	200	ASN
1	Au	70	HIS
1	Au	112	ASN

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Mol	Chain	Res	Type
1	Au	129	ASN
1	Au	149	ASN
1	Au	156	ASN
1	Au	158	ASN
1	Au	167	ASN
1	Au	200	ASN
1	Av	112	ASN
1	Av	129	ASN
1	Av	156	ASN
1	Av	158	ASN
1	Av	167	ASN
1	Av	200	ASN
1	Aw	112	ASN
1	Aw	129	ASN
1	Aw	156	ASN
1	Aw	158	ASN
1	Aw	167	ASN
1	Aw	200	ASN
1	Ax	70	HIS
1	Ax	112	ASN
1	Ax	129	ASN
1	Ax	149	ASN
1	Ax	156	ASN
1	Ax	158	ASN
1	Ax	167	ASN
1	Ax	200	ASN
1	Ay	112	ASN
1	Ay	129	ASN
1	Ay	156	ASN
1	Ay	158	ASN
1	Ay	167	ASN
1	Ay	200	ASN
1	Ay	255	ASN
1	Az	112	ASN
1	Az	129	ASN
1	Az	156	ASN
1	Az	158	ASN
1	Az	167	ASN
1	Az	200	ASN
2	Ba	238	ASN
2	Ba	284	ASN
2	Ba	286	ASN

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Mol	Chain	Res	Type
2	Ba	346	GLN
2	Bb	134	GLN
2	Bb	263	GLN
2	Bb	284	ASN
2	Bb	286	ASN
2	Bb	346	GLN
2	Bc	242	ASN
2	Bc	263	GLN
2	Bc	284	ASN
2	Bc	289	GLN
2	Bc	346	GLN
2	Bd	68	GLN
2	Bd	134	GLN
2	Bd	284	ASN
2	Bd	289	GLN
2	Bd	346	GLN
2	Be	263	GLN
2	Be	284	ASN
2	Be	346	GLN
2	Bf	284	ASN
2	Bf	289	GLN
2	Bf	346	GLN
2	Bg	134	GLN
2	Bg	284	ASN
2	Bg	286	ASN
2	Bg	346	GLN
2	Bh	68	GLN
2	Bh	264	ASN
2	Bh	284	ASN
2	Bh	286	ASN
2	Bh	346	GLN
2	Bi	284	ASN
2	Bi	286	ASN
2	Bi	289	GLN
2	Bi	346	GLN
2	Bj	119	GLN
2	Bj	134	GLN
2	Bj	238	ASN
2	Bj	284	ASN
2	Bj	289	GLN
2	Bj	346	GLN
2	Bk	263	GLN

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Mol	Chain	Res	Type
2	Bk	284	ASN
2	Bk	346	GLN
2	Bl	68	GLN
2	Bl	242	ASN
2	Bl	263	GLN
2	Bl	284	ASN
2	Bl	286	ASN
2	Bl	346	GLN
2	Bm	119	GLN
2	Bm	284	ASN
2	Bm	286	ASN
2	Bm	346	GLN
2	Bn	253	ASN
2	Bn	286	ASN
2	Bn	289	GLN
2	Bn	346	GLN
2	Bo	238	ASN
2	Bo	284	ASN
2	Bo	286	ASN
2	Bo	289	GLN
2	Bo	346	GLN
2	Bp	68	GLN
2	Bp	263	GLN
2	Bp	284	ASN
2	Bp	286	ASN
2	Bp	289	GLN
2	Bp	346	GLN
2	Bq	263	GLN
2	Bq	284	ASN
2	Bq	286	ASN
2	Bq	289	GLN
2	Bq	346	GLN
2	Br	238	ASN
2	Br	263	GLN
2	Br	284	ASN
2	Br	289	GLN
2	Br	346	GLN
2	Bs	119	GLN
2	Bs	134	GLN
2	Bs	238	ASN
2	Bs	284	ASN
2	Bs	286	ASN

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Mol	Chain	Res	Type
2	Bs	346	GLN
2	Bt	68	GLN
2	Bt	134	GLN
2	Bt	286	ASN
2	Bt	289	GLN
2	Bt	346	GLN
2	Bu	134	GLN
2	Bu	263	GLN
2	Bu	284	ASN
2	Bu	286	ASN
2	Bu	346	GLN
2	Bv	68	GLN
2	Bv	284	ASN
2	Bv	286	ASN
2	Bv	346	GLN
2	Bw	134	GLN
2	Bw	264	ASN
2	Bw	284	ASN
2	Bw	289	GLN
2	Bw	346	GLN
2	Bx	68	GLN
2	Bx	134	GLN
2	Bx	284	ASN
2	Bx	346	GLN
2	By	134	GLN
2	By	264	ASN
2	By	284	ASN
2	By	286	ASN
2	By	289	GLN
2	By	346	GLN
2	Bz	253	ASN
2	Bz	263	GLN
2	Bz	284	ASN
2	Bz	286	ASN
2	Bz	289	GLN
2	Bz	346	GLN
3	Cb	187	GLN
3	Cb	217	ASN
3	Cb	293	GLN
3	Cc	44	HIS
3	Cc	208	GLN
3	Cc	217	ASN

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Mol	Chain	Res	Type
3	Cc	253	GLN
3	Cd	44	HIS
3	Cd	97	ASN
3	Cd	217	ASN
3	Cd	293	GLN
3	Cd	322	HIS
3	Ce	212	GLN
3	Ce	330	GLN
3	Ce	339	GLN
3	Cf	66	ASN
3	Cf	135	GLN
3	Cf	154	ASN
3	Cf	217	ASN
3	Cf	253	GLN
3	Cf	322	HIS
3	Cf	368	GLN
3	Cg	217	ASN
3	Cg	293	GLN
3	Cg	314	GLN
3	Ch	253	GLN
3	Ch	322	HIS
3	Ci	97	ASN
3	Ci	135	GLN
3	Ci	212	GLN
3	Ci	329	GLN
3	Cj	44	HIS
3	Cj	217	ASN
3	Cj	253	GLN
3	Cj	322	HIS
3	Cj	368	GLN
3	Ck	253	GLN
3	Ck	329	GLN
3	Cl	314	GLN
3	Cl	322	HIS
3	Cm	314	GLN
3	Cn	135	GLN
3	Cn	187	GLN
3	Cn	253	GLN
3	Cn	322	HIS
3	Cn	368	GLN
3	Co	44	HIS
3	Co	217	ASN

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Mol	Chain	Res	Type
3	Co	253	GLN
3	Cp	44	HIS
3	Cp	83	HIS
3	Cp	187	GLN
3	Cp	253	GLN
3	Cp	322	HIS
3	Cq	66	ASN
3	Cq	217	ASN
3	Cq	293	GLN
3	Cr	44	HIS
3	Cr	83	HIS
3	Cr	116	HIS
3	Cr	135	GLN
3	Cr	141	GLN
3	Cr	217	ASN
3	Cr	322	HIS
3	Cr	368	GLN
3	Cs	116	HIS
3	Cs	135	GLN
3	Cs	212	GLN
3	Ct	44	HIS
3	Ct	135	GLN
3	Ct	322	HIS
3	Cu	212	GLN
3	Cu	217	ASN
3	Cv	44	HIS
3	Cv	66	ASN
3	Cv	97	ASN
3	Cv	217	ASN
3	Cv	293	GLN
3	Cv	330	GLN
3	Cv	368	GLN
3	Cw	66	ASN
3	Cw	212	GLN
3	Cw	293	GLN
3	Cx	44	HIS
3	Cx	217	ASN
3	Cx	293	GLN
3	Cx	339	GLN
3	Cy	44	HIS
3	Cy	83	HIS
3	Cy	135	GLN

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Mol	Chain	Res	Type
3	Cy	187	GLN
3	Cy	217	ASN
3	Cy	293	GLN
3	Cz	83	HIS
3	Cz	116	HIS
3	Cz	135	GLN
3	Cz	217	ASN
3	Cz	293	GLN
3	Cz	322	HIS
3	Cz	329	GLN
4	Da	106	ASN
4	Da	108	GLN
4	Da	112	GLN
4	Da	143	GLN
4	Da	147	GLN
4	Da	282	ASN
4	Db	50	HIS
4	Db	112	GLN
4	Db	120	GLN
4	Db	143	GLN
4	Db	189	GLN
4	Db	235	GLN
4	Db	293	GLN
4	Dc	106	ASN
4	Dc	108	GLN
4	Dc	112	GLN
4	Dc	143	GLN
4	Dc	147	GLN
4	Dc	282	ASN
4	Dd	32	GLN
4	Dd	50	HIS
4	Dd	112	GLN
4	Dd	120	GLN
4	Dd	235	GLN
4	Dd	293	GLN
4	De	106	ASN
4	De	108	GLN
4	De	112	GLN
4	De	147	GLN
4	De	231	ASN
4	De	282	ASN
4	Df	50	HIS

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Mol	Chain	Res	Type
4	Df	112	GLN
4	Df	120	GLN
4	Df	189	GLN
4	Df	235	GLN
4	Df	293	GLN
4	Dg	106	ASN
4	Dg	112	GLN
4	Dg	147	GLN
4	Dg	231	ASN
4	Dg	282	ASN
4	Dh	50	HIS
4	Dh	112	GLN
4	Dh	120	GLN
4	Dh	143	GLN
4	Dh	189	GLN
4	Dh	235	GLN
4	Dh	293	GLN
4	Di	69	ASN
4	Di	106	ASN
4	Di	108	GLN
4	Di	112	GLN
4	Di	147	GLN
4	Di	231	ASN
4	Di	282	ASN
4	Dj	50	HIS
4	Dj	112	GLN
4	Dj	120	GLN
4	Dj	143	GLN
4	Dj	235	GLN
4	Dj	293	GLN
4	Dk	106	ASN
4	Dk	108	GLN
4	Dk	112	GLN
4	Dk	147	GLN
4	Dk	231	ASN
4	Dk	282	ASN
4	Dl	50	HIS
4	Dl	112	GLN
4	Dl	120	GLN
4	Dl	189	GLN
4	Dl	235	GLN
4	Dl	293	GLN

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Mol	Chain	Res	Type
4	Dm	106	ASN
4	Dm	108	GLN
4	Dm	112	GLN
4	Dm	143	GLN
4	Dm	147	GLN
4	Dm	231	ASN
4	Dm	282	ASN
4	Dn	32	GLN
4	Dn	50	HIS
4	Dn	112	GLN
4	Dn	120	GLN
4	Dn	143	GLN
4	Dn	235	GLN
4	Dn	293	GLN
4	Do	106	ASN
4	Do	108	GLN
4	Do	112	GLN
4	Do	143	GLN
4	Do	147	GLN
4	Do	231	ASN
4	Do	282	ASN
4	Dp	32	GLN
4	Dp	50	HIS
4	Dp	112	GLN
4	Dp	120	GLN
4	Dp	143	GLN
4	Dp	235	GLN
4	Dp	293	GLN
4	Dq	106	ASN
4	Dq	108	GLN
4	Dq	112	GLN
4	Dq	143	GLN
4	Dq	147	GLN
4	Dq	282	ASN
4	Dr	32	GLN
4	Dr	50	HIS
4	Dr	112	GLN
4	Dr	120	GLN
4	Dr	143	GLN
4	Dr	235	GLN
4	Dr	293	GLN
4	Ds	106	ASN

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Mol	Chain	Res	Type
4	Ds	108	GLN
4	Ds	112	GLN
4	Ds	143	GLN
4	Ds	147	GLN
4	Ds	282	ASN
4	Dt	32	GLN
4	Dt	112	GLN
4	Dt	120	GLN
4	Dt	235	GLN
4	Dt	293	GLN
4	Du	106	ASN
4	Du	108	GLN
4	Du	112	GLN
4	Du	143	GLN
4	Du	147	GLN
4	Du	231	ASN
4	Du	282	ASN
4	Dv	32	GLN
4	Dv	50	HIS
4	Dv	112	GLN
4	Dv	120	GLN
4	Dv	235	GLN
4	Dv	293	GLN
4	Dw	106	ASN
4	Dw	108	GLN
4	Dw	112	GLN
4	Dw	147	GLN
4	Dw	231	ASN
4	Dw	282	ASN
4	Dx	32	GLN
4	Dx	50	HIS
4	Dx	112	GLN
4	Dx	120	GLN
4	Dx	235	GLN
4	Dx	293	GLN
4	Dy	106	ASN
4	Dy	108	GLN
4	Dy	112	GLN
4	Dy	143	GLN
4	Dy	147	GLN
4	Dy	282	ASN
4	Dz	50	HIS

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Mol	Chain	Res	Type
4	Dz	112	GLN
4	Dz	120	GLN
4	Dz	235	GLN
4	Dz	293	GLN
5	Gf	141	GLN
5	Gg	135	GLN
5	Gi	134	GLN
5	Gk	135	GLN
5	Gn	141	GLN
5	Go	134	GLN
5	Go	135	GLN
5	Gq	135	GLN
5	Gr	135	GLN
5	Gs	141	GLN
5	Gt	135	GLN
5	Gw	141	GLN
5	Gx	141	GLN
5	Gy	135	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

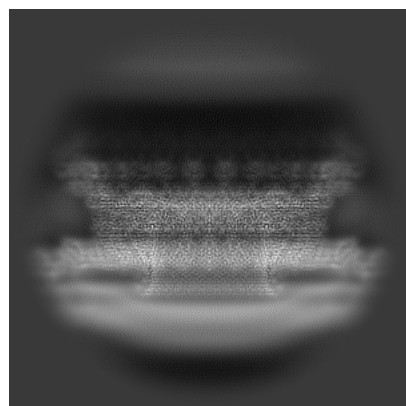
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72834. These allow visual inspection of the internal detail of the map and identification of artifacts.

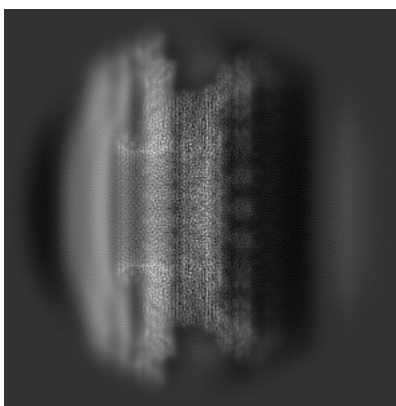
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

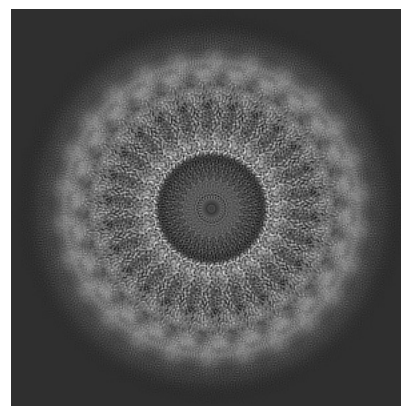
#### 6.1.1 Primary map



X

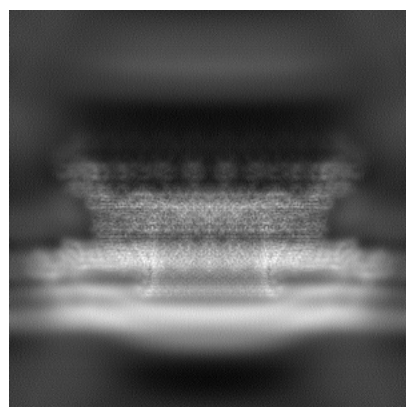


Y

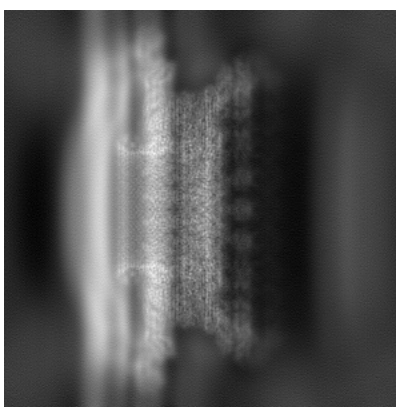


Z

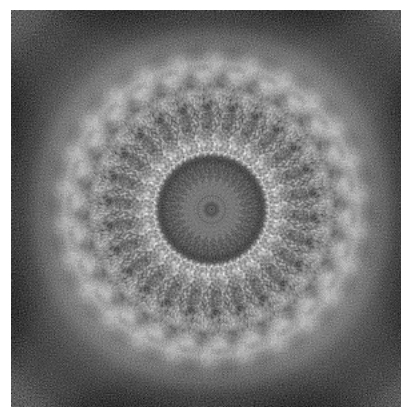
#### 6.1.2 Raw map



X



Y

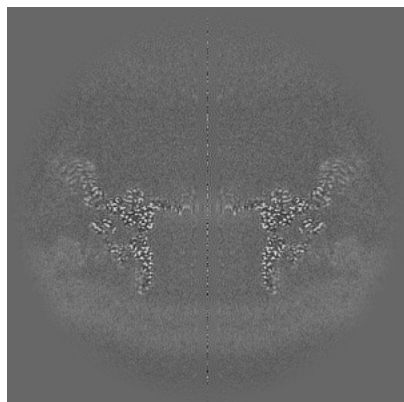


Z

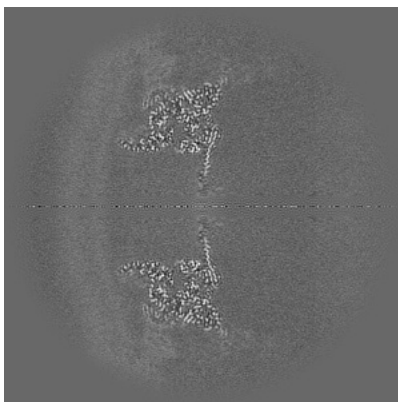
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

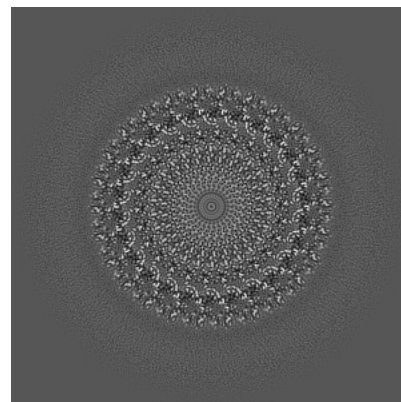
### 6.2.1 Primary map



X Index: 224

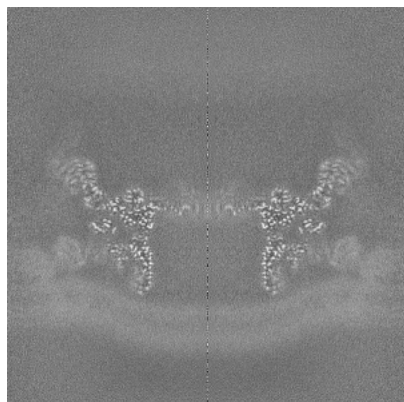


Y Index: 224

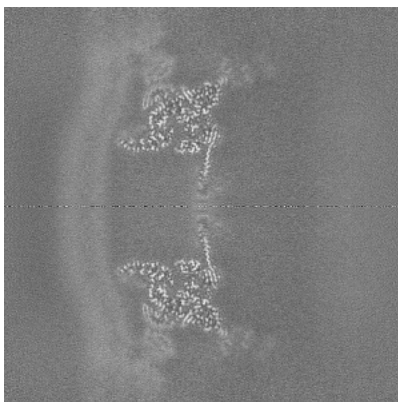


Z Index: 224

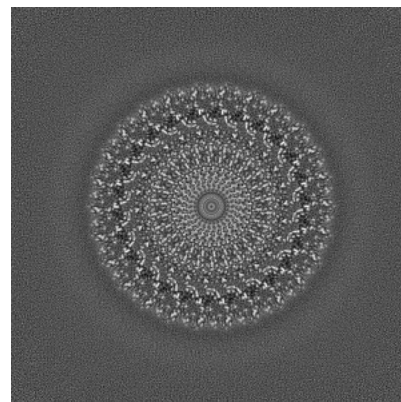
### 6.2.2 Raw map



X Index: 224



Y Index: 224



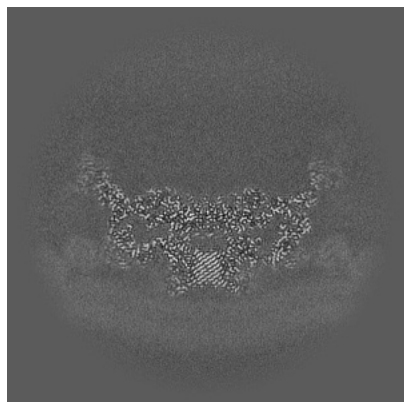
Z Index: 224

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

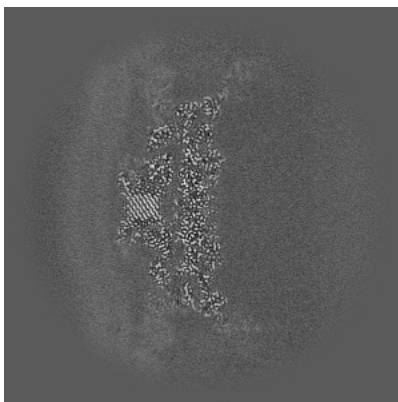


## 6.3 Largest variance slices [i](#)

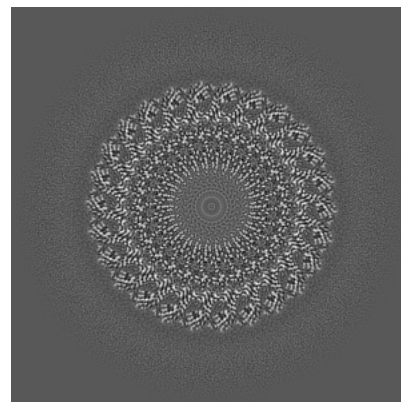
### 6.3.1 Primary map



X Index: 160



Y Index: 160

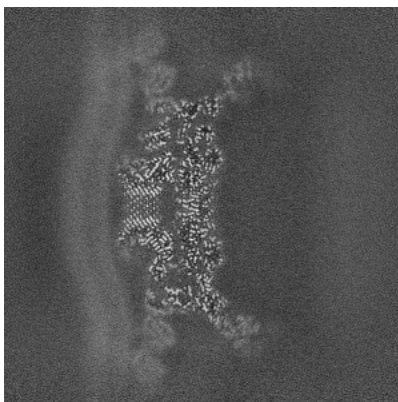


Z Index: 227

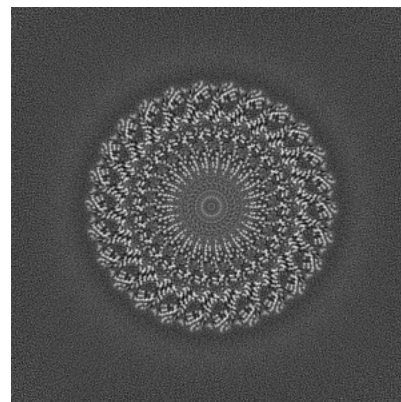
### 6.3.2 Raw map



X Index: 160



Y Index: 162

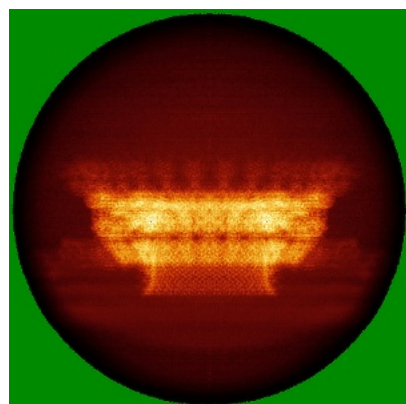


Z Index: 227

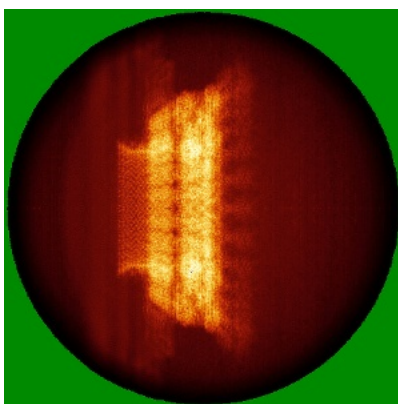
The images above show the largest variance slices of the map in three orthogonal directions.

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

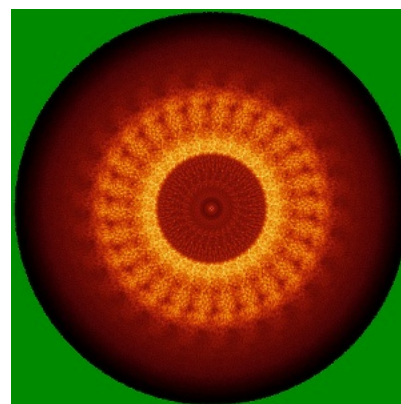
### 6.4.1 Primary map



X

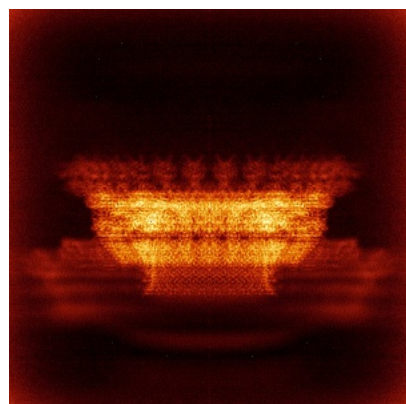


Y

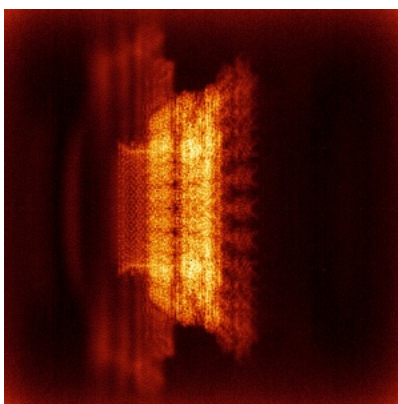


Z

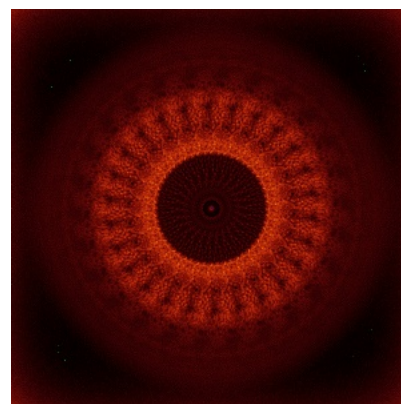
### 6.4.2 Raw map



X



Y



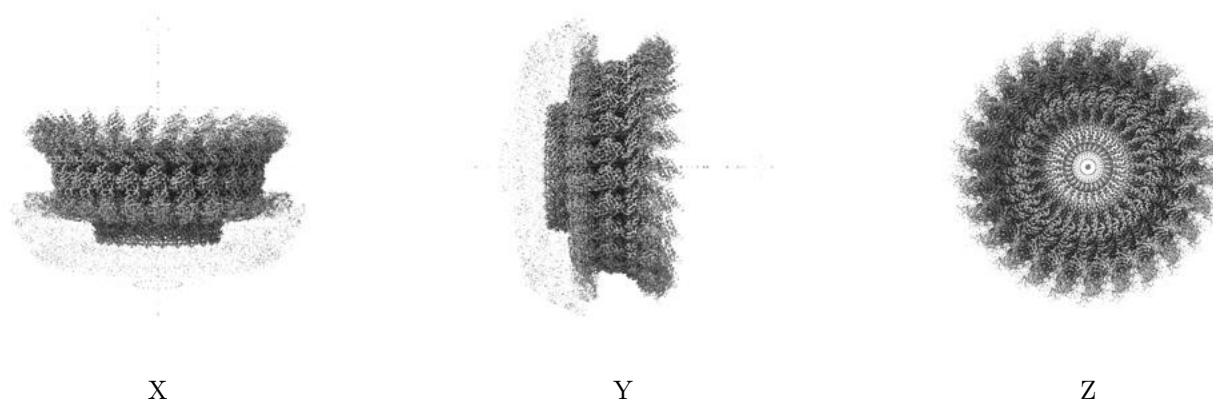
Z

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



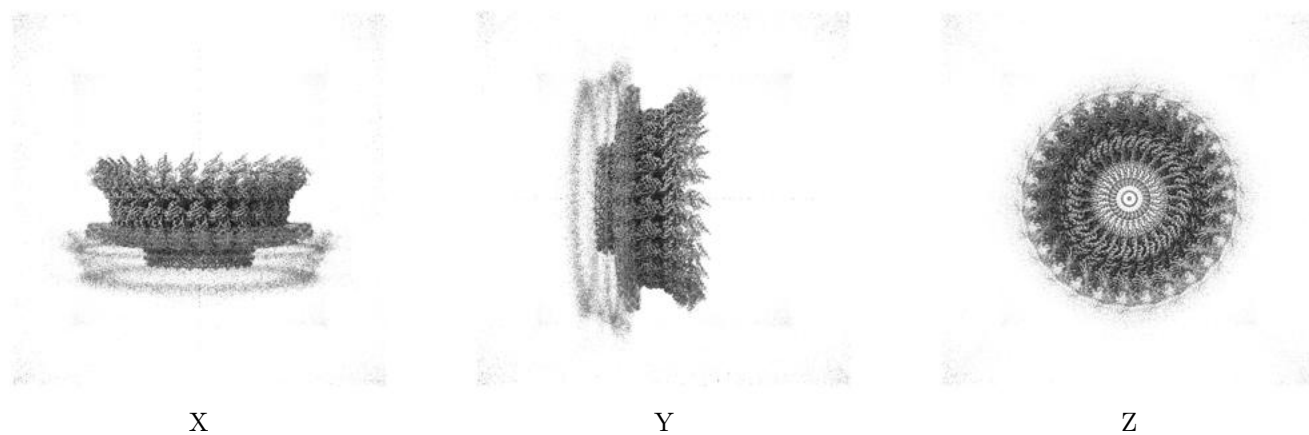
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

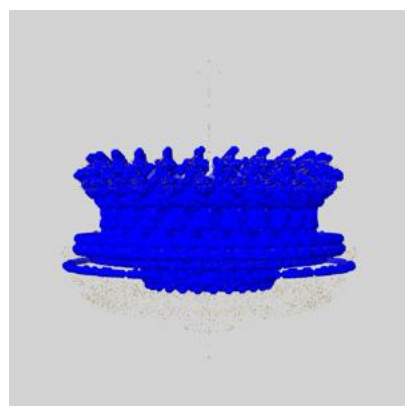
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

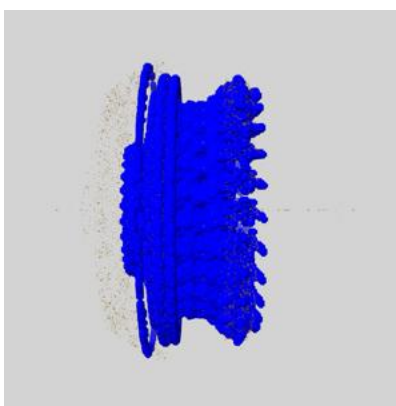
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

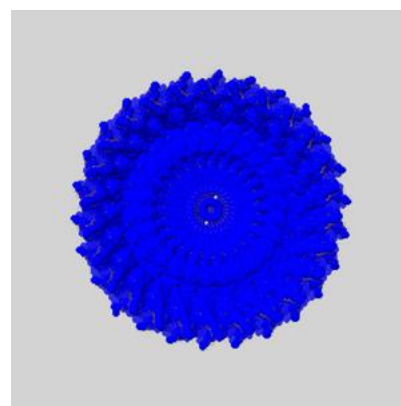
### 6.6.1 emd\_72834\_msk\_1.map [i](#)



X



Y

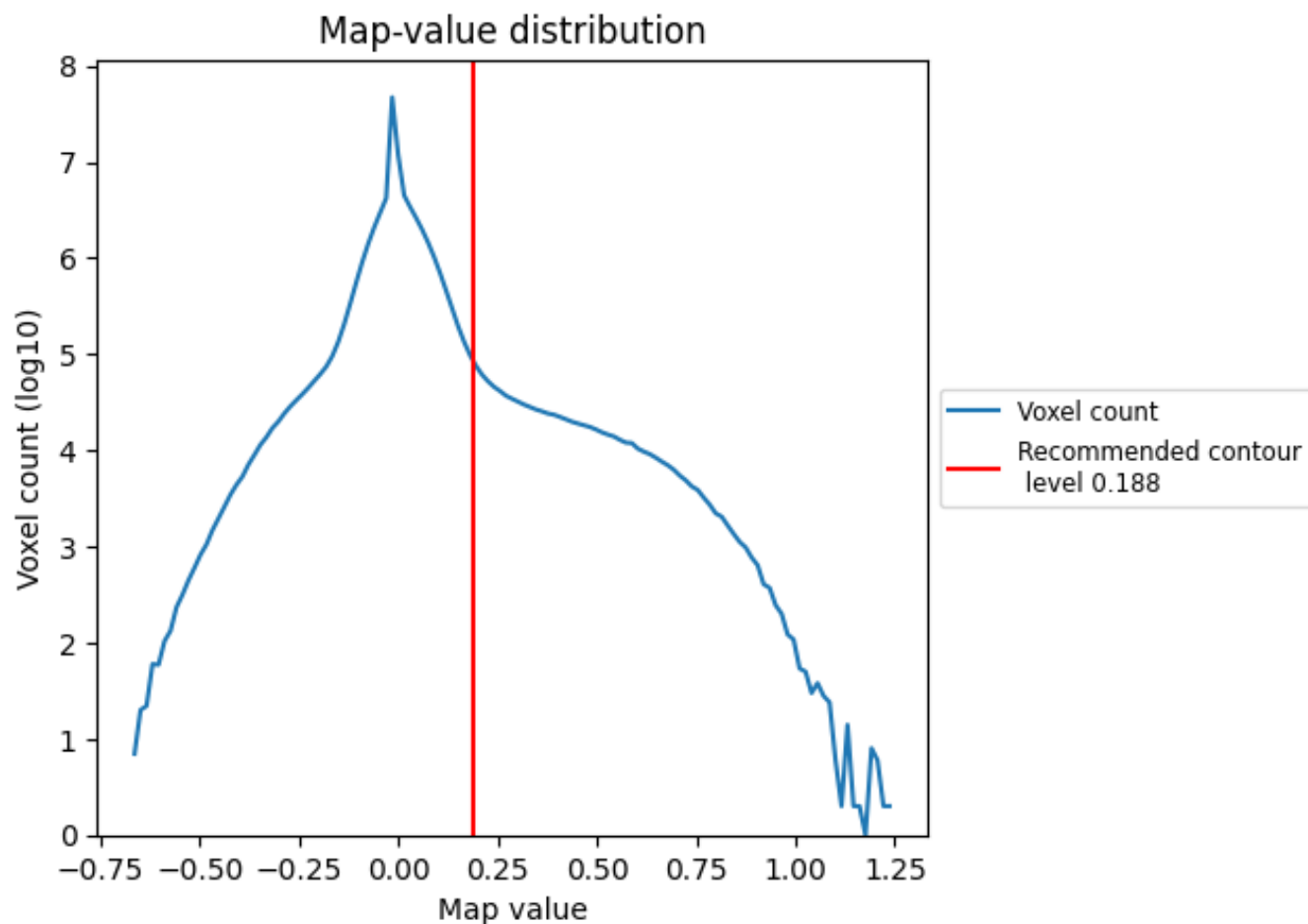


Z

## 7 Map analysis [i](#)

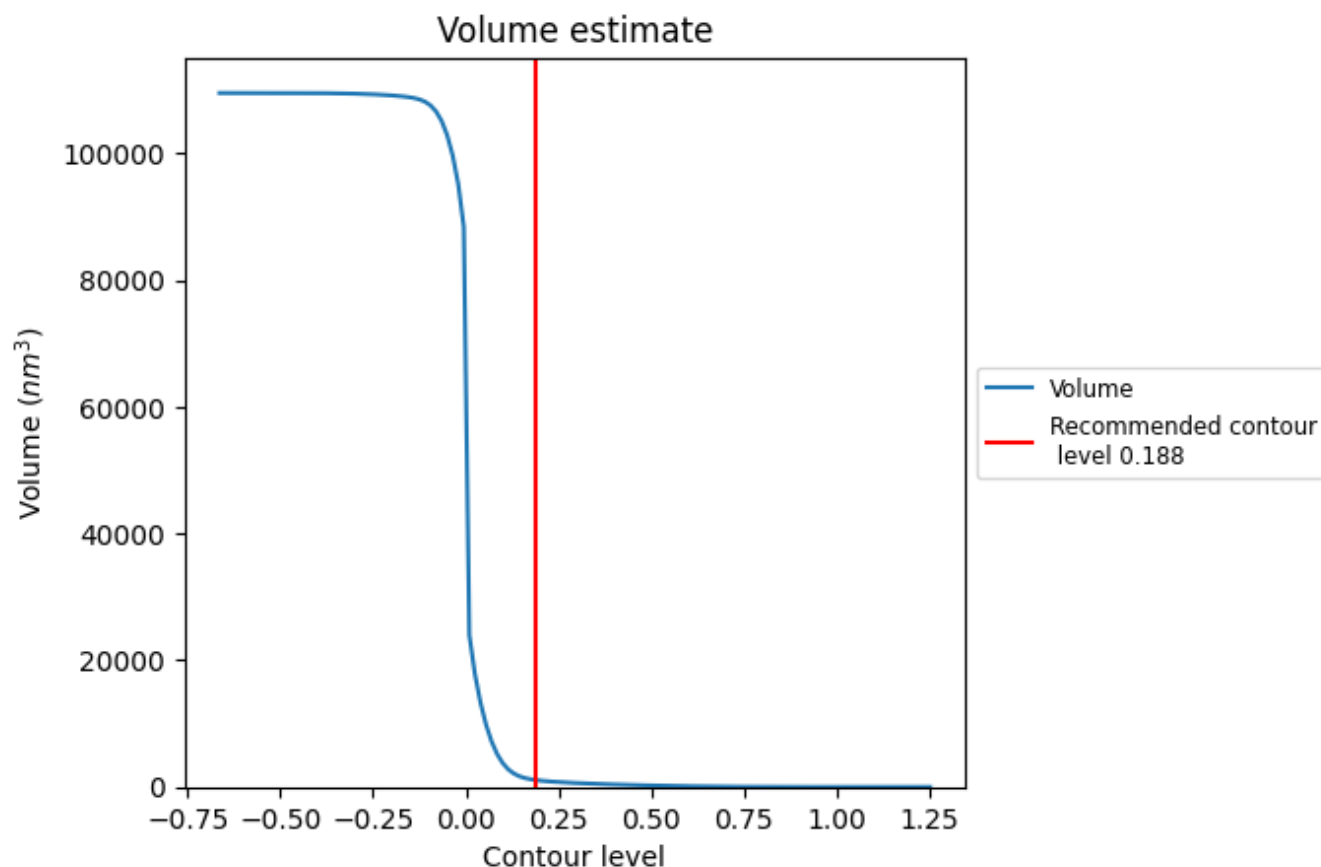
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

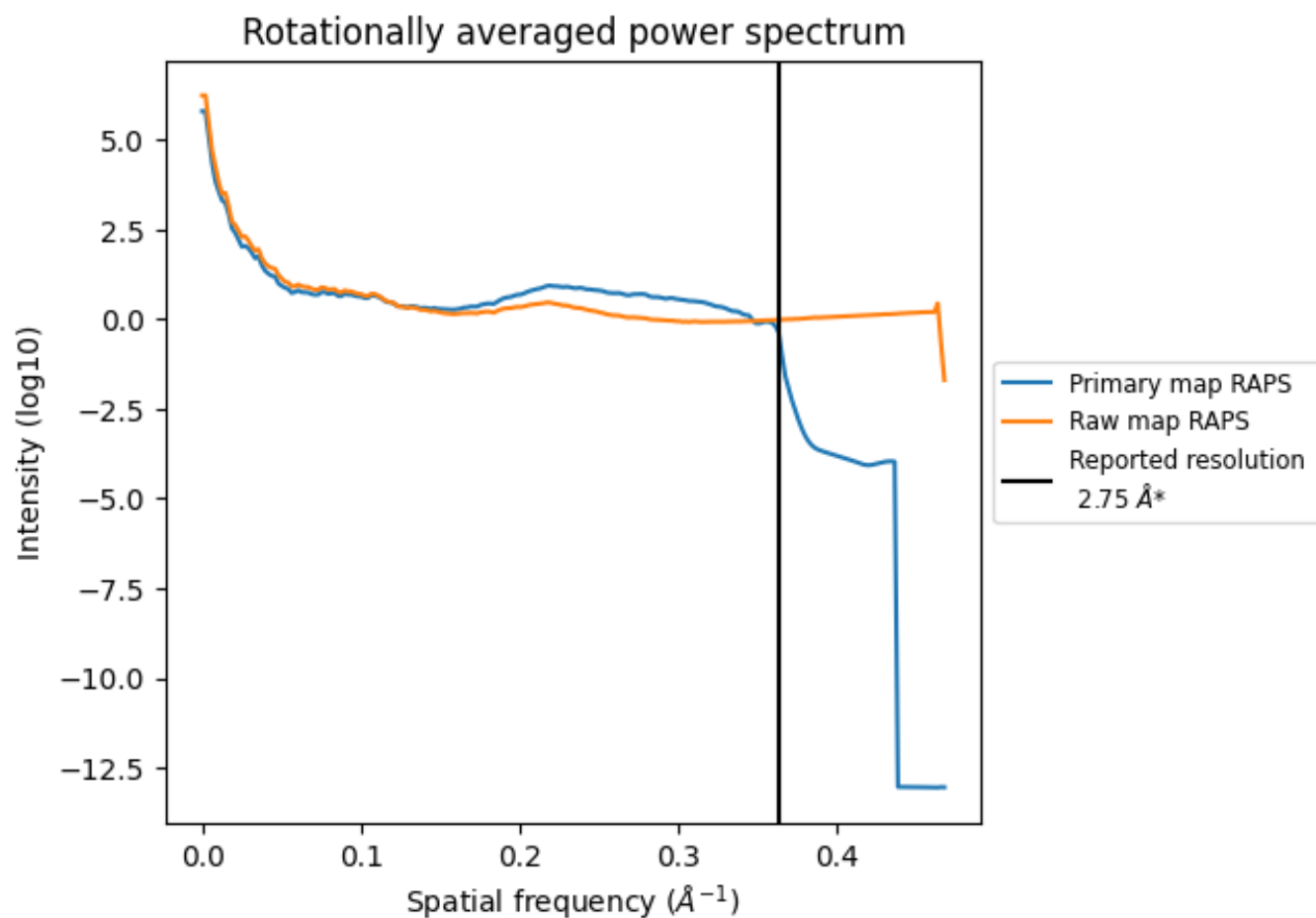
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1097  $\text{nm}^3$ ; this corresponds to an approximate mass of 991 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

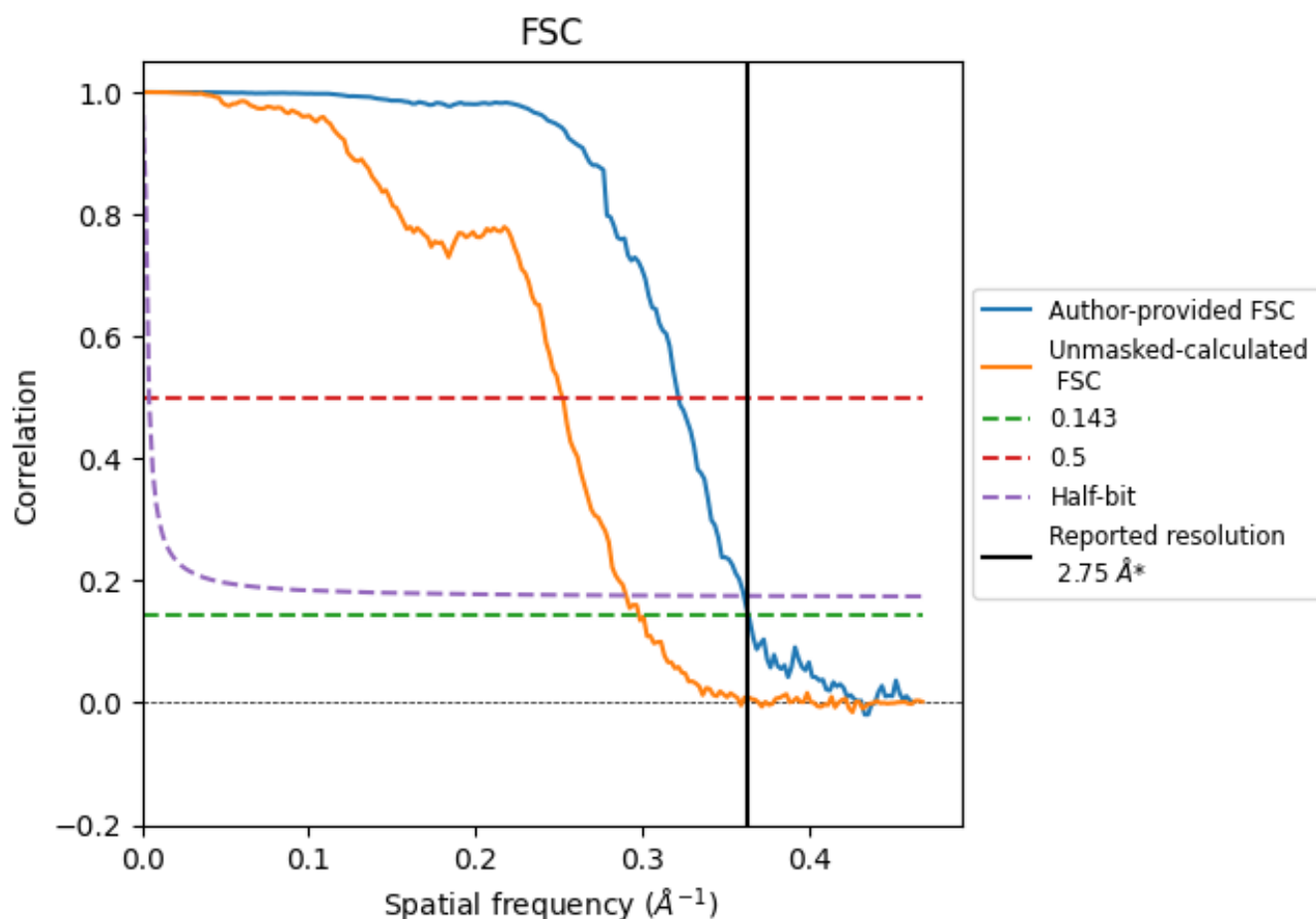


\*Reported resolution corresponds to spatial frequency of 0.364 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.364  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

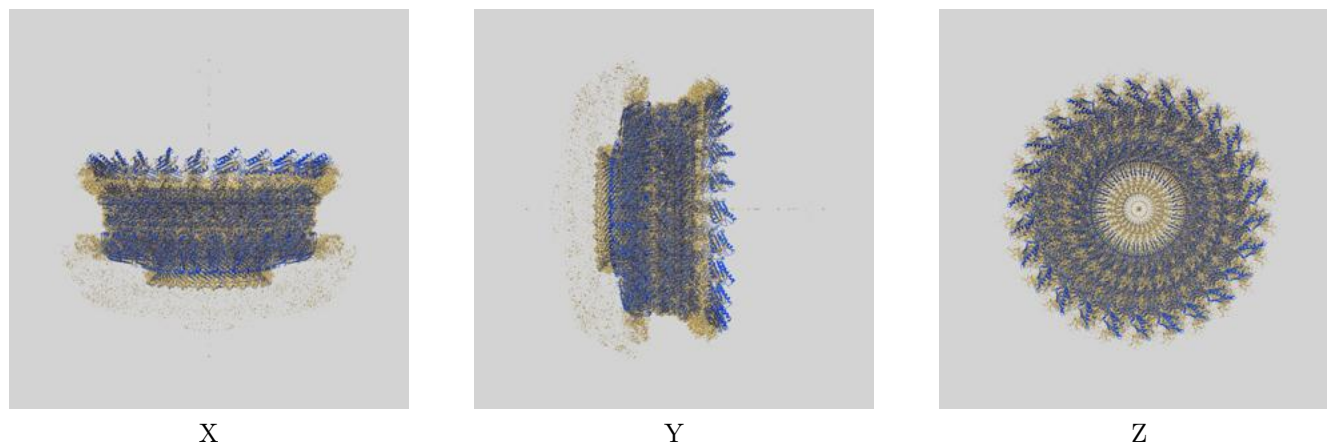
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.75	3.11	2.77
Unmasked-calculated*	3.35	3.97	3.44

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.75 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72834 and PDB model 9YDT. Per-residue inclusion information can be found in section [3](#) on page [18](#).

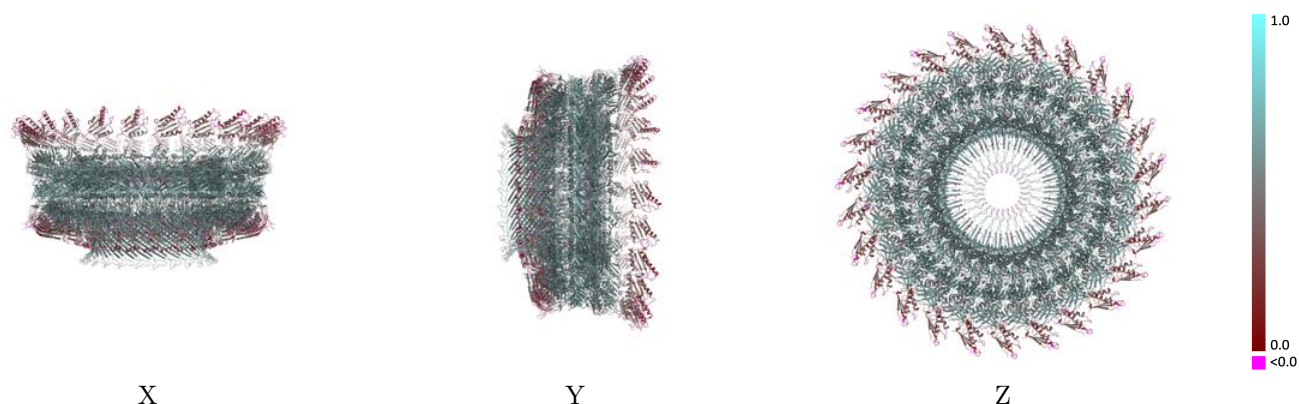
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

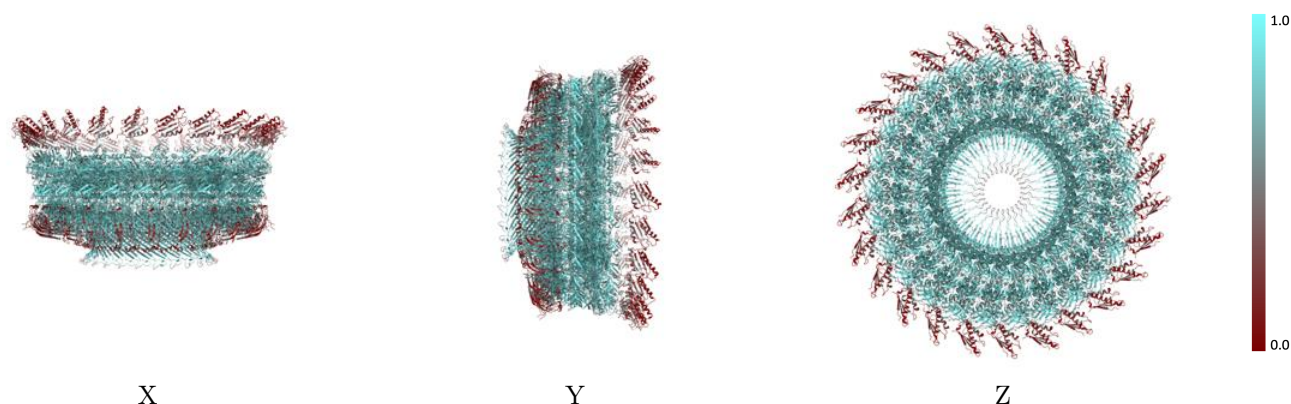


## 9.2 Q-score mapped to coordinate model [i](#)



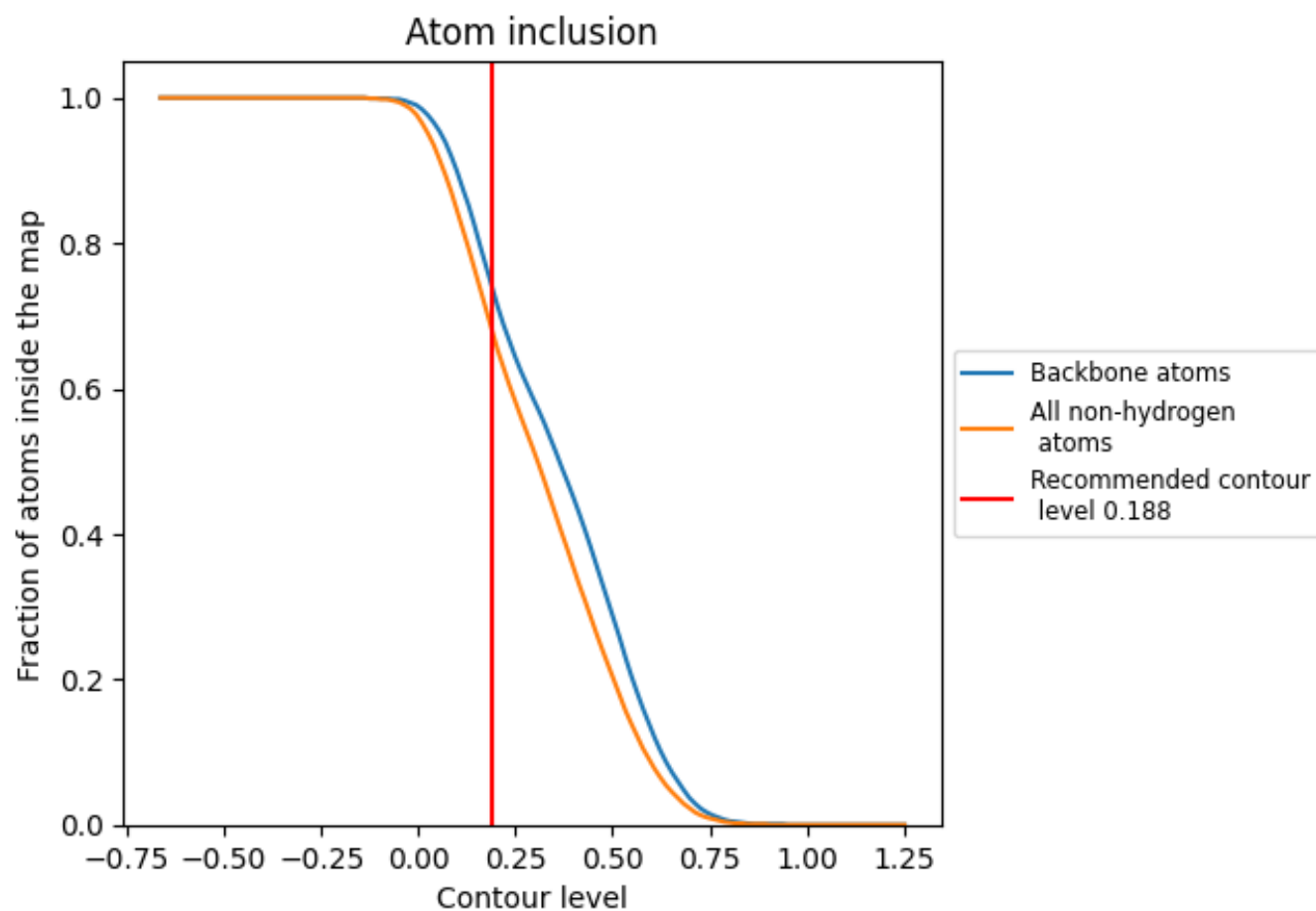
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.188).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6840	 0.5130
Aa	 0.7640	 0.5520
Ab	 0.7580	 0.5510
Ac	 0.7680	 0.5520
Ad	 0.7680	 0.5510
Ae	 0.7680	 0.5520
Af	 0.7660	 0.5510
Ag	 0.7650	 0.5510
Ah	 0.7640	 0.5510
Ai	 0.7640	 0.5510
Aj	 0.7620	 0.5500
Ak	 0.7680	 0.5520
Al	 0.7690	 0.5510
Am	 0.7660	 0.5500
An	 0.7660	 0.5520
Ao	 0.7660	 0.5520
Ap	 0.7630	 0.5520
Aq	 0.7650	 0.5520
Ar	 0.7590	 0.5510
As	 0.7690	 0.5510
At	 0.7640	 0.5520
Au	 0.7650	 0.5510
Av	 0.7660	 0.5510
Aw	 0.7710	 0.5520
Ax	 0.7580	 0.5500
Ay	 0.7680	 0.5500
Az	 0.7680	 0.5510
Ba	 0.8210	 0.5820
Bb	 0.8240	 0.5810
Bc	 0.8210	 0.5810
Bd	 0.8240	 0.5820
Be	 0.8210	 0.5820
Bf	 0.8190	 0.5820
Bg	 0.8220	 0.5810
Bh	 0.8240	 0.5810























































































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Chain	Atom inclusion	Q-score
Bi	 0.8210	 0.5780
Bj	 0.8210	 0.5810
Bk	 0.8250	 0.5810
Bl	 0.8250	 0.5810
Bm	 0.8180	 0.5800
Bn	 0.8160	 0.5780
Bo	 0.8270	 0.5820
Bp	 0.8240	 0.5790
Bq	 0.8240	 0.5780
Br	 0.8170	 0.5780
Bs	 0.8230	 0.5760
Bt	 0.8230	 0.5800
Bu	 0.8230	 0.5840
Bv	 0.8260	 0.5840
Bw	 0.8260	 0.5810
Bx	 0.8230	 0.5800
By	 0.8230	 0.5800
Bz	 0.8190	 0.5790
Ca	 0.6740	 0.5220
Cb	 0.6380	 0.4810
Cc	 0.6770	 0.5280
Cd	 0.6800	 0.5220
Ce	 0.6790	 0.5270
Cf	 0.6790	 0.5250
Cg	 0.6830	 0.5260
Ch	 0.6790	 0.5230
Ci	 0.6800	 0.5230
Cj	 0.6800	 0.5250
Ck	 0.6760	 0.5240
Cl	 0.6780	 0.5260
Cm	 0.6800	 0.5230
Cn	 0.6790	 0.5260
Co	 0.6810	 0.5240
Cp	 0.6790	 0.5230
Cq	 0.6800	 0.5260
Cr	 0.6780	 0.5250
Cs	 0.6760	 0.5220
Ct	 0.6730	 0.5220
Cu	 0.6780	 0.5250
Cv	 0.6830	 0.5270
Cw	 0.6780	 0.5260
Cx	 0.6810	 0.5270

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Chain	Atom inclusion	Q-score
Cy	 0.6810	 0.5250
Cz	 0.6820	 0.5260
Da	 0.5080	 0.4150
Db	 0.5100	 0.4230
Dc	 0.5030	 0.4120
Dd	 0.5030	 0.4230
De	 0.5030	 0.4110
Df	 0.5060	 0.4230
Dg	 0.5060	 0.4120
Dh	 0.5070	 0.4260
Di	 0.5040	 0.4090
Dj	 0.5070	 0.4230
Dk	 0.5070	 0.4100
Dl	 0.5080	 0.4250
Dm	 0.5080	 0.4100
Dn	 0.4970	 0.4200
Do	 0.5010	 0.4060
Dp	 0.5050	 0.4190
Dq	 0.5040	 0.4130
Dr	 0.5030	 0.4210
Ds	 0.5010	 0.4100
Dt	 0.5040	 0.4230
Du	 0.4990	 0.4100
Dv	 0.4960	 0.4170
Dw	 0.5060	 0.4120
Dx	 0.5080	 0.4200
Dy	 0.5050	 0.4130
Dz	 0.5090	 0.4240
Fa	 0.2360	 0.2660
Fb	 0.2200	 0.2250
Fc	 0.2600	 0.2680
Fd	 0.2280	 0.2460
Fe	 0.2360	 0.2370
Ff	 0.2280	 0.2130
Fg	 0.2520	 0.2560
Fh	 0.2680	 0.2510
Fi	 0.2520	 0.2630
Fj	 0.2600	 0.2500
Fk	 0.2360	 0.2320
Fl	 0.2520	 0.2470
Fm	 0.2360	 0.2620
Fn	 0.2200	 0.2160

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Chain	Atom inclusion	Q-score
Fo	0.2680	0.2590
Fp	0.2600	0.2120
Fq	0.2600	0.2160
Fr	0.2440	0.2490
Fs	0.2440	0.2150
Ft	0.2440	0.2240
Fu	0.2600	0.2250
Fv	0.2600	0.2380
Fw	0.2360	0.1930
Fx	0.2520	0.2390
Fy	0.2360	0.2180
Fz	0.2360	0.2160
Ga	0.2910	0.2420
Gb	0.2730	0.2650
Gc	0.2730	0.2190
Gd	0.2820	0.2660
Ge	0.2820	0.2270
Gf	0.2910	0.2290
Gg	0.2730	0.3000
Gh	0.2820	0.2950
Gi	0.2910	0.2290
Gj	0.2820	0.2350
Gk	0.3180	0.2300
Gl	0.2820	0.2580
Gm	0.2820	0.2540
Gn	0.2910	0.2620
Go	0.3000	0.2130
Gp	0.2730	0.2410
Gq	0.2640	0.1900
Gr	0.2640	0.2270
Gs	0.2910	0.2670
Gt	0.2820	0.2870
Gu	0.2730	0.2620
Gv	0.3090	0.2760
Gw	0.1730	0.2040
Gx	0.2640	0.2570
Gy	0.3000	0.3110
Gz	0.2360	0.2250