



## Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 04:07 PM EDT

PDB ID : 9YEC / pdb\_00009yec  
EMDB ID : EMD-72847  
Title : LPHT-ring in *Vibrio cholerae* at disassembled, closed state  
Authors : Guo, W.; Yue, J.  
Deposited on : 2025-09-24  
Resolution : 3.57 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

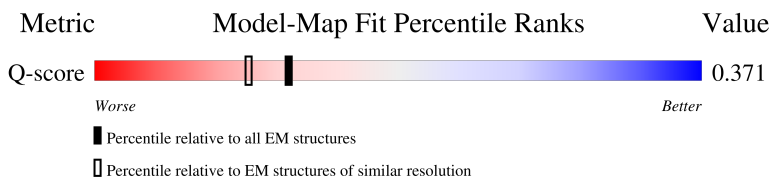
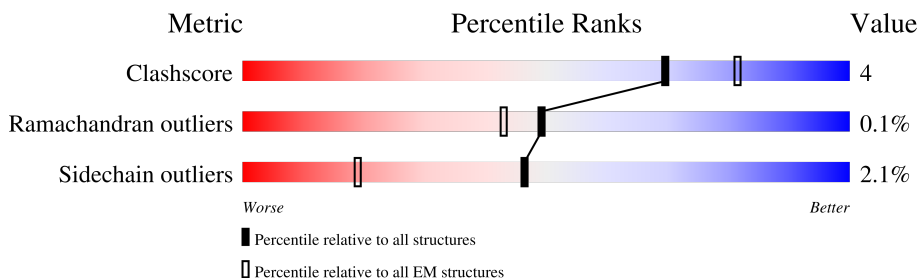
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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





The reported resolution of this entry is 3.57 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.









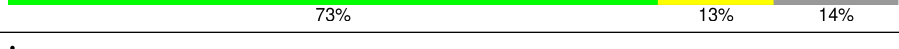
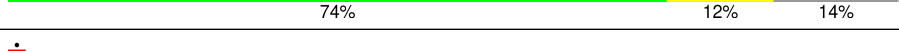
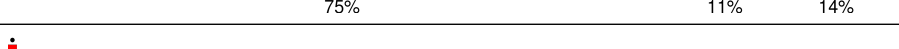
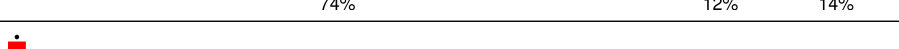
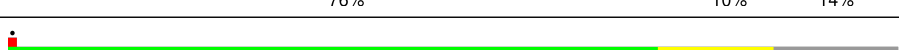

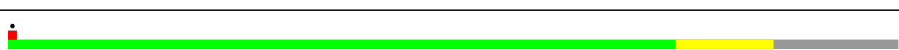

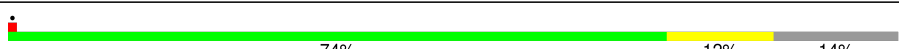





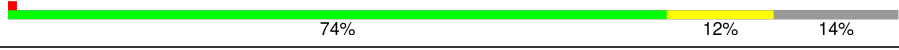
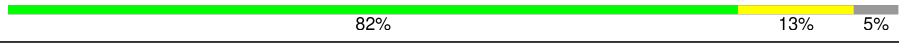



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12682 ( 3.07 - 4.07 )

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

Mol	Chain	Length	Quality of chain
1	Aa	258	
1	Ab	258	
1	Ac	258	
1	Ad	258	



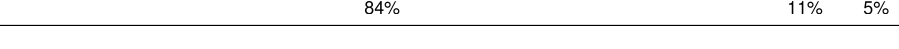
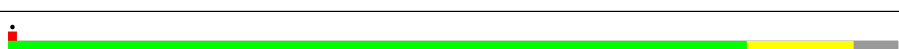



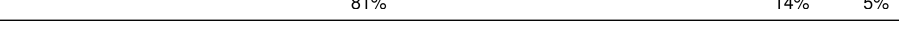



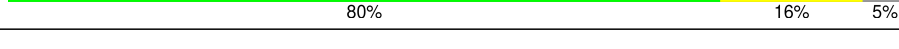

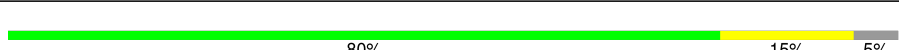


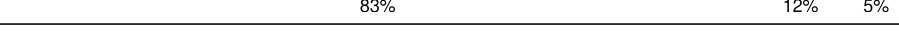







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Mol	Chain	Length	Quality of chain
1	Ae	258	
1	Af	258	
1	Ag	258	
1	Ah	258	
1	Ai	258	
1	Aj	258	
1	Ak	258	
1	Al	258	
1	Am	258	
1	An	258	
1	Ao	258	
1	Ap	258	
1	Aq	258	
1	Ar	258	
1	As	258	
1	At	258	
1	Au	258	
1	Av	258	
1	Aw	258	
1	Ax	258	
1	Ay	258	
1	Az	258	
2	Ba	361	
2	Bb	361	
2	Bc	361	







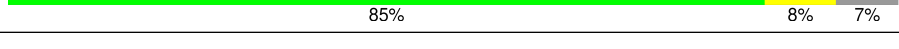
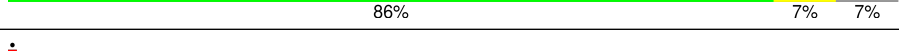
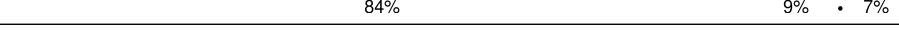
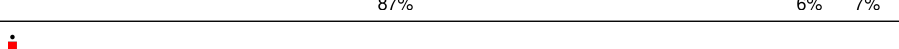
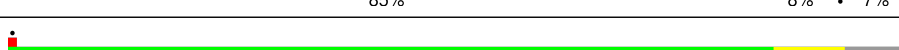

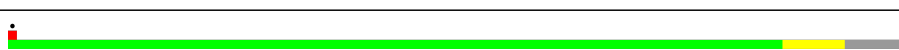

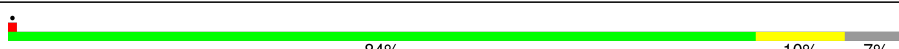





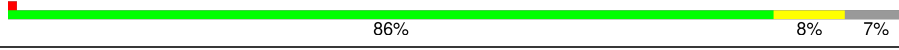
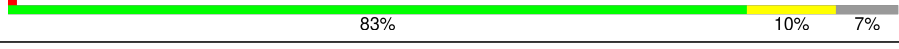



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Mol	Chain	Length	Quality of chain
2	Bd	361	
2	Be	361	
2	Bf	361	
2	Bg	361	
2	Bh	361	
2	Bi	361	
2	Bj	361	
2	Bk	361	
2	Bl	361	
2	Bm	361	
2	Bn	361	
2	Bo	361	
2	Bp	361	
2	Bq	361	
2	Br	361	
2	Bs	361	
2	Bt	361	
2	Bu	361	
2	Bv	361	
2	Bw	361	
2	Bx	361	
2	By	361	
2	Bz	361	
3	Ca	377	
3	Cb	377	







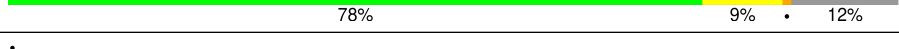
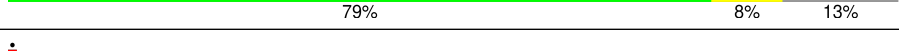
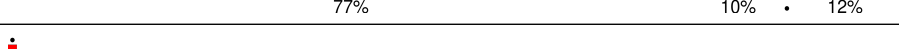
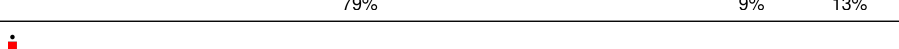
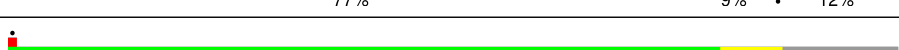

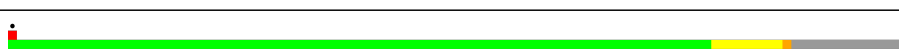

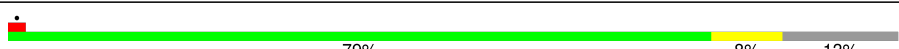





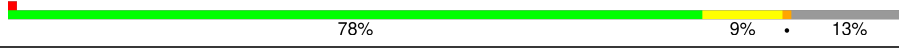
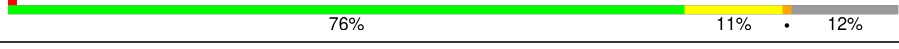



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Mol	Chain	Length	Quality of chain
3	Cc	377	
3	Cd	377	
3	Ce	377	
3	Cf	377	
3	Cg	377	
3	Ch	377	
3	Ci	377	
3	Cj	377	
3	Ck	377	
3	Cl	377	
3	Cm	377	
3	Cn	377	
3	Co	377	
3	Cp	377	
3	Cq	377	
3	Cr	377	
3	Cs	377	
3	Ct	377	
3	Cu	377	
3	Cv	377	
3	Cw	377	
3	Cx	377	
3	Cy	377	
3	Cz	377	
4	Da	294	







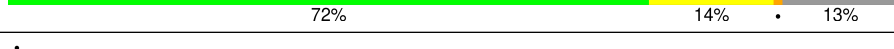
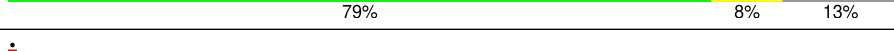
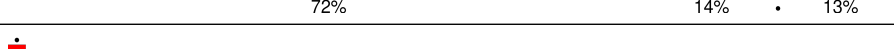
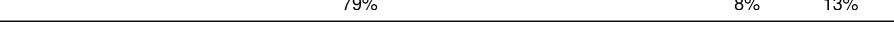
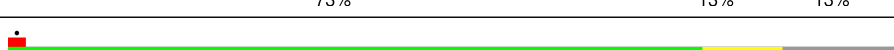

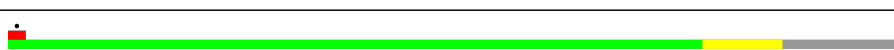

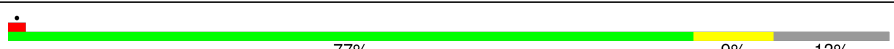





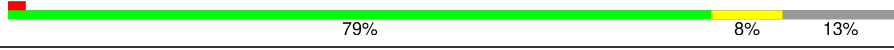
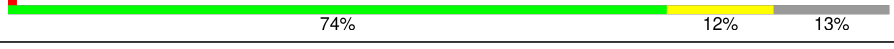



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Mol	Chain	Length	Quality of chain
4	Db	294	
4	Dc	294	
4	Dd	294	
4	De	294	
4	Df	294	
4	Dg	294	
4	Dh	294	
4	Di	294	
4	Dj	294	
4	Dk	294	
4	Dl	294	
4	Dm	294	
4	Dn	294	
4	Do	294	
4	Dp	294	
4	Dq	294	
4	Dr	294	
4	Ds	294	
4	Dt	294	
4	Du	294	
4	Dv	294	
4	Dw	294	
4	Dx	294	
4	Dy	294	
4	Dz	294	






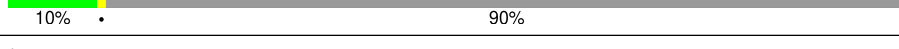

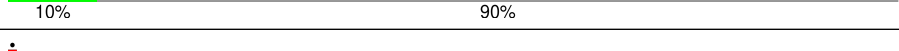
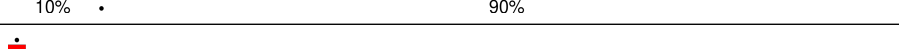
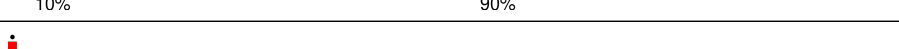















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Mol	Chain	Length	Quality of chain
5	Ea	211	
5	Eb	211	
5	Ec	211	
5	Ed	211	
5	Ee	211	
5	Ef	211	
5	Eg	211	
5	Eh	211	
5	Ei	211	
5	Ej	211	
5	Ek	211	
5	El	211	
5	Em	211	
5	En	211	
5	Eo	211	
5	Ep	211	
5	Eq	211	
5	Er	211	
5	Es	211	
5	Et	211	
5	Eu	211	
5	Ev	211	
5	Ew	211	
5	Ex	211	
5	Ey	211	

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























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Mol	Chain	Length	Quality of chain
5	Ez	211	
6	Fa	145	
6	Fb	145	
6	Fc	145	
6	Fd	145	
6	Fe	145	
6	Ff	145	
6	Fg	145	
6	Fh	145	
6	Fi	145	
6	Fj	145	
6	Fk	145	
6	Fl	145	
6	Fm	145	
6	Fn	145	
6	Fo	145	
6	Fp	145	
6	Fq	145	
6	Fr	145	
6	Fs	145	
6	Ft	145	
6	Fu	145	
6	Fv	145	
6	Fw	145	
6	Fx	145	

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Mol	Chain	Length	Quality of chain	
6	Fy	145		90%
6	Fz	145		90%
6	Ga	145		91%
6	Gb	145		91%
6	Gc	145		91%
6	Gd	145		91%
6	Ge	145		91%
6	Gf	145		91%
6	Gg	145		91%
6	Gh	145		91%
6	Gi	145		91%
6	Gj	145		91%
6	Gk	145		91%
6	Gl	145		91%
6	Gm	145		91%
6	Gn	145		91%
6	Go	145		91%
6	Gp	145		91%
6	Gq	145		91%
6	Gr	145		91%
6	Gs	145		91%
6	Gt	145		91%
6	Gu	145		91%
6	Gv	145		91%
6	Gw	145		91%

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Mol	Chain	Length	Quality of chain
6	Gx	145	 8% 91%
6	Gy	145	 8% 91%
6	Gz	145	 9% 91%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 279357 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar L-ring protein.

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

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

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

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

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

- Molecule 3 is a protein called Flagellar protein FlgT.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Cd	352	Total	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 Lipoprotein.

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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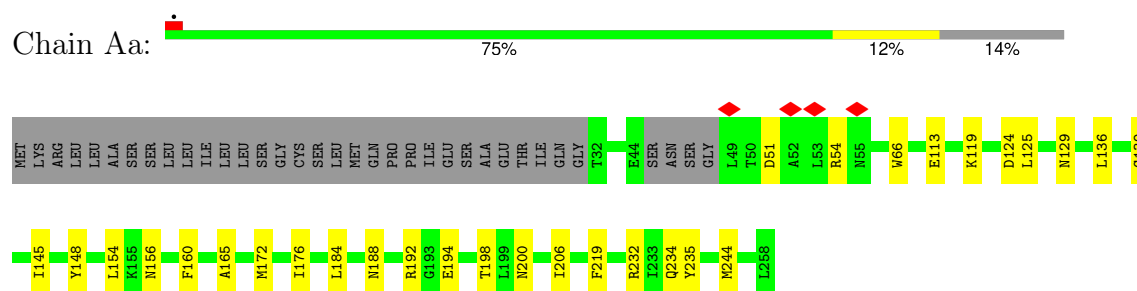
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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Gt	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gu	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gv	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gw	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gx	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gy	13	Total 112	C 71	N 20	O 20	S 1	0	0
6	Gz	13	Total 112	C 71	N 20	O 20	S 1	0	0

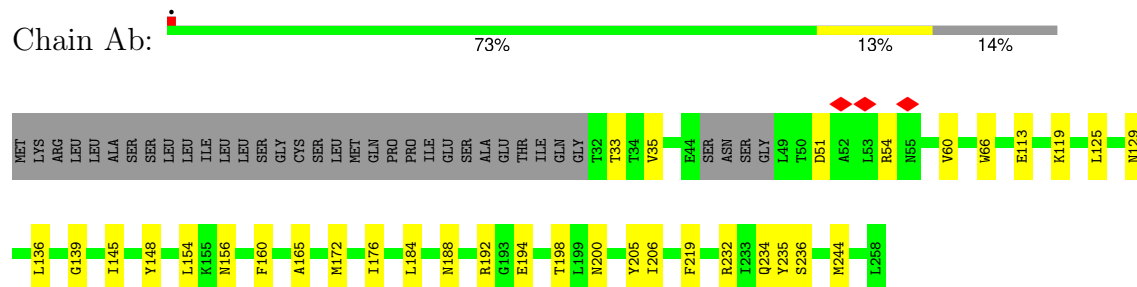
### 3 Residue-property plots [i](#)

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

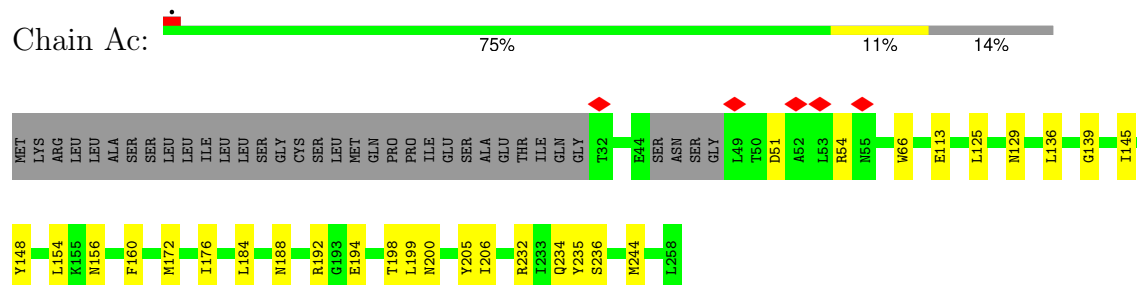
- Molecule 1: Flagellar L-ring protein



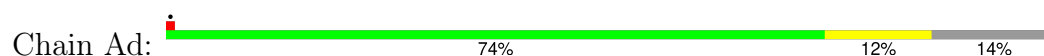
- Molecule 1: Flagellar L-ring protein

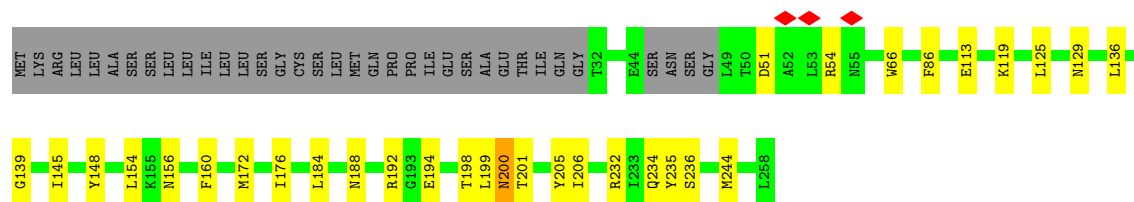


- Molecule 1: Flagellar L-ring protein

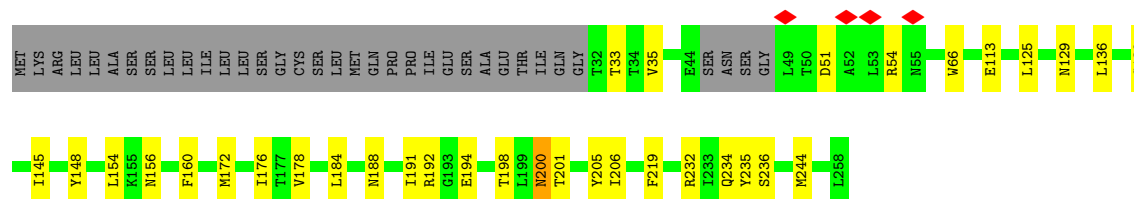
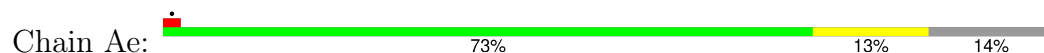


- Molecule 1: Flagellar L-ring protein

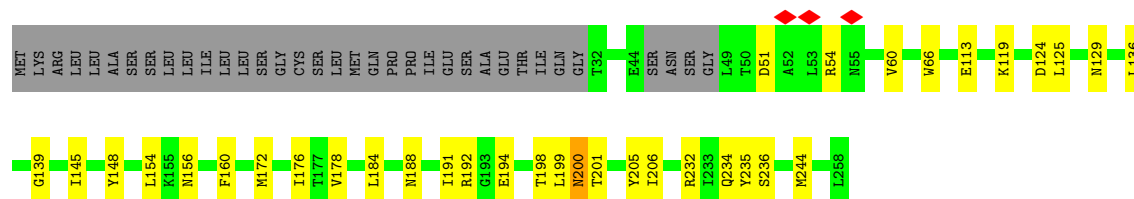




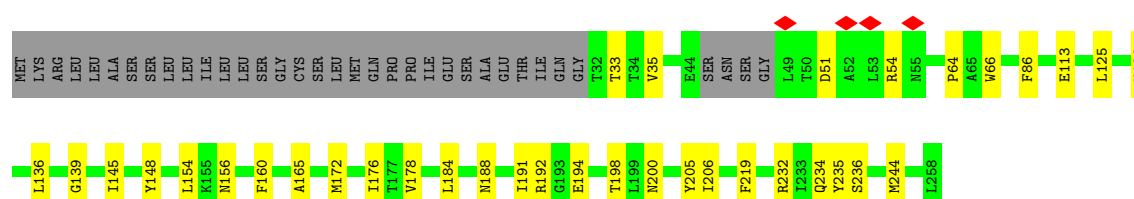
• Molecule 1: Flagellar L-ring protein



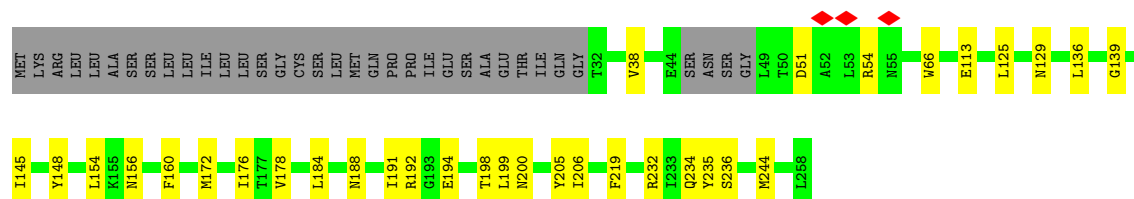
• Molecule 1: Flagellar L-ring protein



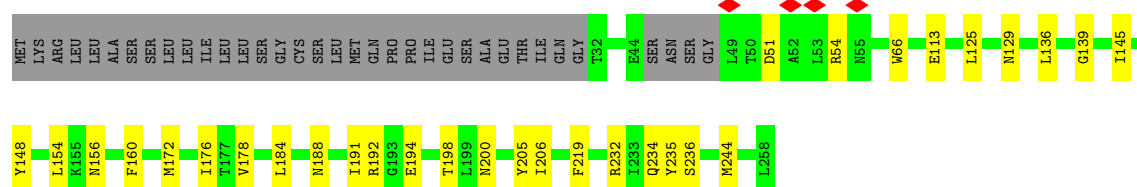

• Molecule 1: Flagellar L-ring protein



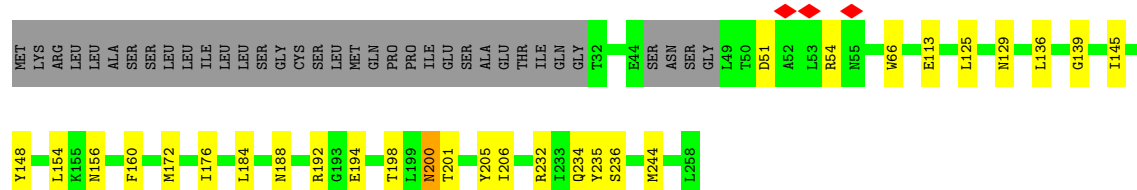

• Molecule 1: Flagellar L-ring protein



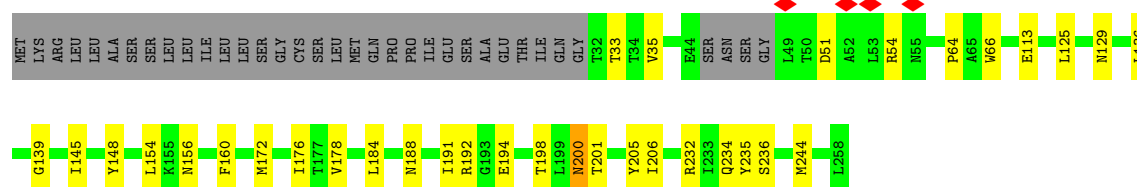

## • Molecule 1: Flagellar L-ring protein

Chain Ai: 

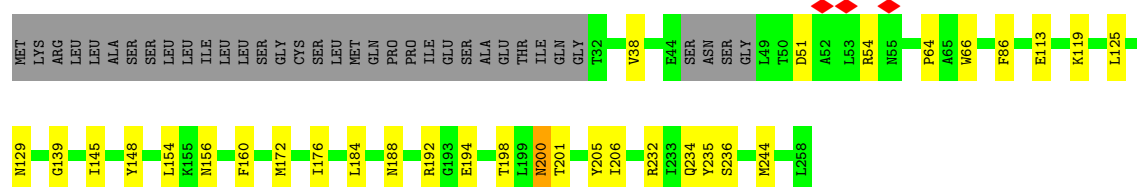

## • Molecule 1: Flagellar L-ring protein

Chain Aj: 


## • Molecule 1: Flagellar L-ring protein

Chain Ak: 

## • Molecule 1: Flagellar L-ring protein

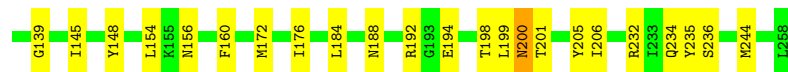
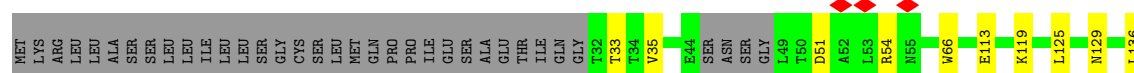
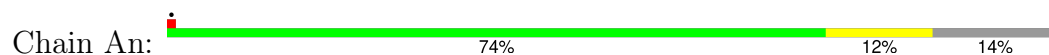
Chain Al: 

## • Molecule 1: Flagellar L-ring protein

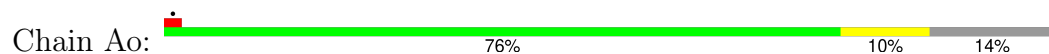
Chain Am: 



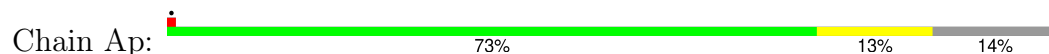
• Molecule 1: Flagellar L-ring protein



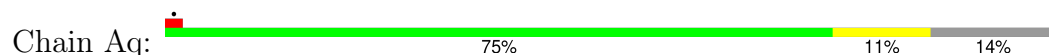
• Molecule 1: Flagellar L-ring protein



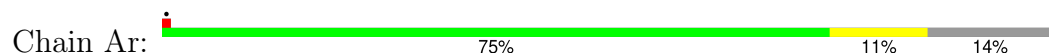
• Molecule 1: Flagellar L-ring protein



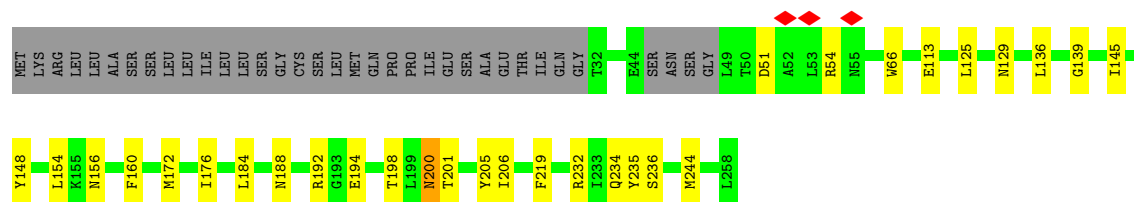
• Molecule 1: Flagellar L-ring protein



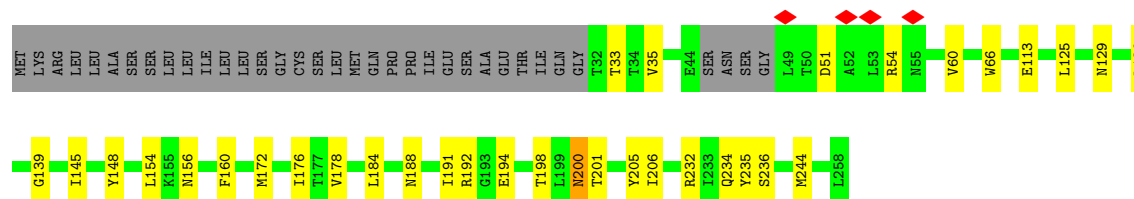
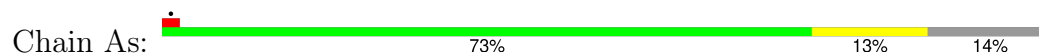
• Molecule 1: Flagellar L-ring protein



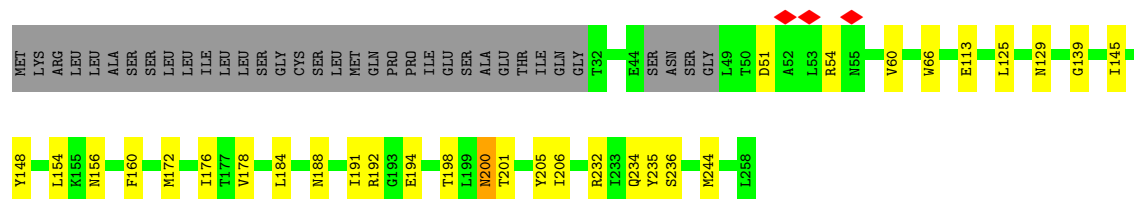
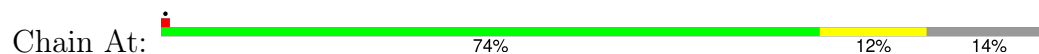




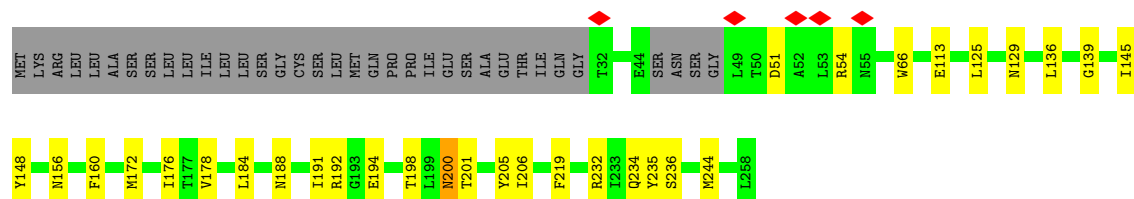
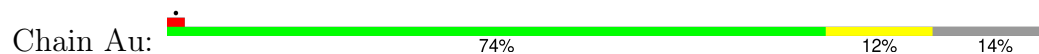
- Molecule 1: Flagellar L-ring protein



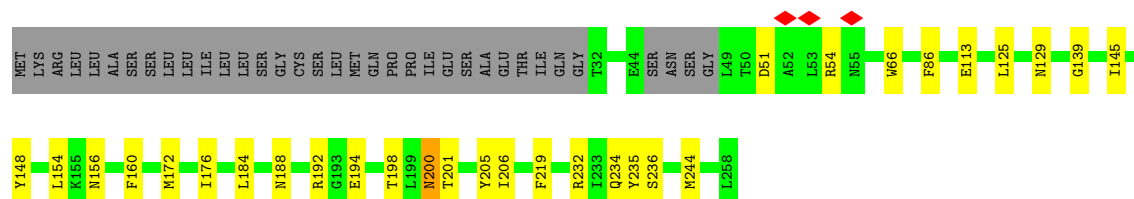
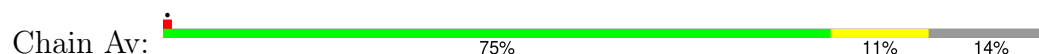
- Molecule 1: Flagellar L-ring protein



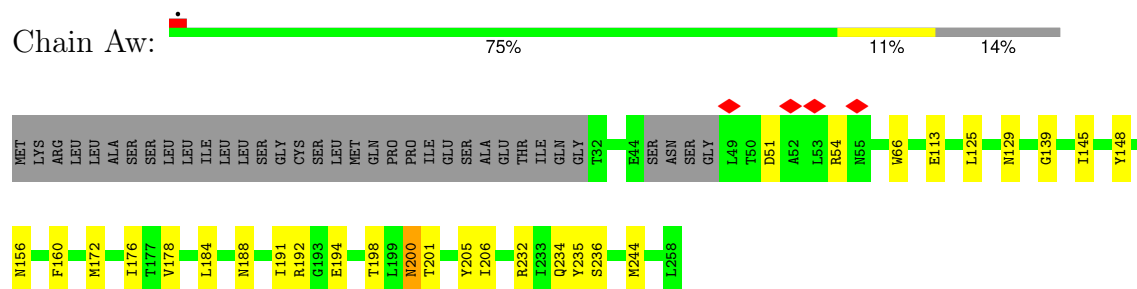
- Molecule 1: Flagellar L-ring protein



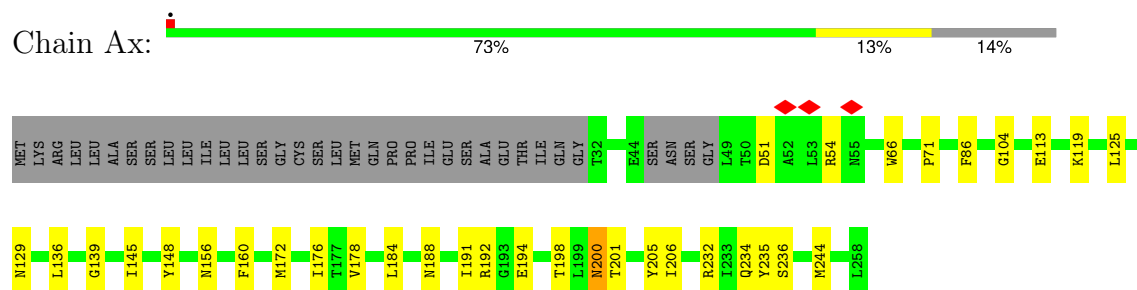
- Molecule 1: Flagellar L-ring protein



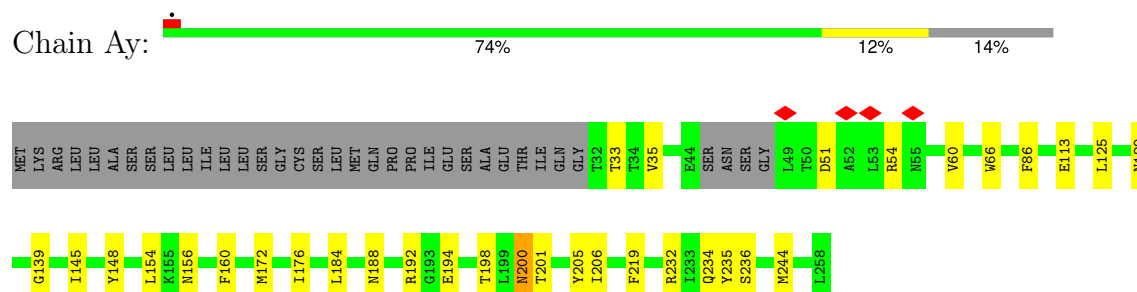
- Molecule 1: Flagellar L-ring protein



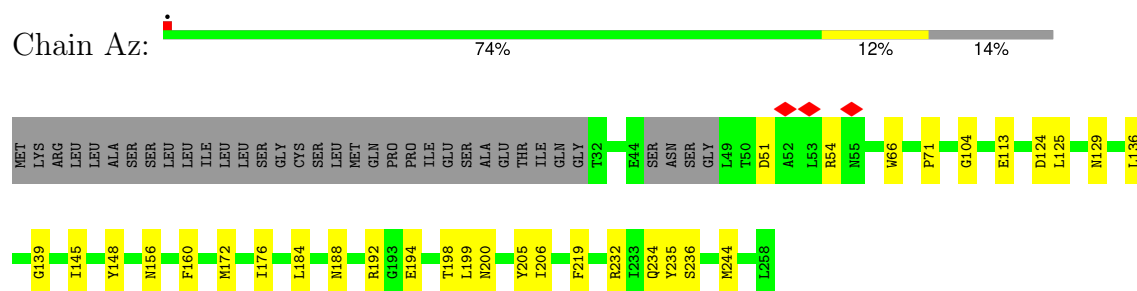
- Molecule 1: Flagellar L-ring protein



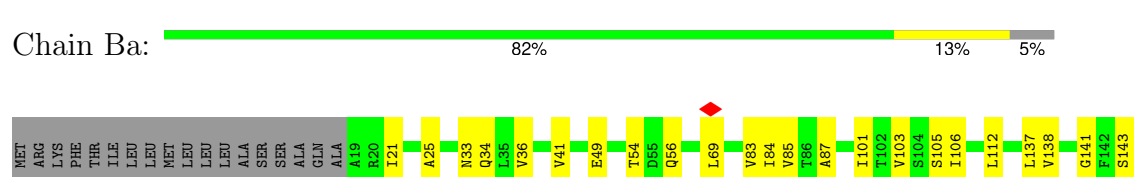
- Molecule 1: Flagellar L-ring protein



- Molecule 1: Flagellar L-ring protein

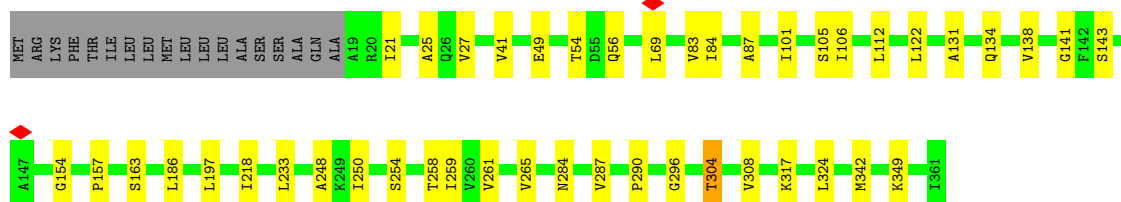
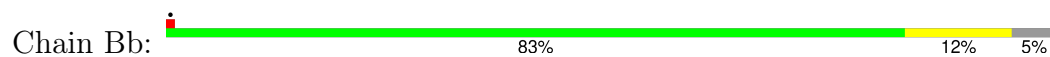


- Molecule 2: Flagellar P-ring protein

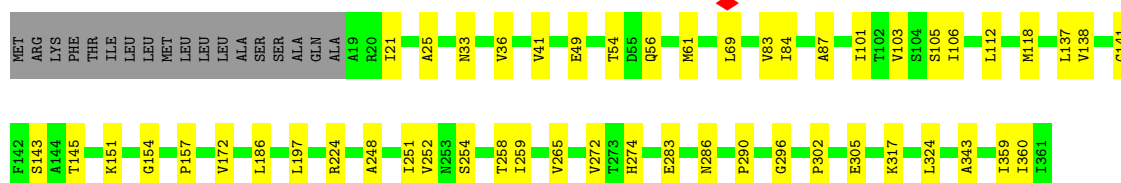
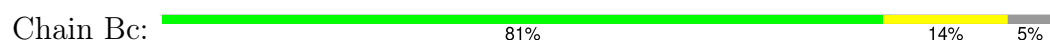




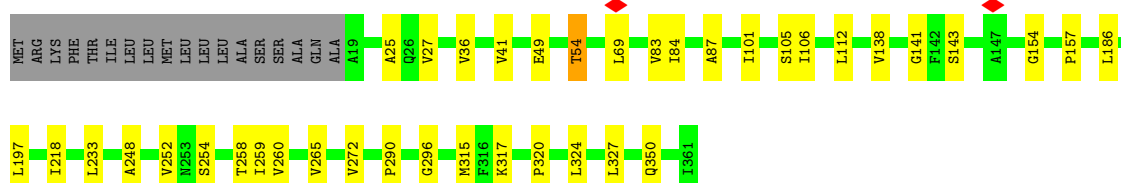
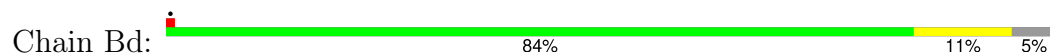
- Molecule 2: Flagellar P-ring protein



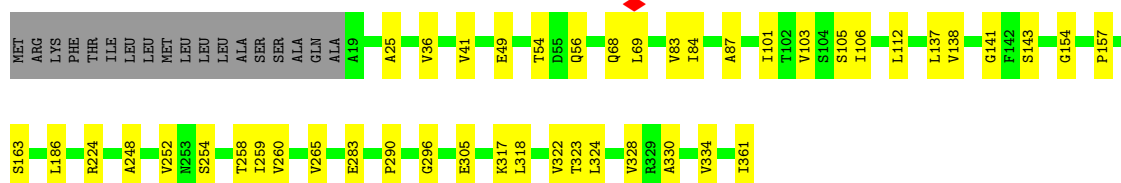
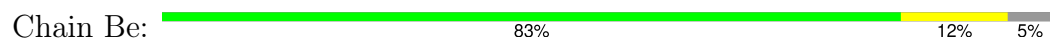
- Molecule 2: Flagellar P-ring protein



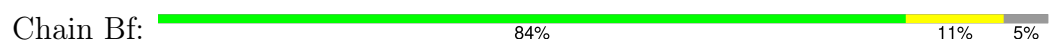
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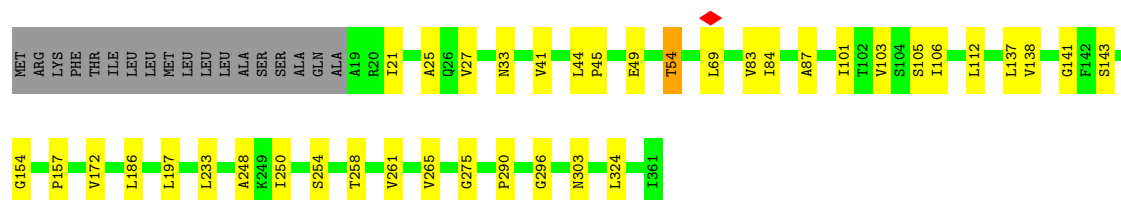


- Molecule 2: Flagellar P-ring protein



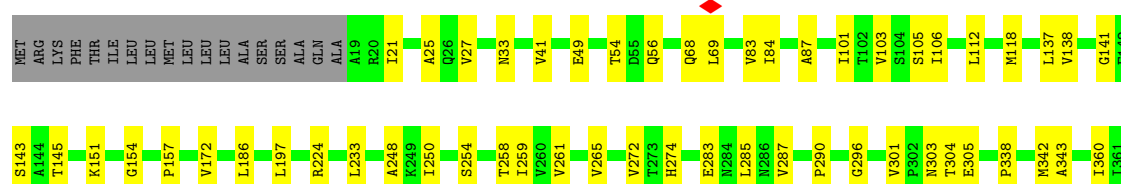
- Molecule 2: Flagellar P-ring protein





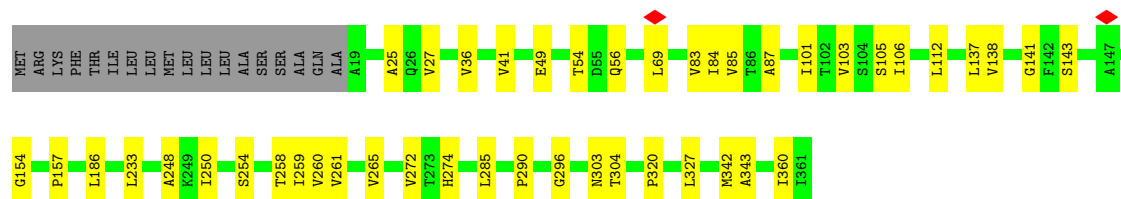
• Molecule 2: Flagellar P-ring protein

Chain Bg: 80% 15% 5%



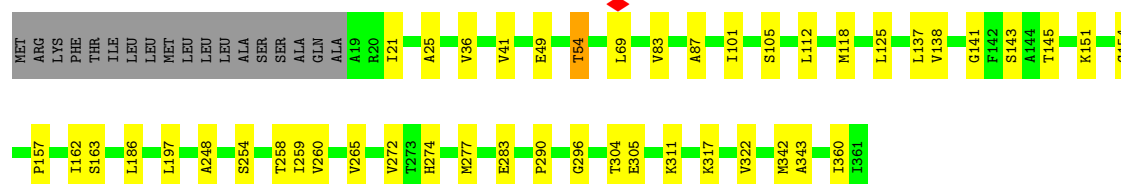
• Molecule 2: Flagellar P-ring protein

Chain Bh: 83% 12% 5%



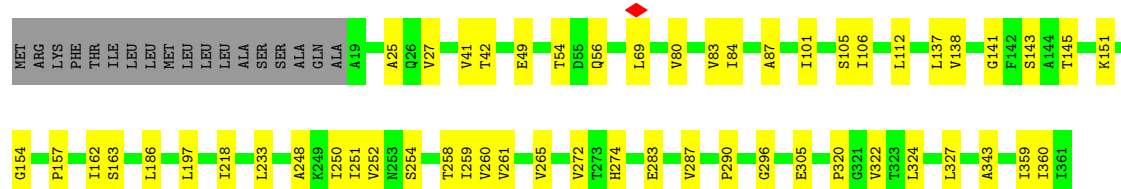
• Molecule 2: Flagellar P-ring protein

Chain Bi: 82% 12% 5%

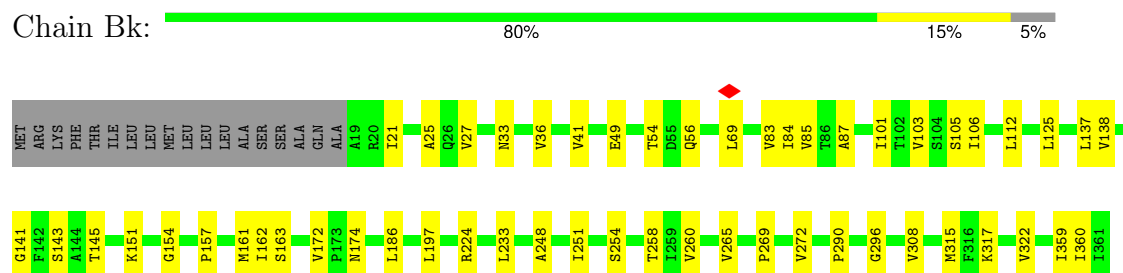


• Molecule 2: Flagellar P-ring protein

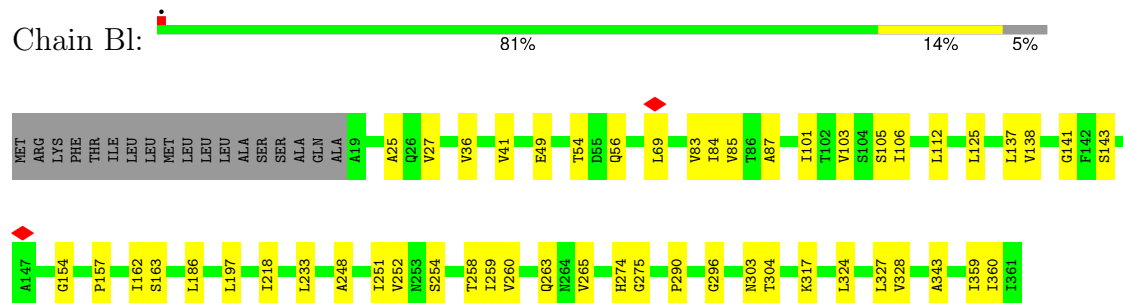
Chain Bj: 80% 15% 5%



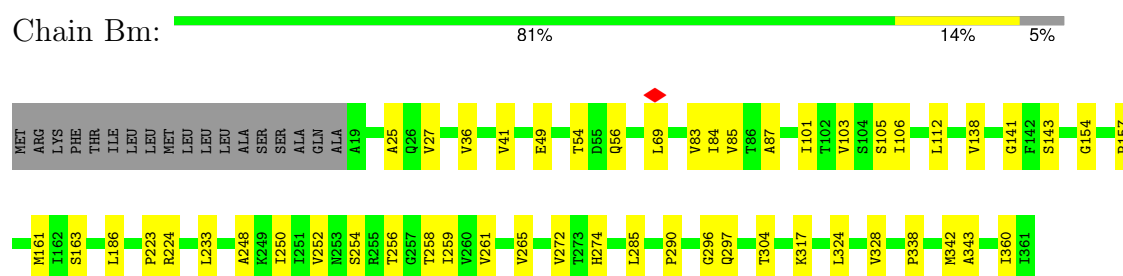
- Molecule 2: Flagellar P-ring protein



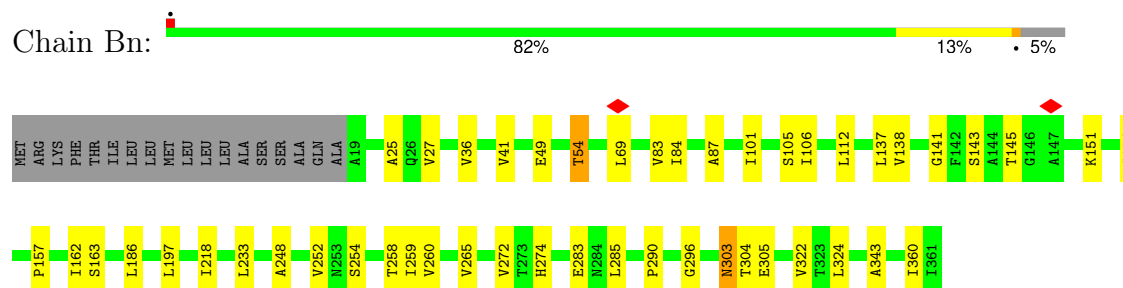
- Molecule 2: Flagellar P-ring protein



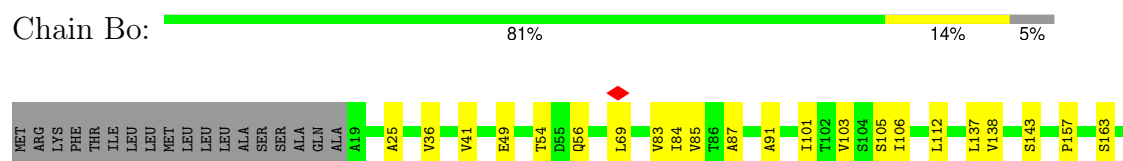
- Molecule 2: Flagellar P-ring protein



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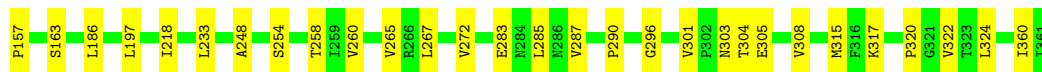
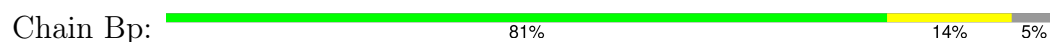


- Molecule 2: Flagellar P-ring protein

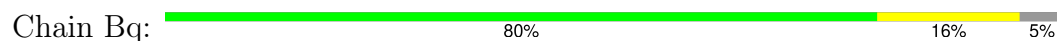




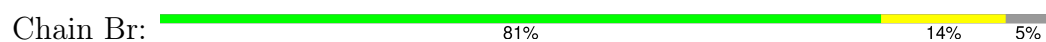
• Molecule 2: Flagellar P-ring protein



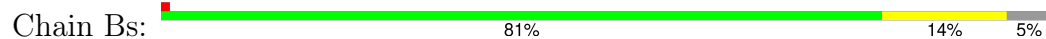
• Molecule 2: Flagellar P-ring protein




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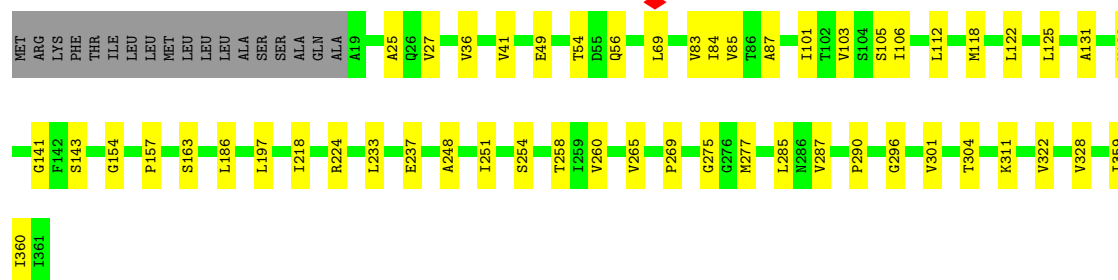


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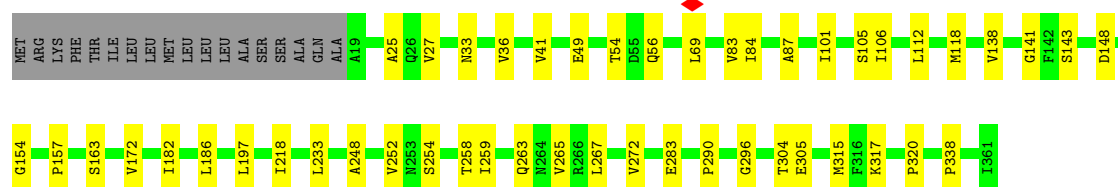
• Molecule 2: Flagellar P-ring protein

Chain Bt: 




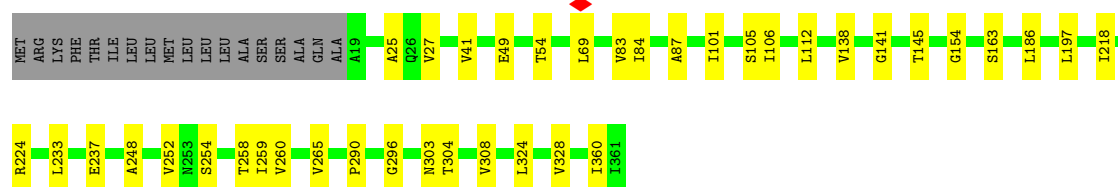
- Molecule 2: Flagellar P-ring protein

Chain Bu: 




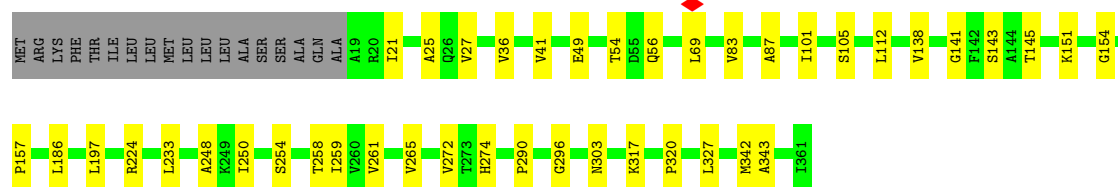
- Molecule 2: Flagellar P-ring protein

Chain Bv: 




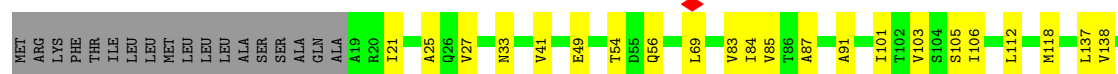
- Molecule 2: Flagellar P-ring protein

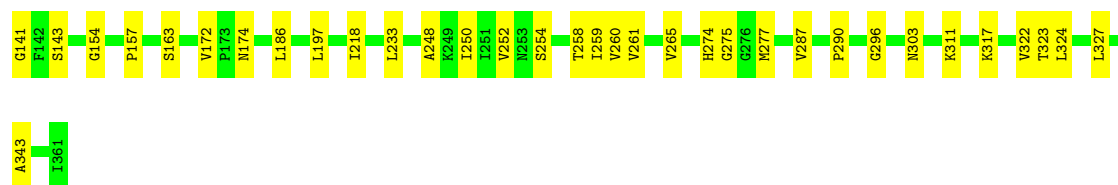
Chain Bw: 



- Molecule 2: Flagellar P-ring protein

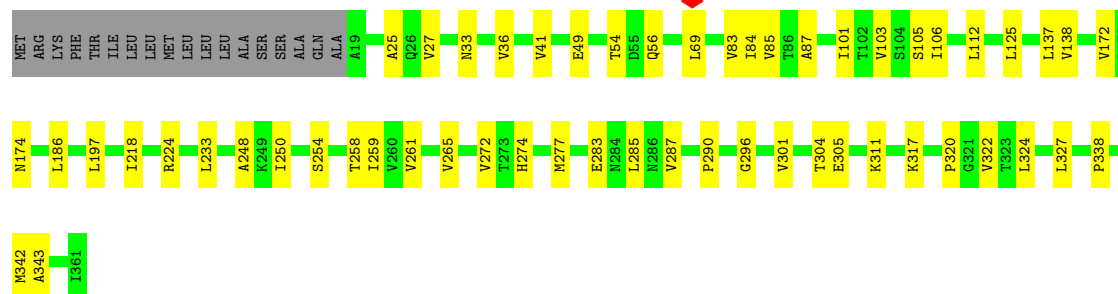
Chain Bx: 





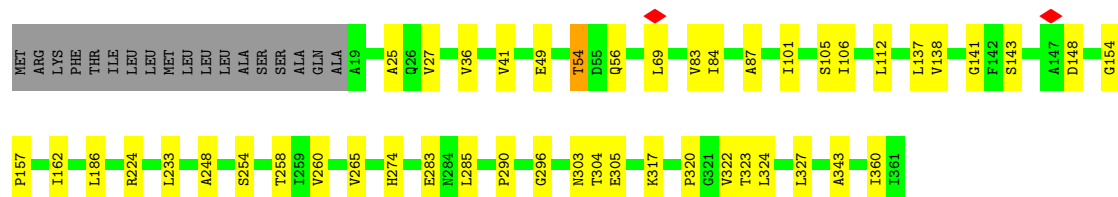
- Molecule 2: Flagellar P-ring protein

Chain By: 80% 15% 5%



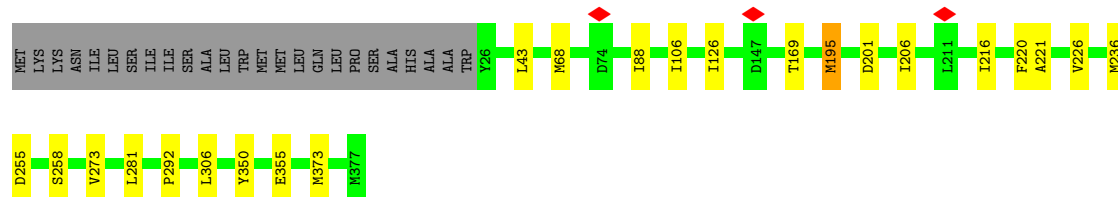
- Molecule 2: Flagellar P-ring protein

Chain Bz: 82% 13% 5%



- Molecule 3: Flagellar protein FlgT

Chain Ca: 87% 6% 7%

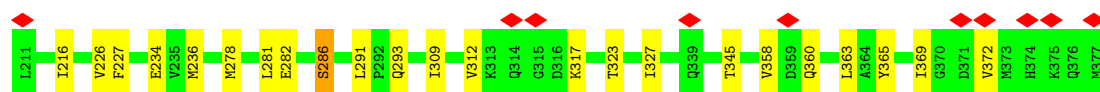


- Molecule 3: Flagellar protein FlgT

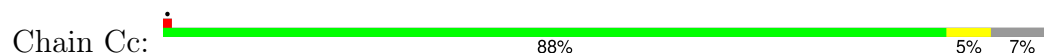
Chain Cb: 82% 10% 7%



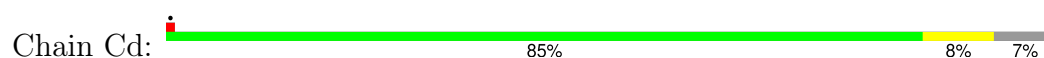




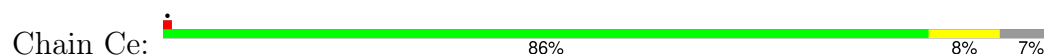
• Molecule 3: Flagellar protein FlgT



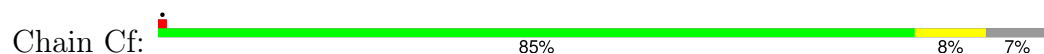
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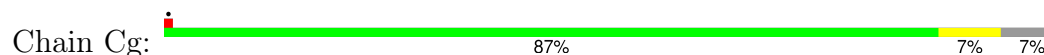
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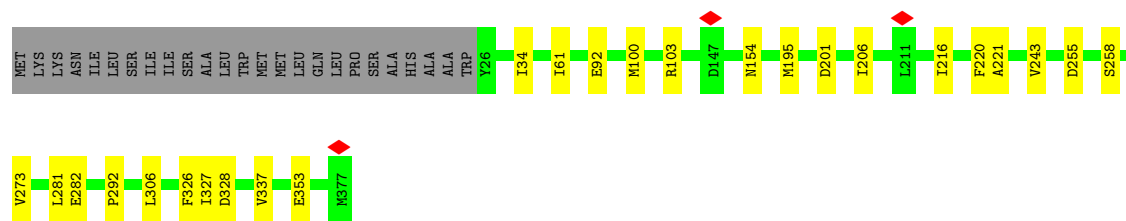


• Molecule 3: Flagellar protein FlgT

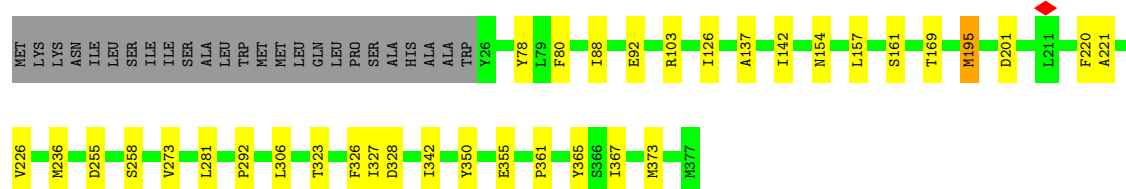
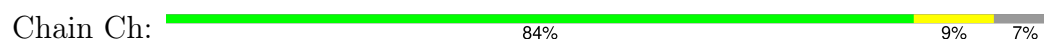


• Molecule 3: Flagellar protein FlgT

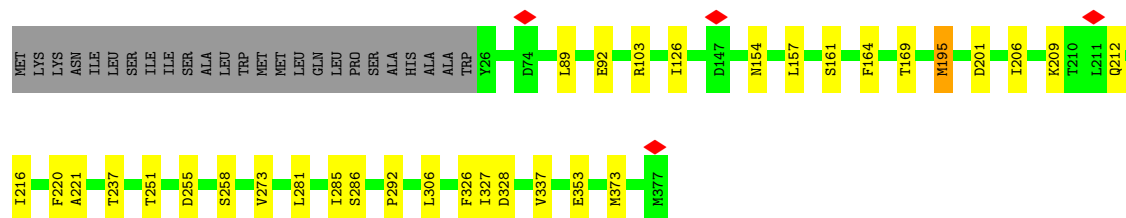
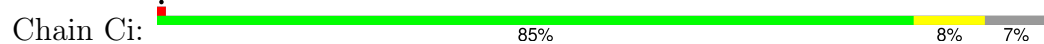




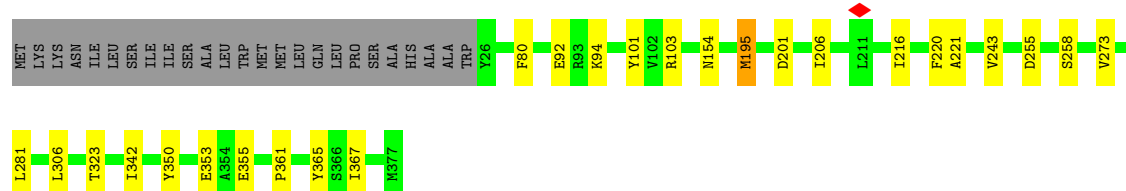
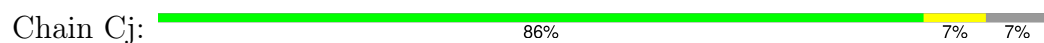
• Molecule 3: Flagellar protein FlgT



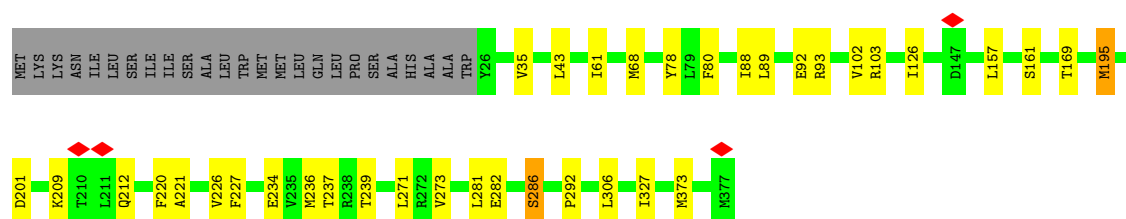
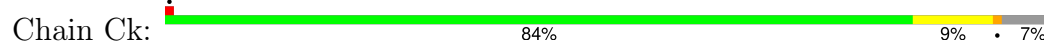
• Molecule 3: Flagellar protein FlgT




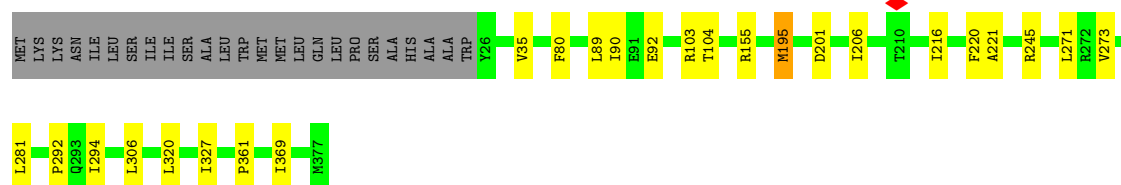
• Molecule 3: Flagellar protein FlgT



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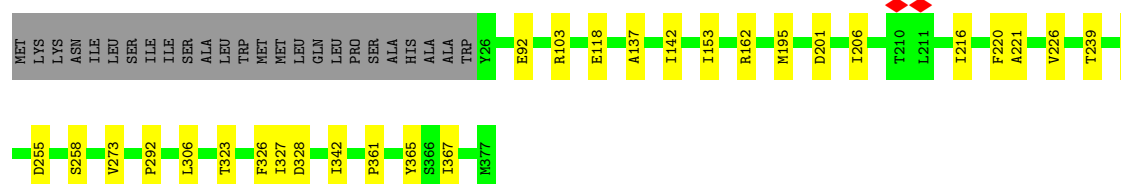
## • Molecule 3: Flagellar protein FlgT

Chain Cl:  87% 6% 7%


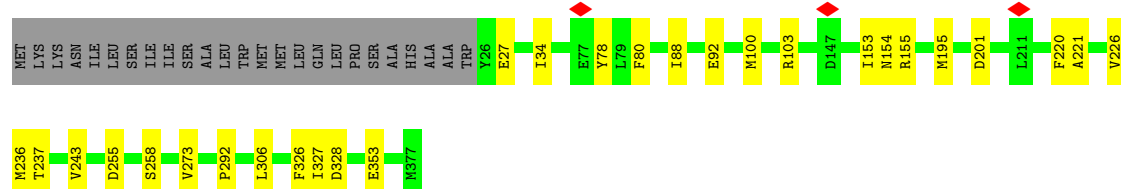
## • Molecule 3: Flagellar protein FlgT

Chain Cm:  85% 8% 7%


## • Molecule 3: Flagellar protein FlgT

Chain Cn:  86% 8% 7%

## • Molecule 3: Flagellar protein FlgT

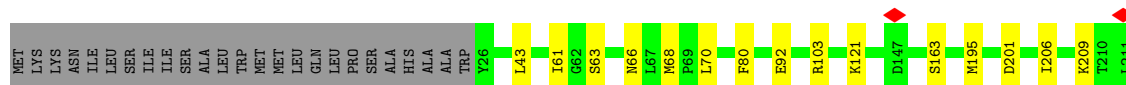
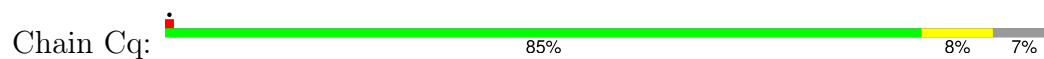
Chain Co:  86% 7% 7%

## • Molecule 3: Flagellar protein FlgT

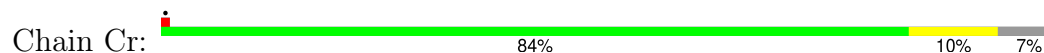
Chain Cp:  87% 7% 7%



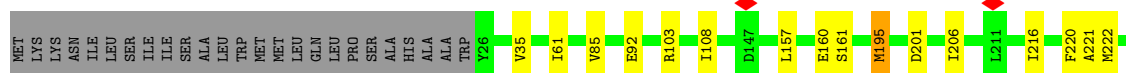
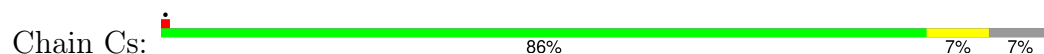
- Molecule 3: Flagellar protein FlgT



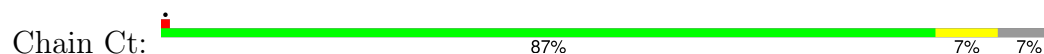
- Molecule 3: Flagellar protein FlgT



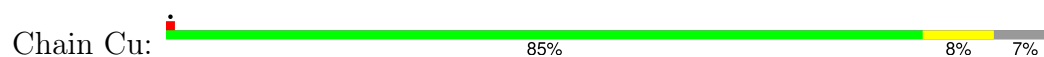
- Molecule 3: Flagellar protein FlgT

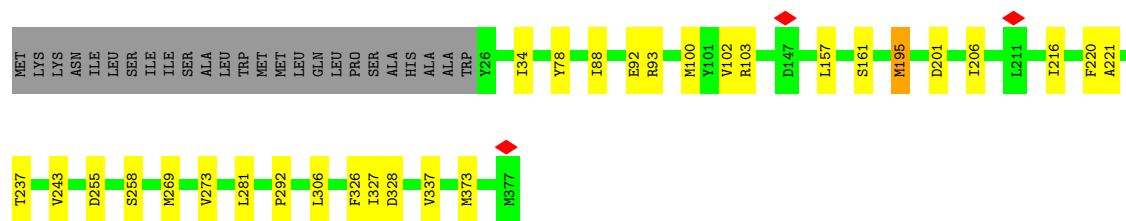


- Molecule 3: Flagellar protein FlgT

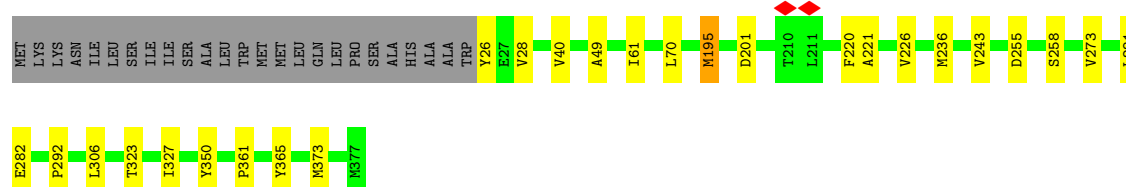
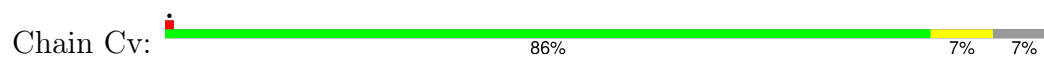


- Molecule 3: Flagellar protein FlgT

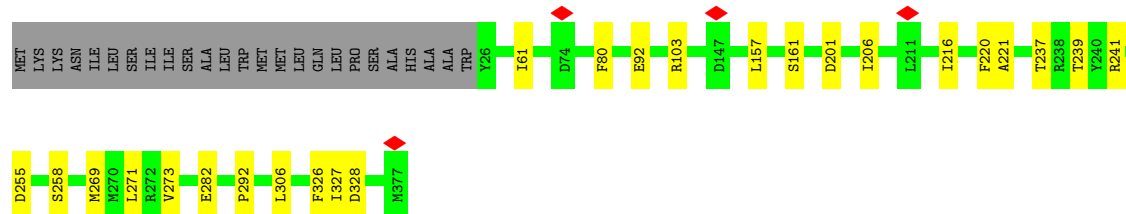
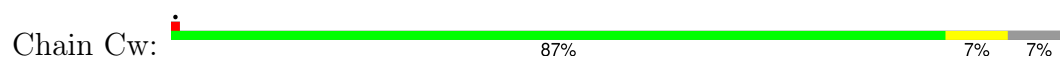




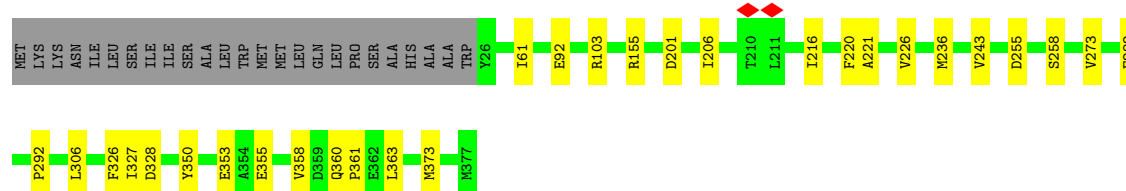
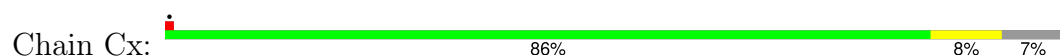
• Molecule 3: Flagellar protein FlgT



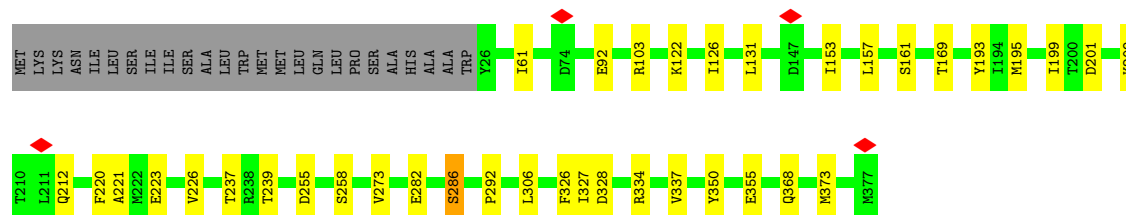
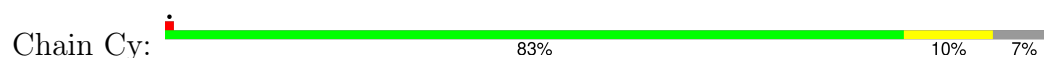
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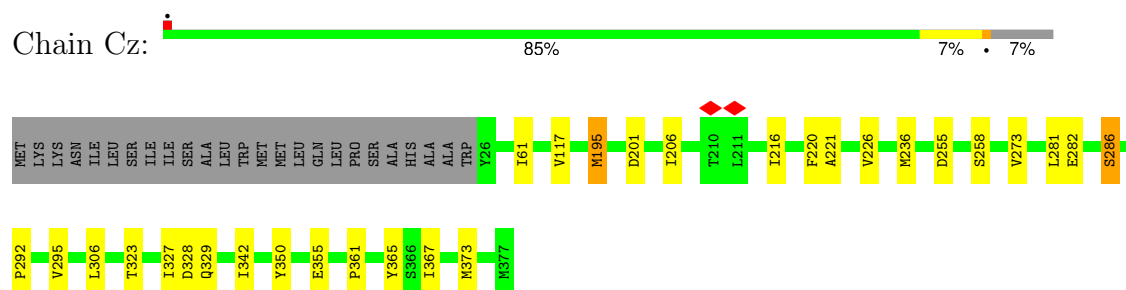
• Molecule 3: Flagellar protein FlgT



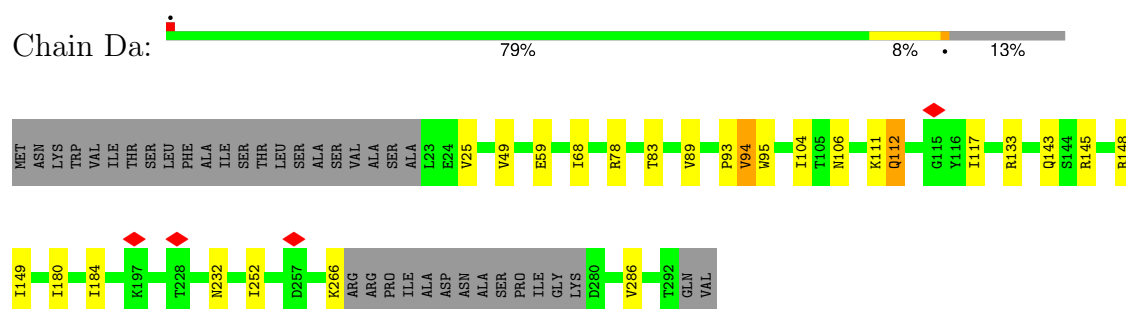
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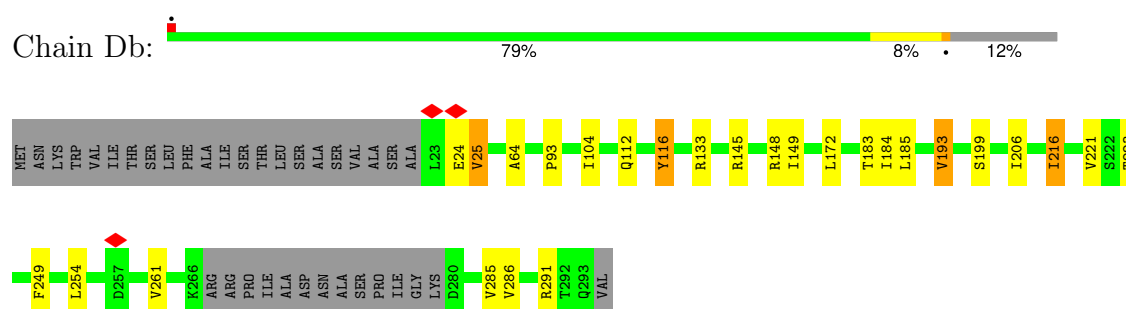
- Molecule 3: Flagellar protein FlgT

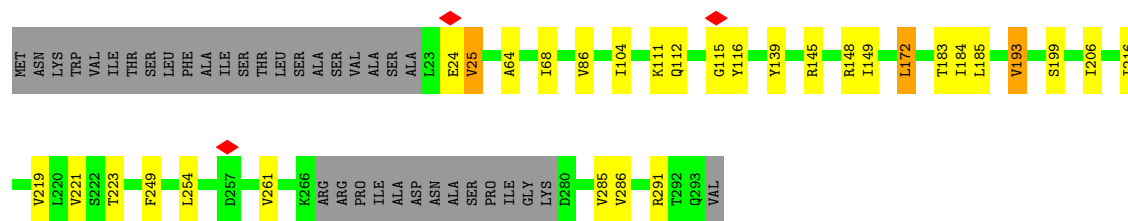


- Molecule 4: Sodium-type flagellar protein MotY

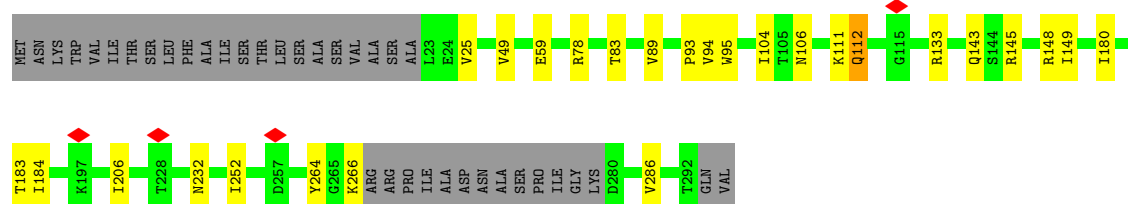
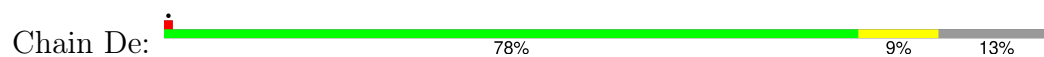


- Molecule 4: Sodium-type flagellar protein MotY

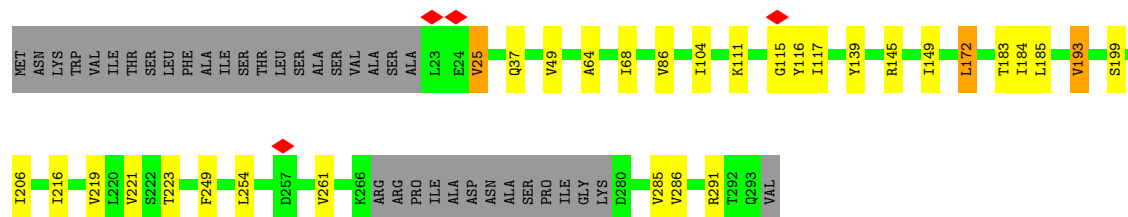
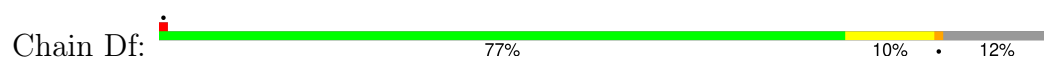




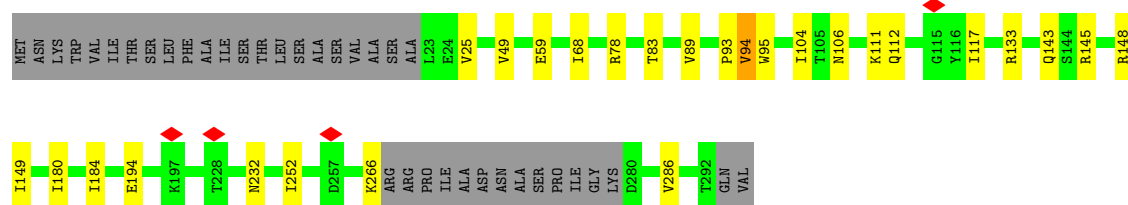
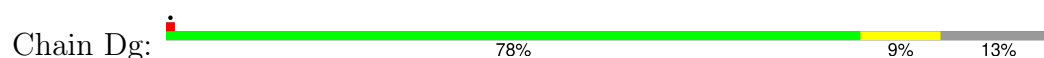
• Molecule 4: Sodium-type flagellar protein MotY



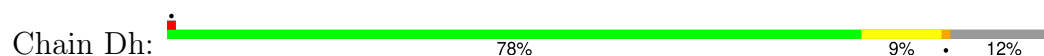
• Molecule 4: Sodium-type flagellar protein MotY

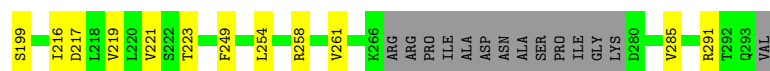


• Molecule 4: Sodium-type flagellar protein MotY

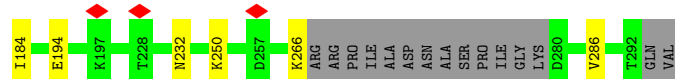
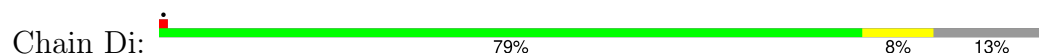


• Molecule 4: Sodium-type flagellar protein MotY

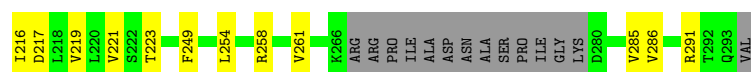
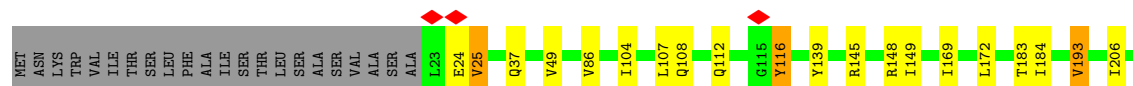
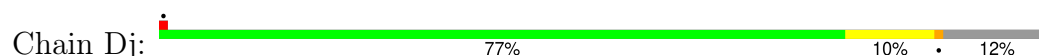




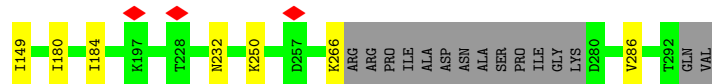
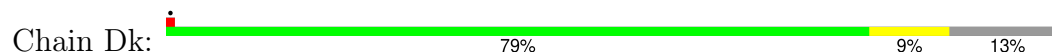
- Molecule 4: Sodium-type flagellar protein MotY



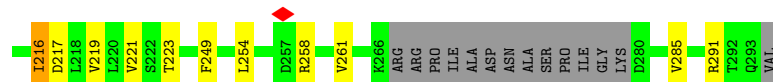
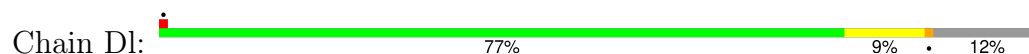
- Molecule 4: Sodium-type flagellar protein MotY



- Molecule 4: Sodium-type flagellar protein MotY




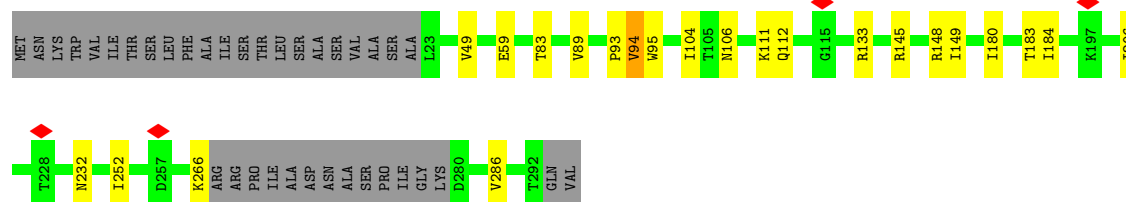
- Molecule 4: Sodium-type flagellar protein MotY




- Molecule 4: Sodium-type flagellar protein MotY

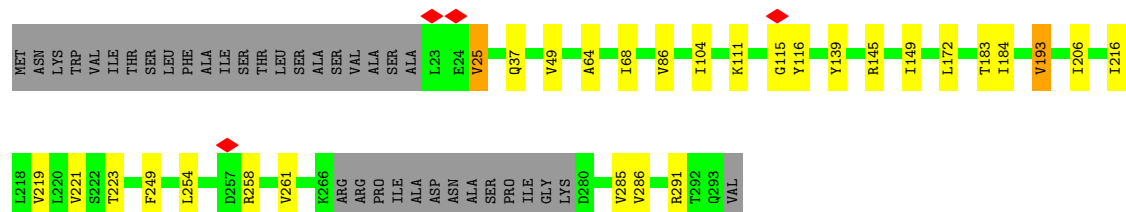


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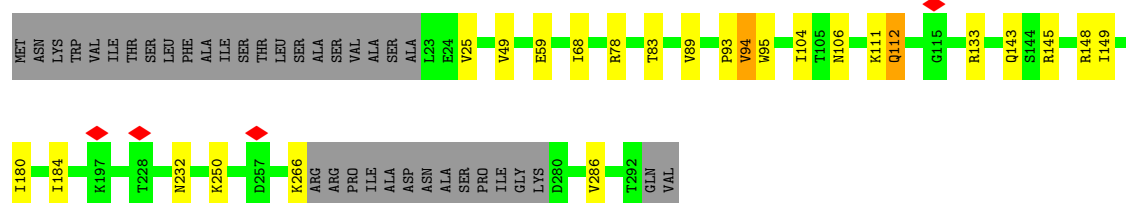
- Molecule 4: Sodium-type flagellar protein MotY

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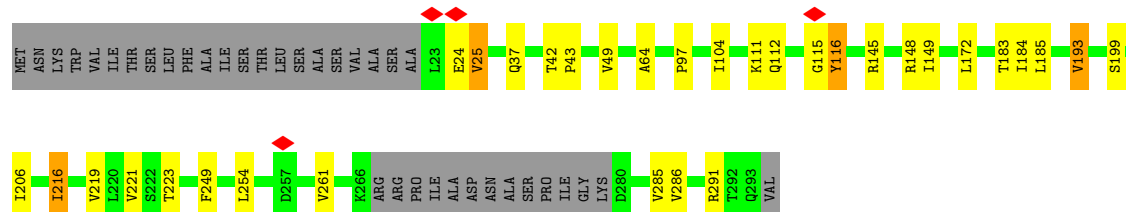
- Molecule 4: Sodium-type flagellar protein MotY

Chain Do: 




- Molecule 4: Sodium-type flagellar protein MotY

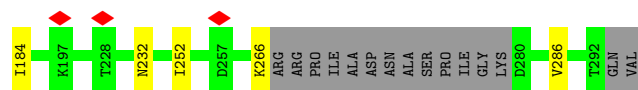
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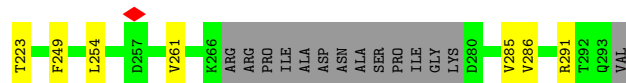
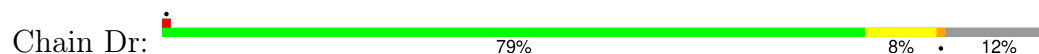
- Molecule 4: Sodium-type flagellar protein MotY

Chain Dq: 

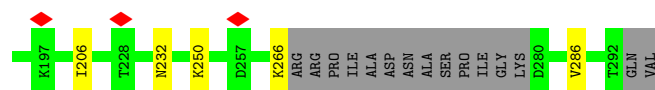
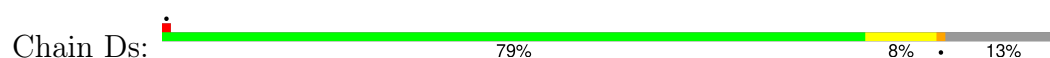




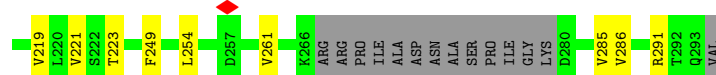
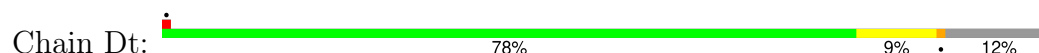
- Molecule 4: Sodium-type flagellar protein MotY



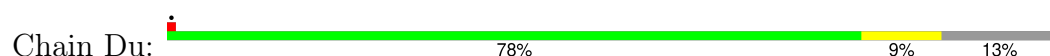
- Molecule 4: Sodium-type flagellar protein MotY




- Molecule 4: Sodium-type flagellar protein MotY

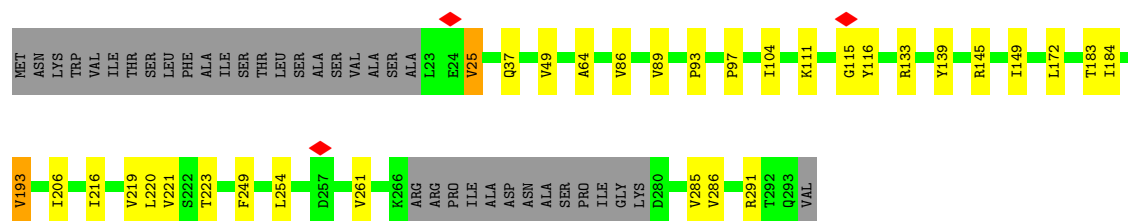


- Molecule 4: Sodium-type flagellar protein MotY




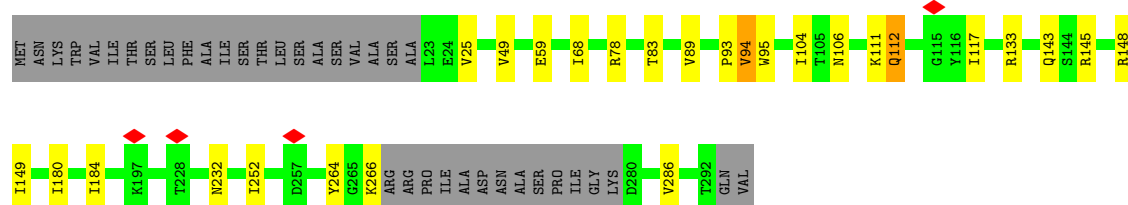
- Molecule 4: Sodium-type flagellar protein MotY

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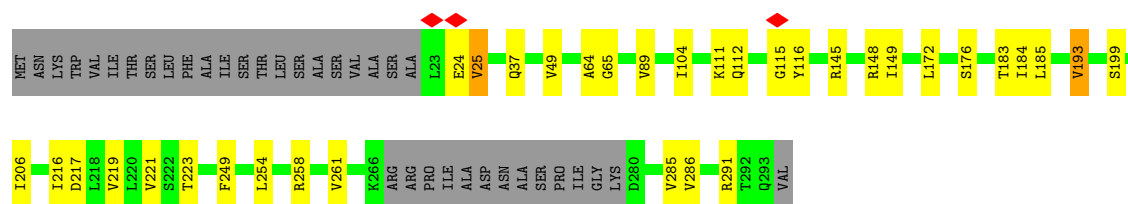
- Molecule 4: Sodium-type flagellar protein MotY

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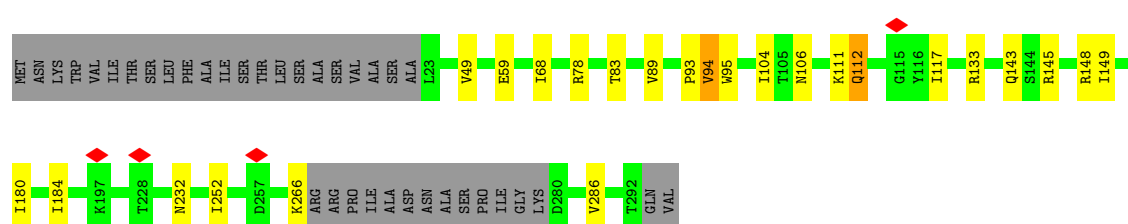
- Molecule 4: Sodium-type flagellar protein MotY

Chain Dx: 




- Molecule 4: Sodium-type flagellar protein MotY

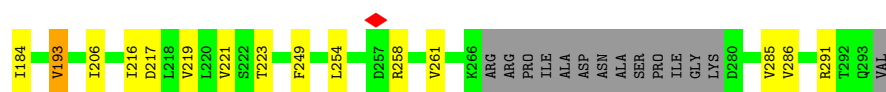
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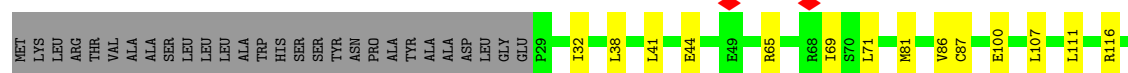
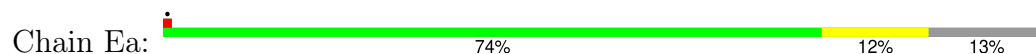
- Molecule 4: Sodium-type flagellar protein MotY

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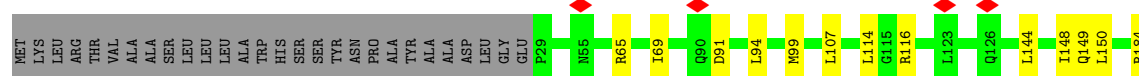
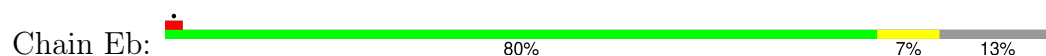




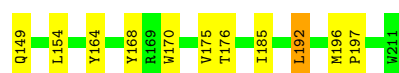
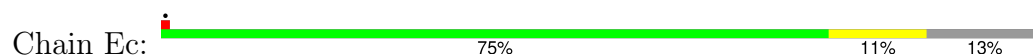
- Molecule 5: Sodium-type flagellar protein MotX



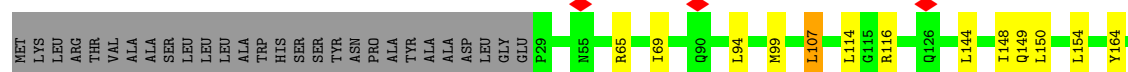
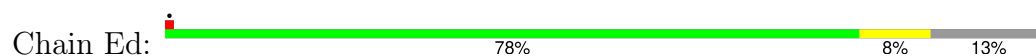
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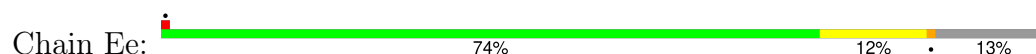
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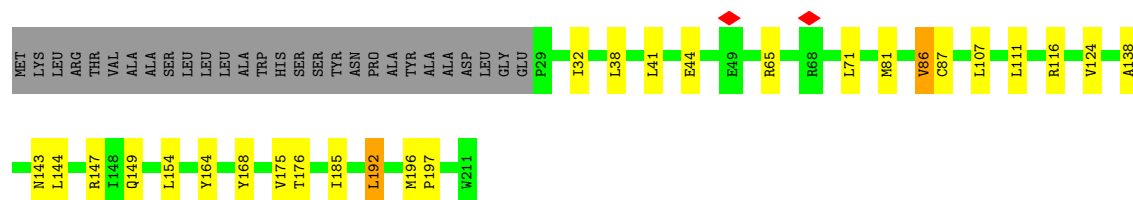


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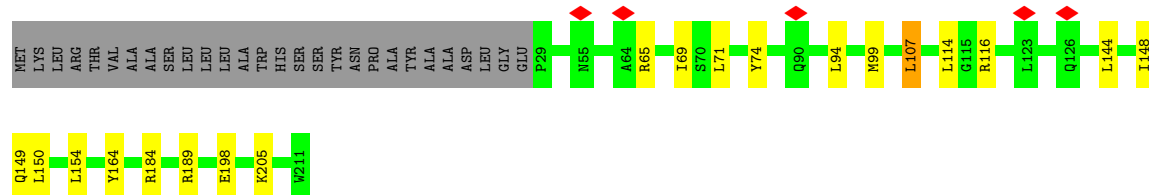
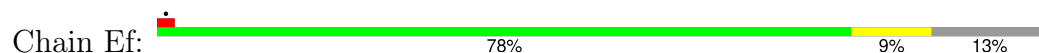


- Molecule 5: Sodium-type flagellar protein MotX

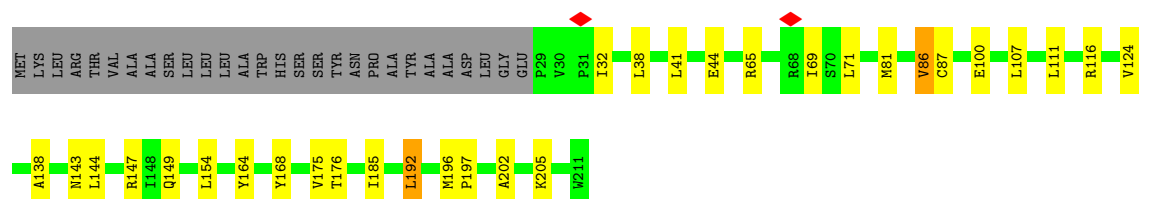
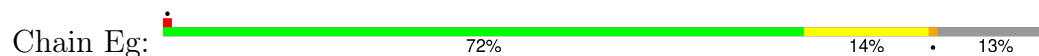




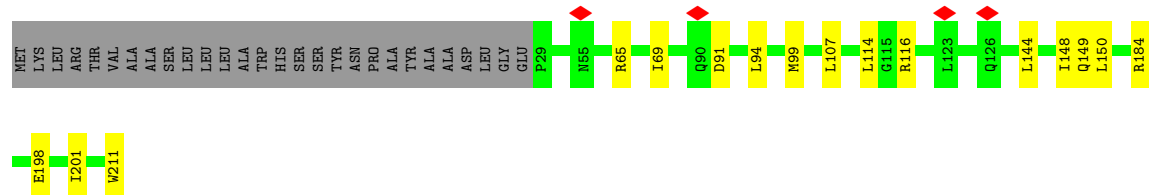
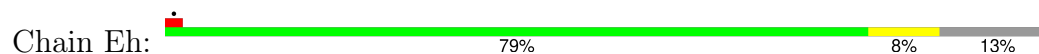
• Molecule 5: Sodium-type flagellar protein MotX



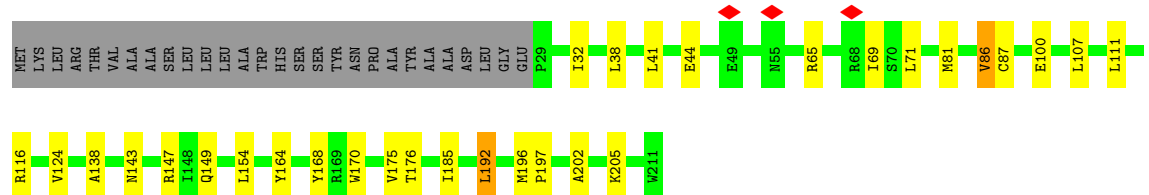
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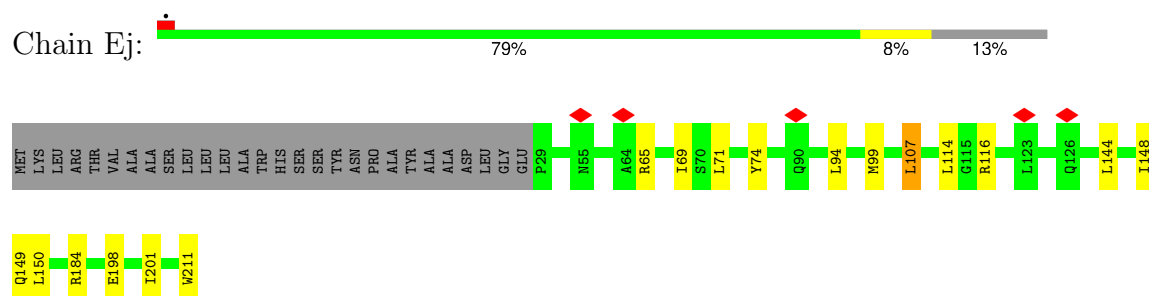
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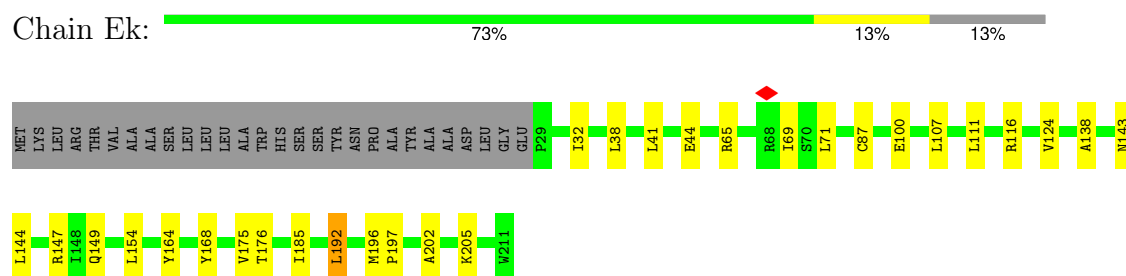
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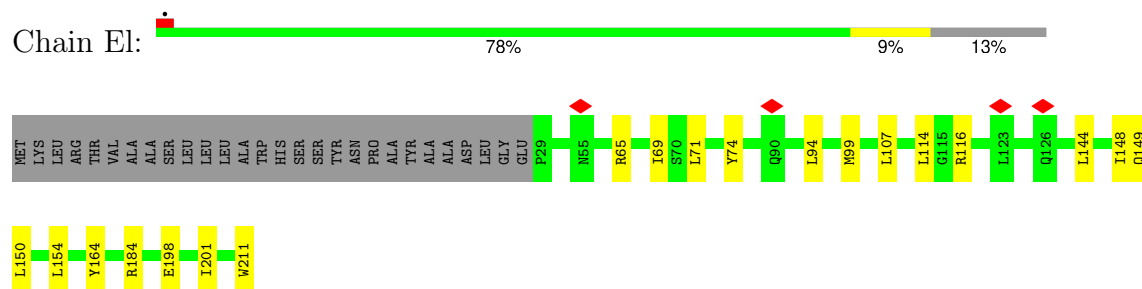
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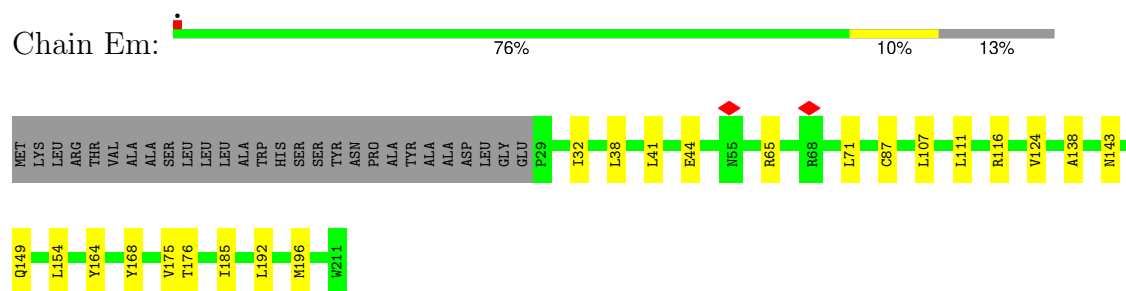
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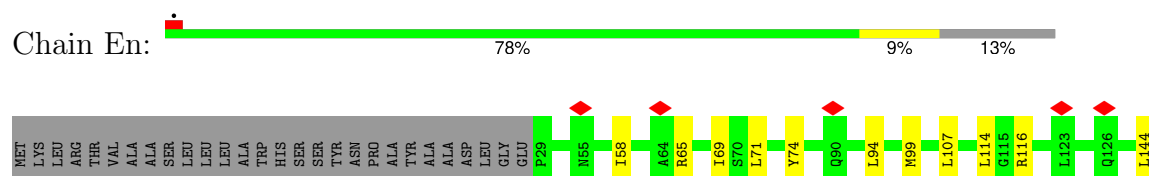
- Molecule 5: Sodium-type flagellar protein MotX



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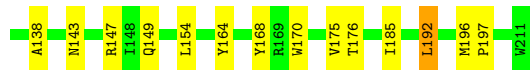
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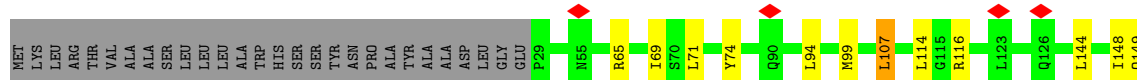
- Molecule 5: Sodium-type flagellar protein MotX

Chain Eo: 73% 13% 13%



- Molecule 5: Sodium-type flagellar protein MotX

Chain Ep: 77% 9% 13%



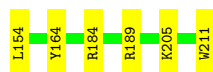
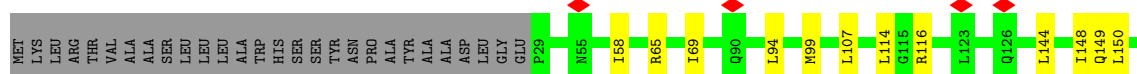
- Molecule 5: Sodium-type flagellar protein MotX

Chain Eq: 74% 13% 13%



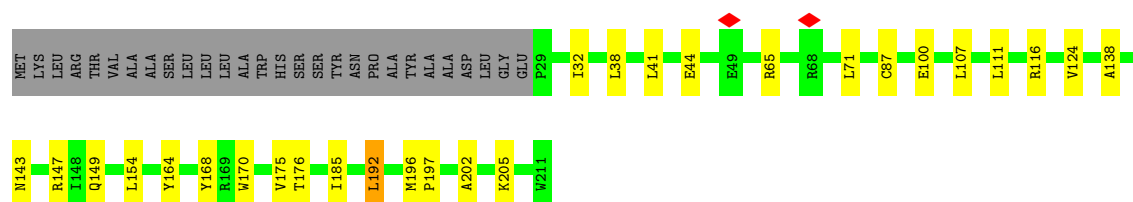
- Molecule 5: Sodium-type flagellar protein MotX

Chain Er: 78% 9% 13%

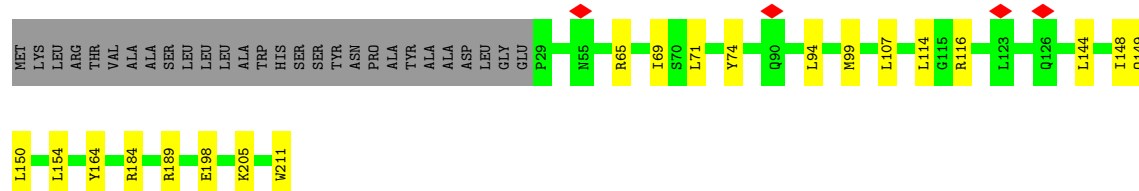
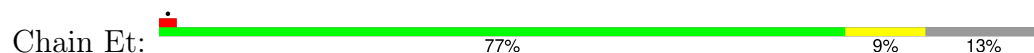


- Molecule 5: Sodium-type flagellar protein MotX

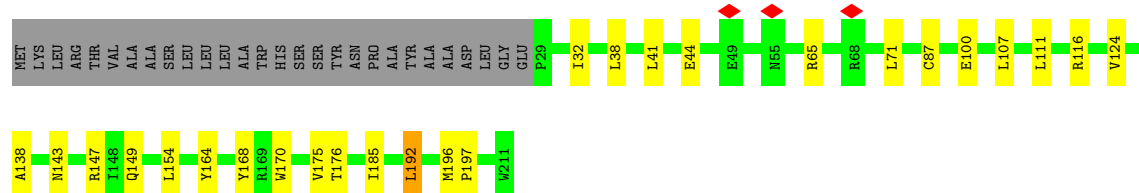
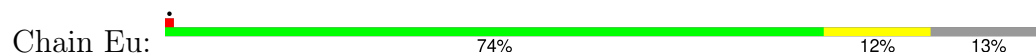
Chain Es: 73% 13% 13%



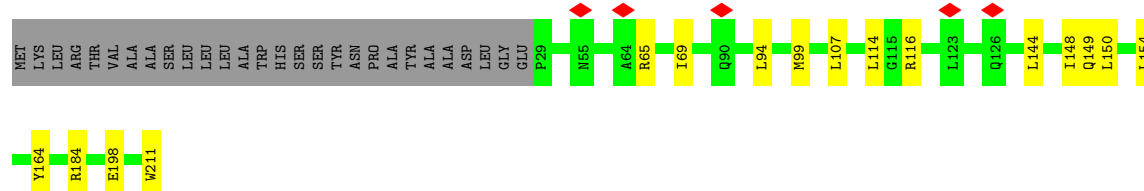
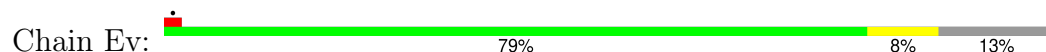
- Molecule 5: Sodium-type flagellar protein MotX



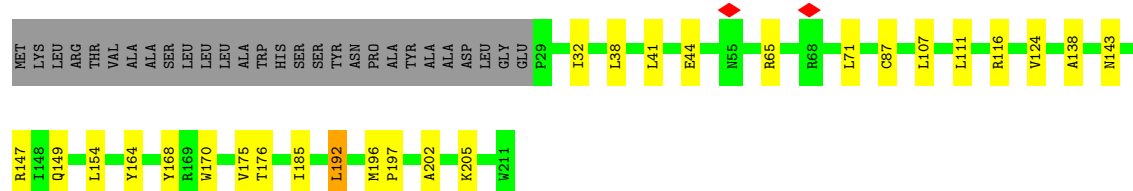
- Molecule 5: Sodium-type flagellar protein MotX



- Molecule 5: Sodium-type flagellar protein MotX




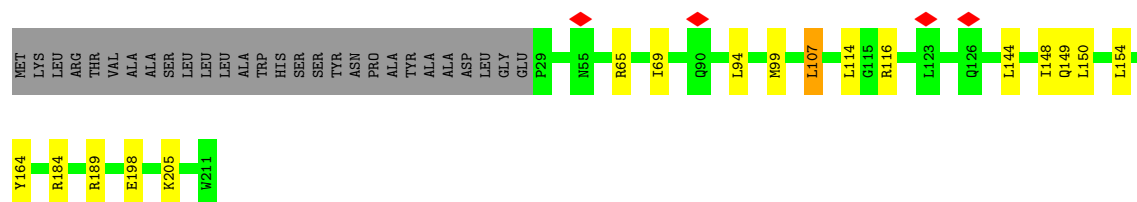
- Molecule 5: Sodium-type flagellar protein MotX



- Molecule 5: Sodium-type flagellar protein MotX

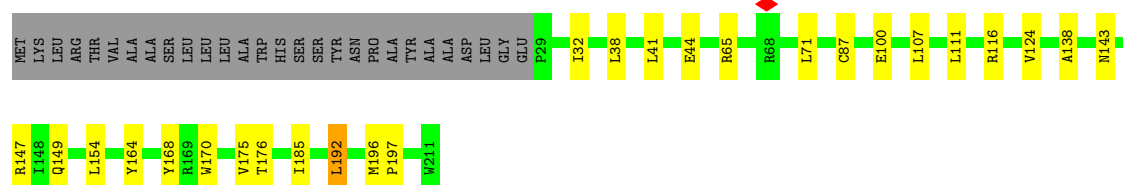


Chain Ex:  79% 8% 13%




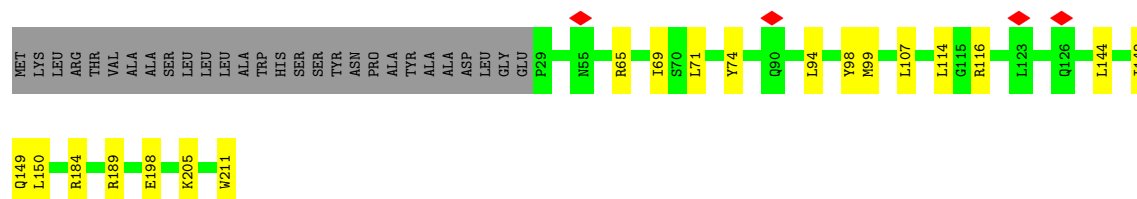
- Molecule 5: Sodium-type flagellar protein MotX

Chain Ey:  74% 12% 13%



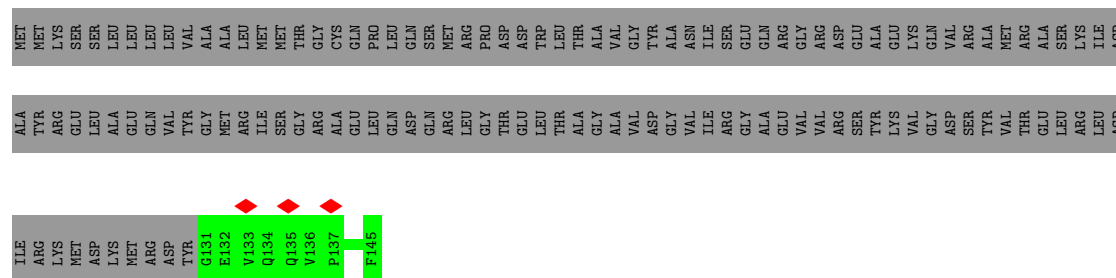
- Molecule 5: Sodium-type flagellar protein MotX

Chain Ez:  78% 9% 13%



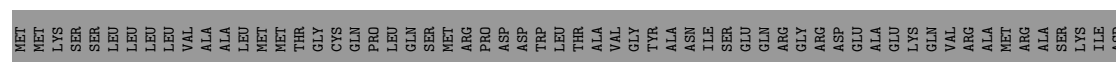
- Molecule 6: Lipoprotein

Chain Fa:  10% 90%

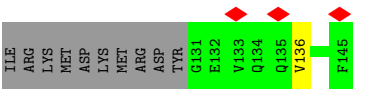


- Molecule 6: Lipoprotein

Chain Fb:  10% 90%



ALA	TYR	ARG	GLU	LEU	ALA	GLU	GLN	VAL	TYR	GLY	MET	ARG	ILE	SER	GLY	ARG	ALA	GLU	LEU	ASP	GLN	ASP	GLN	ASP	GLN	ARG	LEU	GLY	THR	GLU	LEU	THR	THR	ALA	GLY	ALA	VAL	ASP	GLY	VAL	ILE	ARG	GLY	GLN	ALA	GLU	VAL	VAL	ARG	ARG	TYR	LYS	VAL	GLY	ASP	SER	TYR	VAL	THR	THR	LEU	ARG	ILE	LEU	ASP
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• Molecule 6: Lipoprotein



MET	MET	LYS	SER	GLU	LEU	LEU	LEU	VAL	TYR	GLY	ALA	ALA	LEU	MET	MET	THR	GLY	ARG	ALA	CYS	GLN	PRO	GLN	LEU	ASP	GLN	SER	GLN	ARG	LEU	GLY	THR	ASP	GLU	ASP	TRP	LEU	THR	THR	ALA	THR	ALA	VAL	GLY	VAL	TYR	ASP	GLY	ALA	ASN	ILE	SER	GLY	GLN	ALA	ARG	GLY	VAL	VAL	ARG	ASP	GLU	SER	TYR	ALA	ALA	LYS	GLY	VAL	GLN	VAL	ASP	SER	ARG	TYR	VAL	THR	ARG	ALA	SER	LEU	ARG	ILE	LEU	ASP
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ALA	TYR	ARG	GLU	LEU	ALA	GLU	GLN	VAL	TYR	GLY	MET	ARG	ILE	SER	GLY	ARG	ALA	GLU	LEU	PRO	GLN	LEU	ASP	GLN	SER	GLN	ARG	LEU	GLY	THR	ASP	GLU	ASP	TRP	LEU	THR	THR	ALA	THR	ALA	VAL	GLY	VAL	TYR	ASP	GLY	ALA	ASN	ILE	ARG	GLY	GLN	ALA	ARG	GLY	VAL	VAL	ARG	ASP	GLU	SER	TYR	ALA	ALA	LYS	GLY	VAL	GLN	VAL	ASP	SER	ARG	TYR	VAL	THR	ARG	ALA	SER	LEU	ARG	ILE	LEU	ASP
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• Molecule 6: Lipoprotein



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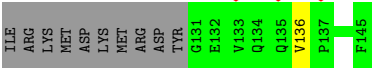


• Molecule 6: Lipoprotein



MET	MET	LYS	SER	GLU	LEU	LEU	LEU	VAL	TYR	GLY	ALA	ALA	LEU	MET	MET	THR	GLY	ARG	ALA	CYS	GLN	PRO	GLN	LEU	ASP	GLN	SER	GLN	ARG	LEU	GLY	THR	ASP	GLU	ASP	TRP	LEU	THR	THR	ALA	THR	ALA	VAL	GLY	VAL	TYR	ASP	GLY	ALA	ASN	ILE	SER	GLY	GLN	ALA	ARG	GLY	VAL	VAL	ARG	ASP	GLU	SER	TYR	ALA	ALA	LYS	GLY	VAL	GLN	VAL	ASP	SER	ARG	TYR	VAL	THR	ARG	ALA	SER	LEU	ARG	ILE	LEU	ASP
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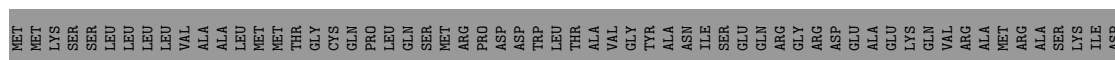
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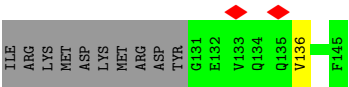
• Molecule 6: Lipoprotein



MET	MET	LYS	SER	GLU	LEU	LEU	LEU	VAL	TYR	GLY	ALA	ALA	LEU	MET	MET	THR	GLY	ARG	ALA	CYS	GLN	PRO	GLN	LEU	ASP	GLN	SER	GLN	ARG	LEU	GLY	THR	ASP	GLU	ASP	TRP	LEU	THR	THR	ALA	THR	ALA	VAL	GLY	VAL	TYR	ASP	GLY	ALA	ASN	ILE	SER	GLY	GLN	ALA	ARG	GLY	VAL	VAL	ARG	ASP	GLU	SER	TYR	ALA	ALA	LYS	GLY	VAL	GLN	VAL	ASP	SER	ARG	TYR	VAL	THR	ARG	ALA	SER	LEU	ARG	ILE	LEU	ASP
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ALA	TYR	ARG	GLU	LEU	ALA	GLU	GLN	VAL	TYR	GLY	MET	ARG	ILE	SER	GLY	ARG	ALA	GLU	LEU	ASP	GLN	ASP	GLN	ASP	ARG	LEU	GLY	THR	GLU	LEU	THR	THR	GLY	ALA	ALA	VAL	ASP	GLY	VAL	ILE	ARG	GLY	ALA	GLU	VAL	ARG	ARG	TYR	LYS	VAL	GLY	ASP	TYR	THR	THR	LEU	ARG	ILE	ASP
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• Molecule 6: Lipoprotein



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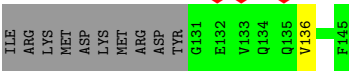


• Molecule 6: Lipoprotein



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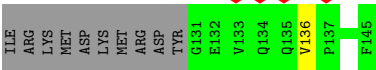


• Molecule 6: Lipoprotein



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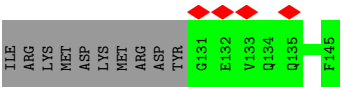


• Molecule 6: Lipoprotein



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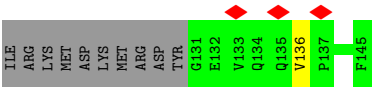


• Molecule 6: Lipoprotein



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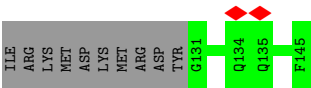


• Molecule 6: Lipoprotein



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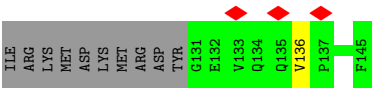


• Molecule 6: Lipoprotein



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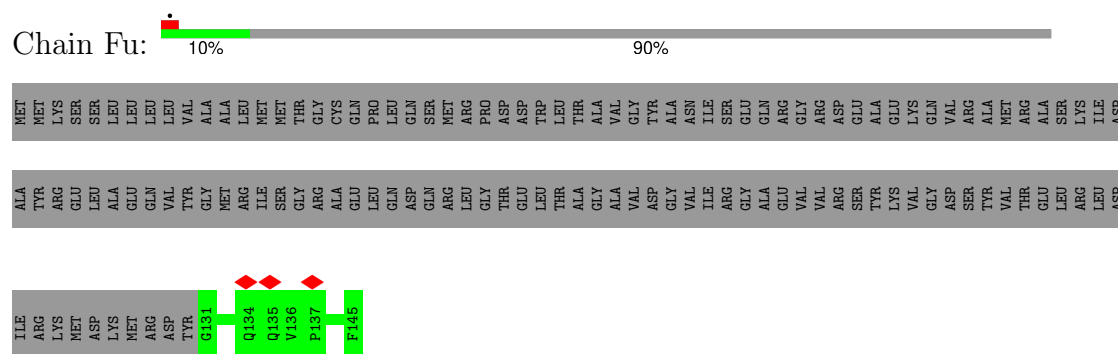
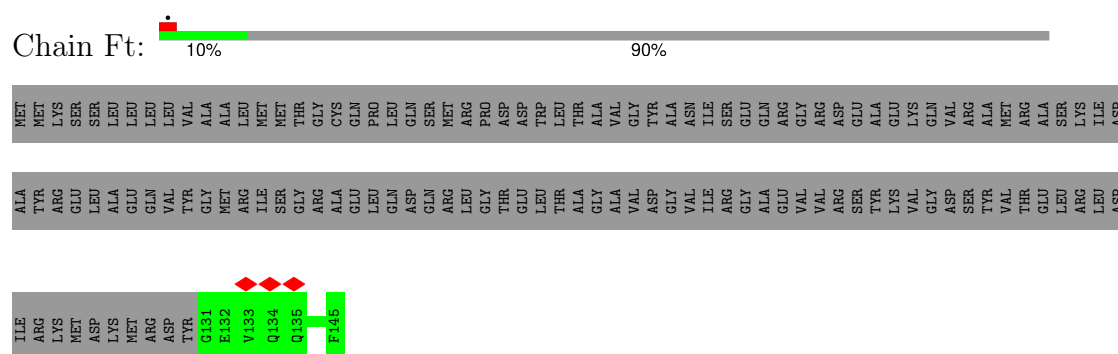
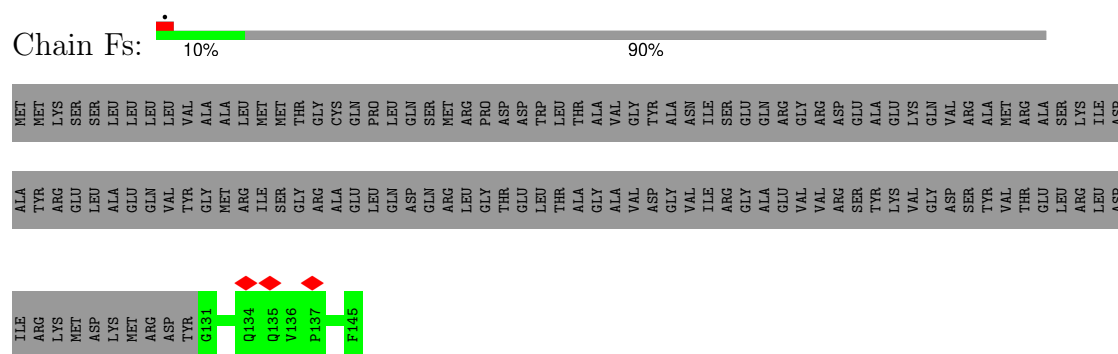
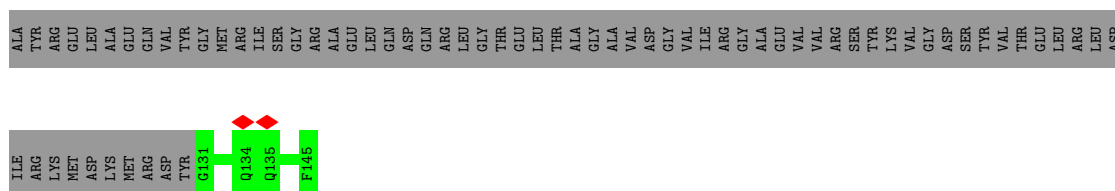
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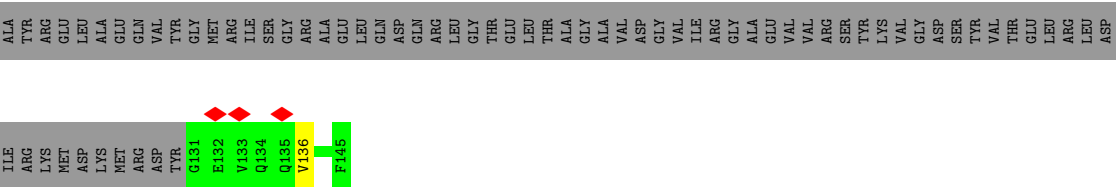


• Molecule 6: Lipoprotein

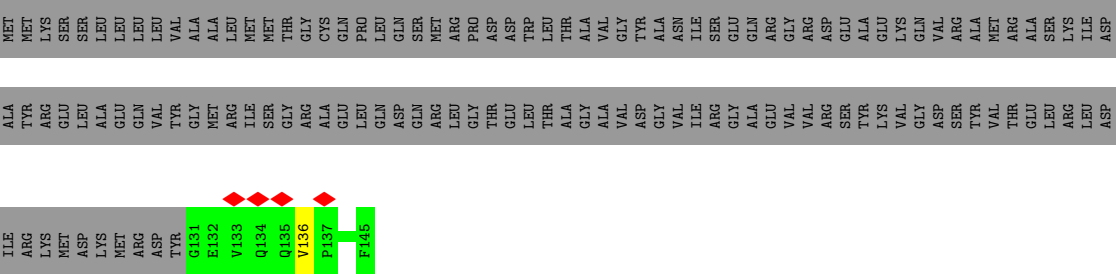


MET	MET	LYS	SER	SER	LEU	LEU	LEU	VAL	LEU	VAL	ALA	ALA	LEU	MET	MET	THR	GLY	CYS	GLN	PRO	ASP	ASP	GLU	TRP	LEU	LEU	THR	THR	ALA	THR	ALA	VAL	GLY	VAL	TYR	ASP	GLY	ALA	ASN	ILE	SER	GLU	GLN	ARG	GLY	VAL	VAL	ARG	ASP	GLU	SER	ALA	TYR	LYS	GLY	VAL	GLN	VAL	ASP	SER	ARG	ALA	TYR	VAL	MET	VAL	THR	ARG	ALA	SER	LYS	LEU	ILE	ASP
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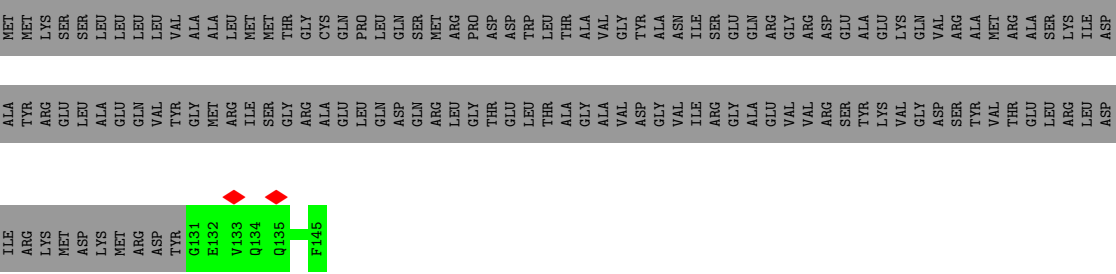




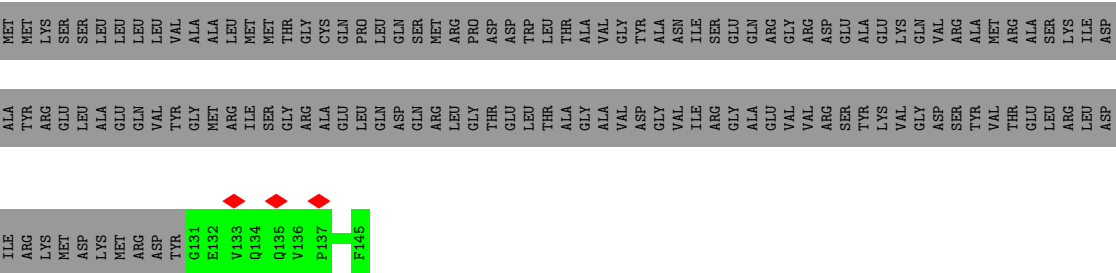
● Molecule 6: Lipoprotein



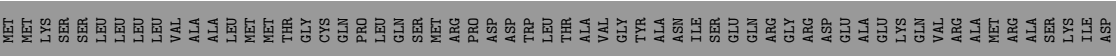
● Molecule 6: Lipoprotein

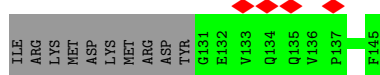


● Molecule 6: Lipoprotein



● Molecule 6: Lipoprotein





- Molecule 6: Lipoprotein



ALA TYR ARG ARG GLU LEU ALA GLU GLN VAL TYR TYR MET GLY ARG ARG ALA GLU LEU GLN ASP ASP GLN ARG LEU GLY THR THR LEU THR ALA ALA VAL ASP GLY ASP VAL VAL ILE ILE ARG ARG GLY GLY TYR TYR LYS VAL GLY ASP SER SER TYR VAL THR GLU LEU ARG LEU

ILE	ARG	LYS	MET	ASP	LYS	MET	ARG	ASP	TYR	GLY	GLU	V133	F145
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- Molecule 6: Lipoprotein



ALA TYR ARG ARG GLU LEU ALA GLU GLN TYR TYR GLY MET ARG ILE SER SER GLY ARG ALA GLU LEU GLN ASP ASP GLN ARG LEU THR GLY THR GLY LEU LEU THR ALA GLY ALA VAL ASP GLY VAL VAL ILE ARG ARG GLY GLY ALA GLU VAL VAL ARG SER TYR LYS VAL GLY ASP SER TYR VAL THR GLU LEU ARG LEU

ILE  
ARG  
LYS  
MET  
ASP  
LYS  
MET  
ARG  
ASP  
TYR  
GLY  
GLU  
V133  
Q141  
F145

- Molecule 6: Lipoprotein



ALA TYR ARG ARG GLU LEU ALA GLU GLN VAL VAL GLY MET ARG ARG ILE SER SER GLY ARG ALA ALA GLU LEU LEU GLN ASP ASP GLN ARG LEU LEU THR THR ALA ALA VAL VAL ASP GLY VAL VAL ILE ARG ARG GLY GLY ALA GLU VAL VAL VAL ARG ARG SER TYR LYS VAL GLY ASP SER TYR VAL THR GLU LEU ARG LEU

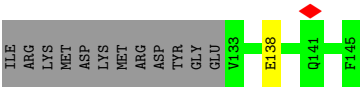
ILE	ARG	LYS	MET	ASP	LYS	MET	ARG	ASP	TYR	GLY	GLU	V133	F145
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- Molecule 6: Lipoprotein

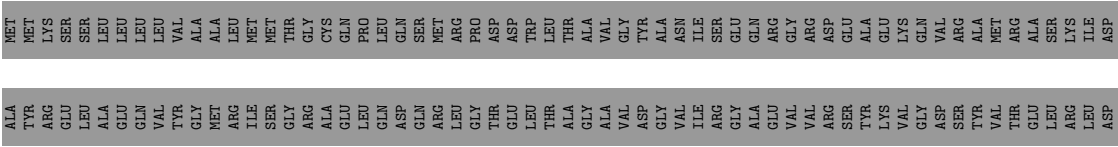


ALA TYR ARG GLU LEU ALA GLU GLN VAL VAL GLY MET ARG ILE SER GLY ARG ALA GLU LEU GLN ASP GLN ARG LEU LEU GLY THR ALA ALA VAL ASP GLY VAL ILE ARG ALA GLY GLY THR VAL VAL VAL ARG SER TYR LYS VAL GLY ASP SER TYR VAL THR GLU LEU ARG LEU

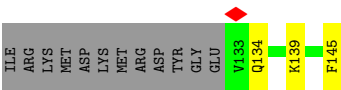
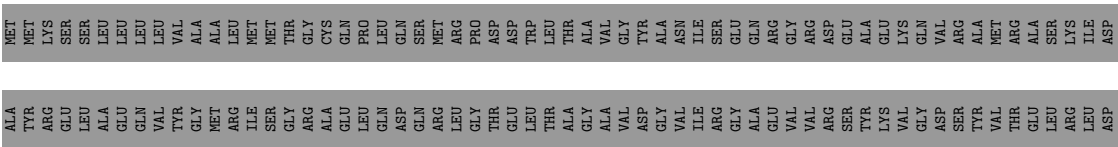




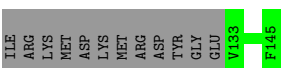
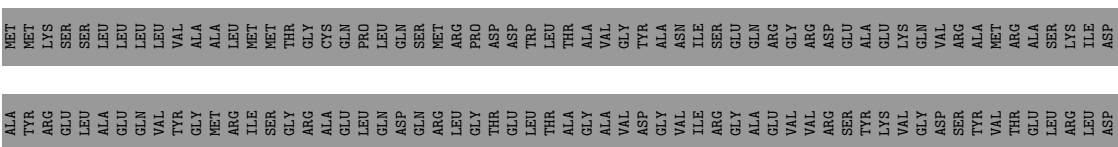
• Molecule 6: Lipoprotein



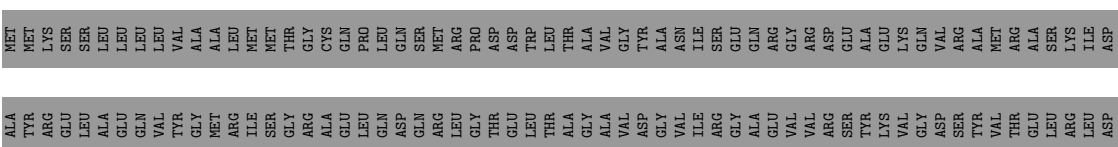
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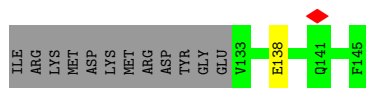


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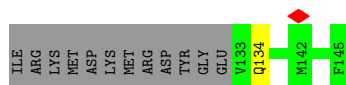
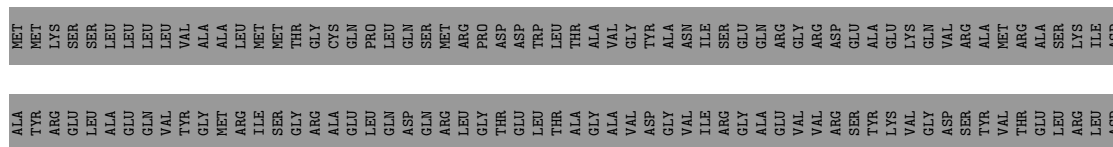


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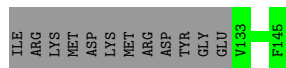
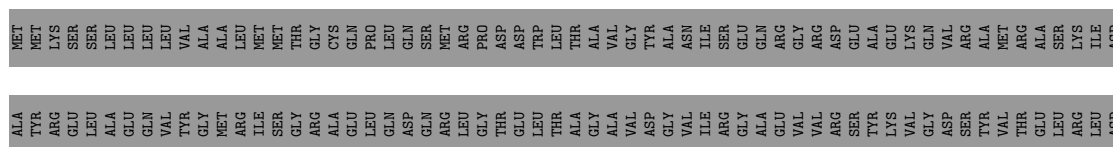




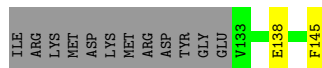
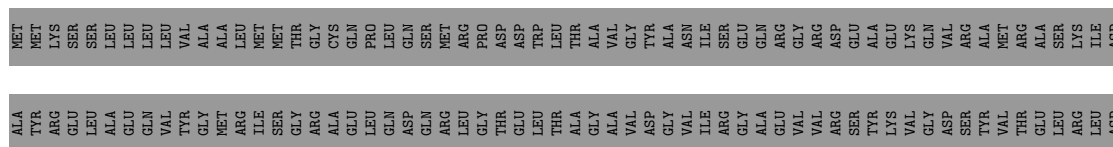
- Molecule 6: Lipoprotein



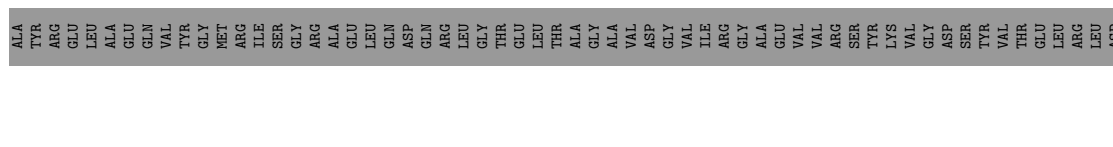
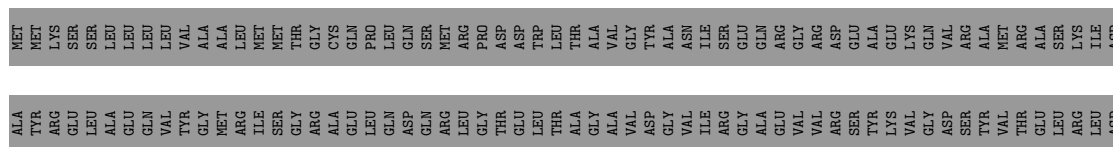
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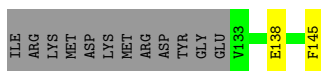


- Molecule 6: Lipoprotein



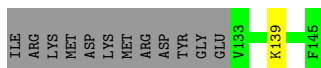
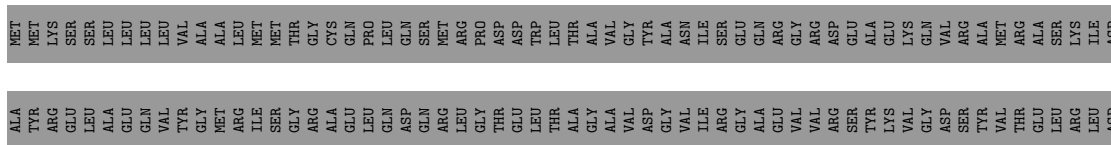
- Molecule 6: Lipoprotein





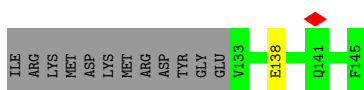
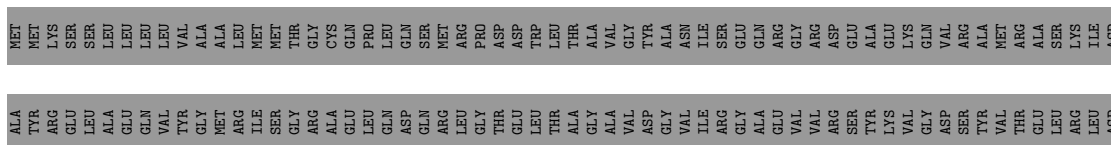
- Molecule 6: Lipoprotein

Chain Gm:  8% 91%



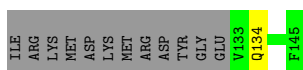
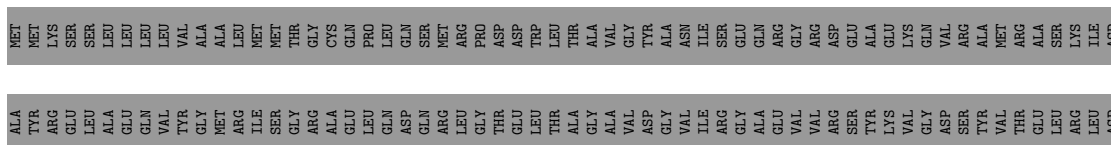
- Molecule 6: Lipoprotein

Chain Gn:  8% 91%



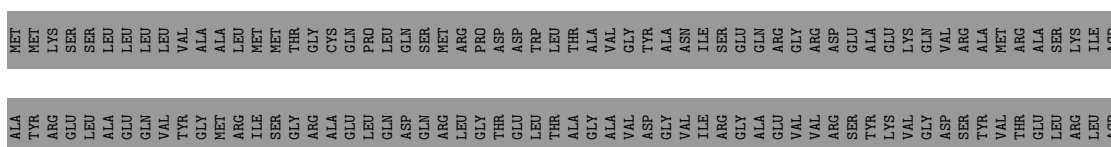
- Molecule 6: Lipoprotein

Chain Go:  8% . 91%



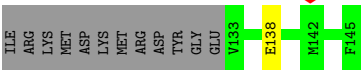
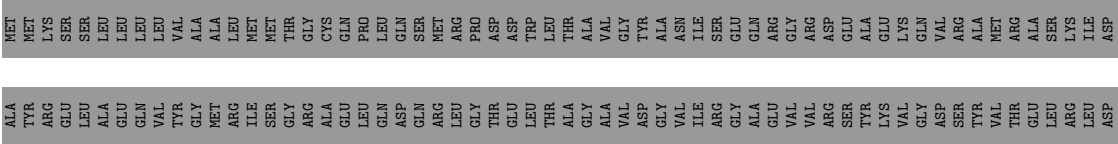
- Molecule 6: Lipoprotein

Chain Gp:  9% 91%

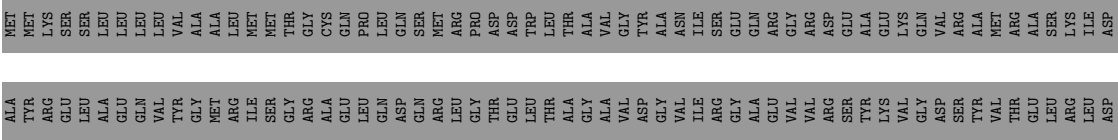




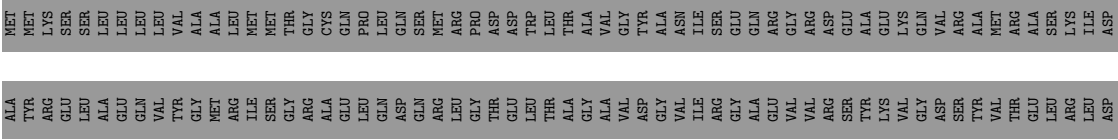
● Molecule 6: Lipoprotein



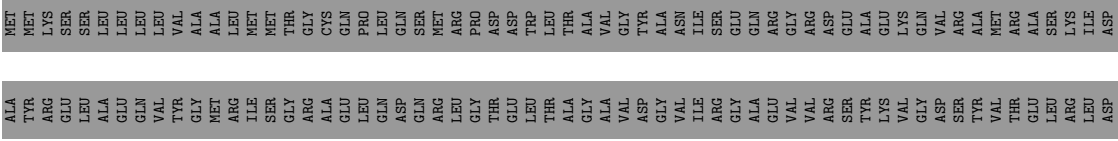
● Molecule 6: Lipoprotein

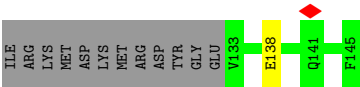


● Molecule 6: Lipoprotein

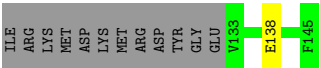
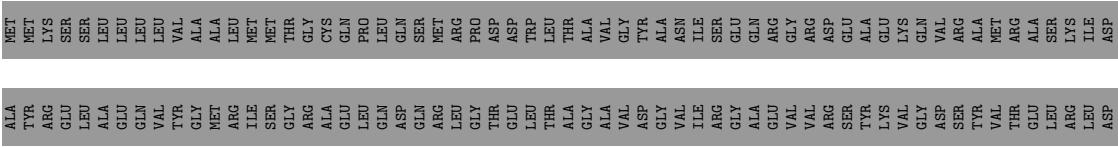


● Molecule 6: Lipoprotein

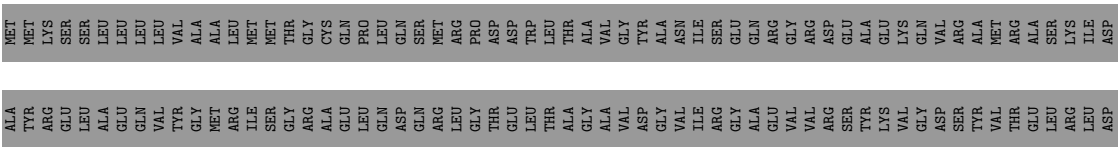




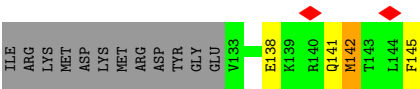
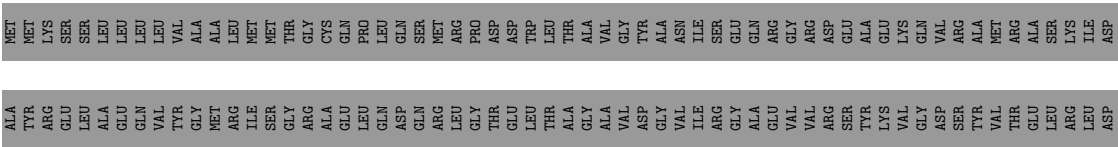
• Molecule 6: Lipoprotein



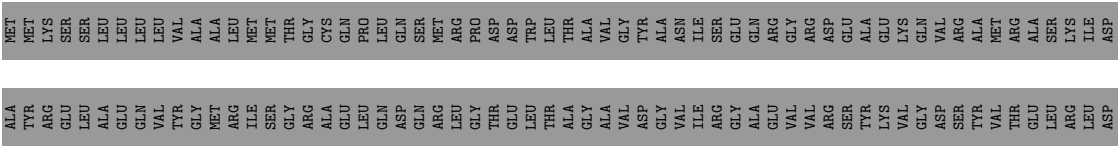
• Molecule 6: Lipoprotein

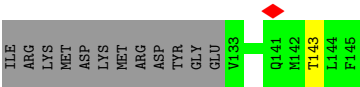


• Molecule 6: Lipoprotein

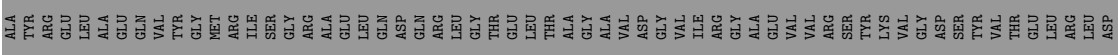
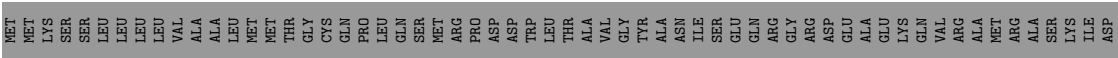


• Molecule 6: Lipoprotein

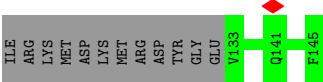
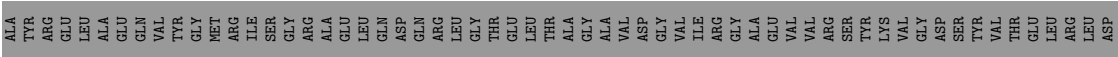
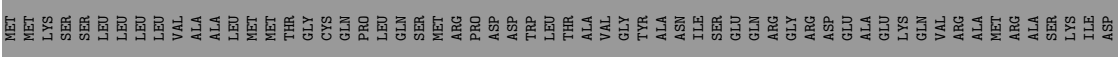




● Molecule 6: Lipoprotein



● Molecule 6: Lipoprotein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C13	Depositor
Number of particles used	25553	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	0.847	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	478.464, 478.464, 478.464	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	Aa	0.11	0/1699	0.31	0/2303
1	Ab	0.11	0/1699	0.30	0/2303
1	Ac	0.11	0/1699	0.31	0/2303
1	Ad	0.11	0/1699	0.30	0/2303
1	Ae	0.11	0/1699	0.31	0/2303
1	Af	0.11	0/1699	0.31	0/2303
1	Ag	0.11	0/1699	0.29	0/2303
1	Ah	0.11	0/1699	0.30	0/2303
1	Ai	0.11	0/1699	0.30	0/2303
1	Aj	0.11	0/1699	0.30	0/2303
1	Ak	0.11	0/1699	0.30	0/2303
1	Al	0.11	0/1699	0.30	0/2303
1	Am	0.11	0/1699	0.30	0/2303
1	An	0.11	0/1699	0.31	0/2303
1	Ao	0.11	0/1699	0.31	0/2303
1	Ap	0.11	0/1699	0.31	0/2303
1	Aq	0.11	0/1699	0.31	0/2303
1	Ar	0.11	0/1699	0.30	0/2303
1	As	0.11	0/1699	0.30	0/2303
1	At	0.11	0/1699	0.30	0/2303
1	Au	0.11	0/1699	0.29	0/2303
1	Av	0.11	0/1699	0.30	0/2303
1	Aw	0.11	0/1699	0.30	0/2303
1	Ax	0.11	0/1699	0.30	0/2303
1	Ay	0.11	0/1699	0.30	0/2303
1	Az	0.11	0/1699	0.30	0/2303
2	Ba	0.11	0/2535	0.28	0/3442
2	Bb	0.11	0/2535	0.28	0/3442
2	Bc	0.11	0/2535	0.28	0/3442
2	Bd	0.11	0/2535	0.28	0/3442
2	Be	0.10	0/2535	0.28	0/3442
2	Bf	0.11	0/2535	0.28	0/3442
2	Bg	0.10	0/2535	0.27	0/3442
2	Bh	0.11	0/2535	0.28	0/3442



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Bi	0.11	0/2535	0.28	0/3442
2	Bj	0.10	0/2535	0.28	0/3442
2	Bk	0.11	0/2535	0.28	0/3442
2	Bl	0.11	0/2535	0.28	0/3442
2	Bm	0.11	0/2535	0.29	1/3442 (0.0%)
2	Bn	0.11	0/2535	0.28	0/3442
2	Bo	0.11	0/2535	0.27	0/3442
2	Bp	0.11	0/2535	0.30	0/3442
2	Bq	0.11	0/2535	0.28	0/3442
2	Br	0.11	0/2535	0.28	0/3442
2	Bs	0.11	0/2535	0.29	0/3442
2	Bt	0.11	0/2535	0.28	0/3442
2	Bu	0.11	0/2535	0.28	0/3442
2	Bv	0.11	0/2535	0.28	0/3442
2	Bw	0.11	0/2535	0.28	0/3442
2	Bx	0.11	0/2535	0.29	0/3442
2	By	0.11	0/2535	0.28	0/3442
2	Bz	0.10	0/2535	0.28	0/3442
3	Ca	0.12	0/2816	0.30	0/3809
3	Cb	0.12	0/2816	0.31	0/3809
3	Cc	0.12	0/2816	0.30	0/3809
3	Cd	0.11	0/2816	0.31	0/3809
3	Ce	0.12	0/2816	0.30	0/3809
3	Cf	0.12	0/2816	0.30	0/3809
3	Cg	0.11	0/2816	0.29	0/3809
3	Ch	0.11	0/2816	0.29	0/3809
3	Ci	0.11	0/2816	0.31	0/3809
3	Cj	0.12	0/2816	0.30	0/3809
3	Ck	0.11	0/2816	0.30	0/3809
3	Cl	0.12	0/2816	0.31	0/3809
3	Cm	0.11	0/2816	0.30	0/3809
3	Cn	0.11	0/2816	0.29	0/3809
3	Co	0.11	0/2816	0.30	0/3809
3	Cp	0.12	0/2816	0.29	0/3809
3	Cq	0.11	0/2816	0.30	0/3809
3	Cr	0.12	0/2816	0.29	0/3809
3	Cs	0.12	0/2816	0.31	0/3809
3	Ct	0.12	0/2816	0.32	0/3809
3	Cu	0.12	0/2816	0.30	0/3809
3	Cv	0.11	0/2816	0.29	0/3809
3	Cw	0.14	0/2816	0.30	0/3809
3	Cx	0.11	0/2816	0.29	0/3809
3	Cy	0.11	0/2816	0.29	0/3809

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	Cz	0.11	0/2816	0.28	0/3809
4	Da	0.14	0/2129	0.35	0/2882
4	Db	0.14	0/2124	0.35	0/2877
4	Dc	0.14	0/2129	0.35	0/2882
4	Dd	0.14	0/2124	0.39	2/2877 (0.1%)
4	De	0.14	0/2129	0.35	0/2882
4	Df	0.14	0/2124	0.39	2/2877 (0.1%)
4	Dg	0.14	0/2129	0.36	0/2882
4	Dh	0.13	0/2124	0.35	0/2877
4	Di	0.14	0/2129	0.35	0/2882
4	Dj	0.14	0/2124	0.36	0/2877
4	Dk	0.14	0/2129	0.35	0/2882
4	Dl	0.13	0/2124	0.35	0/2877
4	Dm	0.14	0/2129	0.36	0/2882
4	Dn	0.13	0/2124	0.35	0/2877
4	Do	0.14	0/2129	0.35	0/2882
4	Dp	0.14	0/2124	0.35	0/2877
4	Dq	0.14	0/2129	0.36	0/2882
4	Dr	0.14	0/2124	0.38	2/2877 (0.1%)
4	Ds	0.14	0/2129	0.34	0/2882
4	Dt	0.14	0/2124	0.36	0/2877
4	Du	0.14	0/2129	0.36	0/2882
4	Dv	0.14	0/2124	0.38	0/2877
4	Dw	0.14	0/2129	0.36	0/2882
4	Dx	0.13	0/2124	0.35	0/2877
4	Dy	0.14	0/2129	0.36	0/2882
4	Dz	0.13	0/2124	0.36	0/2877
5	Ea	0.14	0/1494	0.37	0/2027
5	Eb	0.13	0/1523	0.32	0/2062
5	Ec	0.14	0/1494	0.37	0/2027
5	Ed	0.13	0/1523	0.32	0/2062
5	Ee	0.14	0/1494	0.37	0/2027
5	Ef	0.13	0/1523	0.32	0/2062
5	Eg	0.14	0/1494	0.37	0/2027
5	Uh	0.13	0/1523	0.32	0/2062
5	Ei	0.14	0/1494	0.39	0/2027
5	Ej	0.14	0/1523	0.32	0/2062
5	Ek	0.14	0/1494	0.37	0/2027
5	El	0.13	0/1523	0.32	0/2062
5	Em	0.14	0/1494	0.37	0/2027
5	En	0.13	0/1523	0.32	0/2062
5	Eo	0.14	0/1494	0.37	0/2027
5	Ep	0.13	0/1523	0.32	0/2062

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	Eq	0.14	0/1494	0.37	0/2027
5	Er	0.13	0/1523	0.32	0/2062
5	Es	0.14	0/1494	0.37	0/2027
5	Et	0.13	0/1523	0.32	0/2062
5	Eu	0.14	0/1494	0.37	0/2027
5	Ev	0.13	0/1523	0.32	0/2062
5	Ew	0.14	0/1494	0.37	0/2027
5	Ex	0.13	0/1523	0.32	0/2062
5	Ey	0.14	0/1494	0.36	0/2027
5	Ez	0.13	0/1523	0.32	0/2062
6	Fa	0.18	0/126	0.43	0/166
6	Fb	0.13	0/126	0.36	0/166
6	Fc	0.20	0/126	0.43	0/166
6	Fd	0.19	0/126	0.40	0/166
6	Fe	0.16	0/126	0.38	0/166
6	Ff	0.17	0/126	0.39	0/166
6	Fg	0.15	0/126	0.37	0/166
6	Fh	0.17	0/126	0.42	0/166
6	Fi	0.15	0/126	0.36	0/166
6	Fj	0.15	0/126	0.38	0/166
6	Fk	0.15	0/126	0.36	0/166
6	Fl	0.16	0/126	0.40	0/166
6	Fm	0.14	0/126	0.39	0/166
6	Fn	0.16	0/126	0.38	0/166
6	Fo	0.16	0/126	0.39	0/166
6	Fp	0.19	0/126	0.41	0/166
6	Fq	0.16	0/126	0.41	0/166
6	Fr	0.16	0/126	0.40	0/166
6	Fs	0.17	0/126	0.39	0/166
6	Ft	0.17	0/126	0.39	0/166
6	Fu	0.14	0/126	0.37	0/166
6	Fv	0.18	0/126	0.43	0/166
6	Fw	0.17	0/126	0.41	0/166
6	Fx	0.16	0/126	0.39	0/166
6	Fy	0.18	0/126	0.43	0/166
6	Fz	0.18	0/126	0.47	0/166
6	Ga	0.17	0/113	0.44	0/149
6	Gb	0.16	0/113	0.54	0/149
6	Gc	0.15	0/113	0.49	0/149
6	Gd	0.13	0/113	0.49	0/149
6	Ge	0.19	0/113	0.57	0/149
6	Gf	0.18	0/113	0.48	0/149
6	Gg	0.15	0/113	0.42	0/149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	Gh	0.16	0/113	0.45	0/149
6	Gi	0.14	0/113	0.53	0/149
6	Gj	0.17	0/113	0.48	0/149
6	Gk	0.13	0/113	0.44	0/149
6	Gl	0.14	0/113	0.42	0/149
6	Gm	0.16	0/113	0.49	0/149
6	Gn	0.14	0/113	0.42	0/149
6	Go	0.15	0/113	0.43	0/149
6	Gp	0.15	0/113	0.50	0/149
6	Gq	0.17	0/113	0.52	0/149
6	Gr	0.16	0/113	0.52	0/149
6	Gs	0.13	0/113	0.49	0/149
6	Gt	0.16	0/113	0.54	0/149
6	Gu	0.15	0/113	0.42	0/149
6	Gv	0.13	0/113	0.52	0/149
6	Gw	0.22	0/113	0.64	0/149
6	Gx	0.16	0/113	0.51	0/149
6	Gy	0.14	0/113	0.56	0/149
6	Gz	0.17	0/113	0.45	0/149
All	All	0.12	0/284024	0.32	7/384618 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Df	172	LEU	CA-C-N	5.26	127.72	120.67
4	Df	172	LEU	C-N-CA	5.26	127.72	120.67
4	Dd	172	LEU	CA-C-N	5.22	127.67	120.67
4	Dd	172	LEU	C-N-CA	5.22	127.67	120.67
4	Dr	172	LEU	CA-C-N	5.06	127.44	120.67
4	Dr	172	LEU	C-N-CA	5.06	127.44	120.67
2	Bm	297	GLN	CB-CA-C	-5.02	110.40	117.23

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	21	0
1	Ab	1674	0	1609	23	0
1	Ac	1674	0	1609	19	0
1	Ad	1674	0	1609	22	0
1	Ae	1674	0	1609	22	0
1	Af	1674	0	1609	23	0
1	Ag	1674	0	1609	24	0
1	Ah	1674	0	1609	22	0
1	Ai	1674	0	1609	20	0
1	Aj	1674	0	1609	19	0
1	Ak	1674	0	1609	22	0
1	Al	1674	0	1609	22	0
1	Am	1674	0	1609	20	0
1	An	1674	0	1609	22	0
1	Ao	1674	0	1609	18	0
1	Ap	1674	0	1609	22	0
1	Aq	1674	0	1609	20	0
1	Ar	1674	0	1609	20	0
1	As	1674	0	1609	22	0
1	At	1674	0	1609	19	0
1	Au	1674	0	1609	20	0
1	Av	1674	0	1609	20	0
1	Aw	1674	0	1609	18	0
1	Ax	1674	0	1609	22	0
1	Ay	1674	0	1609	21	0
1	Az	1674	0	1609	21	0
2	Ba	2501	0	2549	27	0
2	Bb	2501	0	2549	27	0
2	Bc	2501	0	2549	30	0
2	Bd	2501	0	2549	24	0
2	Be	2501	0	2549	26	0
2	Bf	2501	0	2549	24	0
2	Bg	2501	0	2549	32	0
2	Bh	2501	0	2549	26	0
2	Bi	2501	0	2549	27	0
2	Bj	2501	0	2549	30	0
2	Bk	2501	0	2549	33	0
2	Bl	2501	0	2549	35	0
2	Bm	2501	0	2549	33	0
2	Bn	2501	0	2549	30	0
2	Bo	2501	0	2549	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bp	2501	0	2549	31	0
2	Bq	2501	0	2549	34	0
2	Br	2501	0	2549	34	0
2	Bs	2501	0	2549	34	0
2	Bt	2501	0	2549	37	0
2	Bu	2501	0	2549	29	0
2	Bv	2501	0	2549	24	0
2	Bw	2501	0	2549	26	0
2	Bx	2501	0	2549	34	0
2	By	2501	0	2549	32	0
2	Bz	2501	0	2549	26	0
3	Ca	2770	0	2749	12	0
3	Cb	2770	0	2749	23	0
3	Cc	2770	0	2749	11	0
3	Cd	2770	0	2749	18	0
3	Ce	2770	0	2749	14	0
3	Cf	2770	0	2749	19	0
3	Cg	2770	0	2749	10	0
3	Ch	2770	0	2749	19	0
3	Ci	2770	0	2749	15	0
3	Cj	2770	0	2749	14	0
3	Ck	2770	0	2749	19	0
3	Cl	2770	0	2749	13	0
3	Cm	2770	0	2749	15	0
3	Cn	2770	0	2749	16	0
3	Co	2770	0	2749	13	0
3	Cp	2770	0	2749	14	0
3	Cq	2770	0	2749	18	0
3	Cr	2770	0	2749	20	0
3	Cs	2770	0	2749	13	0
3	Ct	2770	0	2749	12	0
3	Cu	2770	0	2749	15	0
3	Cv	2770	0	2749	15	0
3	Cw	2770	0	2749	14	0
3	Cx	2770	0	2749	14	0
3	Cy	2770	0	2749	21	0
3	Cz	2770	0	2749	18	0
4	Da	2085	0	2022	13	0
4	Db	2080	0	2003	15	0
4	Dc	2085	0	2022	14	0
4	Dd	2080	0	2003	17	0
4	De	2085	0	2022	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Df	2080	0	2003	17	0
4	Dg	2085	0	2022	13	0
4	Dh	2080	0	2003	17	0
4	Di	2085	0	2022	13	0
4	Dj	2080	0	2003	19	0
4	Dk	2085	0	2022	13	0
4	Dl	2080	0	2003	18	0
4	Dm	2085	0	2022	11	0
4	Dn	2080	0	2003	16	0
4	Do	2085	0	2022	12	0
4	Dp	2080	0	2003	19	0
4	Dq	2085	0	2022	11	0
4	Dr	2080	0	2003	15	0
4	Ds	2085	0	2022	12	0
4	Dt	2080	0	2003	16	0
4	Du	2085	0	2022	13	0
4	Dv	2080	0	2003	17	0
4	Dw	2085	0	2022	14	0
4	Dx	2080	0	2003	19	0
4	Dy	2085	0	2022	13	0
4	Dz	2080	0	2003	21	0
5	Ea	1466	0	1434	10	0
5	Eb	1494	0	1478	6	0
5	Ec	1466	0	1434	10	0
5	Ed	1494	0	1478	9	0
5	Ee	1466	0	1434	11	0
5	Ef	1494	0	1478	9	0
5	Eg	1466	0	1434	13	0
5	Eh	1494	0	1478	7	0
5	Ei	1466	0	1434	13	0
5	Ej	1494	0	1478	9	0
5	Ek	1466	0	1434	12	0
5	El	1494	0	1478	9	0
5	Em	1466	0	1434	8	0
5	En	1494	0	1478	8	0
5	Eo	1466	0	1434	13	0
5	Ep	1494	0	1478	10	0
5	Eq	1466	0	1434	11	0
5	Er	1494	0	1478	8	0
5	Es	1466	0	1434	12	0
5	Et	1494	0	1478	9	0
5	Eu	1466	0	1434	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Ev	1494	0	1478	7	0
5	Ew	1466	0	1434	11	0
5	Ex	1494	0	1478	8	0
5	Ey	1466	0	1434	11	0
5	Ez	1494	0	1478	9	0
6	Fa	125	0	125	0	0
6	Fb	125	0	125	1	0
6	Fc	125	0	125	0	0
6	Fd	125	0	125	1	0
6	Fe	125	0	125	1	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	1	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	0	0
6	Fu	125	0	125	0	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	0	0
6	Gc	112	0	116	1	0
6	Gd	112	0	116	0	0
6	Ge	112	0	116	0	0
6	Gf	112	0	116	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1	0
6	Gw	112	0	116	2	0
6	Gx	112	0	116	1	0
6	Gy	112	0	116	0	0
6	Gz	112	0	116	0	0
All	All	279357	0	276029	1973	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 (1973) 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)
3:Cb:92:GLU:HB2	3:Cb:103:ARG:HB3	1.78	0.64
5:Eh:99:MET:HB3	5:Eh:114:LEU:HD21	1.80	0.64
1:Ai:125:LEU:HB3	1:Al:244:MET:HE3	1.80	0.63
2:Br:317:LYS:HB2	2:Bs:328:VAL:HG21	1.79	0.63
1:Aa:125:LEU:HB3	1:Ad:244:MET:HE3	1.81	0.63
1:As:125:LEU:HB3	1:Av:244:MET:HE3	1.80	0.63
1:Aa:125:LEU:HB2	1:Aa:160:PHE:HB3	1.81	0.63
1:Ab:125:LEU:HB3	1:Ae:244:MET:HE3	1.81	0.63
1:Ao:125:LEU:HB2	1:Ao:160:PHE:HB3	1.81	0.63
1:Ay:125:LEU:HB2	1:Ay:160:PHE:HB3	1.81	0.63
5:Eb:99:MET:HB3	5:Eb:114:LEU:HD21	1.79	0.63
1:Ac:125:LEU:HB3	1:Af:244:MET:HE3	1.81	0.62
1:Aq:125:LEU:HB3	1:At:244:MET:HE3	1.81	0.62
1:Ab:244:MET:HE3	1:Ay:125:LEU:HB3	1.82	0.62
2:Bk:25:ALA:HB2	2:Bk:186:LEU:HD23	1.81	0.62
1:Ai:125:LEU:HB2	1:Ai:160:PHE:HB3	1.81	0.62
1:An:125:LEU:HB3	1:Aq:244:MET:HE3	1.82	0.62
1:Ar:125:LEU:HB3	1:Au:244:MET:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Av:125:LEU:HB3	1:Ay:244:MET:HE3	1.81	0.62
2:Ba:25:ALA:HB2	2:Ba:186:LEU:HD23	1.80	0.62
1:Ac:244:MET:HE3	1:Az:125:LEU:HB3	1.82	0.62
1:Ad:125:LEU:HB3	1:Ag:244:MET:HE3	1.82	0.62
1:Ao:125:LEU:HB3	1:Ar:244:MET:HE3	1.82	0.62
1:Ap:125:LEU:HB3	1:As:244:MET:HE3	1.82	0.62
1:Au:125:LEU:HB3	1:Ax:244:MET:HE3	1.82	0.62
1:Aa:244:MET:HE3	1:Ax:125:LEU:HB3	1.81	0.62
1:Am:125:LEU:HB3	1:Ap:244:MET:HE3	1.82	0.62
2:Be:25:ALA:HB2	2:Be:186:LEU:HD23	1.82	0.62
2:Bh:56:GLN:HE22	2:Bi:69:LEU:H	1.48	0.62
1:Ae:125:LEU:HB3	1:Ah:244:MET:HE3	1.81	0.62
1:Ag:125:LEU:HB2	1:Ag:160:PHE:HB3	1.82	0.62
1:As:125:LEU:HB2	1:As:160:PHE:HB3	1.81	0.62
3:Cy:92:GLU:HB2	3:Cy:103:ARG:HB3	1.80	0.62
1:Af:125:LEU:HB3	1:Ai:244:MET:HE3	1.81	0.62
1:Ag:125:LEU:HB3	1:Aj:244:MET:HE3	1.82	0.62
1:At:125:LEU:HB3	1:Aw:244:MET:HE3	1.82	0.62
1:Au:125:LEU:HB2	1:Au:160:PHE:HB3	1.82	0.62
2:Bi:25:ALA:HB2	2:Bi:186:LEU:HD23	1.82	0.62
1:Ak:125:LEU:HB3	1:An:244:MET:HE3	1.82	0.62
1:Al:125:LEU:HB3	1:Ao:244:MET:HE3	1.82	0.62
1:Am:125:LEU:HB2	1:Am:160:PHE:HB3	1.82	0.62
1:An:125:LEU:HB2	1:An:160:PHE:HB3	1.82	0.62
1:Ay:86:PHE:HB2	2:Bl:125:LEU:HD13	1.82	0.62
2:Bj:25:ALA:HB2	2:Bj:186:LEU:HD23	1.82	0.62
1:Ab:125:LEU:HB2	1:Ab:160:PHE:HB3	1.82	0.62
1:Az:125:LEU:HB2	1:Az:160:PHE:HB3	1.82	0.62
2:Bc:25:ALA:HB2	2:Bc:186:LEU:HD23	1.81	0.62
3:Ci:92:GLU:HB2	3:Ci:103:ARG:HB3	1.82	0.62
3:Cw:92:GLU:HB2	3:Cw:103:ARG:HB3	1.82	0.62
1:Aj:125:LEU:HB3	1:Am:244:MET:HE3	1.82	0.61
1:Aq:125:LEU:HB2	1:Aq:160:PHE:HB3	1.81	0.61
2:Bd:25:ALA:HB2	2:Bd:186:LEU:HD23	1.82	0.61
2:Bn:25:ALA:HB2	2:Bn:186:LEU:HD23	1.82	0.61
1:Ab:232:ARG:HH22	1:Ac:194:GLU:HG3	1.65	0.61
1:Ap:125:LEU:HB2	1:Ap:160:PHE:HB3	1.82	0.61
1:Av:125:LEU:HB2	1:Av:160:PHE:HB3	1.82	0.61
1:Aw:125:LEU:HB3	1:Az:244:MET:HE3	1.82	0.61
2:Bg:25:ALA:HB2	2:Bg:186:LEU:HD23	1.82	0.61
3:Cp:92:GLU:HB2	3:Cp:103:ARG:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:125:LEU:HB2	1:Ae:160:PHE:HB3	1.81	0.61
1:Aj:125:LEU:HB2	1:Aj:160:PHE:HB3	1.82	0.61
1:At:125:LEU:HB2	1:At:160:PHE:HB3	1.82	0.61
2:Bw:25:ALA:HB2	2:Bw:186:LEU:HD23	1.81	0.61
1:Ac:125:LEU:HB2	1:Ac:160:PHE:HB3	1.81	0.61
1:Ac:232:ARG:HH22	1:Ad:194:GLU:HG3	1.66	0.61
1:Ak:125:LEU:HB2	1:Ak:160:PHE:HB3	1.81	0.61
3:Cn:92:GLU:HB2	3:Cn:103:ARG:HB3	1.81	0.61
1:Ah:125:LEU:HB2	1:Ah:160:PHE:HB3	1.83	0.61
1:Ah:125:LEU:HB3	1:Ak:244:MET:HE3	1.82	0.61
2:Bf:25:ALA:HB2	2:Bf:186:LEU:HD23	1.83	0.61
1:Aa:232:ARG:HH22	1:Ab:194:GLU:HG3	1.65	0.61
2:Bz:25:ALA:HB2	2:Bz:186:LEU:HD23	1.83	0.61
3:Cc:92:GLU:HB2	3:Cc:103:ARG:HB3	1.83	0.61
1:Af:125:LEU:HB2	1:Af:160:PHE:HB3	1.82	0.61
2:Bm:25:ALA:HB2	2:Bm:186:LEU:HD23	1.83	0.61
2:Bq:25:ALA:HB2	2:Bq:186:LEU:HD23	1.82	0.61
5:En:99:MET:HB3	5:En:114:LEU:HD21	1.83	0.61
2:Bx:290:PRO:HB3	2:Bx:296:GLY:HA3	1.82	0.61
1:Aw:125:LEU:HB2	1:Aw:160:PHE:HB3	1.82	0.61
2:Bx:25:ALA:HB2	2:Bx:186:LEU:HD23	1.83	0.61
1:Al:125:LEU:HB2	1:Al:160:PHE:HB3	1.82	0.60
1:Ad:125:LEU:HB2	1:Ad:160:PHE:HB3	1.82	0.60
2:Bl:25:ALA:HB2	2:Bl:186:LEU:HD23	1.82	0.60
2:Bo:25:ALA:HB2	2:Bo:186:LEU:HD23	1.83	0.60
2:Bq:56:GLN:HE22	2:Br:69:LEU:H	1.49	0.60
3:Ch:92:GLU:HB2	3:Ch:103:ARG:HB3	1.81	0.60
3:Cl:92:GLU:HB2	3:Cl:103:ARG:HB3	1.81	0.60
1:Af:232:ARG:HH22	1:Ag:194:GLU:HG3	1.66	0.60
1:Ax:125:LEU:HB2	1:Ax:160:PHE:HB3	1.82	0.60
2:Br:25:ALA:HB2	2:Br:186:LEU:HD23	1.82	0.60
1:Ao:232:ARG:HH22	1:Ap:194:GLU:HG3	1.65	0.60
1:Ar:232:ARG:HH22	1:As:194:GLU:HG3	1.66	0.60
2:By:25:ALA:HB2	2:By:186:LEU:HD23	1.82	0.60
1:Aj:232:ARG:HH22	1:Ak:194:GLU:HG3	1.65	0.60
2:Bb:25:ALA:HB2	2:Bb:186:LEU:HD23	1.83	0.60
2:Bp:25:ALA:HB2	2:Bp:186:LEU:HD23	1.83	0.60
2:Bh:25:ALA:HB2	2:Bh:186:LEU:HD23	1.84	0.60
1:Ae:232:ARG:HH22	1:Af:194:GLU:HG3	1.66	0.60
1:Am:232:ARG:HH22	1:An:194:GLU:HG3	1.66	0.60
1:Ap:232:ARG:HH22	1:Aq:194:GLU:HG3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:232:ARG:HH22	1:Al:194:GLU:HG3	1.66	0.60
1:Ar:125:LEU:HB2	1:Ar:160:PHE:HB3	1.82	0.60
5:Ep:99:MET:HB3	5:Ep:114:LEU:HD21	1.83	0.60
1:Ad:232:ARG:HH22	1:Ae:194:GLU:HG3	1.66	0.60
4:Do:49:VAL:HG12	4:Do:59:GLU:HG2	1.84	0.60
1:An:232:ARG:HH22	1:Ao:194:GLU:HG3	1.66	0.60
2:Bs:25:ALA:HB2	2:Bs:186:LEU:HD23	1.82	0.60
1:Av:232:ARG:HH22	1:Aw:194:GLU:HG3	1.65	0.59
2:Bo:56:GLN:HE22	2:Bp:69:LEU:H	1.49	0.59
3:Cw:239:THR:HG21	3:Cx:155:ARG:HD3	1.84	0.59
4:Dm:49:VAL:HG12	4:Dm:59:GLU:HG2	1.84	0.59
5:Ej:99:MET:HB3	5:Ej:114:LEU:HD21	1.84	0.59
1:Al:232:ARG:HH22	1:Am:194:GLU:HG3	1.66	0.59
2:Bp:317:LYS:HB2	2:Bq:328:VAL:HG21	1.84	0.59
2:Bu:25:ALA:HB2	2:Bu:186:LEU:HD23	1.82	0.59
3:Ct:92:GLU:HB2	3:Ct:103:ARG:HB3	1.83	0.59
4:Dq:49:VAL:HG12	4:Dq:59:GLU:HG2	1.84	0.59
5:Ev:99:MET:HB3	5:Ev:114:LEU:HD21	1.83	0.59
5:Ex:99:MET:HB3	5:Ex:114:LEU:HD21	1.84	0.59
1:Aq:232:ARG:HH22	1:Ar:194:GLU:HG3	1.66	0.59
2:Bm:56:GLN:HE22	2:Bn:69:LEU:H	1.50	0.59
3:Cg:92:GLU:HB2	3:Cg:103:ARG:HB3	1.83	0.59
3:Cm:92:GLU:HB2	3:Cm:103:ARG:HB3	1.82	0.59
5:Ez:99:MET:HB3	5:Ez:114:LEU:HD21	1.84	0.59
1:At:232:ARG:HH22	1:Au:194:GLU:HG3	1.66	0.59
1:Ay:232:ARG:HH22	1:Az:194:GLU:HG3	1.66	0.59
1:Ai:232:ARG:HH22	1:Aj:194:GLU:HG3	1.66	0.59
1:Au:232:ARG:HH22	1:Av:194:GLU:HG3	1.66	0.59
1:Aw:232:ARG:HH22	1:Ax:194:GLU:HG3	1.65	0.59
4:Di:49:VAL:HG12	4:Di:59:GLU:HG2	1.84	0.59
4:Dk:49:VAL:HG12	4:Dk:59:GLU:HG2	1.84	0.59
5:El:99:MET:HB3	5:El:114:LEU:HD21	1.83	0.59
1:Ag:232:ARG:HH22	1:Ah:194:GLU:HG3	1.66	0.59
2:Be:56:GLN:HE22	2:Bf:69:LEU:H	1.49	0.59
1:As:232:ARG:HH22	1:At:194:GLU:HG3	1.67	0.59
4:De:49:VAL:HG12	4:De:59:GLU:HG2	1.84	0.59
5:Ef:99:MET:HB3	5:Ef:114:LEU:HD21	1.83	0.59
2:Bh:87:ALA:HB2	2:Bh:101:ILE:HG22	1.85	0.59
3:Co:92:GLU:HB2	3:Co:103:ARG:HB3	1.83	0.59
5:Ed:99:MET:HB3	5:Ed:114:LEU:HD21	1.84	0.59
4:Dg:49:VAL:HG12	4:Dg:59:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bj:56:GLN:HE22	2:Bk:69:LEU:H	1.50	0.58
2:Bq:283:GLU:HG2	2:Bq:305:GLU:HB3	1.85	0.58
2:By:56:GLN:HE22	2:Bz:69:LEU:H	1.51	0.58
4:Ds:49:VAL:HG12	4:Ds:59:GLU:HG2	1.84	0.58
5:Et:99:MET:HB3	5:Et:114:LEU:HD21	1.84	0.58
1:Aa:194:GLU:HG3	1:Az:232:ARG:HH22	1.66	0.58
2:Bv:25:ALA:HB2	2:Bv:186:LEU:HD23	1.83	0.58
3:Cr:92:GLU:HB2	3:Cr:103:ARG:HB3	1.85	0.58
2:Bl:290:PRO:HB3	2:Bl:296:GLY:HA3	1.85	0.58
2:Bt:25:ALA:HB2	2:Bt:186:LEU:HD23	1.84	0.58
2:Bx:91:ALA:HB1	2:Bx:174:ASN:HD21	1.69	0.58
2:Bz:290:PRO:HB3	2:Bz:296:GLY:HA3	1.86	0.58
2:Bt:287:VAL:HG22	2:Bt:301:VAL:HG13	1.85	0.58
3:Ck:92:GLU:HB2	3:Ck:103:ARG:HB3	1.85	0.58
2:Bc:56:GLN:HE22	2:Bd:69:LEU:H	1.50	0.58
2:Bj:87:ALA:HB2	2:Bj:101:ILE:HG22	1.85	0.58
3:Cv:361:PRO:HB2	4:Do:148:ARG:HD2	1.86	0.58
3:Cx:92:GLU:HB2	3:Cx:103:ARG:HB3	1.85	0.58
4:Du:49:VAL:HG12	4:Du:59:GLU:HG2	1.84	0.58
2:Bu:56:GLN:HE22	2:Bv:69:LEU:H	1.51	0.58
2:Bk:56:GLN:HE22	2:Bl:69:LEU:H	1.52	0.58
3:Ch:361:PRO:HB2	4:Da:148:ARG:HD2	1.86	0.58
4:Dc:49:VAL:HG12	4:Dc:59:GLU:HG2	1.84	0.58
2:Bc:87:ALA:HB2	2:Bc:101:ILE:HG22	1.86	0.58
2:Bu:87:ALA:HB2	2:Bu:101:ILE:HG22	1.86	0.58
2:Bw:317:LYS:HE3	2:Bx:324:LEU:HD23	1.84	0.58
3:Cz:361:PRO:HB2	4:Ds:148:ARG:HD2	1.86	0.58
5:Eh:148:ILE:HD12	5:Eh:184:ARG:HE	1.68	0.58
5:Er:99:MET:HB3	5:Er:114:LEU:HD21	1.83	0.58
1:Ax:232:ARG:HH22	1:Ay:194:GLU:HG3	1.66	0.58
2:Bw:56:GLN:HE22	2:Bx:69:LEU:H	1.51	0.58
2:Bx:56:GLN:HE22	2:By:69:LEU:H	1.51	0.58
3:Cn:361:PRO:HB2	4:Dg:148:ARG:HD2	1.86	0.58
5:En:148:ILE:HD12	5:En:184:ARG:HE	1.69	0.58
1:Ah:232:ARG:HH22	1:Ai:194:GLU:HG3	1.67	0.57
2:Bv:87:ALA:HB2	2:Bv:101:ILE:HG22	1.86	0.57
5:El:148:ILE:HD12	5:El:184:ARG:HE	1.69	0.57
2:Bx:87:ALA:HB2	2:Bx:101:ILE:HG22	1.86	0.57
3:Cf:105:ARG:HG3	6:Gf:134:GLN:HE22	1.69	0.57
4:Da:49:VAL:HG12	4:Da:59:GLU:HG2	1.84	0.57
4:Dw:49:VAL:HG12	4:Dw:59:GLU:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Eb:148:ILE:HD12	5:Eb:184:ARG:HE	1.69	0.57
2:Ba:87:ALA:HB2	2:Ba:101:ILE:HG22	1.87	0.57
2:Bb:56:GLN:HE22	2:Bc:69:LEU:H	1.53	0.57
2:Br:87:ALA:HB2	2:Br:101:ILE:HG22	1.86	0.57
5:Ex:148:ILE:HD12	5:Ex:184:ARG:HE	1.69	0.57
2:Bg:283:GLU:HG2	2:Bg:305:GLU:HG2	1.87	0.57
3:Cr:361:PRO:HB2	4:Dk:148:ARG:HD2	1.86	0.57
4:Dy:49:VAL:HG12	4:Dy:59:GLU:HG2	1.84	0.57
5:Et:148:ILE:HD12	5:Et:184:ARG:HE	1.70	0.57
3:Cr:43:LEU:HD21	3:Cr:68:MET:HE1	1.86	0.57
5:Ej:148:ILE:HD12	5:Ej:184:ARG:HE	1.69	0.57
2:Bo:87:ALA:HB2	2:Bo:101:ILE:HG22	1.87	0.57
2:Bp:87:ALA:HB2	2:Bp:101:ILE:HG22	1.87	0.57
2:Bs:56:GLN:HE22	2:Bt:69:LEU:H	1.53	0.57
3:Cf:92:GLU:HB2	3:Cf:103:ARG:HB3	1.85	0.57
3:Cq:92:GLU:HB2	3:Cq:103:ARG:HB3	1.86	0.57
1:Az:219:PHE:HA	2:Bo:69:LEU:HD13	1.87	0.57
5:Ed:148:ILE:HD12	5:Ed:184:ARG:HE	1.70	0.57
2:Br:56:GLN:HE22	2:Bs:69:LEU:H	1.53	0.57
2:Bt:56:GLN:HE22	2:Bu:69:LEU:H	1.53	0.56
2:Br:303:ASN:HB2	2:Bu:148:ASP:HB2	1.88	0.56
3:Cq:43:LEU:HD21	3:Cq:68:MET:HE1	1.85	0.56
5:Ep:148:ILE:HD12	5:Ep:184:ARG:HE	1.69	0.56
5:Er:148:ILE:HD12	5:Er:184:ARG:HE	1.70	0.56
5:Ev:148:ILE:HD12	5:Ev:184:ARG:HE	1.70	0.56
5:Ez:148:ILE:HD12	5:Ez:184:ARG:HE	1.70	0.56
2:Ba:69:LEU:H	2:Bz:56:GLN:HE22	1.53	0.56
5:Em:168:TYR:HB2	5:Em:196:MET:HE1	1.86	0.56
2:Bk:290:PRO:HB3	2:Bk:296:GLY:HA3	1.87	0.56
2:Bs:87:ALA:HB2	2:Bs:101:ILE:HG22	1.88	0.56
3:Cj:92:GLU:HB2	3:Cj:103:ARG:HB3	1.87	0.56
3:Cj:361:PRO:HB2	4:Dc:148:ARG:HD2	1.87	0.56
3:Ca:43:LEU:HD21	3:Ca:68:MET:HE1	1.87	0.56
2:Bb:87:ALA:HB2	2:Bb:101:ILE:HG22	1.88	0.56
3:Ct:153:ILE:HG21	3:Ct:195:MET:HE1	1.86	0.56
5:Ef:148:ILE:HD12	5:Ef:184:ARG:HE	1.70	0.56
2:Bd:87:ALA:HB2	2:Bd:101:ILE:HG22	1.87	0.56
2:Bg:290:PRO:HB3	2:Bg:296:GLY:HA3	1.88	0.56
2:By:317:LYS:HE3	2:Bz:324:LEU:HD23	1.87	0.56
3:Cb:85:VAL:HG22	3:Cb:108:ILE:HG12	1.87	0.56
2:Be:254:SER:HB2	2:Bg:138:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bl:87:ALA:HB2	2:Bl:101:ILE:HG22	1.88	0.56
2:By:87:ALA:HB2	2:By:101:ILE:HG22	1.88	0.56
5:Ea:168:TYR:HB2	5:Ea:196:MET:HE1	1.87	0.56
1:Ab:219:PHE:HA	2:Bq:69:LEU:HD13	1.87	0.55
2:Bi:254:SER:HB2	2:Bk:138:VAL:HG22	1.88	0.55
2:Bn:87:ALA:HB2	2:Bn:101:ILE:HG22	1.88	0.55
3:Cl:361:PRO:HB2	4:De:148:ARG:HD2	1.87	0.55
2:Bg:41:VAL:HG23	2:Bg:83:VAL:HG21	1.88	0.55
2:Bq:290:PRO:HB3	2:Bq:296:GLY:HA3	1.88	0.55
2:Bc:41:VAL:HG23	2:Bc:83:VAL:HG21	1.87	0.55
2:Bh:41:VAL:HG23	2:Bh:83:VAL:HG21	1.88	0.55
2:Bh:254:SER:HB2	2:Bj:138:VAL:HG22	1.88	0.55
2:Bm:41:VAL:HG23	2:Bm:83:VAL:HG21	1.88	0.55
2:Bq:87:ALA:HB2	2:Bq:101:ILE:HG22	1.88	0.55
2:Bs:286:ASN:HB2	2:Bs:302:PRO:HG2	1.88	0.55
4:Dr:111:LYS:H	4:Dr:115:GLY:HA2	1.70	0.55
2:Bc:283:GLU:HG2	2:Bc:305:GLU:HG2	1.88	0.55
2:Bc:290:PRO:HB3	2:Bc:296:GLY:HA3	1.87	0.55
2:Bt:87:ALA:HB2	2:Bt:101:ILE:HG22	1.88	0.55
2:Bw:87:ALA:HB2	2:Bw:101:ILE:HG22	1.89	0.55
3:Ct:361:PRO:HB2	4:Dm:148:ARG:HD2	1.89	0.55
2:Bv:41:VAL:HG23	2:Bv:83:VAL:HG21	1.87	0.55
3:Cf:361:PRO:HB2	4:Dy:148:ARG:HD2	1.86	0.55
4:Dj:219:VAL:HG21	4:Dj:254:LEU:HD21	1.87	0.55
2:Bo:91:ALA:HB1	2:Bo:174:ASN:HD21	1.72	0.55
2:Bo:254:SER:HB2	2:Bq:138:VAL:HG22	1.87	0.55
2:Bw:41:VAL:HG23	2:Bw:83:VAL:HG21	1.88	0.55
3:Cp:361:PRO:HB2	4:Di:148:ARG:HD2	1.89	0.55
2:Be:87:ALA:HB2	2:Be:101:ILE:HG22	1.88	0.55
2:Bg:254:SER:HB2	2:Bi:138:VAL:HG22	1.88	0.55
2:Bo:317:LYS:HE3	2:Bp:324:LEU:HD23	1.89	0.55
4:Dn:111:LYS:H	4:Dn:115:GLY:HA2	1.71	0.55
1:Ai:139:GLY:HA3	1:Aj:148:TYR:HD1	1.72	0.55
2:Bj:254:SER:HB2	2:Bl:138:VAL:HG22	1.89	0.55
2:Bk:224:ARG:HH22	3:Cn:323:THR:HB	1.72	0.55
2:Bo:290:PRO:HB3	2:Bo:296:GLY:HA3	1.89	0.55
5:Eq:168:TYR:HB2	5:Eq:196:MET:HE1	1.87	0.55
2:Bo:41:VAL:HG23	2:Bo:83:VAL:HG21	1.88	0.55
2:Be:41:VAL:HG23	2:Be:83:VAL:HG21	1.89	0.54
2:Bp:283:GLU:HG2	2:Bp:305:GLU:HG2	1.88	0.54
3:Ck:201:ASP:HB3	3:Ck:221:ALA:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ba:56:GLN:HE22	2:Bb:69:LEU:H	1.55	0.54
4:Dg:68:ILE:HD11	4:Dh:112:GLN:HE21	1.71	0.54
4:Dk:68:ILE:HD11	4:Dl:112:GLN:HE21	1.72	0.54
4:Dt:111:LYS:H	4:Dt:115:GLY:HA2	1.71	0.54
5:Ex:189:ARG:HH21	5:Ex:205:LYS:HZ1	1.56	0.54
3:Cx:361:PRO:HB2	4:Dq:148:ARG:HD2	1.90	0.54
4:Df:111:LYS:H	4:Df:115:GLY:HA2	1.71	0.54
2:Bi:290:PRO:HB3	2:Bi:296:GLY:HA3	1.90	0.54
2:Bp:41:VAL:HG23	2:Bp:83:VAL:HG21	1.88	0.54
2:By:290:PRO:HB3	2:By:296:GLY:HA3	1.89	0.54
2:Ba:324:LEU:HD23	2:Bz:317:LYS:HE3	1.89	0.54
2:Bj:41:VAL:HG23	2:Bj:83:VAL:HG21	1.90	0.54
1:Ap:139:GLY:HA3	1:Aq:148:TYR:HD1	1.73	0.54
2:By:287:VAL:HG22	2:By:301:VAL:HG13	1.88	0.54
3:Cd:361:PRO:HB2	4:Dw:148:ARG:HD2	1.88	0.54
3:Cp:220:PHE:HE2	3:Cp:273:VAL:HG11	1.73	0.54
4:Dz:219:VAL:HG21	4:Dz:254:LEU:HD21	1.89	0.54
5:En:65:ARG:HD3	5:En:69:ILE:HD13	1.90	0.54
1:Al:66:TRP:HA	1:Al:192:ARG:HD3	1.89	0.54
1:Au:219:PHE:HA	2:Bj:69:LEU:HD13	1.90	0.54
2:Bd:41:VAL:HG23	2:Bd:83:VAL:HG21	1.89	0.54
2:Br:41:VAL:HG23	2:Br:83:VAL:HG21	1.89	0.54
5:Ez:116:ARG:HA	5:Ez:149:GLN:HE22	1.73	0.54
1:Aa:66:TRP:HA	1:Aa:192:ARG:HD3	1.90	0.54
2:Bf:41:VAL:HG23	2:Bf:83:VAL:HG21	1.89	0.54
2:Bm:87:ALA:HB2	2:Bm:101:ILE:HG22	1.89	0.54
2:Bz:283:GLU:HG2	2:Bz:305:GLU:HG2	1.90	0.54
1:Ar:66:TRP:HA	1:Ar:192:ARG:HD3	1.89	0.54
1:Ax:139:GLY:HA3	1:Ay:148:TYR:HD1	1.73	0.54
2:Bd:317:LYS:HE3	2:Be:324:LEU:HD23	1.89	0.54
5:Ed:65:ARG:HD3	5:Ed:69:ILE:HD13	1.90	0.54
5:Er:65:ARG:HD3	5:Er:69:ILE:HD13	1.90	0.54
1:Ax:66:TRP:HA	1:Ax:192:ARG:HD3	1.90	0.54
2:Ba:41:VAL:HG23	2:Ba:83:VAL:HG21	1.90	0.54
2:Bf:87:ALA:HB2	2:Bf:101:ILE:HG22	1.90	0.54
2:Bk:41:VAL:HG23	2:Bk:83:VAL:HG21	1.90	0.54
3:Ca:226:VAL:HB	3:Ca:236:MET:HB3	1.89	0.54
3:Cs:220:PHE:HE2	3:Cs:273:VAL:HG11	1.73	0.54
4:Dp:111:LYS:H	4:Dp:115:GLY:HA2	1.73	0.54
5:Ef:116:ARG:HA	5:Ef:149:GLN:HE22	1.73	0.54
2:Be:252:VAL:HG22	2:Be:259:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:219:PHE:HD1	2:Bx:69:LEU:HD13	1.73	0.53
1:Am:66:TRP:HA	1:Am:192:ARG:HD3	1.90	0.53
1:Au:66:TRP:HA	1:Au:192:ARG:HD3	1.90	0.53
1:Aw:139:GLY:HA3	1:Ax:148:TYR:HD1	1.73	0.53
2:Bl:41:VAL:HG23	2:Bl:83:VAL:HG21	1.90	0.53
2:By:41:VAL:HG23	2:By:83:VAL:HG21	1.89	0.53
4:Dh:219:VAL:HG21	4:Dh:254:LEU:HD21	1.90	0.53
5:Ep:65:ARG:HD3	5:Ep:69:ILE:HD13	1.91	0.53
1:Av:66:TRP:HA	1:Av:192:ARG:HD3	1.91	0.53
1:Aw:66:TRP:HA	1:Aw:192:ARG:HD3	1.89	0.53
1:Az:66:TRP:HA	1:Az:192:ARG:HD3	1.91	0.53
2:Bc:317:LYS:HE3	2:Bd:324:LEU:HD23	1.89	0.53
3:Ci:255:ASP:HB3	3:Ci:258:SER:HB3	1.91	0.53
3:Cy:220:PHE:HE2	3:Cy:273:VAL:HG11	1.73	0.53
4:Dx:184:ILE:HG12	4:Dx:286:VAL:HG22	1.91	0.53
5:Ee:154:LEU:HB3	5:Ee:164:TYR:HE1	1.73	0.53
5:Ej:116:ARG:HA	5:Ej:149:GLN:HE22	1.73	0.53
1:Ad:139:GLY:HA3	1:Ae:148:TYR:HD1	1.74	0.53
1:Aq:66:TRP:HA	1:Aq:192:ARG:HD3	1.91	0.53
1:Aq:139:GLY:HA3	1:Ar:148:TYR:HD1	1.74	0.53
1:Ar:139:GLY:HA3	1:As:148:TYR:HD1	1.73	0.53
2:Bm:290:PRO:HB3	2:Bm:296:GLY:HA3	1.91	0.53
2:Bs:41:VAL:HG23	2:Bs:83:VAL:HG21	1.89	0.53
3:Cc:239:THR:HG21	3:Cd:155:ARG:HD3	1.91	0.53
4:Da:104:ILE:HG23	4:Db:145:ARG:HD3	1.90	0.53
4:Dy:68:ILE:HD11	4:Dz:112:GLN:HE21	1.74	0.53
1:Ae:139:GLY:HA3	1:Af:148:TYR:HD1	1.74	0.53
1:Af:139:GLY:HA3	1:Ag:148:TYR:HD1	1.73	0.53
1:Ao:139:GLY:HA3	1:Ap:148:TYR:HD1	1.74	0.53
2:Bl:254:SER:HB2	2:Bn:138:VAL:HG22	1.91	0.53
2:Bv:290:PRO:HB3	2:Bv:296:GLY:HA3	1.89	0.53
2:Bx:41:VAL:HG23	2:Bx:83:VAL:HG21	1.89	0.53
3:Cr:206:ILE:HG13	3:Cr:216:ILE:HG12	1.90	0.53
4:Dk:104:ILE:HG23	4:Dl:145:ARG:HD3	1.90	0.53
4:Dp:24:GLU:HG3	4:Dp:148:ARG:HH22	1.73	0.53
4:Dt:184:ILE:HG12	4:Dt:286:VAL:HG22	1.91	0.53
4:Dz:217:ASP:HA	4:Dz:258:ARG:HD3	1.91	0.53
5:Ei:154:LEU:HB3	5:Ei:164:TYR:HE1	1.74	0.53
5:El:65:ARG:HD3	5:El:69:ILE:HD13	1.91	0.53
1:Av:139:GLY:HA3	1:Aw:148:TYR:HD1	1.74	0.53
1:Ay:139:GLY:HA3	1:Az:148:TYR:HD1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bi:87:ALA:HB2	2:Bi:101:ILE:HG22	1.91	0.53
2:Bz:87:ALA:HB2	2:Bz:101:ILE:HG22	1.91	0.53
4:Da:83:THR:HG22	4:Da:111:LYS:HA	1.91	0.53
4:Dr:184:ILE:HG12	4:Dr:286:VAL:HG22	1.91	0.53
5:Ek:154:LEU:HB3	5:Ek:164:TYR:HE1	1.74	0.53
5:Es:154:LEU:HB3	5:Es:164:TYR:HE1	1.73	0.53
1:Ac:139:GLY:HA3	1:Ad:148:TYR:HD1	1.73	0.53
1:Ag:66:TRP:HA	1:Ag:192:ARG:HD3	1.91	0.53
1:Aj:139:GLY:HA3	1:Ak:148:TYR:HD1	1.74	0.53
1:An:139:GLY:HA3	1:Ao:148:TYR:HD1	1.73	0.53
2:Bb:41:VAL:HG23	2:Bb:83:VAL:HG21	1.89	0.53
2:Bc:286:ASN:HB2	2:Bc:302:PRO:HG2	1.91	0.53
2:Bu:41:VAL:HG23	2:Bu:83:VAL:HG21	1.91	0.53
3:Cr:126:ILE:HB	3:Cr:169:THR:HG22	1.91	0.53
4:Dd:184:ILE:HG12	4:Dd:286:VAL:HG22	1.91	0.53
5:Ej:65:ARG:HD3	5:Ej:69:ILE:HD13	1.91	0.53
5:Ez:65:ARG:HD3	5:Ez:69:ILE:HD13	1.91	0.53
1:Ah:139:GLY:HA3	1:Ai:148:TYR:HD1	1.73	0.53
1:Aj:66:TRP:HA	1:Aj:192:ARG:HD3	1.91	0.53
2:Be:317:LYS:HE3	2:Bf:324:LEU:HD23	1.89	0.53
2:Bn:254:SER:HB2	2:Bp:138:VAL:HG22	1.91	0.53
2:Bp:287:VAL:HG13	2:Bp:301:VAL:HG22	1.91	0.53
3:Cl:80:PHE:HA	6:Fl:136:VAL:HG21	1.91	0.53
4:Da:68:ILE:HD11	4:Db:112:GLN:HE21	1.74	0.53
4:De:104:ILE:HG23	4:Df:145:ARG:HD3	1.91	0.53
4:Dj:217:ASP:HA	4:Dj:258:ARG:HD3	1.91	0.53
4:Dv:184:ILE:HG12	4:Dv:286:VAL:HG22	1.91	0.53
5:Es:168:TYR:HB2	5:Es:196:MET:HE1	1.91	0.53
1:Aa:148:TYR:HD1	1:Az:139:GLY:HA3	1.74	0.53
1:Ab:139:GLY:HA3	1:Ac:148:TYR:HD1	1.73	0.53
1:At:139:GLY:HA3	1:Au:148:TYR:HD1	1.73	0.53
2:Bd:254:SER:HB2	2:Bf:138:VAL:HG22	1.91	0.53
2:Bw:254:SER:HB2	2:By:138:VAL:HG22	1.89	0.53
3:Ca:126:ILE:HB	3:Ca:169:THR:HG22	1.91	0.53
3:Cm:126:ILE:HB	3:Cm:169:THR:HG22	1.91	0.53
4:Dy:104:ILE:HG23	4:Dz:145:ARG:HD3	1.91	0.53
4:Dz:184:ILE:HG12	4:Dz:286:VAL:HG22	1.91	0.53
1:Al:139:GLY:HA3	1:Am:148:TYR:HD1	1.73	0.53
1:Am:139:GLY:HA3	1:An:148:TYR:HD1	1.74	0.53
2:Br:290:PRO:HB3	2:Br:296:GLY:HA3	1.89	0.53
5:Eg:154:LEU:HB3	5:Eg:164:TYR:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ep:116:ARG:HA	5:Ep:149:GLN:HE22	1.74	0.53
5:Et:65:ARG:HD3	5:Et:69:ILE:HD13	1.90	0.53
5:Ev:116:ARG:HA	5:Ev:149:GLN:HE22	1.74	0.53
5:Ex:116:ARG:HA	5:Ex:149:GLN:HE22	1.74	0.53
1:Ak:139:GLY:HA3	1:Al:148:TYR:HD1	1.74	0.52
2:Bm:254:SER:HB2	2:Bo:138:VAL:HG22	1.91	0.52
2:Bp:290:PRO:HB3	2:Bp:296:GLY:HA3	1.90	0.52
4:Dp:184:ILE:HG12	4:Dp:286:VAL:HG22	1.91	0.52
4:Dw:68:ILE:HD11	4:Dx:112:GLN:HE21	1.74	0.52
5:Ef:65:ARG:HD3	5:Ef:69:ILE:HD13	1.91	0.52
5:Ev:65:ARG:HD3	5:Ev:69:ILE:HD13	1.91	0.52
5:Ey:168:TYR:HB2	5:Ey:196:MET:HE1	1.92	0.52
1:Ab:66:TRP:HA	1:Ab:192:ARG:HD3	1.91	0.52
1:Ae:66:TRP:HA	1:Ae:192:ARG:HD3	1.90	0.52
2:Ba:138:VAL:HG22	2:By:254:SER:HB2	1.91	0.52
2:Be:49:GLU:HG3	2:Be:54:THR:HG21	1.91	0.52
2:Bg:56:GLN:HE22	2:Bh:69:LEU:H	1.55	0.52
2:Bk:254:SER:HB2	2:Bm:138:VAL:HG22	1.92	0.52
2:Bo:49:GLU:HG3	2:Bo:54:THR:HG21	1.92	0.52
1:Ac:66:TRP:HA	1:Ac:192:ARG:HD3	1.90	0.52
2:Bx:254:SER:HB2	2:Bz:138:VAL:HG22	1.90	0.52
3:Cj:201:ASP:HB3	3:Cj:221:ALA:HB3	1.90	0.52
5:Ex:65:ARG:HD3	5:Ex:69:ILE:HD13	1.91	0.52
1:Aa:139:GLY:HA3	1:Ab:148:TYR:HD1	1.73	0.52
1:Au:139:GLY:HA3	1:Av:148:TYR:HD1	1.74	0.52
2:Bq:317:LYS:HB2	2:Br:328:VAL:HG21	1.90	0.52
2:Br:254:SER:HB2	2:Bt:138:VAL:HG22	1.91	0.52
3:Cb:195:MET:HE2	3:Cb:281:LEU:HD11	1.92	0.52
3:Cb:206:ILE:HG13	3:Cb:216:ILE:HG12	1.90	0.52
3:Cr:61:ILE:HD11	3:Cr:282:GLU:HG3	1.92	0.52
4:De:83:THR:HG22	4:De:111:LYS:HA	1.92	0.52
4:Dv:111:LYS:H	4:Dv:115:GLY:HA2	1.74	0.52
5:Eo:168:TYR:HB2	5:Eo:196:MET:HE1	1.91	0.52
5:Eu:154:LEU:HB3	5:Eu:164:TYR:HE1	1.74	0.52
1:Ai:66:TRP:HA	1:Ai:192:ARG:HD3	1.91	0.52
2:Bb:138:VAL:HG22	2:Bz:254:SER:HB2	1.91	0.52
2:Bc:254:SER:HB2	2:Be:138:VAL:HG22	1.90	0.52
2:Bf:254:SER:HB2	2:Bh:138:VAL:HG22	1.92	0.52
2:Bk:87:ALA:HB2	2:Bk:101:ILE:HG22	1.90	0.52
2:Bk:317:LYS:HB2	2:Bl:328:VAL:HG21	1.92	0.52
4:Dg:104:ILE:HG23	4:Dh:145:ARG:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dl:24:GLU:HG3	4:Dl:148:ARG:HH22	1.75	0.52
4:Dr:24:GLU:HG3	4:Dr:148:ARG:HH22	1.75	0.52
1:Ah:66:TRP:HA	1:Ah:192:ARG:HD3	1.91	0.52
2:Ba:49:GLU:HG3	2:Ba:54:THR:HG21	1.91	0.52
2:Bj:283:GLU:HG2	2:Bj:305:GLU:HG2	1.90	0.52
2:Bp:254:SER:HB2	2:Br:138:VAL:HG22	1.92	0.52
2:Bp:267:LEU:HB2	2:Bp:320:PRO:HB2	1.91	0.52
5:Er:116:ARG:HA	5:Er:149:GLN:HE22	1.75	0.52
1:Ak:66:TRP:HA	1:Ak:192:ARG:HD3	1.91	0.52
2:Bt:41:VAL:HG23	2:Bt:83:VAL:HG21	1.90	0.52
2:Bt:254:SER:HB2	2:Bv:138:VAL:HG22	1.91	0.52
2:Bx:143:SER:HB2	2:Bx:157:PRO:HG3	1.92	0.52
2:Bz:143:SER:HB2	2:Bz:157:PRO:HG3	1.92	0.52
5:En:116:ARG:HA	5:En:149:GLN:HE22	1.75	0.52
5:Et:116:ARG:HA	5:Et:149:GLN:HE22	1.74	0.52
2:Bb:254:SER:HB2	2:Bd:138:VAL:HG22	1.92	0.52
2:Bn:143:SER:HB2	2:Bn:157:PRO:HG3	1.92	0.52
2:Bp:141:GLY:HA3	2:Bp:154:GLY:O	2.10	0.52
2:Br:315:MET:HG3	2:Bs:328:VAL:HG13	1.91	0.52
3:Cl:292:PRO:HB3	3:Cl:306:LEU:HD13	1.91	0.52
3:Co:153:ILE:HG21	3:Co:195:MET:HE1	1.92	0.52
4:Dg:83:THR:HG22	4:Dg:111:LYS:HA	1.92	0.52
5:El:116:ARG:HA	5:El:149:GLN:HE22	1.74	0.52
5:Ew:154:LEU:HB3	5:Ew:164:TYR:HE1	1.75	0.52
2:Bx:317:LYS:HE3	2:By:324:LEU:HD23	1.91	0.52
4:Db:24:GLU:HG3	4:Db:148:ARG:HH22	1.74	0.52
4:Dh:217:ASP:HA	4:Dh:258:ARG:HD3	1.92	0.52
4:Dn:184:ILE:HG12	4:Dn:286:VAL:HG22	1.90	0.52
5:Em:192:LEU:HD12	5:Em:196:MET:HE2	1.92	0.52
4:Dy:83:THR:HG22	4:Dy:111:LYS:HA	1.91	0.52
5:Ew:168:TYR:HB2	5:Ew:196:MET:HE1	1.92	0.52
5:Ey:154:LEU:HB3	5:Ey:164:TYR:HE1	1.75	0.52
4:Dc:68:ILE:HD11	4:Dd:112:GLN:HE21	1.75	0.51
4:Dj:184:ILE:HG12	4:Dj:286:VAL:HG22	1.92	0.51
1:Ad:66:TRP:HA	1:Ad:192:ARG:HD3	1.91	0.51
2:Bb:290:PRO:HB3	2:Bb:296:GLY:HA3	1.92	0.51
2:Bk:272:VAL:HG22	2:Bl:260:VAL:HG22	1.92	0.51
3:Cb:365:TYR:HB3	4:Du:91:MET:HE1	1.92	0.51
3:Cy:223:GLU:HG2	3:Cy:239:THR:HG22	1.90	0.51
4:Di:68:ILE:HD11	4:Dj:112:GLN:HE21	1.75	0.51
5:Eo:154:LEU:HB3	5:Eo:164:TYR:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:139:GLY:HA3	1:Ah:148:TYR:HD1	1.74	0.51
1:Ar:234:GLN:HA	1:As:198:THR:HB	1.92	0.51
2:Bf:290:PRO:HB3	2:Bf:296:GLY:HA3	1.93	0.51
3:Ct:223:GLU:HG2	3:Ct:239:THR:HG22	1.92	0.51
4:Di:83:THR:HG22	4:Di:111:LYS:HA	1.92	0.51
2:Bc:143:SER:HB2	2:Bc:157:PRO:HG3	1.93	0.51
2:Bi:41:VAL:HG23	2:Bi:83:VAL:HG21	1.93	0.51
2:Bn:41:VAL:HG23	2:Bn:83:VAL:HG21	1.91	0.51
2:Bt:143:SER:HB2	2:Bt:157:PRO:HG3	1.92	0.51
3:Ca:220:PHE:HE2	3:Ca:273:VAL:HG11	1.75	0.51
3:Ce:334:ARG:HE	3:Cf:295:VAL:HG21	1.76	0.51
3:Cr:223:GLU:HG2	3:Cr:239:THR:HG22	1.93	0.51
1:Ae:234:GLN:HA	1:Af:198:THR:HB	1.92	0.51
1:Af:66:TRP:HA	1:Af:192:ARG:HD3	1.92	0.51
1:Ap:66:TRP:HA	1:Ap:192:ARG:HD3	1.93	0.51
2:Bu:272:VAL:HG22	2:Bv:260:VAL:HG22	1.92	0.51
3:Ch:126:ILE:HB	3:Ch:169:THR:HG22	1.92	0.51
4:Dc:104:ILE:HG23	4:Dd:145:ARG:HD3	1.92	0.51
1:Ao:66:TRP:HA	1:Ao:192:ARG:HD3	1.92	0.51
2:Bg:87:ALA:HB2	2:Bg:101:ILE:HG22	1.92	0.51
2:Br:283:GLU:HG2	2:Br:305:GLU:HG2	1.93	0.51
3:Co:255:ASP:HB3	3:Co:258:SER:HB3	1.93	0.51
4:Dq:83:THR:HG22	4:Dq:111:LYS:HA	1.93	0.51
4:Du:83:THR:HG22	4:Du:111:LYS:HA	1.92	0.51
5:Ed:116:ARG:HA	5:Ed:149:GLN:HE22	1.75	0.51
5:Eu:168:TYR:HB2	5:Eu:196:MET:HE1	1.93	0.51
1:An:113:GLU:HB2	1:An:172:MET:HB3	1.93	0.51
1:At:66:TRP:HA	1:At:192:ARG:HD3	1.92	0.51
2:Bo:272:VAL:HG22	2:Bp:260:VAL:HG22	1.93	0.51
2:Bp:317:LYS:HE3	2:Bq:324:LEU:HD23	1.92	0.51
2:Bs:254:SER:HB2	2:Bu:138:VAL:HG22	1.93	0.51
3:Cc:209:LYS:HD2	3:Cc:212:GLN:HB2	1.93	0.51
4:Du:104:ILE:HG23	4:Dv:145:ARG:HD3	1.92	0.51
1:Ad:234:GLN:HA	1:Ae:198:THR:HB	1.93	0.51
1:Ah:234:GLN:HA	1:Ai:198:THR:HB	1.92	0.51
2:Br:317:LYS:HE3	2:Bs:324:LEU:HD23	1.92	0.51
3:Ck:209:LYS:HD2	3:Ck:212:GLN:HB2	1.92	0.51
4:Dm:104:ILE:HG23	4:Dn:145:ARG:HD3	1.92	0.51
5:Eo:192:LEU:HD12	5:Eo:196:MET:HE2	1.93	0.51
1:Aa:198:THR:HB	1:Az:234:GLN:HA	1.92	0.51
1:Ai:234:GLN:HA	1:Aj:198:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bv:254:SER:HB2	2:Bx:138:VAL:HG22	1.93	0.51
3:Cp:255:ASP:HB3	3:Cp:258:SER:HB3	1.92	0.51
4:Dc:83:THR:HG22	4:Dc:111:LYS:HA	1.93	0.51
4:Do:83:THR:HG22	4:Do:111:LYS:HA	1.93	0.51
1:Af:234:GLN:HA	1:Ag:198:THR:HB	1.92	0.51
1:Ap:234:GLN:HA	1:Aq:198:THR:HB	1.93	0.51
2:Br:143:SER:HB2	2:Br:157:PRO:HG3	1.93	0.51
2:Bt:269:PRO:HB2	2:Bu:263:GLN:HE21	1.75	0.51
2:By:49:GLU:HG3	2:By:54:THR:HG21	1.93	0.51
3:Cb:165:VAL:HG11	3:Cb:309:ILE:HD12	1.93	0.51
4:Dw:83:THR:HG22	4:Dw:111:LYS:HA	1.92	0.51
1:Ap:113:GLU:HB2	1:Ap:172:MET:HB3	1.94	0.50
1:As:139:GLY:HA3	1:At:148:TYR:HD1	1.75	0.50
2:Bg:49:GLU:HG3	2:Bg:54:THR:HG21	1.93	0.50
4:Ds:104:ILE:HG23	4:Dt:145:ARG:HD3	1.93	0.50
2:Ba:224:ARG:HH22	3:Cd:323:THR:HB	1.76	0.50
2:Be:290:PRO:HB3	2:Be:296:GLY:HA3	1.93	0.50
2:Bi:272:VAL:HG22	2:Bj:260:VAL:HG22	1.92	0.50
2:Bj:272:VAL:HG22	2:Bk:260:VAL:HG22	1.93	0.50
2:Bu:254:SER:HB2	2:Bw:138:VAL:HG22	1.92	0.50
3:Ch:80:PHE:HA	6:Fh:136:VAL:HG21	1.94	0.50
4:Dd:111:LYS:H	4:Dd:115:GLY:HA2	1.76	0.50
5:Ea:192:LEU:HD12	5:Ea:196:MET:HE2	1.93	0.50
5:Ec:154:LEU:HB3	5:Ec:164:TYR:HE1	1.75	0.50
1:Al:234:GLN:HA	1:Am:198:THR:HB	1.92	0.50
1:An:234:GLN:HA	1:Ao:198:THR:HB	1.93	0.50
1:Aq:234:GLN:HA	1:Ar:198:THR:HB	1.92	0.50
2:Bl:360:ILE:HD12	2:Bn:163:SER:H	1.76	0.50
2:Bq:41:VAL:HG23	2:Bq:83:VAL:HG21	1.92	0.50
2:Bq:360:ILE:HD12	2:Bs:163:SER:H	1.77	0.50
2:Bw:224:ARG:HH22	3:Cz:323:THR:HB	1.76	0.50
3:Ch:195:MET:HE2	3:Ch:281:LEU:HD11	1.94	0.50
3:Ci:126:ILE:HB	3:Ci:169:THR:HG22	1.93	0.50
3:Cj:195:MET:HE2	3:Cj:281:LEU:HD11	1.93	0.50
3:Cn:292:PRO:HB3	3:Cn:306:LEU:HD13	1.93	0.50
4:Dd:24:GLU:HG3	4:Dd:148:ARG:HH22	1.74	0.50
1:Ad:113:GLU:HB2	1:Ad:172:MET:HB3	1.93	0.50
1:As:234:GLN:HA	1:At:198:THR:HB	1.92	0.50
1:At:234:GLN:HA	1:Au:198:THR:HB	1.93	0.50
2:Bk:143:SER:HB2	2:Bk:157:PRO:HG3	1.93	0.50
2:Bq:318:LEU:HD11	2:Bq:330:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bz:41:VAL:HG23	2:Bz:83:VAL:HG21	1.94	0.50
2:Bz:320:PRO:HB2	2:Bz:327:LEU:HD12	1.93	0.50
3:Ch:292:PRO:HB3	3:Ch:306:LEU:HD13	1.93	0.50
4:Dr:216:ILE:HA	4:Dr:291:ARG:HA	1.93	0.50
4:Ds:83:THR:HG22	4:Ds:111:LYS:HA	1.93	0.50
4:Dw:104:ILE:HG23	4:Dx:145:ARG:HD3	1.94	0.50
5:Ec:168:TYR:HB2	5:Ec:196:MET:HE1	1.93	0.50
5:Eq:192:LEU:HD12	5:Eq:196:MET:HE2	1.93	0.50
5:Ey:192:LEU:HD12	5:Ey:196:MET:HE2	1.93	0.50
1:Ab:234:GLN:HA	1:Ac:198:THR:HB	1.93	0.50
1:At:113:GLU:HB2	1:At:172:MET:HB3	1.93	0.50
1:Au:234:GLN:HA	1:Av:198:THR:HB	1.93	0.50
1:Ay:234:GLN:HA	1:Az:198:THR:HB	1.92	0.50
1:Az:113:GLU:HB2	1:Az:172:MET:HB3	1.94	0.50
2:Bn:290:PRO:HB3	2:Bn:296:GLY:HA3	1.92	0.50
3:Cs:85:VAL:HG22	3:Cs:108:ILE:HG12	1.94	0.50
4:Dp:216:ILE:HA	4:Dp:291:ARG:HA	1.93	0.50
1:Aa:234:GLN:HA	1:Ab:198:THR:HB	1.93	0.50
1:Ar:113:GLU:HB2	1:Ar:172:MET:HB3	1.94	0.50
1:Av:234:GLN:HA	1:Aw:198:THR:HB	1.93	0.50
1:Ax:234:GLN:HA	1:Ay:198:THR:HB	1.92	0.50
2:Bc:248:ALA:HB1	2:Bc:265:VAL:HG22	1.94	0.50
2:By:272:VAL:HG22	2:Bz:260:VAL:HG22	1.94	0.50
3:Cf:61:ILE:HD11	3:Cf:282:GLU:HG3	1.93	0.50
3:Cv:201:ASP:HB3	3:Cv:221:ALA:HB3	1.93	0.50
1:Ac:234:GLN:HA	1:Ad:198:THR:HB	1.93	0.50
1:An:66:TRP:HA	1:An:192:ARG:HD3	1.93	0.50
2:Bl:56:GLN:HE22	2:Bm:69:LEU:H	1.60	0.50
2:Bq:254:SER:HB2	2:Bs:138:VAL:HG22	1.94	0.50
2:Bs:49:GLU:HG3	2:Bs:54:THR:HG21	1.94	0.50
3:Cj:206:ILE:HG13	3:Cj:216:ILE:HG12	1.94	0.50
3:Cs:61:ILE:HD11	3:Cs:282:GLU:HG3	1.94	0.50
3:Cs:292:PRO:HB3	3:Cs:306:LEU:HD13	1.94	0.50
4:Dm:83:THR:HG22	4:Dm:111:LYS:HA	1.93	0.50
5:Es:192:LEU:HD12	5:Es:196:MET:HE2	1.93	0.50
1:Aj:234:GLN:HA	1:Ak:198:THR:HB	1.93	0.50
2:Bd:272:VAL:HG22	2:Be:260:VAL:HG22	1.93	0.50
2:Bp:272:VAL:HG22	2:Bq:260:VAL:HG22	1.93	0.50
2:Bp:285:LEU:HD23	2:Bp:303:ASN:HB3	1.94	0.50
3:Cf:220:PHE:HE2	3:Cf:273:VAL:HG11	1.76	0.50
4:Dk:83:THR:HG22	4:Dk:111:LYS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Eh:116:ARG:HA	5:Eh:149:GLN:HE22	1.76	0.50
2:Bt:290:PRO:HB3	2:Bt:296:GLY:HA3	1.94	0.50
3:Ct:220:PHE:HE2	3:Ct:273:VAL:HG11	1.76	0.50
5:Eb:116:ARG:HA	5:Eb:149:GLN:HE22	1.77	0.50
1:Ac:206:ILE:HG12	1:Ac:235:TYR:HD1	1.77	0.49
1:Aw:234:GLN:HA	1:Ax:198:THR:HB	1.93	0.49
2:Be:318:LEU:HD22	2:Be:330:ALA:HB1	1.94	0.49
2:Bg:360:ILE:HD12	2:Bi:163:SER:H	1.76	0.49
2:Bl:324:LEU:HD12	2:Bl:327:LEU:HD23	1.94	0.49
3:Cw:61:ILE:HD11	3:Cw:282:GLU:HG3	1.94	0.49
4:Du:93:PRO:HB2	4:Du:95:TRP:HE3	1.75	0.49
1:Ab:113:GLU:HB2	1:Ab:172:MET:HB3	1.94	0.49
1:Am:234:GLN:HA	1:An:198:THR:HB	1.93	0.49
3:Ce:195:MET:HE2	3:Ce:281:LEU:HD11	1.93	0.49
3:Ce:220:PHE:HE2	3:Ce:273:VAL:HG11	1.76	0.49
3:Cv:195:MET:HE2	3:Cv:281:LEU:HD11	1.93	0.49
3:Cy:153:ILE:HG21	3:Cy:195:MET:HE1	1.92	0.49
4:Df:216:ILE:HA	4:Df:291:ARG:HA	1.93	0.49
1:Ad:206:ILE:HG12	1:Ad:235:TYR:HD1	1.78	0.49
1:Am:206:ILE:HG12	1:Am:235:TYR:HD1	1.77	0.49
1:Ao:234:GLN:HA	1:Ap:198:THR:HB	1.93	0.49
1:Au:113:GLU:HB2	1:Au:172:MET:HB3	1.94	0.49
1:Av:113:GLU:HB2	1:Av:172:MET:HB3	1.95	0.49
2:Ba:254:SER:HB2	2:Bc:138:VAL:HG22	1.94	0.49
2:Ba:283:GLU:HG2	2:Ba:305:GLU:HG2	1.94	0.49
2:Br:272:VAL:HG22	2:Bs:260:VAL:HG22	1.94	0.49
2:Bs:224:ARG:HH22	3:Cv:323:THR:HB	1.77	0.49
2:Bv:248:ALA:HB1	2:Bv:265:VAL:HG22	1.94	0.49
3:Ck:61:ILE:HD11	3:Ck:282:GLU:HG3	1.93	0.49
4:Di:104:ILE:HG23	4:Dj:145:ARG:HD3	1.92	0.49
5:Eb:65:ARG:HD3	5:Eb:69:ILE:HD13	1.94	0.49
2:Bg:103:VAL:HB	2:Bg:137:LEU:HD21	1.94	0.49
2:Bl:303:ASN:H	2:Bm:285:LEU:HD12	1.76	0.49
2:Bp:315:MET:HG3	2:Bq:328:VAL:HG13	1.95	0.49
3:Cb:70:LEU:HG	6:Fb:136:VAL:HG13	1.94	0.49
3:Cw:220:PHE:HE2	3:Cw:273:VAL:HG11	1.77	0.49
4:Dx:217:ASP:HA	4:Dx:258:ARG:HD3	1.93	0.49
1:As:206:ILE:HG12	1:As:235:TYR:HD1	1.78	0.49
1:Ay:66:TRP:HA	1:Ay:192:ARG:HD3	1.93	0.49
1:Ay:206:ILE:HG12	1:Ay:235:TYR:HD1	1.78	0.49
1:Az:206:ILE:HG12	1:Az:235:TYR:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bb:248:ALA:HB1	2:Bb:265:VAL:HG22	1.94	0.49
2:Bl:143:SER:HB2	2:Bl:157:PRO:HG3	1.94	0.49
2:Bm:49:GLU:HG3	2:Bm:54:THR:HG21	1.95	0.49
2:Bs:272:VAL:HG22	2:Bt:260:VAL:HG22	1.95	0.49
4:Db:216:ILE:HA	4:Db:291:ARG:HA	1.93	0.49
4:Do:104:ILE:HG23	4:Dp:145:ARG:HD3	1.93	0.49
4:Dv:219:VAL:HG21	4:Dv:254:LEU:HD21	1.95	0.49
5:Ee:168:TYR:HB2	5:Ee:196:MET:HE1	1.94	0.49
1:Ag:113:GLU:HB2	1:Ag:172:MET:HB3	1.94	0.49
1:Ag:234:GLN:HA	1:Ah:198:THR:HB	1.94	0.49
1:Ah:206:ILE:HG12	1:Ah:235:TYR:HD1	1.78	0.49
1:Ai:206:ILE:HG12	1:Ai:235:TYR:HD1	1.77	0.49
1:Al:113:GLU:HB2	1:Al:172:MET:HB3	1.95	0.49
2:Bj:141:GLY:HA3	2:Bj:154:GLY:O	2.11	0.49
2:Bl:317:LYS:HE3	2:Bm:324:LEU:HD23	1.95	0.49
5:Ee:144:LEU:HA	5:Ee:147:ARG:HD2	1.95	0.49
5:Em:154:LEU:HB3	5:Em:164:TYR:HE1	1.78	0.49
1:Aj:206:ILE:HG12	1:Aj:235:TYR:HD1	1.78	0.49
2:Ba:286:ASN:HB2	2:Ba:302:PRO:HG2	1.95	0.49
2:Bu:49:GLU:HG3	2:Bu:54:THR:HG21	1.95	0.49
3:Ca:292:PRO:HB3	3:Ca:306:LEU:HD13	1.95	0.49
3:Cq:195:MET:HE2	3:Cq:281:LEU:HD11	1.94	0.49
4:Dj:216:ILE:HA	4:Dj:291:ARG:HA	1.94	0.49
5:Eq:154:LEU:HB3	5:Eq:164:TYR:HE1	1.77	0.49
1:Ac:113:GLU:HB2	1:Ac:172:MET:HB3	1.95	0.49
1:Ae:206:ILE:HG12	1:Ae:235:TYR:HD1	1.78	0.49
1:Aj:113:GLU:HB2	1:Aj:172:MET:HB3	1.95	0.49
1:Ak:206:ILE:HG12	1:Ak:235:TYR:HD1	1.77	0.49
2:Bl:49:GLU:HG3	2:Bl:54:THR:HG21	1.95	0.49
2:Bx:49:GLU:HG3	2:Bx:54:THR:HG21	1.95	0.49
3:Cg:255:ASP:HB3	3:Cg:258:SER:HB3	1.95	0.49
3:Cn:220:PHE:HE2	3:Cn:273:VAL:HG11	1.77	0.49
5:Ek:144:LEU:HA	5:Ek:147:ARG:HD2	1.94	0.49
1:Al:64:PRO:HB2	1:Am:38:VAL:HG13	1.95	0.49
2:Be:318:LEU:HD11	2:Be:334:VAL:HG21	1.95	0.49
3:Cd:206:ILE:HG13	3:Cd:216:ILE:HG12	1.95	0.49
3:Cu:78:TYR:HD2	3:Cu:88:ILE:HB	1.77	0.49
3:Cu:92:GLU:HB2	3:Cu:103:ARG:HB3	1.95	0.49
3:Cy:334:ARG:HE	3:Cz:295:VAL:HG21	1.78	0.49
4:Dd:216:ILE:HA	4:Dd:291:ARG:HA	1.95	0.49
5:Ei:168:TYR:HB2	5:Ei:196:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:206:ILE:HG12	1:Al:235:TYR:HD1	1.78	0.49
1:Ar:206:ILE:HG12	1:Ar:235:TYR:HD1	1.78	0.49
1:Au:206:ILE:HG12	1:Au:235:TYR:HD1	1.78	0.49
1:Ax:206:ILE:HG12	1:Ax:235:TYR:HD1	1.78	0.49
2:Bd:290:PRO:HB3	2:Bd:296:GLY:HA3	1.95	0.49
2:Bh:360:ILE:HD12	2:Bj:163:SER:H	1.78	0.49
2:Bs:141:GLY:HA3	2:Bs:154:GLY:O	2.13	0.49
2:Bt:49:GLU:HG3	2:Bt:54:THR:HG21	1.95	0.49
2:Bz:248:ALA:HB1	2:Bz:265:VAL:HG22	1.95	0.49
3:Cb:317:LYS:HG2	3:Cb:345:THR:HB	1.93	0.49
3:Ck:126:ILE:HB	3:Ck:169:THR:HG22	1.94	0.49
4:Da:111:LYS:HD2	5:Ey:197:PRO:HD3	1.95	0.49
4:Dt:216:ILE:HA	4:Dt:291:ARG:HA	1.93	0.49
5:Eh:65:ARG:HD3	5:Eh:69:ILE:HD13	1.95	0.49
1:Aa:206:ILE:HG12	1:Aa:235:TYR:HD1	1.78	0.48
1:An:206:ILE:HG12	1:An:235:TYR:HD1	1.78	0.48
2:Br:141:GLY:HA3	2:Br:154:GLY:O	2.13	0.48
3:Cb:61:ILE:HD11	3:Cb:282:GLU:HG3	1.94	0.48
3:Cg:220:PHE:HE2	3:Cg:273:VAL:HG11	1.78	0.48
3:Ci:209:LYS:HD3	3:Ci:212:GLN:HE21	1.77	0.48
4:Dj:221:VAL:HB	4:Dj:261:VAL:HG12	1.95	0.48
5:Eg:144:LEU:HA	5:Eg:147:ARG:HD2	1.95	0.48
5:Er:154:LEU:HB3	5:Er:164:TYR:HE1	1.78	0.48
1:At:206:ILE:HG12	1:At:235:TYR:HD1	1.78	0.48
1:Ax:113:GLU:HB2	1:Ax:172:MET:HB3	1.96	0.48
1:Ay:184:LEU:HD12	1:Ay:188:ASN:HB2	1.95	0.48
2:Be:248:ALA:HB1	2:Be:265:VAL:HG22	1.95	0.48
2:Br:49:GLU:HG3	2:Br:54:THR:HG21	1.95	0.48
2:Br:103:VAL:HB	2:Br:137:LEU:HD21	1.95	0.48
1:Ag:206:ILE:HG12	1:Ag:235:TYR:HD1	1.78	0.48
1:Ah:113:GLU:HB2	1:Ah:172:MET:HB3	1.95	0.48
1:Ak:234:GLN:HA	1:Al:198:THR:HB	1.93	0.48
2:Bb:317:LYS:HE3	2:Bc:324:LEU:HD23	1.95	0.48
2:Bd:315:MET:HG3	2:Be:328:VAL:HG13	1.95	0.48
2:Bf:275:GLY:HA3	2:Bg:338:PRO:HG2	1.95	0.48
2:Bu:317:LYS:HE3	2:Bv:324:LEU:HD23	1.95	0.48
2:Bw:141:GLY:HA3	2:Bw:154:GLY:O	2.13	0.48
3:Cc:201:ASP:HB3	3:Cc:221:ALA:HB3	1.96	0.48
4:Dn:217:ASP:HA	4:Dn:258:ARG:HD3	1.95	0.48
4:Du:111:LYS:HD2	5:Es:197:PRO:HD3	1.95	0.48
4:Dy:111:LYS:HD2	5:Ew:197:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ea:116:ARG:HD3	5:Ea:149:GLN:HE22	1.78	0.48
5:Ek:116:ARG:HD3	5:Ek:149:GLN:HE22	1.79	0.48
5:Es:116:ARG:HD3	5:Es:149:GLN:HE22	1.78	0.48
2:Bc:272:VAL:HG22	2:Bd:260:VAL:HG22	1.95	0.48
2:Be:283:GLU:HG2	2:Be:305:GLU:HG2	1.95	0.48
2:Bh:272:VAL:HG22	2:Bi:260:VAL:HG22	1.94	0.48
2:Bq:49:GLU:HG3	2:Bq:54:THR:HG21	1.96	0.48
2:Br:318:LEU:HD11	2:Br:330:ALA:HB1	1.96	0.48
3:Cf:206:ILE:HG13	3:Cf:216:ILE:HG12	1.95	0.48
3:Cp:206:ILE:HG13	3:Cp:216:ILE:HG12	1.95	0.48
3:Cs:195:MET:HE2	3:Cs:281:LEU:HD11	1.94	0.48
3:Cy:131:LEU:HD23	3:Cy:199:ILE:HB	1.96	0.48
4:Dh:249:PHE:HB3	4:Dh:254:LEU:HD23	1.95	0.48
4:Dj:249:PHE:HB3	4:Dj:254:LEU:HD23	1.95	0.48
4:Dk:111:LYS:HD2	5:Ei:197:PRO:HD3	1.96	0.48
4:Dq:111:LYS:HD2	5:Eo:197:PRO:HD3	1.95	0.48
4:Dx:111:LYS:H	4:Dx:115:GLY:HA2	1.78	0.48
5:Ec:116:ARG:HD3	5:Ec:149:GLN:HE22	1.79	0.48
5:Em:116:ARG:HD3	5:Em:149:GLN:HE22	1.79	0.48
5:Eq:116:ARG:HD3	5:Eq:149:GLN:HE22	1.77	0.48
1:Ao:184:LEU:HD12	1:Ao:188:ASN:HB2	1.95	0.48
1:Av:206:ILE:HG12	1:Av:235:TYR:HD1	1.78	0.48
2:Be:103:VAL:HB	2:Be:137:LEU:HD21	1.95	0.48
3:Ce:292:PRO:HB3	3:Ce:306:LEU:HD13	1.95	0.48
3:Cm:206:ILE:HG13	3:Cm:216:ILE:HG12	1.96	0.48
3:Cz:220:PHE:HE2	3:Cz:273:VAL:HG11	1.78	0.48
5:Ed:154:LEU:HB3	5:Ed:164:TYR:HE1	1.78	0.48
1:Ae:184:LEU:HD12	1:Ae:188:ASN:HB2	1.96	0.48
1:Af:113:GLU:HB2	1:Af:172:MET:HB3	1.95	0.48
1:Af:206:ILE:HG12	1:Af:235:TYR:HD1	1.78	0.48
1:Ak:113:GLU:HB2	1:Ak:172:MET:HB3	1.96	0.48
1:Am:113:GLU:HB2	1:Am:172:MET:HB3	1.96	0.48
1:Ap:206:ILE:HG12	1:Ap:235:TYR:HD1	1.78	0.48
1:Au:184:LEU:HD12	1:Au:188:ASN:HB2	1.95	0.48
1:Ay:113:GLU:HB2	1:Ay:172:MET:HB3	1.96	0.48
2:Bw:49:GLU:HG3	2:Bw:54:THR:HG21	1.96	0.48
2:Bw:272:VAL:HG22	2:Bx:260:VAL:HG22	1.96	0.48
3:Co:220:PHE:HE2	3:Co:273:VAL:HG11	1.78	0.48
3:Cr:201:ASP:HB3	3:Cr:221:ALA:HB3	1.94	0.48
5:Ev:154:LEU:HB3	5:Ev:164:TYR:HE1	1.79	0.48
1:Ac:184:LEU:HD12	1:Ac:188:ASN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aq:206:ILE:HG12	1:Aq:235:TYR:HD1	1.78	0.48
1:Ar:219:PHE:HA	2:Bg:69:LEU:HD13	1.95	0.48
1:Aw:206:ILE:HG12	1:Aw:235:TYR:HD1	1.77	0.48
2:Bd:320:PRO:HB2	2:Bd:327:LEU:HD12	1.95	0.48
4:Dl:216:ILE:HA	4:Dl:291:ARG:HA	1.96	0.48
4:Dw:111:LYS:HD2	5:Eu:197:PRO:HD3	1.96	0.48
5:Ea:81:MET:HG3	5:Ea:86:VAL:HB	1.96	0.48
5:Ea:154:LEU:HB3	5:Ea:164:TYR:HE1	1.78	0.48
5:Ek:168:TYR:HB2	5:Ek:196:MET:HE1	1.95	0.48
1:Ag:184:LEU:HD12	1:Ag:188:ASN:HB2	1.95	0.48
1:Ao:206:ILE:HG12	1:Ao:235:TYR:HD1	1.78	0.48
1:As:113:GLU:HB2	1:As:172:MET:HB3	1.95	0.48
1:Aw:113:GLU:HB2	1:Aw:172:MET:HB3	1.96	0.48
2:Bk:49:GLU:HG3	2:Bk:54:THR:HG21	1.95	0.48
2:Bm:317:LYS:HE3	2:Bn:324:LEU:HD23	1.96	0.48
2:Bz:84:ILE:HG13	2:Bz:106:ILE:HD13	1.96	0.48
3:Ca:201:ASP:HB3	3:Ca:221:ALA:HB3	1.96	0.48
3:Co:27:GLU:HG3	6:Go:134:GLN:HE22	1.77	0.48
5:Ew:192:LEU:HD12	5:Ew:196:MET:HE2	1.95	0.48
1:Aa:113:GLU:HB2	1:Aa:172:MET:HB3	1.96	0.48
1:Ap:219:PHE:HA	2:Be:69:LEU:HD13	1.95	0.48
2:Bb:49:GLU:HG3	2:Bb:54:THR:HG21	1.95	0.48
2:Bm:272:VAL:HG22	2:Bn:260:VAL:HG22	1.95	0.48
2:Bo:285:LEU:HD23	2:Bo:303:ASN:HB3	1.95	0.48
2:Bv:105:SER:HB2	2:Bv:112:LEU:HD11	1.95	0.48
3:Cc:195:MET:HE2	3:Cc:281:LEU:HD11	1.96	0.48
3:Ci:292:PRO:HB3	3:Ci:306:LEU:HD13	1.94	0.48
3:Cn:195:MET:HG3	3:Cn:226:VAL:HG22	1.96	0.48
3:Cr:220:PHE:HE2	3:Cr:273:VAL:HG11	1.79	0.48
3:Cr:255:ASP:HB3	3:Cr:258:SER:HB3	1.95	0.48
1:Ab:206:ILE:HG12	1:Ab:235:TYR:HD1	1.78	0.48
1:Ak:184:LEU:HD12	1:Ak:188:ASN:HB2	1.96	0.48
1:As:66:TRP:HA	1:As:192:ARG:HD3	1.94	0.48
2:Bj:252:VAL:HG22	2:Bj:259:ILE:HG12	1.96	0.48
2:Bm:143:SER:HB2	2:Bm:157:PRO:HG3	1.95	0.48
2:Bm:248:ALA:HB1	2:Bm:265:VAL:HG22	1.96	0.48
2:Br:85:VAL:HG13	2:Br:103:VAL:HG22	1.96	0.48
2:Bw:143:SER:HB2	2:Bw:157:PRO:HG3	1.96	0.48
2:By:105:SER:HB2	2:By:112:LEU:HD11	1.95	0.48
3:Cc:220:PHE:HE2	3:Cc:273:VAL:HG11	1.78	0.48
3:Cg:201:ASP:HB3	3:Cg:221:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cp:342:ILE:HG21	3:Cp:367:ILE:HD11	1.96	0.48
3:Cq:70:LEU:HG	6:Fq:136:VAL:HG13	1.96	0.48
3:Cy:282:GLU:HA	3:Cy:286:SER:HB3	1.96	0.48
4:Dl:219:VAL:HG21	4:Dl:254:LEU:HD21	1.96	0.48
1:Aa:184:LEU:HD12	1:Aa:188:ASN:HB2	1.95	0.47
1:Ap:184:LEU:HD12	1:Ap:188:ASN:HB2	1.96	0.47
2:Ba:290:PRO:HB3	2:Ba:296:GLY:HA3	1.96	0.47
2:Bs:360:ILE:HD12	2:Bu:163:SER:H	1.79	0.47
2:Bv:141:GLY:HA3	2:Bv:154:GLY:O	2.14	0.47
2:Bw:250:ILE:HG12	2:Bw:261:VAL:HG13	1.96	0.47
3:Cw:201:ASP:HB3	3:Cw:221:ALA:HB3	1.96	0.47
3:Cy:292:PRO:HB3	3:Cy:306:LEU:HD13	1.96	0.47
3:Cz:201:ASP:HB3	3:Cz:221:ALA:HB3	1.96	0.47
5:Ew:116:ARG:HD3	5:Ew:149:GLN:HE22	1.79	0.47
5:Ex:154:LEU:HB3	5:Ex:164:TYR:HE1	1.79	0.47
1:Aq:113:GLU:HB2	1:Aq:172:MET:HB3	1.96	0.47
2:Bf:143:SER:HB2	2:Bf:157:PRO:HG3	1.95	0.47
2:Bo:105:SER:HB2	2:Bo:112:LEU:HD11	1.95	0.47
2:Bu:141:GLY:HA3	2:Bu:154:GLY:O	2.14	0.47
3:Ce:201:ASP:HB3	3:Ce:221:ALA:HB3	1.96	0.47
3:Cf:201:ASP:HB3	3:Cf:221:ALA:HB3	1.96	0.47
3:Cl:220:PHE:HE2	3:Cl:273:VAL:HG11	1.77	0.47
4:Dz:249:PHE:HB3	4:Dz:254:LEU:HD23	1.96	0.47
1:At:184:LEU:HD12	1:At:188:ASN:HB2	1.96	0.47
2:Bf:248:ALA:HB1	2:Bf:265:VAL:HG22	1.95	0.47
2:Br:105:SER:HB2	2:Br:112:LEU:HD11	1.95	0.47
2:Bx:103:VAL:HB	2:Bx:137:LEU:HD21	1.96	0.47
3:Cp:292:PRO:HB3	3:Cp:306:LEU:HD13	1.95	0.47
3:Cv:61:ILE:HD11	3:Cv:282:GLU:HG3	1.96	0.47
4:Dg:111:LYS:HD2	5:Ee:197:PRO:HD3	1.96	0.47
4:Du:93:PRO:HD3	4:Du:133:ARG:HA	1.97	0.47
5:Eu:192:LEU:HD12	5:Eu:196:MET:HE2	1.96	0.47
1:Aw:184:LEU:HD12	1:Aw:188:ASN:HB2	1.97	0.47
2:Bg:272:VAL:HG22	2:Bh:260:VAL:HG22	1.96	0.47
2:Bj:290:PRO:HB3	2:Bj:296:GLY:HA3	1.96	0.47
2:Bt:141:GLY:HA3	2:Bt:154:GLY:O	2.14	0.47
3:Co:326:PHE:HD1	3:Co:328:ASP:H	1.63	0.47
3:Cq:292:PRO:HB3	3:Cq:306:LEU:HD13	1.96	0.47
3:Cu:201:ASP:HB3	3:Cu:221:ALA:HB3	1.96	0.47
3:Cx:292:PRO:HB3	3:Cx:306:LEU:HD13	1.96	0.47
4:Dh:216:ILE:HA	4:Dh:291:ARG:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dv:64:ALA:HB2	4:Dv:172:LEU:HD22	1.95	0.47
4:Dv:216:ILE:HA	4:Dv:291:ARG:HA	1.96	0.47
1:Ai:113:GLU:HB2	1:Ai:172:MET:HB3	1.96	0.47
1:Ao:113:GLU:HB2	1:Ao:172:MET:HB3	1.97	0.47
1:Ax:184:LEU:HD12	1:Ax:188:ASN:HB2	1.97	0.47
2:Bh:84:ILE:HG13	2:Bh:106:ILE:HD13	1.96	0.47
2:Bh:105:SER:HB2	2:Bh:112:LEU:HD11	1.96	0.47
2:Bj:105:SER:HB2	2:Bj:112:LEU:HD11	1.96	0.47
3:Cb:293:GLN:HB2	3:Cb:369:ILE:HG23	1.95	0.47
3:Cd:220:PHE:HE2	3:Cd:273:VAL:HG11	1.79	0.47
3:Ck:292:PRO:HB3	3:Ck:306:LEU:HD13	1.96	0.47
4:Dh:221:VAL:HB	4:Dh:261:VAL:HG12	1.97	0.47
5:Eg:116:ARG:HD3	5:Eg:149:GLN:HE22	1.79	0.47
1:Ae:113:GLU:HB2	1:Ae:172:MET:HB3	1.96	0.47
1:Aj:184:LEU:HD12	1:Aj:188:ASN:HB2	1.97	0.47
1:Al:184:LEU:HD12	1:Al:188:ASN:HB2	1.96	0.47
2:Bc:360:ILE:HD12	2:Be:163:SER:H	1.80	0.47
2:Bn:141:GLY:HA3	2:Bn:154:GLY:O	2.15	0.47
2:Bu:248:ALA:HB1	2:Bu:265:VAL:HG22	1.97	0.47
3:Ca:255:ASP:HB3	3:Ca:258:SER:HB3	1.97	0.47
3:Cn:342:ILE:HG21	3:Cn:367:ILE:HD11	1.97	0.47
3:Ct:292:PRO:HB3	3:Ct:306:LEU:HD13	1.95	0.47
4:Dx:219:VAL:HG21	4:Dx:254:LEU:HD21	1.95	0.47
5:Ee:176:THR:HG22	5:Ee:185:ILE:HD12	1.96	0.47
5:Ei:116:ARG:HD3	5:Ei:149:GLN:HE22	1.79	0.47
1:An:184:LEU:HD12	1:An:188:ASN:HB2	1.96	0.47
1:Aq:184:LEU:HD12	1:Aq:188:ASN:HB2	1.97	0.47
1:Az:184:LEU:HD12	1:Az:188:ASN:HB2	1.96	0.47
2:Ba:248:ALA:HB1	2:Ba:265:VAL:HG22	1.97	0.47
2:Bc:21:ILE:HG23	2:Bc:197:LEU:HD11	1.97	0.47
2:Bl:248:ALA:HB1	2:Bl:265:VAL:HG22	1.96	0.47
2:Bm:252:VAL:HG22	2:Bm:259:ILE:HG12	1.97	0.47
3:Cb:282:GLU:HA	3:Cb:286:SER:HB3	1.95	0.47
3:Cj:220:PHE:HE2	3:Cj:273:VAL:HG11	1.79	0.47
3:Cn:206:ILE:HG13	3:Cn:216:ILE:HG12	1.96	0.47
3:Ct:365:TYR:HE2	4:Dm:94:VAL:HG22	1.79	0.47
3:Cw:206:ILE:HG13	3:Cw:216:ILE:HG12	1.97	0.47
3:Cw:292:PRO:HB3	3:Cw:306:LEU:HD13	1.95	0.47
3:Cx:201:ASP:HB3	3:Cx:221:ALA:HB3	1.97	0.47
4:De:111:LYS:HD2	5:Ec:197:PRO:HD3	1.95	0.47
4:Dp:223:THR:HG22	4:Dp:285:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dr:223:THR:HG22	4:Dr:285:VAL:HG22	1.97	0.47
4:Dv:223:THR:HG22	4:Dv:285:VAL:HG22	1.97	0.47
5:Ee:192:LEU:HD12	5:Ee:196:MET:HE2	1.96	0.47
5:Eg:176:THR:HG22	5:Eg:185:ILE:HD12	1.97	0.47
1:Ah:219:PHE:HA	2:Bw:69:LEU:HD13	1.97	0.47
1:Ar:184:LEU:HD12	1:Ar:188:ASN:HB2	1.97	0.47
2:Bg:143:SER:HB2	2:Bg:157:PRO:HG3	1.96	0.47
2:Bj:49:GLU:HG3	2:Bj:54:THR:HG21	1.96	0.47
3:Ce:78:TYR:HD2	3:Ce:88:ILE:HB	1.80	0.47
3:Cl:201:ASP:HB3	3:Cl:221:ALA:HB3	1.97	0.47
3:Cp:93:ARG:HG2	3:Cp:102:VAL:HG23	1.97	0.47
4:Dd:64:ALA:HB2	4:Dd:172:LEU:HD22	1.95	0.47
4:Dd:221:VAL:HB	4:Dd:261:VAL:HG12	1.97	0.47
4:Dz:24:GLU:HG3	4:Dz:148:ARG:HH22	1.80	0.47
5:Ec:176:THR:HG22	5:Ec:185:ILE:HD12	1.97	0.47
5:Ey:176:THR:HG22	5:Ey:185:ILE:HD12	1.97	0.47
2:Bg:105:SER:HB2	2:Bg:112:LEU:HD11	1.96	0.47
2:Bk:360:ILE:HD12	2:Bm:163:SER:H	1.80	0.47
2:Bs:84:ILE:HG13	2:Bs:106:ILE:HD13	1.97	0.47
3:Ci:201:ASP:HB3	3:Ci:221:ALA:HB3	1.97	0.47
3:Cv:220:PHE:HE2	3:Cv:273:VAL:HG11	1.80	0.47
4:Dk:78:ARG:HB3	4:Dk:143:GLN:HE22	1.80	0.47
4:Dr:64:ALA:HB2	4:Dr:172:LEU:HD22	1.97	0.47
1:Af:184:LEU:HD12	1:Af:188:ASN:HB2	1.97	0.47
2:Bc:105:SER:HB2	2:Bc:112:LEU:HD11	1.96	0.47
2:Bh:49:GLU:HG3	2:Bh:54:THR:HG21	1.96	0.47
2:Bx:324:LEU:HD12	2:Bx:327:LEU:HD23	1.97	0.47
3:Cc:373:MET:HE3	3:Cc:373:MET:HB2	1.85	0.47
3:Cm:255:ASP:HB3	3:Cm:258:SER:HB3	1.96	0.47
3:Cy:201:ASP:HB3	3:Cy:221:ALA:HB3	1.97	0.47
4:Di:111:LYS:HD2	5:Eg:197:PRO:HD3	1.97	0.47
4:Di:184:ILE:HG12	4:Di:286:VAL:HG22	1.96	0.47
4:Dn:64:ALA:HB2	4:Dn:172:LEU:HD22	1.96	0.47
4:Dn:249:PHE:HB3	4:Dn:254:LEU:HD23	1.97	0.47
4:Dx:249:PHE:HB3	4:Dx:254:LEU:HD23	1.97	0.47
5:Ey:116:ARG:HD3	5:Ey:149:GLN:HE22	1.79	0.47
2:Bb:84:ILE:HG13	2:Bb:106:ILE:HD13	1.97	0.46
2:Bl:105:SER:HB2	2:Bl:112:LEU:HD11	1.97	0.46
2:Bl:275:GLY:HA3	2:Bm:338:PRO:HG2	1.96	0.46
2:Bp:105:SER:HB2	2:Bp:112:LEU:HD11	1.96	0.46
2:Bw:105:SER:HB2	2:Bw:112:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cv:292:PRO:HB3	3:Cv:306:LEU:HD13	1.96	0.46
4:Dj:223:THR:HG22	4:Dj:285:VAL:HG22	1.97	0.46
4:Dm:111:LYS:HD2	5:Ek:197:PRO:HD3	1.97	0.46
5:Ee:116:ARG:HD3	5:Ee:149:GLN:HE22	1.80	0.46
5:Ek:192:LEU:HD12	5:Ek:196:MET:HE2	1.96	0.46
1:Am:184:LEU:HD12	1:Am:188:ASN:HB2	1.96	0.46
1:Av:184:LEU:HD12	1:Av:188:ASN:HB2	1.97	0.46
2:Bn:105:SER:HB2	2:Bn:112:LEU:HD11	1.97	0.46
3:Cg:206:ILE:HG13	3:Cg:216:ILE:HG12	1.96	0.46
3:Cn:239:THR:HG21	3:Co:155:ARG:HD3	1.97	0.46
3:Cu:255:ASP:HB3	3:Cu:258:SER:HB3	1.97	0.46
4:Dc:184:ILE:HG12	4:Dc:286:VAL:HG22	1.97	0.46
4:Dl:221:VAL:HB	4:Dl:261:VAL:HG12	1.98	0.46
4:Ds:184:ILE:HG12	4:Ds:286:VAL:HG22	1.97	0.46
4:Dt:249:PHE:HB3	4:Dt:254:LEU:HD23	1.98	0.46
4:Dx:64:ALA:HB2	4:Dx:172:LEU:HD22	1.97	0.46
5:Eo:116:ARG:HD3	5:Eo:149:GLN:HE22	1.79	0.46
5:Ew:176:THR:HG22	5:Ew:185:ILE:HD12	1.97	0.46
2:Bx:105:SER:HB2	2:Bx:112:LEU:HD11	1.96	0.46
3:Cp:195:MET:HE2	3:Cp:281:LEU:HD11	1.97	0.46
4:Dp:64:ALA:HB2	4:Dp:172:LEU:HD22	1.96	0.46
4:Dt:223:THR:HG22	4:Dt:285:VAL:HG22	1.97	0.46
4:Dx:216:ILE:HA	4:Dx:291:ARG:HA	1.97	0.46
1:As:184:LEU:HD12	1:As:188:ASN:HB2	1.97	0.46
2:Bg:274:HIS:HE1	2:Bg:343:ALA:HB3	1.80	0.46
3:Cd:201:ASP:HB3	3:Cd:221:ALA:HB3	1.98	0.46
3:Cf:292:PRO:HB3	3:Cf:306:LEU:HD13	1.96	0.46
3:Cm:292:PRO:HB3	3:Cm:306:LEU:HD13	1.98	0.46
3:Cn:326:PHE:HD1	3:Cn:328:ASP:H	1.64	0.46
3:Co:78:TYR:HD2	3:Co:88:ILE:HB	1.81	0.46
3:Cq:201:ASP:HB3	3:Cq:221:ALA:HB3	1.96	0.46
3:Cx:358:VAL:HG12	3:Cx:360:GLN:H	1.80	0.46
3:Cy:126:ILE:HB	3:Cy:169:THR:HG22	1.96	0.46
4:Dl:249:PHE:HB3	4:Dl:254:LEU:HD23	1.97	0.46
4:Dt:221:VAL:HB	4:Dt:261:VAL:HG12	1.96	0.46
5:Ec:192:LEU:HD12	5:Ec:196:MET:HE2	1.97	0.46
5:Ed:189:ARG:HH21	5:Ed:205:LYS:HZ1	1.64	0.46
5:Eg:168:TYR:HB2	5:Eg:196:MET:HE1	1.96	0.46
5:Eq:176:THR:HG22	5:Eq:185:ILE:HD12	1.97	0.46
5:Eu:116:ARG:HD3	5:Eu:149:GLN:HE22	1.80	0.46
5:Eu:176:THR:HG22	5:Eu:185:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bc:49:GLU:HG3	2:Bc:54:THR:HG21	1.97	0.46
2:Be:105:SER:HB2	2:Be:112:LEU:HD11	1.97	0.46
2:Bk:21:ILE:HG23	2:Bk:197:LEU:HD11	1.98	0.46
2:Bu:252:VAL:HG22	2:Bu:259:ILE:HG12	1.96	0.46
2:Bw:248:ALA:HB1	2:Bw:265:VAL:HG22	1.97	0.46
3:Ck:195:MET:HE2	3:Ck:281:LEU:HD11	1.97	0.46
3:Cm:78:TYR:HD2	3:Cm:88:ILE:HB	1.80	0.46
3:Cn:365:TYR:HE2	4:Dg:94:VAL:HG22	1.80	0.46
3:Cz:292:PRO:HB3	3:Cz:306:LEU:HD13	1.97	0.46
4:Db:221:VAL:HB	4:Db:261:VAL:HG12	1.97	0.46
4:Dt:64:ALA:HB2	4:Dt:172:LEU:HD22	1.97	0.46
4:Dv:104:ILE:HA	4:Dw:145:ARG:HD3	1.98	0.46
5:Ea:41:LEU:HA	5:Ea:44:GLU:HG2	1.98	0.46
5:Er:189:ARG:HH21	5:Er:205:LYS:HZ1	1.63	0.46
2:Ba:141:GLY:HA3	2:Ba:154:GLY:O	2.14	0.46
2:Bl:84:ILE:HG13	2:Bl:106:ILE:HD13	1.97	0.46
2:Bm:84:ILE:HG13	2:Bm:106:ILE:HD13	1.97	0.46
2:Bp:143:SER:HB2	2:Bp:157:PRO:HG3	1.97	0.46
2:By:274:HIS:HE1	2:By:343:ALA:HB3	1.81	0.46
3:Cg:61:ILE:HD11	3:Cg:282:GLU:HG3	1.97	0.46
3:Ch:220:PHE:HE2	3:Ch:273:VAL:HG11	1.80	0.46
3:Ck:43:LEU:HD21	3:Ck:68:MET:HE1	1.97	0.46
3:Ck:271:LEU:HD11	6:Gk:145:PHE:HE2	1.81	0.46
3:Cq:63:SER:HA	3:Cq:66:ASN:HD21	1.81	0.46
3:Cq:209:LYS:HD2	3:Cq:212:GLN:HB2	1.98	0.46
3:Cu:206:ILE:HG13	3:Cu:216:ILE:HG12	1.96	0.46
3:Cz:342:ILE:HG21	3:Cz:367:ILE:HD11	1.96	0.46
4:Dh:169:ILE:HG13	4:Dh:172:LEU:HD12	1.98	0.46
4:Di:116:TYR:HE2	5:El:198:GLU:HB3	1.80	0.46
5:Ei:81:MET:HG3	5:Ei:86:VAL:HB	1.98	0.46
1:Ai:184:LEU:HD12	1:Ai:188:ASN:HB2	1.97	0.46
2:Bd:252:VAL:HG22	2:Bd:259:ILE:HG12	1.98	0.46
2:Bj:320:PRO:HB2	2:Bj:327:LEU:HD12	1.98	0.46
3:Ch:342:ILE:HG21	3:Ch:367:ILE:HD11	1.97	0.46
3:Cu:373:MET:HE3	3:Cu:373:MET:HB2	1.85	0.46
4:Dd:223:THR:HG22	4:Dd:285:VAL:HG22	1.97	0.46
4:Df:64:ALA:HB2	4:Df:172:LEU:HD22	1.97	0.46
4:Dw:184:ILE:HG12	4:Dw:286:VAL:HG22	1.96	0.46
4:Dx:223:THR:HG22	4:Dx:285:VAL:HG22	1.97	0.46
4:Dz:221:VAL:HB	4:Dz:261:VAL:HG12	1.97	0.46
5:Ek:176:THR:HG22	5:Ek:185:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bg:224:ARG:HH22	3:Cj:323:THR:HB	1.80	0.46
2:Bn:272:VAL:HG22	2:Bo:260:VAL:HG22	1.97	0.46
2:Bq:84:ILE:HG13	2:Bq:106:ILE:HD13	1.97	0.46
2:Bz:49:GLU:HG3	2:Bz:54:THR:HG21	1.97	0.46
3:Cc:93:ARG:HG2	3:Cc:102:VAL:HG23	1.97	0.46
3:Ch:201:ASP:HB3	3:Ch:221:ALA:HB3	1.98	0.46
3:Cj:255:ASP:HB3	3:Cj:258:SER:HB3	1.98	0.46
3:Cn:201:ASP:HB3	3:Cn:221:ALA:HB3	1.96	0.46
3:Co:80:PHE:HA	6:Fo:136:VAL:HG21	1.97	0.46
4:De:78:ARG:HB3	4:De:143:GLN:HE22	1.81	0.46
4:Dn:221:VAL:HB	4:Dn:261:VAL:HG12	1.98	0.46
4:Dp:249:PHE:HB3	4:Dp:254:LEU:HD23	1.98	0.46
4:Dz:116:TYR:HE2	5:Ez:198:GLU:HB3	1.80	0.46
5:Ea:176:THR:HG22	5:Ea:185:ILE:HD12	1.97	0.46
5:Eg:192:LEU:HD12	5:Eg:196:MET:HE2	1.97	0.46
5:Ei:176:THR:HG22	5:Ei:185:ILE:HD12	1.97	0.46
2:Bc:103:VAL:HB	2:Bc:137:LEU:HD21	1.97	0.46
2:Be:224:ARG:HH22	3:Ch:323:THR:HB	1.80	0.46
2:Bl:137:LEU:HA	2:Bl:162:ILE:HG12	1.98	0.46
2:Bt:248:ALA:HB1	2:Bt:265:VAL:HG22	1.98	0.46
2:Bw:290:PRO:HB3	2:Bw:296:GLY:HA3	1.98	0.46
2:Bx:250:ILE:HG12	2:Bx:261:VAL:HG13	1.98	0.46
2:Bx:275:GLY:HA3	2:By:338:PRO:HG2	1.97	0.46
3:Cb:93:ARG:HG2	3:Cb:102:VAL:HG23	1.97	0.46
3:Cv:26:TYR:HA	6:Gv:134:GLN:HA	1.98	0.46
3:Cw:271:LEU:HD11	6:Gw:145:PHE:HD2	1.81	0.46
4:Db:64:ALA:HB2	4:Db:172:LEU:HD22	1.97	0.46
4:Db:116:TYR:HE2	5:Eb:198:GLU:HB3	1.81	0.46
4:Df:221:VAL:HB	4:Df:261:VAL:HG12	1.98	0.46
4:Dj:24:GLU:HG3	4:Dj:148:ARG:HH22	1.81	0.46
4:Du:184:ILE:HG12	4:Du:286:VAL:HG22	1.97	0.46
4:Dw:78:ARG:HB3	4:Dw:143:GLN:HE22	1.80	0.46
5:Ee:41:LEU:HA	5:Ee:44:GLU:HG2	1.98	0.46
1:Ad:184:LEU:HD12	1:Ad:188:ASN:HB2	1.98	0.46
2:Ba:143:SER:HB2	2:Ba:157:PRO:HG3	1.98	0.46
2:Bf:105:SER:HB2	2:Bf:112:LEU:HD11	1.97	0.46
2:Bk:141:GLY:HA3	2:Bk:154:GLY:O	2.16	0.46
2:Bq:248:ALA:HB1	2:Bq:265:VAL:HG22	1.97	0.46
2:Br:84:ILE:HG13	2:Br:106:ILE:HD13	1.98	0.46
2:Br:85:VAL:HG22	2:Br:103:VAL:HG13	1.98	0.46
2:Bs:103:VAL:HB	2:Bs:137:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bt:118:MET:HE3	2:Bt:118:MET:HB3	1.84	0.46
3:Cj:342:ILE:HG21	3:Cj:367:ILE:HD11	1.97	0.46
3:Cr:292:PRO:HB3	3:Cr:306:LEU:HD13	1.98	0.46
5:Ef:154:LEU:HB3	5:Ef:164:TYR:HE1	1.80	0.46
5:Eg:81:MET:HG3	5:Eg:86:VAL:HB	1.98	0.46
2:Bi:105:SER:HB2	2:Bi:112:LEU:HD11	1.97	0.45
2:Bj:248:ALA:HB1	2:Bj:265:VAL:HG22	1.97	0.45
2:Bx:248:ALA:HB1	2:Bx:265:VAL:HG22	1.96	0.45
3:Cg:34:ILE:HD11	3:Cg:100:MET:HB2	1.98	0.45
3:Ci:206:ILE:HG13	3:Ci:216:ILE:HG12	1.98	0.45
3:Cu:195:MET:HE2	3:Cu:281:LEU:HD11	1.98	0.45
1:Ab:184:LEU:HD12	1:Ab:188:ASN:HB2	1.97	0.45
2:Bh:320:PRO:HB2	2:Bh:327:LEU:HD12	1.99	0.45
2:Bx:84:ILE:HG13	2:Bx:106:ILE:HD13	1.98	0.45
3:Ci:220:PHE:HE2	3:Ci:273:VAL:HG11	1.80	0.45
3:Ct:342:ILE:HG21	3:Ct:367:ILE:HD11	1.98	0.45
3:Cz:365:TYR:HE2	4:Ds:94:VAL:HG22	1.80	0.45
4:Df:104:ILE:HA	4:Dg:145:ARG:HD3	1.99	0.45
4:Dn:216:ILE:HA	4:Dn:291:ARG:HA	1.97	0.45
4:Dn:223:THR:HG22	4:Dn:285:VAL:HG22	1.98	0.45
4:Dr:37:GLN:HG3	4:Dr:49:VAL:HG23	1.98	0.45
4:Dx:221:VAL:HB	4:Dx:261:VAL:HG12	1.97	0.45
4:Dz:117:ILE:HD12	4:Dz:117:ILE:HA	1.86	0.45
5:Es:176:THR:HG22	5:Es:185:ILE:HD12	1.97	0.45
1:Ap:200:ASN:HB3	1:Ap:201:THR:H	1.64	0.45
2:Bb:163:SER:H	2:Bz:360:ILE:HD12	1.81	0.45
2:Bk:145:THR:HB	2:Bk:151:LYS:HG3	1.99	0.45
3:Ci:195:MET:HE2	3:Ci:281:LEU:HD11	1.98	0.45
4:Dc:78:ARG:HB3	4:Dc:143:GLN:HE22	1.82	0.45
4:Dd:249:PHE:HB3	4:Dd:254:LEU:HD23	1.98	0.45
4:Dj:116:TYR:HE2	5:Ej:198:GLU:HB3	1.80	0.45
4:Dm:93:PRO:HB2	4:Dm:95:TRP:HE3	1.82	0.45
4:Dp:221:VAL:HB	4:Dp:261:VAL:HG12	1.98	0.45
1:Ac:51:ASP:HA	1:Ac:54:ARG:HE	1.82	0.45
2:Bb:105:SER:HB2	2:Bb:112:LEU:HD11	1.97	0.45
2:Bh:141:GLY:HA3	2:Bh:154:GLY:O	2.16	0.45
2:Bk:105:SER:HB2	2:Bk:112:LEU:HD11	1.97	0.45
2:Bo:224:ARG:HH22	3:Cr:323:THR:HB	1.81	0.45
2:Bw:259:ILE:HD11	2:Bw:342:MET:HG3	1.98	0.45
3:Ca:195:MET:HE2	3:Ca:281:LEU:HD11	1.98	0.45
3:Cl:195:MET:HE2	3:Cl:281:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cx:220:PHE:HE2	3:Cx:273:VAL:HG11	1.80	0.45
4:Dz:223:THR:HG22	4:Dz:285:VAL:HG22	1.97	0.45
5:Ei:192:LEU:HD12	5:Ei:196:MET:HE2	1.97	0.45
5:En:154:LEU:HB3	5:En:164:TYR:HE1	1.82	0.45
5:Eo:81:MET:HG3	5:Eo:86:VAL:HB	1.99	0.45
5:Ew:41:LEU:HA	5:Ew:44:GLU:HG2	1.98	0.45
1:Ah:184:LEU:HD12	1:Ah:188:ASN:HB2	1.97	0.45
2:Bd:105:SER:HB2	2:Bd:112:LEU:HD11	1.98	0.45
2:Bi:137:LEU:HA	2:Bi:162:ILE:HG12	1.99	0.45
2:Bm:105:SER:HB2	2:Bm:112:LEU:HD11	1.97	0.45
2:Bt:85:VAL:HG22	2:Bt:103:VAL:HG13	1.99	0.45
3:Cc:292:PRO:HB3	3:Cc:306:LEU:HD13	1.98	0.45
3:Cd:239:THR:HG21	3:Ce:155:ARG:HD3	1.99	0.45
3:Co:34:ILE:HD11	3:Co:100:MET:HB2	1.99	0.45
3:Co:292:PRO:HB3	3:Co:306:LEU:HD13	1.97	0.45
3:Cz:282:GLU:HA	3:Cz:286:SER:HB3	1.98	0.45
4:Dh:116:TYR:HE2	5:Eh:198:GLU:HB3	1.80	0.45
4:Dx:104:ILE:HA	4:Dy:145:ARG:HD3	1.99	0.45
5:Ec:41:LEU:HA	5:Ec:44:GLU:HG2	1.98	0.45
2:Bs:303:ASN:H	2:Bt:285:LEU:HD12	1.81	0.45
3:Ch:255:ASP:HB3	3:Ch:258:SER:HB3	1.99	0.45
3:Cl:294:ILE:HG22	3:Cl:369:ILE:HG22	1.98	0.45
3:Cu:93:ARG:HG2	3:Cu:102:VAL:HG22	1.99	0.45
4:Db:184:ILE:HG12	4:Db:286:VAL:HG22	1.98	0.45
4:Dg:184:ILE:HG12	4:Dg:286:VAL:HG22	1.98	0.45
4:Dn:104:ILE:HA	4:Do:145:ARG:HD3	1.99	0.45
4:Dr:249:PHE:HB3	4:Dr:254:LEU:HD23	1.99	0.45
5:Ek:41:LEU:HA	5:Ek:44:GLU:HG2	1.97	0.45
1:Ay:51:ASP:HA	1:Ay:54:ARG:HE	1.81	0.45
1:Az:129:ASN:HB2	1:Az:156:ASN:HB3	1.99	0.45
2:Bv:360:ILE:HD12	2:Bx:163:SER:H	1.80	0.45
2:By:248:ALA:HB1	2:By:265:VAL:HG22	1.99	0.45
3:Ca:206:ILE:HG13	3:Ca:216:ILE:HG12	1.99	0.45
3:Cf:56:PHE:HD1	6:Gf:139:LYS:HE2	1.81	0.45
3:Cf:93:ARG:HG2	3:Cf:102:VAL:HG22	1.99	0.45
3:Cf:365:TYR:HE2	4:Dy:94:VAL:HG22	1.82	0.45
3:Cq:206:ILE:HG13	3:Cq:216:ILE:HG12	1.99	0.45
3:Cr:78:TYR:HD2	3:Cr:88:ILE:HB	1.81	0.45
3:Cz:206:ILE:HG13	3:Cz:216:ILE:HG12	1.97	0.45
4:Dp:104:ILE:HA	4:Dq:145:ARG:HD3	1.99	0.45
5:Em:41:LEU:HA	5:Em:44:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Eo:176:THR:HG22	5:Eo:185:ILE:HD12	1.97	0.45
1:Ar:200:ASN:HB3	1:Ar:201:THR:H	1.64	0.45
2:Bg:248:ALA:HB1	2:Bg:265:VAL:HG22	1.98	0.45
2:Bo:85:VAL:HG22	2:Bo:103:VAL:HG13	1.99	0.45
2:Bt:105:SER:HB2	2:Bt:112:LEU:HD11	1.98	0.45
3:Cb:90:ILE:HG13	3:Cb:104:THR:HB	1.99	0.45
3:Cj:365:TYR:HE2	4:Dc:94:VAL:HG22	1.80	0.45
4:Dn:219:VAL:HG21	4:Dn:254:LEU:HD21	1.98	0.45
4:Dr:221:VAL:HB	4:Dr:261:VAL:HG12	1.97	0.45
4:Dy:78:ARG:HB3	4:Dy:143:GLN:HE22	1.81	0.45
1:Ae:51:ASP:HA	1:Ae:54:ARG:HE	1.82	0.45
1:Af:200:ASN:HB3	1:Af:201:THR:H	1.63	0.45
1:Aj:129:ASN:HB2	1:Aj:156:ASN:HB3	1.99	0.45
1:Ay:200:ASN:HB3	1:Ay:201:THR:H	1.63	0.45
2:Bh:248:ALA:HB1	2:Bh:265:VAL:HG22	1.97	0.45
2:Bl:85:VAL:HG22	2:Bl:103:VAL:HG13	1.99	0.45
2:Bs:27:VAL:HG21	2:Bs:233:LEU:HD21	1.99	0.45
2:Bs:317:LYS:HB2	2:Bt:328:VAL:HG21	1.99	0.45
2:Bu:105:SER:HB2	2:Bu:112:LEU:HD11	1.99	0.45
2:Bv:141:GLY:CA	2:Bv:154:GLY:O	2.65	0.45
2:Bx:141:GLY:HA3	2:Bx:154:GLY:O	2.17	0.45
2:By:320:PRO:HB2	2:By:327:LEU:HD12	1.98	0.45
3:Ce:209:LYS:HD2	3:Ce:212:GLN:HB2	1.99	0.45
5:Ea:32:ILE:HD13	5:Ea:65:ARG:HH22	1.82	0.45
5:Ee:81:MET:HG3	5:Ee:86:VAL:HB	1.99	0.45
5:Eo:41:LEU:HA	5:Eo:44:GLU:HG2	1.98	0.45
1:Aa:51:ASP:HA	1:Aa:54:ARG:HE	1.82	0.45
1:An:200:ASN:HB3	1:An:201:THR:H	1.64	0.45
1:Ax:129:ASN:HB2	1:Ax:156:ASN:HB3	1.99	0.45
2:Bb:259:ILE:HD11	2:Bb:342:MET:HG3	1.99	0.45
2:Bi:83:VAL:HG12	2:Bi:105:SER:HA	1.99	0.45
2:Bj:274:HIS:HE1	2:Bj:343:ALA:HB3	1.82	0.45
2:Bk:269:PRO:HB2	2:Bl:263:GLN:HE21	1.82	0.45
2:Bs:105:SER:HB2	2:Bs:112:LEU:HD11	1.98	0.45
2:Bu:118:MET:HE2	2:Bu:118:MET:HB3	1.80	0.45
3:Ce:206:ILE:HG13	3:Ce:216:ILE:HG12	1.99	0.45
3:Cg:292:PRO:HB3	3:Cg:306:LEU:HD13	1.97	0.45
3:Ct:201:ASP:HB3	3:Ct:221:ALA:HB3	1.99	0.45
3:Cu:292:PRO:HB3	3:Cu:306:LEU:HD13	1.97	0.45
3:Cv:365:TYR:HE2	4:Do:94:VAL:HG22	1.81	0.45
4:Dz:216:ILE:HA	4:Dz:291:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Et:41:LEU:HA	5:Et:44:GLU:HG2	1.98	0.45
1:Ah:129:ASN:HB2	1:Ah:156:ASN:HB3	1.99	0.44
1:Al:129:ASN:HB2	1:Al:156:ASN:HB3	1.99	0.44
1:Ao:200:ASN:HB3	1:Ao:201:THR:H	1.64	0.44
1:At:200:ASN:HB3	1:At:201:THR:H	1.64	0.44
2:Ba:259:ILE:HD11	2:Ba:342:MET:HG3	2.00	0.44
2:Bc:274:HIS:HE1	2:Bc:343:ALA:HB3	1.81	0.44
2:Bd:143:SER:HB2	2:Bd:157:PRO:HG3	1.98	0.44
2:Bh:285:LEU:HD23	2:Bh:303:ASN:HB3	1.99	0.44
2:Bp:27:VAL:HG21	2:Bp:233:LEU:HD21	1.99	0.44
2:Bv:49:GLU:HG3	2:Bv:54:THR:HG21	1.99	0.44
3:Ch:365:TYR:HE2	4:Da:94:VAL:HG22	1.82	0.44
3:Cj:94:LYS:HG3	3:Cj:101:TYR:HB2	1.99	0.44
3:Cn:255:ASP:HB3	3:Cn:258:SER:HB3	1.99	0.44
3:Co:201:ASP:HB3	3:Co:221:ALA:HB3	1.98	0.44
3:Cv:70:LEU:HD22	6:Fv:136:VAL:HG13	1.99	0.44
3:Cy:61:ILE:HD11	3:Cy:282:GLU:HG3	1.99	0.44
4:Db:249:PHE:HB3	4:Db:254:LEU:HD23	1.99	0.44
4:Dy:93:PRO:HB2	4:Dy:95:TRP:HE3	1.82	0.44
1:Ab:51:ASP:HA	1:Ab:54:ARG:HE	1.83	0.44
1:Av:129:ASN:HB2	1:Av:156:ASN:HB3	1.99	0.44
2:Bw:274:HIS:HE1	2:Bw:343:ALA:HB3	1.81	0.44
3:Cf:63:SER:HA	3:Cf:66:ASN:HD21	1.81	0.44
3:Ct:206:ILE:HG13	3:Ct:216:ILE:HG12	1.99	0.44
3:Cv:255:ASP:HB3	3:Cv:258:SER:HB3	1.99	0.44
4:Dg:78:ARG:HB3	4:Dg:143:GLN:HE22	1.81	0.44
4:Dv:249:PHE:HB3	4:Dv:254:LEU:HD23	1.99	0.44
5:Et:154:LEU:HB3	5:Et:164:TYR:HE1	1.80	0.44
1:Aq:200:ASN:HB3	1:Aq:201:THR:H	1.64	0.44
1:Av:219:PHE:HD1	2:Bk:69:LEU:HD13	1.82	0.44
1:Ax:200:ASN:HB3	1:Ax:201:THR:H	1.64	0.44
2:Ba:105:SER:HB2	2:Ba:112:LEU:HD11	1.98	0.44
2:Bn:283:GLU:HG2	2:Bn:305:GLU:HB3	1.99	0.44
2:Bo:143:SER:HB2	2:Bo:157:PRO:HG3	1.99	0.44
2:Bp:360:ILE:HD12	2:Br:163:SER:H	1.82	0.44
2:Bt:85:VAL:HG13	2:Bt:103:VAL:HG22	2.00	0.44
3:Cd:326:PHE:HD1	3:Cd:328:ASP:H	1.65	0.44
3:Cm:80:PHE:HA	6:Fm:136:VAL:HG21	1.99	0.44
3:Cn:153:ILE:HG21	3:Cn:195:MET:HE1	1.99	0.44
3:Cr:350:TYR:HE2	3:Cr:355:GLU:HG3	1.82	0.44
4:Da:78:ARG:HB3	4:Da:143:GLN:HE22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dl:169:ILE:HG13	4:Dl:172:LEU:HD12	1.99	0.44
4:Dq:184:ILE:HG12	4:Dq:286:VAL:HG22	1.99	0.44
5:Ey:41:LEU:HA	5:Ey:44:GLU:HG2	1.98	0.44
1:Az:51:ASP:HA	1:Az:54:ARG:HE	1.83	0.44
2:Ba:34:GLN:HG2	2:Bb:134:GLN:HB3	1.99	0.44
2:Bd:84:ILE:HG13	2:Bd:106:ILE:HD13	1.99	0.44
2:Bm:250:ILE:HG12	2:Bm:261:VAL:HG13	1.98	0.44
2:Bo:248:ALA:HB1	2:Bo:265:VAL:HG22	1.98	0.44
2:Bz:27:VAL:HG21	2:Bz:233:LEU:HD21	1.99	0.44
3:Cg:195:MET:HE2	3:Cg:281:LEU:HD11	1.98	0.44
3:Cs:160:GLU:HG3	6:Gs:144:LEU:HD11	1.98	0.44
4:Dd:104:ILE:HA	4:De:145:ARG:HD3	1.99	0.44
4:Do:184:ILE:HG12	4:Do:286:VAL:HG22	1.99	0.44
4:Dy:184:ILE:HG12	4:Dy:286:VAL:HG22	1.99	0.44
5:Em:176:THR:HG22	5:Em:185:ILE:HD12	1.98	0.44
5:Es:41:LEU:HA	5:Es:44:GLU:HG2	1.98	0.44
2:Bj:27:VAL:HG21	2:Bj:233:LEU:HD21	2.00	0.44
2:Bx:277:MET:HE2	2:Bx:311:LYS:HD2	1.99	0.44
3:Cf:195:MET:HE2	3:Cf:281:LEU:HD11	1.99	0.44
3:Ck:93:ARG:HG2	3:Ck:102:VAL:HG22	1.98	0.44
3:Ck:226:VAL:HB	3:Ck:236:MET:HB3	2.00	0.44
4:Dc:93:PRO:HD3	4:Dc:133:ARG:HA	1.99	0.44
4:Dq:104:ILE:HG23	4:Dr:145:ARG:HD3	1.98	0.44
4:Dr:104:ILE:HA	4:Ds:145:ARG:HD3	1.99	0.44
4:Dv:221:VAL:HB	4:Dv:261:VAL:HG12	1.98	0.44
5:Eg:41:LEU:HA	5:Eg:44:GLU:HG2	1.98	0.44
1:Ad:129:ASN:HB2	1:Ad:156:ASN:HB3	1.99	0.44
1:Au:200:ASN:HB3	1:Au:201:THR:H	1.64	0.44
2:Bb:141:GLY:HA3	2:Bb:154:GLY:O	2.17	0.44
2:Bc:84:ILE:HG13	2:Bc:106:ILE:HD13	1.99	0.44
2:Bh:250:ILE:HG12	2:Bh:261:VAL:HG13	2.00	0.44
2:Bi:248:ALA:HB1	2:Bi:265:VAL:HG22	1.98	0.44
2:Bo:85:VAL:HG13	2:Bo:103:VAL:HG22	2.00	0.44
2:Bo:267:LEU:HB2	2:Bo:320:PRO:HG2	1.99	0.44
2:Bq:105:SER:HB2	2:Bq:112:LEU:HD11	1.99	0.44
2:Bt:27:VAL:HG21	2:Bt:233:LEU:HD21	2.00	0.44
2:Bu:267:LEU:HB2	2:Bu:320:PRO:HG2	1.99	0.44
3:Cy:255:ASP:HB3	3:Cy:258:SER:HB3	1.99	0.44
4:Dh:104:ILE:HA	4:Di:145:ARG:HD3	2.00	0.44
4:Do:93:PRO:HB2	4:Do:95:TRP:HE3	1.83	0.44
4:Dx:24:GLU:HG3	4:Dx:148:ARG:HH22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Eq:41:LEU:HA	5:Eq:44:GLU:HG2	1.98	0.44
1:Ab:129:ASN:HB2	1:Ab:156:ASN:HB3	2.00	0.44
2:Bj:84:ILE:HG13	2:Bj:106:ILE:HD13	1.99	0.44
2:Bw:320:PRO:HB2	2:Bw:327:LEU:HD12	1.99	0.44
2:Bz:137:LEU:HA	2:Bz:162:ILE:HG12	1.99	0.44
3:Cq:373:MET:HE3	3:Cq:373:MET:HB2	1.92	0.44
3:Ct:255:ASP:HB3	3:Ct:258:SER:HB3	1.99	0.44
3:Cv:337:VAL:HG22	3:Cv:350:TYR:HE1	1.83	0.44
3:Cw:255:ASP:HB3	3:Cw:258:SER:HB3	1.99	0.44
3:Cz:328:ASP:HB3	3:Cz:329:GLN:H	1.66	0.44
4:Df:249:PHE:HB3	4:Df:254:LEU:HD23	1.99	0.44
4:Dt:104:ILE:HA	4:Du:145:ARG:HD3	2.00	0.44
5:Eg:32:ILE:HD13	5:Eg:65:ARG:HH22	1.81	0.44
5:Eq:32:ILE:HD13	5:Eq:65:ARG:HH22	1.83	0.44
1:Al:200:ASN:HB3	1:Al:201:THR:H	1.63	0.44
1:Av:200:ASN:HB3	1:Av:201:THR:H	1.64	0.44
1:Aw:200:ASN:HB3	1:Aw:201:THR:H	1.64	0.44
2:Ba:84:ILE:HG13	2:Ba:106:ILE:HD13	2.00	0.44
2:Bi:49:GLU:HG3	2:Bi:54:THR:HG21	1.99	0.44
2:Bl:141:GLY:HA3	2:Bl:154:GLY:O	2.18	0.44
2:Bn:49:GLU:HG3	2:Bn:54:THR:HG21	1.99	0.44
2:Bo:84:ILE:HG13	2:Bo:106:ILE:HD13	1.99	0.44
2:Bp:248:ALA:HB1	2:Bp:265:VAL:HG22	2.00	0.44
2:Bq:272:VAL:HG22	2:Br:260:VAL:HG22	1.99	0.44
2:Bu:315:MET:HG3	2:Bv:328:VAL:HG13	2.00	0.44
3:Ca:373:MET:HE3	3:Ca:373:MET:HB2	1.87	0.44
3:Cp:365:TYR:HE2	4:Di:94:VAL:HG22	1.81	0.44
3:Cz:195:MET:HE2	3:Cz:281:LEU:HD11	1.99	0.44
4:Dk:184:ILE:HG12	4:Dk:286:VAL:HG22	2.00	0.44
4:Dm:184:ILE:HG12	4:Dm:286:VAL:HG22	1.99	0.44
4:Ds:93:PRO:HD3	4:Ds:133:ARG:HA	1.99	0.44
5:Ec:111:LEU:HB3	5:Ec:138:ALA:HB2	2.00	0.44
5:Ep:154:LEU:HB3	5:Ep:164:TYR:HE1	1.81	0.44
5:Eu:41:LEU:HA	5:Eu:44:GLU:HG2	1.98	0.44
1:An:129:ASN:HB2	1:An:156:ASN:HB3	2.00	0.44
1:As:51:ASP:HA	1:As:54:ARG:HE	1.82	0.44
1:As:200:ASN:HB3	1:As:201:THR:H	1.64	0.44
2:Bf:27:VAL:HG21	2:Bf:233:LEU:HD21	1.99	0.44
2:Bh:274:HIS:HE1	2:Bh:343:ALA:HB3	1.83	0.44
2:Bm:141:GLY:HA3	2:Bm:154:GLY:O	2.18	0.44
2:Bn:360:ILE:HD12	2:Bp:163:SER:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Br:33:ASN:HD21	2:Br:172:VAL:HG11	1.83	0.44
2:Bs:21:ILE:HG23	2:Bs:197:LEU:HD11	1.99	0.44
3:Ca:350:TYR:HE2	3:Ca:355:GLU:HG3	1.83	0.44
3:Cd:255:ASP:HB3	3:Cd:258:SER:HB3	2.00	0.44
4:Db:223:THR:HG22	4:Db:285:VAL:HG22	1.99	0.44
4:De:184:ILE:HG12	4:De:286:VAL:HG22	1.99	0.44
4:Dh:25:VAL:HG13	4:Dh:149:ILE:HA	2.00	0.44
4:Dq:93:PRO:HB2	4:Dq:95:TRP:HE3	1.83	0.44
4:Dr:183:THR:HG21	4:Dr:206:ILE:HD11	2.00	0.44
4:Dz:64:ALA:HB2	4:Dz:172:LEU:HD22	2.00	0.44
5:Es:147:ARG:HD3	5:Es:170:TRP:HB3	1.99	0.44
1:Ag:86:PHE:HB2	2:Bt:125:LEU:HD12	1.99	0.43
2:Bd:141:GLY:HA3	2:Bd:154:GLY:O	2.18	0.43
2:Bf:141:GLY:HA3	2:Bf:154:GLY:O	2.17	0.43
2:Bh:27:VAL:HG21	2:Bh:233:LEU:HD21	2.00	0.43
2:Bl:252:VAL:HG22	2:Bl:259:ILE:HG12	2.00	0.43
2:Br:259:ILE:HD11	2:Br:342:MET:HG3	2.00	0.43
3:Ck:220:PHE:HE2	3:Ck:273:VAL:HG11	1.81	0.43
3:Cu:157:LEU:HA	3:Cu:161:SER:HB2	2.00	0.43
4:Do:78:ARG:HB3	4:Do:143:GLN:HE22	1.83	0.43
1:An:51:ASP:HA	1:An:54:ARG:HE	1.82	0.43
2:Bi:274:HIS:HE1	2:Bi:343:ALA:HB3	1.84	0.43
2:Bm:274:HIS:HE1	2:Bm:343:ALA:HB3	1.83	0.43
3:Cp:34:ILE:HD11	3:Cp:100:MET:HB2	2.00	0.43
3:Cu:220:PHE:HE2	3:Cu:273:VAL:HG11	1.83	0.43
4:Do:93:PRO:HD3	4:Do:133:ARG:HA	1.99	0.43
4:Dr:219:VAL:HG21	4:Dr:254:LEU:HD21	1.98	0.43
1:Af:51:ASP:HA	1:Af:54:ARG:HE	1.82	0.43
1:Ak:51:ASP:HA	1:Ak:54:ARG:HE	1.82	0.43
1:Am:200:ASN:HB3	1:Am:201:THR:H	1.64	0.43
2:Bd:49:GLU:HG3	2:Bd:54:THR:HG21	1.99	0.43
2:Bj:42:THR:HG22	2:Bj:80:VAL:HG22	2.00	0.43
2:Bt:83:VAL:HG12	2:Bt:105:SER:HA	2.00	0.43
2:Bx:27:VAL:HG21	2:Bx:233:LEU:HD21	2.00	0.43
2:By:250:ILE:HG12	2:By:261:VAL:HG13	2.00	0.43
3:Cm:61:ILE:HD11	3:Cm:282:GLU:HG3	2.00	0.43
3:Cr:226:VAL:HB	3:Cr:236:MET:HB3	2.00	0.43
3:Ct:121:LYS:HG2	3:Ct:163:SER:HA	2.01	0.43
3:Cx:226:VAL:HB	3:Cx:236:MET:HB3	2.00	0.43
4:Da:184:ILE:HG12	4:Da:286:VAL:HG22	1.99	0.43
4:Df:25:VAL:HG13	4:Df:149:ILE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Dg:93:PRO:HD3	4:Dg:133:ARG:HA	1.99	0.43
4:Dp:183:THR:HG21	4:Dp:206:ILE:HD11	2.01	0.43
5:Eu:32:ILE:HD13	5:Eu:65:ARG:HH22	1.83	0.43
5:Eu:100:GLU:HG3	5:Ev:211:TRP:HB3	2.00	0.43
1:Ag:51:ASP:HA	1:Ag:54:ARG:HE	1.82	0.43
1:An:33:THR:HG23	1:An:35:VAL:H	1.83	0.43
1:Aw:129:ASN:HB2	1:Aw:156:ASN:HB3	2.00	0.43
2:Bd:248:ALA:HB1	2:Bd:265:VAL:HG22	1.99	0.43
2:Bn:248:ALA:HB1	2:Bn:265:VAL:HG22	1.99	0.43
2:Bu:27:VAL:HG21	2:Bu:233:LEU:HD21	2.01	0.43
3:Cq:255:ASP:HB3	3:Cq:258:SER:HB3	2.01	0.43
4:Db:183:THR:HG21	4:Db:206:ILE:HD11	2.01	0.43
4:Dc:93:PRO:HB2	4:Dc:95:TRP:HE3	1.84	0.43
4:Dh:223:THR:HG22	4:Dh:285:VAL:HG22	2.00	0.43
4:Dj:169:ILE:HG13	4:Dj:172:LEU:HD12	2.00	0.43
4:Dk:93:PRO:HD3	4:Dk:133:ARG:HA	2.00	0.43
4:Ds:93:PRO:HB2	4:Ds:95:TRP:HE3	1.83	0.43
4:Dv:25:VAL:HG13	4:Dv:149:ILE:HA	2.00	0.43
4:Dv:37:GLN:HG3	4:Dv:49:VAL:HG23	2.00	0.43
5:Ei:32:ILE:HD13	5:Ei:65:ARG:HH22	1.83	0.43
1:Aa:129:ASN:HB2	1:Aa:156:ASN:HB3	2.01	0.43
1:Ad:51:ASP:HA	1:Ad:54:ARG:HE	1.83	0.43
1:Af:129:ASN:HB2	1:Af:156:ASN:HB3	1.99	0.43
1:Ao:51:ASP:HA	1:Ao:54:ARG:HE	1.82	0.43
1:Ap:51:ASP:HA	1:Ap:54:ARG:HE	1.82	0.43
1:Aq:51:ASP:HA	1:Aq:54:ARG:HE	1.82	0.43
1:Ax:51:ASP:HA	1:Ax:54:ARG:HE	1.83	0.43
2:Ba:274:HIS:HE1	2:Ba:343:ALA:HB3	1.83	0.43
2:Bd:27:VAL:HG21	2:Bd:233:LEU:HD21	2.00	0.43
2:Bg:84:ILE:HG13	2:Bg:106:ILE:HD13	1.99	0.43
2:Bj:137:LEU:HA	2:Bj:162:ILE:HG12	2.00	0.43
2:Bl:317:LYS:HB2	2:Bm:328:VAL:HG21	1.99	0.43
2:Bn:27:VAL:HG21	2:Bn:233:LEU:HD21	2.01	0.43
3:Cm:350:TYR:HE2	3:Cm:355:GLU:HG3	1.83	0.43
3:Cq:220:PHE:HE2	3:Cq:273:VAL:HG11	1.84	0.43
3:Cr:365:TYR:HE2	4:Dk:94:VAL:HG22	1.83	0.43
3:Cs:206:ILE:HG13	3:Cs:216:ILE:HG12	2.00	0.43
3:Cx:255:ASP:HB3	3:Cx:258:SER:HB3	2.01	0.43
4:Dk:93:PRO:HB2	4:Dk:95:TRP:HE3	1.82	0.43
4:Dp:219:VAL:HG21	4:Dp:254:LEU:HD21	1.98	0.43
4:Dt:219:VAL:HG21	4:Dt:254:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Eu:147:ARG:HD3	5:Eu:170:TRP:HB3	2.00	0.43
5:Eu:147:ARG:HD3	5:Eu:170:TRP:HB3	2.00	0.43
1:Am:51:ASP:HA	1:Am:54:ARG:HE	1.82	0.43
2:Bn:274:HIS:HE1	2:Bn:343:ALA:HB3	1.83	0.43
2:Bs:85:VAL:HG22	2:Bs:103:VAL:HG13	2.01	0.43
2:Bs:274:HIS:HE1	2:Bs:343:ALA:HB3	1.83	0.43
2:Bv:84:ILE:HG13	2:Bv:106:ILE:HD13	2.00	0.43
2:Bw:21:ILE:HG23	2:Bw:197:LEU:HD11	1.99	0.43
3:Cb:120:TYR:HE1	3:Cb:312:VAL:HA	1.83	0.43
3:Cw:157:LEU:HA	3:Cw:161:SER:HB2	2.00	0.43
4:Dg:93:PRO:HB2	4:Dg:95:TRP:HE3	1.84	0.43
4:Dl:104:ILE:HA	4:Dm:145:ARG:HD3	2.01	0.43
5:Ey:111:LEU:HB3	5:Ey:138:ALA:HB2	2.01	0.43
5:Ez:189:ARG:HH21	5:Ez:205:LYS:HZ1	1.67	0.43
1:Al:51:ASP:HA	1:Al:54:ARG:HE	1.83	0.43
1:Ap:129:ASN:HB2	1:Ap:156:ASN:HB3	2.00	0.43
1:Au:51:ASP:HA	1:Au:54:ARG:HE	1.83	0.43
2:Ba:21:ILE:HG23	2:Ba:197:LEU:HD11	2.01	0.43
2:Bc:118:MET:HE3	2:Bc:118:MET:HB2	1.91	0.43
2:Bf:49:GLU:HG3	2:Bf:54:THR:HG21	1.99	0.43
2:Bl:27:VAL:HG21	2:Bl:233:LEU:HD21	2.01	0.43
3:Cb:227:PHE:HD1	3:Cb:234:GLU:HA	1.84	0.43
3:Cc:61:ILE:HD11	3:Cc:282:GLU:HG3	2.00	0.43
3:Ci:164:PHE:HZ	3:Ci:285:ILE:HB	1.84	0.43
3:Cl:206:ILE:HG13	3:Cl:216:ILE:HG12	2.01	0.43
3:Cq:337:VAL:HG22	3:Cr:350:TYR:HE1	1.83	0.43
3:Cs:92:GLU:HB2	3:Cs:103:ARG:HB2	2.00	0.43
3:Cz:373:MET:HE3	3:Cz:373:MET:HB2	1.87	0.43
4:Da:145:ARG:HD3	4:Dz:104:ILE:HA	2.01	0.43
4:Db:104:ILE:HA	4:Dc:145:ARG:HD3	2.01	0.43
4:Db:185:LEU:HD22	4:Db:199:SER:HB3	2.01	0.43
4:Df:37:GLN:HG3	4:Df:49:VAL:HG23	2.01	0.43
4:Dy:93:PRO:HD3	4:Dy:133:ARG:HA	2.00	0.43
5:Eg:111:LEU:HB3	5:Eg:138:ALA:HB2	2.01	0.43
5:Eo:100:GLU:HG3	5:Ep:211:TRP:HB3	2.01	0.43
5:Eo:147:ARG:HD3	5:Eo:170:TRP:HB3	2.00	0.43
2:Bj:143:SER:HB2	2:Bj:157:PRO:HG3	2.00	0.43
2:Bm:27:VAL:HG21	2:Bm:233:LEU:HD21	2.01	0.43
2:Bm:259:ILE:HD11	2:Bm:342:MET:HG3	2.01	0.43
2:Bz:105:SER:HB2	2:Bz:112:LEU:HD11	2.00	0.43
3:Cb:358:VAL:HG12	3:Cb:360:GLN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cu:34:ILE:HD11	3:Cu:100:MET:HB2	1.99	0.43
3:Cv:28:VAL:HG13	3:Cv:49:ALA:HB1	2.01	0.43
3:Cy:209:LYS:HD2	3:Cy:212:GLN:HB2	2.00	0.43
4:Dd:183:THR:HG21	4:Dd:206:ILE:HD11	2.01	0.43
4:Df:86:VAL:HG13	4:Df:139:TYR:HB3	2.01	0.43
4:Dj:25:VAL:HG13	4:Dj:149:ILE:HA	2.01	0.43
4:Dt:25:VAL:HG13	4:Dt:149:ILE:HA	2.00	0.43
4:Du:78:ARG:HB3	4:Du:143:GLN:HE22	1.83	0.43
5:Ea:111:LEU:HB3	5:Ea:138:ALA:HB2	2.01	0.43
5:Ee:111:LEU:HB3	5:Ee:138:ALA:HB2	2.00	0.43
1:Ak:129:ASN:HB2	1:Ak:156:ASN:HB3	2.01	0.43
1:Aw:51:ASP:HA	1:Aw:54:ARG:HE	1.83	0.43
2:Ba:317:LYS:HE3	2:Bb:324:LEU:HD23	2.00	0.43
2:Bn:84:ILE:HG13	2:Bn:106:ILE:HD13	2.00	0.43
2:Bn:137:LEU:HA	2:Bn:162:ILE:HG12	2.00	0.43
2:Bq:137:LEU:HA	2:Bq:162:ILE:HG12	2.00	0.43
2:Bq:252:VAL:HG22	2:Bq:259:ILE:HG12	2.01	0.43
3:Ce:269:MET:HE3	3:Ce:269:MET:HB3	1.94	0.43
3:Cq:226:VAL:HB	3:Cq:236:MET:HB3	2.01	0.43
4:Df:183:THR:HG21	4:Df:206:ILE:HD11	2.00	0.43
4:Dv:183:THR:HG21	4:Dv:206:ILE:HD11	2.01	0.43
4:Dz:169:ILE:HG13	4:Dz:172:LEU:HD12	2.00	0.43
5:Em:32:ILE:HD13	5:Em:65:ARG:HH22	1.83	0.43
5:Eu:111:LEU:HB3	5:Eu:138:ALA:HB2	2.00	0.43
5:Ex:107:LEU:HD22	5:Ex:107:LEU:HA	1.93	0.43
1:Ar:129:ASN:HB2	1:Ar:156:ASN:HB3	1.99	0.43
1:At:129:ASN:HB2	1:At:156:ASN:HB3	2.00	0.43
2:Bb:27:VAL:HG21	2:Bb:233:LEU:HD21	2.00	0.43
2:Bc:141:GLY:HA3	2:Bc:154:GLY:O	2.18	0.43
2:Bf:21:ILE:HG23	2:Bf:197:LEU:HD11	2.01	0.43
2:Bi:141:GLY:HA3	2:Bi:154:GLY:O	2.18	0.43
2:Br:85:VAL:HB	2:Br:122:LEU:HD21	2.01	0.43
2:Bv:252:VAL:HG22	2:Bv:259:ILE:HG12	2.01	0.43
3:Cd:195:MET:HE2	3:Cd:281:LEU:HD11	2.00	0.43
3:Cd:292:PRO:HB3	3:Cd:306:LEU:HD13	1.99	0.43
3:Ce:350:TYR:HE2	3:Ce:355:GLU:HG3	1.83	0.43
3:Cp:201:ASP:HB3	3:Cp:221:ALA:HB3	2.01	0.43
3:Cz:61:ILE:HD11	3:Cz:282:GLU:HG3	2.00	0.43
4:Dd:86:VAL:HG13	4:Dd:139:TYR:HB3	2.01	0.43
4:Df:223:THR:HG22	4:Df:285:VAL:HG22	1.99	0.43
4:Ds:111:LYS:HD2	5:Eq:197:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ek:100:GLU:HG3	5:El:211:TRP:HB3	2.01	0.43
1:Ae:200:ASN:HB3	1:Ae:201:THR:H	1.64	0.42
1:Ar:51:ASP:HA	1:Ar:54:ARG:HE	1.83	0.42
1:Ay:129:ASN:HB2	1:Ay:156:ASN:HB3	2.01	0.42
2:Bb:143:SER:HB2	2:Bb:157:PRO:HG3	2.00	0.42
2:Bj:360:ILE:HD12	2:Bl:163:SER:H	1.84	0.42
2:Bk:27:VAL:HG21	2:Bk:233:LEU:HD21	2.01	0.42
2:Bq:27:VAL:HG21	2:Bq:233:LEU:HD21	2.01	0.42
2:Bs:85:VAL:HG13	2:Bs:103:VAL:HG22	2.00	0.42
2:Bt:285:LEU:HD22	2:Bt:301:VAL:HG12	2.01	0.42
2:Bu:33:ASN:HD21	2:Bu:172:VAL:HG11	1.83	0.42
2:Bu:290:PRO:HB3	2:Bu:296:GLY:HA3	2.01	0.42
2:Bw:145:THR:HB	2:Bw:151:LYS:HG3	2.00	0.42
2:Bx:252:VAL:HG22	2:Bx:259:ILE:HG12	2.01	0.42
3:Cb:71:LEU:HD11	3:Cb:88:ILE:HD12	2.01	0.42
3:Cc:271:LEU:HD11	6:Gc:145:PHE:HE2	1.83	0.42
3:Cm:137:ALA:HB1	3:Cm:142:ILE:HG13	2.00	0.42
3:Cr:137:ALA:HB1	3:Cr:142:ILE:HG13	2.00	0.42
3:Cs:201:ASP:HB3	3:Cs:221:ALA:HB3	2.01	0.42
4:Dp:37:GLN:HG3	4:Dp:49:VAL:HG23	2.01	0.42
4:Du:264:TYR:HD1	4:Du:264:TYR:HA	1.78	0.42
5:Ec:147:ARG:HD3	5:Ec:170:TRP:HB3	2.00	0.42
5:Eo:111:LEU:HB3	5:Eo:138:ALA:HB2	2.00	0.42
5:Es:32:ILE:HD13	5:Es:65:ARG:HH22	1.84	0.42
1:Ai:129:ASN:HB2	1:Ai:156:ASN:HB3	2.01	0.42
1:Am:129:ASN:HB2	1:Am:156:ASN:HB3	2.01	0.42
1:Ax:86:PHE:HB2	2:Bk:125:LEU:HD12	2.02	0.42
2:Bf:84:ILE:HG13	2:Bf:106:ILE:HD13	2.01	0.42
2:Bg:145:THR:HB	2:Bg:151:LYS:HG3	2.01	0.42
2:By:33:ASN:HD21	2:By:172:VAL:HG11	1.84	0.42
2:By:224:ARG:HH22	3:Cb:323:THR:HB	1.84	0.42
3:Cm:195:MET:HE2	3:Cm:281:LEU:HD11	2.01	0.42
3:Cy:373:MET:HE3	3:Cy:373:MET:HB2	1.85	0.42
4:Dj:37:GLN:HG3	4:Dj:49:VAL:HG23	2.02	0.42
4:Ds:112:GLN:HE21	4:Ds:112:GLN:HB3	1.63	0.42
5:Ef:107:LEU:HD22	5:Ef:107:LEU:HA	1.93	0.42
5:Ef:189:ARG:HH21	5:Ef:205:LYS:HZ1	1.67	0.42
5:Ei:111:LEU:HB3	5:Ei:138:ALA:HB2	2.01	0.42
1:Ai:51:ASP:HA	1:Ai:54:ARG:HE	1.82	0.42
1:Ak:64:PRO:HB2	1:Al:38:VAL:HG13	2.01	0.42
2:Ba:85:VAL:HG13	2:Ba:103:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bg:27:VAL:HG21	2:Bg:233:LEU:HD21	2.01	0.42
2:Bg:118:MET:HE2	2:Bg:118:MET:HB3	1.89	0.42
2:Bk:33:ASN:HD21	2:Bk:172:VAL:HG11	1.84	0.42
2:Bm:224:ARG:HH22	3:Cp:323:THR:HB	1.84	0.42
2:Bo:274:HIS:HE1	2:Bo:343:ALA:HB3	1.84	0.42
2:Br:360:ILE:HD12	2:Bt:163:SER:H	1.83	0.42
2:Bs:85:VAL:HB	2:Bs:122:LEU:HD21	2.01	0.42
2:Bt:251:ILE:HD13	2:Bt:359:ILE:HB	2.01	0.42
2:By:84:ILE:HG13	2:By:106:ILE:HD13	2.01	0.42
3:Ck:157:LEU:HA	3:Ck:161:SER:HB2	2.01	0.42
3:Cl:271:LEU:HD11	6:Gl:145:PHE:HE2	1.84	0.42
3:Cn:118:GLU:HB3	3:Cn:162:ARG:HH22	1.84	0.42
4:Db:25:VAL:HG13	4:Db:149:ILE:HA	2.00	0.42
4:Dl:223:THR:HG22	4:Dl:285:VAL:HG22	2.01	0.42
4:Dm:93:PRO:HD3	4:Dm:133:ARG:HA	2.01	0.42
5:Em:111:LEU:HB3	5:Em:138:ALA:HB2	2.01	0.42
5:Ep:71:LEU:HB3	5:Ep:74:TYR:HB2	2.01	0.42
5:Ey:147:ARG:HD3	5:Ey:170:TRP:HB3	2.01	0.42
1:Ag:33:THR:HG23	1:Ag:35:VAL:H	1.83	0.42
2:Bf:250:ILE:HG12	2:Bf:261:VAL:HG13	2.01	0.42
2:Bl:83:VAL:HG12	2:Bl:105:SER:HA	2.02	0.42
2:Bo:283:GLU:HG2	2:Bo:305:GLU:HB3	2.00	0.42
2:Bp:84:ILE:HG13	2:Bp:106:ILE:HD13	2.00	0.42
2:Bq:141:GLY:HA3	2:Bq:154:GLY:O	2.19	0.42
2:Bv:27:VAL:HG21	2:Bv:233:LEU:HD21	2.01	0.42
2:Bx:33:ASN:HD21	2:Bx:172:VAL:HG11	1.84	0.42
3:Ch:350:TYR:HE2	3:Ch:355:GLU:HG3	1.84	0.42
3:Cm:34:ILE:HD11	3:Cm:100:MET:HB2	2.02	0.42
3:Cx:206:ILE:HG13	3:Cx:216:ILE:HG12	2.01	0.42
3:Cy:157:LEU:HA	3:Cy:161:SER:HB2	2.01	0.42
3:Cz:255:ASP:HB3	3:Cz:258:SER:HB3	2.02	0.42
4:Df:117:ILE:HD12	4:Df:117:ILE:HA	1.88	0.42
4:Df:185:LEU:HD22	4:Df:199:SER:HB3	2.00	0.42
4:Dl:93:PRO:HD3	4:Dl:133:ARG:HA	2.01	0.42
5: Ei:202:ALA:HA	5: Ei:205:LYS:HZ2	1.85	0.42
5:En:71:LEU:HB3	5:En:74:TYR:HB2	2.02	0.42
5:Ep:189:ARG:HH21	5:Ep:205:LYS:HZ1	1.68	0.42
1:Al:86:PHE:HB2	2:By:125:LEU:HD12	2.01	0.42
1:As:60:VAL:HG13	3: Ci:251:THR:HG21	2.01	0.42
1:At:51:ASP:HA	1:At:54:ARG:HE	1.83	0.42
2:Bj:250:ILE:HG12	2:Bj:261:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bq:285:LEU:HD23	2:Bq:303:ASN:HB3	2.02	0.42
4:Dn:25:VAL:HG13	4:Dn:149:ILE:HA	2.01	0.42
5:Eo:71:LEU:HB3	5:Eo:74:TYR:HB2	2.01	0.42
5:Ew:147:ARG:HD3	5:Ew:170:TRP:HB3	2.01	0.42
1:Aj:51:ASP:HA	1:Aj:54:ARG:HE	1.83	0.42
1:Ak:33:THR:HG23	1:Ak:35:VAL:H	1.84	0.42
2:Be:84:ILE:HG13	2:Be:106:ILE:HD13	2.01	0.42
2:Bf:33:ASN:HD21	2:Bf:172:VAL:HG11	1.84	0.42
2:Bo:324:LEU:HD12	2:Bo:327:LEU:HD23	2.01	0.42
2:Bt:277:MET:HE2	2:Bt:311:LYS:HD2	2.00	0.42
2:By:103:VAL:HB	2:By:137:LEU:HD21	2.00	0.42
3:Ch:78:TYR:HD2	3:Ch:88:ILE:HB	1.85	0.42
3:Ch:137:ALA:HB1	3:Ch:142:ILE:HG13	2.01	0.42
3:Cq:61:ILE:HD11	3:Cq:282:GLU:HG3	2.01	0.42
4:De:93:PRO:HB2	4:De:95:TRP:HE3	1.85	0.42
4:Dj:107:LEU:HD13	4:Dj:107:LEU:HA	1.98	0.42
4:Dl:64:ALA:HB2	4:Dl:172:LEU:HD22	2.00	0.42
4:Dp:116:TYR:HE2	5:Ep:198:GLU:HB3	1.85	0.42
4:Dt:117:ILE:HD12	4:Dt:117:ILE:HA	1.90	0.42
4:Dx:25:VAL:HG13	4:Dx:149:ILE:HA	2.02	0.42
4:Dx:183:THR:HG21	4:Dx:206:ILE:HD11	2.02	0.42
5:Ew:32:ILE:HD13	5:Ew:65:ARG:HH22	1.84	0.42
1:Ag:219:PHE:HD1	2:Bv:69:LEU:HD13	1.84	0.42
1:Ah:51:ASP:HA	1:Ah:54:ARG:HE	1.83	0.42
1:Al:205:TYR:CZ	1:Al:236:SER:HB3	2.55	0.42
1:Av:51:ASP:HA	1:Av:54:ARG:HE	1.83	0.42
2:Bb:141:GLY:CA	2:Bb:154:GLY:O	2.67	0.42
2:Bb:284:ASN:HB2	2:Bb:304:THR:HG23	2.01	0.42
2:Bc:252:VAL:HG22	2:Bc:259:ILE:HG12	2.00	0.42
2:Bd:141:GLY:CA	2:Bd:154:GLY:O	2.67	0.42
2:Bj:145:THR:HB	2:Bj:151:LYS:HG3	2.01	0.42
2:Bm:360:ILE:HD12	2:Bo:163:SER:H	1.85	0.42
2:Bp:141:GLY:CA	2:Bp:154:GLY:O	2.67	0.42
3:Cd:111:SER:HB3	3:Cd:113:THR:HG22	2.01	0.42
3:Cl:35:VAL:HG23	3:Cl:245:ARG:HG3	2.00	0.42
3:Cw:80:PHE:HA	6:Fw:136:VAL:HG21	2.01	0.42
3:Cw:241:ARG:HB3	6:Gx:143:THR:HG21	2.02	0.42
4:Da:93:PRO:HB2	4:Da:95:TRP:HE3	1.84	0.42
4:Df:116:TYR:HE2	5:Ef:198:GLU:HB3	1.85	0.42
4:Dj:183:THR:HG21	4:Dj:206:ILE:HD11	2.01	0.42
1:An:205:TYR:CZ	1:An:236:SER:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bc:145:THR:HB	2:Bc:151:LYS:HG3	2.00	0.42
2:Bg:33:ASN:HD21	2:Bg:172:VAL:HG11	1.85	0.42
2:Bg:287:VAL:HG22	2:Bg:301:VAL:HG13	2.02	0.42
2:Bh:85:VAL:HG13	2:Bh:103:VAL:HG22	2.01	0.42
2:Bh:143:SER:HB2	2:Bh:157:PRO:HG3	2.00	0.42
2:Bi:143:SER:HB2	2:Bi:157:PRO:HG3	2.01	0.42
2:Bq:269:PRO:HB2	2:Br:263:GLN:HE21	1.85	0.42
2:Bt:122:LEU:HB2	2:Bt:131:ALA:HB3	2.00	0.42
3:Ck:282:GLU:HA	3:Ck:286:SER:HB3	2.02	0.42
3:Cw:326:PHE:HD1	3:Cw:328:ASP:H	1.68	0.42
3:Cy:350:TYR:HE2	3:Cy:355:GLU:HG3	1.84	0.42
4:Dn:183:THR:HG21	4:Dn:206:ILE:HD11	2.01	0.42
4:Dt:183:THR:HG21	4:Dt:206:ILE:HD11	2.01	0.42
4:Dx:116:TYR:HE2	5:Ex:198:GLU:HB3	1.85	0.42
4:Dy:112:GLN:HE21	4:Dy:112:GLN:HB3	1.63	0.42
1:At:178:VAL:HG21	1:At:191:ILE:HD12	2.02	0.42
2:Bf:303:ASN:H	2:Bg:285:LEU:HD12	1.85	0.42
2:Bi:118:MET:HE3	2:Bi:118:MET:HB3	1.87	0.42
2:Bw:27:VAL:HG21	2:Bw:233:LEU:HD21	2.01	0.42
2:Bz:274:HIS:HE1	2:Bz:343:ALA:HB3	1.85	0.42
3:Cf:28:VAL:HG13	3:Cf:49:ALA:HB1	2.02	0.42
3:Cj:350:TYR:HE2	3:Cj:355:GLU:HG3	1.85	0.42
3:Cv:373:MET:HE3	3:Cv:373:MET:HB2	1.86	0.42
4:Dd:116:TYR:HE2	5:Ed:198:GLU:HB3	1.85	0.42
4:Di:93:PRO:HB2	4:Di:95:TRP:HE3	1.84	0.42
4:Dl:25:VAL:HG13	4:Dl:149:ILE:HA	2.02	0.42
4:Dn:116:TYR:HE2	5:En:198:GLU:HB3	1.85	0.42
4:Dr:25:VAL:HG13	4:Dr:149:ILE:HA	2.01	0.42
5:Ek:32:ILE:HD13	5:Ek:65:ARG:HH22	1.84	0.42
5:Es:111:LEU:HB3	5:Es:138:ALA:HB2	2.01	0.42
1:Ag:129:ASN:HB2	1:Ag:156:ASN:HB3	2.02	0.42
1:Ak:200:ASN:HB3	1:Ak:201:THR:H	1.64	0.42
1:Aq:205:TYR:CZ	1:Aq:236:SER:HB3	2.55	0.42
1:Ay:219:PHE:CD1	2:Bn:69:LEU:HD13	2.55	0.42
2:Bi:317:LYS:HE3	2:Bj:324:LEU:HD23	2.01	0.42
2:Bk:84:ILE:HG13	2:Bk:106:ILE:HD13	2.02	0.42
2:Bl:197:LEU:HD22	2:Bl:218:ILE:HD13	2.02	0.42
3:Cd:121:LYS:HG2	3:Cd:163:SER:HA	2.02	0.42
3:Ch:226:VAL:HB	3:Ch:236:MET:HB3	2.02	0.42
3:Ci:326:PHE:HD1	3:Ci:328:ASP:H	1.68	0.42
3:Ck:78:TYR:HD2	3:Ck:88:ILE:HB	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ck:373:MET:HE3	3:Ck:373:MET:HB2	1.91	0.42
3:Cs:157:LEU:HA	3:Cs:161:SER:HB2	2.02	0.42
4:Da:112:GLN:HE21	4:Da:112:GLN:HB3	1.63	0.42
4:De:183:THR:HG21	4:De:206:ILE:HD11	2.02	0.42
4:De:264:TYR:HD1	4:De:264:TYR:HA	1.78	0.42
4:Dh:93:PRO:HD3	4:Dh:133:ARG:HA	2.00	0.42
4:Dv:93:PRO:HD3	4:Dv:133:ARG:HA	2.02	0.42
4:Dw:93:PRO:HD3	4:Dw:133:ARG:HA	2.01	0.42
4:Dz:25:VAL:HG13	4:Dz:149:ILE:HA	2.01	0.42
5:Eg:202:ALA:HA	5:Eg:205:LYS:HZ2	1.85	0.42
1:Aa:219:PHE:CD1	2:Bp:69:LEU:HD13	2.55	0.41
1:Ac:129:ASN:HB2	1:Ac:156:ASN:HB3	2.02	0.41
1:Ad:86:PHE:HB2	2:Bq:125:LEU:HD12	2.02	0.41
1:Ai:205:TYR:CZ	1:Ai:236:SER:HB3	2.55	0.41
1:Ax:205:TYR:CZ	1:Ax:236:SER:HB3	2.55	0.41
2:Bm:250:ILE:HG23	2:Bm:261:VAL:HG22	2.02	0.41
2:Bn:252:VAL:HG22	2:Bn:259:ILE:HG12	2.02	0.41
2:Bq:141:GLY:CA	2:Bq:154:GLY:O	2.68	0.41
2:Bu:283:GLU:HG2	2:Bu:305:GLU:HG2	2.02	0.41
2:Bw:250:ILE:HG23	2:Bw:261:VAL:HG22	2.01	0.41
3:Co:226:VAL:HB	3:Co:236:MET:HB3	2.02	0.41
3:Cq:70:LEU:HB3	3:Cq:80:PHE:HE1	1.84	0.41
4:Da:93:PRO:HD3	4:Da:133:ARG:HA	2.02	0.41
5:Ek:111:LEU:HB3	5:Ek:138:ALA:HB2	2.01	0.41
5:Eq:100:GLU:HG3	5:Er:211:TRP:HB3	2.02	0.41
1:Ab:33:THR:HG23	1:Ab:35:VAL:H	1.84	0.41
1:Ag:205:TYR:CZ	1:Ag:236:SER:HB3	2.55	0.41
1:Aj:200:ASN:HB3	1:Aj:201:THR:H	1.64	0.41
1:Aj:205:TYR:CZ	1:Aj:236:SER:HB3	2.55	0.41
1:Am:205:TYR:CZ	1:Am:236:SER:HB3	2.55	0.41
1:At:205:TYR:CZ	1:At:236:SER:HB3	2.55	0.41
1:Au:129:ASN:HB2	1:Au:156:ASN:HB3	2.01	0.41
2:Bg:141:GLY:HA3	2:Bg:154:GLY:O	2.21	0.41
2:Bh:259:ILE:HD11	2:Bh:342:MET:HG3	2.02	0.41
2:Bi:259:ILE:HD11	2:Bi:342:MET:HG3	2.02	0.41
2:Bm:161:MET:HE3	2:Bm:161:MET:HB2	1.91	0.41
2:Bp:197:LEU:HD22	2:Bp:218:ILE:HD13	2.03	0.41
2:Br:318:LEU:HD12	2:Br:318:LEU:HA	1.86	0.41
2:Bt:141:GLY:CA	2:Bt:154:GLY:O	2.67	0.41
2:By:85:VAL:HG22	2:By:103:VAL:HG13	2.01	0.41
2:Bz:224:ARG:HH21	4:Dv:97:PRO:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cd:78:TYR:HD2	3:Cd:88:ILE:HB	1.86	0.41
3:Ch:373:MET:HE3	3:Ch:373:MET:HB2	1.85	0.41
5:Ec:100:GLU:HG3	5:Ed:211:TRP:HB3	2.02	0.41
6:Gw:141:GLN:HG2	6:Gw:142:MET:HG2	2.02	0.41
1:Ad:205:TYR:CZ	1:Ad:236:SER:HB3	2.55	0.41
1:Ao:129:ASN:HB2	1:Ao:156:ASN:HB3	2.01	0.41
1:Ap:205:TYR:CZ	1:Ap:236:SER:HB3	2.55	0.41
1:As:205:TYR:CZ	1:As:236:SER:HB3	2.56	0.41
2:Bb:21:ILE:HG23	2:Bb:197:LEU:HD11	2.02	0.41
2:Bn:141:GLY:CA	2:Bn:154:GLY:O	2.68	0.41
2:Bp:42:THR:HG22	2:Bp:80:VAL:HG22	2.02	0.41
2:Bq:143:SER:HB2	2:Bq:157:PRO:HG3	2.01	0.41
2:Bt:84:ILE:HG13	2:Bt:106:ILE:HD13	2.01	0.41
2:Bu:84:ILE:HG13	2:Bu:106:ILE:HD13	2.01	0.41
2:Bv:197:LEU:HD22	2:Bv:218:ILE:HD13	2.02	0.41
2:Bw:141:GLY:CA	2:Bw:154:GLY:O	2.67	0.41
3:Cu:269:MET:HE3	3:Cu:269:MET:HB3	1.93	0.41
3:Cv:226:VAL:HB	3:Cv:236:MET:HB3	2.03	0.41
4:Dd:219:VAL:HG21	4:Dd:254:LEU:HD21	2.02	0.41
4:Du:183:THR:HG21	4:Du:206:ILE:HD11	2.02	0.41
4:Dw:93:PRO:HB2	4:Dw:95:TRP:HE3	1.84	0.41
4:Dx:37:GLN:HG3	4:Dx:49:VAL:HG23	2.02	0.41
5:Eo:32:ILE:HD13	5:Eo:65:ARG:HH22	1.85	0.41
5:Ep:107:LEU:HD22	5:Ep:107:LEU:HA	1.94	0.41
5:Eq:202:ALA:HA	5:Eq:205:LYS:HZ2	1.84	0.41
1:Aa:136:LEU:HD13	1:Ab:154:LEU:HD13	2.03	0.41
1:Aa:154:LEU:HD13	1:Az:136:LEU:HD13	2.02	0.41
1:Ae:205:TYR:CZ	1:Ae:236:SER:HB3	2.55	0.41
1:Af:205:TYR:CZ	1:Af:236:SER:HB3	2.55	0.41
1:Ax:178:VAL:HG21	1:Ax:191:ILE:HD12	2.03	0.41
2:Bg:285:LEU:HD23	2:Bg:303:ASN:HB3	2.03	0.41
2:Bk:85:VAL:HG22	2:Bk:103:VAL:HG13	2.03	0.41
2:Bl:251:ILE:HD13	2:Bl:359:ILE:HB	2.01	0.41
2:Bt:197:LEU:HD22	2:Bt:218:ILE:HD13	2.02	0.41
3:Cd:167:VAL:HG21	3:Cd:191:ALA:HB2	2.01	0.41
3:Ch:326:PHE:HD1	3:Ch:328:ASP:H	1.68	0.41
4:Dh:37:GLN:HG3	4:Dh:49:VAL:HG23	2.03	0.41
4:Di:93:PRO:HD3	4:Di:133:ARG:HA	2.03	0.41
5:Eq:111:LEU:HB3	5:Eq:138:ALA:HB2	2.01	0.41
5:Es:202:ALA:HA	5:Es:205:LYS:HZ2	1.85	0.41
5:Ew:111:LEU:HB3	5:Ew:138:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ab:136:LEU:HD13	1:Ac:154:LEU:HD13	2.03	0.41
1:Ac:136:LEU:HD13	1:Ad:154:LEU:HD13	2.03	0.41
1:Ae:129:ASN:HB2	1:Ae:156:ASN:HB3	2.01	0.41
1:Ah:178:VAL:HG21	1:Ah:191:ILE:HD12	2.03	0.41
1:Aq:129:ASN:HB2	1:Aq:156:ASN:HB3	2.01	0.41
1:Ax:119:LYS:HB3	1:Az:199:LEU:HD12	2.02	0.41
2:Bg:21:ILE:HG23	2:Bg:197:LEU:HD11	2.03	0.41
2:Bk:137:LEU:HA	2:Bk:162:ILE:HG12	2.02	0.41
3:Cd:80:PHE:HA	6:Fd:136:VAL:HG21	2.02	0.41
3:Cd:373:MET:HE3	3:Cd:373:MET:HB2	1.91	0.41
3:Ci:373:MET:HE3	3:Ci:373:MET:HB2	1.86	0.41
3:Cu:326:PHE:HD1	3:Cu:328:ASP:H	1.69	0.41
4:Dp:25:VAL:HG13	4:Dp:149:ILE:HA	2.01	0.41
4:Dq:78:ARG:HB3	4:Dq:143:GLN:HE22	1.84	0.41
4:Ds:183:THR:HG21	4:Ds:206:ILE:HD11	2.02	0.41
4:Dv:86:VAL:HG13	4:Dv:139:TYR:HB3	2.02	0.41
4:Dv:116:TYR:HE2	5:Ev:198:GLU:HB3	1.85	0.41
5:Ek:202:ALA:HA	5:Ek:205:LYS:HZ2	1.86	0.41
5:Et:189:ARG:HH21	5:Et:205:LYS:HZ1	1.68	0.41
1:Ad:136:LEU:HD13	1:Ae:154:LEU:HD13	2.03	0.41
1:Ag:136:LEU:HD13	1:Ah:154:LEU:HD13	2.03	0.41
1:Ag:178:VAL:HG21	1:Ag:191:ILE:HD12	2.03	0.41
1:Aj:136:LEU:HD13	1:Ak:154:LEU:HD13	2.03	0.41
1:Ak:136:LEU:HD13	1:Al:154:LEU:HD13	2.03	0.41
1:Ak:205:TYR:CZ	1:Ak:236:SER:HB3	2.55	0.41
1:An:119:LYS:HB3	1:Ap:199:LEU:HD12	2.02	0.41
1:Ao:205:TYR:CZ	1:Ao:236:SER:HB3	2.55	0.41
1:As:33:THR:HG23	1:As:35:VAL:H	1.86	0.41
1:Au:205:TYR:CZ	1:Au:236:SER:HB3	2.55	0.41
1:Av:205:TYR:CZ	1:Av:236:SER:HB3	2.55	0.41
1:Ay:205:TYR:CZ	1:Ay:236:SER:HB3	2.55	0.41
1:Az:205:TYR:CZ	1:Az:236:SER:HB3	2.55	0.41
2:Bc:224:ARG:HH22	3:Cf:323:THR:HB	1.86	0.41
2:Be:143:SER:HB2	2:Be:157:PRO:HG3	2.02	0.41
2:Bg:141:GLY:CA	2:Bg:154:GLY:O	2.68	0.41
2:Bh:103:VAL:HB	2:Bh:137:LEU:HD21	2.01	0.41
2:Bk:85:VAL:HG13	2:Bk:103:VAL:HG22	2.03	0.41
2:Bk:248:ALA:HB1	2:Bk:265:VAL:HG22	2.01	0.41
2:Bk:315:MET:HG3	2:Bl:328:VAL:HG13	2.02	0.41
2:By:259:ILE:HD11	2:By:342:MET:HG3	2.02	0.41
3:Cj:80:PHE:HD1	6:Fj:136:VAL:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cx:61:ILE:HD11	3:Cx:282:GLU:HG3	2.02	0.41
4:Dc:112:GLN:HE21	4:Dc:112:GLN:HB3	1.63	0.41
4:Dn:37:GLN:HG3	4:Dn:49:VAL:HG23	2.03	0.41
4:Dr:107:LEU:HD13	4:Dr:107:LEU:HA	1.98	0.41
4:Dz:183:THR:HG21	4:Dz:206:ILE:HD11	2.02	0.41
5:Ej:71:LEU:HB3	5:Ej:74:TYR:HB2	2.03	0.41
5:Es:100:GLU:HG3	5:Et:211:TRP:HB3	2.03	0.41
5:Ey:32:ILE:HD13	5:Ey:65:ARG:HH22	1.84	0.41
1:Ac:205:TYR:CZ	1:Ac:236:SER:HB3	2.55	0.41
1:Ai:178:VAL:HG21	1:Ai:191:ILE:HD12	2.03	0.41
1:Am:136:LEU:HD13	1:An:154:LEU:HD13	2.03	0.41
2:Bb:197:LEU:HD22	2:Bb:218:ILE:HD13	2.02	0.41
2:Bf:44:LEU:HA	2:Bf:45:PRO:HD3	1.94	0.41
2:Bi:21:ILE:HG23	2:Bi:197:LEU:HD11	2.03	0.41
2:Bp:49:GLU:HG3	2:Bp:54:THR:HG21	2.02	0.41
2:Bq:251:ILE:HD13	2:Bq:359:ILE:HB	2.02	0.41
2:Bs:118:MET:HE3	2:Bs:118:MET:HB3	1.85	0.41
2:Bv:233:LEU:O	2:Bv:237:GLU:HB2	2.20	0.41
3:Cb:70:LEU:HB3	3:Cb:80:PHE:HE1	1.85	0.41
3:Ck:227:PHE:HD1	3:Ck:234:GLU:HA	1.85	0.41
3:Ck:239:THR:HG21	3:Cl:155:ARG:HD3	2.03	0.41
3:Cq:121:LYS:HA	3:Cq:163:SER:HB3	2.03	0.41
3:Cs:222:MET:HE2	3:Cs:222:MET:HB3	1.86	0.41
4:Db:93:PRO:HD3	4:Db:133:ARG:HA	2.02	0.41
4:Dh:64:ALA:HB2	4:Dh:172:LEU:HD22	2.01	0.41
4:Dt:93:PRO:HD3	4:Dt:133:ARG:HA	2.03	0.41
4:Dw:112:GLN:HE21	4:Dw:112:GLN:HB3	1.64	0.41
4:Dw:264:TYR:HD1	4:Dw:264:TYR:HA	1.78	0.41
5:Ee:32:ILE:HD13	5:Ee:65:ARG:HH22	1.84	0.41
5:Eh:198:GLU:HA	5:Eh:201:ILE:HG12	2.03	0.41
5:El:198:GLU:HA	5:El:201:ILE:HG12	2.03	0.41
5:Ez:98:TYR:HD1	5:Ez:98:TYR:HA	1.77	0.41
1:Ab:119:LYS:HB3	1:Ad:199:LEU:HD12	2.03	0.41
1:Ab:205:TYR:CZ	1:Ab:236:SER:HB3	2.55	0.41
1:Af:136:LEU:HD13	1:Ag:154:LEU:HD13	2.03	0.41
1:Ag:64:PRO:HB2	1:Ah:38:VAL:HG13	2.02	0.41
1:Ah:136:LEU:HD13	1:Ai:154:LEU:HD13	2.03	0.41
1:As:129:ASN:HB2	1:As:156:ASN:HB3	2.01	0.41
2:Be:141:GLY:CA	2:Be:154:GLY:O	2.69	0.41
2:Bj:251:ILE:HD13	2:Bj:359:ILE:HB	2.02	0.41
2:Bq:197:LEU:HD22	2:Bq:218:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bu:118:MET:H	2:Bu:118:MET:HG2	1.60	0.41
2:Bx:85:VAL:HG13	2:Bx:103:VAL:HG22	2.03	0.41
2:Bx:197:LEU:HD22	2:Bx:218:ILE:HD13	2.01	0.41
3:Ce:255:ASP:HB3	3:Ce:258:SER:HB3	2.03	0.41
3:Cm:56:PHE:HD1	6:Gm:139:LYS:HE2	1.86	0.41
3:Cn:137:ALA:HB1	3:Cn:142:ILE:HG13	2.02	0.41
3:Cs:320:LEU:HD22	3:Cs:342:ILE:HD12	2.03	0.41
3:Cy:195:MET:HG3	3:Cy:226:VAL:HG22	2.02	0.41
4:Dd:25:VAL:HG13	4:Dd:149:ILE:HA	2.02	0.41
4:Dd:185:LEU:HD22	4:Dd:199:SER:HB3	2.03	0.41
4:Dn:86:VAL:HG13	4:Dn:139:TYR:HB3	2.03	0.41
4:Do:68:ILE:HD11	4:Dp:112:GLN:HE21	1.85	0.41
4:Dp:42:THR:HA	4:Dp:43:PRO:HD3	1.92	0.41
5:Ej:198:GLU:HA	5:Ej:201:ILE:HG12	2.03	0.41
5:En:58:ILE:HD12	5:En:58:ILE:HA	1.94	0.41
1:Ad:119:LYS:HB3	1:Af:199:LEU:HD12	2.03	0.41
1:Ae:33:THR:HG23	1:Ae:35:VAL:H	1.85	0.41
1:Ae:136:LEU:HD13	1:Af:154:LEU:HD13	2.03	0.41
1:Ah:205:TYR:CZ	1:Ah:236:SER:HB3	2.55	0.41
1:Av:86:PHE:HB2	2:Bi:125:LEU:HD12	2.03	0.41
1:Aw:205:TYR:CZ	1:Aw:236:SER:HB3	2.56	0.41
1:Az:71:PRO:HB3	1:Az:104:GLY:HA3	2.02	0.41
2:Ba:33:ASN:HD21	2:Ba:172:VAL:HG11	1.85	0.41
2:Ba:141:GLY:CA	2:Ba:154:GLY:O	2.69	0.41
2:Bf:103:VAL:HB	2:Bf:137:LEU:HD21	2.02	0.41
2:Bg:259:ILE:HD11	2:Bg:342:MET:HG3	2.03	0.41
2:Bi:145:THR:HB	2:Bi:151:LYS:HG3	2.02	0.41
2:Bi:277:MET:HE2	2:Bi:311:LYS:HD2	2.02	0.41
2:Bn:83:VAL:HG12	2:Bn:105:SER:HA	2.03	0.41
2:Bn:197:LEU:HD22	2:Bn:218:ILE:HD13	2.02	0.41
2:Bn:285:LEU:HD22	2:Bn:303:ASN:HD22	1.86	0.41
2:Bo:223:PRO:HB3	4:Dk:94:VAL:HG12	2.03	0.41
2:Br:145:THR:HB	2:Br:151:LYS:HG3	2.02	0.41
2:Bt:233:LEU:O	2:Bt:237:GLU:HB2	2.21	0.41
2:Bv:224:ARG:HD2	3:Cy:368:GLN:HB2	2.02	0.41
2:Bx:274:HIS:HE1	2:Bx:343:ALA:HB3	1.86	0.41
3:Cb:226:VAL:HB	3:Cb:236:MET:HB3	2.03	0.41
3:Cg:326:PHE:HD1	3:Cg:328:ASP:H	1.69	0.41
3:Ci:337:VAL:HG22	3:Cj:350:TYR:HE1	1.85	0.41
3:Cw:269:MET:HE3	3:Cw:269:MET:HB3	1.89	0.41
3:Cx:326:PHE:HD1	3:Cx:328:ASP:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Cx:350:TYR:HE2	3:Cx:355:GLU:HG3	1.85	0.41
3:Cx:373:MET:HE3	3:Cx:373:MET:HB2	1.86	0.41
3:Cy:326:PHE:HD1	3:Cy:328:ASP:H	1.69	0.41
3:Cy:337:VAL:HG22	3:Cz:350:TYR:HE1	1.86	0.41
4:Df:219:VAL:HG21	4:Df:254:LEU:HD21	2.02	0.41
4:Di:194:GLU:H	4:Di:194:GLU:HG3	1.72	0.41
4:Dj:107:LEU:HB3	4:Dj:108:GLN:H	1.74	0.41
4:Dl:65:GLY:HA2	4:Dl:176:SER:HB2	2.02	0.41
4:Dl:183:THR:HG21	4:Dl:206:ILE:HD11	2.02	0.41
4:Dl:217:ASP:HA	4:Dl:258:ARG:HD3	2.03	0.41
4:Dq:112:GLN:HE21	4:Dq:112:GLN:HB3	1.64	0.41
5:Ey:100:GLU:HG3	5:Ez:211:TRP:HB3	2.02	0.41
1:Ae:219:PHE:CD1	2:Bt:69:LEU:HD13	2.55	0.41
1:An:136:LEU:HD13	1:Ao:154:LEU:HD13	2.03	0.41
1:Ap:136:LEU:HD13	1:Aq:154:LEU:HD13	2.03	0.41
1:Aq:219:PHE:CD1	2:Bf:69:LEU:HD13	2.55	0.41
2:Ba:103:VAL:HB	2:Ba:137:LEU:HD21	2.03	0.41
2:Bb:250:ILE:HG12	2:Bb:261:VAL:HG13	2.02	0.41
2:Bf:250:ILE:HG23	2:Bf:261:VAL:HG22	2.02	0.41
2:Bm:223:PRO:HB3	4:Di:94:VAL:HG12	2.03	0.41
2:Bq:145:THR:HB	2:Bq:151:LYS:HG3	2.02	0.41
2:Bt:224:ARG:HH21	4:Dp:97:PRO:HB2	1.86	0.41
2:Bt:360:ILE:HD12	2:Bv:163:SER:H	1.85	0.41
2:Bu:143:SER:HB2	2:Bu:157:PRO:HG3	2.02	0.41
2:Bu:197:LEU:HD22	2:Bu:218:ILE:HD13	2.03	0.41
2:Bz:141:GLY:HA3	2:Bz:154:GLY:O	2.20	0.41
3:Ca:88:ILE:HG12	3:Ca:106:ILE:HG12	2.03	0.41
3:Cb:291:LEU:HD22	3:Cb:372:VAL:HA	2.02	0.41
4:Dc:264:TYR:HD1	4:Dc:264:TYR:HA	1.78	0.41
4:Dj:86:VAL:HG13	4:Dj:139:TYR:HB3	2.03	0.41
4:Do:112:GLN:HE21	4:Do:112:GLN:HB3	1.63	0.41
4:Dq:93:PRO:HD3	4:Dq:133:ARG:HA	2.02	0.41
4:Dz:37:GLN:HG3	4:Dz:49:VAL:HG23	2.02	0.41
4:Dz:65:GLY:HA2	4:Dz:176:SER:HB2	2.03	0.41
4:Dz:93:PRO:HD3	4:Dz:133:ARG:HA	2.02	0.41
5:Ed:107:LEU:HD22	5:Ed:107:LEU:HA	1.94	0.41
1:Ap:33:THR:HG23	1:Ap:35:VAL:H	1.86	0.40
1:Ap:178:VAL:HG21	1:Ap:191:ILE:HD12	2.03	0.40
1:Ar:136:LEU:HD13	1:As:154:LEU:HD13	2.02	0.40
2:Bc:33:ASN:HD21	2:Bc:172:VAL:HG11	1.86	0.40
2:Bk:251:ILE:HD13	2:Bk:359:ILE:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bo:103:VAL:HB	2:Bo:137:LEU:HD21	2.03	0.40
2:Bx:21:ILE:HG23	2:Bx:197:LEU:HD11	2.03	0.40
2:By:277:MET:HE2	2:By:311:LYS:HD2	2.03	0.40
2:Bz:285:LEU:HD23	2:Bz:303:ASN:HB3	2.04	0.40
3:Cb:278:MET:HE2	3:Cb:278:MET:HB3	1.99	0.40
3:Cc:70:LEU:HG	6:Fe:136:VAL:HG13	2.03	0.40
3:Ch:157:LEU:HA	3:Ch:161:SER:HB2	2.03	0.40
3:Cp:222:MET:HE2	3:Cp:222:MET:HB3	1.92	0.40
3:Cr:157:LEU:HA	3:Cr:161:SER:HB2	2.04	0.40
3:Cs:326:PHE:HD1	3:Cs:328:ASP:H	1.69	0.40
3:Cz:226:VAL:HB	3:Cz:236:MET:HB3	2.04	0.40
4:De:112:GLN:HE21	4:De:112:GLN:HB3	1.64	0.40
4:Dg:194:GLU:H	4:Dg:194:GLU:HG3	1.72	0.40
5:Ef:71:LEU:HB3	5:Ef:74:TYR:HB2	2.03	0.40
5:El:71:LEU:HB3	5:El:74:TYR:HB2	2.03	0.40
1:Af:178:VAL:HG21	1:Af:191:ILE:HD12	2.03	0.40
1:Al:119:LYS:HB3	1:An:199:LEU:HD12	2.02	0.40
1:As:136:LEU:HD13	1:At:154:LEU:HD13	2.03	0.40
2:Bc:61:MET:HE2	2:Bc:61:MET:HB3	1.98	0.40
2:Bd:197:LEU:HD22	2:Bd:218:ILE:HD13	2.02	0.40
2:Bs:145:THR:HB	2:Bs:151:LYS:HG3	2.03	0.40
2:Bw:303:ASN:HB2	2:Bz:148:ASP:HB2	2.03	0.40
2:Bx:118:MET:HE2	2:Bx:118:MET:HB3	1.94	0.40
3:Cf:377:MET:HE2	6:Ff:142:MET:HE1	2.03	0.40
3:Cq:239:THR:HG21	3:Cr:155:ARG:HD3	2.03	0.40
4:Dc:31:PRO:HB3	4:Dc:156:VAL:HG21	2.03	0.40
4:Dm:183:THR:HG21	4:Dm:206:ILE:HD11	2.03	0.40
4:Dt:37:GLN:HG3	4:Dt:49:VAL:HG23	2.04	0.40
4:Dx:65:GLY:HA2	4:Dx:176:SER:HB2	2.03	0.40
5:Er:58:ILE:HD12	5:Er:58:ILE:HA	1.94	0.40
5:Ez:71:LEU:HB3	5:Ez:74:TYR:HB2	2.02	0.40
1:Aa:124:ASP:HB2	1:Ab:165:ALA:HB3	2.04	0.40
1:Ad:200:ASN:HB3	1:Ad:201:THR:H	1.64	0.40
1:Af:124:ASP:HB2	1:Ag:165:ALA:HB3	2.04	0.40
1:Ak:178:VAL:HG21	1:Ak:191:ILE:HD12	2.03	0.40
1:Am:219:PHE:CD1	2:Bb:69:LEU:HD13	2.56	0.40
1:As:178:VAL:HG21	1:As:191:ILE:HD12	2.04	0.40
1:Au:136:LEU:HD13	1:Av:154:LEU:HD13	2.03	0.40
1:Au:178:VAL:HG21	1:Au:191:ILE:HD12	2.03	0.40
1:Aw:178:VAL:HG21	1:Aw:191:ILE:HD12	2.04	0.40
1:Ay:33:THR:HG23	1:Ay:35:VAL:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bc:251:ILE:HD13	2:Bc:359:ILE:HB	2.02	0.40
2:Bg:250:ILE:HG12	2:Bg:261:VAL:HG13	2.03	0.40
2:Bk:161:MET:HE3	2:Bk:161:MET:HB2	1.93	0.40
2:Bl:141:GLY:CA	2:Bl:154:GLY:O	2.69	0.40
2:Bn:303:ASN:H	2:Bo:285:LEU:HD12	1.86	0.40
2:Bs:143:SER:HB2	2:Bs:157:PRO:HG3	2.02	0.40
2:By:250:ILE:HG23	2:By:261:VAL:HG22	2.03	0.40
2:By:283:GLU:HG2	2:By:305:GLU:HG2	2.03	0.40
3:Cf:222:MET:HE3	3:Cf:222:MET:HB2	1.94	0.40
3:Cm:157:LEU:HA	3:Cm:161:SER:HB2	2.04	0.40
4:Dh:185:LEU:HD22	4:Dh:199:SER:HB3	2.03	0.40
4:Dj:104:ILE:HA	4:Dk:145:ARG:HD3	2.03	0.40
4:Dt:116:TYR:HE2	5:Et:198:GLU:HB3	1.85	0.40
4:Dx:185:LEU:HD22	4:Dx:199:SER:HB3	2.03	0.40
5:Ej:107:LEU:HD22	5:Ej:107:LEU:HA	1.94	0.40
5:El:154:LEU:HB3	5:El:164:TYR:HE1	1.87	0.40
5:Et:71:LEU:HB3	5:Et:74:TYR:HB2	2.02	0.40
1:Aa:119:LYS:HB3	1:Ac:199:LEU:HD12	2.03	0.40
1:Ab:206:ILE:HG23	1:Ab:235:TYR:HB2	2.04	0.40
1:Ae:178:VAL:HG21	1:Ae:191:ILE:HD12	2.04	0.40
1:Ar:205:TYR:CZ	1:Ar:236:SER:HB3	2.55	0.40
1:Ax:71:PRO:HB3	1:Ax:104:GLY:HA3	2.03	0.40
1:Ax:136:LEU:HD13	1:Ay:154:LEU:HD13	2.03	0.40
2:Bd:350:GLN:HG3	2:Be:361:ILE:HG21	2.04	0.40
2:Bh:141:GLY:CA	2:Bh:154:GLY:O	2.70	0.40
2:Bh:290:PRO:HB3	2:Bh:296:GLY:HA3	2.03	0.40
2:Bi:360:ILE:HD12	2:Bk:163:SER:H	1.85	0.40
2:Bj:197:LEU:HD22	2:Bj:218:ILE:HD13	2.03	0.40
2:Bl:274:HIS:HE1	2:Bl:343:ALA:HB3	1.86	0.40
2:Bm:85:VAL:HG22	2:Bm:103:VAL:HG13	2.04	0.40
2:Bo:259:ILE:HD11	2:Bo:342:MET:HG3	2.03	0.40
2:Br:251:ILE:HD13	2:Br:359:ILE:HB	2.03	0.40
2:Bt:275:GLY:HA3	2:Bu:338:PRO:HG2	2.02	0.40
3:Cb:78:TYR:HD2	3:Cb:88:ILE:HB	1.85	0.40
3:Cf:271:LEU:HD11	6:Gf:145:PHE:HE2	1.85	0.40
3:Cy:122:LYS:HD2	3:Cy:193:TYR:HE2	1.86	0.40
3:Cz:350:TYR:HE2	3:Cz:355:GLU:HG3	1.86	0.40
4:De:93:PRO:HD3	4:De:133:ARG:HA	2.02	0.40
4:Dp:185:LEU:HD22	4:Dp:199:SER:HB3	2.03	0.40
4:Dz:107:LEU:HD13	4:Dz:107:LEU:HA	1.98	0.40
5:Ew:202:ALA:HA	5:Ew:205:LYS:HZ2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:165:ALA:HB3	1:Az:124:ASP:HB2	2.04	0.40
1:Af:119:LYS:HB3	1:Ah:199:LEU:HD12	2.03	0.40
1:Ai:136:LEU:HD13	1:Aj:154:LEU:HD13	2.04	0.40
1:Aq:136:LEU:HD13	1:Ar:154:LEU:HD13	2.03	0.40
2:Bb:122:LEU:HB2	2:Bb:131:ALA:HB3	2.04	0.40
2:Bi:283:GLU:HG2	2:Bi:305:GLU:HG2	2.04	0.40
2:Bm:85:VAL:HG13	2:Bm:103:VAL:HG22	2.03	0.40
2:Bn:145:THR:HB	2:Bn:151:LYS:HG3	2.03	0.40
2:Bp:85:VAL:HG13	2:Bp:103:VAL:HG22	2.03	0.40
2:Bq:83:VAL:HG12	2:Bq:105:SER:HA	2.04	0.40
2:Bs:239:LEU:HD23	2:Bs:239:LEU:HA	1.94	0.40
2:Bs:252:VAL:HG22	2:Bs:259:ILE:HG12	2.04	0.40
2:Bx:303:ASN:H	2:By:285:LEU:HD12	1.87	0.40
2:By:27:VAL:HG21	2:By:233:LEU:HD21	2.03	0.40
2:By:197:LEU:HD22	2:By:218:ILE:HD13	2.02	0.40
3:Cc:269:MET:HE3	3:Cc:269:MET:HB3	1.98	0.40
3:Cd:365:TYR:HE2	4:Dw:94:VAL:HG22	1.86	0.40
3:Ci:157:LEU:HA	3:Ci:161:SER:HB2	2.03	0.40
3:Ck:80:PHE:HD1	6:Fk:136:VAL:HG21	1.87	0.40
3:Cl:90:ILE:HG13	3:Cl:104:THR:HB	2.03	0.40
3:Cm:35:VAL:HG21	3:Cm:243:VAL:HG22	2.03	0.40
4:Df:184:ILE:HG12	4:Df:286:VAL:HG22	2.03	0.40
4:Dh:107:LEU:HB3	4:Dh:108:GLN:H	1.74	0.40
4:Dl:185:LEU:HD22	4:Dl:199:SER:HB3	2.03	0.40
4:Du:266:LYS:HE3	4:Du:266:LYS:HB3	1.98	0.40
5:Ea:100:GLU:HG3	5:Eb:211:TRP:HB3	2.03	0.40
5:Eg:100:GLU:HG3	5:Eh:211:TRP:HB3	2.02	0.40
5:Ei:100:GLU:HG3	5:Ej:211:TRP:HB3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	219/258 (85%)	214 (98%)	5 (2%)	0	100	100
1	Ab	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Ac	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Ad	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Ae	219/258 (85%)	214 (98%)	5 (2%)	0	100	100
1	Af	219/258 (85%)	214 (98%)	5 (2%)	0	100	100
1	Ag	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	Ah	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	Ai	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	Aj	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Ak	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Al	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	Am	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	An	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	Ao	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Ap	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	Aq	219/258 (85%)	214 (98%)	5 (2%)	0	100	100
1	Ar	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	As	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	At	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Au	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Av	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	Aw	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Ax	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Ay	219/258 (85%)	215 (98%)	4 (2%)	0	100	100
1	Az	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
2	Ba	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bb	341/361 (94%)	327 (96%)	14 (4%)	0	100	100
2	Bc	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bd	341/361 (94%)	329 (96%)	12 (4%)	0	100	100
2	Be	341/361 (94%)	333 (98%)	8 (2%)	0	100	100
2	Bf	341/361 (94%)	330 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bg	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bh	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bi	341/361 (94%)	332 (97%)	9 (3%)	0	100	100
2	Bj	341/361 (94%)	332 (97%)	9 (3%)	0	100	100
2	Bk	341/361 (94%)	331 (97%)	10 (3%)	0	100	100
2	Bl	341/361 (94%)	329 (96%)	12 (4%)	0	100	100
2	Bm	341/361 (94%)	329 (96%)	12 (4%)	0	100	100
2	Bn	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bo	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bp	341/361 (94%)	331 (97%)	10 (3%)	0	100	100
2	Bq	341/361 (94%)	332 (97%)	9 (3%)	0	100	100
2	Br	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bs	341/361 (94%)	328 (96%)	13 (4%)	0	100	100
2	Bt	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bu	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bv	341/361 (94%)	324 (95%)	17 (5%)	0	100	100
2	Bw	341/361 (94%)	329 (96%)	12 (4%)	0	100	100
2	Bx	341/361 (94%)	329 (96%)	12 (4%)	0	100	100
2	By	341/361 (94%)	330 (97%)	11 (3%)	0	100	100
2	Bz	341/361 (94%)	329 (96%)	12 (4%)	0	100	100
3	Ca	350/377 (93%)	341 (97%)	9 (3%)	0	100	100
3	Cb	350/377 (93%)	336 (96%)	14 (4%)	0	100	100
3	Cc	350/377 (93%)	340 (97%)	10 (3%)	0	100	100
3	Cd	350/377 (93%)	343 (98%)	7 (2%)	0	100	100
3	Ce	350/377 (93%)	339 (97%)	11 (3%)	0	100	100
3	Cf	350/377 (93%)	344 (98%)	6 (2%)	0	100	100
3	Cg	350/377 (93%)	340 (97%)	10 (3%)	0	100	100
3	Ch	350/377 (93%)	343 (98%)	7 (2%)	0	100	100
3	Ci	350/377 (93%)	341 (97%)	9 (3%)	0	100	100
3	Cj	350/377 (93%)	344 (98%)	6 (2%)	0	100	100
3	Ck	350/377 (93%)	343 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Cl	350/377 (93%)	339 (97%)	11 (3%)	0	100	100
3	Cm	350/377 (93%)	342 (98%)	8 (2%)	0	100	100
3	Cn	350/377 (93%)	345 (99%)	5 (1%)	0	100	100
3	Co	350/377 (93%)	341 (97%)	9 (3%)	0	100	100
3	Cp	350/377 (93%)	343 (98%)	7 (2%)	0	100	100
3	Cq	350/377 (93%)	340 (97%)	10 (3%)	0	100	100
3	Cr	350/377 (93%)	343 (98%)	7 (2%)	0	100	100
3	Cs	350/377 (93%)	342 (98%)	8 (2%)	0	100	100
3	Ct	350/377 (93%)	338 (97%)	12 (3%)	0	100	100
3	Cu	350/377 (93%)	339 (97%)	11 (3%)	0	100	100
3	Cv	350/377 (93%)	343 (98%)	7 (2%)	0	100	100
3	Cw	350/377 (93%)	344 (98%)	6 (2%)	0	100	100
3	Cx	350/377 (93%)	343 (98%)	7 (2%)	0	100	100
3	Cy	350/377 (93%)	340 (97%)	10 (3%)	0	100	100
3	Cz	350/377 (93%)	345 (99%)	5 (1%)	0	100	100
4	Da	253/294 (86%)	236 (93%)	17 (7%)	0	100	100
4	Db	254/294 (86%)	233 (92%)	19 (8%)	2 (1%)	16	49
4	Dc	253/294 (86%)	236 (93%)	17 (7%)	0	100	100
4	Dd	254/294 (86%)	237 (93%)	16 (6%)	1 (0%)	30	60
4	De	253/294 (86%)	239 (94%)	14 (6%)	0	100	100
4	Df	254/294 (86%)	237 (93%)	16 (6%)	1 (0%)	30	60
4	Dg	253/294 (86%)	235 (93%)	18 (7%)	0	100	100
4	Dh	254/294 (86%)	235 (92%)	17 (7%)	2 (1%)	16	49
4	Di	253/294 (86%)	236 (93%)	17 (7%)	0	100	100
4	Dj	254/294 (86%)	236 (93%)	16 (6%)	2 (1%)	16	49
4	Dk	253/294 (86%)	235 (93%)	18 (7%)	0	100	100
4	Dl	254/294 (86%)	235 (92%)	17 (7%)	2 (1%)	16	49
4	Dm	253/294 (86%)	236 (93%)	17 (7%)	0	100	100
4	Dn	254/294 (86%)	237 (93%)	16 (6%)	1 (0%)	30	60
4	Do	253/294 (86%)	237 (94%)	16 (6%)	0	100	100
4	Dp	254/294 (86%)	235 (92%)	17 (7%)	2 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Dq	253/294 (86%)	237 (94%)	16 (6%)	0	100	100
4	Dr	254/294 (86%)	235 (92%)	18 (7%)	1 (0%)	30	60
4	Ds	253/294 (86%)	235 (93%)	18 (7%)	0	100	100
4	Dt	254/294 (86%)	236 (93%)	17 (7%)	1 (0%)	30	60
4	Du	253/294 (86%)	238 (94%)	15 (6%)	0	100	100
4	Dv	254/294 (86%)	237 (93%)	16 (6%)	1 (0%)	30	60
4	Dw	253/294 (86%)	238 (94%)	15 (6%)	0	100	100
4	Dx	254/294 (86%)	236 (93%)	17 (7%)	1 (0%)	30	60
4	Dy	253/294 (86%)	237 (94%)	16 (6%)	0	100	100
4	Dz	254/294 (86%)	237 (93%)	15 (6%)	2 (1%)	16	49
5	Ea	181/211 (86%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	Eb	181/211 (86%)	178 (98%)	3 (2%)	0	100	100
5	Ec	181/211 (86%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	Ed	181/211 (86%)	176 (97%)	5 (3%)	0	100	100
5	Ee	181/211 (86%)	169 (93%)	11 (6%)	1 (1%)	21	54
5	Ef	181/211 (86%)	176 (97%)	5 (3%)	0	100	100
5	Eg	181/211 (86%)	170 (94%)	10 (6%)	1 (1%)	21	54
5	Eh	181/211 (86%)	178 (98%)	3 (2%)	0	100	100
5	Ei	181/211 (86%)	169 (93%)	11 (6%)	1 (1%)	21	54
5	Ej	181/211 (86%)	177 (98%)	4 (2%)	0	100	100
5	Ek	181/211 (86%)	172 (95%)	8 (4%)	1 (1%)	21	54
5	El	181/211 (86%)	176 (97%)	5 (3%)	0	100	100
5	Em	181/211 (86%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	En	181/211 (86%)	176 (97%)	5 (3%)	0	100	100
5	Eo	181/211 (86%)	170 (94%)	10 (6%)	1 (1%)	21	54
5	Ep	181/211 (86%)	177 (98%)	4 (2%)	0	100	100
5	Eq	181/211 (86%)	171 (94%)	9 (5%)	1 (1%)	21	54
5	Er	181/211 (86%)	177 (98%)	4 (2%)	0	100	100
5	Es	181/211 (86%)	170 (94%)	10 (6%)	1 (1%)	21	54
5	Et	181/211 (86%)	176 (97%)	5 (3%)	0	100	100
5	Eu	181/211 (86%)	169 (93%)	11 (6%)	1 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ev	181/211 (86%)	176 (97%)	5 (3%)	0	100	100
5	Ew	181/211 (86%)	170 (94%)	10 (6%)	1 (1%)	21	54
5	Ex	181/211 (86%)	176 (97%)	5 (3%)	0	100	100
5	Ey	181/211 (86%)	169 (93%)	11 (6%)	1 (1%)	21	54
5	Ez	181/211 (86%)	177 (98%)	4 (2%)	0	100	100
6	Fa	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fb	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fc	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fd	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fe	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Ff	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fg	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fh	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fi	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fj	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fk	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fl	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fm	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fn	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fo	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fp	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fq	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fr	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fs	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Ft	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fu	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fv	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fw	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fx	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fy	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
6	Fz	13/145 (9%)	12 (92%)	1 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Ga	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gb	11/145 (8%)	8 (73%)	3 (27%)	0	100	100
6	Gc	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gd	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Ge	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gf	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gg	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gh	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gi	11/145 (8%)	8 (73%)	3 (27%)	0	100	100
6	Gj	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gk	11/145 (8%)	8 (73%)	3 (27%)	0	100	100
6	Gl	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gm	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gn	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Go	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gp	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gq	11/145 (8%)	8 (73%)	3 (27%)	0	100	100
6	Gr	11/145 (8%)	8 (73%)	3 (27%)	0	100	100
6	Gs	11/145 (8%)	8 (73%)	3 (27%)	0	100	100
6	Gt	11/145 (8%)	8 (73%)	3 (27%)	0	100	100
6	Gu	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gv	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gw	11/145 (8%)	9 (82%)	1 (9%)	1 (9%)	0	7
6	Gx	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gy	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
6	Gz	11/145 (8%)	9 (82%)	2 (18%)	0	100	100
All	All	35581/46566 (76%)	34238 (96%)	1310 (4%)	33 (0%)	49	79

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	Db	193	VAL
4	Df	193	VAL

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Mol	Chain	Res	Type
4	Dh	193	VAL
4	DI	193	VAL
4	Dj	193	VAL
4	Dn	193	VAL
4	Dr	193	VAL
4	Dt	193	VAL
4	Dh	116	TYR
4	Dj	116	TYR
4	DI	116	TYR
4	Dx	193	VAL
4	Dz	116	TYR
4	Db	116	TYR
4	Dp	116	TYR
5	Ea	87	CYS
5	Ec	87	CYS
5	Ee	87	CYS
5	Eg	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
6	Gw	142	MET
4	Dd	193	VAL
4	Dp	193	VAL
4	Dv	193	VAL
4	Dz	193	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ab	182/213 (85%)	178 (98%)	4 (2%)	45	65
1	Ac	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ad	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ae	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Af	182/213 (85%)	178 (98%)	4 (2%)	45	65
1	Ag	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ah	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ai	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Aj	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ak	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Al	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Am	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	An	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ao	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ap	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Aq	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ar	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	As	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	At	182/213 (85%)	178 (98%)	4 (2%)	45	65
1	Au	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Av	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Aw	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ax	182/213 (85%)	179 (98%)	3 (2%)	55	69
1	Ay	182/213 (85%)	178 (98%)	4 (2%)	45	65
1	Az	182/213 (85%)	179 (98%)	3 (2%)	55	69
2	Ba	267/284 (94%)	263 (98%)	4 (2%)	57	70
2	Bb	267/284 (94%)	262 (98%)	5 (2%)	50	67
2	Bc	267/284 (94%)	265 (99%)	2 (1%)	76	78
2	Bd	267/284 (94%)	264 (99%)	3 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Be	267/284 (94%)	262 (98%)	5 (2%)	50	67
2	Bf	267/284 (94%)	265 (99%)	2 (1%)	76	78
2	Bg	267/284 (94%)	264 (99%)	3 (1%)	65	74
2	Bh	267/284 (94%)	264 (99%)	3 (1%)	65	74
2	Bi	267/284 (94%)	262 (98%)	5 (2%)	50	67
2	Bj	267/284 (94%)	264 (99%)	3 (1%)	65	74
2	Bk	267/284 (94%)	262 (98%)	5 (2%)	50	67
2	Bl	267/284 (94%)	264 (99%)	3 (1%)	65	74
2	Bm	267/284 (94%)	263 (98%)	4 (2%)	57	70
2	Bn	267/284 (94%)	261 (98%)	6 (2%)	45	65
2	Bo	267/284 (94%)	262 (98%)	5 (2%)	50	67
2	Bp	267/284 (94%)	261 (98%)	6 (2%)	45	65
2	Bq	267/284 (94%)	261 (98%)	6 (2%)	45	65
2	Br	267/284 (94%)	264 (99%)	3 (1%)	65	74
2	Bs	267/284 (94%)	263 (98%)	4 (2%)	57	70
2	Bt	267/284 (94%)	263 (98%)	4 (2%)	57	70
2	Bu	267/284 (94%)	263 (98%)	4 (2%)	57	70
2	Bv	267/284 (94%)	262 (98%)	5 (2%)	50	67
2	Bw	267/284 (94%)	265 (99%)	2 (1%)	76	78
2	Bx	267/284 (94%)	263 (98%)	4 (2%)	57	70
2	By	267/284 (94%)	262 (98%)	5 (2%)	50	67
2	Bz	267/284 (94%)	261 (98%)	6 (2%)	45	65
3	Ca	299/324 (92%)	298 (100%)	1 (0%)	86	83
3	Cb	299/324 (92%)	295 (99%)	4 (1%)	61	72
3	Cc	299/324 (92%)	298 (100%)	1 (0%)	86	83
3	Cd	299/324 (92%)	294 (98%)	5 (2%)	53	69
3	Ce	299/324 (92%)	294 (98%)	5 (2%)	53	69
3	Cf	299/324 (92%)	296 (99%)	3 (1%)	68	75
3	Cg	299/324 (92%)	294 (98%)	5 (2%)	53	69
3	Ch	299/324 (92%)	296 (99%)	3 (1%)	68	75
3	Ci	299/324 (92%)	292 (98%)	7 (2%)	44	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Cj	299/324 (92%)	294 (98%)	5 (2%)	53	69
3	Ck	299/324 (92%)	293 (98%)	6 (2%)	48	66
3	Cl	299/324 (92%)	295 (99%)	4 (1%)	61	72
3	Cm	299/324 (92%)	294 (98%)	5 (2%)	53	69
3	Cn	299/324 (92%)	297 (99%)	2 (1%)	76	78
3	Co	299/324 (92%)	294 (98%)	5 (2%)	53	69
3	Cp	299/324 (92%)	298 (100%)	1 (0%)	86	83
3	Cq	299/324 (92%)	298 (100%)	1 (0%)	86	83
3	Cr	299/324 (92%)	296 (99%)	3 (1%)	68	75
3	Cs	299/324 (92%)	295 (99%)	4 (1%)	61	72
3	Ct	299/324 (92%)	296 (99%)	3 (1%)	68	75
3	Cu	299/324 (92%)	295 (99%)	4 (1%)	61	72
3	Cv	299/324 (92%)	295 (99%)	4 (1%)	61	72
3	Cw	299/324 (92%)	297 (99%)	2 (1%)	76	78
3	Cx	299/324 (92%)	295 (99%)	4 (1%)	61	72
3	Cy	299/324 (92%)	296 (99%)	3 (1%)	68	75
3	Cz	299/324 (92%)	295 (99%)	4 (1%)	61	72
4	Da	231/262 (88%)	220 (95%)	11 (5%)	23	49
4	Db	229/262 (87%)	226 (99%)	3 (1%)	61	72
4	Dc	231/262 (88%)	220 (95%)	11 (5%)	23	49
4	Dd	229/262 (87%)	226 (99%)	3 (1%)	61	72
4	De	231/262 (88%)	221 (96%)	10 (4%)	26	52
4	Df	229/262 (87%)	226 (99%)	3 (1%)	61	72
4	Dg	231/262 (88%)	220 (95%)	11 (5%)	23	49
4	Dh	229/262 (87%)	226 (99%)	3 (1%)	61	72
4	Di	231/262 (88%)	220 (95%)	11 (5%)	23	49
4	Dj	229/262 (87%)	227 (99%)	2 (1%)	70	76
4	Dk	231/262 (88%)	220 (95%)	11 (5%)	23	49
4	Dl	229/262 (87%)	226 (99%)	3 (1%)	61	72
4	Dm	231/262 (88%)	222 (96%)	9 (4%)	28	54
4	Dn	229/262 (87%)	226 (99%)	3 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Do	231/262 (88%)	221 (96%)	10 (4%)	26	52
4	Dp	229/262 (87%)	226 (99%)	3 (1%)	61	72
4	Dq	231/262 (88%)	221 (96%)	10 (4%)	26	52
4	Dr	229/262 (87%)	227 (99%)	2 (1%)	70	76
4	Ds	231/262 (88%)	220 (95%)	11 (5%)	23	49
4	Dt	229/262 (87%)	225 (98%)	4 (2%)	53	69
4	Du	231/262 (88%)	221 (96%)	10 (4%)	26	52
4	Dv	229/262 (87%)	225 (98%)	4 (2%)	53	69
4	Dw	231/262 (88%)	220 (95%)	11 (5%)	23	49
4	Dx	229/262 (87%)	226 (99%)	3 (1%)	61	72
4	Dy	231/262 (88%)	221 (96%)	10 (4%)	26	52
4	Dz	229/262 (87%)	226 (99%)	3 (1%)	61	72
5	Ea	149/175 (85%)	142 (95%)	7 (5%)	23	50
5	Eb	154/175 (88%)	149 (97%)	5 (3%)	34	58
5	Ec	149/175 (85%)	142 (95%)	7 (5%)	23	50
5	Ed	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Ee	149/175 (85%)	141 (95%)	8 (5%)	20	47
5	Ef	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Eg	149/175 (85%)	140 (94%)	9 (6%)	17	44
5	Eh	154/175 (88%)	149 (97%)	5 (3%)	34	58
5	Ei	149/175 (85%)	140 (94%)	9 (6%)	17	44
5	Ej	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Ek	149/175 (85%)	141 (95%)	8 (5%)	20	47
5	El	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Em	149/175 (85%)	143 (96%)	6 (4%)	28	53
5	En	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Eo	149/175 (85%)	142 (95%)	7 (5%)	23	50
5	Ep	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Eq	149/175 (85%)	142 (95%)	7 (5%)	23	50
5	Er	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Es	149/175 (85%)	142 (95%)	7 (5%)	23	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Et	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Eu	149/175 (85%)	142 (95%)	7 (5%)	23	50
5	Ev	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Ew	149/175 (85%)	142 (95%)	7 (5%)	23	50
5	Ex	154/175 (88%)	150 (97%)	4 (3%)	40	62
5	Ey	149/175 (85%)	142 (95%)	7 (5%)	23	50
5	Ez	154/175 (88%)	150 (97%)	4 (3%)	40	62
6	Fa	14/121 (12%)	14 (100%)	0	100	100
6	Fb	14/121 (12%)	14 (100%)	0	100	100
6	Fc	14/121 (12%)	14 (100%)	0	100	100
6	Fd	14/121 (12%)	14 (100%)	0	100	100
6	Fe	14/121 (12%)	14 (100%)	0	100	100
6	Ff	14/121 (12%)	13 (93%)	1 (7%)	13	40
6	Fg	14/121 (12%)	14 (100%)	0	100	100
6	Fh	14/121 (12%)	14 (100%)	0	100	100
6	Fi	14/121 (12%)	14 (100%)	0	100	100
6	Fj	14/121 (12%)	14 (100%)	0	100	100
6	Fk	14/121 (12%)	14 (100%)	0	100	100
6	Fl	14/121 (12%)	14 (100%)	0	100	100
6	Fm	14/121 (12%)	14 (100%)	0	100	100
6	Fn	14/121 (12%)	14 (100%)	0	100	100
6	Fo	14/121 (12%)	14 (100%)	0	100	100
6	Fp	14/121 (12%)	14 (100%)	0	100	100
6	Fq	14/121 (12%)	14 (100%)	0	100	100
6	Fr	14/121 (12%)	14 (100%)	0	100	100
6	Fs	14/121 (12%)	14 (100%)	0	100	100
6	Ft	14/121 (12%)	14 (100%)	0	100	100
6	Fu	14/121 (12%)	14 (100%)	0	100	100
6	Fv	14/121 (12%)	14 (100%)	0	100	100
6	Fw	14/121 (12%)	14 (100%)	0	100	100
6	Fx	14/121 (12%)	14 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Fy	14/121 (12%)	14 (100%)	0	100	100
6	Fz	14/121 (12%)	14 (100%)	0	100	100
6	Ga	13/121 (11%)	13 (100%)	0	100	100
6	Gb	13/121 (11%)	13 (100%)	0	100	100
6	Gc	13/121 (11%)	13 (100%)	0	100	100
6	Gd	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Ge	13/121 (11%)	13 (100%)	0	100	100
6	Gf	13/121 (11%)	13 (100%)	0	100	100
6	Gg	13/121 (11%)	13 (100%)	0	100	100
6	Gh	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gi	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gj	13/121 (11%)	13 (100%)	0	100	100
6	Gk	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gl	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gm	13/121 (11%)	13 (100%)	0	100	100
6	Gn	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Go	13/121 (11%)	13 (100%)	0	100	100
6	Gp	13/121 (11%)	13 (100%)	0	100	100
6	Gq	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gr	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gs	13/121 (11%)	13 (100%)	0	100	100
6	Gt	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gu	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gv	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gw	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gx	13/121 (11%)	13 (100%)	0	100	100
6	Gy	13/121 (11%)	12 (92%)	1 (8%)	12	37
6	Gz	13/121 (11%)	13 (100%)	0	100	100
All	All	30069/39000 (77%)	29447 (98%)	622 (2%)	46	65

All (622) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	145	ILE
1	Aa	176	ILE
1	Aa	200	ASN
1	Ab	60	VAL
1	Ab	145	ILE
1	Ab	176	ILE
1	Ab	200	ASN
1	Ac	145	ILE
1	Ac	176	ILE
1	Ac	200	ASN
1	Ad	145	ILE
1	Ad	176	ILE
1	Ad	200	ASN
1	Ae	145	ILE
1	Ae	176	ILE
1	Ae	200	ASN
1	Af	60	VAL
1	Af	145	ILE
1	Af	176	ILE
1	Af	200	ASN
1	Ag	145	ILE
1	Ag	176	ILE
1	Ag	200	ASN
1	Ah	145	ILE
1	Ah	176	ILE
1	Ah	200	ASN
1	Ai	145	ILE
1	Ai	176	ILE
1	Ai	200	ASN
1	Aj	145	ILE
1	Aj	176	ILE
1	Aj	200	ASN
1	Ak	145	ILE
1	Ak	176	ILE
1	Ak	200	ASN
1	Al	145	ILE
1	Al	176	ILE
1	Al	200	ASN
1	Am	145	ILE
1	Am	176	ILE
1	Am	200	ASN
1	An	145	ILE
1	An	176	ILE

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Mol	Chain	Res	Type
1	An	200	ASN
1	Ao	145	ILE
1	Ao	176	ILE
1	Ao	200	ASN
1	Ap	145	ILE
1	Ap	176	ILE
1	Ap	200	ASN
1	Aq	145	ILE
1	Aq	176	ILE
1	Aq	200	ASN
1	Ar	145	ILE
1	Ar	176	ILE
1	Ar	200	ASN
1	As	145	ILE
1	As	176	ILE
1	As	200	ASN
1	At	60	VAL
1	At	145	ILE
1	At	176	ILE
1	At	200	ASN
1	Au	145	ILE
1	Au	176	ILE
1	Au	200	ASN
1	Av	145	ILE
1	Av	176	ILE
1	Av	200	ASN
1	Aw	145	ILE
1	Aw	176	ILE
1	Aw	200	ASN
1	Ax	145	ILE
1	Ax	176	ILE
1	Ax	200	ASN
1	Ay	60	VAL
1	Ay	145	ILE
1	Ay	176	ILE
1	Ay	200	ASN
1	Az	145	ILE
1	Az	176	ILE
1	Az	200	ASN
2	Ba	36	VAL
2	Ba	258	THR
2	Ba	303	ASN

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Mol	Chain	Res	Type
2	Ba	304	THR
2	Bb	258	THR
2	Bb	287	VAL
2	Bb	304	THR
2	Bb	308	VAL
2	Bb	349	LYS
2	Bc	36	VAL
2	Bc	258	THR
2	Bd	36	VAL
2	Bd	54	THR
2	Bd	258	THR
2	Be	36	VAL
2	Be	68	GLN
2	Be	258	THR
2	Be	322	VAL
2	Be	323	THR
2	Bf	54	THR
2	Bf	258	THR
2	Bg	68	GLN
2	Bg	258	THR
2	Bg	304	THR
2	Bh	36	VAL
2	Bh	258	THR
2	Bh	304	THR
2	Bi	36	VAL
2	Bi	54	THR
2	Bi	258	THR
2	Bi	304	THR
2	Bi	322	VAL
2	Bj	258	THR
2	Bj	287	VAL
2	Bj	322	VAL
2	Bk	36	VAL
2	Bk	174	ASN
2	Bk	258	THR
2	Bk	308	VAL
2	Bk	322	VAL
2	Bl	36	VAL
2	Bl	258	THR
2	Bl	304	THR
2	Bm	36	VAL
2	Bm	256	THR

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Mol	Chain	Res	Type
2	Bm	258	THR
2	Bm	304	THR
2	Bn	36	VAL
2	Bn	54	THR
2	Bn	258	THR
2	Bn	303	ASN
2	Bn	304	THR
2	Bn	322	VAL
2	Bo	36	VAL
2	Bo	258	THR
2	Bo	304	THR
2	Bo	308	VAL
2	Bo	323	THR
2	Bp	36	VAL
2	Bp	54	THR
2	Bp	258	THR
2	Bp	304	THR
2	Bp	308	VAL
2	Bp	322	VAL
2	Bq	36	VAL
2	Bq	68	GLN
2	Bq	148	ASP
2	Bq	258	THR
2	Bq	304	THR
2	Bq	322	VAL
2	Br	36	VAL
2	Br	258	THR
2	Br	322	VAL
2	Bs	36	VAL
2	Bs	258	THR
2	Bs	304	THR
2	Bs	322	VAL
2	Bt	36	VAL
2	Bt	258	THR
2	Bt	304	THR
2	Bt	322	VAL
2	Bu	36	VAL
2	Bu	182	ILE
2	Bu	258	THR
2	Bu	304	THR
2	Bv	145	THR
2	Bv	258	THR

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Mol	Chain	Res	Type
2	Bv	303	ASN
2	Bv	304	THR
2	Bv	308	VAL
2	Bw	36	VAL
2	Bw	258	THR
2	Bx	258	THR
2	Bx	287	VAL
2	Bx	322	VAL
2	Bx	323	THR
2	By	36	VAL
2	By	174	ASN
2	By	258	THR
2	By	304	THR
2	By	322	VAL
2	Bz	36	VAL
2	Bz	54	THR
2	Bz	258	THR
2	Bz	304	THR
2	Bz	322	VAL
2	Bz	323	THR
3	Ca	195	MET
3	Cb	102	VAL
3	Cb	286	SER
3	Cb	327	ILE
3	Cb	363	LEU
3	Cc	327	ILE
3	Cd	164	PHE
3	Cd	195	MET
3	Cd	243	VAL
3	Cd	327	ILE
3	Cd	353	GLU
3	Ce	35	VAL
3	Ce	102	VAL
3	Ce	154	ASN
3	Ce	327	ILE
3	Ce	337	VAL
3	Cf	195	MET
3	Cf	243	VAL
3	Cf	328	ASP
3	Cg	154	ASN
3	Cg	243	VAL
3	Cg	327	ILE

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Mol	Chain	Res	Type
3	Cg	337	VAL
3	Cg	353	GLU
3	Ch	154	ASN
3	Ch	195	MET
3	Ch	327	ILE
3	Ci	89	LEU
3	Ci	154	ASN
3	Ci	195	MET
3	Ci	237	THR
3	Ci	286	SER
3	Ci	327	ILE
3	Ci	353	GLU
3	Cj	154	ASN
3	Cj	195	MET
3	Cj	243	VAL
3	Cj	306	LEU
3	Cj	353	GLU
3	Ck	35	VAL
3	Ck	89	LEU
3	Ck	195	MET
3	Ck	237	THR
3	Ck	286	SER
3	Ck	327	ILE
3	Cl	89	LEU
3	Cl	195	MET
3	Cl	320	LEU
3	Cl	327	ILE
3	Cm	35	VAL
3	Cm	117	VAL
3	Cm	243	VAL
3	Cm	353	GLU
3	Cm	374	HIS
3	Cn	243	VAL
3	Cn	327	ILE
3	Co	154	ASN
3	Co	237	THR
3	Co	243	VAL
3	Co	327	ILE
3	Co	353	GLU
3	Cp	327	ILE
3	Cq	243	VAL
3	Cr	237	THR

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Mol	Chain	Res	Type
3	Cr	327	ILE
3	Cr	337	VAL
3	Cs	35	VAL
3	Cs	195	MET
3	Cs	237	THR
3	Cs	327	ILE
3	Ct	35	VAL
3	Ct	209	LYS
3	Ct	243	VAL
3	Cu	195	MET
3	Cu	237	THR
3	Cu	243	VAL
3	Cu	327	ILE
3	Cv	40	VAL
3	Cv	195	MET
3	Cv	243	VAL
3	Cv	327	ILE
3	Cw	237	THR
3	Cw	327	ILE
3	Cx	243	VAL
3	Cx	327	ILE
3	Cx	353	GLU
3	Cx	363	LEU
3	Cy	237	THR
3	Cy	286	SER
3	Cy	327	ILE
3	Cz	117	VAL
3	Cz	195	MET
3	Cz	286	SER
3	Cz	327	ILE
4	Da	25	VAL
4	Da	89	VAL
4	Da	94	VAL
4	Da	106	ASN
4	Da	112	GLN
4	Da	117	ILE
4	Da	149	ILE
4	Da	180	ILE
4	Da	232	ASN
4	Da	252	ILE
4	Da	266	LYS
4	Db	25	VAL

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Mol	Chain	Res	Type
4	Db	193	VAL
4	Db	216	ILE
4	Dc	25	VAL
4	Dc	89	VAL
4	Dc	94	VAL
4	Dc	106	ASN
4	Dc	112	GLN
4	Dc	117	ILE
4	Dc	149	ILE
4	Dc	180	ILE
4	Dc	232	ASN
4	Dc	250	LYS
4	Dc	266	LYS
4	Dd	25	VAL
4	Dd	68	ILE
4	Dd	193	VAL
4	De	25	VAL
4	De	89	VAL
4	De	94	VAL
4	De	106	ASN
4	De	112	GLN
4	De	149	ILE
4	De	180	ILE
4	De	232	ASN
4	De	252	ILE
4	De	266	LYS
4	Df	25	VAL
4	Df	68	ILE
4	Df	193	VAL
4	Dg	25	VAL
4	Dg	89	VAL
4	Dg	94	VAL
4	Dg	106	ASN
4	Dg	112	GLN
4	Dg	117	ILE
4	Dg	149	ILE
4	Dg	180	ILE
4	Dg	232	ASN
4	Dg	252	ILE
4	Dg	266	LYS
4	Dh	25	VAL
4	Dh	68	ILE

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Mol	Chain	Res	Type
4	Dh	193	VAL
4	Di	25	VAL
4	Di	89	VAL
4	Di	94	VAL
4	Di	106	ASN
4	Di	112	GLN
4	Di	117	ILE
4	Di	149	ILE
4	Di	180	ILE
4	Di	232	ASN
4	Di	250	LYS
4	Di	266	LYS
4	Dj	25	VAL
4	Dj	193	VAL
4	Dk	25	VAL
4	Dk	89	VAL
4	Dk	94	VAL
4	Dk	106	ASN
4	Dk	112	GLN
4	Dk	117	ILE
4	Dk	149	ILE
4	Dk	180	ILE
4	Dk	232	ASN
4	Dk	250	LYS
4	Dk	266	LYS
4	Dl	25	VAL
4	Dl	193	VAL
4	Dl	216	ILE
4	Dm	89	VAL
4	Dm	94	VAL
4	Dm	106	ASN
4	Dm	112	GLN
4	Dm	149	ILE
4	Dm	180	ILE
4	Dm	232	ASN
4	Dm	252	ILE
4	Dm	266	LYS
4	Dn	25	VAL
4	Dn	68	ILE
4	Dn	193	VAL
4	Do	25	VAL
4	Do	89	VAL

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Mol	Chain	Res	Type
4	Do	94	VAL
4	Do	106	ASN
4	Do	112	GLN
4	Do	149	ILE
4	Do	180	ILE
4	Do	232	ASN
4	Do	250	LYS
4	Do	266	LYS
4	Dp	25	VAL
4	Dp	193	VAL
4	Dp	216	ILE
4	Dq	89	VAL
4	Dq	94	VAL
4	Dq	106	ASN
4	Dq	112	GLN
4	Dq	117	ILE
4	Dq	149	ILE
4	Dq	180	ILE
4	Dq	232	ASN
4	Dq	252	ILE
4	Dq	266	LYS
4	Dr	25	VAL
4	Dr	193	VAL
4	Ds	25	VAL
4	Ds	89	VAL
4	Ds	94	VAL
4	Ds	106	ASN
4	Ds	112	GLN
4	Ds	117	ILE
4	Ds	149	ILE
4	Ds	180	ILE
4	Ds	232	ASN
4	Ds	250	LYS
4	Ds	266	LYS
4	Dt	25	VAL
4	Dt	68	ILE
4	Dt	193	VAL
4	Dt	216	ILE
4	Du	89	VAL
4	Du	94	VAL
4	Du	106	ASN
4	Du	112	GLN

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Mol	Chain	Res	Type
4	Du	117	ILE
4	Du	149	ILE
4	Du	180	ILE
4	Du	232	ASN
4	Du	250	LYS
4	Du	266	LYS
4	Dv	25	VAL
4	Dv	89	VAL
4	Dv	193	VAL
4	Dv	220	LEU
4	Dw	25	VAL
4	Dw	89	VAL
4	Dw	94	VAL
4	Dw	106	ASN
4	Dw	112	GLN
4	Dw	117	ILE
4	Dw	149	ILE
4	Dw	180	ILE
4	Dw	232	ASN
4	Dw	252	ILE
4	Dw	266	LYS
4	Dx	25	VAL
4	Dx	89	VAL
4	Dx	193	VAL
4	Dy	89	VAL
4	Dy	94	VAL
4	Dy	106	ASN
4	Dy	112	GLN
4	Dy	117	ILE
4	Dy	149	ILE
4	Dy	180	ILE
4	Dy	232	ASN
4	Dy	252	ILE
4	Dy	266	LYS
4	Dz	25	VAL
4	Dz	89	VAL
4	Dz	193	VAL
5	Ea	38	LEU
5	Ea	69	ILE
5	Ea	71	LEU
5	Ea	107	LEU
5	Ea	124	VAL

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Mol	Chain	Res	Type
5	Ea	143	ASN
5	Ea	175	VAL
5	Eb	91	ASP
5	Eb	94	LEU
5	Eb	107	LEU
5	Eb	144	LEU
5	Eb	150	LEU
5	Ec	38	LEU
5	Ec	71	LEU
5	Ec	107	LEU
5	Ec	124	VAL
5	Ec	143	ASN
5	Ec	175	VAL
5	Ec	192	LEU
5	Ed	94	LEU
5	Ed	107	LEU
5	Ed	144	LEU
5	Ed	150	LEU
5	Ee	38	LEU
5	Ee	71	LEU
5	Ee	86	VAL
5	Ee	107	LEU
5	Ee	124	VAL
5	Ee	143	ASN
5	Ee	175	VAL
5	Ee	192	LEU
5	Ef	94	LEU
5	Ef	107	LEU
5	Ef	144	LEU
5	Ef	150	LEU
5	Eg	38	LEU
5	Eg	69	ILE
5	Eg	71	LEU
5	Eg	86	VAL
5	Eg	107	LEU
5	Eg	124	VAL
5	Eg	143	ASN
5	Eg	175	VAL
5	Eg	192	LEU
5	Eh	91	ASP
5	Eh	94	LEU
5	Eh	107	LEU

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Mol	Chain	Res	Type
5	Eh	144	LEU
5	Eh	150	LEU
5	Ei	38	LEU
5	Ei	69	ILE
5	Ei	71	LEU
5	Ei	86	VAL
5	Ei	107	LEU
5	Ei	124	VAL
5	Ei	143	ASN
5	Ei	175	VAL
5	Ei	192	LEU
5	Ej	94	LEU
5	Ej	107	LEU
5	Ej	144	LEU
5	Ej	150	LEU
5	Ek	38	LEU
5	Ek	69	ILE
5	Ek	71	LEU
5	Ek	107	LEU
5	Ek	124	VAL
5	Ek	143	ASN
5	Ek	175	VAL
5	Ek	192	LEU
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	107	LEU
5	Em	124	VAL
5	Em	143	ASN
5	Em	175	VAL
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	107	LEU
5	Eo	124	VAL
5	Eo	143	ASN

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Mol	Chain	Res	Type
5	Eo	175	VAL
5	Eo	192	LEU
5	Ep	94	LEU
5	Ep	107	LEU
5	Ep	144	LEU
5	Ep	150	LEU
5	Eq	38	LEU
5	Eq	69	ILE
5	Eq	71	LEU
5	Eq	107	LEU
5	Eq	124	VAL
5	Eq	143	ASN
5	Eq	175	VAL
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	107	LEU
5	Es	124	VAL
5	Es	143	ASN
5	Es	175	VAL
5	Es	192	LEU
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	107	LEU
5	Eu	124	VAL
5	Eu	143	ASN
5	Eu	175	VAL
5	Eu	192	LEU
5	Ev	94	LEU
5	Ev	107	LEU
5	Ev	144	LEU
5	Ev	150	LEU
5	Ew	38	LEU
5	Ew	71	LEU
5	Ew	107	LEU

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Mol	Chain	Res	Type
5	Ew	124	VAL
5	Ew	143	ASN
5	Ew	175	VAL
5	Ew	192	LEU
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	107	LEU
5	Ey	124	VAL
5	Ey	143	ASN
5	Ey	175	VAL
5	Ey	192	LEU
5	Ez	94	LEU
5	Ez	107	LEU
5	Ez	144	LEU
5	Ez	150	LEU
6	Ff	133	VAL
6	Gd	138	GLU
6	Gh	138	GLU
6	Gi	134	GLN
6	Gk	138	GLU
6	Gl	138	GLU
6	Gn	138	GLU
6	Gq	138	GLU
6	Gr	138	GLU
6	Gt	138	GLU
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 (672) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	149	ASN
1	Aa	156	ASN
1	Aa	200	ASN
1	Aa	221	ASN
1	Ab	77	HIS

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Mol	Chain	Res	Type
1	Ab	129	ASN
1	Ab	149	ASN
1	Ab	200	ASN
1	Ac	129	ASN
1	Ac	149	ASN
1	Ac	167	ASN
1	Ac	200	ASN
1	Ad	129	ASN
1	Ad	149	ASN
1	Ad	167	ASN
1	Ad	200	ASN
1	Ad	221	ASN
1	Ae	129	ASN
1	Ae	156	ASN
1	Ae	200	ASN
1	Ae	221	ASN
1	Af	149	ASN
1	Af	200	ASN
1	Af	221	ASN
1	Ag	70	HIS
1	Ag	77	HIS
1	Ag	149	ASN
1	Ag	156	ASN
1	Ag	167	ASN
1	Ag	200	ASN
1	Ag	221	ASN
1	Ah	77	HIS
1	Ah	129	ASN
1	Ah	149	ASN
1	Ah	200	ASN
1	Ai	70	HIS
1	Ai	77	HIS
1	Ai	149	ASN
1	Ai	156	ASN
1	Ai	167	ASN
1	Ai	200	ASN
1	Aj	77	HIS
1	Aj	149	ASN
1	Aj	200	ASN
1	Aj	221	ASN
1	Ak	77	HIS
1	Ak	129	ASN

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Mol	Chain	Res	Type
1	Ak	156	ASN
1	Ak	200	ASN
1	Ak	221	ASN
1	Al	77	HIS
1	Al	149	ASN
1	Al	156	ASN
1	Al	200	ASN
1	Al	221	ASN
1	Am	77	HIS
1	Am	129	ASN
1	Am	149	ASN
1	Am	156	ASN
1	Am	167	ASN
1	Am	200	ASN
1	Am	221	ASN
1	An	77	HIS
1	An	129	ASN
1	An	149	ASN
1	An	200	ASN
1	An	221	ASN
1	Ao	149	ASN
1	Ao	156	ASN
1	Ao	167	ASN
1	Ao	200	ASN
1	Ao	221	ASN
1	Ap	156	ASN
1	Ap	200	ASN
1	Ap	221	ASN
1	Aq	77	HIS
1	Aq	112	ASN
1	Aq	129	ASN
1	Aq	149	ASN
1	Aq	156	ASN
1	Aq	167	ASN
1	Aq	200	ASN
1	Ar	77	HIS
1	Ar	129	ASN
1	Ar	149	ASN
1	Ar	167	ASN
1	Ar	200	ASN
1	Ar	221	ASN
1	As	129	ASN

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Mol	Chain	Res	Type
1	As	149	ASN
1	As	200	ASN
1	At	129	ASN
1	At	149	ASN
1	At	167	ASN
1	At	200	ASN
1	At	221	ASN
1	Au	77	HIS
1	Au	112	ASN
1	Au	156	ASN
1	Au	167	ASN
1	Au	200	ASN
1	Au	221	ASN
1	Av	149	ASN
1	Av	156	ASN
1	Av	167	ASN
1	Av	200	ASN
1	Av	221	ASN
1	Aw	77	HIS
1	Aw	149	ASN
1	Aw	156	ASN
1	Aw	167	ASN
1	Aw	200	ASN
1	Aw	221	ASN
1	Ax	77	HIS
1	Ax	149	ASN
1	Ax	167	ASN
1	Ax	200	ASN
1	Ax	221	ASN
1	Ay	149	ASN
1	Ay	156	ASN
1	Ay	200	ASN
1	Ay	221	ASN
1	Az	77	HIS
1	Az	112	ASN
1	Az	149	ASN
1	Az	167	ASN
1	Az	200	ASN
2	Ba	33	ASN
2	Ba	263	GLN
2	Ba	284	ASN
2	Ba	286	ASN

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Mol	Chain	Res	Type
2	Ba	303	ASN
2	Ba	346	GLN
2	Bb	33	ASN
2	Bb	156	ASN
2	Bb	195	GLN
2	Bb	263	GLN
2	Bb	286	ASN
2	Bb	346	GLN
2	Bc	33	ASN
2	Bc	346	GLN
2	Bd	33	ASN
2	Bd	134	GLN
2	Bd	303	ASN
2	Bd	346	GLN
2	Be	33	ASN
2	Be	263	GLN
2	Be	284	ASN
2	Be	346	GLN
2	Bf	33	ASN
2	Bf	284	ASN
2	Bf	286	ASN
2	Bf	346	GLN
2	Bg	33	ASN
2	Bg	134	GLN
2	Bg	156	ASN
2	Bg	284	ASN
2	Bg	286	ASN
2	Bh	33	ASN
2	Bh	264	ASN
2	Bh	286	ASN
2	Bi	33	ASN
2	Bi	286	ASN
2	Bi	303	ASN
2	Bj	33	ASN
2	Bj	119	GLN
2	Bj	286	ASN
2	Bj	289	GLN
2	Bk	33	ASN
2	Bk	263	GLN
2	Bk	284	ASN
2	Bk	286	ASN
2	Bl	33	ASN

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Mol	Chain	Res	Type
2	Bl	195	GLN
2	Bl	286	ASN
2	Bl	346	GLN
2	Bm	33	ASN
2	Bm	119	GLN
2	Bm	156	ASN
2	Bm	286	ASN
2	Bm	346	GLN
2	Bn	33	ASN
2	Bn	195	GLN
2	Bn	264	ASN
2	Bn	284	ASN
2	Bn	286	ASN
2	Bn	303	ASN
2	Bo	33	ASN
2	Bo	286	ASN
2	Bp	33	ASN
2	Bp	263	GLN
2	Bp	284	ASN
2	Bp	286	ASN
2	Bp	346	GLN
2	Bq	33	ASN
2	Bq	156	ASN
2	Bq	286	ASN
2	Bq	346	GLN
2	Br	33	ASN
2	Br	284	ASN
2	Br	286	ASN
2	Bs	33	ASN
2	Bs	119	GLN
2	Bs	263	GLN
2	Bs	286	ASN
2	Bt	33	ASN
2	Bt	156	ASN
2	Bt	195	GLN
2	Bt	286	ASN
2	Bt	303	ASN
2	Bu	33	ASN
2	Bu	156	ASN
2	Bu	263	GLN
2	Bu	286	ASN
2	Bu	346	GLN

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Mol	Chain	Res	Type
2	Bv	33	ASN
2	Bv	286	ASN
2	Bv	289	GLN
2	Bv	346	GLN
2	Bw	33	ASN
2	Bw	289	GLN
2	Bw	346	GLN
2	Bx	33	ASN
2	Bx	34	GLN
2	Bx	195	GLN
2	Bx	264	ASN
2	Bx	284	ASN
2	Bx	346	GLN
2	By	33	ASN
2	By	264	ASN
2	By	284	ASN
2	By	286	ASN
2	Bz	33	ASN
2	Bz	136	ASN
2	Bz	286	ASN
3	Ca	44	HIS
3	Ca	66	ASN
3	Ca	116	HIS
3	Ca	159	GLN
3	Ca	217	ASN
3	Cb	97	ASN
3	Cb	154	ASN
3	Cb	217	ASN
3	Cb	374	HIS
3	Cc	217	ASN
3	Cc	253	GLN
3	Cc	276	ASN
3	Cc	322	HIS
3	Cc	368	GLN
3	Cd	97	ASN
3	Cd	322	HIS
3	Ce	212	GLN
3	Ce	217	ASN
3	Ce	339	GLN
3	Cf	66	ASN
3	Cf	97	ASN
3	Cf	135	GLN

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Mol	Chain	Res	Type
3	Cf	154	ASN
3	Cf	159	GLN
3	Cf	217	ASN
3	Cf	253	GLN
3	Cf	322	HIS
3	Cg	159	GLN
3	Cg	217	ASN
3	Cg	310	HIS
3	Cg	314	GLN
3	Ch	253	GLN
3	Ch	322	HIS
3	Ch	352	HIS
3	Ci	97	ASN
3	Ci	135	GLN
3	Ci	159	GLN
3	Ci	212	GLN
3	Ci	330	GLN
3	Ci	374	HIS
3	Cj	217	ASN
3	Cj	253	GLN
3	Cj	322	HIS
3	Cj	368	GLN
3	Cj	374	HIS
3	Ck	154	ASN
3	Ck	253	GLN
3	Cl	159	GLN
3	Cl	314	GLN
3	Cl	322	HIS
3	Cl	374	HIS
3	Cm	154	ASN
3	Cm	314	GLN
3	Cm	322	HIS
3	Cn	135	GLN
3	Cn	253	GLN
3	Cn	276	ASN
3	Cn	322	HIS
3	Co	97	ASN
3	Co	187	GLN
3	Co	217	ASN
3	Co	253	GLN
3	Co	276	ASN
3	Co	374	HIS

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Mol	Chain	Res	Type
3	Cp	116	HIS
3	Cp	253	GLN
3	Cp	322	HIS
3	Cp	374	HIS
3	Cq	44	HIS
3	Cq	66	ASN
3	Cq	217	ASN
3	Cq	233	ASN
3	Cq	368	GLN
3	Cr	44	HIS
3	Cr	66	ASN
3	Cr	116	HIS
3	Cr	135	GLN
3	Cr	141	GLN
3	Cr	154	ASN
3	Cr	217	ASN
3	Cr	322	HIS
3	Cr	368	GLN
3	Cs	97	ASN
3	Cs	116	HIS
3	Cs	135	GLN
3	Cs	154	ASN
3	Cs	159	GLN
3	Cs	212	GLN
3	Cs	217	ASN
3	Cs	322	HIS
3	Cs	368	GLN
3	Cs	374	HIS
3	Ct	135	GLN
3	Ct	154	ASN
3	Ct	322	HIS
3	Ct	368	GLN
3	Ct	374	HIS
3	Cu	97	ASN
3	Cu	116	HIS
3	Cu	154	ASN
3	Cu	217	ASN
3	Cu	322	HIS
3	Cu	368	GLN
3	Cu	374	HIS
3	Cv	97	ASN
3	Cv	154	ASN

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Mol	Chain	Res	Type
3	Cv	187	GLN
3	Cv	217	ASN
3	Cv	322	HIS
3	Cv	330	GLN
3	Cv	352	HIS
3	Cv	368	GLN
3	Cv	374	HIS
3	Cw	66	ASN
3	Cw	116	HIS
3	Cw	322	HIS
3	Cx	217	ASN
3	Cx	322	HIS
3	Cx	339	GLN
3	Cx	374	HIS
3	Cy	97	ASN
3	Cy	135	GLN
3	Cy	154	ASN
3	Cy	217	ASN
3	Cy	322	HIS
3	Cy	374	HIS
3	Cz	97	ASN
3	Cz	135	GLN
3	Cz	154	ASN
3	Cz	159	GLN
3	Cz	322	HIS
3	Cz	376	GLN
4	Da	108	GLN
4	Da	112	GLN
4	Da	143	GLN
4	Da	147	GLN
4	Da	282	ASN
4	Db	50	HIS
4	Db	112	GLN
4	Db	120	GLN
4	Db	147	GLN
4	Db	189	GLN
4	Db	235	GLN
4	Db	293	GLN
4	Dc	108	GLN
4	Dc	112	GLN
4	Dc	143	GLN
4	Dc	147	GLN

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

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Mol	Chain	Res	Type
4	Dk	112	GLN
4	Dk	143	GLN
4	Dk	147	GLN
4	Dk	282	ASN
4	Dl	50	HIS
4	Dl	85	ASN
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	108	GLN
4	Dm	112	GLN
4	Dm	147	GLN
4	Dm	282	ASN
4	Dn	50	HIS
4	Dn	85	ASN
4	Dn	120	GLN
4	Dn	147	GLN
4	Dn	235	GLN
4	Dn	293	GLN
4	Do	108	GLN
4	Do	112	GLN
4	Do	143	GLN
4	Do	147	GLN
4	Do	282	ASN
4	Dp	32	GLN
4	Dp	50	HIS
4	Dp	112	GLN
4	Dp	120	GLN
4	Dp	147	GLN
4	Dp	235	GLN
4	Dp	293	GLN
4	Dq	108	GLN
4	Dq	112	GLN
4	Dq	143	GLN
4	Dq	147	GLN
4	Dq	282	ASN
4	Dr	50	HIS
4	Dr	120	GLN
4	Dr	147	GLN

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Mol	Chain	Res	Type
4	Dr	235	GLN
4	Dr	293	GLN
4	Ds	108	GLN
4	Ds	112	GLN
4	Ds	143	GLN
4	Ds	147	GLN
4	Ds	282	ASN
4	Dt	32	GLN
4	Dt	50	HIS
4	Dt	85	ASN
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
4	Dv	85	ASN
4	Dv	120	GLN
4	Dv	147	GLN
4	Dv	235	GLN
4	Dv	293	GLN
4	Dw	108	GLN
4	Dw	112	GLN
4	Dw	143	GLN
4	Dw	147	GLN
4	Dw	282	ASN
4	Dx	32	GLN
4	Dx	50	HIS
4	Dx	112	GLN
4	Dx	120	GLN
4	Dx	147	GLN
4	Dx	235	GLN
4	Dx	293	GLN
4	Dy	108	GLN
4	Dy	112	GLN
4	Dy	143	GLN
4	Dy	147	GLN

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Mol	Chain	Res	Type
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	90	GLN
5	Ea	143	ASN
5	Ea	145	ASN
5	Ea	149	GLN
5	Ea	173	ASN
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	Ec	90	GLN
5	Ec	143	ASN
5	Ec	145	ASN
5	Ec	149	GLN
5	Ec	173	ASN
5	Ec	183	ASN
5	Ed	57	GLN
5	Ed	90	GLN
5	Ed	143	ASN
5	Ed	149	GLN
5	Ed	179	GLN
5	Ee	90	GLN
5	Ee	143	ASN
5	Ee	145	ASN
5	Ee	149	GLN
5	Ee	173	ASN
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

*Continued on next page...*

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Mol	Chain	Res	Type
5	Eg	90	GLN
5	Eg	143	ASN
5	Eg	145	ASN
5	Eg	149	GLN
5	Eg	173	ASN
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	Ei	90	GLN
5	Ei	143	ASN
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	Ek	143	ASN
5	Ek	145	ASN
5	Ek	149	GLN
5	Ek	173	ASN
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	Em	143	ASN
5	Em	145	ASN
5	Em	149	GLN
5	Em	173	ASN
5	Em	183	ASN
5	En	57	GLN
5	En	90	GLN
5	En	143	ASN
5	En	149	GLN

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

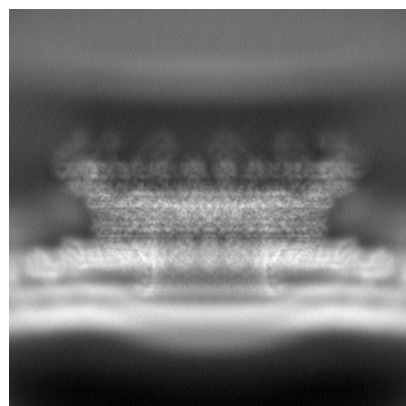
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72847. These allow visual inspection of the internal detail of the map and identification of artifacts.

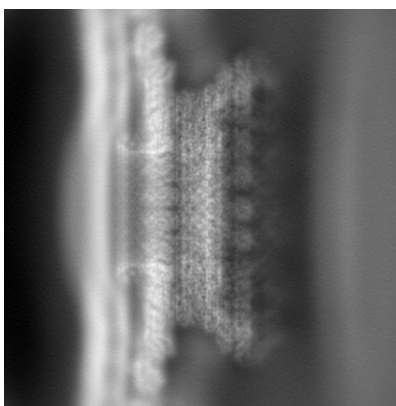
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

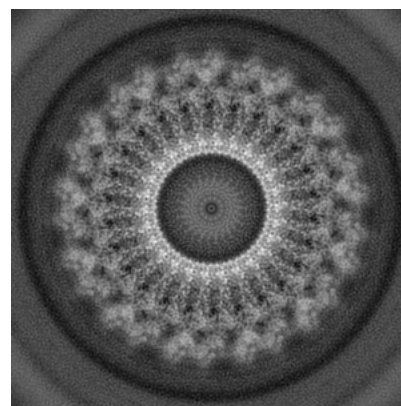
#### 6.1.1 Primary map



X

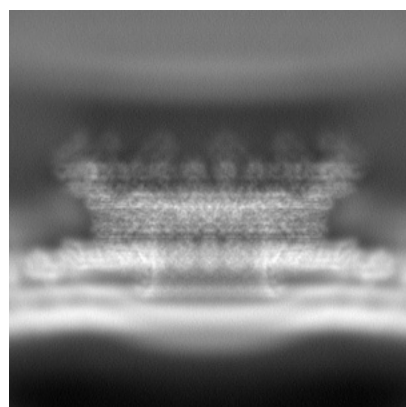


Y

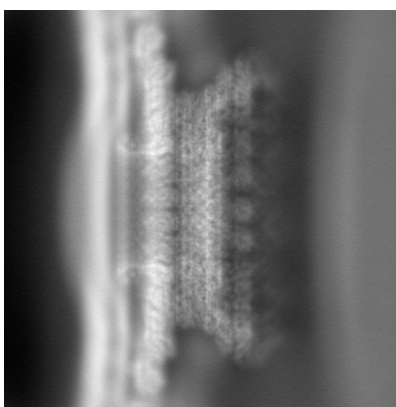


Z

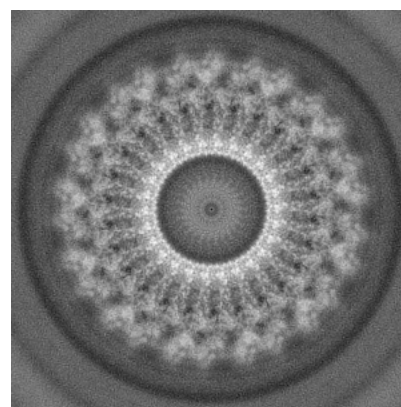
#### 6.1.2 Raw map



X



Y

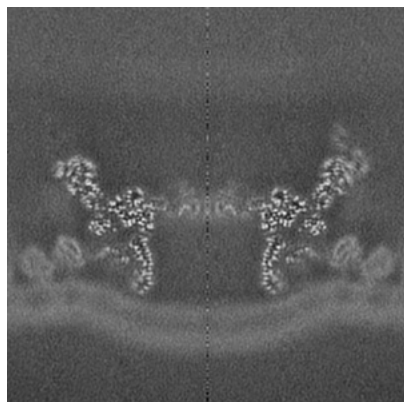


Z

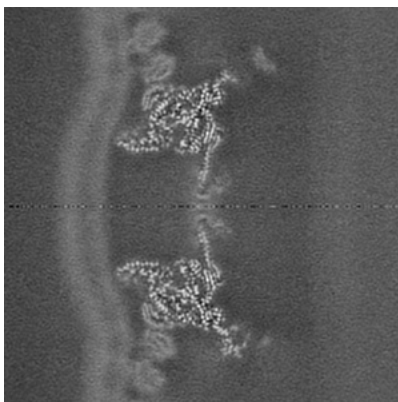
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

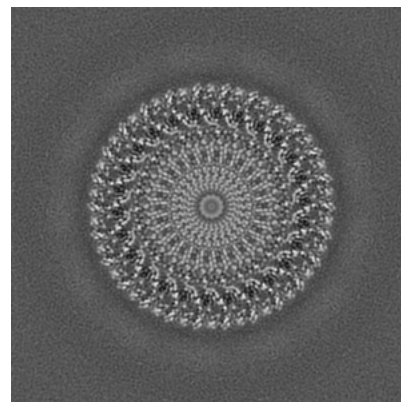
### 6.2.1 Primary map



X Index: 224

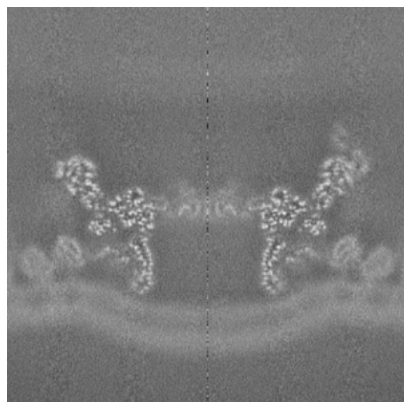


Y Index: 224

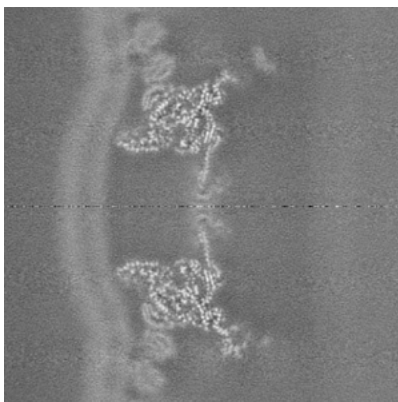


Z Index: 224

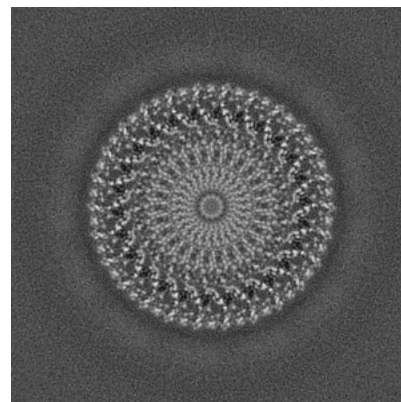
### 6.2.2 Raw map



X Index: 224



Y Index: 224



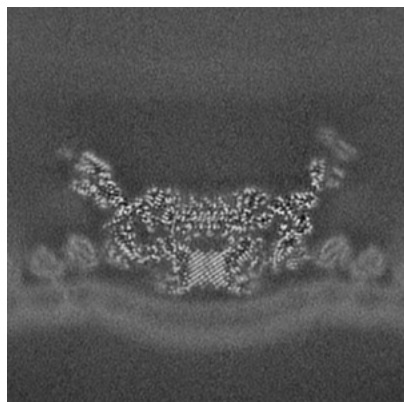
Z Index: 224

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

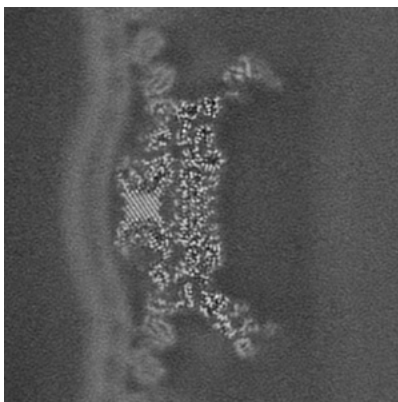


## 6.3 Largest variance slices [i](#)

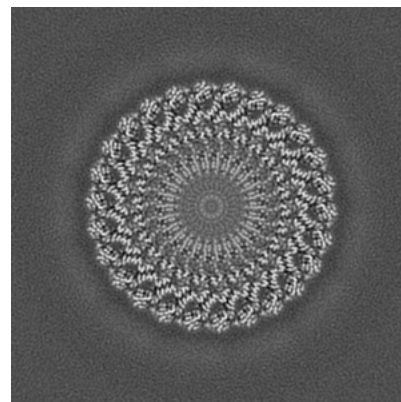
### 6.3.1 Primary map



X Index: 161

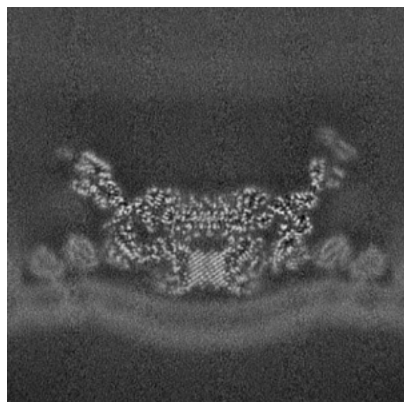


Y Index: 160

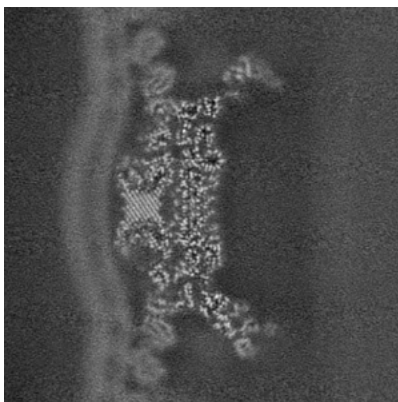


Z Index: 227

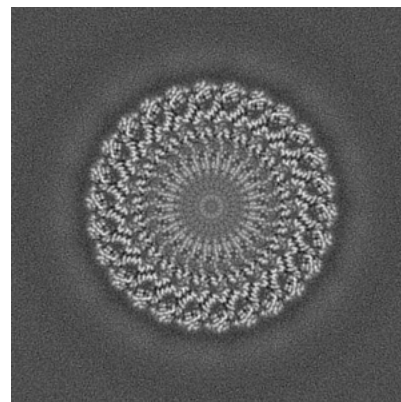
### 6.3.2 Raw map



X Index: 161



Y Index: 160

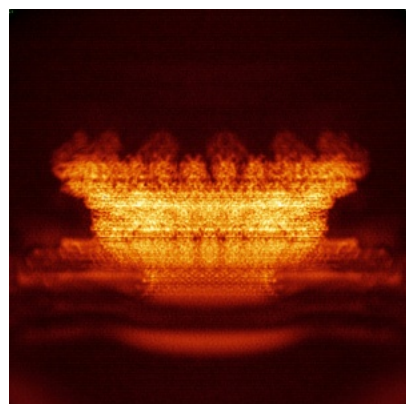


Z Index: 227

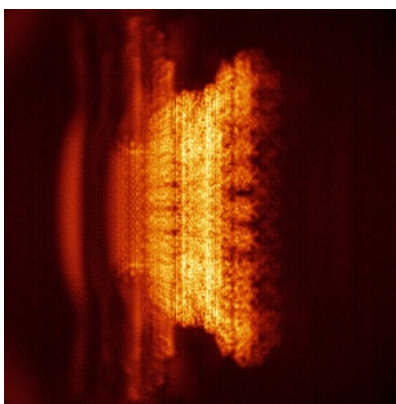
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

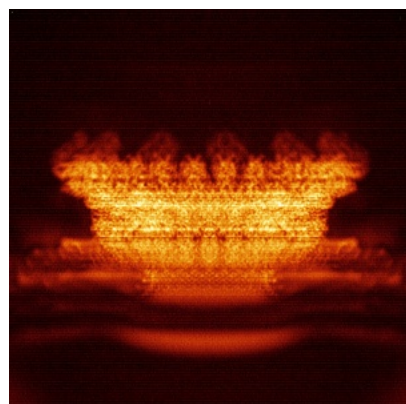


Y

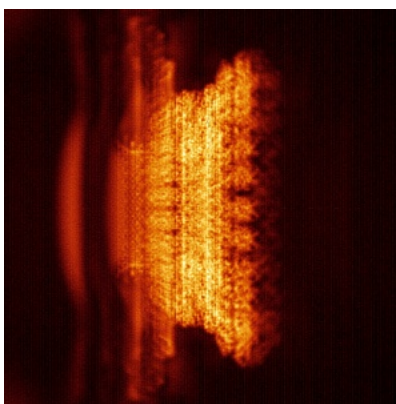


Z

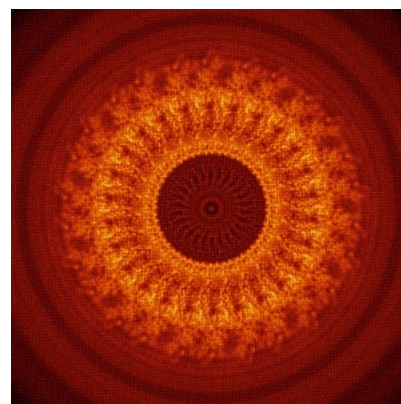
### 6.4.2 Raw map



X



Y

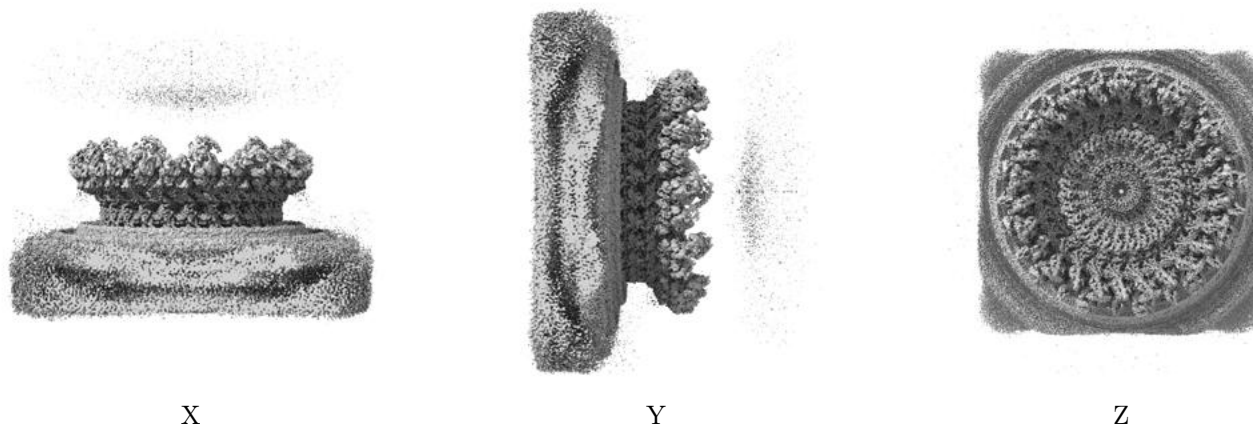


Z

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

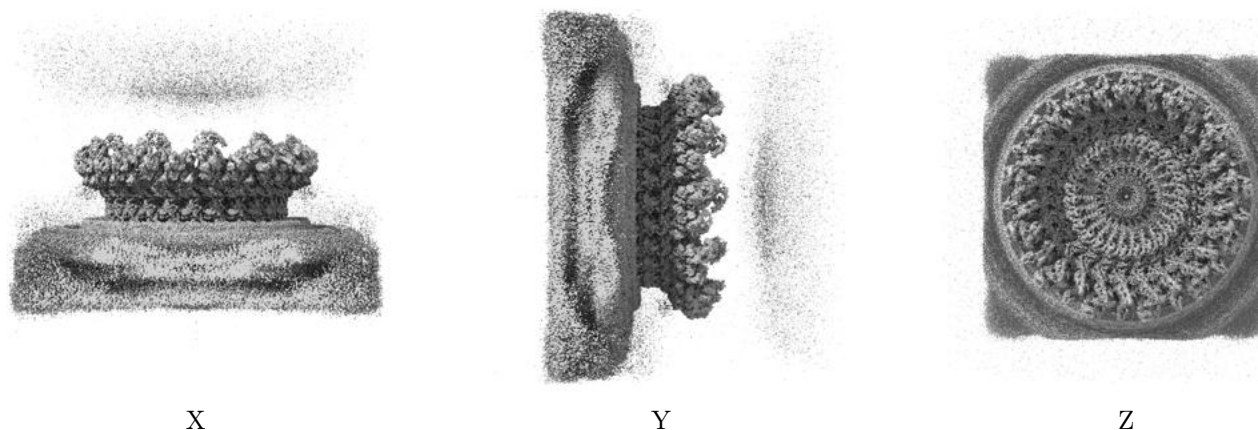
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.



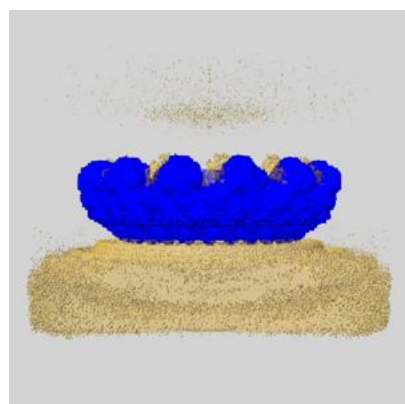
## 6.6 Mask visualisation [i](#)

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

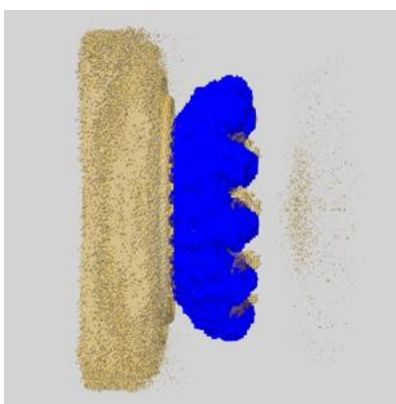
A mask typically either:

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

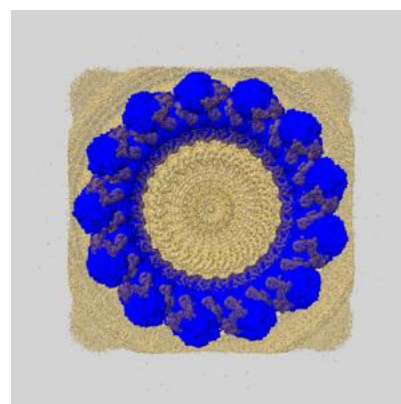
### 6.6.1 emd\_72847\_msk\_1.map [i](#)



X



Y

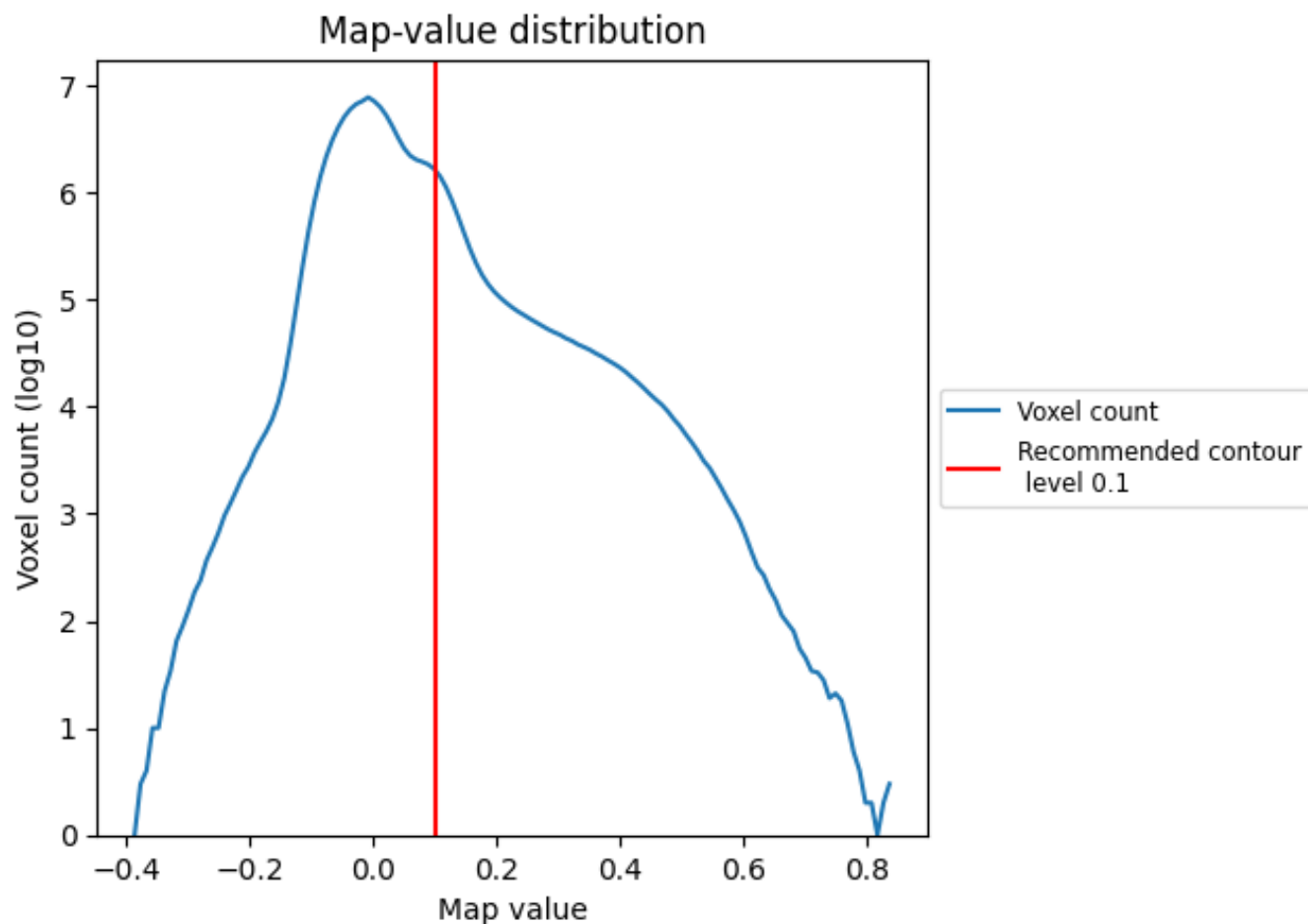


Z

## 7 Map analysis [i](#)

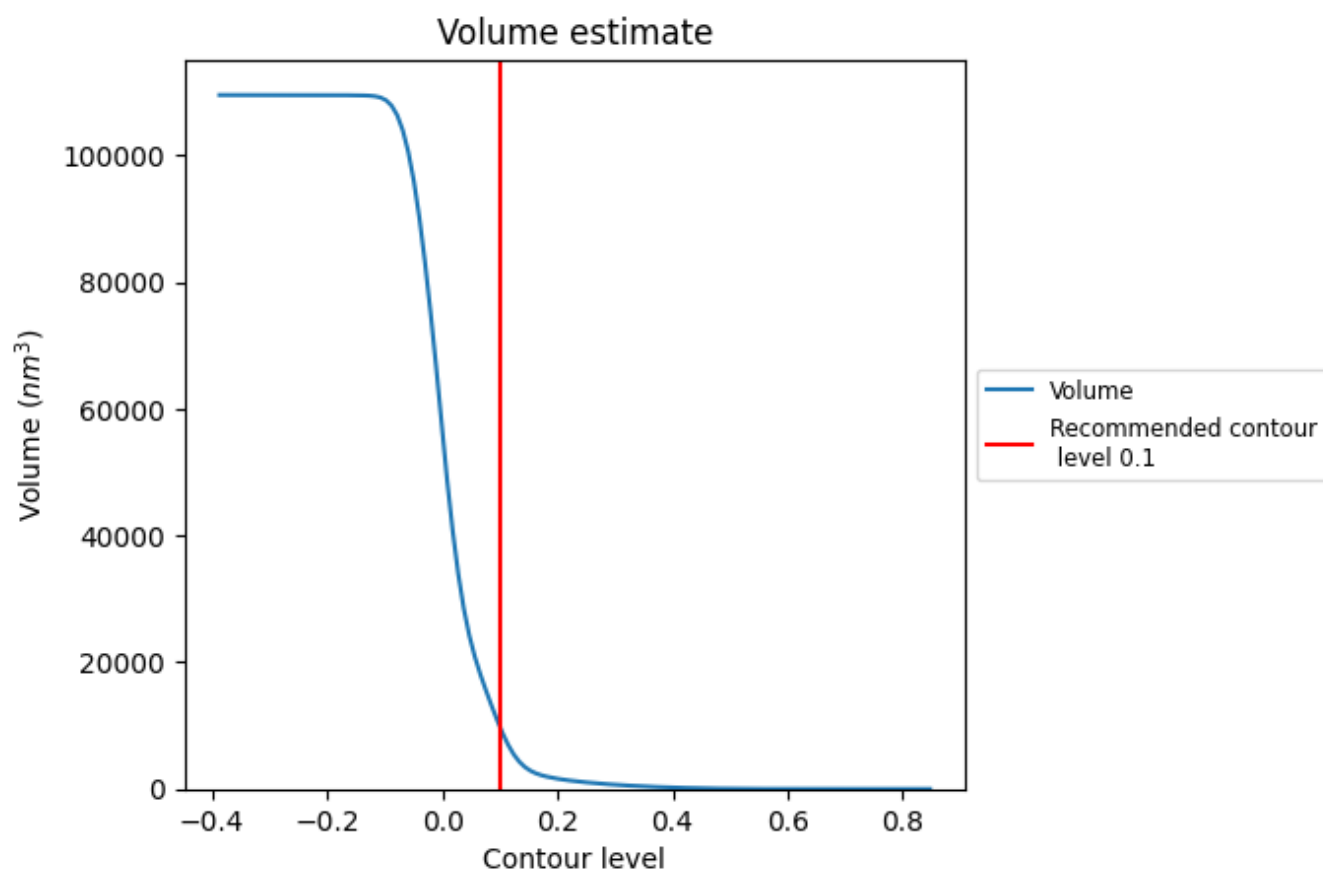
This section contains the results of statistical analysis of the map.

### 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.

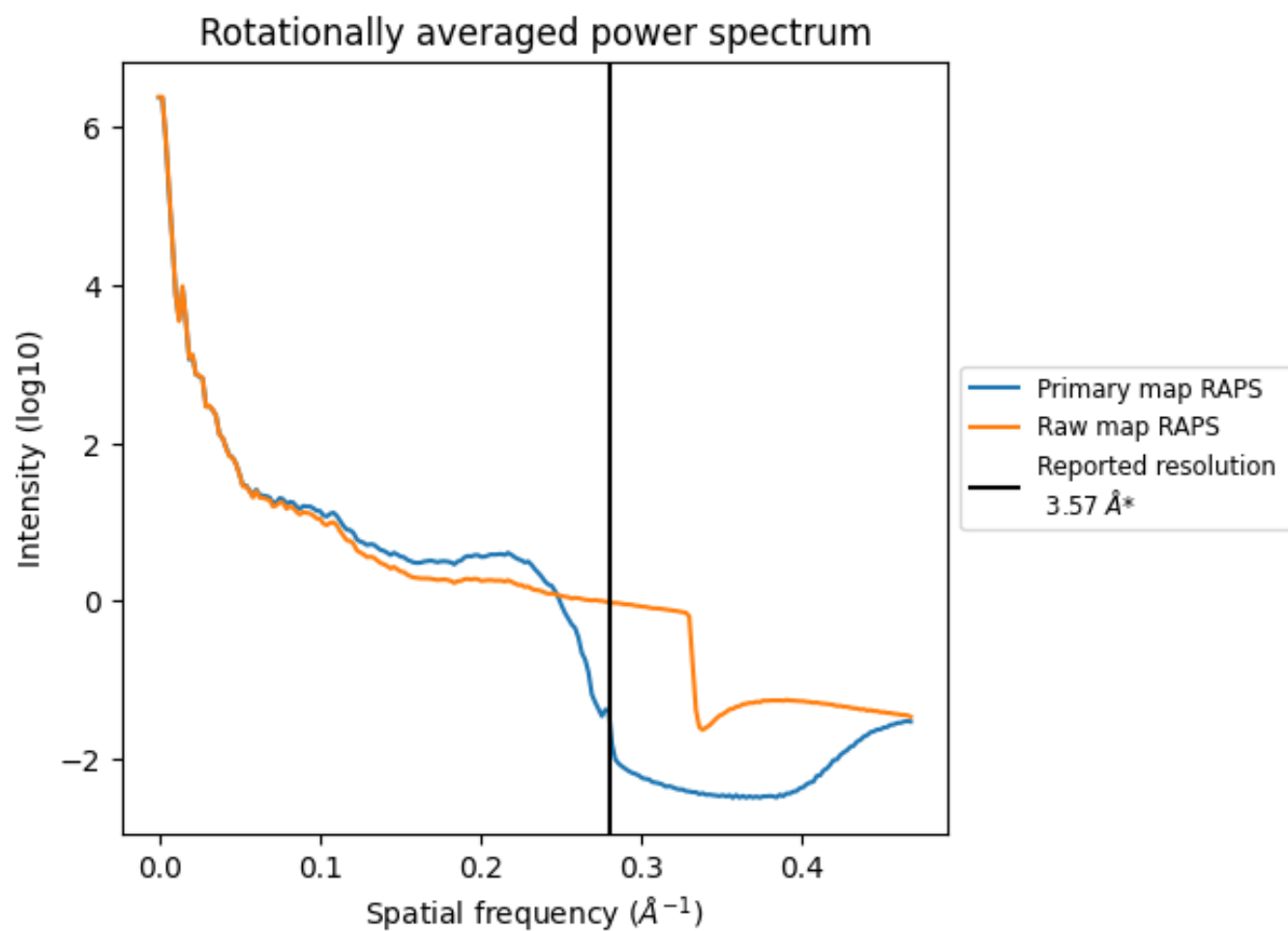
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9845 nm<sup>3</sup>; this corresponds to an approximate mass of 8893 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 ⓘ

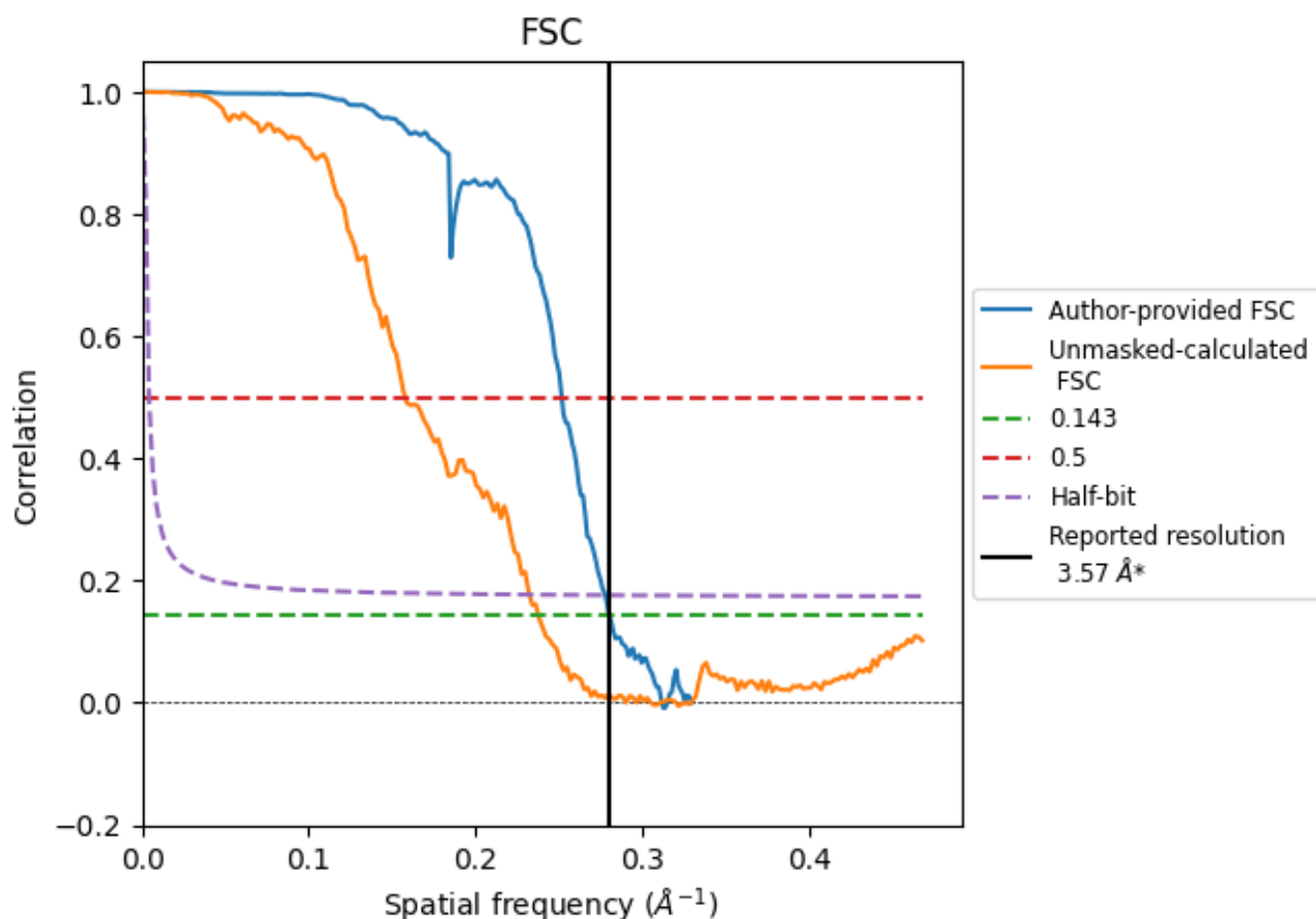


\*Reported resolution corresponds to spatial frequency of 0.280 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.280  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

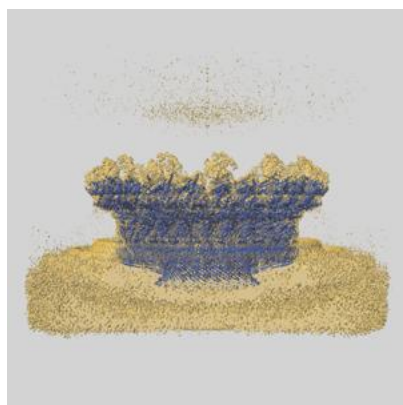
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	3.97	3.60
Unmasked-calculated*	4.21	6.34	4.30

\*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 4.21 differs from the reported value 3.57 by more than 10 %

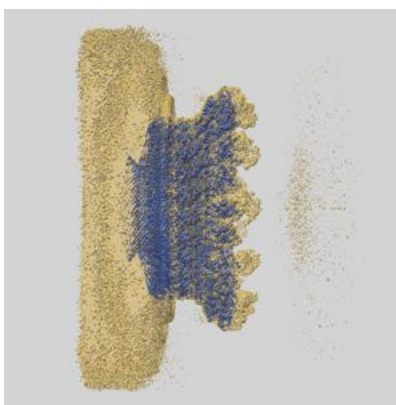
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72847 and PDB model 9YEC. Per-residue inclusion information can be found in section 3 on page 21.

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



X



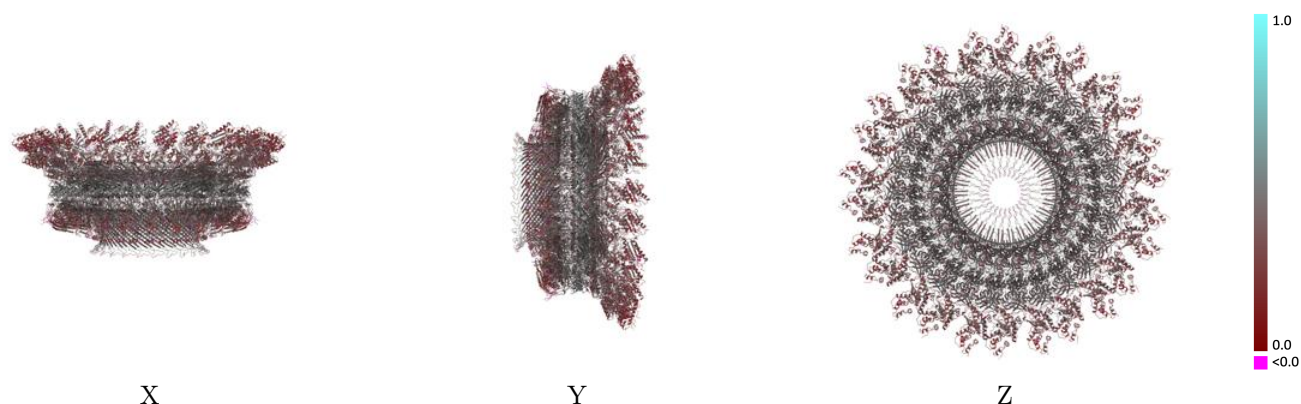
Y



Z

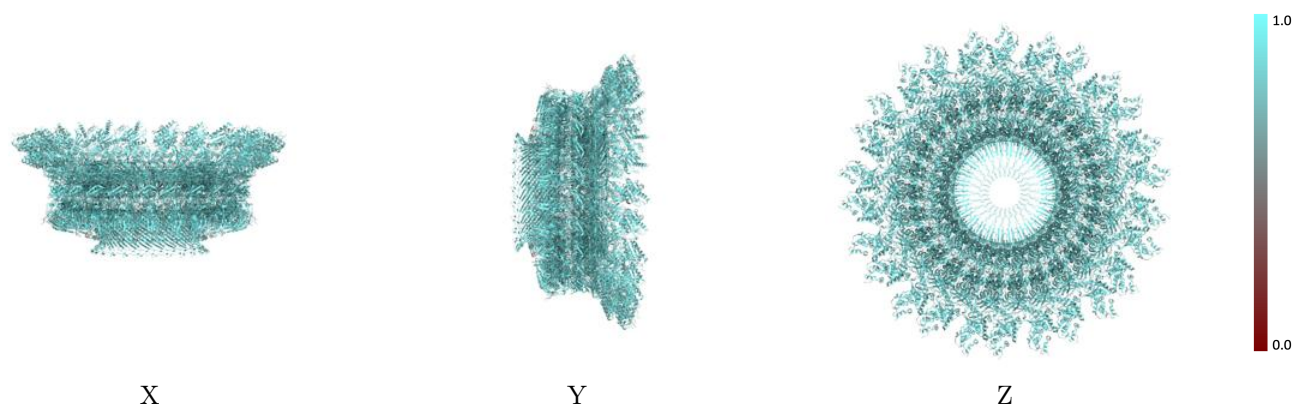
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



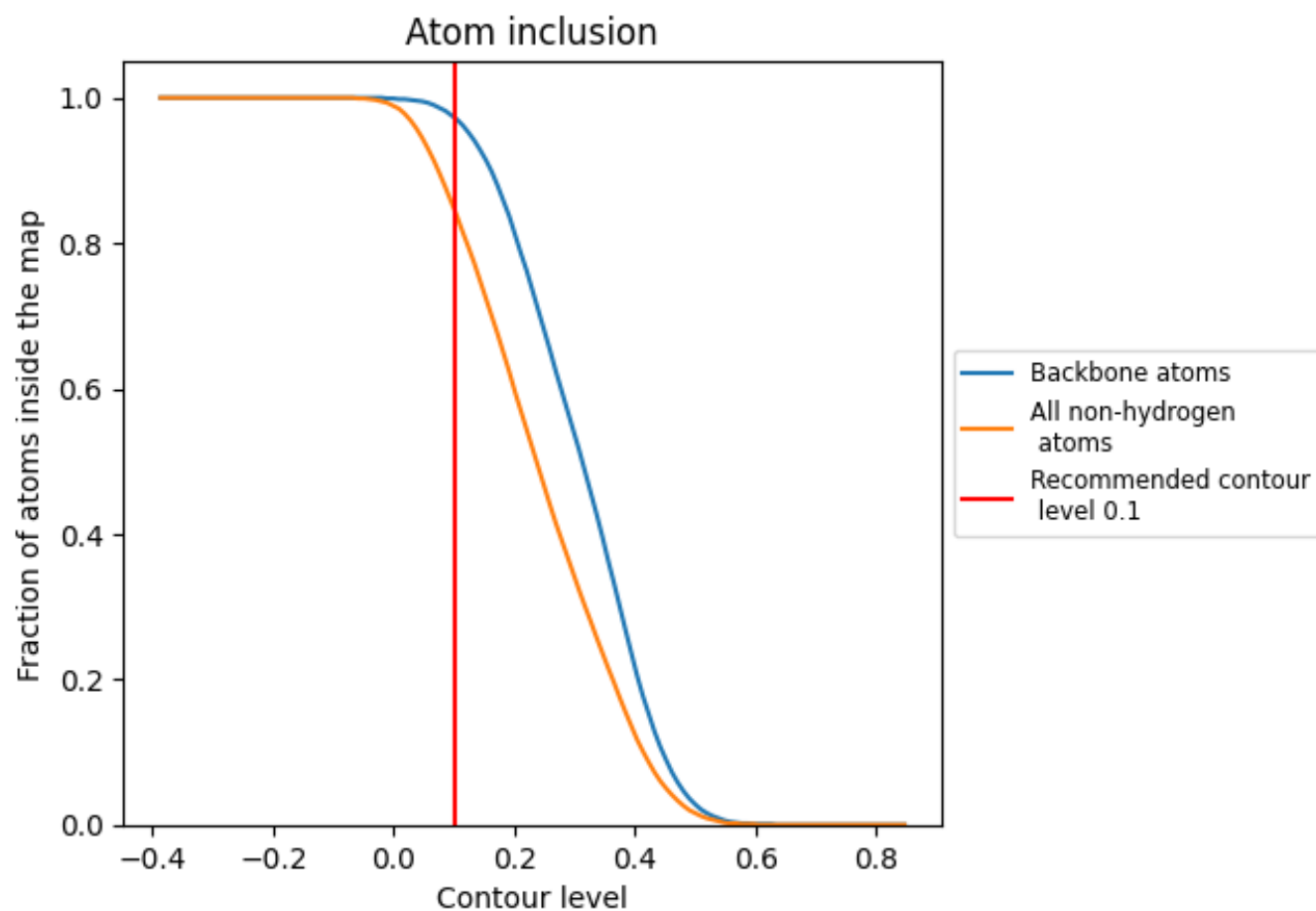
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 85% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.3710
Aa	 0.8530	 0.3850
Ab	 0.8530	 0.3870
Ac	 0.8540	 0.3860
Ad	 0.8560	 0.3880
Ae	 0.8550	 0.3850
Af	 0.8510	 0.3890
Ag	 0.8540	 0.3850
Ah	 0.8560	 0.3880
Ai	 0.8560	 0.3860
Aj	 0.8570	 0.3890
Ak	 0.8510	 0.3860
Al	 0.8530	 0.3890
Am	 0.8580	 0.3860
An	 0.8500	 0.3890
Ao	 0.8540	 0.3860
Ap	 0.8540	 0.3880
Aq	 0.8570	 0.3850
Ar	 0.8560	 0.3870
As	 0.8510	 0.3850
At	 0.8560	 0.3890
Au	 0.8560	 0.3850
Av	 0.8540	 0.3880
Aw	 0.8540	 0.3870
Ax	 0.8550	 0.3890
Ay	 0.8540	 0.3860
Az	 0.8510	 0.3860
Ba	 0.8760	 0.4220
Bb	 0.8740	 0.4240
Bc	 0.8770	 0.4260
Bd	 0.8790	 0.4260
Be	 0.8760	 0.4240
Bf	 0.8840	 0.4290
Bg	 0.8790	 0.4240
Bh	 0.8810	 0.4240




















































































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Chain	Atom inclusion	Q-score
Bi	 0.8770	 0.4250
Bj	 0.8770	 0.4240
Bk	 0.8760	 0.4220
Bl	 0.8840	 0.4260
Bm	 0.8750	 0.4220
Bn	 0.8750	 0.4230
Bo	 0.8740	 0.4220
Bp	 0.8800	 0.4240
Bq	 0.8730	 0.4220
Br	 0.8800	 0.4230
Bs	 0.8770	 0.4230
Bt	 0.8820	 0.4260
Bu	 0.8750	 0.4250
Bv	 0.8800	 0.4260
Bw	 0.8720	 0.4220
Bx	 0.8780	 0.4260
By	 0.8780	 0.4260
Bz	 0.8810	 0.4270
Ca	 0.8570	 0.3850
Cb	 0.8310	 0.3540
Cc	 0.8640	 0.3900
Cd	 0.8560	 0.3890
Ce	 0.8620	 0.3860
Cf	 0.8600	 0.3910
Cg	 0.8580	 0.3870
Ch	 0.8600	 0.3890
Ci	 0.8660	 0.3870
Cj	 0.8620	 0.3900
Ck	 0.8600	 0.3860
Cl	 0.8630	 0.3890
Cm	 0.8600	 0.3870
Cn	 0.8540	 0.3930
Co	 0.8620	 0.3900
Cp	 0.8600	 0.3900
Cq	 0.8600	 0.3870
Cr	 0.8550	 0.3860
Cs	 0.8620	 0.3880
Ct	 0.8520	 0.3900
Cu	 0.8580	 0.3880
Cv	 0.8590	 0.3890
Cw	 0.8590	 0.3900
Cx	 0.8590	 0.3920





















































































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Chain	Atom inclusion	Q-score
Cy	 0.8630	 0.3900
Cz	 0.8550	 0.3910
Da	 0.8370	 0.3490
Db	 0.8470	 0.3620
Dc	 0.8370	 0.3450
Dd	 0.8440	 0.3610
De	 0.8360	 0.3470
Df	 0.8460	 0.3580
Dg	 0.8390	 0.3450
Dh	 0.8450	 0.3600
Di	 0.8380	 0.3440
Dj	 0.8500	 0.3600
Dk	 0.8400	 0.3420
Dl	 0.8460	 0.3590
Dm	 0.8400	 0.3480
Dn	 0.8500	 0.3580
Do	 0.8360	 0.3450
Dp	 0.8500	 0.3590
Dq	 0.8350	 0.3470
Dr	 0.8450	 0.3580
Ds	 0.8380	 0.3490
Dt	 0.8530	 0.3590
Du	 0.8380	 0.3500
Dv	 0.8480	 0.3600
Dw	 0.8370	 0.3500
Dx	 0.8480	 0.3590
Dy	 0.8370	 0.3490
Dz	 0.8480	 0.3600
Ea	 0.8140	 0.2950
Eb	 0.7790	 0.2690
Ec	 0.8180	 0.2960
Ed	 0.7830	 0.2700
Ee	 0.8180	 0.2970
Ef	 0.7840	 0.2680
Eg	 0.8210	 0.2970
Eh	 0.7710	 0.2670
Ei	 0.8180	 0.2970
Ej	 0.7780	 0.2680
Ek	 0.8170	 0.2980
El	 0.7770	 0.2650
Em	 0.8140	 0.2980
En	 0.7740	 0.2670

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








































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Chain	Atom inclusion	Q-score
Eo	 0.8190	 0.2990
Ep	 0.7800	 0.2690
Eq	 0.8170	 0.2980
Er	 0.7790	 0.2680
Es	 0.8180	 0.2990
Et	 0.7760	 0.2700
Eu	 0.8170	 0.2970
Ev	 0.7740	 0.2720
Ew	 0.8170	 0.2970
Ex	 0.7760	 0.2710
Ey	 0.8190	 0.2970
Ez	 0.7740	 0.2720
Fa	 0.6340	 0.1810
Fb	 0.6100	 0.1600
Fc	 0.6340	 0.2110
Fd	 0.6100	 0.1480
Fe	 0.6500	 0.1800
Ff	 0.7480	 0.2190
Fg	 0.6260	 0.1910
Fh	 0.6580	 0.1840
Fi	 0.6340	 0.1870
Fj	 0.6420	 0.1800
Fk	 0.6260	 0.1800
Fl	 0.6260	 0.1730
Fm	 0.6260	 0.1660
Fn	 0.6340	 0.1680
Fo	 0.6260	 0.1810
Fp	 0.6910	 0.1840
Fq	 0.6340	 0.1840
Fr	 0.6990	 0.2050
Fs	 0.6500	 0.1750
Ft	 0.6750	 0.2030
Fu	 0.6670	 0.2130
Fv	 0.6580	 0.1780
Fw	 0.6180	 0.1990
Fx	 0.6500	 0.1880
Fy	 0.6340	 0.1980
Fz	 0.6340	 0.1690
Ga	 0.7820	 0.2530
Gb	 0.7730	 0.2640
Gc	 0.7640	 0.2040
Gd	 0.7000	 0.2580

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Chain	Atom inclusion	Q-score
Ge	 0.7730	 0.2610
Gf	 0.7820	 0.2640
Gg	 0.7460	 0.2620
Gh	 0.7270	 0.2650
Gi	 0.7460	 0.2300
Gj	 0.7460	 0.2660
Gk	 0.7360	 0.2370
Gl	 0.8000	 0.2990
Gm	 0.8090	 0.2590
Gn	 0.7360	 0.2760
Go	 0.7270	 0.2270
Gp	 0.7640	 0.2660
Gq	 0.7000	 0.1820
Gr	 0.7820	 0.2760
Gs	 0.7360	 0.2340
Gt	 0.7820	 0.2580
Gu	 0.7540	 0.2520
Gv	 0.7460	 0.2760
Gw	 0.7000	 0.1580
Gx	 0.7360	 0.2630
Gy	 0.7730	 0.2460
Gz	 0.7640	 0.2680