



## Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 03:44 PM EDT

PDB ID : 9YDO / pdb\_00009ydo  
EMDB ID : EMD-72815  
Title : LPHT-ring in *Vibrio cholerae* at assembled, opened state  
Authors : Guo, W.; Yue, J.  
Deposited on : 2025-09-22  
Resolution : 2.69 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:

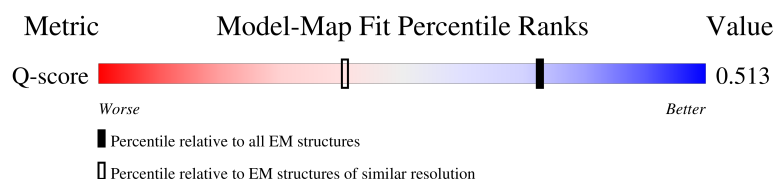
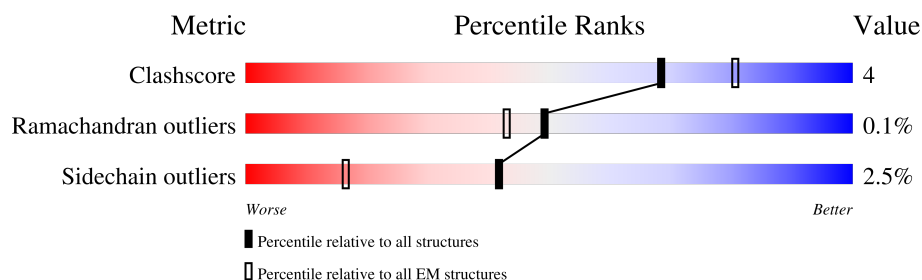
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 2.69 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	9309 ( 2.19 - 3.19 )

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	
1	Ab	227	
1	Ac	227	
1	Ad	227	







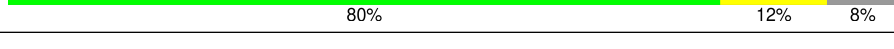
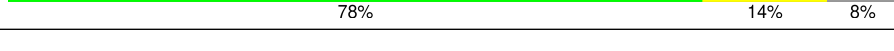
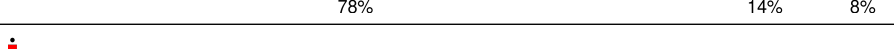
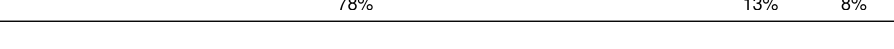
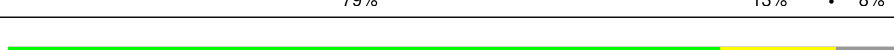

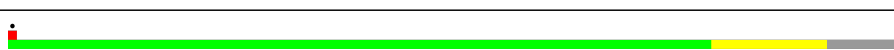

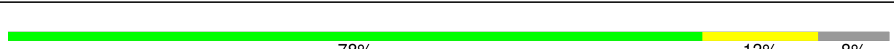





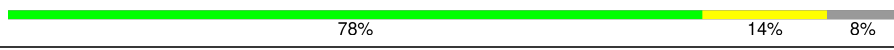
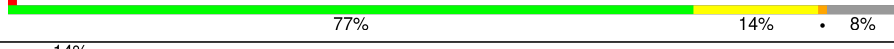
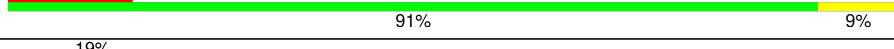
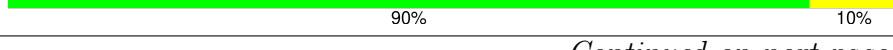

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Mol	Chain	Length	Quality of chain
1	Ae	227	
1	Af	227	
1	Ag	227	
1	Ah	227	
1	Ai	227	
1	Aj	227	
1	Ak	227	
1	Al	227	
1	Am	227	
1	An	227	
1	Ao	227	
1	Ap	227	
1	Aq	227	
1	Ar	227	
1	As	227	
1	At	227	
1	Au	227	
1	Av	227	
1	Aw	227	
1	Ax	227	
1	Ay	227	
1	Az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

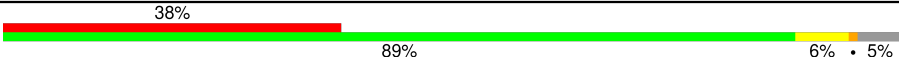

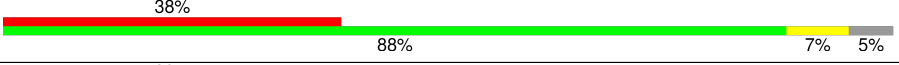

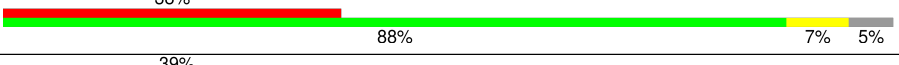
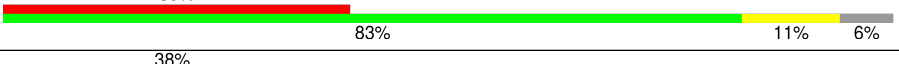
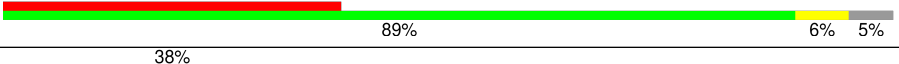

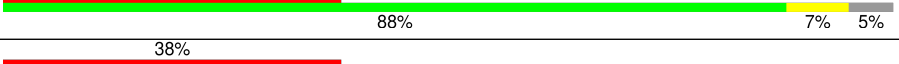

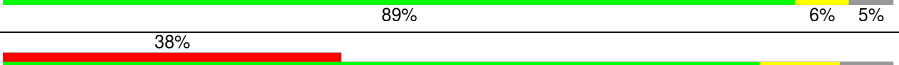
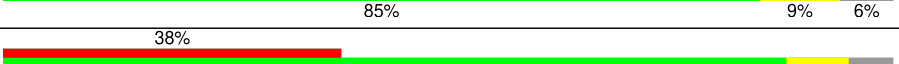
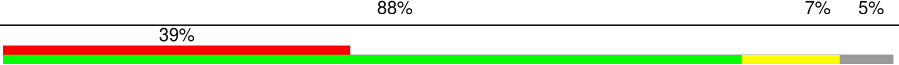
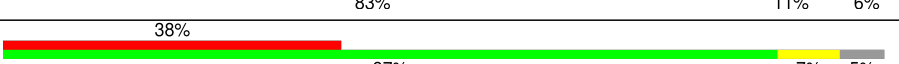

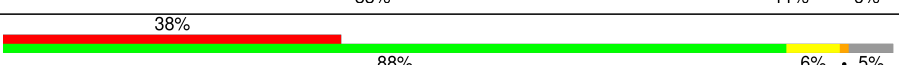
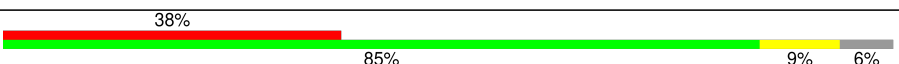
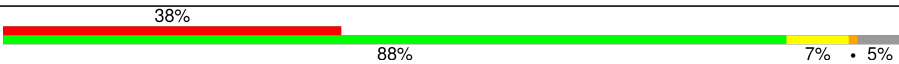
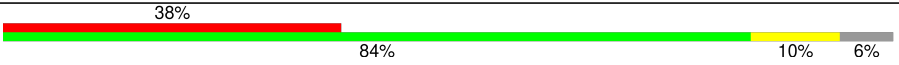


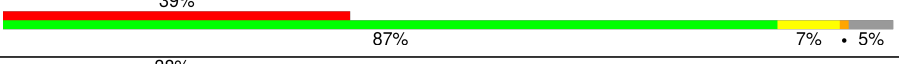
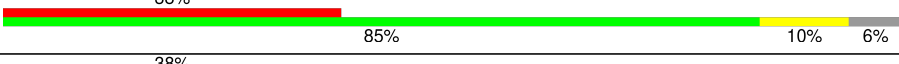


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Mol	Chain	Length	Quality of chain
3	Cc	352	
3	Cd	352	
3	Ce	352	
3	Cf	352	
3	Cg	352	
3	Ch	352	
3	Ci	352	
3	Cj	352	
3	Ck	352	
3	Cl	352	
3	Cm	352	
3	Cn	352	
3	Co	352	
3	Cp	352	
3	Cq	352	
3	Cr	352	
3	Cs	352	
3	Ct	352	
3	Cu	352	
3	Cv	352	
3	Cw	352	
3	Cx	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	<div>60% 93% 7%</div>
5	Fb	15	<div>67% 93% 7%</div>
5	Fc	15	<div>60% 100%</div>
5	Fd	15	<div>60% 87% 13%</div>
5	Fe	15	<div>60% 93% 7%</div>
5	Ff	15	<div>60% 93% 7%</div>
5	Fg	15	<div>60% 100%</div>
5	Fh	15	<div>73% 93% 7%</div>
5	Fi	15	<div>60% 87% 13%</div>
5	Fj	15	<div>67% 93% 7%</div>
5	Fk	15	<div>60% 100%</div>
5	Fl	15	<div>60% 87% 13%</div>
5	Fm	15	<div>60% 93% 7%</div>
5	Fn	15	<div>67% 100%</div>
5	Fo	15	<div>60% 93% 7%</div>
5	Fp	15	<div>60% 93% 7%</div>
5	Fq	15	<div>67% 87% 13%</div>
5	Fr	15	<div>60% 100%</div>
5	Fs	15	<div>60% 100%</div>
5	Ft	15	<div>67% 87% 13%</div>
5	Fu	15	<div>60% 93% 7%</div>
5	Fv	15	<div>67% 100%</div>
5	Fw	15	<div>60% 93% 7%</div>
5	Fx	15	<div>60% 100%</div>
5	Fy	15	<div>67% 93% 7%</div>

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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><div></div><div></div><div></div></div><div>60%80%7%13%</div></div>
5	Gz	15	<div><div><div></div><div></div><div></div><div></div></div><div>60%80%7%13%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 236015 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	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bb	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bc	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bd	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Be	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bf	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bg	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bh	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bi	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bj	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bk	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bl	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bm	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bn	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bo	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bp	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bq	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Br	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bs	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bt	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bu	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bv	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bw	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bx	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	By	316	Total	C	N	O	S	0	0
			2314	1457	404	446	7		
2	Bz	316	Total	C	N	O	S	0	0
			2314	1457	404	446	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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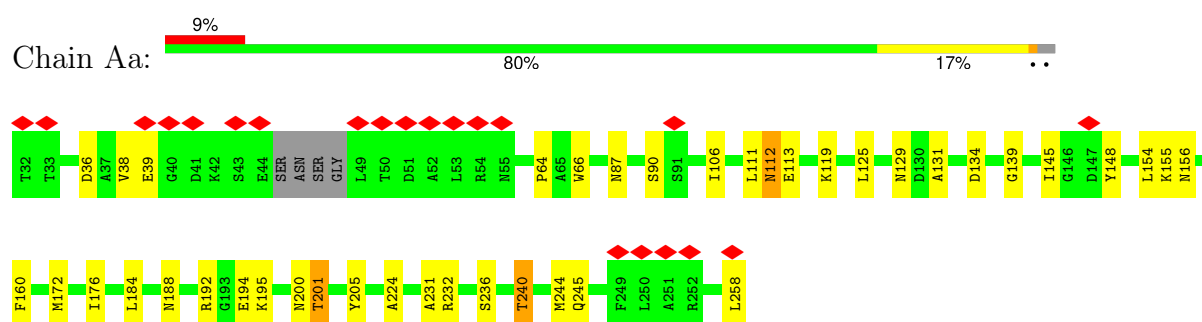
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Mol	Chain	Residues	Atoms					AltConf	Trace
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5	Gh	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gi	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gj	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gk	13	Total 112	C 71	N 20	O 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
5	Gy	13	Total 112	C 71	N 20	O 20	S 1	0	0
5	Gz	13	Total 112	C 71	N 20	O 20	S 1	0	0

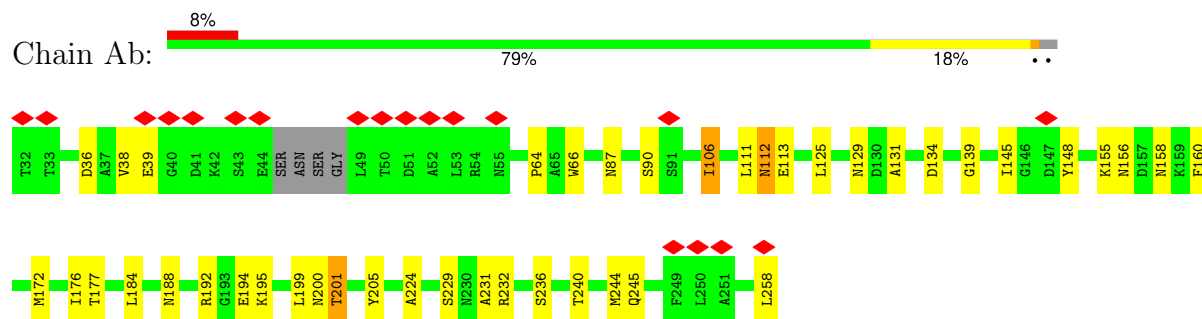
### 3 Residue-property plots

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

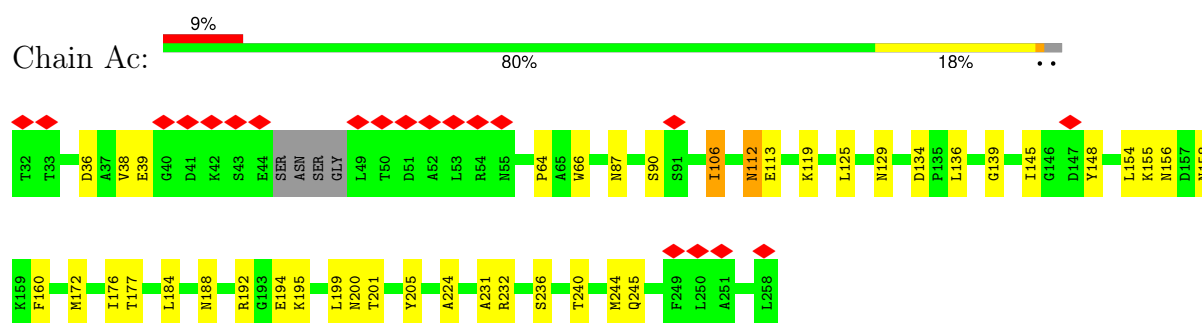
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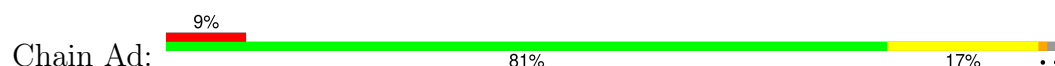
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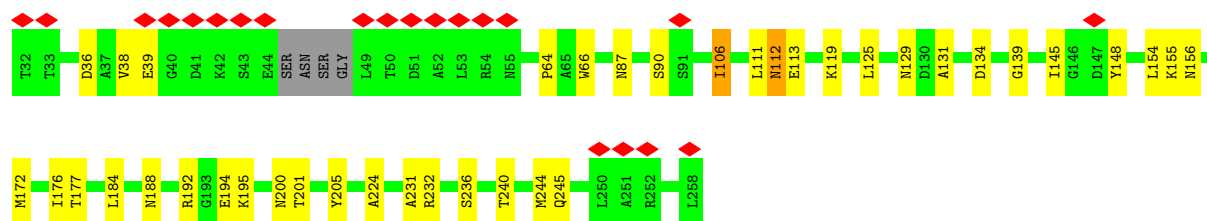


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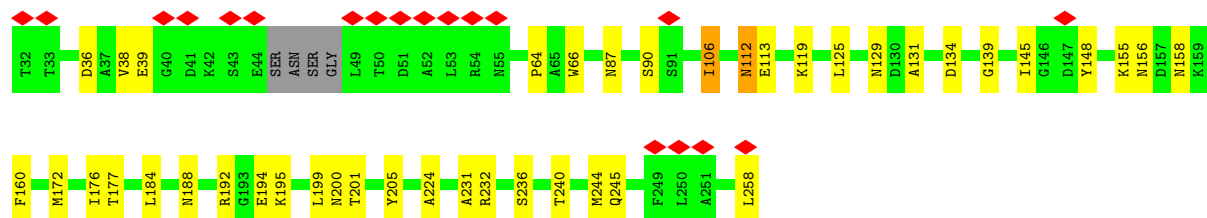
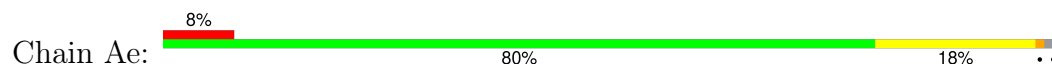


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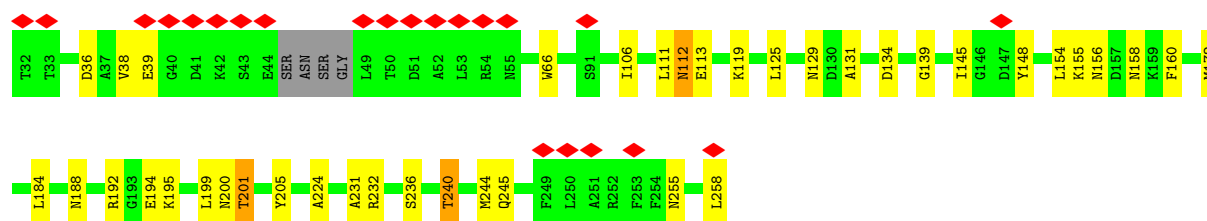
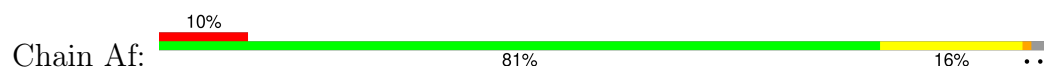




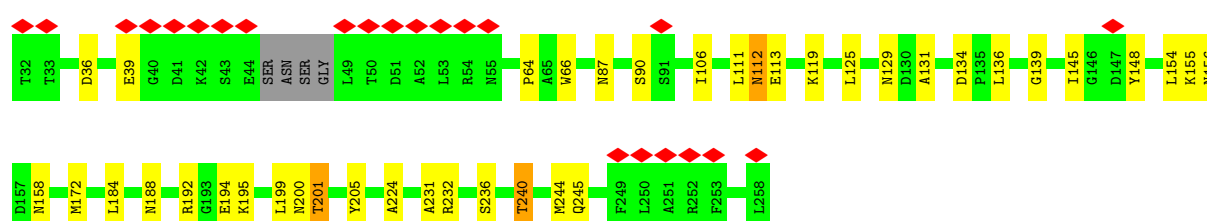
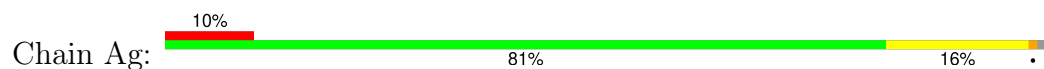
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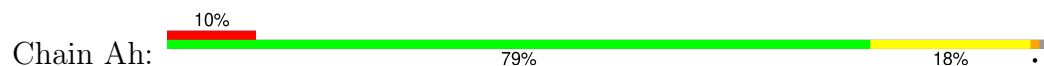
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

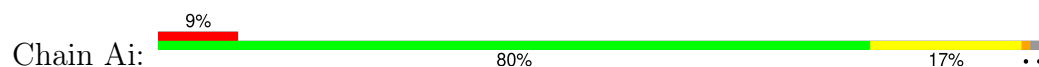


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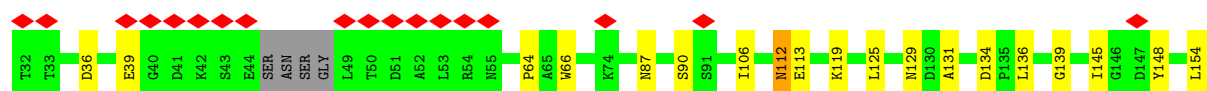
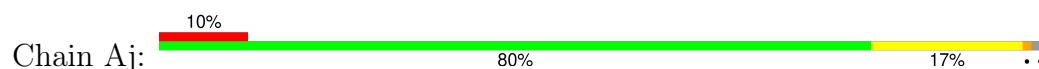




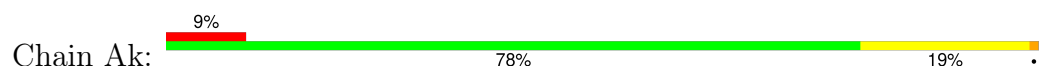
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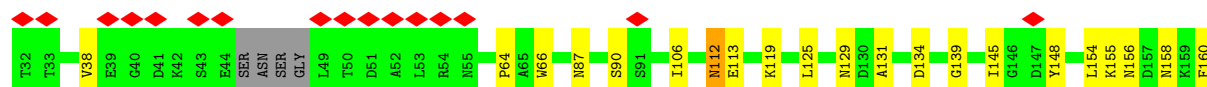
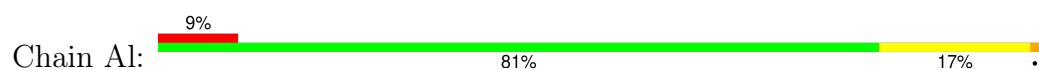
• Molecule 1: Flagellar L-ring protein



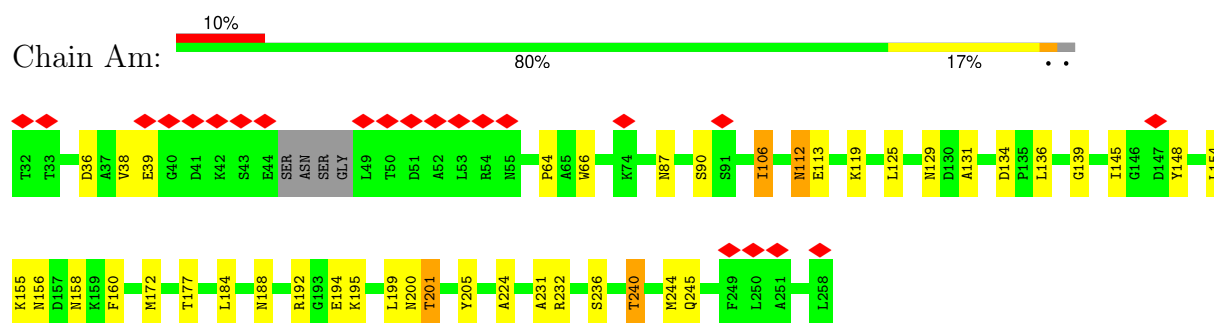
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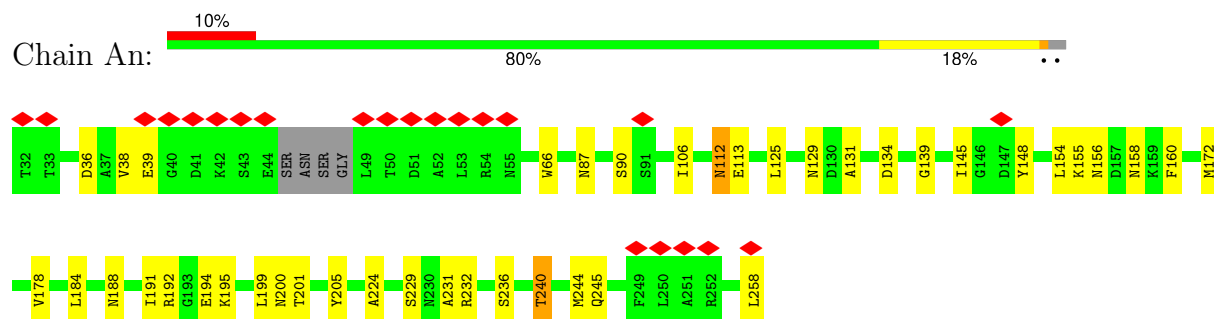
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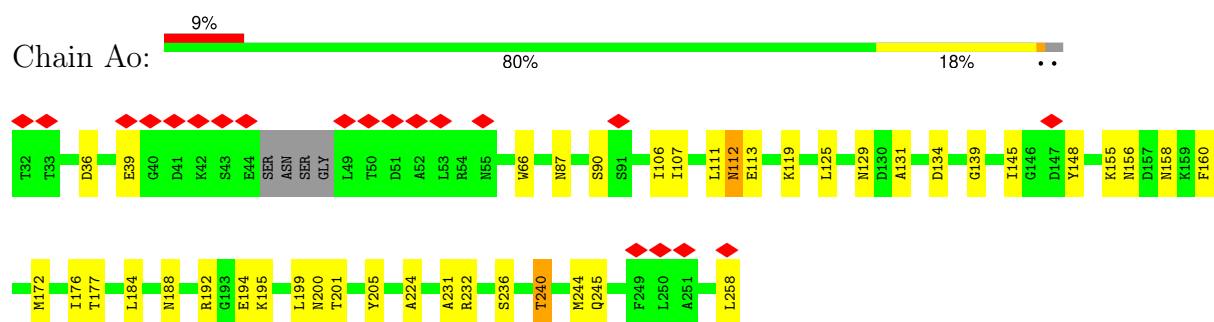
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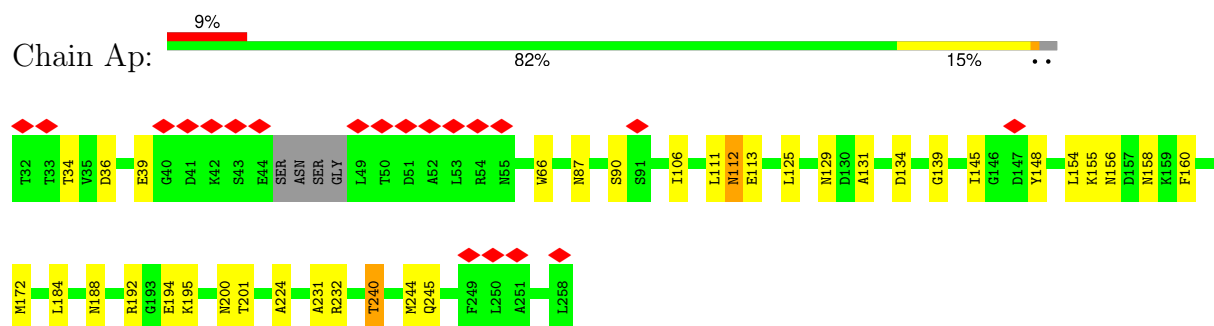
- Molecule 1: Flagellar L-ring protein



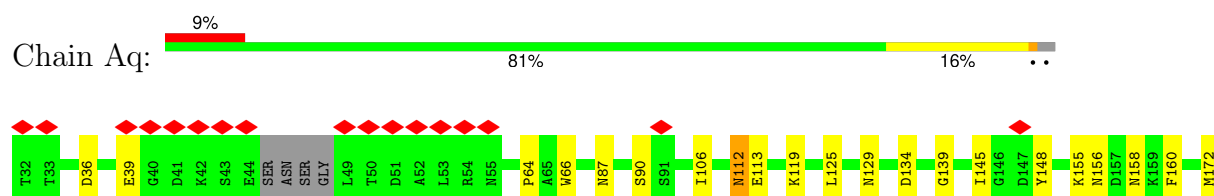
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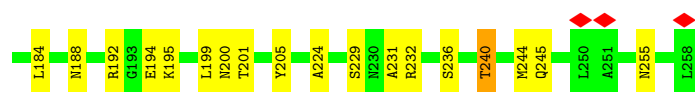


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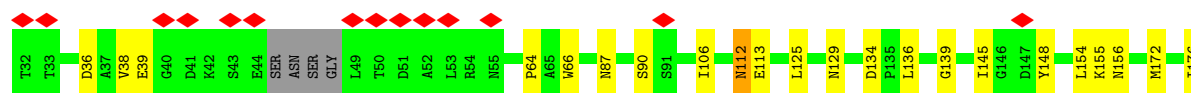
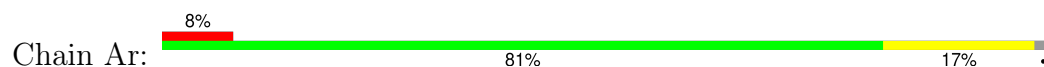


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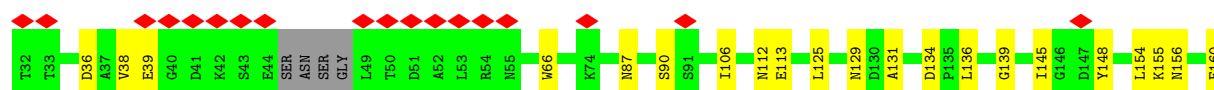
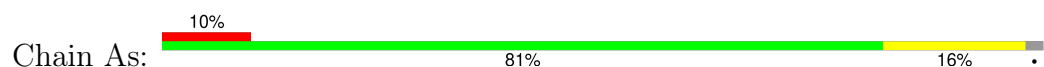




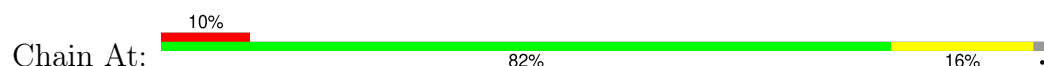
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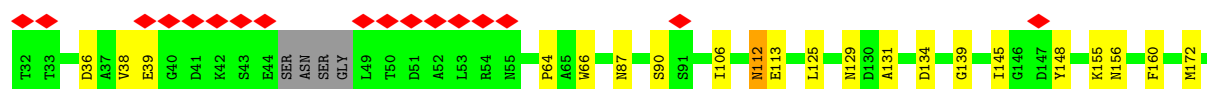
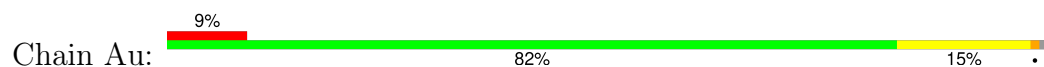
- Molecule 1: Flagellar L-ring protein



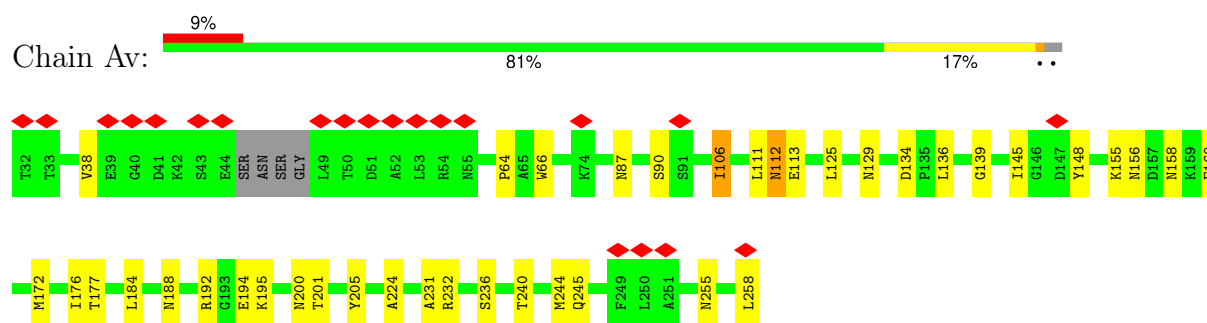
- Molecule 1: Flagellar L-ring protein



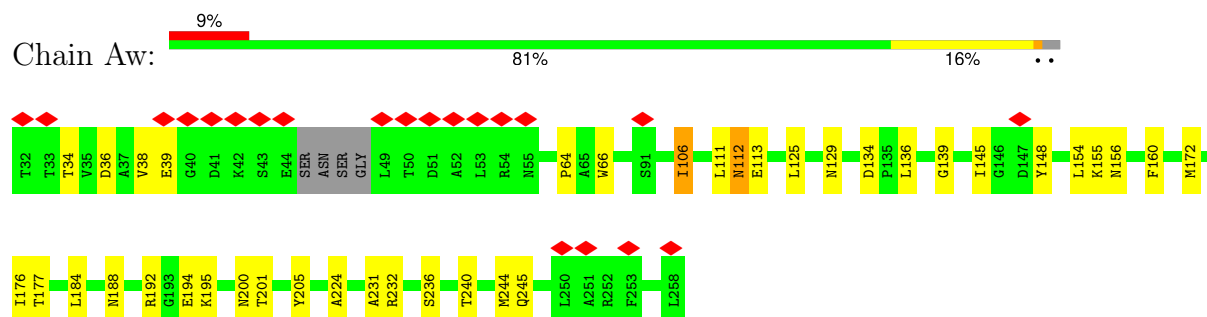
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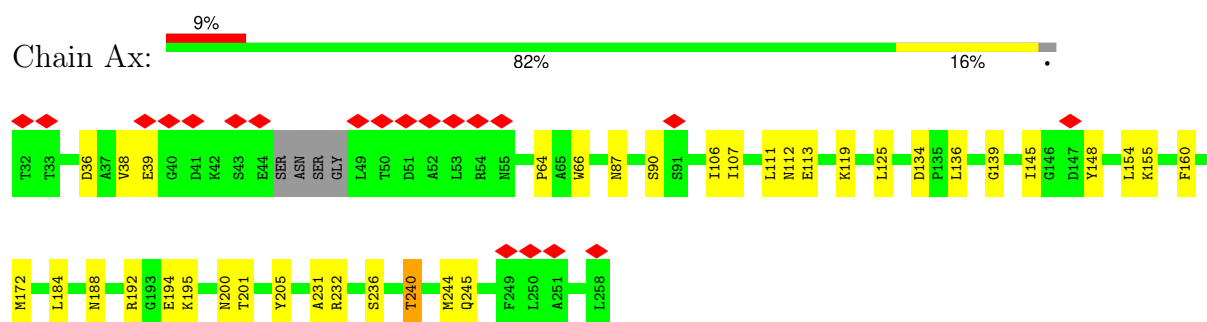
- Molecule 1: Flagellar L-ring protein



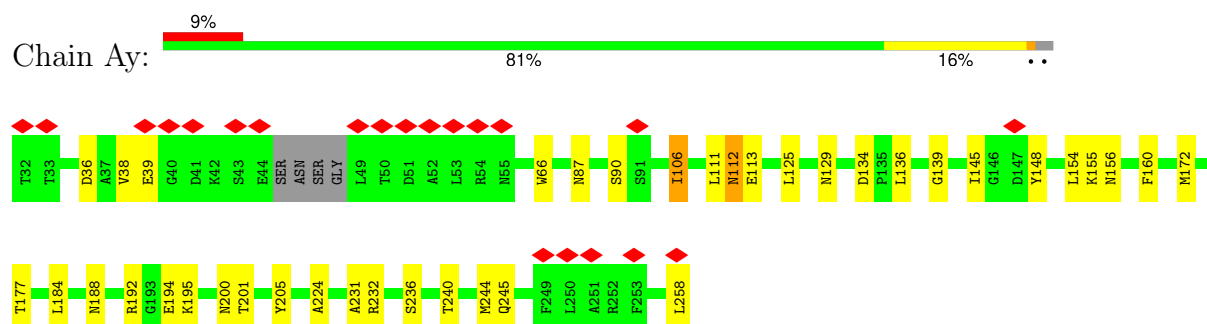
• Molecule 1: Flagellar L-ring protein



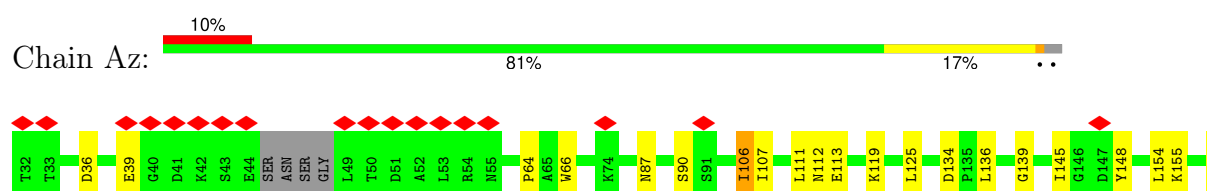
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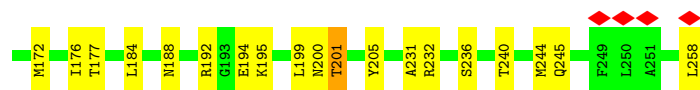


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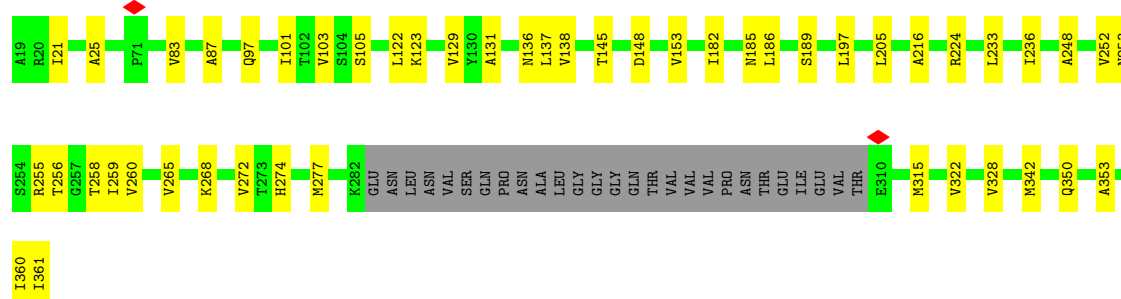
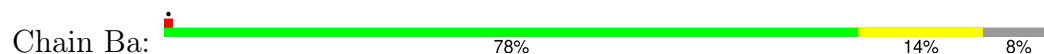


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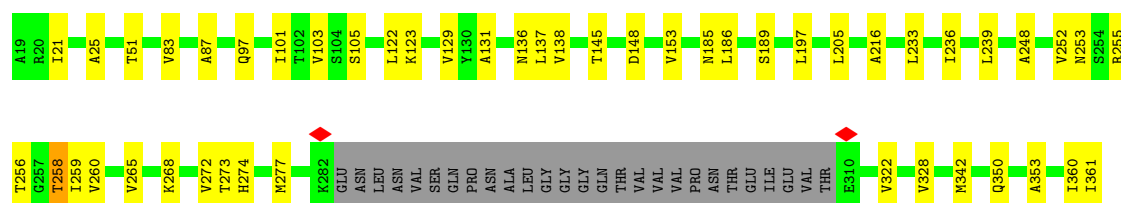
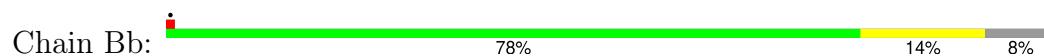




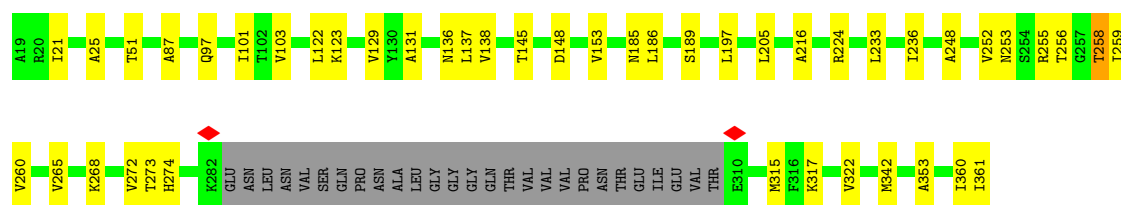
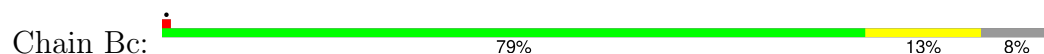
• Molecule 2: Flagellar P-ring protein



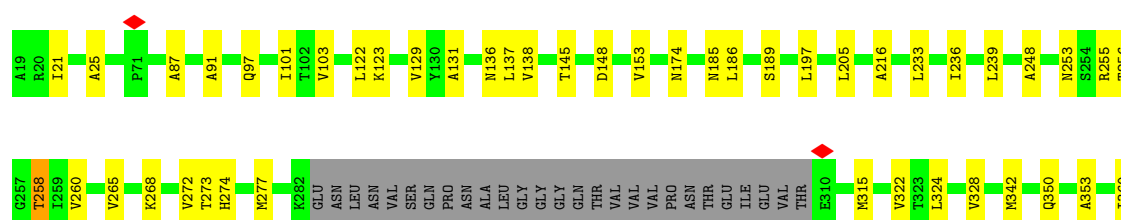
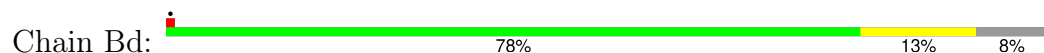
• Molecule 2: Flagellar P-ring protein



• Molecule 2: Flagellar P-ring protein




• Molecule 2: Flagellar P-ring protein

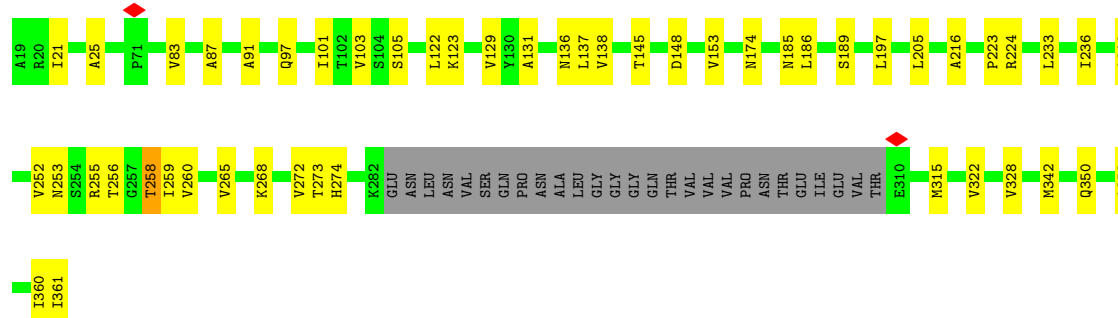





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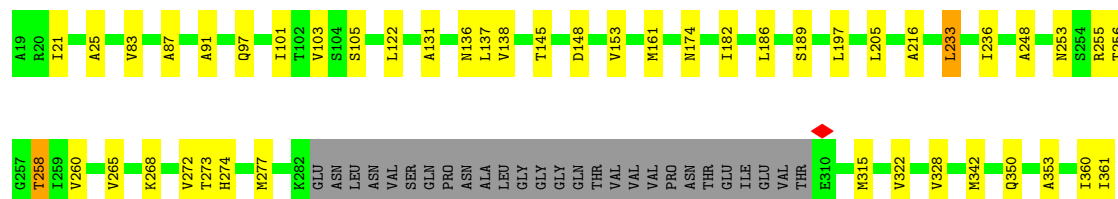
- Molecule 2: Flagellar P-ring protein

Chain Be:  77% 15% 8%




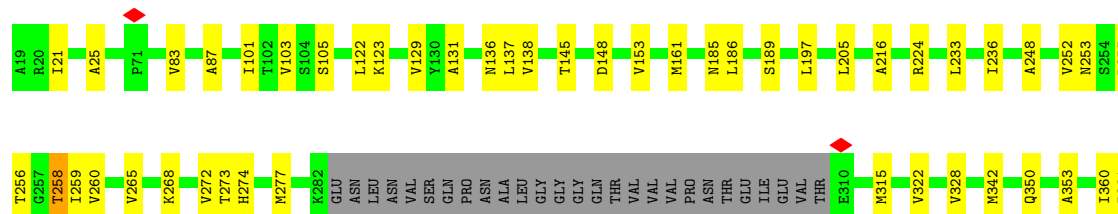
- Molecule 2: Flagellar P-ring protein

Chain Bf:  78% 13% 8%




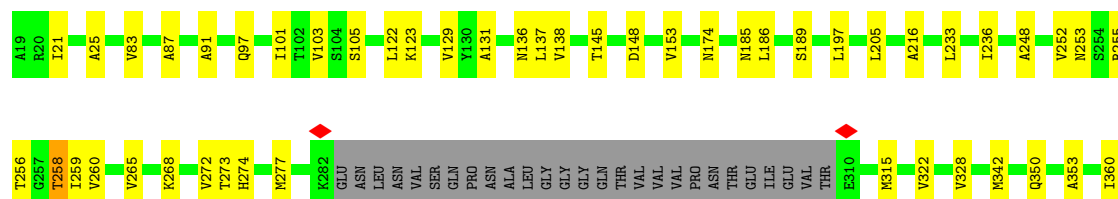
- Molecule 2: Flagellar P-ring protein

Chain Bg:  78% 14% 8%

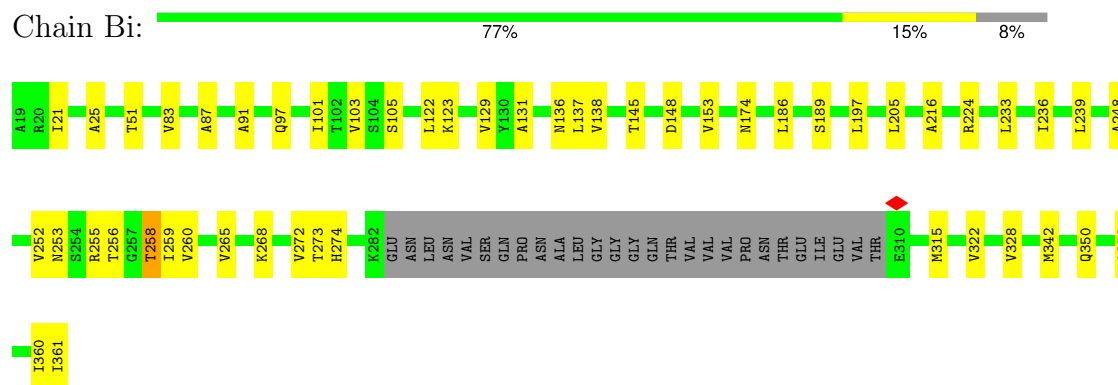


- Molecule 2: Flagellar P-ring protein

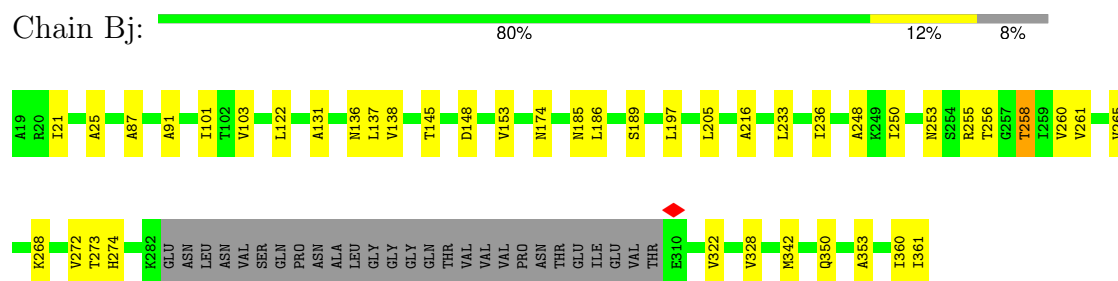
Chain Bh:  78% 14% 8%



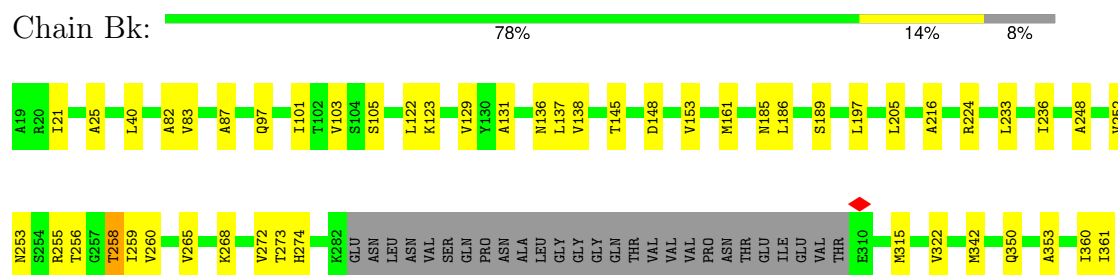
- Molecule 2: Flagellar P-ring protein



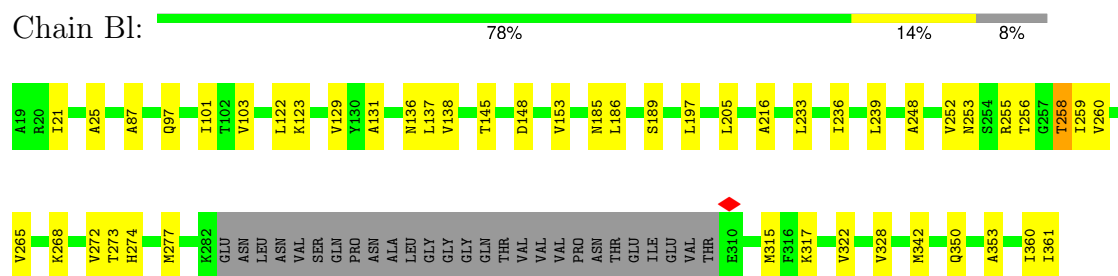
- Molecule 2: Flagellar P-ring protein



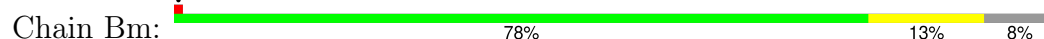
- Molecule 2: Flagellar P-ring protein

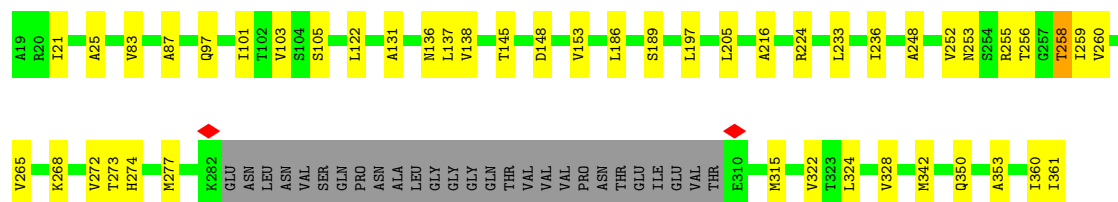


- Molecule 2: Flagellar P-ring protein



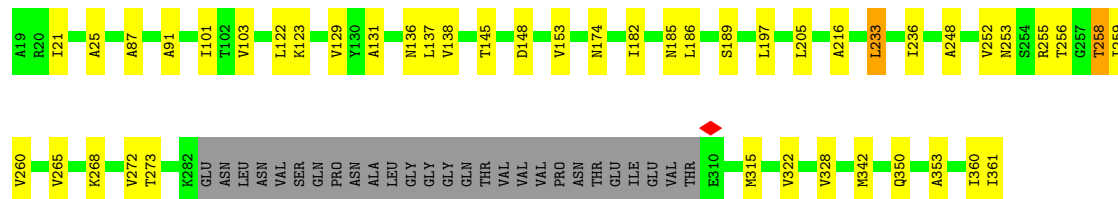
- Molecule 2: Flagellar P-ring protein





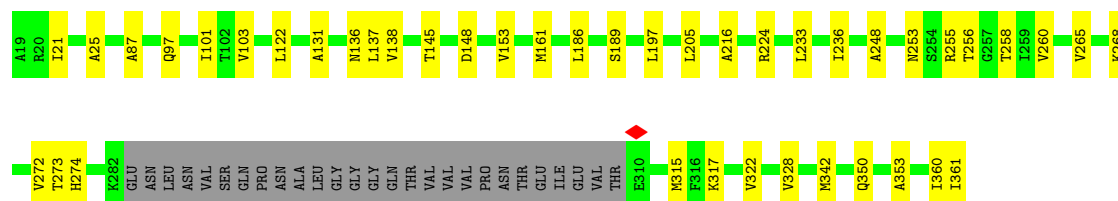
• Molecule 2: Flagellar P-ring protein

Chain Bn: 79% 13% 8%



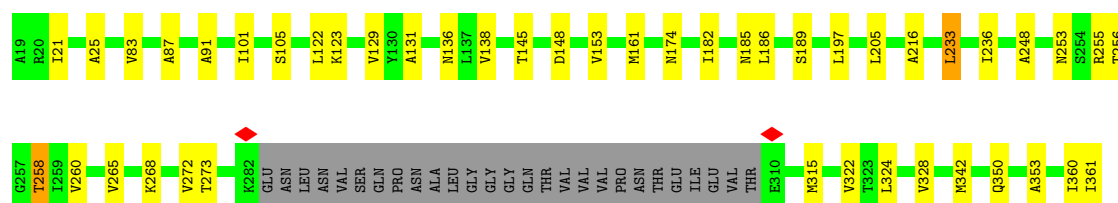
• Molecule 2: Flagellar P-ring protein

Chain Bo: 80% 13% 8%



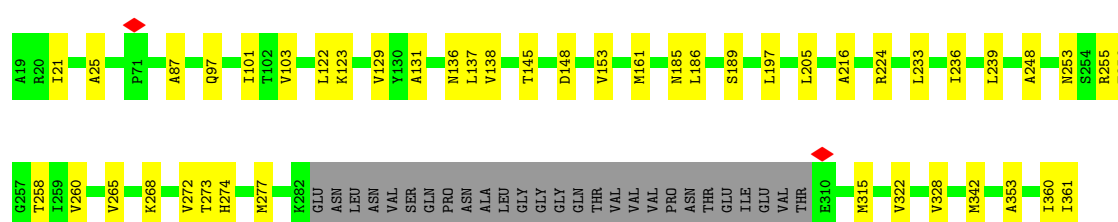
• Molecule 2: Flagellar P-ring protein

Chain Bp: 79% 13% 8%

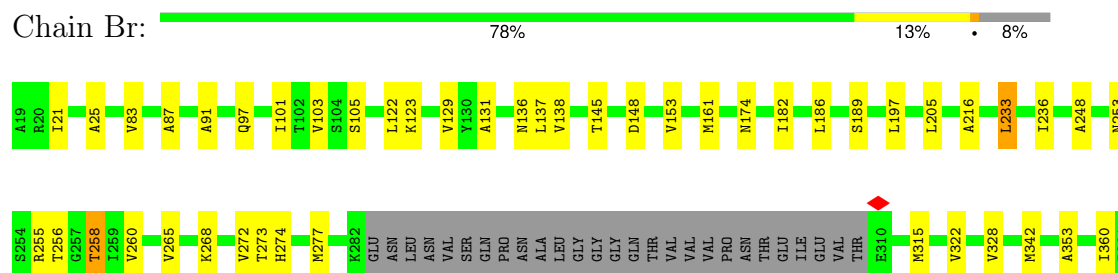


• Molecule 2: Flagellar P-ring protein

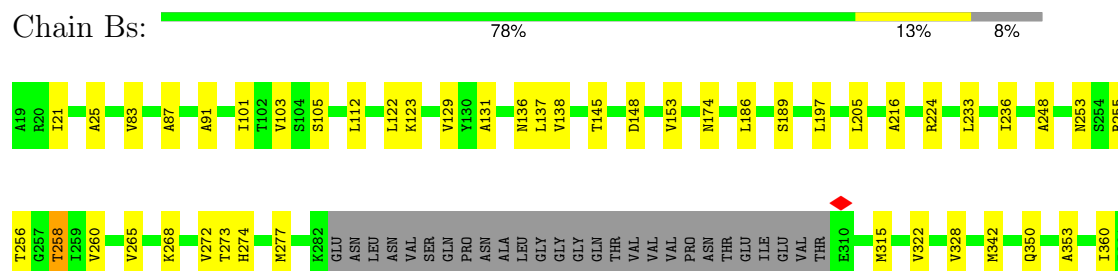
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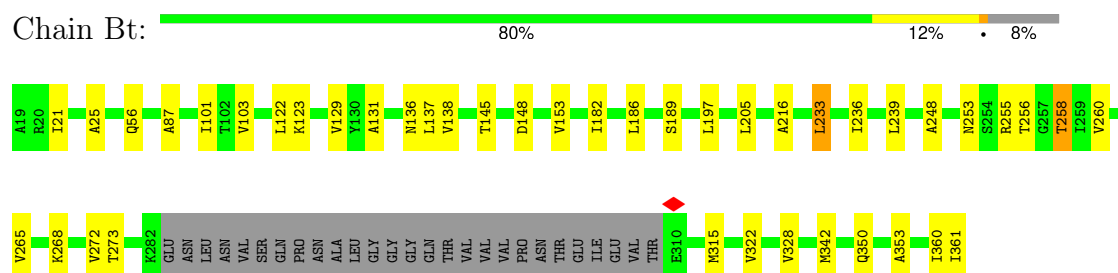
## • Molecule 2: Flagellar P-ring protein



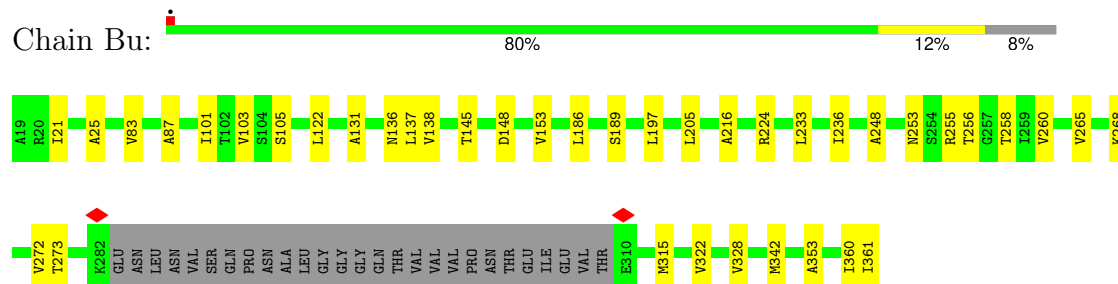
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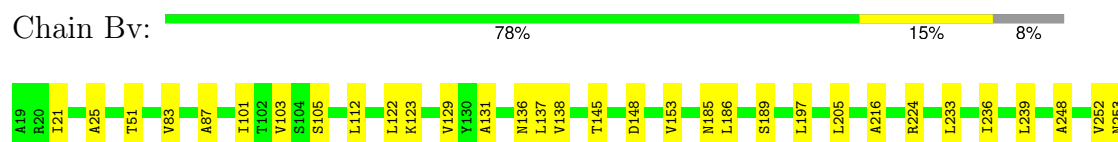
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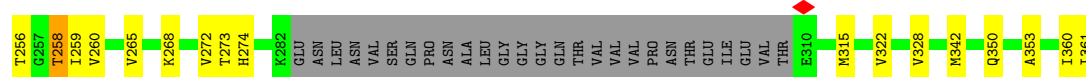
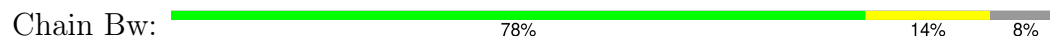
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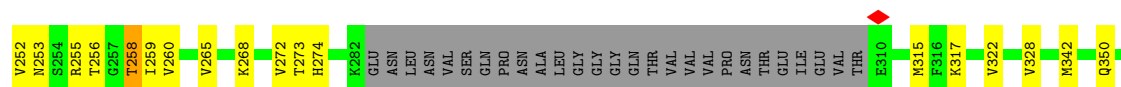
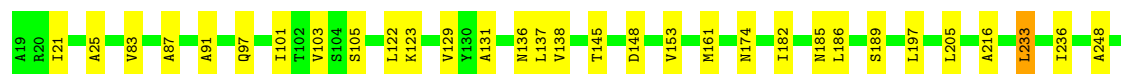
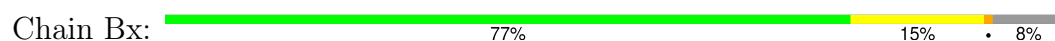
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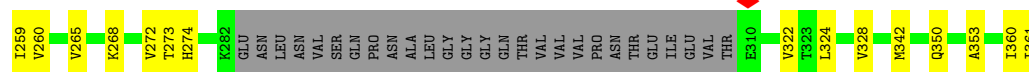
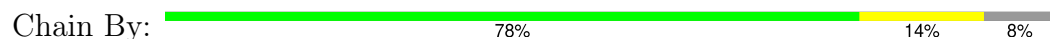
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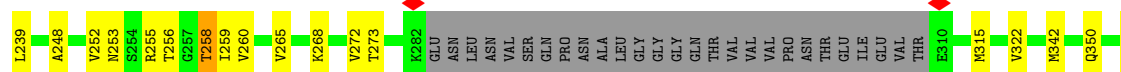
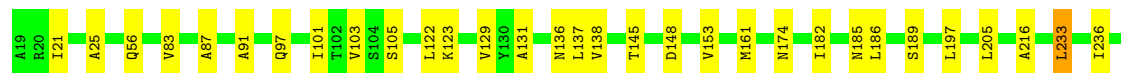
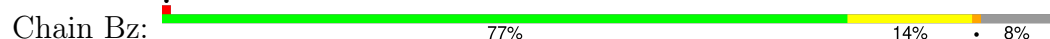
- Molecule 2: Flagellar P-ring protein



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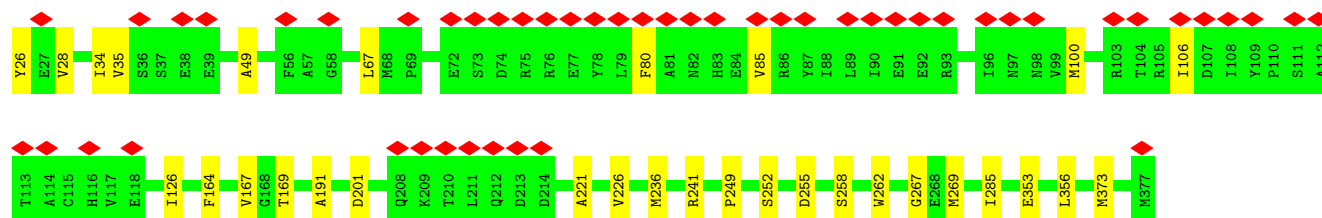


- Molecule 2: Flagellar P-ring protein

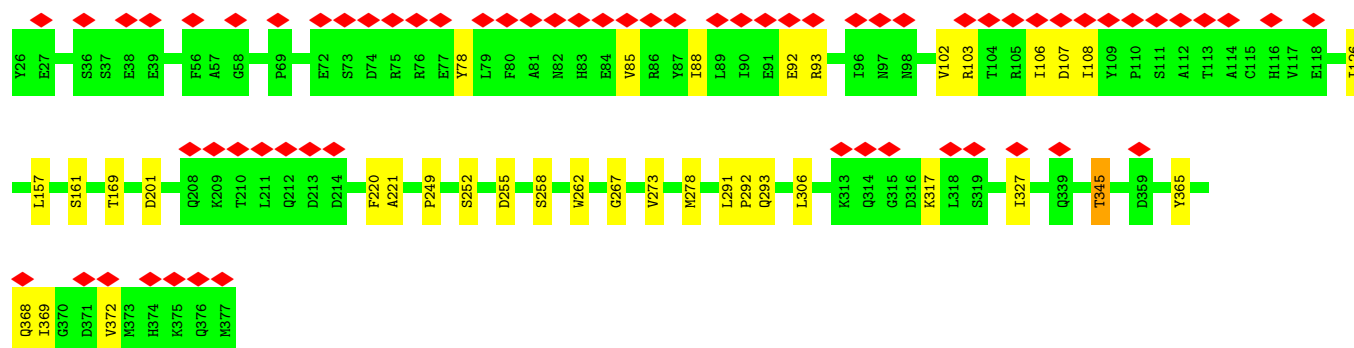
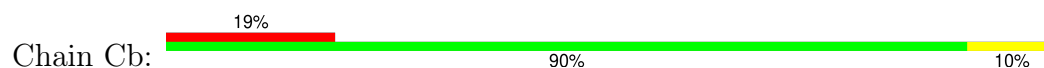




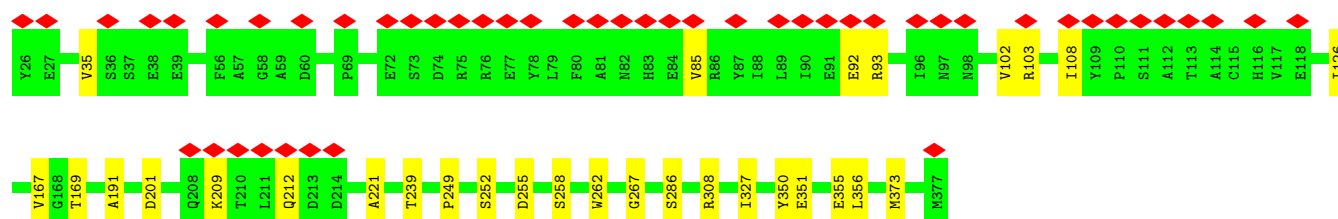
## • Molecule 3: Flagellar protein FlgT



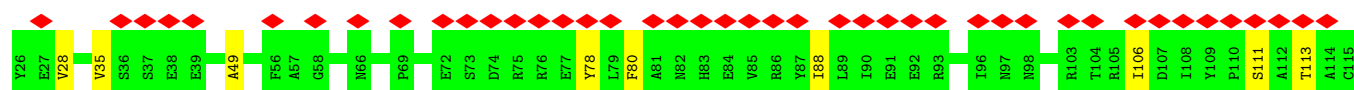
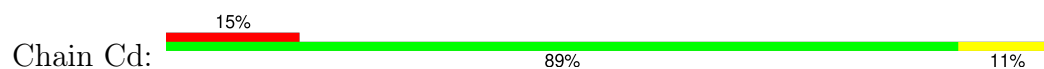
## • Molecule 3: Flagellar protein FlgT

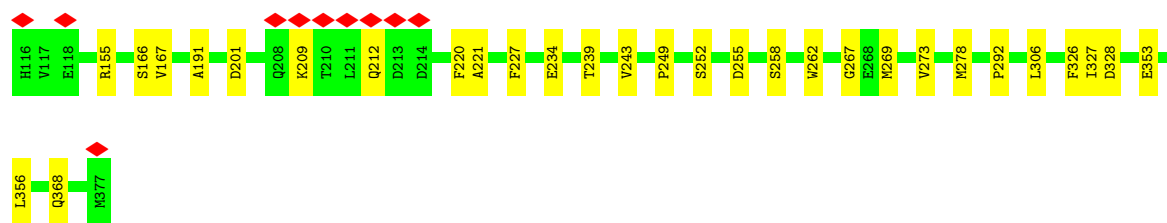


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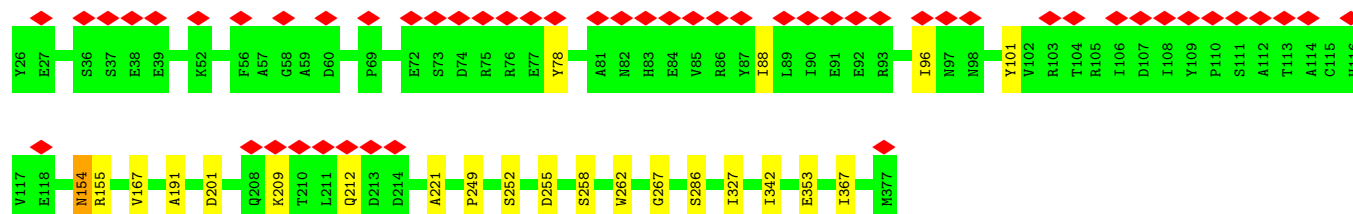


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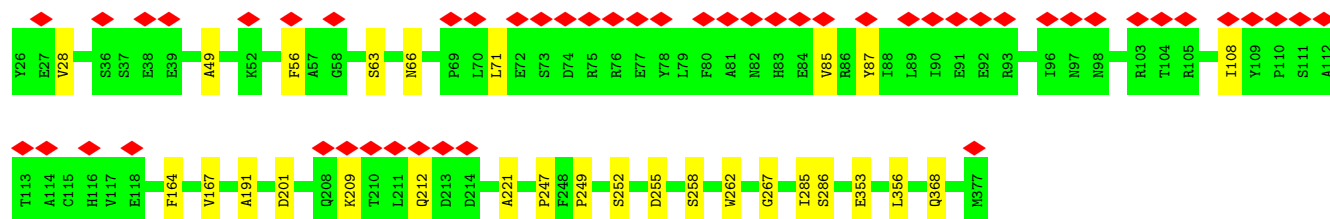




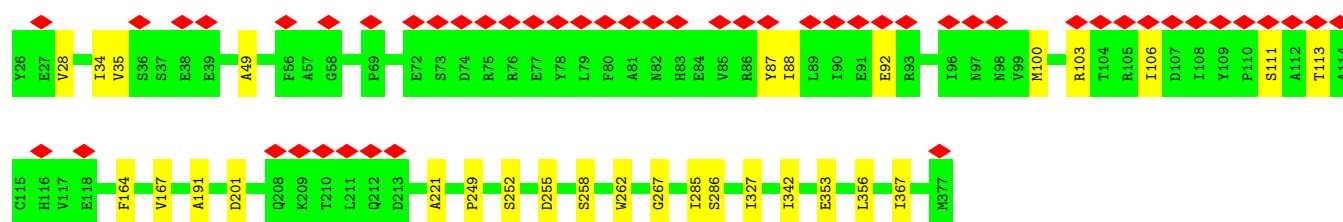
• Molecule 3: Flagellar protein FlgT



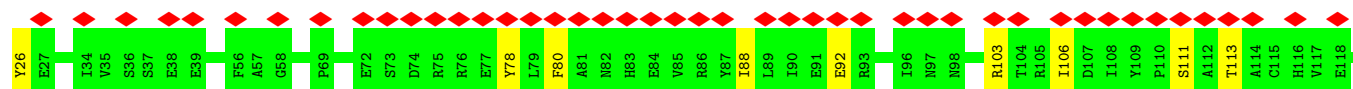
• Molecule 3: Flagellar protein FlgT



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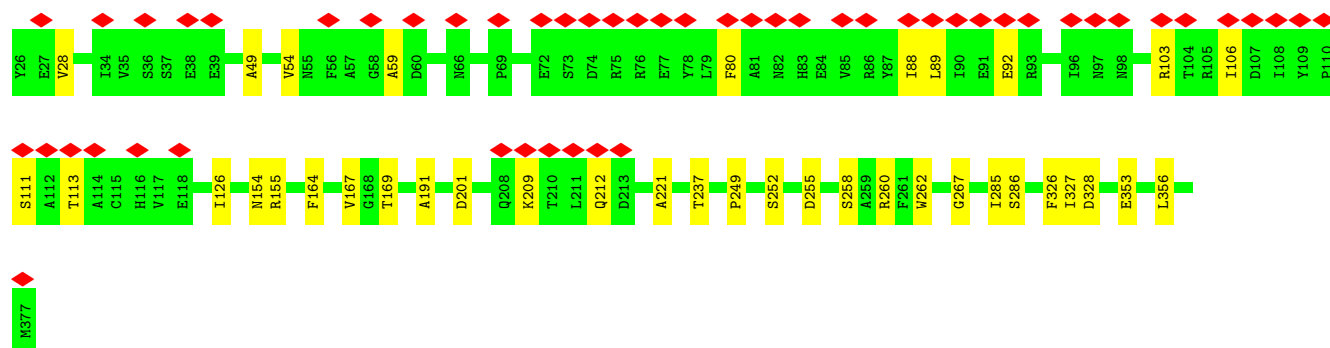
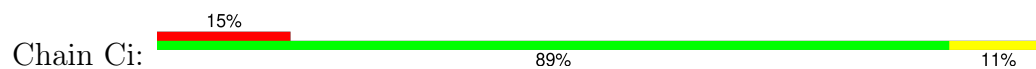


• Molecule 3: Flagellar protein FlgT

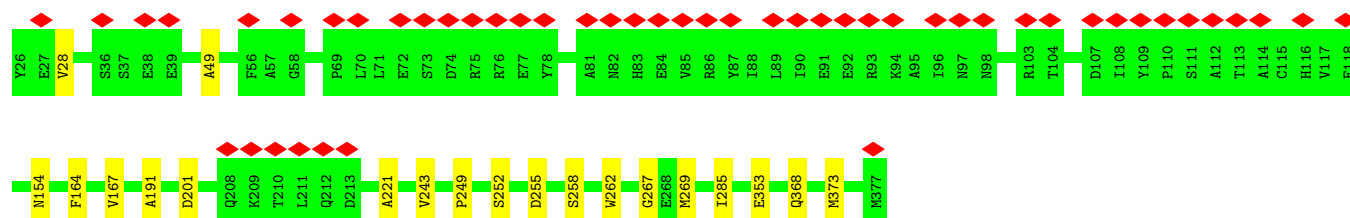




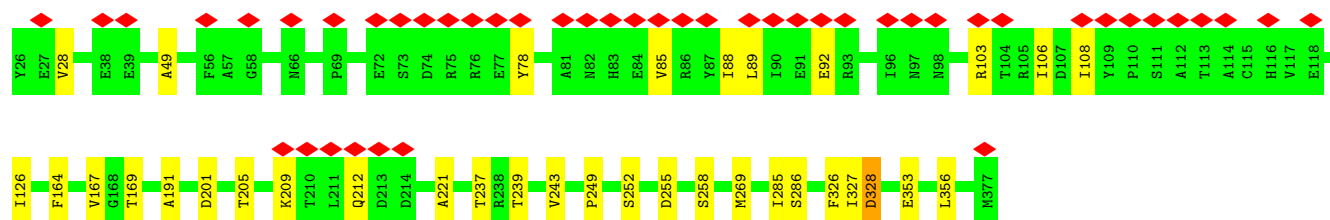
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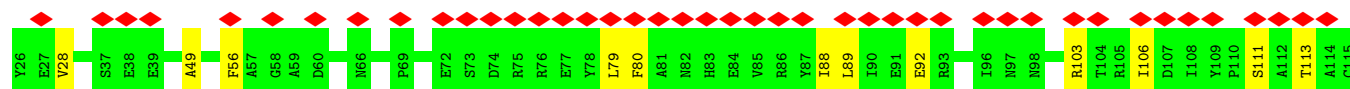
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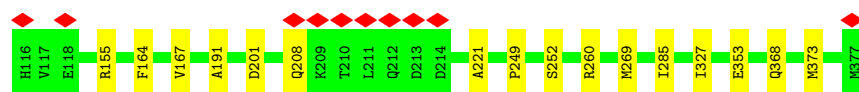
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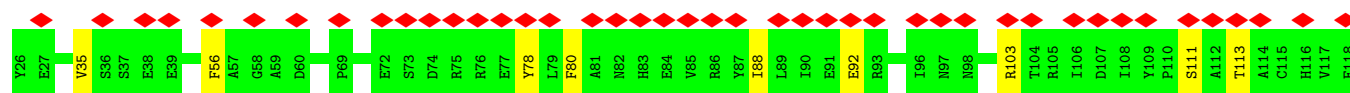
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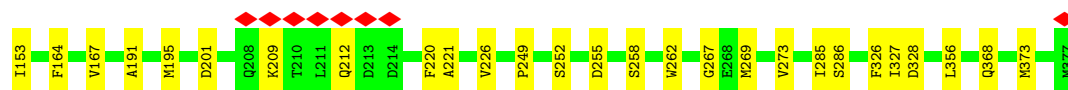




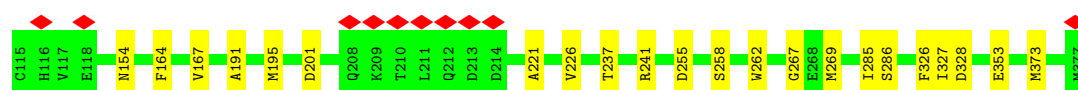
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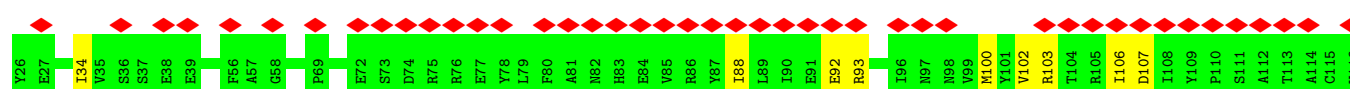
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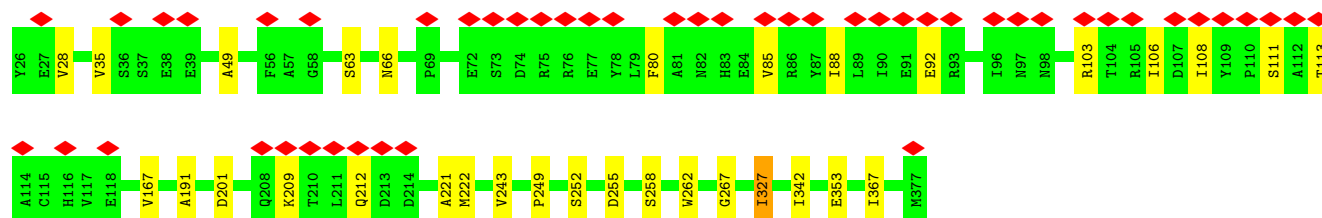
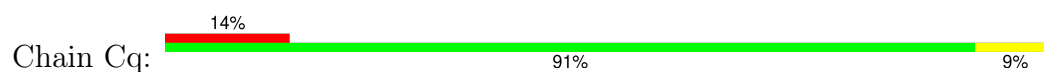
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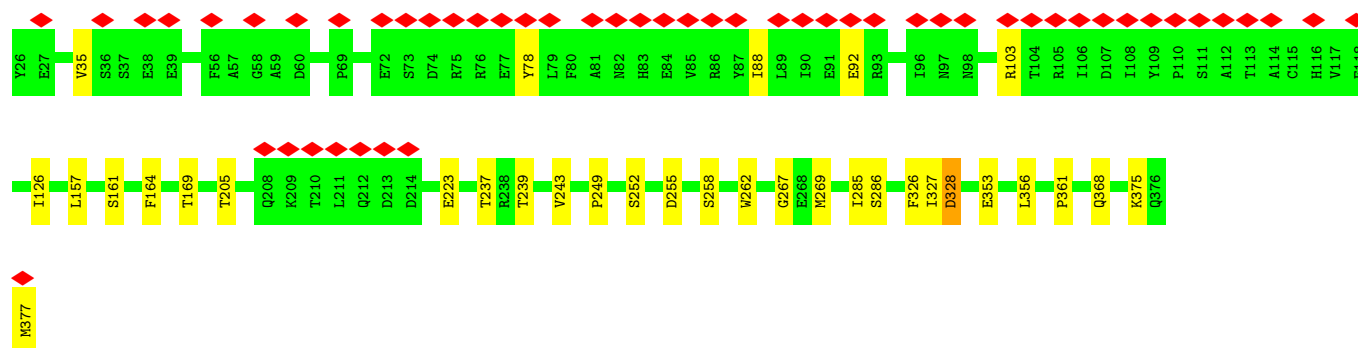
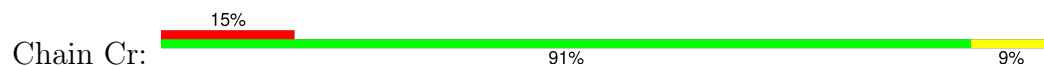
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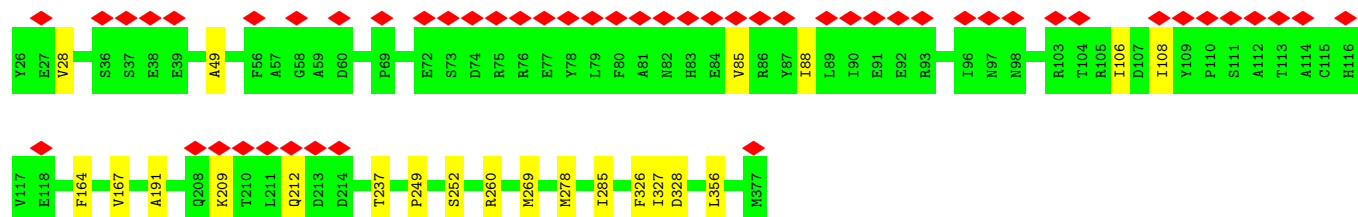
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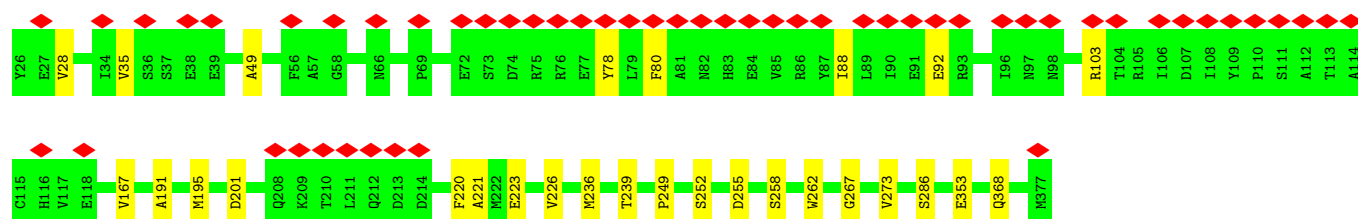
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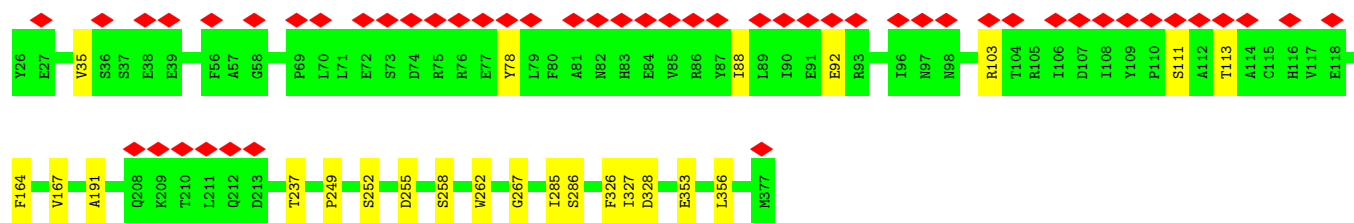


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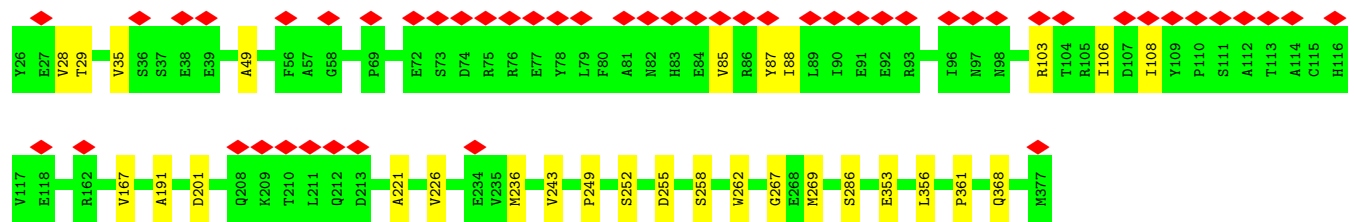


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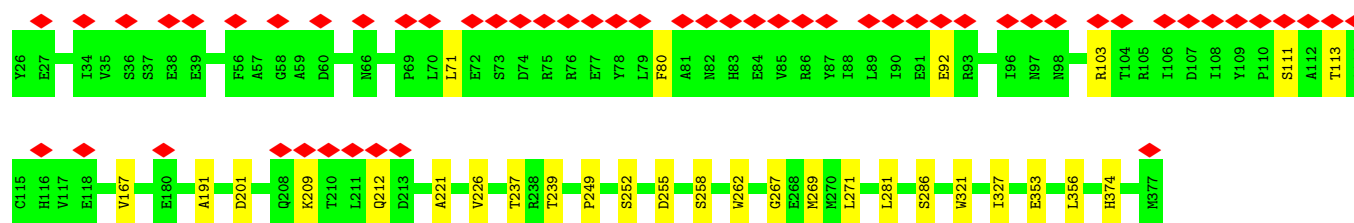




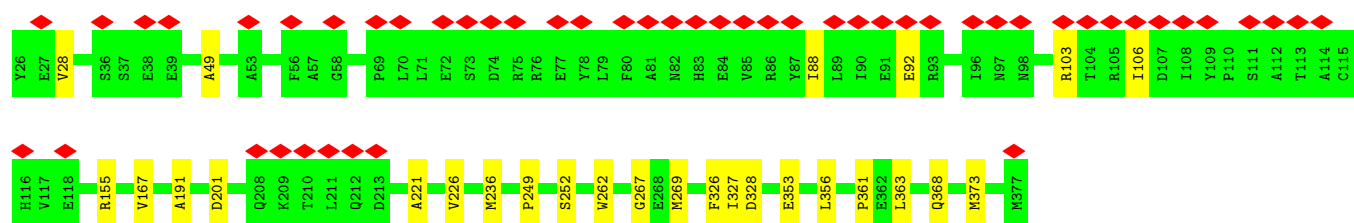
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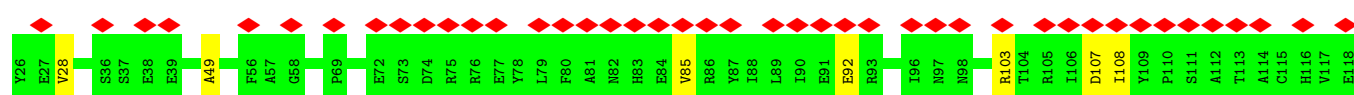
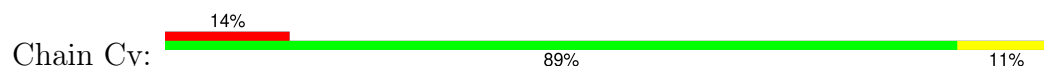
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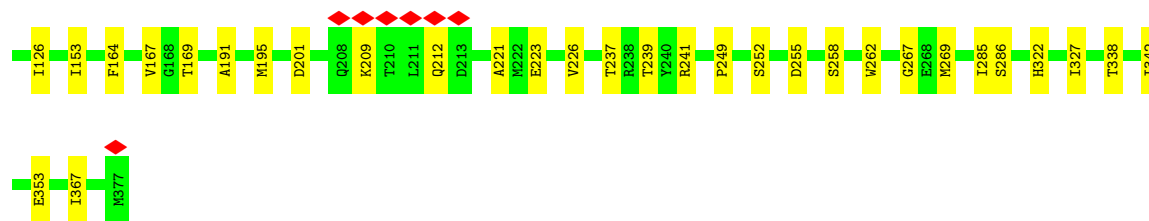


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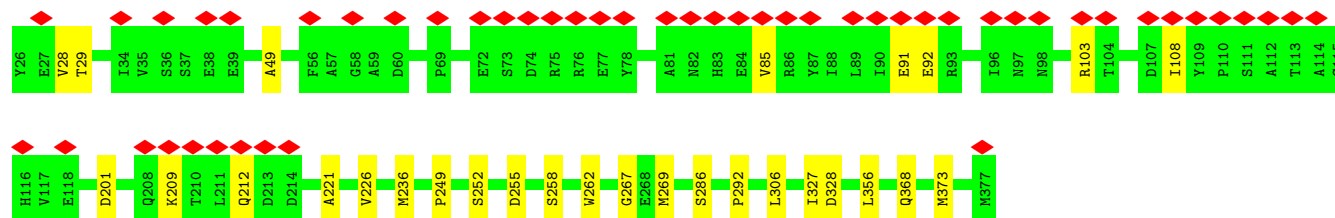
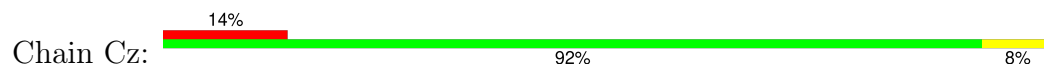


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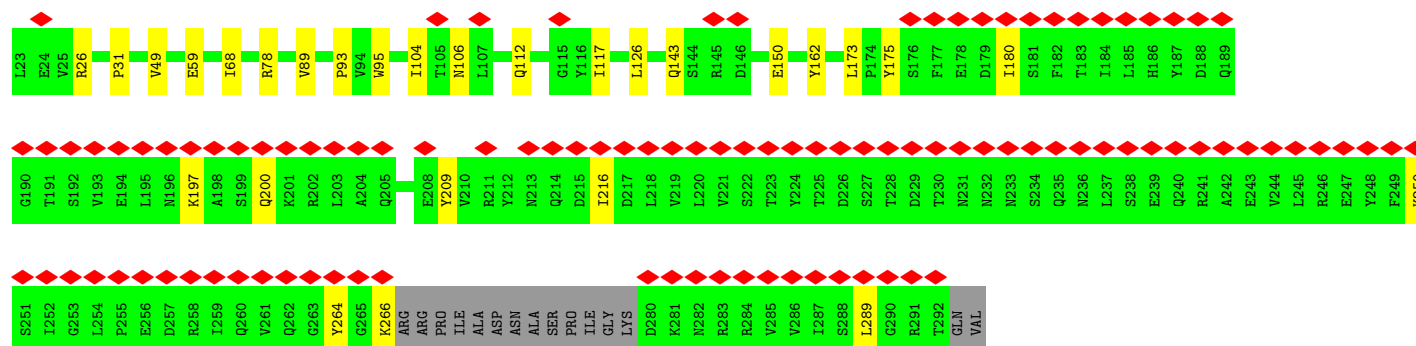
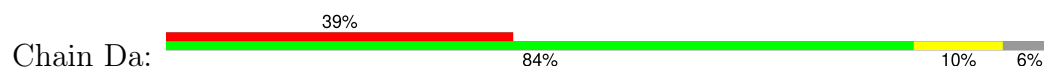




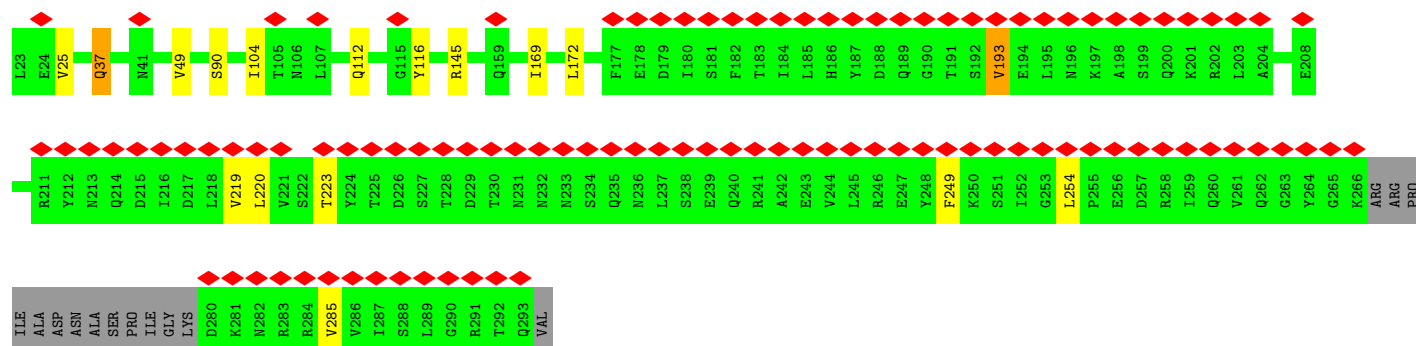
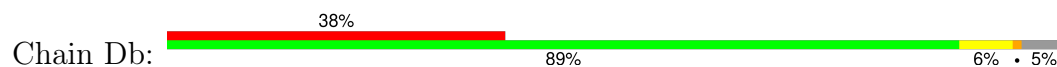
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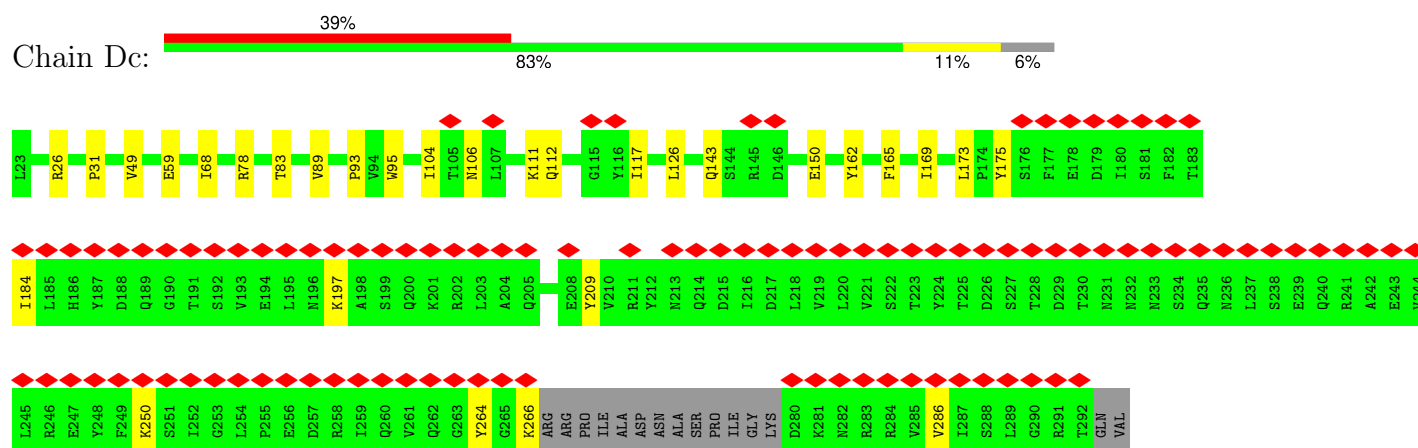
• Molecule 4: Sodium-type flagellar protein MotY



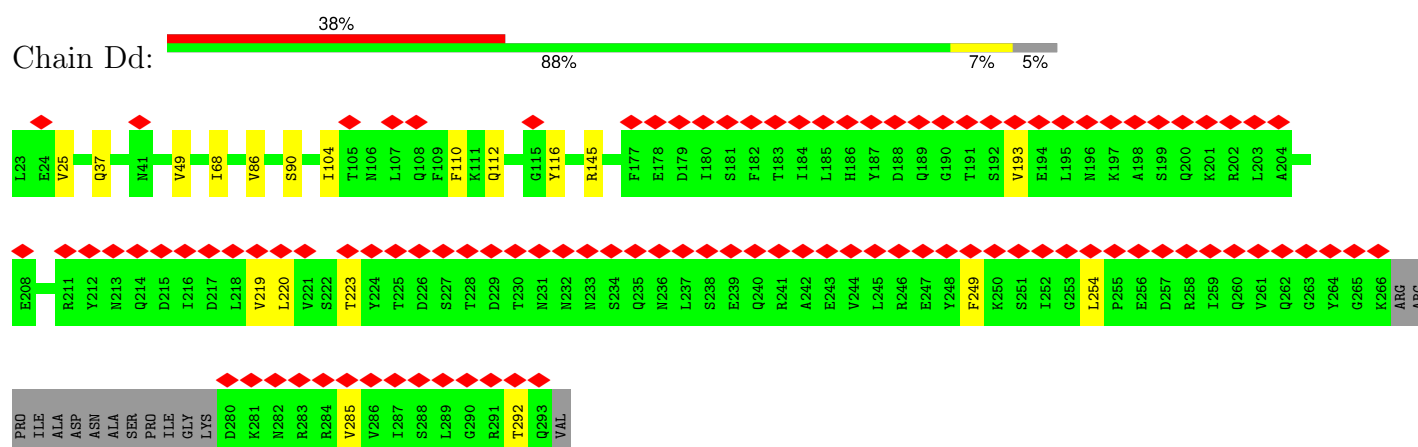
• Molecule 4: Sodium-type flagellar protein MotY



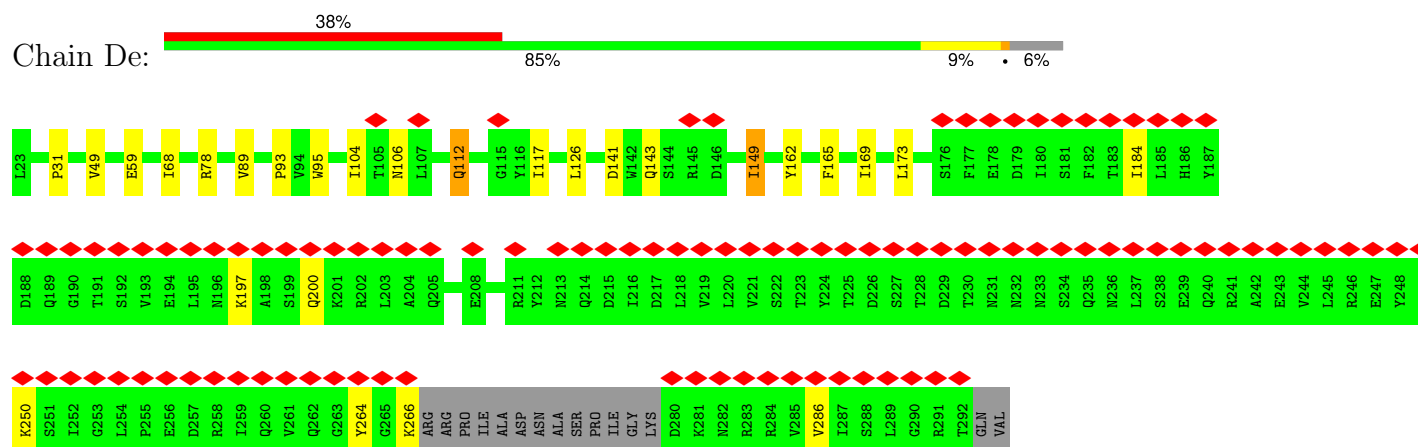
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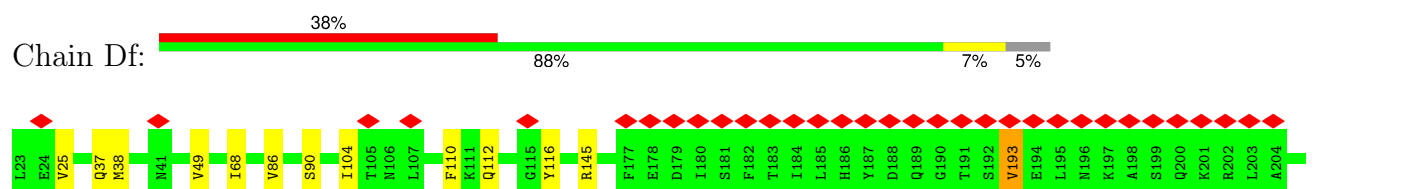
- Molecule 4: Sodium-type flagellar protein MotY

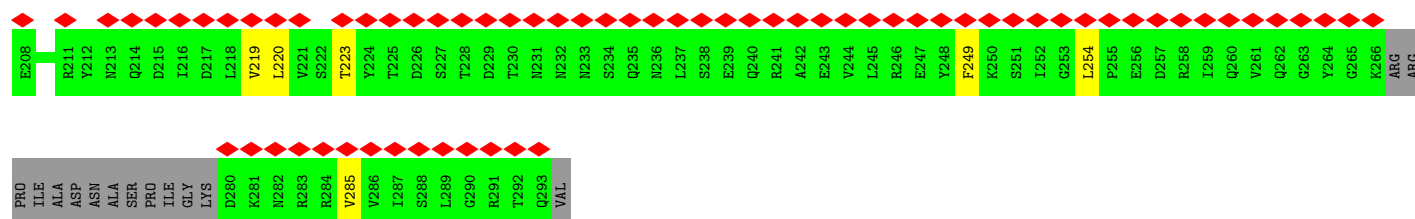


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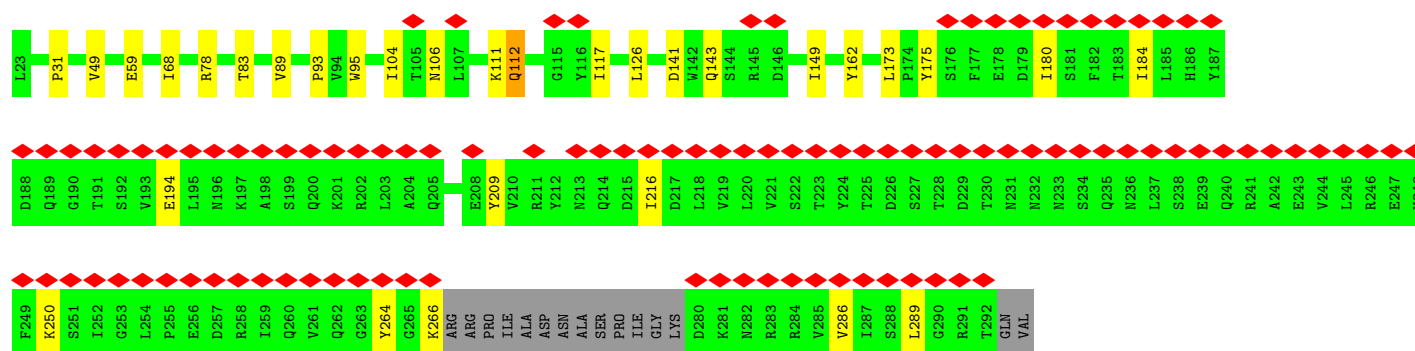
- Molecule 4: Sodium-type flagellar protein MotY





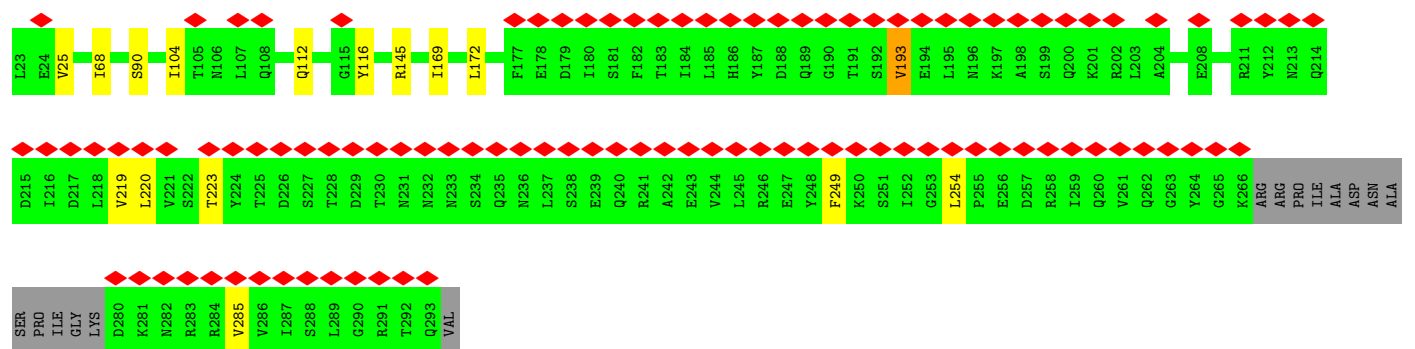
• Molecule 4: Sodium-type flagellar protein MotY

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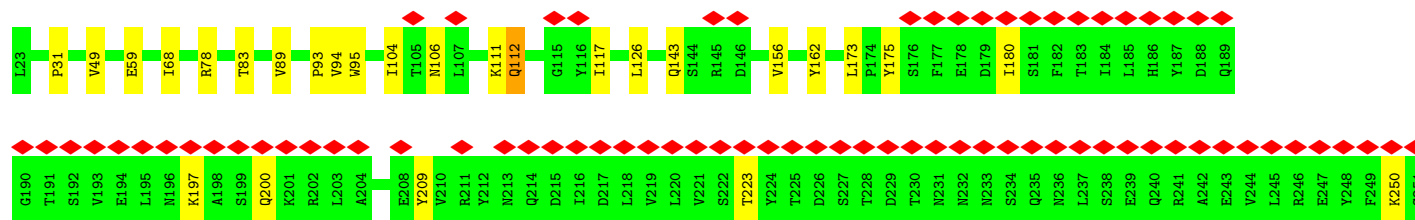
• Molecule 4: Sodium-type flagellar protein MotY

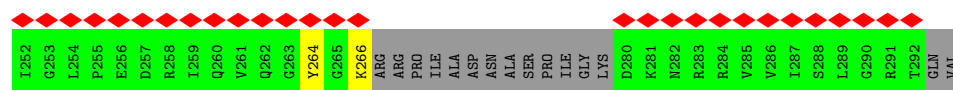
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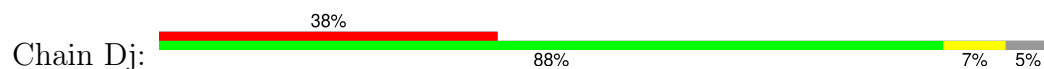
• Molecule 4: Sodium-type flagellar protein MotY

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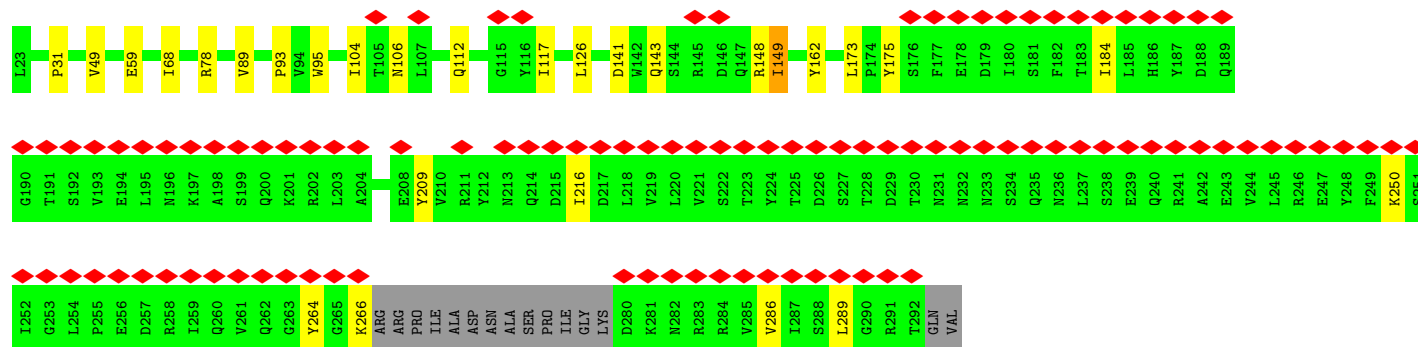
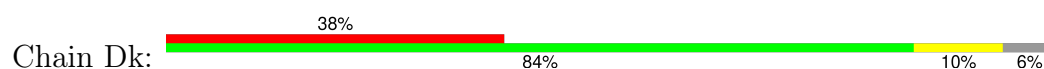




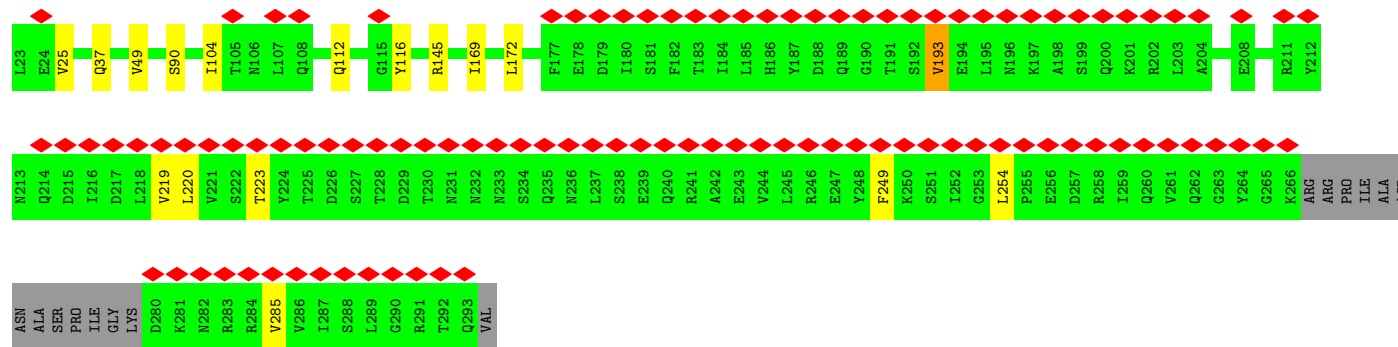
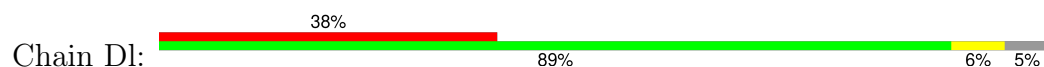
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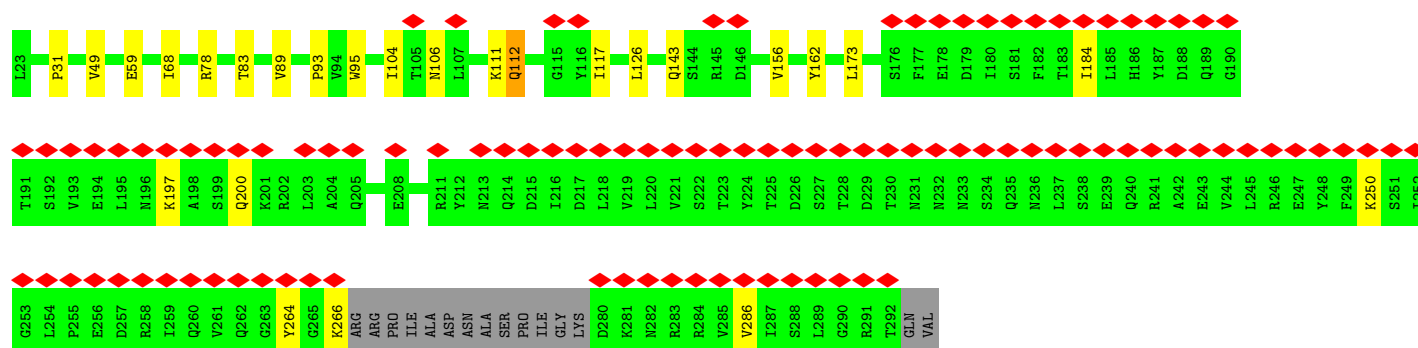


• Molecule 4: Sodium-type flagellar protein MotY




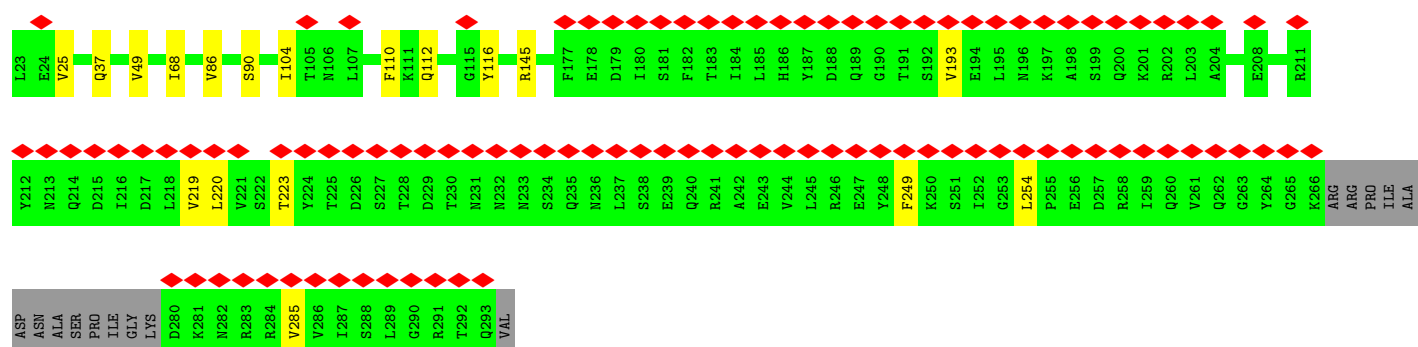
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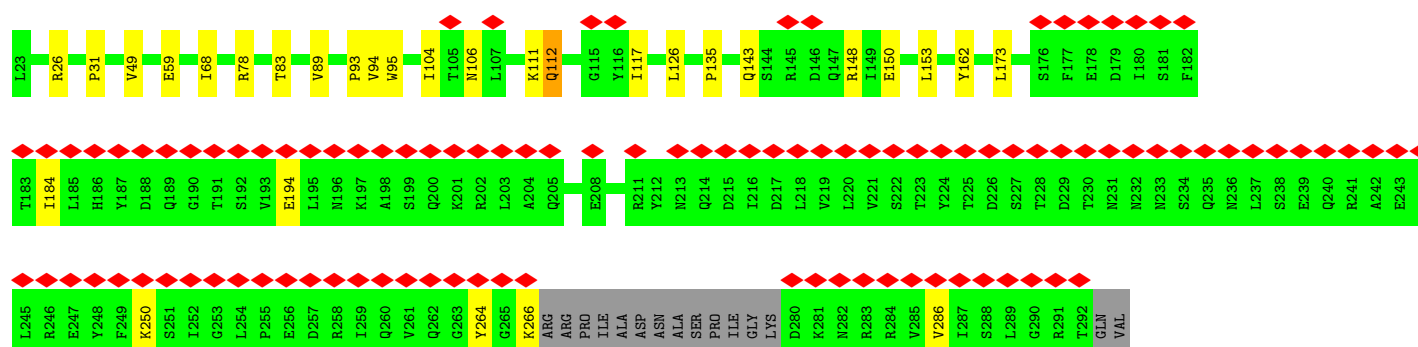
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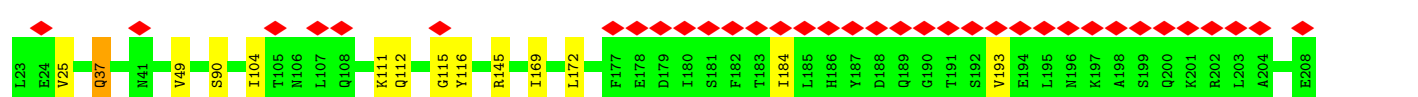
• Molecule 4: Sodium-type flagellar protein MotY

Chain Do: 



• Molecule 4: Sodium-type flagellar protein MotY

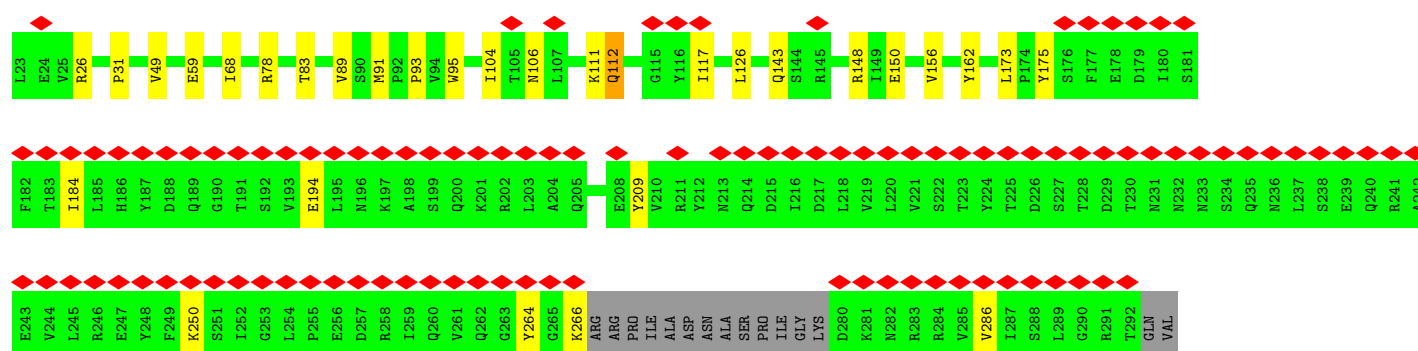
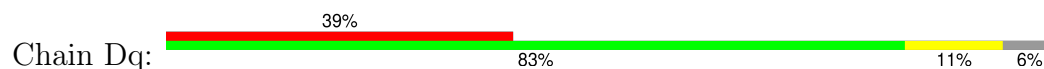
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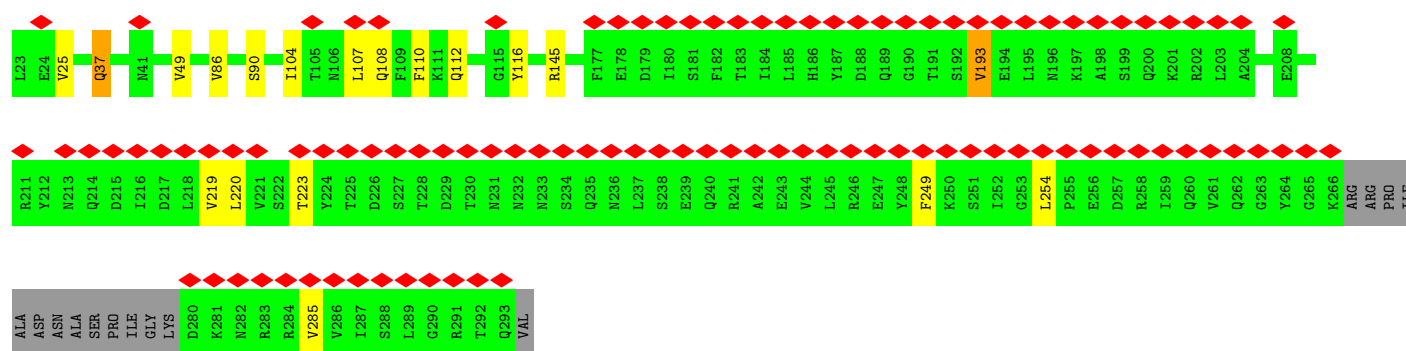
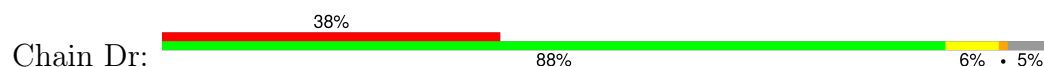




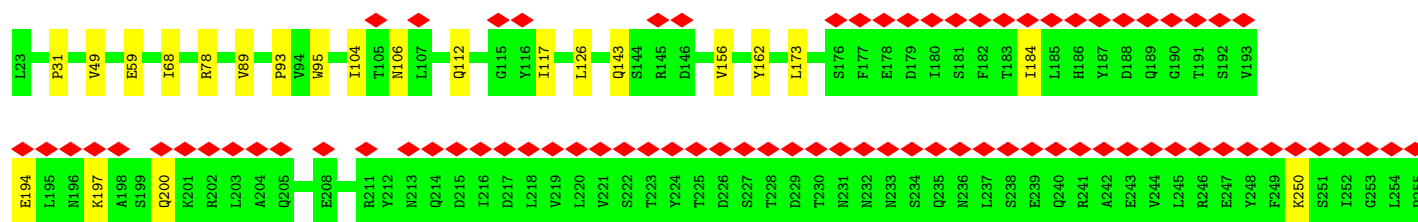
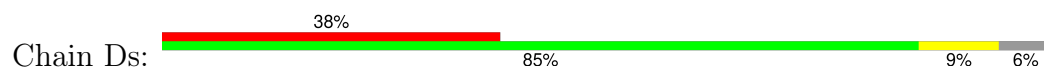
• Molecule 4: Sodium-type flagellar protein MotY

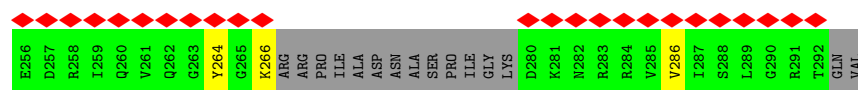


• Molecule 4: Sodium-type flagellar protein MotY

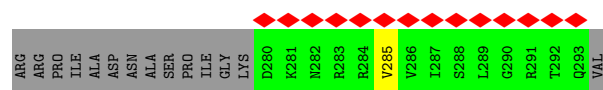
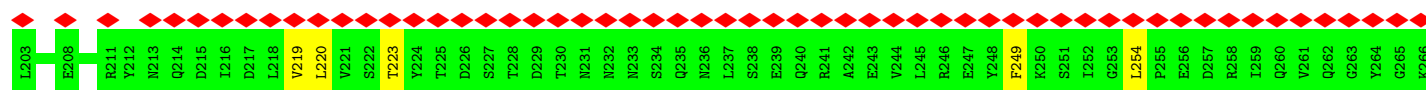
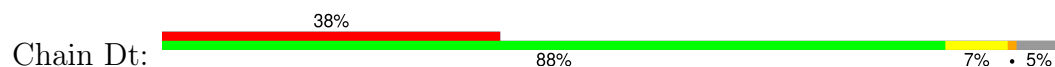


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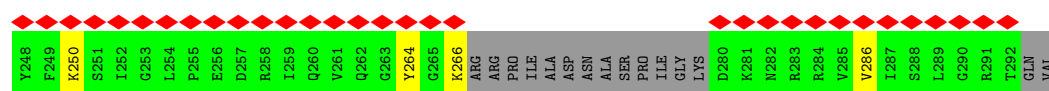
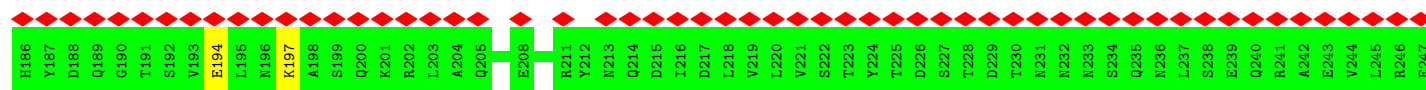
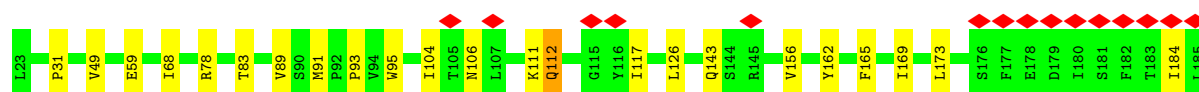
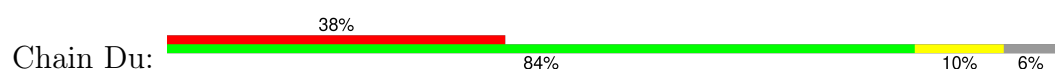




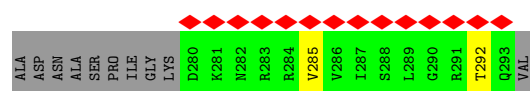
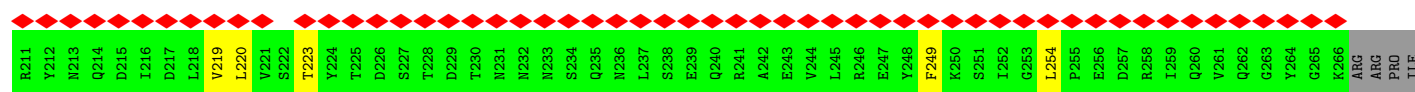
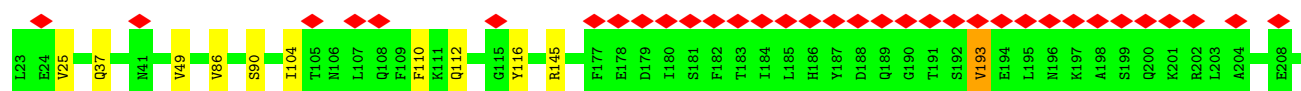
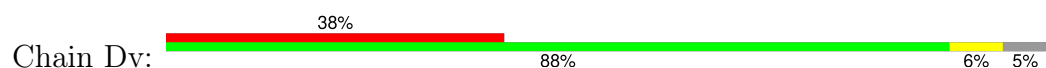
• Molecule 4: Sodium-type flagellar protein MotY




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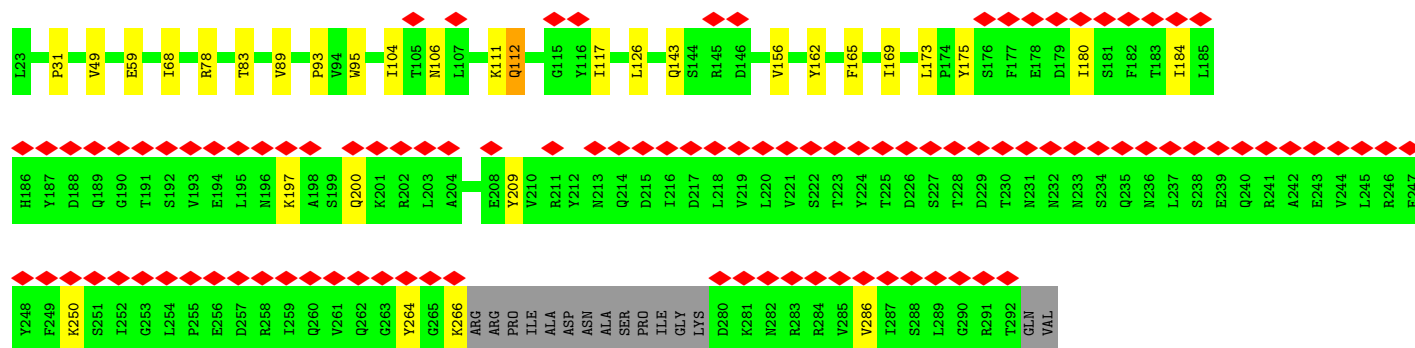


• Molecule 4: Sodium-type flagellar protein MotY




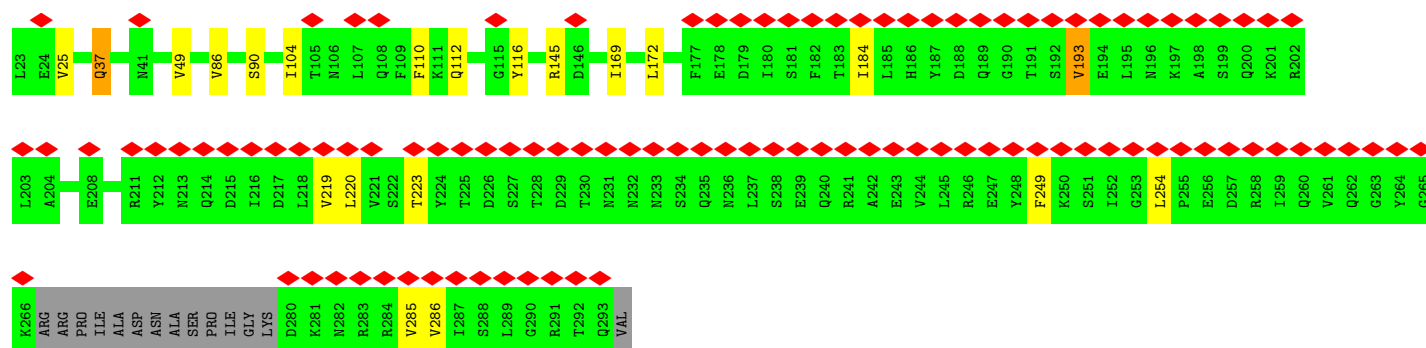
• Molecule 4: Sodium-type flagellar protein MotY

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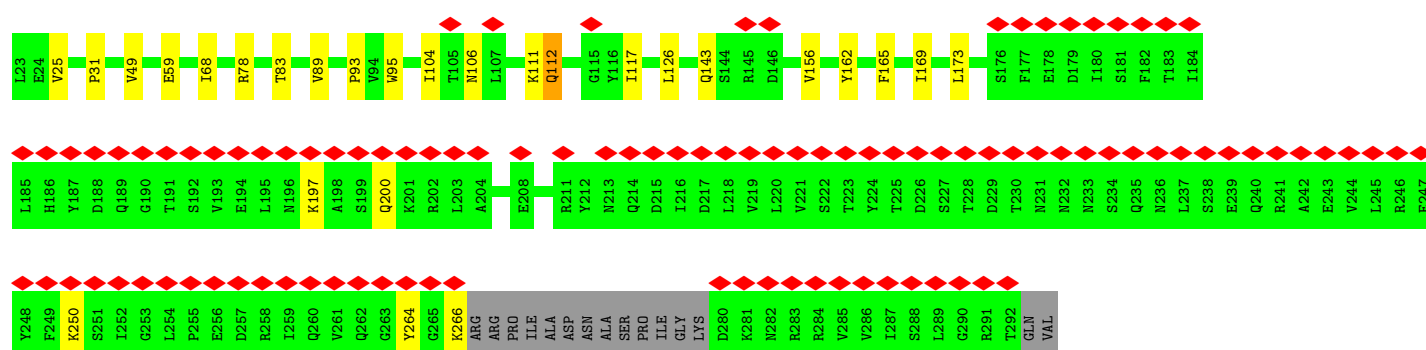
• Molecule 4: Sodium-type flagellar protein MotY

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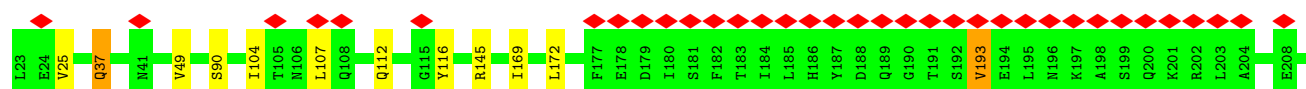
• Molecule 4: Sodium-type flagellar protein MotY

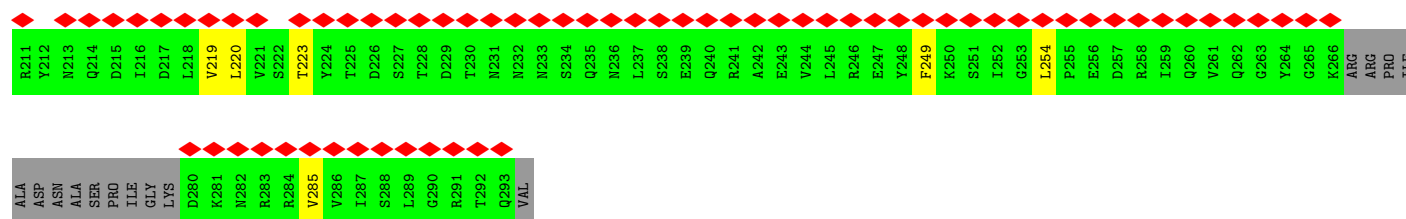
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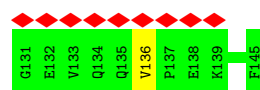
• Molecule 4: Sodium-type flagellar protein MotY

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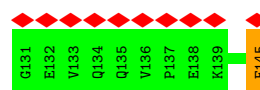




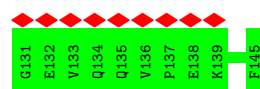
• Molecule 5: Flagellar assembly lipoprotein FlgP



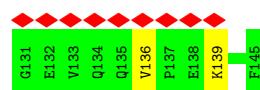
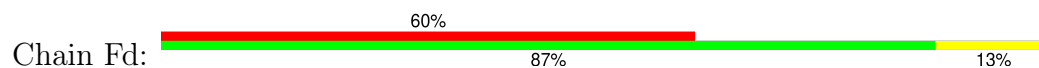
• Molecule 5: Flagellar assembly lipoprotein FlgP



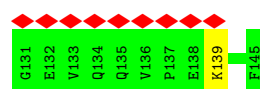
• Molecule 5: Flagellar assembly lipoprotein FlgP



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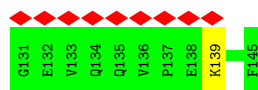


• Molecule 5: Flagellar assembly lipoprotein FlgP

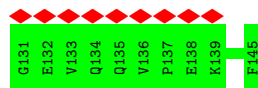


• Molecule 5: Flagellar assembly lipoprotein FlgP

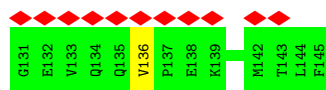
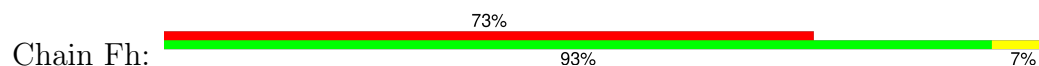




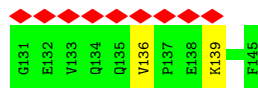
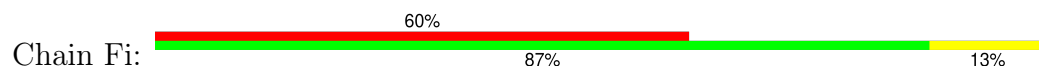
- Molecule 5: Flagellar assembly lipoprotein FlgP



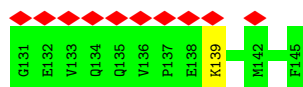
- Molecule 5: Flagellar assembly lipoprotein FlgP



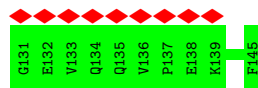
- Molecule 5: Flagellar assembly lipoprotein FlgP



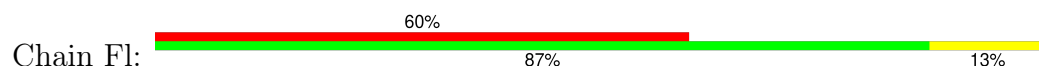
- Molecule 5: Flagellar assembly lipoprotein FlgP



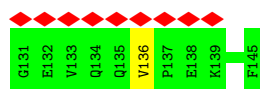
- Molecule 5: Flagellar assembly lipoprotein FlgP



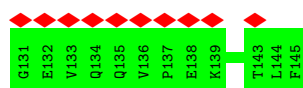
- Molecule 5: Flagellar assembly lipoprotein FlgP



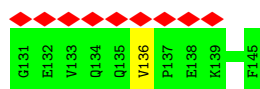
- Molecule 5: Flagellar assembly lipoprotein FlgP



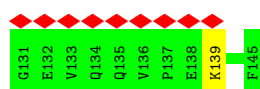
- Molecule 5: Flagellar assembly lipoprotein FlgP



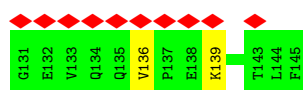
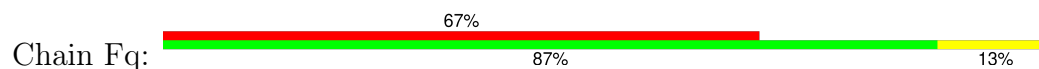
- Molecule 5: Flagellar assembly lipoprotein FlgP



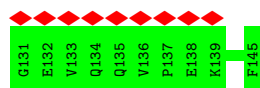
- Molecule 5: Flagellar assembly lipoprotein FlgP



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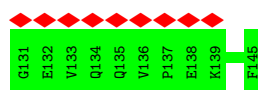


- Molecule 5: Flagellar assembly lipoprotein FlgP

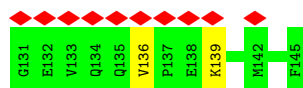
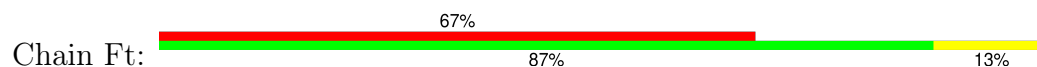


- Molecule 5: Flagellar assembly lipoprotein FlgP

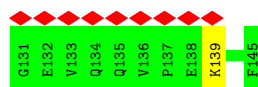




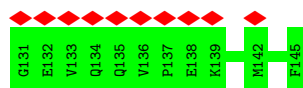
- Molecule 5: Flagellar assembly lipoprotein FlgP



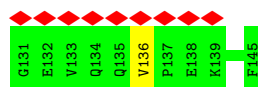
- Molecule 5: Flagellar assembly lipoprotein FlgP



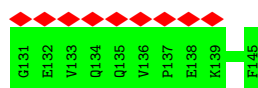
- Molecule 5: Flagellar assembly lipoprotein FlgP



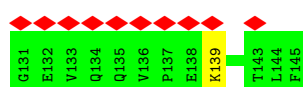
- Molecule 5: Flagellar assembly lipoprotein FlgP



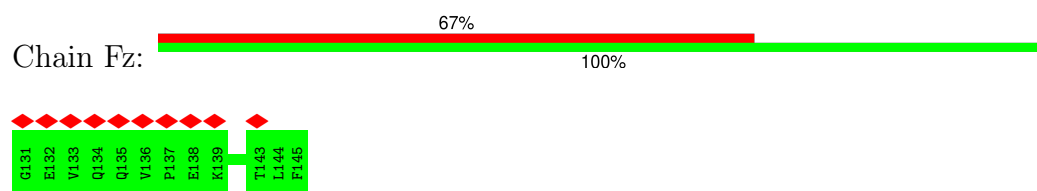
- Molecule 5: Flagellar assembly lipoprotein FlgP



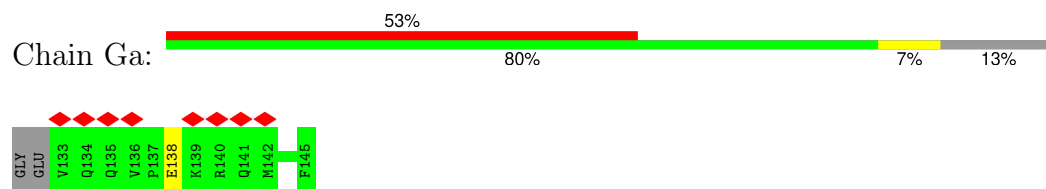
- Molecule 5: Flagellar assembly lipoprotein FlgP



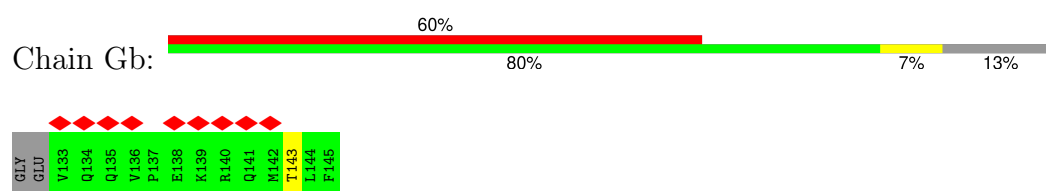
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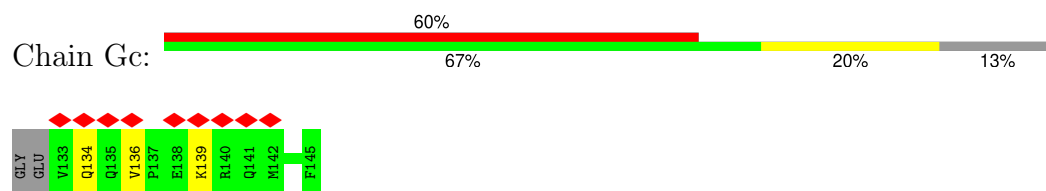
- Molecule 5: Flagellar assembly lipoprotein FlgP



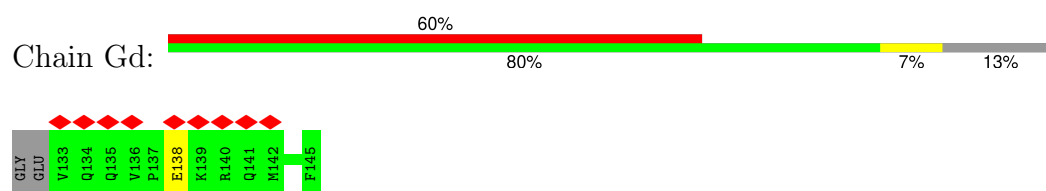
- Molecule 5: Flagellar assembly lipoprotein FlgP



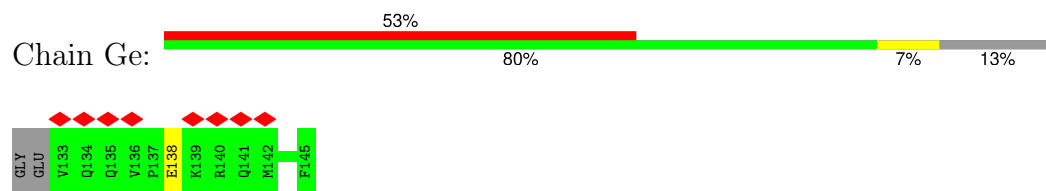
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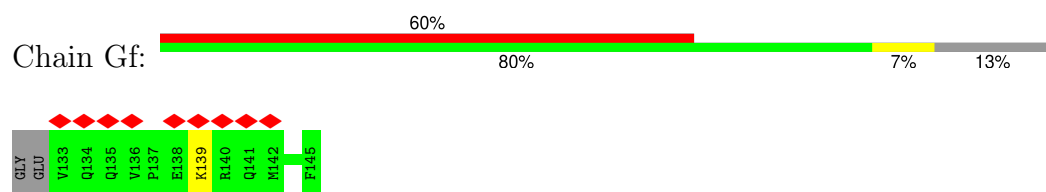
- Molecule 5: Flagellar assembly lipoprotein FlgP



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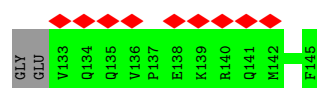
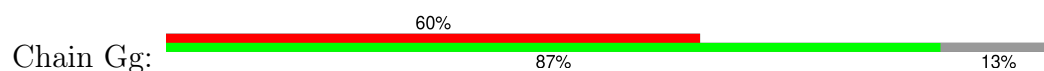


- Molecule 5: Flagellar assembly lipoprotein FlgP

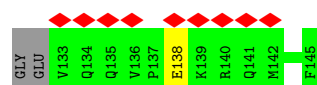
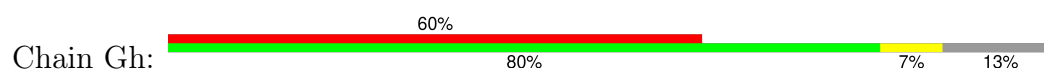




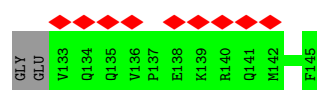
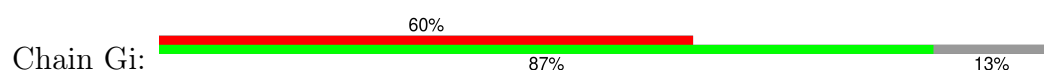
## ● Molecule 5: Flagellar assembly lipoprotein FlgP



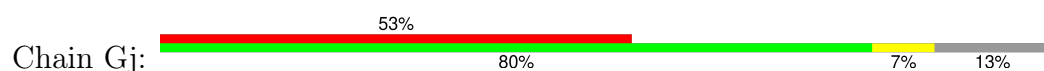
## ● Molecule 5: Flagellar assembly lipoprotein FlgP



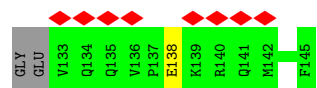
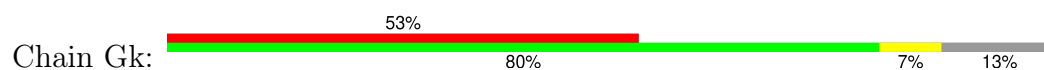
## ● Molecule 5: Flagellar assembly lipoprotein FlgP



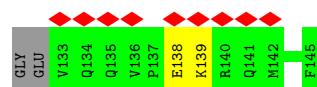
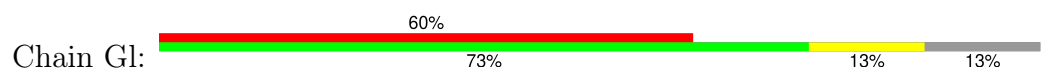
## ● Molecule 5: Flagellar assembly lipoprotein FlgP



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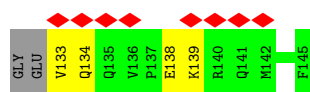


## ● Molecule 5: Flagellar assembly lipoprotein FlgP

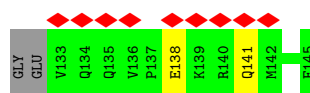
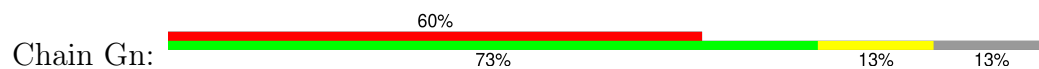


## ● Molecule 5: Flagellar assembly lipoprotein FlgP

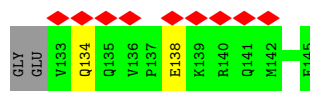
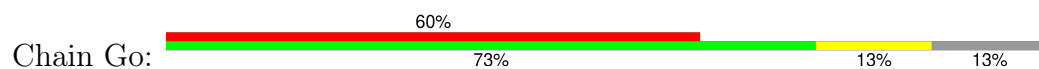




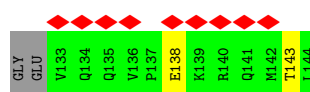
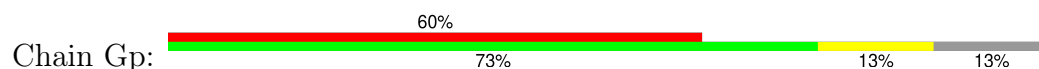
- Molecule 5: Flagellar assembly lipoprotein FlgP



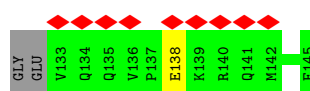
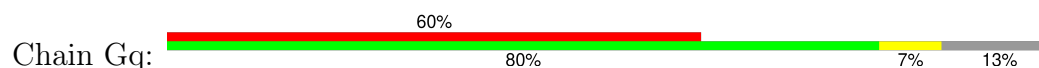
- Molecule 5: Flagellar assembly lipoprotein FlgP



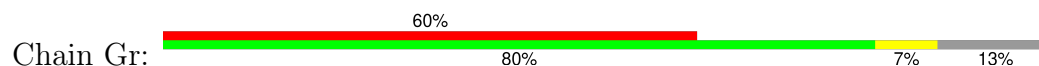
- Molecule 5: Flagellar assembly lipoprotein FlgP



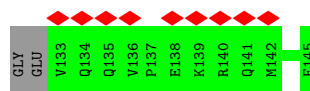
- Molecule 5: Flagellar assembly lipoprotein FlgP



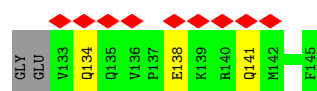
- Molecule 5: Flagellar assembly lipoprotein FlgP



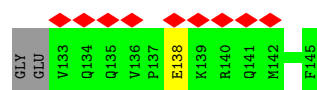
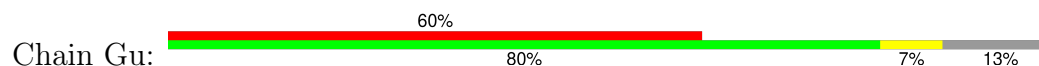
- Molecule 5: Flagellar assembly lipoprotein FlgP



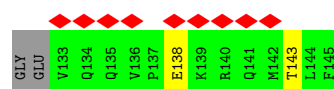
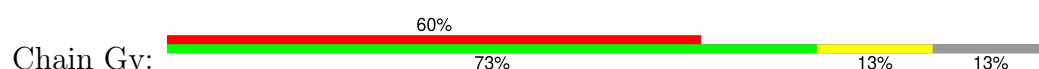
- Molecule 5: Flagellar assembly lipoprotein FlgP



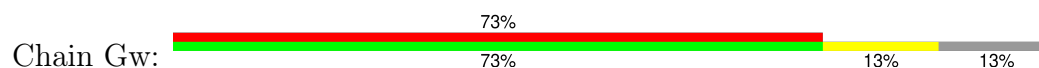
• Molecule 5: Flagellar assembly lipoprotein FlgP



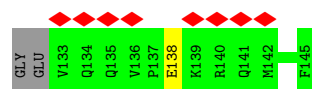
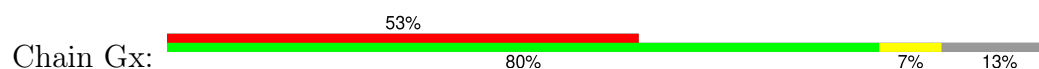
• Molecule 5: Flagellar assembly lipoprotein FlgP



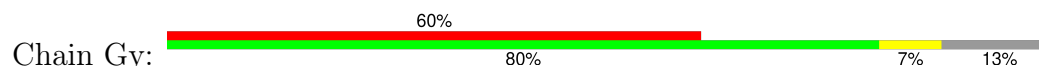
• Molecule 5: Flagellar assembly lipoprotein FlgP



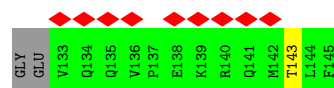
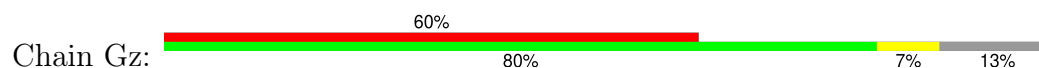
• Molecule 5: Flagellar assembly lipoprotein FlgP



• Molecule 5: Flagellar assembly lipoprotein FlgP



• 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	112879	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	1.250	Depositor
Minimum map value	-0.672	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.15	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	0.28	0/2303
1	Ab	0.11	0/1699	0.28	0/2303
1	Ac	0.12	0/1699	0.28	0/2303
1	Ad	0.11	0/1699	0.28	0/2303
1	Ae	0.11	0/1699	0.28	0/2303
1	Af	0.11	0/1699	0.28	0/2303
1	Ag	0.12	0/1699	0.28	0/2303
1	Ah	0.11	0/1699	0.28	0/2303
1	Ai	0.11	0/1699	0.28	0/2303
1	Aj	0.12	0/1699	0.28	0/2303
1	Ak	0.12	0/1699	0.28	0/2303
1	Al	0.12	0/1699	0.28	0/2303
1	Am	0.12	0/1699	0.28	0/2303
1	An	0.11	0/1699	0.28	0/2303
1	Ao	0.11	0/1699	0.28	0/2303
1	Ap	0.11	0/1699	0.28	0/2303
1	Aq	0.11	0/1699	0.28	0/2303
1	Ar	0.12	0/1699	0.29	0/2303
1	As	0.11	0/1699	0.28	0/2303
1	At	0.11	0/1699	0.29	0/2303
1	Au	0.12	0/1699	0.28	0/2303
1	Av	0.11	0/1699	0.28	0/2303
1	Aw	0.11	0/1699	0.28	0/2303
1	Ax	0.12	0/1699	0.28	0/2303
1	Ay	0.12	0/1699	0.28	0/2303
1	Az	0.11	0/1699	0.29	0/2303
2	Ba	0.12	0/2345	0.32	0/3177
2	Bb	0.12	0/2345	0.32	0/3177
2	Bc	0.12	0/2345	0.32	0/3177
2	Bd	0.12	0/2345	0.32	0/3177
2	Be	0.12	0/2345	0.32	0/3177
2	Bf	0.13	0/2345	0.32	0/3177
2	Bg	0.12	0/2345	0.31	0/3177
2	Bh	0.13	0/2345	0.32	0/3177

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Bi	0.13	0/2345	0.31	0/3177
2	Bj	0.12	0/2345	0.32	0/3177
2	Bk	0.13	0/2345	0.32	0/3177
2	Bl	0.13	0/2345	0.32	0/3177
2	Bm	0.13	0/2345	0.32	0/3177
2	Bn	0.13	0/2345	0.32	0/3177
2	Bo	0.12	0/2345	0.32	0/3177
2	Bp	0.13	0/2345	0.32	0/3177
2	Bq	0.12	0/2345	0.32	0/3177
2	Br	0.13	0/2345	0.32	0/3177
2	Bs	0.12	0/2345	0.32	0/3177
2	Bt	0.13	0/2345	0.32	0/3177
2	Bu	0.12	0/2345	0.32	0/3177
2	Bv	0.12	0/2345	0.32	0/3177
2	Bw	0.12	0/2345	0.32	0/3177
2	Bx	0.12	0/2345	0.32	0/3177
2	By	0.12	0/2345	0.32	0/3177
2	Bz	0.13	0/2345	0.32	0/3177
3	Ca	0.12	0/2816	0.30	0/3809
3	Cb	0.12	0/2816	0.32	0/3809
3	Cc	0.12	0/2816	0.30	0/3809
3	Cd	0.12	0/2816	0.31	0/3809
3	Ce	0.12	0/2816	0.31	0/3809
3	Cf	0.12	0/2816	0.30	0/3809
3	Cg	0.12	0/2816	0.30	0/3809
3	Ch	0.12	0/2816	0.30	0/3809
3	Ci	0.11	0/2816	0.31	0/3809
3	Cj	0.11	0/2816	0.29	0/3809
3	Ck	0.12	0/2816	0.30	0/3809
3	Cl	0.12	0/2816	0.32	0/3809
3	Cm	0.12	0/2816	0.30	0/3809
3	Cn	0.12	0/2816	0.29	0/3809
3	Co	0.12	0/2816	0.30	0/3809
3	Cp	0.12	0/2816	0.31	0/3809
3	Cq	0.12	0/2816	0.30	0/3809
3	Cr	0.12	0/2816	0.30	0/3809
3	Cs	0.12	0/2816	0.30	0/3809
3	Ct	0.12	0/2816	0.32	0/3809
3	Cu	0.12	0/2816	0.30	0/3809
3	Cv	0.12	0/2816	0.29	0/3809
3	Cw	0.12	0/2816	0.30	0/3809
3	Cx	0.12	0/2816	0.29	0/3809
3	Cy	0.11	0/2816	0.29	0/3809

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	Cz	0.12	0/2816	0.29	0/3809
4	Da	0.14	0/2129	0.34	0/2882
4	Db	0.14	0/2124	0.36	0/2877
4	Dc	0.14	0/2129	0.34	0/2882
4	Dd	0.14	0/2124	0.37	0/2877
4	De	0.13	0/2129	0.33	0/2882
4	Df	0.14	0/2124	0.37	0/2877
4	Dg	0.14	0/2129	0.34	0/2882
4	Dh	0.14	0/2124	0.36	0/2877
4	Di	0.14	0/2129	0.34	0/2882
4	Dj	0.13	0/2124	0.36	0/2877
4	Dk	0.14	0/2129	0.34	0/2882
4	Dl	0.14	0/2124	0.36	0/2877
4	Dm	0.14	0/2129	0.33	0/2882
4	Dn	0.13	0/2124	0.35	0/2877
4	Do	0.14	0/2129	0.33	0/2882
4	Dp	0.14	0/2124	0.35	0/2877
4	Dq	0.14	0/2129	0.34	0/2882
4	Dr	0.13	0/2124	0.35	0/2877
4	Ds	0.14	0/2129	0.34	0/2882
4	Dt	0.13	0/2124	0.35	0/2877
4	Du	0.14	0/2129	0.34	0/2882
4	Dv	0.14	0/2124	0.35	0/2877
4	Dw	0.14	0/2129	0.33	0/2882
4	Dx	0.13	0/2124	0.35	0/2877
4	Dy	0.14	0/2129	0.32	0/2882
4	Dz	0.13	0/2124	0.35	0/2877
5	Fa	0.17	0/126	0.43	0/166
5	Fb	0.15	0/126	0.34	0/166
5	Fc	0.16	0/126	0.42	0/166
5	Fd	0.16	0/126	0.46	0/166
5	Fe	0.17	0/126	0.41	0/166
5	Ff	0.16	0/126	0.43	0/166
5	Fg	0.16	0/126	0.43	0/166
5	Fh	0.17	0/126	0.45	0/166
5	Fi	0.17	0/126	0.40	0/166
5	Fj	0.16	0/126	0.44	0/166
5	Fk	0.17	0/126	0.41	0/166
5	Fl	0.17	0/126	0.43	0/166
5	Fm	0.17	0/126	0.44	0/166
5	Fn	0.15	0/126	0.44	0/166
5	Fo	0.17	0/126	0.43	0/166
5	Fp	0.17	0/126	0.41	0/166

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	Fq	0.18	0/126	0.44	0/166
5	Fr	0.16	0/126	0.41	0/166
5	Fs	0.16	0/126	0.41	0/166
5	Ft	0.16	0/126	0.44	0/166
5	Fu	0.17	0/126	0.44	0/166
5	Fv	0.17	0/126	0.44	0/166
5	Fw	0.16	0/126	0.44	0/166
5	Fx	0.17	0/126	0.44	0/166
5	Fy	0.16	0/126	0.43	0/166
5	Fz	0.16	0/126	0.45	0/166
5	Ga	0.16	0/113	0.47	0/149
5	Gb	0.15	0/113	0.43	0/149
5	Gc	0.16	0/113	0.44	0/149
5	Gd	0.13	0/113	0.40	0/149
5	Ge	0.14	0/113	0.43	0/149
5	Gf	0.15	0/113	0.45	0/149
5	Gg	0.16	0/113	0.47	0/149
5	Gh	0.15	0/113	0.45	0/149
5	Gi	0.13	0/113	0.44	0/149
5	Gj	0.14	0/113	0.44	0/149
5	Gk	0.16	0/113	0.46	0/149
5	Gl	0.15	0/113	0.45	0/149
5	Gm	0.15	0/113	0.45	0/149
5	Gn	0.15	0/113	0.46	0/149
5	Go	0.14	0/113	0.43	0/149
5	Gp	0.15	0/113	0.46	0/149
5	Gq	0.13	0/113	0.44	0/149
5	Gr	0.17	0/113	0.43	0/149
5	Gs	0.14	0/113	0.49	0/149
5	Gt	0.16	0/113	0.50	0/149
5	Gu	0.12	0/113	0.42	0/149
5	Gv	0.18	0/113	0.51	0/149
5	Gw	0.21	0/113	0.59	0/149
5	Gx	0.17	0/113	0.41	0/149
5	Gy	0.13	0/113	0.44	0/149
5	Gz	0.16	0/113	0.43	0/149
All	All	0.12	0/239863	0.32	0/324571

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	31	0
1	Ab	1674	0	1609	32	0
1	Ac	1674	0	1609	32	0
1	Ad	1674	0	1609	29	0
1	Ae	1674	0	1609	31	0
1	Af	1674	0	1609	31	0
1	Ag	1674	0	1609	32	0
1	Ah	1674	0	1609	33	0
1	Ai	1674	0	1609	32	0
1	Aj	1674	0	1609	29	0
1	Ak	1674	0	1609	34	0
1	Al	1674	0	1609	32	0
1	Am	1674	0	1609	32	0
1	An	1674	0	1609	30	0
1	Ao	1674	0	1609	29	0
1	Ap	1674	0	1609	26	0
1	Aq	1674	0	1609	28	0
1	Ar	1674	0	1609	28	0
1	As	1674	0	1609	27	0
1	At	1674	0	1609	27	0
1	Au	1674	0	1609	27	0
1	Av	1674	0	1609	30	0
1	Aw	1674	0	1609	30	0
1	Ax	1674	0	1609	27	0
1	Ay	1674	0	1609	29	0
1	Az	1674	0	1609	30	0
2	Ba	2314	0	2373	32	0
2	Bb	2314	0	2373	31	0
2	Bc	2314	0	2373	29	0
2	Bd	2314	0	2373	31	0
2	Be	2314	0	2373	34	0
2	Bf	2314	0	2373	32	0
2	Bg	2314	0	2373	32	0
2	Bh	2314	0	2373	32	0
2	Bi	2314	0	2373	32	0
2	Bj	2314	0	2373	28	0
2	Bk	2314	0	2373	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bl	2314	0	2373	32	0
2	Bm	2314	0	2373	31	0
2	Bn	2314	0	2373	30	0
2	Bo	2314	0	2373	29	0
2	Bp	2314	0	2373	31	0
2	Bq	2314	0	2373	31	0
2	Br	2314	0	2373	30	0
2	Bs	2314	0	2373	30	0
2	Bt	2314	0	2373	28	0
2	Bu	2314	0	2373	24	0
2	Bv	2314	0	2373	31	0
2	Bw	2314	0	2373	33	0
2	Bx	2314	0	2373	35	0
2	By	2314	0	2373	33	0
2	Bz	2314	0	2373	33	0
3	Ca	2770	0	2749	16	0
3	Cb	2770	0	2749	20	0
3	Cc	2770	0	2749	14	0
3	Cd	2770	0	2749	20	0
3	Ce	2770	0	2749	11	0
3	Cf	2770	0	2749	13	0
3	Cg	2770	0	2749	12	0
3	Ch	2770	0	2749	18	0
3	Ci	2770	0	2749	17	0
3	Cj	2770	0	2749	10	0
3	Ck	2770	0	2749	16	0
3	Cl	2770	0	2749	16	0
3	Cm	2770	0	2749	15	0
3	Cn	2770	0	2749	17	0
3	Co	2770	0	2749	16	0
3	Cp	2770	0	2749	16	0
3	Cq	2770	0	2749	17	0
3	Cr	2770	0	2749	15	0
3	Cs	2770	0	2749	11	0
3	Ct	2770	0	2749	14	0
3	Cu	2770	0	2749	9	0
3	Cv	2770	0	2749	13	0
3	Cw	2770	0	2749	14	0
3	Cx	2770	0	2749	14	0
3	Cy	2770	0	2749	18	0
3	Cz	2770	0	2749	14	0
4	Da	2085	0	2022	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Db	2080	0	2003	8	0
4	Dc	2085	0	2022	14	0
4	Dd	2080	0	2003	9	0
4	De	2085	0	2022	12	0
4	Df	2080	0	2003	9	0
4	Dg	2085	0	2022	14	0
4	Dh	2080	0	2003	7	0
4	Di	2085	0	2022	13	0
4	Dj	2080	0	2003	9	0
4	Dk	2085	0	2022	12	0
4	Dl	2080	0	2003	8	0
4	Dm	2085	0	2022	12	0
4	Dn	2080	0	2003	8	0
4	Do	2085	0	2022	15	0
4	Dp	2080	0	2003	10	0
4	Dq	2085	0	2022	16	0
4	Dr	2080	0	2003	9	0
4	Ds	2085	0	2022	11	0
4	Dt	2080	0	2003	9	0
4	Du	2085	0	2022	16	0
4	Dv	2080	0	2003	9	0
4	Dw	2085	0	2022	14	0
4	Dx	2080	0	2003	10	0
4	Dy	2085	0	2022	12	0
4	Dz	2080	0	2003	9	0
5	Fa	125	0	125	1	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	0	0
5	Fg	125	0	125	0	0
5	Fh	125	0	125	1	0
5	Fi	125	0	125	1	0
5	Fj	125	0	125	0	0
5	Fk	125	0	125	0	0
5	Fl	125	0	125	2	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	1	0
5	Fu	125	0	125	0	0
5	Fv	125	0	125	0	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	2	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	0	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	1	0
5	Gp	112	0	116	1	0
5	Gq	112	0	116	0	0
5	Gr	112	0	116	0	0
5	Gs	112	0	116	0	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	1	0
5	Gx	112	0	116	0	0
5	Gy	112	0	116	0	0
5	Gz	112	0	116	1	0
All	All	236015	0	233597	1723	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 (1723) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bb:185:ASN:HB3	2:Bc:97:GLN:HE21	1.59	0.68
3:Cw:271:LEU:HD21	5:Gw:145:PHE:HB3	1.80	0.63
2:Bs:25:ALA:HB2	2:Bs:186:LEU:HD23	1.82	0.62
2:Bv:25:ALA:HB2	2:Bv:186:LEU:HD23	1.82	0.62
2:By:25:ALA:HB2	2:By:186:LEU:HD23	1.81	0.61
2:Ba:97:GLN:HE21	2:Bz:185:ASN:HB3	1.65	0.61
2:Bu:25:ALA:HB2	2:Bu:186:LEU:HD23	1.82	0.61
4:Dc:78:ARG:HB3	4:Dc:143:GLN:HE22	1.65	0.61
2:Bq:25:ALA:HB2	2:Bq:186:LEU:HD23	1.83	0.61
4:Dm:78:ARG:HB3	4:Dm:143:GLN:HE22	1.66	0.61
2:Bn:25:ALA:HB2	2:Bn:186:LEU:HD23	1.81	0.61
2:Bo:25:ALA:HB2	2:Bo:186:LEU:HD23	1.83	0.61
3:Cb:291:LEU:HD22	3:Cb:372:VAL:HA	1.83	0.61
2:Bg:25:ALA:HB2	2:Bg:186:LEU:HD23	1.82	0.60
2:Bp:25:ALA:HB2	2:Bp:186:LEU:HD23	1.83	0.60
1:Ak:112:ASN:HD21	1:Ak:224:ALA:HB1	1.65	0.60
2:Be:25:ALA:HB2	2:Be:186:LEU:HD23	1.83	0.60
2:Bi:25:ALA:HB2	2:Bi:186:LEU:HD23	1.83	0.60
2:Bw:25:ALA:HB2	2:Bw:186:LEU:HD23	1.83	0.60
1:Ap:112:ASN:HD21	1:Ap:224:ALA:HB1	1.66	0.60
4:Dq:78:ARG:HB3	4:Dq:143:GLN:HE22	1.66	0.60
1:Ar:112:ASN:HD21	1:Ar:224:ALA:HB1	1.66	0.60
4:Di:68:ILE:HD11	4:Dj:112:GLN:HE21	1.67	0.60
2:Bm:25:ALA:HB2	2:Bm:186:LEU:HD23	1.82	0.59
4:Do:68:ILE:HD11	4:Dp:112:GLN:HE21	1.67	0.59
1:Aq:125:LEU:HB3	1:At:244:MET:HE3	1.84	0.59
2:Ba:25:ALA:HB2	2:Ba:186:LEU:HD23	1.84	0.59
2:Bx:25:ALA:HB2	2:Bx:186:LEU:HD23	1.83	0.59
3:Ci:126:ILE:HB	3:Ci:169:THR:HG22	1.84	0.59
3:Ck:126:ILE:HB	3:Ck:169:THR:HG22	1.84	0.59
1:Au:125:LEU:HB3	1:Ax:244:MET:HE3	1.85	0.59
1:Am:66:TRP:HA	1:Am:192:ARG:HD3	1.84	0.59
2:Bb:25:ALA:HB2	2:Bb:186:LEU:HD23	1.84	0.59
2:Bk:25:ALA:HB2	2:Bk:186:LEU:HD23	1.85	0.59
2:Bz:25:ALA:HB2	2:Bz:186:LEU:HD23	1.84	0.59
3:Cb:293:GLN:HB2	3:Cb:369:ILE:HG23	1.84	0.59
3:Ch:126:ILE:HB	3:Ch:169:THR:HG22	1.85	0.59
4:Da:68:ILE:HD11	4:Db:112:GLN:HE21	1.68	0.59
4:Do:78:ARG:HB3	4:Do:143:GLN:HE22	1.66	0.59
1:Af:112:ASN:HD21	1:Af:224:ALA:HB1	1.68	0.59
2:Br:25:ALA:HB2	2:Br:186:LEU:HD23	1.84	0.59
3:Cz:85:VAL:HG22	3:Cz:108:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:112:ASN:HD21	1:Am:224:ALA:HB1	1.67	0.59
4:Dg:68:ILE:HD11	4:Dh:112:GLN:HE21	1.67	0.59
1:Ab:66:TRP:HA	1:Ab:192:ARG:HD3	1.84	0.59
1:Al:112:ASN:HD21	1:Al:224:ALA:HB1	1.67	0.59
2:Bj:25:ALA:HB2	2:Bj:186:LEU:HD23	1.84	0.59
4:Dk:68:ILE:HD11	4:Dl:112:GLN:HE21	1.68	0.59
2:Bt:25:ALA:HB2	2:Bt:186:LEU:HD23	1.84	0.59
4:Dy:68:ILE:HD11	4:Dz:112:GLN:HE21	1.68	0.59
1:Ac:244:MET:HE3	1:Az:125:LEU:HB3	1.85	0.58
2:Bc:25:ALA:HB2	2:Bc:186:LEU:HD23	1.84	0.58
4:Dy:78:ARG:HB3	4:Dy:143:GLN:HE22	1.67	0.58
1:Al:66:TRP:HA	1:Al:192:ARG:HD3	1.85	0.58
1:As:125:LEU:HB3	1:Av:244:MET:HE3	1.85	0.58
1:Ac:66:TRP:HA	1:Ac:192:ARG:HD3	1.85	0.58
3:Ca:126:ILE:HB	3:Ca:169:THR:HG22	1.85	0.58
1:Ap:125:LEU:HB3	1:As:244:MET:HE3	1.86	0.58
2:Bd:25:ALA:HB2	2:Bd:186:LEU:HD23	1.84	0.58
3:Cc:85:VAL:HG22	3:Cc:108:ILE:HG12	1.86	0.58
1:Ao:112:ASN:HD21	1:Ao:224:ALA:HB1	1.69	0.58
1:Ab:244:MET:HE3	1:Ay:125:LEU:HB3	1.86	0.58
1:Af:66:TRP:HA	1:Af:192:ARG:HD3	1.85	0.58
1:Ai:112:ASN:HD21	1:Ai:224:ALA:HB1	1.69	0.58
1:At:125:LEU:HB3	1:Aw:244:MET:HE3	1.86	0.58
3:Cr:126:ILE:HB	3:Cr:169:THR:HG22	1.86	0.58
4:De:68:ILE:HD11	4:Df:112:GLN:HE21	1.69	0.58
4:Du:93:PRO:HB2	4:Du:95:TRP:HE3	1.68	0.58
1:Ae:66:TRP:HA	1:Ae:192:ARG:HD3	1.85	0.58
4:Ds:78:ARG:HB3	4:Ds:143:GLN:HE22	1.68	0.58
1:Aa:113:GLU:HB2	1:Aa:172:MET:HB3	1.86	0.58
2:Bk:185:ASN:HB3	2:Bl:97:GLN:HE21	1.69	0.58
3:Cm:126:ILE:HB	3:Cm:169:THR:HG22	1.86	0.58
1:Aa:66:TRP:HA	1:Aa:192:ARG:HD3	1.86	0.57
2:Bh:25:ALA:HB2	2:Bh:186:LEU:HD23	1.85	0.57
4:Di:78:ARG:HB3	4:Di:143:GLN:HE22	1.67	0.57
1:Ak:66:TRP:HA	1:Ak:192:ARG:HD3	1.85	0.57
1:As:66:TRP:HA	1:As:192:ARG:HD3	1.86	0.57
1:Aw:125:LEU:HB3	1:Az:244:MET:HE3	1.86	0.57
2:Bn:185:ASN:HB3	2:Bo:97:GLN:HE21	1.69	0.57
3:Cy:126:ILE:HB	3:Cy:169:THR:HG22	1.86	0.57
4:Do:93:PRO:HB2	4:Do:95:TRP:HE3	1.69	0.57
4:Da:104:ILE:HG23	4:Db:145:ARG:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:112:ASN:HD21	1:An:224:ALA:HB1	1.68	0.57
1:Au:66:TRP:HA	1:Au:192:ARG:HD3	1.86	0.57
1:Aw:66:TRP:HA	1:Aw:192:ARG:HD3	1.86	0.57
2:Bf:25:ALA:HB2	2:Bf:186:LEU:HD23	1.84	0.57
3:Ca:226:VAL:HB	3:Ca:236:MET:HB3	1.85	0.57
4:Dq:68:ILE:HD11	4:Dr:112:GLN:HE21	1.70	0.57
4:Du:68:ILE:HD11	4:Dv:112:GLN:HE21	1.69	0.57
4:De:49:VAL:HG12	4:De:59:GLU:HG2	1.87	0.57
4:Dk:49:VAL:HG12	4:Dk:59:GLU:HG2	1.87	0.57
4:Dm:93:PRO:HB2	4:Dm:95:TRP:HE3	1.69	0.57
1:Av:66:TRP:HA	1:Av:192:ARG:HD3	1.86	0.57
3:Ce:262:TRP:HA	3:Ce:267:GLY:HA3	1.87	0.57
1:Ad:66:TRP:HA	1:Ad:192:ARG:HD3	1.86	0.57
4:Dc:49:VAL:HG12	4:Dc:59:GLU:HG2	1.87	0.57
4:Dc:93:PRO:HB2	4:Dc:95:TRP:HE3	1.70	0.57
1:An:125:LEU:HB3	1:Aq:244:MET:HE3	1.87	0.56
1:Aq:245:GLN:HG3	1:Ar:200:ASN:HD21	1.70	0.56
3:Ck:85:VAL:HG22	3:Ck:108:ILE:HG12	1.86	0.56
2:Bk:205:LEU:HD11	2:Bk:236:ILE:HD11	1.86	0.56
4:Dg:49:VAL:HG12	4:Dg:59:GLU:HG2	1.87	0.56
4:Dk:78:ARG:HB3	4:Dk:143:GLN:HE22	1.70	0.56
4:Dw:78:ARG:HB3	4:Dw:143:GLN:HE22	1.70	0.56
4:Dw:93:PRO:HB2	4:Dw:95:TRP:HE3	1.71	0.56
1:Ai:66:TRP:HA	1:Ai:192:ARG:HD3	1.86	0.56
1:At:66:TRP:HA	1:At:192:ARG:HD3	1.87	0.56
2:Bl:25:ALA:HB2	2:Bl:186:LEU:HD23	1.87	0.56
1:Ar:125:LEU:HB3	1:Au:244:MET:HE3	1.88	0.56
2:Bj:185:ASN:HB3	2:Bk:97:GLN:HE21	1.71	0.56
1:Ao:245:GLN:HG3	1:Ap:200:ASN:HD21	1.71	0.56
1:Ay:66:TRP:HA	1:Ay:192:ARG:HD3	1.87	0.56
2:By:205:LEU:HD11	2:By:236:ILE:HD11	1.88	0.56
4:Dc:68:ILE:HD11	4:Dd:112:GLN:HE21	1.70	0.56
1:Ai:125:LEU:HB3	1:Al:244:MET:HE3	1.87	0.56
1:Az:66:TRP:HA	1:Az:192:ARG:HD3	1.86	0.56
4:Dm:49:VAL:HG12	4:Dm:59:GLU:HG2	1.88	0.56
4:Dw:68:ILE:HD11	4:Dx:112:GLN:HE21	1.70	0.56
4:Dy:93:PRO:HB2	4:Dy:95:TRP:HE3	1.71	0.56
1:Ai:113:GLU:HB2	1:Ai:172:MET:HB3	1.87	0.56
1:Ap:66:TRP:HA	1:Ap:192:ARG:HD3	1.87	0.56
1:Ay:112:ASN:HD21	1:Ay:224:ALA:HB1	1.71	0.56
4:Da:93:PRO:HB2	4:Da:95:TRP:HE3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cs:85:VAL:HG22	3:Cs:108:ILE:HG12	1.87	0.56
4:Dy:49:VAL:HG12	4:Dy:59:GLU:HG2	1.88	0.56
1:Ak:125:LEU:HB3	1:An:244:MET:HE3	1.87	0.56
1:As:245:GLN:HG3	1:At:200:ASN:HD21	1.70	0.56
4:Dc:104:ILE:HG23	4:Dd:145:ARG:HD3	1.88	0.56
4:Di:49:VAL:HG12	4:Di:59:GLU:HG2	1.88	0.56
4:Ds:93:PRO:HB2	4:Ds:95:TRP:HE3	1.71	0.56
4:Du:104:ILE:HG23	4:Dv:145:ARG:HD3	1.88	0.56
1:Ai:245:GLN:HG3	1:Aj:200:ASN:HD21	1.71	0.55
1:Ao:125:LEU:HB3	1:Ar:244:MET:HE3	1.88	0.55
1:Av:125:LEU:HB3	1:Ay:244:MET:HE3	1.88	0.55
2:Bu:87:ALA:HB2	2:Bu:101:ILE:HG22	1.88	0.55
4:Ds:49:VAL:HG12	4:Ds:59:GLU:HG2	1.88	0.55
2:Bw:185:ASN:HB3	2:Bx:97:GLN:HE21	1.71	0.55
3:Cg:262:TRP:HA	3:Cg:267:GLY:HA3	1.88	0.55
1:An:66:TRP:HA	1:An:192:ARG:HD3	1.87	0.55
1:Ax:66:TRP:HA	1:Ax:192:ARG:HD3	1.87	0.55
2:Bu:153:VAL:HG21	2:Bv:148:ASP:HB3	1.89	0.55
4:Dg:93:PRO:HB2	4:Dg:95:TRP:HE3	1.71	0.55
4:Dm:68:ILE:HD11	4:Dn:112:GLN:HE21	1.69	0.55
1:Ac:125:LEU:HB3	1:Af:244:MET:HE3	1.88	0.55
1:Ax:245:GLN:HG3	1:Ay:200:ASN:HD21	1.72	0.55
2:Ba:205:LEU:HD11	2:Ba:236:ILE:HD11	1.88	0.55
2:Bq:248:ALA:HB1	2:Bq:265:VAL:HG22	1.88	0.55
4:Da:49:VAL:HG12	4:Da:59:GLU:HG2	1.88	0.55
4:Dw:49:VAL:HG12	4:Dw:59:GLU:HG2	1.88	0.55
1:Aa:125:LEU:HB3	1:Ad:244:MET:HE3	1.89	0.55
1:Aj:66:TRP:HA	1:Aj:192:ARG:HD3	1.86	0.55
1:Av:232:ARG:HH22	1:Aw:194:GLU:HG3	1.72	0.55
1:Az:113:GLU:HB2	1:Az:172:MET:HB3	1.89	0.55
2:Bk:248:ALA:HB1	2:Bk:265:VAL:HG22	1.89	0.55
2:Bl:248:ALA:HB1	2:Bl:265:VAL:HG22	1.89	0.55
2:Bo:248:ALA:HB1	2:Bo:265:VAL:HG22	1.88	0.55
4:Di:104:ILE:HG23	4:Dj:145:ARG:HD3	1.88	0.55
1:Aq:66:TRP:HA	1:Aq:192:ARG:HD3	1.87	0.55
1:As:231:ALA:HB3	1:At:195:LYS:HG3	1.89	0.55
2:Bc:205:LEU:HD11	2:Bc:236:ILE:HD11	1.89	0.55
2:Bj:248:ALA:HB1	2:Bj:265:VAL:HG22	1.89	0.55
4:Dd:219:VAL:HG21	4:Dd:254:LEU:HD21	1.88	0.55
4:Ds:68:ILE:HD11	4:Dt:112:GLN:HE21	1.71	0.55
1:Ab:112:ASN:HD21	1:Ab:224:ALA:HB1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:245:GLN:HG3	1:As:200:ASN:HD21	1.71	0.55
2:Ba:87:ALA:HB2	2:Ba:101:ILE:HG22	1.89	0.55
3:Cc:92:GLU:HB2	3:Cc:103:ARG:HB3	1.89	0.55
1:Am:245:GLN:HG3	1:An:200:ASN:HD21	1.72	0.55
4:De:104:ILE:HG23	4:Df:145:ARG:HD3	1.88	0.55
4:Dg:104:ILE:HG23	4:Dh:145:ARG:HD3	1.88	0.55
4:Do:49:VAL:HG12	4:Do:59:GLU:HG2	1.89	0.55
1:Ao:66:TRP:HA	1:Ao:192:ARG:HD3	1.89	0.55
1:As:240:THR:HG22	1:As:244:MET:HE2	1.89	0.55
1:Au:245:GLN:HG3	1:Av:200:ASN:HD21	1.72	0.55
1:Av:112:ASN:HD21	1:Av:224:ALA:HB1	1.72	0.55
1:Ay:245:GLN:HG3	1:Az:200:ASN:HD21	1.71	0.55
2:Bh:248:ALA:HB1	2:Bh:265:VAL:HG22	1.89	0.55
1:Ag:112:ASN:HD21	1:Ag:224:ALA:HB1	1.72	0.55
1:Av:245:GLN:HG3	1:Aw:200:ASN:HD21	1.72	0.55
1:Az:184:LEU:HD12	1:Az:188:ASN:HB2	1.88	0.55
1:Ab:125:LEU:HB3	1:Ae:244:MET:HE3	1.89	0.54
1:Ac:245:GLN:HG3	1:Ad:200:ASN:HD21	1.72	0.54
1:Ah:66:TRP:HA	1:Ah:192:ARG:HD3	1.87	0.54
1:Ar:113:GLU:HB2	1:Ar:172:MET:HB3	1.88	0.54
3:Cc:262:TRP:HA	3:Cc:267:GLY:HA3	1.88	0.54
4:Dq:49:VAL:HG12	4:Dq:59:GLU:HG2	1.90	0.54
1:Aa:245:GLN:HG3	1:Ab:200:ASN:HD21	1.73	0.54
1:Al:231:ALA:HB3	1:Am:195:LYS:HG3	1.89	0.54
2:Be:248:ALA:HB1	2:Be:265:VAL:HG22	1.89	0.54
2:Bf:248:ALA:HB1	2:Bf:265:VAL:HG22	1.89	0.54
2:Bg:224:ARG:HH21	3:Cx:368:GLN:HB2	1.73	0.54
2:Bq:87:ALA:HB2	2:Bq:101:ILE:HG22	1.89	0.54
4:Dq:93:PRO:HB2	4:Dq:95:TRP:HE3	1.72	0.54
4:Dy:104:ILE:HG23	4:Dz:145:ARG:HD3	1.89	0.54
1:Ag:125:LEU:HB3	1:Aj:244:MET:HE3	1.89	0.54
1:Aj:245:GLN:HG3	1:Ak:200:ASN:HD21	1.72	0.54
1:Ap:245:GLN:HG3	1:Aq:200:ASN:HD21	1.72	0.54
1:Aq:112:ASN:HD21	1:Aq:224:ALA:HB1	1.72	0.54
1:Ar:66:TRP:HA	1:Ar:192:ARG:HD3	1.89	0.54
2:Bm:205:LEU:HD11	2:Bm:236:ILE:HD11	1.88	0.54
2:Bp:248:ALA:HB1	2:Bp:265:VAL:HG22	1.89	0.54
3:Cl:80:PHE:HA	5:Fl:136:VAL:HG21	1.88	0.54
1:Ae:245:GLN:HG3	1:Af:200:ASN:HD21	1.72	0.54
1:Ak:245:GLN:HG3	1:Al:200:ASN:HD21	1.73	0.54
1:At:113:GLU:HB2	1:At:172:MET:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:36:ASP:HB3	1:Az:39:GLU:HG2	1.90	0.54
2:Bg:248:ALA:HB1	2:Bg:265:VAL:HG22	1.89	0.54
3:Cp:255:ASP:HB3	3:Cp:258:SER:HB3	1.90	0.54
3:Cy:262:TRP:HA	3:Cy:267:GLY:HA3	1.89	0.54
3:Cz:262:TRP:HA	3:Cz:267:GLY:HA3	1.89	0.54
1:Aj:125:LEU:HB3	1:Am:244:MET:HE3	1.89	0.54
2:Bn:248:ALA:HB1	2:Bn:265:VAL:HG22	1.90	0.54
4:Dw:104:ILE:HG23	4:Dx:145:ARG:HD3	1.88	0.54
1:Ac:240:THR:HG22	1:Ac:244:MET:HE2	1.90	0.54
1:Ad:112:ASN:HD21	1:Ad:224:ALA:HB1	1.72	0.54
1:Ao:231:ALA:HB3	1:Ap:195:LYS:HG3	1.90	0.54
1:Av:231:ALA:HB3	1:Aw:195:LYS:HG3	1.90	0.54
1:Ax:240:THR:HG22	1:Ax:244:MET:HE2	1.89	0.54
2:Be:205:LEU:HD11	2:Be:236:ILE:HD11	1.88	0.54
2:Bo:153:VAL:HG21	2:Bp:148:ASP:HB3	1.89	0.54
3:Cq:255:ASP:HB3	3:Cq:258:SER:HB3	1.89	0.54
4:Df:219:VAL:HG21	4:Df:254:LEU:HD21	1.90	0.54
1:Aa:244:MET:HE3	1:Ax:125:LEU:HB3	1.90	0.54
1:Ag:66:TRP:HA	1:Ag:192:ARG:HD3	1.89	0.54
1:Ag:245:GLN:HG3	1:Ah:200:ASN:HD21	1.73	0.54
1:Ar:240:THR:HG22	1:Ar:244:MET:HE2	1.90	0.54
2:Bb:248:ALA:HB1	2:Bb:265:VAL:HG22	1.89	0.54
2:Bq:205:LEU:HD11	2:Bq:236:ILE:HD11	1.89	0.54
2:Bs:205:LEU:HD11	2:Bs:236:ILE:HD11	1.89	0.54
2:Bu:205:LEU:HD11	2:Bu:236:ILE:HD11	1.90	0.54
4:De:78:ARG:HB3	4:De:143:GLN:HE22	1.73	0.54
4:Dk:104:ILE:HG23	4:Dl:145:ARG:HD3	1.88	0.54
4:Du:78:ARG:HB3	4:Du:143:GLN:HE22	1.72	0.54
1:Ab:184:LEU:HD12	1:Ab:188:ASN:HB2	1.90	0.54
1:Af:125:LEU:HB3	1:Ai:244:MET:HE3	1.89	0.54
1:Aq:240:THR:HG22	1:Aq:244:MET:HE2	1.90	0.54
1:At:245:GLN:HG3	1:Au:200:ASN:HD21	1.73	0.54
2:Bf:87:ALA:HB2	2:Bf:101:ILE:HG22	1.90	0.54
2:Bg:205:LEU:HD11	2:Bg:236:ILE:HD11	1.89	0.54
2:Bu:248:ALA:HB1	2:Bu:265:VAL:HG22	1.88	0.54
2:Bv:153:VAL:HG21	2:Bw:148:ASP:HB3	1.89	0.54
2:By:223:PRO:HB3	4:Di:94:VAL:HB	1.90	0.54
3:Ci:262:TRP:HA	3:Ci:267:GLY:HA3	1.90	0.54
1:Ad:184:LEU:HD12	1:Ad:188:ASN:HB2	1.90	0.54
2:Be:21:ILE:HG23	2:Be:197:LEU:HD11	1.90	0.54
2:Bm:248:ALA:HB1	2:Bm:265:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bp:87:ALA:HB2	2:Bp:101:ILE:HG22	1.90	0.54
2:Br:248:ALA:HB1	2:Br:265:VAL:HG22	1.90	0.54
4:De:93:PRO:HB2	4:De:95:TRP:HE3	1.72	0.54
4:Dm:104:ILE:HG23	4:Dn:145:ARG:HD3	1.88	0.54
1:Ak:113:GLU:HB2	1:Ak:172:MET:HB3	1.90	0.54
2:Bd:248:ALA:HB1	2:Bd:265:VAL:HG22	1.90	0.54
2:Be:223:PRO:HB3	4:Do:94:VAL:HB	1.90	0.54
2:Bf:122:LEU:HB2	2:Bf:131:ALA:HB3	1.90	0.54
2:Bo:205:LEU:HD11	2:Bo:236:ILE:HD11	1.90	0.54
2:Bv:185:ASN:HB3	2:Bw:97:GLN:HE21	1.72	0.54
4:Ds:104:ILE:HG23	4:Dt:145:ARG:HD3	1.88	0.54
1:Ae:125:LEU:HB3	1:Ah:244:MET:HE3	1.88	0.53
1:Ae:231:ALA:HB3	1:Af:195:LYS:HG3	1.89	0.53
1:Al:113:GLU:HB2	1:Al:172:MET:HB3	1.90	0.53
1:Ao:113:GLU:HB2	1:Ao:172:MET:HB3	1.90	0.53
1:Ax:113:GLU:HB2	1:Ax:172:MET:HB3	1.90	0.53
2:Ba:248:ALA:HB1	2:Ba:265:VAL:HG22	1.89	0.53
2:Bz:122:LEU:HB2	2:Bz:131:ALA:HB3	1.90	0.53
3:Cb:92:GLU:HB2	3:Cb:103:ARG:HB3	1.90	0.53
3:Cb:126:ILE:HB	3:Cb:169:THR:HG22	1.90	0.53
3:Cf:85:VAL:HG22	3:Cf:108:ILE:HG12	1.90	0.53
4:Dk:93:PRO:HB2	4:Dk:95:TRP:HE3	1.71	0.53
4:Do:104:ILE:HG23	4:Dp:145:ARG:HD3	1.89	0.53
4:Dq:104:ILE:HG23	4:Dr:145:ARG:HD3	1.89	0.53
1:Ad:113:GLU:HB2	1:Ad:172:MET:HB3	1.90	0.53
1:Ae:184:LEU:HD12	1:Ae:188:ASN:HB2	1.91	0.53
2:Bb:136:ASN:HB2	2:Bz:360:ILE:HG22	1.90	0.53
2:Bg:360:ILE:HG22	2:Bi:136:ASN:HB2	1.89	0.53
2:Bm:153:VAL:HG21	2:Bn:148:ASP:HB3	1.89	0.53
2:Bs:248:ALA:HB1	2:Bs:265:VAL:HG22	1.91	0.53
3:Ck:209:LYS:HD2	3:Ck:212:GLN:HB2	1.91	0.53
1:Aj:231:ALA:HB3	1:Ak:195:LYS:HG3	1.90	0.53
1:Aw:231:ALA:HB3	1:Ax:195:LYS:HG3	1.90	0.53
1:Aw:240:THR:HG22	1:Aw:244:MET:HE2	1.90	0.53
2:Bc:87:ALA:HB2	2:Bc:101:ILE:HG22	1.90	0.53
2:Bc:122:LEU:HB2	2:Bc:131:ALA:HB3	1.90	0.53
2:Bi:248:ALA:HB1	2:Bi:265:VAL:HG22	1.91	0.53
2:Bq:21:ILE:HG23	2:Bq:197:LEU:HD11	1.90	0.53
2:Bv:87:ALA:HB2	2:Bv:101:ILE:HG22	1.91	0.53
2:Bz:248:ALA:HB1	2:Bz:265:VAL:HG22	1.90	0.53
3:Ct:255:ASP:HB3	3:Ct:258:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Di:93:PRO:HB2	4:Di:95:TRP:HE3	1.71	0.53
1:Am:240:THR:HG22	1:Am:244:MET:HE2	1.90	0.53
1:Aw:245:GLN:HG3	1:Ax:200:ASN:HD21	1.72	0.53
2:Bc:248:ALA:HB1	2:Bc:265:VAL:HG22	1.89	0.53
2:Bd:122:LEU:HB2	2:Bd:131:ALA:HB3	1.90	0.53
2:Bf:360:ILE:HG22	2:Bh:136:ASN:HB2	1.91	0.53
2:Bh:360:ILE:HG22	2:Bj:136:ASN:HB2	1.91	0.53
2:Bw:205:LEU:HD11	2:Bw:236:ILE:HD11	1.91	0.53
4:Dn:219:VAL:HG21	4:Dn:254:LEU:HD21	1.91	0.53
1:Aa:200:ASN:HD21	1:Az:245:GLN:HG3	1.73	0.53
1:An:245:GLN:HG3	1:Ao:200:ASN:HD21	1.72	0.53
1:Au:113:GLU:HB2	1:Au:172:MET:HB3	1.89	0.53
1:Au:240:THR:HG22	1:Au:244:MET:HE2	1.90	0.53
1:Av:240:THR:HG22	1:Av:244:MET:HE2	1.89	0.53
2:Ba:122:LEU:HB2	2:Ba:131:ALA:HB3	1.91	0.53
2:Bb:87:ALA:HB2	2:Bb:101:ILE:HG22	1.90	0.53
2:Bx:87:ALA:HB2	2:Bx:101:ILE:HG22	1.91	0.53
3:Cx:262:TRP:HA	3:Cx:267:GLY:HA3	1.90	0.53
1:Ah:240:THR:HG22	1:Ah:244:MET:HE2	1.91	0.53
1:An:232:ARG:HH22	1:Ao:194:GLU:HG3	1.74	0.53
1:At:231:ALA:HB3	1:Au:195:LYS:HG3	1.91	0.53
2:Ba:21:ILE:HG23	2:Ba:197:LEU:HD11	1.89	0.53
2:Bc:360:ILE:HG22	2:Be:136:ASN:HB2	1.90	0.53
2:Be:360:ILE:HG22	2:Bg:136:ASN:HB2	1.90	0.53
2:Bh:185:ASN:HB3	2:Bi:97:GLN:HE21	1.74	0.53
2:Bv:21:ILE:HG23	2:Bv:197:LEU:HD11	1.89	0.53
2:Bw:224:ARG:HH21	3:Cn:368:GLN:HB2	1.74	0.53
3:Cb:262:TRP:HA	3:Cb:267:GLY:HA3	1.89	0.53
3:Cw:80:PHE:HA	5:Fw:136:VAL:HG21	1.90	0.53
1:Ad:245:GLN:HG3	1:Ae:200:ASN:HD21	1.73	0.53
1:Aq:232:ARG:HH22	1:Ar:194:GLU:HG3	1.73	0.53
2:Bb:360:ILE:HG22	2:Bd:136:ASN:HB2	1.89	0.53
2:Bd:360:ILE:HG22	2:Bf:136:ASN:HB2	1.91	0.53
2:Bi:205:LEU:HD11	2:Bi:236:ILE:HD11	1.89	0.53
2:Bo:360:ILE:HG22	2:Bq:136:ASN:HB2	1.91	0.53
1:Ac:184:LEU:HD12	1:Ac:188:ASN:HB2	1.90	0.53
1:Ah:245:GLN:HG3	1:Ai:200:ASN:HD21	1.72	0.53
1:Al:245:GLN:HG3	1:Am:200:ASN:HD21	1.72	0.53
1:Au:112:ASN:HD21	1:Au:224:ALA:HB1	1.74	0.53
1:Ay:232:ARG:HH22	1:Az:194:GLU:HG3	1.73	0.53
2:Bi:360:ILE:HG22	2:Bk:136:ASN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Br:87:ALA:HB2	2:Br:101:ILE:HG22	1.91	0.53
2:Bt:248:ALA:HB1	2:Bt:265:VAL:HG22	1.90	0.53
3:Cp:145:VAL:HA	3:Cp:256:THR:HG21	1.88	0.53
1:Aa:195:LYS:HG3	1:Az:231:ALA:HB3	1.91	0.53
1:Ac:232:ARG:HH22	1:Ad:194:GLU:HG3	1.74	0.53
1:Ah:184:LEU:HD12	1:Ah:188:ASN:HB2	1.91	0.53
1:Aj:184:LEU:HD12	1:Aj:188:ASN:HB2	1.89	0.53
1:An:240:THR:HG22	1:An:244:MET:HE2	1.91	0.53
1:As:232:ARG:HH22	1:At:194:GLU:HG3	1.73	0.53
2:Bj:360:ILE:HG22	2:Bl:136:ASN:HB2	1.91	0.53
4:Dh:223:THR:HG22	4:Dh:285:VAL:HG22	1.91	0.53
1:Ac:231:ALA:HB3	1:Ad:195:LYS:HG3	1.90	0.53
1:Af:245:GLN:HG3	1:Ag:200:ASN:HD21	1.73	0.53
1:Aj:113:GLU:HB2	1:Aj:172:MET:HB3	1.91	0.53
1:Au:231:ALA:HB3	1:Av:195:LYS:HG3	1.91	0.53
1:Ax:231:ALA:HB3	1:Ay:195:LYS:HG3	1.91	0.53
2:Bq:153:VAL:HG21	2:Br:148:ASP:HB3	1.91	0.53
1:Ad:125:LEU:HB3	1:Ag:244:MET:HE3	1.91	0.52
1:Ap:231:ALA:HB3	1:Aq:195:LYS:HG3	1.92	0.52
1:Aq:231:ALA:HB3	1:Ar:195:LYS:HG3	1.91	0.52
2:Bw:248:ALA:HB1	2:Bw:265:VAL:HG22	1.90	0.52
1:Ag:113:GLU:HB2	1:Ag:172:MET:HB3	1.91	0.52
1:Al:240:THR:HG22	1:Al:244:MET:HE2	1.90	0.52
1:Am:113:GLU:HB2	1:Am:172:MET:HB3	1.91	0.52
1:An:231:ALA:HB3	1:Ao:195:LYS:HG3	1.92	0.52
1:Ao:232:ARG:HH22	1:Ap:194:GLU:HG3	1.74	0.52
1:As:113:GLU:HB2	1:As:172:MET:HB3	1.91	0.52
1:Aw:113:GLU:HB2	1:Aw:172:MET:HB3	1.91	0.52
2:Bf:21:ILE:HG23	2:Bf:197:LEU:HD11	1.91	0.52
2:Bh:122:LEU:HB2	2:Bh:131:ALA:HB3	1.91	0.52
2:Bn:360:ILE:HG22	2:Bp:136:ASN:HB2	1.89	0.52
2:Bt:153:VAL:HG21	2:Bu:148:ASP:HB3	1.91	0.52
3:Cw:262:TRP:HA	3:Cw:267:GLY:HA3	1.91	0.52
1:Ag:232:ARG:HH22	1:Ah:194:GLU:HG3	1.75	0.52
1:Am:125:LEU:HB3	1:Ap:244:MET:HE3	1.90	0.52
1:Ao:240:THR:HG22	1:Ao:244:MET:HE2	1.91	0.52
2:Be:122:LEU:HB2	2:Be:131:ALA:HB3	1.91	0.52
2:Bi:87:ALA:HB2	2:Bi:101:ILE:HG22	1.91	0.52
2:Bk:360:ILE:HG22	2:Bm:136:ASN:HB2	1.91	0.52
2:Bl:87:ALA:HB2	2:Bl:101:ILE:HG22	1.91	0.52
2:Bx:248:ALA:HB1	2:Bx:265:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bx:360:ILE:HG22	2:Bz:136:ASN:HB2	1.90	0.52
2:By:248:ALA:HB1	2:By:265:VAL:HG22	1.90	0.52
1:Ap:232:ARG:HH22	1:Aq:194:GLU:HG3	1.74	0.52
2:Bi:224:ARG:HH21	3:Cz:368:GLN:HB2	1.75	0.52
2:Bm:360:ILE:HG22	2:Bo:136:ASN:HB2	1.90	0.52
2:Bv:248:ALA:HB1	2:Bv:265:VAL:HG22	1.90	0.52
3:Cn:85:VAL:HG22	3:Cn:108:ILE:HG12	1.91	0.52
4:Da:78:ARG:HB3	4:Da:143:GLN:HE22	1.75	0.52
4:Du:49:VAL:HG12	4:Du:59:GLU:HG2	1.92	0.52
1:Ab:232:ARG:HH22	1:Ac:194:GLU:HG3	1.75	0.52
1:Ab:245:GLN:HG3	1:Ac:200:ASN:HD21	1.74	0.52
1:Ae:232:ARG:HH22	1:Af:194:GLU:HG3	1.74	0.52
1:Ai:184:LEU:HD12	1:Ai:188:ASN:HB2	1.90	0.52
1:Ak:184:LEU:HD12	1:Ak:188:ASN:HB2	1.90	0.52
2:Ba:138:VAL:HG21	2:By:342:MET:HE2	1.92	0.52
2:Bl:360:ILE:HG22	2:Bn:136:ASN:HB2	1.91	0.52
4:Dl:223:THR:HG22	4:Dl:285:VAL:HG22	1.92	0.52
1:Ag:139:GLY:HA3	1:Ah:148:TYR:HD1	1.75	0.52
1:Al:139:GLY:HA3	1:Am:148:TYR:HD1	1.75	0.52
1:Ap:113:GLU:HB2	1:Ap:172:MET:HB3	1.92	0.52
2:Bu:21:ILE:HG23	2:Bu:197:LEU:HD11	1.91	0.52
2:Bu:360:ILE:HG22	2:Bw:136:ASN:HB2	1.90	0.52
3:Cw:255:ASP:HB3	3:Cw:258:SER:HB3	1.91	0.52
4:Dr:219:VAL:HG21	4:Dr:254:LEU:HD21	1.92	0.52
1:Af:113:GLU:HB2	1:Af:172:MET:HB3	1.92	0.52
1:Aj:232:ARG:HH22	1:Ak:194:GLU:HG3	1.74	0.52
1:Aq:113:GLU:HB2	1:Aq:172:MET:HB3	1.91	0.52
2:Bj:87:ALA:HB2	2:Bj:101:ILE:HG22	1.91	0.52
2:Bp:360:ILE:HG22	2:Br:136:ASN:HB2	1.90	0.52
2:Bq:224:ARG:HH21	3:Ch:368:GLN:HB2	1.74	0.52
1:Aa:240:THR:HG22	1:Aa:244:MET:HE2	1.91	0.52
1:At:240:THR:HG22	1:At:244:MET:HE2	1.92	0.52
2:Ba:224:ARG:HH21	3:Cr:368:GLN:HB2	1.74	0.52
2:Bg:122:LEU:HB2	2:Bg:131:ALA:HB3	1.92	0.52
2:Bl:122:LEU:HB2	2:Bl:131:ALA:HB3	1.90	0.52
2:Bm:87:ALA:HB2	2:Bm:101:ILE:HG22	1.90	0.52
2:Bo:87:ALA:HB2	2:Bo:101:ILE:HG22	1.92	0.52
2:Bs:87:ALA:HB2	2:Bs:101:ILE:HG22	1.92	0.52
2:Bv:360:ILE:HG22	2:Bx:136:ASN:HB2	1.91	0.52
2:Bz:87:ALA:HB2	2:Bz:101:ILE:HG22	1.92	0.52
1:Ab:113:GLU:HB2	1:Ab:172:MET:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:240:THR:HG22	1:Aj:244:MET:HE2	1.92	0.52
1:At:125:LEU:HB2	1:At:160:PHE:HB3	1.92	0.52
2:Bn:153:VAL:HG21	2:Bo:148:ASP:HB3	1.91	0.52
2:Br:360:ILE:HG22	2:Bt:136:ASN:HB2	1.90	0.52
3:Cp:262:TRP:HA	3:Cp:267:GLY:HA3	1.91	0.52
4:Db:223:THR:HG22	4:Db:285:VAL:HG22	1.92	0.52
1:Ac:113:GLU:HB2	1:Ac:172:MET:HB3	1.91	0.52
1:Ag:240:THR:HG22	1:Ag:244:MET:HE2	1.91	0.52
1:Ah:231:ALA:HB3	1:Ai:195:LYS:HG3	1.91	0.52
1:Ay:113:GLU:HB2	1:Ay:172:MET:HB3	1.92	0.52
2:Bb:21:ILE:HG23	2:Bb:197:LEU:HD11	1.90	0.52
2:Bs:153:VAL:HG21	2:Bt:148:ASP:HB3	1.91	0.52
2:Bs:360:ILE:HG22	2:Bu:136:ASN:HB2	1.91	0.52
2:Bt:87:ALA:HB2	2:Bt:101:ILE:HG22	1.92	0.52
3:Cf:262:TRP:HA	3:Cf:267:GLY:HA3	1.91	0.52
1:Ah:232:ARG:HH22	1:Ai:194:GLU:HG3	1.75	0.51
1:Al:232:ARG:HH22	1:Am:194:GLU:HG3	1.75	0.51
2:Ba:136:ASN:HB2	2:By:360:ILE:HG22	1.91	0.51
2:Ba:153:VAL:HG21	2:Bb:148:ASP:HB3	1.91	0.51
2:Be:342:MET:HE2	2:Bg:138:VAL:HG21	1.92	0.51
2:Bh:21:ILE:HG23	2:Bh:197:LEU:HD11	1.92	0.51
2:Bh:255:ARG:HH12	2:Bj:136:ASN:HB3	1.75	0.51
2:Bo:122:LEU:HB2	2:Bo:131:ALA:HB3	1.91	0.51
2:Bq:360:ILE:HG22	2:Bs:136:ASN:HB2	1.91	0.51
2:Bw:153:VAL:HG21	2:Bx:148:ASP:HB3	1.92	0.51
3:Cm:262:TRP:HA	3:Cm:267:GLY:HA3	1.90	0.51
3:Co:262:TRP:HA	3:Co:267:GLY:HA3	1.91	0.51
1:Ae:112:ASN:HD21	1:Ae:224:ALA:HB1	1.75	0.51
2:Ba:148:ASP:HB3	2:Bz:153:VAL:HG21	1.92	0.51
3:Cd:262:TRP:HA	3:Cd:267:GLY:HA3	1.91	0.51
3:Cj:262:TRP:HA	3:Cj:267:GLY:HA3	1.91	0.51
3:Cp:92:GLU:HB2	3:Cp:103:ARG:HB3	1.91	0.51
4:Df:223:THR:HG22	4:Df:285:VAL:HG22	1.92	0.51
1:Aa:194:GLU:HG3	1:Az:232:ARG:HH22	1.75	0.51
1:Ah:125:LEU:HB3	1:Ak:244:MET:HE3	1.92	0.51
2:Bb:138:VAL:HG21	2:Bz:342:MET:HE2	1.92	0.51
3:Cd:78:TYR:HD2	3:Cd:88:ILE:HB	1.75	0.51
3:Cr:361:PRO:HB2	4:Dk:148:ARG:HD2	1.92	0.51
3:Ct:262:TRP:HA	3:Ct:267:GLY:HA3	1.93	0.51
4:Dd:249:PHE:HB3	4:Dd:254:LEU:HD23	1.92	0.51
4:Dv:219:VAL:HG21	4:Dv:254:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ab:231:ALA:HB3	1:Ac:195:LYS:HG3	1.91	0.51
1:Af:184:LEU:HD12	1:Af:188:ASN:HB2	1.92	0.51
1:At:232:ARG:HH22	1:Au:194:GLU:HG3	1.75	0.51
2:Bd:87:ALA:HB2	2:Bd:101:ILE:HG22	1.92	0.51
2:Bd:185:ASN:HB3	2:Be:97:GLN:HE21	1.75	0.51
2:Be:153:VAL:HG21	2:Bf:148:ASP:HB3	1.91	0.51
3:Cr:255:ASP:HB3	3:Cr:258:SER:HB3	1.92	0.51
4:Dh:219:VAL:HG21	4:Dh:254:LEU:HD21	1.93	0.51
2:Bc:342:MET:HE2	2:Be:138:VAL:HG21	1.92	0.51
2:Bi:255:ARG:HH12	2:Bk:136:ASN:HB3	1.76	0.51
2:Bl:255:ARG:HH12	2:Bn:136:ASN:HB3	1.75	0.51
2:Bx:153:VAL:HG21	2:By:148:ASP:HB3	1.92	0.51
3:Ch:80:PHE:HA	5:Fh:136:VAL:HG21	1.92	0.51
4:Db:219:VAL:HG21	4:Db:254:LEU:HD21	1.93	0.51
4:Db:249:PHE:HB3	4:Db:254:LEU:HD23	1.93	0.51
4:Dp:219:VAL:HG21	4:Dp:254:LEU:HD21	1.92	0.51
4:Dr:223:THR:HG22	4:Dr:285:VAL:HG22	1.92	0.51
4:Dz:223:THR:HG22	4:Dz:285:VAL:HG22	1.93	0.51
1:Ad:231:ALA:HB3	1:Ae:195:LYS:HG3	1.91	0.51
1:Al:64:PRO:HB2	1:Am:38:VAL:HG13	1.92	0.51
1:Al:184:LEU:HD12	1:Al:188:ASN:HB2	1.92	0.51
1:Am:232:ARG:HH22	1:An:194:GLU:HG3	1.76	0.51
1:Ar:232:ARG:HH22	1:As:194:GLU:HG3	1.75	0.51
1:Ay:231:ALA:HB3	1:Az:195:LYS:HG3	1.93	0.51
2:Be:87:ALA:HB2	2:Be:101:ILE:HG22	1.93	0.51
2:Bf:342:MET:HE2	2:Bh:138:VAL:HG21	1.91	0.51
2:Bk:122:LEU:HB2	2:Bk:131:ALA:HB3	1.91	0.51
2:Bw:122:LEU:HB2	2:Bw:131:ALA:HB3	1.92	0.51
3:Ca:241:ARG:HB3	5:Gb:143:THR:HG21	1.92	0.51
3:Cu:262:TRP:HA	3:Cu:267:GLY:HA3	1.92	0.51
3:Cy:195:MET:HG3	3:Cy:226:VAL:HG22	1.93	0.51
4:Dd:223:THR:HG22	4:Dd:285:VAL:HG22	1.92	0.51
4:Dv:223:THR:HG22	4:Dv:285:VAL:HG22	1.93	0.51
1:Aa:231:ALA:HB3	1:Ab:195:LYS:HG3	1.92	0.51
1:Ac:112:ASN:HD21	1:Ac:224:ALA:HB1	1.75	0.51
1:Ao:139:GLY:HA3	1:Ap:148:TYR:HD1	1.74	0.51
1:Ay:240:THR:HG22	1:Ay:244:MET:HE2	1.93	0.51
2:Bt:360:ILE:HG22	2:Bv:136:ASN:HB2	1.91	0.51
3:Cp:93:ARG:HG2	3:Cp:102:VAL:HG23	1.92	0.51
4:Dx:249:PHE:HB3	4:Dx:254:LEU:HD23	1.93	0.51
1:Aa:112:ASN:HD21	1:Aa:224:ALA:HB1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:231:ALA:HB3	1:Ah:195:LYS:HG3	1.92	0.51
1:An:113:GLU:HB2	1:An:172:MET:HB3	1.93	0.51
2:Ba:360:ILE:HG22	2:Bc:136:ASN:HB2	1.90	0.51
2:Bw:21:ILE:HG23	2:Bw:197:LEU:HD11	1.92	0.51
2:Bw:360:ILE:HG22	2:By:136:ASN:HB2	1.91	0.51
2:By:21:ILE:HG23	2:By:197:LEU:HD11	1.92	0.51
4:Dj:223:THR:HG22	4:Dj:285:VAL:HG22	1.93	0.51
1:Aa:184:LEU:HD12	1:Aa:188:ASN:HB2	1.93	0.51
1:Af:240:THR:HG22	1:Af:244:MET:HE2	1.92	0.51
1:At:184:LEU:HD12	1:At:188:ASN:HB2	1.92	0.51
1:Aw:232:ARG:HH22	1:Ax:194:GLU:HG3	1.75	0.51
1:Ay:184:LEU:HD12	1:Ay:188:ASN:HB2	1.93	0.51
2:Ba:136:ASN:HB3	2:By:255:ARG:HH12	1.76	0.51
2:Bd:342:MET:HE2	2:Bf:138:VAL:HG21	1.92	0.51
2:Bk:224:ARG:HH21	3:Cb:368:GLN:HB3	1.75	0.51
3:Ch:262:TRP:HA	3:Ch:267:GLY:HA3	1.93	0.51
4:Dg:78:ARG:HB3	4:Dg:143:GLN:HE22	1.75	0.51
4:Dt:223:THR:HG22	4:Dt:285:VAL:HG22	1.93	0.51
1:Aj:112:ASN:HD21	1:Aj:224:ALA:HB1	1.76	0.51
1:Ak:231:ALA:HB3	1:Al:195:LYS:HG3	1.93	0.51
1:Ak:240:THR:HG22	1:Ak:244:MET:HE2	1.93	0.51
2:Bc:153:VAL:HG21	2:Bd:148:ASP:HB3	1.93	0.51
2:Bh:87:ALA:HB2	2:Bh:101:ILE:HG22	1.92	0.51
2:Bv:255:ARG:HH12	2:Bx:136:ASN:HB3	1.76	0.51
2:Bv:342:MET:HE2	2:Bx:138:VAL:HG21	1.92	0.51
2:Bw:87:ALA:HB2	2:Bw:101:ILE:HG22	1.93	0.51
3:Ca:262:TRP:HA	3:Ca:267:GLY:HA3	1.92	0.51
3:Cn:262:TRP:HA	3:Cn:267:GLY:HA3	1.92	0.51
3:Co:78:TYR:HD2	3:Co:88:ILE:HB	1.76	0.51
3:Cv:262:TRP:HA	3:Cv:267:GLY:HA3	1.93	0.51
4:Df:249:PHE:HB3	4:Df:254:LEU:HD23	1.93	0.51
1:Ah:112:ASN:HD21	1:Ah:224:ALA:HB1	1.76	0.50
2:Bd:153:VAL:HG21	2:Be:148:ASP:HB3	1.93	0.50
2:Bh:153:VAL:HG21	2:Bi:148:ASP:HB3	1.93	0.50
2:Bv:122:LEU:HB2	2:Bv:131:ALA:HB3	1.92	0.50
2:By:87:ALA:HB2	2:By:101:ILE:HG22	1.93	0.50
3:Cn:92:GLU:HB2	3:Cn:103:ARG:HB3	1.92	0.50
4:Dx:223:THR:HG22	4:Dx:285:VAL:HG22	1.93	0.50
1:Ad:232:ARG:HH22	1:Ae:194:GLU:HG3	1.76	0.50
1:Ah:113:GLU:HB2	1:Ah:172:MET:HB3	1.93	0.50
1:Ai:232:ARG:HH22	1:Aj:194:GLU:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:232:ARG:HH22	1:Al:194:GLU:HG3	1.76	0.50
1:Aq:139:GLY:HA3	1:Ar:148:TYR:HD1	1.76	0.50
1:Ay:36:ASP:HB3	1:Ay:39:GLU:HG2	1.93	0.50
2:Bp:21:ILE:HG23	2:Bp:197:LEU:HD11	1.92	0.50
2:Bs:122:LEU:HB2	2:Bs:131:ALA:HB3	1.93	0.50
3:Cc:93:ARG:HG2	3:Cc:102:VAL:HG23	1.93	0.50
3:Cf:255:ASP:HB3	3:Cf:258:SER:HB3	1.93	0.50
1:Af:231:ALA:HB3	1:Ag:195:LYS:HG3	1.93	0.50
1:Am:139:GLY:HA3	1:An:148:TYR:HD1	1.76	0.50
1:An:184:LEU:HD12	1:An:188:ASN:HB2	1.92	0.50
1:Ar:139:GLY:HA3	1:As:148:TYR:HD1	1.76	0.50
1:Av:64:PRO:HB2	1:Aw:38:VAL:HG13	1.94	0.50
2:Bp:153:VAL:HG21	2:Bq:148:ASP:HB3	1.93	0.50
2:Bq:342:MET:HE2	2:Bs:138:VAL:HG21	1.93	0.50
2:Bw:342:MET:HE2	2:By:138:VAL:HG21	1.94	0.50
3:Cr:249:PRO:HG2	3:Cr:252:SER:HB3	1.94	0.50
3:Cz:255:ASP:HB3	3:Cz:258:SER:HB3	1.92	0.50
1:Af:232:ARG:HH22	1:Ag:194:GLU:HG3	1.76	0.50
1:Aw:125:LEU:HB2	1:Aw:160:PHE:HB3	1.94	0.50
2:Bj:122:LEU:HB2	2:Bj:131:ALA:HB3	1.92	0.50
3:Cm:56:PHE:HD1	5:Gm:139:LYS:HE2	1.76	0.50
3:Co:80:PHE:HA	5:Fo:136:VAL:HG21	1.93	0.50
3:Cs:249:PRO:HG2	3:Cs:252:SER:HB3	1.93	0.50
4:Dp:249:PHE:HB3	4:Dp:254:LEU:HD23	1.93	0.50
1:Ae:113:GLU:HB2	1:Ae:172:MET:HB3	1.93	0.50
1:Ai:240:THR:HG22	1:Ai:244:MET:HE2	1.94	0.50
1:Am:231:ALA:HB3	1:An:195:LYS:HG3	1.93	0.50
2:Bj:153:VAL:HG21	2:Bk:148:ASP:HB3	1.93	0.50
2:Bo:224:ARG:HH21	3:Cf:368:GLN:HB2	1.77	0.50
3:Cv:85:VAL:HG22	3:Cv:108:ILE:HG12	1.93	0.50
1:Aa:139:GLY:HA3	1:Ab:148:TYR:HD1	1.76	0.50
1:Al:125:LEU:HB3	1:Ao:244:MET:HE3	1.92	0.50
2:Bc:224:ARG:HH21	3:Ct:368:GLN:HB2	1.77	0.50
2:Be:255:ARG:HH12	2:Bg:136:ASN:HB3	1.77	0.50
2:Bg:255:ARG:HH12	2:Bi:136:ASN:HB3	1.77	0.50
3:Cm:78:TYR:HD2	3:Cm:88:ILE:HB	1.76	0.50
3:Cm:249:PRO:HG2	3:Cm:252:SER:HB3	1.94	0.50
4:Dz:219:VAL:HG21	4:Dz:254:LEU:HD21	1.93	0.50
1:Ab:139:GLY:HA3	1:Ac:148:TYR:HD1	1.77	0.50
1:Ab:240:THR:HG22	1:Ab:244:MET:HE2	1.93	0.50
1:Ad:240:THR:HG22	1:Ad:244:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:184:LEU:HD12	1:Ao:188:ASN:HB2	1.92	0.50
1:Ap:34:THR:HG21	3:Cf:247:PRO:HB2	1.93	0.50
1:Ar:231:ALA:HB3	1:As:195:LYS:HG3	1.94	0.50
2:Bj:255:ARG:HH12	2:Bl:136:ASN:HB3	1.77	0.50
2:Bk:21:ILE:HG23	2:Bk:197:LEU:HD11	1.93	0.50
2:Bl:153:VAL:HG21	2:Bm:148:ASP:HB3	1.93	0.50
2:Bq:255:ARG:HH12	2:Bs:136:ASN:HB3	1.76	0.50
2:Br:122:LEU:HB2	2:Br:131:ALA:HB3	1.92	0.50
3:Ca:249:PRO:HG2	3:Ca:252:SER:HB3	1.94	0.50
4:Dp:223:THR:HG22	4:Dp:285:VAL:HG22	1.93	0.50
4:Dt:249:PHE:HB3	4:Dt:254:LEU:HD23	1.93	0.50
4:Dx:219:VAL:HG21	4:Dx:254:LEU:HD21	1.93	0.50
1:Ad:87:ASN:HB3	1:Ad:90:SER:HB2	1.93	0.50
1:As:36:ASP:HB3	1:As:39:GLU:HG2	1.94	0.50
1:Ax:139:GLY:HA3	1:Ay:148:TYR:HD1	1.76	0.50
1:Ax:232:ARG:HH22	1:Ay:194:GLU:HG3	1.75	0.50
2:Bn:87:ALA:HB2	2:Bn:101:ILE:HG22	1.93	0.50
2:Bq:185:ASN:HB3	2:Br:97:GLN:HE21	1.77	0.50
3:Cb:78:TYR:HD2	3:Cb:88:ILE:HB	1.76	0.50
4:Dt:219:VAL:HG21	4:Dt:254:LEU:HD21	1.94	0.50
1:Aa:232:ARG:HH22	1:Ab:194:GLU:HG3	1.77	0.50
2:Bg:87:ALA:HB2	2:Bg:101:ILE:HG22	1.93	0.50
2:Bk:87:ALA:HB2	2:Bk:101:ILE:HG22	1.94	0.50
2:Bk:342:MET:HE2	2:Bm:138:VAL:HG21	1.93	0.50
2:Bt:342:MET:HE2	2:Bv:138:VAL:HG21	1.94	0.50
1:Ai:231:ALA:HB3	1:Aj:195:LYS:HG3	1.93	0.49
2:Bk:255:ARG:HH12	2:Bm:136:ASN:HB3	1.77	0.49
2:Bs:224:ARG:HH21	3:Cj:368:GLN:HB2	1.77	0.49
2:Bt:21:ILE:HG23	2:Bt:197:LEU:HD11	1.93	0.49
2:Bx:21:ILE:HG23	2:Bx:197:LEU:HD11	1.93	0.49
3:Cf:56:PHE:HD1	5:Gf:139:LYS:HE2	1.76	0.49
3:Cr:78:TYR:HD2	3:Cr:88:ILE:HB	1.76	0.49
3:Cy:153:ILE:HG21	3:Cy:195:MET:HE1	1.94	0.49
3:Cy:223:GLU:HG2	3:Cy:239:THR:HG22	1.94	0.49
4:Dr:249:PHE:HB3	4:Dr:254:LEU:HD23	1.93	0.49
1:Ad:139:GLY:HA3	1:Ae:148:TYR:HD1	1.76	0.49
1:Ak:87:ASN:HB3	1:Ak:90:SER:HB2	1.94	0.49
1:Au:139:GLY:HA3	1:Av:148:TYR:HD1	1.76	0.49
1:Av:184:LEU:HD12	1:Av:188:ASN:HB2	1.94	0.49
2:By:122:LEU:HB2	2:By:131:ALA:HB3	1.94	0.49
4:Dl:219:VAL:HG21	4:Dl:254:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aq:36:ASP:HB3	1:Aq:39:GLU:HG2	1.94	0.49
2:Bb:255:ARG:HH12	2:Bd:136:ASN:HB3	1.77	0.49
2:Bm:122:LEU:HB2	2:Bm:131:ALA:HB3	1.93	0.49
2:Bp:185:ASN:HB3	2:Bq:97:GLN:HE21	1.76	0.49
2:Br:255:ARG:HH12	2:Bt:136:ASN:HB3	1.76	0.49
2:Bs:21:ILE:HG23	2:Bs:197:LEU:HD11	1.94	0.49
2:By:153:VAL:HG21	2:Bz:148:ASP:HB3	1.93	0.49
2:By:224:ARG:HH21	3:Cp:368:GLN:HB2	1.77	0.49
3:Cz:91:GLU:HG2	3:Cz:92:GLU:HG3	1.94	0.49
4:Dz:249:PHE:HB3	4:Dz:254:LEU:HD23	1.94	0.49
2:Bg:153:VAL:HG21	2:Bh:148:ASP:HB3	1.92	0.49
2:Bg:189:SER:HA	2:Bg:216:ALA:HB2	1.95	0.49
2:Bh:189:SER:HA	2:Bh:216:ALA:HB2	1.95	0.49
1:Ap:184:LEU:HD12	1:Ap:188:ASN:HB2	1.93	0.49
2:Bd:255:ARG:HH12	2:Bf:136:ASN:HB3	1.77	0.49
2:Bi:122:LEU:HB2	2:Bi:131:ALA:HB3	1.94	0.49
3:Cb:85:VAL:HG22	3:Cb:108:ILE:HG12	1.94	0.49
3:Ce:78:TYR:HD2	3:Ce:88:ILE:HB	1.78	0.49
4:Dn:223:THR:HG22	4:Dn:285:VAL:HG22	1.94	0.49
1:As:184:LEU:HD12	1:As:188:ASN:HB2	1.95	0.49
2:Ba:342:MET:HE2	2:Bc:138:VAL:HG21	1.93	0.49
2:Bc:21:ILE:HG23	2:Bc:197:LEU:HD11	1.93	0.49
2:Bg:21:ILE:HG23	2:Bg:197:LEU:HD11	1.94	0.49
2:Bh:272:VAL:HG22	2:Bi:260:VAL:HG22	1.94	0.49
4:Dp:37:GLN:HG3	4:Dp:49:VAL:HG23	1.94	0.49
4:Dv:249:PHE:HB3	4:Dv:254:LEU:HD23	1.94	0.49
1:Am:129:ASN:HB2	1:Am:156:ASN:HB3	1.95	0.49
1:At:36:ASP:HB3	1:At:39:GLU:HG2	1.95	0.49
2:Bh:342:MET:HE2	2:Bj:138:VAL:HG21	1.93	0.49
3:Co:27:GLU:HG3	5:Go:134:GLN:HE22	1.77	0.49
3:Cu:255:ASP:HB3	3:Cu:258:SER:HB3	1.94	0.49
1:Aj:139:GLY:HA3	1:Ak:148:TYR:HD1	1.77	0.49
1:At:64:PRO:HB2	1:Au:38:VAL:HG13	1.95	0.49
2:Bb:153:VAL:HG21	2:Bc:148:ASP:HB3	1.94	0.49
2:Bf:255:ARG:HH12	2:Bh:136:ASN:HB3	1.78	0.49
2:Bj:21:ILE:HG23	2:Bj:197:LEU:HD11	1.94	0.49
2:Bs:342:MET:HE2	2:Bu:138:VAL:HG21	1.94	0.49
2:Bx:122:LEU:HB2	2:Bx:131:ALA:HB3	1.94	0.49
2:Bx:272:VAL:HG22	2:By:260:VAL:HG22	1.95	0.49
3:Cm:80:PHE:HA	5:Fm:136:VAL:HG21	1.93	0.49
4:Dh:249:PHE:HB3	4:Dh:254:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:129:ASN:HB2	1:Ak:156:ASN:HB3	1.95	0.49
1:Ap:240:THR:HG22	1:Ap:244:MET:HE2	1.93	0.49
1:Aw:112:ASN:HD21	1:Aw:224:ALA:HB1	1.78	0.49
1:Ay:139:GLY:HA3	1:Az:148:TYR:HD1	1.78	0.49
2:Bg:342:MET:HE2	2:Bi:138:VAL:HG21	1.93	0.49
2:Bl:342:MET:HE2	2:Bn:138:VAL:HG21	1.94	0.49
2:Bt:122:LEU:HB2	2:Bt:131:ALA:HB3	1.94	0.49
3:Ct:223:GLU:HG2	3:Ct:239:THR:HG22	1.95	0.49
3:Cw:167:VAL:HG21	3:Cw:191:ALA:HB2	1.95	0.49
1:Ae:125:LEU:HB2	1:Ae:160:PHE:HB3	1.95	0.49
2:Bc:272:VAL:HG22	2:Bd:260:VAL:HG22	1.95	0.49
2:Bk:153:VAL:HG21	2:Bl:148:ASP:HB3	1.93	0.49
2:Bz:21:ILE:HG23	2:Bz:197:LEU:HD11	1.94	0.49
3:Cq:167:VAL:HG21	3:Cq:191:ALA:HB2	1.94	0.49
4:De:141:ASP:HB2	4:De:149:ILE:HG12	1.94	0.49
1:Ak:36:ASP:HB3	1:Ak:39:GLU:HG2	1.95	0.48
1:Au:232:ARG:HH22	1:Av:194:GLU:HG3	1.77	0.48
1:Av:113:GLU:HB2	1:Av:172:MET:HB3	1.95	0.48
2:Bb:342:MET:HE2	2:Bd:138:VAL:HG21	1.94	0.48
2:Bp:342:MET:HE2	2:Br:138:VAL:HG21	1.95	0.48
3:Cg:92:GLU:HB2	3:Cg:103:ARG:HB3	1.94	0.48
4:Dj:219:VAL:HG21	4:Dj:254:LEU:HD21	1.95	0.48
2:Bn:122:LEU:HB2	2:Bn:131:ALA:HB3	1.94	0.48
2:Bn:255:ARG:HH12	2:Bp:136:ASN:HB3	1.78	0.48
2:Br:342:MET:HE2	2:Bt:138:VAL:HG21	1.95	0.48
3:Ca:80:PHE:HA	5:Fa:136:VAL:HG21	1.94	0.48
3:Cm:92:GLU:HB2	3:Cm:103:ARG:HB3	1.94	0.48
3:Cr:223:GLU:HG2	3:Cr:239:THR:HG22	1.94	0.48
3:Ct:80:PHE:HA	5:Ft:136:VAL:HG21	1.95	0.48
4:Dl:249:PHE:HB3	4:Dl:254:LEU:HD23	1.94	0.48
1:Aq:64:PRO:HB2	1:Ar:38:VAL:HG13	1.96	0.48
2:Bm:255:ARG:HH12	2:Bo:136:ASN:HB3	1.78	0.48
2:Bs:255:ARG:HH12	2:Bu:136:ASN:HB3	1.77	0.48
2:Bu:224:ARG:HH21	3:Cl:368:GLN:HB2	1.78	0.48
1:Ap:87:ASN:HB3	1:Ap:90:SER:HB2	1.95	0.48
1:Av:125:LEU:HB2	1:Av:160:PHE:HB3	1.94	0.48
2:Bf:153:VAL:HG21	2:Bg:148:ASP:HB3	1.94	0.48
2:Bp:255:ARG:HH12	2:Br:136:ASN:HB3	1.78	0.48
2:Bq:122:LEU:HB2	2:Bq:131:ALA:HB3	1.94	0.48
2:Br:21:ILE:HG23	2:Br:197:LEU:HD11	1.95	0.48
2:Bt:272:VAL:HG22	2:Bu:260:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ck:92:GLU:HB2	3:Ck:103:ARG:HB3	1.95	0.48
1:Aa:36:ASP:HB3	1:Aa:39:GLU:HG2	1.94	0.48
1:Ae:139:GLY:HA3	1:Af:148:TYR:HD1	1.79	0.48
1:Au:184:LEU:HD12	1:Au:188:ASN:HB2	1.95	0.48
2:Bb:122:LEU:HB2	2:Bb:131:ALA:HB3	1.96	0.48
2:Bg:185:ASN:HB3	2:Bh:97:GLN:HE21	1.79	0.48
2:Bi:21:ILE:HG23	2:Bi:197:LEU:HD11	1.95	0.48
2:Bo:255:ARG:HH12	2:Bq:136:ASN:HB3	1.79	0.48
2:Bw:255:ARG:HH12	2:By:136:ASN:HB3	1.78	0.48
3:Cl:92:GLU:HB2	3:Cl:103:ARG:HB3	1.93	0.48
3:Cn:255:ASP:HB3	3:Cn:258:SER:HB3	1.95	0.48
3:Cv:255:ASP:HB3	3:Cv:258:SER:HB3	1.94	0.48
3:Cy:255:ASP:HB3	3:Cy:258:SER:HB3	1.95	0.48
1:Ai:139:GLY:HA3	1:Aj:148:TYR:HD1	1.78	0.48
1:At:112:ASN:HD21	1:At:224:ALA:HB1	1.79	0.48
1:Az:240:THR:HG22	1:Az:244:MET:HE2	1.95	0.48
2:Bm:21:ILE:HG23	2:Bm:197:LEU:HD11	1.94	0.48
2:Bv:224:ARG:HH21	3:Cm:368:GLN:HB2	1.77	0.48
4:Dg:141:ASP:HB2	4:Dg:149:ILE:HG12	1.94	0.48
1:Ah:125:LEU:HB2	1:Ah:160:PHE:HB3	1.96	0.48
1:Ap:139:GLY:HA3	1:Aq:148:TYR:HD1	1.79	0.48
3:Cw:239:THR:HG21	3:Cx:155:ARG:HD3	1.95	0.48
1:Ax:125:LEU:HB2	1:Ax:160:PHE:HB3	1.96	0.48
2:Bi:153:VAL:HG21	2:Bj:148:ASP:HB3	1.94	0.48
2:Bl:272:VAL:HG22	2:Bm:260:VAL:HG22	1.96	0.48
2:Br:153:VAL:HG21	2:Bs:148:ASP:HB3	1.96	0.48
2:Bx:255:ARG:HH12	2:Bz:136:ASN:HB3	1.79	0.48
3:Cu:78:TYR:HD2	3:Cu:88:ILE:HB	1.77	0.48
4:Dz:37:GLN:HG3	4:Dz:49:VAL:HG23	1.96	0.48
1:Ae:119:LYS:HB3	1:Ag:199:LEU:HD12	1.96	0.48
1:Ae:240:THR:HG22	1:Ae:244:MET:HE2	1.95	0.48
1:Af:36:ASP:HB3	1:Af:39:GLU:HG2	1.95	0.48
1:At:139:GLY:HA3	1:Au:148:TYR:HD1	1.79	0.48
2:Bn:272:VAL:HG22	2:Bo:260:VAL:HG22	1.96	0.48
3:Cn:249:PRO:HG2	3:Cn:252:SER:HB3	1.95	0.48
1:Ae:129:ASN:HB2	1:Ae:156:ASN:HB3	1.96	0.48
1:Ah:139:GLY:HA3	1:Ai:148:TYR:HD1	1.79	0.48
2:Bp:272:VAL:HG22	2:Bq:260:VAL:HG22	1.96	0.48
3:Cq:92:GLU:HB2	3:Cq:103:ARG:HB3	1.95	0.48
3:Cx:92:GLU:HB2	3:Cx:103:ARG:HB2	1.95	0.48
1:Av:139:GLY:HA3	1:Aw:148:TYR:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Br:189:SER:HA	2:Br:216:ALA:HB2	1.96	0.47
3:Ca:255:ASP:HB3	3:Ca:258:SER:HB3	1.96	0.47
3:Cq:262:TRP:HA	3:Cq:267:GLY:HA3	1.95	0.47
3:Cv:28:VAL:HG13	3:Cv:49:ALA:HB1	1.96	0.47
1:Ad:129:ASN:HB2	1:Ad:156:ASN:HB3	1.96	0.47
1:An:129:ASN:HB2	1:An:156:ASN:HB3	1.97	0.47
1:Ax:154:LEU:HD21	1:Az:258:LEU:HD11	1.96	0.47
2:Ba:255:ARG:HH12	2:Bc:136:ASN:HB3	1.79	0.47
2:Bi:189:SER:HA	2:Bi:216:ALA:HB2	1.96	0.47
2:Bq:272:VAL:HG22	2:Br:260:VAL:HG22	1.95	0.47
3:Cb:88:ILE:HG12	3:Cb:106:ILE:HG23	1.96	0.47
3:Ci:92:GLU:HB2	3:Ci:103:ARG:HB3	1.96	0.47
3:Cl:56:PHE:HD1	5:Gl:139:LYS:HE2	1.79	0.47
4:Dj:169:ILE:HG13	4:Dj:172:LEU:HD12	1.95	0.47
1:Aa:64:PRO:HB2	1:Ab:38:VAL:HG13	1.96	0.47
1:Al:125:LEU:HB2	1:Al:160:PHE:HB3	1.96	0.47
1:Al:129:ASN:HB2	1:Al:156:ASN:HB3	1.96	0.47
1:Ar:184:LEU:HD12	1:Ar:188:ASN:HB2	1.96	0.47
1:Aw:64:PRO:HB2	1:Ax:38:VAL:HG13	1.96	0.47
2:Bm:189:SER:HA	2:Bm:216:ALA:HB2	1.97	0.47
2:Bo:272:VAL:HG22	2:Bp:260:VAL:HG22	1.95	0.47
2:Bu:342:MET:HE2	2:Bw:138:VAL:HG21	1.95	0.47
1:Ak:64:PRO:HB2	1:Al:38:VAL:HG13	1.95	0.47
1:Ar:36:ASP:HB3	1:Ar:39:GLU:HG2	1.96	0.47
1:At:129:ASN:HB2	1:At:156:ASN:HB3	1.97	0.47
2:Bh:268:LYS:HB2	2:Bh:353:ALA:HB1	1.96	0.47
2:Bi:272:VAL:HG22	2:Bj:260:VAL:HG22	1.96	0.47
2:Bv:272:VAL:HG22	2:Bw:260:VAL:HG22	1.97	0.47
3:Cd:255:ASP:HB3	3:Cd:258:SER:HB3	1.96	0.47
4:Dn:249:PHE:HB3	4:Dn:254:LEU:HD23	1.95	0.47
1:Ai:129:ASN:HB2	1:Ai:156:ASN:HB3	1.96	0.47
2:Bc:185:ASN:HB3	2:Bd:97:GLN:HE21	1.79	0.47
2:Be:272:VAL:HG22	2:Bf:260:VAL:HG22	1.97	0.47
2:Bu:272:VAL:HG22	2:Bv:260:VAL:HG22	1.96	0.47
3:Cb:255:ASP:HB3	3:Cb:258:SER:HB3	1.96	0.47
3:Co:255:ASP:HB3	3:Co:258:SER:HB3	1.95	0.47
3:Cq:209:LYS:HD2	3:Cq:212:GLN:HB2	1.97	0.47
2:Bg:272:VAL:HG22	2:Bh:260:VAL:HG22	1.97	0.47
2:Bm:272:VAL:HG22	2:Bn:260:VAL:HG22	1.95	0.47
1:Ao:129:ASN:HB2	1:Ao:156:ASN:HB3	1.97	0.47
2:Bb:136:ASN:HB3	2:Bz:255:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bf:272:VAL:HG22	2:Bg:260:VAL:HG22	1.97	0.47
2:Bj:272:VAL:HG22	2:Bk:260:VAL:HG22	1.97	0.47
2:Bm:224:ARG:HH21	3:Cd:368:GLN:HB2	1.79	0.47
2:Bo:342:MET:HE2	2:Bq:138:VAL:HG21	1.95	0.47
2:Bu:255:ARG:HH12	2:Bw:136:ASN:HB3	1.80	0.47
3:Cb:88:ILE:HG23	3:Cb:106:ILE:HG12	1.96	0.47
3:Cc:249:PRO:HG2	3:Cc:252:SER:HB3	1.97	0.47
3:Ch:92:GLU:HB2	3:Ch:103:ARG:HB3	1.95	0.47
3:Cy:92:GLU:HB2	3:Cy:103:ARG:HB3	1.96	0.47
4:Dj:217:ASP:HA	4:Dj:258:ARG:HD3	1.97	0.47
2:Bf:268:LYS:HB2	2:Bf:353:ALA:HB1	1.96	0.47
2:Bj:342:MET:HE2	2:Bl:138:VAL:HG21	1.96	0.47
2:Bl:21:ILE:HG23	2:Bl:197:LEU:HD11	1.97	0.47
2:Bn:189:SER:HA	2:Bn:216:ALA:HB2	1.97	0.47
2:Bn:342:MET:HE2	2:Bp:138:VAL:HG21	1.96	0.47
3:Cu:249:PRO:HG2	3:Cu:252:SER:HB3	1.95	0.47
4:Dp:90:SER:HB2	4:Dp:104:ILE:HD11	1.97	0.47
1:As:87:ASN:HB3	1:As:90:SER:HB2	1.96	0.47
2:Bc:255:ARG:HH12	2:Be:136:ASN:HB3	1.79	0.47
2:Bl:189:SER:HA	2:Bl:216:ALA:HB2	1.97	0.47
2:Bo:189:SER:HA	2:Bo:216:ALA:HB2	1.96	0.47
2:Bu:122:LEU:HB2	2:Bu:131:ALA:HB3	1.96	0.47
2:Bx:185:ASN:HB3	2:By:97:GLN:HE21	1.80	0.47
2:Bx:189:SER:HA	2:Bx:216:ALA:HB2	1.97	0.47
3:Cw:92:GLU:HB2	3:Cw:103:ARG:HB3	1.96	0.47
1:Ab:87:ASN:HB3	1:Ab:90:SER:HB2	1.95	0.47
1:Ab:129:ASN:HB2	1:Ab:156:ASN:HB3	1.97	0.47
1:Ah:154:LEU:HD21	1:Aj:258:LEU:HD11	1.96	0.47
1:At:87:ASN:HB3	1:At:90:SER:HB2	1.97	0.47
2:Bj:189:SER:HA	2:Bj:216:ALA:HB2	1.96	0.47
2:By:189:SER:HA	2:By:216:ALA:HB2	1.98	0.47
3:Cc:209:LYS:HD2	3:Cc:212:GLN:HB2	1.97	0.47
3:Cr:262:TRP:HA	3:Cr:267:GLY:HA3	1.95	0.47
3:Cy:85:VAL:HG22	3:Cy:108:ILE:HG12	1.97	0.47
1:Ab:125:LEU:HB2	1:Ab:160:PHE:HB3	1.96	0.46
1:Ag:87:ASN:HB3	1:Ag:90:SER:HB2	1.96	0.46
1:Aj:154:LEU:HD21	1:Al:258:LEU:HD11	1.96	0.46
1:Al:87:ASN:HB3	1:Al:90:SER:HB2	1.97	0.46
2:Bm:342:MET:HE2	2:Bo:138:VAL:HG21	1.96	0.46
2:Br:272:VAL:HG22	2:Bs:260:VAL:HG22	1.97	0.46
2:Bt:255:ARG:HH12	2:Bv:136:ASN:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cg:167:VAL:HG21	3:Cg:191:ALA:HB2	1.98	0.46
4:Dn:37:GLN:HG3	4:Dn:49:VAL:HG23	1.97	0.46
1:Ac:36:ASP:HB3	1:Ac:39:GLU:HG2	1.96	0.46
1:Ac:129:ASN:HB2	1:Ac:156:ASN:HB3	1.98	0.46
1:Ad:36:ASP:HB3	1:Ad:39:GLU:HG2	1.96	0.46
1:Ai:154:LEU:HD21	1:Ak:258:LEU:HD11	1.95	0.46
1:Aw:36:ASP:HB3	1:Aw:39:GLU:HG2	1.96	0.46
2:Bb:83:VAL:HG12	2:Bb:105:SER:HA	1.97	0.46
2:Bd:268:LYS:HB2	2:Bd:353:ALA:HB1	1.97	0.46
2:Bh:91:ALA:HB1	2:Bh:174:ASN:HD21	1.80	0.46
1:Ab:36:ASP:HB3	1:Ab:39:GLU:HG2	1.96	0.46
1:Ah:36:ASP:HB3	1:Ah:39:GLU:HG2	1.96	0.46
1:Av:87:ASN:HB3	1:Av:90:SER:HB2	1.97	0.46
2:Ba:185:ASN:HB3	2:Bb:97:GLN:HE21	1.80	0.46
2:Bs:272:VAL:HG22	2:Bt:260:VAL:HG22	1.97	0.46
2:Bt:268:LYS:HB2	2:Bt:353:ALA:HB1	1.96	0.46
2:Bv:205:LEU:HD11	2:Bv:236:ILE:HD11	1.97	0.46
2:Bx:342:MET:HE2	2:Bz:138:VAL:HG21	1.97	0.46
3:Cb:93:ARG:HG2	3:Cb:102:VAL:HG23	1.96	0.46
1:Ae:87:ASN:HB3	1:Ae:90:SER:HB2	1.95	0.46
1:Af:154:LEU:HD21	1:Ah:258:LEU:HD11	1.98	0.46
2:Bd:272:VAL:HG22	2:Be:260:VAL:HG22	1.96	0.46
2:Bp:189:SER:HA	2:Bp:216:ALA:HB2	1.96	0.46
2:Bz:189:SER:HA	2:Bz:216:ALA:HB2	1.97	0.46
3:Cd:249:PRO:HG2	3:Cd:252:SER:HB3	1.95	0.46
3:Ci:209:LYS:HD3	3:Ci:212:GLN:HE21	1.81	0.46
3:Cx:226:VAL:HB	3:Cx:236:MET:HB3	1.98	0.46
1:Aa:125:LEU:HB2	1:Aa:160:PHE:HB3	1.98	0.46
2:Bf:315:MET:HG2	2:Bg:328:VAL:HG22	1.98	0.46
2:Bo:21:ILE:HG23	2:Bo:197:LEU:HD11	1.97	0.46
2:Bu:189:SER:HA	2:Bu:216:ALA:HB2	1.96	0.46
2:Bw:272:VAL:HG22	2:Bx:260:VAL:HG22	1.96	0.46
3:Cd:269:MET:HE3	3:Cd:269:MET:HB3	1.79	0.46
3:Ce:249:PRO:HG2	3:Ce:252:SER:HB3	1.97	0.46
1:Aa:148:TYR:HD1	1:Az:139:GLY:HA3	1.80	0.46
1:Af:119:LYS:HD2	1:Ah:199:LEU:HB2	1.98	0.46
1:Ah:87:ASN:HB3	1:Ah:90:SER:HB2	1.97	0.46
1:Aj:87:ASN:HB3	1:Aj:90:SER:HB2	1.97	0.46
1:Aj:129:ASN:HB2	1:Aj:156:ASN:HB3	1.97	0.46
1:Ao:36:ASP:HB3	1:Ao:39:GLU:HG2	1.97	0.46
1:As:125:LEU:HB2	1:As:160:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cc:167:VAL:HG21	3:Cc:191:ALA:HB2	1.98	0.46
3:Cq:249:PRO:HG2	3:Cq:252:SER:HB3	1.97	0.46
1:Ak:139:GLY:HA3	1:Al:148:TYR:HD1	1.81	0.46
1:Aw:139:GLY:HA3	1:Ax:148:TYR:HD1	1.80	0.46
1:Ay:125:LEU:HB2	1:Ay:160:PHE:HB3	1.98	0.46
2:Bc:268:LYS:HB2	2:Bc:353:ALA:HB1	1.98	0.46
2:Bv:189:SER:HA	2:Bv:216:ALA:HB2	1.97	0.46
3:Ca:28:VAL:HG13	3:Ca:49:ALA:HB1	1.98	0.46
4:Dj:90:SER:HB2	4:Dj:104:ILE:HD11	1.98	0.46
1:Ap:129:ASN:HB2	1:Ap:156:ASN:HB3	1.97	0.46
1:Aq:87:ASN:HB3	1:Aq:90:SER:HB2	1.97	0.46
3:Cd:167:VAL:HG21	3:Cd:191:ALA:HB2	1.98	0.46
3:Cg:249:PRO:HG2	3:Cg:252:SER:HB3	1.97	0.46
3:Cv:201:ASP:HB3	3:Cv:221:ALA:HB3	1.98	0.46
3:Cw:209:LYS:HD2	3:Cw:212:GLN:HB2	1.98	0.46
4:Dj:249:PHE:HB3	4:Dj:254:LEU:HD23	1.97	0.46
1:Aa:129:ASN:HB2	1:Aa:156:ASN:HB3	1.98	0.46
1:Ag:154:LEU:HD21	1:Ai:258:LEU:HD11	1.98	0.46
1:As:139:GLY:HA3	1:At:148:TYR:HD1	1.81	0.46
1:Au:87:ASN:HB3	1:Au:90:SER:HB2	1.97	0.46
1:Ay:87:ASN:HB3	1:Ay:90:SER:HB2	1.98	0.46
2:Bd:205:LEU:HD11	2:Bd:236:ILE:HD11	1.97	0.46
2:By:272:VAL:HG22	2:Bz:260:VAL:HG22	1.97	0.46
3:Cc:255:ASP:HB3	3:Cc:258:SER:HB3	1.97	0.46
3:Ci:255:ASP:HB3	3:Ci:258:SER:HB3	1.96	0.46
3:Cl:249:PRO:HG2	3:Cl:252:SER:HB3	1.96	0.46
3:Cv:269:MET:HE3	3:Cv:269:MET:HB3	1.88	0.46
3:Cw:249:PRO:HG2	3:Cw:252:SER:HB3	1.97	0.46
1:Aa:87:ASN:HB3	1:Aa:90:SER:HB2	1.97	0.46
1:Ai:87:ASN:HB3	1:Ai:90:SER:HB2	1.97	0.46
1:Ax:87:ASN:HB3	1:Ax:90:SER:HB2	1.97	0.46
2:Ba:272:VAL:HG22	2:Bb:260:VAL:HG22	1.98	0.46
2:Bb:272:VAL:HG22	2:Bc:260:VAL:HG22	1.97	0.46
2:Bv:268:LYS:HB2	2:Bv:353:ALA:HB1	1.98	0.46
3:Co:241:ARG:HB3	5:Gp:143:THR:HG21	1.98	0.46
3:Cp:88:ILE:HG23	3:Cp:106:ILE:HG12	1.97	0.46
3:Cy:249:PRO:HG2	3:Cy:252:SER:HB3	1.98	0.46
1:An:139:GLY:HA3	1:Ao:148:TYR:HD1	1.81	0.45
1:As:129:ASN:HB2	1:As:156:ASN:HB3	1.98	0.45
1:Ax:119:LYS:HD2	1:Az:199:LEU:HB2	1.97	0.45
3:Cx:249:PRO:HG2	3:Cx:252:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dm:126:LEU:HD13	4:Dm:162:TYR:HE1	1.81	0.45
1:Af:139:GLY:HA3	1:Ag:148:TYR:HD1	1.81	0.45
1:Al:154:LEU:HD21	1:An:258:LEU:HD11	1.97	0.45
1:Ar:87:ASN:HB3	1:Ar:90:SER:HB2	1.97	0.45
2:Bk:268:LYS:HB2	2:Bk:353:ALA:HB1	1.98	0.45
3:Cb:249:PRO:HG2	3:Cb:252:SER:HB3	1.98	0.45
4:Dp:169:ILE:HG13	4:Dp:172:LEU:HD12	1.97	0.45
1:An:87:ASN:HB3	1:An:90:SER:HB2	1.98	0.45
1:Ax:64:PRO:HB2	1:Ay:38:VAL:HG13	1.98	0.45
1:Az:87:ASN:HB3	1:Az:90:SER:HB2	1.98	0.45
2:Be:350:GLN:HG3	2:Bf:361:ILE:HG21	1.98	0.45
2:Bt:189:SER:HA	2:Bt:216:ALA:HB2	1.98	0.45
3:Cf:28:VAL:HG13	3:Cf:49:ALA:HB1	1.98	0.45
3:Cx:167:VAL:HG21	3:Cx:191:ALA:HB2	1.97	0.45
4:Dk:126:LEU:HD13	4:Dk:162:TYR:HE1	1.82	0.45
4:Do:126:LEU:HD13	4:Do:162:TYR:HE1	1.82	0.45
4:Dz:169:ILE:HG13	4:Dz:172:LEU:HD12	1.99	0.45
5:Gc:134:GLN:HE21	5:Gc:136:VAL:HG22	1.81	0.45
1:Af:129:ASN:HB2	1:Af:156:ASN:HB3	1.98	0.45
1:Av:129:ASN:HB2	1:Av:156:ASN:HB3	1.98	0.45
2:Be:268:LYS:HB2	2:Be:353:ALA:HB1	1.97	0.45
2:Bl:103:VAL:HB	2:Bl:137:LEU:HD21	1.98	0.45
2:Bp:83:VAL:HG12	2:Bp:105:SER:HA	1.99	0.45
2:Bq:315:MET:HG2	2:Br:328:VAL:HG22	1.98	0.45
2:Bw:83:VAL:HG12	2:Bw:105:SER:HA	1.99	0.45
3:Cr:269:MET:HE3	3:Cr:269:MET:HB3	1.88	0.45
3:Cx:326:PHE:HD1	3:Cx:328:ASP:H	1.64	0.45
1:Au:129:ASN:HB2	1:Au:156:ASN:HB3	1.97	0.45
1:Aw:184:LEU:HD12	1:Aw:188:ASN:HB2	1.99	0.45
2:Ba:260:VAL:HG22	2:Bz:272:VAL:HG22	1.98	0.45
2:Bb:189:SER:HA	2:Bb:216:ALA:HB2	1.98	0.45
2:Bj:91:ALA:HB1	2:Bj:174:ASN:HD21	1.82	0.45
2:Bk:272:VAL:HG22	2:Bl:260:VAL:HG22	1.98	0.45
2:Bl:185:ASN:HB3	2:Bm:97:GLN:HE21	1.81	0.45
2:Bq:268:LYS:HB2	2:Bq:353:ALA:HB1	1.99	0.45
3:Ck:239:THR:HG21	3:Cl:155:ARG:HD3	1.98	0.45
3:Ck:269:MET:HE3	3:Ck:269:MET:HB3	1.87	0.45
3:Cp:167:VAL:HG21	3:Cp:191:ALA:HB2	1.98	0.45
3:Cs:269:MET:HE3	3:Cs:269:MET:HB3	1.89	0.45
1:Ac:139:GLY:HA3	1:Ad:148:TYR:HD1	1.82	0.45
1:Ax:184:LEU:HD12	1:Ax:188:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ba:103:VAL:HB	2:Ba:137:LEU:HD21	1.98	0.45
2:Bb:350:GLN:HG3	2:Bc:361:ILE:HG21	1.97	0.45
2:Bd:189:SER:HA	2:Bd:216:ALA:HB2	1.99	0.45
3:Cb:292:PRO:HB3	3:Cb:306:LEU:HD22	1.97	0.45
3:Ch:255:ASP:HB3	3:Ch:258:SER:HB3	1.98	0.45
3:Cx:201:ASP:HB3	3:Cx:221:ALA:HB3	1.99	0.45
4:Dk:175:TYR:HE1	4:Dk:209:TYR:HB2	1.80	0.45
4:Dq:126:LEU:HD13	4:Dq:162:TYR:HE1	1.81	0.45
4:Dx:37:GLN:HG3	4:Dx:49:VAL:HG23	1.98	0.45
2:Bb:268:LYS:HB2	2:Bb:353:ALA:HB1	1.99	0.45
2:Bf:189:SER:HA	2:Bf:216:ALA:HB2	1.99	0.45
2:Bf:350:GLN:HG3	2:Bg:361:ILE:HG21	1.99	0.45
2:Bg:103:VAL:HB	2:Bg:137:LEU:HD21	1.99	0.45
2:Bi:342:MET:HE2	2:Bk:138:VAL:HG21	1.98	0.45
2:Bw:189:SER:HA	2:Bw:216:ALA:HB2	1.99	0.45
3:Ca:164:PHE:HZ	3:Ca:285:ILE:HB	1.81	0.45
3:Cf:249:PRO:HG2	3:Cf:252:SER:HB3	1.97	0.45
3:Cm:255:ASP:HB3	3:Cm:258:SER:HB3	1.99	0.45
3:Ct:28:VAL:HG13	3:Ct:49:ALA:HB1	1.99	0.45
3:Cw:226:VAL:HG21	3:Cw:281:LEU:HD21	1.99	0.45
4:Dm:112:GLN:HE21	4:Dm:112:GLN:HB3	1.59	0.45
4:Dy:112:GLN:HE21	4:Dy:112:GLN:HB3	1.61	0.45
1:Ag:184:LEU:HD12	1:Ag:188:ASN:HB2	1.98	0.45
1:Ah:205:TYR:CZ	1:Ah:236:SER:HB3	2.52	0.45
1:Ap:36:ASP:HB3	1:Ap:39:GLU:HG2	1.98	0.45
1:Aw:134:ASP:HB2	1:Ax:155:LYS:HB2	1.99	0.45
2:Bf:182:ILE:HD12	2:Bf:233:LEU:HD23	1.99	0.45
2:Bs:189:SER:HA	2:Bs:216:ALA:HB2	1.98	0.45
2:Bx:91:ALA:HB1	2:Bx:174:ASN:HD21	1.80	0.45
2:Bz:268:LYS:HB2	2:Bz:353:ALA:HB1	1.98	0.45
3:Ce:167:VAL:HG21	3:Ce:191:ALA:HB2	1.98	0.45
3:Cx:361:PRO:HB2	4:Dq:148:ARG:HD2	1.98	0.45
4:Dd:37:GLN:HG3	4:Dd:49:VAL:HG23	1.99	0.45
4:Dg:175:TYR:HE1	4:Dg:209:TYR:HB2	1.82	0.45
4:Dr:90:SER:HB2	4:Dr:104:ILE:HD11	1.98	0.45
1:Ac:64:PRO:HB2	1:Ad:38:VAL:HG13	1.99	0.45
1:Ae:36:ASP:HB3	1:Ae:39:GLU:HG2	1.98	0.45
1:Ai:36:ASP:HB3	1:Ai:39:GLU:HG2	1.97	0.45
1:Ai:131:ALA:HA	1:Aj:158:ASN:HA	1.99	0.45
1:An:36:ASP:HB3	1:An:39:GLU:HG2	1.98	0.45
2:Bk:189:SER:HA	2:Bk:216:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bn:182:ILE:HD12	2:Bn:233:LEU:HD23	1.99	0.45
2:Bq:189:SER:HA	2:Bq:216:ALA:HB2	1.98	0.45
2:Bu:103:VAL:HB	2:Bu:137:LEU:HD21	1.97	0.45
3:Ce:154:ASN:HD22	3:Ce:154:ASN:HA	1.59	0.45
3:Ck:164:PHE:HZ	3:Ck:285:ILE:HB	1.81	0.45
1:Am:119:LYS:HD2	1:Ao:199:LEU:HB2	1.99	0.45
1:Am:125:LEU:HB2	1:Am:160:PHE:HB3	1.99	0.45
2:Be:224:ARG:HH21	3:Cv:368:GLN:HB2	1.81	0.45
2:Bf:361:ILE:HD12	2:Bg:161:MET:HE1	1.99	0.45
2:Bj:103:VAL:HB	2:Bj:137:LEU:HD21	1.99	0.45
2:Bn:268:LYS:HB2	2:Bn:353:ALA:HB1	1.98	0.45
2:Bz:91:ALA:HB1	2:Bz:174:ASN:HD21	1.82	0.45
3:Cm:164:PHE:HZ	3:Cm:285:ILE:HB	1.81	0.45
3:Cv:249:PRO:HG2	3:Cv:252:SER:HB3	1.98	0.45
3:Cy:269:MET:HE3	3:Cy:269:MET:HB3	1.89	0.45
4:Du:31:PRO:HG3	4:Du:95:TRP:HZ2	1.81	0.45
1:Ab:199:LEU:HB2	1:Az:119:LYS:HD2	1.98	0.44
1:Ac:134:ASP:HB2	1:Ad:155:LYS:HB2	1.99	0.44
1:Ae:131:ALA:HA	1:Af:158:ASN:HA	2.00	0.44
1:Ag:36:ASP:HB3	1:Ag:39:GLU:HG2	1.99	0.44
1:An:125:LEU:HB2	1:An:160:PHE:HB3	2.00	0.44
1:Au:131:ALA:HA	1:Av:158:ASN:HA	1.99	0.44
2:Ba:328:VAL:HG22	2:Bz:315:MET:HG2	1.99	0.44
2:Bd:103:VAL:HB	2:Bd:137:LEU:HD21	1.99	0.44
2:Bj:268:LYS:HB2	2:Bj:353:ALA:HB1	1.99	0.44
2:Bx:123:LYS:HG2	2:Bx:129:VAL:HG22	1.99	0.44
3:Cd:111:SER:HB3	3:Cd:113:THR:HG22	2.00	0.44
3:Ch:26:TYR:HB2	3:Ch:106:ILE:O	2.17	0.44
3:Ck:78:TYR:HD2	3:Ck:88:ILE:HB	1.82	0.44
3:Cy:241:ARG:HB3	5:Gz:143:THR:HG21	1.99	0.44
3:Cy:342:ILE:HG21	3:Cy:367:ILE:HD11	2.00	0.44
1:Aq:129:ASN:HB2	1:Aq:156:ASN:HB3	1.99	0.44
2:Ba:83:VAL:HG12	2:Ba:105:SER:HA	1.99	0.44
2:Bh:315:MET:HG2	2:Bi:328:VAL:HG22	1.99	0.44
2:Bl:268:LYS:HB2	2:Bl:353:ALA:HB1	1.99	0.44
2:By:185:ASN:HB3	2:Bz:97:GLN:HE21	1.82	0.44
3:Cz:28:VAL:HG13	3:Cz:49:ALA:HB1	1.99	0.44
4:Dg:184:ILE:HG12	4:Dg:286:VAL:HG22	1.99	0.44
4:Du:31:PRO:HB3	4:Du:156:VAL:HG21	2.00	0.44
2:Ba:189:SER:HA	2:Ba:216:ALA:HB2	1.98	0.44
2:Bm:103:VAL:HB	2:Bm:137:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bs:123:LYS:HG2	2:Bs:129:VAL:HG22	2.00	0.44
2:Bt:182:ILE:HD12	2:Bt:233:LEU:HD23	2.00	0.44
3:Cg:255:ASP:HB3	3:Cg:258:SER:HB3	1.99	0.44
3:Cq:63:SER:HA	3:Cq:66:ASN:HD21	1.82	0.44
1:Ac:205:TYR:CZ	1:Ac:236:SER:HB3	2.52	0.44
1:Aj:131:ALA:HA	1:Ak:158:ASN:HA	1.99	0.44
1:At:134:ASP:HB2	1:Au:155:LYS:HB2	2.00	0.44
2:Bb:103:VAL:HB	2:Bb:137:LEU:HD21	1.99	0.44
2:Bd:21:ILE:HG23	2:Bd:197:LEU:HD11	1.99	0.44
2:Bi:268:LYS:HB2	2:Bi:353:ALA:HB1	2.00	0.44
2:Bp:122:LEU:HB2	2:Bp:131:ALA:HB3	1.97	0.44
2:Bv:123:LYS:HG2	2:Bv:129:VAL:HG22	2.00	0.44
2:Bx:350:GLN:HG3	2:By:361:ILE:HG21	1.98	0.44
3:Cf:201:ASP:HB3	3:Cf:221:ALA:HB3	1.99	0.44
3:Cj:167:VAL:HG21	3:Cj:191:ALA:HB2	2.00	0.44
3:Cl:373:MET:HE3	3:Cl:373:MET:HB2	1.84	0.44
3:Cn:209:LYS:HD2	3:Cn:212:GLN:HB2	1.98	0.44
3:Cq:342:ILE:HG21	3:Cq:367:ILE:HD11	1.98	0.44
4:Dg:31:PRO:HG3	4:Dg:95:TRP:HZ2	1.83	0.44
4:Dr:37:GLN:HG3	4:Dr:49:VAL:HG23	1.98	0.44
4:Ds:184:ILE:HG12	4:Ds:286:VAL:HG22	1.99	0.44
4:Du:197:LYS:HD3	4:Dv:292:THR:HB	1.99	0.44
1:Ai:200:ASN:HB3	1:Ai:201:THR:H	1.70	0.44
1:An:205:TYR:CZ	1:An:236:SER:HB3	2.53	0.44
2:Be:123:LYS:HG2	2:Be:129:VAL:HG22	1.99	0.44
2:Br:182:ILE:HD12	2:Br:233:LEU:HD23	2.00	0.44
2:Bx:205:LEU:HD11	2:Bx:236:ILE:HD11	2.00	0.44
3:Cb:317:LYS:HG2	3:Cb:345:THR:HB	1.99	0.44
3:Cd:239:THR:HG21	3:Ce:155:ARG:HD3	1.99	0.44
3:Cf:167:VAL:HG21	3:Cf:191:ALA:HB2	2.00	0.44
3:Cn:153:ILE:HG21	3:Cn:195:MET:HE1	1.99	0.44
3:Co:269:MET:HE3	3:Co:269:MET:HB3	1.87	0.44
3:Cr:375:LYS:HE3	3:Cr:377:MET:HE2	2.00	0.44
4:Dm:31:PRO:HB3	4:Dm:156:VAL:HG21	1.99	0.44
4:Ds:126:LEU:HD13	4:Ds:162:TYR:HE1	1.82	0.44
2:Be:185:ASN:HB3	2:Bf:97:GLN:HE21	1.82	0.44
2:Bs:103:VAL:HB	2:Bs:137:LEU:HD21	1.99	0.44
3:Ci:28:VAL:HG13	3:Ci:49:ALA:HB1	2.00	0.44
3:Cj:255:ASP:HB3	3:Cj:258:SER:HB3	1.99	0.44
3:Cn:201:ASP:HB3	3:Cn:221:ALA:HB3	2.00	0.44
3:Cp:269:MET:HE3	3:Cp:269:MET:HB3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dg:126:LEU:HD13	4:Dg:162:TYR:HE1	1.83	0.44
4:Di:112:GLN:HE21	4:Di:112:GLN:HB3	1.60	0.44
1:Ag:131:ALA:HA	1:Ah:158:ASN:HA	2.00	0.44
1:Aj:205:TYR:CZ	1:Aj:236:SER:HB3	2.53	0.44
2:Bc:189:SER:HA	2:Bc:216:ALA:HB2	1.99	0.44
2:Bp:182:ILE:HD12	2:Bp:233:LEU:HD23	2.00	0.44
2:Bu:83:VAL:HG12	2:Bu:105:SER:HA	2.00	0.44
2:Bw:361:ILE:HD12	2:Bx:161:MET:HE1	2.00	0.44
4:Dq:26:ARG:HG3	4:Dq:150:GLU:HB2	1.98	0.44
1:Ag:64:PRO:HB2	1:Ah:38:VAL:HG13	2.00	0.44
2:Be:189:SER:HA	2:Be:216:ALA:HB2	2.00	0.44
2:Bi:91:ALA:HB1	2:Bi:174:ASN:HD21	1.83	0.44
2:Bo:268:LYS:HB2	2:Bo:353:ALA:HB1	1.99	0.44
2:Bv:83:VAL:HG12	2:Bv:105:SER:HA	2.00	0.44
3:Cf:63:SER:HA	3:Cf:66:ASN:HD21	1.82	0.44
3:Ck:201:ASP:HB3	3:Ck:221:ALA:HB3	2.00	0.44
4:Dm:31:PRO:HG3	4:Dm:95:TRP:HZ2	1.83	0.44
4:Dq:31:PRO:HG3	4:Dq:95:TRP:HZ2	1.83	0.44
2:Ba:123:LYS:HG2	2:Ba:129:VAL:HG22	1.99	0.44
2:Bc:103:VAL:HB	2:Bc:137:LEU:HD21	2.00	0.44
3:Cn:326:PHE:HD1	3:Cn:328:ASP:H	1.65	0.44
1:Ag:129:ASN:HB2	1:Ag:156:ASN:HB3	1.99	0.43
1:Al:131:ALA:HA	1:Am:158:ASN:HA	2.00	0.43
1:Au:134:ASP:HB2	1:Av:155:LYS:HB2	2.00	0.43
2:Bb:123:LYS:HG2	2:Bb:129:VAL:HG22	1.99	0.43
2:Be:361:ILE:HD12	2:Bf:161:MET:HE1	1.99	0.43
2:Bg:123:LYS:HG2	2:Bg:129:VAL:HG22	1.99	0.43
2:Bh:205:LEU:HD11	2:Bh:236:ILE:HD11	1.98	0.43
2:Bn:91:ALA:HB1	2:Bn:174:ASN:HD21	1.83	0.43
2:Br:315:MET:HG2	2:Bs:328:VAL:HG22	2.00	0.43
3:Co:92:GLU:HB2	3:Co:103:ARG:HB3	1.99	0.43
3:Ct:220:PHE:HE2	3:Ct:273:VAL:HG11	1.83	0.43
3:Cy:209:LYS:HD2	3:Cy:212:GLN:HB2	1.99	0.43
4:Da:126:LEU:HD13	4:Da:162:TYR:HE1	1.82	0.43
4:Dc:175:TYR:HE1	4:Dc:209:TYR:HB2	1.83	0.43
4:Dk:31:PRO:HG3	4:Dk:95:TRP:HZ2	1.83	0.43
1:Ar:205:TYR:CZ	1:Ar:236:SER:HB3	2.53	0.43
1:Au:36:ASP:HB3	1:Au:39:GLU:HG2	1.99	0.43
1:Ax:134:ASP:HB2	1:Ay:155:LYS:HB2	2.00	0.43
1:Ay:129:ASN:HB2	1:Ay:156:ASN:HB3	1.99	0.43
1:Ay:134:ASP:HB2	1:Az:155:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ba:361:ILE:HG21	2:Bz:350:GLN:HG3	1.99	0.43
2:Bg:83:VAL:HG12	2:Bg:105:SER:HA	2.00	0.43
3:Cg:28:VAL:HG13	3:Cg:49:ALA:HB1	2.01	0.43
3:Cm:201:ASP:HB3	3:Cm:221:ALA:HB3	2.01	0.43
3:Cu:92:GLU:HB2	3:Cu:103:ARG:HB3	2.00	0.43
3:Cz:249:PRO:HG2	3:Cz:252:SER:HB3	2.00	0.43
4:Dh:90:SER:HB2	4:Dh:104:ILE:HD11	2.00	0.43
4:Dk:184:ILE:HG12	4:Dk:286:VAL:HG22	2.00	0.43
1:Ac:125:LEU:HB2	1:Ac:160:PHE:HB3	1.99	0.43
1:Ae:134:ASP:HB2	1:Af:155:LYS:HB2	2.00	0.43
1:Aj:64:PRO:HB2	1:Ak:38:VAL:HG13	1.99	0.43
1:Aj:119:LYS:HD2	1:Al:199:LEU:HB2	1.99	0.43
1:Am:154:LEU:HD21	1:Ao:258:LEU:HD11	1.99	0.43
1:At:154:LEU:HD21	1:Av:258:LEU:HD11	1.98	0.43
1:Aw:129:ASN:HB2	1:Aw:156:ASN:HB3	1.99	0.43
2:Be:315:MET:HG2	2:Bf:328:VAL:HG22	2.00	0.43
2:Bp:91:ALA:HB1	2:Bp:174:ASN:HD21	1.83	0.43
2:Bp:268:LYS:HB2	2:Bp:353:ALA:HB1	2.00	0.43
3:Cd:326:PHE:HD1	3:Cd:328:ASP:H	1.65	0.43
3:Cn:373:MET:HE3	3:Cn:373:MET:HB2	1.80	0.43
3:Cs:326:PHE:HD1	3:Cs:328:ASP:H	1.64	0.43
4:Db:90:SER:HB2	4:Db:104:ILE:HD11	2.00	0.43
4:Dq:175:TYR:HE1	4:Dq:209:TYR:HB2	1.82	0.43
4:Dt:90:SER:HB2	4:Dt:104:ILE:HD11	2.00	0.43
1:Aa:131:ALA:HA	1:Ab:158:ASN:HA	2.01	0.43
1:Ag:205:TYR:CZ	1:Ag:236:SER:HB3	2.54	0.43
1:Ah:129:ASN:HB2	1:Ah:156:ASN:HB3	2.00	0.43
1:Aj:36:ASP:HB3	1:Aj:39:GLU:HG2	1.99	0.43
1:Ax:36:ASP:HB3	1:Ax:39:GLU:HG2	2.00	0.43
2:Bi:123:LYS:HG2	2:Bi:129:VAL:HG22	2.00	0.43
2:Bn:103:VAL:HB	2:Bn:137:LEU:HD21	2.00	0.43
2:Bo:361:ILE:HD12	2:Bp:161:MET:HE1	2.00	0.43
2:Bp:205:LEU:HD11	2:Bp:236:ILE:HD11	2.00	0.43
3:Ce:201:ASP:HB3	3:Ce:221:ALA:HB3	2.00	0.43
3:Cj:201:ASP:HB3	3:Cj:221:ALA:HB3	2.00	0.43
3:Ct:167:VAL:HG21	3:Ct:191:ALA:HB2	2.00	0.43
3:Cu:326:PHE:HD1	3:Cu:328:ASP:H	1.66	0.43
3:Cx:28:VAL:HG13	3:Cx:49:ALA:HB1	2.00	0.43
3:Cz:29:THR:HG22	3:Cz:103:ARG:HG2	2.01	0.43
4:Dq:112:GLN:HE21	4:Dq:112:GLN:HB3	1.60	0.43
4:Dt:169:ILE:HG13	4:Dt:172:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:38:VAL:HG13	1:Az:64:PRO:HB2	1.99	0.43
1:Au:125:LEU:HB2	1:Au:160:PHE:HB3	2.01	0.43
2:Be:252:VAL:HG22	2:Be:259:ILE:HG12	2.00	0.43
2:Bx:361:ILE:HD12	2:By:161:MET:HE1	2.01	0.43
2:Bz:123:LYS:HG2	2:Bz:129:VAL:HG22	1.99	0.43
3:Cb:220:PHE:HE2	3:Cb:273:VAL:HG11	1.83	0.43
3:Cc:308:ARG:HD2	3:Cc:351:GLU:HA	2.00	0.43
3:Ch:167:VAL:HG21	3:Ch:191:ALA:HB2	2.01	0.43
3:Ch:205:THR:HG22	3:Ci:260:ARG:HD3	2.01	0.43
3:Cl:111:SER:HB3	3:Cl:113:THR:HG22	2.00	0.43
3:Cn:167:VAL:HG21	3:Cn:191:ALA:HB2	2.00	0.43
3:Co:326:PHE:HD1	3:Co:328:ASP:H	1.65	0.43
3:Cr:92:GLU:HB2	3:Cr:103:ARG:HB3	1.99	0.43
3:Cx:269:MET:HE3	3:Cx:269:MET:HB3	1.84	0.43
4:Dl:37:GLN:HG3	4:Dl:49:VAL:HG23	2.01	0.43
1:Aa:155:LYS:HB2	1:Az:134:ASP:HB2	2.01	0.43
1:Ab:64:PRO:HB2	1:Ac:38:VAL:HG13	1.99	0.43
1:Ab:131:ALA:HA	1:Ac:158:ASN:HA	2.00	0.43
1:Ab:205:TYR:CZ	1:Ab:236:SER:HB3	2.54	0.43
1:Ad:154:LEU:HD21	1:Af:258:LEU:HD11	2.01	0.43
1:Af:125:LEU:HB2	1:Af:160:PHE:HB3	2.01	0.43
1:Ah:200:ASN:HB3	1:Ah:201:THR:H	1.68	0.43
1:Ai:119:LYS:HD2	1:Ak:199:LEU:HB2	2.00	0.43
1:Aq:134:ASP:HB2	1:Ar:155:LYS:HB2	2.00	0.43
1:Av:134:ASP:HB2	1:Aw:155:LYS:HB2	2.01	0.43
1:Az:125:LEU:HB2	1:Az:160:PHE:HB3	2.01	0.43
2:Ba:350:GLN:HG3	2:Bb:361:ILE:HG21	2.00	0.43
2:Bk:315:MET:HG2	2:Bl:328:VAL:HG22	2.01	0.43
2:Bt:315:MET:HG2	2:Bu:328:VAL:HG22	2.00	0.43
2:Bw:268:LYS:HB2	2:Bw:353:ALA:HB1	2.00	0.43
2:By:268:LYS:HB2	2:By:353:ALA:HB1	1.99	0.43
3:Cd:201:ASP:HB3	3:Cd:221:ALA:HB3	2.00	0.43
3:Ci:167:VAL:HG21	3:Ci:191:ALA:HB2	2.01	0.43
3:Cq:111:SER:HB3	3:Cq:113:THR:HG22	2.01	0.43
3:Cs:28:VAL:HG13	3:Cs:49:ALA:HB1	2.01	0.43
4:Dw:112:GLN:HE21	4:Dw:112:GLN:HB3	1.60	0.43
1:Aa:258:LEU:HD11	1:Ay:154:LEU:HD21	2.00	0.43
1:Ab:258:LEU:HD11	1:Az:154:LEU:HD21	2.01	0.43
1:Ag:200:ASN:HB3	1:Ag:201:THR:H	1.68	0.43
1:Ai:205:TYR:CZ	1:Ai:236:SER:HB3	2.54	0.43
1:Am:36:ASP:HB3	1:Am:39:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:134:ASP:HB2	1:Ap:155:LYS:HB2	2.00	0.43
1:Ar:134:ASP:HB2	1:As:155:LYS:HB2	2.00	0.43
2:Bl:315:MET:HG2	2:Bm:328:VAL:HG22	2.00	0.43
2:Bq:361:ILE:HD12	2:Br:161:MET:HE1	2.01	0.43
2:Bx:103:VAL:HB	2:Bx:137:LEU:HD21	2.00	0.43
2:Bz:103:VAL:HB	2:Bz:137:LEU:HD21	2.00	0.43
3:Ce:255:ASP:HB3	3:Ce:258:SER:HB3	2.00	0.43
3:Ci:249:PRO:HG2	3:Ci:252:SER:HB3	1.99	0.43
3:Cn:111:SER:HB3	3:Cn:113:THR:HG22	1.99	0.43
1:Ac:119:LYS:HD2	1:Ae:199:LEU:HB2	2.00	0.43
1:Af:134:ASP:HB2	1:Ag:155:LYS:HB2	2.01	0.43
1:Ao:125:LEU:HB2	1:Ao:160:PHE:HB3	2.01	0.43
2:Bf:83:VAL:HG12	2:Bf:105:SER:HA	2.00	0.43
2:Bj:205:LEU:HD11	2:Bj:236:ILE:HD11	2.00	0.43
2:Bn:361:ILE:HD12	2:Bo:161:MET:HE1	2.00	0.43
2:Br:123:LYS:HG2	2:Br:129:VAL:HG22	2.01	0.43
2:Bv:239:LEU:HD23	2:Bv:239:LEU:HA	1.92	0.43
2:By:361:ILE:HD12	2:Bz:161:MET:HE1	2.01	0.43
3:Ci:164:PHE:HZ	3:Ci:285:ILE:HB	1.84	0.43
3:Cl:167:VAL:HG21	3:Cl:191:ALA:HB2	2.00	0.43
3:Cy:164:PHE:HZ	3:Cy:285:ILE:HB	1.84	0.43
4:Dv:37:GLN:HG3	4:Dv:49:VAL:HG23	2.01	0.43
4:Dv:90:SER:HB2	4:Dv:104:ILE:HD11	2.00	0.43
4:Dx:169:ILE:HG13	4:Dx:172:LEU:HD12	2.00	0.43
1:Ac:87:ASN:HB3	1:Ac:90:SER:HB2	2.00	0.43
1:Ad:119:LYS:HD2	1:Af:199:LEU:HB2	2.01	0.43
1:Ai:111:LEU:HB3	1:Ai:172:MET:HG3	2.01	0.43
1:An:134:ASP:HB2	1:Ao:155:LYS:HB2	2.00	0.43
1:Ao:111:LEU:HB3	1:Ao:172:MET:HG3	2.01	0.43
1:As:205:TYR:CZ	1:As:236:SER:HB3	2.54	0.43
2:Ba:274:HIS:CD2	2:Bb:258:THR:HB	2.54	0.43
2:Bc:252:VAL:HG22	2:Bc:259:ILE:HG12	2.00	0.43
3:Cg:342:ILE:HG21	3:Cg:367:ILE:HD11	1.99	0.43
3:Ch:249:PRO:HG2	3:Ch:252:SER:HB3	2.00	0.43
3:Cn:164:PHE:HZ	3:Cn:285:ILE:HB	1.84	0.43
4:Ds:31:PRO:HG3	4:Ds:95:TRP:HZ2	1.84	0.43
4:Dy:31:PRO:HG3	4:Dy:95:TRP:HZ2	1.84	0.43
1:Ad:134:ASP:HB2	1:Ae:155:LYS:HB2	2.01	0.43
1:Am:134:ASP:HB2	1:An:155:LYS:HB2	2.00	0.43
1:Av:106:ILE:HD12	1:Av:177:THR:HG21	2.01	0.43
2:Bd:91:ALA:HB1	2:Bd:174:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bf:205:LEU:HD11	2:Bf:236:ILE:HD11	2.01	0.43
2:Br:268:LYS:HB2	2:Br:353:ALA:HB1	2.01	0.43
3:Ce:342:ILE:HG21	3:Ce:367:ILE:HD11	2.00	0.43
3:Cp:222:MET:HE2	3:Cp:222:MET:HB3	1.82	0.43
3:Cq:85:VAL:HG22	3:Cq:108:ILE:HG12	1.99	0.43
3:Ct:201:ASP:HB3	3:Ct:221:ALA:HB3	2.01	0.43
4:Dx:90:SER:HB2	4:Dx:104:ILE:HD11	2.01	0.43
1:Ae:119:LYS:HD2	1:Ag:199:LEU:HB2	2.01	0.42
1:Al:205:TYR:CZ	1:Al:236:SER:HB3	2.54	0.42
1:Av:136:LEU:HD13	1:Aw:154:LEU:HD13	2.01	0.42
2:Bd:350:GLN:HG3	2:Be:361:ILE:HG21	2.00	0.42
2:Bl:252:VAL:HG22	2:Bl:259:ILE:HG12	2.00	0.42
2:Bn:21:ILE:HG23	2:Bn:197:LEU:HD11	2.00	0.42
3:Ci:111:SER:HB3	3:Ci:113:THR:HG22	2.01	0.42
3:Cn:195:MET:HG3	3:Cn:226:VAL:HG22	2.01	0.42
3:Cq:88:ILE:HG12	3:Cq:106:ILE:HG23	2.01	0.42
3:Cs:164:PHE:HZ	3:Cs:285:ILE:HB	1.84	0.42
4:Dd:90:SER:HB2	4:Dd:104:ILE:HD11	2.01	0.42
4:Df:37:GLN:HG3	4:Df:49:VAL:HG23	2.01	0.42
1:Aa:134:ASP:HB2	1:Ab:155:LYS:HB2	2.02	0.42
1:Ab:134:ASP:HB2	1:Ac:155:LYS:HB2	2.01	0.42
1:Ad:205:TYR:CZ	1:Ad:236:SER:HB3	2.54	0.42
1:Ag:119:LYS:HD2	1:Ai:199:LEU:HB2	2.01	0.42
1:Ah:111:LEU:HB3	1:Ah:172:MET:HG3	2.01	0.42
1:Al:119:LYS:HD2	1:An:199:LEU:HB2	2.00	0.42
2:Ba:315:MET:HG2	2:Bb:328:VAL:HG22	2.00	0.42
2:Bg:350:GLN:HG3	2:Bh:361:ILE:HG21	2.01	0.42
2:Bh:274:HIS:HB3	2:Bh:277:MET:HE2	2.01	0.42
2:Bl:350:GLN:HG3	2:Bm:361:ILE:HG21	2.00	0.42
2:Bo:350:GLN:HG3	2:Bp:361:ILE:HG21	2.01	0.42
2:Bp:350:GLN:HG3	2:Bq:361:ILE:HG21	2.00	0.42
2:Bs:268:LYS:HB2	2:Bs:353:ALA:HB1	2.01	0.42
2:Bw:123:LYS:HG2	2:Bw:129:VAL:HG22	2.02	0.42
2:Bz:83:VAL:HG12	2:Bz:105:SER:HA	2.01	0.42
3:Ca:373:MET:HE3	3:Ca:373:MET:HB2	1.85	0.42
3:Co:28:VAL:HG13	3:Co:49:ALA:HB1	2.01	0.42
3:Co:167:VAL:HG21	3:Co:191:ALA:HB2	2.00	0.42
3:Cr:326:PHE:HD1	3:Cr:328:ASP:H	1.66	0.42
4:Da:31:PRO:HG3	4:Da:95:TRP:HZ2	1.84	0.42
4:Dc:126:LEU:HD13	4:Dc:162:TYR:HE1	1.84	0.42
4:Di:83:THR:HG22	4:Di:111:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Di:126:LEU:HD13	4:Di:162:TYR:HE1	1.83	0.42
1:Ac:154:LEU:HD21	1:Ae:258:LEU:HD11	2.01	0.42
1:Aj:134:ASP:HB2	1:Ak:155:LYS:HB2	2.00	0.42
1:Am:205:TYR:CZ	1:Am:236:SER:HB3	2.54	0.42
2:Bf:103:VAL:HB	2:Bf:137:LEU:HD21	2.02	0.42
2:Bo:315:MET:HG2	2:Bp:328:VAL:HG22	2.01	0.42
2:Bp:315:MET:HG2	2:Bq:328:VAL:HG22	2.02	0.42
2:Bv:105:SER:HB2	2:Bv:112:LEU:HD11	2.01	0.42
3:Cc:350:TYR:HE2	3:Cc:355:GLU:HG3	1.84	0.42
3:Cj:164:PHE:HZ	3:Cj:285:ILE:HB	1.84	0.42
3:Cj:373:MET:HE3	3:Cj:373:MET:HB2	1.82	0.42
3:Cl:164:PHE:HZ	3:Cl:285:ILE:HB	1.84	0.42
3:Cv:167:VAL:HG21	3:Cv:191:ALA:HB2	2.01	0.42
4:Db:169:ILE:HG13	4:Db:172:LEU:HD12	2.00	0.42
4:De:31:PRO:HG3	4:De:95:TRP:HZ2	1.84	0.42
4:Dy:126:LEU:HD13	4:Dy:162:TYR:HE1	1.82	0.42
1:Ao:87:ASN:HB3	1:Ao:90:SER:HB2	2.00	0.42
1:Ap:125:LEU:HB2	1:Ap:160:PHE:HB3	2.00	0.42
1:Ap:134:ASP:HB2	1:Aq:155:LYS:HB2	2.00	0.42
1:Aq:184:LEU:HD12	1:Aq:188:ASN:HB2	2.01	0.42
1:Aq:205:TYR:CZ	1:Aq:236:SER:HB3	2.54	0.42
2:Bb:274:HIS:HB3	2:Bb:277:MET:HE2	2.02	0.42
2:Bc:315:MET:HG2	2:Bd:328:VAL:HG22	2.01	0.42
2:Be:103:VAL:HB	2:Be:137:LEU:HD21	2.02	0.42
2:Bi:103:VAL:HB	2:Bi:137:LEU:HD21	2.01	0.42
2:Bl:205:LEU:HD11	2:Bl:236:ILE:HD11	2.00	0.42
2:Bn:205:LEU:HD11	2:Bn:236:ILE:HD11	2.01	0.42
2:Bn:350:GLN:HG3	2:Bo:361:ILE:HG21	2.00	0.42
2:Bz:182:ILE:HD12	2:Bz:233:LEU:HD23	2.00	0.42
3:Ca:167:VAL:HG21	3:Ca:191:ALA:HB2	2.00	0.42
3:Cj:249:PRO:HG2	3:Cj:252:SER:HB3	2.00	0.42
3:Ck:88:ILE:HG12	3:Ck:106:ILE:HG23	2.01	0.42
3:Co:373:MET:HE3	3:Co:373:MET:HB2	1.81	0.42
3:Cp:34:ILE:HD11	3:Cp:100:MET:HB2	2.02	0.42
3:Ct:92:GLU:HB2	3:Ct:103:ARG:HB3	2.01	0.42
4:Dc:31:PRO:HG3	4:Dc:95:TRP:HZ2	1.83	0.42
1:Ae:205:TYR:CZ	1:Ae:236:SER:HB3	2.55	0.42
1:Af:131:ALA:HA	1:Ag:158:ASN:HA	2.01	0.42
1:Ak:205:TYR:CZ	1:Ak:236:SER:HB3	2.54	0.42
1:Am:87:ASN:HB3	1:Am:90:SER:HB2	2.00	0.42
1:Aw:34:THR:HG21	3:Cm:247:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bg:274:HIS:CD2	2:Bh:258:THR:HB	2.55	0.42
2:Bi:239:LEU:HD23	2:Bi:239:LEU:HA	1.92	0.42
2:Bj:350:GLN:HG3	2:Bk:361:ILE:HG21	2.00	0.42
2:Bm:83:VAL:HG12	2:Bm:105:SER:HA	2.02	0.42
2:Bt:205:LEU:HD11	2:Bt:236:ILE:HD11	2.02	0.42
2:Bw:315:MET:HG2	2:Bx:328:VAL:HG22	1.99	0.42
3:Ce:96:ILE:HB	3:Ce:101:TYR:HE2	1.85	0.42
3:Cj:28:VAL:HG13	3:Cj:49:ALA:HB1	2.02	0.42
3:Cs:167:VAL:HG21	3:Cs:191:ALA:HB2	2.02	0.42
3:Cu:111:SER:HB3	3:Cu:113:THR:HG22	2.02	0.42
3:Cy:201:ASP:HB3	3:Cy:221:ALA:HB3	2.01	0.42
3:Cz:373:MET:HE3	3:Cz:373:MET:HB2	1.82	0.42
4:Da:26:ARG:HG3	4:Da:150:GLU:HB2	2.00	0.42
4:De:126:LEU:HD13	4:De:162:TYR:HE1	1.85	0.42
4:Di:31:PRO:HB3	4:Di:156:VAL:HG21	2.02	0.42
4:Dn:86:VAL:HG21	4:Dn:110:PHE:CG	2.54	0.42
4:Do:112:GLN:HE21	4:Do:112:GLN:HB3	1.60	0.42
5:Ge:139:LYS:HD2	5:Ge:139:LYS:HA	1.75	0.42
1:Ai:134:ASP:HB2	1:Aj:155:LYS:HB2	2.01	0.42
1:Ar:129:ASN:HB2	1:Ar:156:ASN:HB3	2.01	0.42
2:Bk:123:LYS:HG2	2:Bk:129:VAL:HG22	2.00	0.42
3:Cv:29:THR:HB	3:Cv:103:ARG:HG2	2.01	0.42
3:Cx:88:ILE:HG12	3:Cx:106:ILE:HG12	2.00	0.42
4:Dc:184:ILE:HG12	4:Dc:286:VAL:HG22	2.02	0.42
4:Dg:83:THR:HG22	4:Dg:111:LYS:HA	2.00	0.42
4:Dk:141:ASP:HB2	4:Dk:149:ILE:HG12	2.00	0.42
4:Do:26:ARG:HG3	4:Do:150:GLU:HB2	2.01	0.42
4:Dz:90:SER:HB2	4:Dz:104:ILE:HD11	2.00	0.42
1:Af:111:LEU:HB3	1:Af:172:MET:HG3	2.02	0.42
1:Ak:119:LYS:HD2	1:Am:199:LEU:HB2	2.00	0.42
1:As:131:ALA:HA	1:At:158:ASN:HA	2.01	0.42
1:As:134:ASP:HB2	1:At:155:LYS:HB2	2.01	0.42
1:Ay:111:LEU:HB3	1:Ay:172:MET:HG3	2.02	0.42
2:Ba:274:HIS:HB3	2:Ba:277:MET:HE2	2.02	0.42
2:Bh:83:VAL:HG12	2:Bh:105:SER:HA	2.02	0.42
2:Br:103:VAL:HB	2:Br:137:LEU:HD21	2.01	0.42
2:Bt:123:LYS:HG2	2:Bt:129:VAL:HG22	2.02	0.42
2:Bx:317:LYS:HE2	2:By:324:LEU:HB2	2.02	0.42
3:Cb:201:ASP:HB3	3:Cb:221:ALA:HB3	2.01	0.42
3:Cd:278:MET:HE2	3:Cd:278:MET:HB3	1.95	0.42
3:Ck:249:PRO:HG2	3:Ck:252:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cp:201:ASP:HB3	3:Cp:221:ALA:HB3	2.02	0.42
3:Cw:111:SER:HB3	3:Cw:113:THR:HG22	2.02	0.42
4:Da:175:TYR:HE1	4:Da:209:TYR:HB2	1.85	0.42
4:De:197:LYS:HA	4:De:200:GLN:HB2	2.02	0.42
4:Dg:194:GLU:H	4:Dg:194:GLU:HG3	1.71	0.42
4:Dq:91:MET:HE2	4:Dq:91:MET:HB3	1.80	0.42
4:Dw:31:PRO:HB3	4:Dw:156:VAL:HG21	2.02	0.42
4:Dw:31:PRO:HG3	4:Dw:95:TRP:HZ2	1.84	0.42
4:Dw:83:THR:HG22	4:Dw:111:LYS:HA	2.01	0.42
1:Ab:229:SER:HB3	1:Ac:177:THR:HG22	2.01	0.42
1:Ai:125:LEU:HB2	1:Ai:160:PHE:HB3	2.01	0.42
2:Bb:252:VAL:HG22	2:Bb:259:ILE:HG12	2.01	0.42
2:Bd:274:HIS:CD2	2:Be:258:THR:HB	2.55	0.42
2:Bm:268:LYS:HB2	2:Bm:353:ALA:HB1	2.02	0.42
2:Bp:123:LYS:HG2	2:Bp:129:VAL:HG22	2.01	0.42
2:Br:83:VAL:HG12	2:Br:105:SER:HA	2.02	0.42
2:Bs:91:ALA:HB1	2:Bs:174:ASN:HD21	1.84	0.42
3:Cd:209:LYS:HD2	3:Cd:212:GLN:HB2	2.02	0.42
3:Cg:111:SER:HB3	3:Cg:113:THR:HG22	2.01	0.42
3:Ck:205:THR:HG22	3:Cl:260:ARG:HD3	2.01	0.42
3:Cl:269:MET:HE3	3:Cl:269:MET:HB3	1.96	0.42
3:Cq:80:PHE:HA	5:Fq:136:VAL:HG21	2.01	0.42
3:Cu:167:VAL:HG21	3:Cu:191:ALA:HB2	2.02	0.42
4:Dj:37:GLN:HG3	4:Dj:49:VAL:HG23	2.02	0.42
4:Do:83:THR:HG22	4:Do:111:LYS:HA	2.01	0.42
4:Dy:31:PRO:HB3	4:Dy:156:VAL:HG21	2.02	0.42
4:Dy:83:THR:HG22	4:Dy:111:LYS:HA	2.01	0.42
1:Ag:134:ASP:HB2	1:Ah:155:LYS:HB2	2.02	0.42
1:An:229:SER:HB3	1:Ao:177:THR:HG22	2.02	0.42
1:Ap:111:LEU:HB3	1:Ap:172:MET:HG3	2.01	0.42
1:Aw:154:LEU:HD21	1:Ay:258:LEU:HD11	2.02	0.42
1:Ax:205:TYR:CZ	1:Ax:236:SER:HB3	2.54	0.42
2:Bb:205:LEU:HD11	2:Bb:236:ILE:HD11	2.02	0.42
2:Bo:103:VAL:HB	2:Bo:137:LEU:HD21	2.01	0.42
2:Bp:361:ILE:HD12	2:Bq:161:MET:HE1	2.02	0.42
2:Bq:123:LYS:HG2	2:Bq:129:VAL:HG22	2.01	0.42
2:Br:274:HIS:CD2	2:Bs:258:THR:HB	2.55	0.42
3:Cm:111:SER:HB3	3:Cm:113:THR:HG22	2.01	0.42
3:Ct:78:TYR:HD2	3:Ct:88:ILE:HB	1.84	0.42
3:Cv:226:VAL:HB	3:Cv:236:MET:HB3	2.01	0.42
4:Du:91:MET:HE2	4:Du:91:MET:HB3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Du:126:LEU:HD13	4:Du:162:TYR:HE1	1.85	0.42
1:Ae:64:PRO:HB2	1:Af:38:VAL:HG13	2.02	0.42
1:Ak:229:SER:HB3	1:Al:177:THR:HG22	2.02	0.42
1:Av:111:LEU:HB3	1:Av:172:MET:HG3	2.02	0.42
1:Aw:111:LEU:HB3	1:Aw:172:MET:HG3	2.02	0.42
2:Bi:315:MET:HG2	2:Bj:328:VAL:HG22	2.01	0.42
3:Cd:80:PHE:HA	5:Fd:136:VAL:HG21	2.02	0.42
3:Ci:201:ASP:HB3	3:Ci:221:ALA:HB3	2.02	0.42
3:Cm:269:MET:HE3	3:Cm:269:MET:HB3	1.95	0.42
3:Cz:209:LYS:HD2	3:Cz:212:GLN:HB2	2.01	0.42
4:Df:90:SER:HB2	4:Df:104:ILE:HD11	2.01	0.42
4:Di:175:TYR:HE1	4:Di:209:TYR:HB2	1.84	0.42
4:Dt:86:VAL:HG21	4:Dt:110:PHE:CG	2.55	0.42
4:Dw:197:LYS:HA	4:Dw:200:GLN:HB2	2.02	0.42
1:Aa:119:LYS:HB3	1:Ac:199:LEU:HD12	2.02	0.41
1:Av:205:TYR:CZ	1:Av:236:SER:HB3	2.55	0.41
2:Ba:268:LYS:HB2	2:Ba:353:ALA:HB1	2.00	0.41
2:Bn:123:LYS:HG2	2:Bn:129:VAL:HG22	2.01	0.41
2:Bo:317:LYS:HE2	2:Bp:324:LEU:HB2	2.03	0.41
2:Bs:274:HIS:CD2	2:Bt:258:THR:HB	2.55	0.41
2:Bs:350:GLN:HG3	2:Bt:361:ILE:HG21	2.01	0.41
2:Bz:56:GLN:HE21	2:Bz:56:GLN:HB3	1.65	0.41
3:Ca:34:ILE:HD11	3:Ca:100:MET:HB2	2.02	0.41
3:Ch:220:PHE:HE2	3:Ch:273:VAL:HG11	1.84	0.41
3:Ck:326:PHE:HD1	3:Ck:328:ASP:H	1.68	0.41
3:Cp:373:MET:HE3	3:Cp:373:MET:HB2	1.84	0.41
3:Cq:201:ASP:HB3	3:Cq:221:ALA:HB3	2.02	0.41
3:Cv:361:PRO:HB2	4:Do:148:ARG:HD2	2.01	0.41
3:Cw:201:ASP:HB3	3:Cw:221:ALA:HB3	2.02	0.41
4:Dm:197:LYS:HA	4:Dm:200:GLN:HB2	2.02	0.41
4:Do:135:PRO:HD2	4:Do:153:LEU:HB2	2.02	0.41
4:Dq:184:ILE:HG12	4:Dq:286:VAL:HG22	2.01	0.41
4:Dw:126:LEU:HD13	4:Dw:162:TYR:HE1	1.83	0.41
1:Ac:136:LEU:HD13	1:Ad:154:LEU:HD13	2.00	0.41
1:Ah:136:LEU:HD13	1:Ai:154:LEU:HD13	2.01	0.41
1:Aq:229:SER:HB3	1:Ar:177:THR:HG22	2.03	0.41
1:Aw:205:TYR:CZ	1:Aw:236:SER:HB3	2.55	0.41
1:Ay:136:LEU:HD13	1:Az:154:LEU:HD13	2.01	0.41
2:Bd:239:LEU:HD23	2:Bd:239:LEU:HA	1.92	0.41
2:Bi:83:VAL:HG12	2:Bi:105:SER:HA	2.02	0.41
2:Bw:252:VAL:HG22	2:Bw:259:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:By:274:HIS:CD2	2:Bz:258:THR:HB	2.55	0.41
3:Ca:201:ASP:HB3	3:Ca:221:ALA:HB3	2.02	0.41
3:Ci:54:VAL:HG13	3:Ci:59:ALA:HB3	2.02	0.41
3:Cl:88:ILE:HG23	3:Cl:106:ILE:HG12	2.02	0.41
3:Cs:88:ILE:HG12	3:Cs:106:ILE:HG23	2.01	0.41
3:Cy:28:VAL:HG13	3:Cy:49:ALA:HB1	2.03	0.41
4:Dc:26:ARG:HG3	4:Dc:150:GLU:HB2	2.01	0.41
4:Do:31:PRO:HG3	4:Do:95:TRP:HZ2	1.84	0.41
1:Ah:229:SER:HB3	1:Ai:177:THR:HG22	2.01	0.41
1:Az:205:TYR:CZ	1:Az:236:SER:HB3	2.55	0.41
2:Bh:274:HIS:CD2	2:Bi:258:THR:HB	2.55	0.41
2:Bl:274:HIS:HB3	2:Bl:277:MET:HE2	2.02	0.41
2:Bn:315:MET:HG2	2:Bo:328:VAL:HG22	2.02	0.41
2:Bv:315:MET:HG2	2:Bw:328:VAL:HG22	2.02	0.41
2:Bx:274:HIS:CD2	2:By:258:THR:HB	2.55	0.41
3:Cb:157:LEU:HA	3:Cb:161:SER:HB2	2.01	0.41
3:Ch:226:VAL:HB	3:Ch:236:MET:HB3	2.02	0.41
4:Dd:86:VAL:HG21	4:Dd:110:PHE:CG	2.55	0.41
4:Df:86:VAL:HG21	4:Df:110:PHE:CG	2.55	0.41
4:Du:112:GLN:HE21	4:Du:112:GLN:HB3	1.60	0.41
1:Ad:111:LEU:HB3	1:Ad:172:MET:HG3	2.03	0.41
1:Ak:134:ASP:HB2	1:Al:155:LYS:HB2	2.02	0.41
1:Ao:205:TYR:CZ	1:Ao:236:SER:HB3	2.55	0.41
2:Bb:239:LEU:HD23	2:Bb:239:LEU:HA	1.93	0.41
2:Bh:103:VAL:HB	2:Bh:137:LEU:HD21	2.02	0.41
2:Bm:274:HIS:HB3	2:Bm:277:MET:HE2	2.01	0.41
2:Bv:103:VAL:HB	2:Bv:137:LEU:HD21	2.01	0.41
2:Bx:315:MET:HG2	2:By:328:VAL:HG22	2.02	0.41
2:Bz:205:LEU:HD11	2:Bz:236:ILE:HD11	2.02	0.41
3:Ch:111:SER:HB3	3:Ch:113:THR:HG22	2.02	0.41
3:Cp:249:PRO:HG2	3:Cp:252:SER:HB3	2.01	0.41
3:Cq:222:MET:HE3	3:Cq:222:MET:HB2	1.95	0.41
3:Cr:164:PHE:HZ	3:Cr:285:ILE:HB	1.85	0.41
3:Cs:209:LYS:HD2	3:Cs:212:GLN:HB2	2.01	0.41
4:Dc:83:THR:HG22	4:Dc:111:LYS:HA	2.02	0.41
4:Di:31:PRO:HG3	4:Di:95:TRP:HZ2	1.84	0.41
4:Dp:111:LYS:H	4:Dp:115:GLY:HA2	1.85	0.41
4:Dy:197:LYS:HA	4:Dy:200:GLN:HB2	2.03	0.41
1:Ah:134:ASP:HB2	1:Ai:155:LYS:HB2	2.02	0.41
1:Aj:229:SER:HB3	1:Ak:177:THR:HG22	2.02	0.41
1:Ak:106:ILE:HD12	1:Ak:177:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:131:ALA:HA	1:Al:158:ASN:HA	2.02	0.41
1:Aw:106:ILE:HD12	1:Aw:177:THR:HG21	2.02	0.41
2:Bf:274:HIS:HB3	2:Bf:277:MET:HE2	2.02	0.41
2:Bg:268:LYS:HB2	2:Bg:353:ALA:HB1	2.02	0.41
2:Bj:250:ILE:HG23	2:Bj:261:VAL:HG22	2.03	0.41
2:Bl:123:LYS:HG2	2:Bl:129:VAL:HG22	2.01	0.41
2:Bm:274:HIS:CD2	2:Bn:258:THR:HB	2.55	0.41
2:Bq:239:LEU:HD23	2:Bq:239:LEU:HA	1.94	0.41
2:Br:205:LEU:HD11	2:Br:236:ILE:HD11	2.02	0.41
2:Bw:274:HIS:CD2	2:Bx:258:THR:HB	2.55	0.41
2:Bx:268:LYS:HB2	2:Bx:353:ALA:HB1	2.02	0.41
2:By:103:VAL:HB	2:By:137:LEU:HD21	2.01	0.41
2:By:350:GLN:HG3	2:Bz:361:ILE:HG21	2.02	0.41
3:Ca:269:MET:HE3	3:Ca:269:MET:HB3	1.89	0.41
3:Cb:278:MET:HE2	3:Cb:278:MET:HB3	1.96	0.41
3:Cg:34:ILE:HD11	3:Cg:100:MET:HB2	2.02	0.41
3:Ci:80:PHE:HA	5:Fi:136:VAL:HG21	2.02	0.41
3:Ck:28:VAL:HG13	3:Ck:49:ALA:HB1	2.03	0.41
3:Cw:269:MET:HE3	3:Cw:269:MET:HB3	1.82	0.41
4:Db:37:GLN:HG3	4:Db:49:VAL:HG23	2.01	0.41
1:Aa:119:LYS:HD2	1:Ac:199:LEU:HB2	2.02	0.41
1:Aa:154:LEU:HD13	1:Az:136:LEU:HD13	2.03	0.41
1:An:131:ALA:HA	1:Ao:158:ASN:HA	2.02	0.41
1:Az:111:LEU:HB3	1:Az:172:MET:HG3	2.03	0.41
2:Be:83:VAL:HG12	2:Be:105:SER:HA	2.02	0.41
2:Be:274:HIS:CD2	2:Bf:258:THR:HB	2.56	0.41
2:Bg:252:VAL:HG22	2:Bg:259:ILE:HG12	2.01	0.41
2:Bh:252:VAL:HG22	2:Bh:259:ILE:HG12	2.02	0.41
2:Bi:252:VAL:HG22	2:Bi:259:ILE:HG12	2.01	0.41
2:Bi:274:HIS:CD2	2:Bj:258:THR:HB	2.56	0.41
2:Bi:350:GLN:HG3	2:Bj:361:ILE:HG21	2.02	0.41
2:Bm:350:GLN:HG3	2:Bn:361:ILE:HG21	2.01	0.41
2:Bs:83:VAL:HG12	2:Bs:105:SER:HA	2.03	0.41
2:Bt:239:LEU:HD23	2:Bt:239:LEU:HA	1.93	0.41
2:Bx:83:VAL:HG12	2:Bx:105:SER:HA	2.03	0.41
2:Bx:182:ILE:HD12	2:Bx:233:LEU:HD23	2.02	0.41
2:By:123:LYS:HG2	2:By:129:VAL:HG22	2.02	0.41
3:Ca:26:TYR:HB2	3:Ca:106:ILE:O	2.20	0.41
3:Cg:88:ILE:HG12	3:Cg:106:ILE:HG23	2.03	0.41
3:Cl:201:ASP:HB3	3:Cl:221:ALA:HB3	2.03	0.41
3:Cm:167:VAL:HG21	3:Cm:191:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cn:269:MET:HE3	3:Cn:269:MET:HB3	1.94	0.41
3:Co:201:ASP:HB3	3:Co:221:ALA:HB3	2.03	0.41
3:Cp:321:TRP:HE1	3:Cp:374:HIS:CE1	2.38	0.41
4:Dg:216:ILE:HG21	4:Dg:289:LEU:HD22	2.03	0.41
4:Dt:37:GLN:HG3	4:Dt:49:VAL:HG23	2.02	0.41
5:Fb:145:PHE:HD1	5:Fb:145:PHE:HA	1.68	0.41
1:Ag:111:LEU:HB3	1:Ag:172:MET:HG3	2.03	0.41
1:Ak:136:LEU:HD13	1:Al:154:LEU:HD13	2.02	0.41
2:Ba:252:VAL:HG22	2:Ba:259:ILE:HG12	2.02	0.41
2:Bc:317:LYS:HE2	2:Bd:324:LEU:HB2	2.03	0.41
2:Bf:274:HIS:CD2	2:Bg:258:THR:HB	2.56	0.41
2:Bk:83:VAL:HG12	2:Bk:105:SER:HA	2.03	0.41
2:Bt:103:VAL:HB	2:Bt:137:LEU:HD21	2.01	0.41
2:Bx:252:VAL:HG22	2:Bx:259:ILE:HG12	2.02	0.41
3:Ca:67:LEU:HD22	3:Ca:85:VAL:HG21	2.03	0.41
3:Cd:220:PHE:HE2	3:Cd:273:VAL:HG11	1.85	0.41
3:Ch:373:MET:HE3	3:Ch:373:MET:HB2	1.81	0.41
3:Co:195:MET:HG3	3:Co:226:VAL:HG22	2.02	0.41
3:Cr:157:LEU:HA	3:Cr:161:SER:HB2	2.02	0.41
3:Cw:321:TRP:HE1	3:Cw:374:HIS:CE1	2.38	0.41
4:De:165:PHE:O	4:De:169:ILE:HG12	2.20	0.41
4:Dg:112:GLN:HE21	4:Dg:112:GLN:HB3	1.61	0.41
4:Dm:184:ILE:HG12	4:Dm:286:VAL:HG22	2.03	0.41
4:Dp:184:ILE:HG12	4:Dp:286:VAL:HG22	2.02	0.41
4:Dx:184:ILE:HG12	4:Dx:286:VAL:HG22	2.03	0.41
5:Gm:133:VAL:HG12	5:Gm:134:GLN:HG2	2.01	0.41
1:Aa:200:ASN:HB3	1:Aa:201:THR:H	1.69	0.41
1:Ad:64:PRO:HB2	1:Ae:38:VAL:HG13	2.02	0.41
1:Aq:255:ASN:ND2	1:Ar:244:MET:HE1	2.36	0.41
2:Bd:315:MET:HG2	2:Be:328:VAL:HG22	2.02	0.41
2:Bh:123:LYS:HG2	2:Bh:129:VAL:HG22	2.02	0.41
2:Bj:361:ILE:HD12	2:Bk:161:MET:HE1	2.02	0.41
2:Bq:274:HIS:CD2	2:Br:258:THR:HB	2.56	0.41
2:Bv:274:HIS:CD2	2:Bw:258:THR:HB	2.55	0.41
2:Bw:350:GLN:HG3	2:Bx:361:ILE:HG21	2.02	0.41
2:By:252:VAL:HG22	2:By:259:ILE:HG12	2.03	0.41
3:Cd:88:ILE:HG23	3:Cd:106:ILE:HG12	2.03	0.41
3:Ce:209:LYS:HD2	3:Ce:212:GLN:HB2	2.02	0.41
3:Cg:201:ASP:HB3	3:Cg:221:ALA:HB3	2.02	0.41
3:Ck:255:ASP:HB3	3:Ck:258:SER:HB3	2.01	0.41
3:Cl:79:LEU:HD23	5:Fl:134:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cr:205:THR:HG22	3:Cs:260:ARG:HD3	2.02	0.41
3:Cu:164:PHE:HZ	3:Cu:285:ILE:HB	1.86	0.41
3:Cv:88:ILE:HG12	3:Cv:106:ILE:HG12	2.02	0.41
3:Cz:201:ASP:HB3	3:Cz:221:ALA:HB3	2.03	0.41
3:Cz:292:PRO:HB3	3:Cz:306:LEU:HD22	2.02	0.41
4:De:112:GLN:HE21	4:De:112:GLN:HB3	1.60	0.41
4:Du:83:THR:HG22	4:Du:111:LYS:HA	2.02	0.41
4:Dv:86:VAL:HG21	4:Dv:110:PHE:CG	2.56	0.41
1:Aa:111:LEU:HB3	1:Aa:172:MET:HG3	2.03	0.41
1:Ab:200:ASN:HB3	1:Ab:201:THR:H	1.69	0.41
1:Ac:106:ILE:HD12	1:Ac:177:THR:HG21	2.03	0.41
1:Ad:106:ILE:HD12	1:Ad:177:THR:HG21	2.03	0.41
1:Ad:131:ALA:HA	1:Ae:158:ASN:HA	2.03	0.41
1:Af:200:ASN:HB3	1:Af:201:THR:H	1.69	0.41
1:Af:205:TYR:CZ	1:Af:236:SER:HB3	2.56	0.41
1:Am:106:ILE:HD12	1:Am:177:THR:HG21	2.02	0.41
1:Am:200:ASN:HB3	1:Am:201:THR:H	1.69	0.41
1:Ao:131:ALA:HA	1:Ap:158:ASN:HA	2.01	0.41
1:Aq:125:LEU:HB2	1:Aq:160:PHE:HB3	2.02	0.41
1:Au:64:PRO:HB2	1:Av:38:VAL:HG13	2.03	0.41
1:Ax:111:LEU:HB3	1:Ax:172:MET:HG3	2.03	0.41
1:Az:200:ASN:HB3	1:Az:201:THR:H	1.68	0.41
2:Bf:91:ALA:HB1	2:Bf:174:ASN:HD21	1.85	0.41
2:Bn:252:VAL:HG22	2:Bn:259:ILE:HG12	2.02	0.41
2:Br:91:ALA:HB1	2:Br:174:ASN:HD21	1.85	0.41
2:Bs:315:MET:HG2	2:Bt:328:VAL:HG22	2.02	0.41
2:Bt:350:GLN:HG3	2:Bu:361:ILE:HG21	2.01	0.41
2:Bu:315:MET:HG2	2:Bv:328:VAL:HG22	2.02	0.41
2:Bv:350:GLN:HG3	2:Bw:361:ILE:HG21	2.02	0.41
2:Bw:103:VAL:HB	2:Bw:137:LEU:HD21	2.02	0.41
2:Bz:252:VAL:HG22	2:Bz:259:ILE:HG12	2.03	0.41
3:Cc:373:MET:HE3	3:Cc:373:MET:HB2	1.86	0.41
3:Ci:88:ILE:HG12	3:Ci:106:ILE:HG23	2.03	0.41
3:Cj:269:MET:HE3	3:Cj:269:MET:HB3	1.86	0.41
3:Cn:220:PHE:HE2	3:Cn:273:VAL:HG11	1.86	0.41
3:Co:164:PHE:HZ	3:Co:285:ILE:HB	1.86	0.41
3:Cs:278:MET:HE2	3:Cs:278:MET:HB3	2.00	0.41
3:Cx:373:MET:HE3	3:Cx:373:MET:HB2	1.82	0.41
3:Cy:322:HIS:HB2	3:Cy:338:THR:HB	2.03	0.41
3:Cz:226:VAL:HB	3:Cz:236:MET:HB3	2.03	0.41
4:Dn:90:SER:HB2	4:Dn:104:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Do:194:GLU:H	4:Do:194:GLU:HG3	1.71	0.41
4:Dq:31:PRO:HB3	4:Dq:156:VAL:HG21	2.03	0.41
4:Dr:86:VAL:HG21	4:Dr:110:PHE:CG	2.55	0.41
4:Ds:31:PRO:HB3	4:Ds:156:VAL:HG21	2.03	0.41
4:Ds:194:GLU:H	4:Ds:194:GLU:HG3	1.71	0.41
4:Dw:175:TYR:HE1	4:Dw:209:TYR:HB2	1.86	0.41
4:Dx:86:VAL:HG21	4:Dx:110:PHE:CG	2.55	0.41
1:Am:64:PRO:HB2	1:An:38:VAL:HG13	2.03	0.41
1:Am:184:LEU:HD12	1:Am:188:ASN:HB2	2.01	0.41
1:Aq:119:LYS:HB3	1:As:199:LEU:HD12	2.03	0.41
1:As:154:LEU:HD21	1:Au:258:LEU:HD11	2.02	0.41
1:Ax:136:LEU:HD13	1:Ay:154:LEU:HD13	2.03	0.41
2:Bb:274:HIS:CD2	2:Bc:258:THR:HB	2.56	0.41
2:Bg:274:HIS:HB3	2:Bg:277:MET:HE2	2.03	0.41
2:Bh:350:GLN:HG3	2:Bi:361:ILE:HG21	2.02	0.41
2:Bl:274:HIS:CD2	2:Bm:258:THR:HB	2.56	0.41
2:Bs:105:SER:HB2	2:Bs:112:LEU:HD11	2.03	0.41
3:Ci:326:PHE:HD1	3:Ci:328:ASP:H	1.68	0.41
3:Cq:88:ILE:HG23	3:Cq:106:ILE:HG12	2.02	0.41
3:Ct:249:PRO:HG2	3:Ct:252:SER:HB3	2.01	0.41
1:Aa:205:TYR:CZ	1:Aa:236:SER:HB3	2.56	0.40
1:Ab:111:LEU:HB3	1:Ab:172:MET:HG3	2.04	0.40
1:Ag:136:LEU:HD13	1:Ah:154:LEU:HD13	2.02	0.40
1:Ah:64:PRO:HB2	1:Ai:38:VAL:HG13	2.02	0.40
1:Aj:136:LEU:HD13	1:Ak:154:LEU:HD13	2.03	0.40
1:Ar:64:PRO:HB2	1:As:38:VAL:HG13	2.03	0.40
1:As:136:LEU:HD13	1:At:154:LEU:HD13	2.02	0.40
1:Ay:106:ILE:HD12	1:Ay:177:THR:HG21	2.03	0.40
2:Bg:315:MET:HG2	2:Bh:328:VAL:HG22	2.02	0.40
2:Bj:274:HIS:CD2	2:Bk:258:THR:HB	2.56	0.40
2:Bk:103:VAL:HB	2:Bk:137:LEU:HD21	2.04	0.40
2:Bk:274:HIS:CD2	2:Bl:258:THR:HB	2.56	0.40
2:Bm:315:MET:HG2	2:Bn:328:VAL:HG22	2.03	0.40
2:Bo:274:HIS:CD2	2:Bp:258:THR:HB	2.55	0.40
3:Cb:365:TYR:HB3	4:Du:91:MET:HE1	2.03	0.40
3:Cf:209:LYS:HD2	3:Cf:212:GLN:HB2	2.02	0.40
3:Ch:78:TYR:HD2	3:Ch:88:ILE:HB	1.86	0.40
3:Ch:201:ASP:HB3	3:Ch:221:ALA:HB3	2.03	0.40
3:Ch:239:THR:HG21	3:Ci:155:ARG:HD3	2.03	0.40
3:Ck:167:VAL:HG21	3:Ck:191:ALA:HB2	2.03	0.40
3:Co:54:VAL:HG13	3:Co:59:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ct:195:MET:HG3	3:Ct:226:VAL:HG22	2.03	0.40
4:Da:197:LYS:HA	4:Da:200:GLN:HB2	2.04	0.40
4:Da:216:ILE:HG21	4:Da:289:LEU:HD22	2.03	0.40
4:De:184:ILE:HG12	4:De:286:VAL:HG22	2.03	0.40
4:Dq:83:THR:HG22	4:Dq:111:LYS:HA	2.02	0.40
1:Al:134:ASP:HB2	1:Am:155:LYS:HB2	2.02	0.40
1:Ar:136:LEU:HD13	1:As:154:LEU:HD13	2.04	0.40
1:At:255:ASN:ND2	1:Au:244:MET:HE1	2.37	0.40
2:Ba:259:ILE:HD11	2:Ba:342:MET:HB2	2.03	0.40
2:Be:91:ALA:HB1	2:Be:174:ASN:HD21	1.86	0.40
2:Bk:40:LEU:HD23	2:Bk:82:ALA:HA	2.03	0.40
2:Bl:239:LEU:HD23	2:Bl:239:LEU:HA	1.92	0.40
2:Bl:317:LYS:HE2	2:Bm:324:LEU:HB2	2.04	0.40
2:Br:274:HIS:HB3	2:Br:277:MET:HE2	2.02	0.40
2:Bt:56:GLN:HE21	2:Bt:56:GLN:HB3	1.63	0.40
3:Cc:201:ASP:HB3	3:Cc:221:ALA:HB3	2.03	0.40
3:Cq:327:ILE:H	3:Cq:327:ILE:HG13	1.66	0.40
3:Cy:167:VAL:HG21	3:Cy:191:ALA:HB2	2.03	0.40
4:Dm:83:THR:HG22	4:Dm:111:LYS:HA	2.03	0.40
4:Dy:165:PHE:O	4:Dy:169:ILE:HG12	2.21	0.40
4:Dz:107:LEU:HD13	4:Dz:107:LEU:HA	1.98	0.40
1:Ae:106:ILE:HD12	1:Ae:177:THR:HG21	2.04	0.40
1:Am:131:ALA:HA	1:An:158:ASN:HA	2.02	0.40
1:Au:255:ASN:ND2	1:Av:244:MET:HE1	2.36	0.40
2:Bc:123:LYS:HG2	2:Bc:129:VAL:HG22	2.02	0.40
2:Bk:350:GLN:HG3	2:Bl:361:ILE:HG21	2.03	0.40
3:Cd:28:VAL:HG13	3:Cd:49:ALA:HB1	2.04	0.40
3:Cd:292:PRO:HB3	3:Cd:306:LEU:HD22	2.04	0.40
4:Dc:165:PHE:O	4:Dc:169:ILE:HG12	2.21	0.40
4:Dh:169:ILE:HG13	4:Dh:172:LEU:HD12	2.02	0.40
4:Di:197:LYS:HA	4:Di:200:GLN:HB2	2.04	0.40
4:Dq:194:GLU:H	4:Dq:194:GLU:HG3	1.72	0.40
1:Ab:106:ILE:HD12	1:Ab:177:THR:HG21	2.02	0.40
1:Am:136:LEU:HD13	1:An:154:LEU:HD13	2.03	0.40
1:An:178:VAL:HG21	1:An:191:ILE:HD12	2.03	0.40
1:Ao:119:LYS:HD2	1:Aq:199:LEU:HB2	2.02	0.40
1:Ar:154:LEU:HD21	1:At:258:LEU:HD11	2.03	0.40
1:Av:255:ASN:ND2	1:Aw:244:MET:HE1	2.37	0.40
2:Bc:274:HIS:CD2	2:Bd:258:THR:HB	2.56	0.40
2:Bd:123:LYS:HG2	2:Bd:129:VAL:HG22	2.02	0.40
2:Bk:252:VAL:HG22	2:Bk:259:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bq:103:VAL:HB	2:Bq:137:LEU:HD21	2.03	0.40
2:Bs:274:HIS:HB3	2:Bs:277:MET:HE2	2.03	0.40
2:Bz:239:LEU:HD23	2:Bz:239:LEU:HA	1.92	0.40
3:Cc:239:THR:HG21	3:Cd:155:ARG:HD3	2.03	0.40
3:Cf:164:PHE:HZ	3:Cf:285:ILE:HB	1.87	0.40
3:Ch:88:ILE:HG23	3:Ch:106:ILE:HG12	2.04	0.40
3:Cp:126:ILE:O	3:Cp:169:THR:HA	2.22	0.40
3:Ct:226:VAL:HB	3:Ct:236:MET:HB3	2.03	0.40
3:Cz:269:MET:HE3	3:Cz:269:MET:HB3	1.82	0.40
4:Dk:216:ILE:HG21	4:Dk:289:LEU:HD22	2.03	0.40
4:Dl:90:SER:HB2	4:Dl:104:ILE:HD11	2.04	0.40
4:Dl:169:ILE:HG13	4:Dl:172:LEU:HD12	2.02	0.40
4:Ds:197:LYS:HA	4:Ds:200:GLN:HB2	2.03	0.40
4:Du:165:PHE:O	4:Du:169:ILE:HG12	2.22	0.40
4:Du:184:ILE:HG12	4:Du:286:VAL:HG22	2.04	0.40
1:Af:255:ASN:ND2	1:Ag:244:MET:HE1	2.36	0.40
1:Ak:255:ASN:ND2	1:Al:244:MET:HE1	2.36	0.40
1:Ap:131:ALA:HA	1:Aq:158:ASN:HA	2.02	0.40
1:Ap:154:LEU:HD21	1:Ar:258:LEU:HD11	2.03	0.40
1:Aw:136:LEU:HD13	1:Ax:154:LEU:HD13	2.03	0.40
1:Ay:205:TYR:CZ	1:Ay:236:SER:HB3	2.56	0.40
1:Az:106:ILE:HD12	1:Az:177:THR:HG21	2.04	0.40
2:Bd:274:HIS:HB3	2:Bd:277:MET:HE2	2.02	0.40
2:Bm:252:VAL:HG22	2:Bm:259:ILE:HG12	2.02	0.40
2:Bq:274:HIS:HB3	2:Bq:277:MET:HE2	2.02	0.40
2:Bu:268:LYS:HB2	2:Bu:353:ALA:HB1	2.01	0.40
2:Bv:252:VAL:HG22	2:Bv:259:ILE:HG12	2.04	0.40
2:Bv:361:ILE:HD12	2:Bw:161:MET:HE1	2.04	0.40
3:Cc:126:ILE:O	3:Cc:169:THR:HA	2.21	0.40
3:Cd:227:PHE:HD1	3:Cd:234:GLU:HA	1.86	0.40
3:Cg:164:PHE:HZ	3:Cg:285:ILE:HB	1.87	0.40
3:Cl:28:VAL:HG13	3:Cl:49:ALA:HB1	2.03	0.40
3:Cq:28:VAL:HG13	3:Cq:49:ALA:HB1	2.03	0.40
4:Dc:93:PRO:HB2	4:Dc:95:TRP:CE3	2.54	0.40
4:Dc:197:LYS:HD3	4:Dd:292:THR:HB	2.02	0.40
4:Df:38:MET:HE2	4:Df:38:MET:HB2	1.95	0.40
4:Do:184:ILE:HG12	4:Do:286:VAL:HG22	2.03	0.40
4:Dr:107:LEU:HB3	4:Dr:108:GLN:H	1.81	0.40
4:Du:194:GLU:H	4:Du:194:GLU:HG3	1.71	0.40
4:Dw:165:PHE:O	4:Dw:169:ILE:HG12	2.22	0.40
4:Dw:184:ILE:HG12	4:Dw:286:VAL:HG22	2.04	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%)	215 (98%)	4 (2%)	0	100	100
1	Ac	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ad	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
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%)	212 (97%)	7 (3%)	0	100	100
1	Ah	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ai	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Aj	219/227 (96%)	216 (99%)	3 (1%)	0	100	100
1	Ak	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Al	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Am	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	An	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Ao	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ap	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Aq	219/227 (96%)	215 (98%)	4 (2%)	0	100	100
1	Ar	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	As	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	At	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Au	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Av	219/227 (96%)	215 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aw	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ax	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ay	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Az	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
2	Ba	312/343 (91%)	304 (97%)	8 (3%)	0	100	100
2	Bb	312/343 (91%)	302 (97%)	10 (3%)	0	100	100
2	Bc	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bd	312/343 (91%)	302 (97%)	10 (3%)	0	100	100
2	Be	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bf	312/343 (91%)	302 (97%)	10 (3%)	0	100	100
2	Bg	312/343 (91%)	304 (97%)	8 (3%)	0	100	100
2	Bh	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bi	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bj	312/343 (91%)	302 (97%)	10 (3%)	0	100	100
2	Bk	312/343 (91%)	304 (97%)	8 (3%)	0	100	100
2	Bl	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bm	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bn	312/343 (91%)	304 (97%)	8 (3%)	0	100	100
2	Bo	312/343 (91%)	304 (97%)	8 (3%)	0	100	100
2	Bp	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bq	312/343 (91%)	304 (97%)	8 (3%)	0	100	100
2	Br	312/343 (91%)	301 (96%)	11 (4%)	0	100	100
2	Bs	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bt	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bu	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bv	312/343 (91%)	304 (97%)	8 (3%)	0	100	100
2	Bw	312/343 (91%)	302 (97%)	10 (3%)	0	100	100
2	Bx	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	By	312/343 (91%)	303 (97%)	9 (3%)	0	100	100
2	Bz	312/343 (91%)	302 (97%)	10 (3%)	0	100	100
3	Ca	350/352 (99%)	342 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Cb	350/352 (99%)	332 (95%)	18 (5%)	0	100	100
3	Cc	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	Cd	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Ce	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Cf	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Cg	350/352 (99%)	342 (98%)	8 (2%)	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%)	339 (97%)	11 (3%)	0	100	100
3	Ck	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Cl	350/352 (99%)	339 (97%)	11 (3%)	0	100	100
3	Cm	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	Cn	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Co	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Cp	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Cq	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	Cr	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Cs	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Ct	350/352 (99%)	339 (97%)	11 (3%)	0	100	100
3	Cu	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Cv	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	Cw	350/352 (99%)	338 (97%)	12 (3%)	0	100	100
3	Cx	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Cy	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Cz	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
4	Da	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
4	Db	254/272 (93%)	234 (92%)	18 (7%)	2 (1%)	16	37
4	Dc	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
4	Dd	254/272 (93%)	234 (92%)	18 (7%)	2 (1%)	16	37
4	De	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
4	Df	254/272 (93%)	234 (92%)	18 (7%)	2 (1%)	16	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Dg	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
4	Dh	254/272 (93%)	235 (92%)	17 (7%)	2 (1%)	16	37
4	Di	253/272 (93%)	238 (94%)	15 (6%)	0	100	100
4	Dj	254/272 (93%)	234 (92%)	18 (7%)	2 (1%)	16	37
4	Dk	253/272 (93%)	236 (93%)	17 (7%)	0	100	100
4	Dl	254/272 (93%)	233 (92%)	19 (8%)	2 (1%)	16	37
4	Dm	253/272 (93%)	238 (94%)	15 (6%)	0	100	100
4	Dn	254/272 (93%)	233 (92%)	19 (8%)	2 (1%)	16	37
4	Do	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
4	Dp	254/272 (93%)	235 (92%)	17 (7%)	2 (1%)	16	37
4	Dq	253/272 (93%)	237 (94%)	16 (6%)	0	100	100
4	Dr	254/272 (93%)	232 (91%)	20 (8%)	2 (1%)	16	37
4	Ds	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
4	Dt	254/272 (93%)	234 (92%)	18 (7%)	2 (1%)	16	37
4	Du	253/272 (93%)	238 (94%)	15 (6%)	0	100	100
4	Dv	254/272 (93%)	233 (92%)	19 (8%)	2 (1%)	16	37
4	Dw	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
4	Dx	254/272 (93%)	233 (92%)	19 (8%)	2 (1%)	16	37
4	Dy	253/272 (93%)	240 (95%)	13 (5%)	0	100	100
4	Dz	254/272 (93%)	234 (92%)	18 (7%)	2 (1%)	16	37
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%)	12 (92%)	1 (8%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	12 (92%)	1 (8%)	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
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%)	9 (82%)	2 (18%)	0	100	100
5	Gc	11/15 (73%)	9 (82%)	2 (18%)	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%)	9 (82%)	2 (18%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	8 (73%)	3 (27%)	0	100	100
5	Gw	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
5	Gx	11/15 (73%)	8 (73%)	3 (27%)	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	30121/31824 (95%)	28961 (96%)	1134 (4%)	26 (0%)	49	73

All (26) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
4	Dv	193	VAL
4	Dx	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%)	176 (97%)	6 (3%)	33	63
1	Ab	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ac	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ad	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ae	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Af	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ag	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ah	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ai	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Aj	182/186 (98%)	176 (97%)	6 (3%)	33	63
1	Ak	182/186 (98%)	176 (97%)	6 (3%)	33	63
1	Al	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Am	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	An	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ao	182/186 (98%)	175 (96%)	7 (4%)	29	58
1	Ap	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Aq	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ar	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	As	182/186 (98%)	176 (97%)	6 (3%)	33	63
1	At	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Au	182/186 (98%)	176 (97%)	6 (3%)	33	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Av	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Aw	182/186 (98%)	177 (97%)	5 (3%)	39	69
1	Ax	182/186 (98%)	176 (97%)	6 (3%)	33	63
1	Ay	182/186 (98%)	178 (98%)	4 (2%)	45	74
1	Az	182/186 (98%)	176 (97%)	6 (3%)	33	63
2	Ba	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bb	246/269 (91%)	238 (97%)	8 (3%)	33	63
2	Bc	246/269 (91%)	238 (97%)	8 (3%)	33	63
2	Bd	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Be	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bf	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bg	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bh	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bi	246/269 (91%)	238 (97%)	8 (3%)	33	63
2	Bj	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bk	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bl	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bm	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bn	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bo	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bp	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bq	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Br	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bs	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bt	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bu	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bv	246/269 (91%)	238 (97%)	8 (3%)	33	63
2	Bw	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bx	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	By	246/269 (91%)	239 (97%)	7 (3%)	38	68
2	Bz	246/269 (91%)	239 (97%)	7 (3%)	38	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ca	299/303 (99%)	296 (99%)	3 (1%)	68	86
3	Cb	299/303 (99%)	296 (99%)	3 (1%)	68	86
3	Cc	299/303 (99%)	295 (99%)	4 (1%)	61	83
3	Cd	299/303 (99%)	293 (98%)	6 (2%)	48	76
3	Ce	299/303 (99%)	295 (99%)	4 (1%)	61	83
3	Cf	299/303 (99%)	294 (98%)	5 (2%)	53	79
3	Cg	299/303 (99%)	293 (98%)	6 (2%)	48	76
3	Ch	299/303 (99%)	294 (98%)	5 (2%)	53	79
3	Ci	299/303 (99%)	292 (98%)	7 (2%)	44	73
3	Cj	299/303 (99%)	296 (99%)	3 (1%)	68	86
3	Ck	299/303 (99%)	291 (97%)	8 (3%)	39	69
3	Cl	299/303 (99%)	295 (99%)	4 (1%)	61	83
3	Cm	299/303 (99%)	294 (98%)	5 (2%)	53	79
3	Cn	299/303 (99%)	296 (99%)	3 (1%)	68	86
3	Co	299/303 (99%)	293 (98%)	6 (2%)	48	76
3	Cp	299/303 (99%)	295 (99%)	4 (1%)	61	83
3	Cq	299/303 (99%)	295 (99%)	4 (1%)	61	83
3	Cr	299/303 (99%)	291 (97%)	8 (3%)	39	69
3	Cs	299/303 (99%)	296 (99%)	3 (1%)	68	86
3	Ct	299/303 (99%)	296 (99%)	3 (1%)	68	86
3	Cu	299/303 (99%)	293 (98%)	6 (2%)	48	76
3	Cv	299/303 (99%)	293 (98%)	6 (2%)	48	76
3	Cw	299/303 (99%)	293 (98%)	6 (2%)	48	76
3	Cx	299/303 (99%)	295 (99%)	4 (1%)	61	83
3	Cy	299/303 (99%)	294 (98%)	5 (2%)	53	79
3	Cz	299/303 (99%)	295 (99%)	4 (1%)	61	83
4	Da	231/244 (95%)	222 (96%)	9 (4%)	28	57
4	Db	229/244 (94%)	225 (98%)	4 (2%)	53	79
4	Dc	231/244 (95%)	223 (96%)	8 (4%)	32	61
4	Dd	229/244 (94%)	226 (99%)	3 (1%)	61	83
4	De	231/244 (95%)	222 (96%)	9 (4%)	28	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Df	229/244 (94%)	225 (98%)	4 (2%)	53	79
4	Dg	231/244 (95%)	222 (96%)	9 (4%)	28	57
4	Dh	229/244 (94%)	225 (98%)	4 (2%)	53	79
4	Di	231/244 (95%)	221 (96%)	10 (4%)	26	54
4	Dj	229/244 (94%)	227 (99%)	2 (1%)	70	87
4	Dk	231/244 (95%)	222 (96%)	9 (4%)	28	57
4	Dl	229/244 (94%)	226 (99%)	3 (1%)	61	83
4	Dm	231/244 (95%)	223 (96%)	8 (4%)	32	61
4	Dn	229/244 (94%)	226 (99%)	3 (1%)	61	83
4	Do	231/244 (95%)	223 (96%)	8 (4%)	32	61
4	Dp	229/244 (94%)	226 (99%)	3 (1%)	61	83
4	Dq	231/244 (95%)	223 (96%)	8 (4%)	32	61
4	Dr	229/244 (94%)	225 (98%)	4 (2%)	53	79
4	Ds	231/244 (95%)	223 (96%)	8 (4%)	32	61
4	Dt	229/244 (94%)	224 (98%)	5 (2%)	45	74
4	Du	231/244 (95%)	223 (96%)	8 (4%)	32	61
4	Dv	229/244 (94%)	226 (99%)	3 (1%)	61	83
4	Dw	231/244 (95%)	222 (96%)	9 (4%)	28	57
4	Dx	229/244 (94%)	225 (98%)	4 (2%)	53	79
4	Dy	231/244 (95%)	222 (96%)	9 (4%)	28	57
4	Dz	229/244 (94%)	225 (98%)	4 (2%)	53	79
5	Fa	14/14 (100%)	14 (100%)	0	100	100
5	Fb	14/14 (100%)	13 (93%)	1 (7%)	13	33
5	Fc	14/14 (100%)	14 (100%)	0	100	100
5	Fd	14/14 (100%)	13 (93%)	1 (7%)	13	33
5	Fe	14/14 (100%)	13 (93%)	1 (7%)	13	33
5	Ff	14/14 (100%)	13 (93%)	1 (7%)	13	33
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%)	13 (93%)	1 (7%)	13	33
5	Fj	14/14 (100%)	13 (93%)	1 (7%)	13	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	13 (93%)	1 (7%)	13	33
5	Fq	14/14 (100%)	13 (93%)	1 (7%)	13	33
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%)	13 (93%)	1 (7%)	13	33
5	Fu	14/14 (100%)	13 (93%)	1 (7%)	13	33
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%)	13 (93%)	1 (7%)	13	33
5	Fz	14/14 (100%)	14 (100%)	0	100	100
5	Ga	13/14 (93%)	12 (92%)	1 (8%)	12	30
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	30
5	Ge	13/14 (93%)	12 (92%)	1 (8%)	12	30
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	30
5	Gi	13/14 (93%)	13 (100%)	0	100	100
5	Gj	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gk	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gl	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gm	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gn	13/14 (93%)	11 (85%)	2 (15%)	2	7
5	Go	13/14 (93%)	12 (92%)	1 (8%)	12	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Gp	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gq	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gr	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gs	13/14 (93%)	13 (100%)	0	100	100
5	Gt	13/14 (93%)	10 (77%)	3 (23%)	1	2
5	Gu	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gv	13/14 (93%)	11 (85%)	2 (15%)	2	7
5	Gw	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gx	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gy	13/14 (93%)	12 (92%)	1 (8%)	12	30
5	Gz	13/14 (93%)	13 (100%)	0	100	100
All	All	25584/26780 (96%)	24943 (98%)	641 (2%)	42	71

All (641) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	106	ILE
1	Aa	112	ASN
1	Aa	145	ILE
1	Aa	176	ILE
1	Aa	201	THR
1	Aa	240	THR
1	Ab	106	ILE
1	Ab	112	ASN
1	Ab	145	ILE
1	Ab	176	ILE
1	Ab	201	THR
1	Ac	106	ILE
1	Ac	112	ASN
1	Ac	145	ILE
1	Ac	176	ILE
1	Ac	201	THR
1	Ad	106	ILE
1	Ad	112	ASN
1	Ad	145	ILE
1	Ad	176	ILE
1	Ad	201	THR
1	Ae	106	ILE

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Mol	Chain	Res	Type
1	Ae	112	ASN
1	Ae	145	ILE
1	Ae	176	ILE
1	Ae	201	THR
1	Af	106	ILE
1	Af	112	ASN
1	Af	145	ILE
1	Af	201	THR
1	Af	240	THR
1	Ag	106	ILE
1	Ag	112	ASN
1	Ag	145	ILE
1	Ag	201	THR
1	Ag	240	THR
1	Ah	106	ILE
1	Ah	112	ASN
1	Ah	145	ILE
1	Ah	176	ILE
1	Ah	201	THR
1	Ai	106	ILE
1	Ai	112	ASN
1	Ai	145	ILE
1	Ai	201	THR
1	Ai	240	THR
1	Aj	106	ILE
1	Aj	112	ASN
1	Aj	145	ILE
1	Aj	176	ILE
1	Aj	201	THR
1	Aj	240	THR
1	Ak	106	ILE
1	Ak	112	ASN
1	Ak	145	ILE
1	Ak	176	ILE
1	Ak	201	THR
1	Ak	240	THR
1	Al	106	ILE
1	Al	112	ASN
1	Al	145	ILE
1	Al	201	THR
1	Al	240	THR
1	Am	106	ILE

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Mol	Chain	Res	Type
1	Am	112	ASN
1	Am	145	ILE
1	Am	201	THR
1	Am	240	THR
1	An	106	ILE
1	An	112	ASN
1	An	145	ILE
1	An	201	THR
1	An	240	THR
1	Ao	106	ILE
1	Ao	107	ILE
1	Ao	112	ASN
1	Ao	145	ILE
1	Ao	176	ILE
1	Ao	201	THR
1	Ao	240	THR
1	Ap	106	ILE
1	Ap	112	ASN
1	Ap	145	ILE
1	Ap	201	THR
1	Ap	240	THR
1	Aq	106	ILE
1	Aq	112	ASN
1	Aq	145	ILE
1	Aq	201	THR
1	Aq	240	THR
1	Ar	106	ILE
1	Ar	112	ASN
1	Ar	145	ILE
1	Ar	176	ILE
1	Ar	201	THR
1	As	106	ILE
1	As	112	ASN
1	As	145	ILE
1	As	176	ILE
1	As	201	THR
1	As	240	THR
1	At	106	ILE
1	At	112	ASN
1	At	145	ILE
1	At	176	ILE
1	At	201	THR

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Mol	Chain	Res	Type
1	Au	106	ILE
1	Au	112	ASN
1	Au	145	ILE
1	Au	176	ILE
1	Au	201	THR
1	Au	240	THR
1	Av	106	ILE
1	Av	112	ASN
1	Av	145	ILE
1	Av	176	ILE
1	Av	201	THR
1	Aw	106	ILE
1	Aw	112	ASN
1	Aw	145	ILE
1	Aw	176	ILE
1	Aw	201	THR
1	Ax	106	ILE
1	Ax	107	ILE
1	Ax	112	ASN
1	Ax	145	ILE
1	Ax	201	THR
1	Ax	240	THR
1	Ay	106	ILE
1	Ay	112	ASN
1	Ay	145	ILE
1	Ay	201	THR
1	Az	106	ILE
1	Az	107	ILE
1	Az	112	ASN
1	Az	145	ILE
1	Az	176	ILE
1	Az	201	THR
2	Ba	145	THR
2	Ba	182	ILE
2	Ba	233	LEU
2	Ba	253	ASN
2	Ba	256	THR
2	Ba	258	THR
2	Ba	322	VAL
2	Bb	51	THR
2	Bb	145	THR
2	Bb	233	LEU

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Mol	Chain	Res	Type
2	Bb	253	ASN
2	Bb	256	THR
2	Bb	258	THR
2	Bb	273	THR
2	Bb	322	VAL
2	Bc	51	THR
2	Bc	145	THR
2	Bc	233	LEU
2	Bc	253	ASN
2	Bc	256	THR
2	Bc	258	THR
2	Bc	273	THR
2	Bc	322	VAL
2	Bd	145	THR
2	Bd	233	LEU
2	Bd	253	ASN
2	Bd	256	THR
2	Bd	258	THR
2	Bd	273	THR
2	Bd	322	VAL
2	Be	145	THR
2	Be	233	LEU
2	Be	253	ASN
2	Be	256	THR
2	Be	258	THR
2	Be	273	THR
2	Be	322	VAL
2	Bf	145	THR
2	Bf	233	LEU
2	Bf	253	ASN
2	Bf	256	THR
2	Bf	258	THR
2	Bf	273	THR
2	Bf	322	VAL
2	Bg	145	THR
2	Bg	233	LEU
2	Bg	253	ASN
2	Bg	256	THR
2	Bg	258	THR
2	Bg	273	THR
2	Bg	322	VAL
2	Bh	145	THR

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Mol	Chain	Res	Type
2	Bh	233	LEU
2	Bh	253	ASN
2	Bh	256	THR
2	Bh	258	THR
2	Bh	273	THR
2	Bh	322	VAL
2	Bi	51	THR
2	Bi	145	THR
2	Bi	233	LEU
2	Bi	253	ASN
2	Bi	256	THR
2	Bi	258	THR
2	Bi	273	THR
2	Bi	322	VAL
2	Bj	145	THR
2	Bj	233	LEU
2	Bj	253	ASN
2	Bj	256	THR
2	Bj	258	THR
2	Bj	273	THR
2	Bj	322	VAL
2	Bk	145	THR
2	Bk	233	LEU
2	Bk	253	ASN
2	Bk	256	THR
2	Bk	258	THR
2	Bk	273	THR
2	Bk	322	VAL
2	Bl	145	THR
2	Bl	233	LEU
2	Bl	253	ASN
2	Bl	256	THR
2	Bl	258	THR
2	Bl	273	THR
2	Bl	322	VAL
2	Bm	145	THR
2	Bm	233	LEU
2	Bm	253	ASN
2	Bm	256	THR
2	Bm	258	THR
2	Bm	273	THR
2	Bm	322	VAL

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Mol	Chain	Res	Type
2	Bn	145	THR
2	Bn	233	LEU
2	Bn	253	ASN
2	Bn	256	THR
2	Bn	258	THR
2	Bn	273	THR
2	Bn	322	VAL
2	Bo	145	THR
2	Bo	233	LEU
2	Bo	253	ASN
2	Bo	256	THR
2	Bo	258	THR
2	Bo	273	THR
2	Bo	322	VAL
2	Bp	145	THR
2	Bp	233	LEU
2	Bp	253	ASN
2	Bp	256	THR
2	Bp	258	THR
2	Bp	273	THR
2	Bp	322	VAL
2	Bq	145	THR
2	Bq	233	LEU
2	Bq	253	ASN
2	Bq	256	THR
2	Bq	258	THR
2	Bq	273	THR
2	Bq	322	VAL
2	Br	145	THR
2	Br	233	LEU
2	Br	253	ASN
2	Br	256	THR
2	Br	258	THR
2	Br	273	THR
2	Br	322	VAL
2	Bs	145	THR
2	Bs	233	LEU
2	Bs	253	ASN
2	Bs	256	THR
2	Bs	258	THR
2	Bs	273	THR
2	Bs	322	VAL

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Mol	Chain	Res	Type
2	Bt	145	THR
2	Bt	233	LEU
2	Bt	253	ASN
2	Bt	256	THR
2	Bt	258	THR
2	Bt	273	THR
2	Bt	322	VAL
2	Bu	145	THR
2	Bu	233	LEU
2	Bu	253	ASN
2	Bu	256	THR
2	Bu	258	THR
2	Bu	273	THR
2	Bu	322	VAL
2	Bv	51	THR
2	Bv	145	THR
2	Bv	233	LEU
2	Bv	253	ASN
2	Bv	256	THR
2	Bv	258	THR
2	Bv	273	THR
2	Bv	322	VAL
2	Bw	145	THR
2	Bw	233	LEU
2	Bw	253	ASN
2	Bw	256	THR
2	Bw	258	THR
2	Bw	273	THR
2	Bw	322	VAL
2	Bx	145	THR
2	Bx	233	LEU
2	Bx	253	ASN
2	Bx	256	THR
2	Bx	258	THR
2	Bx	273	THR
2	Bx	322	VAL
2	By	145	THR
2	By	233	LEU
2	By	253	ASN
2	By	256	THR
2	By	258	THR
2	By	273	THR

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Mol	Chain	Res	Type
2	By	322	VAL
2	Bz	145	THR
2	Bz	233	LEU
2	Bz	253	ASN
2	Bz	256	THR
2	Bz	258	THR
2	Bz	273	THR
2	Bz	322	VAL
3	Ca	35	VAL
3	Ca	353	GLU
3	Ca	356	LEU
3	Cb	107	ASP
3	Cb	327	ILE
3	Cb	345	THR
3	Cc	35	VAL
3	Cc	286	SER
3	Cc	327	ILE
3	Cc	356	LEU
3	Cd	35	VAL
3	Cd	166	SER
3	Cd	243	VAL
3	Cd	327	ILE
3	Cd	353	GLU
3	Cd	356	LEU
3	Ce	154	ASN
3	Ce	286	SER
3	Ce	327	ILE
3	Ce	353	GLU
3	Cf	71	LEU
3	Cf	87	TYR
3	Cf	286	SER
3	Cf	353	GLU
3	Cf	356	LEU
3	Cg	35	VAL
3	Cg	87	TYR
3	Cg	286	SER
3	Cg	327	ILE
3	Cg	353	GLU
3	Cg	356	LEU
3	Ch	154	ASN
3	Ch	286	SER
3	Ch	327	ILE

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Mol	Chain	Res	Type
3	Ch	353	GLU
3	Ch	356	LEU
3	Ci	89	LEU
3	Ci	154	ASN
3	Ci	237	THR
3	Ci	286	SER
3	Ci	327	ILE
3	Ci	353	GLU
3	Ci	356	LEU
3	Cj	154	ASN
3	Cj	243	VAL
3	Cj	353	GLU
3	Ck	89	LEU
3	Ck	237	THR
3	Ck	243	VAL
3	Ck	286	SER
3	Ck	327	ILE
3	Ck	328	ASP
3	Ck	353	GLU
3	Ck	356	LEU
3	Cl	89	LEU
3	Cl	208	GLN
3	Cl	327	ILE
3	Cl	353	GLU
3	Cm	35	VAL
3	Cm	286	SER
3	Cm	327	ILE
3	Cm	353	GLU
3	Cm	356	LEU
3	Cn	286	SER
3	Cn	327	ILE
3	Cn	356	LEU
3	Co	35	VAL
3	Co	154	ASN
3	Co	237	THR
3	Co	286	SER
3	Co	327	ILE
3	Co	353	GLU
3	Cp	107	ASP
3	Cp	286	SER
3	Cp	327	ILE
3	Cp	353	GLU

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Mol	Chain	Res	Type
3	Cq	35	VAL
3	Cq	243	VAL
3	Cq	327	ILE
3	Cq	353	GLU
3	Cr	35	VAL
3	Cr	237	THR
3	Cr	243	VAL
3	Cr	286	SER
3	Cr	327	ILE
3	Cr	328	ASP
3	Cr	353	GLU
3	Cr	356	LEU
3	Cs	237	THR
3	Cs	327	ILE
3	Cs	356	LEU
3	Ct	35	VAL
3	Ct	286	SER
3	Ct	353	GLU
3	Cu	35	VAL
3	Cu	237	THR
3	Cu	286	SER
3	Cu	327	ILE
3	Cu	353	GLU
3	Cu	356	LEU
3	Cv	35	VAL
3	Cv	87	TYR
3	Cv	243	VAL
3	Cv	286	SER
3	Cv	353	GLU
3	Cv	356	LEU
3	Cw	71	LEU
3	Cw	237	THR
3	Cw	286	SER
3	Cw	327	ILE
3	Cw	353	GLU
3	Cw	356	LEU
3	Cx	327	ILE
3	Cx	353	GLU
3	Cx	356	LEU
3	Cx	363	LEU
3	Cy	107	ASP
3	Cy	237	THR

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Mol	Chain	Res	Type
3	Cy	286	SER
3	Cy	327	ILE
3	Cy	353	GLU
3	Cz	286	SER
3	Cz	327	ILE
3	Cz	328	ASP
3	Cz	356	LEU
4	Da	89	VAL
4	Da	106	ASN
4	Da	112	GLN
4	Da	117	ILE
4	Da	173	LEU
4	Da	180	ILE
4	Da	250	LYS
4	Da	264	TYR
4	Da	266	LYS
4	Db	25	VAL
4	Db	37	GLN
4	Db	193	VAL
4	Db	220	LEU
4	Dc	89	VAL
4	Dc	106	ASN
4	Dc	112	GLN
4	Dc	117	ILE
4	Dc	173	LEU
4	Dc	250	LYS
4	Dc	264	TYR
4	Dc	266	LYS
4	Dd	25	VAL
4	Dd	68	ILE
4	Dd	220	LEU
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	250	LYS
4	De	264	TYR
4	De	266	LYS
4	Df	25	VAL
4	Df	68	ILE

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Mol	Chain	Res	Type
4	Df	193	VAL
4	Df	220	LEU
4	Dg	89	VAL
4	Dg	106	ASN
4	Dg	112	GLN
4	Dg	117	ILE
4	Dg	173	LEU
4	Dg	180	ILE
4	Dg	250	LYS
4	Dg	264	TYR
4	Dg	266	LYS
4	Dh	25	VAL
4	Dh	68	ILE
4	Dh	193	VAL
4	Dh	220	LEU
4	Di	89	VAL
4	Di	106	ASN
4	Di	112	GLN
4	Di	117	ILE
4	Di	173	LEU
4	Di	180	ILE
4	Di	223	THR
4	Di	250	LYS
4	Di	264	TYR
4	Di	266	LYS
4	Dj	25	VAL
4	Dj	220	LEU
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	250	LYS
4	Dk	264	TYR
4	Dk	266	LYS
4	Dl	25	VAL
4	Dl	193	VAL
4	Dl	220	LEU
4	Dm	89	VAL
4	Dm	106	ASN
4	Dm	112	GLN

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Mol	Chain	Res	Type
4	Dm	117	ILE
4	Dm	173	LEU
4	Dm	250	LYS
4	Dm	264	TYR
4	Dm	266	LYS
4	Dn	25	VAL
4	Dn	68	ILE
4	Dn	220	LEU
4	Do	89	VAL
4	Do	106	ASN
4	Do	112	GLN
4	Do	117	ILE
4	Do	173	LEU
4	Do	250	LYS
4	Do	264	TYR
4	Do	266	LYS
4	Dp	25	VAL
4	Dp	37	GLN
4	Dp	220	LEU
4	Dq	89	VAL
4	Dq	106	ASN
4	Dq	112	GLN
4	Dq	117	ILE
4	Dq	173	LEU
4	Dq	250	LYS
4	Dq	264	TYR
4	Dq	266	LYS
4	Dr	25	VAL
4	Dr	37	GLN
4	Dr	193	VAL
4	Dr	220	LEU
4	Ds	89	VAL
4	Ds	106	ASN
4	Ds	112	GLN
4	Ds	117	ILE
4	Ds	173	LEU
4	Ds	250	LYS
4	Ds	264	TYR
4	Ds	266	LYS
4	Dt	25	VAL
4	Dt	37	GLN
4	Dt	68	ILE

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Mol	Chain	Res	Type
4	Dt	193	VAL
4	Dt	220	LEU
4	Du	89	VAL
4	Du	106	ASN
4	Du	112	GLN
4	Du	117	ILE
4	Du	173	LEU
4	Du	250	LYS
4	Du	264	TYR
4	Du	266	LYS
4	Dv	25	VAL
4	Dv	193	VAL
4	Dv	220	LEU
4	Dw	89	VAL
4	Dw	106	ASN
4	Dw	112	GLN
4	Dw	117	ILE
4	Dw	173	LEU
4	Dw	180	ILE
4	Dw	250	LYS
4	Dw	264	TYR
4	Dw	266	LYS
4	Dx	25	VAL
4	Dx	37	GLN
4	Dx	193	VAL
4	Dx	220	LEU
4	Dy	25	VAL
4	Dy	89	VAL
4	Dy	106	ASN
4	Dy	112	GLN
4	Dy	117	ILE
4	Dy	173	LEU
4	Dy	250	LYS
4	Dy	264	TYR
4	Dy	266	LYS
4	Dz	25	VAL
4	Dz	37	GLN
4	Dz	193	VAL
4	Dz	220	LEU
5	Fb	145	PHE
5	Fd	139	LYS
5	Fe	139	LYS

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Mol	Chain	Res	Type
5	Ff	139	LYS
5	Fi	139	LYS
5	Fj	139	LYS
5	Fp	139	LYS
5	Fq	139	LYS
5	Ft	139	LYS
5	Fu	139	LYS
5	Fy	139	LYS
5	Ga	138	GLU
5	Gd	138	GLU
5	Ge	138	GLU
5	Gh	138	GLU
5	Gj	138	GLU
5	Gk	138	GLU
5	Gl	138	GLU
5	Gm	138	GLU
5	Gn	138	GLU
5	Gn	141	GLN
5	Go	138	GLU
5	Gp	138	GLU
5	Gq	138	GLU
5	Gr	138	GLU
5	Gt	134	GLN
5	Gt	138	GLU
5	Gt	141	GLN
5	Gu	138	GLU
5	Gv	138	GLU
5	Gv	143	THR
5	Gw	138	GLU
5	Gx	138	GLU
5	Gy	138	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (529) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	112	ASN
1	Aa	200	ASN
1	Aa	226	ASN
1	Aa	255	ASN
1	Ab	70	HIS
1	Ab	112	ASN
1	Ab	200	ASN

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Mol	Chain	Res	Type
1	Ab	226	ASN
1	Ab	255	ASN
1	Ac	112	ASN
1	Ac	200	ASN
1	Ac	226	ASN
1	Ac	255	ASN
1	Ad	112	ASN
1	Ad	200	ASN
1	Ad	226	ASN
1	Ad	255	ASN
1	Ae	112	ASN
1	Ae	129	ASN
1	Ae	200	ASN
1	Ae	226	ASN
1	Ae	255	ASN
1	Af	112	ASN
1	Af	129	ASN
1	Af	158	ASN
1	Af	167	ASN
1	Af	200	ASN
1	Af	226	ASN
1	Af	255	ASN
1	Ag	112	ASN
1	Ag	129	ASN
1	Ag	158	ASN
1	Ag	200	ASN
1	Ag	226	ASN
1	Ag	255	ASN
1	Ah	112	ASN
1	Ah	200	ASN
1	Ah	226	ASN
1	Ah	255	ASN
1	Ai	112	ASN
1	Ai	200	ASN
1	Ai	226	ASN
1	Ai	242	GLN
1	Ai	255	ASN
1	Aj	112	ASN
1	Aj	200	ASN
1	Aj	226	ASN
1	Aj	255	ASN
1	Ak	112	ASN

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Mol	Chain	Res	Type
1	Ak	167	ASN
1	Ak	200	ASN
1	Ak	226	ASN
1	Ak	255	ASN
1	Al	112	ASN
1	Al	129	ASN
1	Al	200	ASN
1	Al	226	ASN
1	Al	255	ASN
1	Am	112	ASN
1	Am	129	ASN
1	Am	200	ASN
1	Am	226	ASN
1	Am	255	ASN
1	An	112	ASN
1	An	129	ASN
1	An	167	ASN
1	An	200	ASN
1	An	226	ASN
1	An	255	ASN
1	Ao	112	ASN
1	Ao	129	ASN
1	Ao	200	ASN
1	Ao	226	ASN
1	Ao	255	ASN
1	Ap	112	ASN
1	Ap	129	ASN
1	Ap	158	ASN
1	Ap	200	ASN
1	Ap	226	ASN
1	Ap	255	ASN
1	Aq	112	ASN
1	Aq	129	ASN
1	Aq	200	ASN
1	Aq	226	ASN
1	Aq	255	ASN
1	Ar	112	ASN
1	Ar	129	ASN
1	Ar	158	ASN
1	Ar	200	ASN
1	Ar	226	ASN
1	Ar	255	ASN

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Mol	Chain	Res	Type
1	As	112	ASN
1	As	200	ASN
1	As	226	ASN
1	As	242	GLN
1	As	255	ASN
1	At	112	ASN
1	At	200	ASN
1	At	226	ASN
1	At	255	ASN
1	Au	112	ASN
1	Au	167	ASN
1	Au	200	ASN
1	Au	226	ASN
1	Au	255	ASN
1	Av	112	ASN
1	Av	200	ASN
1	Av	226	ASN
1	Av	255	ASN
1	Aw	112	ASN
1	Aw	129	ASN
1	Aw	200	ASN
1	Aw	226	ASN
1	Aw	255	ASN
1	Ax	112	ASN
1	Ax	129	ASN
1	Ax	200	ASN
1	Ax	226	ASN
1	Ax	255	ASN
1	Ay	112	ASN
1	Ay	129	ASN
1	Ay	200	ASN
1	Ay	226	ASN
1	Az	112	ASN
1	Az	129	ASN
1	Az	158	ASN
1	Az	200	ASN
1	Az	226	ASN
1	Az	255	ASN
2	Ba	26	GLN
2	Ba	56	GLN
2	Ba	97	GLN
2	Ba	134	GLN

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Mol	Chain	Res	Type
2	Ba	253	ASN
2	Ba	357	GLN
2	Bb	26	GLN
2	Bb	56	GLN
2	Bb	134	GLN
2	Bb	228	GLN
2	Bb	253	ASN
2	Bb	264	ASN
2	Bb	346	GLN
2	Bb	357	GLN
2	Bc	26	GLN
2	Bc	56	GLN
2	Bc	97	GLN
2	Bc	238	ASN
2	Bc	253	ASN
2	Bc	264	ASN
2	Bc	346	GLN
2	Bc	357	GLN
2	Bd	26	GLN
2	Bd	56	GLN
2	Bd	195	GLN
2	Bd	253	ASN
2	Bd	357	GLN
2	Be	26	GLN
2	Be	56	GLN
2	Be	134	GLN
2	Be	228	GLN
2	Be	253	ASN
2	Be	357	GLN
2	Bf	26	GLN
2	Bf	56	GLN
2	Bf	134	GLN
2	Bf	253	ASN
2	Bf	264	ASN
2	Bf	346	GLN
2	Bf	357	GLN
2	Bg	26	GLN
2	Bg	56	GLN
2	Bg	134	GLN
2	Bg	253	ASN
2	Bg	346	GLN
2	Bg	357	GLN

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Mol	Chain	Res	Type
2	Bh	26	GLN
2	Bh	56	GLN
2	Bh	134	GLN
2	Bh	253	ASN
2	Bh	264	ASN
2	Bh	357	GLN
2	Bi	26	GLN
2	Bi	56	GLN
2	Bi	97	GLN
2	Bi	253	ASN
2	Bi	357	GLN
2	Bj	26	GLN
2	Bj	56	GLN
2	Bj	134	GLN
2	Bj	228	GLN
2	Bj	253	ASN
2	Bj	357	GLN
2	Bk	26	GLN
2	Bk	56	GLN
2	Bk	97	GLN
2	Bk	253	ASN
2	Bk	264	ASN
2	Bk	357	GLN
2	Bl	26	GLN
2	Bl	56	GLN
2	Bl	97	GLN
2	Bl	253	ASN
2	Bl	264	ASN
2	Bm	26	GLN
2	Bm	56	GLN
2	Bm	134	GLN
2	Bm	253	ASN
2	Bm	264	ASN
2	Bm	357	GLN
2	Bn	26	GLN
2	Bn	56	GLN
2	Bn	134	GLN
2	Bn	238	ASN
2	Bn	253	ASN
2	Bn	264	ASN
2	Bn	357	GLN
2	Bo	26	GLN

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Mol	Chain	Res	Type
2	Bo	56	GLN
2	Bo	97	GLN
2	Bo	195	GLN
2	Bo	253	ASN
2	Bo	357	GLN
2	Bp	26	GLN
2	Bp	56	GLN
2	Bp	134	GLN
2	Bp	253	ASN
2	Bp	357	GLN
2	Bq	26	GLN
2	Bq	56	GLN
2	Bq	134	GLN
2	Bq	238	ASN
2	Bq	253	ASN
2	Bq	346	GLN
2	Bq	357	GLN
2	Br	26	GLN
2	Br	56	GLN
2	Br	97	GLN
2	Br	195	GLN
2	Br	253	ASN
2	Br	264	ASN
2	Br	357	GLN
2	Bs	26	GLN
2	Bs	56	GLN
2	Bs	134	GLN
2	Bs	253	ASN
2	Bs	264	ASN
2	Bs	357	GLN
2	Bt	26	GLN
2	Bt	56	GLN
2	Bt	134	GLN
2	Bt	253	ASN
2	Bt	264	ASN
2	Bu	26	GLN
2	Bu	56	GLN
2	Bu	134	GLN
2	Bu	253	ASN
2	Bu	357	GLN
2	Bv	26	GLN
2	Bv	56	GLN

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Mol	Chain	Res	Type
2	Bv	134	GLN
2	Bv	195	GLN
2	Bv	253	ASN
2	Bv	264	ASN
2	Bv	357	GLN
2	Bw	26	GLN
2	Bw	56	GLN
2	Bw	97	GLN
2	Bw	134	GLN
2	Bw	253	ASN
2	Bw	264	ASN
2	Bw	357	GLN
2	Bx	26	GLN
2	Bx	56	GLN
2	Bx	97	GLN
2	Bx	134	GLN
2	Bx	228	GLN
2	Bx	253	ASN
2	Bx	264	ASN
2	Bx	357	GLN
2	By	26	GLN
2	By	56	GLN
2	By	134	GLN
2	By	228	GLN
2	By	253	ASN
2	By	264	ASN
2	By	357	GLN
2	Bz	26	GLN
2	Bz	56	GLN
2	Bz	134	GLN
2	Bz	253	ASN
2	Bz	357	GLN
3	Ca	128	ASN
3	Cb	97	ASN
3	Cb	116	HIS
3	Cb	154	ASN
3	Cb	217	ASN
3	Cb	329	GLN
3	Cb	374	HIS
3	Cc	154	ASN
3	Cc	208	GLN
3	Cc	253	GLN

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Mol	Chain	Res	Type
3	Cc	276	ASN
3	Cc	329	GLN
3	Cd	154	ASN
3	Cd	293	GLN
3	Cd	322	HIS
3	Ce	97	ASN
3	Ce	154	ASN
3	Ce	212	GLN
3	Ce	339	GLN
3	Cf	66	ASN
3	Cf	128	ASN
3	Cf	135	GLN
3	Cf	154	ASN
3	Cf	159	GLN
3	Cf	217	ASN
3	Cf	253	GLN
3	Cf	322	HIS
3	Cg	128	ASN
3	Cg	293	GLN
3	Cg	314	GLN
3	Cg	322	HIS
3	Ch	253	GLN
3	Ch	322	HIS
3	Ci	128	ASN
3	Ci	135	GLN
3	Ci	212	GLN
3	Cj	97	ASN
3	Cj	253	GLN
3	Cj	322	HIS
3	Ck	97	ASN
3	Ck	253	GLN
3	Cl	314	GLN
3	Cl	322	HIS
3	Cm	314	GLN
3	Cn	135	GLN
3	Cn	212	GLN
3	Cn	253	GLN
3	Cn	322	HIS
3	Co	97	ASN
3	Co	128	ASN
3	Co	253	GLN
3	Co	276	ASN

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Mol	Chain	Res	Type
3	Cp	253	GLN
3	Cp	322	HIS
3	Cq	66	ASN
3	Cq	322	HIS
3	Cr	135	GLN
3	Cr	322	HIS
3	Cs	116	HIS
3	Cs	135	GLN
3	Cs	212	GLN
3	Ct	97	ASN
3	Ct	135	GLN
3	Ct	322	HIS
3	Cu	276	ASN
3	Cu	329	GLN
3	Cv	97	ASN
3	Cv	116	HIS
3	Cv	322	HIS
3	Cw	66	ASN
3	Cw	154	ASN
3	Cw	212	GLN
3	Cx	97	ASN
3	Cx	322	HIS
3	Cx	339	GLN
3	Cy	97	ASN
3	Cy	135	GLN
3	Cz	97	ASN
3	Cz	135	GLN
3	Cz	159	GLN
3	Cz	322	HIS
3	Cz	376	GLN
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	189	GLN
4	Db	235	GLN
4	Db	293	GLN
4	Dc	33	GLN

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Mol	Chain	Res	Type
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	108	GLN
4	De	112	GLN
4	De	143	GLN
4	De	147	GLN
4	De	282	ASN
4	Df	50	HIS
4	Df	112	GLN
4	Df	120	GLN
4	Df	189	GLN
4	Df	235	GLN
4	Df	293	GLN
4	Dg	108	GLN
4	Dg	112	GLN
4	Dg	143	GLN
4	Dg	147	GLN
4	Dg	282	ASN
4	Dh	50	HIS
4	Dh	112	GLN
4	Dh	120	GLN
4	Dh	189	GLN
4	Dh	235	GLN
4	Dh	293	GLN
4	Di	33	GLN
4	Di	108	GLN
4	Di	112	GLN
4	Di	143	GLN
4	Di	147	GLN
4	Di	282	ASN
4	Dj	50	HIS
4	Dj	112	GLN
4	Dj	120	GLN

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Mol	Chain	Res	Type
4	Dj	235	GLN
4	Dj	293	GLN
4	Dk	33	GLN
4	Dk	108	GLN
4	Dk	112	GLN
4	Dk	143	GLN
4	Dk	147	GLN
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
4	Dm	108	GLN
4	Dm	112	GLN
4	Dm	143	GLN
4	Dm	147	GLN
4	Dm	282	ASN
4	Dn	32	GLN
4	Dn	112	GLN
4	Dn	120	GLN
4	Dn	235	GLN
4	Dn	293	GLN
4	Do	108	GLN
4	Do	112	GLN
4	Do	143	GLN
4	Do	147	GLN
4	Do	282	ASN
4	Dp	32	GLN
4	Dp	50	HIS
4	Dp	112	GLN
4	Dp	120	GLN
4	Dp	235	GLN
4	Dp	293	GLN
4	Dq	108	GLN
4	Dq	112	GLN
4	Dq	143	GLN
4	Dq	147	GLN
4	Dq	282	ASN
4	Dr	112	GLN
4	Dr	120	GLN

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Mol	Chain	Res	Type
4	Dr	235	GLN
4	Dr	293	GLN
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	50	HIS
4	Dt	112	GLN
4	Dt	120	GLN
4	Dt	235	GLN
4	Dt	293	GLN
4	Du	33	GLN
4	Du	108	GLN
4	Du	112	GLN
4	Du	143	GLN
4	Du	147	GLN
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	33	GLN
4	Dw	108	GLN
4	Dw	112	GLN
4	Dw	143	GLN
4	Dw	147	GLN
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	108	GLN
4	Dy	112	GLN
4	Dy	143	GLN
4	Dy	147	GLN
4	Dy	282	ASN

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Mol	Chain	Res	Type
4	Dz	50	HIS
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	Gi	135	GLN
5	Gk	135	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	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.

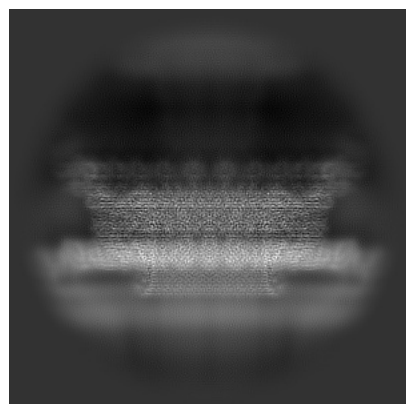
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72815. These allow visual inspection of the internal detail of the map and identification of artifacts.

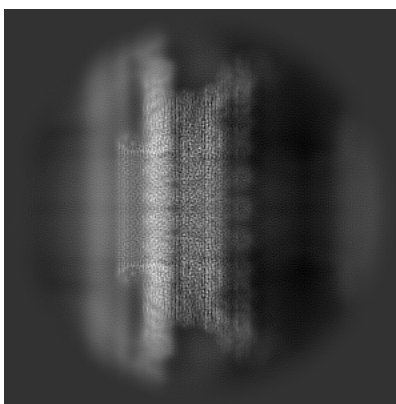
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

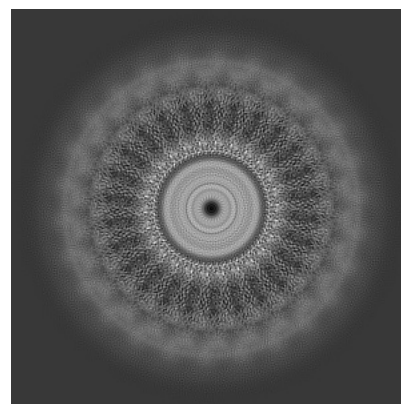
#### 6.1.1 Primary map



X

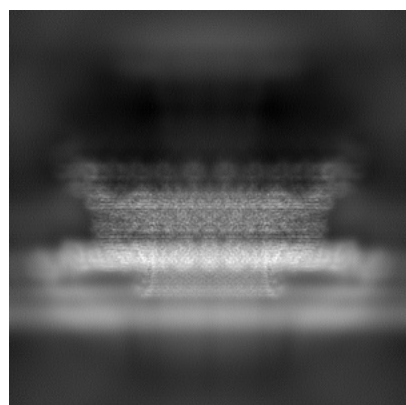


Y

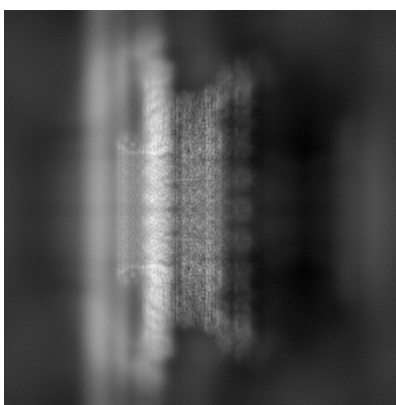


Z

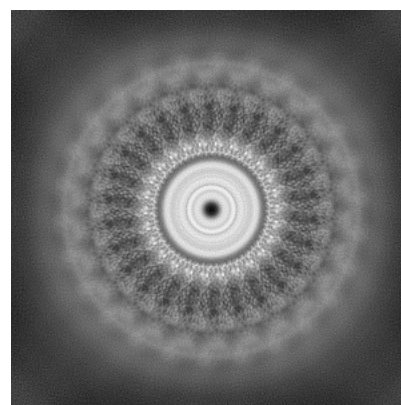
#### 6.1.2 Raw map



X



Y



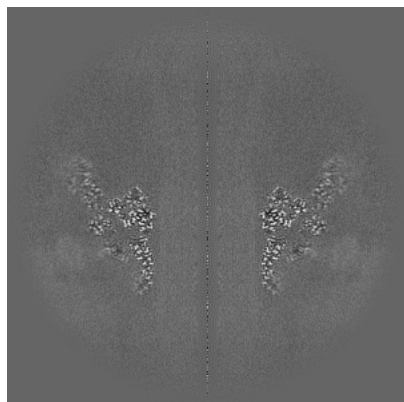
Z

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

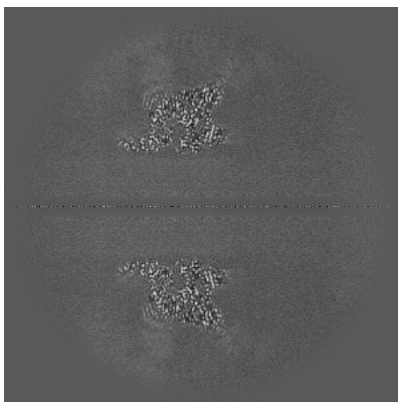


## 6.2 Central slices [i](#)

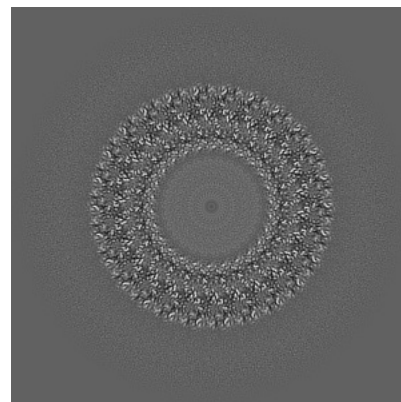
### 6.2.1 Primary map



X Index: 224

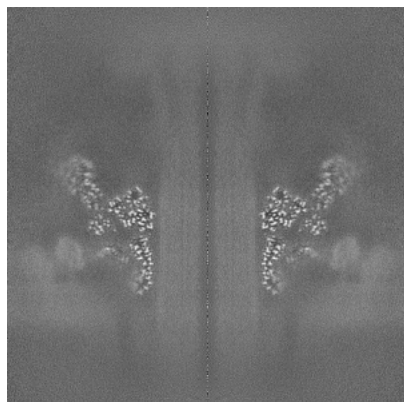


Y Index: 224

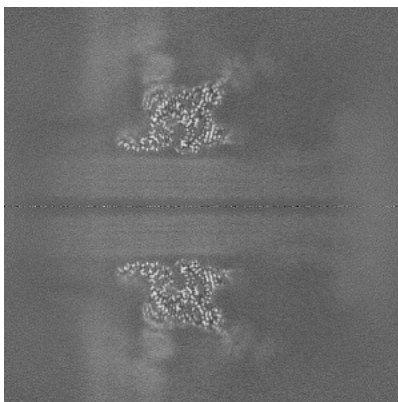


Z Index: 224

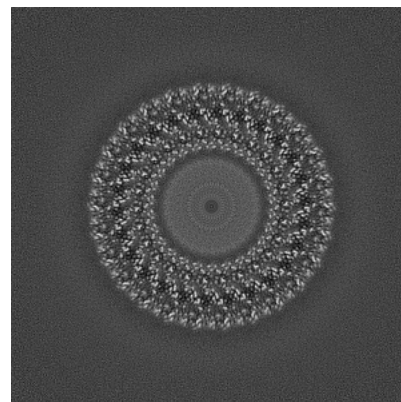
### 6.2.2 Raw map



X Index: 224



Y Index: 224

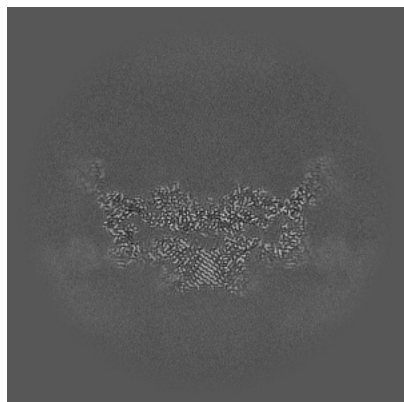


Z Index: 224

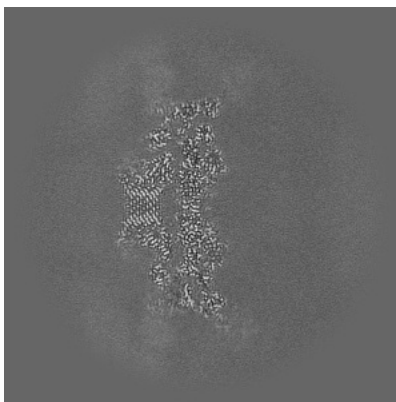
The images above show central slices of the map in three orthogonal directions.

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

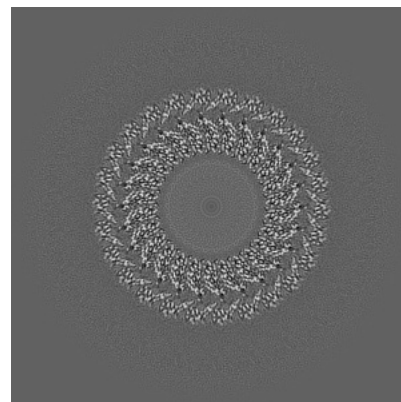
### 6.3.1 Primary map



X Index: 289

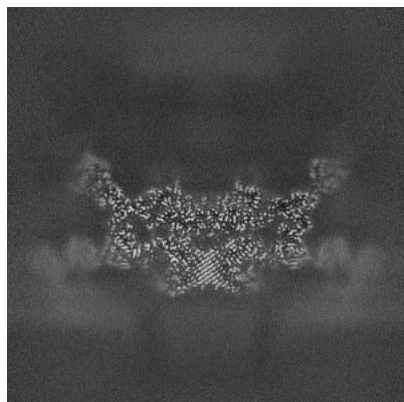


Y Index: 161

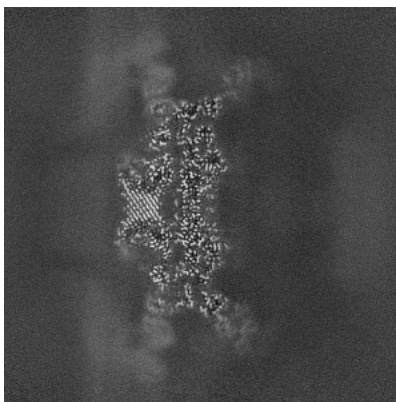


Z Index: 208

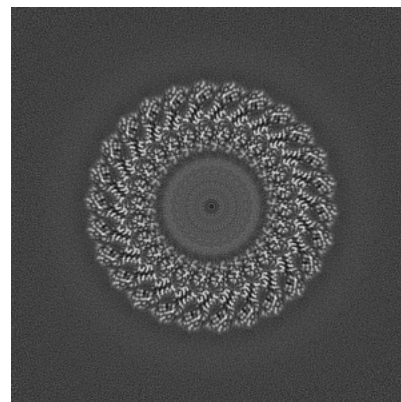
### 6.3.2 Raw map



X Index: 159



Y Index: 160

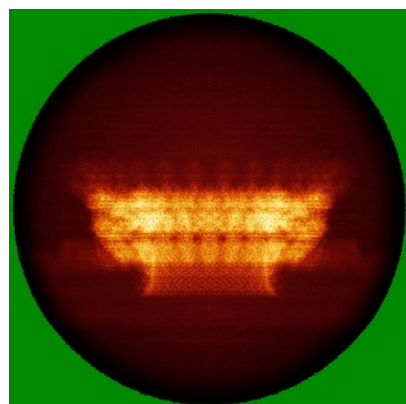


Z Index: 227

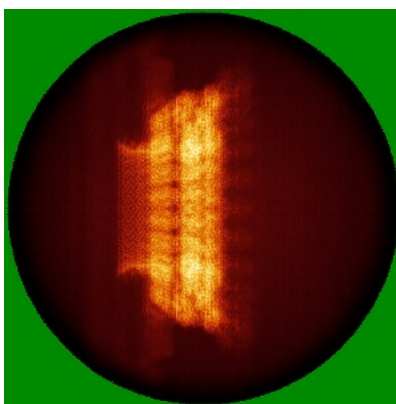
The images above show the largest variance slices of the map in three orthogonal directions.

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

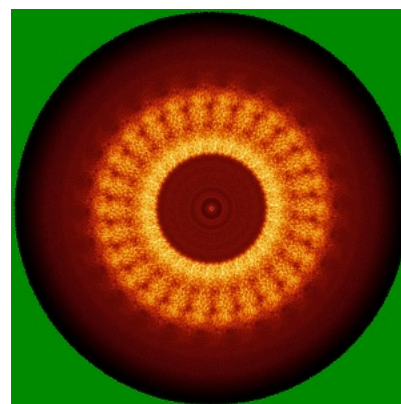
### 6.4.1 Primary map



X

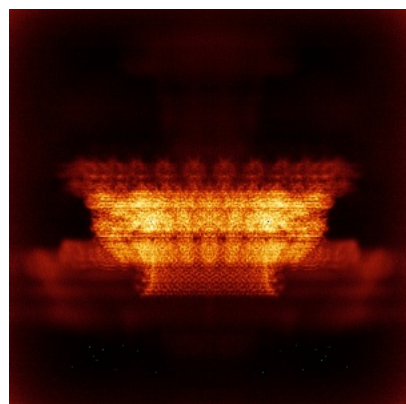


Y

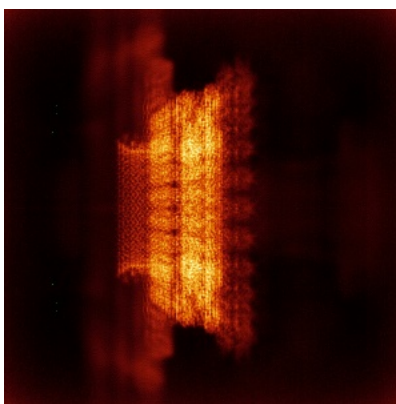


Z

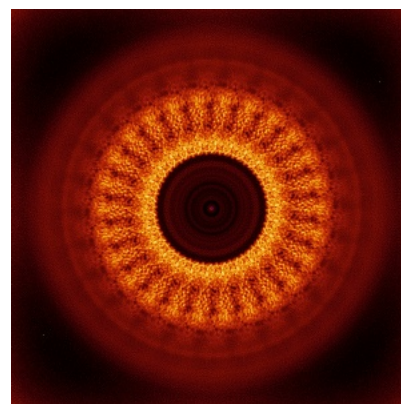
### 6.4.2 Raw map



X



Y

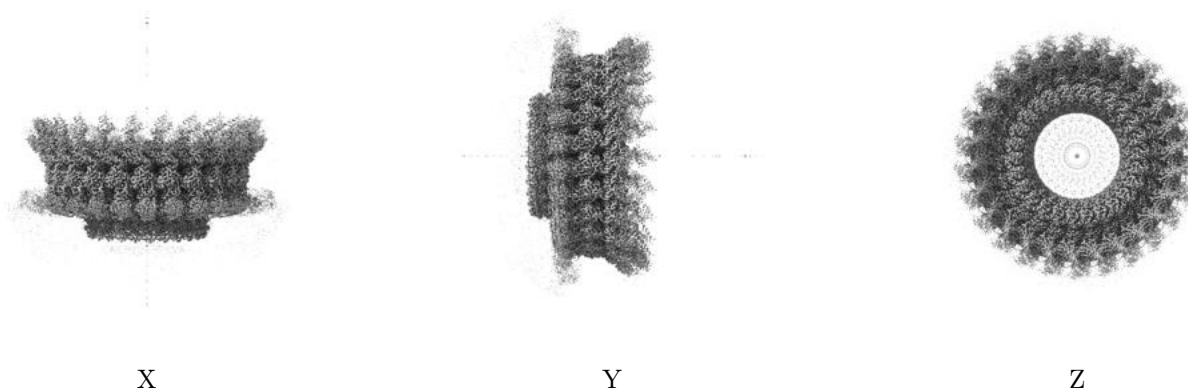


Z

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.

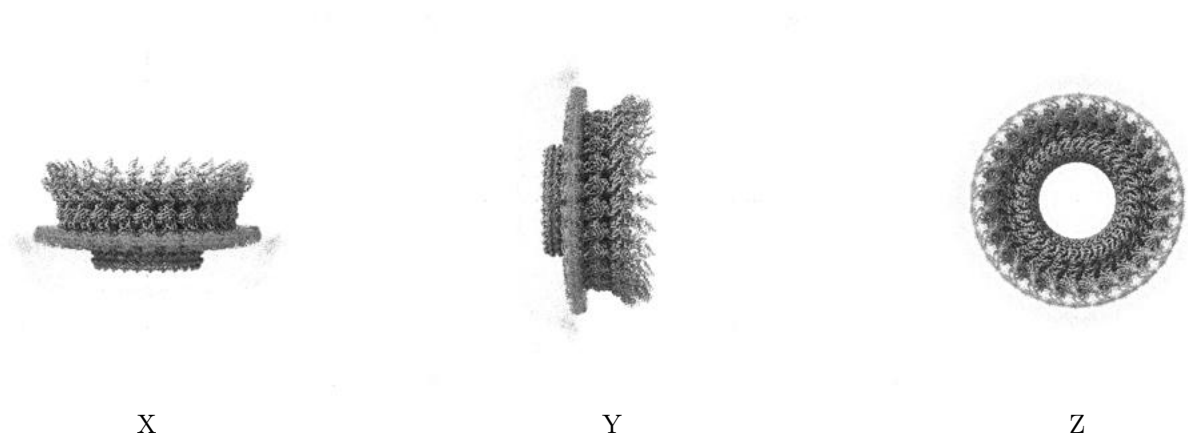
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.



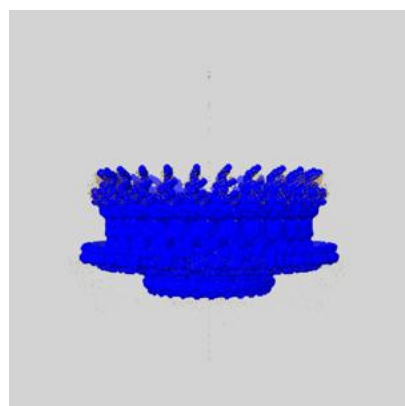
## 6.6 Mask visualisation [i](#)

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

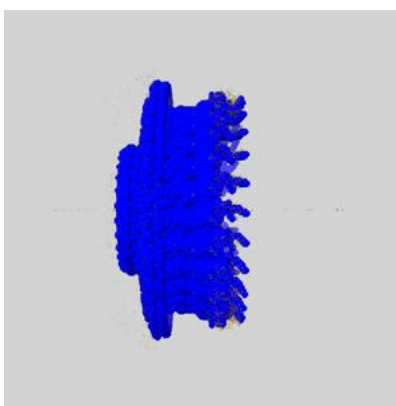
A mask typically either:

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

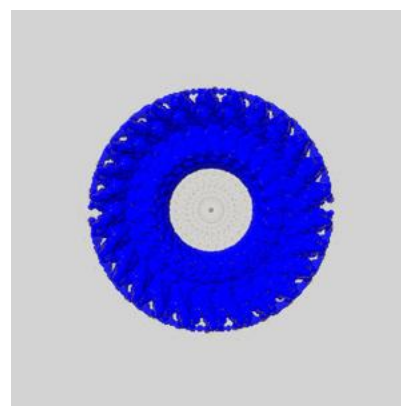
### 6.6.1 emd\_72815\_msk\_1.map [i](#)



X



Y

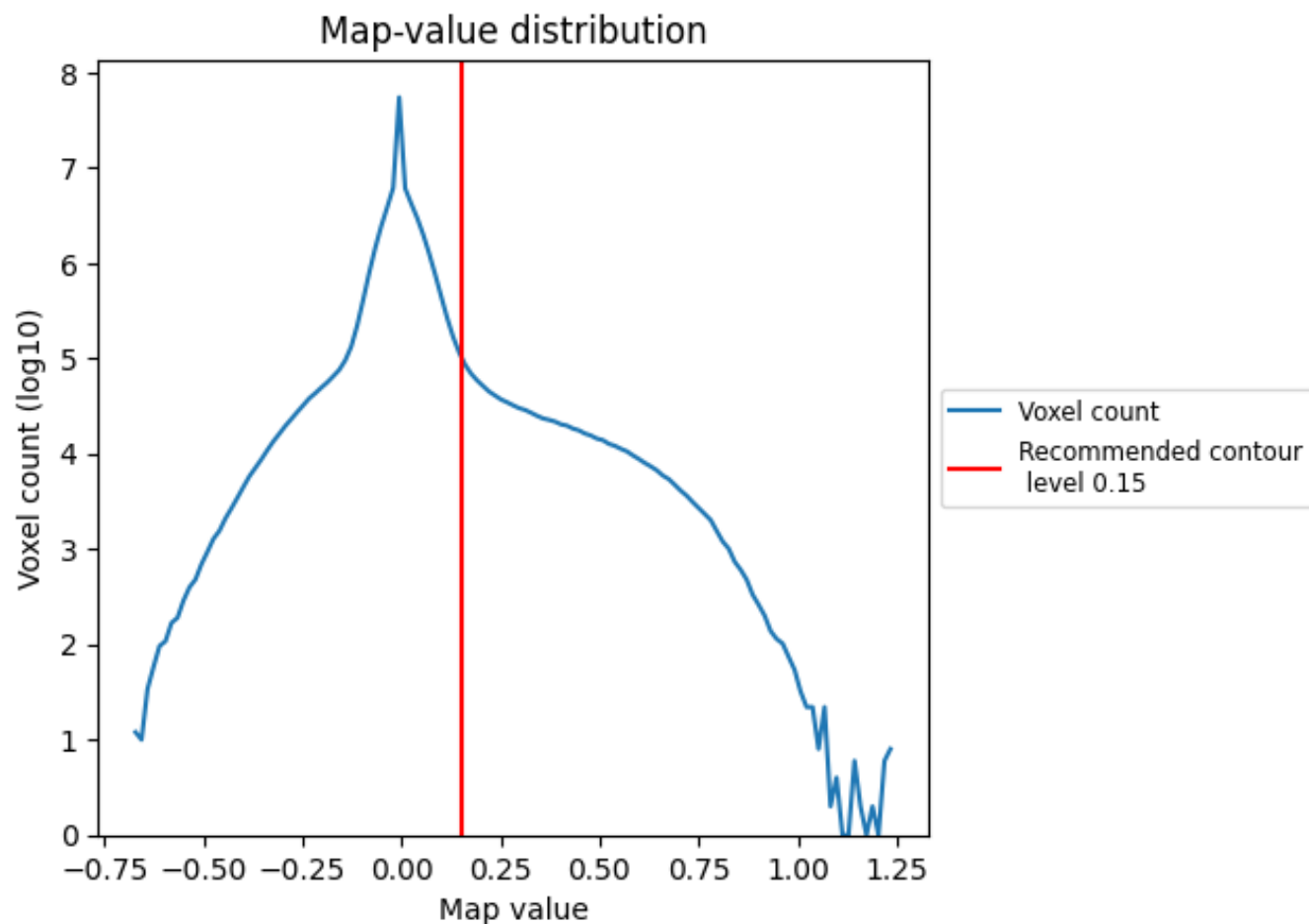


Z

## 7 Map analysis [i](#)

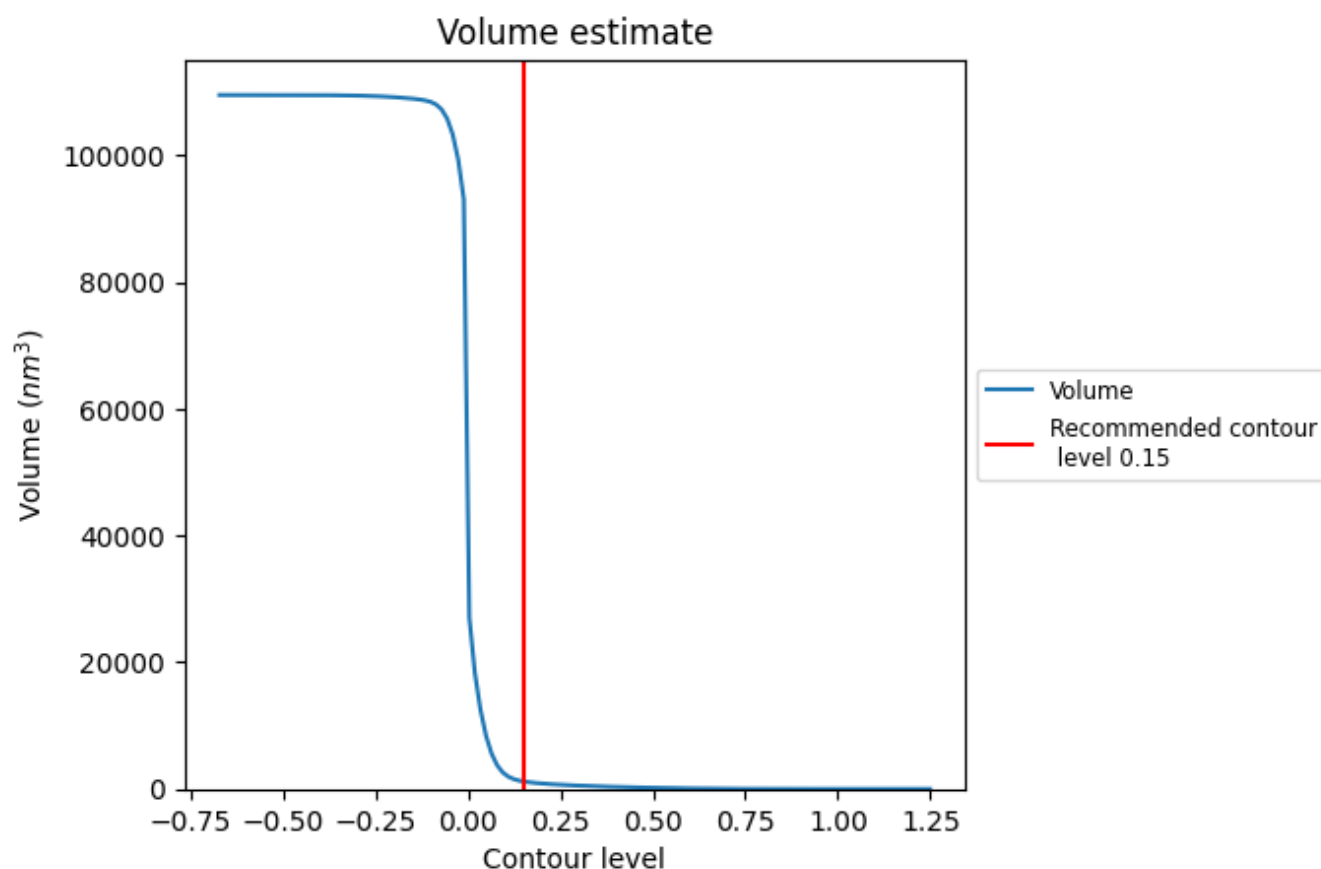
This section contains the results of statistical analysis of the map.

### 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.

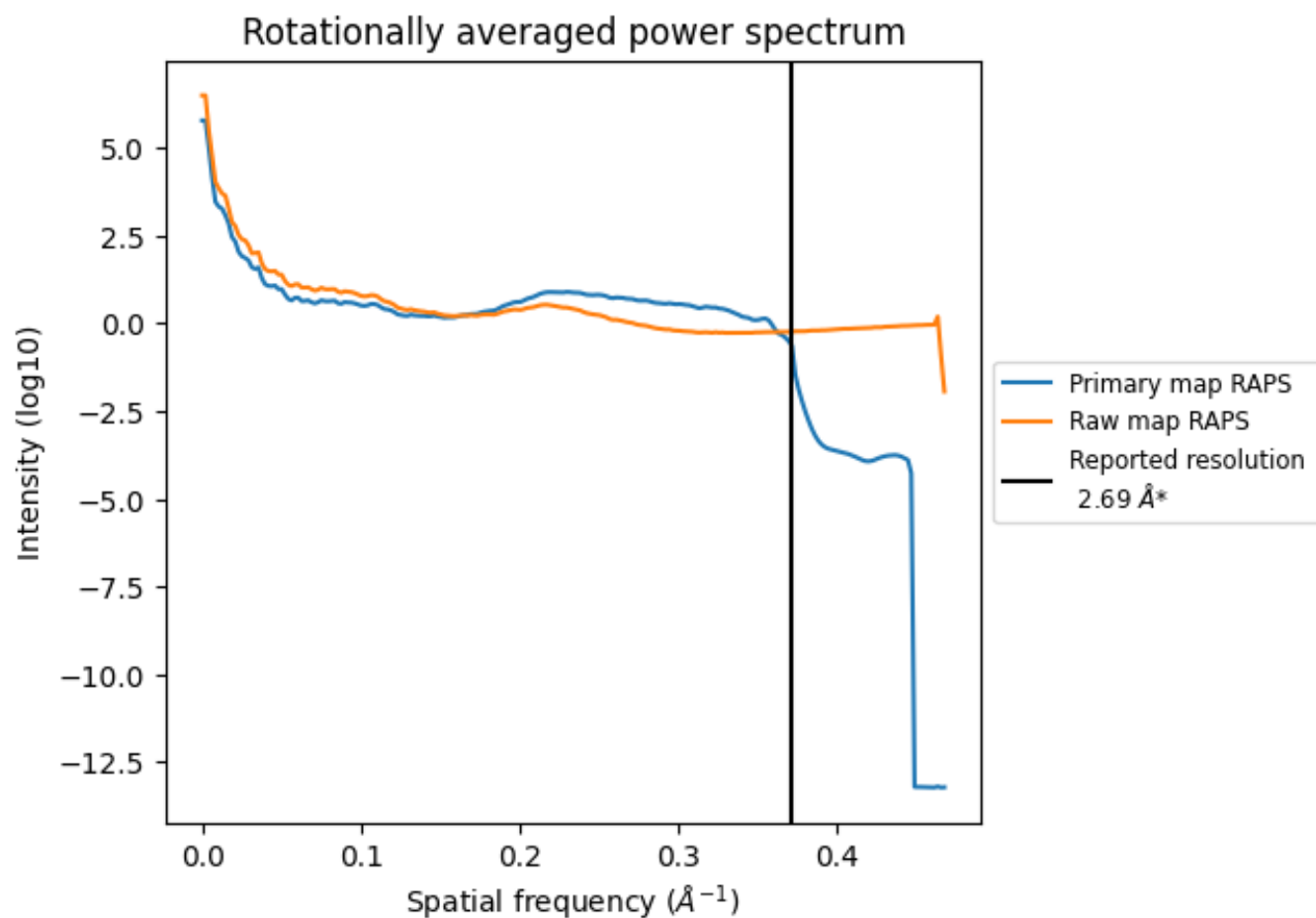
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1189  $\text{nm}^3$ ; this corresponds to an approximate mass of 1074 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 ⓘ



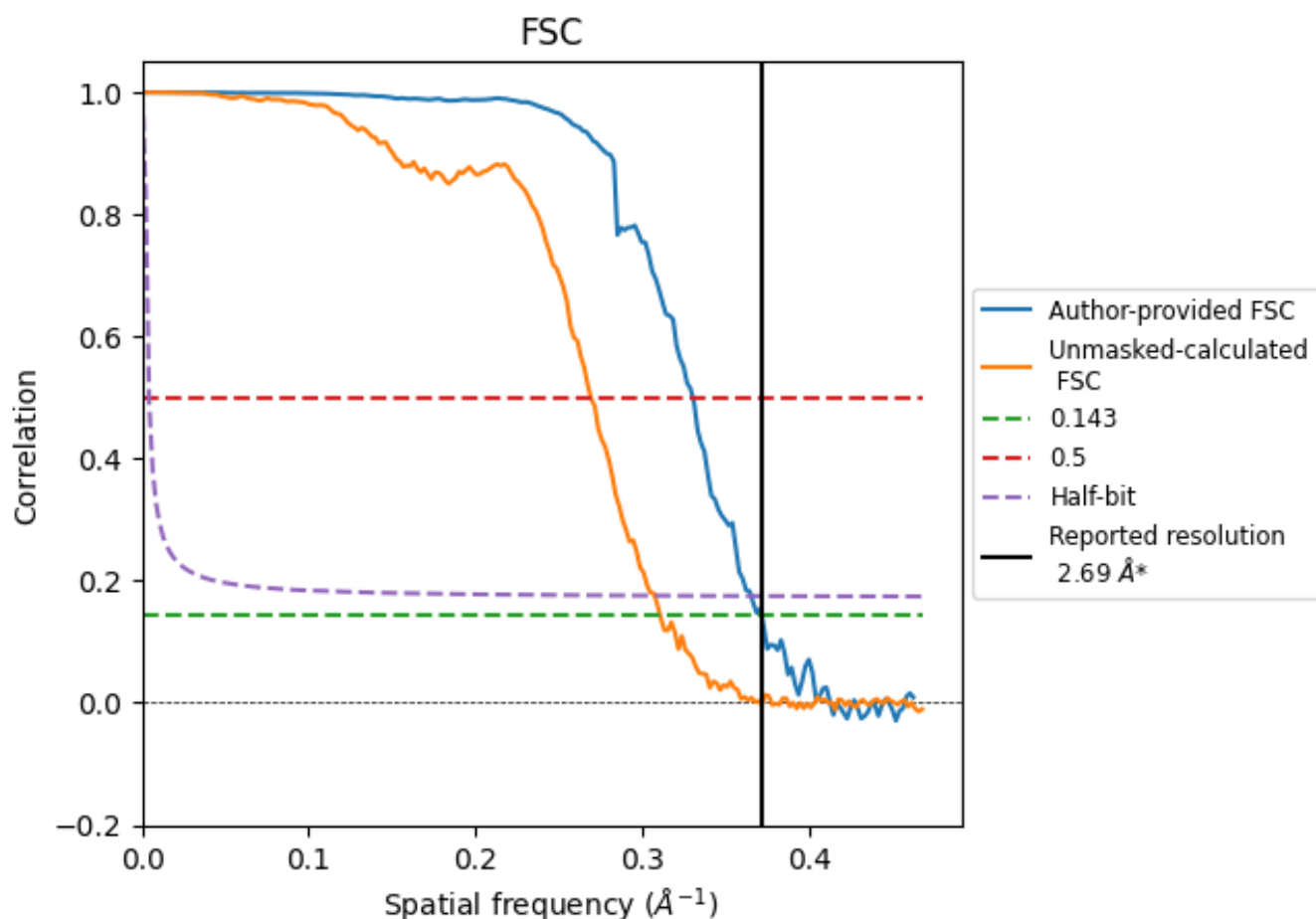
\*Reported resolution corresponds to spatial frequency of 0.372 Å<sup>-1</sup>



## 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  $0.372 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

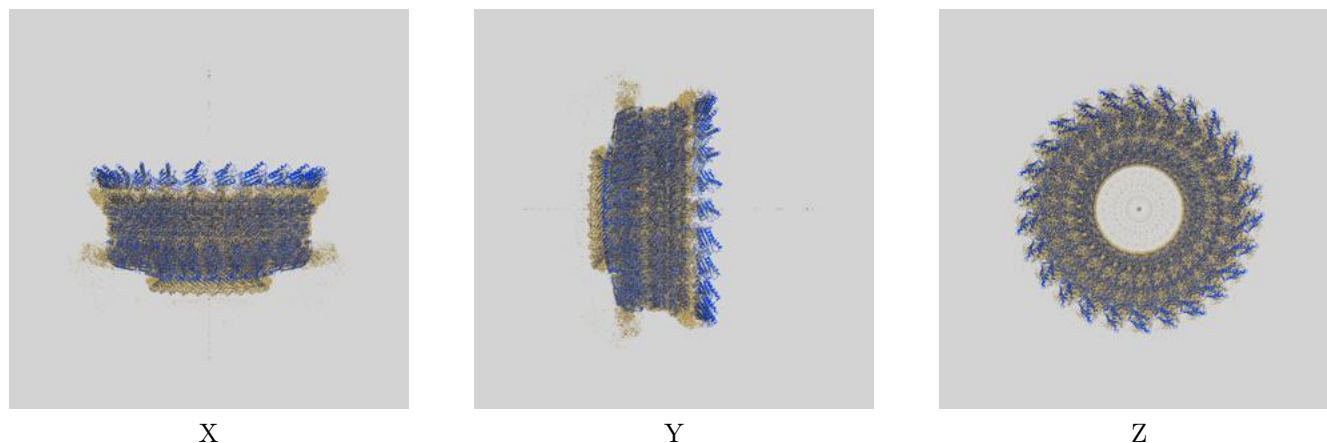
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	3.03	2.74
Unmasked-calculated*	3.22	3.71	3.25

\*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 3.22 differs from the reported value 2.69 by more than 10 %

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

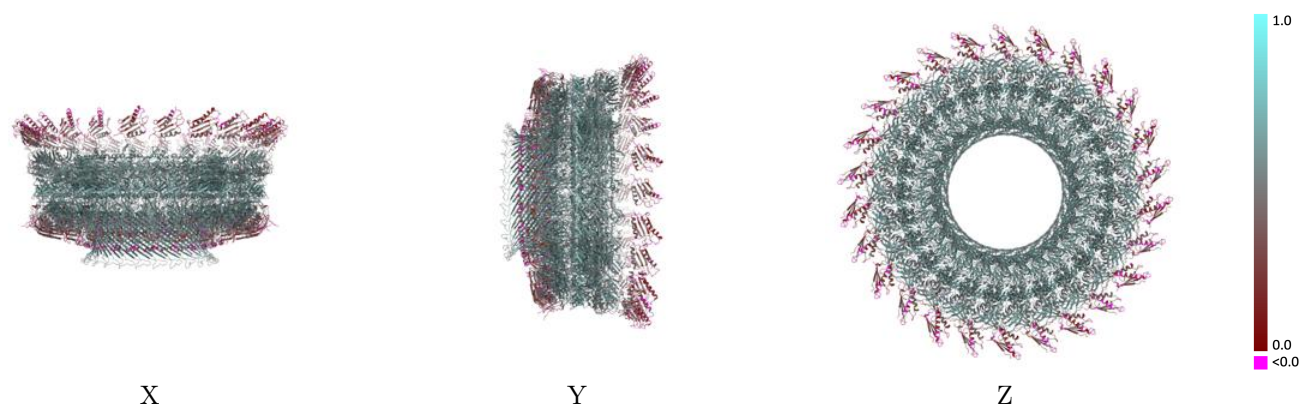
This section contains information regarding the fit between EMDB map EMD-72815 and PDB model 9YDO. Per-residue inclusion information can be found in section [3](#) on page [18](#).

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



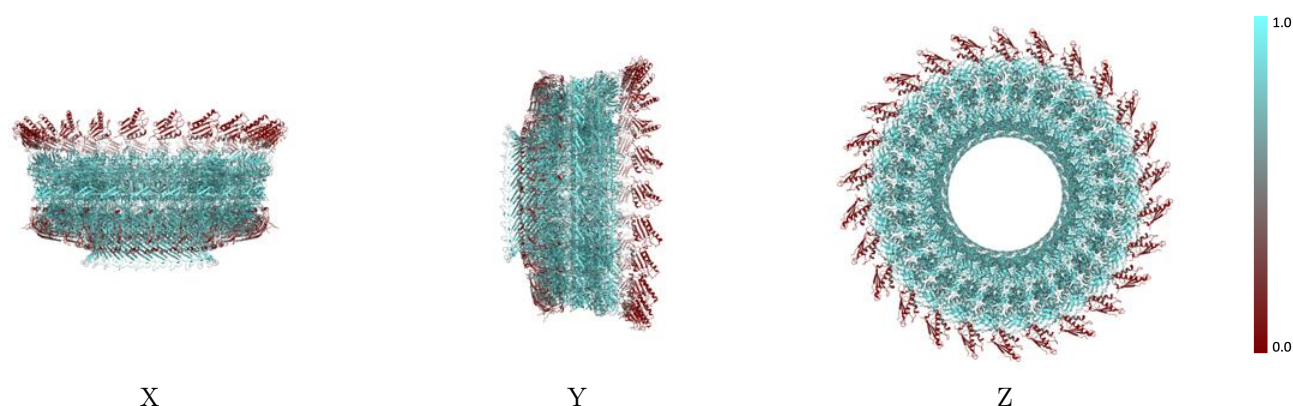
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



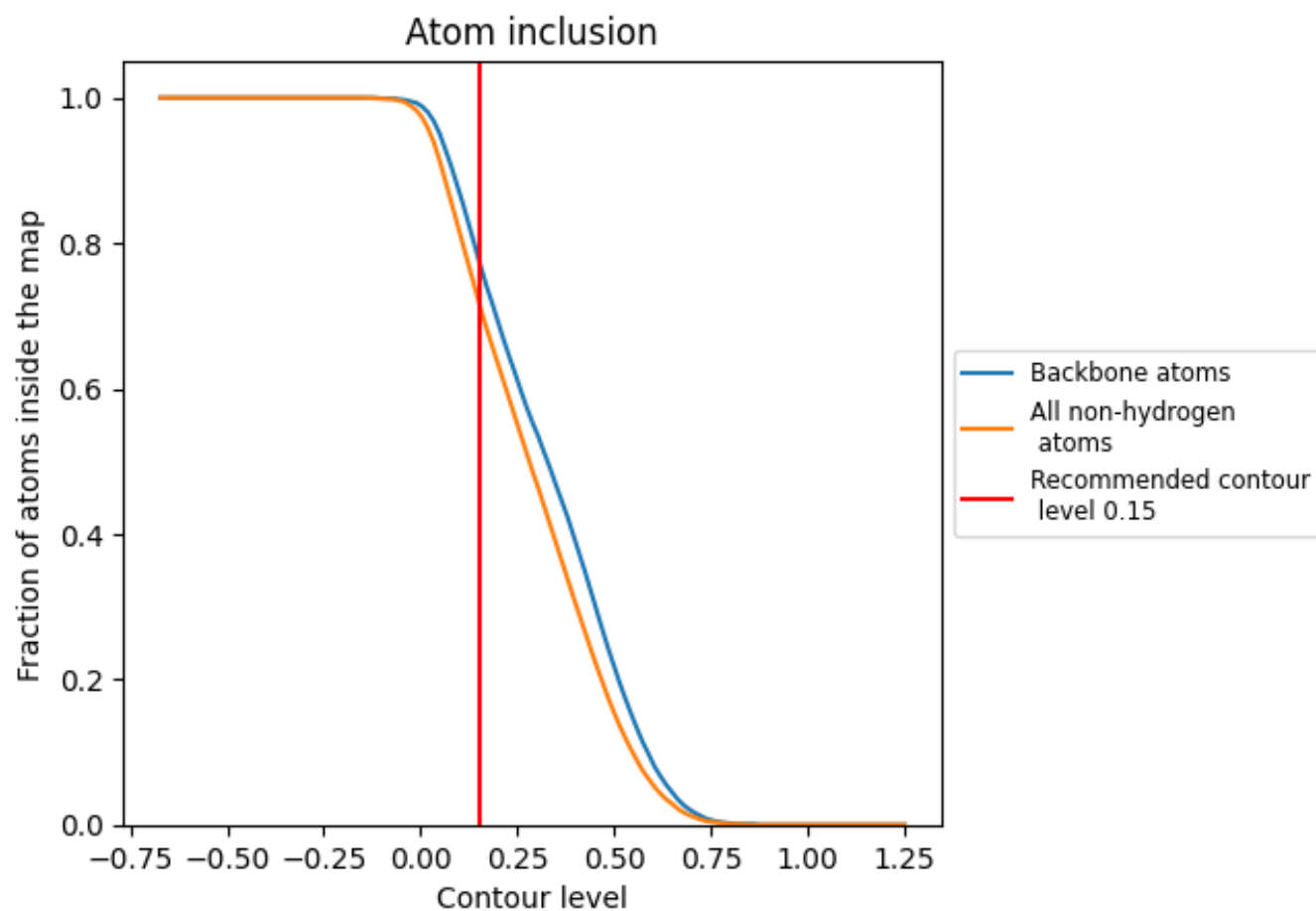
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.5130
Aa	 0.7940	 0.5590
Ab	 0.8020	 0.5610
Ac	 0.7980	 0.5600
Ad	 0.7950	 0.5600
Ae	 0.7940	 0.5610
Af	 0.7920	 0.5600
Ag	 0.7940	 0.5590
Ah	 0.7950	 0.5590
Ai	 0.7970	 0.5600
Aj	 0.7940	 0.5590
Ak	 0.7940	 0.5600
Al	 0.7940	 0.5610
Am	 0.7940	 0.5590
An	 0.7940	 0.5590
Ao	 0.8020	 0.5610
Ap	 0.7970	 0.5600
Aq	 0.7950	 0.5610
Ar	 0.7970	 0.5620
As	 0.7900	 0.5590
At	 0.7950	 0.5610
Au	 0.7970	 0.5620
Av	 0.7940	 0.5600
Aw	 0.7940	 0.5600
Ax	 0.8000	 0.5610
Ay	 0.7990	 0.5610
Az	 0.7970	 0.5600
Ba	 0.8850	 0.6030
Bb	 0.8810	 0.6020
Bc	 0.8810	 0.6020
Bd	 0.8790	 0.6010
Be	 0.8810	 0.6010
Bf	 0.8790	 0.6040
Bg	 0.8830	 0.6030
Bh	 0.8850	 0.6020























































































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Chain	Atom inclusion	Q-score
Bi	 0.8800	 0.6030
Bj	 0.8790	 0.6020
Bk	 0.8750	 0.6010
Bl	 0.8810	 0.6020
Bm	 0.8850	 0.6030
Bn	 0.8870	 0.6020
Bo	 0.8830	 0.6010
Bp	 0.8810	 0.6010
Bq	 0.8800	 0.6010
Br	 0.8810	 0.6010
Bs	 0.8820	 0.6020
Bt	 0.8810	 0.6000
Bu	 0.8870	 0.6000
Bv	 0.8810	 0.6010
Bw	 0.8820	 0.6010
Bx	 0.8790	 0.6020
By	 0.8790	 0.6020
Bz	 0.8830	 0.6020
Ca	 0.7330	 0.5160
Cb	 0.6900	 0.4750
Cc	 0.7300	 0.5200
Cd	 0.7310	 0.5170
Ce	 0.7340	 0.5160
Cf	 0.7380	 0.5180
Cg	 0.7330	 0.5230
Ch	 0.7250	 0.5180
Ci	 0.7310	 0.5170
Cj	 0.7360	 0.5210
Ck	 0.7360	 0.5210
Cl	 0.7320	 0.5170
Cm	 0.7320	 0.5130
Cn	 0.7340	 0.5170
Co	 0.7310	 0.5180
Cp	 0.7280	 0.5170
Cq	 0.7340	 0.5200
Cr	 0.7310	 0.5190
Cs	 0.7310	 0.5150
Ct	 0.7270	 0.5180
Cu	 0.7270	 0.5130
Cv	 0.7300	 0.5200
Cw	 0.7270	 0.5150
Cx	 0.7350	 0.5230

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Chain	Atom inclusion	Q-score
Cy	 0.7310	 0.5170
Cz	 0.7340	 0.5190
Da	 0.5000	 0.3930
Db	 0.5080	 0.4160
Dc	 0.5070	 0.3930
Dd	 0.5110	 0.4150
De	 0.5030	 0.3920
Df	 0.5100	 0.4160
Dg	 0.4970	 0.3900
Dh	 0.5100	 0.4170
Di	 0.5030	 0.3910
Dj	 0.5060	 0.4150
Dk	 0.5030	 0.3910
Dl	 0.5130	 0.4150
Dm	 0.5040	 0.3920
Dn	 0.5090	 0.4140
Do	 0.5010	 0.3910
Dp	 0.5110	 0.4120
Dq	 0.5020	 0.3900
Dr	 0.5130	 0.4120
Ds	 0.5020	 0.3920
Dt	 0.5070	 0.4150
Du	 0.4990	 0.3910
Dv	 0.5090	 0.4130
Dw	 0.5000	 0.3930
Dx	 0.5060	 0.4140
Dy	 0.5020	 0.3950
Dz	 0.5100	 0.4170
Fa	 0.3090	 0.2680
Fb	 0.2850	 0.2610
Fc	 0.3010	 0.2470
Fd	 0.3010	 0.2690
Fe	 0.2930	 0.2500
Ff	 0.3090	 0.2670
Fg	 0.3090	 0.2670
Fh	 0.2680	 0.2390
Fi	 0.3090	 0.2200
Fj	 0.2850	 0.2890
Fk	 0.3250	 0.2050
Fl	 0.3090	 0.2520
Fm	 0.3170	 0.2590
Fn	 0.2850	 0.2450

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Chain	Atom inclusion	Q-score
Fo	 0.3010	 0.2360
Fp	 0.2850	 0.2260
Fq	 0.2930	 0.2750
Fr	 0.3010	 0.2440
Fs	 0.3170	 0.1930
Ft	 0.2930	 0.2480
Fu	 0.3010	 0.2330
Fv	 0.3010	 0.2520
Fw	 0.3010	 0.2710
Fx	 0.3330	 0.2720
Fy	 0.2850	 0.2590
Fz	 0.2850	 0.1910
Ga	 0.3180	 0.2600
Gb	 0.3000	 0.2230
Gc	 0.3270	 0.2060
Gd	 0.3090	 0.2480
Ge	 0.3090	 0.2240
Gf	 0.3360	 0.2240
Gg	 0.3000	 0.2460
Gh	 0.3180	 0.2590
Gi	 0.3090	 0.2340
Gj	 0.3450	 0.2570
Gk	 0.3540	 0.2410
Gl	 0.3360	 0.2090
Gm	 0.3450	 0.2380
Gn	 0.3640	 0.2800
Go	 0.3180	 0.2690
Gp	 0.2730	 0.2510
Gq	 0.3270	 0.2330
Gr	 0.2910	 0.2540
Gs	 0.3090	 0.2390
Gt	 0.3180	 0.2720
Gu	 0.3270	 0.2790
Gv	 0.3360	 0.2600
Gw	 0.2450	 0.1440
Gx	 0.3540	 0.2400
Gy	 0.3540	 0.2750
Gz	 0.2910	 0.2460