



Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 04:06 PM EDT

PDB ID : 9YH0 / pdb_00009yh0
EMDB ID : EMD-72947
Title : LPHT-ring subunit with C13 MotX in Vibrio cholerae at assembled state
Authors : Guo, W.; Yue, J.; Liu, J.
Deposited on : 2025-09-29
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

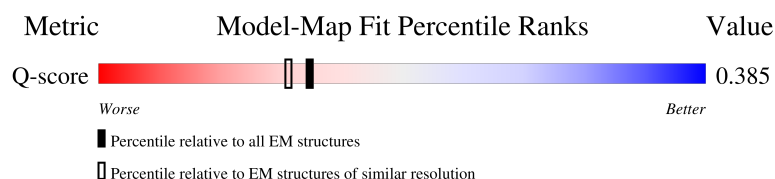
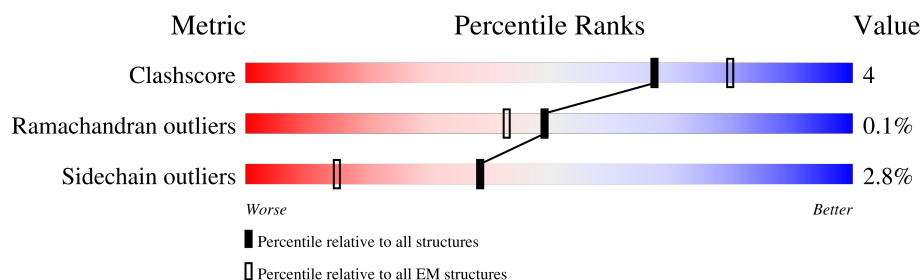
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	Aa	227	<div> <div>9%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	Ab	227	<div> <div>11%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	Ac	227	<div> <div>10%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	Ad	227	<div> <div>10%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>







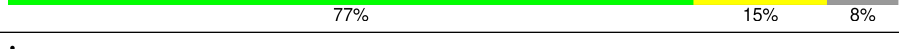
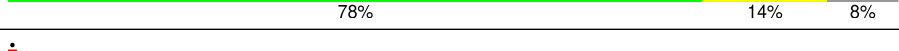
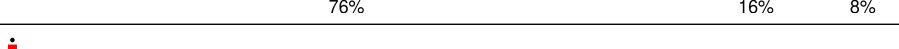
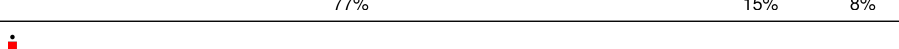
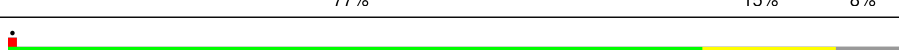

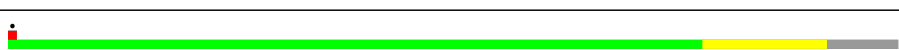

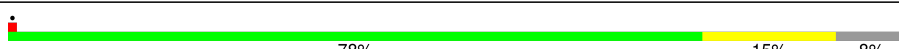





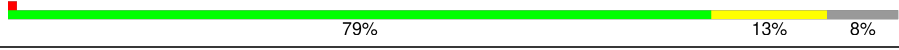
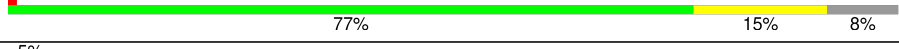
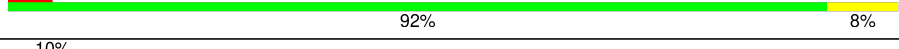
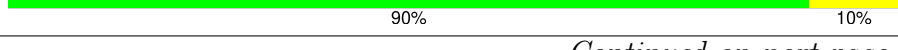

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Mol	Chain	Length	Quality of chain
1	Ae	227	
1	Af	227	
1	Ag	227	
1	Ah	227	
1	Ai	227	
1	Aj	227	
1	Ak	227	
1	Al	227	
1	Am	227	
1	An	227	
1	Ao	227	
1	Ap	227	
1	Aq	227	
1	Ar	227	
1	As	227	
1	At	227	
1	Au	227	
1	Av	227	
1	Aw	227	
1	Ax	227	
1	Ay	227	
1	Az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

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







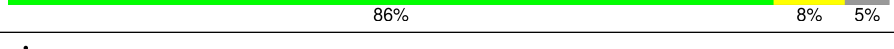
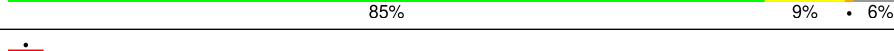
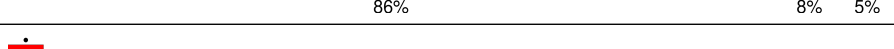
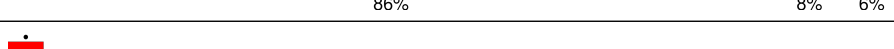
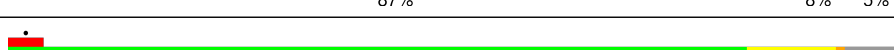

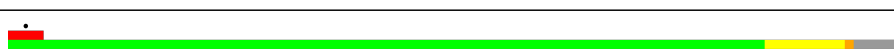

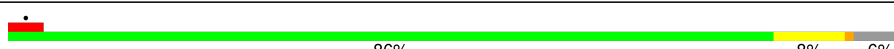





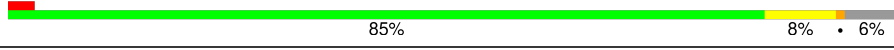
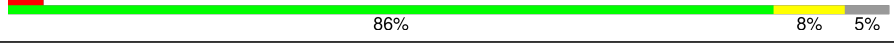



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Mol	Chain	Length	Quality of chain
3	Cc	352	
3	Cd	352	
3	Ce	352	
3	Cf	352	
3	Cg	352	
3	Ch	352	
3	Ci	352	
3	Cj	352	
3	Ck	352	
3	Cl	352	
3	Cm	352	
3	Cn	352	
3	Co	352	
3	Cp	352	
3	Cq	352	
3	Cr	352	
3	Cs	352	
3	Ct	352	
3	Cu	352	
3	Cv	352	
3	Cw	352	
3	Cx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

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

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Mol	Chain	Length	Quality of chain
5	Ea	188	<div> <div>12%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
5	Eb	188	<div> <div>15%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
5	Ec	188	<div> <div>11%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
5	Ed	188	<div> <div>15%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
5	Ee	188	<div> <div>11%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
5	Ef	188	<div> <div>15%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
5	Eg	188	<div> <div>11%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
5	Eh	188	<div> <div>15%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
5	Ei	188	<div> <div>12%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
5	Ej	188	<div> <div>16%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
5	Ek	188	<div> <div>11%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
5	El	188	<div> <div>14%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
5	Em	188	<div> <div>13%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
5	En	188	<div> <div>16%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
5	Eo	188	<div> <div>13%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
5	Ep	188	<div> <div>15%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
5	Eq	188	<div> <div>13%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
5	Er	188	<div> <div>15%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
5	Es	188	<div> <div>11%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
5	Et	188	<div> <div>13%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
5	Eu	188	<div> <div>10%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
5	Ev	188	<div> <div>14%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
5	Ew	188	<div> <div>11%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
5	Ex	188	<div> <div>14%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
5	Ey	188	<div> <div>10%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
5	Ez	188	
6	Fa	15	
6	Fb	15	
6	Fc	15	
6	Fd	15	
6	Fe	15	
6	Ff	15	
6	Fg	15	
6	Fh	15	
6	Fi	15	
6	Fj	15	
6	Fk	15	
6	Fl	15	
6	Fm	15	
6	Fn	15	
6	Fo	15	
6	Fp	15	
6	Fq	15	
6	Fr	15	
6	Fs	15	
6	Ft	15	
6	Fu	15	
6	Fv	15	
6	Fw	15	
6	Fx	15	

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Mol	Chain	Length	Quality of chain
6	Fy	15	<div> <div>40%</div> <div>100%</div> </div>
6	Fz	15	<div> <div>47%</div> <div>100%</div> </div>
6	Ga	15	<div> <div>33%</div> <div>87%</div> <div>13%</div> </div>
6	Gb	15	<div> <div>27%</div> <div>67%</div> <div>20%</div> <div>13%</div> </div>
6	Gc	15	<div> <div>40%</div> <div>67%</div> <div>20%</div> <div>13%</div> </div>
6	Gd	15	<div> <div>27%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Ge	15	<div> <div>27%</div> <div>87%</div> <div>13%</div> </div>
6	Gf	15	<div> <div>27%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
6	Gg	15	<div> <div>20%</div> <div>87%</div> <div>13%</div> </div>
6	Gh	15	<div> <div>27%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Gi	15	<div> <div>27%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
6	Gj	15	<div> <div>33%</div> <div>87%</div> <div>13%</div> </div>
6	Gk	15	<div> <div>27%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Gl	15	<div> <div>33%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
6	Gm	15	<div> <div>33%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
6	Gn	15	<div> <div>20%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Go	15	<div> <div>27%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Gp	15	<div> <div>27%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Gq	15	<div> <div>33%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Gr	15	<div> <div>20%</div> <div>87%</div> <div>13%</div> </div>
6	Gs	15	<div> <div>27%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
6	Gt	15	<div> <div>27%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
6	Gu	15	<div> <div>27%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Gv	15	<div> <div>27%</div> <div>80%</div> <div>7%</div> <div>13%</div> </div>
6	Gw	15	<div> <div>47%</div> <div>60%</div> <div>27%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
6	Gx	15	<div><div>27%</div><div><div></div><div>80%</div><div>7%</div><div>13%</div></div></div>
6	Gy	15	<div><div>27%</div><div><div></div><div>80%</div><div>7%</div><div>13%</div></div></div>
6	Gz	15	<div><div>40%</div><div><div></div><div>80%</div><div>7%</div><div>13%</div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 274495 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	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Ce	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cf	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cg	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Ch	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Ci	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cj	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Ck	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cl	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cm	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cn	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Co	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cp	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cq	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cr	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cs	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Ct	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cu	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cv	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cw	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		
3	Cx	352	Total	C	N	O	S	0	0
			2770	1741	477	535	17		

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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 Sodium-type flagellar protein MotX.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ea	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Eb	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Ec	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Ed	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Ee	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Ef	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Eg	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Eh	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Ei	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Ej	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ek	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	El	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Em	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	En	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Eo	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Ep	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Eq	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Er	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Es	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Et	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Eu	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Ev	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Ew	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Ex	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		
5	Ey	183	Total	C	N	O	S	0	0
			1466	926	259	275	6		
5	Ez	183	Total	C	N	O	S	0	0
			1494	943	268	277	6		

- Molecule 6 is a protein called Flagellar assembly lipoprotein FlgP.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Fa	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
6	Fb	15	Total	C	N	O	S	0	0
			125	78	22	24	1		
6	Fc	15	Total	C	N	O	S	0	0
			125	78	22	24	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Fd	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fe	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Ff	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fg	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fh	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fi	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fj	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fk	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fl	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fm	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fn	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fo	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fp	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fq	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fr	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fs	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Ft	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fu	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fv	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fw	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fx	15	Total 125	C 78	N 22	O 24	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Fy	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Fz	15	Total 125	C 78	N 22	O 24	S 1	0	0
6	Ga	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gb	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gc	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gd	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Ge	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gf	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gg	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gh	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gi	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gj	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gk	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gl	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gm	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gn	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Go	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gp	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gq	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gr	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gs	13	Total 112	C 71	N 20	O 20	S 1	0	0

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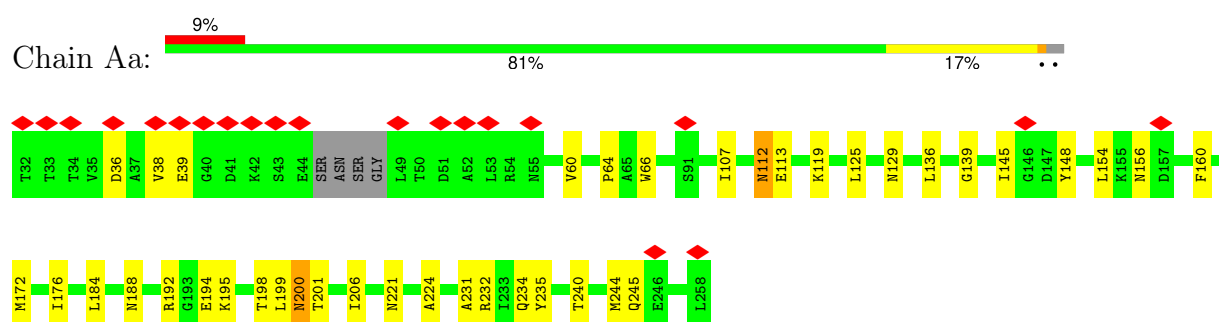
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Mol	Chain	Residues	Atoms					AltConf	Trace
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6	Gu	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gv	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gw	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gx	13	Total 112	C 71	N 20	O 20	S 1	0	0
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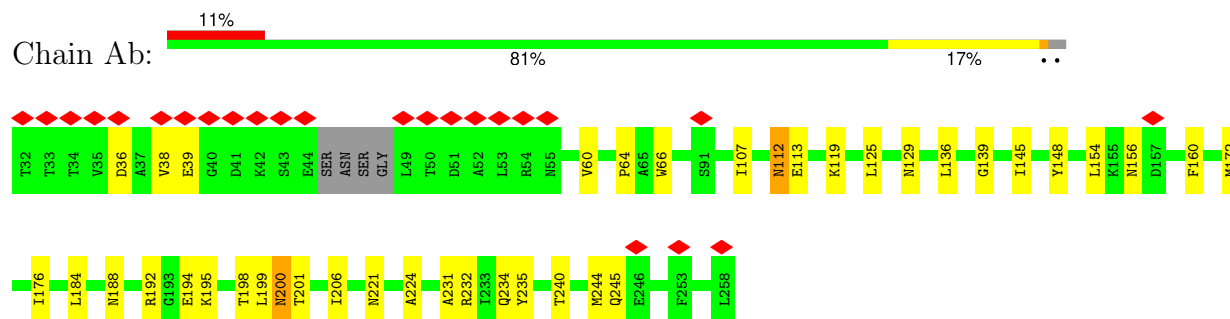
3 Residue-property plots [i](#)

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

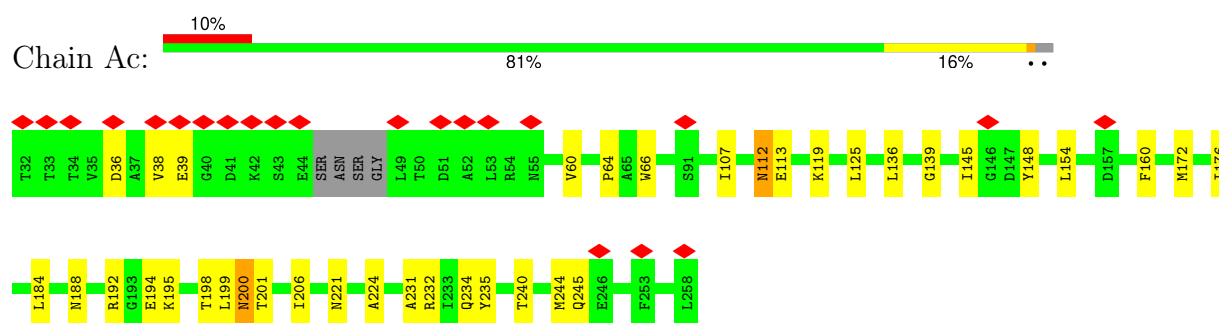
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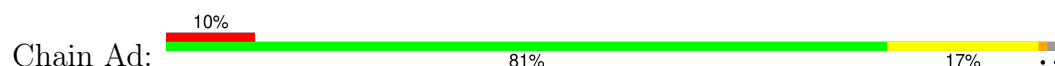
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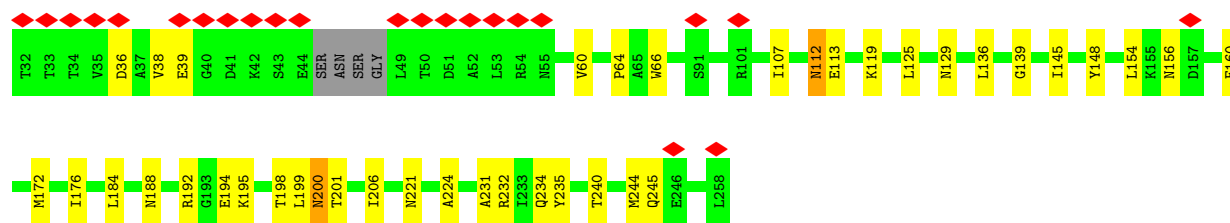


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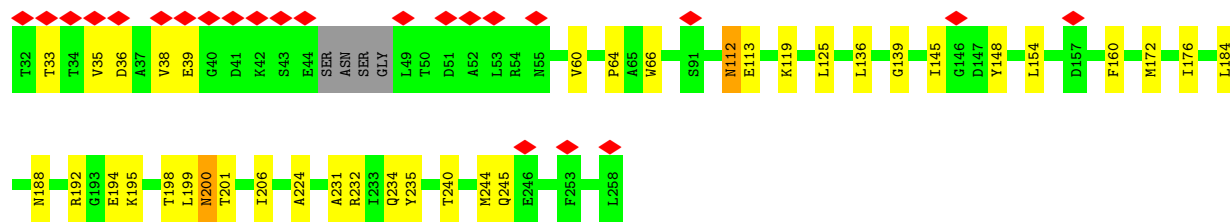
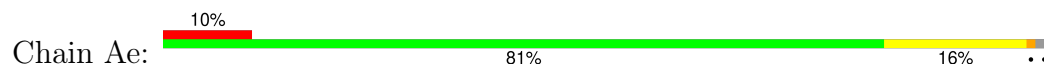


- Molecule 1: Flagellar L-ring protein

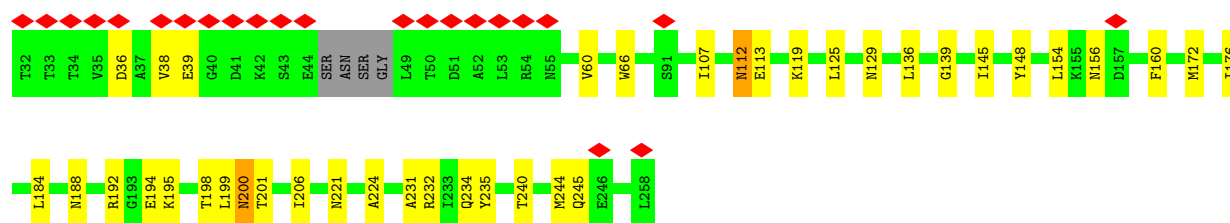
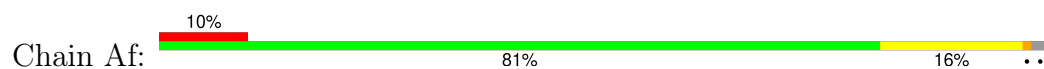




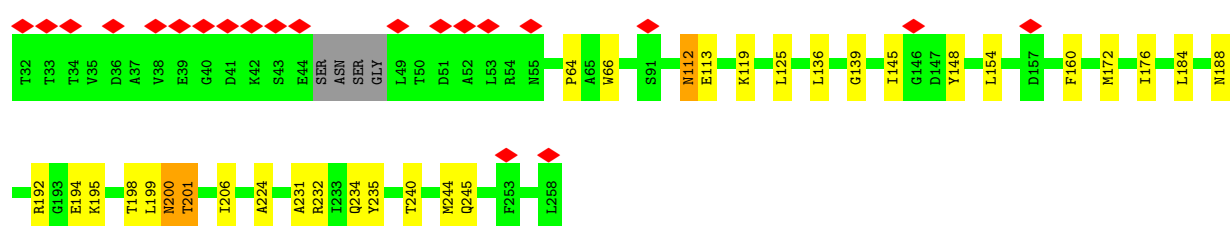
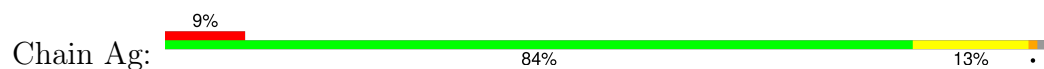
• Molecule 1: Flagellar L-ring protein



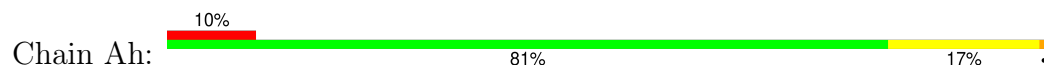
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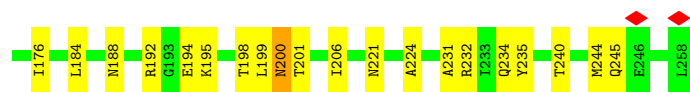


• Molecule 1: Flagellar L-ring protein

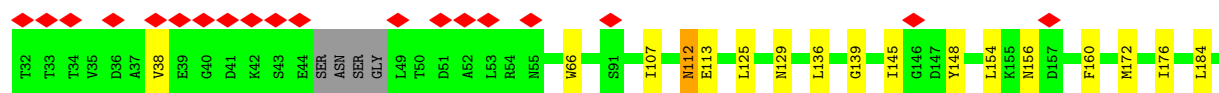
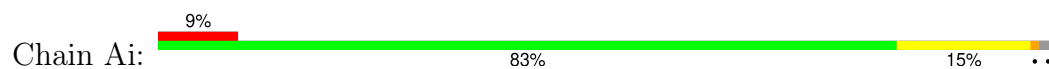


• Molecule 1: Flagellar L-ring protein

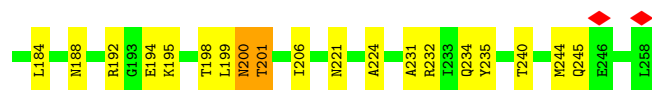
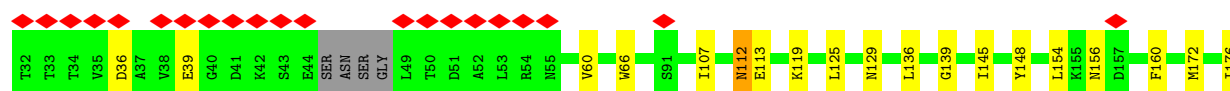
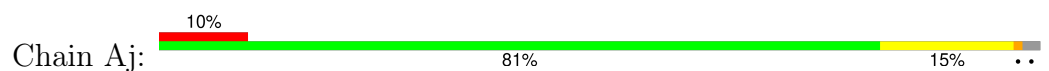




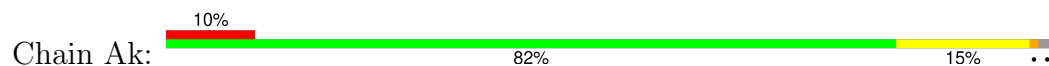
- Molecule 1: Flagellar L-ring protein



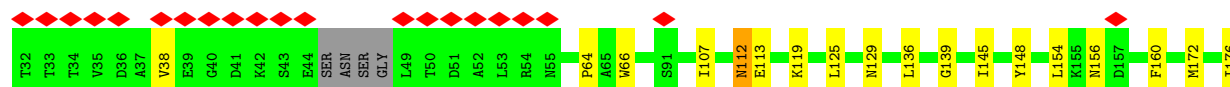
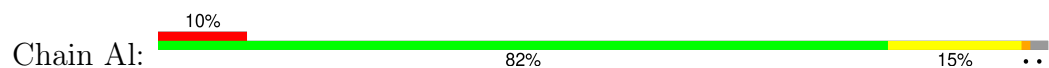
- Molecule 1: Flagellar L-ring protein



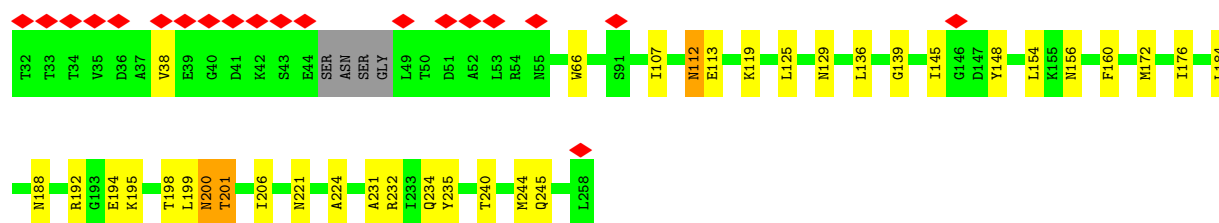
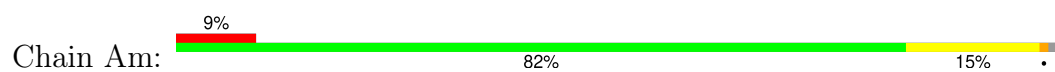
- Molecule 1: Flagellar L-ring protein



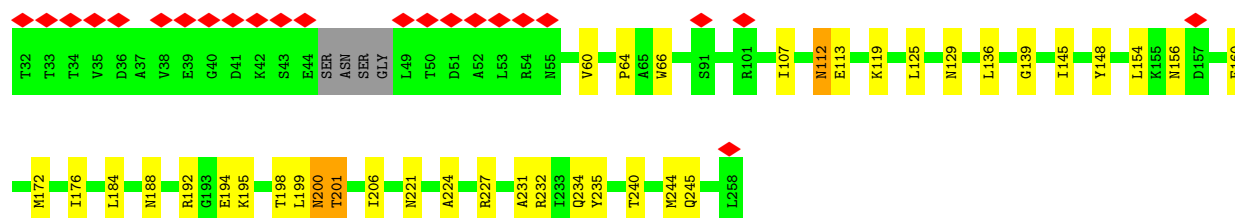
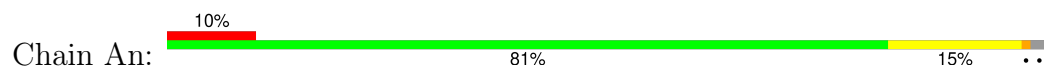
- Molecule 1: Flagellar L-ring protein



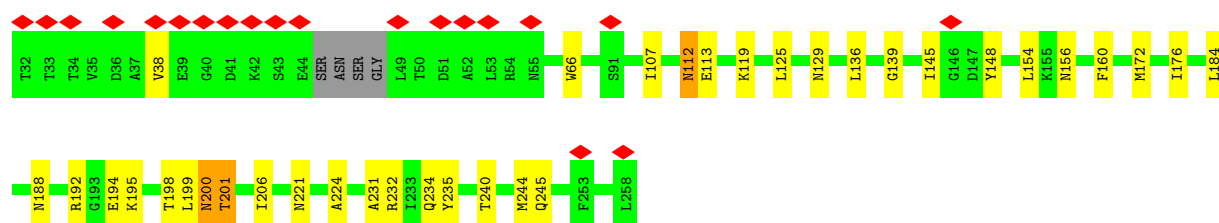
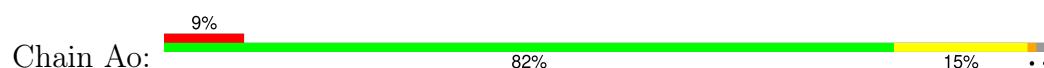
- Molecule 1: Flagellar L-ring protein



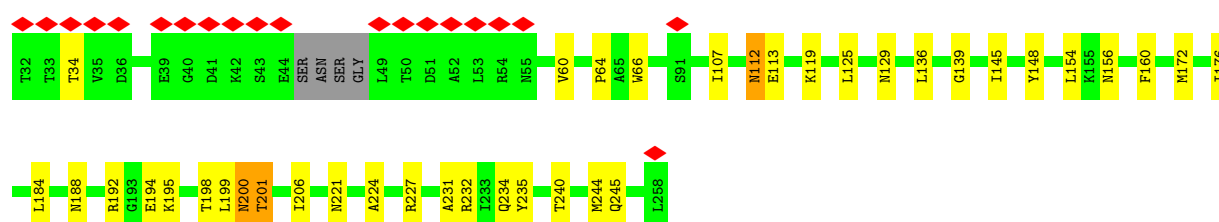
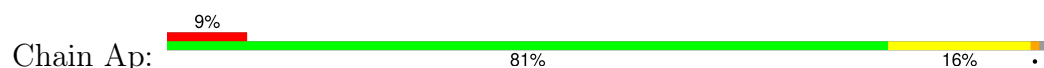
• Molecule 1: Flagellar L-ring protein



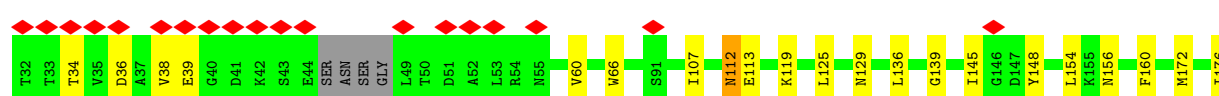
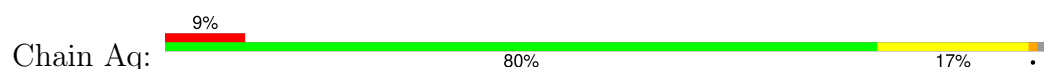
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

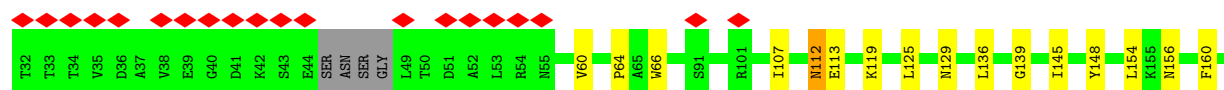
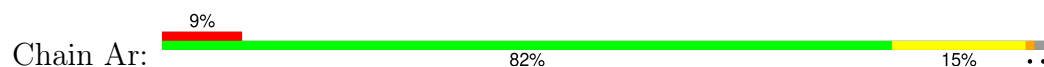


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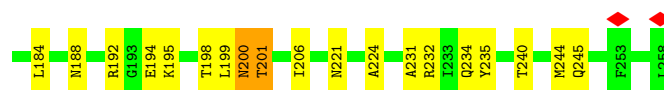
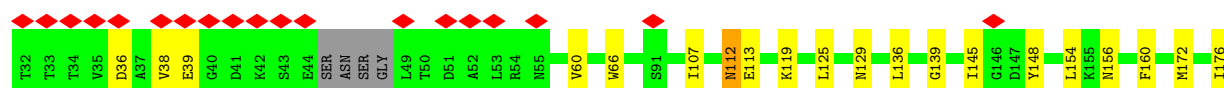
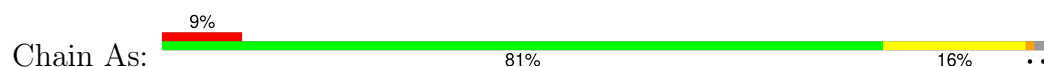




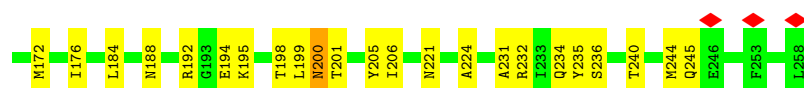
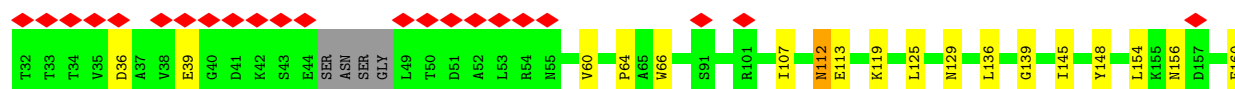
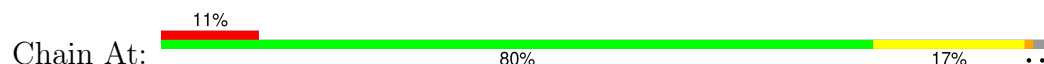
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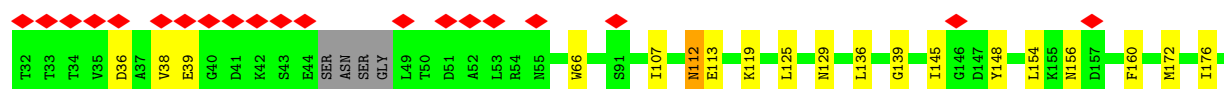
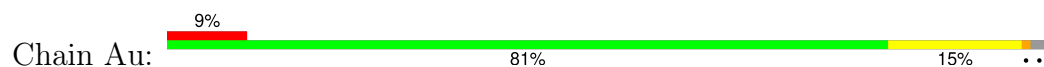
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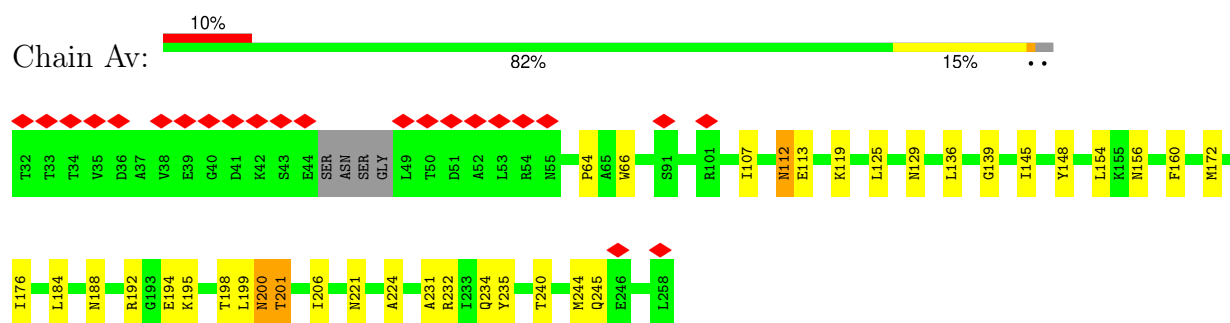
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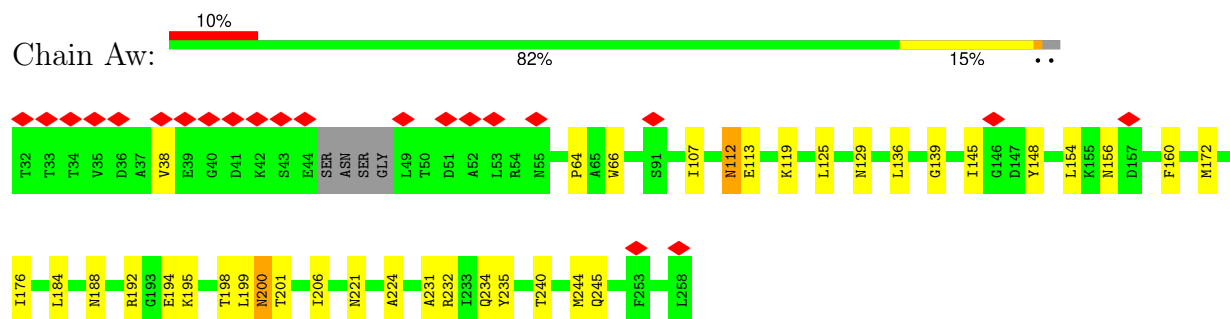
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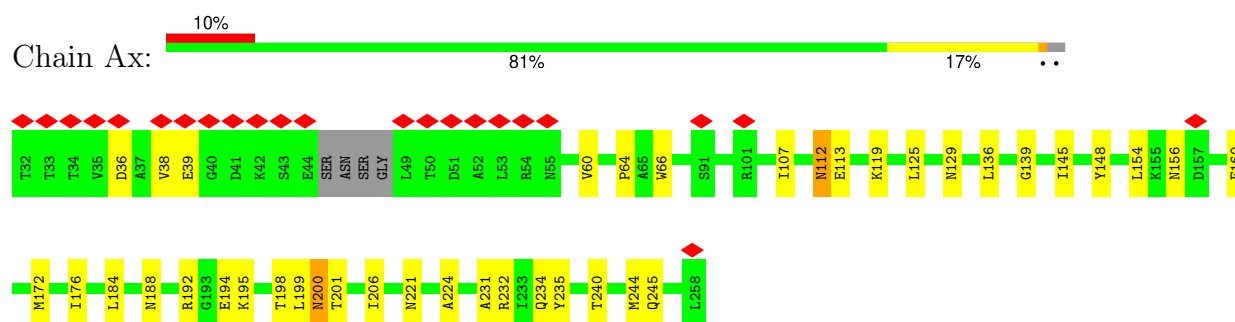
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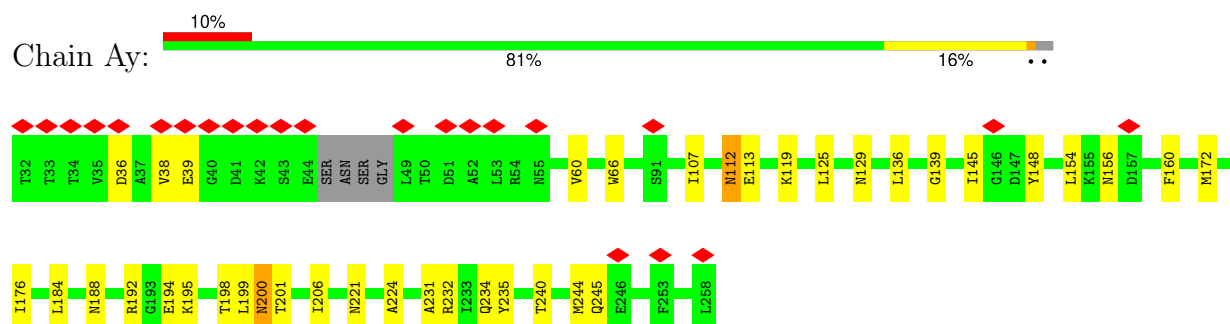
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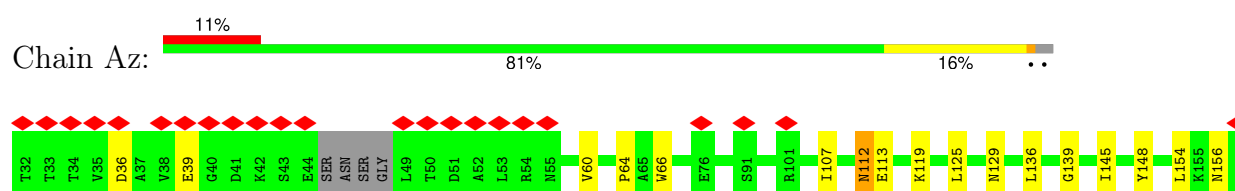
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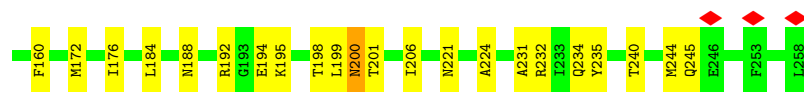


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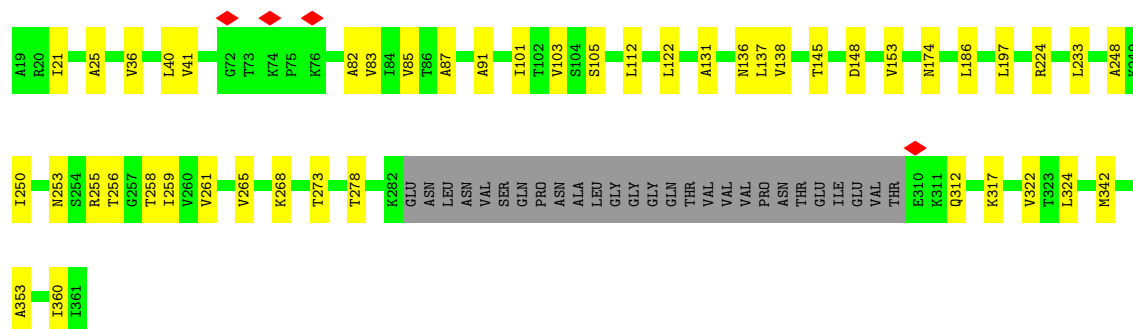
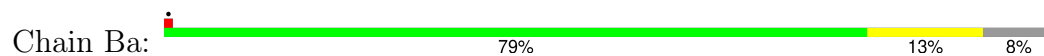


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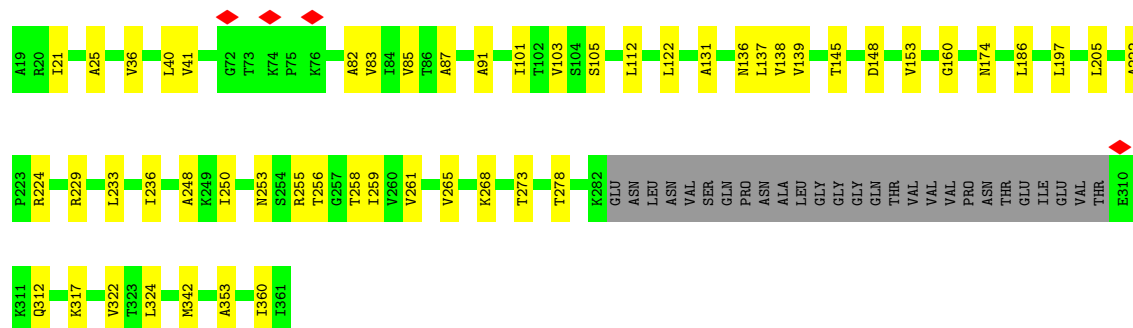
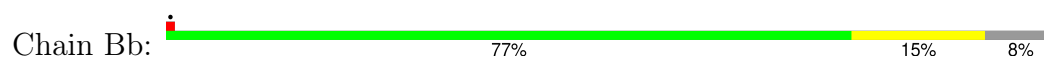




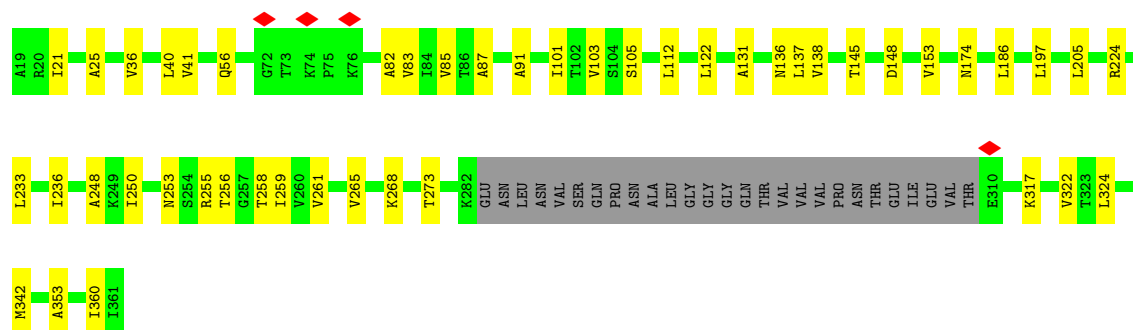
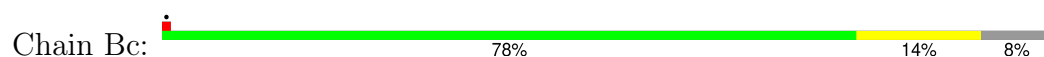
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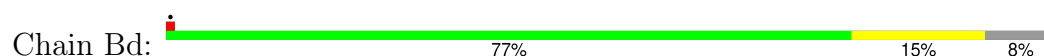
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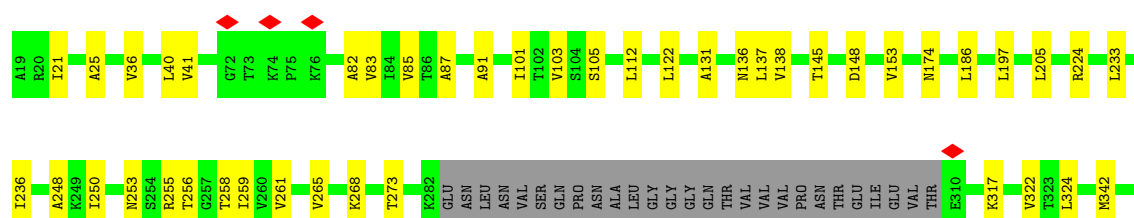


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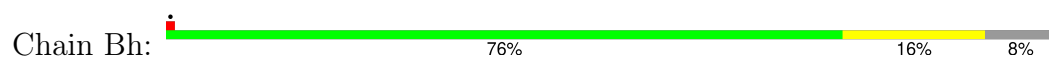
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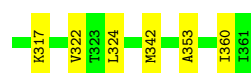
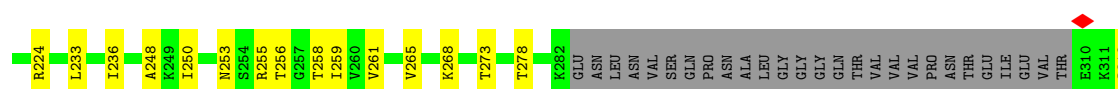
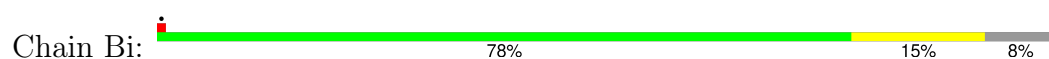




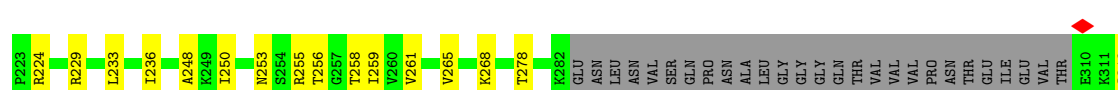
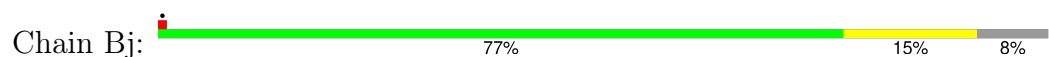
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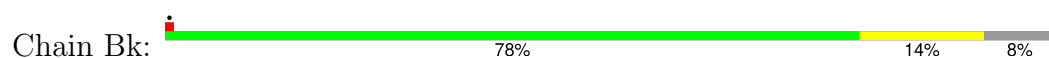
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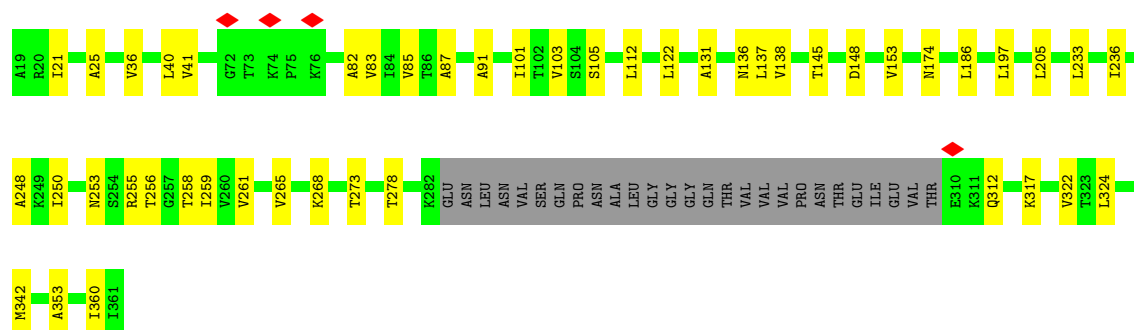


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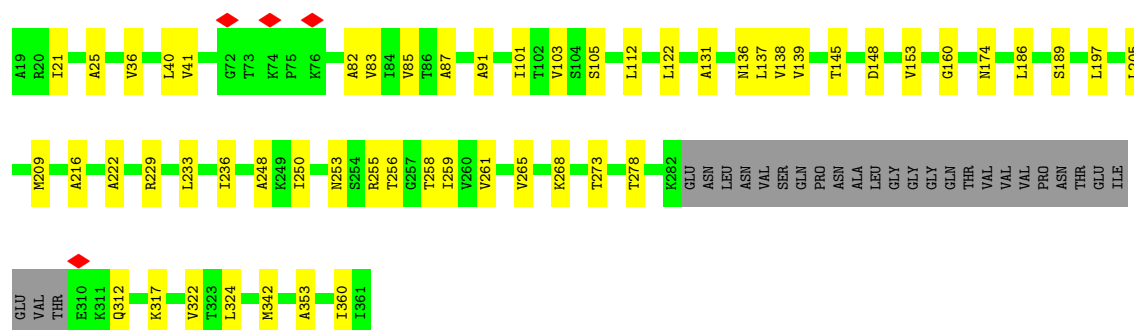
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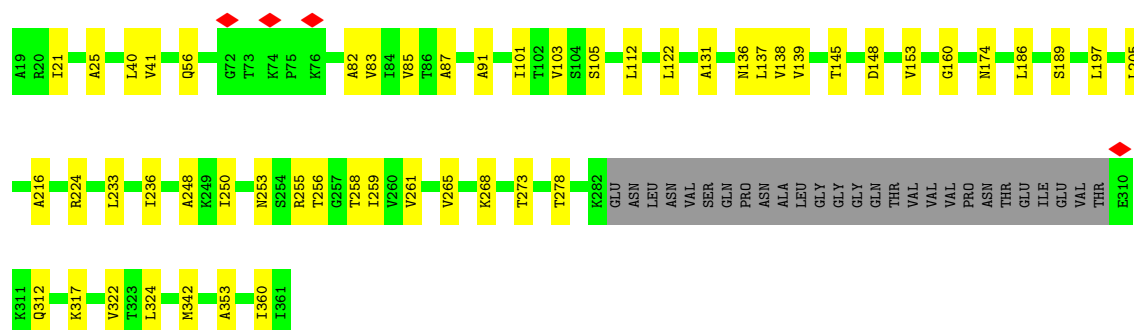
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Chain Bl: 76% 16% 8%



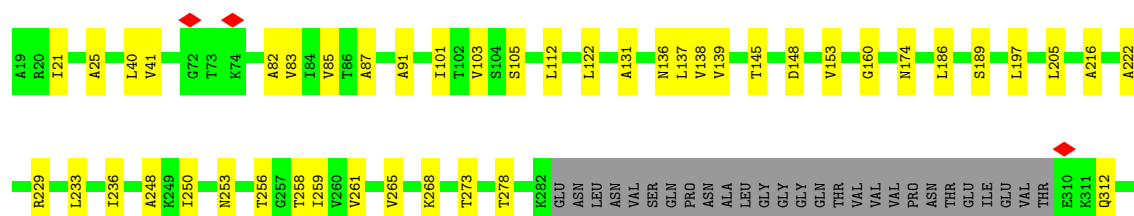
• Molecule 2: Flagellar P-ring protein

Chain Bm: 77% 15% 8%



• Molecule 2: Flagellar P-ring protein

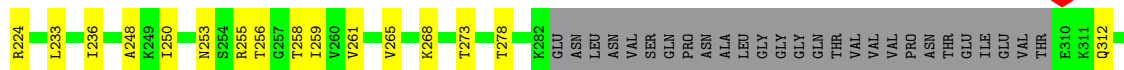
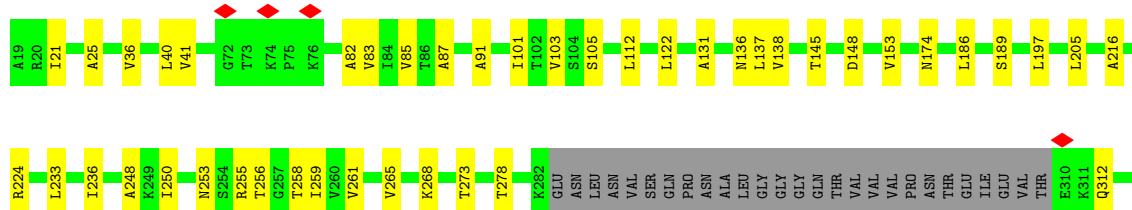
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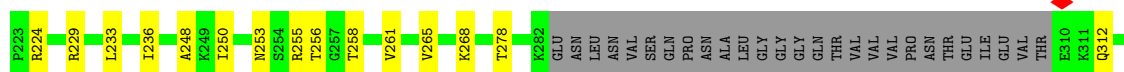
• Molecule 2: Flagellar P-ring protein

Chain Bo: 78% 15% 8%



• Molecule 2: Flagellar P-ring protein

Chain Bp: 77% 15% 8%



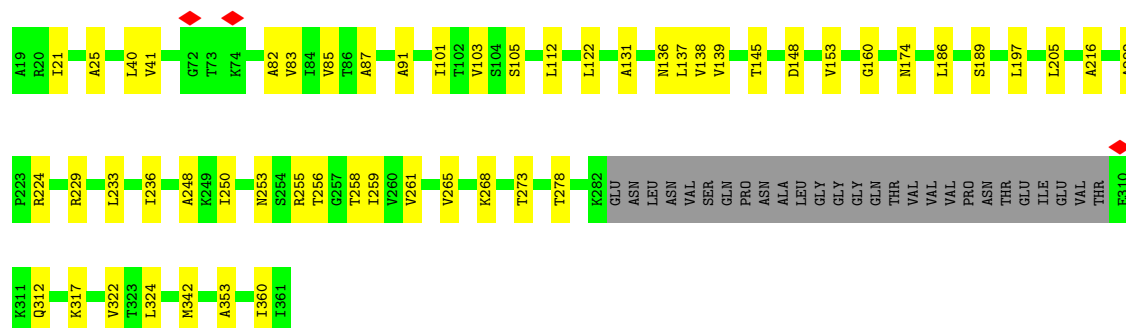
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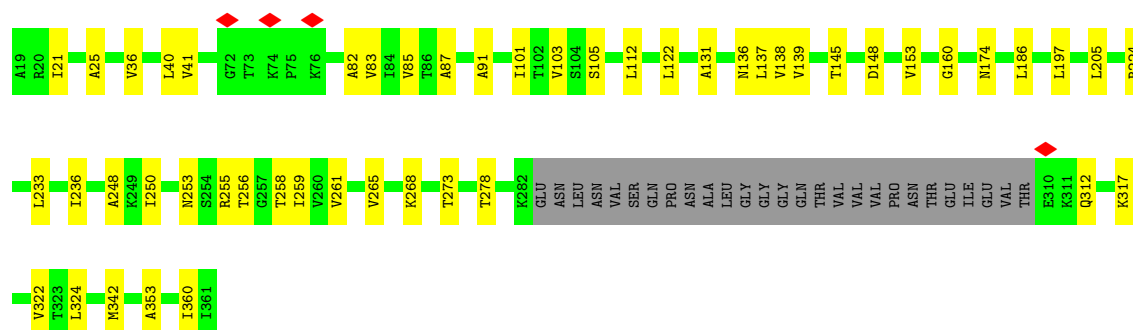
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Chain Br: 77% 15% 8%



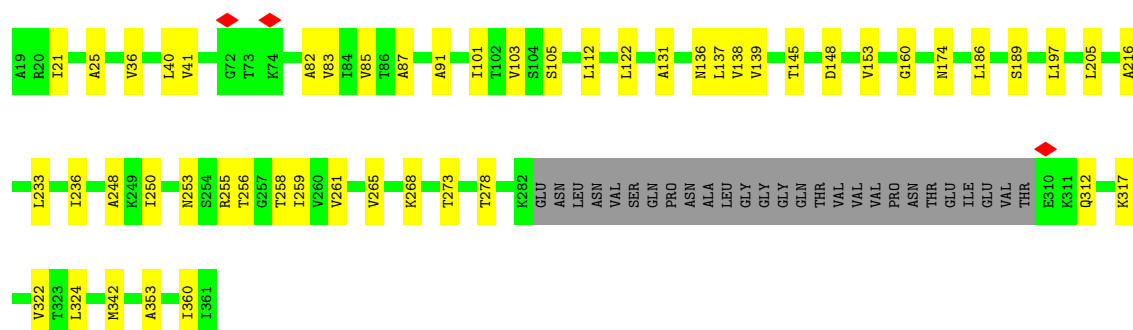
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Chain Bs: 78% 15% 8%



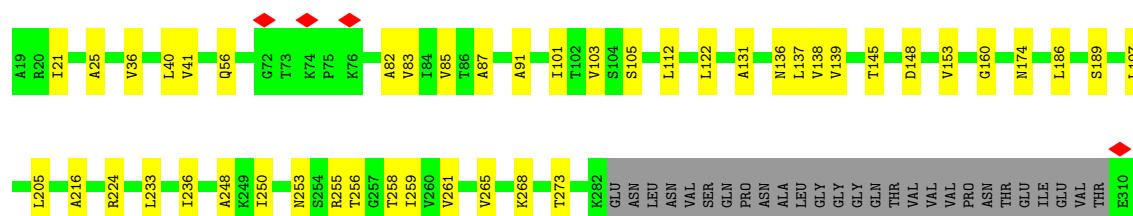
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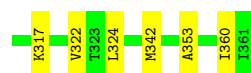
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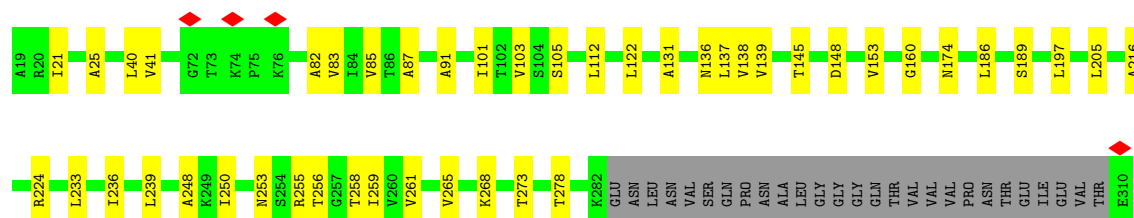
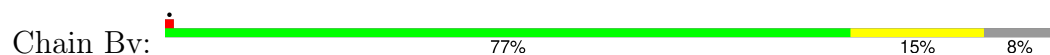
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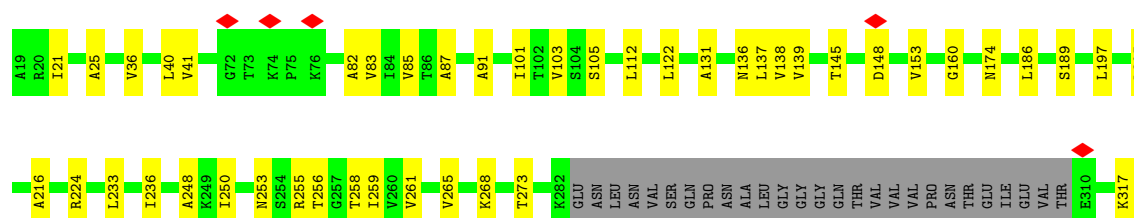
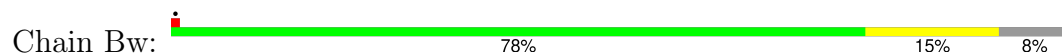




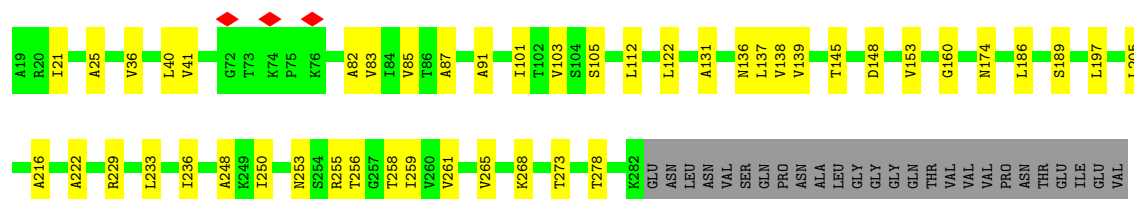
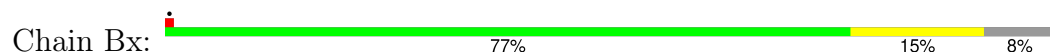
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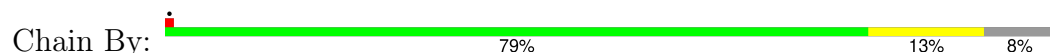
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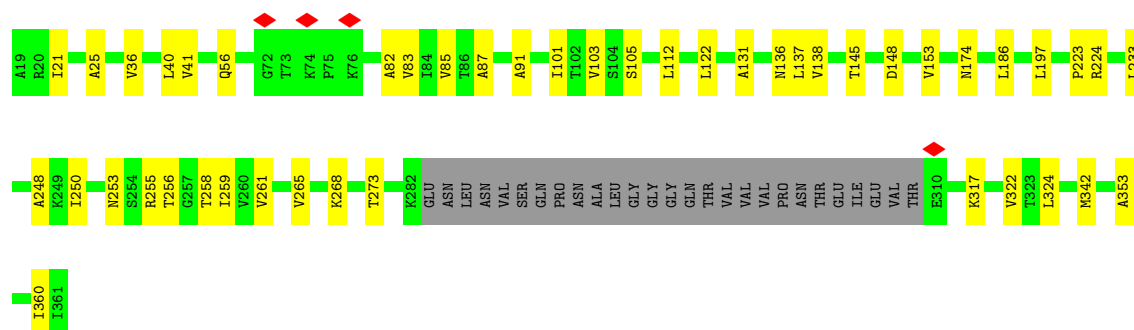


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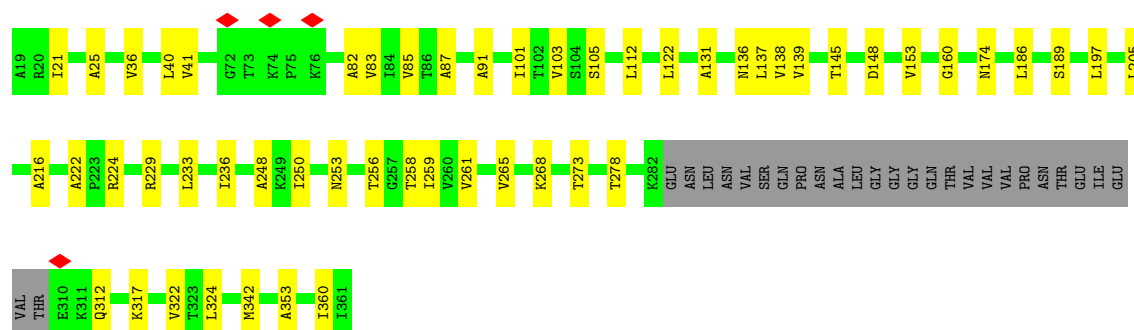
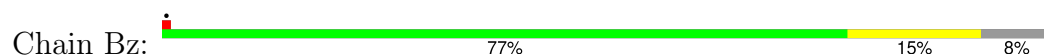


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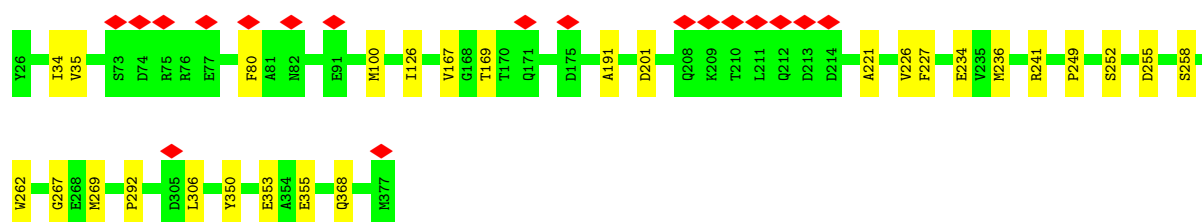




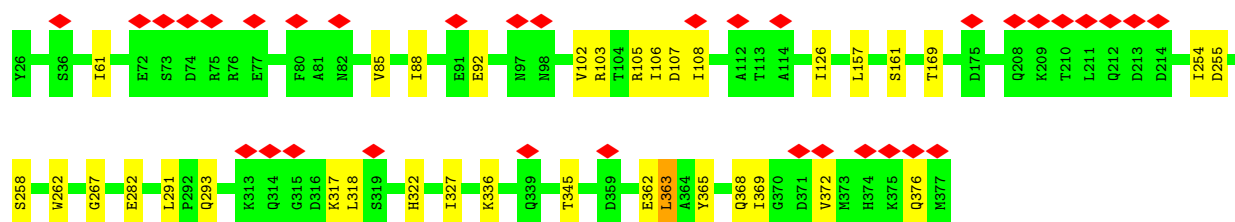
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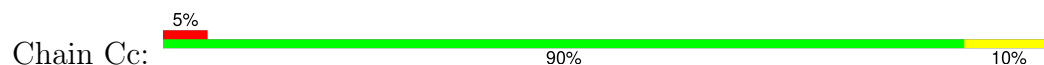
• Molecule 3: Flagellar protein FlgT

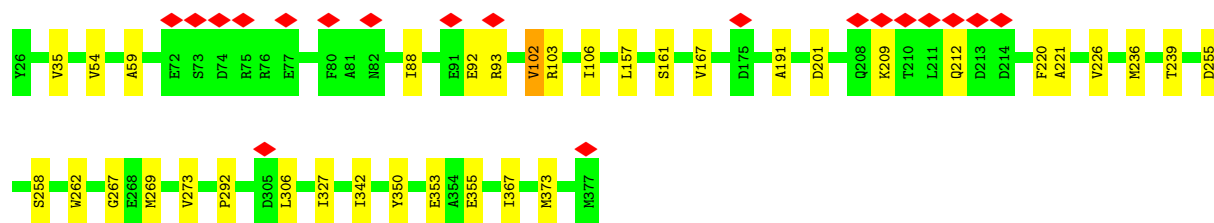


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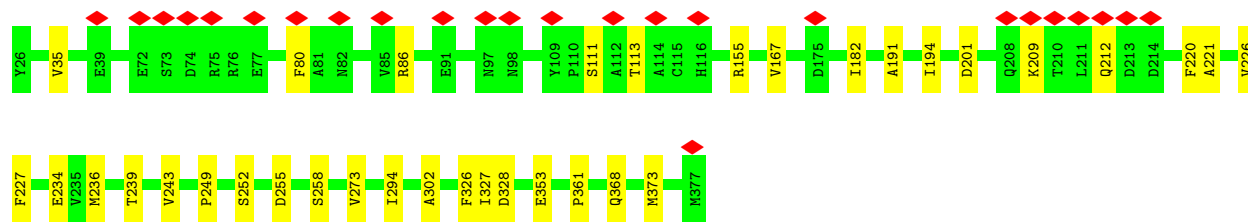
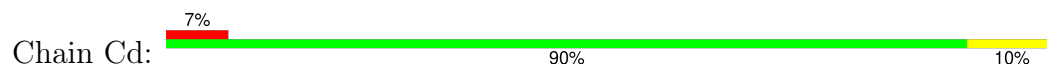


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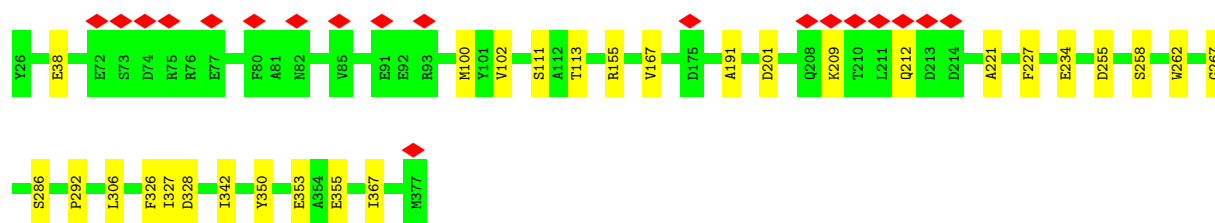




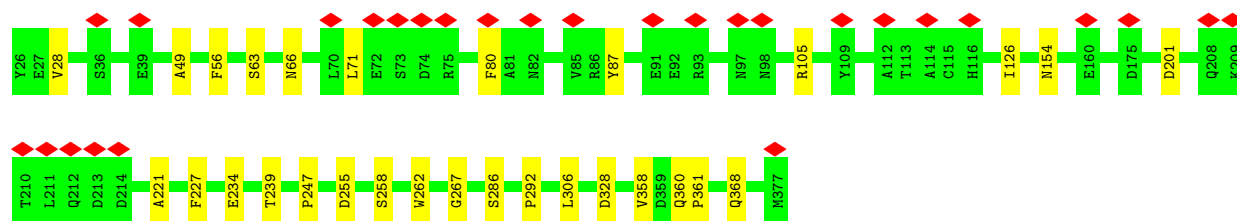
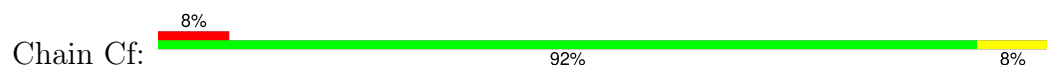
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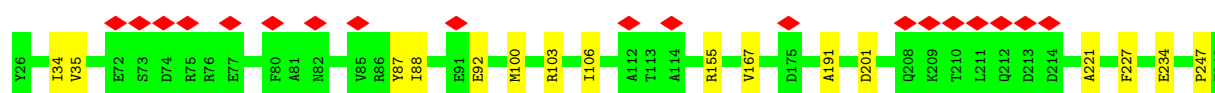
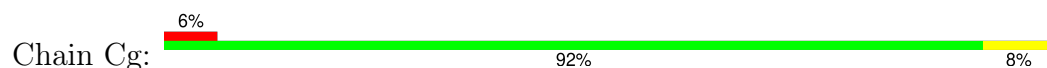
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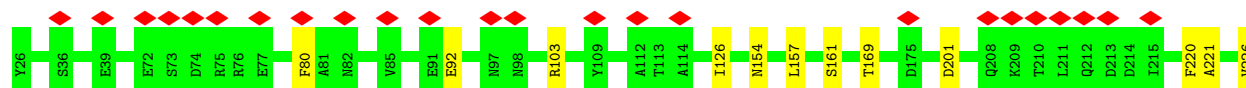


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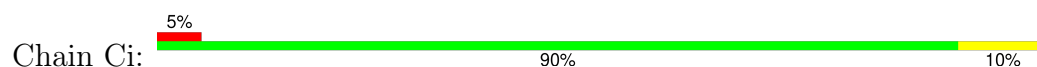




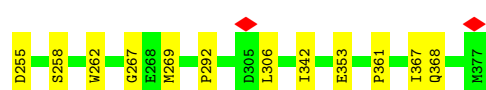
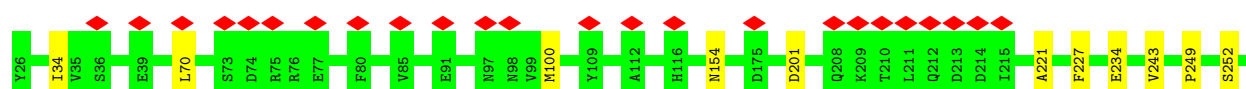
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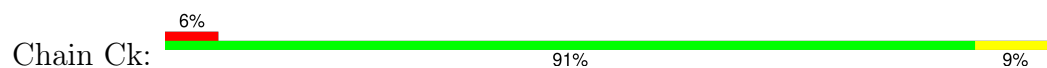
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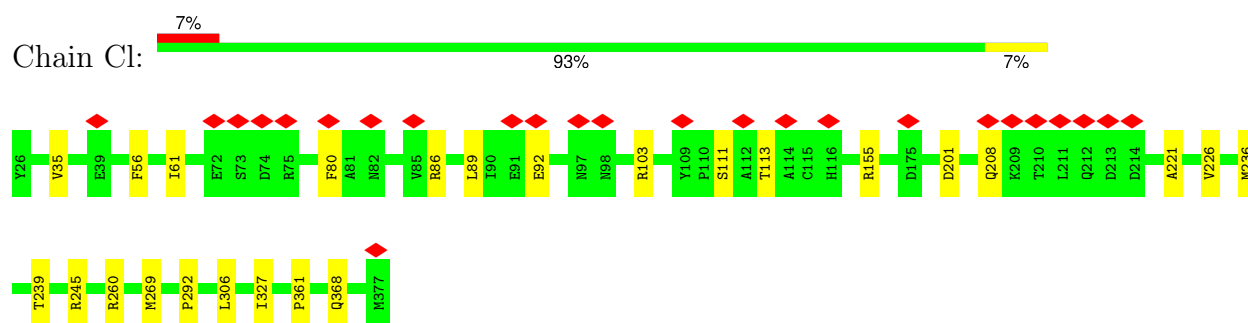
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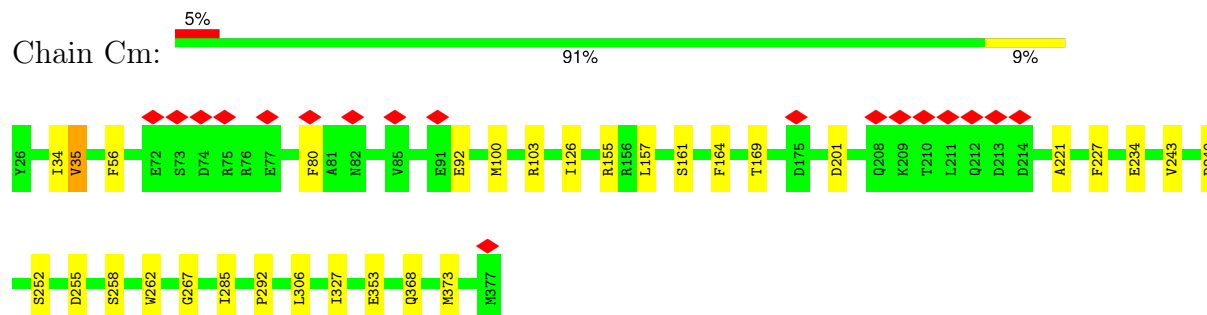
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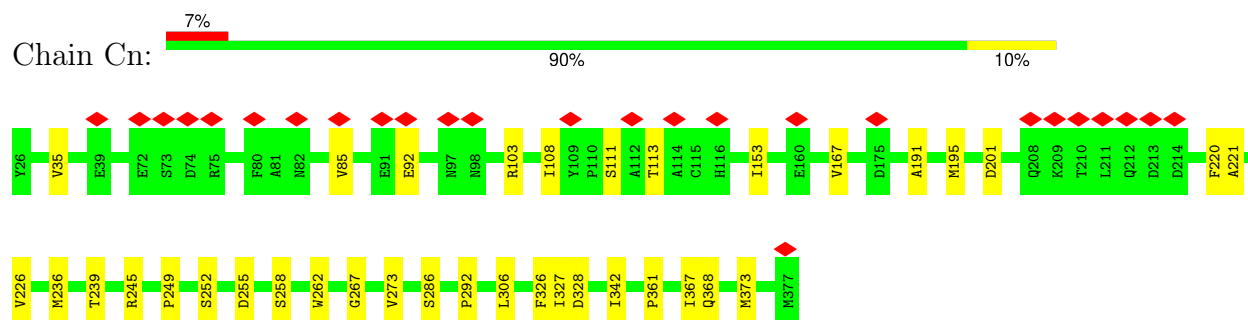
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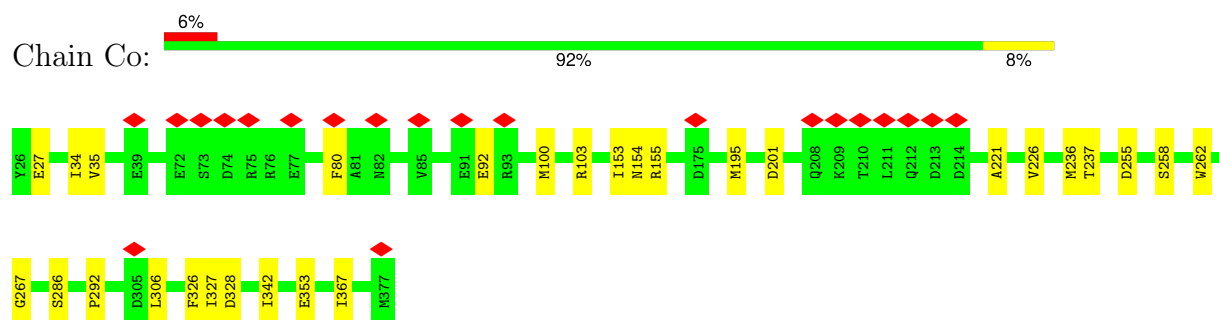
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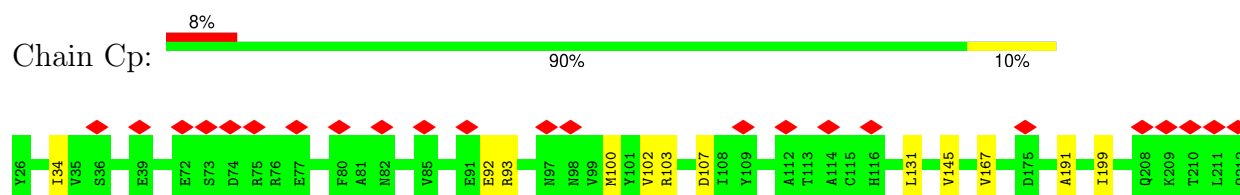
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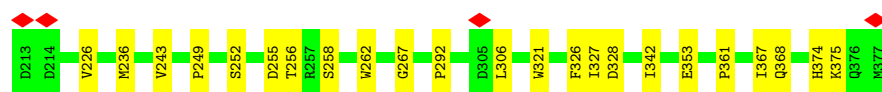


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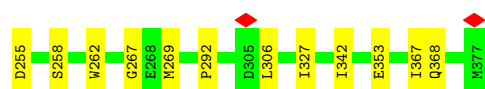


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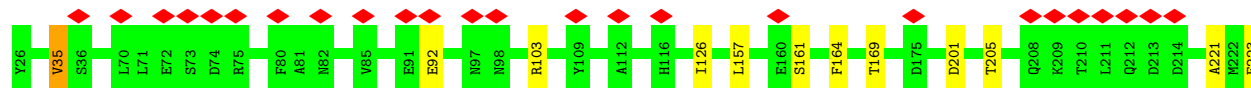
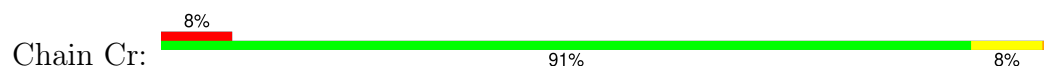




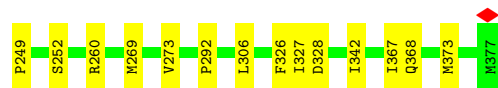
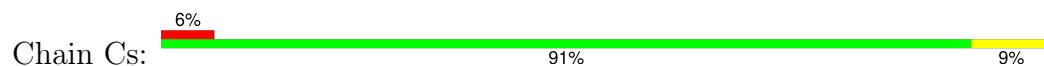
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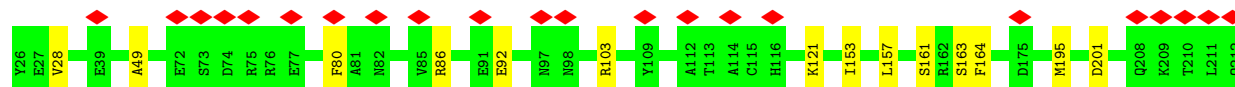
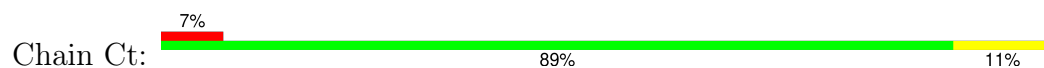
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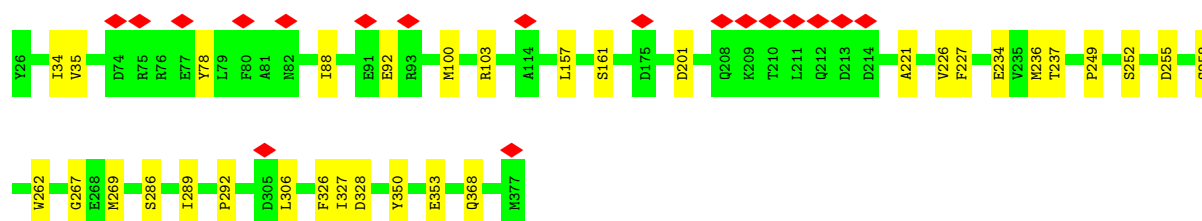
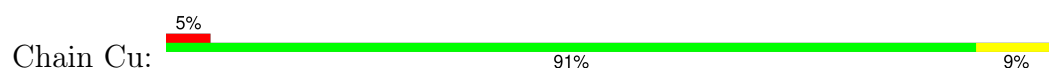
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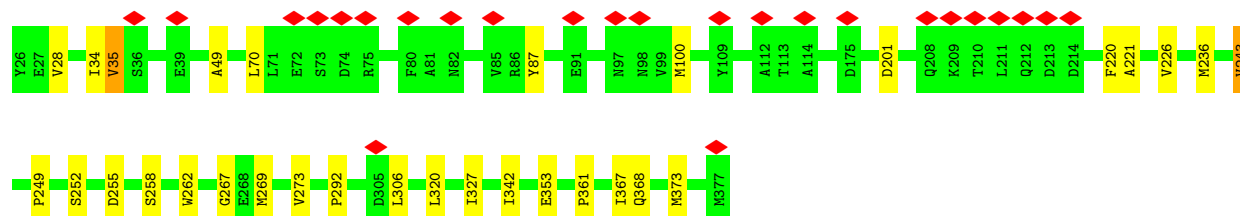
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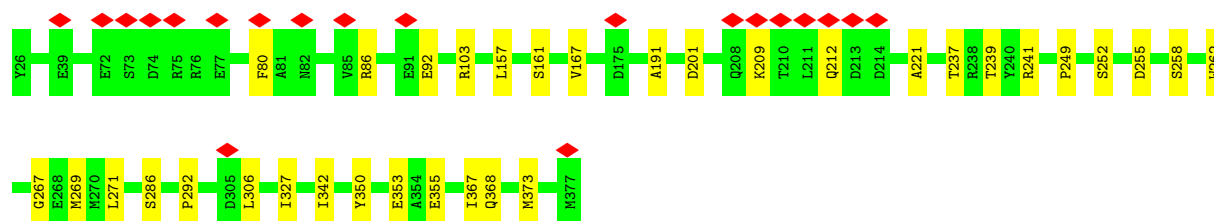
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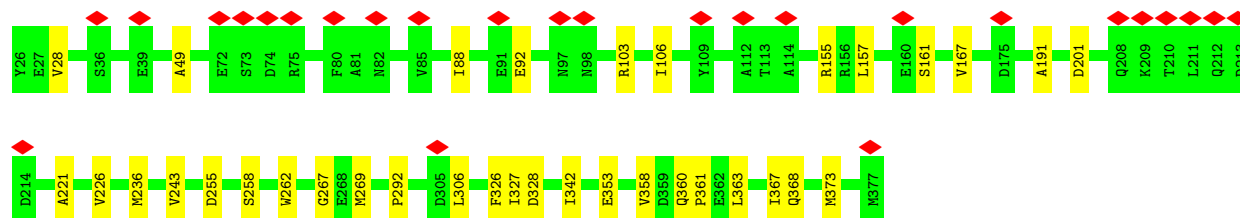
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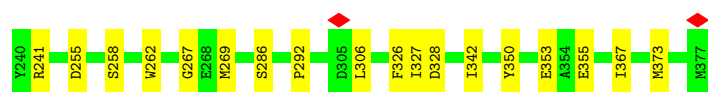


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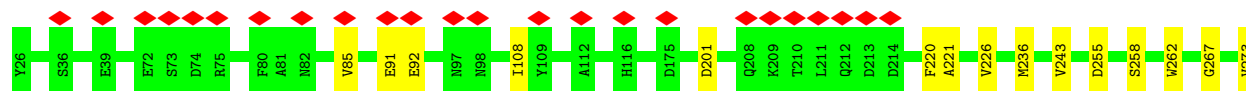


• Molecule 3: Flagellar protein FlgT

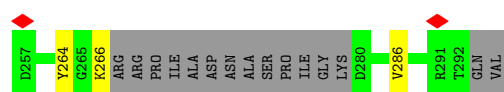
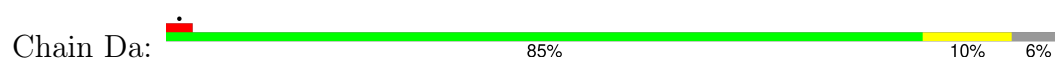




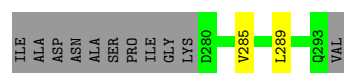
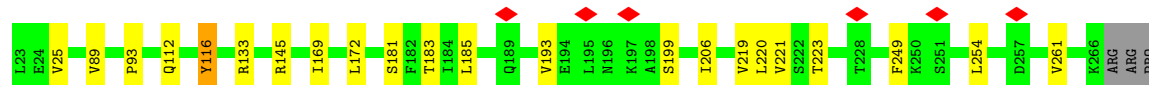
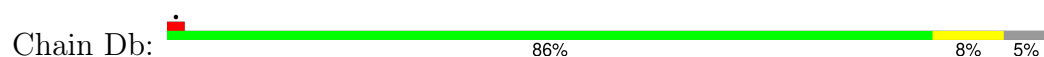
- Molecule 3: Flagellar protein FlgT



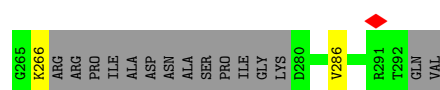
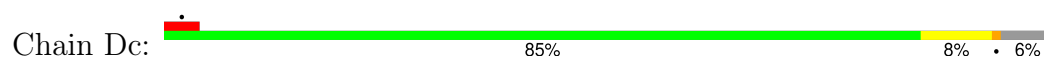
- Molecule 4: Sodium-type flagellar protein MotY




- Molecule 4: Sodium-type flagellar protein MotY

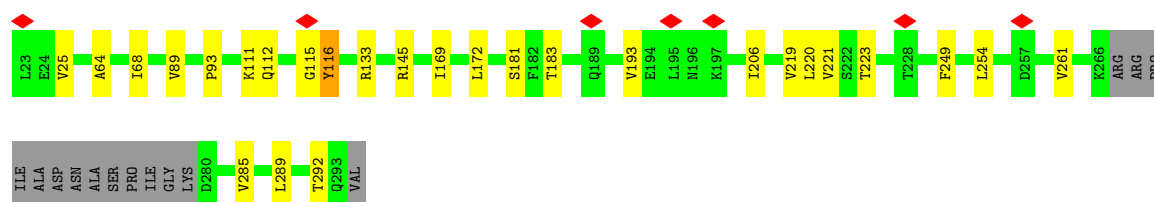


- Molecule 4: Sodium-type flagellar protein MotY




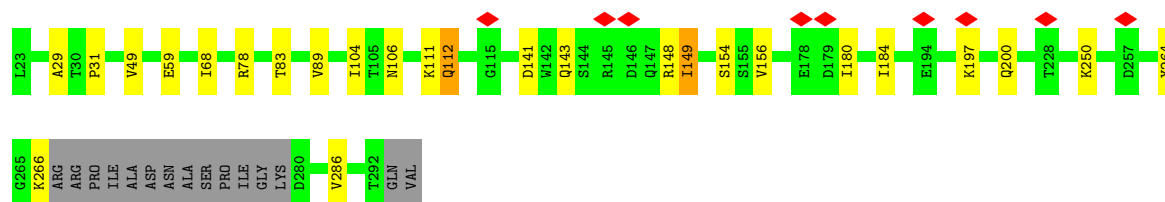
- Molecule 4: Sodium-type flagellar protein MotY

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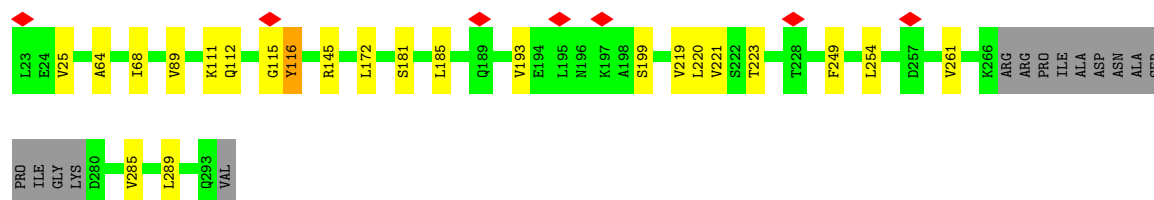
• Molecule 4: Sodium-type flagellar protein MotY

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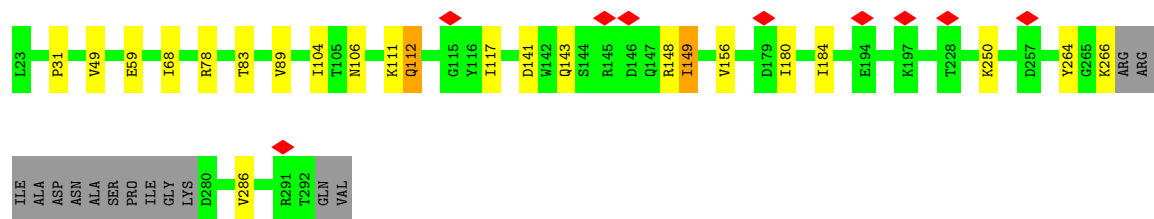
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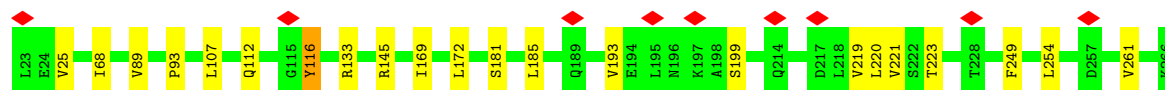
• Molecule 4: Sodium-type flagellar protein MotY

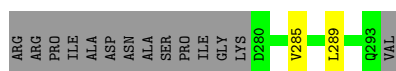
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• Molecule 4: Sodium-type flagellar protein MotY

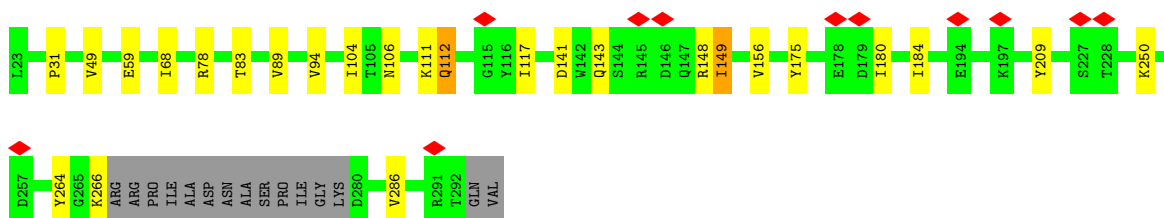
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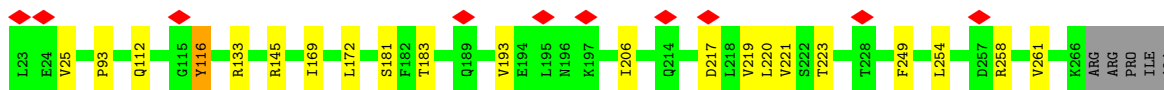
- Molecule 4: Sodium-type flagellar protein MotY

Chain Di: 85% 9% 6%



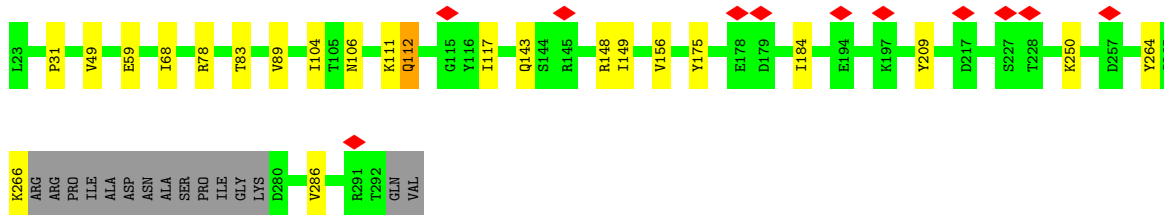
- Molecule 4: Sodium-type flagellar protein MotY

Chain Dj: 86% 8% 5%



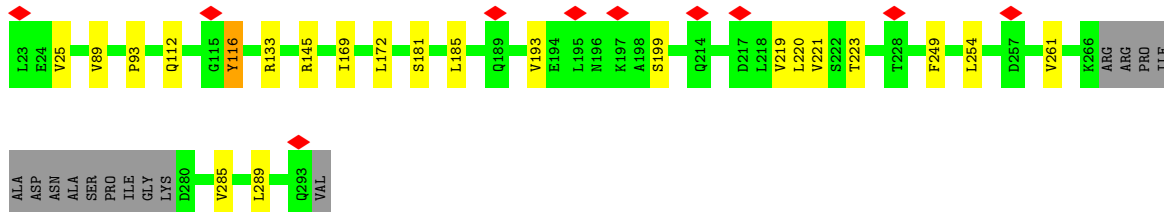
- Molecule 4: Sodium-type flagellar protein MotY

Chain Dk: 86% 8% 6%




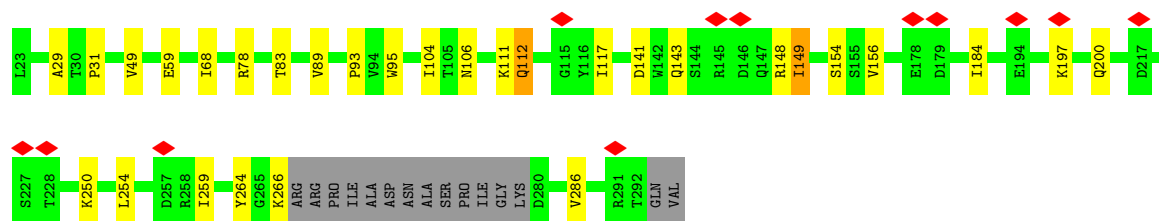
- Molecule 4: Sodium-type flagellar protein MotY

Chain Dl: 87% 8% 5%




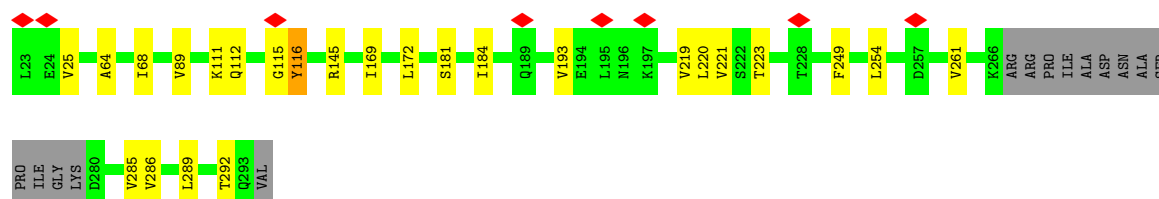
- Molecule 4: Sodium-type flagellar protein MotY

Chain Dm:  83% 10% • 6%




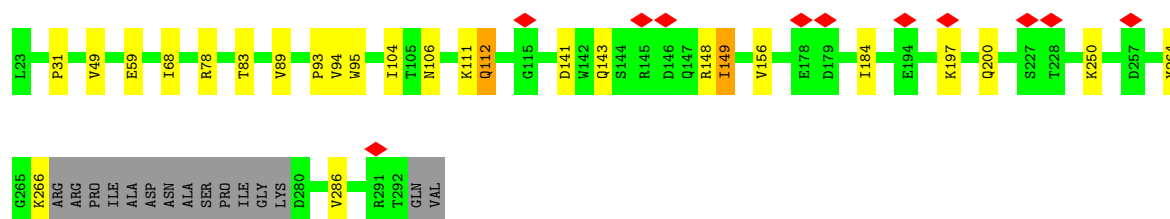
• Molecule 4: Sodium-type flagellar protein MotY

Chain Dn:  86% 9% 5%




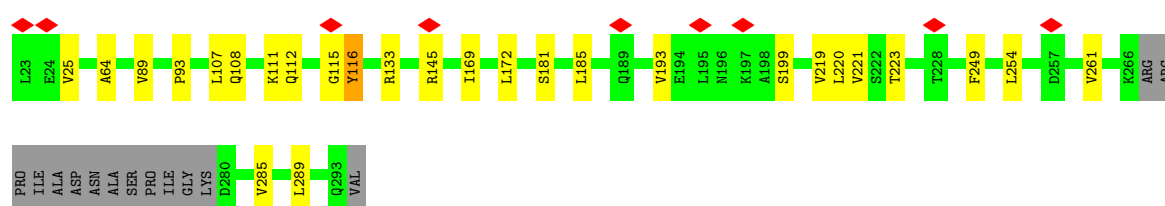
• Molecule 4: Sodium-type flagellar protein MotY

Chain Do:  85% 9% • 6%




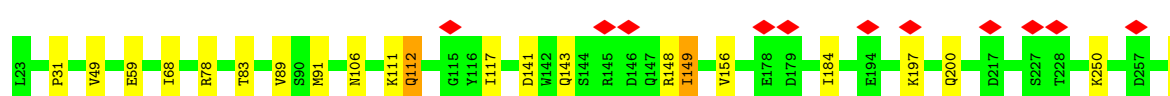
• Molecule 4: Sodium-type flagellar protein MotY

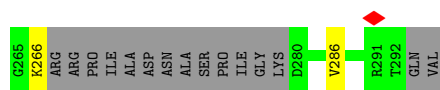
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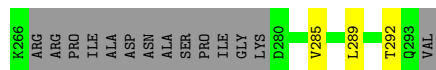
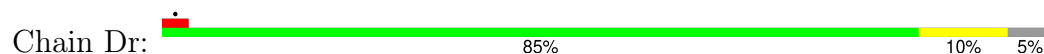
• Molecule 4: Sodium-type flagellar protein MotY

Chain Dq:  86% 8% • 6%

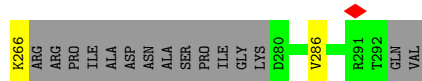
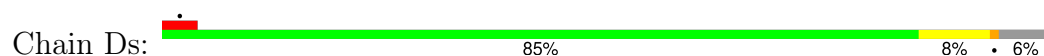




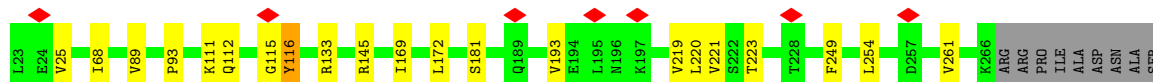
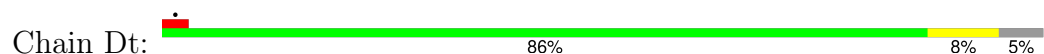
- Molecule 4: Sodium-type flagellar protein MotY



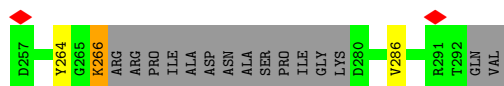
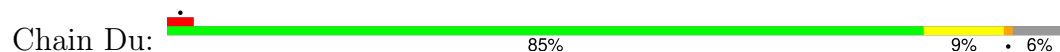
- Molecule 4: Sodium-type flagellar protein MotY




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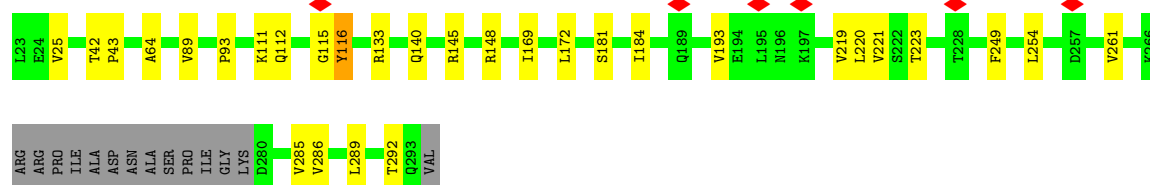


- Molecule 4: Sodium-type flagellar protein MotY




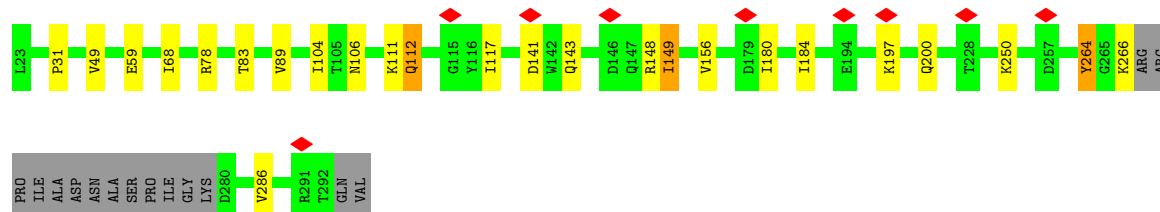
- Molecule 4: Sodium-type flagellar protein MotY

Chain Dv: 



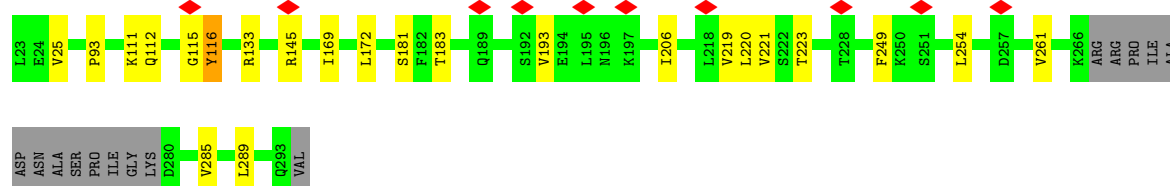
- Molecule 4: Sodium-type flagellar protein MotY

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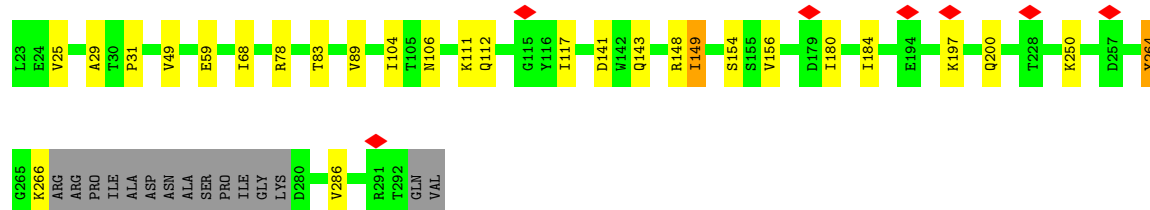
- Molecule 4: Sodium-type flagellar protein MotY

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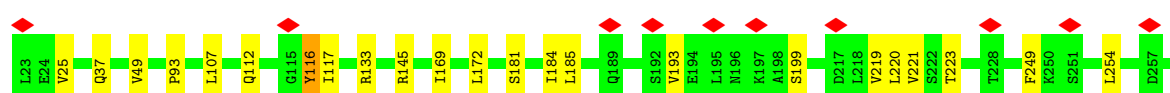
- Molecule 4: Sodium-type flagellar protein MotY

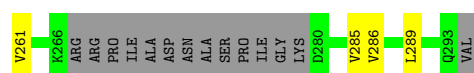
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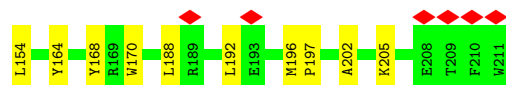
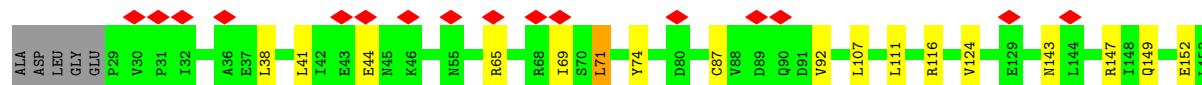
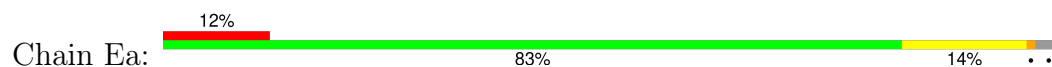
- Molecule 4: Sodium-type flagellar protein MotY

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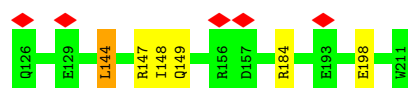
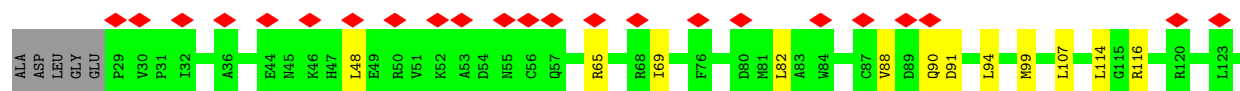
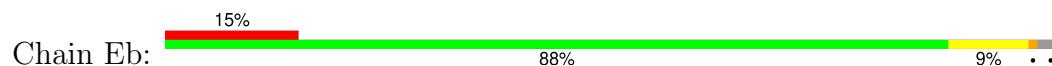




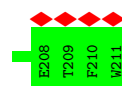
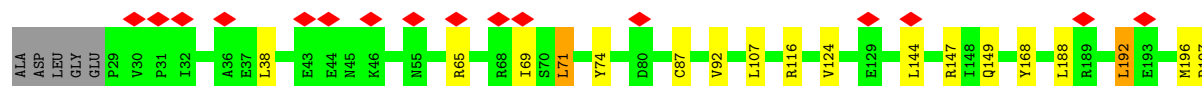
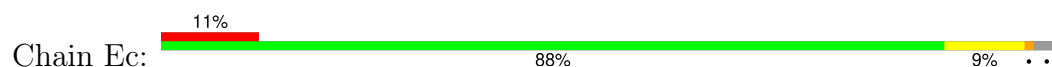
- Molecule 5: Sodium-type flagellar protein MotX



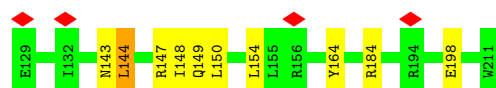
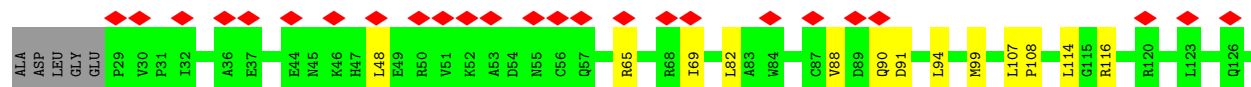
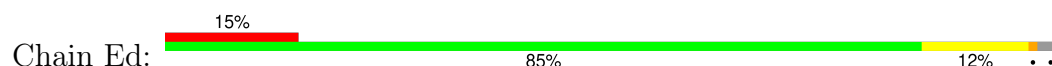
- Molecule 5: Sodium-type flagellar protein MotX




- Molecule 5: Sodium-type flagellar protein MotX

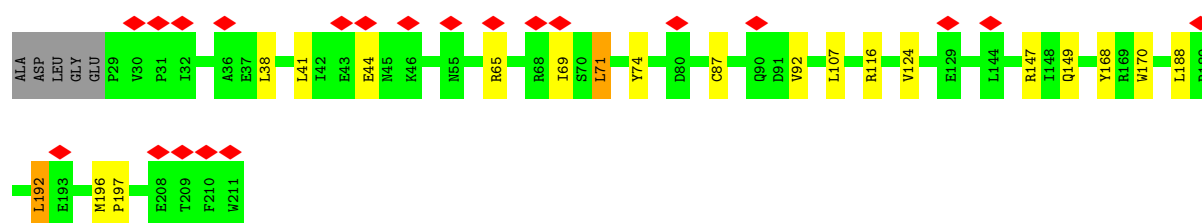


- Molecule 5: Sodium-type flagellar protein MotX




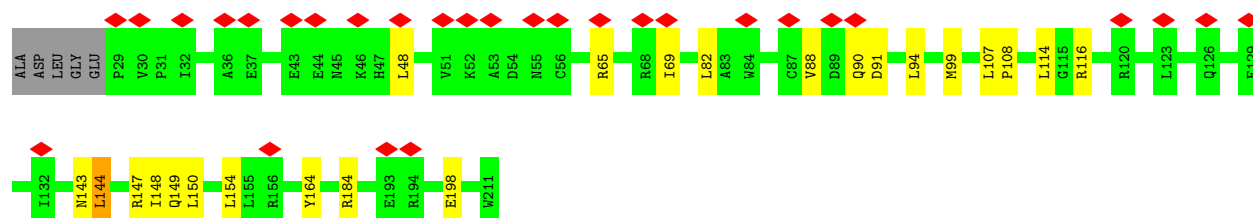
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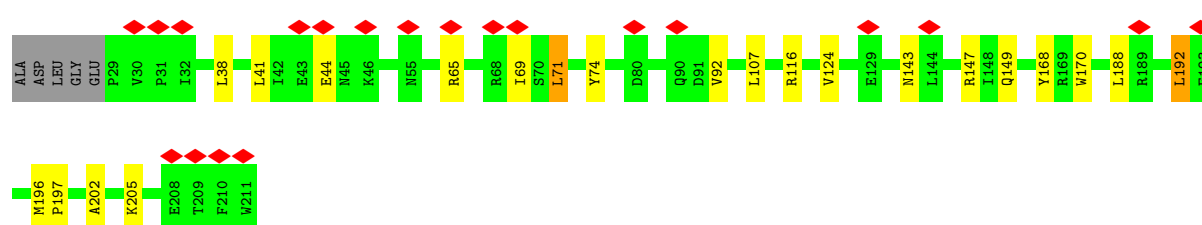
- Molecule 5: Sodium-type flagellar protein MotX

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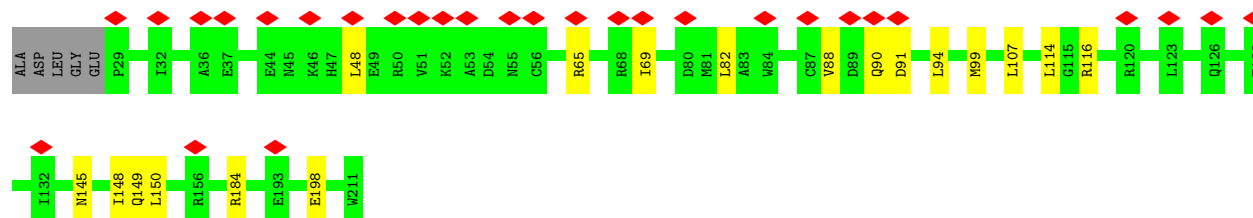
- Molecule 5: Sodium-type flagellar protein MotX

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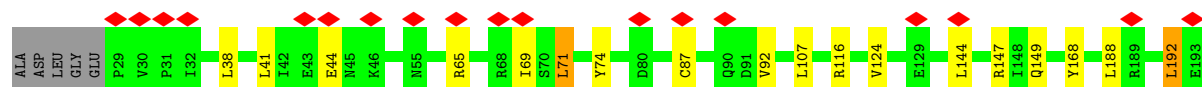
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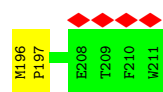
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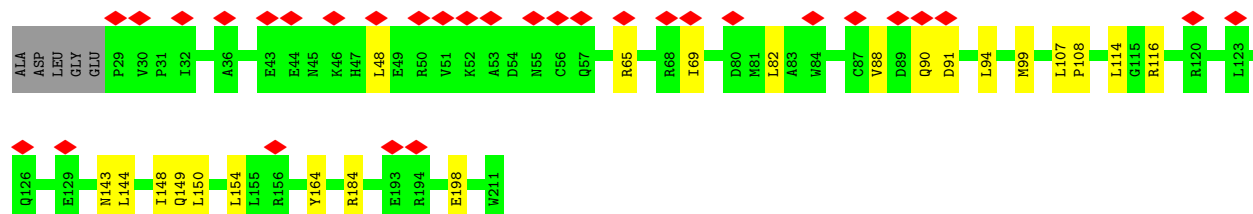
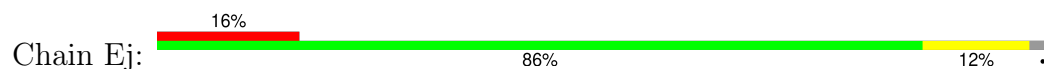
- Molecule 5: Sodium-type flagellar protein MotX

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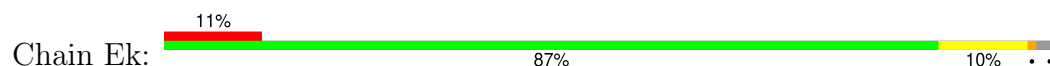




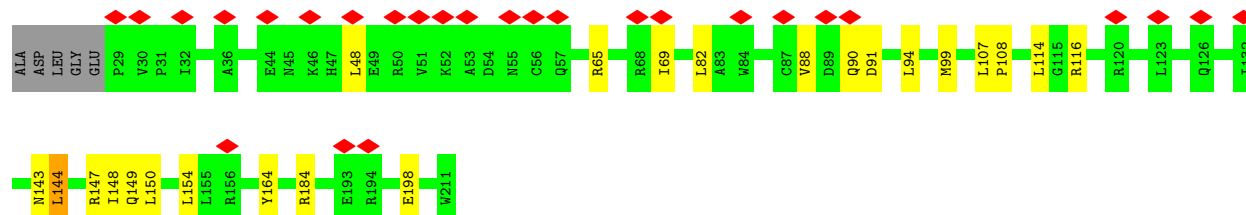
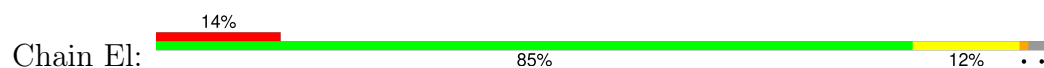
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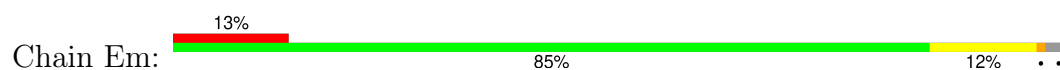
- Molecule 5: Sodium-type flagellar protein MotX



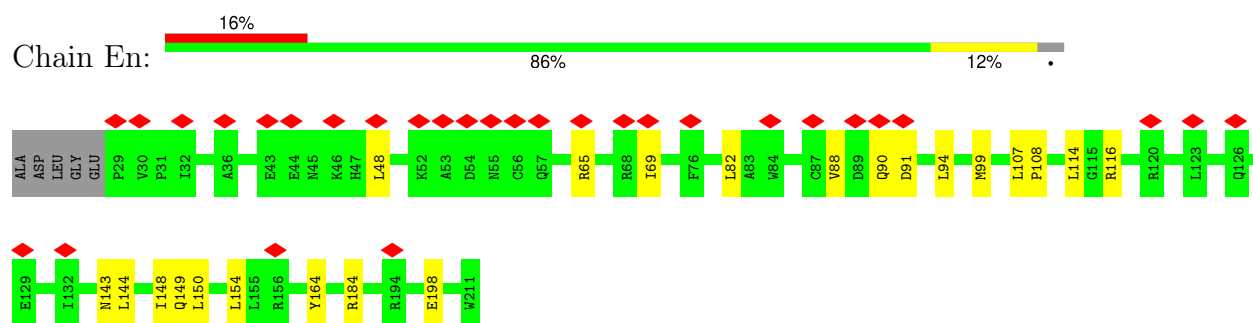
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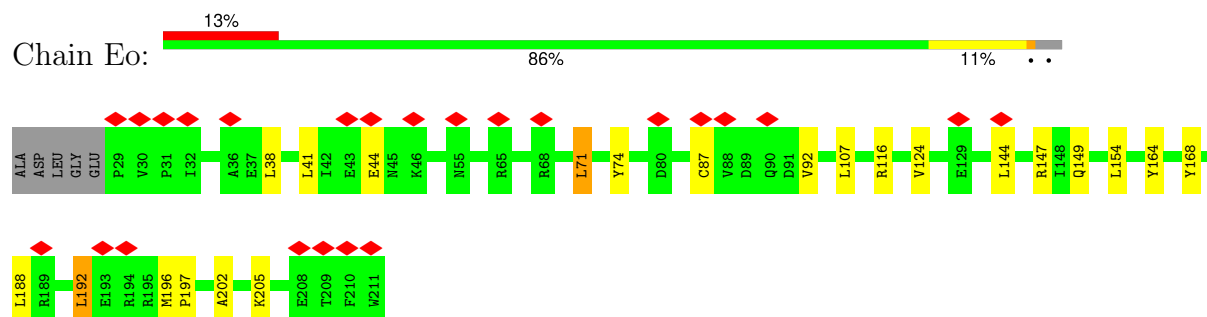
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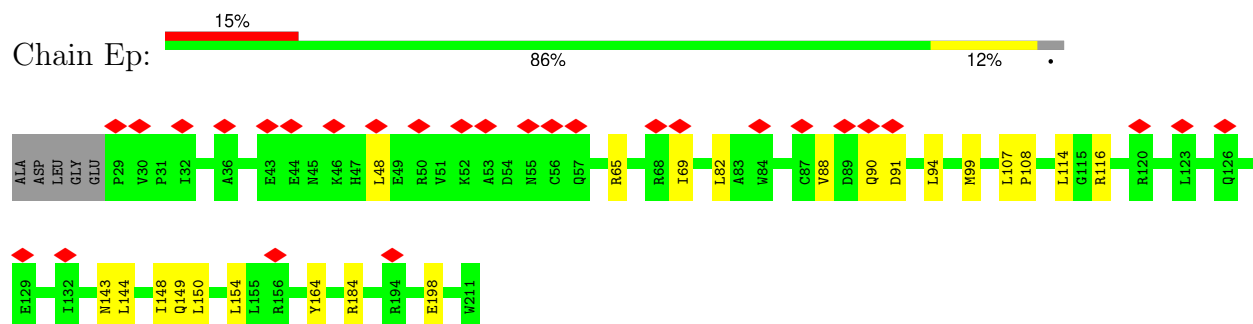
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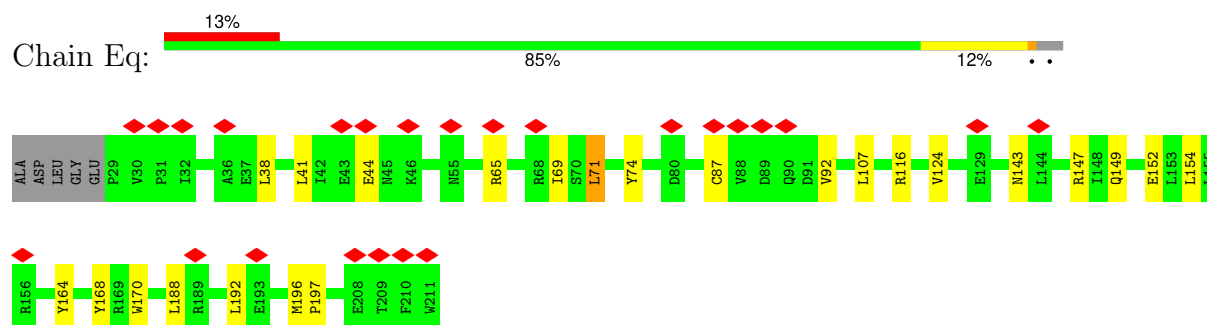
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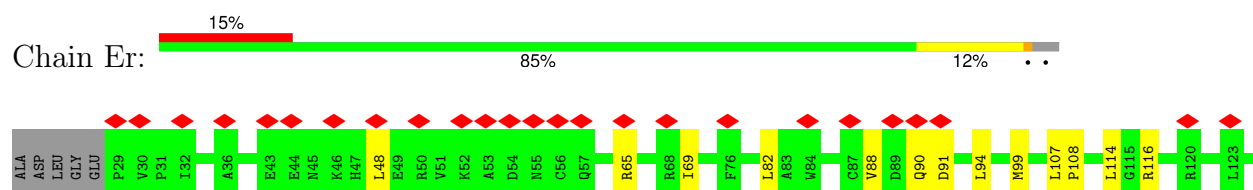
- Molecule 5: Sodium-type flagellar protein MotX

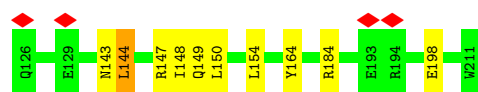


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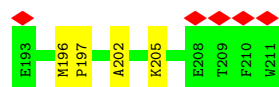
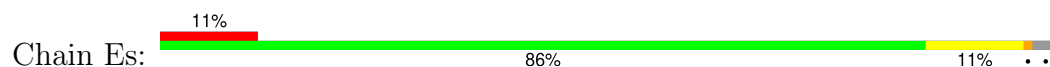


- Molecule 5: Sodium-type flagellar protein MotX

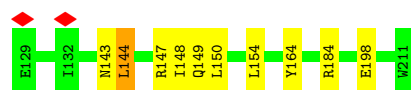
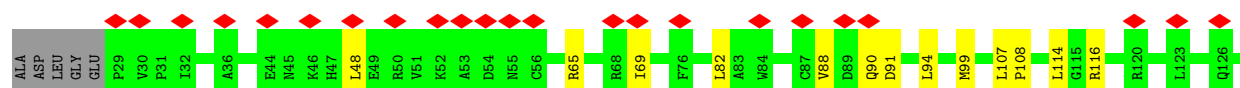
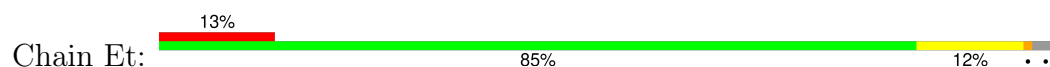




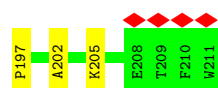
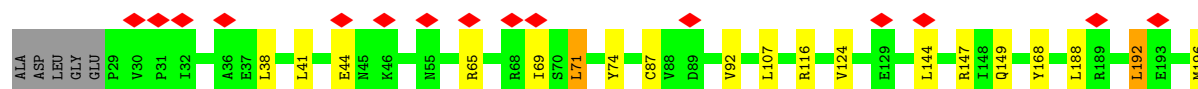
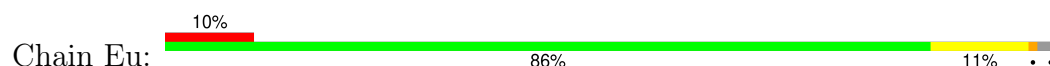
- Molecule 5: Sodium-type flagellar protein MotX



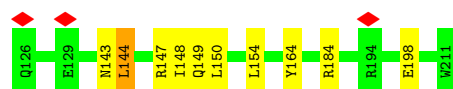
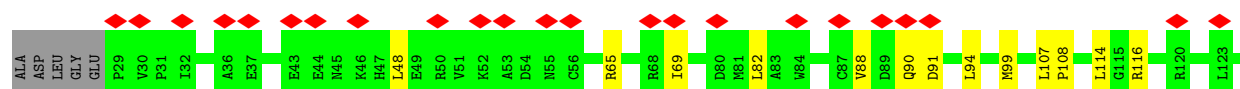
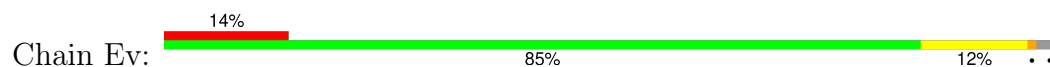
- Molecule 5: Sodium-type flagellar protein MotX



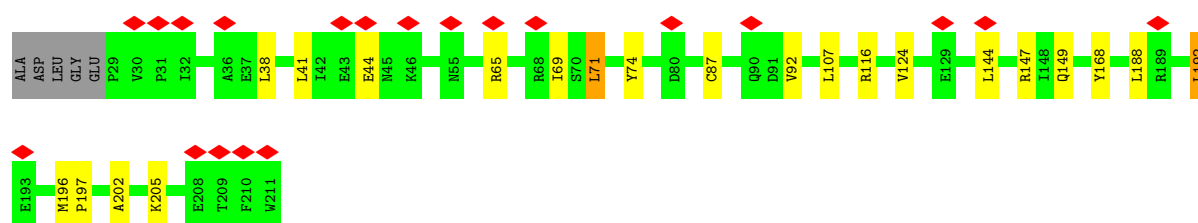
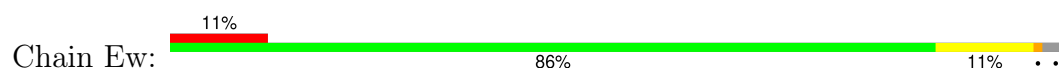
- Molecule 5: Sodium-type flagellar protein MotX



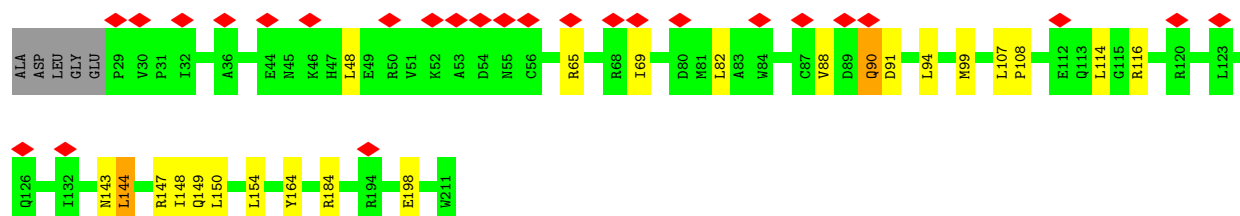
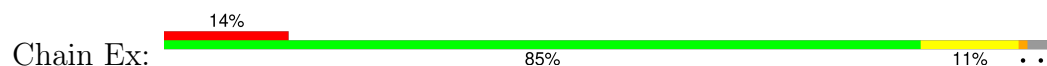
- Molecule 5: Sodium-type flagellar protein MotX



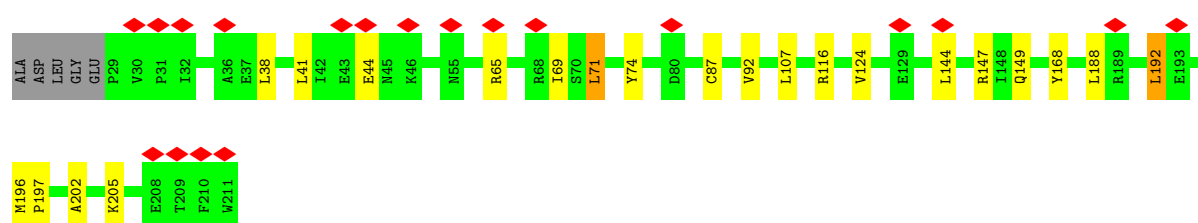
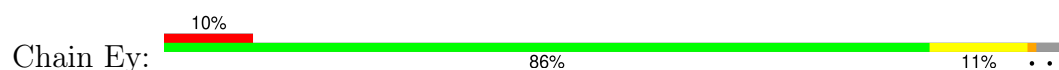
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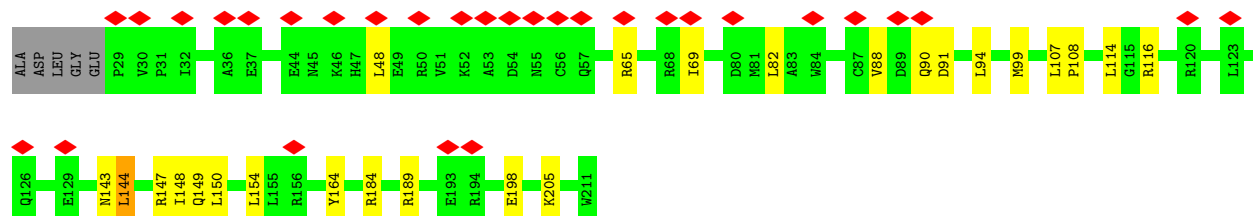
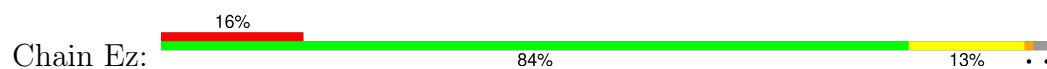
- Molecule 5: Sodium-type flagellar protein MotX



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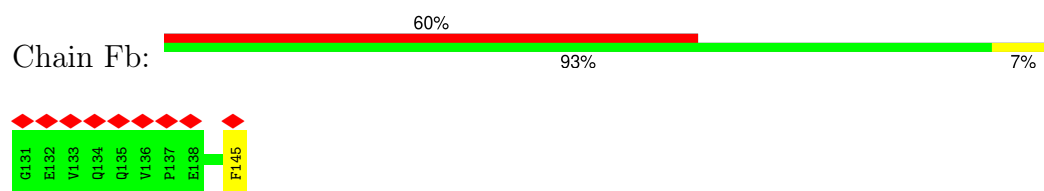
- Molecule 5: Sodium-type flagellar protein MotX



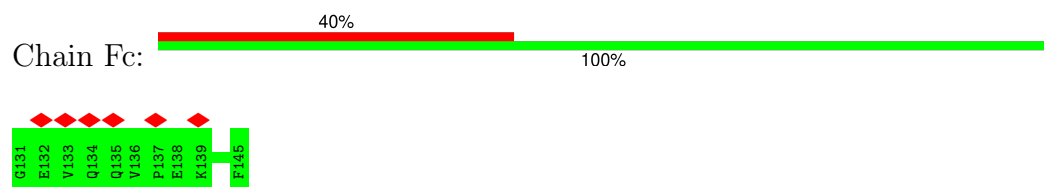
- Molecule 6: Flagellar assembly lipoprotein FlgP



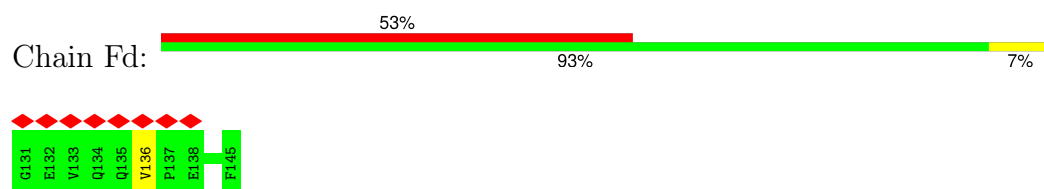
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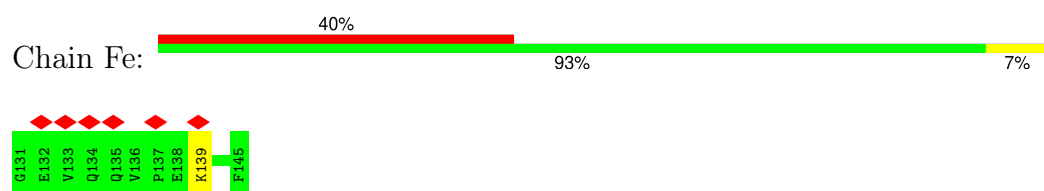
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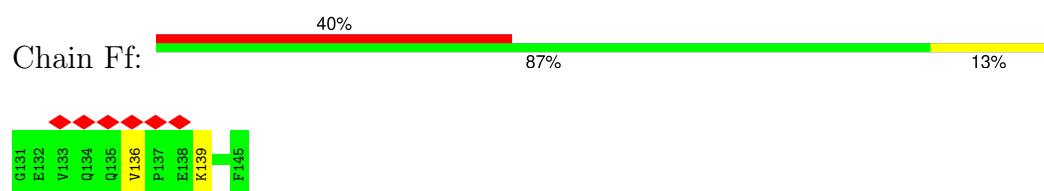
• Molecule 6: Flagellar assembly lipoprotein FlgP



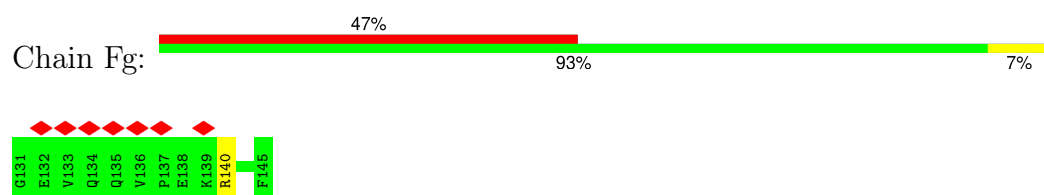
• Molecule 6: Flagellar assembly lipoprotein FlgP



• Molecule 6: Flagellar assembly lipoprotein FlgP

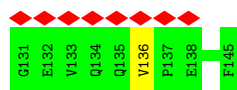


• Molecule 6: Flagellar assembly lipoprotein FlgP

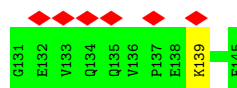
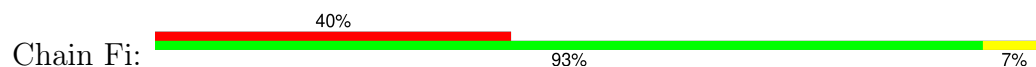


• Molecule 6: Flagellar assembly lipoprotein FlgP

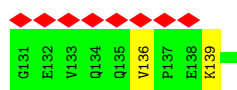
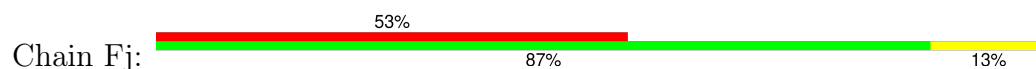




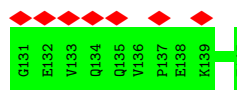
- Molecule 6: Flagellar assembly lipoprotein FlgP



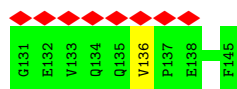
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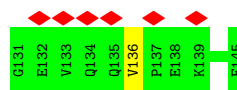
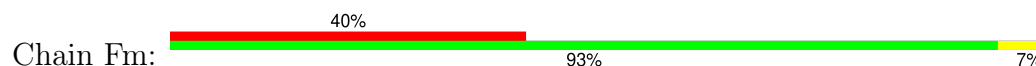
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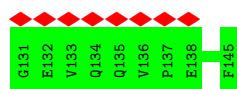
- Molecule 6: Flagellar assembly lipoprotein FlgP



- Molecule 6: Flagellar assembly lipoprotein FlgP



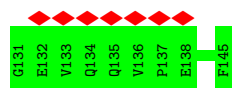
- Molecule 6: Flagellar assembly lipoprotein FlgP



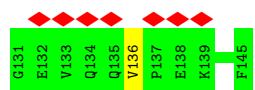
- Molecule 6: Flagellar assembly lipoprotein FlgP



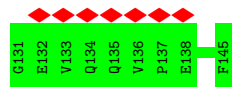
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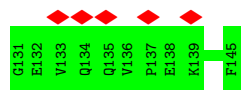
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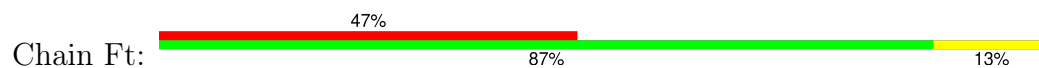
- Molecule 6: Flagellar assembly lipoprotein FlgP



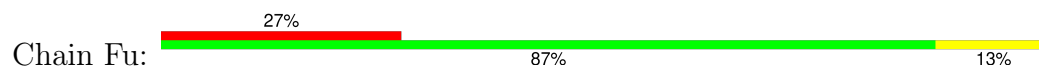
- Molecule 6: Flagellar assembly lipoprotein FlgP

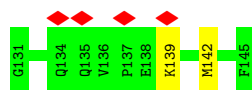


- Molecule 6: Flagellar assembly lipoprotein FlgP

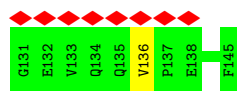


- Molecule 6: Flagellar assembly lipoprotein FlgP

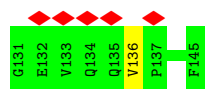




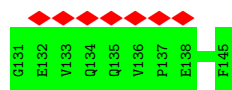
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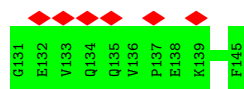
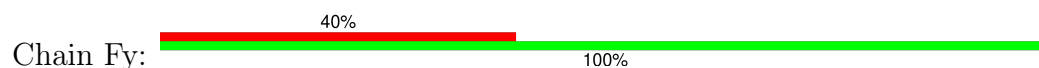
- Molecule 6: Flagellar assembly lipoprotein FlgP



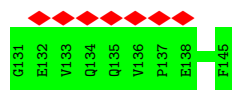
- Molecule 6: Flagellar assembly lipoprotein FlgP



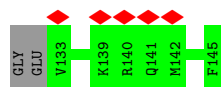
- Molecule 6: Flagellar assembly lipoprotein FlgP



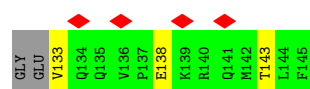
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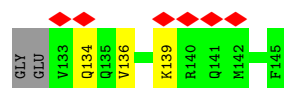
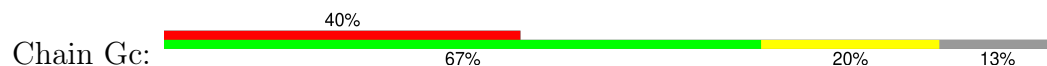
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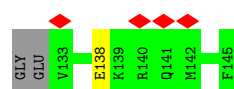
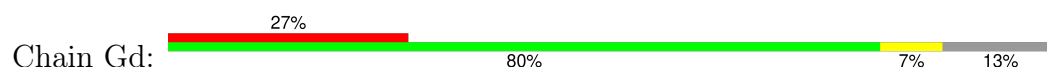
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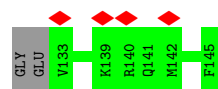
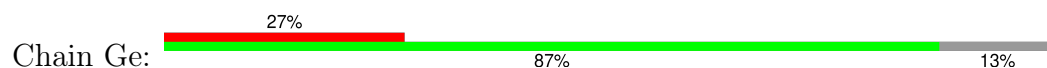
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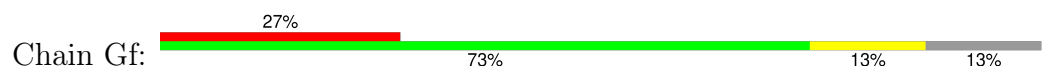
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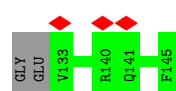
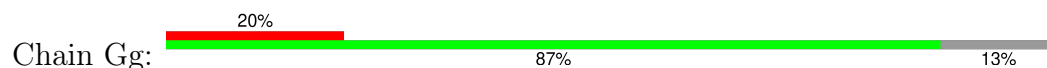
- Molecule 6: Flagellar assembly lipoprotein FlgP



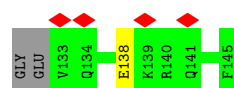
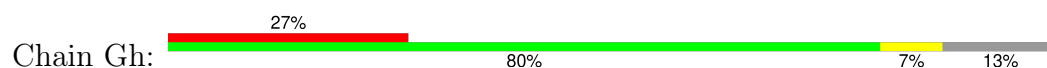
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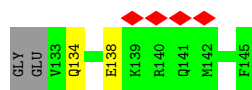
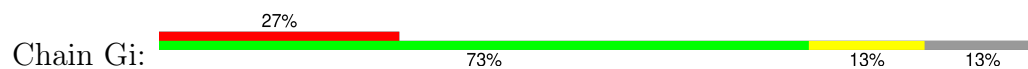
- Molecule 6: Flagellar assembly lipoprotein FlgP



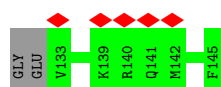
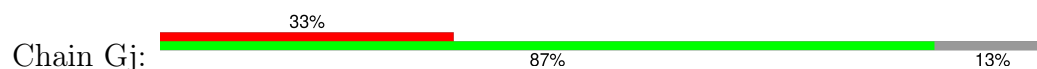
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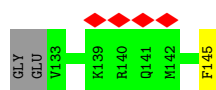
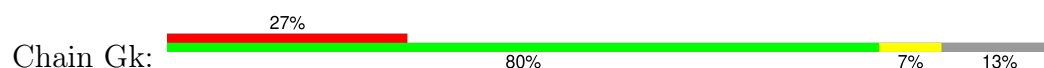
• Molecule 6: Flagellar assembly lipoprotein FlgP



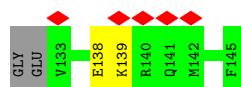
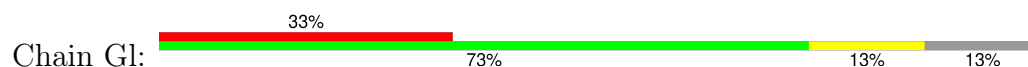
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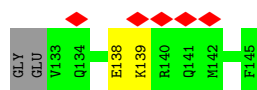
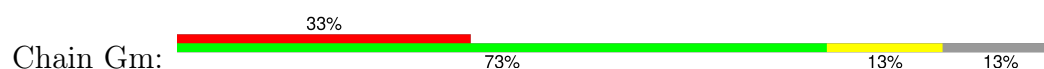
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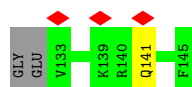
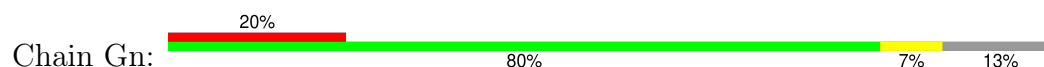
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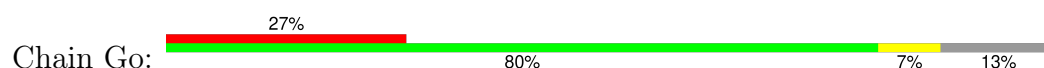
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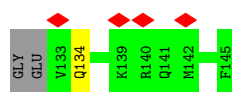


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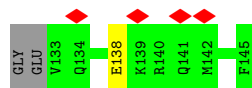
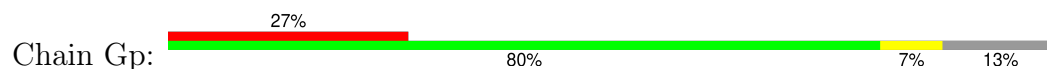


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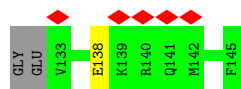
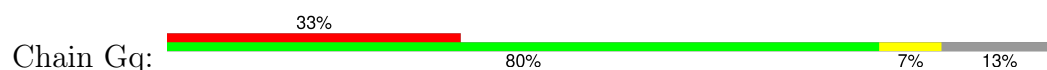




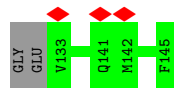
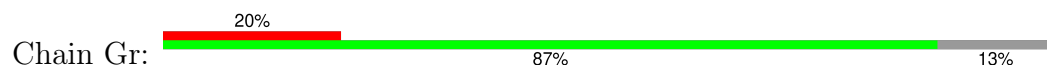
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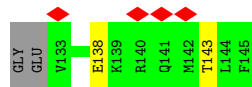
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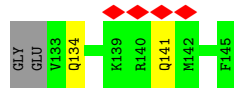
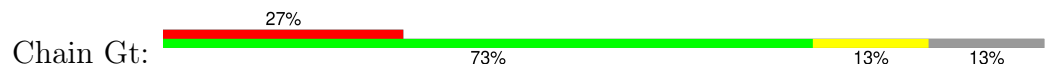
- Molecule 6: Flagellar assembly lipoprotein FlgP



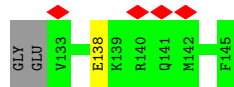
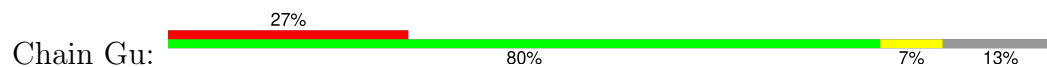
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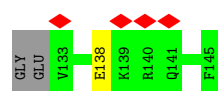
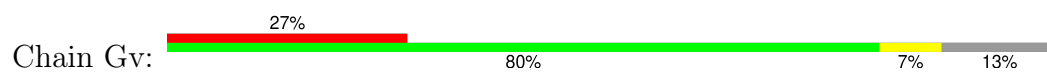
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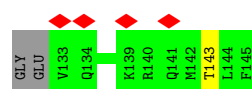
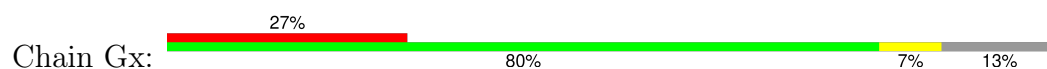
- Molecule 6: Flagellar assembly lipoprotein FlgP



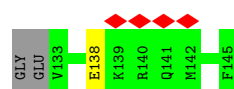
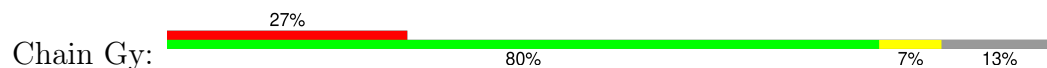
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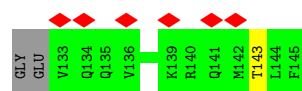
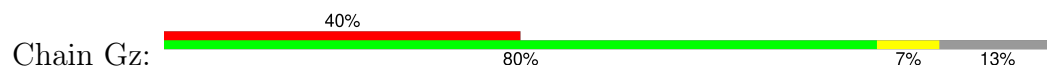
- Molecule 6: Flagellar assembly lipoprotein FlgP



- Molecule 6: Flagellar assembly lipoprotein FlgP



- Molecule 6: Flagellar assembly lipoprotein FlgP



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53628	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	0.811	Depositor
Minimum map value	-0.389	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	477.636, 477.636, 477.636	wwPDB
Map dimensions	318, 318, 318	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.502, 1.502, 1.502	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Aa	0.09	0/1699	0.27	0/2303
1	Ab	0.10	0/1699	0.27	0/2303
1	Ac	0.10	0/1699	0.27	0/2303
1	Ad	0.10	0/1699	0.27	0/2303
1	Ae	0.09	0/1699	0.27	0/2303
1	Af	0.09	0/1699	0.27	0/2303
1	Ag	0.10	0/1699	0.26	0/2303
1	Ah	0.09	0/1699	0.27	0/2303
1	Ai	0.09	0/1699	0.27	0/2303
1	Aj	0.10	0/1699	0.27	0/2303
1	Ak	0.09	0/1699	0.27	0/2303
1	Al	0.09	0/1699	0.27	0/2303
1	Am	0.09	0/1699	0.27	0/2303
1	An	0.09	0/1699	0.27	0/2303
1	Ao	0.09	0/1699	0.26	0/2303
1	Ap	0.09	0/1699	0.27	0/2303
1	Aq	0.09	0/1699	0.27	0/2303
1	Ar	0.10	0/1699	0.27	0/2303
1	As	0.09	0/1699	0.27	0/2303
1	At	0.09	0/1699	0.26	0/2303
1	Au	0.09	0/1699	0.27	0/2303
1	Av	0.09	0/1699	0.27	0/2303
1	Aw	0.09	0/1699	0.27	0/2303
1	Ax	0.10	0/1699	0.26	0/2303
1	Ay	0.09	0/1699	0.27	0/2303
1	Az	0.09	0/1699	0.27	0/2303
2	Ba	0.11	0/2345	0.29	0/3177
2	Bb	0.11	0/2345	0.29	0/3177
2	Bc	0.11	0/2345	0.29	0/3177
2	Bd	0.11	0/2345	0.29	0/3177
2	Be	0.11	0/2345	0.29	0/3177
2	Bf	0.11	0/2345	0.29	0/3177
2	Bg	0.11	0/2345	0.29	0/3177
2	Bh	0.11	0/2345	0.29	0/3177

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Bi	0.11	0/2345	0.29	0/3177
2	Bj	0.11	0/2345	0.29	0/3177
2	Bk	0.11	0/2345	0.29	0/3177
2	Bl	0.10	0/2345	0.29	0/3177
2	Bm	0.11	0/2345	0.29	0/3177
2	Bn	0.11	0/2345	0.29	0/3177
2	Bo	0.11	0/2345	0.29	0/3177
2	Bp	0.11	0/2345	0.29	0/3177
2	Bq	0.11	0/2345	0.29	0/3177
2	Br	0.11	0/2345	0.29	0/3177
2	Bs	0.11	0/2345	0.29	0/3177
2	Bt	0.11	0/2345	0.29	0/3177
2	Bu	0.11	0/2345	0.29	0/3177
2	Bv	0.11	0/2345	0.29	0/3177
2	Bw	0.11	0/2345	0.29	0/3177
2	Bx	0.11	0/2345	0.29	0/3177
2	By	0.11	0/2345	0.29	0/3177
2	Bz	0.11	0/2345	0.29	0/3177
3	Ca	0.11	0/2816	0.29	0/3809
3	Cb	0.14	0/2816	0.30	0/3809
3	Cc	0.11	0/2816	0.28	0/3809
3	Cd	0.11	0/2816	0.29	0/3809
3	Ce	0.11	0/2816	0.28	0/3809
3	Cf	0.11	0/2816	0.29	0/3809
3	Cg	0.11	0/2816	0.29	0/3809
3	Ch	0.12	0/2816	0.30	0/3809
3	Ci	0.11	0/2816	0.29	0/3809
3	Cj	0.11	0/2816	0.29	0/3809
3	Ck	0.11	0/2816	0.29	0/3809
3	Cl	0.12	0/2816	0.30	0/3809
3	Cm	0.11	0/2816	0.29	0/3809
3	Cn	0.11	0/2816	0.28	0/3809
3	Co	0.11	0/2816	0.29	0/3809
3	Cp	0.11	0/2816	0.29	0/3809
3	Cq	0.11	0/2816	0.28	0/3809
3	Cr	0.11	0/2816	0.28	0/3809
3	Cs	0.11	0/2816	0.30	0/3809
3	Ct	0.12	0/2816	0.31	0/3809
3	Cu	0.11	0/2816	0.30	0/3809
3	Cv	0.11	0/2816	0.28	0/3809
3	Cw	0.11	0/2816	0.29	0/3809
3	Cx	0.11	0/2816	0.28	0/3809
3	Cy	0.11	0/2816	0.28	0/3809

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Cz	0.11	0/2816	0.29	0/3809
4	Da	0.13	0/2129	0.32	0/2882
4	Db	0.13	0/2124	0.35	0/2877
4	Dc	0.13	0/2129	0.31	0/2882
4	Dd	0.13	0/2124	0.36	0/2877
4	De	0.13	0/2129	0.32	0/2882
4	Df	0.13	0/2124	0.36	0/2877
4	Dg	0.13	0/2129	0.32	0/2882
4	Dh	0.13	0/2124	0.36	0/2877
4	Di	0.13	0/2129	0.32	0/2882
4	Dj	0.13	0/2124	0.34	0/2877
4	Dk	0.13	0/2129	0.32	0/2882
4	Dl	0.13	0/2124	0.35	0/2877
4	Dm	0.12	0/2129	0.31	0/2882
4	Dn	0.13	0/2124	0.34	0/2877
4	Do	0.13	0/2129	0.31	0/2882
4	Dp	0.13	0/2124	0.35	0/2877
4	Dq	0.13	0/2129	0.32	0/2882
4	Dr	0.13	0/2124	0.34	0/2877
4	Ds	0.12	0/2129	0.31	0/2882
4	Dt	0.13	0/2124	0.35	0/2877
4	Du	0.13	0/2129	0.32	0/2882
4	Dv	0.13	0/2124	0.36	0/2877
4	Dw	0.13	0/2129	0.32	0/2882
4	Dx	0.13	0/2124	0.34	0/2877
4	Dy	0.13	0/2129	0.32	0/2882
4	Dz	0.14	0/2124	0.35	0/2877
5	Ea	0.12	0/1494	0.32	0/2027
5	Eb	0.13	0/1523	0.34	0/2062
5	Ec	0.12	0/1494	0.32	0/2027
5	Ed	0.13	0/1523	0.34	0/2062
5	Ee	0.12	0/1494	0.32	0/2027
5	Ef	0.13	0/1523	0.34	0/2062
5	Eg	0.12	0/1494	0.33	0/2027
5	Eh	0.13	0/1523	0.34	0/2062
5	Ei	0.12	0/1494	0.32	0/2027
5	Ej	0.13	0/1523	0.34	0/2062
5	Ek	0.12	0/1494	0.33	0/2027
5	El	0.13	0/1523	0.34	0/2062
5	Em	0.12	0/1494	0.33	0/2027
5	En	0.13	0/1523	0.34	0/2062
5	Eo	0.12	0/1494	0.32	0/2027
5	Ep	0.13	0/1523	0.34	0/2062

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	Eq	0.12	0/1494	0.32	0/2027
5	Er	0.13	0/1523	0.34	0/2062
5	Es	0.12	0/1494	0.32	0/2027
5	Et	0.13	0/1523	0.34	0/2062
5	Eu	0.12	0/1494	0.33	0/2027
5	Ev	0.13	0/1523	0.34	0/2062
5	Ew	0.12	0/1494	0.32	0/2027
5	Ex	0.12	0/1523	0.34	0/2062
5	Ey	0.12	0/1494	0.32	0/2027
5	Ez	0.13	0/1523	0.34	0/2062
6	Fa	0.15	0/126	0.37	0/166
6	Fb	0.15	0/126	0.35	0/166
6	Fc	0.17	0/126	0.41	0/166
6	Fd	0.13	0/126	0.39	0/166
6	Fe	0.15	0/126	0.37	0/166
6	Ff	0.15	0/126	0.41	0/166
6	Fg	0.13	0/126	0.39	0/166
6	Fh	0.15	0/126	0.41	0/166
6	Fi	0.16	0/126	0.41	0/166
6	Fj	0.15	0/126	0.39	0/166
6	Fk	0.16	0/126	0.39	0/166
6	Fl	0.15	0/126	0.40	0/166
6	Fm	0.16	0/126	0.41	0/166
6	Fn	0.13	0/126	0.38	0/166
6	Fo	0.15	0/126	0.37	0/166
6	Fp	0.15	0/126	0.38	0/166
6	Fq	0.13	0/126	0.37	0/166
6	Fr	0.12	0/126	0.35	0/166
6	Fs	0.13	0/126	0.35	0/166
6	Ft	0.14	0/126	0.38	0/166
6	Fu	0.13	0/126	0.39	0/166
6	Fv	0.16	0/126	0.39	0/166
6	Fw	0.13	0/126	0.37	0/166
6	Fx	0.14	0/126	0.38	0/166
6	Fy	0.14	0/126	0.40	0/166
6	Fz	0.15	0/126	0.40	0/166
6	Ga	0.15	0/113	0.44	0/149
6	Gb	0.15	0/113	0.44	0/149
6	Gc	0.16	0/113	0.45	0/149
6	Gd	0.14	0/113	0.40	0/149
6	Ge	0.14	0/113	0.42	0/149
6	Gf	0.15	0/113	0.45	0/149
6	Gg	0.16	0/113	0.45	0/149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Gh	0.15	0/113	0.43	0/149
6	Gi	0.14	0/113	0.44	0/149
6	Gj	0.13	0/113	0.42	0/149
6	Gk	0.16	0/113	0.45	0/149
6	Gl	0.14	0/113	0.42	0/149
6	Gm	0.15	0/113	0.43	0/149
6	Gn	0.16	0/113	0.44	0/149
6	Go	0.14	0/113	0.42	0/149
6	Gp	0.14	0/113	0.44	0/149
6	Gq	0.13	0/113	0.44	0/149
6	Gr	0.15	0/113	0.43	0/149
6	Gs	0.15	0/113	0.40	0/149
6	Gt	0.15	0/113	0.45	0/149
6	Gu	0.13	0/113	0.41	0/149
6	Gv	0.14	0/113	0.48	0/149
6	Gw	0.20	0/113	0.59	0/149
6	Gx	0.17	0/113	0.45	0/149
6	Gy	0.13	0/113	0.43	0/149
6	Gz	0.17	0/113	0.44	0/149
All	All	0.12	0/279084	0.31	0/377728

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	1674	0	1609	30	0
1	Ab	1674	0	1609	29	0
1	Ac	1674	0	1609	28	0
1	Ad	1674	0	1609	29	0
1	Ae	1674	0	1609	27	0
1	Af	1674	0	1609	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ag	1674	0	1609	26	0
1	Ah	1674	0	1609	28	0
1	Ai	1674	0	1609	26	0
1	Aj	1674	0	1609	27	0
1	Ak	1674	0	1609	28	0
1	Al	1674	0	1609	30	0
1	Am	1674	0	1609	28	0
1	An	1674	0	1609	29	0
1	Ao	1674	0	1609	29	0
1	Ap	1674	0	1609	30	0
1	Aq	1674	0	1609	33	0
1	Ar	1674	0	1609	29	0
1	As	1674	0	1609	30	0
1	At	1674	0	1609	29	0
1	Au	1674	0	1609	29	0
1	Av	1674	0	1609	28	0
1	Aw	1674	0	1609	27	0
1	Ax	1674	0	1609	28	0
1	Ay	1674	0	1609	28	0
1	Az	1674	0	1609	28	0
2	Ba	2314	0	2373	28	0
2	Bb	2314	0	2373	30	0
2	Bc	2314	0	2373	30	0
2	Bd	2314	0	2373	30	0
2	Be	2314	0	2373	32	0
2	Bf	2314	0	2373	29	0
2	Bg	2314	0	2373	28	0
2	Bh	2314	0	2373	32	0
2	Bi	2314	0	2373	30	0
2	Bj	2314	0	2373	31	0
2	Bk	2314	0	2373	28	0
2	Bl	2314	0	2373	31	0
2	Bm	2314	0	2373	32	0
2	Bn	2314	0	2373	30	0
2	Bo	2314	0	2373	29	0
2	Bp	2314	0	2373	30	0
2	Bq	2314	0	2373	30	0
2	Br	2314	0	2373	32	0
2	Bs	2314	0	2373	30	0
2	Bt	2314	0	2373	30	0
2	Bu	2314	0	2373	32	0
2	Bv	2314	0	2373	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bw	2314	0	2373	30	0
2	Bx	2314	0	2373	31	0
2	By	2314	0	2373	29	0
2	Bz	2314	0	2373	31	0
3	Ca	2770	0	2749	15	0
3	Cb	2770	0	2749	18	0
3	Cc	2770	0	2749	18	0
3	Cd	2770	0	2749	19	0
3	Ce	2770	0	2749	13	0
3	Cf	2770	0	2749	16	0
3	Cg	2770	0	2749	15	0
3	Ch	2770	0	2749	16	0
3	Ci	2770	0	2749	16	0
3	Cj	2770	0	2749	12	0
3	Ck	2770	0	2749	16	0
3	Cl	2770	0	2749	15	0
3	Cm	2770	0	2749	17	0
3	Cn	2770	0	2749	19	0
3	Co	2770	0	2749	13	0
3	Cp	2770	0	2749	16	0
3	Cq	2770	0	2749	16	0
3	Cr	2770	0	2749	17	0
3	Cs	2770	0	2749	16	0
3	Ct	2770	0	2749	21	0
3	Cu	2770	0	2749	16	0
3	Cv	2770	0	2749	16	0
3	Cw	2770	0	2749	20	0
3	Cx	2770	0	2749	18	0
3	Cy	2770	0	2749	17	0
3	Cz	2770	0	2749	11	0
4	Da	2085	0	2022	12	0
4	Db	2080	0	2003	12	0
4	Dc	2085	0	2022	13	0
4	Dd	2080	0	2003	14	0
4	De	2085	0	2022	13	0
4	Df	2080	0	2003	11	0
4	Dg	2085	0	2022	11	0
4	Dh	2080	0	2003	12	0
4	Di	2085	0	2022	13	0
4	Dj	2080	0	2003	12	0
4	Dk	2085	0	2022	11	0
4	Dl	2080	0	2003	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Dm	2085	0	2022	16	0
4	Dn	2080	0	2003	13	0
4	Do	2085	0	2022	14	0
4	Dp	2080	0	2003	15	0
4	Dq	2085	0	2022	13	0
4	Dr	2080	0	2003	15	0
4	Ds	2085	0	2022	13	0
4	Dt	2080	0	2003	12	0
4	Du	2085	0	2022	16	0
4	Dv	2080	0	2003	16	0
4	Dw	2085	0	2022	13	0
4	Dx	2080	0	2003	12	0
4	Dy	2085	0	2022	13	0
4	Dz	2080	0	2003	15	0
5	Ea	1466	0	1434	11	0
5	Eb	1494	0	1478	7	0
5	Ec	1466	0	1434	7	0
5	Ed	1494	0	1478	9	0
5	Ee	1466	0	1434	9	0
5	Ef	1494	0	1478	9	0
5	Eg	1466	0	1434	9	0
5	Eh	1494	0	1478	6	0
5	Ei	1466	0	1434	8	0
5	Ej	1494	0	1478	8	0
5	Ek	1466	0	1434	8	0
5	El	1494	0	1478	9	0
5	Em	1466	0	1434	10	0
5	En	1494	0	1478	8	0
5	Eo	1466	0	1434	9	0
5	Ep	1494	0	1478	8	0
5	Eq	1466	0	1434	10	0
5	Er	1494	0	1478	9	0
5	Es	1466	0	1434	9	0
5	Et	1494	0	1478	9	0
5	Eu	1466	0	1434	9	0
5	Ev	1494	0	1478	9	0
5	Ew	1466	0	1434	9	0
5	Ex	1494	0	1478	10	0
5	Ey	1466	0	1434	9	0
5	Ez	1494	0	1478	10	0
6	Fa	125	0	125	1	0
6	Fb	125	0	125	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Fc	125	0	125	0	0
6	Fd	125	0	125	1	0
6	Fe	125	0	125	0	0
6	Ff	125	0	125	1	0
6	Fg	125	0	125	0	0
6	Fh	125	0	125	1	0
6	Fi	125	0	125	0	0
6	Fj	125	0	125	1	0
6	Fk	125	0	125	0	0
6	Fl	125	0	125	1	0
6	Fm	125	0	125	1	0
6	Fn	125	0	125	0	0
6	Fo	125	0	125	1	0
6	Fp	125	0	125	0	0
6	Fq	125	0	125	1	0
6	Fr	125	0	125	0	0
6	Fs	125	0	125	0	0
6	Ft	125	0	125	1	0
6	Fu	125	0	125	1	0
6	Fv	125	0	125	1	0
6	Fw	125	0	125	1	0
6	Fx	125	0	125	0	0
6	Fy	125	0	125	0	0
6	Fz	125	0	125	0	0
6	Ga	112	0	116	0	0
6	Gb	112	0	116	2	0
6	Gc	112	0	116	2	0
6	Gd	112	0	116	0	0
6	Ge	112	0	116	0	0
6	Gf	112	0	116	2	0
6	Gg	112	0	116	0	0
6	Gh	112	0	116	0	0
6	Gi	112	0	116	0	0
6	Gj	112	0	116	0	0
6	Gk	112	0	116	1	0
6	Gl	112	0	116	1	0
6	Gm	112	0	116	1	0
6	Gn	112	0	116	0	0
6	Go	112	0	116	1	0
6	Gp	112	0	116	0	0
6	Gq	112	0	116	0	0
6	Gr	112	0	116	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Gs	112	0	116	1	0
6	Gt	112	0	116	0	0
6	Gu	112	0	116	0	0
6	Gv	112	0	116	0	0
6	Gw	112	0	116	3	0
6	Gx	112	0	116	1	0
6	Gy	112	0	116	0	0
6	Gz	112	0	116	1	0
All	All	274495	0	271453	2051	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 (2051) 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:Bj:25:ALA:HB2	2:Bj:186:LEU:HD23	1.79	0.65
2:Bi:25:ALA:HB2	2:Bi:186:LEU:HD23	1.79	0.65
2:Bg:25:ALA:HB2	2:Bg:186:LEU:HD23	1.79	0.64
2:Bk:25:ALA:HB2	2:Bk:186:LEU:HD23	1.79	0.64
2:Bh:25:ALA:HB2	2:Bh:186:LEU:HD23	1.79	0.64
2:Bl:25:ALA:HB2	2:Bl:186:LEU:HD23	1.79	0.64
2:Bf:25:ALA:HB2	2:Bf:186:LEU:HD23	1.79	0.64
2:By:25:ALA:HB2	2:By:186:LEU:HD23	1.79	0.64
2:Bw:25:ALA:HB2	2:Bw:186:LEU:HD23	1.79	0.64
2:Bt:25:ALA:HB2	2:Bt:186:LEU:HD23	1.79	0.63
2:Bz:25:ALA:HB2	2:Bz:186:LEU:HD23	1.79	0.63
2:Ba:25:ALA:HB2	2:Ba:186:LEU:HD23	1.79	0.63
2:Bd:25:ALA:HB2	2:Bd:186:LEU:HD23	1.79	0.63
2:Bm:25:ALA:HB2	2:Bm:186:LEU:HD23	1.79	0.63
2:Bu:25:ALA:HB2	2:Bu:186:LEU:HD23	1.79	0.63
2:Bb:25:ALA:HB2	2:Bb:186:LEU:HD23	1.79	0.63
2:Bc:25:ALA:HB2	2:Bc:186:LEU:HD23	1.79	0.63
2:Br:25:ALA:HB2	2:Br:186:LEU:HD23	1.79	0.63
2:Bs:25:ALA:HB2	2:Bs:186:LEU:HD23	1.79	0.63
2:Bn:25:ALA:HB2	2:Bn:186:LEU:HD23	1.79	0.63
2:Be:25:ALA:HB2	2:Be:186:LEU:HD23	1.79	0.63
2:Bo:25:ALA:HB2	2:Bo:186:LEU:HD23	1.79	0.63
2:Bx:25:ALA:HB2	2:Bx:186:LEU:HD23	1.80	0.63
2:Bq:25:ALA:HB2	2:Bq:186:LEU:HD23	1.79	0.62
2:Bv:25:ALA:HB2	2:Bv:186:LEU:HD23	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bp:25:ALA:HB2	2:Bp:186:LEU:HD23	1.79	0.62
4:Do:49:VAL:HG12	4:Do:59:GLU:HG2	1.83	0.61
5:Eb:65:ARG:HD3	5:Eb:69:ILE:HD13	1.83	0.61
4:Dm:49:VAL:HG12	4:Dm:59:GLU:HG2	1.83	0.61
5:Eh:65:ARG:HD3	5:Eh:69:ILE:HD13	1.83	0.61
5:En:65:ARG:HD3	5:En:69:ILE:HD13	1.83	0.61
5:Ej:65:ARG:HD3	5:Ej:69:ILE:HD13	1.83	0.60
5:El:65:ARG:HD3	5:El:69:ILE:HD13	1.83	0.60
4:Dk:49:VAL:HG12	4:Dk:59:GLU:HG2	1.84	0.60
4:Di:49:VAL:HG12	4:Di:59:GLU:HG2	1.84	0.60
5:Ed:65:ARG:HD3	5:Ed:69:ILE:HD13	1.83	0.60
5:Ef:65:ARG:HD3	5:Ef:69:ILE:HD13	1.83	0.60
5:Ez:65:ARG:HD3	5:Ez:69:ILE:HD13	1.84	0.60
5:Ex:65:ARG:HD3	5:Ex:69:ILE:HD13	1.84	0.60
4:Dg:49:VAL:HG12	4:Dg:59:GLU:HG2	1.84	0.60
5:Ep:65:ARG:HD3	5:Ep:69:ILE:HD13	1.84	0.60
5:Er:65:ARG:HD3	5:Er:69:ILE:HD13	1.84	0.60
4:Dn:219:VAL:HG21	4:Dn:254:LEU:HD21	1.84	0.60
4:Dq:49:VAL:HG12	4:Dq:59:GLU:HG2	1.84	0.60
4:Dl:219:VAL:HG21	4:Dl:254:LEU:HD21	1.84	0.60
5:Em:168:TYR:HB2	5:Em:196:MET:HE1	1.84	0.59
3:Ca:226:VAL:HB	3:Ca:236:MET:HB3	1.83	0.59
4:Ds:49:VAL:HG12	4:Ds:59:GLU:HG2	1.84	0.59
5:Et:65:ARG:HD3	5:Et:69:ILE:HD13	1.84	0.59
5:Ev:65:ARG:HD3	5:Ev:69:ILE:HD13	1.84	0.59
4:Dy:49:VAL:HG12	4:Dy:59:GLU:HG2	1.84	0.59
4:Dz:219:VAL:HG21	4:Dz:254:LEU:HD21	1.85	0.59
3:Cw:271:LEU:HD21	6:Gw:145:PHE:HB3	1.84	0.59
4:De:49:VAL:HG12	4:De:59:GLU:HG2	1.84	0.59
5:Eq:168:TYR:HB2	5:Eq:196:MET:HE1	1.84	0.59
5:Ea:168:TYR:HB2	5:Ea:196:MET:HE1	1.84	0.59
3:Ca:126:ILE:HB	3:Ca:169:THR:HG22	1.85	0.58
4:Da:49:VAL:HG12	4:Da:59:GLU:HG2	1.85	0.58
4:Dq:68:ILE:HD11	4:Dr:112:GLN:HE21	1.68	0.58
4:Dw:49:VAL:HG12	4:Dw:59:GLU:HG2	1.85	0.58
1:Ay:232:ARG:HH22	1:Az:194:GLU:HG3	1.68	0.58
4:Dc:49:VAL:HG12	4:Dc:59:GLU:HG2	1.85	0.58
4:Df:219:VAL:HG21	4:Df:254:LEU:HD21	1.85	0.58
4:Du:49:VAL:HG12	4:Du:59:GLU:HG2	1.85	0.58
4:Dv:219:VAL:HG21	4:Dv:254:LEU:HD21	1.85	0.58
5:Es:168:TYR:HB2	5:Es:196:MET:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aw:232:ARG:HH22	1:Ax:194:GLU:HG3	1.68	0.58
4:Dh:219:VAL:HG21	4:Dh:254:LEU:HD21	1.84	0.58
4:Dp:219:VAL:HG21	4:Dp:254:LEU:HD21	1.85	0.58
5:Eo:168:TYR:HB2	5:Eo:196:MET:HE1	1.86	0.58
1:As:232:ARG:HH22	1:At:194:GLU:HG3	1.68	0.58
3:Ci:126:ILE:HB	3:Ci:169:THR:HG22	1.86	0.58
1:Aa:232:ARG:HH22	1:Ab:194:GLU:HG3	1.68	0.58
1:Av:232:ARG:HH22	1:Aw:194:GLU:HG3	1.69	0.58
4:Dj:219:VAL:HG21	4:Dj:254:LEU:HD21	1.85	0.58
4:Dx:219:VAL:HG21	4:Dx:254:LEU:HD21	1.84	0.58
5:Ey:168:TYR:HB2	5:Ey:196:MET:HE1	1.86	0.58
1:Ap:232:ARG:HH22	1:Aq:194:GLU:HG3	1.68	0.58
4:De:68:ILE:HD11	4:Df:112:GLN:HE21	1.68	0.58
4:Dr:219:VAL:HG21	4:Dr:254:LEU:HD21	1.86	0.58
1:Ao:232:ARG:HH22	1:Ap:194:GLU:HG3	1.69	0.57
1:Aq:232:ARG:HH22	1:Ar:194:GLU:HG3	1.69	0.57
1:Ax:232:ARG:HH22	1:Ay:194:GLU:HG3	1.69	0.57
4:Dk:68:ILE:HD11	4:Dl:112:GLN:HE21	1.70	0.57
4:Dm:68:ILE:HD11	4:Dn:112:GLN:HE21	1.69	0.57
4:Du:68:ILE:HD11	4:Dv:112:GLN:HE21	1.70	0.57
5:Eu:168:TYR:HB2	5:Eu:196:MET:HE1	1.86	0.57
1:Au:232:ARG:HH22	1:Av:194:GLU:HG3	1.69	0.57
4:Dt:219:VAL:HG21	4:Dt:254:LEU:HD21	1.86	0.57
5:Ec:168:TYR:HB2	5:Ec:196:MET:HE1	1.86	0.57
1:Ai:66:TRP:HA	1:Ai:192:ARG:HD3	1.87	0.57
5:Ew:168:TYR:HB2	5:Ew:196:MET:HE1	1.86	0.57
1:Aa:194:GLU:HG3	1:Az:232:ARG:HH22	1.69	0.57
1:Ac:232:ARG:HH22	1:Ad:194:GLU:HG3	1.68	0.57
3:Cb:92:GLU:HB2	3:Cb:103:ARG:HB3	1.86	0.57
3:Cb:365:TYR:HB3	4:Du:91:MET:HE1	1.86	0.57
4:Dc:68:ILE:HD11	4:Dd:112:GLN:HE21	1.69	0.57
1:Ab:232:ARG:HH22	1:Ac:194:GLU:HG3	1.68	0.57
1:Ae:66:TRP:HA	1:Ae:192:ARG:HD3	1.87	0.57
1:Af:232:ARG:HH22	1:Ag:194:GLU:HG3	1.68	0.57
1:At:232:ARG:HH22	1:Au:194:GLU:HG3	1.69	0.57
3:Cr:361:PRO:HB2	4:Dk:148:ARG:HD2	1.86	0.57
1:Ar:232:ARG:HH22	1:As:194:GLU:HG3	1.69	0.57
4:Da:68:ILE:HD11	4:Db:112:GLN:HE21	1.70	0.57
5:Ee:168:TYR:HB2	5:Ee:196:MET:HE1	1.87	0.57
1:Ab:244:MET:HE3	1:Ay:125:LEU:HB3	1.87	0.57
3:Ck:209:LYS:HD2	3:Ck:212:GLN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Do:68:ILE:HD11	4:Dp:112:GLN:HE21	1.70	0.57
1:As:125:LEU:HB3	1:Av:244:MET:HE3	1.87	0.57
1:Aa:125:LEU:HB3	1:Ad:244:MET:HE3	1.87	0.57
1:An:232:ARG:HH22	1:Ao:194:GLU:HG3	1.69	0.57
4:Db:219:VAL:HG21	4:Db:254:LEU:HD21	1.86	0.57
1:Aa:66:TRP:HA	1:Aa:192:ARG:HD3	1.87	0.56
1:Am:232:ARG:HH22	1:An:194:GLU:HG3	1.69	0.56
4:Dd:219:VAL:HG21	4:Dd:254:LEU:HD21	1.85	0.56
4:Ds:68:ILE:HD11	4:Dt:112:GLN:HE21	1.70	0.56
5:Ei:168:TYR:HB2	5:Ei:196:MET:HE1	1.87	0.56
1:Am:66:TRP:HA	1:Am:192:ARG:HD3	1.87	0.56
1:Ag:232:ARG:HH22	1:Ah:194:GLU:HG3	1.69	0.56
1:Ao:66:TRP:HA	1:Ao:192:ARG:HD3	1.87	0.56
1:Aw:125:LEU:HB3	1:Az:244:MET:HE3	1.88	0.56
5:Et:148:ILE:HD12	5:Et:184:ARG:HE	1.71	0.56
1:Ac:125:LEU:HB3	1:Af:244:MET:HE3	1.87	0.56
1:Ad:232:ARG:HH22	1:Ae:194:GLU:HG3	1.69	0.56
1:Ae:232:ARG:HH22	1:Af:194:GLU:HG3	1.70	0.56
4:Dw:68:ILE:HD11	4:Dx:112:GLN:HE21	1.70	0.56
3:Ck:126:ILE:HB	3:Ck:169:THR:HG22	1.88	0.56
4:Dg:68:ILE:HD11	4:Dh:112:GLN:HE21	1.70	0.56
5:Eg:168:TYR:HB2	5:Eg:196:MET:HE1	1.87	0.56
1:Ab:125:LEU:HB3	1:Ae:244:MET:HE3	1.88	0.56
1:Aj:232:ARG:HH22	1:Ak:194:GLU:HG3	1.68	0.56
1:Au:125:LEU:HB3	1:Ax:244:MET:HE3	1.87	0.56
3:Ch:126:ILE:HB	3:Ch:169:THR:HG22	1.87	0.56
5:Ek:168:TYR:HB2	5:Ek:196:MET:HE1	1.87	0.56
1:Au:66:TRP:HA	1:Au:192:ARG:HD3	1.87	0.56
1:Aa:244:MET:HE3	1:Ax:125:LEU:HB3	1.88	0.56
1:Ar:125:LEU:HB3	1:Au:244:MET:HE3	1.88	0.56
1:Ae:125:LEU:HB3	1:Ah:244:MET:HE3	1.87	0.56
1:Af:66:TRP:HA	1:Af:192:ARG:HD3	1.88	0.56
1:Ag:66:TRP:HA	1:Ag:192:ARG:HD3	1.88	0.56
1:Ac:244:MET:HE3	1:Az:125:LEU:HB3	1.88	0.56
1:Al:66:TRP:HA	1:Al:192:ARG:HD3	1.88	0.56
2:Bk:248:ALA:HB1	2:Bk:265:VAL:HG22	1.88	0.56
2:Bt:153:VAL:HG21	2:Bu:148:ASP:HB3	1.88	0.56
5:Ej:148:ILE:HD12	5:Ej:184:ARG:HE	1.71	0.56
1:Ah:232:ARG:HH22	1:Ai:194:GLU:HG3	1.70	0.55
1:Ai:232:ARG:HH22	1:Aj:194:GLU:HG3	1.69	0.55
1:At:125:LEU:HB3	1:Aw:244:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:122:LEU:HB2	2:Bd:131:ALA:HB3	1.88	0.55
2:Bj:248:ALA:HB1	2:Bj:265:VAL:HG22	1.88	0.55
2:Bl:122:LEU:HB2	2:Bl:131:ALA:HB3	1.88	0.55
5:Ep:148:ILE:HD12	5:Ep:184:ARG:HE	1.70	0.55
1:Ah:66:TRP:HA	1:Ah:192:ARG:HD3	1.88	0.55
1:Ak:66:TRP:HA	1:Ak:192:ARG:HD3	1.89	0.55
2:Bh:122:LEU:HB2	2:Bh:131:ALA:HB3	1.89	0.55
2:Bj:122:LEU:HB2	2:Bj:131:ALA:HB3	1.88	0.55
2:Bo:122:LEU:HB2	2:Bo:131:ALA:HB3	1.88	0.55
3:Cf:105:ARG:HG3	6:Gf:134:GLN:HE22	1.72	0.55
5:En:148:ILE:HD12	5:En:184:ARG:HE	1.71	0.55
1:Ak:232:ARG:HH22	1:Al:194:GLU:HG3	1.69	0.55
1:Ay:66:TRP:HA	1:Ay:192:ARG:HD3	1.87	0.55
2:Bv:122:LEU:HB2	2:Bv:131:ALA:HB3	1.89	0.55
1:Al:232:ARG:HH22	1:Am:194:GLU:HG3	1.69	0.55
1:Ao:125:LEU:HB3	1:Ar:244:MET:HE3	1.88	0.55
1:Aq:125:LEU:HB3	1:At:244:MET:HE3	1.88	0.55
2:Bf:122:LEU:HB2	2:Bf:131:ALA:HB3	1.89	0.55
2:Bg:122:LEU:HB2	2:Bg:131:ALA:HB3	1.89	0.55
2:Bn:122:LEU:HB2	2:Bn:131:ALA:HB3	1.88	0.55
2:Bo:248:ALA:HB1	2:Bo:265:VAL:HG22	1.88	0.55
2:Bt:122:LEU:HB2	2:Bt:131:ALA:HB3	1.89	0.55
2:Bu:122:LEU:HB2	2:Bu:131:ALA:HB3	1.89	0.55
1:Ac:66:TRP:HA	1:Ac:192:ARG:HD3	1.88	0.55
1:Aj:66:TRP:HA	1:Aj:192:ARG:HD3	1.89	0.55
1:Av:125:LEU:HB3	1:Ay:244:MET:HE3	1.89	0.55
2:Bi:248:ALA:HB1	2:Bi:265:VAL:HG22	1.89	0.55
2:Br:122:LEU:HB2	2:Br:131:ALA:HB3	1.89	0.55
2:Bx:122:LEU:HB2	2:Bx:131:ALA:HB3	1.89	0.55
2:Bz:122:LEU:HB2	2:Bz:131:ALA:HB3	1.89	0.55
1:An:66:TRP:HA	1:An:192:ARG:HD3	1.88	0.55
2:Bt:248:ALA:HB1	2:Bt:265:VAL:HG22	1.88	0.55
3:Cp:92:GLU:HB2	3:Cp:103:ARG:HB3	1.87	0.55
1:Ak:125:LEU:HB3	1:An:244:MET:HE3	1.88	0.55
1:Ap:125:LEU:HB3	1:As:244:MET:HE3	1.88	0.55
1:As:66:TRP:HA	1:As:192:ARG:HD3	1.87	0.55
2:Bj:153:VAL:HG21	2:Bk:148:ASP:HB3	1.89	0.55
2:Bl:248:ALA:HB1	2:Bl:265:VAL:HG22	1.88	0.55
2:Bn:248:ALA:HB1	2:Bn:265:VAL:HG22	1.89	0.55
3:Cy:126:ILE:HB	3:Cy:169:THR:HG22	1.88	0.55
1:Ag:125:LEU:HB3	1:Aj:244:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:125:LEU:HB3	1:Ap:244:MET:HE3	1.88	0.55
1:An:125:LEU:HB3	1:Aq:244:MET:HE3	1.88	0.55
2:Be:122:LEU:HB2	2:Be:131:ALA:HB3	1.89	0.55
2:Bk:122:LEU:HB2	2:Bk:131:ALA:HB3	1.89	0.55
2:Bp:248:ALA:HB1	2:Bp:265:VAL:HG22	1.88	0.55
2:By:122:LEU:HB2	2:By:131:ALA:HB3	1.89	0.55
2:Bz:248:ALA:HB1	2:Bz:265:VAL:HG22	1.88	0.55
1:Af:125:LEU:HB3	1:Ai:244:MET:HE3	1.88	0.55
1:Aj:125:LEU:HB3	1:Am:244:MET:HE3	1.88	0.55
2:Bf:248:ALA:HB1	2:Bf:265:VAL:HG22	1.88	0.55
2:Bm:122:LEU:HB2	2:Bm:131:ALA:HB3	1.89	0.55
2:Bw:122:LEU:HB2	2:Bw:131:ALA:HB3	1.89	0.55
3:Cc:92:GLU:HB2	3:Cc:103:ARG:HB3	1.89	0.55
5:Ef:148:ILE:HD12	5:Ef:184:ARG:HE	1.71	0.55
2:Bc:122:LEU:HB2	2:Bc:131:ALA:HB3	1.89	0.55
2:Bh:153:VAL:HG21	2:Bi:148:ASP:HB3	1.89	0.55
2:Bo:153:VAL:HG21	2:Bp:148:ASP:HB3	1.89	0.55
2:Bp:122:LEU:HB2	2:Bp:131:ALA:HB3	1.89	0.55
2:Bx:248:ALA:HB1	2:Bx:265:VAL:HG22	1.88	0.55
5:El:148:ILE:HD12	5:El:184:ARG:HE	1.72	0.55
2:Ba:248:ALA:HB1	2:Ba:265:VAL:HG22	1.88	0.54
3:Cx:361:PRO:HB2	4:Dq:148:ARG:HD2	1.89	0.54
5:Er:148:ILE:HD12	5:Er:184:ARG:HE	1.72	0.54
1:Ad:125:LEU:HB3	1:Ag:244:MET:HE3	1.88	0.54
1:Ai:125:LEU:HB3	1:Al:244:MET:HE3	1.88	0.54
2:Bv:250:ILE:HG12	2:Bv:261:VAL:HG13	1.90	0.54
4:Di:68:ILE:HD11	4:Dj:112:GLN:HE21	1.72	0.54
4:Dy:68:ILE:HD11	4:Dz:112:GLN:HE21	1.71	0.54
2:Bb:248:ALA:HB1	2:Bb:265:VAL:HG22	1.88	0.54
2:Bc:153:VAL:HG21	2:Bd:148:ASP:HB3	1.89	0.54
2:Bi:122:LEU:HB2	2:Bi:131:ALA:HB3	1.90	0.54
2:Bm:248:ALA:HB1	2:Bm:265:VAL:HG22	1.88	0.54
2:Bq:248:ALA:HB1	2:Bq:265:VAL:HG22	1.88	0.54
2:Bv:248:ALA:HB1	2:Bv:265:VAL:HG22	1.89	0.54
2:Bw:248:ALA:HB1	2:Bw:265:VAL:HG22	1.89	0.54
2:By:248:ALA:HB1	2:By:265:VAL:HG22	1.89	0.54
3:Cm:126:ILE:HB	3:Cm:169:THR:HG22	1.89	0.54
5:Ez:148:ILE:HD12	5:Ez:184:ARG:HE	1.72	0.54
1:Ap:66:TRP:HA	1:Ap:192:ARG:HD3	1.89	0.54
2:Bb:122:LEU:HB2	2:Bb:131:ALA:HB3	1.89	0.54
2:Be:248:ALA:HB1	2:Be:265:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bq:122:LEU:HB2	2:Bq:131:ALA:HB3	1.89	0.54
1:Aq:66:TRP:HA	1:Aq:192:ARG:HD3	1.89	0.54
2:Bs:122:LEU:HB2	2:Bs:131:ALA:HB3	1.90	0.54
2:Bz:250:ILE:HG12	2:Bz:261:VAL:HG13	1.90	0.54
1:Aw:66:TRP:HA	1:Aw:192:ARG:HD3	1.89	0.54
2:Ba:122:LEU:HB2	2:Ba:131:ALA:HB3	1.89	0.54
2:Bd:248:ALA:HB1	2:Bd:265:VAL:HG22	1.88	0.54
2:Bu:248:ALA:HB1	2:Bu:265:VAL:HG22	1.88	0.54
1:Ah:125:LEU:HB3	1:Ak:244:MET:HE3	1.88	0.54
2:Bh:248:ALA:HB1	2:Bh:265:VAL:HG22	1.89	0.54
2:Bm:153:VAL:HG21	2:Bn:148:ASP:HB3	1.90	0.54
2:Bv:153:VAL:HG21	2:Bw:148:ASP:HB3	1.90	0.54
3:Cl:80:PHE:HA	6:Fl:136:VAL:HG21	1.89	0.54
5:Eb:148:ILE:HD12	5:Eb:184:ARG:HE	1.72	0.54
1:Ad:184:LEU:HD12	1:Ad:188:ASN:HB2	1.90	0.54
2:Bc:248:ALA:HB1	2:Bc:265:VAL:HG22	1.88	0.54
2:Be:153:VAL:HG21	2:Bf:148:ASP:HB3	1.89	0.54
2:Be:250:ILE:HG12	2:Be:261:VAL:HG13	1.90	0.54
2:Br:153:VAL:HG21	2:Bs:148:ASP:HB3	1.90	0.54
5:Ee:65:ARG:HG2	5:Ee:69:ILE:HD13	1.90	0.54
5:Em:65:ARG:HG2	5:Em:69:ILE:HD13	1.90	0.54
1:Ad:66:TRP:HA	1:Ad:192:ARG:HD3	1.89	0.54
1:At:184:LEU:HD12	1:At:188:ASN:HB2	1.90	0.54
2:Ba:148:ASP:HB3	2:Bz:153:VAL:HG21	1.90	0.54
2:Bc:250:ILE:HG12	2:Bc:261:VAL:HG13	1.90	0.54
2:Bf:360:ILE:HG22	2:Bh:136:ASN:HB2	1.90	0.54
2:Bg:248:ALA:HB1	2:Bg:265:VAL:HG22	1.88	0.54
2:Bj:250:ILE:HG12	2:Bj:261:VAL:HG13	1.90	0.54
2:Bs:248:ALA:HB1	2:Bs:265:VAL:HG22	1.89	0.54
2:By:21:ILE:HG23	2:By:197:LEU:HD11	1.90	0.54
1:Al:125:LEU:HB3	1:Ao:244:MET:HE3	1.88	0.54
2:Bp:153:VAL:HG21	2:Bq:148:ASP:HB3	1.88	0.54
5:Ev:148:ILE:HD12	5:Ev:184:ARG:HE	1.72	0.54
5:Ex:148:ILE:HD12	5:Ex:184:ARG:HE	1.73	0.54
2:Bb:250:ILE:HG12	2:Bb:261:VAL:HG13	1.90	0.53
2:Bl:153:VAL:HG21	2:Bm:148:ASP:HB3	1.89	0.53
2:Bs:153:VAL:HG21	2:Bt:148:ASP:HB3	1.90	0.53
5:Ei:65:ARG:HG2	5:Ei:69:ILE:HD13	1.91	0.53
1:Av:184:LEU:HD12	1:Av:188:ASN:HB2	1.90	0.53
2:Bb:153:VAL:HG21	2:Bc:148:ASP:HB3	1.90	0.53
2:Bh:250:ILE:HG12	2:Bh:261:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bh:360:ILE:HG22	2:Bj:136:ASN:HB2	1.91	0.53
3:Cb:126:ILE:HB	3:Cb:169:THR:HG22	1.91	0.53
5:Eh:148:ILE:HD12	5:Eh:184:ARG:HE	1.73	0.53
1:Az:184:LEU:HD12	1:Az:188:ASN:HB2	1.89	0.53
5:Eg:65:ARG:HG2	5:Eg:69:ILE:HD13	1.91	0.53
2:Ba:250:ILE:HG12	2:Ba:261:VAL:HG13	1.90	0.53
2:Bd:360:ILE:HG22	2:Bf:136:ASN:HB2	1.91	0.53
2:Bg:21:ILE:HG23	2:Bg:197:LEU:HD11	1.91	0.53
2:Bg:250:ILE:HG12	2:Bg:261:VAL:HG13	1.90	0.53
2:Bl:250:ILE:HG12	2:Bl:261:VAL:HG13	1.90	0.53
2:Bl:360:ILE:HG22	2:Bn:136:ASN:HB2	1.91	0.53
3:Cb:291:LEU:HD22	3:Cb:372:VAL:HA	1.89	0.53
3:Ci:209:LYS:HD3	3:Ci:212:GLN:HE21	1.72	0.53
5:Ec:65:ARG:HG2	5:Ec:69:ILE:HD13	1.90	0.53
5:Eq:65:ARG:HG2	5:Eq:69:ILE:HD13	1.90	0.53
2:Be:21:ILE:HG23	2:Be:197:LEU:HD11	1.91	0.53
2:Bp:250:ILE:HG12	2:Bp:261:VAL:HG13	1.89	0.53
2:Br:248:ALA:HB1	2:Br:265:VAL:HG22	1.88	0.53
3:Cr:126:ILE:HB	3:Cr:169:THR:HG22	1.90	0.53
3:Ct:255:ASP:HB3	3:Ct:258:SER:HB3	1.91	0.53
1:Ab:184:LEU:HD12	1:Ab:188:ASN:HB2	1.90	0.53
1:Ax:184:LEU:HD12	1:Ax:188:ASN:HB2	1.90	0.53
2:Ba:153:VAL:HG21	2:Bb:148:ASP:HB3	1.90	0.53
2:Bj:360:ILE:HG22	2:Bl:136:ASN:HB2	1.91	0.53
2:Bt:250:ILE:HG12	2:Bt:261:VAL:HG13	1.90	0.53
3:Cb:363:LEU:HD13	4:Du:101:ALA:HB3	1.90	0.53
4:Dt:111:LYS:H	4:Dt:115:GLY:HA2	1.74	0.53
5:Ew:65:ARG:HG2	5:Ew:69:ILE:HD13	1.90	0.53
1:Az:66:TRP:HA	1:Az:192:ARG:HD3	1.89	0.53
2:Ba:21:ILE:HG23	2:Ba:197:LEU:HD11	1.91	0.53
2:Bf:250:ILE:HG12	2:Bf:261:VAL:HG13	1.90	0.53
5:Ed:154:LEU:HB3	5:Ed:164:TYR:HE1	1.73	0.53
1:At:66:TRP:HA	1:At:192:ARG:HD3	1.90	0.53
1:Au:184:LEU:HD12	1:Au:188:ASN:HB2	1.91	0.53
1:Av:66:TRP:HA	1:Av:192:ARG:HD3	1.89	0.53
1:Aw:184:LEU:HD12	1:Aw:188:ASN:HB2	1.91	0.53
2:Bd:21:ILE:HG23	2:Bd:197:LEU:HD11	1.91	0.53
2:Bh:87:ALA:HB2	2:Bh:101:ILE:HG22	1.91	0.53
3:Cw:239:THR:HG21	3:Cx:155:ARG:HD3	1.90	0.53
4:Dn:111:LYS:H	4:Dn:115:GLY:HA2	1.73	0.53
5:Ek:65:ARG:HG2	5:Ek:69:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:184:LEU:HD12	1:Ac:188:ASN:HB2	1.91	0.53
2:Bb:21:ILE:HG23	2:Bb:197:LEU:HD11	1.91	0.53
2:Bb:360:ILE:HG22	2:Bd:136:ASN:HB2	1.91	0.53
2:Bk:250:ILE:HG12	2:Bk:261:VAL:HG13	1.90	0.53
2:Bn:360:ILE:HG22	2:Bp:136:ASN:HB2	1.91	0.53
2:Bx:153:VAL:HG21	2:By:148:ASP:HB3	1.91	0.53
2:Bx:250:ILE:HG12	2:Bx:261:VAL:HG13	1.91	0.53
3:Ci:92:GLU:HB2	3:Ci:103:ARG:HB3	1.91	0.53
3:Cl:361:PRO:HB2	4:De:148:ARG:HD2	1.91	0.53
3:Cr:223:GLU:HG2	3:Cr:239:THR:HG22	1.91	0.53
3:Ct:223:GLU:HG2	3:Ct:239:THR:HG22	1.91	0.53
4:Dv:111:LYS:H	4:Dv:115:GLY:HA2	1.74	0.53
5:Eo:71:LEU:HB3	5:Eo:74:TYR:HB2	1.91	0.53
5:Es:65:ARG:HG2	5:Es:69:ILE:HD13	1.90	0.53
6:Gw:139:LYS:HB3	6:Gw:141:GLN:HE22	1.74	0.53
1:Ae:184:LEU:HD12	1:Ae:188:ASN:HB2	1.90	0.53
2:Bd:250:ILE:HG12	2:Bd:261:VAL:HG13	1.90	0.53
2:Bj:21:ILE:HG23	2:Bj:197:LEU:HD11	1.91	0.53
2:Bn:153:VAL:HG21	2:Bo:148:ASP:HB3	1.90	0.53
2:Bs:21:ILE:HG23	2:Bs:197:LEU:HD11	1.90	0.53
5:Ey:65:ARG:HG2	5:Ey:69:ILE:HD13	1.91	0.53
1:Ab:66:TRP:HA	1:Ab:192:ARG:HD3	1.90	0.52
1:Ah:184:LEU:HD12	1:Ah:188:ASN:HB2	1.90	0.52
1:Aj:184:LEU:HD12	1:Aj:188:ASN:HB2	1.90	0.52
1:Ak:184:LEU:HD12	1:Ak:188:ASN:HB2	1.90	0.52
2:Bd:153:VAL:HG21	2:Be:148:ASP:HB3	1.90	0.52
2:Bf:153:VAL:HG21	2:Bg:148:ASP:HB3	1.90	0.52
2:Bi:250:ILE:HG12	2:Bi:261:VAL:HG13	1.91	0.52
2:Bn:21:ILE:HG23	2:Bn:197:LEU:HD11	1.91	0.52
5:Ed:148:ILE:HD12	5:Ed:184:ARG:HE	1.74	0.52
1:Ai:184:LEU:HD12	1:Ai:188:ASN:HB2	1.90	0.52
1:Ap:184:LEU:HD12	1:Ap:188:ASN:HB2	1.90	0.52
2:Bj:87:ALA:HB2	2:Bj:101:ILE:HG22	1.92	0.52
2:Bn:250:ILE:HG12	2:Bn:261:VAL:HG13	1.90	0.52
2:Bp:360:ILE:HG22	2:Br:136:ASN:HB2	1.90	0.52
2:Br:250:ILE:HG12	2:Br:261:VAL:HG13	1.91	0.52
2:Bs:250:ILE:HG12	2:Bs:261:VAL:HG13	1.90	0.52
2:Bb:136:ASN:HB2	2:Bz:360:ILE:HG22	1.91	0.52
2:Bc:21:ILE:HG23	2:Bc:197:LEU:HD11	1.91	0.52
2:Bi:21:ILE:HG23	2:Bi:197:LEU:HD11	1.92	0.52
2:Bq:250:ILE:HG12	2:Bq:261:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bu:153:VAL:HG21	2:Bv:148:ASP:HB3	1.91	0.52
2:By:250:ILE:HG12	2:By:261:VAL:HG13	1.91	0.52
1:Aa:184:LEU:HD12	1:Aa:188:ASN:HB2	1.91	0.52
3:Cf:361:PRO:HB2	4:Dy:148:ARG:HD2	1.92	0.52
4:Dy:111:LYS:HD2	5:Ew:197:PRO:HD3	1.92	0.52
1:Af:184:LEU:HD12	1:Af:188:ASN:HB2	1.90	0.52
1:Al:184:LEU:HD12	1:Al:188:ASN:HB2	1.90	0.52
1:Ax:66:TRP:HA	1:Ax:192:ARG:HD3	1.90	0.52
2:Bl:87:ALA:HB2	2:Bl:101:ILE:HG22	1.92	0.52
2:Bq:153:VAL:HG21	2:Br:148:ASP:HB3	1.92	0.52
2:Bw:360:ILE:HG22	2:By:136:ASN:HB2	1.90	0.52
3:Cd:361:PRO:HB2	4:Dw:148:ARG:HD2	1.92	0.52
4:Du:111:LYS:HD2	5:Es:197:PRO:HD3	1.91	0.52
5:Ew:144:LEU:HA	5:Ew:147:ARG:HD2	1.92	0.52
2:Bg:360:ILE:HG22	2:Bi:136:ASN:HB2	1.90	0.52
2:Bm:21:ILE:HG23	2:Bm:197:LEU:HD11	1.92	0.52
2:Bm:360:ILE:HG22	2:Bo:136:ASN:HB2	1.90	0.52
2:Bs:360:ILE:HG22	2:Bu:136:ASN:HB2	1.91	0.52
2:Bu:250:ILE:HG12	2:Bu:261:VAL:HG13	1.91	0.52
2:Bw:153:VAL:HG21	2:Bx:148:ASP:HB3	1.91	0.52
2:Bx:360:ILE:HG22	2:Bz:136:ASN:HB2	1.91	0.52
2:By:153:VAL:HG21	2:Bz:148:ASP:HB3	1.92	0.52
5:Eu:65:ARG:HG2	5:Eu:69:ILE:HD13	1.90	0.52
1:An:184:LEU:HD12	1:An:188:ASN:HB2	1.90	0.52
2:Ba:360:ILE:HG22	2:Bc:136:ASN:HB2	1.90	0.52
2:Bk:21:ILE:HG23	2:Bk:197:LEU:HD11	1.92	0.52
2:Bo:87:ALA:HB2	2:Bo:101:ILE:HG22	1.92	0.52
2:Bo:360:ILE:HG22	2:Bq:136:ASN:HB2	1.91	0.52
2:Bp:21:ILE:HG23	2:Bp:197:LEU:HD11	1.92	0.52
2:Br:360:ILE:HG22	2:Bt:136:ASN:HB2	1.90	0.52
2:Bw:250:ILE:HG12	2:Bw:261:VAL:HG13	1.91	0.52
2:Bx:21:ILE:HG23	2:Bx:197:LEU:HD11	1.92	0.52
2:Bx:87:ALA:HB2	2:Bx:101:ILE:HG22	1.91	0.52
2:Bz:21:ILE:HG23	2:Bz:197:LEU:HD11	1.92	0.52
3:Cm:80:PHE:HA	6:Fm:136:VAL:HG21	1.92	0.52
4:Dp:111:LYS:H	4:Dp:115:GLY:HA2	1.74	0.52
5:Ea:65:ARG:HG2	5:Ea:69:ILE:HD13	1.91	0.52
1:Ay:184:LEU:HD12	1:Ay:188:ASN:HB2	1.90	0.52
2:Ba:136:ASN:HB2	2:By:360:ILE:HG22	1.91	0.52
2:Bd:87:ALA:HB2	2:Bd:101:ILE:HG22	1.92	0.52
2:Be:360:ILE:HG22	2:Bg:136:ASN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bf:87:ALA:HB2	2:Bf:101:ILE:HG22	1.92	0.52
2:Bh:21:ILE:HG23	2:Bh:197:LEU:HD11	1.92	0.52
2:Bk:360:ILE:HG22	2:Bm:136:ASN:HB2	1.91	0.52
2:Bq:360:ILE:HG22	2:Bs:136:ASN:HB2	1.90	0.52
2:Bv:21:ILE:HG23	2:Bv:197:LEU:HD11	1.92	0.52
3:Ck:201:ASP:HB3	3:Ck:221:ALA:HB3	1.91	0.52
1:Ar:66:TRP:HA	1:Ar:192:ARG:HD3	1.91	0.52
2:Bg:87:ALA:HB2	2:Bg:101:ILE:HG22	1.92	0.52
2:Bk:87:ALA:HB2	2:Bk:101:ILE:HG22	1.92	0.52
2:Bm:250:ILE:HG12	2:Bm:261:VAL:HG13	1.91	0.52
2:Bn:87:ALA:HB2	2:Bn:101:ILE:HG22	1.92	0.52
2:Bu:360:ILE:HG22	2:Bw:136:ASN:HB2	1.91	0.52
3:Cy:223:GLU:HG2	3:Cy:239:THR:HG22	1.91	0.52
4:Da:111:LYS:HD2	5:Ey:197:PRO:HD3	1.92	0.52
4:Dr:111:LYS:H	4:Dr:115:GLY:HA2	1.75	0.52
4:Dw:111:LYS:HD2	5:Eu:197:PRO:HD3	1.92	0.52
1:Ag:184:LEU:HD12	1:Ag:188:ASN:HB2	1.91	0.51
1:Aq:184:LEU:HD12	1:Aq:188:ASN:HB2	1.91	0.51
1:Ar:184:LEU:HD12	1:Ar:188:ASN:HB2	1.90	0.51
2:Bc:87:ALA:HB2	2:Bc:101:ILE:HG22	1.92	0.51
2:Bc:360:ILE:HG22	2:Be:136:ASN:HB2	1.90	0.51
2:Bf:21:ILE:HG23	2:Bf:197:LEU:HD11	1.92	0.51
2:Bi:360:ILE:HG22	2:Bk:136:ASN:HB2	1.91	0.51
2:Bt:360:ILE:HG22	2:Bv:136:ASN:HB2	1.91	0.51
3:Cs:85:VAL:HG22	3:Cs:108:ILE:HG12	1.92	0.51
3:Cv:201:ASP:HB3	3:Cv:221:ALA:HB3	1.92	0.51
3:Cz:361:PRO:HB2	4:Ds:148:ARG:HD2	1.92	0.51
4:Dx:111:LYS:H	4:Dx:115:GLY:HA2	1.74	0.51
5:Ev:154:LEU:HB3	5:Ev:164:TYR:HE1	1.75	0.51
1:Al:64:PRO:HB2	1:Am:38:VAL:HG13	1.92	0.51
1:Ao:184:LEU:HD12	1:Ao:188:ASN:HB2	1.91	0.51
1:As:184:LEU:HD12	1:As:188:ASN:HB2	1.91	0.51
2:Bb:87:ALA:HB2	2:Bb:101:ILE:HG22	1.92	0.51
2:Bk:153:VAL:HG21	2:Bl:148:ASP:HB3	1.92	0.51
2:Bo:250:ILE:HG12	2:Bo:261:VAL:HG13	1.91	0.51
2:Br:21:ILE:HG23	2:Br:197:LEU:HD11	1.92	0.51
2:Br:87:ALA:HB2	2:Br:101:ILE:HG22	1.92	0.51
3:Ca:241:ARG:HB3	6:Gb:143:THR:HG21	1.92	0.51
3:Cm:201:ASP:HB3	3:Cm:221:ALA:HB3	1.92	0.51
2:Bu:21:ILE:HG23	2:Bu:197:LEU:HD11	1.92	0.51
2:Bz:87:ALA:HB2	2:Bz:101:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ch:361:PRO:HB2	4:Da:148:ARG:HD2	1.93	0.51
3:Cq:255:ASP:HB3	3:Cq:258:SER:HB3	1.92	0.51
4:Df:111:LYS:H	4:Df:115:GLY:HA2	1.75	0.51
1:Am:184:LEU:HD12	1:Am:188:ASN:HB2	1.91	0.51
2:Be:87:ALA:HB2	2:Be:101:ILE:HG22	1.93	0.51
2:Bi:87:ALA:HB2	2:Bi:101:ILE:HG22	1.93	0.51
2:Bq:87:ALA:HB2	2:Bq:101:ILE:HG22	1.93	0.51
2:Bw:21:ILE:HG23	2:Bw:197:LEU:HD11	1.92	0.51
3:Cw:80:PHE:HA	6:Fw:136:VAL:HG21	1.93	0.51
4:Dk:111:LYS:HD2	5:Ei:197:PRO:HD3	1.92	0.51
1:Ap:34:THR:HG21	3:Cf:247:PRO:HB2	1.93	0.51
2:Bl:21:ILE:HG23	2:Bl:197:LEU:HD11	1.93	0.51
2:Bm:87:ALA:HB2	2:Bm:101:ILE:HG22	1.93	0.51
3:Cj:201:ASP:HB3	3:Cj:221:ALA:HB3	1.93	0.51
3:Ck:92:GLU:HB2	3:Ck:103:ARG:HB3	1.92	0.51
3:Cl:92:GLU:HB2	3:Cl:103:ARG:HB3	1.91	0.51
3:Co:27:GLU:HG3	6:Go:134:GLN:HE22	1.74	0.51
2:Ba:87:ALA:HB2	2:Ba:101:ILE:HG22	1.92	0.51
2:Bq:21:ILE:HG23	2:Bq:197:LEU:HD11	1.93	0.51
2:Bt:21:ILE:HG23	2:Bt:197:LEU:HD11	1.92	0.51
3:Cx:92:GLU:HB2	3:Cx:103:ARG:HB2	1.92	0.51
4:Dd:111:LYS:H	4:Dd:115:GLY:HA2	1.76	0.51
2:Bg:153:VAL:HG21	2:Bh:148:ASP:HB3	1.92	0.51
3:Cc:209:LYS:HD2	3:Cc:212:GLN:HB2	1.92	0.51
3:Cj:361:PRO:HB2	4:Dc:148:ARG:HD2	1.93	0.51
3:Cp:342:ILE:HG21	3:Cp:367:ILE:HD11	1.93	0.51
4:Dq:111:LYS:HD2	5:Eo:197:PRO:HD3	1.92	0.51
1:Ac:112:ASN:HD21	1:Ac:224:ALA:HB1	1.75	0.51
2:Bi:268:LYS:HB2	2:Bi:353:ALA:HB1	1.93	0.51
2:Bo:21:ILE:HG23	2:Bo:197:LEU:HD11	1.93	0.51
2:Bp:87:ALA:HB2	2:Bp:101:ILE:HG22	1.93	0.51
3:Cb:255:ASP:HB3	3:Cb:258:SER:HB3	1.92	0.51
4:Df:223:THR:HG22	4:Df:285:VAL:HG22	1.93	0.51
4:Dm:111:LYS:HD2	5:Ek:197:PRO:HD3	1.92	0.51
2:Bk:268:LYS:HB2	2:Bk:353:ALA:HB1	1.93	0.51
2:Bv:87:ALA:HB2	2:Bv:101:ILE:HG22	1.92	0.51
3:Ch:80:PHE:HA	6:Fh:136:VAL:HG21	1.93	0.51
3:Cm:92:GLU:HB2	3:Cm:103:ARG:HB3	1.91	0.51
3:Cn:255:ASP:HB3	3:Cn:258:SER:HB3	1.93	0.51
5:Eh:99:MET:HB3	5:Eh:114:LEU:HD21	1.92	0.51
5:Er:154:LEU:HB3	5:Er:164:TYR:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ey:144:LEU:HA	5:Ey:147:ARG:HD2	1.93	0.51
2:Bi:153:VAL:HG21	2:Bj:148:ASP:HB3	1.92	0.51
2:Bv:360:ILE:HG22	2:Bx:136:ASN:HB2	1.91	0.51
3:Ce:262:TRP:HA	3:Ce:267:GLY:HA3	1.93	0.51
3:Cn:361:PRO:HB2	4:Dg:148:ARG:HD2	1.93	0.51
3:Cq:92:GLU:HB2	3:Cq:103:ARG:HB3	1.92	0.51
3:Cs:88:ILE:HG12	3:Cs:106:ILE:HG23	1.93	0.51
4:De:111:LYS:HD2	5:Ec:197:PRO:HD3	1.92	0.51
4:Dv:223:THR:HG22	4:Dv:285:VAL:HG22	1.93	0.51
5:Ec:144:LEU:HA	5:Ec:147:ARG:HD2	1.93	0.51
2:Bw:87:ALA:HB2	2:Bw:101:ILE:HG22	1.92	0.50
3:Cb:293:GLN:HB2	3:Cb:369:ILE:HG23	1.93	0.50
3:Cb:317:LYS:HG2	3:Cb:345:THR:HB	1.92	0.50
4:Dq:78:ARG:HB3	4:Dq:143:GLN:HE22	1.76	0.50
5:Es:144:LEU:HA	5:Es:147:ARG:HD2	1.93	0.50
2:Bg:268:LYS:HB2	2:Bg:353:ALA:HB1	1.94	0.50
5:Eu:144:LEU:HA	5:Eu:147:ARG:HD2	1.93	0.50
1:Ah:139:GLY:HA3	1:Ai:148:TYR:HD1	1.77	0.50
2:Bd:268:LYS:HB2	2:Bd:353:ALA:HB1	1.93	0.50
3:Cn:342:ILE:HG21	3:Cn:367:ILE:HD11	1.94	0.50
3:Cp:255:ASP:HB3	3:Cp:258:SER:HB3	1.93	0.50
4:Dh:223:THR:HG22	4:Dh:285:VAL:HG22	1.94	0.50
4:Dj:217:ASP:HA	4:Dj:258:ARG:HD3	1.94	0.50
2:Bf:268:LYS:HB2	2:Bf:353:ALA:HB1	1.94	0.50
2:Bs:317:LYS:HE2	2:Bt:324:LEU:HB2	1.94	0.50
2:Bt:87:ALA:HB2	2:Bt:101:ILE:HG22	1.93	0.50
3:Cf:201:ASP:HB3	3:Cf:221:ALA:HB3	1.93	0.50
4:Dd:223:THR:HG22	4:Dd:285:VAL:HG22	1.93	0.50
4:Dg:111:LYS:HD2	5:Ee:197:PRO:HD3	1.92	0.50
4:Dj:223:THR:HG22	4:Dj:285:VAL:HG22	1.94	0.50
4:Dp:249:PHE:HB3	4:Dp:254:LEU:HD23	1.92	0.50
5:Ex:154:LEU:HB3	5:Ex:164:TYR:HE1	1.75	0.50
2:Bc:268:LYS:HB2	2:Bc:353:ALA:HB1	1.93	0.50
2:Bo:268:LYS:HB2	2:Bo:353:ALA:HB1	1.94	0.50
2:By:87:ALA:HB2	2:By:101:ILE:HG22	1.93	0.50
3:Cx:201:ASP:HB3	3:Cx:221:ALA:HB3	1.94	0.50
4:Db:223:THR:HG22	4:Db:285:VAL:HG22	1.94	0.50
5:Eo:144:LEU:HA	5:Eo:147:ARG:HD2	1.92	0.50
1:Au:112:ASN:HD21	1:Au:224:ALA:HB1	1.77	0.50
2:Be:268:LYS:HB2	2:Be:353:ALA:HB1	1.93	0.50
2:Bj:268:LYS:HB2	2:Bj:353:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bl:268:LYS:HB2	2:Bl:353:ALA:HB1	1.94	0.50
2:Bn:268:LYS:HB2	2:Bn:353:ALA:HB1	1.94	0.50
2:Bs:87:ALA:HB2	2:Bs:101:ILE:HG22	1.93	0.50
3:Co:80:PHE:HA	6:Fo:136:VAL:HG21	1.93	0.50
4:Dt:223:THR:HG22	4:Dt:285:VAL:HG22	1.93	0.50
5:Eb:99:MET:HB3	5:Eb:114:LEU:HD21	1.92	0.50
1:Am:206:ILE:HG12	1:Am:235:TYR:HD1	1.77	0.50
1:Ay:112:ASN:HD21	1:Ay:224:ALA:HB1	1.77	0.50
2:Bh:268:LYS:HB2	2:Bh:353:ALA:HB1	1.94	0.50
2:Bq:268:LYS:HB2	2:Bq:353:ALA:HB1	1.94	0.50
2:Bu:87:ALA:HB2	2:Bu:101:ILE:HG22	1.93	0.50
4:Di:111:LYS:HD2	5:Eg:197:PRO:HD3	1.93	0.50
1:Ad:125:LEU:HB2	1:Ad:160:PHE:HB3	1.94	0.50
2:Bm:268:LYS:HB2	2:Bm:353:ALA:HB1	1.94	0.50
3:Cl:201:ASP:HB3	3:Cl:221:ALA:HB3	1.94	0.50
3:Ct:342:ILE:HG21	3:Ct:367:ILE:HD11	1.93	0.50
4:De:184:ILE:HG12	4:De:286:VAL:HG22	1.93	0.50
4:Dr:223:THR:HG22	4:Dr:285:VAL:HG22	1.93	0.50
1:Ax:139:GLY:HA3	1:Ay:148:TYR:HD1	1.77	0.50
2:Bt:268:LYS:HB2	2:Bt:353:ALA:HB1	1.94	0.50
3:Cy:241:ARG:HB3	6:Gz:143:THR:HG21	1.94	0.50
4:Dg:78:ARG:HB3	4:Dg:143:GLN:HE22	1.77	0.50
5:Ei:144:LEU:HA	5:Ei:147:ARG:HD2	1.93	0.50
1:Af:139:GLY:HA3	1:Ag:148:TYR:HD1	1.77	0.49
1:Am:112:ASN:HD21	1:Am:224:ALA:HB1	1.78	0.49
1:Aq:206:ILE:HG12	1:Aq:235:TYR:HD1	1.77	0.49
2:Bu:317:LYS:HE2	2:Bv:324:LEU:HB2	1.94	0.49
2:Bv:268:LYS:HB2	2:Bv:353:ALA:HB1	1.94	0.49
3:Cl:35:VAL:HG23	3:Cl:245:ARG:HG3	1.94	0.49
3:Cz:255:ASP:HB3	3:Cz:258:SER:HB3	1.93	0.49
4:Dx:223:THR:HG22	4:Dx:285:VAL:HG22	1.94	0.49
5:Eo:192:LEU:HD12	5:Eo:196:MET:HE2	1.94	0.49
5:Es:116:ARG:HD3	5:Es:149:GLN:HE22	1.77	0.49
1:Ab:139:GLY:HA3	1:Ac:148:TYR:HD1	1.77	0.49
1:Ap:139:GLY:HA3	1:Aq:148:TYR:HD1	1.77	0.49
1:Ap:206:ILE:HG12	1:Ap:235:TYR:HD1	1.77	0.49
1:At:206:ILE:HG12	1:At:235:TYR:HD1	1.77	0.49
2:Bp:268:LYS:HB2	2:Bp:353:ALA:HB1	1.94	0.49
3:Cg:255:ASP:HB3	3:Cg:258:SER:HB3	1.94	0.49
3:Cn:92:GLU:HB2	3:Cn:103:ARG:HB3	1.93	0.49
3:Ct:153:ILE:HG21	3:Ct:195:MET:HE1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:112:ASN:HD21	1:As:224:ALA:HB1	1.77	0.49
1:Aw:206:ILE:HG12	1:Aw:235:TYR:HD1	1.78	0.49
2:Bw:268:LYS:HB2	2:Bw:353:ALA:HB1	1.93	0.49
3:Cn:201:ASP:HB3	3:Cn:221:ALA:HB3	1.93	0.49
4:Dp:223:THR:HG22	4:Dp:285:VAL:HG22	1.93	0.49
4:Dy:78:ARG:HB3	4:Dy:143:GLN:HE22	1.78	0.49
4:Dz:223:THR:HG22	4:Dz:285:VAL:HG22	1.95	0.49
5:Ek:116:ARG:HD3	5:Ek:149:GLN:HE22	1.78	0.49
5:Eq:116:ARG:HD3	5:Eq:149:GLN:HE22	1.76	0.49
1:Aa:148:TYR:HD1	1:Az:139:GLY:HA3	1.77	0.49
1:Aj:139:GLY:HA3	1:Ak:148:TYR:HD1	1.77	0.49
1:Ak:112:ASN:HD21	1:Ak:224:ALA:HB1	1.77	0.49
1:An:206:ILE:HG12	1:An:235:TYR:HD1	1.77	0.49
1:Ay:206:ILE:HG12	1:Ay:235:TYR:HD1	1.78	0.49
2:Bs:268:LYS:HB2	2:Bs:353:ALA:HB1	1.94	0.49
3:Cy:255:ASP:HB3	3:Cy:258:SER:HB3	1.95	0.49
3:Cz:91:GLU:HG2	3:Cz:92:GLU:HG3	1.93	0.49
3:Cz:342:ILE:HG21	3:Cz:367:ILE:HD11	1.94	0.49
4:Dc:111:LYS:HD2	5:Ea:197:PRO:HD3	1.95	0.49
4:Dk:184:ILE:HG12	4:Dk:286:VAL:HG22	1.94	0.49
1:Aa:206:ILE:HG12	1:Aa:235:TYR:HD1	1.77	0.49
1:Ae:206:ILE:HG12	1:Ae:235:TYR:HD1	1.78	0.49
1:An:139:GLY:HA3	1:Ao:148:TYR:HD1	1.78	0.49
1:Aw:231:ALA:HB3	1:Ax:195:LYS:HG3	1.95	0.49
1:Ax:64:PRO:HB2	1:Ay:38:VAL:HG13	1.93	0.49
2:Bb:268:LYS:HB2	2:Bb:353:ALA:HB1	1.94	0.49
2:Be:317:LYS:HE2	2:Bf:324:LEU:HB2	1.94	0.49
2:By:268:LYS:HB2	2:By:353:ALA:HB1	1.94	0.49
3:Cg:92:GLU:HB2	3:Cg:103:ARG:HB3	1.94	0.49
3:Ch:255:ASP:HB3	3:Ch:258:SER:HB3	1.94	0.49
4:Db:249:PHE:HB3	4:Db:254:LEU:HD23	1.94	0.49
5:Ea:116:ARG:HD3	5:Ea:149:GLN:HE22	1.76	0.49
1:Aa:113:GLU:HB2	1:Aa:172:MET:HB3	1.95	0.49
1:Ab:125:LEU:HB2	1:Ab:160:PHE:HB3	1.95	0.49
1:Ab:206:ILE:HG12	1:Ab:235:TYR:HD1	1.78	0.49
1:Aj:206:ILE:HG12	1:Aj:235:TYR:HD1	1.78	0.49
1:At:139:GLY:HA3	1:Au:148:TYR:HD1	1.77	0.49
1:Av:231:ALA:HB3	1:Aw:195:LYS:HG3	1.95	0.49
2:Bz:268:LYS:HB2	2:Bz:353:ALA:HB1	1.94	0.49
3:Cw:255:ASP:HB3	3:Cw:258:SER:HB3	1.94	0.49
1:Ag:206:ILE:HG12	1:Ag:235:TYR:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:206:ILE:HG12	1:Ak:235:TYR:HD1	1.78	0.49
1:As:206:ILE:HG12	1:As:235:TYR:HD1	1.78	0.49
3:Co:255:ASP:HB3	3:Co:258:SER:HB3	1.95	0.49
4:Dc:78:ARG:HB3	4:Dc:143:GLN:HE22	1.77	0.49
4:Dn:223:THR:HG22	4:Dn:285:VAL:HG22	1.94	0.49
1:Ac:139:GLY:HA3	1:Ad:148:TYR:HD1	1.78	0.49
1:Ah:206:ILE:HG12	1:Ah:235:TYR:HD1	1.78	0.49
1:Ar:139:GLY:HA3	1:As:148:TYR:HD1	1.77	0.49
1:Av:206:ILE:HG12	1:Av:235:TYR:HD1	1.78	0.49
1:Az:206:ILE:HG12	1:Az:235:TYR:HD1	1.78	0.49
3:Co:201:ASP:HB3	3:Co:221:ALA:HB3	1.94	0.49
4:De:78:ARG:HB3	4:De:143:GLN:HE22	1.78	0.49
1:Aa:139:GLY:HA3	1:Ab:148:TYR:HD1	1.78	0.49
1:Ak:139:GLY:HA3	1:Al:148:TYR:HD1	1.78	0.49
1:Ao:113:GLU:HB2	1:Ao:172:MET:HB3	1.95	0.49
1:As:231:ALA:HB3	1:At:195:LYS:HG3	1.95	0.49
1:Au:139:GLY:HA3	1:Av:148:TYR:HD1	1.78	0.49
3:Cq:201:ASP:HB3	3:Cq:221:ALA:HB3	1.95	0.49
3:Cr:255:ASP:HB3	3:Cr:258:SER:HB3	1.94	0.49
1:Ac:206:ILE:HG12	1:Ac:235:TYR:HD1	1.77	0.49
1:Am:125:LEU:HB2	1:Am:160:PHE:HB3	1.95	0.49
1:Aq:231:ALA:HB3	1:Ar:195:LYS:HG3	1.95	0.49
1:Av:139:GLY:HA3	1:Aw:148:TYR:HD1	1.78	0.49
1:Aw:112:ASN:HD21	1:Aw:224:ALA:HB1	1.76	0.49
2:Ba:268:LYS:HB2	2:Ba:353:ALA:HB1	1.94	0.49
4:Da:78:ARG:HB3	4:Da:143:GLN:HE22	1.77	0.49
4:Dh:116:TYR:HE2	5:Eh:198:GLU:HB3	1.78	0.49
4:Dl:223:THR:HG22	4:Dl:285:VAL:HG22	1.95	0.49
5:Ec:116:ARG:HD3	5:Ec:149:GLN:HE22	1.78	0.49
5:Ei:116:ARG:HD3	5:Ei:149:GLN:HE22	1.78	0.49
1:Aa:125:LEU:HB2	1:Aa:160:PHE:HB3	1.95	0.48
1:Ae:139:GLY:HA3	1:Af:148:TYR:HD1	1.78	0.48
1:Af:125:LEU:HB2	1:Af:160:PHE:HB3	1.94	0.48
1:Am:113:GLU:HB2	1:Am:172:MET:HB3	1.95	0.48
1:Aq:125:LEU:HB2	1:Aq:160:PHE:HB3	1.95	0.48
1:Aw:113:GLU:HB2	1:Aw:172:MET:HB3	1.95	0.48
1:Aw:125:LEU:HB2	1:Aw:160:PHE:HB3	1.95	0.48
2:Bd:317:LYS:HE2	2:Be:324:LEU:HB2	1.94	0.48
2:Bf:342:MET:HE2	2:Bh:138:VAL:HG21	1.95	0.48
2:Bg:317:LYS:HE2	2:Bh:324:LEU:HB2	1.94	0.48
2:Bp:342:MET:HE2	2:Br:138:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Br:268:LYS:HB2	2:Br:353:ALA:HB1	1.95	0.48
2:Bt:317:LYS:HE2	2:Bu:324:LEU:HB2	1.95	0.48
3:Cx:226:VAL:HB	3:Cx:236:MET:HB3	1.95	0.48
4:Dr:249:PHE:HB3	4:Dr:254:LEU:HD23	1.94	0.48
5:Ea:154:LEU:HB3	5:Ea:164:TYR:HE1	1.78	0.48
5:Em:192:LEU:HD12	5:Em:196:MET:HE2	1.95	0.48
5:Eq:154:LEU:HB3	5:Eq:164:TYR:HE1	1.78	0.48
1:Ad:139:GLY:HA3	1:Ae:148:TYR:HD1	1.77	0.48
1:Ae:112:ASN:HD21	1:Ae:224:ALA:HB1	1.78	0.48
1:Ak:113:GLU:HB2	1:Ak:172:MET:HB3	1.95	0.48
1:Ao:206:ILE:HG12	1:Ao:235:TYR:HD1	1.78	0.48
1:Ap:231:ALA:HB3	1:Aq:195:LYS:HG3	1.95	0.48
1:Ay:139:GLY:HA3	1:Az:148:TYR:HD1	1.78	0.48
2:Bm:317:LYS:HE2	2:Bn:324:LEU:HB2	1.95	0.48
2:Bn:85:VAL:HG22	2:Bn:103:VAL:HG22	1.95	0.48
2:Bq:317:LYS:HE2	2:Br:324:LEU:HB2	1.95	0.48
2:Bu:268:LYS:HB2	2:Bu:353:ALA:HB1	1.95	0.48
3:Ck:85:VAL:HG22	3:Ck:108:ILE:HG12	1.95	0.48
3:Cu:92:GLU:HB2	3:Cu:103:ARG:HB3	1.95	0.48
4:Ds:111:LYS:HD2	5:Eq:197:PRO:HD3	1.94	0.48
5:Ee:116:ARG:HD3	5:Ee:149:GLN:HE22	1.78	0.48
5:Eh:116:ARG:HA	5:Eh:149:GLN:HE22	1.78	0.48
5:Ek:192:LEU:HD12	5:Ek:196:MET:HE2	1.95	0.48
1:Ac:125:LEU:HB2	1:Ac:160:PHE:HB3	1.96	0.48
1:Ad:206:ILE:HG12	1:Ad:235:TYR:HD1	1.77	0.48
1:Af:206:ILE:HG12	1:Af:235:TYR:HD1	1.78	0.48
1:Al:125:LEU:HB2	1:Al:160:PHE:HB3	1.96	0.48
2:Br:317:LYS:HE2	2:Bs:324:LEU:HB2	1.95	0.48
3:Cp:145:VAL:HA	3:Cp:256:THR:HG21	1.95	0.48
3:Cy:92:GLU:HB2	3:Cy:103:ARG:HB3	1.94	0.48
4:Dk:78:ARG:HB3	4:Dk:143:GLN:HE22	1.77	0.48
4:Dw:184:ILE:HG12	4:Dw:286:VAL:HG22	1.94	0.48
5:Em:116:ARG:HD3	5:Em:149:GLN:HE22	1.77	0.48
5:Ep:154:LEU:HB3	5:Ep:164:TYR:HE1	1.78	0.48
1:Ac:113:GLU:HB2	1:Ac:172:MET:HB3	1.95	0.48
1:Ai:113:GLU:HB2	1:Ai:172:MET:HB3	1.94	0.48
1:Aj:125:LEU:HB2	1:Aj:160:PHE:HB3	1.95	0.48
1:Ar:206:ILE:HG12	1:Ar:235:TYR:HD1	1.77	0.48
1:Ar:231:ALA:HB3	1:As:195:LYS:HG3	1.96	0.48
1:Av:125:LEU:HB2	1:Av:160:PHE:HB3	1.96	0.48
1:Aw:139:GLY:HA3	1:Ax:148:TYR:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:231:ALA:HB3	1:Az:195:LYS:HG3	1.95	0.48
2:Bc:317:LYS:HE2	2:Bd:324:LEU:HB2	1.94	0.48
2:Bk:317:LYS:HE2	2:Bl:324:LEU:HB2	1.94	0.48
3:Ck:88:ILE:HG12	3:Ck:106:ILE:HG23	1.94	0.48
3:Cp:361:PRO:HB2	4:Di:148:ARG:HD2	1.95	0.48
3:Cq:209:LYS:HD2	3:Cq:212:GLN:HB2	1.95	0.48
3:Cx:358:VAL:HG12	3:Cx:360:GLN:H	1.79	0.48
3:Cz:226:VAL:HB	3:Cz:236:MET:HB3	1.95	0.48
1:Ai:139:GLY:HA3	1:Aj:148:TYR:HD1	1.78	0.48
1:Ak:125:LEU:HB2	1:Ak:160:PHE:HB3	1.96	0.48
2:Bt:342:MET:HE2	2:Bv:138:VAL:HG21	1.95	0.48
2:By:317:LYS:HE2	2:Bz:324:LEU:HB2	1.94	0.48
3:Ch:92:GLU:HB2	3:Ch:103:ARG:HB3	1.95	0.48
3:Cw:201:ASP:HB3	3:Cw:221:ALA:HB3	1.95	0.48
1:Aa:112:ASN:HD21	1:Aa:224:ALA:HB1	1.78	0.48
1:Ab:64:PRO:HB2	1:Ac:38:VAL:HG13	1.95	0.48
1:Al:139:GLY:HA3	1:Am:148:TYR:HD1	1.77	0.48
1:Aq:113:GLU:HB2	1:Aq:172:MET:HB3	1.95	0.48
1:Aq:139:GLY:HA3	1:Ar:148:TYR:HD1	1.78	0.48
2:Bb:138:VAL:HG21	2:Bz:342:MET:HE2	1.96	0.48
2:Bv:342:MET:HE2	2:Bx:138:VAL:HG21	1.95	0.48
2:Bw:317:LYS:HE2	2:Bx:324:LEU:HB2	1.94	0.48
3:Cf:56:PHE:HD1	6:Gf:139:LYS:HE2	1.77	0.48
4:Du:184:ILE:HG12	4:Du:286:VAL:HG22	1.95	0.48
5:Em:154:LEU:HB3	5:Em:164:TYR:HE1	1.79	0.48
5:Eo:202:ALA:HA	5:Eo:205:LYS:HZ2	1.78	0.48
1:Ag:112:ASN:HD21	1:Ag:224:ALA:HB1	1.78	0.48
1:Ai:206:ILE:HG12	1:Ai:235:TYR:HD1	1.77	0.48
1:Al:206:ILE:HG12	1:Al:235:TYR:HD1	1.78	0.48
1:An:231:ALA:HB3	1:Ao:195:LYS:HG3	1.96	0.48
1:Aq:112:ASN:HD21	1:Aq:224:ALA:HB1	1.77	0.48
2:Ba:324:LEU:HB2	2:Bz:317:LYS:HE2	1.95	0.48
2:Be:342:MET:HE2	2:Bg:138:VAL:HG21	1.96	0.48
2:Bg:224:ARG:HH21	3:Cx:368:GLN:HB2	1.79	0.48
3:Cn:326:PHE:HD2	3:Cn:328:ASP:H	1.61	0.48
5:Ey:116:ARG:HD3	5:Ey:149:GLN:HE22	1.78	0.48
1:Aa:231:ALA:HB3	1:Ab:195:LYS:HG3	1.95	0.48
1:Ai:112:ASN:HD21	1:Ai:224:ALA:HB1	1.78	0.48
1:Am:139:GLY:HA3	1:An:148:TYR:HD1	1.79	0.48
1:Ap:125:LEU:HB2	1:Ap:160:PHE:HB3	1.96	0.48
1:Ar:125:LEU:HB2	1:Ar:160:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: Au:206: ILE: HG12	1: Au:235: TYR: HD1	1.77	0.48
2: Ba:317: LYS: HE2	2: Bb:324: LEU: HB2	1.95	0.48
2: Bd:342: MET: HE2	2: Bf:138: VAL: HG21	1.95	0.48
2: Bh:85: VAL: HG22	2: Bh:103: VAL: HG22	1.96	0.48
2: Bh:317: LYS: HE2	2: Bi:324: LEU: HB2	1.95	0.48
2: Bh:342: MET: HE2	2: Bj:138: VAL: HG21	1.96	0.48
2: Bj:342: MET: HE2	2: Bl:138: VAL: HG21	1.95	0.48
2: Bl:317: LYS: HE2	2: Bm:324: LEU: HB2	1.95	0.48
3: Cg:201: ASP: HB3	3: Cg:221: ALA: HB3	1.96	0.48
4: Du:78: ARG: HB3	4: Du:143: GLN: HE22	1.79	0.48
5: Ee:192: LEU: HD12	5: Ee:196: MET: HE2	1.95	0.48
5: Eg:116: ARG: HD3	5: Eg:149: GLN: HE22	1.77	0.48
1: Ab:231: ALA: HB3	1: Ac:195: LYS: HG3	1.95	0.48
1: As:139: GLY: HA3	1: At:148: TYR: HD1	1.78	0.48
1: Ax:125: LEU: HB2	1: Ax:160: PHE: HB3	1.96	0.48
1: Ax:231: ALA: HB3	1: Ay:195: LYS: HG3	1.95	0.48
2: Bx:317: LYS: HE2	2: By:324: LEU: HB2	1.95	0.48
4: Df:249: PHE: HB3	4: Df:254: LEU: HD23	1.95	0.48
4: Di:78: ARG: HB3	4: Di:143: GLN: HE22	1.79	0.48
5: Ea:202: ALA: HA	5: Ea:205: LYS: HZ2	1.78	0.48
1: Ah:125: LEU: HB2	1: Ah:160: PHE: HB3	1.95	0.48
2: Be:205: LEU: HD11	2: Be:236: ILE: HD11	1.95	0.48
3: Ca:80: PHE: HA	6: Fa:136: VAL: HG21	1.96	0.48
3: Cv:361: PRO: HB2	4: Do:148: ARG: HD2	1.94	0.48
5: Eq:192: LEU: HD12	5: Eq:196: MET: HE2	1.96	0.48
5: Es:192: LEU: HD12	5: Es:196: MET: HE2	1.96	0.48
5: Ew:116: ARG: HD3	5: Ew:149: GLN: HE22	1.79	0.48
1: An:240: THR: HG22	1: An:244: MET: HE2	1.96	0.47
1: Ax:206: ILE: HG12	1: Ax:235: TYR: HD1	1.78	0.47
1: Ay:113: GLU: HB2	1: Ay:172: MET: HB3	1.96	0.47
2: Bl:85: VAL: HG22	2: Bl:103: VAL: HG22	1.96	0.47
2: Bl:342: MET: HE2	2: Bn:138: VAL: HG21	1.95	0.47
2: Bn:342: MET: HE2	2: Bp:138: VAL: HG21	1.96	0.47
2: Bo:342: MET: HE2	2: Bq:138: VAL: HG21	1.97	0.47
3: Co:326: PHE: HD2	3: Co:328: ASP: H	1.62	0.47
4: Db:116: TYR: HE2	5: Eb:198: GLU: HB3	1.79	0.47
4: Dt:249: PHE: HB3	4: Dt:254: LEU: HD23	1.95	0.47
5: Eg:192: LEU: HD12	5: Eg:196: MET: HE2	1.96	0.47
5: Eu:116: ARG: HD3	5: Eu:149: GLN: HE22	1.79	0.47
1: Ac:231: ALA: HB3	1: Ad:195: LYS: HG3	1.95	0.47
1: Ae:125: LEU: HB2	1: Ae:160: PHE: HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ah:240:THR:HG22	1:Ah:244:MET:HE2	1.96	0.47
1:An:113:GLU:HB2	1:An:172:MET:HB3	1.96	0.47
1:Ao:139:GLY:HA3	1:Ap:148:TYR:HD1	1.78	0.47
1:Ao:231:ALA:HB3	1:Ap:195:LYS:HG3	1.96	0.47
2:Bb:317:LYS:HE2	2:Bc:324:LEU:HB2	1.95	0.47
2:Bi:317:LYS:HE2	2:Bj:324:LEU:HB2	1.95	0.47
2:Bx:268:LYS:HB2	2:Bx:353:ALA:HB1	1.95	0.47
3:Cn:35:VAL:HG23	3:Cn:245:ARG:HG3	1.96	0.47
3:Ct:361:PRO:HB2	4:Dm:148:ARG:HD2	1.95	0.47
5:Em:71:LEU:HB3	5:Em:74:TYR:HB2	1.96	0.47
1:Al:113:GLU:HB2	1:Al:172:MET:HB3	1.96	0.47
1:Ao:125:LEU:HB2	1:Ao:160:PHE:HB3	1.96	0.47
1:At:231:ALA:HB3	1:Au:195:LYS:HG3	1.97	0.47
2:Bf:317:LYS:HE2	2:Bg:324:LEU:HB2	1.95	0.47
2:Bg:342:MET:HE2	2:Bi:138:VAL:HG21	1.97	0.47
2:Bx:85:VAL:HG22	2:Bx:103:VAL:HG22	1.95	0.47
3:Cc:201:ASP:HB3	3:Cc:221:ALA:HB3	1.96	0.47
3:Cc:262:TRP:HA	3:Cc:267:GLY:HA3	1.97	0.47
3:Cj:342:ILE:HG21	3:Cj:367:ILE:HD11	1.96	0.47
3:Cs:326:PHE:HD2	3:Cs:328:ASP:H	1.63	0.47
3:Cu:201:ASP:HB3	3:Cu:221:ALA:HB3	1.96	0.47
4:Do:184:ILE:HG12	4:Do:286:VAL:HG22	1.96	0.47
4:Ds:184:ILE:HG12	4:Ds:286:VAL:HG22	1.95	0.47
1:Ai:125:LEU:HB2	1:Ai:160:PHE:HB3	1.96	0.47
1:Al:240:THR:HG22	1:Al:244:MET:HE2	1.97	0.47
1:Au:113:GLU:HB2	1:Au:172:MET:HB3	1.96	0.47
2:Bb:85:VAL:HG22	2:Bb:103:VAL:HG22	1.96	0.47
2:Bb:342:MET:HE2	2:Bd:138:VAL:HG21	1.96	0.47
3:Ca:249:PRO:HG2	3:Ca:252:SER:HB3	1.96	0.47
3:Cc:292:PRO:HB3	3:Cc:306:LEU:HD13	1.96	0.47
3:Cy:153:ILE:HG21	3:Cy:195:MET:HE1	1.96	0.47
4:Dm:141:ASP:HB2	4:Dm:149:ILE:HG12	1.97	0.47
4:Dq:184:ILE:HG12	4:Dq:286:VAL:HG22	1.96	0.47
1:Ag:139:GLY:HA3	1:Ah:148:TYR:HD1	1.78	0.47
1:Aj:231:ALA:HB3	1:Ak:195:LYS:HG3	1.95	0.47
1:Aj:240:THR:HG22	1:Aj:244:MET:HE2	1.97	0.47
1:Ak:240:THR:HG22	1:Ak:244:MET:HE2	1.97	0.47
1:Am:240:THR:HG22	1:Am:244:MET:HE2	1.97	0.47
1:As:125:LEU:HB2	1:As:160:PHE:HB3	1.96	0.47
2:Bn:103:VAL:HB	2:Bn:137:LEU:HD21	1.97	0.47
3:Cc:93:ARG:HG2	3:Cc:102:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cr:201:ASP:HB3	3:Cr:221:ALA:HB3	1.96	0.47
4:Dd:249:PHE:HB3	4:Dd:254:LEU:HD23	1.96	0.47
4:Dw:78:ARG:HB3	4:Dw:143:GLN:HE22	1.79	0.47
1:Au:125:LEU:HB2	1:Au:160:PHE:HB3	1.96	0.47
2:Bd:85:VAL:HG22	2:Bd:103:VAL:HG22	1.96	0.47
2:Bj:317:LYS:HE2	2:Bk:324:LEU:HB2	1.96	0.47
2:Bm:85:VAL:HG22	2:Bm:103:VAL:HG22	1.97	0.47
2:Bn:317:LYS:HE2	2:Bo:324:LEU:HB2	1.96	0.47
2:Bo:317:LYS:HE2	2:Bp:324:LEU:HB2	1.95	0.47
3:Cd:239:THR:HG21	3:Ce:155:ARG:HD3	1.97	0.47
3:Ch:226:VAL:HB	3:Ch:236:MET:HB3	1.97	0.47
3:Ci:201:ASP:HB3	3:Ci:221:ALA:HB3	1.97	0.47
3:Cx:342:ILE:HG21	3:Cx:367:ILE:HD11	1.97	0.47
4:Di:116:TYR:HE2	5:El:198:GLU:HB3	1.79	0.47
4:Do:111:LYS:HD2	5:Em:197:PRO:HD3	1.96	0.47
4:Dp:64:ALA:HB2	4:Dp:172:LEU:HD22	1.97	0.47
4:Dz:93:PRO:HD3	4:Dz:133:ARG:HA	1.96	0.47
5:Ea:192:LEU:HD12	5:Ea:196:MET:HE2	1.96	0.47
5:Eb:116:ARG:HA	5:Eb:149:GLN:HE22	1.79	0.47
1:Ad:113:GLU:HB2	1:Ad:172:MET:HB3	1.96	0.47
1:Ae:113:GLU:HB2	1:Ae:172:MET:HB3	1.96	0.47
1:Af:231:ALA:HB3	1:Ag:195:LYS:HG3	1.95	0.47
1:Ag:113:GLU:HB2	1:Ag:172:MET:HB3	1.95	0.47
1:Ag:240:THR:HG22	1:Ag:244:MET:HE2	1.97	0.47
1:Am:231:ALA:HB3	1:An:195:LYS:HG3	1.96	0.47
1:Ao:240:THR:HG22	1:Ao:244:MET:HE2	1.97	0.47
1:Ao:245:GLN:HG3	1:Ap:200:ASN:HD21	1.80	0.47
1:Ap:113:GLU:HB2	1:Ap:172:MET:HB3	1.97	0.47
1:Aq:240:THR:HG22	1:Aq:244:MET:HE2	1.97	0.47
1:Av:240:THR:HG22	1:Av:244:MET:HE2	1.97	0.47
1:Aw:64:PRO:HB2	1:Ax:38:VAL:HG13	1.96	0.47
1:Az:125:LEU:HB2	1:Az:160:PHE:HB3	1.96	0.47
2:Ba:138:VAL:HG21	2:By:342:MET:HE2	1.97	0.47
2:Bi:85:VAL:HG22	2:Bi:103:VAL:HG22	1.97	0.47
2:Bn:250:ILE:HG23	2:Bn:261:VAL:HG22	1.97	0.47
2:Bo:85:VAL:HG22	2:Bo:103:VAL:HG22	1.96	0.47
2:Bq:342:MET:HE2	2:Bs:138:VAL:HG21	1.96	0.47
3:Cm:56:PHE:HD1	6:Gm:139:LYS:HE2	1.79	0.47
3:Cm:249:PRO:HG2	3:Cm:252:SER:HB3	1.96	0.47
3:Cz:201:ASP:HB3	3:Cz:221:ALA:HB3	1.97	0.47
4:De:104:ILE:HG23	4:Df:145:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dg:184:ILE:HG12	4:Dg:286:VAL:HG22	1.95	0.47
4:Dj:116:TYR:HE2	5:Ej:198:GLU:HB3	1.80	0.47
5:Eo:116:ARG:HD3	5:Eo:149:GLN:HE22	1.80	0.47
5:Ev:99:MET:HB3	5:Ev:114:LEU:HD21	1.97	0.47
5:Ez:99:MET:HB3	5:Ez:114:LEU:HD21	1.97	0.47
1:Aa:195:LYS:HG3	1:Az:231:ALA:HB3	1.97	0.47
1:Al:231:ALA:HB3	1:Am:195:LYS:HG3	1.96	0.47
1:As:113:GLU:HB2	1:As:172:MET:HB3	1.96	0.47
1:At:125:LEU:HB2	1:At:160:PHE:HB3	1.95	0.47
1:Aw:240:THR:HG22	1:Aw:244:MET:HE2	1.97	0.47
2:Bc:85:VAL:HG22	2:Bc:103:VAL:HG22	1.96	0.47
2:Bg:85:VAL:HG22	2:Bg:103:VAL:HG22	1.97	0.47
2:Bm:342:MET:HE2	2:Bo:138:VAL:HG21	1.97	0.47
3:Cb:85:VAL:HG22	3:Cb:108:ILE:HG12	1.96	0.47
3:Cd:201:ASP:HB3	3:Cd:221:ALA:HB3	1.97	0.47
3:Ch:342:ILE:HG21	3:Ch:367:ILE:HD11	1.96	0.47
3:Ct:80:PHE:HA	6:Ft:136:VAL:HG21	1.97	0.47
4:Dm:184:ILE:HG12	4:Dm:286:VAL:HG22	1.97	0.47
5:El:99:MET:HB3	5:El:114:LEU:HD21	1.96	0.47
1:Ab:113:GLU:HB2	1:Ab:172:MET:HB3	1.97	0.47
1:Ao:112:ASN:HD21	1:Ao:224:ALA:HB1	1.80	0.47
1:Ap:240:THR:HG22	1:Ap:244:MET:HE2	1.97	0.47
1:As:240:THR:HG22	1:As:244:MET:HE2	1.97	0.47
2:Be:85:VAL:HG22	2:Be:103:VAL:HG22	1.96	0.47
2:Br:342:MET:HE2	2:Bt:138:VAL:HG21	1.96	0.47
2:Bv:85:VAL:HG22	2:Bv:103:VAL:HG22	1.96	0.47
2:Bw:85:VAL:HG22	2:Bw:103:VAL:HG22	1.96	0.47
3:Ca:255:ASP:HB3	3:Ca:258:SER:HB3	1.97	0.47
3:Cy:209:LYS:HD2	3:Cy:212:GLN:HB2	1.97	0.47
4:Dm:83:THR:HG22	4:Dm:111:LYS:HA	1.97	0.47
5:Eu:202:ALA:HA	5:Eu:205:LYS:HZ2	1.79	0.47
1:Ae:240:THR:HG22	1:Ae:244:MET:HE2	1.97	0.47
1:Af:240:THR:HG22	1:Af:244:MET:HE2	1.97	0.47
1:Ar:113:GLU:HB2	1:Ar:172:MET:HB3	1.97	0.47
1:Ay:240:THR:HG22	1:Ay:244:MET:HE2	1.97	0.47
1:Az:240:THR:HG22	1:Az:244:MET:HE2	1.97	0.47
2:Br:205:LEU:HD11	2:Br:236:ILE:HD11	1.97	0.47
2:Br:250:ILE:HG23	2:Br:261:VAL:HG22	1.97	0.47
2:Bv:91:ALA:HB1	2:Bv:174:ASN:HD21	1.80	0.47
2:Bz:85:VAL:HG22	2:Bz:103:VAL:HG22	1.96	0.47
3:Cb:105:ARG:HH21	6:Gb:133:VAL:HG13	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cj:292:PRO:HB3	3:Cj:306:LEU:HD13	1.97	0.47
4:Do:78:ARG:HB3	4:Do:143:GLN:HE22	1.80	0.47
4:Dv:64:ALA:HB2	4:Dv:172:LEU:HD22	1.97	0.47
5:Ek:147:ARG:HD3	5:Ek:170:TRP:HB3	1.97	0.47
5:Et:99:MET:HB3	5:Et:114:LEU:HD21	1.97	0.47
1:Ae:231:ALA:HB3	1:Af:195:LYS:HG3	1.96	0.46
1:Ai:240:THR:HG22	1:Ai:244:MET:HE2	1.97	0.46
2:Ba:224:ARG:HH21	3:Cr:368:GLN:HB2	1.79	0.46
2:Bk:250:ILE:HG23	2:Bk:261:VAL:HG22	1.97	0.46
2:Bl:103:VAL:HB	2:Bl:137:LEU:HD21	1.97	0.46
2:Bq:85:VAL:HG22	2:Bq:103:VAL:HG22	1.96	0.46
2:Br:85:VAL:HG22	2:Br:103:VAL:HG22	1.96	0.46
2:Bs:105:SER:HB2	2:Bs:112:LEU:HD11	1.97	0.46
2:Bt:85:VAL:HG22	2:Bt:103:VAL:HG22	1.96	0.46
3:Cu:255:ASP:HB3	3:Cu:258:SER:HB3	1.95	0.46
3:Cx:292:PRO:HB3	3:Cx:306:LEU:HD13	1.97	0.46
4:Dc:184:ILE:HG12	4:Dc:286:VAL:HG22	1.95	0.46
4:Dg:31:PRO:HB3	4:Dg:156:VAL:HG21	1.96	0.46
4:Dk:83:THR:HG22	4:Dk:111:LYS:HA	1.98	0.46
4:Dy:184:ILE:HG12	4:Dy:286:VAL:HG22	1.96	0.46
5:Ey:192:LEU:HD12	5:Ey:196:MET:HE2	1.96	0.46
1:Ab:240:THR:HG22	1:Ab:244:MET:HE2	1.97	0.46
1:An:125:LEU:HB2	1:An:160:PHE:HB3	1.97	0.46
1:As:245:GLN:HG3	1:At:200:ASN:HD21	1.80	0.46
1:At:240:THR:HG22	1:At:244:MET:HE2	1.98	0.46
1:Ay:245:GLN:HG3	1:Az:200:ASN:HD21	1.80	0.46
2:Ba:342:MET:HE2	2:Bc:138:VAL:HG21	1.97	0.46
2:Bc:205:LEU:HD11	2:Bc:236:ILE:HD11	1.98	0.46
2:Bp:85:VAL:HG22	2:Bp:103:VAL:HG22	1.96	0.46
2:Bp:317:LYS:HE2	2:Bq:324:LEU:HB2	1.96	0.46
2:Bu:342:MET:HE2	2:Bw:138:VAL:HG21	1.97	0.46
4:Di:83:THR:HG22	4:Di:111:LYS:HA	1.97	0.46
4:Do:83:THR:HG22	4:Do:111:LYS:HA	1.97	0.46
5:Ei:192:LEU:HD12	5:Ei:196:MET:HE2	1.97	0.46
5:El:154:LEU:HB3	5:El:164:TYR:HE1	1.80	0.46
5:Ep:99:MET:HB3	5:Ep:114:LEU:HD21	1.97	0.46
5:Ev:116:ARG:HA	5:Ev:149:GLN:HE22	1.81	0.46
5:Ex:99:MET:HB3	5:Ex:114:LEU:HD21	1.98	0.46
1:Aa:245:GLN:HG3	1:Ab:200:ASN:HD21	1.80	0.46
1:Au:231:ALA:HB3	1:Av:195:LYS:HG3	1.97	0.46
1:Au:240:THR:HG22	1:Au:244:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ax:113:GLU:HB2	1:Ax:172:MET:HB3	1.97	0.46
1:Ax:240:THR:HG22	1:Ax:244:MET:HE2	1.98	0.46
1:Az:113:GLU:HB2	1:Az:172:MET:HB3	1.97	0.46
2:Bd:103:VAL:HB	2:Bd:137:LEU:HD21	1.97	0.46
2:Bf:85:VAL:HG22	2:Bf:103:VAL:HG22	1.97	0.46
2:Bg:250:ILE:HG23	2:Bg:261:VAL:HG22	1.98	0.46
2:Bi:342:MET:HE2	2:Bk:138:VAL:HG21	1.97	0.46
2:Bj:91:ALA:HB1	2:Bj:174:ASN:HD21	1.80	0.46
2:Bj:103:VAL:HB	2:Bj:137:LEU:HD21	1.97	0.46
2:Bk:85:VAL:HG22	2:Bk:103:VAL:HG22	1.97	0.46
2:Bp:103:VAL:HB	2:Bp:137:LEU:HD21	1.97	0.46
2:Bp:105:SER:HB2	2:Bp:112:LEU:HD11	1.97	0.46
2:Bv:317:LYS:HE2	2:Bw:324:LEU:HB2	1.96	0.46
2:Bx:342:MET:HE2	2:Bz:138:VAL:HG21	1.96	0.46
2:By:85:VAL:HG22	2:By:103:VAL:HG22	1.96	0.46
3:Cc:226:VAL:HB	3:Cc:236:MET:HB3	1.97	0.46
3:Ch:201:ASP:HB3	3:Ch:221:ALA:HB3	1.98	0.46
3:Ci:292:PRO:HB3	3:Ci:306:LEU:HD13	1.96	0.46
3:Cw:92:GLU:HB2	3:Cw:103:ARG:HB3	1.96	0.46
1:Ad:64:PRO:HB2	1:Ae:38:VAL:HG13	1.97	0.46
1:Am:245:GLN:HG3	1:An:200:ASN:HD21	1.81	0.46
1:Av:113:GLU:HB2	1:Av:172:MET:HB3	1.97	0.46
2:Ba:85:VAL:HG22	2:Ba:103:VAL:HG22	1.96	0.46
2:Bl:250:ILE:HG23	2:Bl:261:VAL:HG22	1.97	0.46
2:Bo:250:ILE:HG23	2:Bo:261:VAL:HG22	1.98	0.46
2:Bu:85:VAL:HG22	2:Bu:103:VAL:HG22	1.96	0.46
3:Cc:269:MET:HE3	3:Cc:269:MET:HB3	1.87	0.46
3:Cl:226:VAL:HB	3:Cl:236:MET:HB3	1.98	0.46
3:Cw:262:TRP:HA	3:Cw:267:GLY:HA3	1.97	0.46
5:Ek:71:LEU:HB3	5:Ek:74:TYR:HB2	1.97	0.46
5:Er:99:MET:HB3	5:Er:114:LEU:HD21	1.97	0.46
1:Af:113:GLU:HB2	1:Af:172:MET:HB3	1.96	0.46
1:Ar:240:THR:HG22	1:Ar:244:MET:HE2	1.98	0.46
2:Bd:224:ARG:HH21	3:Cu:368:GLN:HB2	1.80	0.46
2:Bh:105:SER:HB2	2:Bh:112:LEU:HD11	1.97	0.46
2:Bj:85:VAL:HG22	2:Bj:103:VAL:HG22	1.97	0.46
2:Bj:105:SER:HB2	2:Bj:112:LEU:HD11	1.97	0.46
2:Bk:342:MET:HE2	2:Bm:138:VAL:HG21	1.96	0.46
3:Cc:342:ILE:HG21	3:Cc:367:ILE:HD11	1.98	0.46
4:Dz:116:TYR:HE2	5:Ez:198:GLU:HB3	1.80	0.46
5:Ew:192:LEU:HD12	5:Ew:196:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:240:THR:HG22	1:Aa:244:MET:HE2	1.98	0.46
1:Ag:125:LEU:HB2	1:Ag:160:PHE:HB3	1.96	0.46
2:Be:105:SER:HB2	2:Be:112:LEU:HD11	1.97	0.46
2:Bs:250:ILE:HG23	2:Bs:261:VAL:HG22	1.98	0.46
4:Da:184:ILE:HG12	4:Da:286:VAL:HG22	1.97	0.46
4:Di:184:ILE:HG12	4:Di:286:VAL:HG22	1.97	0.46
5:Eg:202:ALA:HA	5:Eg:205:LYS:HZ2	1.81	0.46
1:Ac:240:THR:HG22	1:Ac:244:MET:HE2	1.97	0.46
1:Aw:245:GLN:HG3	1:Ax:200:ASN:HD21	1.80	0.46
1:Ay:125:LEU:HB2	1:Ay:160:PHE:HB3	1.97	0.46
2:Bq:105:SER:HB2	2:Bq:112:LEU:HD11	1.98	0.46
2:Bv:250:ILE:HG23	2:Bv:261:VAL:HG22	1.97	0.46
3:Cu:157:LEU:HA	3:Cu:161:SER:HB2	1.98	0.46
3:Cy:292:PRO:HB3	3:Cy:306:LEU:HD13	1.97	0.46
4:Ds:78:ARG:HB3	4:Ds:143:GLN:HE22	1.81	0.46
5:Ea:147:ARG:HD3	5:Ea:170:TRP:HB3	1.98	0.46
5:Ed:99:MET:HB3	5:Ed:114:LEU:HD21	1.98	0.46
5:Em:147:ARG:HD3	5:Em:170:TRP:HB3	1.97	0.46
5:Eq:147:ARG:HD3	5:Eq:170:TRP:HB3	1.98	0.46
1:Aq:245:GLN:HG3	1:Ar:200:ASN:HD21	1.81	0.46
2:Bt:250:ILE:HG23	2:Bt:261:VAL:HG22	1.97	0.46
3:Ci:255:ASP:HB3	3:Ci:258:SER:HB3	1.97	0.46
3:Co:292:PRO:HB3	3:Co:306:LEU:HD13	1.98	0.46
3:Cr:157:LEU:HA	3:Cr:161:SER:HB2	1.98	0.46
3:Cv:269:MET:HE3	3:Cv:269:MET:HB3	1.85	0.46
4:Dc:197:LYS:HD3	4:Dd:292:THR:HB	1.98	0.46
5:Ef:99:MET:HB3	5:Ef:114:LEU:HD21	1.98	0.46
5:Ev:108:PRO:HB2	5:Ev:143:ASN:HD22	1.81	0.46
1:Ad:231:ALA:HB3	1:Ae:195:LYS:HG3	1.97	0.46
1:Ah:231:ALA:HB3	1:Ai:195:LYS:HG3	1.97	0.46
1:Ar:64:PRO:HB2	1:As:38:VAL:HG13	1.97	0.46
2:Bf:250:ILE:HG23	2:Bf:261:VAL:HG22	1.98	0.46
2:Bq:250:ILE:HG23	2:Bq:261:VAL:HG22	1.97	0.46
2:Bs:85:VAL:HG22	2:Bs:103:VAL:HG22	1.97	0.46
2:Bs:342:MET:HE2	2:Bu:138:VAL:HG21	1.98	0.46
3:Cc:255:ASP:HB3	3:Cc:258:SER:HB3	1.98	0.46
3:Ci:269:MET:HE3	3:Ci:269:MET:HB3	1.84	0.46
3:Ck:239:THR:HG21	3:Cl:155:ARG:HD3	1.98	0.46
4:Db:93:PRO:HD3	4:Db:133:ARG:HA	1.98	0.46
4:Dy:31:PRO:HB3	4:Dy:156:VAL:HG21	1.97	0.46
5:Eu:192:LEU:HD12	5:Eu:196:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ew:202:ALA:HA	5:Ew:205:LYS:HZ2	1.80	0.46
5:Ey:202:ALA:HA	5:Ey:205:LYS:HZ2	1.80	0.46
1:Ad:240:THR:HG22	1:Ad:244:MET:HE2	1.98	0.46
1:Ad:245:GLN:HG3	1:Ae:200:ASN:HD21	1.81	0.46
1:Ag:245:GLN:HG3	1:Ah:200:ASN:HD21	1.80	0.46
1:Ah:245:GLN:HG3	1:Ai:200:ASN:HD21	1.81	0.46
1:At:113:GLU:HB2	1:At:172:MET:HB3	1.97	0.46
2:Bc:105:SER:HB2	2:Bc:112:LEU:HD11	1.97	0.46
2:Bm:224:ARG:HH21	3:Cd:368:GLN:HB2	1.80	0.46
2:Bu:105:SER:HB2	2:Bu:112:LEU:HD11	1.97	0.46
3:Ch:269:MET:HE3	3:Ch:269:MET:HB3	1.92	0.46
3:Ci:262:TRP:HA	3:Ci:267:GLY:HA3	1.97	0.46
5:El:108:PRO:HB2	5:El:143:ASN:HD22	1.80	0.46
1:Aj:113:GLU:HB2	1:Aj:172:MET:HB3	1.97	0.45
2:Br:41:VAL:HG23	2:Br:83:VAL:HG21	1.98	0.45
2:Bw:250:ILE:HG23	2:Bw:261:VAL:HG22	1.98	0.45
3:Cl:292:PRO:HB3	3:Cl:306:LEU:HD13	1.97	0.45
4:Da:104:ILE:HG23	4:Db:145:ARG:HD3	1.98	0.45
4:Dx:249:PHE:HB3	4:Dx:254:LEU:HD23	1.97	0.45
1:Ak:231:ALA:HB3	1:Al:195:LYS:HG3	1.98	0.45
1:Ak:245:GLN:HG3	1:Al:200:ASN:HD21	1.81	0.45
1:Ar:200:ASN:HB3	1:Ar:201:THR:H	1.68	0.45
2:Bc:342:MET:HE2	2:Be:138:VAL:HG21	1.97	0.45
2:Bd:41:VAL:HG23	2:Bd:83:VAL:HG21	1.98	0.45
2:Bg:41:VAL:HG23	2:Bg:83:VAL:HG21	1.99	0.45
2:Bh:205:LEU:HD11	2:Bh:236:ILE:HD11	1.98	0.45
2:Bo:103:VAL:HB	2:Bo:137:LEU:HD21	1.98	0.45
2:Bp:250:ILE:HG23	2:Bp:261:VAL:HG22	1.98	0.45
2:Br:105:SER:HB2	2:Br:112:LEU:HD11	1.98	0.45
2:By:223:PRO:HB3	4:Di:94:VAL:HB	1.97	0.45
3:Ch:373:MET:HE3	3:Ch:373:MET:HB2	1.82	0.45
5:Ey:71:LEU:HB3	5:Ey:74:TYR:HB2	1.98	0.45
1:Az:112:ASN:HD21	1:Az:224:ALA:HB1	1.81	0.45
2:Bb:103:VAL:HB	2:Bb:137:LEU:HD21	1.99	0.45
2:Bc:250:ILE:HG23	2:Bc:261:VAL:HG22	1.99	0.45
2:Bg:103:VAL:HB	2:Bg:137:LEU:HD21	1.99	0.45
2:Bl:41:VAL:HG23	2:Bl:83:VAL:HG21	1.99	0.45
2:Bv:103:VAL:HB	2:Bv:137:LEU:HD21	1.99	0.45
2:Bv:105:SER:HB2	2:Bv:112:LEU:HD11	1.97	0.45
2:Bw:342:MET:HE2	2:By:138:VAL:HG21	1.97	0.45
2:By:224:ARG:HH21	3:Cp:368:GLN:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cr:241:ARG:HB3	6:Gs:143:THR:HG21	1.98	0.45
3:Cv:269:MET:HE3	3:Cv:269:MET:HB3	1.86	0.45
3:Cw:292:PRO:HB3	3:Cw:306:LEU:HD13	1.98	0.45
4:Di:141:ASP:HB2	4:Di:149:ILE:HG12	1.98	0.45
5:Eb:82:LEU:HD23	5:Eb:88:VAL:HG21	1.98	0.45
5:Ec:192:LEU:HD12	5:Ec:196:MET:HE2	1.97	0.45
5:Ej:82:LEU:HD23	5:Ej:88:VAL:HG21	1.98	0.45
5:Ej:99:MET:HB3	5:Ej:114:LEU:HD21	1.97	0.45
5:Et:154:LEU:HB3	5:Et:164:TYR:HE1	1.82	0.45
1:Ai:231:ALA:HB3	1:Aj:195:LYS:HG3	1.97	0.45
1:As:200:ASN:HB3	1:As:201:THR:H	1.68	0.45
2:Ba:250:ILE:HG23	2:Ba:261:VAL:HG22	1.98	0.45
2:Bf:103:VAL:HB	2:Bf:137:LEU:HD21	1.98	0.45
2:Bj:250:ILE:HG23	2:Bj:261:VAL:HG22	1.98	0.45
3:Cg:262:TRP:HA	3:Cg:267:GLY:HA3	1.98	0.45
3:Cs:220:PHE:HE2	3:Cs:273:VAL:HG11	1.81	0.45
3:Cs:342:ILE:HG21	3:Cs:367:ILE:HD11	1.97	0.45
3:Cz:373:MET:HE3	3:Cz:373:MET:HB2	1.84	0.45
1:Ag:64:PRO:HB2	1:Ah:38:VAL:HG13	1.99	0.45
1:Ag:231:ALA:HB3	1:Ah:195:LYS:HG3	1.97	0.45
1:Au:200:ASN:HB3	1:Au:201:THR:H	1.68	0.45
1:Au:245:GLN:HG3	1:Av:200:ASN:HD21	1.81	0.45
1:Av:200:ASN:HB3	1:Av:201:THR:H	1.68	0.45
1:Av:245:GLN:HG3	1:Aw:200:ASN:HD21	1.81	0.45
2:Bf:91:ALA:HB1	2:Bf:174:ASN:HD21	1.82	0.45
2:Bk:105:SER:HB2	2:Bk:112:LEU:HD11	1.97	0.45
2:Bm:41:VAL:HG23	2:Bm:83:VAL:HG21	1.99	0.45
2:By:105:SER:HB2	2:By:112:LEU:HD11	1.97	0.45
2:Bz:103:VAL:HB	2:Bz:137:LEU:HD21	1.98	0.45
3:Cb:88:ILE:HG23	3:Cb:106:ILE:HG12	1.98	0.45
3:Cv:342:ILE:HG21	3:Cv:367:ILE:HD11	1.98	0.45
4:Df:221:VAL:HB	4:Df:261:VAL:HG12	1.99	0.45
4:Dq:141:ASP:HB2	4:Dq:149:ILE:HG12	1.99	0.45
4:Ds:112:GLN:HE21	4:Ds:112:GLN:HB3	1.61	0.45
5:Ee:147:ARG:HD3	5:Ee:170:TRP:HB3	1.97	0.45
5:Es:202:ALA:HA	5:Es:205:LYS:HZ2	1.81	0.45
5:Ex:82:LEU:HD23	5:Ex:88:VAL:HG21	1.98	0.45
5:Ez:82:LEU:HD23	5:Ez:88:VAL:HG21	1.98	0.45
1:Ah:113:GLU:HB2	1:Ah:172:MET:HB3	1.97	0.45
1:Ai:245:GLN:HG3	1:Aj:200:ASN:HD21	1.81	0.45
1:Ap:200:ASN:HB3	1:Ap:201:THR:H	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aq:200:ASN:HB3	1:Aq:201:THR:H	1.68	0.45
2:Bb:105:SER:HB2	2:Bb:112:LEU:HD11	1.98	0.45
2:Bb:222:ALA:HB3	2:Bb:229:ARG:HH21	1.82	0.45
2:Bh:103:VAL:HB	2:Bh:137:LEU:HD21	1.99	0.45
2:Bo:41:VAL:HG23	2:Bo:83:VAL:HG21	1.99	0.45
2:Bp:205:LEU:HD11	2:Bp:236:ILE:HD11	1.98	0.45
2:Bq:205:LEU:HD11	2:Bq:236:ILE:HD11	1.98	0.45
3:Cj:255:ASP:HB3	3:Cj:258:SER:HB3	1.98	0.45
3:Co:92:GLU:HB2	3:Co:103:ARG:HB3	1.98	0.45
4:Ds:83:THR:HG22	4:Ds:111:LYS:HA	1.98	0.45
4:Dy:83:THR:HG22	4:Dy:111:LYS:HA	1.97	0.45
5:Eh:82:LEU:HD23	5:Eh:88:VAL:HG21	1.98	0.45
5:En:99:MET:HB3	5:En:114:LEU:HD21	1.97	0.45
1:Ac:245:GLN:HG3	1:Ad:200:ASN:HD21	1.81	0.45
1:Al:245:GLN:HG3	1:Am:200:ASN:HD21	1.81	0.45
2:Bb:250:ILE:HG23	2:Bb:261:VAL:HG22	1.99	0.45
2:Bc:224:ARG:HH21	3:Ct:368:GLN:HB2	1.82	0.45
2:Bh:250:ILE:HG23	2:Bh:261:VAL:HG22	1.99	0.45
2:Bw:91:ALA:HB1	2:Bw:174:ASN:HD21	1.82	0.45
3:Co:342:ILE:HG21	3:Co:367:ILE:HD11	1.99	0.45
3:Cw:157:LEU:HA	3:Cw:161:SER:HB2	1.99	0.45
4:Du:83:THR:HG22	4:Du:111:LYS:HA	1.98	0.45
1:Af:245:GLN:HG3	1:Ag:200:ASN:HD21	1.81	0.45
1:Ap:245:GLN:HG3	1:Aq:200:ASN:HD21	1.81	0.45
2:Bb:41:VAL:HG23	2:Bb:83:VAL:HG21	1.99	0.45
2:Bg:105:SER:HB2	2:Bg:112:LEU:HD11	1.99	0.45
2:Bh:41:VAL:HG23	2:Bh:83:VAL:HG21	1.99	0.45
2:Bi:250:ILE:HG23	2:Bi:261:VAL:HG22	1.98	0.45
2:Bj:41:VAL:HG23	2:Bj:83:VAL:HG21	1.99	0.45
2:Bm:91:ALA:HB1	2:Bm:174:ASN:HD21	1.82	0.45
2:Bm:103:VAL:HB	2:Bm:137:LEU:HD21	1.99	0.45
2:Bn:41:VAL:HG23	2:Bn:83:VAL:HG21	1.99	0.45
2:Bp:41:VAL:HG23	2:Bp:83:VAL:HG21	1.99	0.45
2:Bx:250:ILE:HG23	2:Bx:261:VAL:HG22	1.99	0.45
3:Cd:326:PHE:HD2	3:Cd:328:ASP:H	1.63	0.45
3:Ce:292:PRO:HB3	3:Ce:306:LEU:HD13	1.99	0.45
3:Cw:241:ARG:HB3	6:Gx:143:THR:HG21	1.98	0.45
3:Cy:157:LEU:HA	3:Cy:161:SER:HB2	1.99	0.45
4:Do:31:PRO:HB3	4:Do:156:VAL:HG21	1.99	0.45
4:Ds:31:PRO:HB3	4:Ds:156:VAL:HG21	1.99	0.45
5:Eg:147:ARG:HD3	5:Eg:170:TRP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Em:135:LEU:HB3	5:Em:150:LEU:HB2	1.98	0.45
5:Eq:71:LEU:HB3	5:Eq:74:TYR:HB2	1.98	0.45
1:Av:64:PRO:HB2	1:Aw:38:VAL:HG13	1.99	0.45
1:Ax:245:GLN:HG3	1:Ay:200:ASN:HD21	1.81	0.45
2:Ba:41:VAL:HG23	2:Ba:83:VAL:HG21	1.99	0.45
2:Bf:105:SER:HB2	2:Bf:112:LEU:HD11	1.99	0.45
2:Br:103:VAL:HB	2:Br:137:LEU:HD21	1.98	0.45
2:Bt:91:ALA:HB1	2:Bt:174:ASN:HD21	1.82	0.45
2:Bx:41:VAL:HG23	2:Bx:83:VAL:HG21	1.98	0.45
3:Co:262:TRP:HA	3:Co:267:GLY:HA3	1.98	0.45
3:Cq:63:SER:HA	3:Cq:66:ASN:HD21	1.81	0.45
4:Dd:221:VAL:HB	4:Dd:261:VAL:HG12	1.99	0.45
4:Do:141:ASP:HB2	4:Do:149:ILE:HG12	1.99	0.45
4:Dq:83:THR:HG22	4:Dq:111:LYS:HA	1.97	0.45
4:Dw:83:THR:HG22	4:Dw:111:LYS:HA	1.98	0.45
5:Ef:82:LEU:HD23	5:Ef:88:VAL:HG21	1.98	0.45
5:El:82:LEU:HD23	5:El:88:VAL:HG21	1.98	0.45
5:Ep:116:ARG:HA	5:Ep:149:GLN:HE22	1.82	0.45
5:Ev:82:LEU:HD23	5:Ev:88:VAL:HG21	1.98	0.45
1:Aj:245:GLN:HG3	1:Ak:200:ASN:HD21	1.82	0.45
1:Al:64:PRO:HB2	1:Al:38:VAL:HG13	1.99	0.45
1:Ax:112:ASN:HD21	1:Ax:224:ALA:HB1	1.82	0.45
2:Ba:105:SER:HB2	2:Ba:112:LEU:HD11	1.98	0.45
2:Bc:41:VAL:HG23	2:Bc:83:VAL:HG21	1.99	0.45
2:Be:41:VAL:HG23	2:Be:83:VAL:HG21	1.99	0.45
2:Bn:105:SER:HB2	2:Bn:112:LEU:HD11	1.98	0.45
2:Bq:41:VAL:HG23	2:Bq:83:VAL:HG21	1.99	0.45
2:Bs:41:VAL:HG23	2:Bs:83:VAL:HG21	1.99	0.45
3:Cf:262:TRP:HA	3:Cf:267:GLY:HA3	1.99	0.45
3:Ci:373:MET:HE3	3:Ci:373:MET:HB2	1.85	0.45
3:Cs:292:PRO:HB3	3:Cs:306:LEU:HD13	1.97	0.45
3:Cy:227:PHE:HD1	3:Cy:234:GLU:HA	1.82	0.45
4:Da:83:THR:HG22	4:Da:111:LYS:HA	1.98	0.45
4:Da:141:ASP:HB2	4:Da:149:ILE:HG12	1.99	0.45
4:Dw:112:GLN:HE21	4:Dw:112:GLN:HB3	1.61	0.45
1:Ab:245:GLN:HG3	1:Ac:200:ASN:HD21	1.82	0.44
1:Ae:245:GLN:HG3	1:Af:200:ASN:HD21	1.81	0.44
2:Bd:105:SER:HB2	2:Bd:112:LEU:HD11	1.99	0.44
2:Bd:250:ILE:HG23	2:Bd:261:VAL:HG22	1.98	0.44
2:Bf:41:VAL:HG23	2:Bf:83:VAL:HG21	1.99	0.44
2:Bj:224:ARG:HH21	3:Ca:368:GLN:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bt:103:VAL:HB	2:Bt:137:LEU:HD21	1.99	0.44
2:Bv:41:VAL:HG23	2:Bv:83:VAL:HG21	1.99	0.44
2:Bw:41:VAL:HG23	2:Bw:83:VAL:HG21	1.99	0.44
2:Bz:250:ILE:HG23	2:Bz:261:VAL:HG22	1.97	0.44
3:Cd:220:PHE:HE2	3:Cd:273:VAL:HG11	1.82	0.44
3:Cf:63:SER:HA	3:Cf:66:ASN:HD21	1.81	0.44
3:Cl:56:PHE:HD1	6:Gl:139:LYS:HE2	1.80	0.44
4:Db:221:VAL:HB	4:Db:261:VAL:HG12	1.99	0.44
5:Ej:116:ARG:HA	5:Ej:149:GLN:HE22	1.82	0.44
1:An:245:GLN:HG3	1:Ao:200:ASN:HD21	1.82	0.44
1:Ar:245:GLN:HG3	1:As:200:ASN:HD21	1.81	0.44
2:Bk:205:LEU:HD11	2:Bk:236:ILE:HD11	1.98	0.44
2:Bo:105:SER:HB2	2:Bo:112:LEU:HD11	1.99	0.44
2:Bo:205:LEU:HD11	2:Bo:236:ILE:HD11	1.99	0.44
2:Bw:103:VAL:HB	2:Bw:137:LEU:HD21	1.99	0.44
2:By:91:ALA:HB1	2:By:174:ASN:HD21	1.82	0.44
2:By:250:ILE:HG23	2:By:261:VAL:HG22	1.98	0.44
3:Ce:255:ASP:HB3	3:Ce:258:SER:HB3	1.99	0.44
5:Ez:116:ARG:HA	5:Ez:149:GLN:HE22	1.82	0.44
1:Ar:112:ASN:HD21	1:Ar:224:ALA:HB1	1.82	0.44
2:Bx:103:VAL:HB	2:Bx:137:LEU:HD21	1.99	0.44
3:Ca:292:PRO:HB3	3:Ca:306:LEU:HD13	1.98	0.44
3:Cc:373:MET:HE3	3:Cc:373:MET:HB2	1.88	0.44
3:Cd:255:ASP:HB3	3:Cd:258:SER:HB3	1.99	0.44
3:Cm:157:LEU:HA	3:Cm:161:SER:HB2	2.00	0.44
3:Cs:227:PHE:HD1	3:Cs:234:GLU:HA	1.83	0.44
3:Cs:249:PRO:HG2	3:Cs:252:SER:HB3	1.99	0.44
3:Ct:262:TRP:HA	3:Ct:267:GLY:HA3	1.98	0.44
3:Cv:226:VAL:HB	3:Cv:236:MET:HB3	2.00	0.44
3:Cx:373:MET:HE3	3:Cx:373:MET:HB2	1.84	0.44
4:Df:64:ALA:HB2	4:Df:172:LEU:HD22	2.00	0.44
4:Dh:93:PRO:HD3	4:Dh:133:ARG:HA	1.99	0.44
4:Dt:181:SER:HA	4:Dt:289:LEU:HD12	2.00	0.44
5:Ew:71:LEU:HB3	5:Ew:74:TYR:HB2	1.99	0.44
1:Ao:200:ASN:HB3	1:Ao:201:THR:H	1.68	0.44
2:Be:91:ALA:HB1	2:Be:174:ASN:HD21	1.82	0.44
2:Bu:41:VAL:HG23	2:Bu:83:VAL:HG21	1.99	0.44
2:Bu:250:ILE:HG23	2:Bu:261:VAL:HG22	1.98	0.44
3:Cj:227:PHE:HD1	3:Cj:234:GLU:HA	1.83	0.44
3:Ck:292:PRO:HB3	3:Ck:306:LEU:HD13	1.99	0.44
3:Cn:226:VAL:HB	3:Cn:236:MET:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cq:85:VAL:HG22	3:Cq:108:ILE:HG12	1.99	0.44
4:Dr:64:ALA:HB2	4:Dr:172:LEU:HD22	1.99	0.44
5:Ed:82:LEU:HD23	5:Ed:88:VAL:HG21	1.98	0.44
5:Ez:189:ARG:HH21	5:Ez:205:LYS:HZ1	1.64	0.44
1:At:112:ASN:HD21	1:At:224:ALA:HB1	1.83	0.44
1:Ay:234:GLN:HA	1:Az:198:THR:HB	1.99	0.44
2:Bd:205:LEU:HD11	2:Bd:236:ILE:HD11	1.99	0.44
2:Be:250:ILE:HG23	2:Be:261:VAL:HG22	1.98	0.44
2:Bk:91:ALA:HB1	2:Bk:174:ASN:HD21	1.82	0.44
2:Bm:250:ILE:HG23	2:Bm:261:VAL:HG22	1.99	0.44
3:Cv:28:VAL:HG13	3:Cv:49:ALA:HB1	2.00	0.44
4:Dc:141:ASP:HB2	4:Dc:149:ILE:HG12	1.98	0.44
4:Dg:104:ILE:HG23	4:Dh:145:ARG:HD3	2.00	0.44
5:Er:82:LEU:HD23	5:Er:88:VAL:HG21	1.98	0.44
5:Et:116:ARG:HA	5:Et:149:GLN:HE22	1.83	0.44
1:Ah:112:ASN:HD21	1:Ah:224:ALA:HB1	1.82	0.44
2:Bi:41:VAL:HG23	2:Bi:83:VAL:HG21	2.00	0.44
2:Bi:105:SER:HB2	2:Bi:112:LEU:HD11	1.99	0.44
2:Bk:41:VAL:HG23	2:Bk:83:VAL:HG21	2.00	0.44
2:Bw:105:SER:HB2	2:Bw:112:LEU:HD11	1.98	0.44
2:By:41:VAL:HG23	2:By:83:VAL:HG21	1.99	0.44
2:Bz:41:VAL:HG23	2:Bz:83:VAL:HG21	1.99	0.44
2:Bz:205:LEU:HD11	2:Bz:236:ILE:HD11	1.98	0.44
3:Cf:227:PHE:HD1	3:Cf:234:GLU:HA	1.83	0.44
3:Cs:157:LEU:HA	3:Cs:161:SER:HB2	2.00	0.44
3:Cs:222:MET:HE2	3:Cs:222:MET:HB3	1.78	0.44
3:Cu:292:PRO:HB3	3:Cu:306:LEU:HD13	1.99	0.44
3:Cx:255:ASP:HB3	3:Cx:258:SER:HB3	1.99	0.44
3:Cy:373:MET:HE3	3:Cy:373:MET:HB2	1.86	0.44
4:De:83:THR:HG22	4:De:111:LYS:HA	1.98	0.44
4:Dg:83:THR:HG22	4:Dg:111:LYS:HA	1.98	0.44
4:Dp:169:ILE:HG13	4:Dp:172:LEU:HD12	1.98	0.44
4:Dr:181:SER:HA	4:Dr:289:LEU:HD12	2.00	0.44
4:Du:93:PRO:HB2	4:Du:95:TRP:HE3	1.82	0.44
4:Dv:116:TYR:HE2	5:Ev:198:GLU:HB3	1.83	0.44
4:Dx:93:PRO:HD3	4:Dx:133:ARG:HA	1.99	0.44
4:Dy:104:ILE:HG23	4:Dz:145:ARG:HD3	2.00	0.44
5:En:82:LEU:HD23	5:En:88:VAL:HG21	1.98	0.44
5:En:154:LEU:HB3	5:En:164:TYR:HE1	1.83	0.44
1:An:200:ASN:HB3	1:An:201:THR:H	1.68	0.44
1:Au:234:GLN:HA	1:Av:198:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aw:234:GLN:HA	1:Ax:198:THR:HB	2.00	0.44
2:Bk:103:VAL:HB	2:Bk:137:LEU:HD21	1.99	0.44
2:Bl:105:SER:HB2	2:Bl:112:LEU:HD11	1.98	0.44
2:Bq:224:ARG:HH21	3:Ch:368:GLN:HB2	1.82	0.44
2:Bw:224:ARG:HH21	3:Cn:368:GLN:HB2	1.83	0.44
2:Bx:91:ALA:HB1	2:Bx:174:ASN:HD21	1.83	0.44
3:Cc:239:THR:HG21	3:Cd:155:ARG:HD3	1.99	0.44
3:Ce:227:PHE:HD1	3:Ce:234:GLU:HA	1.82	0.44
3:Cf:292:PRO:HB3	3:Cf:306:LEU:HD13	1.99	0.44
3:Ci:326:PHE:HD2	3:Ci:328:ASP:H	1.66	0.44
3:Cl:111:SER:HB3	3:Cl:113:THR:HG22	2.00	0.44
3:Cr:249:PRO:HG2	3:Cr:252:SER:HB3	1.99	0.44
4:De:31:PRO:HB3	4:De:156:VAL:HG21	1.98	0.44
4:Dj:221:VAL:HB	4:Dj:261:VAL:HG12	2.00	0.44
4:Dm:31:PRO:HB3	4:Dm:156:VAL:HG21	2.00	0.44
4:Dt:221:VAL:HB	4:Dt:261:VAL:HG12	2.00	0.44
5:Et:82:LEU:HD23	5:Et:88:VAL:HG21	1.98	0.44
1:Aa:200:ASN:HD21	1:Az:245:GLN:HG3	1.81	0.44
1:Ah:64:PRO:HB2	1:Ai:38:VAL:HG13	2.00	0.44
2:Bb:224:ARG:HH21	3:Cs:368:GLN:HB2	1.83	0.44
2:Bi:224:ARG:HH21	3:Cz:368:GLN:HB2	1.83	0.44
2:Bp:91:ALA:HB1	2:Bp:174:ASN:HD21	1.82	0.44
2:Bq:103:VAL:HB	2:Bq:137:LEU:HD21	1.99	0.44
2:Bt:41:VAL:HG23	2:Bt:83:VAL:HG21	2.00	0.44
2:Bv:205:LEU:HD11	2:Bv:236:ILE:HD11	1.99	0.44
2:Bx:222:ALA:HB3	2:Bx:229:ARG:HH21	1.83	0.44
2:By:56:GLN:HE21	2:By:56:GLN:HB3	1.71	0.44
3:Cq:292:PRO:HB3	3:Cq:306:LEU:HD13	2.00	0.44
3:Cr:92:GLU:HB2	3:Cr:103:ARG:HB3	1.99	0.44
3:Ct:226:VAL:HB	3:Ct:236:MET:HB3	2.00	0.44
4:Dn:221:VAL:HB	4:Dn:261:VAL:HG12	2.00	0.44
4:Ds:104:ILE:HG23	4:Dt:145:ARG:HD3	2.00	0.44
4:Du:112:GLN:HE21	4:Du:112:GLN:HB3	1.61	0.44
5:Ec:71:LEU:HB3	5:Ec:74:TYR:HB2	1.98	0.44
5:Ep:82:LEU:HD23	5:Ep:88:VAL:HG21	1.98	0.44
1:Aa:234:GLN:HA	1:Ab:198:THR:HB	1.99	0.44
1:Ae:119:LYS:HB3	1:Ag:199:LEU:HD12	2.00	0.44
1:Al:112:ASN:HD21	1:Al:224:ALA:HB1	1.83	0.44
2:Bf:205:LEU:HD11	2:Bf:236:ILE:HD11	2.00	0.44
2:Bn:189:SER:HA	2:Bn:216:ALA:HB2	2.00	0.44
2:Bu:103:VAL:HB	2:Bu:137:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bw:205:LEU:HD11	2:Bw:236:ILE:HD11	1.99	0.44
3:Ci:342:ILE:HG21	3:Ci:367:ILE:HD11	1.99	0.44
3:Cp:131:LEU:HD23	3:Cp:199:ILE:HB	1.98	0.44
3:Cr:292:PRO:HB3	3:Cr:306:LEU:HD13	1.99	0.44
3:Cy:342:ILE:HG21	3:Cy:367:ILE:HD11	2.00	0.44
5:En:116:ARG:HA	5:En:149:GLN:HE22	1.83	0.44
2:Bn:205:LEU:HD11	2:Bn:236:ILE:HD11	1.99	0.43
2:Bs:91:ALA:HB1	2:Bs:174:ASN:HD21	1.83	0.43
3:Ca:227:PHE:HD1	3:Ca:234:GLU:HA	1.83	0.43
3:Cm:227:PHE:HD1	3:Cm:234:GLU:HA	1.83	0.43
3:Ct:121:LYS:HG2	3:Ct:163:SER:HA	1.99	0.43
3:Cx:269:MET:HE3	3:Cx:269:MET:HB3	1.88	0.43
4:Dh:221:VAL:HB	4:Dh:261:VAL:HG12	2.00	0.43
4:Dp:93:PRO:HD3	4:Dp:133:ARG:HA	2.00	0.43
4:Dt:93:PRO:HD3	4:Dt:133:ARG:HA	2.00	0.43
4:Dw:104:ILE:HG23	4:Dx:145:ARG:HD3	1.99	0.43
1:Az:129:ASN:HB2	1:Az:156:ASN:HB3	1.99	0.43
2:Bv:224:ARG:HH21	3:Cm:368:GLN:HB2	1.82	0.43
2:Bz:105:SER:HB2	2:Bz:112:LEU:HD11	1.99	0.43
3:Cc:54:VAL:HG13	3:Cc:59:ALA:HB3	1.99	0.43
3:Ch:292:PRO:HB3	3:Ch:306:LEU:HD13	1.99	0.43
3:Cr:269:MET:HE3	3:Cr:269:MET:HB3	1.87	0.43
3:Cw:342:ILE:HG21	3:Cw:367:ILE:HD11	2.00	0.43
4:Dc:83:THR:HG22	4:Dc:111:LYS:HA	1.99	0.43
4:Dn:64:ALA:HB2	4:Dn:172:LEU:HD22	2.00	0.43
4:Dr:221:VAL:HB	4:Dr:261:VAL:HG12	2.00	0.43
4:Ds:141:ASP:HB2	4:Ds:149:ILE:HG12	2.00	0.43
4:Du:31:PRO:HB3	4:Du:156:VAL:HG21	2.01	0.43
5:Eu:71:LEU:HB3	5:Eu:74:TYR:HB2	1.99	0.43
1:Aq:234:GLN:HA	1:Ar:198:THR:HB	2.00	0.43
1:At:245:GLN:HG3	1:Au:200:ASN:HD21	1.82	0.43
2:Ba:103:VAL:HB	2:Ba:137:LEU:HD21	2.00	0.43
2:Bb:91:ALA:HB1	2:Bb:174:ASN:HD21	1.83	0.43
2:Bl:205:LEU:HD11	2:Bl:236:ILE:HD11	1.99	0.43
2:Bl:222:ALA:HB3	2:Bl:229:ARG:HH21	1.84	0.43
2:Bm:105:SER:HB2	2:Bm:112:LEU:HD11	1.99	0.43
2:Bt:205:LEU:HD11	2:Bt:236:ILE:HD11	1.99	0.43
2:Bz:91:ALA:HB1	2:Bz:174:ASN:HD21	1.84	0.43
3:Ch:262:TRP:HA	3:Ch:267:GLY:HA3	1.99	0.43
3:Cu:227:PHE:HD1	3:Cu:234:GLU:HA	1.83	0.43
3:Cw:269:MET:HE3	3:Cw:269:MET:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dp:181:SER:HA	4:Dp:289:LEU:HD12	2.00	0.43
4:Dq:31:PRO:HB3	4:Dq:156:VAL:HG21	2.00	0.43
4:Dt:116:TYR:HE2	5:Et:198:GLU:HB3	1.84	0.43
6:Gc:139:LYS:HD2	6:Gc:139:LYS:HA	1.77	0.43
1:Ad:112:ASN:HD21	1:Ad:224:ALA:HB1	1.84	0.43
1:Ae:136:LEU:HD13	1:Af:154:LEU:HD13	2.01	0.43
2:Bj:205:LEU:HD11	2:Bj:236:ILE:HD11	2.00	0.43
2:Bl:91:ALA:HB1	2:Bl:174:ASN:HD21	1.83	0.43
2:Bo:224:ARG:HH21	3:Cf:368:GLN:HB2	1.83	0.43
3:Ca:201:ASP:HB3	3:Ca:221:ALA:HB3	1.99	0.43
3:Cc:167:VAL:HG21	3:Cc:191:ALA:HB2	2.01	0.43
3:Ce:342:ILE:HG21	3:Ce:367:ILE:HD11	1.99	0.43
3:Cn:85:VAL:HG22	3:Cn:108:ILE:HG12	2.00	0.43
3:Co:34:ILE:HD11	3:Co:100:MET:HB2	2.00	0.43
3:Ct:337:VAL:HG22	3:Cu:350:TYR:HE1	1.84	0.43
3:Cy:262:TRP:HA	3:Cy:267:GLY:HA3	1.99	0.43
3:Cz:262:TRP:HA	3:Cz:267:GLY:HA3	2.00	0.43
4:Dl:93:PRO:HD3	4:Dl:133:ARG:HA	2.00	0.43
4:Dm:104:ILE:HG23	4:Dn:145:ARG:HD3	2.00	0.43
4:Dn:249:PHE:HB3	4:Dn:254:LEU:HD23	1.99	0.43
4:Do:104:ILE:HG23	4:Dp:145:ARG:HD3	2.00	0.43
4:Dv:221:VAL:HB	4:Dv:261:VAL:HG12	2.00	0.43
4:Dv:249:PHE:HB3	4:Dv:254:LEU:HD23	1.99	0.43
5:Ed:108:PRO:HB2	5:Ed:143:ASN:HD22	1.83	0.43
5:Ep:108:PRO:HB2	5:Ep:143:ASN:HD22	1.83	0.43
1:Ae:234:GLN:HA	1:Af:198:THR:HB	1.99	0.43
1:Ag:136:LEU:HD13	1:Ah:154:LEU:HD13	2.01	0.43
2:Br:91:ALA:HB1	2:Br:174:ASN:HD21	1.83	0.43
2:Br:189:SER:HA	2:Br:216:ALA:HB2	2.00	0.43
2:Bs:224:ARG:HH21	3:Cj:368:GLN:HB2	1.83	0.43
3:Ci:157:LEU:HA	3:Ci:161:SER:HB2	2.00	0.43
3:Cn:239:THR:HG21	3:Co:155:ARG:HD3	2.01	0.43
3:Cq:226:VAL:HB	3:Cq:236:MET:HB3	2.00	0.43
3:Cs:373:MET:HE3	3:Cs:373:MET:HB2	1.83	0.43
3:Cz:85:VAL:HG22	3:Cz:108:ILE:HG12	1.99	0.43
3:Cz:220:PHE:HE2	3:Cz:273:VAL:HG11	1.83	0.43
4:Df:181:SER:HA	4:Df:289:LEU:HD12	2.00	0.43
4:Dx:169:ILE:HG13	4:Dx:172:LEU:HD12	2.00	0.43
5:Ea:71:LEU:HB3	5:Ea:74:TYR:HB2	2.00	0.43
5:Ex:116:ARG:HA	5:Ex:149:GLN:HE22	1.82	0.43
1:Aa:136:LEU:HD13	1:Ab:154:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bn:91:ALA:HB1	2:Bn:174:ASN:HD21	1.82	0.43
3:Cg:227:PHE:HD1	3:Cg:234:GLU:HA	1.83	0.43
3:Cm:292:PRO:HB3	3:Cm:306:LEU:HD13	2.00	0.43
3:Ct:220:PHE:HE2	3:Ct:273:VAL:HG11	1.82	0.43
3:Cw:373:MET:HE3	3:Cw:373:MET:HB2	1.84	0.43
3:Cx:262:TRP:HA	3:Cx:267:GLY:HA3	2.00	0.43
4:Da:31:PRO:HB3	4:Da:156:VAL:HG21	2.00	0.43
4:Dk:104:ILE:HG23	4:Dl:145:ARG:HD3	1.99	0.43
1:Ar:129:ASN:HB2	1:Ar:156:ASN:HB3	2.00	0.43
1:As:234:GLN:HA	1:At:198:THR:HB	2.01	0.43
2:Bi:103:VAL:HB	2:Bi:137:LEU:HD21	2.01	0.43
2:Bp:222:ALA:HB3	2:Bp:229:ARG:HH21	1.84	0.43
2:Bq:91:ALA:HB1	2:Bq:174:ASN:HD21	1.84	0.43
3:Cb:262:TRP:HA	3:Cb:267:GLY:HA3	2.01	0.43
3:Ch:157:LEU:HA	3:Ch:161:SER:HB2	2.00	0.43
3:Cn:262:TRP:HA	3:Cn:267:GLY:HA3	2.00	0.43
3:Cn:292:PRO:HB3	3:Cn:306:LEU:HD13	1.99	0.43
3:Ct:292:PRO:HB3	3:Ct:306:LEU:HD13	2.00	0.43
4:Dv:93:PRO:HD3	4:Dv:133:ARG:HA	2.01	0.43
4:Dv:181:SER:HA	4:Dv:289:LEU:HD12	2.01	0.43
5:Ef:108:PRO:HB2	5:Ef:143:ASN:HD22	1.83	0.43
5:En:108:PRO:HB2	5:En:143:ASN:HD22	1.83	0.43
5:Es:71:LEU:HB3	5:Es:74:TYR:HB2	1.99	0.43
1:Ab:112:ASN:HD21	1:Ab:224:ALA:HB1	1.83	0.43
1:An:112:ASN:HD21	1:An:224:ALA:HB1	1.84	0.43
1:Ao:234:GLN:HA	1:Ap:198:THR:HB	2.00	0.43
2:Bd:222:ALA:HB3	2:Bd:229:ARG:HH21	1.84	0.43
2:Bh:91:ALA:HB1	2:Bh:174:ASN:HD21	1.84	0.43
2:Bl:189:SER:HA	2:Bl:216:ALA:HB2	2.01	0.43
2:Bo:91:ALA:HB1	2:Bo:174:ASN:HD21	1.84	0.43
2:Bp:189:SER:HA	2:Bp:216:ALA:HB2	2.01	0.43
2:Bs:205:LEU:HD11	2:Bs:236:ILE:HD11	2.00	0.43
3:Cc:350:TYR:HE2	3:Cc:355:GLU:HG3	1.84	0.43
3:Ce:201:ASP:HB3	3:Ce:221:ALA:HB3	1.99	0.43
3:Cg:292:PRO:HB3	3:Cg:306:LEU:HD13	1.99	0.43
3:Cg:342:ILE:HG21	3:Cg:367:ILE:HD11	2.00	0.43
3:Cj:34:ILE:HD11	3:Cj:100:MET:HB2	2.00	0.43
3:Ck:350:TYR:HE2	3:Ck:355:GLU:HG3	1.84	0.43
3:Cu:78:TYR:HD2	3:Cu:88:ILE:HB	1.83	0.43
4:Dr:116:TYR:HE2	5:Er:198:GLU:HB3	1.83	0.43
4:Du:197:LYS:HD3	4:Dv:292:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dx:181:SER:HA	4:Dx:289:LEU:HD12	2.01	0.43
4:Dz:221:VAL:HB	4:Dz:261:VAL:HG12	2.00	0.43
5:Ed:116:ARG:HA	5:Ed:149:GLN:HE22	1.84	0.43
5:Ez:154:LEU:HB3	5:Ez:164:TYR:HE1	1.84	0.43
1:Aq:36:ASP:HB3	1:Aq:39:GLU:HG2	2.00	0.43
2:Ba:91:ALA:HB1	2:Ba:174:ASN:HD21	1.84	0.43
2:Bb:205:LEU:HD11	2:Bb:236:ILE:HD11	1.99	0.43
2:Bt:105:SER:HB2	2:Bt:112:LEU:HD11	2.00	0.43
4:Dd:64:ALA:HB2	4:Dd:172:LEU:HD22	2.01	0.43
4:Dl:221:VAL:HB	4:Dl:261:VAL:HG12	2.01	0.43
4:Dr:93:PRO:HD3	4:Dr:133:ARG:HA	2.00	0.43
4:Dw:31:PRO:HB3	4:Dw:156:VAL:HG21	2.01	0.43
4:Dx:116:TYR:HE2	5:Ex:198:GLU:HB3	1.84	0.43
5:Ei:71:LEU:HB3	5:Ei:74:TYR:HB2	2.00	0.43
1:Ai:136:LEU:HD13	1:Aj:154:LEU:HD13	2.01	0.43
1:Am:200:ASN:HB3	1:Am:201:THR:H	1.68	0.43
1:Ap:129:ASN:HB2	1:Ap:156:ASN:HB3	2.01	0.43
3:Ck:226:VAL:HB	3:Ck:236:MET:HB3	2.01	0.43
3:Cp:262:TRP:HA	3:Cp:267:GLY:HA3	2.01	0.43
3:Cq:262:TRP:HA	3:Cq:267:GLY:HA3	2.00	0.43
4:Db:169:ILE:HG13	4:Db:172:LEU:HD12	2.01	0.43
4:Dh:169:ILE:HG13	4:Dh:172:LEU:HD12	2.01	0.43
4:Dl:181:SER:HA	4:Dl:289:LEU:HD12	2.00	0.43
4:Dw:264:TYR:HD1	4:Dw:264:TYR:HA	1.76	0.43
4:Dx:221:VAL:HB	4:Dx:261:VAL:HG12	2.00	0.43
5:Ee:71:LEU:HB3	5:Ee:74:TYR:HB2	2.00	0.43
5:Eg:71:LEU:HB3	5:Eg:74:TYR:HB2	2.00	0.43
5:Ez:108:PRO:HB2	5:Ez:143:ASN:HD22	1.84	0.43
6:Gc:134:GLN:HE21	6:Gc:136:VAL:HG22	1.83	0.43
1:Ac:136:LEU:HD13	1:Ad:154:LEU:HD13	2.01	0.42
2:Bx:205:LEU:HD11	2:Bx:236:ILE:HD11	1.99	0.42
3:Ca:34:ILE:HD11	3:Ca:100:MET:HB2	2.00	0.42
3:Cf:80:PHE:HD1	6:Ff:136:VAL:HG11	1.84	0.42
3:Cm:34:ILE:HD11	3:Cm:100:MET:HB2	2.00	0.42
3:Cu:34:ILE:HD11	3:Cu:100:MET:HB2	2.01	0.42
3:Cy:326:PHE:HD2	3:Cy:328:ASP:H	1.67	0.42
4:Db:185:LEU:HD22	4:Db:199:SER:HB3	2.01	0.42
4:Dc:104:ILE:HG23	4:Dd:145:ARG:HD3	2.00	0.42
4:Di:104:ILE:HG23	4:Dj:145:ARG:HD3	2.01	0.42
4:Dn:169:ILE:HG13	4:Dn:172:LEU:HD12	2.01	0.42
4:Do:112:GLN:HE21	4:Do:112:GLN:HB3	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Du:141:ASP:HB2	4:Du:149:ILE:HG12	2.00	0.42
4:Dy:141:ASP:HB2	4:Dy:149:ILE:HG12	2.00	0.42
4:Dz:169:ILE:HG13	4:Dz:172:LEU:HD12	2.01	0.42
4:Dz:249:PHE:HB3	4:Dz:254:LEU:HD23	2.00	0.42
5:Ef:116:ARG:HA	5:Ef:149:GLN:HE22	1.83	0.42
5:Et:108:PRO:HB2	5:Et:143:ASN:HD22	1.83	0.42
1:Ag:234:GLN:HA	1:Ah:198:THR:HB	2.00	0.42
1:Aj:129:ASN:HB2	1:Aj:156:ASN:HB3	2.00	0.42
1:Al:129:ASN:HB2	1:Al:156:ASN:HB3	2.01	0.42
2:Bg:205:LEU:HD11	2:Bg:236:ILE:HD11	2.00	0.42
2:Bh:40:LEU:HD23	2:Bh:82:ALA:HA	2.01	0.42
2:Bj:40:LEU:HD23	2:Bj:82:ALA:HA	2.01	0.42
2:Bt:189:SER:HA	2:Bt:216:ALA:HB2	2.01	0.42
2:Bz:224:ARG:HH21	3:Cq:368:GLN:HB2	1.85	0.42
3:Cj:249:PRO:HG2	3:Cj:252:SER:HB3	2.00	0.42
3:Cv:292:PRO:HB3	3:Cv:306:LEU:HD13	2.00	0.42
4:Db:181:SER:HA	4:Db:289:LEU:HD12	2.00	0.42
4:Dh:181:SER:HA	4:Dh:289:LEU:HD12	2.01	0.42
4:Dp:116:TYR:HE2	5:Ep:198:GLU:HB3	1.83	0.42
4:Dw:141:ASP:HB2	4:Dw:149:ILE:HG12	1.99	0.42
5:Ef:154:LEU:HB3	5:Ef:164:TYR:HE1	1.84	0.42
1:Ai:234:GLN:HA	1:Aj:198:THR:HB	2.00	0.42
1:At:234:GLN:HA	1:Au:198:THR:HB	2.01	0.42
1:Av:112:ASN:HD21	1:Av:224:ALA:HB1	1.83	0.42
1:Ax:129:ASN:HB2	1:Ax:156:ASN:HB3	2.01	0.42
2:Bc:91:ALA:HB1	2:Bc:174:ASN:HD21	1.84	0.42
2:Bd:40:LEU:HD23	2:Bd:82:ALA:HA	2.01	0.42
2:Bf:189:SER:HA	2:Bf:216:ALA:HB2	2.00	0.42
2:Bj:222:ALA:HB3	2:Bj:229:ARG:HH21	1.84	0.42
2:Bu:56:GLN:HE21	2:Bu:56:GLN:HB3	1.70	0.42
2:Bz:189:SER:HA	2:Bz:216:ALA:HB2	2.00	0.42
3:Cb:61:ILE:HD11	3:Cb:282:GLU:HG3	2.00	0.42
3:Cd:86:ARG:HA	3:Cd:86:ARG:HD3	1.84	0.42
3:Ce:209:LYS:HD2	3:Ce:212:GLN:HB2	2.01	0.42
3:Co:226:VAL:HB	3:Co:236:MET:HB3	2.01	0.42
4:Df:116:TYR:HE2	5:Ef:198:GLU:HB3	1.83	0.42
1:Ad:129:ASN:HB2	1:Ad:156:ASN:HB3	2.00	0.42
1:Af:129:ASN:HB2	1:Af:156:ASN:HB3	2.01	0.42
1:Ay:129:ASN:HB2	1:Ay:156:ASN:HB3	2.00	0.42
2:Bf:40:LEU:HD23	2:Bf:82:ALA:HA	2.01	0.42
2:Bn:222:ALA:HB3	2:Bn:229:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bv:189:SER:HA	2:Bv:216:ALA:HB2	2.01	0.42
3:Cc:157:LEU:HA	3:Cc:161:SER:HB2	2.00	0.42
3:Cf:28:VAL:HG13	3:Cf:49:ALA:HB1	2.02	0.42
3:Cg:167:VAL:HG21	3:Cg:191:ALA:HB2	2.01	0.42
3:Cm:262:TRP:HA	3:Cm:267:GLY:HA3	2.00	0.42
4:Dj:93:PRO:HD3	4:Dj:133:ARG:HA	2.00	0.42
4:Dj:169:ILE:HG13	4:Dj:172:LEU:HD12	2.00	0.42
4:Dj:181:SER:HA	4:Dj:289:LEU:HD12	2.00	0.42
4:Dk:31:PRO:HB3	4:Dk:156:VAL:HG21	2.01	0.42
4:Dq:112:GLN:HE21	4:Dq:112:GLN:HB3	1.60	0.42
4:Dt:169:ILE:HG13	4:Dt:172:LEU:HD12	2.00	0.42
5:El:116:ARG:HA	5:El:149:GLN:HE22	1.83	0.42
1:Aa:129:ASN:HB2	1:Aa:156:ASN:HB3	2.00	0.42
1:Ab:199:LEU:HB2	1:Az:119:LYS:HD2	2.02	0.42
1:Ah:136:LEU:HD13	1:Ai:154:LEU:HD13	2.02	0.42
1:Ak:129:ASN:HB2	1:Ak:156:ASN:HB3	2.00	0.42
1:Ak:136:LEU:HD13	1:Al:154:LEU:HD13	2.02	0.42
1:Av:234:GLN:HA	1:Aw:198:THR:HB	2.01	0.42
2:Bc:56:GLN:HE21	2:Bc:56:GLN:HB3	1.72	0.42
2:Bd:91:ALA:HB1	2:Bd:174:ASN:HD21	1.84	0.42
2:Bg:40:LEU:HD23	2:Bg:82:ALA:HA	2.02	0.42
2:Bh:255:ARG:HH12	2:Bj:136:ASN:HB3	1.85	0.42
2:Bh:259:ILE:HD11	2:Bh:342:MET:HB2	2.02	0.42
2:Bs:139:VAL:HG22	2:Bs:160:GLY:HA3	2.02	0.42
2:Bu:91:ALA:HB1	2:Bu:174:ASN:HD21	1.84	0.42
3:Ce:326:PHE:HD2	3:Ce:328:ASP:H	1.67	0.42
3:Ch:220:PHE:HE2	3:Ch:273:VAL:HG11	1.85	0.42
3:Cn:111:SER:HB3	3:Cn:113:THR:HG22	2.00	0.42
3:Cx:326:PHE:HD2	3:Cx:328:ASP:H	1.68	0.42
4:Dd:116:TYR:HE2	5:Ed:198:GLU:HB3	1.84	0.42
4:Dd:181:SER:HA	4:Dd:289:LEU:HD12	2.01	0.42
4:Di:249:PHE:HB3	4:Di:254:LEU:HD23	2.01	0.42
4:Dm:197:LYS:HD3	4:Dn:292:THR:HB	2.01	0.42
1:Aa:119:LYS:HB3	1:Ac:199:LEU:HD12	2.02	0.42
1:Aj:112:ASN:HD21	1:Aj:224:ALA:HB1	1.84	0.42
1:Am:136:LEU:HD13	1:An:154:LEU:HD13	2.01	0.42
1:Ao:129:ASN:HB2	1:Ao:156:ASN:HB3	2.01	0.42
1:Ar:234:GLN:HA	1:As:198:THR:HB	2.01	0.42
1:Ax:119:LYS:HD2	1:Az:199:LEU:HB2	2.02	0.42
2:Bk:40:LEU:HD23	2:Bk:82:ALA:HA	2.02	0.42
2:Bm:40:LEU:HD23	2:Bm:82:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cd:80:PHE:HA	6:Fd:136:VAL:HG21	2.02	0.42
3:Cd:167:VAL:HG21	3:Cd:191:ALA:HB2	2.01	0.42
3:Cf:126:ILE:HG13	3:Cf:154:ASN:HB2	2.02	0.42
3:Ck:157:LEU:HA	3:Ck:161:SER:HB2	2.02	0.42
3:Cn:249:PRO:HG2	3:Cn:252:SER:HB3	2.00	0.42
3:Cs:92:GLU:HB2	3:Cs:103:ARG:HB2	2.01	0.42
3:Cu:249:PRO:HG2	3:Cu:252:SER:HB3	2.02	0.42
3:Cx:157:LEU:HA	3:Cx:161:SER:HB2	2.01	0.42
4:Dc:31:PRO:HB3	4:Dc:156:VAL:HG21	2.01	0.42
4:Dr:107:LEU:HD13	4:Dr:107:LEU:HA	1.95	0.42
5:Er:108:PRO:HB2	5:Er:143:ASN:HD22	1.84	0.42
1:Aa:64:PRO:HB2	1:Ab:38:VAL:HG13	2.00	0.42
1:Ab:136:LEU:HD13	1:Ac:154:LEU:HD13	2.02	0.42
1:Ac:64:PRO:HB2	1:Ad:38:VAL:HG13	2.02	0.42
1:Ac:234:GLN:HA	1:Ad:198:THR:HB	2.01	0.42
1:Ae:36:ASP:HB3	1:Ae:39:GLU:HG2	2.02	0.42
1:Af:36:ASP:HB3	1:Af:39:GLU:HG2	2.01	0.42
1:Af:112:ASN:HD21	1:Af:224:ALA:HB1	1.84	0.42
1:Af:136:LEU:HD13	1:Ag:154:LEU:HD13	2.02	0.42
1:Ai:129:ASN:HB2	1:Ai:156:ASN:HB3	2.01	0.42
1:Aj:136:LEU:HD13	1:Ak:154:LEU:HD13	2.02	0.42
1:An:119:LYS:HD2	1:Ap:199:LEU:HB2	2.02	0.42
1:Ax:234:GLN:HA	1:Ay:198:THR:HB	2.01	0.42
2:Bb:139:VAL:HG22	2:Bb:160:GLY:HA3	2.02	0.42
2:Bj:259:ILE:HD11	2:Bj:342:MET:HB2	2.02	0.42
2:Bn:40:LEU:HD23	2:Bn:82:ALA:HA	2.01	0.42
2:Bu:139:VAL:HG22	2:Bu:160:GLY:HA3	2.02	0.42
2:Bx:105:SER:HB2	2:Bx:112:LEU:HD11	2.00	0.42
3:Cd:111:SER:HB3	3:Cd:113:THR:HG22	2.02	0.42
3:Cd:227:PHE:HD1	3:Cd:234:GLU:HA	1.84	0.42
3:Cf:255:ASP:HB3	3:Cf:258:SER:HB3	2.02	0.42
3:Cl:239:THR:HG21	3:Cm:155:ARG:HD3	2.02	0.42
3:Cx:28:VAL:HG13	3:Cx:49:ALA:HB1	2.01	0.42
4:Dm:197:LYS:HA	4:Dm:200:GLN:HB2	2.02	0.42
4:Dn:116:TYR:HE2	5:En:198:GLU:HB3	1.83	0.42
4:Dp:221:VAL:HB	4:Dp:261:VAL:HG12	2.02	0.42
5:Ex:108:PRO:HB2	5:Ex:143:ASN:HD22	1.85	0.42
1:Ab:36:ASP:HB3	1:Ab:39:GLU:HG2	2.01	0.42
1:Ad:136:LEU:HD13	1:Ae:154:LEU:HD13	2.02	0.42
1:Af:234:GLN:HA	1:Ag:198:THR:HB	2.00	0.42
1:Al:136:LEU:HD13	1:Am:154:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:136:LEU:HD13	1:Ap:154:LEU:HD13	2.01	0.42
1:Ar:119:LYS:HD2	1:At:199:LEU:HB2	2.01	0.42
1:As:36:ASP:HB3	1:As:39:GLU:HG2	2.01	0.42
1:As:136:LEU:HD13	1:At:154:LEU:HD13	2.01	0.42
1:At:107:ILE:HA	1:At:221:ASN:HD21	1.85	0.42
2:Bc:40:LEU:HD23	2:Bc:82:ALA:HA	2.02	0.42
2:Bd:259:ILE:HD11	2:Bd:342:MET:HB2	2.02	0.42
2:Be:40:LEU:HD23	2:Be:82:ALA:HA	2.02	0.42
2:Be:223:PRO:HB3	4:Do:94:VAL:HB	2.01	0.42
2:Bi:259:ILE:HD11	2:Bi:342:MET:HB2	2.02	0.42
2:Bl:40:LEU:HD23	2:Bl:82:ALA:HA	2.01	0.42
2:Bp:139:VAL:HG22	2:Bp:160:GLY:HA3	2.02	0.42
2:Bq:255:ARG:HH12	2:Bs:136:ASN:HB3	1.85	0.42
2:Bz:259:ILE:HD11	2:Bz:342:MET:HB2	2.02	0.42
3:Ce:38:GLU:HB2	3:Ce:100:MET:HE1	2.00	0.42
3:Cg:249:PRO:HG2	3:Cg:252:SER:HB3	2.01	0.42
3:Ch:249:PRO:HG2	3:Ch:252:SER:HB3	2.02	0.42
3:Ci:220:PHE:HE2	3:Ci:273:VAL:HG11	1.85	0.42
3:Ck:34:ILE:HD11	3:Ck:100:MET:HB2	2.00	0.42
3:Cw:249:PRO:HG2	3:Cw:252:SER:HB3	2.02	0.42
4:Dm:93:PRO:HB2	4:Dm:95:TRP:HE3	1.84	0.42
5:Ek:41:LEU:HA	5:Ek:44:GLU:HG2	2.02	0.42
1:Aj:119:LYS:HD2	1:Al:199:LEU:HB2	2.02	0.42
1:Al:119:LYS:HD2	1:An:199:LEU:HB2	2.02	0.42
1:Am:234:GLN:HA	1:An:198:THR:HB	2.01	0.42
1:Av:119:LYS:HD2	1:Ax:199:LEU:HB2	2.02	0.42
1:Ay:136:LEU:HD13	1:Az:154:LEU:HD13	2.02	0.42
1:Az:36:ASP:HB3	1:Az:39:GLU:HG2	2.00	0.42
2:Bb:40:LEU:HD23	2:Bb:82:ALA:HA	2.02	0.42
2:Bc:259:ILE:HD11	2:Bc:342:MET:HB2	2.02	0.42
2:Be:103:VAL:HB	2:Be:137:LEU:HD21	2.01	0.42
2:Be:224:ARG:HH21	3:Cv:368:GLN:HB2	1.85	0.42
2:Br:224:ARG:HH21	3:Ci:368:GLN:HB2	1.84	0.42
2:Bu:255:ARG:HH12	2:Bw:136:ASN:HB3	1.85	0.42
2:Bz:222:ALA:HB3	2:Bz:229:ARG:HH21	1.85	0.42
3:Cd:209:LYS:HD2	3:Cd:212:GLN:HB2	2.02	0.42
3:Ck:373:MET:HE3	3:Ck:373:MET:HB2	1.86	0.42
3:Co:153:ILE:HG21	3:Co:195:MET:HE1	2.01	0.42
3:Cv:34:ILE:HD11	3:Cv:100:MET:HB2	2.01	0.42
4:Dh:107:LEU:HD13	4:Dh:107:LEU:HA	1.95	0.42
4:Di:31:PRO:HB3	4:Di:156:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Es:41:LEU:HA	5:Es:44:GLU:HG2	2.02	0.42
5:Eu:41:LEU:HA	5:Eu:44:GLU:HG2	2.02	0.42
5:Ev:144:LEU:HA	5:Ev:147:ARG:HG2	2.02	0.42
1:Ad:119:LYS:HB3	1:Af:199:LEU:HD12	2.02	0.42
1:Af:107:ILE:HA	1:Af:221:ASN:HD21	1.85	0.42
1:Ah:234:GLN:HA	1:Ai:198:THR:HB	2.01	0.42
1:Al:200:ASN:HB3	1:Al:201:THR:H	1.68	0.42
1:An:136:LEU:HD13	1:Ao:154:LEU:HD13	2.02	0.42
1:Au:119:LYS:HD2	1:Aw:199:LEU:HB2	2.02	0.42
1:Aw:119:LYS:HD2	1:Ay:199:LEU:HB2	2.02	0.42
2:Bb:259:ILE:HD11	2:Bb:342:MET:HB2	2.02	0.42
2:Bi:40:LEU:HD23	2:Bi:82:ALA:HA	2.02	0.42
2:Bm:278:THR:HB	2:Bm:312:GLN:HB3	2.02	0.42
2:Bv:139:VAL:HG22	2:Bv:160:GLY:HA3	2.02	0.42
2:Bv:255:ARG:HH12	2:Bx:136:ASN:HB3	1.85	0.42
3:Ca:350:TYR:HE2	3:Ca:355:GLU:HG3	1.85	0.42
3:Cc:220:PHE:HE2	3:Cc:273:VAL:HG11	1.85	0.42
3:Cg:88:ILE:HG23	3:Cg:106:ILE:HG12	2.01	0.42
3:Cp:93:ARG:HG2	3:Cp:102:VAL:HG23	2.00	0.42
3:Cx:88:ILE:HG12	3:Cx:106:ILE:HG12	2.02	0.42
5:Er:116:ARG:HA	5:Er:149:GLN:HE22	1.84	0.42
1:Aa:199:LEU:HB2	1:Ay:119:LYS:HD2	2.02	0.41
1:Ah:129:ASN:HB2	1:Ah:156:ASN:HB3	2.01	0.41
1:Al:119:LYS:HB3	1:An:199:LEU:HD12	2.01	0.41
1:An:129:ASN:HB2	1:An:156:ASN:HB3	2.02	0.41
1:Ap:119:LYS:HB3	1:Ar:199:LEU:HD12	2.01	0.41
1:Ap:234:GLN:HA	1:Aq:198:THR:HB	2.02	0.41
1:Aq:119:LYS:HD2	1:As:199:LEU:HB2	2.02	0.41
1:Ar:107:ILE:HA	1:Ar:221:ASN:HD21	1.85	0.41
1:Ay:36:ASP:HB3	1:Ay:39:GLU:HG2	2.01	0.41
1:Az:107:ILE:HA	1:Az:221:ASN:HD21	1.85	0.41
2:Bb:278:THR:HB	2:Bb:312:GLN:HB3	2.02	0.41
2:Bd:139:VAL:HG22	2:Bd:160:GLY:HA3	2.02	0.41
2:Bw:83:VAL:HG12	2:Bw:105:SER:HA	2.02	0.41
3:Cc:88:ILE:HG12	3:Cc:106:ILE:HG23	2.01	0.41
3:Cf:239:THR:HG21	3:Cg:155:ARG:HD3	2.02	0.41
3:Ci:164:PHE:HZ	3:Ci:285:ILE:HB	1.84	0.41
3:Ci:350:TYR:HE2	3:Ci:355:GLU:HG3	1.85	0.41
3:Cq:88:ILE:HG23	3:Cq:106:ILE:HG12	2.02	0.41
3:Cx:167:VAL:HG21	3:Cx:191:ALA:HB2	2.02	0.41
4:Dn:184:ILE:HG12	4:Dn:286:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:234:GLN:HA	1:Ae:198:THR:HB	2.01	0.41
1:Ah:107:ILE:HA	1:Ah:221:ASN:HD21	1.85	0.41
1:Ak:119:LYS:HD2	1:Am:199:LEU:HB2	2.03	0.41
1:An:234:GLN:HA	1:Ao:198:THR:HB	2.01	0.41
1:Ap:112:ASN:HD21	1:Ap:224:ALA:HB1	1.84	0.41
1:Au:136:LEU:HD13	1:Av:154:LEU:HD13	2.01	0.41
1:Aw:136:LEU:HD13	1:Ax:154:LEU:HD13	2.01	0.41
2:Ba:40:LEU:HD23	2:Ba:82:ALA:HA	2.02	0.41
2:Ba:259:ILE:HD11	2:Ba:342:MET:HB2	2.02	0.41
2:Bf:259:ILE:HD11	2:Bf:342:MET:HB2	2.02	0.41
2:Bh:139:VAL:HG22	2:Bh:160:GLY:HA3	2.02	0.41
2:Bj:278:THR:HB	2:Bj:312:GLN:HB3	2.03	0.41
2:Bl:259:ILE:HD11	2:Bl:342:MET:HB2	2.01	0.41
2:Bl:278:THR:HB	2:Bl:312:GLN:HB3	2.03	0.41
2:Br:139:VAL:HG22	2:Br:160:GLY:HA3	2.03	0.41
2:Bt:139:VAL:HG22	2:Bt:160:GLY:HA3	2.02	0.41
2:Bx:259:ILE:HD11	2:Bx:342:MET:HB2	2.02	0.41
2:By:259:ILE:HD11	2:By:342:MET:HB2	2.02	0.41
3:Cp:326:PHE:HD2	3:Cp:328:ASP:H	1.68	0.41
3:Cq:80:PHE:HA	6:Fq:136:VAL:HG21	2.02	0.41
3:Cq:269:MET:HE3	3:Cq:269:MET:HB3	1.88	0.41
3:Ct:28:VAL:HG13	3:Ct:49:ALA:HB1	2.02	0.41
4:Dd:93:PRO:HD3	4:Dd:133:ARG:HA	2.02	0.41
4:Dh:185:LEU:HD22	4:Dh:199:SER:HB3	2.01	0.41
4:Dj:249:PHE:HB3	4:Dj:254:LEU:HD23	2.02	0.41
4:Dv:140:GLN:HA	4:Dv:148:ARG:HA	2.03	0.41
4:Dy:264:TYR:HD1	4:Dy:264:TYR:HA	1.76	0.41
4:Dz:107:LEU:HD13	4:Dz:107:LEU:HA	1.95	0.41
1:Aa:154:LEU:HD13	1:Az:136:LEU:HD13	2.02	0.41
1:Ab:107:ILE:HA	1:Ab:221:ASN:HD21	1.85	0.41
1:Ad:107:ILE:HA	1:Ad:221:ASN:HD21	1.86	0.41
1:Ak:234:GLN:HA	1:Al:198:THR:HB	2.01	0.41
1:Ap:136:LEU:HD13	1:Aq:154:LEU:HD13	2.02	0.41
1:Au:107:ILE:HA	1:Au:221:ASN:HD21	1.85	0.41
1:Aw:107:ILE:HA	1:Aw:221:ASN:HD21	1.85	0.41
1:Ax:136:LEU:HD13	1:Ay:154:LEU:HD13	2.02	0.41
2:Ba:255:ARG:HH12	2:Bc:136:ASN:HB3	1.85	0.41
2:Be:259:ILE:HD11	2:Be:342:MET:HB2	2.02	0.41
2:Bk:259:ILE:HD11	2:Bk:342:MET:HB2	2.02	0.41
2:Bo:40:LEU:HD23	2:Bo:82:ALA:HA	2.02	0.41
2:Bu:224:ARG:HH21	3:Cl:368:GLN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bz:83:VAL:HG12	2:Bz:105:SER:HA	2.03	0.41
3:Cj:269:MET:HE3	3:Cj:269:MET:HB3	1.85	0.41
3:Cl:86:ARG:HD3	3:Cl:86:ARG:HA	1.79	0.41
3:Cn:153:ILE:HG21	3:Cn:195:MET:HE1	2.02	0.41
3:Cn:220:PHE:HE2	3:Cn:273:VAL:HG11	1.84	0.41
3:Cr:205:THR:HG22	3:Cs:260:ARG:HD3	2.02	0.41
3:Cw:209:LYS:HD2	3:Cw:212:GLN:HB2	2.02	0.41
3:Cy:350:TYR:HE2	3:Cy:355:GLU:HG3	1.85	0.41
5:Ej:154:LEU:HB3	5:Ej:164:TYR:HE1	1.85	0.41
5:El:144:LEU:HA	5:El:147:ARG:HG2	2.02	0.41
5:Ex:144:LEU:HA	5:Ex:147:ARG:HG2	2.01	0.41
1:Aa:119:LYS:HD2	1:Ac:199:LEU:HB2	2.03	0.41
1:Ab:119:LYS:HD2	1:Ad:199:LEU:HB2	2.03	0.41
1:Ab:199:LEU:HD12	1:Az:119:LYS:HB3	2.02	0.41
1:Ac:119:LYS:HD2	1:Ae:199:LEU:HB2	2.03	0.41
1:Aj:107:ILE:HA	1:Aj:221:ASN:HD21	1.85	0.41
1:Al:234:GLN:HA	1:Am:198:THR:HB	2.01	0.41
1:Aq:107:ILE:HA	1:Aq:221:ASN:HD21	1.85	0.41
1:At:36:ASP:HB3	1:At:39:GLU:HG2	2.01	0.41
1:At:119:LYS:HD2	1:Av:199:LEU:HB2	2.02	0.41
1:Av:129:ASN:HB2	1:Av:156:ASN:HB3	2.01	0.41
1:Ay:107:ILE:HA	1:Ay:221:ASN:HD21	1.85	0.41
2:Bb:83:VAL:HG12	2:Bb:105:SER:HA	2.03	0.41
2:Bg:255:ARG:HH12	2:Bi:136:ASN:HB3	1.85	0.41
2:Bk:255:ARG:HH12	2:Bm:136:ASN:HB3	1.86	0.41
2:Bl:255:ARG:HH12	2:Bn:136:ASN:HB3	1.86	0.41
2:Br:83:VAL:HG12	2:Br:105:SER:HA	2.02	0.41
3:Cb:322:HIS:CD2	3:Cb:368:GLN:H	2.39	0.41
3:Ck:205:THR:HG22	3:Cl:260:ARG:HD3	2.01	0.41
3:Cp:34:ILE:HD11	3:Cp:100:MET:HB2	2.03	0.41
3:Ct:157:LEU:HA	3:Ct:161:SER:HB2	2.03	0.41
3:Ct:249:PRO:HG2	3:Ct:252:SER:HB3	2.02	0.41
3:Cv:262:TRP:HA	3:Cv:267:GLY:HA3	2.02	0.41
4:Da:175:TYR:HE1	4:Da:209:TYR:HB2	1.86	0.41
4:Df:185:LEU:HD22	4:Df:199:SER:HB3	2.01	0.41
4:Dg:141:ASP:HB2	4:Dg:149:ILE:HG12	2.02	0.41
4:Dh:249:PHE:HB3	4:Dh:254:LEU:HD23	2.01	0.41
4:Dx:183:THR:HG21	4:Dx:206:ILE:HD11	2.03	0.41
5:Em:41:LEU:HA	5:Em:44:GLU:HG2	2.02	0.41
1:Aa:198:THR:HB	1:Az:234:GLN:HA	2.01	0.41
1:An:227:ARG:HH22	1:Ao:221:ASN:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:107:ILE:HA	1:Ao:221:ASN:HD21	1.85	0.41
1:As:119:LYS:HB3	1:Au:199:LEU:HD12	2.01	0.41
1:At:64:PRO:HB2	1:Au:38:VAL:HG13	2.02	0.41
1:Av:107:ILE:HA	1:Av:221:ASN:HD21	1.85	0.41
2:Bc:83:VAL:HG12	2:Bc:105:SER:HA	2.03	0.41
2:Bd:83:VAL:HG12	2:Bd:105:SER:HA	2.03	0.41
2:Bg:259:ILE:HD11	2:Bg:342:MET:HB2	2.02	0.41
2:Bh:222:ALA:HB3	2:Bh:229:ARG:HH21	1.86	0.41
2:Bi:205:LEU:HD11	2:Bi:236:ILE:HD11	2.01	0.41
2:Bk:278:THR:HB	2:Bk:312:GLN:HB3	2.03	0.41
2:Bu:236:ILE:HD13	2:Bu:236:ILE:HA	1.95	0.41
2:Bv:83:VAL:HG12	2:Bv:105:SER:HA	2.03	0.41
2:Bx:40:LEU:HD23	2:Bx:82:ALA:HA	2.01	0.41
2:Bx:83:VAL:HG12	2:Bx:105:SER:HA	2.03	0.41
2:By:83:VAL:HG12	2:By:105:SER:HA	2.03	0.41
3:Cb:88:ILE:HG12	3:Cb:106:ILE:HG23	2.02	0.41
3:Ct:164:PHE:HZ	3:Ct:285:ILE:HB	1.85	0.41
3:Cu:226:VAL:HB	3:Cu:236:MET:HB3	2.02	0.41
3:Cv:220:PHE:HE2	3:Cv:273:VAL:HG11	1.84	0.41
4:Db:183:THR:HG21	4:Db:206:ILE:HD11	2.02	0.41
4:De:141:ASP:HB2	4:De:149:ILE:HG12	2.01	0.41
4:Dl:169:ILE:HG13	4:Dl:172:LEU:HD12	2.02	0.41
4:Dm:29:ALA:HB3	4:Dm:154:SER:HB2	2.02	0.41
4:Dm:78:ARG:HB3	4:Dm:143:GLN:HE22	1.86	0.41
4:Du:104:ILE:HG23	4:Dv:145:ARG:HD3	2.03	0.41
4:Dz:184:ILE:HG12	4:Dz:286:VAL:HG22	2.01	0.41
5:Ej:108:PRO:HB2	5:Ej:143:ASN:HD22	1.85	0.41
1:Aa:107:ILE:HA	1:Aa:221:ASN:HD21	1.86	0.41
1:Aa:199:LEU:HD12	1:Ay:119:LYS:HB3	2.02	0.41
1:Ah:119:LYS:HD2	1:Aj:199:LEU:HB2	2.03	0.41
1:Ak:200:ASN:HB3	1:Ak:201:THR:H	1.68	0.41
1:An:64:PRO:HB2	1:Ao:38:VAL:HG13	2.01	0.41
1:Ap:227:ARG:HH22	1:Aq:221:ASN:HB3	1.86	0.41
1:Aq:136:LEU:HD13	1:Ar:154:LEU:HD13	2.01	0.41
1:As:107:ILE:HA	1:As:221:ASN:HD21	1.86	0.41
1:At:129:ASN:HB2	1:At:156:ASN:HB3	2.02	0.41
2:Ba:278:THR:HB	2:Ba:312:GLN:HB3	2.02	0.41
2:Bd:278:THR:HB	2:Bd:312:GLN:HB3	2.02	0.41
2:Be:255:ARG:HH12	2:Bg:136:ASN:HB3	1.85	0.41
2:Bg:91:ALA:HB1	2:Bg:174:ASN:HD21	1.84	0.41
2:Bh:83:VAL:HG12	2:Bh:105:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bh:189:SER:HA	2:Bh:216:ALA:HB2	2.01	0.41
2:Bi:83:VAL:HG12	2:Bi:105:SER:HA	2.03	0.41
2:Bn:278:THR:HB	2:Bn:312:GLN:HB3	2.03	0.41
2:Bo:189:SER:HA	2:Bo:216:ALA:HB2	2.03	0.41
2:Bq:56:GLN:HE21	2:Bq:56:GLN:HB3	1.71	0.41
2:Br:40:LEU:HD23	2:Br:82:ALA:HA	2.01	0.41
2:Bs:83:VAL:HG12	2:Bs:105:SER:HA	2.02	0.41
2:Bv:239:LEU:HD23	2:Bv:239:LEU:HA	1.94	0.41
2:By:40:LEU:HD23	2:By:82:ALA:HA	2.02	0.41
3:Cg:34:ILE:HD11	3:Cg:100:MET:HB2	2.02	0.41
3:Ck:269:MET:HE3	3:Ck:269:MET:HB3	1.88	0.41
3:Cp:321:TRP:HE1	3:Cp:374:HIS:CE1	2.39	0.41
3:Ct:358:VAL:HG12	3:Ct:360:GLN:H	1.86	0.41
4:Da:29:ALA:HB3	4:Da:154:SER:HB2	2.03	0.41
4:Dm:112:GLN:HE21	4:Dm:112:GLN:HB3	1.61	0.41
4:Dq:91:MET:HE2	4:Dq:91:MET:HB3	1.84	0.41
5:Eo:41:LEU:HA	5:Eo:44:GLU:HG2	2.02	0.41
5:Ew:41:LEU:HA	5:Ew:44:GLU:HG2	2.02	0.41
1:Ap:64:PRO:HB2	1:Aq:38:VAL:HG13	2.02	0.41
1:Ap:107:ILE:HA	1:Ap:221:ASN:HD21	1.85	0.41
1:As:119:LYS:HD2	1:Au:199:LEU:HB2	2.03	0.41
1:Ax:107:ILE:HA	1:Ax:221:ASN:HD21	1.86	0.41
2:Bf:278:THR:HB	2:Bf:312:GLN:HB3	2.03	0.41
2:Bj:255:ARG:HH12	2:Bl:136:ASN:HB3	1.86	0.41
2:Bn:83:VAL:HG12	2:Bn:105:SER:HA	2.03	0.41
2:Bn:259:ILE:HD11	2:Bn:342:MET:HB2	2.01	0.41
2:Bu:189:SER:HA	2:Bu:216:ALA:HB2	2.03	0.41
2:Bx:189:SER:HA	2:Bx:216:ALA:HB2	2.02	0.41
2:Bz:40:LEU:HD23	2:Bz:82:ALA:HA	2.02	0.41
3:Ce:167:VAL:HG21	3:Ce:191:ALA:HB2	2.01	0.41
3:Cg:88:ILE:HG12	3:Cg:106:ILE:HG23	2.03	0.41
3:Cm:373:MET:HE3	3:Cm:373:MET:HB2	1.97	0.41
3:Cs:269:MET:HE3	3:Cs:269:MET:HB3	1.91	0.41
3:Cu:326:PHE:HD2	3:Cu:328:ASP:H	1.69	0.41
4:Dv:42:THR:HA	4:Dv:43:PRO:HD3	1.93	0.41
5:Ei:41:LEU:HA	5:Ei:44:GLU:HG2	2.02	0.41
5:Ex:90:GLN:HE21	5:Ex:90:GLN:HB2	1.72	0.41
1:Ac:107:ILE:HA	1:Ac:221:ASN:HD21	1.85	0.41
1:Ag:200:ASN:HB3	1:Ag:201:THR:H	1.68	0.41
2:Bc:236:ILE:HD13	2:Bc:236:ILE:HA	1.94	0.41
2:Bo:259:ILE:HD11	2:Bo:342:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bp:83:VAL:HG12	2:Bp:105:SER:HA	2.03	0.41
2:Br:255:ARG:HH12	2:Bt:136:ASN:HB3	1.86	0.41
2:Br:278:THR:HB	2:Br:312:GLN:HB3	2.02	0.41
2:Bv:259:ILE:HD11	2:Bv:342:MET:HB2	2.02	0.41
2:Bw:40:LEU:HD23	2:Bw:82:ALA:HA	2.02	0.41
2:Bw:255:ARG:HH12	2:By:136:ASN:HB3	1.86	0.41
3:Ca:167:VAL:HG21	3:Ca:191:ALA:HB2	2.03	0.41
3:Cb:318:LEU:HD21	3:Cb:376:GLN:HE21	1.85	0.41
3:Cd:182:ILE:HG23	3:Cd:194:ILE:HD12	2.02	0.41
3:Cd:249:PRO:HG2	3:Cd:252:SER:HB3	2.03	0.41
3:Cn:167:VAL:HG21	3:Cn:191:ALA:HB2	2.01	0.41
3:Cr:375:LYS:HE3	3:Cr:377:MET:HE2	2.02	0.41
3:Cy:201:ASP:HB3	3:Cy:221:ALA:HB3	2.02	0.41
4:De:197:LYS:HA	4:De:200:GLN:HB2	2.03	0.41
4:Du:197:LYS:HA	4:Du:200:GLN:HB2	2.03	0.41
4:Dz:185:LEU:HD22	4:Dz:199:SER:HB3	2.02	0.41
5:Eb:144:LEU:HA	5:Eb:147:ARG:HG2	2.02	0.41
1:Aa:36:ASP:HB3	1:Aa:39:GLU:HG2	2.03	0.41
1:Ac:36:ASP:HB3	1:Ac:39:GLU:HG2	2.03	0.41
1:Ad:36:ASP:HB3	1:Ad:39:GLU:HG2	2.03	0.41
1:Af:119:LYS:HD2	1:Ah:199:LEU:HB2	2.03	0.41
1:Aj:234:GLN:HA	1:Ak:198:THR:HB	2.02	0.41
1:Am:107:ILE:HA	1:Am:221:ASN:HD21	1.86	0.41
1:Ap:119:LYS:HD2	1:Ar:199:LEU:HB2	2.03	0.41
1:Aq:34:THR:HG21	3:Cg:247:PRO:HB2	2.01	0.41
1:Aq:129:ASN:HB2	1:Aq:156:ASN:HB3	2.03	0.41
1:Ar:136:LEU:HD13	1:As:154:LEU:HD13	2.02	0.41
1:Av:136:LEU:HD13	1:Aw:154:LEU:HD13	2.02	0.41
2:Bi:91:ALA:HB1	2:Bi:174:ASN:HD21	1.85	0.41
2:Bi:139:VAL:HG22	2:Bi:160:GLY:HA3	2.03	0.41
2:Bj:139:VAL:HG22	2:Bj:160:GLY:HA3	2.03	0.41
2:Bl:139:VAL:HG22	2:Bl:160:GLY:HA3	2.03	0.41
2:Bm:205:LEU:HD11	2:Bm:236:ILE:HD11	2.02	0.41
2:Bm:255:ARG:HH12	2:Bo:136:ASN:HB3	1.86	0.41
2:Bm:259:ILE:HD11	2:Bm:342:MET:HB2	2.02	0.41
2:Bo:255:ARG:HH12	2:Bq:136:ASN:HB3	1.86	0.41
2:Bo:278:THR:HB	2:Bo:312:GLN:HB3	2.03	0.41
2:Bp:40:LEU:HD23	2:Bp:82:ALA:HA	2.02	0.41
2:Bp:278:THR:HB	2:Bp:312:GLN:HB3	2.03	0.41
2:Bq:139:VAL:HG22	2:Bq:160:GLY:HA3	2.03	0.41
2:Bs:40:LEU:HD23	2:Bs:82:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bs:103:VAL:HB	2:Bs:137:LEU:HD21	2.02	0.41
2:Bu:83:VAL:HG12	2:Bu:105:SER:HA	2.03	0.41
2:Bu:259:ILE:HD11	2:Bu:342:MET:HB2	2.02	0.41
2:Bv:40:LEU:HD23	2:Bv:82:ALA:HA	2.01	0.41
2:Bv:278:THR:HB	2:Bv:312:GLN:HB3	2.02	0.41
2:Bx:255:ARG:HH12	2:Bz:136:ASN:HB3	1.86	0.41
2:Bz:139:VAL:HG22	2:Bz:160:GLY:HA3	2.03	0.41
3:Cb:157:LEU:HA	3:Cb:161:SER:HB2	2.02	0.41
3:Cd:226:VAL:HB	3:Cd:236:MET:HB3	2.03	0.41
3:Cd:294:ILE:HD12	3:Cd:302:ALA:HB1	2.03	0.41
3:Ce:111:SER:HB3	3:Ce:113:THR:HG22	2.03	0.41
3:Cj:70:LEU:HG	6:Fj:136:VAL:HG13	2.03	0.41
3:Cj:262:TRP:HA	3:Cj:267:GLY:HA3	2.02	0.41
3:Cl:269:MET:HE3	3:Cl:269:MET:HB3	1.96	0.41
3:Cm:35:VAL:HG21	3:Cm:243:VAL:HG22	2.03	0.41
3:Cn:373:MET:HE3	3:Cn:373:MET:HB2	1.82	0.41
3:Cp:249:PRO:HG2	3:Cp:252:SER:HB3	2.01	0.41
3:Cp:292:PRO:HB3	3:Cp:306:LEU:HD13	2.02	0.41
3:Cq:249:PRO:HG2	3:Cq:252:SER:HB3	2.03	0.41
3:Cr:35:VAL:HG21	3:Cr:243:VAL:HG22	2.02	0.41
3:Ct:201:ASP:HB3	3:Ct:221:ALA:HB3	2.03	0.41
3:Cv:35:VAL:HG21	3:Cv:243:VAL:HG22	2.03	0.41
3:Cy:269:MET:HE3	3:Cy:269:MET:HB3	1.91	0.41
4:Dc:264:TYR:HD1	4:Dc:264:TYR:HA	1.76	0.41
4:Dd:169:ILE:HG13	4:Dd:172:LEU:HD12	2.03	0.41
4:De:29:ALA:HB3	4:De:154:SER:HB2	2.03	0.41
4:Dn:181:SER:HA	4:Dn:289:LEU:HD12	2.02	0.41
4:Dr:183:THR:HG21	4:Dr:206:ILE:HD11	2.02	0.41
4:Dz:181:SER:HA	4:Dz:289:LEU:HD12	2.03	0.41
5:Eg:41:LEU:HA	5:Eg:44:GLU:HG2	2.02	0.41
5:Eq:41:LEU:HA	5:Eq:44:GLU:HG2	2.02	0.41
5:Et:144:LEU:HA	5:Et:147:ARG:HG2	2.03	0.41
5:Ez:144:LEU:HA	5:Ez:147:ARG:HG2	2.03	0.41
1:Ae:33:THR:HG23	1:Ae:35:VAL:H	1.86	0.41
1:Aj:36:ASP:HB3	1:Aj:39:GLU:HG2	2.02	0.41
1:Ak:107:ILE:HA	1:Ak:221:ASN:HD21	1.85	0.41
1:Ao:119:LYS:HD2	1:Aq:199:LEU:HB2	2.03	0.41
1:Aw:129:ASN:HB2	1:Aw:156:ASN:HB3	2.02	0.41
2:Bi:255:ARG:HH12	2:Bk:136:ASN:HB3	1.86	0.41
2:Bj:83:VAL:HG12	2:Bj:105:SER:HA	2.03	0.41
2:Bn:139:VAL:HG22	2:Bn:160:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bq:40:LEU:HD23	2:Bq:82:ALA:HA	2.02	0.41
2:Bu:40:LEU:HD23	2:Bu:82:ALA:HA	2.02	0.41
2:Bw:259:ILE:HD11	2:Bw:342:MET:HB2	2.02	0.41
3:Cp:167:VAL:HG21	3:Cp:191:ALA:HB2	2.02	0.41
3:Cq:88:ILE:HG12	3:Cq:106:ILE:HG23	2.03	0.41
3:Cr:326:PHE:HD2	3:Cr:328:ASP:H	1.69	0.41
3:Cv:249:PRO:HG2	3:Cv:252:SER:HB3	2.03	0.41
3:Cv:255:ASP:HB3	3:Cv:258:SER:HB3	2.01	0.41
3:Cw:86:ARG:HA	3:Cw:86:ARG:HD3	1.88	0.41
4:Di:112:GLN:HE21	4:Di:112:GLN:HB3	1.61	0.41
4:Dl:185:LEU:HD22	4:Dl:199:SER:HB3	2.02	0.41
4:Do:197:LYS:HA	4:Do:200:GLN:HB2	2.03	0.41
4:Dy:197:LYS:HA	4:Dy:200:GLN:HB2	2.03	0.41
5:Ea:41:LEU:HA	5:Ea:44:GLU:HG2	2.02	0.41
5:Ef:144:LEU:HA	5:Ef:147:ARG:HG2	2.02	0.41
5:Er:144:LEU:HA	5:Er:147:ARG:HG2	2.03	0.41
1:Aa:38:VAL:HG13	1:Aa:64:PRO:HB2	2.03	0.40
1:Ab:129:ASN:HB2	1:Ab:156:ASN:HB3	2.02	0.40
1:Ag:119:LYS:HB3	1:Ai:199:LEU:HD12	2.03	0.40
1:Ak:227:ARG:HH22	1:Al:221:ASN:HB3	1.86	0.40
1:Al:107:ILE:HA	1:Al:221:ASN:HD21	1.85	0.40
1:Am:119:LYS:HD2	1:Ao:199:LEU:HB2	2.04	0.40
1:Ao:119:LYS:HB3	1:Aq:199:LEU:HD12	2.02	0.40
1:Au:36:ASP:HB3	1:Au:39:GLU:HG2	2.03	0.40
1:Ax:36:ASP:HB3	1:Ax:39:GLU:HG2	2.03	0.40
2:Bb:255:ARG:HH12	2:Bd:136:ASN:HB3	1.86	0.40
2:Be:83:VAL:HG12	2:Be:105:SER:HA	2.03	0.40
2:Bf:255:ARG:HH12	2:Bh:136:ASN:HB3	1.86	0.40
2:Bl:205:LEU:HD13	2:Bl:209:MET:HE2	2.03	0.40
2:Bm:189:SER:HA	2:Bm:216:ALA:HB2	2.03	0.40
2:Br:222:ALA:HB3	2:Br:229:ARG:HH21	1.86	0.40
2:Bt:259:ILE:HD11	2:Bt:342:MET:HB2	2.02	0.40
2:Bt:278:THR:HB	2:Bt:312:GLN:HB3	2.02	0.40
2:Bx:278:THR:HB	2:Bx:312:GLN:HB3	2.03	0.40
3:Cm:164:PHE:HZ	3:Cm:285:ILE:HB	1.86	0.40
3:Cq:342:ILE:HG21	3:Cq:367:ILE:HD11	2.02	0.40
3:Cs:28:VAL:HG13	3:Cs:49:ALA:HB1	2.03	0.40
3:Ct:86:ARG:HD3	3:Ct:86:ARG:HA	1.84	0.40
3:Ct:92:GLU:HB2	3:Ct:103:ARG:HB3	2.03	0.40
3:Cv:70:LEU:HD22	6:Fv:136:VAL:HG13	2.03	0.40
3:Cw:167:VAL:HG21	3:Cw:191:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dc:29:ALA:HB3	4:Dc:154:SER:HB2	2.03	0.40
4:De:112:GLN:HE21	4:De:112:GLN:HB3	1.61	0.40
4:Dg:112:GLN:HE21	4:Dg:112:GLN:HB3	1.61	0.40
4:Dp:107:LEU:HD13	4:Dp:107:LEU:HA	1.95	0.40
4:Dp:185:LEU:HD22	4:Dp:199:SER:HB3	2.03	0.40
4:Dr:169:ILE:HG13	4:Dr:172:LEU:HD12	2.04	0.40
4:Ds:197:LYS:HD3	4:Dt:292:THR:HB	2.02	0.40
4:Du:266:LYS:HE3	4:Du:266:LYS:HB3	1.97	0.40
4:Dw:197:LYS:HA	4:Dw:200:GLN:HB2	2.03	0.40
4:Dz:117:ILE:HD12	4:Dz:117:ILE:HA	1.94	0.40
5:Ee:41:LEU:HA	5:Ee:44:GLU:HG2	2.02	0.40
5:Ey:41:LEU:HA	5:Ey:44:GLU:HG2	2.02	0.40
1:Ah:36:ASP:HB3	1:Ah:39:GLU:HG2	2.02	0.40
1:Am:129:ASN:HB2	1:Am:156:ASN:HB3	2.03	0.40
1:Aq:119:LYS:HB3	1:As:199:LEU:HD12	2.03	0.40
1:As:129:ASN:HB2	1:As:156:ASN:HB3	2.03	0.40
1:Au:129:ASN:HB2	1:Au:156:ASN:HB3	2.02	0.40
2:Bf:139:VAL:HG22	2:Bf:160:GLY:HA3	2.04	0.40
2:Bf:224:ARG:HH21	3:Cw:368:GLN:HB2	1.85	0.40
2:Bh:56:GLN:HE21	2:Bh:56:GLN:HB3	1.74	0.40
2:Bs:255:ARG:HH12	2:Bu:136:ASN:HB3	1.85	0.40
2:Bs:259:ILE:HD11	2:Bs:342:MET:HB2	2.02	0.40
2:Bw:189:SER:HA	2:Bw:216:ALA:HB2	2.03	0.40
2:Bz:278:THR:HB	2:Bz:312:GLN:HB3	2.03	0.40
3:Ca:262:TRP:HA	3:Ca:267:GLY:HA3	2.02	0.40
3:Ce:350:TYR:HE2	3:Ce:355:GLU:HG3	1.86	0.40
3:Ck:271:LEU:HD11	6:Gk:145:PHE:HE2	1.86	0.40
3:Cw:350:TYR:HE2	3:Cw:355:GLU:HG3	1.86	0.40
4:Dm:254:LEU:HB3	4:Dm:259:ILE:HD11	2.03	0.40
5:Ee:192:LEU:HD13	5:Ee:192:LEU:HA	1.91	0.40
1:Ab:234:GLN:HA	1:Ac:198:THR:HB	2.01	0.40
1:Ad:119:LYS:HD2	1:Af:199:LEU:HB2	2.03	0.40
1:Aj:200:ASN:HB3	1:Aj:201:THR:H	1.68	0.40
1:At:119:LYS:HB3	1:Av:199:LEU:HD12	2.02	0.40
2:Be:278:THR:HB	2:Be:312:GLN:HB3	2.03	0.40
2:Bk:83:VAL:HG12	2:Bk:105:SER:HA	2.04	0.40
2:Bm:139:VAL:HG22	2:Bm:160:GLY:HA3	2.03	0.40
2:Bp:255:ARG:HH12	2:Br:136:ASN:HB3	1.87	0.40
2:Bt:83:VAL:HG12	2:Bt:105:SER:HA	2.03	0.40
2:Bt:255:ARG:HH12	2:Bv:136:ASN:HB3	1.86	0.40
3:Cb:336:LYS:HE3	3:Cb:336:LYS:HB3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cf:358:VAL:HG12	3:Cf:360:GLN:H	1.86	0.40
3:Cm:255:ASP:HB3	3:Cm:258:SER:HB3	2.03	0.40
3:Cr:164:PHE:HZ	3:Cr:285:ILE:HB	1.87	0.40
4:Di:175:TYR:HE1	4:Di:209:TYR:HB2	1.86	0.40
4:Dk:112:GLN:HE21	4:Dk:112:GLN:HB3	1.61	0.40
4:Dq:197:LYS:HA	4:Dq:200:GLN:HB2	2.03	0.40
4:Dr:37:GLN:HG3	4:Dr:49:VAL:HG23	2.03	0.40
4:Ds:197:LYS:HA	4:Ds:200:GLN:HB2	2.03	0.40
4:Dv:169:ILE:HG13	4:Dv:172:LEU:HD12	2.03	0.40
4:Dy:29:ALA:HB3	4:Dy:154:SER:HB2	2.03	0.40
4:Dz:37:GLN:HG3	4:Dz:49:VAL:HG23	2.03	0.40
5:Ea:152:GLU:HG3	5:Ea:188:LEU:HD21	2.03	0.40
5:Ed:144:LEU:HA	5:Ed:147:ARG:HG2	2.02	0.40
5:Eo:154:LEU:HB3	5:Eo:164:TYR:HE1	1.86	0.40
1:Ag:119:LYS:HD2	1:Ai:199:LEU:HB2	2.03	0.40
1:Ai:107:ILE:HA	1:Ai:221:ASN:HD21	1.85	0.40
1:Ak:119:LYS:HB3	1:Am:199:LEU:HD12	2.02	0.40
1:At:136:LEU:HD13	1:Au:154:LEU:HD13	2.02	0.40
1:At:205:TYR:CZ	1:At:236:SER:HB3	2.57	0.40
2:Ba:83:VAL:HG12	2:Ba:105:SER:HA	2.04	0.40
2:Bc:255:ARG:HH12	2:Be:136:ASN:HB3	1.86	0.40
2:Be:139:VAL:HG22	2:Be:160:GLY:HA3	2.04	0.40
2:Bg:83:VAL:HG12	2:Bg:105:SER:HA	2.04	0.40
2:Bh:278:THR:HB	2:Bh:312:GLN:HB3	2.04	0.40
2:Bm:56:GLN:HE21	2:Bm:56:GLN:HB3	1.75	0.40
2:Bq:189:SER:HA	2:Bq:216:ALA:HB2	2.04	0.40
2:Br:259:ILE:HD11	2:Br:342:MET:HB2	2.02	0.40
2:Bt:40:LEU:HD23	2:Bt:82:ALA:HA	2.02	0.40
2:Bw:139:VAL:HG22	2:Bw:160:GLY:HA3	2.04	0.40
3:Cp:226:VAL:HB	3:Cp:236:MET:HB3	2.03	0.40
3:Cu:289:ILE:HG12	6:Fu:142:MET:HE2	2.03	0.40
3:Cw:271:LEU:HD11	6:Gw:145:PHE:HD1	1.85	0.40
4:Dd:183:THR:HG21	4:Dd:206:ILE:HD11	2.02	0.40
4:Dq:197:LYS:HD3	4:Dr:292:THR:HB	2.02	0.40
4:Dv:184:ILE:HG12	4:Dv:286:VAL:HG22	2.03	0.40
5:Eq:152:GLU:HG3	5:Eq:188:LEU:HD21	2.03	0.40
1:Ae:64:PRO:HB2	1:Af:38:VAL:HG13	2.04	0.40
1:An:107:ILE:HA	1:An:221:ASN:HD21	1.85	0.40
1:Aq:227:ARG:HH22	1:Ar:221:ASN:HB3	1.86	0.40
2:Ba:136:ASN:HB3	2:By:255:ARG:HH12	1.85	0.40
2:Bc:103:VAL:HB	2:Bc:137:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Be:56:GLN:HE21	2:Be:56:GLN:HB3	1.74	0.40
2:Bi:278:THR:HB	2:Bi:312:GLN:HB3	2.04	0.40
2:Bm:83:VAL:HG12	2:Bm:105:SER:HA	2.04	0.40
2:Bp:224:ARG:HH21	3:Cg:368:GLN:HB2	1.87	0.40
2:Bq:83:VAL:HG12	2:Bq:105:SER:HA	2.04	0.40
2:Bs:278:THR:HB	2:Bs:312:GLN:HB3	2.03	0.40
2:Bu:205:LEU:HD11	2:Bu:236:ILE:HD11	2.03	0.40
2:Bx:139:VAL:HG22	2:Bx:160:GLY:HA3	2.04	0.40
2:By:103:VAL:HB	2:By:137:LEU:HD21	2.02	0.40
3:Ca:269:MET:HE3	3:Ca:269:MET:HB3	1.94	0.40
3:Cd:373:MET:HE3	3:Cd:373:MET:HB2	1.85	0.40
3:Cu:262:TRP:HA	3:Cu:267:GLY:HA3	2.03	0.40
3:Cv:373:MET:HE3	3:Cv:373:MET:HB2	1.85	0.40
4:Dj:183:THR:HG21	4:Dj:206:ILE:HD11	2.02	0.40
4:Dk:175:TYR:HE1	4:Dk:209:TYR:HB2	1.86	0.40
4:Do:93:PRO:HB2	4:Do:95:TRP:HE3	1.86	0.40
4:Dp:107:LEU:HB3	4:Dp:108:GLN:H	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ab	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ac	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ad	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Ae	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Af	219/227 (96%)	212 (97%)	7 (3%)	0	100	100
1	Ag	219/227 (96%)	213 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ah	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ai	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Aj	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ak	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Al	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Am	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	An	219/227 (96%)	213 (97%)	6 (3%)	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%)	214 (98%)	5 (2%)	0	100	100
1	Ar	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	As	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	At	219/227 (96%)	212 (97%)	7 (3%)	0	100	100
1	Au	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Av	219/227 (96%)	214 (98%)	5 (2%)	0	100	100
1	Aw	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ax	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Ay	219/227 (96%)	213 (97%)	6 (3%)	0	100	100
1	Az	219/227 (96%)	212 (97%)	7 (3%)	0	100	100
2	Ba	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
2	Bb	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bc	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
2	Bd	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Be	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bf	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bg	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bh	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bi	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bj	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bk	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bl	312/343 (91%)	306 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bm	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bn	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bo	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
2	Bp	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
2	Bq	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
2	Br	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bs	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bt	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
2	Bu	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
2	Bv	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bw	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	Bx	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
2	By	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
2	Bz	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
3	Ca	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	Cb	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
3	Cc	350/352 (99%)	346 (99%)	4 (1%)	0	100	100
3	Cd	350/352 (99%)	345 (99%)	5 (1%)	0	100	100
3	Ce	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Cf	350/352 (99%)	345 (99%)	5 (1%)	0	100	100
3	Cg	350/352 (99%)	344 (98%)	6 (2%)	0	100	100
3	Ch	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Ci	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Cj	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Ck	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Cl	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Cm	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Cn	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Co	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	Cp	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Cq	350/352 (99%)	342 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Cr	350/352 (99%)	344 (98%)	6 (2%)	0	100	100
3	Cs	350/352 (99%)	341 (97%)	9 (3%)	0	100	100
3	Ct	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
3	Cu	350/352 (99%)	339 (97%)	11 (3%)	0	100	100
3	Cv	350/352 (99%)	345 (99%)	5 (1%)	0	100	100
3	Cw	350/352 (99%)	340 (97%)	10 (3%)	0	100	100
3	Cx	350/352 (99%)	343 (98%)	7 (2%)	0	100	100
3	Cy	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
3	Cz	350/352 (99%)	344 (98%)	6 (2%)	0	100	100
4	Da	253/272 (93%)	236 (93%)	17 (7%)	0	100	100
4	Db	254/272 (93%)	229 (90%)	23 (9%)	2 (1%)	16	49
4	Dc	253/272 (93%)	236 (93%)	17 (7%)	0	100	100
4	Dd	254/272 (93%)	230 (91%)	22 (9%)	2 (1%)	16	49
4	De	253/272 (93%)	235 (93%)	18 (7%)	0	100	100
4	Df	254/272 (93%)	231 (91%)	21 (8%)	2 (1%)	16	49
4	Dg	253/272 (93%)	237 (94%)	16 (6%)	0	100	100
4	Dh	254/272 (93%)	231 (91%)	21 (8%)	2 (1%)	16	49
4	Di	253/272 (93%)	236 (93%)	17 (7%)	0	100	100
4	Dj	254/272 (93%)	230 (91%)	22 (9%)	2 (1%)	16	49
4	Dk	253/272 (93%)	234 (92%)	19 (8%)	0	100	100
4	Dl	254/272 (93%)	230 (91%)	22 (9%)	2 (1%)	16	49
4	Dm	253/272 (93%)	237 (94%)	16 (6%)	0	100	100
4	Dn	254/272 (93%)	232 (91%)	20 (8%)	2 (1%)	16	49
4	Do	253/272 (93%)	238 (94%)	15 (6%)	0	100	100
4	Dp	254/272 (93%)	231 (91%)	21 (8%)	2 (1%)	16	49
4	Dq	253/272 (93%)	236 (93%)	17 (7%)	0	100	100
4	Dr	254/272 (93%)	230 (91%)	22 (9%)	2 (1%)	16	49
4	Ds	253/272 (93%)	237 (94%)	16 (6%)	0	100	100
4	Dt	254/272 (93%)	231 (91%)	21 (8%)	2 (1%)	16	49
4	Du	253/272 (93%)	239 (94%)	14 (6%)	0	100	100
4	Dv	254/272 (93%)	230 (91%)	22 (9%)	2 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Dw	253/272 (93%)	238 (94%)	15 (6%)	0	100	100
4	Dx	254/272 (93%)	229 (90%)	23 (9%)	2 (1%)	16	49
4	Dy	253/272 (93%)	237 (94%)	16 (6%)	0	100	100
4	Dz	254/272 (93%)	230 (91%)	22 (9%)	2 (1%)	16	49
5	Ea	181/188 (96%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	Eb	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Ec	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	21	54
5	Ed	181/188 (96%)	177 (98%)	4 (2%)	0	100	100
5	Ee	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	21	54
5	Ef	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Eg	181/188 (96%)	171 (94%)	10 (6%)	0	100	100
5	Eh	181/188 (96%)	177 (98%)	4 (2%)	0	100	100
5	Ei	181/188 (96%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	Ej	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Ek	181/188 (96%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	El	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Em	181/188 (96%)	173 (96%)	7 (4%)	1 (1%)	21	54
5	En	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Eo	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	21	54
5	Ep	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Eq	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	21	54
5	Er	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Es	181/188 (96%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	Et	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Eu	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	21	54
5	Ev	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Ew	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	21	54
5	Ex	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
5	Ey	181/188 (96%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	Ez	181/188 (96%)	177 (98%)	4 (2%)	0	100	100
6	Fa	13/15 (87%)	12 (92%)	1 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Fb	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fc	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fd	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fe	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Ff	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fg	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fh	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fi	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fj	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fk	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fl	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fm	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fn	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
6	Fo	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fp	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fq	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fr	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fs	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Ft	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fu	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fv	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fw	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fx	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fy	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Fz	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
6	Ga	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gb	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gc	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gd	11/15 (73%)	7 (64%)	4 (36%)	0	100	100
6	Ge	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gf	11/15 (73%)	9 (82%)	2 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Gg	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gh	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gi	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gj	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gk	11/15 (73%)	7 (64%)	4 (36%)	0	100	100
6	Gl	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gm	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gn	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Go	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gp	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gq	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gr	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gs	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gt	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gu	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gv	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gw	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
6	Gx	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gy	11/15 (73%)	8 (73%)	3 (27%)	0	100	100
6	Gz	11/15 (73%)	9 (82%)	2 (18%)	0	100	100
All	All	34827/36712 (95%)	33524 (96%)	1265 (4%)	38 (0%)	49	79

All (38) 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

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Mol	Chain	Res	Type
4	Dv	116	TYR
4	Dx	116	TYR
4	Dz	116	TYR
5	Ea	87	CYS
5	Ec	87	CYS
5	Ee	87	CYS
5	Ei	87	CYS
5	Ek	87	CYS
5	Em	87	CYS
5	Eo	87	CYS
5	Eq	87	CYS
5	Es	87	CYS
5	Eu	87	CYS
5	Ew	87	CYS
5	Ey	87	CYS
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
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	58
1	Ab	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Ac	182/186 (98%)	176 (97%)	6 (3%)	33	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ad	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Ae	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Af	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Ag	182/186 (98%)	177 (97%)	5 (3%)	39	61
1	Ah	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Ai	182/186 (98%)	177 (97%)	5 (3%)	39	61
1	Aj	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Ak	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Al	182/186 (98%)	177 (97%)	5 (3%)	39	61
1	Am	182/186 (98%)	177 (97%)	5 (3%)	39	61
1	An	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Ao	182/186 (98%)	177 (97%)	5 (3%)	39	61
1	Ap	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Aq	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Ar	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	As	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	At	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Au	182/186 (98%)	177 (97%)	5 (3%)	39	61
1	Av	182/186 (98%)	177 (97%)	5 (3%)	39	61
1	Aw	182/186 (98%)	177 (97%)	5 (3%)	39	61
1	Ax	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Ay	182/186 (98%)	176 (97%)	6 (3%)	33	58
1	Az	182/186 (98%)	176 (97%)	6 (3%)	33	58
2	Ba	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bb	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bc	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bd	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Be	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bf	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bg	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bh	246/269 (91%)	238 (97%)	8 (3%)	33	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bi	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bj	246/269 (91%)	239 (97%)	7 (3%)	38	60
2	Bk	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bl	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bm	246/269 (91%)	239 (97%)	7 (3%)	38	60
2	Bn	246/269 (91%)	239 (97%)	7 (3%)	38	60
2	Bo	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bp	246/269 (91%)	240 (98%)	6 (2%)	43	63
2	Bq	246/269 (91%)	239 (97%)	7 (3%)	38	60
2	Br	246/269 (91%)	239 (97%)	7 (3%)	38	60
2	Bs	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bt	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bu	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bv	246/269 (91%)	239 (97%)	7 (3%)	38	60
2	Bw	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bx	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	By	246/269 (91%)	238 (97%)	8 (3%)	33	58
2	Bz	246/269 (91%)	238 (97%)	8 (3%)	33	58
3	Ca	299/303 (99%)	297 (99%)	2 (1%)	76	78
3	Cb	299/303 (99%)	293 (98%)	6 (2%)	48	66
3	Cc	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Cd	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Ce	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Cf	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Cg	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Ch	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Ci	299/303 (99%)	292 (98%)	7 (2%)	44	64
3	Cj	299/303 (99%)	296 (99%)	3 (1%)	68	75
3	Ck	299/303 (99%)	293 (98%)	6 (2%)	48	66
3	Cl	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Cm	299/303 (99%)	296 (99%)	3 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Cn	299/303 (99%)	297 (99%)	2 (1%)	76	78
3	Co	299/303 (99%)	293 (98%)	6 (2%)	48	66
3	Cp	299/303 (99%)	294 (98%)	5 (2%)	53	69
3	Cq	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Cr	299/303 (99%)	294 (98%)	5 (2%)	53	69
3	Cs	299/303 (99%)	296 (99%)	3 (1%)	68	75
3	Ct	299/303 (99%)	297 (99%)	2 (1%)	76	78
3	Cu	299/303 (99%)	294 (98%)	5 (2%)	53	69
3	Cv	299/303 (99%)	293 (98%)	6 (2%)	48	66
3	Cw	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Cx	299/303 (99%)	295 (99%)	4 (1%)	61	72
3	Cy	299/303 (99%)	294 (98%)	5 (2%)	53	69
3	Cz	299/303 (99%)	296 (99%)	3 (1%)	68	75
4	Da	231/244 (95%)	222 (96%)	9 (4%)	28	54
4	Db	229/244 (94%)	226 (99%)	3 (1%)	61	72
4	Dc	231/244 (95%)	223 (96%)	8 (4%)	32	57
4	Dd	229/244 (94%)	225 (98%)	4 (2%)	53	69
4	De	231/244 (95%)	223 (96%)	8 (4%)	32	57
4	Df	229/244 (94%)	225 (98%)	4 (2%)	53	69
4	Dg	231/244 (95%)	222 (96%)	9 (4%)	28	54
4	Dh	229/244 (94%)	225 (98%)	4 (2%)	53	69
4	Di	231/244 (95%)	222 (96%)	9 (4%)	28	54
4	Dj	229/244 (94%)	227 (99%)	2 (1%)	70	76
4	Dk	231/244 (95%)	223 (96%)	8 (4%)	32	57
4	Dl	229/244 (94%)	226 (99%)	3 (1%)	61	72
4	Dm	231/244 (95%)	223 (96%)	8 (4%)	32	57
4	Dn	229/244 (94%)	225 (98%)	4 (2%)	53	69
4	Do	231/244 (95%)	224 (97%)	7 (3%)	36	59
4	Dp	229/244 (94%)	226 (99%)	3 (1%)	61	72
4	Dq	231/244 (95%)	223 (96%)	8 (4%)	32	57
4	Dr	229/244 (94%)	226 (99%)	3 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Ds	231/244 (95%)	222 (96%)	9 (4%)	28	54
4	Dt	229/244 (94%)	225 (98%)	4 (2%)	53	69
4	Du	231/244 (95%)	223 (96%)	8 (4%)	32	57
4	Dv	229/244 (94%)	226 (99%)	3 (1%)	61	72
4	Dw	231/244 (95%)	222 (96%)	9 (4%)	28	54
4	Dx	229/244 (94%)	227 (99%)	2 (1%)	70	76
4	Dy	231/244 (95%)	221 (96%)	10 (4%)	26	52
4	Dz	229/244 (94%)	227 (99%)	2 (1%)	70	76
5	Ea	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	Eb	154/157 (98%)	148 (96%)	6 (4%)	28	54
5	Ec	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	Ed	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Ee	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	Ef	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Eg	149/157 (95%)	141 (95%)	8 (5%)	20	47
5	Eh	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Ei	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	Ej	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Ek	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	El	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Em	149/157 (95%)	144 (97%)	5 (3%)	32	57
5	En	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Eo	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	Ep	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Eq	149/157 (95%)	143 (96%)	6 (4%)	28	54
5	Er	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Es	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	Et	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Eu	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	Ev	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Ew	149/157 (95%)	142 (95%)	7 (5%)	23	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Ex	154/157 (98%)	147 (96%)	7 (4%)	24	51
5	Ey	149/157 (95%)	142 (95%)	7 (5%)	23	50
5	Ez	154/157 (98%)	147 (96%)	7 (4%)	24	51
6	Fa	14/14 (100%)	14 (100%)	0	100	100
6	Fb	14/14 (100%)	13 (93%)	1 (7%)	13	40
6	Fc	14/14 (100%)	14 (100%)	0	100	100
6	Fd	14/14 (100%)	14 (100%)	0	100	100
6	Fe	14/14 (100%)	13 (93%)	1 (7%)	13	40
6	Ff	14/14 (100%)	13 (93%)	1 (7%)	13	40
6	Fg	14/14 (100%)	13 (93%)	1 (7%)	13	40
6	Fh	14/14 (100%)	14 (100%)	0	100	100
6	Fi	14/14 (100%)	13 (93%)	1 (7%)	13	40
6	Fj	14/14 (100%)	13 (93%)	1 (7%)	13	40
6	Fk	14/14 (100%)	14 (100%)	0	100	100
6	Fl	14/14 (100%)	14 (100%)	0	100	100
6	Fm	14/14 (100%)	14 (100%)	0	100	100
6	Fn	14/14 (100%)	14 (100%)	0	100	100
6	Fo	14/14 (100%)	14 (100%)	0	100	100
6	Fp	14/14 (100%)	14 (100%)	0	100	100
6	Fq	14/14 (100%)	14 (100%)	0	100	100
6	Fr	14/14 (100%)	14 (100%)	0	100	100
6	Fs	14/14 (100%)	14 (100%)	0	100	100
6	Ft	14/14 (100%)	13 (93%)	1 (7%)	13	40
6	Fu	14/14 (100%)	13 (93%)	1 (7%)	13	40
6	Fv	14/14 (100%)	14 (100%)	0	100	100
6	Fw	14/14 (100%)	14 (100%)	0	100	100
6	Fx	14/14 (100%)	14 (100%)	0	100	100
6	Fy	14/14 (100%)	14 (100%)	0	100	100
6	Fz	14/14 (100%)	14 (100%)	0	100	100
6	Ga	13/14 (93%)	13 (100%)	0	100	100
6	Gb	13/14 (93%)	12 (92%)	1 (8%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Gc	13/14 (93%)	13 (100%)	0	100	100
6	Gd	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Ge	13/14 (93%)	13 (100%)	0	100	100
6	Gf	13/14 (93%)	13 (100%)	0	100	100
6	Gg	13/14 (93%)	13 (100%)	0	100	100
6	Gh	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gi	13/14 (93%)	11 (85%)	2 (15%)	2	16
6	Gj	13/14 (93%)	13 (100%)	0	100	100
6	Gk	13/14 (93%)	13 (100%)	0	100	100
6	Gl	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gm	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gn	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Go	13/14 (93%)	13 (100%)	0	100	100
6	Gp	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gq	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gr	13/14 (93%)	13 (100%)	0	100	100
6	Gs	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gt	13/14 (93%)	11 (85%)	2 (15%)	2	16
6	Gu	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gv	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gw	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gx	13/14 (93%)	13 (100%)	0	100	100
6	Gy	13/14 (93%)	12 (92%)	1 (8%)	12	38
6	Gz	13/14 (93%)	13 (100%)	0	100	100
All	All	29523/30862 (96%)	28711 (97%)	812 (3%)	38	60

All (812) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	60	VAL
1	Aa	112	ASN
1	Aa	145	ILE
1	Aa	176	ILE
1	Aa	200	ASN

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Mol	Chain	Res	Type
1	Aa	201	THR
1	Ab	60	VAL
1	Ab	112	ASN
1	Ab	145	ILE
1	Ab	176	ILE
1	Ab	200	ASN
1	Ab	201	THR
1	Ac	60	VAL
1	Ac	112	ASN
1	Ac	145	ILE
1	Ac	176	ILE
1	Ac	200	ASN
1	Ac	201	THR
1	Ad	60	VAL
1	Ad	112	ASN
1	Ad	145	ILE
1	Ad	176	ILE
1	Ad	200	ASN
1	Ad	201	THR
1	Ae	60	VAL
1	Ae	112	ASN
1	Ae	145	ILE
1	Ae	176	ILE
1	Ae	200	ASN
1	Ae	201	THR
1	Af	60	VAL
1	Af	112	ASN
1	Af	145	ILE
1	Af	176	ILE
1	Af	200	ASN
1	Af	201	THR
1	Ag	112	ASN
1	Ag	145	ILE
1	Ag	176	ILE
1	Ag	200	ASN
1	Ag	201	THR
1	Ah	60	VAL
1	Ah	112	ASN
1	Ah	145	ILE
1	Ah	176	ILE
1	Ah	200	ASN
1	Ah	201	THR

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Mol	Chain	Res	Type
1	Ai	112	ASN
1	Ai	145	ILE
1	Ai	176	ILE
1	Ai	200	ASN
1	Ai	201	THR
1	Aj	60	VAL
1	Aj	112	ASN
1	Aj	145	ILE
1	Aj	176	ILE
1	Aj	200	ASN
1	Aj	201	THR
1	Ak	60	VAL
1	Ak	112	ASN
1	Ak	145	ILE
1	Ak	176	ILE
1	Ak	200	ASN
1	Ak	201	THR
1	Al	112	ASN
1	Al	145	ILE
1	Al	176	ILE
1	Al	200	ASN
1	Al	201	THR
1	Am	112	ASN
1	Am	145	ILE
1	Am	176	ILE
1	Am	200	ASN
1	Am	201	THR
1	An	60	VAL
1	An	112	ASN
1	An	145	ILE
1	An	176	ILE
1	An	200	ASN
1	An	201	THR
1	Ao	112	ASN
1	Ao	145	ILE
1	Ao	176	ILE
1	Ao	200	ASN
1	Ao	201	THR
1	Ap	60	VAL
1	Ap	112	ASN
1	Ap	145	ILE
1	Ap	176	ILE

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Mol	Chain	Res	Type
1	Ap	200	ASN
1	Ap	201	THR
1	Aq	60	VAL
1	Aq	112	ASN
1	Aq	145	ILE
1	Aq	176	ILE
1	Aq	200	ASN
1	Aq	201	THR
1	Ar	60	VAL
1	Ar	112	ASN
1	Ar	145	ILE
1	Ar	176	ILE
1	Ar	200	ASN
1	Ar	201	THR
1	As	60	VAL
1	As	112	ASN
1	As	145	ILE
1	As	176	ILE
1	As	200	ASN
1	As	201	THR
1	At	60	VAL
1	At	112	ASN
1	At	145	ILE
1	At	176	ILE
1	At	200	ASN
1	At	201	THR
1	Au	112	ASN
1	Au	145	ILE
1	Au	176	ILE
1	Au	200	ASN
1	Au	201	THR
1	Av	112	ASN
1	Av	145	ILE
1	Av	176	ILE
1	Av	200	ASN
1	Av	201	THR
1	Aw	112	ASN
1	Aw	145	ILE
1	Aw	176	ILE
1	Aw	200	ASN
1	Aw	201	THR
1	Ax	60	VAL

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Mol	Chain	Res	Type
1	Ax	112	ASN
1	Ax	145	ILE
1	Ax	176	ILE
1	Ax	200	ASN
1	Ax	201	THR
1	Ay	60	VAL
1	Ay	112	ASN
1	Ay	145	ILE
1	Ay	176	ILE
1	Ay	200	ASN
1	Ay	201	THR
1	Az	60	VAL
1	Az	112	ASN
1	Az	145	ILE
1	Az	176	ILE
1	Az	200	ASN
1	Az	201	THR
2	Ba	36	VAL
2	Ba	145	THR
2	Ba	233	LEU
2	Ba	253	ASN
2	Ba	256	THR
2	Ba	258	THR
2	Ba	273	THR
2	Ba	322	VAL
2	Bb	36	VAL
2	Bb	145	THR
2	Bb	233	LEU
2	Bb	253	ASN
2	Bb	256	THR
2	Bb	258	THR
2	Bb	273	THR
2	Bb	322	VAL
2	Bc	36	VAL
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	36	VAL

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Mol	Chain	Res	Type
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	36	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	36	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	36	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	36	VAL
2	Bh	145	THR
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	36	VAL
2	Bi	145	THR
2	Bi	233	LEU

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Mol	Chain	Res	Type
2	Bi	253	ASN
2	Bi	256	THR
2	Bi	258	THR
2	Bi	273	THR
2	Bi	322	VAL
2	Bj	36	VAL
2	Bj	145	THR
2	Bj	233	LEU
2	Bj	253	ASN
2	Bj	256	THR
2	Bj	258	THR
2	Bj	322	VAL
2	Bk	36	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	36	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
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

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Mol	Chain	Res	Type
2	Bo	36	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	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	36	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
2	Bt	36	VAL
2	Bt	145	THR
2	Bt	233	LEU
2	Bt	253	ASN
2	Bt	256	THR
2	Bt	258	THR

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Mol	Chain	Res	Type
2	Bt	273	THR
2	Bt	322	VAL
2	Bu	36	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	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	36	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	36	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	36	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
2	By	322	VAL
2	Bz	36	VAL

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Mol	Chain	Res	Type
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	Cb	102	VAL
3	Cb	107	ASP
3	Cb	254	ILE
3	Cb	327	ILE
3	Cb	362	GLU
3	Cb	363	LEU
3	Cc	35	VAL
3	Cc	102	VAL
3	Cc	327	ILE
3	Cc	353	GLU
3	Cd	35	VAL
3	Cd	243	VAL
3	Cd	327	ILE
3	Cd	353	GLU
3	Ce	102	VAL
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	328	ASP
3	Cg	35	VAL
3	Cg	87	TYR
3	Cg	327	ILE
3	Cg	353	GLU
3	Ch	154	ASN
3	Ch	243	VAL
3	Ch	327	ILE
3	Ch	353	GLU
3	Ci	89	LEU
3	Ci	117	VAL
3	Ci	154	ASN

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Mol	Chain	Res	Type
3	Ci	237	THR
3	Ci	286	SER
3	Ci	327	ILE
3	Ci	353	GLU
3	Cj	154	ASN
3	Cj	243	VAL
3	Cj	353	GLU
3	Ck	89	LEU
3	Ck	237	THR
3	Ck	243	VAL
3	Ck	286	SER
3	Ck	327	ILE
3	Ck	353	GLU
3	Cl	61	ILE
3	Cl	89	LEU
3	Cl	208	GLN
3	Cl	327	ILE
3	Cm	35	VAL
3	Cm	327	ILE
3	Cm	353	GLU
3	Cn	286	SER
3	Cn	327	ILE
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	243	VAL
3	Cp	327	ILE
3	Cp	353	GLU
3	Cp	375	LYS
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	327	ILE
3	Cr	328	ASP

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Mol	Chain	Res	Type
3	Cs	237	THR
3	Cs	243	VAL
3	Cs	327	ILE
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	Cv	35	VAL
3	Cv	87	TYR
3	Cv	243	VAL
3	Cv	320	LEU
3	Cv	327	ILE
3	Cv	353	GLU
3	Cw	237	THR
3	Cw	286	SER
3	Cw	327	ILE
3	Cw	353	GLU
3	Cx	243	VAL
3	Cx	327	ILE
3	Cx	353	GLU
3	Cx	363	LEU
3	Cy	107	ASP
3	Cy	237	THR
3	Cy	286	SER
3	Cy	327	ILE
3	Cy	353	GLU
3	Cz	243	VAL
3	Cz	286	SER
3	Cz	327	ILE
4	Da	89	VAL
4	Da	106	ASN
4	Da	112	GLN
4	Da	117	ILE
4	Da	149	ILE
4	Da	180	ILE
4	Da	250	LYS
4	Da	264	TYR
4	Da	266	LYS
4	Db	25	VAL

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Mol	Chain	Res	Type
4	Db	89	VAL
4	Db	220	LEU
4	Dc	89	VAL
4	Dc	106	ASN
4	Dc	112	GLN
4	Dc	117	ILE
4	Dc	149	ILE
4	Dc	250	LYS
4	Dc	264	TYR
4	Dc	266	LYS
4	Dd	25	VAL
4	Dd	68	ILE
4	Dd	89	VAL
4	Dd	220	LEU
4	De	89	VAL
4	De	106	ASN
4	De	112	GLN
4	De	149	ILE
4	De	180	ILE
4	De	250	LYS
4	De	264	TYR
4	De	266	LYS
4	Df	25	VAL
4	Df	68	ILE
4	Df	89	VAL
4	Df	220	LEU
4	Dg	89	VAL
4	Dg	106	ASN
4	Dg	112	GLN
4	Dg	117	ILE
4	Dg	149	ILE
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	89	VAL
4	Dh	220	LEU
4	Di	89	VAL
4	Di	106	ASN
4	Di	112	GLN

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Mol	Chain	Res	Type
4	Di	117	ILE
4	Di	149	ILE
4	Di	180	ILE
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	250	LYS
4	Dk	264	TYR
4	Dk	266	LYS
4	Dl	25	VAL
4	Dl	89	VAL
4	Dl	220	LEU
4	Dm	89	VAL
4	Dm	106	ASN
4	Dm	112	GLN
4	Dm	117	ILE
4	Dm	149	ILE
4	Dm	250	LYS
4	Dm	264	TYR
4	Dm	266	LYS
4	Dn	25	VAL
4	Dn	68	ILE
4	Dn	89	VAL
4	Dn	220	LEU
4	Do	89	VAL
4	Do	106	ASN
4	Do	112	GLN
4	Do	149	ILE
4	Do	250	LYS
4	Do	264	TYR
4	Do	266	LYS
4	Dp	25	VAL
4	Dp	89	VAL
4	Dp	220	LEU
4	Dq	89	VAL

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Mol	Chain	Res	Type
4	Dq	106	ASN
4	Dq	112	GLN
4	Dq	117	ILE
4	Dq	149	ILE
4	Dq	250	LYS
4	Dq	264	TYR
4	Dq	266	LYS
4	Dr	25	VAL
4	Dr	89	VAL
4	Dr	220	LEU
4	Ds	89	VAL
4	Ds	106	ASN
4	Ds	112	GLN
4	Ds	117	ILE
4	Ds	149	ILE
4	Ds	180	ILE
4	Ds	250	LYS
4	Ds	264	TYR
4	Ds	266	LYS
4	Dt	25	VAL
4	Dt	68	ILE
4	Dt	89	VAL
4	Dt	220	LEU
4	Du	89	VAL
4	Du	106	ASN
4	Du	112	GLN
4	Du	117	ILE
4	Du	149	ILE
4	Du	250	LYS
4	Du	264	TYR
4	Du	266	LYS
4	Dv	25	VAL
4	Dv	89	VAL
4	Dv	220	LEU
4	Dw	89	VAL
4	Dw	106	ASN
4	Dw	112	GLN
4	Dw	117	ILE
4	Dw	149	ILE
4	Dw	180	ILE
4	Dw	250	LYS
4	Dw	264	TYR

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Mol	Chain	Res	Type
4	Dw	266	LYS
4	Dx	25	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	149	ILE
4	Dy	180	ILE
4	Dy	250	LYS
4	Dy	264	TYR
4	Dy	266	LYS
4	Dz	25	VAL
4	Dz	220	LEU
5	Ea	38	LEU
5	Ea	71	LEU
5	Ea	92	VAL
5	Ea	107	LEU
5	Ea	111	LEU
5	Ea	124	VAL
5	Ea	143	ASN
5	Eb	48	LEU
5	Eb	90	GLN
5	Eb	91	ASP
5	Eb	94	LEU
5	Eb	107	LEU
5	Eb	144	LEU
5	Ec	38	LEU
5	Ec	71	LEU
5	Ec	92	VAL
5	Ec	107	LEU
5	Ec	124	VAL
5	Ec	188	LEU
5	Ec	192	LEU
5	Ed	48	LEU
5	Ed	90	GLN
5	Ed	91	ASP
5	Ed	94	LEU
5	Ed	107	LEU
5	Ed	144	LEU
5	Ed	150	LEU

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Mol	Chain	Res	Type
5	Ee	38	LEU
5	Ee	71	LEU
5	Ee	92	VAL
5	Ee	107	LEU
5	Ee	124	VAL
5	Ee	188	LEU
5	Ee	192	LEU
5	Ef	48	LEU
5	Ef	90	GLN
5	Ef	91	ASP
5	Ef	94	LEU
5	Ef	107	LEU
5	Ef	144	LEU
5	Ef	150	LEU
5	Eg	38	LEU
5	Eg	71	LEU
5	Eg	92	VAL
5	Eg	107	LEU
5	Eg	124	VAL
5	Eg	143	ASN
5	Eg	188	LEU
5	Eg	192	LEU
5	Eh	48	LEU
5	Eh	90	GLN
5	Eh	91	ASP
5	Eh	94	LEU
5	Eh	107	LEU
5	Eh	145	ASN
5	Eh	150	LEU
5	Ei	38	LEU
5	Ei	71	LEU
5	Ei	92	VAL
5	Ei	107	LEU
5	Ei	124	VAL
5	Ei	188	LEU
5	Ei	192	LEU
5	Ej	48	LEU
5	Ej	90	GLN
5	Ej	91	ASP
5	Ej	94	LEU
5	Ej	107	LEU
5	Ej	144	LEU

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Mol	Chain	Res	Type
5	Ej	150	LEU
5	Ek	38	LEU
5	Ek	71	LEU
5	Ek	92	VAL
5	Ek	107	LEU
5	Ek	124	VAL
5	Ek	188	LEU
5	Ek	192	LEU
5	El	48	LEU
5	El	90	GLN
5	El	91	ASP
5	El	94	LEU
5	El	107	LEU
5	El	144	LEU
5	El	150	LEU
5	Em	38	LEU
5	Em	71	LEU
5	Em	92	VAL
5	Em	107	LEU
5	Em	124	VAL
5	En	48	LEU
5	En	90	GLN
5	En	91	ASP
5	En	94	LEU
5	En	107	LEU
5	En	144	LEU
5	En	150	LEU
5	Eo	38	LEU
5	Eo	71	LEU
5	Eo	92	VAL
5	Eo	107	LEU
5	Eo	124	VAL
5	Eo	188	LEU
5	Eo	192	LEU
5	Ep	48	LEU
5	Ep	90	GLN
5	Ep	91	ASP
5	Ep	94	LEU
5	Ep	107	LEU
5	Ep	144	LEU
5	Ep	150	LEU
5	Eq	38	LEU

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Mol	Chain	Res	Type
5	Eq	71	LEU
5	Eq	92	VAL
5	Eq	107	LEU
5	Eq	124	VAL
5	Eq	143	ASN
5	Er	48	LEU
5	Er	90	GLN
5	Er	91	ASP
5	Er	94	LEU
5	Er	107	LEU
5	Er	144	LEU
5	Er	150	LEU
5	Es	38	LEU
5	Es	71	LEU
5	Es	92	VAL
5	Es	107	LEU
5	Es	124	VAL
5	Es	188	LEU
5	Es	192	LEU
5	Et	48	LEU
5	Et	90	GLN
5	Et	91	ASP
5	Et	94	LEU
5	Et	107	LEU
5	Et	144	LEU
5	Et	150	LEU
5	Eu	38	LEU
5	Eu	71	LEU
5	Eu	92	VAL
5	Eu	107	LEU
5	Eu	124	VAL
5	Eu	188	LEU
5	Eu	192	LEU
5	Ev	48	LEU
5	Ev	90	GLN
5	Ev	91	ASP
5	Ev	94	LEU
5	Ev	107	LEU
5	Ev	144	LEU
5	Ev	150	LEU
5	Ew	38	LEU
5	Ew	71	LEU

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Mol	Chain	Res	Type
5	Ew	92	VAL
5	Ew	107	LEU
5	Ew	124	VAL
5	Ew	188	LEU
5	Ew	192	LEU
5	Ex	48	LEU
5	Ex	90	GLN
5	Ex	91	ASP
5	Ex	94	LEU
5	Ex	107	LEU
5	Ex	144	LEU
5	Ex	150	LEU
5	Ey	38	LEU
5	Ey	71	LEU
5	Ey	92	VAL
5	Ey	107	LEU
5	Ey	124	VAL
5	Ey	188	LEU
5	Ey	192	LEU
5	Ez	48	LEU
5	Ez	90	GLN
5	Ez	91	ASP
5	Ez	94	LEU
5	Ez	107	LEU
5	Ez	144	LEU
5	Ez	150	LEU
6	Fb	145	PHE
6	Fe	139	LYS
6	Ff	139	LYS
6	Fg	140	ARG
6	Fi	139	LYS
6	Fj	139	LYS
6	Ft	139	LYS
6	Fu	139	LYS
6	Gb	138	GLU
6	Gd	138	GLU
6	Gh	138	GLU
6	Gi	134	GLN
6	Gi	138	GLU
6	Gl	138	GLU
6	Gm	138	GLU
6	Gn	141	GLN

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Mol	Chain	Res	Type
6	Gp	138	GLU
6	Gq	138	GLU
6	Gs	138	GLU
6	Gt	134	GLN
6	Gt	141	GLN
6	Gu	138	GLU
6	Gv	138	GLU
6	Gw	138	GLU
6	Gy	138	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (735) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	112	ASN
1	Aa	129	ASN
1	Aa	156	ASN
1	Aa	158	ASN
1	Aa	200	ASN
1	Aa	226	ASN
1	Aa	255	ASN
1	Ab	112	ASN
1	Ab	129	ASN
1	Ab	156	ASN
1	Ab	158	ASN
1	Ab	200	ASN
1	Ab	226	ASN
1	Ab	255	ASN
1	Ac	112	ASN
1	Ac	129	ASN
1	Ac	156	ASN
1	Ac	158	ASN
1	Ac	200	ASN
1	Ac	226	ASN
1	Ac	255	ASN
1	Ad	112	ASN
1	Ad	129	ASN
1	Ad	149	ASN
1	Ad	156	ASN
1	Ad	158	ASN
1	Ad	200	ASN
1	Ad	226	ASN
1	Ad	255	ASN

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Mol	Chain	Res	Type
1	Ae	112	ASN
1	Ae	129	ASN
1	Ae	149	ASN
1	Ae	156	ASN
1	Ae	158	ASN
1	Ae	200	ASN
1	Ae	226	ASN
1	Ae	255	ASN
1	Af	112	ASN
1	Af	129	ASN
1	Af	149	ASN
1	Af	156	ASN
1	Af	158	ASN
1	Af	200	ASN
1	Af	226	ASN
1	Af	255	ASN
1	Ag	112	ASN
1	Ag	129	ASN
1	Ag	200	ASN
1	Ag	226	ASN
1	Ag	255	ASN
1	Ah	77	HIS
1	Ah	112	ASN
1	Ah	129	ASN
1	Ah	149	ASN
1	Ah	156	ASN
1	Ah	158	ASN
1	Ah	200	ASN
1	Ah	226	ASN
1	Ah	255	ASN
1	Ai	112	ASN
1	Ai	129	ASN
1	Ai	149	ASN
1	Ai	156	ASN
1	Ai	158	ASN
1	Ai	200	ASN
1	Ai	226	ASN
1	Ai	255	ASN
1	Aj	112	ASN
1	Aj	129	ASN
1	Aj	149	ASN
1	Aj	156	ASN

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Mol	Chain	Res	Type
1	Aj	158	ASN
1	Aj	200	ASN
1	Aj	226	ASN
1	Aj	255	ASN
1	Ak	112	ASN
1	Ak	129	ASN
1	Ak	149	ASN
1	Ak	156	ASN
1	Ak	158	ASN
1	Ak	200	ASN
1	Ak	226	ASN
1	Ak	255	ASN
1	Al	112	ASN
1	Al	129	ASN
1	Al	149	ASN
1	Al	156	ASN
1	Al	158	ASN
1	Al	200	ASN
1	Al	226	ASN
1	Al	255	ASN
1	Am	112	ASN
1	Am	129	ASN
1	Am	149	ASN
1	Am	156	ASN
1	Am	158	ASN
1	Am	200	ASN
1	Am	226	ASN
1	Am	242	GLN
1	Am	255	ASN
1	An	112	ASN
1	An	129	ASN
1	An	156	ASN
1	An	158	ASN
1	An	200	ASN
1	An	226	ASN
1	An	255	ASN
1	Ao	112	ASN
1	Ao	129	ASN
1	Ao	156	ASN
1	Ao	158	ASN
1	Ao	200	ASN
1	Ao	226	ASN

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Mol	Chain	Res	Type
1	Ao	255	ASN
1	Ap	112	ASN
1	Ap	129	ASN
1	Ap	156	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	156	ASN
1	Aq	158	ASN
1	Aq	200	ASN
1	Aq	226	ASN
1	Aq	255	ASN
1	Ar	112	ASN
1	Ar	129	ASN
1	Ar	156	ASN
1	Ar	158	ASN
1	Ar	200	ASN
1	Ar	226	ASN
1	Ar	255	ASN
1	As	112	ASN
1	As	129	ASN
1	As	149	ASN
1	As	156	ASN
1	As	158	ASN
1	As	200	ASN
1	As	226	ASN
1	As	255	ASN
1	At	112	ASN
1	At	129	ASN
1	At	156	ASN
1	At	158	ASN
1	At	200	ASN
1	At	226	ASN
1	At	255	ASN
1	Au	112	ASN
1	Au	129	ASN
1	Au	149	ASN
1	Au	156	ASN
1	Au	158	ASN

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Mol	Chain	Res	Type
1	Au	200	ASN
1	Au	226	ASN
1	Au	255	ASN
1	Av	112	ASN
1	Av	129	ASN
1	Av	156	ASN
1	Av	158	ASN
1	Av	200	ASN
1	Av	226	ASN
1	Av	255	ASN
1	Aw	112	ASN
1	Aw	129	ASN
1	Aw	149	ASN
1	Aw	156	ASN
1	Aw	158	ASN
1	Aw	200	ASN
1	Aw	226	ASN
1	Aw	255	ASN
1	Ax	112	ASN
1	Ax	129	ASN
1	Ax	149	ASN
1	Ax	156	ASN
1	Ax	158	ASN
1	Ax	200	ASN
1	Ax	226	ASN
1	Ax	255	ASN
1	Ay	112	ASN
1	Ay	129	ASN
1	Ay	149	ASN
1	Ay	156	ASN
1	Ay	158	ASN
1	Ay	200	ASN
1	Ay	226	ASN
1	Ay	255	ASN
1	Az	112	ASN
1	Az	129	ASN
1	Az	149	ASN
1	Az	156	ASN
1	Az	158	ASN
1	Az	200	ASN
1	Az	226	ASN
1	Az	255	ASN

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Mol	Chain	Res	Type
2	Ba	26	GLN
2	Ba	56	GLN
2	Ba	253	ASN
2	Ba	264	ASN
2	Ba	357	GLN
2	Bb	26	GLN
2	Bb	56	GLN
2	Bb	195	GLN
2	Bb	253	ASN
2	Bb	264	ASN
2	Bb	357	GLN
2	Bc	26	GLN
2	Bc	56	GLN
2	Bc	242	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	264	ASN
2	Bd	357	GLN
2	Be	26	GLN
2	Be	56	GLN
2	Be	195	GLN
2	Be	228	GLN
2	Be	253	ASN
2	Be	264	ASN
2	Be	346	GLN
2	Be	357	GLN
2	Bf	26	GLN
2	Bf	56	GLN
2	Bf	195	GLN
2	Bf	253	ASN
2	Bf	264	ASN
2	Bf	357	GLN
2	Bg	26	GLN
2	Bg	56	GLN
2	Bg	253	ASN
2	Bg	264	ASN

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Mol	Chain	Res	Type
2	Bg	357	GLN
2	Bh	26	GLN
2	Bh	56	GLN
2	Bh	195	GLN
2	Bh	242	ASN
2	Bh	253	ASN
2	Bh	264	ASN
2	Bh	357	GLN
2	Bi	26	GLN
2	Bi	56	GLN
2	Bi	253	ASN
2	Bi	264	ASN
2	Bi	357	GLN
2	Bj	26	GLN
2	Bj	56	GLN
2	Bj	195	GLN
2	Bj	253	ASN
2	Bj	264	ASN
2	Bj	357	GLN
2	Bk	26	GLN
2	Bk	56	GLN
2	Bk	195	GLN
2	Bk	253	ASN
2	Bk	264	ASN
2	Bk	357	GLN
2	Bl	26	GLN
2	Bl	56	GLN
2	Bl	195	GLN
2	Bl	253	ASN
2	Bl	264	ASN
2	Bl	357	GLN
2	Bm	26	GLN
2	Bm	56	GLN
2	Bm	253	ASN
2	Bm	264	ASN
2	Bm	357	GLN
2	Bn	26	GLN
2	Bn	56	GLN
2	Bn	195	GLN
2	Bn	253	ASN
2	Bn	264	ASN
2	Bn	357	GLN

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Mol	Chain	Res	Type
2	Bo	26	GLN
2	Bo	56	GLN
2	Bo	195	GLN
2	Bo	253	ASN
2	Bo	264	ASN
2	Bo	357	GLN
2	Bp	26	GLN
2	Bp	56	GLN
2	Bp	195	GLN
2	Bp	253	ASN
2	Bp	264	ASN
2	Bp	357	GLN
2	Bq	26	GLN
2	Bq	56	GLN
2	Bq	195	GLN
2	Bq	253	ASN
2	Bq	264	ASN
2	Bq	357	GLN
2	Br	26	GLN
2	Br	56	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	253	ASN
2	Bs	264	ASN
2	Bs	357	GLN
2	Bt	26	GLN
2	Bt	56	GLN
2	Bt	195	GLN
2	Bt	253	ASN
2	Bt	264	ASN
2	Bt	357	GLN
2	Bu	26	GLN
2	Bu	56	GLN
2	Bu	228	GLN
2	Bu	253	ASN
2	Bu	264	ASN
2	Bu	357	GLN
2	Bv	26	GLN

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Mol	Chain	Res	Type
2	Bv	56	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	253	ASN
2	Bw	264	ASN
2	Bw	357	GLN
2	Bx	26	GLN
2	Bx	56	GLN
2	Bx	195	GLN
2	Bx	253	ASN
2	Bx	264	ASN
2	Bx	357	GLN
2	By	26	GLN
2	By	56	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	195	GLN
2	Bz	253	ASN
2	Bz	264	ASN
2	Bz	357	GLN
3	Ca	116	HIS
3	Ca	159	GLN
3	Ca	217	ASN
3	Cb	154	ASN
3	Cb	217	ASN
3	Cb	374	HIS
3	Cb	376	GLN
3	Cc	253	GLN
3	Cc	374	HIS
3	Cd	159	GLN
3	Cd	322	HIS
3	Cd	376	GLN
3	Ce	217	ASN
3	Ce	339	GLN

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Mol	Chain	Res	Type
3	Cf	66	ASN
3	Cf	135	GLN
3	Cf	159	GLN
3	Cf	217	ASN
3	Cf	253	GLN
3	Cf	322	HIS
3	Cg	66	ASN
3	Cg	128	ASN
3	Cg	159	GLN
3	Cg	314	GLN
3	Cg	322	HIS
3	Ch	97	ASN
3	Ch	154	ASN
3	Ch	253	GLN
3	Ch	322	HIS
3	Ch	374	HIS
3	Ci	128	ASN
3	Ci	154	ASN
3	Ci	212	GLN
3	Cj	97	ASN
3	Cj	217	ASN
3	Cj	253	GLN
3	Cj	322	HIS
3	Ck	154	ASN
3	Ck	253	GLN
3	Cl	154	ASN
3	Cl	159	GLN
3	Cl	314	GLN
3	Cl	322	HIS
3	Cm	314	GLN
3	Cn	135	GLN
3	Cn	159	GLN
3	Cn	253	GLN
3	Cn	322	HIS
3	Cn	374	HIS
3	Co	253	GLN
3	Cp	44	HIS
3	Cp	253	GLN
3	Cp	322	HIS
3	Cp	374	HIS
3	Cq	66	ASN
3	Cr	135	GLN

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Mol	Chain	Res	Type
3	Cr	141	GLN
3	Cr	322	HIS
3	Cs	116	HIS
3	Cs	128	ASN
3	Cs	135	GLN
3	Cs	154	ASN
3	Cs	159	GLN
3	Cs	212	GLN
3	Cs	217	ASN
3	Ct	154	ASN
3	Ct	322	HIS
3	Ct	374	HIS
3	Cu	66	ASN
3	Cu	154	ASN
3	Cv	97	ASN
3	Cv	116	HIS
3	Cv	154	ASN
3	Cv	322	HIS
3	Cv	330	GLN
3	Cw	66	ASN
3	Cw	97	ASN
3	Cw	293	GLN
3	Cx	97	ASN
3	Cx	159	GLN
3	Cx	217	ASN
3	Cx	322	HIS
3	Cx	339	GLN
3	Cy	97	ASN
3	Cy	135	GLN
3	Cy	217	ASN
3	Cz	135	GLN
3	Cz	154	ASN
3	Cz	159	GLN
3	Cz	217	ASN
3	Cz	276	ASN
3	Cz	322	HIS
3	Cz	374	HIS
3	Cz	376	GLN
4	Da	106	ASN
4	Da	108	GLN
4	Da	112	GLN
4	Da	143	GLN

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Mol	Chain	Res	Type
4	Da	147	GLN
4	Da	282	ASN
4	Db	50	HIS
4	Db	112	GLN
4	Db	120	GLN
4	Db	147	GLN
4	Db	235	GLN
4	Db	293	GLN
4	Dc	106	ASN
4	Dc	108	GLN
4	Dc	112	GLN
4	Dc	143	GLN
4	Dc	147	GLN
4	Dc	282	ASN
4	Dd	50	HIS
4	Dd	112	GLN
4	Dd	120	GLN
4	Dd	147	GLN
4	Dd	235	GLN
4	Dd	293	GLN
4	De	106	ASN
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	147	GLN
4	Df	189	GLN
4	Df	235	GLN
4	Df	293	GLN
4	Dg	106	ASN
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

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Mol	Chain	Res	Type
4	Dh	147	GLN
4	Dh	189	GLN
4	Dh	235	GLN
4	Dh	293	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
4	Dj	147	GLN
4	Dj	235	GLN
4	Dj	293	GLN
4	Dk	106	ASN
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	147	GLN
4	Dl	189	GLN
4	Dl	235	GLN
4	Dl	293	GLN
4	Dm	106	ASN
4	Dm	108	GLN
4	Dm	112	GLN
4	Dm	143	GLN
4	Dm	147	GLN
4	Dm	282	ASN
4	Dn	50	HIS
4	Dn	112	GLN
4	Dn	120	GLN
4	Dn	147	GLN
4	Dn	235	GLN
4	Dn	293	GLN
4	Do	108	GLN
4	Do	112	GLN

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Mol	Chain	Res	Type
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	147	GLN
4	Dp	235	GLN
4	Dp	293	GLN
4	Dq	106	ASN
4	Dq	108	GLN
4	Dq	112	GLN
4	Dq	143	GLN
4	Dq	147	GLN
4	Dq	282	ASN
4	Dr	50	HIS
4	Dr	112	GLN
4	Dr	120	GLN
4	Dr	147	GLN
4	Dr	235	GLN
4	Dr	293	GLN
4	Ds	106	ASN
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	147	GLN
4	Dt	235	GLN
4	Dt	293	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

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Mol	Chain	Res	Type
4	Dv	112	GLN
4	Dv	120	GLN
4	Dv	147	GLN
4	Dv	235	GLN
4	Dw	106	ASN
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	112	GLN
4	Dx	120	GLN
4	Dx	147	GLN
4	Dx	235	GLN
4	Dx	293	GLN
4	Dy	106	ASN
4	Dy	108	GLN
4	Dy	143	GLN
4	Dy	147	GLN
4	Dy	282	ASN
4	Dz	50	HIS
4	Dz	112	GLN
4	Dz	120	GLN
4	Dz	147	GLN
4	Dz	235	GLN
4	Dz	293	GLN
5	Ea	145	ASN
5	Ea	149	GLN
5	Ea	183	ASN
5	Eb	57	GLN
5	Eb	90	GLN
5	Eb	113	GLN
5	Eb	143	ASN
5	Eb	149	GLN
5	Eb	179	GLN
5	Eb	182	HIS
5	Ec	145	ASN
5	Ec	149	GLN
5	Ec	183	ASN
5	Ed	57	GLN
5	Ed	90	GLN

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Mol	Chain	Res	Type
5	Ed	143	ASN
5	Ed	149	GLN
5	Ed	179	GLN
5	Ed	182	HIS
5	Ee	145	ASN
5	Ee	149	GLN
5	Ee	183	ASN
5	Ef	57	GLN
5	Ef	90	GLN
5	Ef	143	ASN
5	Ef	149	GLN
5	Ef	179	GLN
5	Ef	182	HIS
5	Eg	145	ASN
5	Eg	149	GLN
5	Eg	183	ASN
5	Eh	57	GLN
5	Eh	90	GLN
5	Eh	113	GLN
5	Eh	143	ASN
5	Eh	149	GLN
5	Eh	179	GLN
5	Eh	182	HIS
5	Ei	145	ASN
5	Ei	149	GLN
5	Ei	173	ASN
5	Ei	183	ASN
5	Ej	57	GLN
5	Ej	90	GLN
5	Ej	143	ASN
5	Ej	149	GLN
5	Ej	179	GLN
5	Ej	182	HIS
5	Ek	145	ASN
5	Ek	149	GLN
5	Ek	183	ASN
5	El	57	GLN
5	El	90	GLN
5	El	143	ASN
5	El	149	GLN
5	El	179	GLN
5	El	182	HIS

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Mol	Chain	Res	Type
5	Em	145	ASN
5	Em	149	GLN
5	Em	183	ASN
5	En	57	GLN
5	En	90	GLN
5	En	143	ASN
5	En	149	GLN
5	En	179	GLN
5	En	182	HIS
5	Eo	145	ASN
5	Eo	149	GLN
5	Eo	173	ASN
5	Eo	183	ASN
5	Ep	57	GLN
5	Ep	90	GLN
5	Ep	143	ASN
5	Ep	149	GLN
5	Ep	179	GLN
5	Ep	182	HIS
5	Eq	145	ASN
5	Eq	149	GLN
5	Eq	183	ASN
5	Er	57	GLN
5	Er	90	GLN
5	Er	143	ASN
5	Er	149	GLN
5	Er	179	GLN
5	Er	182	HIS
5	Es	145	ASN
5	Es	149	GLN
5	Es	173	ASN
5	Es	183	ASN
5	Et	57	GLN
5	Et	90	GLN
5	Et	143	ASN
5	Et	149	GLN
5	Et	179	GLN
5	Eu	145	ASN
5	Eu	149	GLN
5	Eu	173	ASN
5	Eu	183	ASN
5	Ev	57	GLN

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Mol	Chain	Res	Type
5	Ev	90	GLN
5	Ev	143	ASN
5	Ev	149	GLN
5	Ev	179	GLN
5	Ev	182	HIS
5	Ew	145	ASN
5	Ew	149	GLN
5	Ew	173	ASN
5	Ew	183	ASN
5	Ex	57	GLN
5	Ex	90	GLN
5	Ex	149	GLN
5	Ex	179	GLN
5	Ex	182	HIS
5	Ey	145	ASN
5	Ey	149	GLN
5	Ey	183	ASN
5	Ez	57	GLN
5	Ez	90	GLN
5	Ez	149	GLN
5	Ez	179	GLN
5	Ez	182	HIS
6	Gb	135	GLN
6	Gi	134	GLN
6	Gi	135	GLN
6	Gk	135	GLN
6	Go	134	GLN
6	Gq	135	GLN
6	Gr	135	GLN
6	Gs	141	GLN
6	Gt	135	GLN
6	Gw	141	GLN
6	Gx	141	GLN
6	Gy	135	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

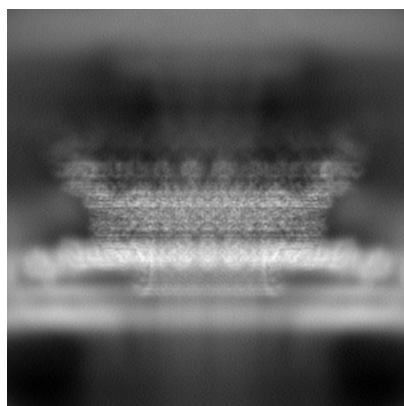
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72947. These allow visual inspection of the internal detail of the map and identification of artifacts.

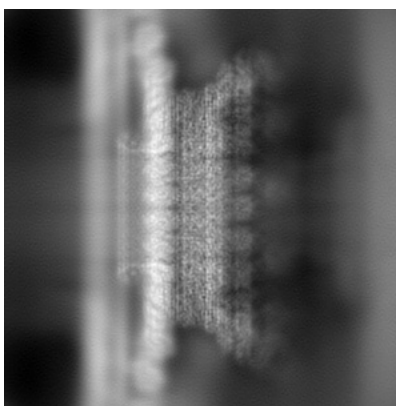
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

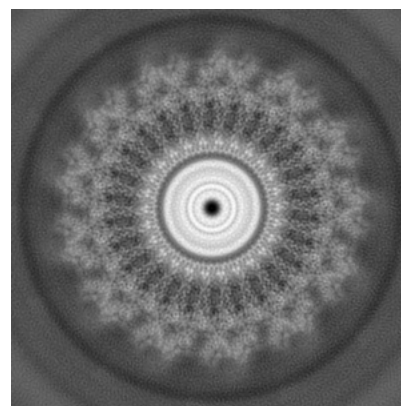
6.1.1 Primary map



X

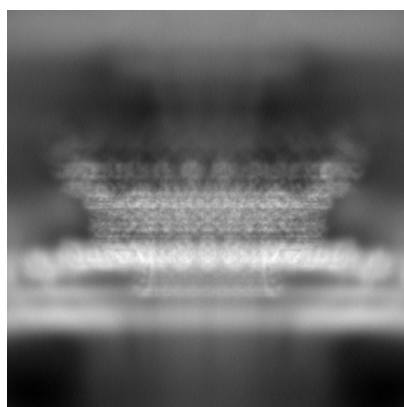


Y

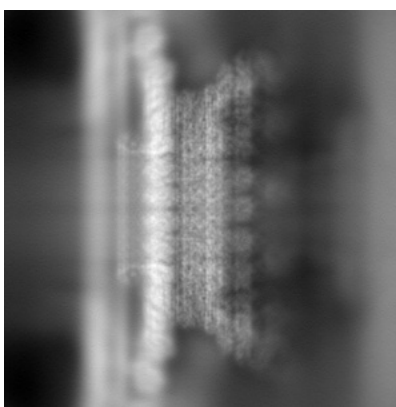


Z

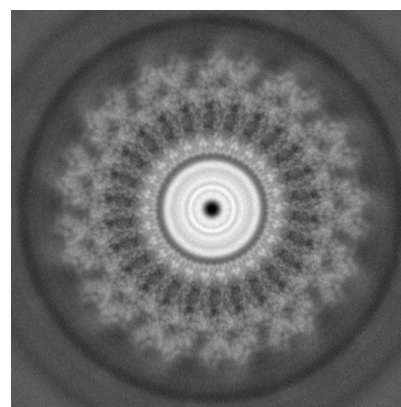
6.1.2 Raw map



X



Y

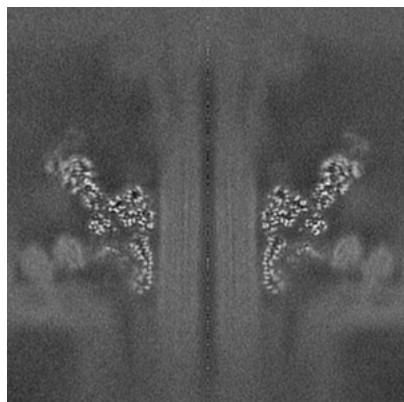


Z

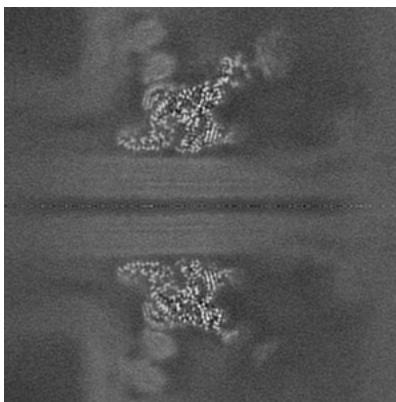
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

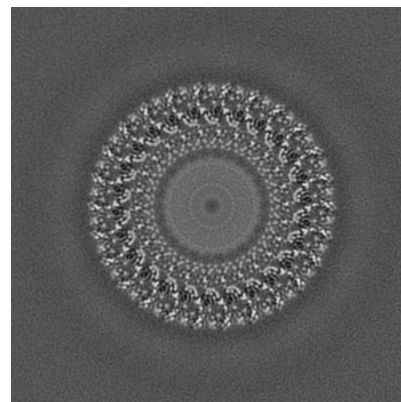
6.2.1 Primary map



X Index: 159

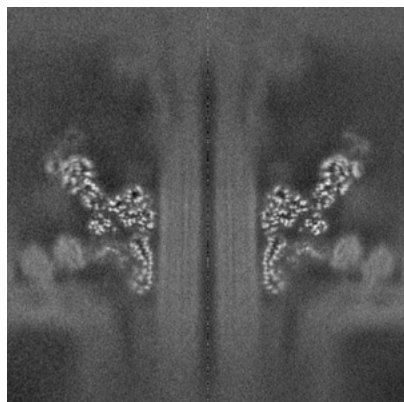


Y Index: 159

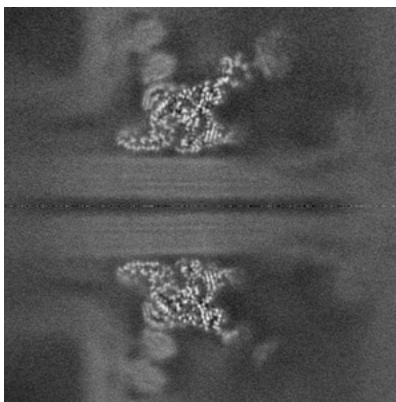


Z Index: 159

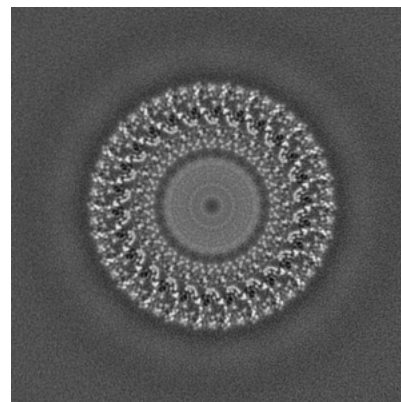
6.2.2 Raw map



X Index: 159



Y Index: 159

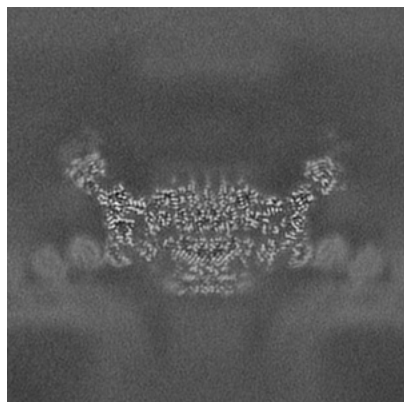


Z Index: 159

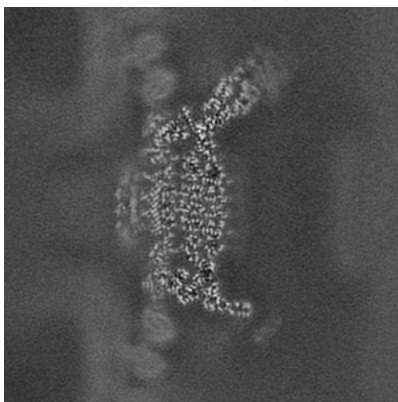
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

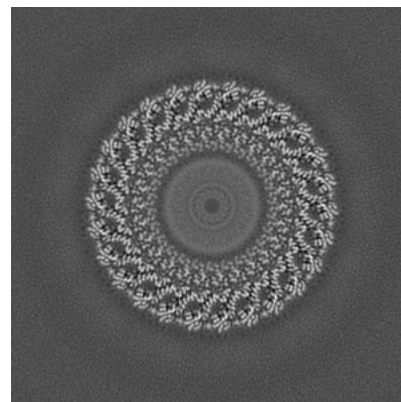
6.3.1 Primary map



X Index: 210

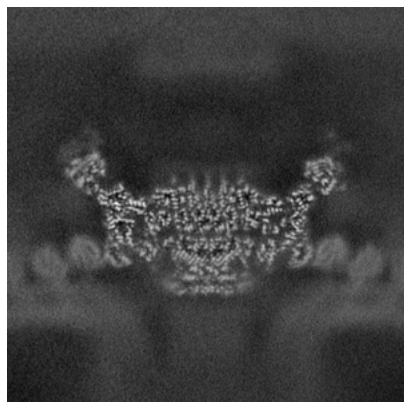


Y Index: 106

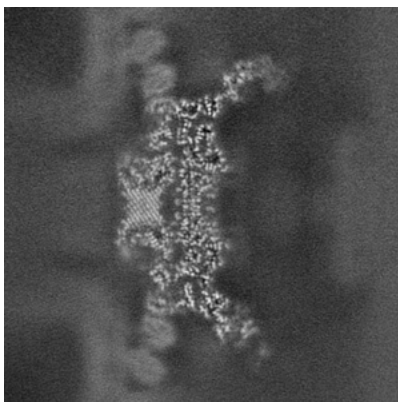


Z Index: 161

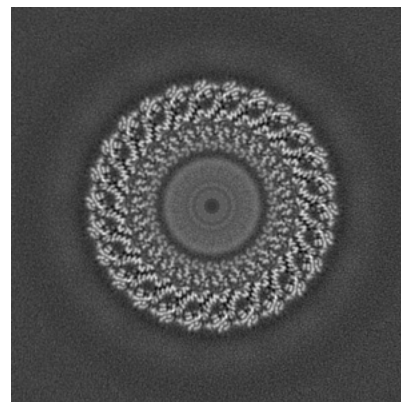
6.3.2 Raw map



X Index: 210



Y Index: 114

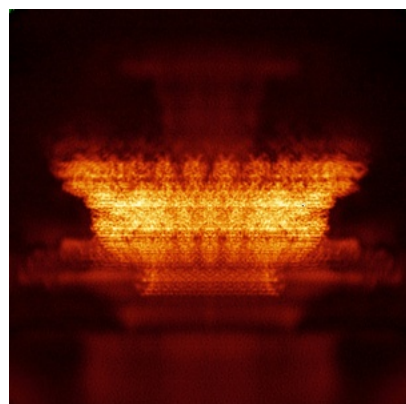


Z Index: 161

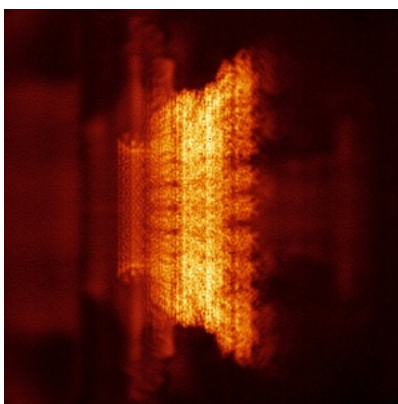
The images above show the largest variance slices of the map in three orthogonal directions.

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

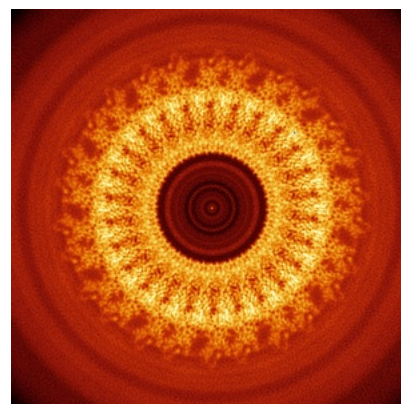
6.4.1 Primary map



X

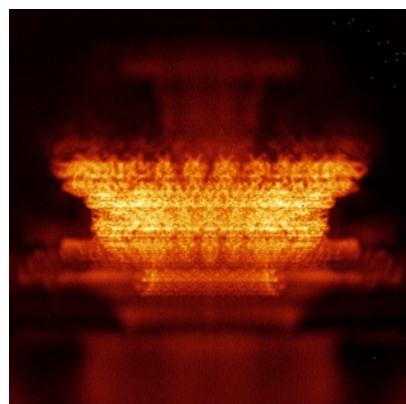


Y

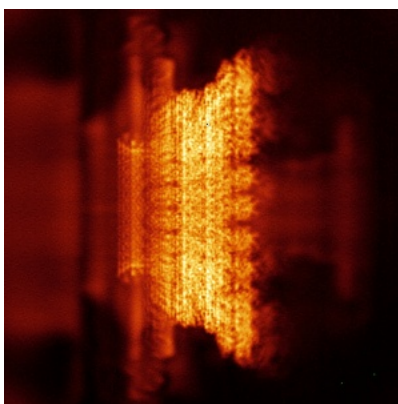


Z

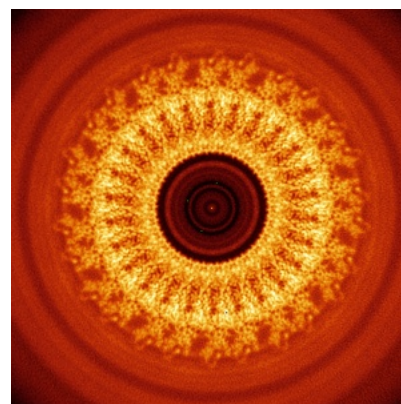
6.4.2 Raw map



X



Y

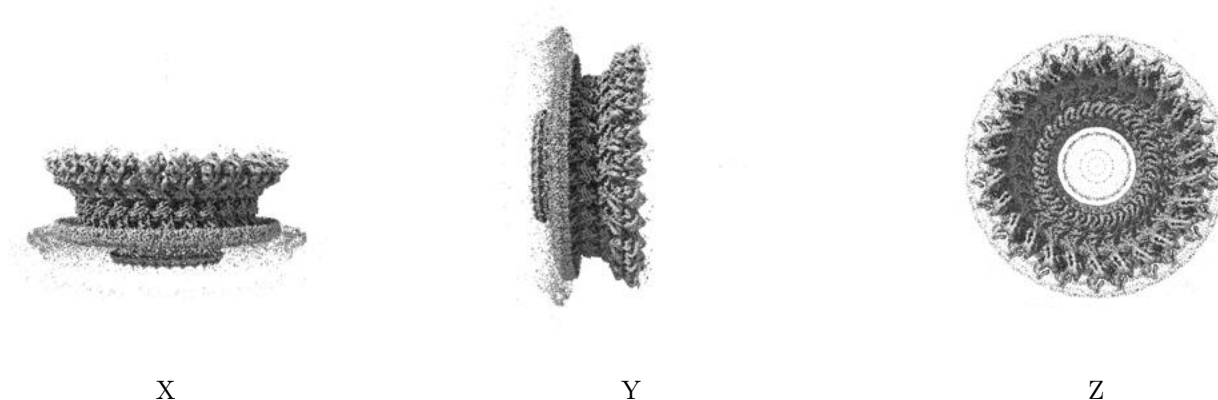


Z

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.

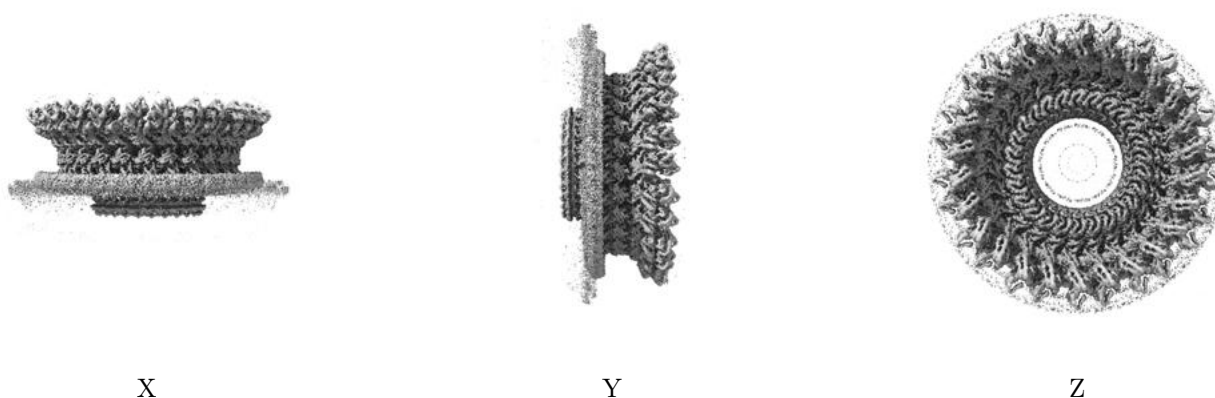
6.5 Orthogonal surface views [i](#)

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.

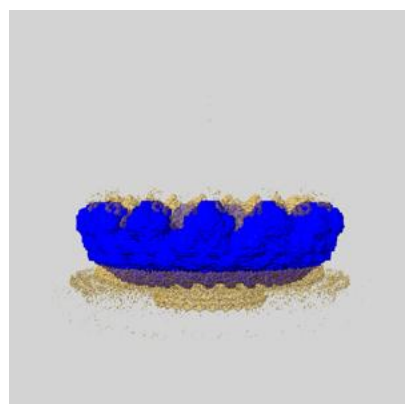
6.6 Mask visualisation [i](#)

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

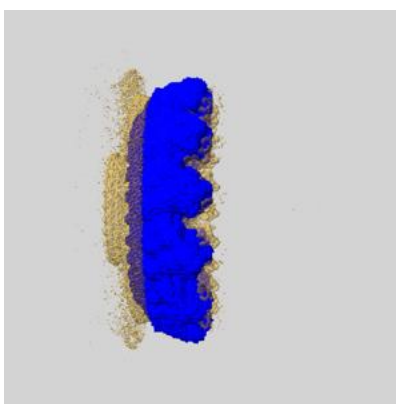
A mask typically either:

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

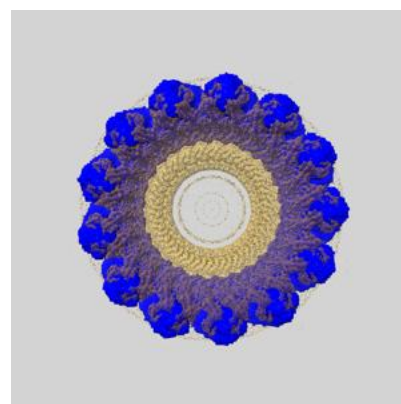
6.6.1 emd_72947_msk_1.map [i](#)



X



Y

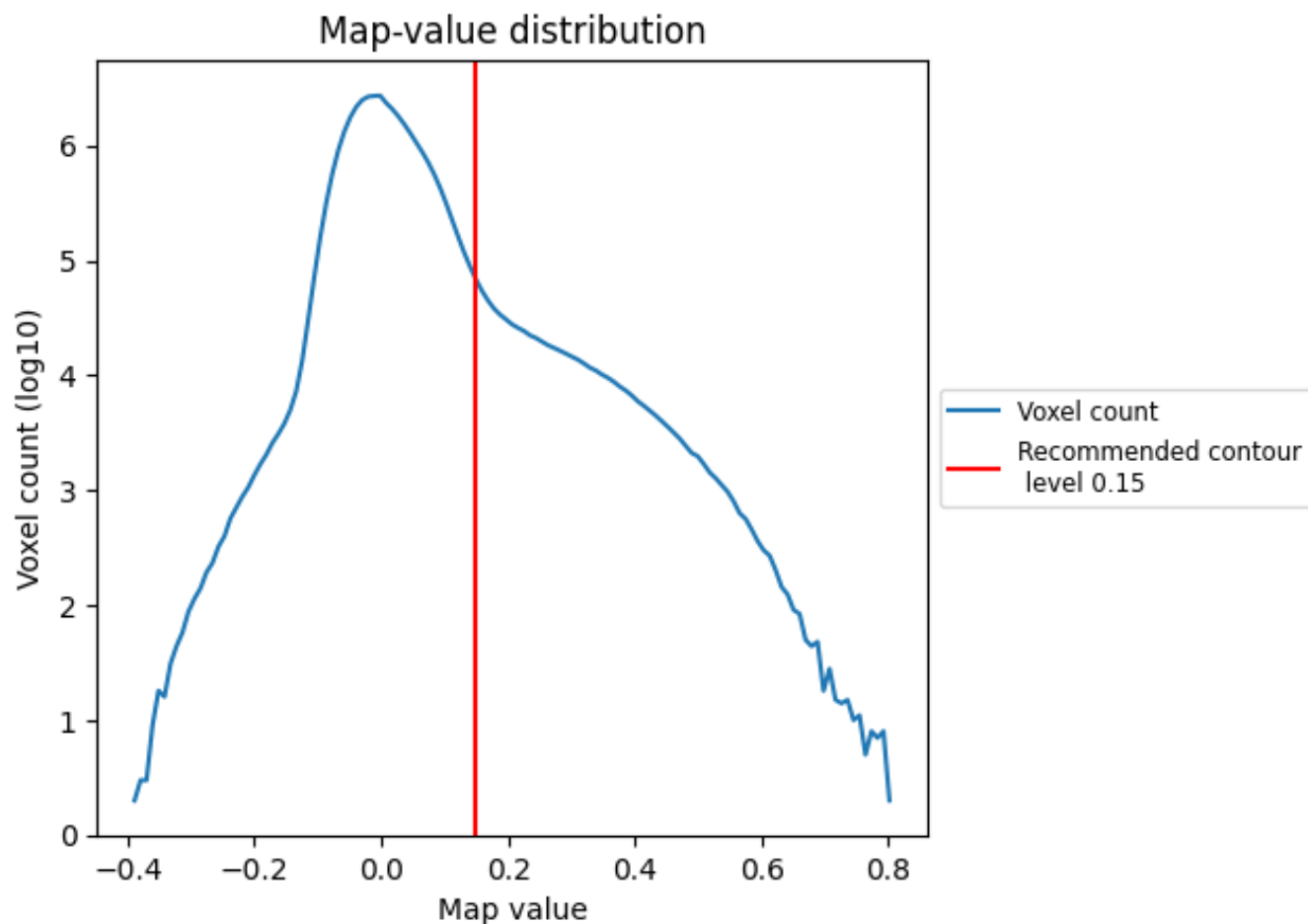


Z

7 Map analysis [i](#)

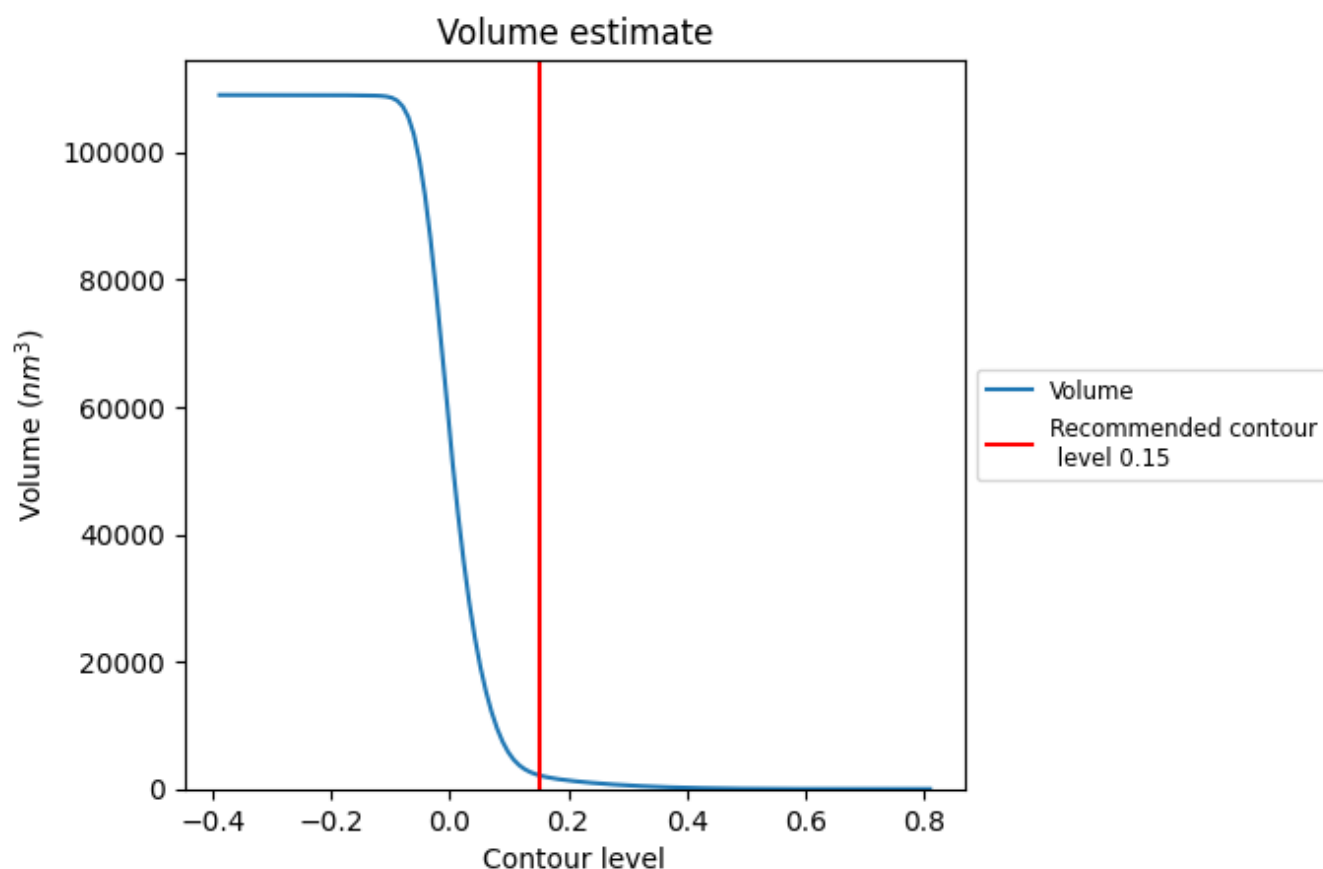
This section contains the results of statistical analysis of the map.

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.

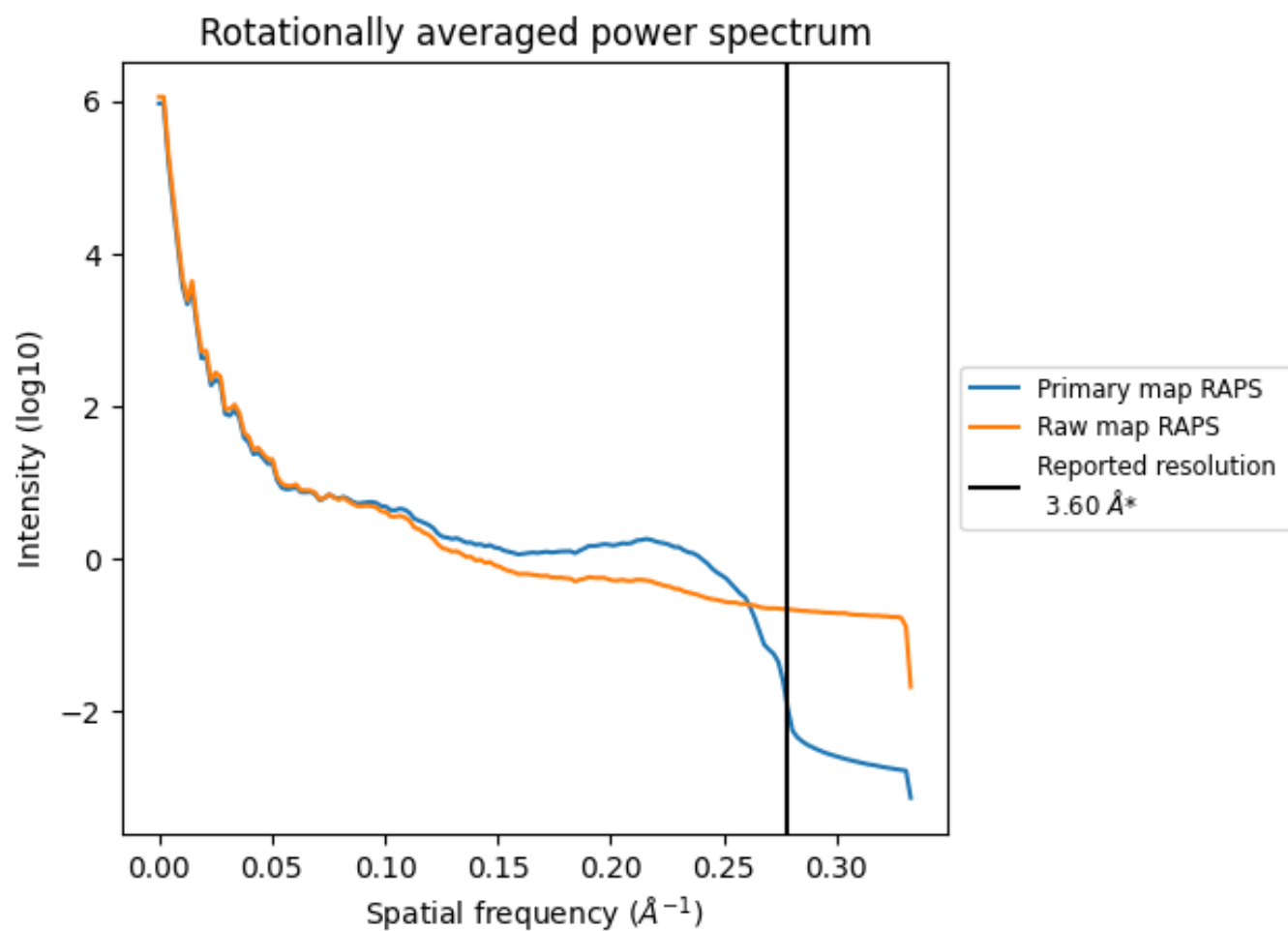
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2181 nm^3 ; this corresponds to an approximate mass of 1971 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 ⓘ

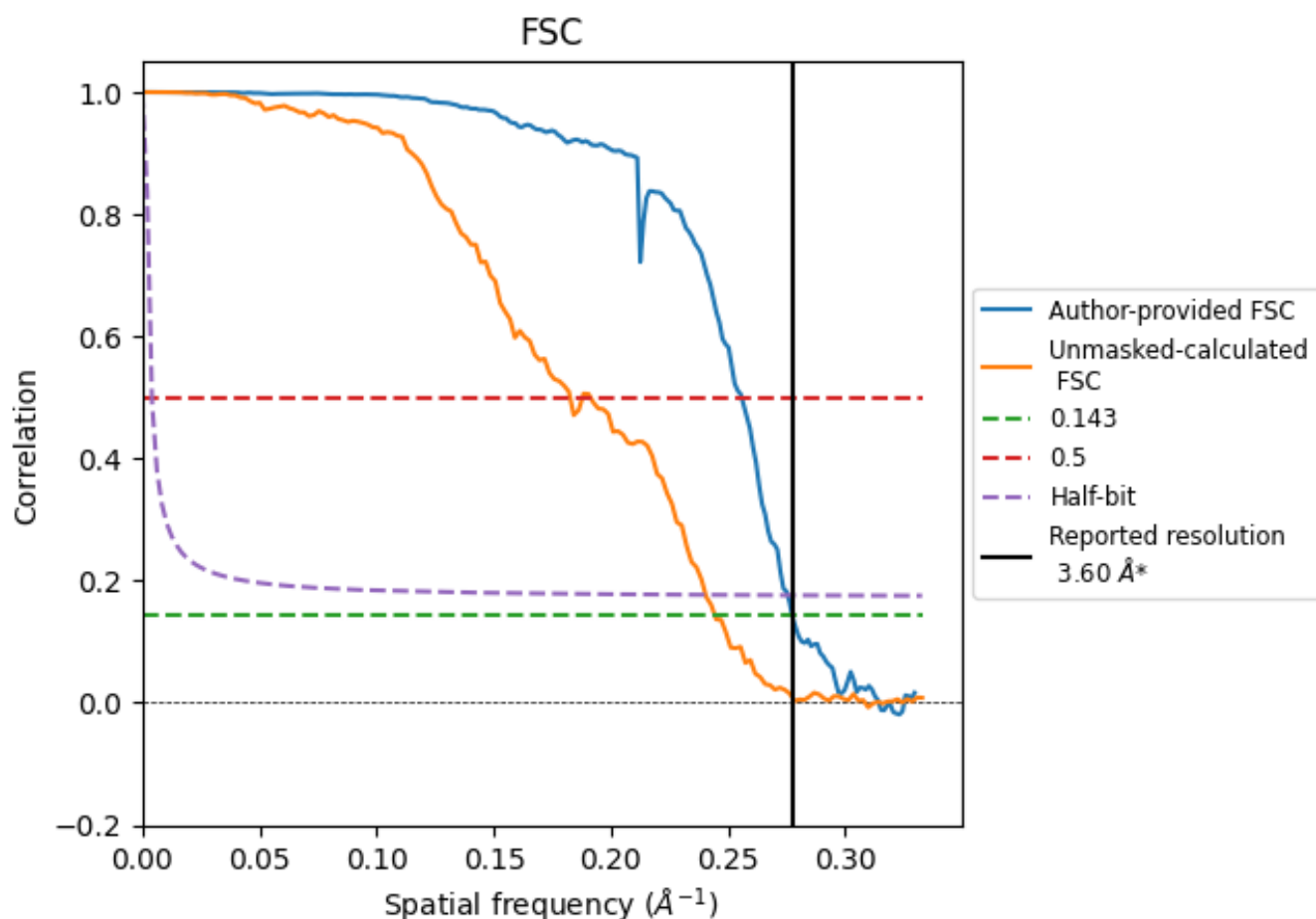


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	3.91	3.63
Unmasked-calculated*	4.09	5.47	4.16

*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 4.09 differs from the reported value 3.6 by more than 10 %

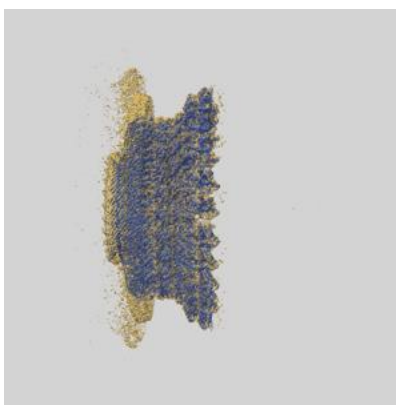
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72947 and PDB model 9YH0. Per-residue inclusion information can be found in section [3](#) on page [21](#).

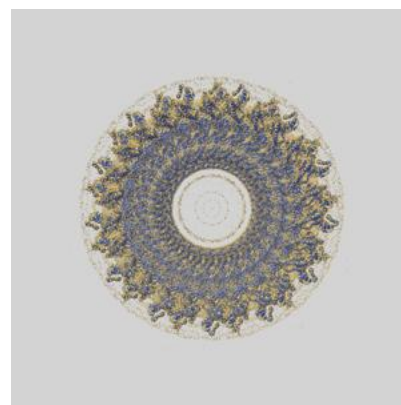
9.1 Map-model overlay [i](#)



X



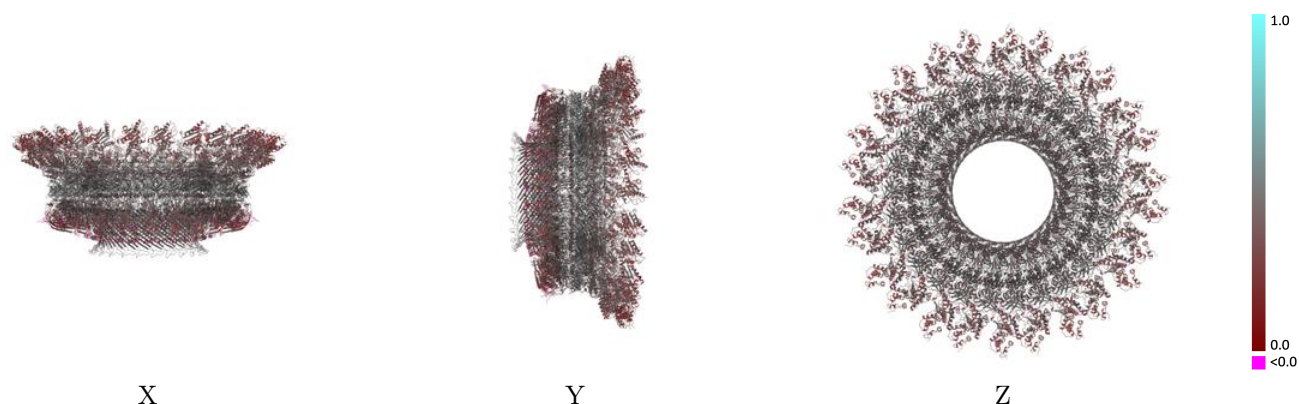
Y



Z

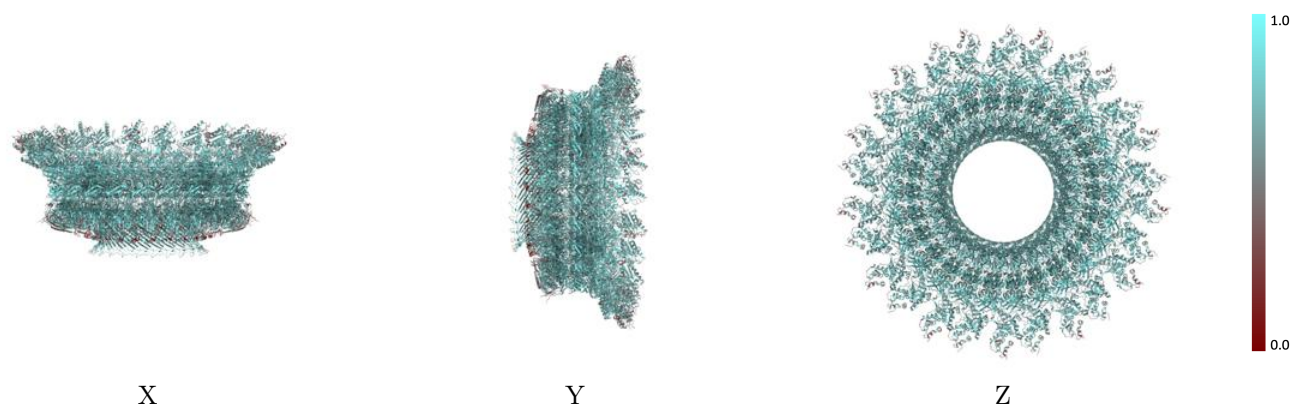
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



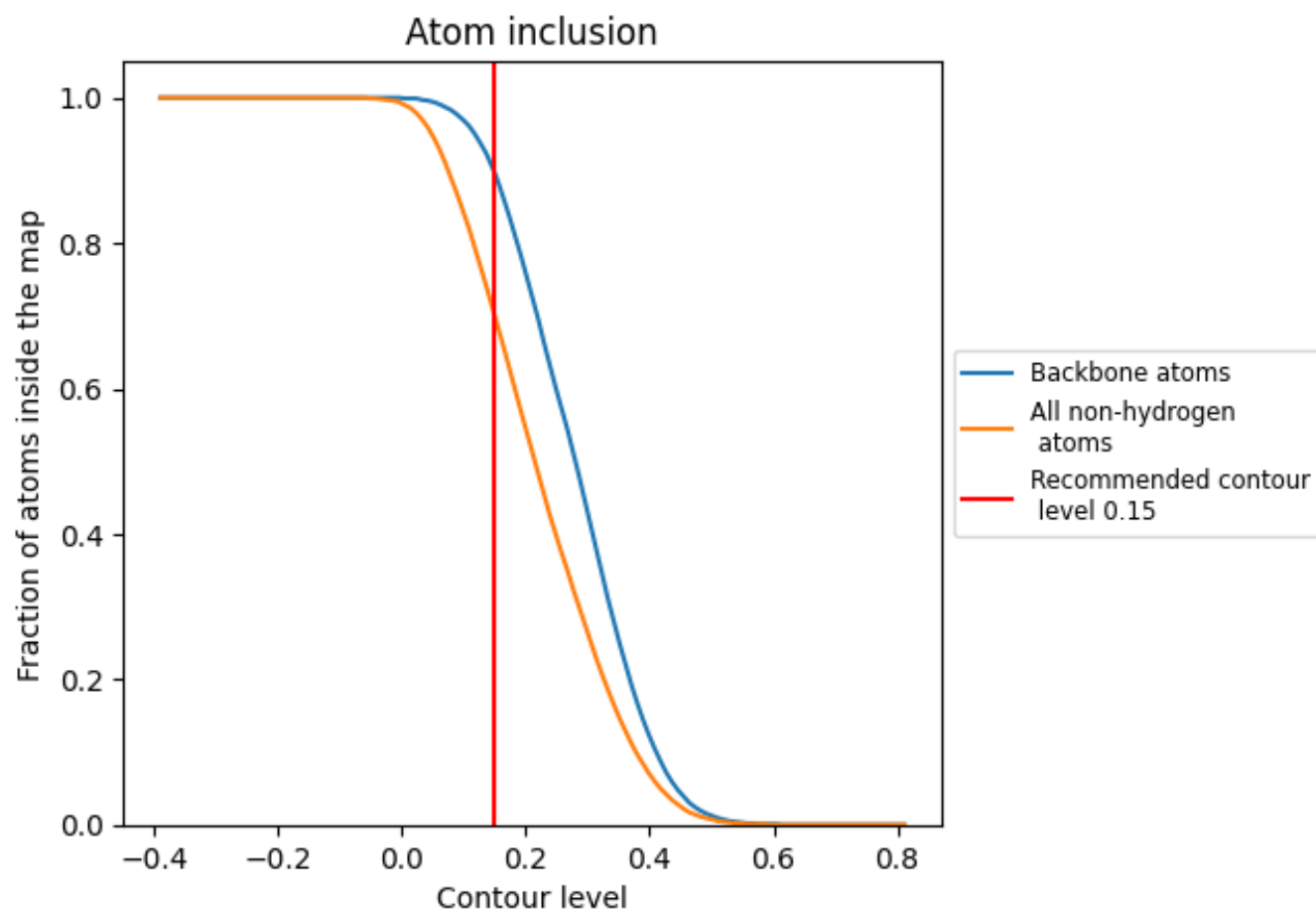
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 70% 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	 0.7010	 0.3850
Aa	 0.6850	 0.4030
Ab	 0.6780	 0.3950
Ac	 0.6830	 0.4040
Ad	 0.6800	 0.3980
Ae	 0.6860	 0.4060
Af	 0.6740	 0.3960
Ag	 0.6840	 0.4050
Ah	 0.6750	 0.3960
Ai	 0.6860	 0.4060
Aj	 0.6810	 0.3970
Ak	 0.6850	 0.4070
Al	 0.6770	 0.3980
Am	 0.6940	 0.4060
An	 0.6800	 0.4000
Ao	 0.6910	 0.4090
Ap	 0.6830	 0.4000
Aq	 0.6910	 0.4070
Ar	 0.6810	 0.3970
As	 0.6900	 0.4050
At	 0.6800	 0.3980
Au	 0.6890	 0.4070
Av	 0.6810	 0.3970
Aw	 0.6920	 0.4060
Ax	 0.6780	 0.3960
Ay	 0.6840	 0.4020
Az	 0.6720	 0.3960
Ba	 0.7470	 0.4340
Bb	 0.7480	 0.4360
Bc	 0.7400	 0.4330
Bd	 0.7500	 0.4350
Be	 0.7470	 0.4320
Bf	 0.7500	 0.4340
Bg	 0.7420	 0.4320
Bh	 0.7450	 0.4360























































































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Chain	Atom inclusion	Q-score
Bi	 0.7420	 0.4290
Bj	 0.7460	 0.4340
Bk	 0.7470	 0.4320
Bl	 0.7530	 0.4360
Bm	 0.7500	 0.4320
Bn	 0.7490	 0.4350
Bo	 0.7500	 0.4310
Bp	 0.7510	 0.4370
Bq	 0.7520	 0.4340
Br	 0.7500	 0.4370
Bs	 0.7500	 0.4350
Bt	 0.7520	 0.4370
Bu	 0.7510	 0.4320
Bv	 0.7540	 0.4380
Bw	 0.7450	 0.4330
Bx	 0.7510	 0.4360
By	 0.7390	 0.4340
Bz	 0.7510	 0.4380
Ca	 0.7110	 0.3830
Cb	 0.6790	 0.3500
Cc	 0.7090	 0.3850
Cd	 0.7070	 0.3840
Ce	 0.7140	 0.3820
Cf	 0.7070	 0.3840
Cg	 0.7150	 0.3850
Ch	 0.7120	 0.3850
Ci	 0.7150	 0.3870
Cj	 0.7130	 0.3860
Ck	 0.7070	 0.3870
Cl	 0.7100	 0.3850
Cm	 0.7090	 0.3830
Cn	 0.7110	 0.3860
Co	 0.7130	 0.3860
Cp	 0.7040	 0.3830
Cq	 0.7120	 0.3860
Cr	 0.7050	 0.3830
Cs	 0.7070	 0.3840
Ct	 0.7080	 0.3820
Cu	 0.7050	 0.3830
Cv	 0.7070	 0.3830
Cw	 0.7110	 0.3820
Cx	 0.7060	 0.3840





















































































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Chain	Atom inclusion	Q-score
Cy	 0.7090	 0.3830
Cz	 0.7070	 0.3840
Da	 0.7380	 0.3840
Db	 0.7430	 0.3960
Dc	 0.7320	 0.3830
Dd	 0.7350	 0.3970
De	 0.7330	 0.3810
Df	 0.7390	 0.3940
Dg	 0.7350	 0.3800
Dh	 0.7370	 0.3950
Di	 0.7330	 0.3790
Dj	 0.7350	 0.3940
Dk	 0.7280	 0.3760
Dl	 0.7330	 0.3920
Dm	 0.7280	 0.3750
Dn	 0.7340	 0.3910
Do	 0.7300	 0.3790
Dp	 0.7320	 0.3910
Dq	 0.7250	 0.3780
Dr	 0.7380	 0.3920
Ds	 0.7270	 0.3770
Dt	 0.7410	 0.3910
Du	 0.7330	 0.3800
Dv	 0.7390	 0.3910
Dw	 0.7340	 0.3820
Dx	 0.7370	 0.3950
Dy	 0.7380	 0.3830
Dz	 0.7410	 0.3970
Ea	 0.6570	 0.3380
Eb	 0.6120	 0.3090
Ec	 0.6580	 0.3350
Ed	 0.6130	 0.3090
Ee	 0.6520	 0.3330
Ef	 0.6100	 0.3090
Eg	 0.6440	 0.3290
Eh	 0.6110	 0.3070
Ei	 0.6440	 0.3280
Ej	 0.6040	 0.3040
Ek	 0.6420	 0.3280
El	 0.6040	 0.3020
Em	 0.6380	 0.3310
En	 0.6060	 0.3020













































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Chain	Atom inclusion	Q-score
Eo	 0.6450	 0.3320
Ep	 0.6050	 0.3030
Eq	 0.6400	 0.3350
Er	 0.6060	 0.3070
Es	 0.6500	 0.3400
Et	 0.6080	 0.3080
Eu	 0.6490	 0.3370
Ev	 0.6150	 0.3090
Ew	 0.6520	 0.3370
Ex	 0.6090	 0.3120
Ey	 0.6580	 0.3370
Ez	 0.6180	 0.3160
Fa	 0.4060	 0.1940
Fb	 0.3250	 0.1520
Fc	 0.4470	 0.1940
Fd	 0.3330	 0.1470
Fe	 0.4390	 0.1910
Ff	 0.4390	 0.2440
Fg	 0.4230	 0.1870
Fh	 0.3420	 0.1790
Fi	 0.4150	 0.1990
Fj	 0.3420	 0.1880
Fk	 0.4150	 0.1830
Fl	 0.3660	 0.1740
Fm	 0.4310	 0.1930
Fn	 0.3500	 0.1540
Fo	 0.3580	 0.1780
Fp	 0.3900	 0.2150
Fq	 0.4470	 0.2100
Fr	 0.4060	 0.1860
Fs	 0.4710	 0.1910
Ft	 0.3980	 0.1980
Fu	 0.5040	 0.2320
Fv	 0.3500	 0.1650
Fw	 0.4390	 0.1930
Fx	 0.3660	 0.2070
Fy	 0.4550	 0.2150
Fz	 0.3980	 0.1770
Ga	 0.5270	 0.2580
Gb	 0.5180	 0.2910
Gc	 0.5090	 0.2370
Gd	 0.5090	 0.2710

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Chain	Atom inclusion	Q-score
Ge	 0.5360	 0.2550
Gf	 0.5540	 0.2560
Gg	 0.5180	 0.2640
Gh	 0.5180	 0.2580
Gi	 0.5000	 0.2560
Gj	 0.5270	 0.2680
Gk	 0.5270	 0.2420
Gl	 0.5180	 0.2900
Gm	 0.5180	 0.2530
Gn	 0.5450	 0.2750
Go	 0.5180	 0.2270
Gp	 0.5180	 0.2550
Gq	 0.4730	 0.2140
Gr	 0.5270	 0.2910
Gs	 0.4820	 0.2230
Gt	 0.5450	 0.2900
Gu	 0.5000	 0.2350
Gv	 0.5360	 0.2460
Gw	 0.4000	 0.1330
Gx	 0.5450	 0.2580
Gy	 0.5090	 0.2560
Gz	 0.5180	 0.2800