



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:37 AM UTC

PDB ID : 6K3I / pdb_00006k3i
EMDB ID : EMD-9909
Title : Salmonella hook in curved state - 66 subunit models
Authors : Shibata, S.; Matsunami, H.; Wolf, M.; Aizawa, S.
Deposited on : 2019-05-19
Resolution : 2.86 Å(reported)
Based on initial model : 1WLG

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

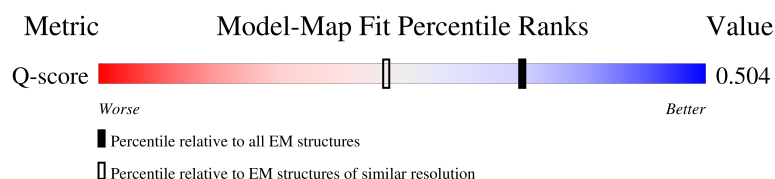
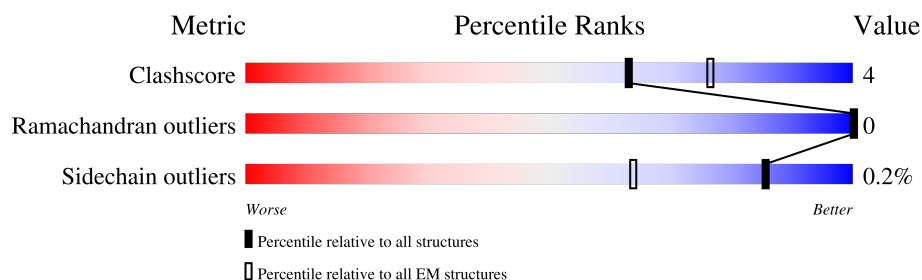
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

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

Mol	Chain	Length	Quality of chain
1	AA	402	25% 88% 12%
1	AB	402	10% 91% 9%
1	AC	402	11% 89% 11%
1	AD	402	17% 88% 12%

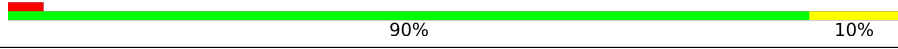
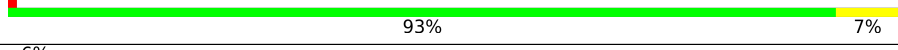
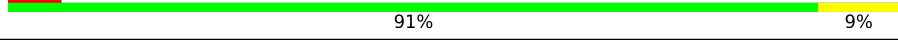
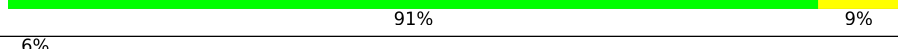
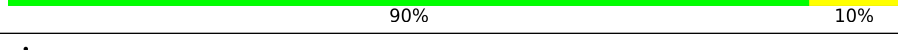
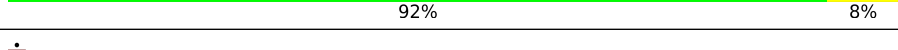
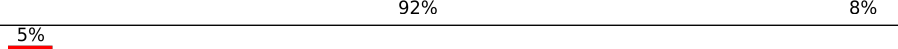
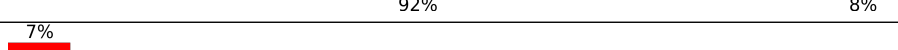
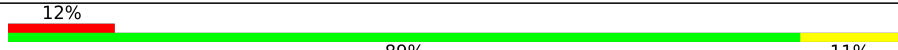
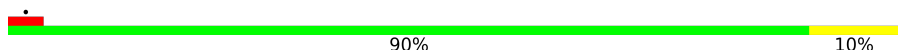
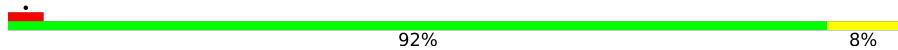
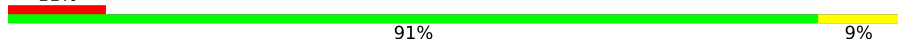
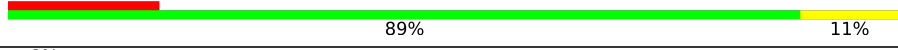
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Mol	Chain	Length	Quality of chain
1	AE	402	
1	AF	402	
1	AG	402	
1	AH	402	
1	AI	402	
1	AJ	402	
1	AK	402	
1	BA	402	
1	BB	402	
1	BC	402	
1	BD	402	
1	BE	402	
1	BF	402	
1	BG	402	
1	BH	402	
1	BI	402	
1	BJ	402	
1	BK	402	
1	CA	402	
1	CB	402	
1	CC	402	
1	CD	402	
1	CE	402	
1	CF	402	
1	CG	402	

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Mol	Chain	Length	Quality of chain
1	CH	402	 90%10%
1	CI	402	 86%14%
1	CJ	402	 90%10%
1	CK	402	 93%7%
1	DA	402	 6%91%9%
1	DB	402	 91%9%
1	DC	402	 6%90%10%
1	DD	402	 92%8%
1	DE	402	 92%8%
1	DF	402	 5%92%8%
1	DG	402	 7%88%12%
1	DH	402	 87%13%
1	DI	402	 6%89%11%
1	DJ	402	 5%89%11%
1	DK	402	 90%10%
1	EA	402	 12%89%11%
1	EB	402	 7%86%14%
1	EC	402	 90%10%
1	ED	402	 92%8%
1	EE	402	 6%88%11%
1	EF	402	 11%91%9%
1	EG	402	 17%89%11%
1	EH	402	 8%88%12%
1	EI	402	 8%89%11%
1	EJ	402	 10%89%11%

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Mol	Chain	Length	Quality of chain
1	EK	402	
1	FA	402	
1	FB	402	
1	FC	402	
1	FD	402	
1	FE	402	
1	FF	402	
1	FG	402	
1	FH	402	
1	FI	402	
1	FJ	402	
1	FK	402	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 195294 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 hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	AK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	BK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	CK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	ED	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

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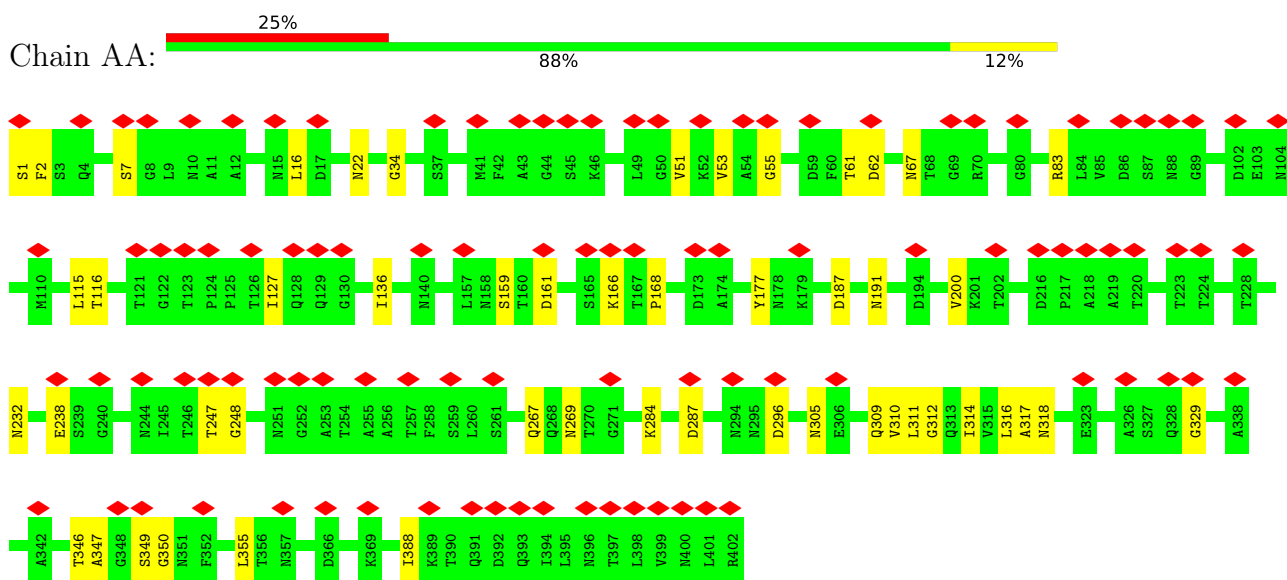
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Mol	Chain	Residues	Atoms					AltConf	Trace
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			2959	1820	511	620	8		
1	FF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

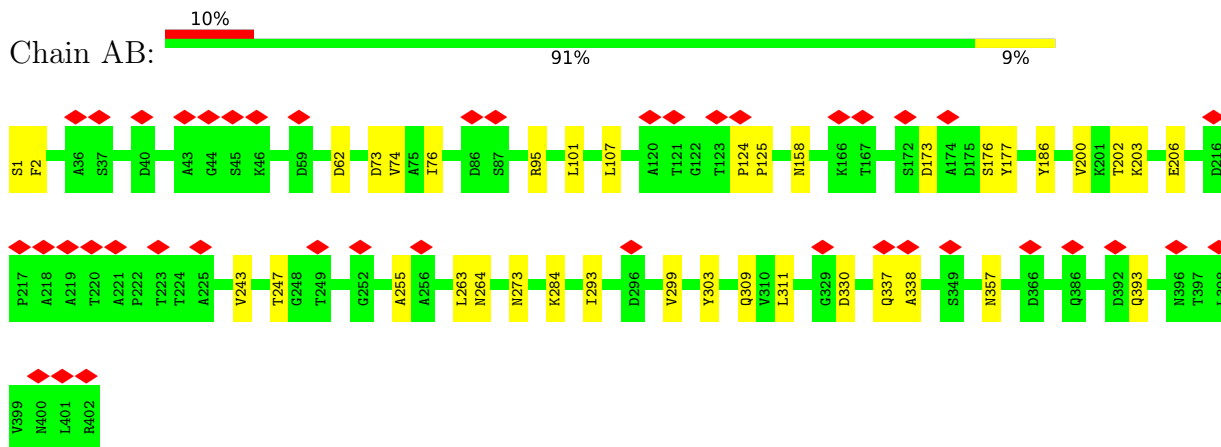
3 Residue-property plots

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

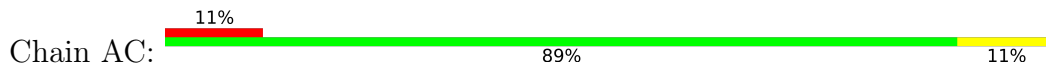
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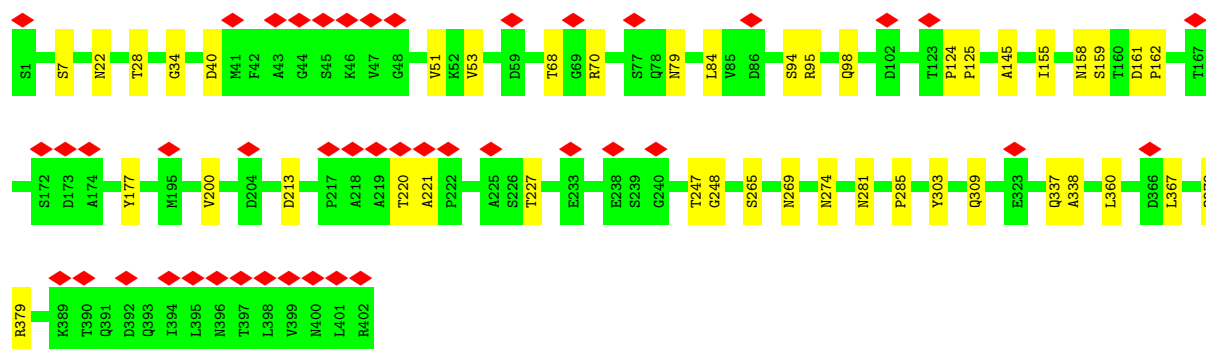


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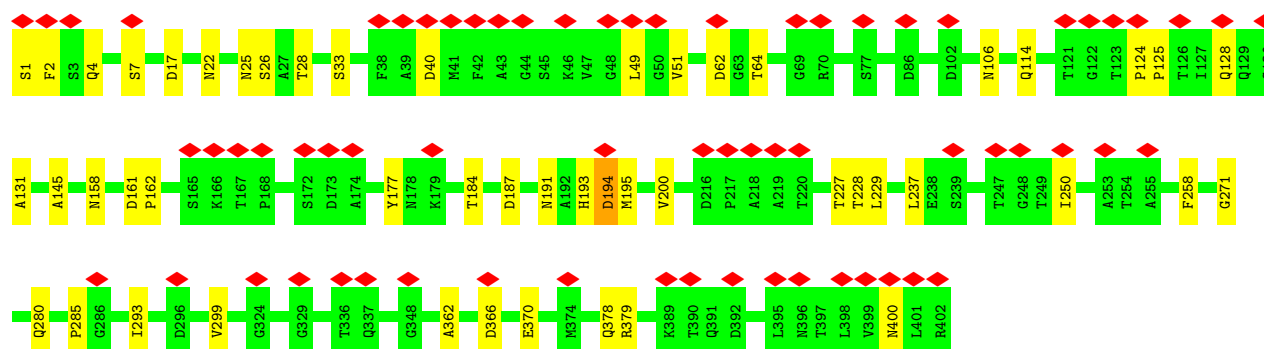


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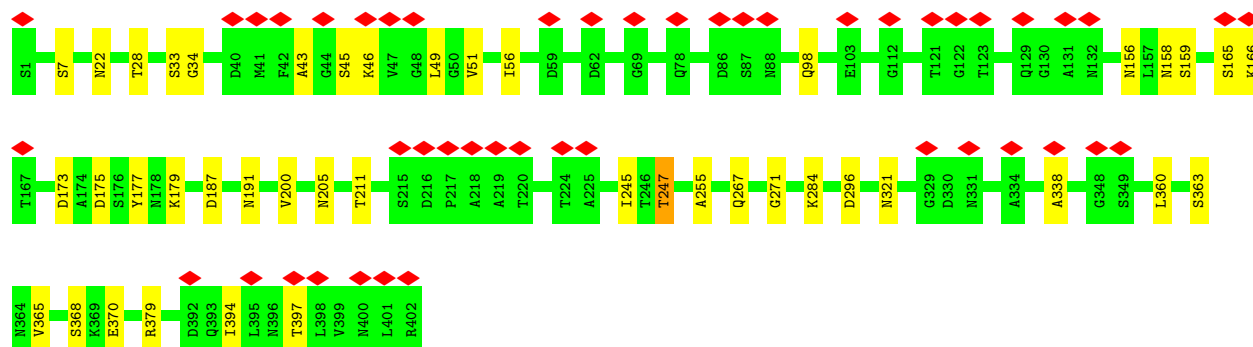




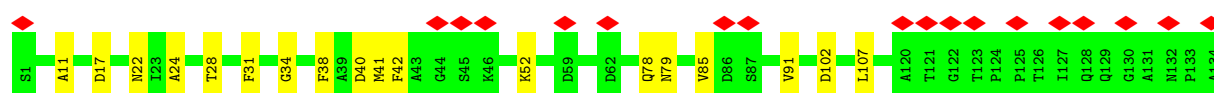
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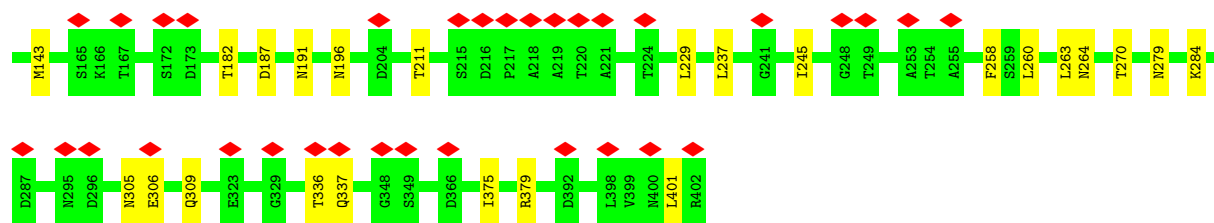


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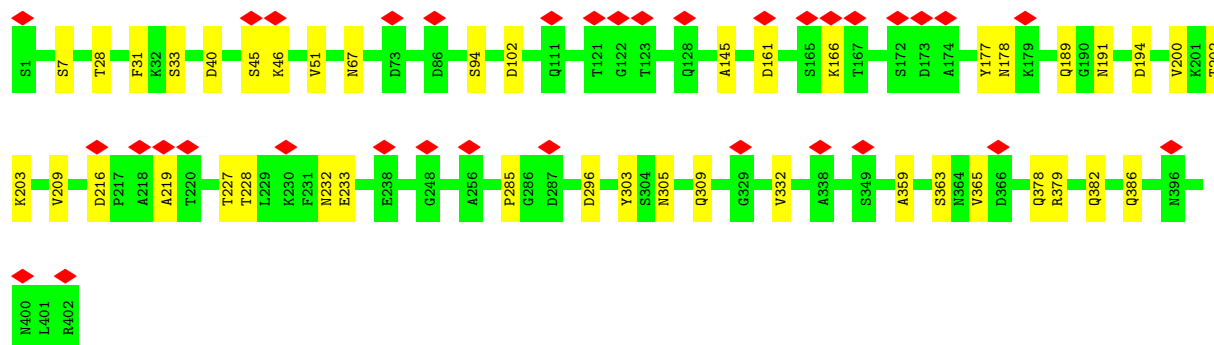
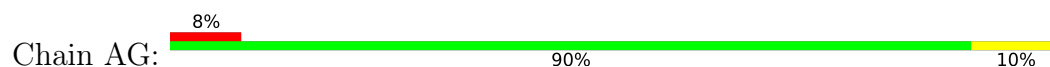


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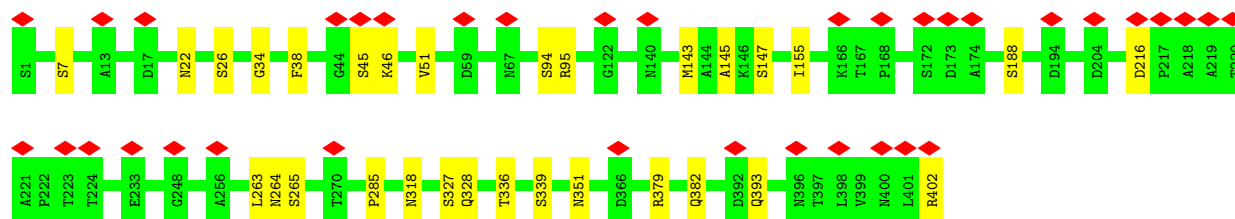




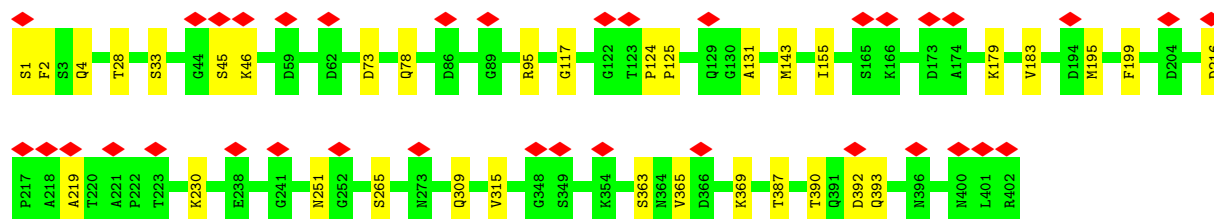
• Molecule 1: Flagellar hook protein FlgE



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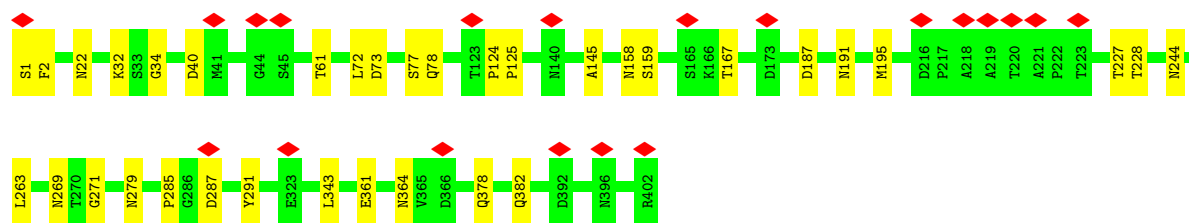


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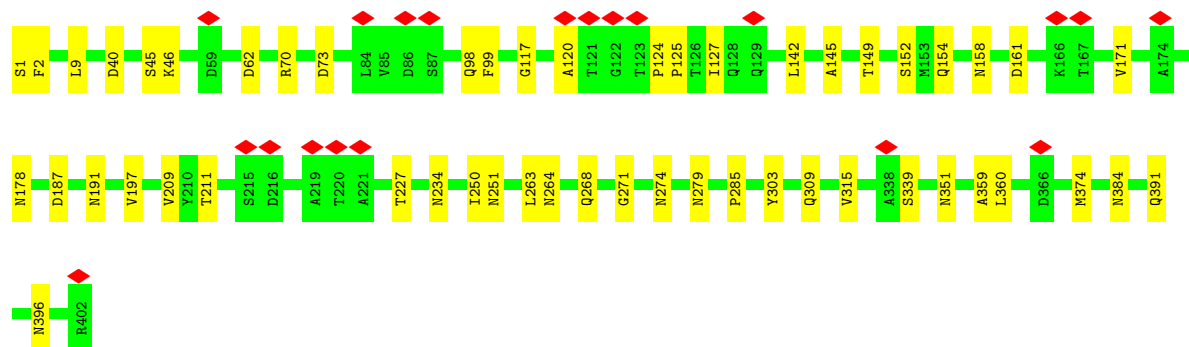
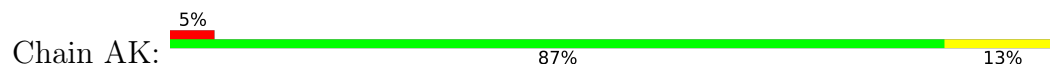


• Molecule 1: Flagellar hook protein FlgE

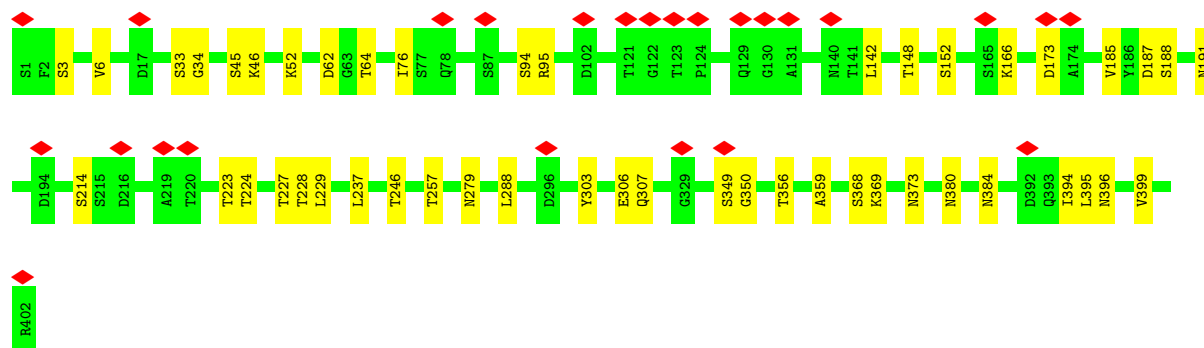
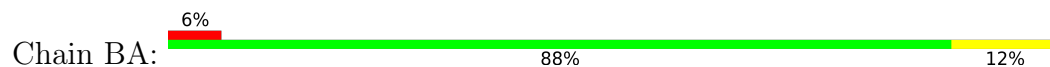




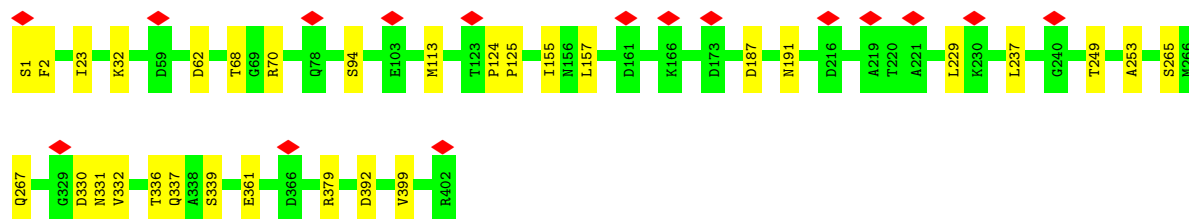
- Molecule 1: Flagellar hook protein FlgE



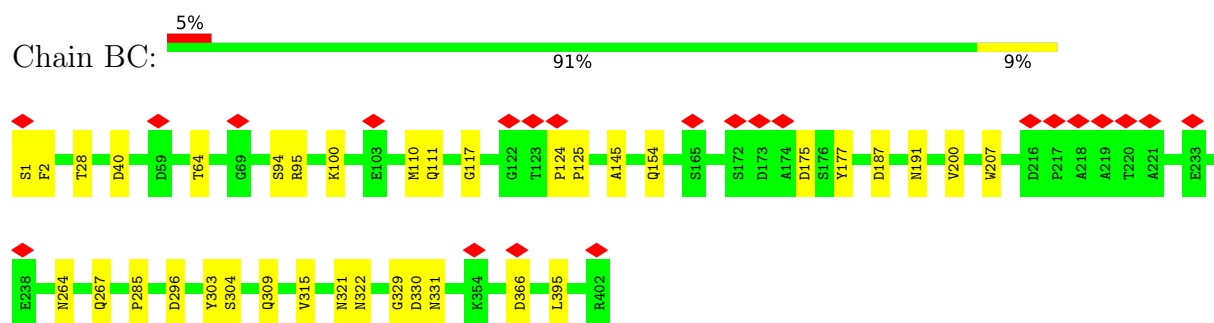
- Molecule 1: Flagellar hook protein FlgE



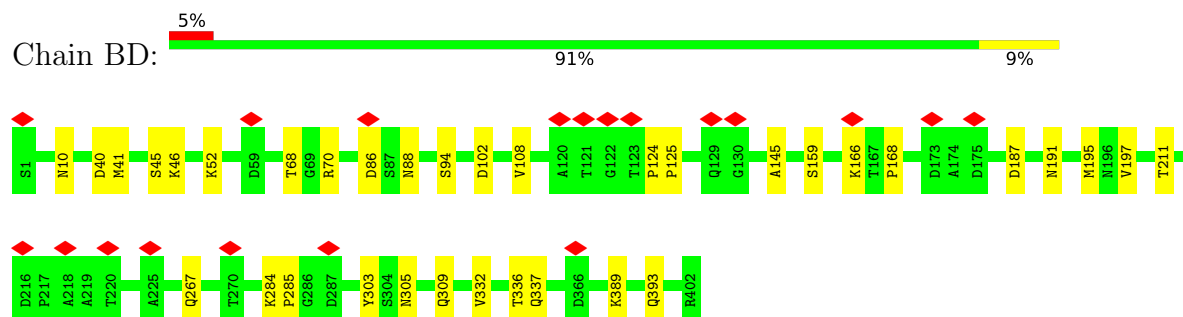
- Molecule 1: Flagellar hook protein FlgE



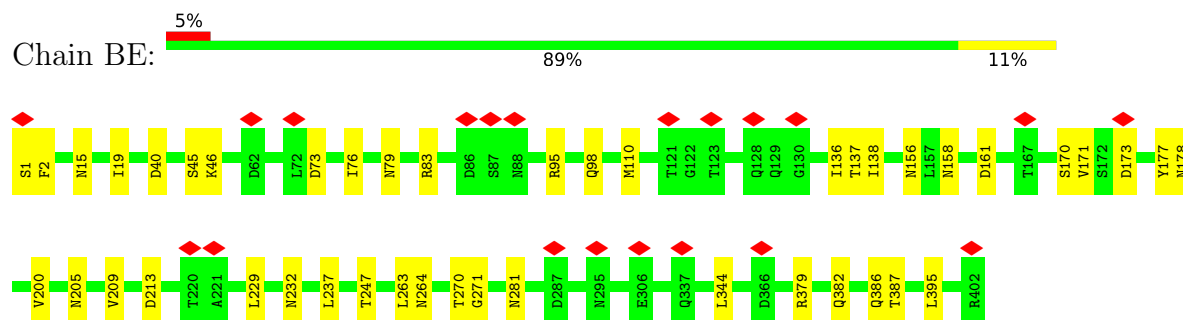
- Molecule 1: Flagellar hook protein FlgE



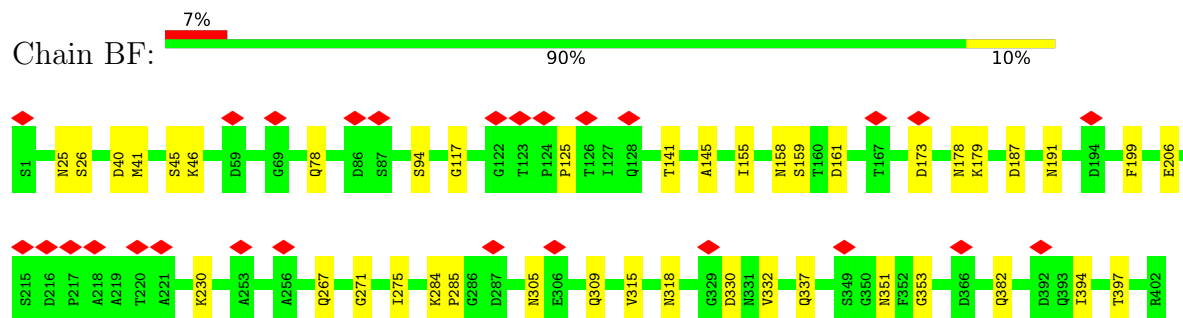
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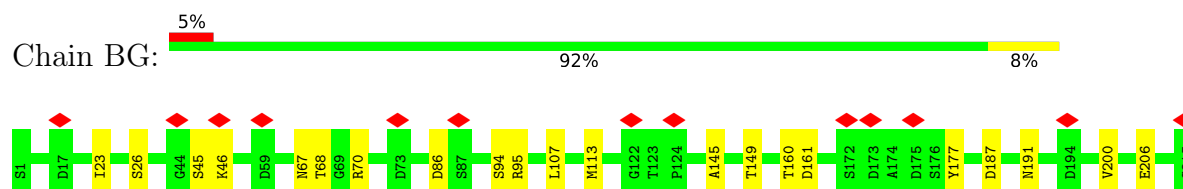
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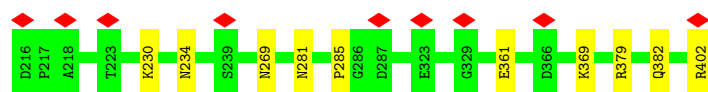


- Molecule 1: Flagellar hook protein FlgE

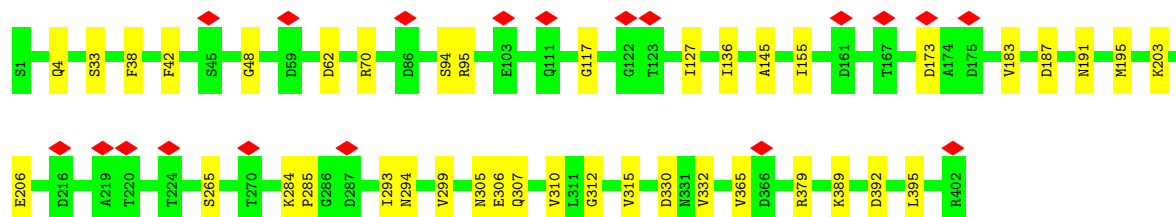
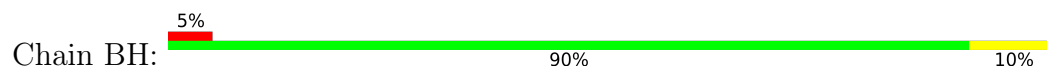


- Molecule 1: Flagellar hook protein FlgE

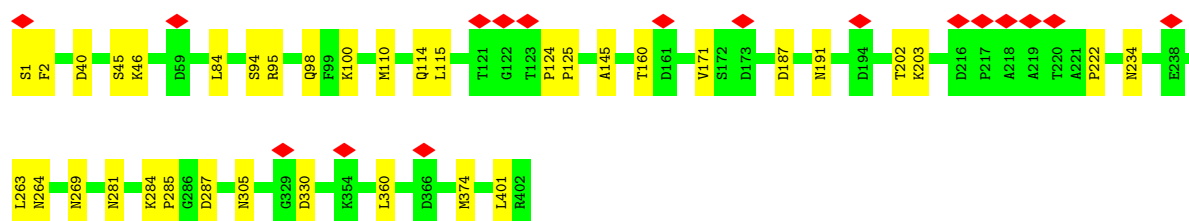




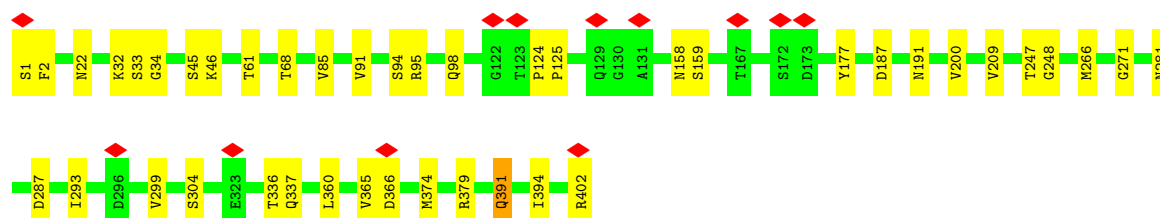
- Molecule 1: Flagellar hook protein FlgE



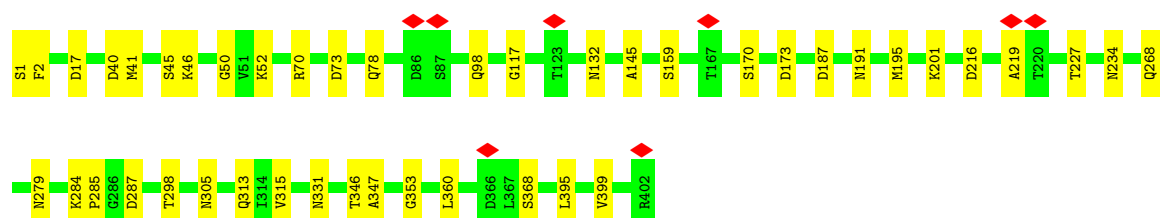
- Molecule 1: Flagellar hook protein FlgE



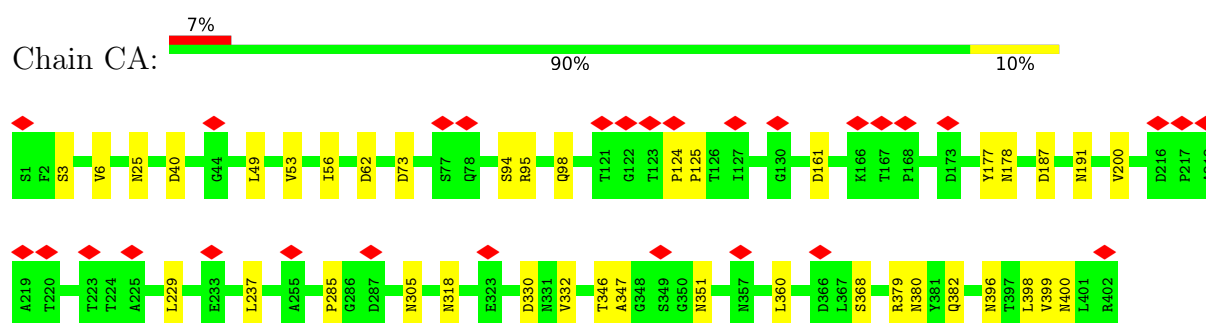
- Molecule 1: Flagellar hook protein FlgE



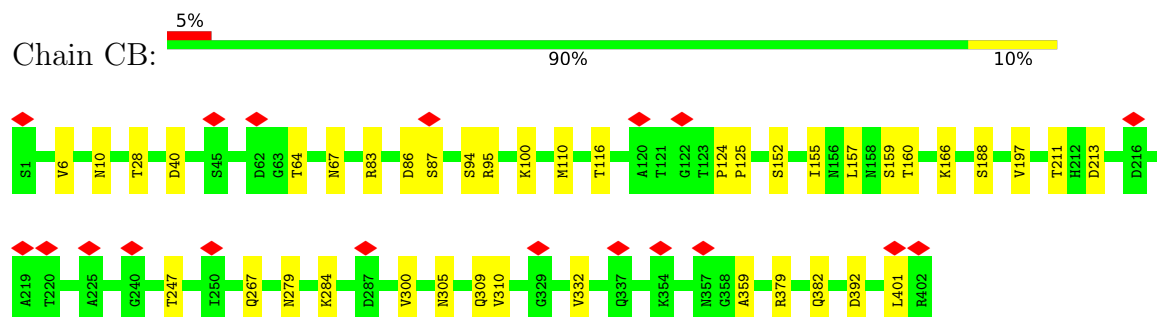
- Molecule 1: Flagellar hook protein FlgE



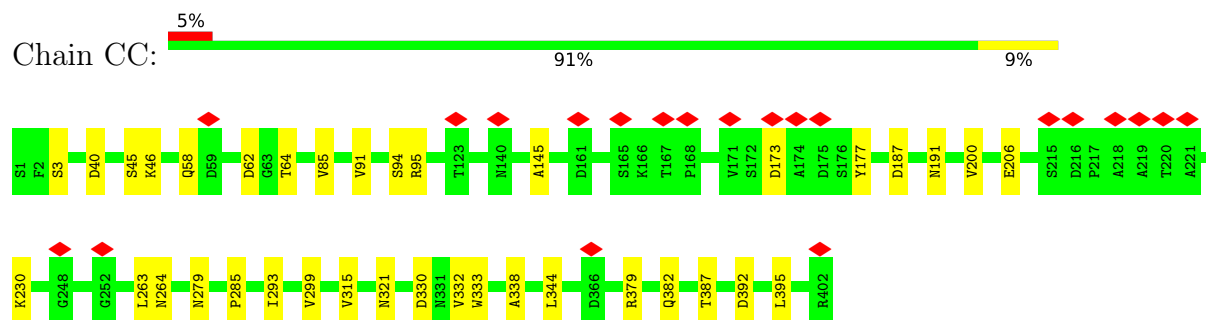
- Molecule 1: Flagellar hook protein FlgE



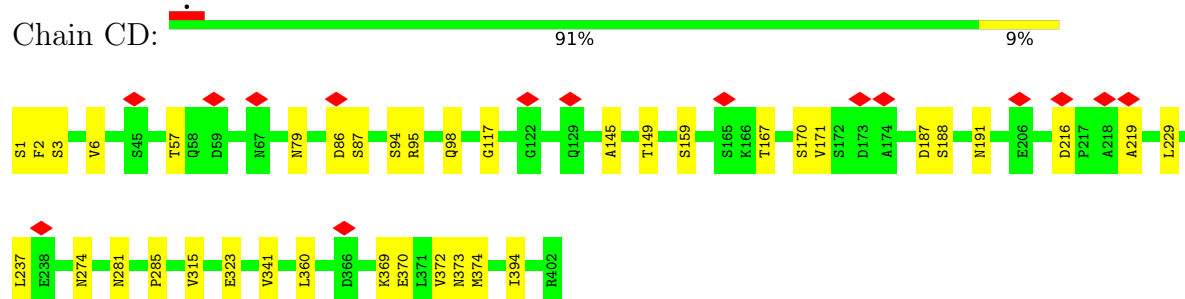
- Molecule 1: Flagellar hook protein FlgE



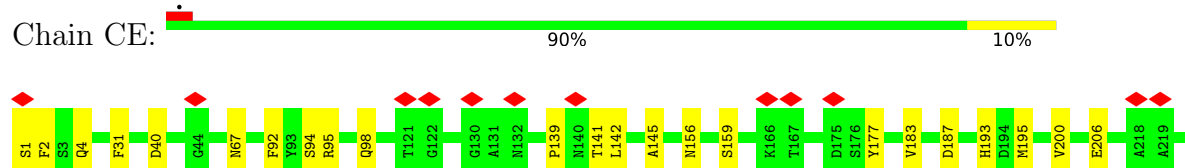
- Molecule 1: Flagellar hook protein FlgE



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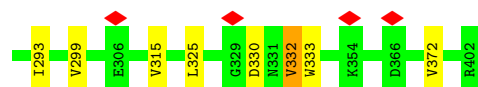


- Molecule 1: Flagellar hook protein FlgE

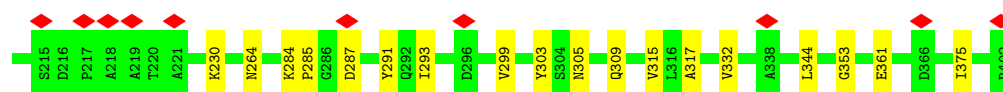
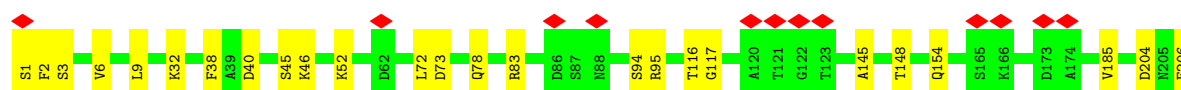
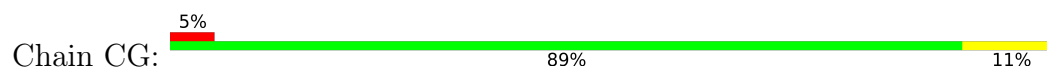




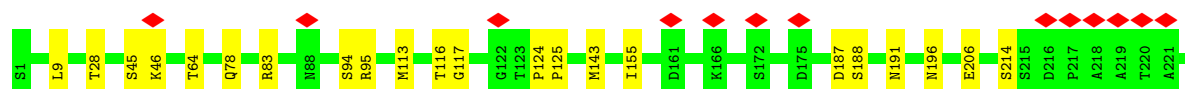
- Molecule 1: Flagellar hook protein FlgE



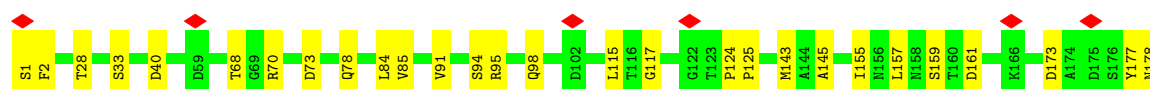
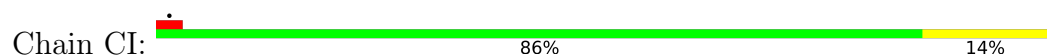
- Molecule 1: Flagellar hook protein FlgE



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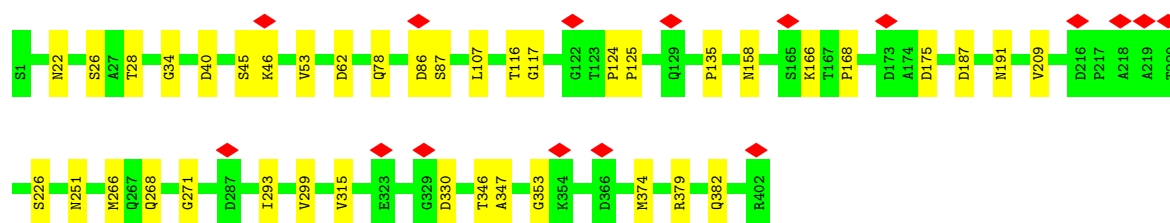


- Molecule 1: Flagellar hook protein FlgE

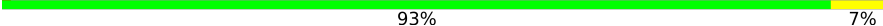


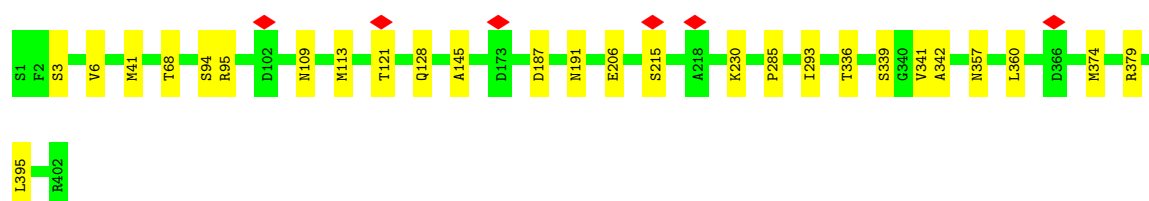
- Molecule 1: Flagellar hook protein FlgE

Chain CJ:  90% 10%



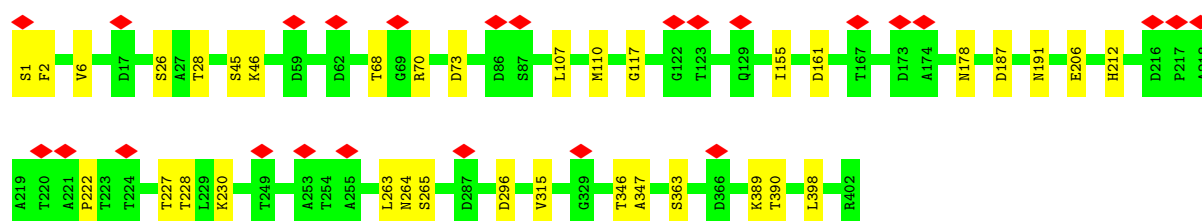
• Molecule 1: Flagellar hook protein FlgE

Chain CK:  93% 7%



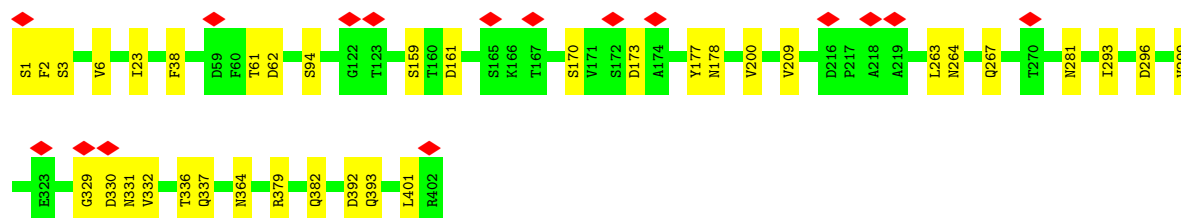
• Molecule 1: Flagellar hook protein FlgE

Chain DA:  91% 6% 9%



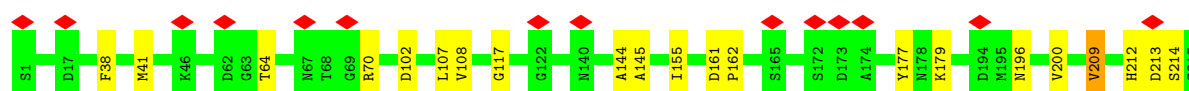
• Molecule 1: Flagellar hook protein FlgE

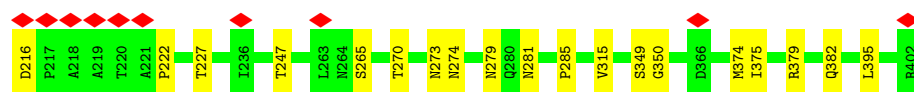
Chain DB:  91% 6% 9%



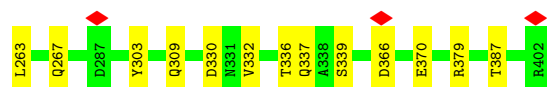
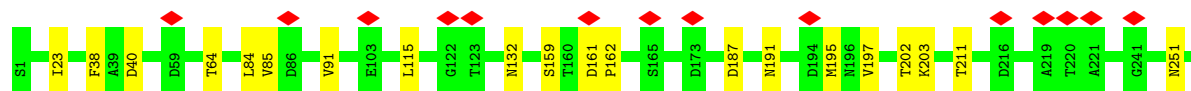
• Molecule 1: Flagellar hook protein FlgE

Chain DC:  90% 6% 10%

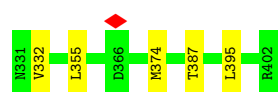
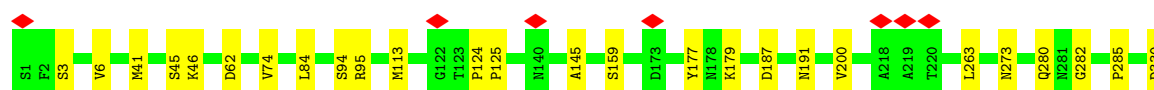




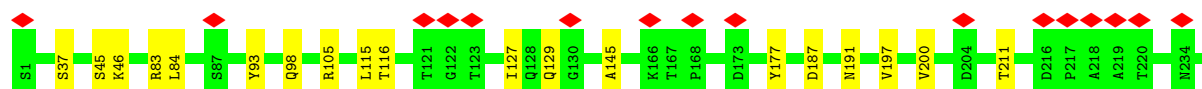
- Molecule 1: Flagellar hook protein FlgE



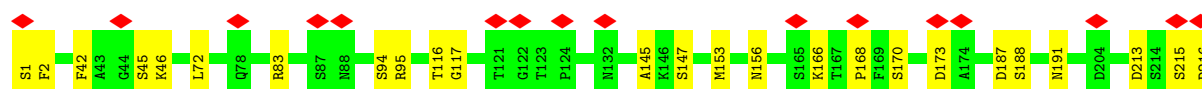
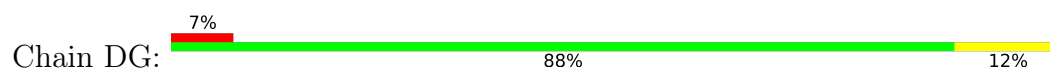
- Molecule 1: Flagellar hook protein FlgE



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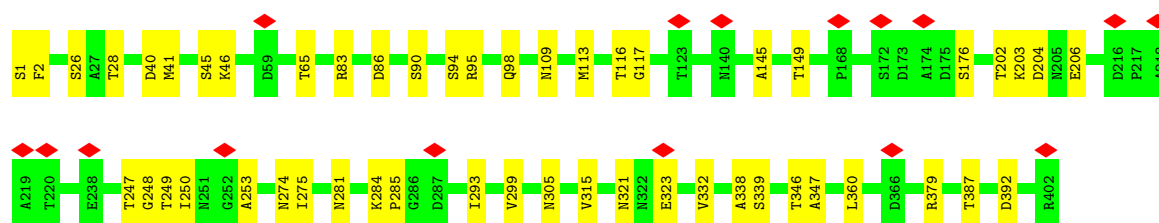


- Molecule 1: Flagellar hook protein FlgE



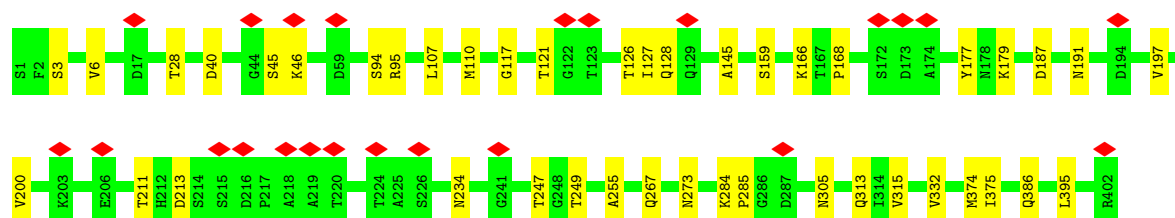
- Molecule 1: Flagellar hook protein FlgE

Chain DH:  87% 13%



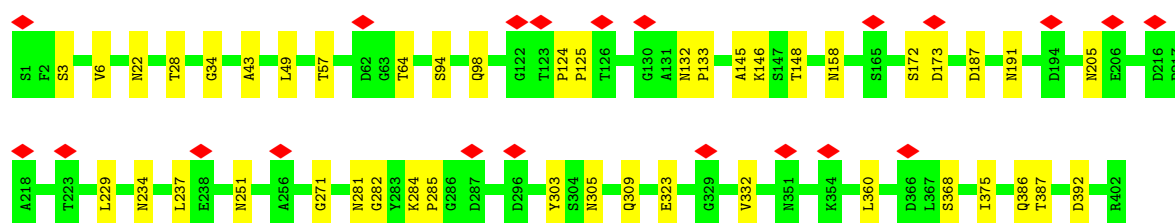
• Molecule 1: Flagellar hook protein FlgE

Chain DI:  6% 89% 11%



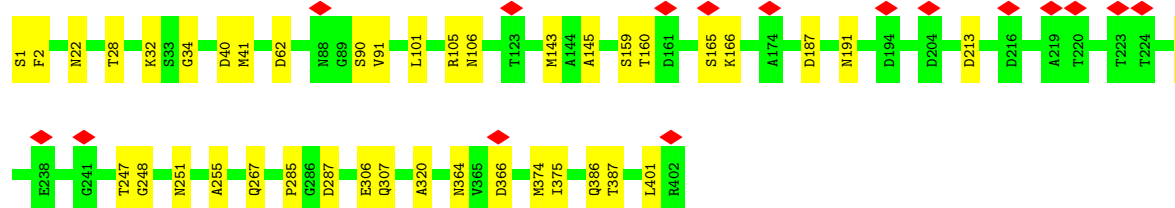
• Molecule 1: Flagellar hook protein FlgE

Chain DJ:  5% 89% 11%



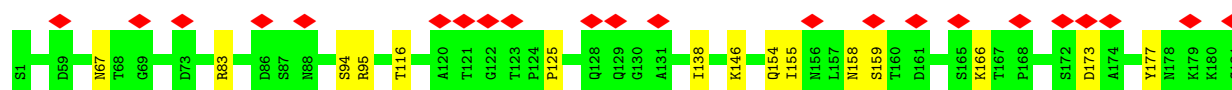
• Molecule 1: Flagellar hook protein FlgE

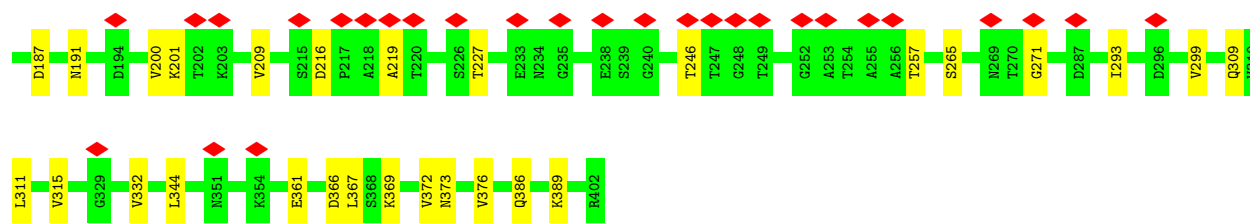
Chain DK:  90% 10%



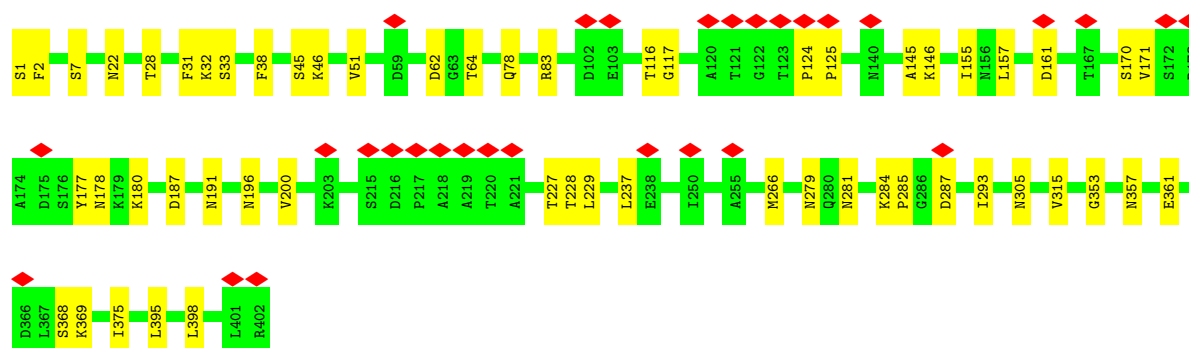
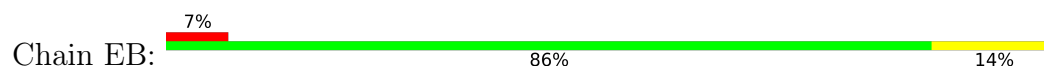
• Molecule 1: Flagellar hook protein FlgE

Chain EA:  12% 89% 11%

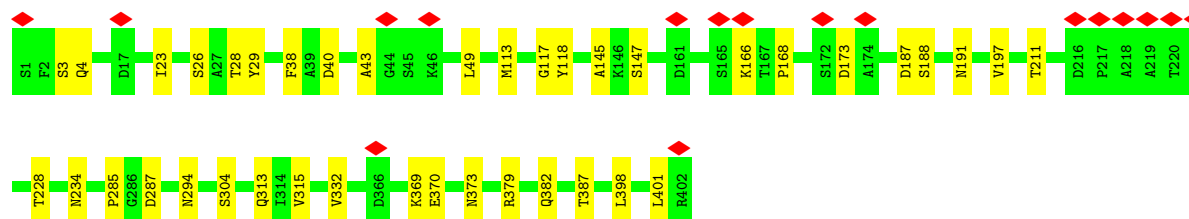




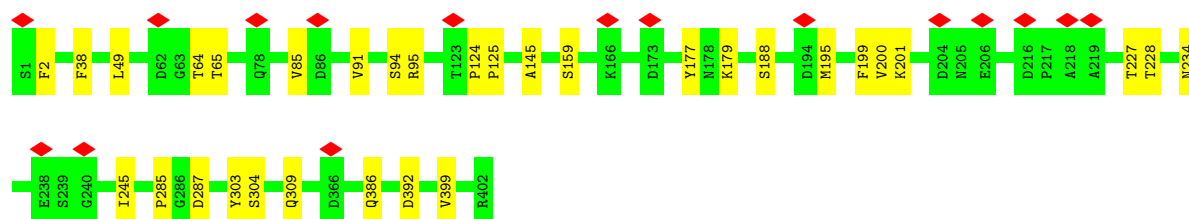
• Molecule 1: Flagellar hook protein FlgE



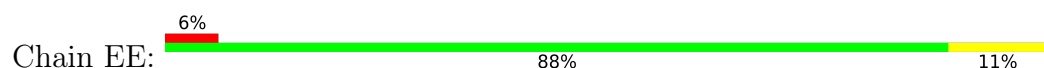
• Molecule 1: Flagellar hook protein FlgE

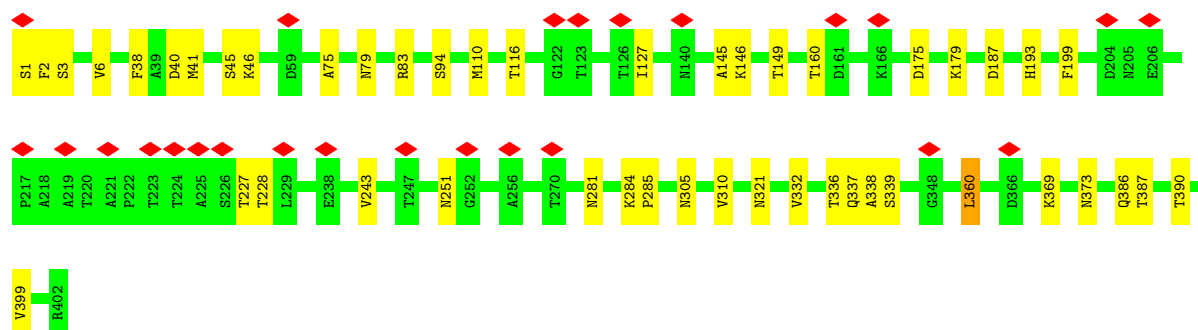


• Molecule 1: Flagellar hook protein FlgE

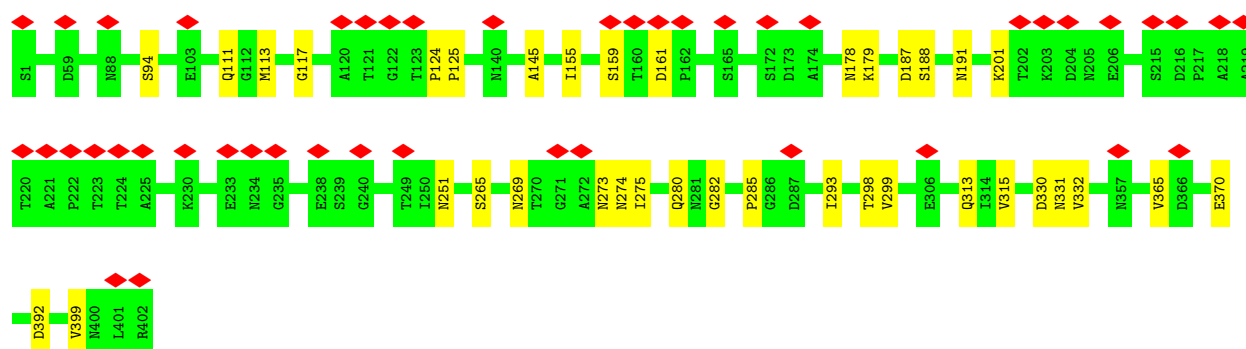
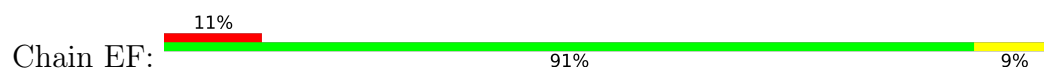


• Molecule 1: Flagellar hook protein FlgE

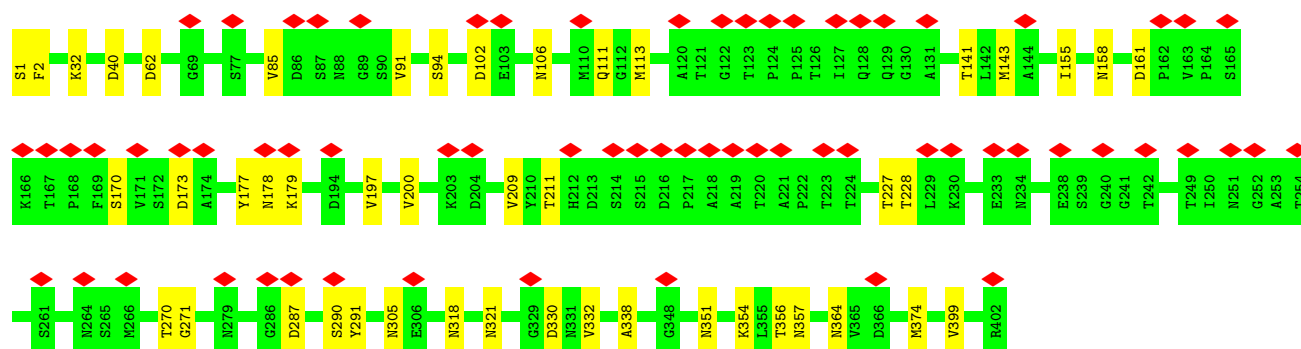
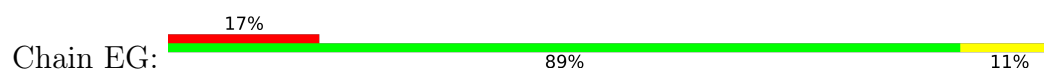




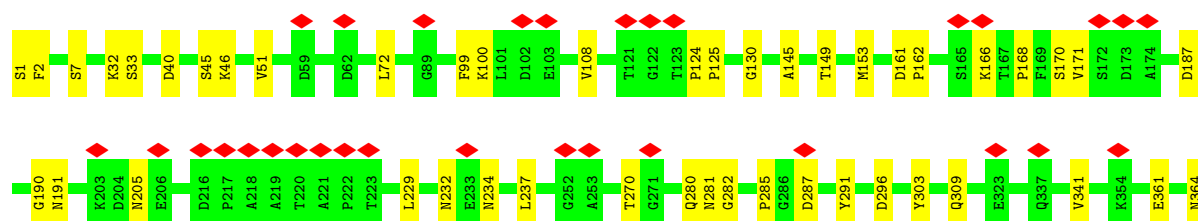
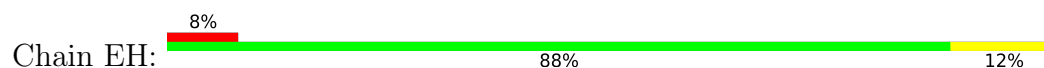
- Molecule 1: Flagellar hook protein FlgE



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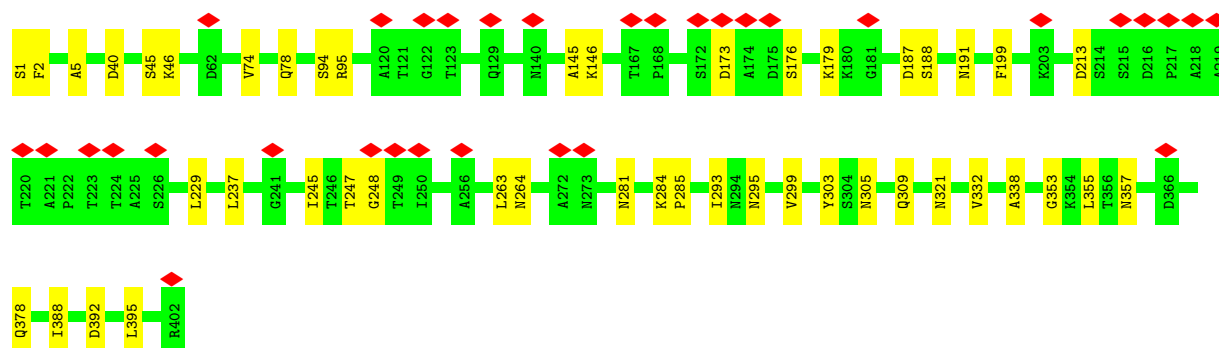
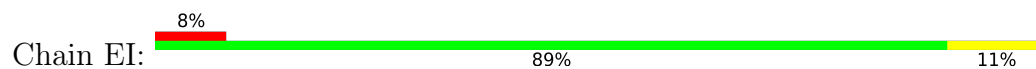


- Molecule 1: Flagellar hook protein FlgE

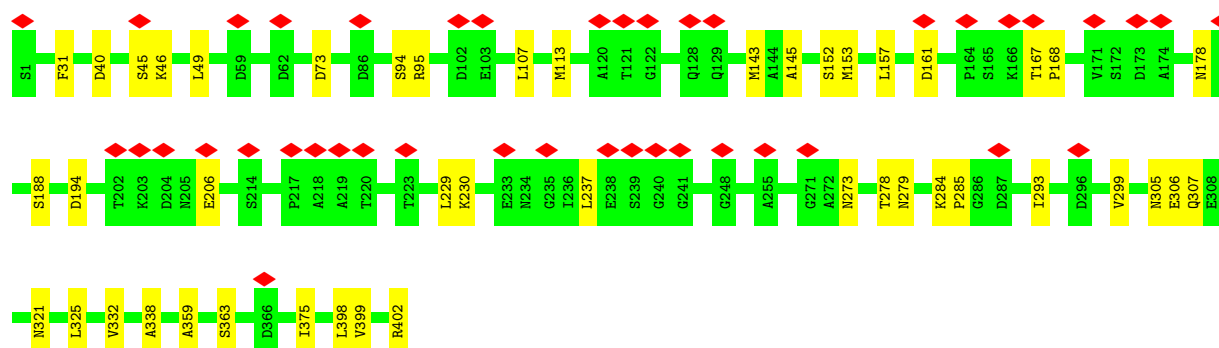
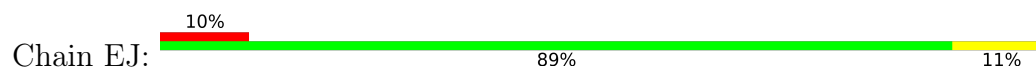




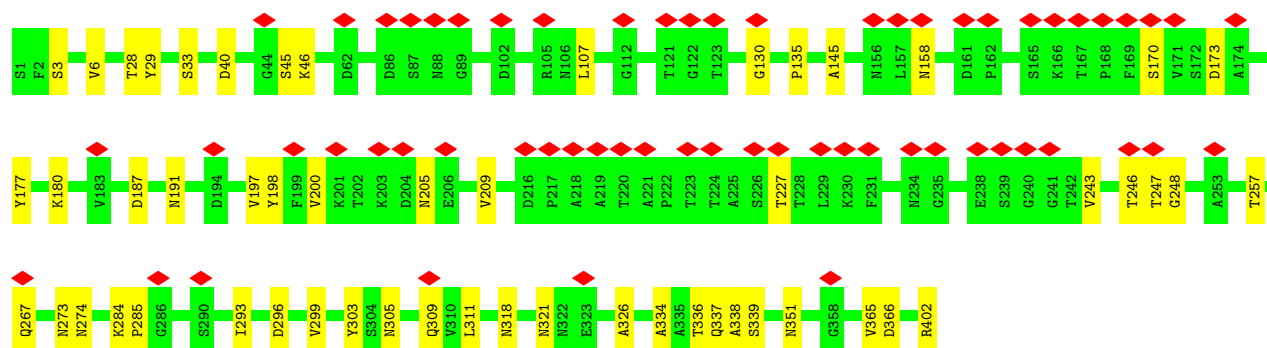
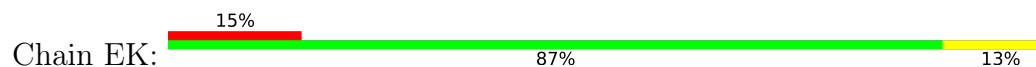
• Molecule 1: Flagellar hook protein FlgE



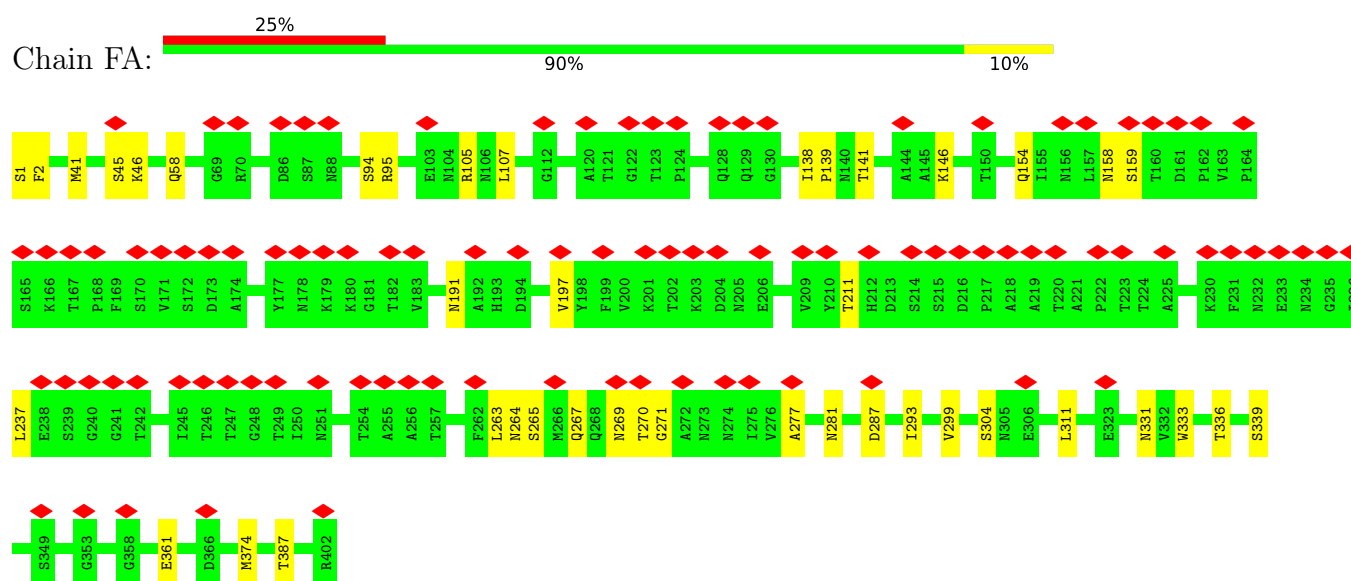
• Molecule 1: Flagellar hook protein FlgE



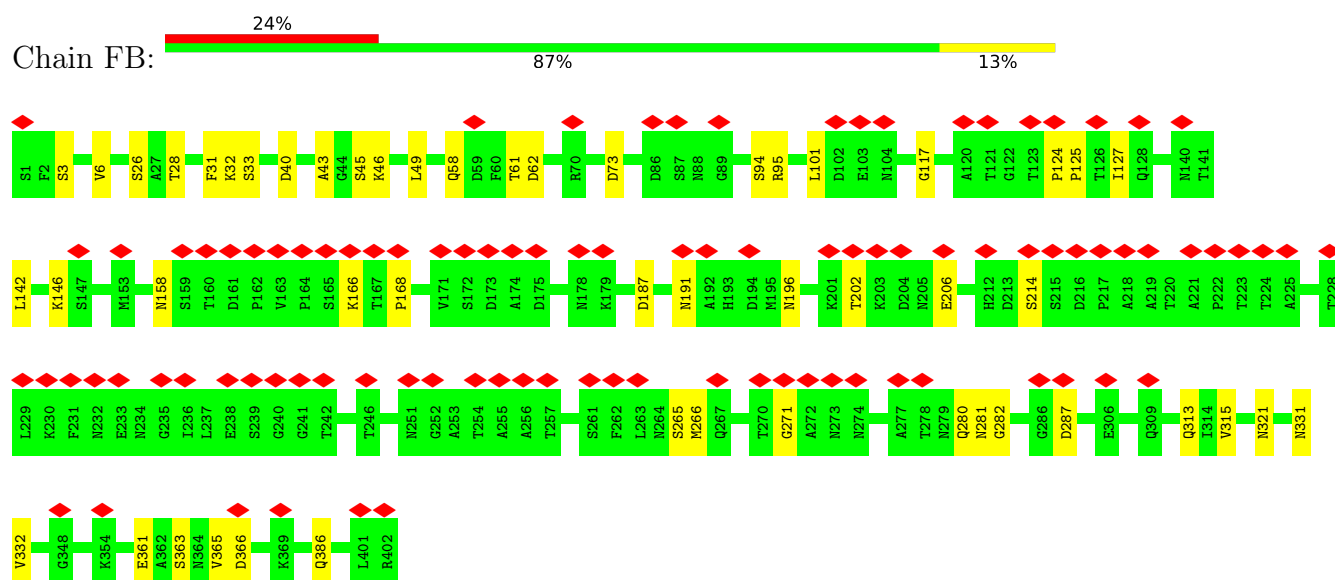
• Molecule 1: Flagellar hook protein FlgE



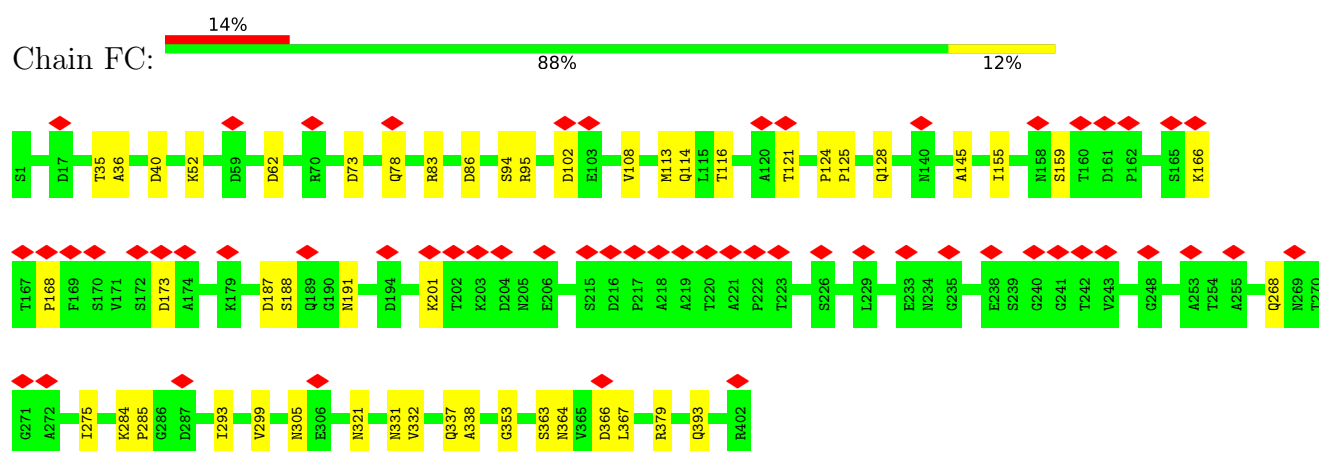
• Molecule 1: Flagellar hook protein FlgE



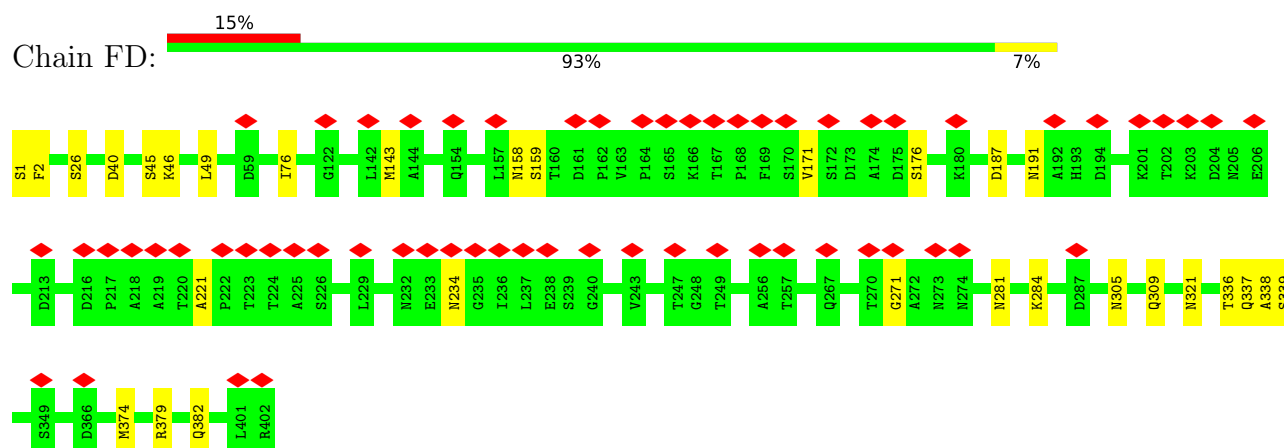
• Molecule 1: Flagellar hook protein FlgE



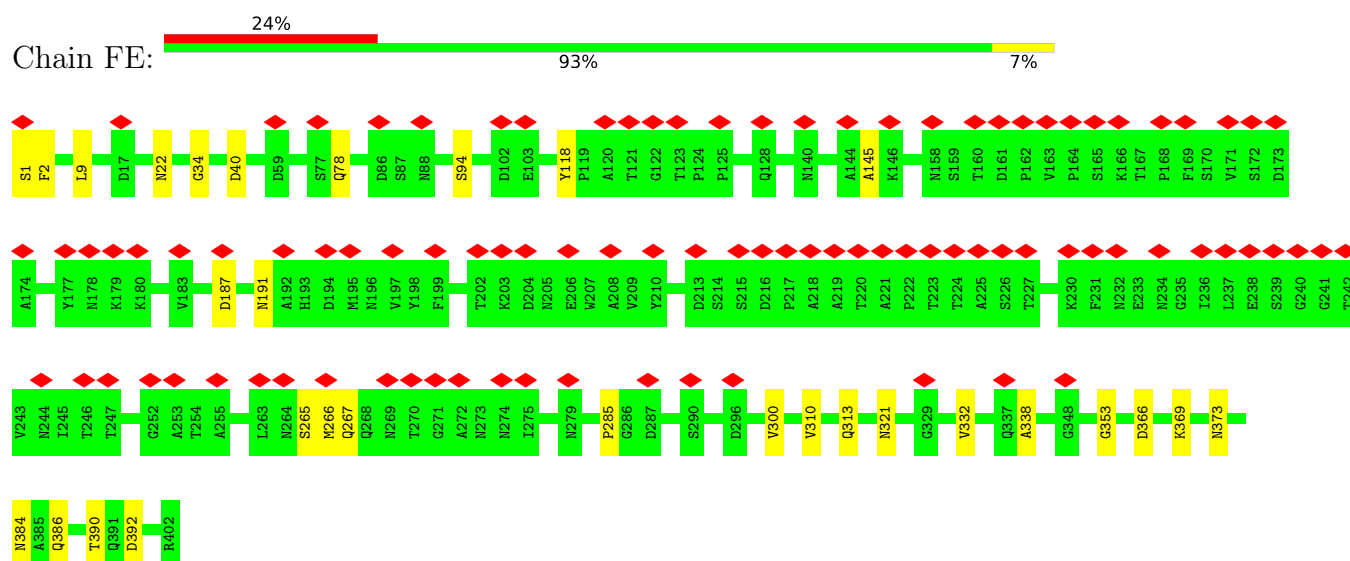
• Molecule 1: Flagellar hook protein FlgE



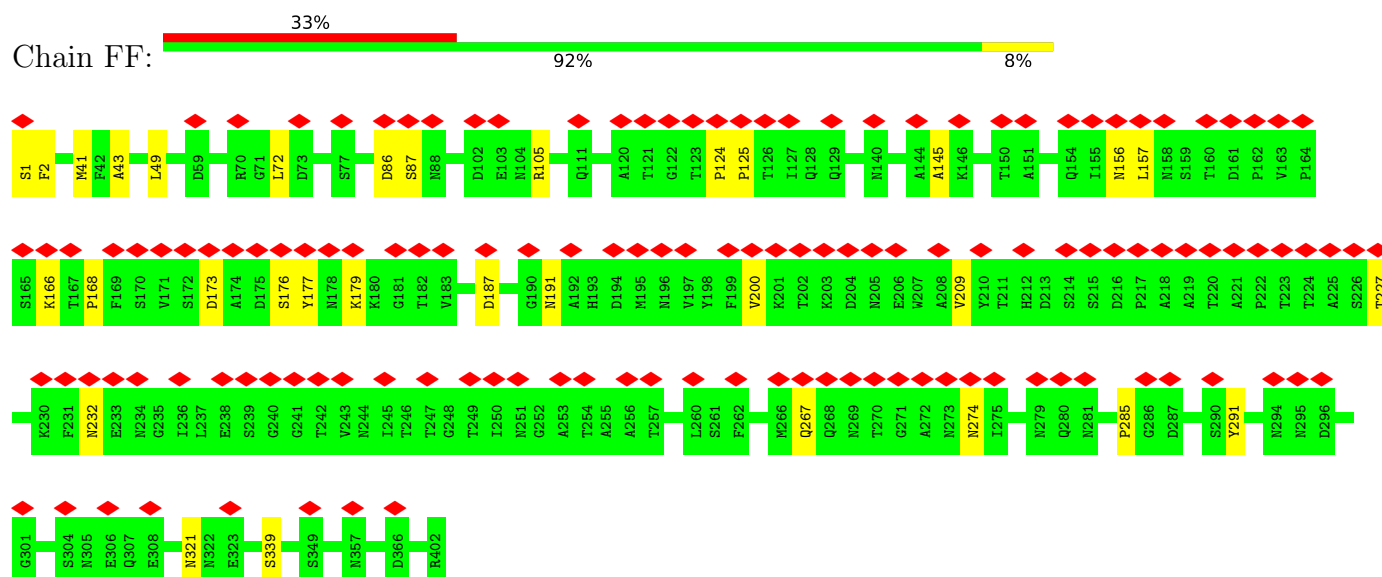
- Molecule 1: Flagellar hook protein FlgE



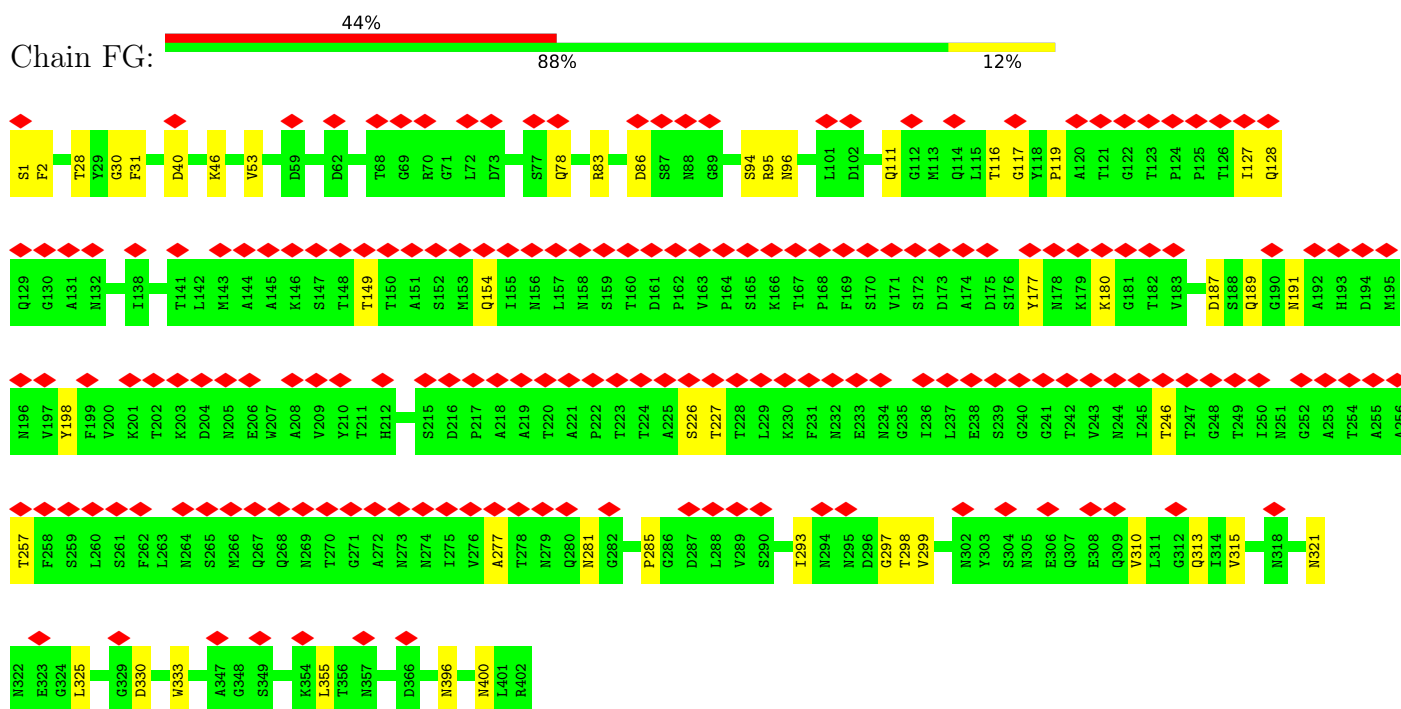
- Molecule 1: Flagellar hook protein FlgE



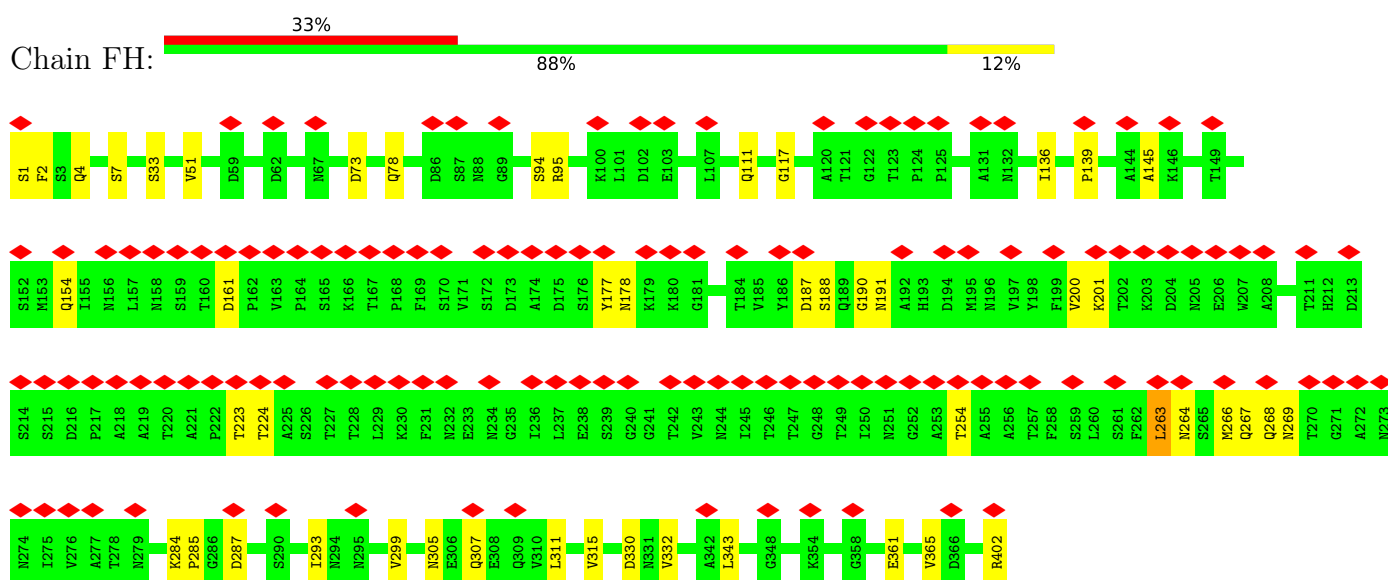
- Molecule 1: Flagellar hook protein FlgE



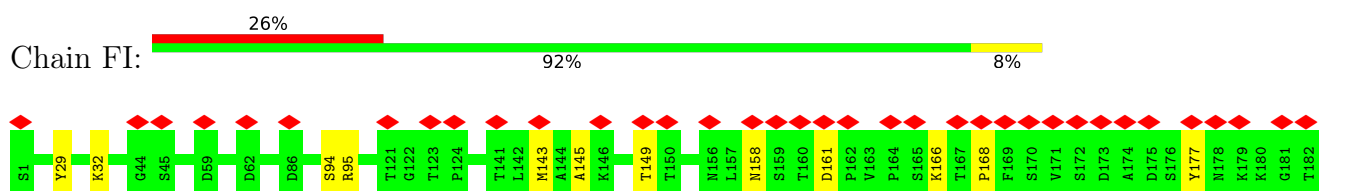
- Molecule 1: Flagellar hook protein FlgE

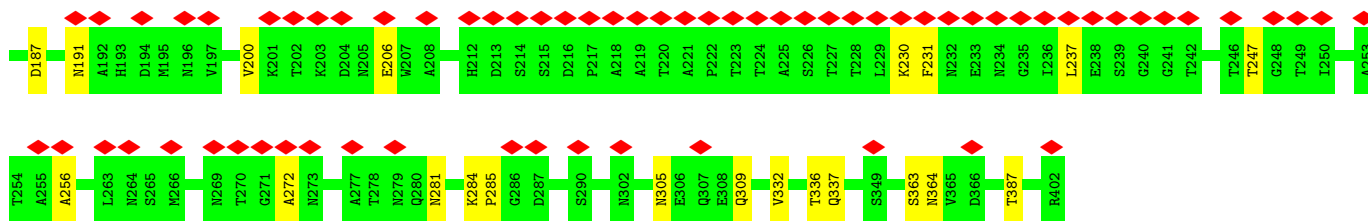


- Molecule 1: Flagellar hook protein FlgE

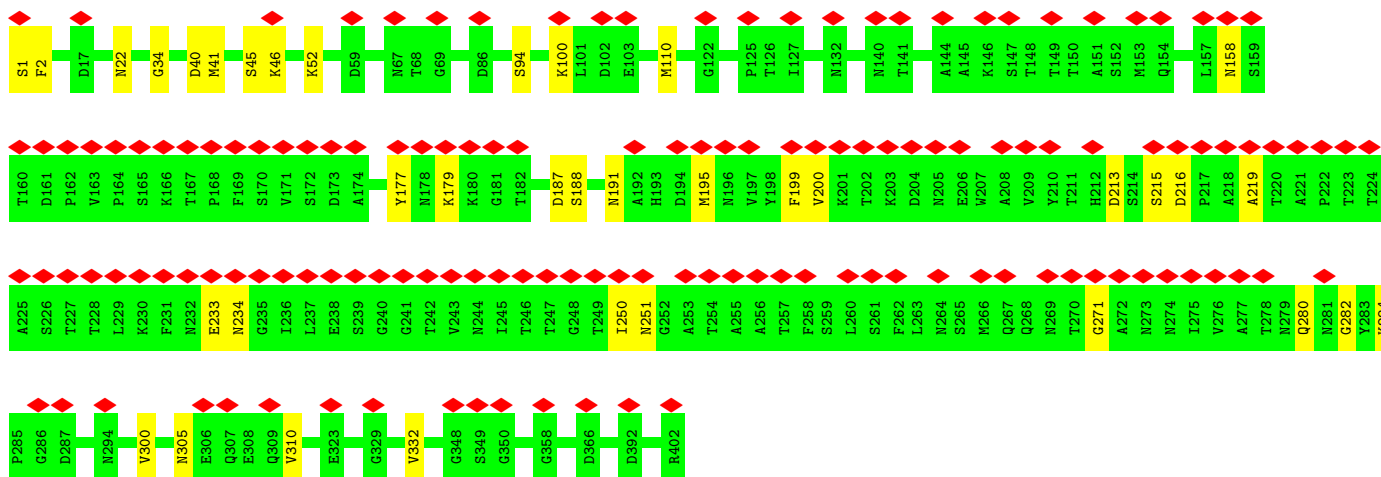


- Molecule 1: Flagellar hook protein FlgE

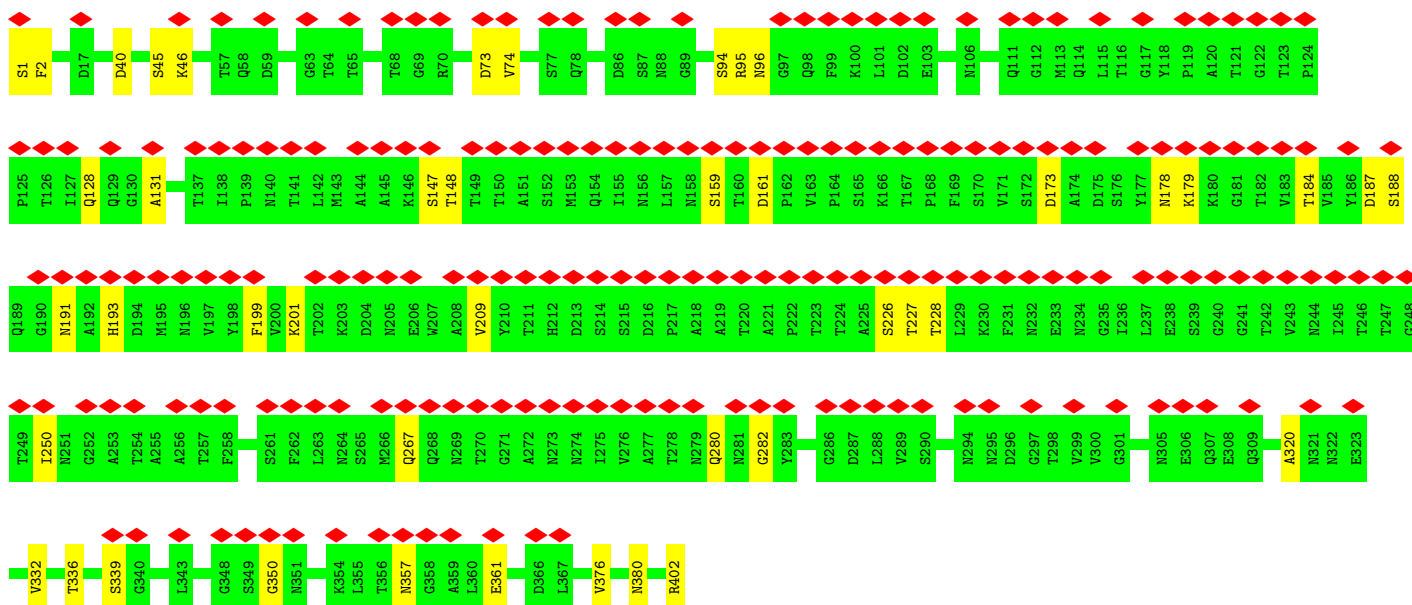
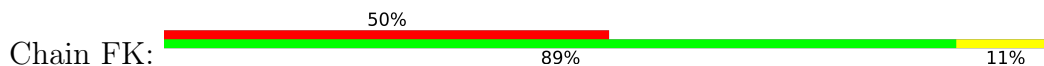




• Molecule 1: Flagellar hook protein FlgE



• Molecule 1: Flagellar hook protein FlgE



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	234536	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; deconvolution in cisTEM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	89	Depositor
Minimum defocus (nm)	430	Depositor
Maximum defocus (nm)	5130	Depositor
Magnification	107914	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	14.197	Depositor
Minimum map value	-9.643	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	533.76, 533.76, 533.76	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.23	0/3003	0.55	0/4090
1	AB	0.26	0/3003	0.54	0/4090
1	AC	0.26	0/3003	0.51	0/4090
1	AD	0.24	0/3003	0.50	0/4090
1	AE	0.25	0/3003	0.54	1/4090 (0.0%)
1	AF	0.25	0/3003	0.54	0/4090
1	AG	0.26	0/3003	0.52	0/4090
1	AH	0.29	0/3003	0.52	0/4090
1	AI	0.28	0/3003	0.54	2/4090 (0.0%)
1	AJ	0.27	0/3003	0.52	0/4090
1	AK	0.27	0/3003	0.55	2/4090 (0.0%)
1	BA	0.27	0/3003	0.50	0/4090
1	BB	0.29	0/3003	0.52	0/4090
1	BC	0.30	0/3003	0.53	0/4090
1	BD	0.29	0/3003	0.54	0/4090
1	BE	0.30	0/3003	0.55	0/4090
1	BF	0.28	0/3003	0.51	0/4090
1	BG	0.28	0/3003	0.54	0/4090
1	BH	0.30	0/3003	0.52	0/4090
1	BI	0.30	0/3003	0.52	0/4090
1	BJ	0.30	0/3003	0.54	0/4090
1	BK	0.31	0/3003	0.51	0/4090
1	CA	0.29	0/3003	0.54	0/4090
1	CB	0.30	0/3003	0.52	0/4090
1	CC	0.31	0/3003	0.54	0/4090
1	CD	0.29	0/3003	0.52	0/4090
1	CE	0.30	0/3003	0.52	0/4090
1	CF	0.31	0/3003	0.52	0/4090
1	CG	0.29	0/3003	0.52	0/4090
1	CH	0.30	0/3003	0.52	0/4090
1	CI	0.30	0/3003	0.51	0/4090
1	CJ	0.30	0/3003	0.55	0/4090
1	CK	0.31	0/3003	0.55	0/4090
1	DA	0.28	0/3003	0.50	0/4090

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DB	0.30	0/3003	0.53	0/4090
1	DC	0.30	0/3003	0.52	0/4090
1	DD	0.29	0/3003	0.49	0/4090
1	DE	0.30	0/3003	0.55	0/4090
1	DF	0.30	0/3003	0.52	0/4090
1	DG	0.28	0/3003	0.53	0/4090
1	DH	0.30	0/3003	0.52	0/4090
1	DI	0.30	0/3003	0.53	0/4090
1	DJ	0.28	0/3003	0.50	0/4090
1	DK	0.28	0/3003	0.52	0/4090
1	EA	0.28	0/3003	0.53	1/4090 (0.0%)
1	EB	0.29	0/3003	0.53	0/4090
1	EC	0.32	0/3003	0.56	0/4090
1	ED	0.30	0/3003	0.53	0/4090
1	EE	0.28	0/3003	0.54	0/4090
1	EF	0.28	0/3003	0.52	0/4090
1	EG	0.27	0/3003	0.50	0/4090
1	EH	0.28	0/3003	0.53	0/4090
1	EI	0.29	0/3003	0.51	0/4090
1	EJ	0.29	0/3003	0.53	0/4090
1	EK	0.32	2/3003 (0.1%)	0.52	0/4090
1	FA	0.29	1/3003 (0.0%)	0.52	0/4090
1	FB	0.26	0/3003	0.51	0/4090
1	FC	0.31	0/3003	0.53	0/4090
1	FD	0.28	0/3003	0.54	0/4090
1	FE	0.25	0/3003	0.48	0/4090
1	FF	0.24	0/3003	0.55	0/4090
1	FG	0.24	0/3003	0.55	0/4090
1	FH	0.26	0/3003	0.51	0/4090
1	FI	0.26	0/3003	0.51	0/4090
1	FJ	0.26	0/3003	0.54	0/4090
1	FK	0.22	0/3003	0.51	0/4090
All	All	0.28	3/198198 (0.0%)	0.53	6/269940 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EK	130	GLY	C-N	8.67	1.44	1.33
1	FA	107	LEU	C-N	-5.99	1.27	1.33
1	EK	135	PRO	C-N	-5.02	1.27	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AK	171	VAL	N-CA-C	-7.99	104.92	112.83
1	EA	372	VAL	N-CA-C	-6.03	106.93	112.96
1	AE	284	LYS	N-CA-C	-5.91	100.49	108.11
1	AK	339	SER	N-CA-C	-5.72	107.29	114.56
1	AI	131	ALA	CA-C-N	5.28	130.97	120.94
1	AI	131	ALA	C-N-CA	5.28	130.97	120.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2959	0	2855	29	0
1	AB	2959	0	2855	22	0
1	AC	2959	0	2855	26	0
1	AD	2959	0	2855	32	0
1	AE	2959	0	2855	24	0
1	AF	2959	0	2855	27	0
1	AG	2959	0	2855	29	0
1	AH	2959	0	2855	18	0
1	AI	2959	0	2855	20	0
1	AJ	2959	0	2855	23	0
1	AK	2959	0	2855	32	0
1	BA	2959	0	2855	29	0
1	BB	2959	0	2855	22	0
1	BC	2959	0	2855	23	0
1	BD	2959	0	2855	21	0
1	BE	2959	0	2855	27	0
1	BF	2959	0	2855	26	0
1	BG	2959	0	2855	24	0
1	BH	2959	0	2855	28	0
1	BI	2959	0	2855	28	0
1	BJ	2959	0	2855	25	0
1	BK	2959	0	2855	30	0
1	CA	2959	0	2855	24	0
1	CB	2959	0	2855	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CC	2959	0	2855	24	0
1	CD	2959	0	2855	21	0
1	CE	2959	0	2855	25	0
1	CF	2959	0	2855	21	0
1	CG	2959	0	2855	27	0
1	CH	2959	0	2855	29	0
1	CI	2959	0	2855	31	0
1	CJ	2959	0	2855	25	0
1	CK	2959	0	2855	18	0
1	DA	2959	0	2855	32	0
1	DB	2959	0	2855	27	0
1	DC	2959	0	2855	29	0
1	DD	2959	0	2855	30	0
1	DE	2959	0	2855	21	0
1	DF	2959	0	2855	21	0
1	DG	2959	0	2855	40	0
1	DH	2959	0	2855	34	0
1	DI	2959	0	2855	27	0
1	DJ	2959	0	2855	30	0
1	DK	2959	0	2855	33	0
1	EA	2959	0	2855	24	0
1	EB	2959	0	2855	34	0
1	EC	2959	0	2855	28	0
1	ED	2959	0	2855	22	0
1	EE	2959	0	2855	31	0
1	EF	2959	0	2855	26	0
1	EG	2959	0	2855	28	0
1	EH	2959	0	2855	33	0
1	EI	2959	0	2855	27	0
1	EJ	2959	0	2855	30	0
1	EK	2959	0	2855	32	0
1	FA	2959	0	2855	28	0
1	FB	2959	0	2855	34	0
1	FC	2959	0	2855	33	0
1	FD	2959	0	2855	20	0
1	FE	2959	0	2855	20	0
1	FF	2959	0	2855	22	0
1	FG	2959	0	2855	33	0
1	FH	2959	0	2855	32	0
1	FI	2959	0	2855	20	0
1	FJ	2959	0	2855	20	0
1	FK	2959	0	2855	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	195294	0	188430	1596	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 (1596) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BI:84:LEU:CD2	1:BI:115:LEU:HA	1.74	1.17
1:DD:84:LEU:CD2	1:DD:115:LEU:HA	1.80	1.12
1:FG:180:LYS:HE2	1:FG:198:TYR:HE1	1.09	1.12
1:DD:84:LEU:HD23	1:DD:115:LEU:HA	1.34	1.09
1:DA:390:THR:HG22	1:DG:402:ARG:HE	1.18	1.06
1:FA:105:ARG:HD3	1:FA:138:ILE:O	1.56	1.03
1:BI:84:LEU:HD23	1:BI:115:LEU:HA	1.41	0.98
1:FG:180:LYS:HE2	1:FG:198:TYR:CE1	2.00	0.97
1:DK:375:ILE:HD13	1:EF:392:ASP:OD2	1.67	0.95
1:FG:177:TYR:OH	1:FG:180:LYS:HE3	1.66	0.94
1:EJ:375:ILE:HD13	1:FE:392:ASP:OD2	1.67	0.94
1:DA:390:THR:HG22	1:DG:402:ARG:NE	1.86	0.90
1:DK:101:LEU:HD12	1:DK:106:ASN:O	1.77	0.84
1:FF:72:LEU:HD21	1:FF:291:TYR:CE2	2.14	0.82
1:BI:84:LEU:CD2	1:BI:115:LEU:CA	2.59	0.80
1:DA:390:THR:HA	1:DG:402:ARG:HH21	1.48	0.79
1:DD:84:LEU:CD2	1:DD:115:LEU:CA	2.62	0.76
1:FA:105:ARG:CD	1:FA:138:ILE:O	2.33	0.76
1:FG:177:TYR:OH	1:FG:180:LYS:CE	2.33	0.76
1:AD:17:ASP:HA	1:AI:4:GLN:HE22	1.52	0.74
1:DK:375:ILE:HG21	1:EF:392:ASP:OD1	1.89	0.72
1:BG:379:ARG:NE	1:CB:392:ASP:OD1	2.24	0.69
1:AD:106:ASN:HD22	1:AD:114:GLN:HE22	1.41	0.69
1:DK:374:MET:HE1	1:EE:387:THR:HG22	1.75	0.69
1:FF:72:LEU:HD21	1:FF:291:TYR:HE2	1.57	0.69
1:EH:2:PHE:HZ	1:EH:392:ASP:OD1	1.75	0.68
1:DI:375:ILE:CG2	1:ED:392:ASP:OD2	2.42	0.68
1:DA:389:LYS:HB3	1:DG:402:ARG:HH12	1.56	0.68
1:DD:84:LEU:HD21	1:DD:115:LEU:HD12	1.73	0.68
1:CK:379:ARG:NH2	1:DF:392:ASP:OD1	2.25	0.67
1:DF:84:LEU:HD23	1:DF:115:LEU:HA	1.76	0.67
1:FJ:280:GLN:HG2	1:FJ:282:GLY:H	1.60	0.66
1:DA:389:LYS:HB3	1:DG:402:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DJ:22:ASN:HD21	1:DJ:34:GLY:H	1.45	0.65
1:DA:389:LYS:CB	1:DG:402:ARG:NH1	2.59	0.64
1:DA:390:THR:HA	1:DG:402:ARG:NH2	2.13	0.64
1:CI:28:THR:HG22	1:DC:38:PHE:HB2	1.78	0.64
1:FC:145:ALA:HB2	1:FC:285:PRO:HD3	1.80	0.64
1:AF:143:MET:SD	1:AF:309:GLN:NE2	2.70	0.63
1:FK:178:ASN:HD21	1:FK:201:LYS:H	1.47	0.63
1:AB:293:ILE:HG12	1:AB:299:VAL:HG12	1.81	0.62
1:EB:180:LYS:HD3	1:EB:196:ASN:HD22	1.64	0.62
1:DA:389:LYS:C	1:DG:402:ARG:NH2	2.58	0.62
1:FB:331:ASN:OD1	1:FB:331:ASN:O	2.18	0.62
1:BH:379:ARG:HD2	1:CC:395:LEU:HD22	1.79	0.62
1:EH:280:GLN:HG2	1:EH:282:GLY:H	1.65	0.62
1:AH:145:ALA:HB2	1:AH:285:PRO:HD3	1.82	0.61
1:CD:229:LEU:HD22	1:CD:237:LEU:HD11	1.81	0.61
1:FA:159:SER:OG	1:FA:267:GLN:NE2	2.33	0.61
1:BB:68:THR:HG23	1:BB:70:ARG:H	1.66	0.61
1:FE:266:MET:HE3	1:FE:267:GLN:H	1.65	0.61
1:BK:17:ASP:OD1	1:CE:4:GLN:NE2	2.32	0.61
1:DJ:94:SER:HB2	1:DJ:332:VAL:HG12	1.82	0.61
1:FF:72:LEU:HD21	1:FF:291:TYR:CD2	2.35	0.61
1:AK:154:GLN:HE22	1:BF:141:THR:HG22	1.64	0.61
1:EA:293:ILE:HG12	1:EA:299:VAL:HG12	1.82	0.61
1:AI:33:SER:HB3	1:AI:365:VAL:HG22	1.83	0.61
1:BG:145:ALA:HB2	1:BG:285:PRO:HD3	1.83	0.61
1:DI:94:SER:HB2	1:DI:332:VAL:HG12	1.81	0.61
1:CA:229:LEU:HD22	1:CA:237:LEU:HD11	1.82	0.61
1:DI:127:ILE:HG21	1:DI:313:GLN:HE21	1.64	0.60
1:EE:145:ALA:HB2	1:EE:285:PRO:HD3	1.83	0.60
1:AE:247:THR:HB	1:AE:255:ALA:HB1	1.83	0.60
1:DE:94:SER:HB2	1:DE:332:VAL:HG12	1.82	0.60
1:DI:28:THR:HG22	1:EC:38:PHE:HB2	1.84	0.60
1:BE:170:SER:OG	1:BE:171:VAL:N	2.35	0.60
1:EK:293:ILE:HG12	1:EK:299:VAL:HG12	1.84	0.60
1:CH:379:ARG:HD2	1:DC:395:LEU:HD22	1.84	0.60
1:EK:205:ASN:HA	1:EK:267:GLN:HE22	1.67	0.60
1:BI:84:LEU:HD22	1:BI:115:LEU:HA	1.78	0.60
1:AC:145:ALA:HB2	1:AC:285:PRO:HD3	1.83	0.59
1:FI:32:LYS:HA	1:FI:364:ASN:HD21	1.67	0.59
1:BH:187:ASP:OD1	1:BH:191:ASN:N	2.35	0.59
1:FI:158:ASN:HD21	1:FI:272:ALA:HA	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FE:78:GLN:HB2	1:FE:353:GLY:HA3	1.84	0.59
1:AK:263:LEU:HD23	1:AK:264:ASN:HB2	1.85	0.59
1:BJ:1:SER:OG	1:BJ:2:PHE:N	2.34	0.59
1:CB:94:SER:HB2	1:CB:332:VAL:HG12	1.84	0.59
1:ED:145:ALA:HB2	1:ED:285:PRO:HD3	1.85	0.59
1:ED:195:MET:HE1	1:ED:245:ILE:HG21	1.85	0.59
1:FG:187:ASP:OD1	1:FG:191:ASN:N	2.36	0.59
1:CI:284:LYS:O	1:CI:305:ASN:ND2	2.32	0.59
1:EK:187:ASP:OD1	1:EK:191:ASN:N	2.36	0.59
1:DH:145:ALA:HB2	1:DH:285:PRO:HD3	1.84	0.59
1:DI:145:ALA:HB2	1:DI:285:PRO:HD3	1.84	0.59
1:EC:145:ALA:HB2	1:EC:285:PRO:HD3	1.85	0.59
1:AG:216:ASP:HB3	1:AG:219:ALA:HB2	1.85	0.59
1:AK:197:VAL:HG12	1:AK:211:THR:HG22	1.84	0.58
1:BD:145:ALA:HB2	1:BD:285:PRO:HD3	1.85	0.58
1:BG:67:ASN:HD21	1:CG:52:LYS:HE2	1.67	0.58
1:DF:105:ARG:NH2	1:DK:320:ALA:O	2.36	0.58
1:FH:7:SER:OG	1:FH:51:VAL:O	2.21	0.58
1:FJ:94:SER:HB2	1:FJ:332:VAL:HG12	1.84	0.58
1:EE:146:LYS:NZ	1:EE:281:ASN:O	2.36	0.58
1:FB:158:ASN:ND2	1:FB:271:GLY:O	2.36	0.58
1:FJ:179:LYS:HB3	1:FJ:199:PHE:HB2	1.85	0.58
1:FG:119:PRO:HD2	1:FG:128:GLN:HE22	1.69	0.58
1:BB:94:SER:HB3	1:BB:332:VAL:HG12	1.86	0.58
1:CF:100:LYS:NZ	1:CF:110:MET:SD	2.76	0.58
1:CG:94:SER:HB2	1:CG:332:VAL:HG12	1.85	0.58
1:DK:375:ILE:HG21	1:EF:392:ASP:CG	2.28	0.58
1:EI:187:ASP:OD1	1:EI:191:ASN:N	2.36	0.58
1:FG:180:LYS:HG3	1:FG:198:TYR:CE1	2.38	0.58
1:FF:232:ASN:O	1:FF:267:GLN:NE2	2.36	0.58
1:AE:187:ASP:OD1	1:AE:191:ASN:N	2.35	0.58
1:BJ:293:ILE:HG12	1:BJ:299:VAL:HG12	1.85	0.58
1:DF:374:MET:HE1	1:DK:387:THR:HG23	1.85	0.58
1:EK:284:LYS:O	1:EK:305:ASN:ND2	2.37	0.58
1:FJ:100:LYS:NZ	1:FJ:110:MET:SD	2.76	0.58
1:CC:62:ASP:OD1	1:CC:62:ASP:N	2.36	0.57
1:BJ:158:ASN:ND2	1:BJ:271:GLY:O	2.36	0.57
1:BK:187:ASP:OD1	1:BK:191:ASN:N	2.37	0.57
1:CH:366:ASP:OD1	1:CH:366:ASP:N	2.35	0.57
1:EJ:157:LEU:HD23	1:EJ:273:ASN:HD21	1.67	0.57
1:CD:159:SER:O	1:CJ:251:ASN:ND2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:390:THR:CG2	1:DG:402:ARG:NE	2.65	0.57
1:AG:378:GLN:HE21	1:AG:382:GLN:HE22	1.52	0.57
1:DB:379:ARG:NH1	1:DB:382:GLN:OE1	2.37	0.57
1:FI:166:LYS:HG3	1:FI:168:PRO:HD2	1.86	0.57
1:BG:45:SER:OG	1:BG:46:LYS:N	2.38	0.57
1:CH:45:SER:OG	1:CH:46:LYS:N	2.36	0.57
1:FH:33:SER:HB3	1:FH:365:VAL:HG22	1.87	0.57
1:FH:293:ILE:HG12	1:FH:299:VAL:HG12	1.87	0.57
1:BF:145:ALA:HB2	1:BF:285:PRO:HG3	1.87	0.57
1:BG:187:ASP:OD1	1:BG:191:ASN:N	2.37	0.57
1:CE:1:SER:OG	1:CE:2:PHE:N	2.38	0.57
1:CH:28:THR:HG22	1:DB:38:PHE:HB2	1.86	0.57
1:EI:378:GLN:NE2	1:FC:393:GLN:OE1	2.37	0.57
1:BD:159:SER:HA	1:BD:267:GLN:HE21	1.70	0.57
1:CB:100:LYS:NZ	1:CB:110:MET:SD	2.78	0.57
1:CA:98:GLN:HG3	1:CA:360:LEU:HD21	1.87	0.57
1:CC:145:ALA:HB2	1:CC:285:PRO:HD3	1.86	0.57
1:CJ:374:MET:HE1	1:DD:387:THR:HG23	1.86	0.57
1:DH:149:THR:HG1	1:DH:281:ASN:HD21	1.52	0.57
1:CJ:166:LYS:HG3	1:CJ:168:PRO:HD2	1.87	0.56
1:AG:227:THR:OG1	1:AG:228:THR:N	2.38	0.56
1:BC:1:SER:OG	1:BC:2:PHE:N	2.38	0.56
1:CD:374:MET:HE1	1:CI:387:THR:HG23	1.86	0.56
1:DH:284:LYS:O	1:DH:305:ASN:ND2	2.37	0.56
1:DI:166:LYS:HG3	1:DI:168:PRO:HD2	1.87	0.56
1:FJ:233:GLU:OE1	1:FJ:234:ASN:ND2	2.37	0.56
1:AD:145:ALA:HB2	1:AD:285:PRO:HD3	1.87	0.56
1:BB:187:ASP:OD1	1:BB:191:ASN:N	2.38	0.56
1:BE:76:ILE:HD11	1:BE:95:ARG:HG3	1.87	0.56
1:BK:1:SER:OG	1:BK:2:PHE:N	2.37	0.56
1:CC:187:ASP:OD2	1:CC:191:ASN:ND2	2.38	0.56
1:CG:293:ILE:HG12	1:CG:299:VAL:HG12	1.87	0.56
1:CK:187:ASP:OD1	1:CK:191:ASN:N	2.38	0.56
1:EG:197:VAL:HG12	1:EG:211:THR:HG22	1.87	0.56
1:FI:187:ASP:OD1	1:FI:191:ASN:N	2.34	0.56
1:DA:206:GLU:HG2	1:DA:230:LYS:HG2	1.88	0.56
1:EB:45:SER:OG	1:EB:46:LYS:N	2.38	0.56
1:CI:145:ALA:HB2	1:CI:285:PRO:HD3	1.86	0.56
1:EJ:145:ALA:HB2	1:EJ:285:PRO:HD3	1.87	0.56
1:FD:45:SER:OG	1:FD:46:LYS:N	2.38	0.56
1:AE:159:SER:O	1:AK:251:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:284:LYS:O	1:CG:305:ASN:ND2	2.37	0.56
1:DA:389:LYS:HB2	1:DG:402:ARG:NH1	2.21	0.56
1:EB:293:ILE:O	1:EB:357:ASN:ND2	2.39	0.56
1:AA:22:ASN:HD21	1:AA:34:GLY:H	1.53	0.56
1:CA:187:ASP:OD1	1:CA:191:ASN:N	2.37	0.56
1:DA:45:SER:OG	1:DA:46:LYS:N	2.38	0.56
1:EG:177:TYR:HA	1:EG:200:VAL:HG12	1.88	0.56
1:FA:197:VAL:HG12	1:FA:211:THR:HG22	1.88	0.56
1:CA:161:ASP:OD1	1:CA:178:ASN:ND2	2.39	0.56
1:CH:379:ARG:NH1	1:CH:382:GLN:OE1	2.39	0.56
1:EG:85:VAL:HG12	1:EG:91:VAL:HG12	1.87	0.56
1:EJ:161:ASP:OD2	1:EJ:178:ASN:ND2	2.39	0.56
1:FD:158:ASN:ND2	1:FD:271:GLY:O	2.39	0.56
1:FF:145:ALA:HB2	1:FF:285:PRO:HD3	1.87	0.56
1:FI:161:ASP:OD1	1:FI:161:ASP:N	2.39	0.56
1:AB:263:LEU:HD23	1:AB:264:ASN:HB2	1.88	0.56
1:AK:374:MET:HE1	1:BE:387:THR:HA	1.87	0.56
1:CD:170:SER:OG	1:CD:171:VAL:N	2.38	0.56
1:CJ:187:ASP:OD1	1:CJ:191:ASN:N	2.38	0.56
1:DH:45:SER:OG	1:DH:46:LYS:N	2.38	0.56
1:EB:145:ALA:HB2	1:EB:285:PRO:HD3	1.87	0.56
1:FD:379:ARG:NH1	1:FD:382:GLN:OE1	2.38	0.56
1:AK:120:ALA:HB2	1:AK:127:ILE:HD13	1.88	0.56
1:BE:386:GLN:NE2	1:BK:399:VAL:O	2.39	0.56
1:DC:374:MET:HE1	1:DH:387:THR:HG23	1.86	0.56
1:EF:187:ASP:OD1	1:EF:191:ASN:N	2.39	0.56
1:BE:382:GLN:HB3	1:BK:399:VAL:HG11	1.87	0.55
1:CB:125:PRO:HG2	1:CB:309:GLN:HE21	1.71	0.55
1:BD:166:LYS:HG3	1:BD:168:PRO:HD2	1.87	0.55
1:CI:216:ASP:N	1:CI:216:ASP:OD1	2.39	0.55
1:CJ:45:SER:OG	1:CJ:46:LYS:N	2.40	0.55
1:DJ:187:ASP:OD1	1:DJ:191:ASN:N	2.39	0.55
1:ED:227:THR:OG1	1:ED:228:THR:N	2.39	0.55
1:AA:7:SER:OG	1:AA:51:VAL:O	2.24	0.55
1:AI:179:LYS:HB3	1:AI:199:PHE:HB2	1.88	0.55
1:CA:379:ARG:NH1	1:CA:382:GLN:OE1	2.39	0.55
1:EC:379:ARG:NH1	1:EC:382:GLN:OE1	2.39	0.55
1:EI:1:SER:OG	1:EI:2:PHE:N	2.39	0.55
1:FJ:45:SER:OG	1:FJ:46:LYS:N	2.38	0.55
1:AF:284:LYS:O	1:AF:305:ASN:ND2	2.34	0.55
1:DJ:205:ASN:OD1	1:EE:251:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EK:45:SER:OG	1:EK:46:LYS:N	2.38	0.55
1:FG:83:ARG:HH11	1:FG:116:THR:HG21	1.71	0.55
1:EC:294:ASN:ND2	1:FC:337:GLN:OE1	2.40	0.55
1:EJ:152:SER:OG	1:EJ:279:ASN:OD1	2.20	0.55
1:FC:73:ASP:OD1	1:FC:73:ASP:N	2.39	0.55
1:AD:158:ASN:ND2	1:AD:271:GLY:O	2.40	0.55
1:BC:145:ALA:HB2	1:BC:285:PRO:HD3	1.88	0.55
1:BE:161:ASP:OD2	1:BE:178:ASN:ND2	2.40	0.55
1:BF:284:LYS:O	1:BF:305:ASN:ND2	2.39	0.55
1:BH:94:SER:HB2	1:BH:332:VAL:HG12	1.87	0.55
1:CA:94:SER:HB2	1:CA:332:VAL:HG12	1.88	0.55
1:DH:293:ILE:HG12	1:DH:299:VAL:HG12	1.88	0.55
1:BC:207:TRP:NE1	1:BC:267:GLN:OE1	2.39	0.55
1:BF:158:ASN:ND2	1:BF:271:GLY:O	2.40	0.55
1:EC:166:LYS:HG3	1:EC:168:PRO:HD2	1.89	0.55
1:FF:187:ASP:OD1	1:FF:191:ASN:N	2.35	0.55
1:FI:206:GLU:HG2	1:FI:230:LYS:HG3	1.88	0.55
1:CC:379:ARG:NH1	1:CC:382:GLN:OE1	2.40	0.55
1:CD:187:ASP:OD1	1:CD:191:ASN:N	2.39	0.55
1:DI:284:LYS:O	1:DI:305:ASN:ND2	2.40	0.55
1:EC:287:ASP:H	1:EC:304:SER:HB3	1.71	0.55
1:EG:158:ASN:ND2	1:EG:271:GLY:O	2.40	0.55
1:FH:111:GLN:NE2	1:FH:330:ASP:OD2	2.40	0.55
1:FG:396:ASN:O	1:FG:400:ASN:ND2	2.40	0.55
1:FK:74:VAL:HG12	1:FK:357:ASN:HA	1.89	0.55
1:AH:379:ARG:NH1	1:AH:382:GLN:OE1	2.40	0.55
1:BB:1:SER:OG	1:BB:2:PHE:N	2.40	0.55
1:CF:40:ASP:OD1	1:CF:40:ASP:N	2.40	0.55
1:FC:293:ILE:HG12	1:FC:299:VAL:HG12	1.88	0.55
1:FH:78:GLN:O	1:FH:95:ARG:NH2	2.40	0.55
1:AG:145:ALA:HB2	1:AG:285:PRO:HD3	1.88	0.54
1:AG:194:ASP:OD1	1:AG:194:ASP:N	2.40	0.54
1:BA:64:THR:HB	1:CA:49:LEU:HD11	1.89	0.54
1:CH:389:LYS:NZ	1:DB:401:LEU:O	2.41	0.54
1:CI:1:SER:OG	1:CI:2:PHE:N	2.40	0.54
1:DF:197:VAL:HG12	1:DF:211:THR:HG22	1.89	0.54
1:EE:127:ILE:HD11	1:EE:310:VAL:HG11	1.89	0.54
1:FA:146:LYS:NZ	1:FA:281:ASN:O	2.40	0.54
1:FC:86:ASP:HB3	1:FC:113:MET:HG2	1.89	0.54
1:FI:284:LYS:O	1:FI:305:ASN:ND2	2.40	0.54
1:AD:293:ILE:HG12	1:AD:299:VAL:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:182:THR:HG22	1:AF:196:ASN:HD22	1.72	0.54
1:AJ:287:ASP:OD1	1:AJ:287:ASP:N	2.40	0.54
1:AK:161:ASP:OD2	1:AK:178:ASN:ND2	2.40	0.54
1:BI:330:ASP:OD1	1:BI:330:ASP:N	2.40	0.54
1:CB:197:VAL:HG12	1:CB:211:THR:HG22	1.89	0.54
1:CC:45:SER:OG	1:CC:46:LYS:N	2.40	0.54
1:DH:321:ASN:ND2	1:DH:338:ALA:O	2.34	0.54
1:EH:187:ASP:OD1	1:EH:191:ASN:N	2.39	0.54
1:FC:121:THR:HB	1:FC:128:GLN:HE22	1.72	0.54
1:FI:145:ALA:HB2	1:FI:285:PRO:HD3	1.89	0.54
1:CE:145:ALA:HB2	1:CE:285:PRO:HD3	1.89	0.54
1:DK:101:LEU:HD11	1:DK:105:ARG:C	2.32	0.54
1:EJ:113:MET:HE1	1:EJ:332:VAL:HG21	1.88	0.54
1:BI:263:LEU:HD23	1:BI:264:ASN:HB2	1.89	0.54
1:CA:40:ASP:OD1	1:CA:40:ASP:N	2.39	0.54
1:DA:1:SER:OG	1:DA:2:PHE:N	2.41	0.54
1:DB:293:ILE:HG12	1:DB:299:VAL:HG12	1.88	0.54
1:DC:379:ARG:NH1	1:DC:382:GLN:OE1	2.41	0.54
1:DG:145:ALA:HB2	1:DG:285:PRO:HD3	1.90	0.54
1:EA:95:ARG:NH1	1:EA:361:GLU:OE2	2.41	0.54
1:EC:173:ASP:N	1:EC:173:ASP:OD1	2.40	0.54
1:EG:1:SER:OG	1:EG:2:PHE:N	2.38	0.54
1:EJ:94:SER:OG	1:EJ:95:ARG:N	2.41	0.54
1:AE:321:ASN:ND2	1:AE:338:ALA:O	2.37	0.54
1:FB:40:ASP:OD1	1:FB:40:ASP:N	2.41	0.54
1:FE:369:LYS:O	1:FE:373:ASN:ND2	2.41	0.54
1:AI:216:ASP:HB3	1:AI:219:ALA:HB2	1.90	0.54
1:BI:145:ALA:HB2	1:BI:285:PRO:HD3	1.90	0.54
1:DB:62:ASP:OD1	1:DB:62:ASP:N	2.40	0.54
1:EE:40:ASP:N	1:EE:40:ASP:OD1	2.41	0.54
1:FD:187:ASP:OD1	1:FD:191:ASN:N	2.40	0.54
1:FH:145:ALA:HB2	1:FH:285:PRO:HD3	1.88	0.54
1:FH:284:LYS:O	1:FH:305:ASN:ND2	2.41	0.54
1:FI:247:THR:HG22	1:FI:256:ALA:H	1.71	0.54
1:AD:184:THR:O	1:AD:280:GLN:NE2	2.41	0.54
1:BG:379:ARG:NH1	1:BG:382:GLN:OE1	2.41	0.54
1:EG:113:MET:HE1	1:EG:332:VAL:HG11	1.87	0.54
1:EI:284:LYS:O	1:EI:305:ASN:ND2	2.41	0.54
1:FB:61:THR:OG1	1:FB:62:ASP:N	2.41	0.54
1:AD:40:ASP:OD1	1:AD:40:ASP:N	2.40	0.54
1:BA:369:LYS:O	1:BA:373:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CE:139:PRO:HB2	1:CE:141:THR:HG22	1.89	0.54
1:DD:379:ARG:NH2	1:DJ:392:ASP:OD1	2.39	0.54
1:DI:197:VAL:HG12	1:DI:211:THR:HG22	1.88	0.54
1:DJ:145:ALA:HB2	1:DJ:285:PRO:HD3	1.88	0.54
1:EI:263:LEU:HD23	1:EI:264:ASN:HB2	1.89	0.54
1:EK:321:ASN:ND2	1:EK:338:ALA:O	2.37	0.54
1:BC:154:GLN:NE2	1:BC:264:ASN:O	2.41	0.54
1:CC:173:ASP:OD1	1:CC:173:ASP:N	2.39	0.54
1:CH:28:THR:O	1:CH:363:SER:OG	2.24	0.54
1:FK:179:LYS:HB3	1:FK:199:PHE:HB2	1.89	0.54
1:BD:389:LYS:HE2	1:BI:401:LEU:HB2	1.90	0.54
1:BE:263:LEU:HD23	1:BE:264:ASN:HB2	1.89	0.54
1:BK:159:SER:O	1:BK:201:LYS:NZ	2.41	0.54
1:CG:45:SER:OG	1:CG:46:LYS:N	2.41	0.54
1:DD:40:ASP:OD1	1:DD:40:ASP:N	2.39	0.54
1:DF:145:ALA:HB2	1:DF:285:PRO:HD3	1.90	0.54
1:EC:113:MET:HE1	1:EC:332:VAL:HG11	1.89	0.54
1:FG:1:SER:OG	1:FG:2:PHE:N	2.40	0.54
1:BH:155:ILE:O	1:BH:265:SER:OG	2.26	0.53
1:DA:161:ASP:OD2	1:DA:178:ASN:ND2	2.40	0.53
1:EA:159:SER:O	1:EA:201:LYS:NZ	2.41	0.53
1:FE:94:SER:HB3	1:FE:332:VAL:HG12	1.90	0.53
1:FJ:177:TYR:HA	1:FJ:200:VAL:HG12	1.90	0.53
1:AE:22:ASN:HD21	1:AE:34:GLY:H	1.54	0.53
1:AH:318:ASN:ND2	1:AH:351:ASN:OD1	2.41	0.53
1:BJ:159:SER:O	1:CE:251:ASN:ND2	2.41	0.53
1:CI:227:THR:OG1	1:CI:228:THR:N	2.41	0.53
1:DI:187:ASP:OD1	1:DI:191:ASN:N	2.40	0.53
1:EA:158:ASN:ND2	1:EA:271:GLY:O	2.41	0.53
1:FK:209:VAL:O	1:FK:226:SER:OG	2.27	0.53
1:BE:45:SER:OG	1:BE:46:LYS:N	2.41	0.53
1:FH:161:ASP:O	1:FH:201:LYS:NZ	2.38	0.53
1:FK:161:ASP:N	1:FK:161:ASP:OD1	2.42	0.53
1:BF:187:ASP:OD2	1:BF:191:ASN:ND2	2.42	0.53
1:CG:204:ASP:N	1:CG:204:ASP:OD1	2.39	0.53
1:DD:159:SER:O	1:DJ:251:ASN:ND2	2.41	0.53
1:EB:170:SER:OG	1:EB:171:VAL:N	2.39	0.53
1:EI:94:SER:HB2	1:EI:332:VAL:HG12	1.90	0.53
1:EJ:229:LEU:HD22	1:EJ:237:LEU:HD11	1.91	0.53
1:FD:374:MET:HE1	1:FI:387:THR:HG23	1.89	0.53
1:AA:269:ASN:ND2	1:AG:191:ASN:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:177:TYR:HA	1:DC:200:VAL:HG12	1.89	0.53
1:DK:165:SER:OG	1:DK:166:LYS:NZ	2.42	0.53
1:EI:229:LEU:HD22	1:EI:237:LEU:HD11	1.90	0.53
1:FB:73:ASP:OD1	1:FB:73:ASP:N	2.39	0.53
1:FK:187:ASP:OD1	1:FK:191:ASN:N	2.42	0.53
1:AJ:40:ASP:OD1	1:AJ:40:ASP:N	2.42	0.53
1:EE:227:THR:OG1	1:EE:228:THR:N	2.40	0.53
1:FA:138:ILE:HG13	1:FA:311:LEU:HD13	1.90	0.53
1:FA:237:LEU:HD11	1:FA:265:SER:H	1.74	0.53
1:AA:161:ASP:OD1	1:AA:161:ASP:N	2.42	0.53
1:AI:183:VAL:HG12	1:AI:195:MET:HB2	1.91	0.53
1:BK:40:ASP:OD1	1:BK:40:ASP:N	2.42	0.53
1:CB:83:ARG:HH11	1:CB:116:THR:HG21	1.73	0.53
1:CE:293:ILE:O	1:CE:357:ASN:ND2	2.38	0.53
1:CH:9:LEU:HD12	1:CH:384:ASN:HB3	1.91	0.53
1:CH:206:GLU:OE2	1:CH:230:LYS:NZ	2.38	0.53
1:DG:318:ASN:ND2	1:DG:351:ASN:O	2.42	0.53
1:EB:284:LYS:O	1:EB:305:ASN:ND2	2.41	0.53
1:EF:94:SER:HB3	1:EF:332:VAL:HG12	1.90	0.53
1:EI:45:SER:OG	1:EI:46:LYS:N	2.42	0.53
1:EI:146:LYS:NZ	1:EI:281:ASN:O	2.42	0.53
1:FD:171:VAL:HG21	1:FD:221:ALA:HB1	1.91	0.53
1:BI:45:SER:OG	1:BI:46:LYS:N	2.42	0.53
1:DG:247:THR:HG23	1:DG:255:ALA:HB1	1.90	0.53
1:DJ:284:LYS:O	1:DJ:305:ASN:ND2	2.39	0.53
1:EA:315:VAL:HG11	1:EA:344:LEU:HD23	1.90	0.53
1:EG:290:SER:OG	1:EG:291:TYR:N	2.42	0.53
1:FC:94:SER:HB2	1:FC:332:VAL:HG12	1.90	0.53
1:FD:1:SER:OG	1:FD:2:PHE:N	2.41	0.53
1:FJ:187:ASP:OD1	1:FJ:191:ASN:N	2.42	0.53
1:AD:187:ASP:OD1	1:AD:191:ASN:N	2.42	0.53
1:AH:45:SER:OG	1:AH:46:LYS:N	2.38	0.53
1:BJ:45:SER:OG	1:BJ:46:LYS:N	2.42	0.53
1:CE:156:ASN:HB3	1:CE:270:THR:HG21	1.90	0.53
1:DA:187:ASP:OD1	1:DA:191:ASN:N	2.40	0.53
1:DG:166:LYS:HG3	1:DG:168:PRO:HD2	1.91	0.53
1:DG:216:ASP:HB3	1:DG:219:ALA:HB2	1.90	0.53
1:DK:32:LYS:HA	1:DK:364:ASN:HD21	1.74	0.53
1:ED:386:GLN:NE2	1:EJ:399:VAL:O	2.41	0.53
1:EI:5:ALA:HB1	1:EI:388:ILE:HG12	1.91	0.53
1:FB:366:ASP:OD1	1:FB:366:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:159:SER:O	1:AI:251:ASN:ND2	2.42	0.53
1:CB:6:VAL:O	1:CB:10:ASN:ND2	2.41	0.53
1:DJ:57:THR:OG1	1:DJ:323:GLU:OE1	2.27	0.53
1:FF:1:SER:OG	1:FF:2:PHE:N	2.42	0.53
1:AA:83:ARG:HD3	1:AA:116:THR:HG21	1.91	0.52
1:DG:94:SER:OG	1:DG:95:ARG:N	2.40	0.52
1:EC:23:ILE:HD11	1:EC:370:GLU:HB2	1.91	0.52
1:EE:369:LYS:O	1:EE:373:ASN:ND2	2.42	0.52
1:FA:293:ILE:HG12	1:FA:299:VAL:HG12	1.92	0.52
1:AE:296:ASP:OD2	1:AE:296:ASP:N	2.42	0.52
1:AK:45:SER:OG	1:AK:46:LYS:N	2.42	0.52
1:CJ:78:GLN:HB2	1:CJ:353:GLY:HA3	1.92	0.52
1:EA:155:ILE:O	1:EA:265:SER:OG	2.27	0.52
1:EA:216:ASP:HB3	1:EA:219:ALA:HB2	1.90	0.52
1:EG:227:THR:OG1	1:EG:228:THR:N	2.42	0.52
1:EI:295:ASN:OD1	1:EI:357:ASN:ND2	2.42	0.52
1:EI:321:ASN:ND2	1:EI:338:ALA:O	2.40	0.52
1:AC:337:GLN:HE21	1:AC:338:ALA:H	1.56	0.52
1:AJ:61:THR:O	1:AJ:364:ASN:ND2	2.42	0.52
1:DA:296:ASP:N	1:DA:296:ASP:OD1	2.43	0.52
1:EE:75:ALA:HB2	1:EE:360:LEU:HA	1.91	0.52
1:AD:22:ASN:ND2	1:AD:33:SER:OG	2.37	0.52
1:AE:379:ARG:NH1	1:AK:396:ASN:OD1	2.43	0.52
1:DA:26:SER:O	1:DA:26:SER:OG	2.27	0.52
1:DA:155:ILE:O	1:DA:265:SER:OG	2.27	0.52
1:EG:111:GLN:NE2	1:EG:330:ASP:OD2	2.42	0.52
1:FB:187:ASP:OD1	1:FB:191:ASN:N	2.41	0.52
1:FE:145:ALA:HB2	1:FE:285:PRO:HD3	1.91	0.52
1:FE:187:ASP:OD1	1:FE:191:ASN:N	2.41	0.52
1:FG:149:THR:OG1	1:FG:281:ASN:ND2	2.39	0.52
1:FJ:158:ASN:ND2	1:FJ:271:GLY:O	2.42	0.52
1:AE:98:GLN:HG3	1:AE:360:LEU:HD21	1.91	0.52
1:AE:165:SER:OG	1:AE:175:ASP:OD2	2.27	0.52
1:AG:28:THR:O	1:AG:363:SER:OG	2.27	0.52
1:AH:216:ASP:N	1:AH:216:ASP:OD1	2.42	0.52
1:DJ:148:THR:HG22	1:DJ:282:GLY:HA3	1.90	0.52
1:ED:177:TYR:HA	1:ED:200:VAL:HG12	1.91	0.52
1:EK:40:ASP:OD1	1:EK:40:ASP:N	2.43	0.52
1:AJ:187:ASP:OD1	1:AJ:191:ASN:N	2.42	0.52
1:CB:379:ARG:NH1	1:CB:382:GLN:OE1	2.43	0.52
1:EB:375:ILE:CG2	1:EH:392:ASP:OD2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EH:1:SER:OG	1:EH:2:PHE:N	2.40	0.52
1:CB:28:THR:HG22	1:CG:38:PHE:HB2	1.91	0.52
1:CD:117:GLY:HA2	1:CD:315:VAL:HG12	1.92	0.52
1:CK:145:ALA:HB2	1:CK:285:PRO:HD3	1.91	0.52
1:DD:330:ASP:N	1:DD:330:ASP:OD1	2.36	0.52
1:EC:379:ARG:NE	1:EI:392:ASP:OD1	2.40	0.52
1:EK:158:ASN:ND2	1:EK:273:ASN:OD1	2.42	0.52
1:AJ:32:LYS:NZ	1:AJ:361:GLU:OE2	2.43	0.52
1:DB:161:ASP:OD2	1:DB:178:ASN:ND2	2.42	0.52
1:EH:166:LYS:HG3	1:EH:168:PRO:HD2	1.92	0.52
1:EK:274:ASN:HD22	1:FK:350:GLY:HA2	1.75	0.52
1:FD:159:SER:O	1:FJ:251:ASN:ND2	2.43	0.52
1:FE:40:ASP:OD1	1:FE:40:ASP:N	2.39	0.52
1:FG:325:LEU:HB3	1:FG:333:TRP:HB3	1.91	0.52
1:FI:143:MET:SD	1:FI:309:GLN:NE2	2.82	0.52
1:AC:98:GLN:HG3	1:AC:360:LEU:HD21	1.91	0.52
1:AI:143:MET:HE3	1:AI:309:GLN:HE21	1.74	0.52
1:CI:94:SER:OG	1:CI:95:ARG:N	2.42	0.52
1:DI:177:TYR:HA	1:DI:200:VAL:HG12	1.92	0.52
1:EH:145:ALA:HB2	1:EH:285:PRO:HD3	1.92	0.52
1:EH:234:ASN:OD1	1:FC:188:SER:OG	2.28	0.52
1:FE:1:SER:OG	1:FE:2:PHE:N	2.42	0.52
1:BI:287:ASP:OD1	1:BI:287:ASP:N	2.41	0.52
1:CE:287:ASP:OD1	1:CE:287:ASP:N	2.42	0.52
1:CF:325:LEU:HB3	1:CF:333:TRP:HB3	1.92	0.52
1:DB:3:SER:HA	1:DB:6:VAL:HG12	1.92	0.52
1:EF:155:ILE:HD13	1:EF:275:ILE:HG13	1.93	0.52
1:EH:7:SER:OG	1:EH:51:VAL:O	2.28	0.52
1:EJ:194:ASP:OD1	1:EJ:194:ASP:N	2.42	0.52
1:EK:180:LYS:NZ	1:EK:198:TYR:OH	2.42	0.52
1:AB:1:SER:OG	1:AB:2:PHE:N	2.41	0.51
1:BJ:287:ASP:OD2	1:BJ:304:SER:OG	2.28	0.51
1:CD:370:GLU:HA	1:CD:373:ASN:HD22	1.75	0.51
1:CK:94:SER:OG	1:CK:95:ARG:N	2.42	0.51
1:EB:161:ASP:OD2	1:EB:178:ASN:ND2	2.43	0.51
1:AE:166:LYS:NZ	1:AE:173:ASP:OD2	2.42	0.51
1:CA:318:ASN:ND2	1:CA:351:ASN:OD1	2.43	0.51
1:CC:177:TYR:HA	1:CC:200:VAL:HG12	1.91	0.51
1:EB:62:ASP:OD1	1:EB:62:ASP:N	2.43	0.51
1:DE:94:SER:OG	1:DE:95:ARG:N	2.43	0.51
1:DK:145:ALA:HB2	1:DK:285:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EG:318:ASN:ND2	1:EG:351:ASN:OD1	2.43	0.51
1:FH:1:SER:OG	1:FH:2:PHE:N	2.43	0.51
1:AD:161:ASP:OD2	1:AD:161:ASP:N	2.38	0.51
1:BA:33:SER:OG	1:BA:34:GLY:N	2.41	0.51
1:BK:331:ASN:OD1	1:BK:331:ASN:N	2.44	0.51
1:CG:78:GLN:HB2	1:CG:353:GLY:HA3	1.93	0.51
1:CI:173:ASP:N	1:CI:173:ASP:OD1	2.43	0.51
1:DB:170:SER:OG	1:DB:173:ASP:OD1	2.29	0.51
1:DK:159:SER:HA	1:DK:267:GLN:HE21	1.75	0.51
1:AE:22:ASN:ND2	1:AE:33:SER:OG	2.44	0.51
1:BG:234:ASN:OD1	1:CB:188:SER:OG	2.28	0.51
1:BI:1:SER:OG	1:BI:2:PHE:N	2.41	0.51
1:CC:206:GLU:HG2	1:CC:230:LYS:HG3	1.91	0.51
1:DD:159:SER:HA	1:DD:267:GLN:HE21	1.76	0.51
1:EH:170:SER:OG	1:EH:171:VAL:N	2.42	0.51
1:EJ:375:ILE:HG21	1:FE:392:ASP:OD1	2.10	0.51
1:AA:177:TYR:HA	1:AA:200:VAL:HG12	1.93	0.51
1:AG:94:SER:HB3	1:AG:332:VAL:HG12	1.91	0.51
1:CA:62:ASP:OD1	1:CA:62:ASP:N	2.44	0.51
1:CF:1:SER:OG	1:CF:2:PHE:N	2.43	0.51
1:DE:159:SER:O	1:DK:251:ASN:ND2	2.44	0.51
1:DF:45:SER:OG	1:DF:46:LYS:N	2.43	0.51
1:DI:159:SER:OG	1:DI:267:GLN:NE2	2.42	0.51
1:AI:155:ILE:O	1:AI:265:SER:OG	2.26	0.51
1:AK:152:SER:OG	1:AK:279:ASN:OD1	2.28	0.51
1:BF:45:SER:OG	1:BF:46:LYS:N	2.44	0.51
1:BH:94:SER:OG	1:BH:95:ARG:N	2.44	0.51
1:BK:145:ALA:HB2	1:BK:285:PRO:HD3	1.92	0.51
1:CE:40:ASP:OD1	1:CE:40:ASP:N	2.43	0.51
1:FF:173:ASP:O	1:FF:176:SER:OG	2.29	0.51
1:FH:73:ASP:N	1:FH:73:ASP:OD1	2.39	0.51
1:BA:45:SER:OG	1:BA:46:LYS:N	2.44	0.51
1:BG:86:ASP:HB3	1:BG:113:MET:HG2	1.92	0.51
1:BG:379:ARG:NH2	1:CB:392:ASP:OD1	2.43	0.51
1:BI:100:LYS:NZ	1:BI:110:MET:SD	2.74	0.51
1:FH:266:MET:HE3	1:FH:267:GLN:H	1.76	0.51
1:BC:321:ASN:ND2	1:BC:322:ASN:O	2.44	0.51
1:CJ:293:ILE:HG12	1:CJ:299:VAL:HG12	1.91	0.51
1:DB:296:ASP:OD1	1:DB:296:ASP:N	2.42	0.51
1:EI:293:ILE:HG12	1:EI:299:VAL:HG12	1.93	0.51
1:AA:67:ASN:HD21	1:BA:52:LYS:HE2	1.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:177:TYR:HA	1:AE:200:VAL:HG22	1.93	0.51
1:CD:149:THR:HG1	1:CD:281:ASN:HD21	1.58	0.51
1:CK:3:SER:HA	1:CK:6:VAL:HG12	1.93	0.51
1:DJ:43:ALA:HB2	1:DJ:49:LEU:HD11	1.92	0.51
1:EH:100:LYS:HE3	1:FB:321:ASN:HD21	1.76	0.51
1:FG:28:THR:HG22	1:FG:30:GLY:H	1.75	0.51
1:BB:379:ARG:HD2	1:BH:395:LEU:HD22	1.92	0.50
1:BD:187:ASP:OD1	1:BD:191:ASN:N	2.44	0.50
1:ED:94:SER:OG	1:ED:95:ARG:N	2.43	0.50
1:EG:40:ASP:OD1	1:EG:40:ASP:N	2.41	0.50
1:EI:213:ASP:OD2	1:EI:247:THR:OG1	2.29	0.50
1:CB:213:ASP:OD2	1:CB:247:THR:OG1	2.28	0.50
1:CE:206:GLU:HG2	1:CE:230:LYS:HG2	1.93	0.50
1:CH:64:THR:HG23	1:DH:41:MET:HE1	1.93	0.50
1:CI:293:ILE:O	1:CI:357:ASN:ND2	2.43	0.50
1:DC:216:ASP:OD1	1:DC:216:ASP:N	2.44	0.50
1:DJ:375:ILE:HG12	1:EJ:402:ARG:HD3	1.93	0.50
1:EG:170:SER:OG	1:EG:173:ASP:OD1	2.29	0.50
1:FC:40:ASP:N	1:FC:40:ASP:OD1	2.39	0.50
1:FD:321:ASN:ND2	1:FD:338:ALA:O	2.44	0.50
1:AB:173:ASP:OD1	1:AB:173:ASP:N	2.40	0.50
1:AB:202:THR:OG1	1:AB:206:GLU:OE2	2.27	0.50
1:BA:380:ASN:O	1:BA:384:ASN:ND2	2.45	0.50
1:BC:40:ASP:OD1	1:BC:40:ASP:N	2.41	0.50
1:CF:145:ALA:HB2	1:CF:285:PRO:HG3	1.92	0.50
1:CG:117:GLY:HA2	1:CG:315:VAL:HG12	1.93	0.50
1:DA:117:GLY:HA2	1:DA:315:VAL:HG12	1.93	0.50
1:EF:111:GLN:NE2	1:EF:330:ASP:OD2	2.45	0.50
1:FF:72:LEU:HD11	1:FF:291:TYR:CE2	2.46	0.50
1:AI:73:ASP:N	1:AI:73:ASP:OD1	2.44	0.50
1:BA:187:ASP:OD2	1:BA:191:ASN:ND2	2.45	0.50
1:BF:318:ASN:HD21	1:BF:351:ASN:HB3	1.76	0.50
1:CF:43:ALA:HB2	1:CF:49:LEU:HD11	1.93	0.50
1:CI:117:GLY:HA2	1:CI:315:VAL:HG12	1.93	0.50
1:DB:159:SER:HA	1:DB:267:GLN:HE21	1.77	0.50
1:DB:263:LEU:HD23	1:DB:264:ASN:HB2	1.93	0.50
1:EH:149:THR:HG22	1:EH:281:ASN:HD21	1.76	0.50
1:AC:68:THR:HG23	1:AC:70:ARG:H	1.77	0.50
1:AD:25:ASN:HD22	1:AD:28:THR:HG21	1.76	0.50
1:AD:378:GLN:NE2	1:AI:393:GLN:OE1	2.44	0.50
1:BD:40:ASP:OD1	1:BD:40:ASP:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BH:62:ASP:N	1:BH:62:ASP:OD1	2.39	0.50
1:CI:298:THR:HG22	1:CI:313:GLN:HG3	1.93	0.50
1:DB:177:TYR:HA	1:DB:200:VAL:HG12	1.92	0.50
1:DG:1:SER:OG	1:DG:2:PHE:N	2.43	0.50
1:DH:94:SER:OG	1:DH:95:ARG:N	2.44	0.50
1:DJ:64:THR:HG23	1:EJ:49:LEU:HD22	1.94	0.50
1:EE:284:LYS:O	1:EE:305:ASN:ND2	2.39	0.50
1:FG:94:SER:OG	1:FG:95:ARG:N	2.44	0.50
1:FK:227:THR:OG1	1:FK:228:THR:N	2.43	0.50
1:AD:7:SER:OG	1:AD:51:VAL:O	2.29	0.50
1:BA:62:ASP:OD1	1:BA:62:ASP:N	2.43	0.50
1:BJ:85:VAL:HG22	1:BJ:91:VAL:HG12	1.94	0.50
1:BK:170:SER:OG	1:BK:173:ASP:OD1	2.29	0.50
1:DC:213:ASP:OD2	1:DC:247:THR:OG1	2.28	0.50
1:EH:32:LYS:NZ	1:EH:361:GLU:OE2	2.41	0.50
1:FD:284:LYS:O	1:FD:305:ASN:ND2	2.45	0.50
1:FE:265:SER:OG	1:FE:266:MET:N	2.45	0.50
1:AE:394:ILE:HA	1:AE:397:THR:HG22	1.93	0.50
1:CA:396:ASN:OD1	1:CA:400:ASN:ND2	2.43	0.50
1:DF:349:SER:OG	1:DF:350:GLY:N	2.45	0.50
1:EB:117:GLY:HA2	1:EB:315:VAL:HG23	1.94	0.50
1:EB:368:SER:OG	1:EH:381:TYR:OH	2.30	0.50
1:EI:179:LYS:HB3	1:EI:199:PHE:HB2	1.92	0.50
1:FA:45:SER:OG	1:FA:46:LYS:N	2.44	0.50
1:AE:158:ASN:ND2	1:AE:271:GLY:O	2.44	0.50
1:AG:67:ASN:HA	1:AG:359:ALA:HA	1.92	0.50
1:CA:285:PRO:O	1:CA:305:ASN:ND2	2.45	0.50
1:DE:62:ASP:OD1	1:DE:62:ASP:N	2.43	0.50
1:DK:22:ASN:HD21	1:DK:34:GLY:H	1.59	0.50
1:EG:94:SER:HB2	1:EG:332:VAL:HG12	1.93	0.50
1:FG:78:GLN:O	1:FG:95:ARG:NH2	2.45	0.50
1:FJ:195:MET:HG2	1:FJ:213:ASP:HB3	1.93	0.50
1:AD:193:HIS:HE1	1:AD:250:ILE:HG22	1.77	0.50
1:BE:73:ASP:OD1	1:BE:73:ASP:N	2.44	0.50
1:CF:293:ILE:HG12	1:CF:299:VAL:HG12	1.93	0.50
1:CI:40:ASP:OD1	1:CI:40:ASP:N	2.38	0.50
1:DC:155:ILE:O	1:DC:265:SER:OG	2.25	0.50
1:EG:161:ASP:OD1	1:EG:178:ASN:ND2	2.44	0.50
1:EH:99:PHE:HB3	1:EH:108:VAL:O	2.12	0.50
1:FB:94:SER:OG	1:FB:95:ARG:N	2.45	0.50
1:FB:127:ILE:HG21	1:FB:313:GLN:HE21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:136:ILE:HD11	1:AA:312:GLY:HA3	1.93	0.49
1:AG:45:SER:OG	1:AG:46:LYS:N	2.45	0.49
1:AK:303:TYR:HE1	1:AK:309:GLN:HB2	1.76	0.49
1:BA:368:SER:HA	1:CA:398:LEU:HD21	1.94	0.49
1:BC:187:ASP:OD1	1:BC:191:ASN:N	2.35	0.49
1:CJ:209:VAL:O	1:CJ:226:SER:OG	2.28	0.49
1:DG:45:SER:OG	1:DG:46:LYS:N	2.42	0.49
1:EA:209:VAL:HB	1:EA:227:THR:HB	1.94	0.49
1:ED:2:PHE:HZ	1:ED:392:ASP:OD1	1.95	0.49
1:AJ:187:ASP:OD2	1:AJ:191:ASN:ND2	2.45	0.49
1:DF:177:TYR:HA	1:DF:200:VAL:HG12	1.93	0.49
1:EB:1:SER:OG	1:EB:2:PHE:N	2.45	0.49
1:ED:303:TYR:HE1	1:ED:309:GLN:HB2	1.75	0.49
1:EE:1:SER:OG	1:EE:2:PHE:N	2.40	0.49
1:EF:269:ASN:ND2	1:FA:191:ASN:OD1	2.45	0.49
1:EH:205:ASN:ND2	1:EH:232:ASN:O	2.44	0.49
1:FC:62:ASP:OD1	1:FC:95:ARG:NH2	2.44	0.49
1:AC:22:ASN:HD21	1:AC:34:GLY:H	1.59	0.49
1:AK:158:ASN:ND2	1:AK:271:GLY:O	2.44	0.49
1:BC:111:GLN:NE2	1:BC:330:ASP:OD2	2.45	0.49
1:BD:94:SER:HB2	1:BD:332:VAL:HG12	1.93	0.49
1:BF:40:ASP:OD1	1:BF:40:ASP:N	2.44	0.49
1:BH:203:LYS:NZ	1:BH:206:GLU:OE1	2.42	0.49
1:CG:154:GLN:NE2	1:CG:264:ASN:O	2.46	0.49
1:CI:159:SER:O	1:DD:251:ASN:ND2	2.45	0.49
1:CJ:62:ASP:OD1	1:CJ:62:ASP:N	2.38	0.49
1:CK:379:ARG:HH21	1:DF:392:ASP:CG	2.18	0.49
1:EB:22:ASN:ND2	1:EB:33:SER:OG	2.44	0.49
1:EB:375:ILE:HG21	1:EH:392:ASP:OD2	2.12	0.49
1:FC:366:ASP:OD1	1:FC:366:ASP:N	2.38	0.49
1:AD:22:ASN:HD21	1:AD:33:SER:HG	1.58	0.49
1:BB:336:THR:O	1:BB:339:SER:OG	2.28	0.49
1:CE:141:THR:OG1	1:CE:142:LEU:N	2.46	0.49
1:CE:187:ASP:OD1	1:CE:193:HIS:NE2	2.39	0.49
1:CJ:266:MET:SD	1:CJ:268:GLN:NE2	2.82	0.49
1:DH:117:GLY:HA2	1:DH:315:VAL:HG23	1.93	0.49
1:DK:62:ASP:OD1	1:DK:62:ASP:N	2.41	0.49
1:EF:280:GLN:OE1	1:EF:282:GLY:N	2.41	0.49
1:EF:298:THR:HG22	1:EF:313:GLN:HG3	1.93	0.49
1:FH:187:ASP:OD1	1:FH:191:ASN:N	2.42	0.49
1:BH:389:LYS:NZ	1:CB:401:LEU:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CD:86:ASP:N	1:CD:86:ASP:OD1	2.45	0.49
1:DC:196:ASN:HD21	1:DC:214:SER:HB3	1.77	0.49
1:DI:374:MET:HE1	1:EC:387:THR:HA	1.94	0.49
1:AB:73:ASP:OD1	1:AB:73:ASP:N	2.42	0.49
1:AF:41:MET:HE3	1:AF:52:LYS:HD2	1.95	0.49
1:BK:298:THR:HG22	1:BK:313:GLN:HB3	1.94	0.49
1:CD:79:ASN:OD1	1:CD:79:ASN:N	2.44	0.49
1:EF:159:SER:O	1:EF:201:LYS:NZ	2.46	0.49
1:FB:3:SER:HA	1:FB:6:VAL:HG12	1.94	0.49
1:AH:22:ASN:HD21	1:AH:34:GLY:H	1.61	0.49
1:CB:40:ASP:OD1	1:CB:40:ASP:N	2.43	0.49
1:EB:287:ASP:OD1	1:EB:287:ASP:N	2.46	0.49
1:FB:202:THR:OG1	1:FB:206:GLU:OE2	2.28	0.49
1:FH:188:SER:HB3	1:FH:254:THR:HB	1.93	0.49
1:AD:4:GLN:HE22	1:AD:49:LEU:HA	1.77	0.49
1:BF:179:LYS:HB3	1:BF:199:PHE:HB2	1.95	0.49
1:BG:160:THR:OG1	1:BG:269:ASN:OD1	2.31	0.49
1:CC:40:ASP:OD1	1:CC:40:ASP:N	2.45	0.49
1:CI:78:GLN:HB2	1:CI:353:GLY:HA3	1.95	0.49
1:DE:145:ALA:HB2	1:DE:285:PRO:HD3	1.94	0.49
1:EB:177:TYR:HA	1:EB:200:VAL:HG12	1.94	0.49
1:EI:145:ALA:HB2	1:EI:285:PRO:HD3	1.95	0.49
1:EK:33:SER:HB3	1:EK:365:VAL:HG22	1.93	0.49
1:FG:111:GLN:NE2	1:FG:330:ASP:OD1	2.46	0.49
1:AE:156:ASN:HD21	1:AK:142:LEU:HB2	1.77	0.49
1:AH:94:SER:OG	1:AH:95:ARG:N	2.46	0.49
1:BE:40:ASP:OD1	1:BE:40:ASP:N	2.43	0.49
1:CF:187:ASP:OD1	1:CF:191:ASN:N	2.37	0.49
1:CG:83:ARG:O	1:CG:116:THR:OG1	2.30	0.49
1:CH:268:GLN:HE22	1:DC:144:ALA:HB1	1.78	0.49
1:DG:215:SER:O	1:DG:215:SER:OG	2.31	0.49
1:EJ:284:LYS:O	1:EJ:305:ASN:ND2	2.46	0.49
1:FF:177:TYR:HA	1:FF:200:VAL:HG12	1.95	0.49
1:FJ:1:SER:OG	1:FJ:2:PHE:N	2.37	0.49
1:AG:28:THR:HG23	1:AG:31:PHE:HB2	1.95	0.49
1:AJ:72:LEU:HD21	1:AJ:291:TYR:HE2	1.77	0.49
1:BK:78:GLN:HB2	1:BK:353:GLY:HA3	1.93	0.49
1:CG:1:SER:OG	1:CG:2:PHE:N	2.46	0.49
1:DB:329:GLY:H	1:DG:42:PHE:HB2	1.77	0.49
1:DC:102:ASP:HB2	1:DC:108:VAL:HG11	1.94	0.49
1:DD:84:LEU:HD21	1:DD:115:LEU:CD1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EF:330:ASP:OD1	1:EF:330:ASP:N	2.39	0.49
1:EJ:40:ASP:OD1	1:EJ:40:ASP:N	2.46	0.49
1:EJ:206:GLU:HG2	1:EJ:230:LYS:HG2	1.95	0.49
1:FF:166:LYS:HG3	1:FF:168:PRO:HD2	1.95	0.49
1:FK:94:SER:HB3	1:FK:332:VAL:HG12	1.94	0.49
1:AG:303:TYR:HE2	1:AG:309:GLN:HB2	1.78	0.48
1:AH:26:SER:O	1:AH:26:SER:OG	2.31	0.48
1:AI:45:SER:OG	1:AI:46:LYS:N	2.46	0.48
1:CG:32:LYS:NZ	1:CG:361:GLU:OE2	2.39	0.48
1:EB:146:LYS:NZ	1:EB:281:ASN:O	2.46	0.48
1:FB:45:SER:OG	1:FB:46:LYS:N	2.45	0.48
1:FC:94:SER:OG	1:FC:95:ARG:N	2.46	0.48
1:FC:166:LYS:HG3	1:FC:168:PRO:HD2	1.94	0.48
1:FK:1:SER:OG	1:FK:2:PHE:N	2.45	0.48
1:AA:159:SER:OG	1:AG:189:GLN:NE2	2.46	0.48
1:AF:279:ASN:OD1	1:AF:279:ASN:N	2.44	0.48
1:BB:336:THR:OG1	1:BB:337:GLN:N	2.46	0.48
1:BE:173:ASP:OD1	1:BE:173:ASP:N	2.46	0.48
1:BK:284:LYS:O	1:BK:305:ASN:ND2	2.40	0.48
1:CE:98:GLN:HG3	1:CE:360:LEU:HD21	1.93	0.48
1:CK:121:THR:OG1	1:CK:128:GLN:NE2	2.41	0.48
1:EB:155:ILE:HG12	1:EB:157:LEU:HG	1.94	0.48
1:DA:263:LEU:HD23	1:DA:264:ASN:HB2	1.95	0.48
1:EE:45:SER:OG	1:EE:46:LYS:N	2.46	0.48
1:FA:158:ASN:ND2	1:FA:271:GLY:O	2.46	0.48
1:FF:72:LEU:HD11	1:FF:291:TYR:HE2	1.78	0.48
1:AB:62:ASP:OD1	1:AB:62:ASP:N	2.45	0.48
1:AC:378:GLN:NE2	1:AH:393:GLN:OE1	2.46	0.48
1:AE:28:THR:O	1:AE:363:SER:OG	2.27	0.48
1:BK:368:SER:HB2	1:CF:9:LEU:HD23	1.94	0.48
1:CF:372:VAL:HG21	1:DA:6:VAL:HG11	1.95	0.48
1:DA:68:THR:HG22	1:DA:70:ARG:H	1.78	0.48
1:DI:234:ASN:OD1	1:ED:188:SER:OG	2.30	0.48
1:EA:67:ASN:OD1	1:EA:67:ASN:N	2.45	0.48
1:AB:202:THR:OG1	1:AB:203:LYS:N	2.46	0.48
1:BA:214:SER:O	1:BA:214:SER:OG	2.29	0.48
1:BI:284:LYS:O	1:BI:305:ASN:ND2	2.46	0.48
1:CG:94:SER:OG	1:CG:95:ARG:N	2.46	0.48
1:CH:187:ASP:OD1	1:CH:191:ASN:N	2.46	0.48
1:EI:78:GLN:HB2	1:EI:353:GLY:HA3	1.94	0.48
1:AA:232:ASN:ND2	1:AA:238:GLU:OE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:101:LEU:HD13	1:AB:107:LEU:HD23	1.96	0.48
1:BH:145:ALA:HB2	1:BH:285:PRO:HD3	1.96	0.48
1:CI:177:TYR:HA	1:CI:200:VAL:HG22	1.94	0.48
1:DG:83:ARG:O	1:DG:116:THR:OG1	2.30	0.48
1:DG:229:LEU:HD22	1:DG:237:LEU:HD11	1.95	0.48
1:DI:45:SER:OG	1:DI:46:LYS:N	2.45	0.48
1:DI:386:GLN:NE2	1:ED:399:VAL:O	2.46	0.48
1:EA:125:PRO:HG2	1:EA:309:GLN:HE21	1.78	0.48
1:EA:366:ASP:HB3	1:EA:369:LYS:HB3	1.95	0.48
1:EF:179:LYS:HD3	1:EF:273:ASN:HB2	1.95	0.48
1:FA:94:SER:OG	1:FA:95:ARG:N	2.47	0.48
1:FB:196:ASN:OD1	1:FB:214:SER:OG	2.32	0.48
1:FG:293:ILE:HG12	1:FG:299:VAL:HG12	1.95	0.48
1:AA:187:ASP:OD1	1:AA:191:ASN:N	2.46	0.48
1:AA:287:ASP:OD2	1:AA:287:ASP:N	2.40	0.48
1:AB:393:GLN:OE1	1:AH:402:ARG:NH1	2.47	0.48
1:AF:85:VAL:HG22	1:AF:91:VAL:HG22	1.94	0.48
1:AG:379:ARG:NE	1:BB:392:ASP:OD1	2.42	0.48
1:BE:205:ASN:ND2	1:BE:232:ASN:O	2.46	0.48
1:BI:84:LEU:HD22	1:BI:114:GLN:C	2.39	0.48
1:BK:45:SER:OG	1:BK:46:LYS:N	2.46	0.48
1:CA:73:ASP:N	1:CA:73:ASP:OD1	2.46	0.48
1:DA:346:THR:OG1	1:DA:347:ALA:N	2.45	0.48
1:EF:117:GLY:HA2	1:EF:315:VAL:HG12	1.95	0.48
1:EF:161:ASP:OD2	1:EF:178:ASN:ND2	2.47	0.48
1:EH:229:LEU:HD22	1:EH:237:LEU:HD11	1.95	0.48
1:AA:115:LEU:HD21	1:AA:314:ILE:HD12	1.96	0.48
1:AB:76:ILE:HD11	1:AB:95:ARG:HG2	1.95	0.48
1:BD:102:ASP:HB3	1:BD:108:VAL:HG11	1.96	0.48
1:BG:379:ARG:CZ	1:CB:392:ASP:OD1	2.61	0.48
1:BK:287:ASP:OD1	1:BK:287:ASP:N	2.45	0.48
1:DH:321:ASN:HB3	1:DH:339:SER:HA	1.95	0.48
1:DK:40:ASP:OD1	1:DK:40:ASP:N	2.44	0.48
1:DK:366:ASP:OD1	1:DK:366:ASP:N	2.40	0.48
1:BG:369:LYS:HE2	1:CB:10:ASN:HB2	1.95	0.48
1:DH:83:ARG:HH11	1:DH:116:THR:HG21	1.79	0.48
1:EG:102:ASP:OD2	1:EG:106:ASN:N	2.41	0.48
1:EK:227:THR:HG21	1:EK:243:VAL:HG21	1.95	0.48
1:FA:154:GLN:NE2	1:FA:263:LEU:O	2.47	0.48
1:FA:154:GLN:HE22	1:FA:264:ASN:HB2	1.78	0.48
1:FA:270:THR:HB	1:FG:285:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:155:ILE:HG13	1:FC:275:ILE:HA	1.95	0.48
1:FF:156:ASN:HD22	1:FF:274:ASN:H	1.60	0.48
1:FG:127:ILE:HD11	1:FG:310:VAL:HG11	1.95	0.48
1:AA:166:LYS:HG3	1:AA:168:PRO:HD2	1.96	0.48
1:AA:349:SER:OG	1:AA:350:GLY:N	2.47	0.48
1:AG:102:ASP:OD1	1:AG:102:ASP:N	2.47	0.48
1:BB:379:ARG:HE	1:BB:392:ASP:HB2	1.78	0.48
1:CI:68:THR:HG23	1:CI:70:ARG:H	1.79	0.48
1:CJ:124:PRO:HA	1:CJ:125:PRO:HD3	1.80	0.48
1:DH:1:SER:OG	1:DH:2:PHE:N	2.46	0.48
1:DJ:303:TYR:HE2	1:DJ:309:GLN:HB2	1.78	0.48
1:FG:246:THR:HG23	1:FG:257:THR:HG22	1.96	0.48
1:AA:127:ILE:HD11	1:AA:310:VAL:HG11	1.95	0.47
1:AJ:159:SER:HB3	1:AJ:269:ASN:HB2	1.96	0.47
1:BE:213:ASP:OD2	1:BE:247:THR:OG1	2.31	0.47
1:BI:187:ASP:OD1	1:BI:191:ASN:N	2.37	0.47
1:BJ:94:SER:OG	1:BJ:95:ARG:N	2.47	0.47
1:CC:58:GLN:HE22	1:CC:333:TRP:HE1	1.62	0.47
1:DC:209:VAL:HG22	1:DC:227:THR:HB	1.95	0.47
1:DG:213:ASP:OD2	1:DG:247:THR:OG1	2.32	0.47
1:FJ:215:SER:HB3	1:FJ:250:ILE:HD11	1.95	0.47
1:AI:28:THR:O	1:AI:363:SER:OG	2.29	0.47
1:CA:25:ASN:HD21	1:CF:40:ASP:HB3	1.79	0.47
1:CB:152:SER:OG	1:CB:279:ASN:OD1	2.30	0.47
1:CH:83:ARG:O	1:CH:116:THR:OG1	2.30	0.47
1:DE:280:GLN:HG2	1:DE:282:GLY:H	1.78	0.47
1:AE:43:ALA:HB2	1:AE:49:LEU:HD11	1.96	0.47
1:AG:7:SER:OG	1:AG:51:VAL:O	2.31	0.47
1:AG:386:GLN:NE2	1:BB:399:VAL:O	2.46	0.47
1:CC:279:ASN:OD1	1:CC:279:ASN:N	2.46	0.47
1:CI:84:LEU:HD23	1:CI:115:LEU:HA	1.96	0.47
1:FC:321:ASN:ND2	1:FC:338:ALA:O	2.43	0.47
1:FG:83:ARG:HB3	1:FG:116:THR:HB	1.97	0.47
1:FK:147:SER:OG	1:FK:148:THR:N	2.47	0.47
1:BI:98:GLN:HG2	1:BI:360:LEU:HD21	1.95	0.47
1:CB:67:ASN:HA	1:CB:359:ALA:HA	1.95	0.47
1:DJ:158:ASN:ND2	1:DJ:271:GLY:O	2.47	0.47
1:EB:229:LEU:HD22	1:EB:237:LEU:HD11	1.96	0.47
1:EF:145:ALA:HB2	1:EF:285:PRO:HD3	1.96	0.47
1:EJ:153:MET:HG3	1:EJ:278:THR:HG22	1.97	0.47
1:EK:28:THR:OG1	1:EK:29:TYR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:152:SER:OG	1:BA:279:ASN:OD1	2.32	0.47
1:BF:159:SER:HA	1:BF:267:GLN:HE21	1.79	0.47
1:BJ:33:SER:HB2	1:BJ:365:VAL:HG12	1.96	0.47
1:CH:113:MET:HE1	1:CH:332:VAL:HG21	1.96	0.47
1:DD:85:VAL:HG12	1:DD:91:VAL:HG12	1.97	0.47
1:DK:386:GLN:NE2	1:EF:399:VAL:O	2.47	0.47
1:EK:145:ALA:HB2	1:EK:285:PRO:HD3	1.95	0.47
1:FB:28:THR:O	1:FB:363:SER:OG	2.30	0.47
1:FE:300:VAL:HG22	1:FE:310:VAL:HG12	1.96	0.47
1:FH:95:ARG:NH1	1:FH:361:GLU:OE1	2.46	0.47
1:BF:25:ASN:ND2	1:BK:50:GLY:O	2.39	0.47
1:DA:390:THR:N	1:DG:402:ARG:NH2	2.62	0.47
1:AC:7:SER:OG	1:AC:51:VAL:O	2.33	0.47
1:AC:84:LEU:HD12	1:AC:84:LEU:N	2.29	0.47
1:AD:195:MET:HG3	1:AD:258:PHE:HZ	1.80	0.47
1:AG:202:THR:OG1	1:AG:203:LYS:N	2.47	0.47
1:AJ:378:GLN:HE21	1:AJ:382:GLN:HE22	1.63	0.47
1:BA:229:LEU:HD22	1:BA:237:LEU:HD11	1.97	0.47
1:BD:197:VAL:HG12	1:BD:211:THR:HG22	1.96	0.47
1:BJ:98:GLN:HG3	1:BJ:360:LEU:HD21	1.97	0.47
1:BK:216:ASP:HB3	1:BK:219:ALA:HB2	1.96	0.47
1:DG:187:ASP:OD1	1:DG:191:ASN:N	2.38	0.47
1:DH:176:SER:O	1:DH:176:SER:OG	2.32	0.47
1:DH:202:THR:OG1	1:DH:206:GLU:OE1	2.33	0.47
1:EA:187:ASP:OD1	1:EA:191:ASN:N	2.48	0.47
1:EA:386:GLN:NE2	1:EG:399:VAL:O	2.47	0.47
1:EC:40:ASP:OD1	1:EC:40:ASP:N	2.44	0.47
1:ED:234:ASN:OD1	1:EJ:188:SER:OG	2.32	0.47
1:EE:321:ASN:ND2	1:EE:338:ALA:O	2.48	0.47
1:EF:293:ILE:HG12	1:EF:299:VAL:HG12	1.96	0.47
1:EH:45:SER:OG	1:EH:46:LYS:N	2.44	0.47
1:EH:287:ASP:OD2	1:EH:287:ASP:N	2.42	0.47
1:FA:336:THR:O	1:FA:339:SER:OG	2.33	0.47
1:AD:62:ASP:OD1	1:AD:62:ASP:N	2.46	0.47
1:BJ:22:ASN:HD21	1:BJ:34:GLY:H	1.62	0.47
1:DK:1:SER:OG	1:DK:2:PHE:N	2.40	0.47
1:EC:26:SER:O	1:EC:26:SER:OG	2.33	0.47
1:ED:2:PHE:CZ	1:ED:392:ASP:OD1	2.68	0.47
1:FA:41:MET:HE3	1:FA:41:MET:HB2	1.77	0.47
1:AF:270:THR:HG21	1:BA:142:LEU:HD21	1.96	0.47
1:BF:117:GLY:HA2	1:BF:315:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BI:84:LEU:HD22	1:BI:115:LEU:CA	2.40	0.47
1:BK:346:THR:OG1	1:BK:347:ALA:N	2.46	0.47
1:DB:1:SER:OG	1:DB:2:PHE:N	2.43	0.47
1:EB:64:THR:HG22	1:FB:49:LEU:HD12	1.96	0.47
1:EG:374:MET:HE1	1:FA:387:THR:HG23	1.97	0.47
1:EK:197:VAL:HG13	1:EK:209:VAL:HG13	1.97	0.47
1:EK:246:THR:HG23	1:EK:257:THR:HG22	1.97	0.47
1:AD:366:ASP:OD2	1:AD:366:ASP:N	2.39	0.47
1:BK:234:ASN:O	1:BK:268:GLN:NE2	2.40	0.47
1:DC:179:LYS:HD3	1:DC:273:ASN:HB2	1.96	0.47
1:EB:28:THR:HB	1:EB:31:PHE:HB2	1.95	0.47
1:EG:270:THR:HG21	1:FB:142:LEU:HD21	1.97	0.47
1:AC:158:ASN:ND2	1:AC:269:ASN:OD1	2.47	0.46
1:AF:17:ASP:OD1	1:AK:1:SER:N	2.47	0.46
1:AJ:22:ASN:HD21	1:AJ:34:GLY:H	1.61	0.46
1:DD:84:LEU:CD2	1:DD:115:LEU:HD12	2.42	0.46
1:EC:187:ASP:OD1	1:EC:191:ASN:N	2.48	0.46
1:FB:32:LYS:O	1:FB:58:GLN:NE2	2.48	0.46
1:FC:83:ARG:O	1:FC:116:THR:OG1	2.32	0.46
1:FG:28:THR:HB	1:FG:31:PHE:HB2	1.97	0.46
1:AD:22:ASN:ND2	1:AD:370:GLU:OE2	2.49	0.46
1:CK:336:THR:O	1:CK:339:SER:OG	2.32	0.46
1:DJ:234:ASN:OD1	1:DJ:234:ASN:N	2.45	0.46
1:EF:274:ASN:N	1:EF:274:ASN:OD1	2.47	0.46
1:FH:161:ASP:OD2	1:FH:178:ASN:ND2	2.48	0.46
1:FK:45:SER:OG	1:FK:46:LYS:N	2.48	0.46
1:AD:177:TYR:HA	1:AD:200:VAL:HG22	1.98	0.46
1:BJ:281:ASN:OD1	1:BJ:281:ASN:N	2.47	0.46
1:CG:3:SER:HA	1:CG:6:VAL:HG12	1.97	0.46
1:CI:85:VAL:HG22	1:CI:91:VAL:HG12	1.97	0.46
1:CJ:158:ASN:ND2	1:CJ:271:GLY:O	2.48	0.46
1:DF:187:ASP:OD1	1:DF:191:ASN:N	2.48	0.46
1:DG:153:MET:HG3	1:DG:278:THR:HG22	1.97	0.46
1:DH:28:THR:HG22	1:EB:38:PHE:HB2	1.98	0.46
1:EG:321:ASN:ND2	1:EG:338:ALA:O	2.44	0.46
1:FA:58:GLN:HE21	1:FA:333:TRP:HH2	1.63	0.46
1:FH:94:SER:OG	1:FH:95:ARG:N	2.48	0.46
1:AK:1:SER:HA	1:AK:391:GLN:HE22	1.80	0.46
1:BI:234:ASN:OD1	1:CD:188:SER:OG	2.34	0.46
1:CK:109:ASN:HD21	1:CK:113:MET:HE3	1.81	0.46
1:ED:179:LYS:HB3	1:ED:199:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EF:365:VAL:HG13	1:EF:370:GLU:HG3	1.98	0.46
1:AE:45:SER:OG	1:AE:46:LYS:N	2.48	0.46
1:AK:274:ASN:OD1	1:AK:274:ASN:N	2.49	0.46
1:BF:330:ASP:O	1:BF:332:VAL:N	2.46	0.46
1:BH:379:ARG:NE	1:CC:392:ASP:OD1	2.46	0.46
1:AA:309:GLN:HE21	1:AA:311:LEU:HD21	1.81	0.46
1:AK:234:ASN:O	1:AK:268:GLN:NE2	2.39	0.46
1:BD:68:THR:HG22	1:BD:70:ARG:H	1.80	0.46
1:BK:117:GLY:HA2	1:BK:315:VAL:HG12	1.97	0.46
1:CD:216:ASP:HB3	1:CD:219:ALA:HB2	1.96	0.46
1:CH:378:GLN:NE2	1:DB:393:GLN:OE1	2.42	0.46
1:DA:390:THR:CA	1:DG:402:ARG:NH2	2.76	0.46
1:DK:234:ASN:OD1	1:EF:188:SER:OG	2.29	0.46
1:EK:274:ASN:N	1:EK:274:ASN:OD1	2.49	0.46
1:FC:284:LYS:O	1:FC:305:ASN:ND2	2.39	0.46
1:FF:105:ARG:NH2	1:FK:320:ALA:O	2.48	0.46
1:FK:148:THR:HG22	1:FK:282:GLY:HA3	1.97	0.46
1:AA:1:SER:OG	1:AA:2:PHE:N	2.45	0.46
1:BB:62:ASP:OD1	1:BB:62:ASP:N	2.49	0.46
1:CK:374:MET:HE1	1:DE:387:THR:HG23	1.96	0.46
1:DG:170:SER:OG	1:DG:173:ASP:OD1	2.28	0.46
1:FF:72:LEU:CD2	1:FF:291:TYR:HE2	2.26	0.46
1:FG:40:ASP:OD1	1:FG:40:ASP:N	2.39	0.46
1:FH:177:TYR:HA	1:FH:200:VAL:HG12	1.97	0.46
1:BB:249:THR:OG1	1:BB:253:ALA:O	2.29	0.46
1:BG:149:THR:HG22	1:BG:281:ASN:HD21	1.80	0.46
1:CC:64:THR:HG23	1:DC:41:MET:HE1	1.97	0.46
1:CE:330:ASP:O	1:CE:332:VAL:N	2.48	0.46
1:CK:379:ARG:HG3	1:DF:395:LEU:HD13	1.98	0.46
1:DA:70:ARG:NH1	1:DA:73:ASP:OD2	2.48	0.46
1:DC:70:ARG:NH2	1:DH:323:GLU:OE2	2.48	0.46
1:DC:379:ARG:HD2	1:DI:395:LEU:HD22	1.97	0.46
1:EH:2:PHE:CZ	1:EH:392:ASP:OD1	2.64	0.46
1:EI:173:ASP:OD1	1:EI:176:SER:OG	2.32	0.46
1:FF:43:ALA:HB2	1:FF:49:LEU:HD11	1.98	0.46
1:AD:128:GLN:HE21	1:AD:131:ALA:HB2	1.80	0.46
1:BH:379:ARG:HA	1:BH:379:ARG:HD3	1.70	0.46
1:CC:85:VAL:HG12	1:CC:91:VAL:HG22	1.98	0.46
1:CE:159:SER:HA	1:CE:267:GLN:HE21	1.81	0.46
1:CG:73:ASP:OD2	1:CG:73:ASP:N	2.49	0.46
1:FE:321:ASN:ND2	1:FE:338:ALA:O	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:73:ASP:OD1	1:AJ:73:ASP:N	2.48	0.46
1:AJ:158:ASN:ND2	1:AJ:271:GLY:O	2.49	0.46
1:BA:288:LEU:HA	1:BA:303:TYR:HD1	1.80	0.46
1:BJ:32:LYS:NZ	1:BJ:61:THR:O	2.43	0.46
1:CD:57:THR:OG1	1:CD:323:GLU:OE1	2.27	0.46
1:CF:117:GLY:HA2	1:CF:315:VAL:HG12	1.98	0.46
1:DG:366:ASP:OD1	1:DG:366:ASP:N	2.41	0.46
1:FD:234:ASN:OD1	1:FJ:188:SER:OG	2.34	0.46
1:FK:159:SER:HA	1:FK:267:GLN:HE21	1.81	0.46
1:AD:64:THR:H	1:AD:362:ALA:HB3	1.79	0.45
1:BD:45:SER:OG	1:BD:46:LYS:N	2.49	0.45
1:BE:177:TYR:HA	1:BE:200:VAL:HG22	1.97	0.45
1:BF:26:SER:O	1:BF:26:SER:OG	2.30	0.45
1:CF:209:VAL:HB	1:CF:227:THR:HG22	1.98	0.45
1:EE:79:ASN:OD1	1:EE:79:ASN:N	2.46	0.45
1:EE:83:ARG:O	1:EE:116:THR:OG1	2.34	0.45
1:FG:86:ASP:OD1	1:FG:86:ASP:N	2.45	0.45
1:FG:94:SER:OG	1:FG:96:ASN:OD1	2.34	0.45
1:AB:299:VAL:HG23	1:AB:311:LEU:HB2	1.98	0.45
1:AB:337:GLN:HE21	1:AB:338:ALA:H	1.62	0.45
1:BB:113:MET:HE1	1:BB:332:VAL:HG11	1.98	0.45
1:CE:31:PHE:HB3	1:CE:363:SER:HB2	1.99	0.45
1:DJ:98:GLN:HG3	1:DJ:360:LEU:HD21	1.97	0.45
1:DK:143:MET:HE1	1:DK:307:GLN:HB2	1.98	0.45
1:FB:32:LYS:NZ	1:FB:361:GLU:OE2	2.41	0.45
1:FI:94:SER:HB2	1:FI:332:VAL:HG12	1.98	0.45
1:AJ:1:SER:OG	1:AJ:2:PHE:N	2.46	0.45
1:AJ:77:SER:OG	1:AJ:78:GLN:OE1	2.25	0.45
1:BH:306:GLU:O	1:BH:307:GLN:NE2	2.49	0.45
1:BK:279:ASN:N	1:BK:279:ASN:OD1	2.48	0.45
1:CD:98:GLN:HG3	1:CD:360:LEU:HD21	1.98	0.45
1:CH:155:ILE:O	1:CH:265:SER:OG	2.27	0.45
1:CJ:346:THR:OG1	1:CJ:347:ALA:N	2.49	0.45
1:EK:336:THR:O	1:EK:339:SER:OG	2.34	0.45
1:FA:1:SER:OG	1:FA:2:PHE:N	2.49	0.45
1:FB:280:GLN:HG2	1:FB:282:GLY:H	1.80	0.45
1:BA:173:ASP:OD1	1:BA:173:ASP:N	2.48	0.45
1:CG:303:TYR:HE2	1:CG:309:GLN:HB2	1.80	0.45
1:DC:270:THR:HG23	1:DI:285:PRO:HG2	1.98	0.45
1:DI:213:ASP:OD2	1:DI:247:THR:OG1	2.35	0.45
1:EK:318:ASN:ND2	1:EK:351:ASN:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EK:326:ALA:HB3	1:EK:334:ALA:HB3	1.98	0.45
1:FB:28:THR:HG23	1:FB:31:PHE:HB2	1.98	0.45
1:AA:296:ASP:OD1	1:AA:296:ASP:N	2.42	0.45
1:BB:32:LYS:NZ	1:BB:361:GLU:OE2	2.40	0.45
1:BE:83:ARG:HD2	1:BE:344:LEU:HD11	1.99	0.45
1:CD:87:SER:O	1:CD:87:SER:OG	2.35	0.45
1:CH:117:GLY:HA2	1:CH:315:VAL:HG12	1.97	0.45
1:CH:196:ASN:OD1	1:CH:214:SER:OG	2.34	0.45
1:CI:336:THR:OG1	1:CI:337:GLN:N	2.48	0.45
1:FB:43:ALA:H	1:FB:49:LEU:HD23	1.82	0.45
1:AD:227:THR:OG1	1:AD:228:THR:N	2.49	0.45
1:BA:306:GLU:O	1:BA:307:GLN:NE2	2.49	0.45
1:BA:394:ILE:HG13	1:BA:395:LEU:HD12	1.99	0.45
1:BG:94:SER:OG	1:BG:95:ARG:N	2.50	0.45
1:DG:117:GLY:HA2	1:DG:315:VAL:HG12	1.98	0.45
1:EC:43:ALA:HB2	1:EC:49:LEU:HD11	1.98	0.45
1:EK:3:SER:HA	1:EK:6:VAL:HG12	1.99	0.45
1:FB:26:SER:O	1:FB:26:SER:OG	2.29	0.45
1:FB:101:LEU:O	1:FG:321:ASN:ND2	2.50	0.45
1:FD:143:MET:HE3	1:FD:309:GLN:HE21	1.81	0.45
1:FK:193:HIS:HE1	1:FK:250:ILE:HD12	1.81	0.45
1:AC:177:TYR:HA	1:AC:200:VAL:HG12	1.97	0.45
1:AF:28:THR:HG23	1:AF:31:PHE:HB2	1.98	0.45
1:BG:95:ARG:NH2	1:BG:361:GLU:OE2	2.45	0.45
1:CE:92:PHE:HB3	1:CE:332:VAL:HG13	1.98	0.45
1:DD:303:TYR:HE2	1:DD:309:GLN:HB2	1.82	0.45
1:DG:228:THR:OG1	1:DG:230:LYS:NZ	2.49	0.45
1:EA:373:ASN:HA	1:EA:376:VAL:HG22	1.98	0.45
1:EJ:143:MET:HE3	1:EJ:309:GLN:HE21	1.82	0.45
1:EK:303:TYR:HE2	1:EK:309:GLN:HB2	1.81	0.45
1:AB:74:VAL:HG12	1:AB:357:ASN:HA	1.98	0.45
1:AF:102:ASP:OD1	1:AF:102:ASP:N	2.48	0.45
1:AF:336:THR:OG1	1:AF:337:GLN:N	2.50	0.45
1:BC:296:ASP:OD1	1:BC:296:ASP:N	2.43	0.45
1:BI:84:LEU:HD21	1:BI:115:LEU:HA	1.88	0.45
1:CE:94:SER:OG	1:CE:95:ARG:N	2.49	0.45
1:DC:117:GLY:HA2	1:DC:315:VAL:HG12	1.98	0.45
1:DI:110:MET:HE3	1:DI:110:MET:HB3	1.85	0.45
1:DJ:229:LEU:HD22	1:DJ:237:LEU:HD11	1.98	0.45
1:EG:173:ASP:OD1	1:EG:173:ASP:N	2.46	0.45
1:FC:268:GLN:HB3	1:FI:285:PRO:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FH:287:ASP:OD2	1:FH:287:ASP:N	2.41	0.45
1:FJ:22:ASN:HD21	1:FJ:34:GLY:H	1.64	0.45
1:AC:94:SER:OG	1:AC:95:ARG:N	2.50	0.45
1:AF:40:ASP:OD1	1:AF:40:ASP:N	2.38	0.45
1:BB:330:ASP:O	1:BB:332:VAL:N	2.49	0.45
1:CD:94:SER:OG	1:CD:95:ARG:N	2.48	0.45
1:CH:287:ASP:N	1:CH:287:ASP:OD1	2.46	0.45
1:CJ:26:SER:O	1:CJ:26:SER:OG	2.32	0.45
1:CJ:330:ASP:N	1:CJ:330:ASP:OD1	2.49	0.45
1:DH:109:ASN:HD21	1:DH:113:MET:HE3	1.81	0.45
1:DI:3:SER:HA	1:DI:6:VAL:HG12	1.99	0.45
1:EI:74:VAL:HB	1:EI:355:LEU:HD12	1.99	0.45
1:EI:303:TYR:HE2	1:EI:309:GLN:HB2	1.82	0.45
1:FK:128:GLN:HE22	1:FK:131:ALA:HB2	1.82	0.45
1:AB:330:ASP:OD1	1:AB:330:ASP:N	2.43	0.45
1:AC:79:ASN:OD1	1:AC:79:ASN:N	2.48	0.45
1:AF:187:ASP:OD1	1:AF:191:ASN:N	2.35	0.45
1:AI:1:SER:OG	1:AI:2:PHE:N	2.48	0.45
1:BD:195:MET:HE3	1:BD:195:MET:HB2	1.87	0.45
1:BJ:177:TYR:HA	1:BJ:200:VAL:HG22	1.97	0.45
1:BK:195:MET:HE3	1:BK:195:MET:HB3	1.73	0.45
1:CC:330:ASP:O	1:CC:332:VAL:N	2.50	0.45
1:DD:202:THR:OG1	1:DD:203:LYS:N	2.50	0.45
1:DG:284:LYS:O	1:DG:305:ASN:ND2	2.44	0.45
1:EB:124:PRO:HA	1:EB:125:PRO:HD3	1.84	0.45
1:FA:105:ARG:O	1:FA:105:ARG:HG2	2.17	0.45
1:AC:155:ILE:O	1:AC:265:SER:OG	2.31	0.44
1:AF:24:ALA:HA	1:AK:384:ASN:HD21	1.80	0.44
1:AG:40:ASP:N	1:AG:40:ASP:OD1	2.44	0.44
1:CJ:379:ARG:NH1	1:CJ:382:GLN:OE1	2.49	0.44
1:DC:349:SER:OG	1:DC:350:GLY:N	2.51	0.44
1:DD:64:THR:HG22	1:ED:49:LEU:HD12	1.99	0.44
1:DJ:386:GLN:NE2	1:EE:399:VAL:O	2.50	0.44
1:EE:94:SER:HB2	1:EE:332:VAL:HG12	1.99	0.44
1:EH:33:SER:H	1:EH:364:ASN:HD22	1.64	0.44
1:EJ:306:GLU:O	1:EJ:307:GLN:NE2	2.50	0.44
1:FD:26:SER:O	1:FD:26:SER:OG	2.35	0.44
1:FH:266:MET:HE2	1:FH:268:GLN:HG3	1.99	0.44
1:FK:184:THR:O	1:FK:280:GLN:NE2	2.50	0.44
1:AF:107:LEU:HD23	1:AF:107:LEU:HA	1.89	0.44
1:AG:296:ASP:N	1:AG:296:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:304:SER:O	1:BC:304:SER:OG	2.34	0.44
1:CB:379:ARG:HA	1:CB:379:ARG:HD3	1.69	0.44
1:DC:279:ASN:OD1	1:DC:279:ASN:N	2.49	0.44
1:DE:84:LEU:HB3	1:DE:113:MET:HB3	1.99	0.44
1:DG:147:SER:HB3	1:DG:188:SER:HA	1.99	0.44
1:ED:65:THR:O	1:ED:65:THR:OG1	2.36	0.44
1:EF:155:ILE:O	1:EF:265:SER:OG	2.28	0.44
1:EH:153:MET:HE3	1:EH:153:MET:HB2	1.91	0.44
1:EK:296:ASP:OD1	1:EK:296:ASP:N	2.42	0.44
1:AG:161:ASP:OD1	1:AG:178:ASN:ND2	2.50	0.44
1:AK:187:ASP:OD1	1:AK:191:ASN:N	2.37	0.44
1:BB:331:ASN:OD1	1:BB:331:ASN:N	2.50	0.44
1:BD:124:PRO:HA	1:BD:125:PRO:HD3	1.85	0.44
1:CD:274:ASN:OD1	1:CD:274:ASN:N	2.51	0.44
1:CG:287:ASP:OD1	1:CG:287:ASP:N	2.44	0.44
1:DA:363:SER:O	1:DA:363:SER:OG	2.35	0.44
1:DH:65:THR:O	1:DH:65:THR:OG1	2.36	0.44
1:DI:94:SER:OG	1:DI:95:ARG:N	2.50	0.44
1:DI:121:THR:OG1	1:DI:128:GLN:NE2	2.51	0.44
1:EA:154:GLN:HE22	1:EG:141:THR:HG22	1.82	0.44
1:EC:234:ASN:OD1	1:EI:188:SER:OG	2.36	0.44
1:EH:296:ASP:N	1:EH:296:ASP:OD1	2.49	0.44
1:EJ:167:THR:HG23	1:EJ:168:PRO:HD3	1.99	0.44
1:FC:173:ASP:OD1	1:FC:173:ASP:N	2.44	0.44
1:FH:94:SER:HB2	1:FH:332:VAL:HG12	1.99	0.44
1:AJ:195:MET:HE3	1:AJ:195:MET:HB3	1.90	0.44
1:BE:79:ASN:OD1	1:BE:79:ASN:N	2.50	0.44
1:BH:284:LYS:O	1:BH:305:ASN:ND2	2.43	0.44
1:CB:300:VAL:HG12	1:CB:310:VAL:HG12	1.99	0.44
1:CC:379:ARG:HD3	1:CC:379:ARG:HA	1.77	0.44
1:AD:26:SER:O	1:AD:26:SER:OG	2.31	0.44
1:BC:28:THR:HG22	1:BH:38:PHE:HB2	2.00	0.44
1:CB:124:PRO:HA	1:CB:125:PRO:HD3	1.83	0.44
1:CD:1:SER:OG	1:CD:2:PHE:N	2.48	0.44
1:DB:379:ARG:HA	1:DB:379:ARG:HD3	1.74	0.44
1:DH:46:LYS:HA	1:DH:46:LYS:HD3	1.72	0.44
1:DI:117:GLY:HA2	1:DI:315:VAL:HG12	2.00	0.44
1:EB:187:ASP:OD1	1:EB:191:ASN:N	2.40	0.44
1:EK:107:LEU:HD23	1:EK:107:LEU:HA	1.85	0.44
1:FA:139:PRO:HB2	1:FA:141:THR:HG23	1.99	0.44
1:FH:263:LEU:HD23	1:FH:264:ASN:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:176:SER:O	1:AB:176:SER:OG	2.34	0.44
1:AE:365:VAL:HG23	1:AE:370:GLU:HG3	2.00	0.44
1:AK:62:ASP:OD1	1:AK:62:ASP:N	2.43	0.44
1:BH:117:GLY:HA2	1:BH:315:VAL:HG12	1.99	0.44
1:BI:187:ASP:OD2	1:BI:191:ASN:ND2	2.42	0.44
1:CB:64:THR:HG21	1:DB:3:SER:HB2	1.99	0.44
1:CH:78:GLN:HB2	1:CH:353:GLY:HA3	2.00	0.44
1:CH:94:SER:OG	1:CH:95:ARG:N	2.49	0.44
1:CJ:28:THR:HG22	1:DD:38:PHE:HB2	1.99	0.44
1:DC:145:ALA:HB2	1:DC:285:PRO:HD3	1.99	0.44
1:DD:336:THR:OG1	1:DD:337:GLN:N	2.49	0.44
1:DE:124:PRO:HA	1:DE:125:PRO:HD3	1.82	0.44
1:DF:83:ARG:HH11	1:DF:116:THR:HG21	1.82	0.44
1:DG:72:LEU:HD21	1:DG:291:TYR:HE2	1.83	0.44
1:EC:379:ARG:HA	1:EC:379:ARG:HD3	1.76	0.44
1:EE:336:THR:O	1:EE:339:SER:OG	2.35	0.44
1:FA:269:ASN:ND2	1:FG:189:GLN:O	2.34	0.44
1:FB:94:SER:HB2	1:FB:332:VAL:HG12	2.00	0.44
1:FH:305:ASN:HB3	1:FH:307:GLN:HB2	1.98	0.44
1:FJ:40:ASP:OD1	1:FJ:40:ASP:N	2.50	0.44
1:AC:220:THR:OG1	1:AC:221:ALA:N	2.50	0.44
1:AE:205:ASN:HA	1:AE:267:GLN:HE22	1.82	0.44
1:BA:246:THR:HG23	1:BA:257:THR:HG22	2.00	0.44
1:BC:177:TYR:HA	1:BC:200:VAL:HG12	1.98	0.44
1:BE:137:THR:OG1	1:BE:138:ILE:N	2.50	0.44
1:BE:229:LEU:HD22	1:BE:237:LEU:HD11	1.99	0.44
1:BH:294:ASN:OD1	1:CH:337:GLN:NE2	2.51	0.44
1:DA:212:HIS:HB2	1:DA:222:PRO:HG3	1.99	0.44
1:DF:98:GLN:HG3	1:DF:360:LEU:HD21	1.99	0.44
1:EB:7:SER:OG	1:EB:51:VAL:O	2.36	0.44
1:EC:147:SER:HB2	1:EC:188:SER:HA	1.98	0.44
1:EK:177:TYR:HA	1:EK:200:VAL:HG22	1.99	0.44
1:FB:386:GLN:O	1:FH:402:ARG:NH2	2.51	0.44
1:FJ:41:MET:HG2	1:FJ:52:LYS:HE3	2.00	0.44
1:AH:263:LEU:HD23	1:AH:264:ASN:HB2	1.99	0.44
1:AK:98:GLN:HG3	1:AK:360:LEU:HD21	1.98	0.44
1:BA:94:SER:OG	1:BA:95:ARG:N	2.51	0.44
1:BA:349:SER:OG	1:BA:350:GLY:N	2.51	0.44
1:BE:158:ASN:ND2	1:BE:271:GLY:O	2.50	0.44
1:BG:68:THR:HG23	1:BG:70:ARG:H	1.81	0.44
1:CI:161:ASP:OD1	1:CI:178:ASN:ND2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:227:THR:OG1	1:DA:228:THR:N	2.51	0.44
1:DB:379:ARG:NE	1:DH:392:ASP:OD1	2.48	0.44
1:DK:159:SER:O	1:EF:251:ASN:ND2	2.51	0.44
1:EK:299:VAL:HG23	1:EK:311:LEU:HB2	1.99	0.44
1:FE:390:THR:OG1	1:FK:402:ARG:NH2	2.51	0.44
1:FG:117:GLY:HA2	1:FG:315:VAL:HG23	2.00	0.44
1:AD:194:ASP:OD1	1:AD:194:ASP:N	2.36	0.44
1:BA:223:THR:OG1	1:BA:224:THR:N	2.51	0.44
1:DE:3:SER:HA	1:DE:6:VAL:HG12	2.00	0.44
1:ED:159:SER:O	1:ED:201:LYS:NZ	2.51	0.44
1:EH:379:ARG:HA	1:EH:379:ARG:HD3	1.89	0.44
1:EJ:293:ILE:HG12	1:EJ:299:VAL:HG22	2.00	0.44
1:EK:170:SER:HB2	1:EK:173:ASP:HB2	2.00	0.44
1:FD:40:ASP:OD1	1:FD:40:ASP:N	2.40	0.44
1:FD:336:THR:O	1:FD:339:SER:OG	2.30	0.44
1:FK:376:VAL:O	1:FK:380:ASN:ND2	2.44	0.44
1:AK:73:ASP:OD2	1:AK:359:ALA:N	2.51	0.43
1:BC:94:SER:OG	1:BC:95:ARG:N	2.51	0.43
1:CB:166:LYS:HD3	1:CB:166:LYS:HA	1.89	0.43
1:CC:315:VAL:HG11	1:CC:344:LEU:HD12	2.00	0.43
1:CI:331:ASN:OD1	1:CI:331:ASN:N	2.50	0.43
1:DB:94:SER:HB2	1:DB:332:VAL:HG12	2.00	0.43
1:DC:107:LEU:HD23	1:DC:107:LEU:HA	1.91	0.43
1:ED:85:VAL:HG12	1:ED:91:VAL:HG12	1.99	0.43
1:ED:124:PRO:HA	1:ED:125:PRO:HD3	1.89	0.43
1:EE:175:ASP:OD1	1:EE:175:ASP:N	2.45	0.43
1:FC:187:ASP:OD1	1:FC:191:ASN:N	2.40	0.43
1:AB:303:TYR:HE1	1:AB:309:GLN:HB2	1.83	0.43
1:AE:7:SER:OG	1:AE:51:VAL:O	2.35	0.43
1:AE:179:LYS:HA	1:AE:179:LYS:HD2	1.87	0.43
1:AK:124:PRO:HA	1:AK:125:PRO:HD3	1.86	0.43
1:BA:396:ASN:HA	1:BA:399:VAL:HG22	1.99	0.43
1:BG:206:GLU:HG2	1:BG:230:LYS:HB3	2.00	0.43
1:CF:185:VAL:HG23	1:CF:193:HIS:HB2	2.00	0.43
1:DD:366:ASP:OD1	1:DD:366:ASP:N	2.36	0.43
1:DJ:281:ASN:OD1	1:DJ:281:ASN:N	2.51	0.43
1:EE:149:THR:OG1	1:EE:281:ASN:ND2	2.45	0.43
1:EJ:73:ASP:OD2	1:EJ:359:ALA:N	2.51	0.43
1:FF:321:ASN:HB3	1:FF:339:SER:HA	2.01	0.43
1:AF:306:GLU:HG3	1:BF:337:GLN:HB2	1.99	0.43
1:AH:7:SER:OG	1:AH:51:VAL:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:78:GLN:HB2	1:BF:353:GLY:HA3	1.99	0.43
1:BG:161:ASP:N	1:BG:161:ASP:OD1	2.51	0.43
1:BG:177:TYR:HA	1:BG:200:VAL:HG12	2.00	0.43
1:BK:73:ASP:N	1:BK:73:ASP:OD1	2.50	0.43
1:DF:93:TYR:O	1:DF:333:TRP:N	2.47	0.43
1:ED:287:ASP:N	1:ED:304:SER:OG	2.49	0.43
1:FH:4:GLN:H	1:FH:4:GLN:HG2	1.59	0.43
1:AK:117:GLY:HA2	1:AK:315:VAL:HG12	2.00	0.43
1:BE:1:SER:OG	1:BE:2:PHE:N	2.51	0.43
1:BF:161:ASP:OD2	1:BF:178:ASN:ND2	2.41	0.43
1:CI:143:MET:HE3	1:CI:309:GLN:HE21	1.82	0.43
1:EC:117:GLY:HA2	1:EC:315:VAL:HG12	2.00	0.43
1:EC:398:LEU:HA	1:EC:401:LEU:HD23	2.00	0.43
1:FK:147:SER:HB2	1:FK:188:SER:HB2	1.99	0.43
1:AB:247:THR:HB	1:AB:255:ALA:HB1	1.99	0.43
1:BD:389:LYS:HD2	1:BJ:402:ARG:HH22	1.84	0.43
1:BH:183:VAL:HG12	1:BH:195:MET:HB2	2.00	0.43
1:BJ:124:PRO:HA	1:BJ:125:PRO:HD3	1.88	0.43
1:CE:67:ASN:ND2	1:DE:41:MET:SD	2.92	0.43
1:CF:132:ASN:OD1	1:CF:132:ASN:N	2.51	0.43
1:CI:124:PRO:HA	1:CI:125:PRO:HD3	1.86	0.43
1:CJ:175:ASP:OD1	1:CJ:175:ASP:N	2.47	0.43
1:DD:132:ASN:OD1	1:DD:132:ASN:N	2.51	0.43
1:EB:32:LYS:NZ	1:EB:361:GLU:OE2	2.48	0.43
1:EG:354:LYS:HE2	1:EG:354:LYS:HB3	1.76	0.43
1:EI:94:SER:OG	1:EI:95:ARG:N	2.51	0.43
1:EJ:45:SER:OG	1:EJ:46:LYS:N	2.52	0.43
1:FC:108:VAL:HG12	1:FC:114:GLN:HA	2.00	0.43
1:FF:209:VAL:HB	1:FF:227:THR:HG22	1.99	0.43
1:FK:193:HIS:CE1	1:FK:250:ILE:HD12	2.54	0.43
1:AC:40:ASP:OD1	1:AC:40:ASP:N	2.51	0.43
1:AC:367:LEU:HD23	1:BC:395:LEU:HD11	2.00	0.43
1:BB:155:ILE:O	1:BB:265:SER:OG	2.32	0.43
1:BC:331:ASN:OD1	1:BC:331:ASN:N	2.50	0.43
1:BD:86:ASP:OD1	1:BD:88:ASN:ND2	2.46	0.43
1:BE:281:ASN:OD1	1:BE:281:ASN:N	2.52	0.43
1:BK:98:GLN:HG3	1:BK:360:LEU:HD21	2.00	0.43
1:CA:94:SER:OG	1:CA:95:ARG:N	2.51	0.43
1:CC:321:ASN:ND2	1:CC:338:ALA:O	2.41	0.43
1:DE:263:LEU:HD23	1:DE:263:LEU:HA	1.87	0.43
1:DF:366:ASP:OD2	1:DF:366:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DH:26:SER:O	1:DH:26:SER:OG	2.28	0.43
1:FF:124:PRO:HA	1:FF:125:PRO:HD3	1.83	0.43
1:AC:213:ASP:OD2	1:AC:247:THR:OG1	2.37	0.43
1:AC:303:TYR:HE2	1:AC:309:GLN:HG2	1.82	0.43
1:CG:40:ASP:OD1	1:CG:40:ASP:N	2.52	0.43
1:EG:143:MET:SD	1:EG:305:ASN:ND2	2.85	0.43
1:AA:317:ALA:O	1:AA:318:ASN:ND2	2.51	0.43
1:AF:263:LEU:HD23	1:AF:264:ASN:HB2	2.01	0.43
1:BE:98:GLN:HB3	1:BE:110:MET:HE3	2.00	0.43
1:BJ:391:GLN:HA	1:BJ:394:ILE:HG12	2.01	0.43
1:CB:86:ASP:OD1	1:CB:87:SER:N	2.52	0.43
1:CJ:22:ASN:HD21	1:CJ:34:GLY:H	1.67	0.43
1:DF:127:ILE:HD12	1:DF:129:GLN:HE21	1.84	0.43
1:FA:331:ASN:OD1	1:FA:331:ASN:N	2.50	0.43
1:FB:281:ASN:OD1	1:FB:281:ASN:N	2.51	0.43
1:FC:159:SER:O	1:FC:201:LYS:NZ	2.51	0.43
1:AG:379:ARG:HH21	1:BG:402:ARG:HH21	1.67	0.43
1:BC:303:TYR:HE2	1:BC:309:GLN:HB2	1.84	0.43
1:BE:156:ASN:HB3	1:BE:270:THR:HG21	2.01	0.43
1:CI:213:ASP:OD1	1:CI:213:ASP:N	2.41	0.43
1:DB:61:THR:O	1:DB:364:ASN:ND2	2.50	0.43
1:DE:41:MET:HE3	1:DE:41:MET:HB2	1.83	0.43
1:DJ:146:LYS:NZ	1:DJ:281:ASN:O	2.41	0.43
1:DK:247:THR:OG1	1:DK:248:GLY:N	2.48	0.43
1:FH:117:GLY:HA2	1:FH:315:VAL:HG12	1.99	0.43
1:AK:1:SER:OG	1:AK:2:PHE:N	2.48	0.43
1:BB:229:LEU:HD22	1:BB:237:LEU:HD11	2.00	0.43
1:BJ:187:ASP:OD1	1:BJ:191:ASN:N	2.51	0.43
1:CE:330:ASP:OD1	1:CE:330:ASP:N	2.45	0.43
1:DB:331:ASN:OD1	1:DB:331:ASN:N	2.50	0.43
1:DJ:172:SER:OG	1:DJ:173:ASP:N	2.52	0.43
1:DK:166:LYS:HA	1:DK:166:LYS:HD3	1.76	0.43
1:EE:149:THR:HG1	1:EE:281:ASN:HD21	1.63	0.43
1:EJ:31:PHE:HB3	1:EJ:363:SER:HB2	2.01	0.43
1:FB:265:SER:OG	1:FB:266:MET:N	2.52	0.43
1:FC:102:ASP:OD1	1:FC:102:ASP:N	2.50	0.43
1:FE:118:TYR:HD2	1:FE:313:GLN:HE21	1.65	0.43
1:FH:269:ASN:OD1	1:FH:269:ASN:N	2.52	0.43
1:AK:351:ASN:OD1	1:AK:351:ASN:N	2.50	0.42
1:BH:330:ASP:O	1:BH:332:VAL:N	2.52	0.42
1:CA:3:SER:HA	1:CA:6:VAL:HG12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:188:SER:O	1:CH:188:SER:OG	2.33	0.42
1:DJ:368:SER:HA	1:EJ:398:LEU:HD21	2.01	0.42
1:FK:73:ASP:OD1	1:FK:73:ASP:N	2.51	0.42
1:AF:211:THR:HG21	1:AF:245:ILE:HD12	2.02	0.42
1:AJ:378:GLN:NE2	1:BD:393:GLN:OE1	2.52	0.42
1:AK:145:ALA:HB2	1:AK:285:PRO:HD3	2.01	0.42
1:BH:127:ILE:HD11	1:BH:310:VAL:HG11	2.01	0.42
1:CB:94:SER:OG	1:CB:95:ARG:N	2.52	0.42
1:CC:263:LEU:HD23	1:CC:264:ASN:HB2	2.01	0.42
1:CG:148:THR:HG21	1:CG:185:VAL:HG12	2.01	0.42
1:DE:45:SER:OG	1:DE:46:LYS:N	2.52	0.42
1:EE:179:LYS:HB3	1:EE:199:PHE:HB2	1.99	0.42
1:EE:336:THR:OG1	1:EE:337:GLN:N	2.52	0.42
1:EF:113:MET:HE1	1:EF:332:VAL:HG11	2.01	0.42
1:EJ:46:LYS:HD3	1:EJ:46:LYS:HA	1.78	0.42
1:FE:9:LEU:HD12	1:FE:384:ASN:HB3	2.00	0.42
1:AD:1:SER:OG	1:AD:2:PHE:N	2.52	0.42
1:AG:177:TYR:HA	1:AG:200:VAL:HG12	2.02	0.42
1:AH:147:SER:HB2	1:AH:188:SER:HA	2.01	0.42
1:AJ:145:ALA:HB2	1:AJ:285:PRO:HD3	2.01	0.42
1:BA:188:SER:O	1:BA:188:SER:OG	2.29	0.42
1:BF:94:SER:HB2	1:BF:332:VAL:HG12	2.01	0.42
1:BF:155:ILE:HG13	1:BF:275:ILE:HG12	2.00	0.42
1:DD:187:ASP:OD1	1:DD:191:ASN:N	2.43	0.42
1:DJ:305:ASN:N	1:DJ:305:ASN:OD1	2.49	0.42
1:EE:386:GLN:NE2	1:EK:402:ARG:OXT	2.53	0.42
1:FG:297:GLY:HA2	1:FG:355:LEU:HD12	2.00	0.42
1:AF:245:ILE:HD13	1:AF:245:ILE:HA	1.93	0.42
1:BC:366:ASP:OD1	1:BC:366:ASP:N	2.50	0.42
1:CG:46:LYS:HA	1:CG:46:LYS:HD3	1.84	0.42
1:DD:84:LEU:HD22	1:DD:115:LEU:CA	2.45	0.42
1:EE:390:THR:HG22	1:EK:402:ARG:HH22	1.85	0.42
1:FD:336:THR:OG1	1:FD:337:GLN:N	2.52	0.42
1:FG:226:SER:OG	1:FG:227:THR:N	2.53	0.42
1:FH:223:THR:HG23	1:FH:224:THR:HG23	1.99	0.42
1:AB:177:TYR:HA	1:AB:200:VAL:HG12	2.00	0.42
1:AC:274:ASN:OD1	1:AC:274:ASN:N	2.53	0.42
1:AJ:343:LEU:HD12	1:AJ:343:LEU:HA	1.89	0.42
1:BC:175:ASP:N	1:BC:175:ASP:OD1	2.44	0.42
1:BF:173:ASP:OD1	1:BF:173:ASP:N	2.44	0.42
1:DD:161:ASP:HA	1:DD:162:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DJ:124:PRO:HA	1:DJ:125:PRO:HD3	1.82	0.42
1:EA:177:TYR:HA	1:EA:200:VAL:HG22	2.02	0.42
1:EE:41:MET:HE3	1:EE:41:MET:HB2	1.91	0.42
1:FI:94:SER:OG	1:FI:95:ARG:N	2.53	0.42
1:BE:15:ASN:O	1:BE:19:ILE:HG12	2.19	0.42
1:BH:4:GLN:NE2	1:BH:48:GLY:O	2.51	0.42
1:BI:281:ASN:OD1	1:BI:281:ASN:N	2.52	0.42
1:CG:375:ILE:HD13	1:DB:392:ASP:OD2	2.19	0.42
1:CH:124:PRO:HA	1:CH:125:PRO:HD3	1.92	0.42
1:DE:187:ASP:OD1	1:DE:191:ASN:N	2.52	0.42
1:EG:32:LYS:HA	1:EG:364:ASN:HD21	1.84	0.42
1:FB:146:LYS:NZ	1:FB:281:ASN:O	2.44	0.42
1:FC:78:GLN:HB2	1:FC:353:GLY:HA3	2.01	0.42
1:FK:173:ASP:OD1	1:FK:173:ASP:N	2.41	0.42
1:AF:11:ALA:HB1	1:AF:38:PHE:HE1	1.85	0.42
1:BA:3:SER:HA	1:BA:6:VAL:HG22	2.02	0.42
1:BF:382:GLN:HB3	1:CA:399:VAL:HG11	2.01	0.42
1:BJ:366:ASP:OD1	1:BJ:366:ASP:N	2.52	0.42
1:BK:52:LYS:HB3	1:BK:52:LYS:HE2	1.86	0.42
1:DC:281:ASN:OD1	1:DC:281:ASN:N	2.52	0.42
1:DH:40:ASP:N	1:DH:40:ASP:OD1	2.48	0.42
1:DH:275:ILE:HD12	1:EH:130:GLY:HA3	2.02	0.42
1:DH:346:THR:OG1	1:DH:347:ALA:N	2.53	0.42
1:EB:78:GLN:HB2	1:EB:353:GLY:HA3	2.01	0.42
1:EB:83:ARG:O	1:EB:116:THR:OG1	2.29	0.42
1:EG:287:ASP:OD1	1:EG:287:ASP:N	2.44	0.42
1:FA:287:ASP:H	1:FA:304:SER:HG	1.62	0.42
1:FB:117:GLY:HA2	1:FB:315:VAL:HG12	2.01	0.42
1:FC:331:ASN:OD1	1:FC:331:ASN:N	2.51	0.42
1:FF:157:LEU:HD23	1:FF:179:LYS:HD2	2.01	0.42
1:AA:247:THR:OG1	1:AA:248:GLY:N	2.52	0.42
1:AB:158:ASN:H	1:AB:273:ASN:ND2	2.18	0.42
1:AF:375:ILE:HB	1:AF:379:ARG:HH21	1.83	0.42
1:AI:117:GLY:HA2	1:AI:315:VAL:HG12	2.01	0.42
1:CE:183:VAL:HG23	1:CE:195:MET:HB2	2.02	0.42
1:DH:249:THR:OG1	1:DH:253:ALA:O	2.36	0.42
1:EA:94:SER:HB3	1:EA:332:VAL:HG12	2.02	0.42
1:EH:40:ASP:OD1	1:EH:40:ASP:N	2.52	0.42
1:EJ:321:ASN:ND2	1:EJ:338:ALA:O	2.47	0.42
1:FB:166:LYS:HG2	1:FB:168:PRO:HD2	2.01	0.42
1:FE:366:ASP:OD1	1:FE:366:ASP:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FG:154:GLN:HB3	1:FG:277:ALA:HB3	2.02	0.42
1:AA:284:LYS:O	1:AA:305:ASN:ND2	2.38	0.42
1:AG:33:SER:HB3	1:AG:365:VAL:HG22	2.02	0.42
1:AJ:227:THR:OG1	1:AJ:228:THR:N	2.53	0.42
1:AK:250:ILE:HD13	1:AK:250:ILE:HA	1.93	0.42
1:BC:64:THR:HG21	1:CC:3:SER:HB2	2.01	0.42
1:BF:187:ASP:OD1	1:BF:191:ASN:N	2.50	0.42
1:BK:132:ASN:OD1	1:BK:132:ASN:N	2.52	0.42
1:CH:143:MET:HE3	1:CH:309:GLN:HE21	1.85	0.42
1:DB:173:ASP:OD1	1:DB:173:ASP:N	2.52	0.42
1:EC:118:TYR:HB2	1:EC:313:GLN:HB3	2.02	0.42
1:EI:247:THR:OG1	1:EI:248:GLY:N	2.53	0.42
1:FD:76:ILE:H	1:FD:76:ILE:HG12	1.69	0.42
1:FI:231:PHE:HE1	1:FI:237:LEU:HD12	1.85	0.42
1:AH:155:ILE:O	1:AH:265:SER:OG	2.28	0.42
1:AH:336:THR:O	1:AH:339:SER:OG	2.31	0.42
1:AJ:124:PRO:HA	1:AJ:125:PRO:HD3	1.90	0.42
1:BH:33:SER:HB2	1:BH:365:VAL:HG22	2.02	0.42
1:BH:70:ARG:HE	1:BH:70:ARG:HB3	1.64	0.42
1:BI:40:ASP:OD1	1:BI:40:ASP:N	2.43	0.42
1:CD:3:SER:HA	1:CD:6:VAL:HG22	2.02	0.42
1:CE:303:TYR:HE1	1:CE:309:GLN:HG2	1.85	0.42
1:CK:206:GLU:HG2	1:CK:230:LYS:HG2	2.01	0.42
1:DC:274:ASN:OD1	1:DC:274:ASN:N	2.52	0.42
1:DE:179:LYS:HD3	1:DE:273:ASN:HB2	2.01	0.42
1:EC:379:ARG:HD2	1:EI:395:LEU:HD23	2.01	0.42
1:ED:64:THR:HG22	1:FD:49:LEU:HD13	2.01	0.42
1:EI:245:ILE:HD13	1:EI:245:ILE:HA	1.93	0.42
1:AA:388:ILE:HG21	1:AF:401:LEU:HD21	2.01	0.41
1:AI:230:LYS:HB3	1:AI:230:LYS:HE2	1.88	0.41
1:BF:125:PRO:HG2	1:BF:309:GLN:HE21	1.84	0.41
1:CE:177:TYR:HA	1:CE:200:VAL:HG22	2.02	0.41
1:DA:107:LEU:HD23	1:DA:107:LEU:HA	1.93	0.41
1:DH:86:ASP:OD1	1:DH:90:SER:N	2.53	0.41
1:EF:124:PRO:HA	1:EF:125:PRO:HD3	1.90	0.41
1:EF:331:ASN:N	1:EF:331:ASN:OD1	2.49	0.41
1:FK:336:THR:O	1:FK:339:SER:OG	2.35	0.41
1:AF:229:LEU:HD22	1:AF:237:LEU:HD11	2.02	0.41
1:BE:136:ILE:HD12	1:BE:136:ILE:HA	1.90	0.41
1:BI:171:VAL:HG11	1:BI:222:PRO:HD2	2.01	0.41
1:CB:284:LYS:O	1:CB:305:ASN:ND2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CJ:40:ASP:OD1	1:CJ:40:ASP:N	2.49	0.41
1:CJ:107:LEU:HD23	1:CJ:107:LEU:HA	1.85	0.41
1:CK:395:LEU:HD23	1:CK:395:LEU:HA	1.93	0.41
1:DF:269:ASN:OD1	1:DF:269:ASN:N	2.53	0.41
1:DG:279:ASN:OD1	1:DG:279:ASN:N	2.54	0.41
1:DI:40:ASP:OD1	1:DI:40:ASP:N	2.47	0.41
1:DK:213:ASP:OD2	1:DK:247:THR:OG1	2.30	0.41
1:FB:33:SER:HB2	1:FB:365:VAL:HG22	2.01	0.41
1:FF:41:MET:HB2	1:FF:49:LEU:HB2	2.03	0.41
1:AA:159:SER:HA	1:AA:267:GLN:HE21	1.85	0.41
1:BA:148:THR:HG21	1:BA:185:VAL:HB	2.01	0.41
1:BB:157:LEU:HB2	1:BB:267:GLN:HB3	2.03	0.41
1:CG:145:ALA:HB2	1:CG:285:PRO:HD3	2.03	0.41
1:CJ:116:THR:HA	1:CJ:135:PRO:HA	2.02	0.41
1:CK:293:ILE:O	1:CK:357:ASN:ND2	2.42	0.41
1:DA:110:MET:SD	1:DF:37:SER:OG	2.72	0.41
1:DG:247:THR:OG1	1:DG:248:GLY:N	2.53	0.41
1:DG:298:THR:HG22	1:DG:313:GLN:HB3	2.02	0.41
1:EG:155:ILE:HD11	1:EG:179:LYS:HG2	2.03	0.41
1:FA:95:ARG:NH2	1:FA:361:GLU:OE2	2.54	0.41
1:FB:124:PRO:HA	1:FB:125:PRO:HD3	1.89	0.41
1:FC:363:SER:O	1:FC:364:ASN:ND2	2.53	0.41
1:AD:229:LEU:HD22	1:AD:237:LEU:HD11	2.01	0.41
1:BD:41:MET:HE2	1:BD:52:LYS:HB2	2.02	0.41
1:BD:303:TYR:HE1	1:BD:309:GLN:HB2	1.84	0.41
1:CF:281:ASN:OD1	1:CF:281:ASN:N	2.53	0.41
1:CF:330:ASP:O	1:CF:332:VAL:N	2.54	0.41
1:DB:336:THR:HG22	1:DB:337:GLN:H	1.84	0.41
1:DH:202:THR:OG1	1:DH:203:LYS:N	2.54	0.41
1:DH:379:ARG:HD3	1:DH:379:ARG:HA	1.83	0.41
1:DK:90:SER:OG	1:DK:91:VAL:N	2.53	0.41
1:EC:369:LYS:O	1:EC:373:ASN:ND2	2.53	0.41
1:FA:374:MET:HE2	1:FA:374:MET:HB3	1.91	0.41
1:FE:386:GLN:NE2	1:FK:402:ARG:OXT	2.54	0.41
1:FH:343:LEU:HD12	1:FH:343:LEU:HA	1.91	0.41
1:FI:336:THR:OG1	1:FI:337:GLN:N	2.53	0.41
1:AA:329:GLY:H	1:AF:42:PHE:HB2	1.85	0.41
1:AB:124:PRO:HA	1:AB:125:PRO:HD3	1.88	0.41
1:AE:368:SER:HB2	1:AK:9:LEU:HD23	2.02	0.41
1:AF:22:ASN:HD21	1:AF:34:GLY:H	1.69	0.41
1:AI:387:THR:HA	1:AI:390:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:124:PRO:HA	1:BB:125:PRO:HD3	1.95	0.41
1:BD:284:LYS:O	1:BD:305:ASN:ND2	2.47	0.41
1:BE:379:ARG:HG3	1:BK:395:LEU:HD23	2.01	0.41
1:BI:124:PRO:HA	1:BI:125:PRO:HD3	1.88	0.41
1:BI:160:THR:OG1	1:BI:269:ASN:OD1	2.38	0.41
1:CC:293:ILE:HG12	1:CC:299:VAL:HG12	2.03	0.41
1:CF:28:THR:HB	1:CF:31:PHE:HB2	2.02	0.41
1:CG:9:LEU:HD12	1:CG:9:LEU:HA	1.93	0.41
1:CK:215:SER:O	1:CK:215:SER:OG	2.34	0.41
1:DE:330:ASP:O	1:DE:332:VAL:N	2.50	0.41
1:EI:40:ASP:OD1	1:EI:40:ASP:N	2.53	0.41
1:EK:366:ASP:OD1	1:EK:366:ASP:N	2.52	0.41
1:FA:154:GLN:HG3	1:FA:277:ALA:HB3	2.02	0.41
1:FG:298:THR:HG22	1:FG:313:GLN:HB3	2.03	0.41
1:FI:177:TYR:HA	1:FI:200:VAL:HG12	2.03	0.41
1:FK:96:ASN:OD1	1:FK:96:ASN:N	2.47	0.41
1:AE:211:THR:HG21	1:AE:245:ILE:HD12	2.02	0.41
1:AF:78:GLN:CD	1:AF:79:ASN:H	2.28	0.41
1:AG:305:ASN:OD1	1:AG:305:ASN:N	2.54	0.41
1:CB:159:SER:HA	1:CB:267:GLN:HE21	1.85	0.41
1:CH:379:ARG:HA	1:CH:379:ARG:HD3	1.70	0.41
1:CI:303:TYR:HE1	1:CI:309:GLN:HB2	1.85	0.41
1:DI:107:LEU:HD23	1:DI:107:LEU:HA	1.91	0.41
1:DI:249:THR:HG22	1:DI:255:ALA:HB2	2.03	0.41
1:EE:187:ASP:OD2	1:EE:193:HIS:NE2	2.42	0.41
1:EG:356:THR:OG1	1:EG:357:ASN:N	2.53	0.41
1:EH:72:LEU:HD21	1:EH:291:TYR:HE2	1.85	0.41
1:FJ:216:ASP:HB3	1:FJ:219:ALA:HB2	2.02	0.41
1:AA:53:VAL:HG12	1:AA:55:GLY:H	1.86	0.41
1:AC:247:THR:OG1	1:AC:248:GLY:N	2.54	0.41
1:AG:232:ASN:OD1	1:AG:233:GLU:N	2.50	0.41
1:AG:379:ARG:NH2	1:BG:402:ARG:HH21	2.18	0.41
1:AI:78:GLN:O	1:AI:95:ARG:NH2	2.53	0.41
1:AJ:279:ASN:OD1	1:AJ:279:ASN:N	2.54	0.41
1:BC:124:PRO:HA	1:BC:125:PRO:HD3	1.94	0.41
1:CF:124:PRO:HA	1:CF:125:PRO:HD3	1.84	0.41
1:CH:227:THR:OG1	1:CH:228:THR:N	2.53	0.41
1:CI:73:ASP:OD1	1:CI:359:ALA:N	2.53	0.41
1:CK:41:MET:HE3	1:CK:41:MET:HB2	1.88	0.41
1:DD:263:LEU:HD23	1:DD:263:LEU:HA	1.91	0.41
1:DF:274:ASN:OD1	1:DF:274:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DG:156:ASN:OD1	1:DG:156:ASN:N	2.53	0.41
1:DH:204:ASP:OD1	1:DH:204:ASP:N	2.53	0.41
1:DJ:173:ASP:N	1:DJ:173:ASP:OD1	2.51	0.41
1:EB:369:LYS:HE3	1:EB:369:LYS:HB2	1.83	0.41
1:FE:22:ASN:HD21	1:FE:34:GLY:H	1.68	0.41
1:AA:316:LEU:HD11	1:AA:355:LEU:HD21	2.02	0.41
1:AF:258:PHE:HE2	1:AF:260:LEU:HD13	1.86	0.41
1:BG:26:SER:OG	1:CA:380:ASN:OD1	2.36	0.41
1:BJ:68:THR:HG21	1:BJ:360:LEU:HD13	2.02	0.41
1:BJ:336:THR:OG1	1:BJ:337:GLN:N	2.53	0.41
1:CA:124:PRO:HA	1:CA:125:PRO:HD3	1.85	0.41
1:CH:304:SER:O	1:CH:304:SER:OG	2.31	0.41
1:CK:68:THR:HG21	1:CK:360:LEU:HD12	2.02	0.41
1:DE:177:TYR:HA	1:DE:200:VAL:HG22	2.03	0.41
1:DG:379:ARG:HA	1:DG:379:ARG:HD3	1.83	0.41
1:EA:146:LYS:HD2	1:EA:146:LYS:HA	1.82	0.41
1:EA:389:LYS:HE2	1:EA:389:LYS:HB3	1.81	0.41
1:EH:124:PRO:HA	1:EH:125:PRO:HD3	1.87	0.41
1:FC:52:LYS:HB2	1:FC:52:LYS:HE3	1.89	0.41
1:FH:187:ASP:OD1	1:FH:190:GLY:N	2.51	0.41
1:FI:363:SER:O	1:FI:364:ASN:ND2	2.54	0.41
1:AA:346:THR:OG1	1:AA:347:ALA:N	2.49	0.41
1:AB:186:TYR:HE2	1:AB:284:LYS:HG3	1.85	0.41
1:AC:124:PRO:HA	1:AC:125:PRO:HD3	1.80	0.41
1:AC:281:ASN:OD1	1:AC:281:ASN:N	2.52	0.41
1:AG:378:GLN:HE21	1:AG:382:GLN:NE2	2.18	0.41
1:AH:143:MET:HE2	1:AH:143:MET:HB3	1.92	0.41
1:AJ:244:ASN:OD1	1:AJ:244:ASN:N	2.49	0.41
1:AK:70:ARG:NH2	1:AK:99:PHE:O	2.54	0.41
1:BA:76:ILE:HD11	1:BA:95:ARG:NH1	2.35	0.41
1:BA:356:THR:HG21	1:BA:359:ALA:HB3	2.01	0.41
1:BB:330:ASP:OD2	1:BB:330:ASP:N	2.54	0.41
1:BE:395:LEU:HD23	1:BE:395:LEU:HA	1.92	0.41
1:BG:23:ILE:HD13	1:BG:23:ILE:HA	1.92	0.41
1:BG:107:LEU:HD23	1:BG:107:LEU:HA	1.85	0.41
1:BH:173:ASP:OD1	1:BH:173:ASP:N	2.54	0.41
1:BI:202:THR:OG1	1:BI:203:LYS:N	2.53	0.41
1:CA:330:ASP:O	1:CA:332:VAL:N	2.50	0.41
1:CJ:379:ARG:HG3	1:DE:395:LEU:HD23	2.03	0.41
1:DB:281:ASN:OD1	1:DB:281:ASN:N	2.53	0.41
1:DC:161:ASP:HA	1:DC:162:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DC:212:HIS:HB2	1:DC:222:PRO:HG3	2.03	0.41
1:DD:23:ILE:HD11	1:DD:370:GLU:HB2	2.03	0.41
1:DD:330:ASP:O	1:DD:332:VAL:N	2.54	0.41
1:DD:336:THR:O	1:DD:339:SER:OG	2.39	0.41
1:DF:389:LYS:HE3	1:DK:401:LEU:HD23	2.02	0.41
1:DH:113:MET:HE1	1:DH:332:VAL:HG21	2.03	0.41
1:DI:179:LYS:HD3	1:DI:273:ASN:HB2	2.02	0.41
1:DK:287:ASP:OD1	1:DK:287:ASP:N	2.53	0.41
1:EA:138:ILE:HG23	1:EA:311:LEU:HD13	2.02	0.41
1:EA:367:LEU:HD23	1:EA:367:LEU:HA	1.94	0.41
1:EB:227:THR:OG1	1:EB:228:THR:N	2.54	0.41
1:EB:266:MET:HE3	1:EB:266:MET:HB2	1.97	0.41
1:EB:398:LEU:HD23	1:EB:398:LEU:HA	1.89	0.41
1:EE:110:MET:HE3	1:EE:110:MET:HB3	1.93	0.41
1:FC:86:ASP:OD1	1:FC:86:ASP:N	2.53	0.41
1:FH:117:GLY:HA3	1:FH:136:ILE:HD11	2.02	0.41
1:FJ:300:VAL:HG12	1:FJ:310:VAL:HG22	2.01	0.41
1:FK:40:ASP:N	1:FK:40:ASP:OD1	2.49	0.41
1:AD:379:ARG:HA	1:AD:379:ARG:HD3	1.76	0.41
1:BF:41:MET:HE3	1:BF:41:MET:HB2	1.94	0.41
1:BI:94:SER:OG	1:BI:95:ARG:N	2.54	0.41
1:BJ:266:MET:HE3	1:BJ:266:MET:HB2	1.96	0.41
1:CD:369:LYS:HE2	1:CD:369:LYS:HB2	1.93	0.41
1:CG:317:ALA:HB2	1:CG:344:LEU:HD23	2.03	0.41
1:CI:98:GLN:HG3	1:CI:360:LEU:HD21	2.02	0.41
1:CK:341:VAL:HG12	1:CK:342:ALA:H	1.85	0.41
1:DB:330:ASP:O	1:DB:332:VAL:N	2.49	0.41
1:DC:375:ILE:HD13	1:EC:401:LEU:HD11	2.03	0.41
1:EE:281:ASN:OD1	1:EE:281:ASN:N	2.54	0.41
1:FB:287:ASP:OD1	1:FB:287:ASP:N	2.51	0.41
1:FC:379:ARG:HA	1:FC:379:ARG:HD3	1.92	0.41
1:FJ:284:LYS:O	1:FJ:305:ASN:ND2	2.54	0.41
1:AC:161:ASP:HA	1:AC:162:PRO:HD3	1.84	0.40
1:CA:368:SER:HA	1:DA:398:LEU:HD21	2.03	0.40
1:DD:195:MET:HE3	1:DD:195:MET:HB3	1.91	0.40
1:DK:187:ASP:OD1	1:DK:191:ASN:N	2.54	0.40
1:DK:247:THR:HG23	1:DK:255:ALA:HB1	2.03	0.40
1:DK:306:GLU:HB3	1:EK:337:GLN:HG2	2.02	0.40
1:EB:395:LEU:HA	1:EB:395:LEU:HD12	1.89	0.40
1:EC:4:GLN:H	1:EC:4:GLN:HG2	1.73	0.40
1:EC:28:THR:OG1	1:EC:29:TYR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EH:161:ASP:HA	1:EH:162:PRO:HD3	1.91	0.40
1:EJ:107:LEU:HD23	1:EJ:107:LEU:HA	1.89	0.40
1:EJ:375:ILE:CG2	1:FE:392:ASP:OD1	2.69	0.40
1:FC:124:PRO:HA	1:FC:125:PRO:HD3	1.94	0.40
1:FC:166:LYS:HD2	1:FC:166:LYS:HA	1.91	0.40
1:FF:86:ASP:OD1	1:FF:87:SER:N	2.48	0.40
1:FG:46:LYS:HA	1:FG:46:LYS:HD2	1.87	0.40
1:AG:166:LYS:HD2	1:AG:166:LYS:HA	1.82	0.40
1:AK:209:VAL:HB	1:AK:227:THR:HG22	2.02	0.40
1:BF:206:GLU:HG2	1:BF:230:LYS:HG2	2.03	0.40
1:BF:394:ILE:HA	1:BF:397:THR:HG22	2.03	0.40
1:BJ:247:THR:OG1	1:BJ:248:GLY:N	2.55	0.40
1:CB:155:ILE:HG12	1:CB:157:LEU:HG	2.04	0.40
1:CD:145:ALA:HB2	1:CD:285:PRO:HD3	2.02	0.40
1:CE:227:THR:OG1	1:CE:228:THR:N	2.54	0.40
1:CF:216:ASP:OD1	1:CF:216:ASP:N	2.46	0.40
1:CF:244:ASN:HD22	1:CF:244:ASN:HA	1.73	0.40
1:CI:229:LEU:HB3	1:CI:237:LEU:HD11	2.03	0.40
1:DB:23:ILE:HD13	1:DB:23:ILE:HA	1.92	0.40
1:DK:41:MET:HE3	1:DK:41:MET:HB2	1.88	0.40
1:EE:3:SER:HA	1:EE:6:VAL:HG12	2.03	0.40
1:FD:176:SER:O	1:FD:176:SER:OG	2.39	0.40
1:FD:281:ASN:OD1	1:FD:281:ASN:N	2.54	0.40
1:AC:379:ARG:NE	1:AI:392:ASP:OD1	2.46	0.40
1:AD:124:PRO:HA	1:AD:125:PRO:HD3	1.87	0.40
1:AD:161:ASP:HA	1:AD:162:PRO:HD3	1.91	0.40
1:AD:400:ASN:HD22	1:AD:400:ASN:HA	1.68	0.40
1:AH:327:SER:O	1:AH:328:GLN:NE2	2.53	0.40
1:AI:369:LYS:HD3	1:BD:10:ASN:HD21	1.86	0.40
1:BI:374:MET:HE1	1:CC:387:THR:HG23	2.03	0.40
1:BK:41:MET:HE3	1:BK:41:MET:HB2	1.84	0.40
1:CC:94:SER:OG	1:CC:95:ARG:N	2.54	0.40
1:CG:206:GLU:HG2	1:CG:230:LYS:HG2	2.03	0.40
1:CI:33:SER:HB3	1:CI:365:VAL:HG22	2.03	0.40
1:CJ:117:GLY:HA2	1:CJ:315:VAL:HG12	2.02	0.40
1:DD:197:VAL:HG12	1:DD:211:THR:HG22	2.03	0.40
1:DE:374:MET:HE1	1:DJ:387:THR:HA	2.04	0.40
1:DJ:28:THR:HG22	1:ED:38:PHE:HB2	2.03	0.40
1:DJ:132:ASN:HA	1:DJ:133:PRO:HD3	1.91	0.40
1:EA:83:ARG:O	1:EA:116:THR:OG1	2.31	0.40
1:EB:279:ASN:OD1	1:EB:279:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:197:VAL:HG12	1:EC:211:THR:HG22	2.03	0.40
1:EG:62:ASP:OD2	1:EG:62:ASP:N	2.55	0.40
1:EH:303:TYR:HE1	1:EH:309:GLN:HB2	1.86	0.40
1:FI:149:THR:HG22	1:FI:281:ASN:HD21	1.85	0.40
1:AI:124:PRO:HA	1:AI:125:PRO:HD3	1.99	0.40
1:AK:40:ASP:OD1	1:AK:40:ASP:N	2.54	0.40
1:BA:227:THR:OG1	1:BA:228:THR:N	2.54	0.40
1:BB:23:ILE:HD13	1:BB:23:ILE:HA	1.93	0.40
1:BC:100:LYS:HE3	1:BC:110:MET:HG2	2.03	0.40
1:BC:329:GLY:H	1:BH:42:PHE:HB2	1.87	0.40
1:BD:336:THR:OG1	1:BD:337:GLN:N	2.54	0.40
1:BH:136:ILE:HD13	1:BH:312:GLY:HA3	2.03	0.40
1:BH:293:ILE:HG12	1:BH:299:VAL:HG12	2.02	0.40
1:BJ:374:MET:HE2	1:BJ:374:MET:HB3	1.76	0.40
1:CA:346:THR:OG1	1:CA:347:ALA:N	2.52	0.40
1:CH:281:ASN:OD1	1:CH:281:ASN:N	2.54	0.40
1:CI:155:ILE:HG12	1:CI:157:LEU:HG	2.02	0.40
1:DC:64:THR:HG21	1:EC:3:SER:HB2	2.04	0.40
1:DC:379:ARG:HA	1:DC:379:ARG:HD3	1.80	0.40
1:DG:262:PHE:O	1:DG:265:SER:OG	2.31	0.40
1:DH:98:GLN:HB2	1:DH:360:LEU:HD21	2.04	0.40
1:DH:274:ASN:N	1:DH:274:ASN:OD1	2.54	0.40
1:EA:166:LYS:NZ	1:EA:173:ASP:OD1	2.55	0.40
1:EH:369:LYS:HE3	1:EH:369:LYS:HB2	1.94	0.40
1:EK:247:THR:OG1	1:EK:248:GLY:N	2.53	0.40
1:AA:61:THR:OG1	1:AA:62:ASP:N	2.51	0.40
1:AC:28:THR:HG22	1:AH:38:PHE:HB2	2.03	0.40
1:AJ:263:LEU:HD23	1:AJ:263:LEU:HA	1.85	0.40
1:BA:166:LYS:HE3	1:BA:166:LYS:HB3	1.93	0.40
1:BC:117:GLY:HA2	1:BC:315:VAL:HG23	2.03	0.40
1:BJ:379:ARG:HG3	1:CE:395:LEU:HD23	2.02	0.40
1:BK:70:ARG:HH22	1:BK:98:GLN:HG2	1.87	0.40
1:CA:177:TYR:HA	1:CA:200:VAL:HG22	2.03	0.40
1:CG:72:LEU:HD21	1:CG:291:TYR:HE2	1.86	0.40
1:CJ:86:ASP:OD1	1:CJ:87:SER:N	2.55	0.40
1:DE:74:VAL:HB	1:DE:355:LEU:HD22	2.03	0.40
1:DH:247:THR:OG1	1:DH:248:GLY:N	2.55	0.40
1:DJ:3:SER:HA	1:DJ:6:VAL:HG12	2.03	0.40
1:DK:28:THR:HG22	1:EE:38:PHE:HB2	2.02	0.40
1:EA:246:THR:HG22	1:EA:257:THR:HG23	2.02	0.40
1:EH:187:ASP:OD1	1:EH:190:GLY:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:35:THR:OG1	1:FC:36:ALA:N	2.55	0.40
1:FH:139:PRO:HD2	1:FH:311:LEU:HD23	2.03	0.40
1:FH:154:GLN:NE2	1:FH:264:ASN:O	2.38	0.40
1:FI:29:TYR:HD1	1:FI:29:TYR:HA	1.82	0.40
1:FK:95:ARG:NH1	1:FK:361:GLU:OE1	2.54	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	400/402 (100%)	366 (92%)	34 (8%)	0	100	100
1	AB	400/402 (100%)	368 (92%)	32 (8%)	0	100	100
1	AC	400/402 (100%)	373 (93%)	27 (7%)	0	100	100
1	AD	400/402 (100%)	370 (92%)	30 (8%)	0	100	100
1	AE	400/402 (100%)	368 (92%)	32 (8%)	0	100	100
1	AF	400/402 (100%)	369 (92%)	31 (8%)	0	100	100
1	AG	400/402 (100%)	364 (91%)	36 (9%)	0	100	100
1	AH	400/402 (100%)	371 (93%)	29 (7%)	0	100	100
1	AI	400/402 (100%)	360 (90%)	40 (10%)	0	100	100
1	AJ	400/402 (100%)	371 (93%)	29 (7%)	0	100	100
1	AK	400/402 (100%)	364 (91%)	36 (9%)	0	100	100
1	BA	400/402 (100%)	371 (93%)	29 (7%)	0	100	100
1	BB	400/402 (100%)	367 (92%)	33 (8%)	0	100	100
1	BC	400/402 (100%)	366 (92%)	34 (8%)	0	100	100
1	BD	400/402 (100%)	369 (92%)	31 (8%)	0	100	100
1	BE	400/402 (100%)	370 (92%)	30 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BF	400/402 (100%)	370 (92%)	30 (8%)	0	100	100
1	BG	400/402 (100%)	370 (92%)	30 (8%)	0	100	100
1	BH	400/402 (100%)	374 (94%)	26 (6%)	0	100	100
1	BI	400/402 (100%)	371 (93%)	29 (7%)	0	100	100
1	BJ	400/402 (100%)	373 (93%)	27 (7%)	0	100	100
1	BK	400/402 (100%)	369 (92%)	31 (8%)	0	100	100
1	CA	400/402 (100%)	367 (92%)	33 (8%)	0	100	100
1	CB	400/402 (100%)	368 (92%)	32 (8%)	0	100	100
1	CC	400/402 (100%)	360 (90%)	40 (10%)	0	100	100
1	CD	400/402 (100%)	368 (92%)	32 (8%)	0	100	100
1	CE	400/402 (100%)	362 (90%)	38 (10%)	0	100	100
1	CF	400/402 (100%)	370 (92%)	30 (8%)	0	100	100
1	CG	400/402 (100%)	362 (90%)	38 (10%)	0	100	100
1	CH	400/402 (100%)	371 (93%)	29 (7%)	0	100	100
1	CI	400/402 (100%)	374 (94%)	26 (6%)	0	100	100
1	CJ	400/402 (100%)	373 (93%)	27 (7%)	0	100	100
1	CK	400/402 (100%)	369 (92%)	31 (8%)	0	100	100
1	DA	400/402 (100%)	371 (93%)	29 (7%)	0	100	100
1	DB	400/402 (100%)	366 (92%)	34 (8%)	0	100	100
1	DC	400/402 (100%)	373 (93%)	27 (7%)	0	100	100
1	DD	400/402 (100%)	370 (92%)	30 (8%)	0	100	100
1	DE	400/402 (100%)	368 (92%)	32 (8%)	0	100	100
1	DF	400/402 (100%)	363 (91%)	37 (9%)	0	100	100
1	DG	400/402 (100%)	361 (90%)	39 (10%)	0	100	100
1	DH	400/402 (100%)	366 (92%)	34 (8%)	0	100	100
1	DI	400/402 (100%)	369 (92%)	31 (8%)	0	100	100
1	DJ	400/402 (100%)	371 (93%)	29 (7%)	0	100	100
1	DK	400/402 (100%)	364 (91%)	36 (9%)	0	100	100
1	EA	400/402 (100%)	364 (91%)	36 (9%)	0	100	100
1	EB	400/402 (100%)	375 (94%)	25 (6%)	0	100	100
1	EC	400/402 (100%)	373 (93%)	27 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ED	400/402 (100%)	366 (92%)	34 (8%)	0	100	100
1	EE	400/402 (100%)	367 (92%)	33 (8%)	0	100	100
1	EF	400/402 (100%)	365 (91%)	35 (9%)	0	100	100
1	EG	400/402 (100%)	363 (91%)	37 (9%)	0	100	100
1	EH	400/402 (100%)	369 (92%)	31 (8%)	0	100	100
1	EI	400/402 (100%)	371 (93%)	29 (7%)	0	100	100
1	EJ	400/402 (100%)	366 (92%)	34 (8%)	0	100	100
1	EK	400/402 (100%)	369 (92%)	31 (8%)	0	100	100
1	FA	400/402 (100%)	374 (94%)	26 (6%)	0	100	100
1	FB	400/402 (100%)	367 (92%)	33 (8%)	0	100	100
1	FC	400/402 (100%)	368 (92%)	32 (8%)	0	100	100
1	FD	400/402 (100%)	378 (94%)	22 (6%)	0	100	100
1	FE	400/402 (100%)	365 (91%)	35 (9%)	0	100	100
1	FF	400/402 (100%)	374 (94%)	26 (6%)	0	100	100
1	FG	400/402 (100%)	361 (90%)	39 (10%)	0	100	100
1	FH	400/402 (100%)	375 (94%)	25 (6%)	0	100	100
1	FI	400/402 (100%)	373 (93%)	27 (7%)	0	100	100
1	FJ	400/402 (100%)	360 (90%)	40 (10%)	0	100	100
1	FK	400/402 (100%)	374 (94%)	26 (6%)	0	100	100
All	All	26400/26532 (100%)	24317 (92%)	2083 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	AB	322/322 (100%)	321 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	322/322 (100%)	320 (99%)	2 (1%)	78	89
1	AD	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	AE	322/322 (100%)	320 (99%)	2 (1%)	78	89
1	AF	322/322 (100%)	322 (100%)	0	100	100
1	AG	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	AH	322/322 (100%)	322 (100%)	0	100	100
1	AI	322/322 (100%)	322 (100%)	0	100	100
1	AJ	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	AK	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	BA	322/322 (100%)	322 (100%)	0	100	100
1	BB	322/322 (100%)	322 (100%)	0	100	100
1	BC	322/322 (100%)	322 (100%)	0	100	100
1	BD	322/322 (100%)	322 (100%)	0	100	100
1	BE	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	BF	322/322 (100%)	322 (100%)	0	100	100
1	BG	322/322 (100%)	322 (100%)	0	100	100
1	BH	322/322 (100%)	322 (100%)	0	100	100
1	BI	322/322 (100%)	322 (100%)	0	100	100
1	BJ	322/322 (100%)	320 (99%)	2 (1%)	78	89
1	BK	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	CA	322/322 (100%)	320 (99%)	2 (1%)	78	89
1	CB	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	CC	322/322 (100%)	322 (100%)	0	100	100
1	CD	322/322 (100%)	318 (99%)	4 (1%)	63	80
1	CE	322/322 (100%)	322 (100%)	0	100	100
1	CF	322/322 (100%)	320 (99%)	2 (1%)	78	89
1	CG	322/322 (100%)	322 (100%)	0	100	100
1	CH	322/322 (100%)	320 (99%)	2 (1%)	78	89
1	CI	322/322 (100%)	320 (99%)	2 (1%)	78	89
1	CJ	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	CK	322/322 (100%)	322 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DA	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	DB	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	DC	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	DD	322/322 (100%)	322 (100%)	0	100	100
1	DE	322/322 (100%)	322 (100%)	0	100	100
1	DF	322/322 (100%)	322 (100%)	0	100	100
1	DG	322/322 (100%)	322 (100%)	0	100	100
1	DH	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	DI	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	DJ	322/322 (100%)	322 (100%)	0	100	100
1	DK	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	EA	322/322 (100%)	322 (100%)	0	100	100
1	EB	322/322 (100%)	322 (100%)	0	100	100
1	EC	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	ED	322/322 (100%)	322 (100%)	0	100	100
1	EE	322/322 (100%)	319 (99%)	3 (1%)	70	84
1	EF	322/322 (100%)	322 (100%)	0	100	100
1	EG	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	EH	322/322 (100%)	320 (99%)	2 (1%)	78	89
1	EI	322/322 (100%)	322 (100%)	0	100	100
1	EJ	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	EK	322/322 (100%)	322 (100%)	0	100	100
1	FA	322/322 (100%)	322 (100%)	0	100	100
1	FB	322/322 (100%)	322 (100%)	0	100	100
1	FC	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	FD	322/322 (100%)	322 (100%)	0	100	100
1	FE	322/322 (100%)	322 (100%)	0	100	100
1	FF	322/322 (100%)	322 (100%)	0	100	100
1	FG	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	FH	322/322 (100%)	321 (100%)	1 (0%)	86	93
1	FI	322/322 (100%)	322 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FJ	322/322 (100%)	322 (100%)	0	100	100
1	FK	322/322 (100%)	322 (100%)	0	100	100
All	All	21252/21252 (100%)	21207 (100%)	45 (0%)	85	95

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	16	LEU
1	AB	243	VAL
1	AC	53	VAL
1	AC	227	THR
1	AD	194	ASP
1	AE	56	ILE
1	AE	247	THR
1	AG	209	VAL
1	AJ	167	THR
1	AK	149	THR
1	BE	209	VAL
1	BJ	209	VAL
1	BJ	391	GLN
1	BK	227	THR
1	CA	53	VAL
1	CA	56	ILE
1	CB	160	THR
1	CD	167	THR
1	CD	341	VAL
1	CD	372	VAL
1	CD	394	ILE
1	CF	35	THR
1	CF	332	VAL
1	CH	332	VAL
1	CH	366	ASP
1	CI	209	VAL
1	CI	346	THR
1	CJ	53	VAL
1	DA	28	THR
1	DB	209	VAL
1	DC	209	VAL
1	DH	250	ILE
1	DI	126	THR
1	DK	160	THR

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Mol	Chain	Res	Type
1	EC	228	THR
1	EE	160	THR
1	EE	243	VAL
1	EE	360	LEU
1	EG	209	VAL
1	EH	270	THR
1	EH	341	VAL
1	EJ	325	LEU
1	FC	367	LEU
1	FG	53	VAL
1	FH	263	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (722) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	21	ASN
1	AA	22	ASN
1	AA	67	ASN
1	AA	154	GLN
1	AA	158	ASN
1	AA	178	ASN
1	AA	193	HIS
1	AA	279	ASN
1	AA	309	GLN
1	AA	318	ASN
1	AA	322	ASN
1	AA	328	GLN
1	AA	331	ASN
1	AA	391	GLN
1	AA	396	ASN
1	AB	4	GLN
1	AB	10	ASN
1	AB	21	ASN
1	AB	22	ASN
1	AB	114	GLN
1	AB	129	GLN
1	AB	154	GLN
1	AB	178	ASN
1	AB	191	ASN
1	AB	273	ASN
1	AB	307	GLN
1	AB	328	GLN

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Mol	Chain	Res	Type
1	AB	337	GLN
1	AC	22	ASN
1	AC	25	ASN
1	AC	98	GLN
1	AC	128	GLN
1	AC	279	ASN
1	AC	337	GLN
1	AC	391	GLN
1	AC	400	ASN
1	AD	4	GLN
1	AD	22	ASN
1	AD	25	ASN
1	AD	104	ASN
1	AD	111	GLN
1	AD	114	GLN
1	AD	128	GLN
1	AD	129	GLN
1	AD	178	ASN
1	AD	189	GLN
1	AD	193	HIS
1	AD	196	ASN
1	AD	295	ASN
1	AD	322	ASN
1	AD	331	ASN
1	AD	391	GLN
1	AD	400	ASN
1	AE	21	ASN
1	AE	22	ASN
1	AE	25	ASN
1	AE	104	ASN
1	AE	109	ASN
1	AE	111	GLN
1	AE	154	GLN
1	AE	156	ASN
1	AE	158	ASN
1	AE	386	GLN
1	AE	396	ASN
1	AF	96	ASN
1	AF	129	GLN
1	AF	154	GLN
1	AF	196	ASN
1	AF	251	ASN

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Mol	Chain	Res	Type
1	AF	307	GLN
1	AF	309	GLN
1	AF	400	ASN
1	AG	21	ASN
1	AG	25	ASN
1	AG	154	GLN
1	AG	178	ASN
1	AG	189	GLN
1	AG	196	ASN
1	AG	244	ASN
1	AG	269	ASN
1	AG	279	ASN
1	AG	307	GLN
1	AG	321	ASN
1	AG	382	GLN
1	AH	10	ASN
1	AH	21	ASN
1	AH	22	ASN
1	AH	98	GLN
1	AH	106	ASN
1	AH	111	GLN
1	AH	132	ASN
1	AH	154	GLN
1	AH	178	ASN
1	AH	205	ASN
1	AH	318	ASN
1	AH	351	ASN
1	AI	4	GLN
1	AI	10	ASN
1	AI	25	ASN
1	AI	58	GLN
1	AI	88	ASN
1	AI	196	ASN
1	AI	295	ASN
1	AI	309	GLN
1	AI	331	ASN
1	AI	396	ASN
1	AJ	22	ASN
1	AJ	88	ASN
1	AJ	104	ASN
1	AJ	111	GLN
1	AJ	158	ASN

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Mol	Chain	Res	Type
1	AJ	269	ASN
1	AJ	305	ASN
1	AJ	309	GLN
1	AJ	322	ASN
1	AJ	337	GLN
1	AJ	378	GLN
1	AK	21	ASN
1	AK	111	GLN
1	AK	128	GLN
1	AK	154	GLN
1	AK	156	ASN
1	AK	196	ASN
1	AK	322	ASN
1	AK	328	GLN
1	AK	331	ASN
1	AK	384	ASN
1	AK	393	GLN
1	BA	25	ASN
1	BA	67	ASN
1	BA	129	GLN
1	BA	132	ASN
1	BA	140	ASN
1	BA	154	GLN
1	BA	178	ASN
1	BA	267	GLN
1	BA	295	ASN
1	BA	307	GLN
1	BA	322	ASN
1	BA	331	ASN
1	BA	337	GLN
1	BB	21	ASN
1	BB	25	ASN
1	BB	129	GLN
1	BB	132	ASN
1	BB	244	ASN
1	BB	251	ASN
1	BB	295	ASN
1	BC	104	ASN
1	BC	106	ASN
1	BC	128	GLN
1	BC	189	GLN
1	BC	193	HIS

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Mol	Chain	Res	Type
1	BC	251	ASN
1	BC	279	ASN
1	BC	295	ASN
1	BC	309	GLN
1	BC	313	GLN
1	BC	328	GLN
1	BC	378	GLN
1	BD	10	ASN
1	BD	25	ASN
1	BD	106	ASN
1	BD	154	GLN
1	BD	205	ASN
1	BD	212	HIS
1	BD	244	ASN
1	BD	295	ASN
1	BD	302	ASN
1	BD	322	ASN
1	BE	21	ASN
1	BE	111	GLN
1	BE	154	GLN
1	BE	196	ASN
1	BE	251	ASN
1	BE	307	GLN
1	BE	322	ASN
1	BE	328	GLN
1	BE	331	ASN
1	BE	384	ASN
1	BF	96	ASN
1	BF	104	ASN
1	BF	111	GLN
1	BF	132	ASN
1	BF	158	ASN
1	BF	251	ASN
1	BF	267	GLN
1	BF	274	ASN
1	BF	318	ASN
1	BF	384	ASN
1	BF	396	ASN
1	BG	4	GLN
1	BG	25	ASN
1	BG	67	ASN
1	BG	88	ASN

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Mol	Chain	Res	Type
1	BG	104	ASN
1	BG	114	GLN
1	BG	132	ASN
1	BG	244	ASN
1	BG	264	ASN
1	BG	295	ASN
1	BG	318	ASN
1	BG	322	ASN
1	BG	331	ASN
1	BG	386	GLN
1	BG	391	GLN
1	BH	10	ASN
1	BH	96	ASN
1	BH	158	ASN
1	BH	279	ASN
1	BH	302	ASN
1	BH	307	GLN
1	BH	328	GLN
1	BH	337	GLN
1	BI	21	ASN
1	BI	104	ASN
1	BI	114	GLN
1	BI	128	GLN
1	BI	132	ASN
1	BI	154	GLN
1	BI	193	HIS
1	BI	279	ASN
1	BI	322	ASN
1	BI	331	ASN
1	BI	391	GLN
1	BJ	22	ASN
1	BJ	25	ASN
1	BJ	154	GLN
1	BJ	302	ASN
1	BJ	318	ASN
1	BJ	337	GLN
1	BK	25	ASN
1	BK	111	GLN
1	BK	114	GLN
1	BK	154	GLN
1	BK	196	ASN
1	BK	328	GLN

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Mol	Chain	Res	Type
1	BK	382	GLN
1	CA	10	ASN
1	CA	21	ASN
1	CA	25	ASN
1	CA	154	GLN
1	CA	212	HIS
1	CA	269	ASN
1	CA	309	GLN
1	CA	328	GLN
1	CA	384	ASN
1	CB	10	ASN
1	CB	25	ASN
1	CB	191	ASN
1	CB	196	ASN
1	CB	251	ASN
1	CB	267	GLN
1	CB	274	ASN
1	CB	295	ASN
1	CB	309	GLN
1	CB	322	ASN
1	CB	378	GLN
1	CB	393	GLN
1	CC	25	ASN
1	CC	58	GLN
1	CC	98	GLN
1	CC	104	ASN
1	CC	106	ASN
1	CC	111	GLN
1	CC	158	ASN
1	CC	178	ASN
1	CC	302	ASN
1	CC	331	ASN
1	CC	351	ASN
1	CD	154	GLN
1	CD	156	ASN
1	CD	196	ASN
1	CD	295	ASN
1	CD	318	ASN
1	CD	322	ASN
1	CD	373	ASN
1	CD	386	GLN
1	CE	4	GLN

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Mol	Chain	Res	Type
1	CE	25	ASN
1	CE	154	GLN
1	CE	158	ASN
1	CE	191	ASN
1	CE	196	ASN
1	CE	267	GLN
1	CE	279	ASN
1	CE	295	ASN
1	CE	307	GLN
1	CE	322	ASN
1	CE	328	GLN
1	CE	331	ASN
1	CE	391	GLN
1	CE	400	ASN
1	CF	21	ASN
1	CF	104	ASN
1	CF	154	GLN
1	CF	156	ASN
1	CF	244	ASN
1	CF	251	ASN
1	CF	269	ASN
1	CF	302	ASN
1	CF	309	GLN
1	CF	328	GLN
1	CF	386	GLN
1	CG	21	ASN
1	CG	78	GLN
1	CG	79	ASN
1	CG	88	ASN
1	CG	104	ASN
1	CG	106	ASN
1	CG	111	GLN
1	CG	129	GLN
1	CG	154	GLN
1	CG	158	ASN
1	CG	269	ASN
1	CG	292	GLN
1	CG	302	ASN
1	CG	393	GLN
1	CH	21	ASN
1	CH	58	GLN
1	CH	88	ASN

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Mol	Chain	Res	Type
1	CH	111	GLN
1	CH	114	GLN
1	CH	251	ASN
1	CH	279	ASN
1	CH	295	ASN
1	CH	321	ASN
1	CH	322	ASN
1	CH	328	GLN
1	CH	380	ASN
1	CI	67	ASN
1	CI	111	GLN
1	CI	154	GLN
1	CI	193	HIS
1	CI	251	ASN
1	CI	281	ASN
1	CJ	25	ASN
1	CJ	114	GLN
1	CJ	154	GLN
1	CJ	158	ASN
1	CJ	205	ASN
1	CJ	234	ASN
1	CJ	251	ASN
1	CJ	269	ASN
1	CJ	279	ASN
1	CJ	328	GLN
1	CJ	400	ASN
1	CK	21	ASN
1	CK	22	ASN
1	CK	67	ASN
1	CK	109	ASN
1	CK	111	GLN
1	CK	154	GLN
1	CK	196	ASN
1	CK	205	ASN
1	CK	307	GLN
1	CK	384	ASN
1	DA	25	ASN
1	DA	96	ASN
1	DA	106	ASN
1	DA	154	GLN
1	DA	302	ASN
1	DB	21	ASN

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Mol	Chain	Res	Type
1	DB	88	ASN
1	DB	111	GLN
1	DB	158	ASN
1	DB	178	ASN
1	DB	251	ASN
1	DB	267	GLN
1	DB	269	ASN
1	DB	305	ASN
1	DB	309	GLN
1	DB	318	ASN
1	DB	328	GLN
1	DB	337	GLN
1	DB	396	ASN
1	DC	25	ASN
1	DC	111	GLN
1	DC	129	GLN
1	DC	156	ASN
1	DC	158	ASN
1	DC	196	ASN
1	DC	322	ASN
1	DC	331	ASN
1	DC	378	GLN
1	DD	25	ASN
1	DD	88	ASN
1	DD	128	GLN
1	DD	129	GLN
1	DD	154	GLN
1	DD	178	ASN
1	DD	191	ASN
1	DD	251	ASN
1	DD	267	GLN
1	DD	322	ASN
1	DD	331	ASN
1	DD	380	ASN
1	DD	382	GLN
1	DE	10	ASN
1	DE	21	ASN
1	DE	78	GLN
1	DE	111	GLN
1	DE	154	GLN
1	DE	191	ASN
1	DE	251	ASN

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Mol	Chain	Res	Type
1	DE	279	ASN
1	DE	322	ASN
1	DE	328	GLN
1	DF	21	ASN
1	DF	78	GLN
1	DF	111	GLN
1	DF	128	GLN
1	DF	129	GLN
1	DF	158	ASN
1	DF	205	ASN
1	DF	251	ASN
1	DF	302	ASN
1	DF	322	ASN
1	DG	22	ASN
1	DG	25	ASN
1	DG	58	GLN
1	DG	67	ASN
1	DG	78	GLN
1	DG	96	ASN
1	DG	111	GLN
1	DG	140	ASN
1	DG	191	ASN
1	DG	212	HIS
1	DG	251	ASN
1	DG	302	ASN
1	DG	307	GLN
1	DG	328	GLN
1	DG	337	GLN
1	DH	21	ASN
1	DH	79	ASN
1	DH	106	ASN
1	DH	132	ASN
1	DH	154	GLN
1	DH	244	ASN
1	DH	251	ASN
1	DH	307	GLN
1	DH	309	GLN
1	DH	322	ASN
1	DH	331	ASN
1	DH	378	GLN
1	DH	391	GLN
1	DI	96	ASN

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Mol	Chain	Res	Type
1	DI	111	GLN
1	DI	128	GLN
1	DI	154	GLN
1	DI	267	GLN
1	DI	307	GLN
1	DI	313	GLN
1	DJ	22	ASN
1	DJ	25	ASN
1	DJ	106	ASN
1	DJ	114	GLN
1	DJ	128	GLN
1	DJ	154	GLN
1	DJ	193	HIS
1	DJ	196	ASN
1	DJ	251	ASN
1	DJ	267	GLN
1	DJ	273	ASN
1	DJ	295	ASN
1	DJ	307	GLN
1	DJ	328	GLN
1	DK	21	ASN
1	DK	22	ASN
1	DK	96	ASN
1	DK	106	ASN
1	DK	128	GLN
1	DK	154	GLN
1	DK	178	ASN
1	DK	191	ASN
1	DK	302	ASN
1	DK	322	ASN
1	DK	328	GLN
1	DK	331	ASN
1	DK	337	GLN
1	DK	364	ASN
1	DK	382	GLN
1	EA	25	ASN
1	EA	96	ASN
1	EA	106	ASN
1	EA	128	GLN
1	EA	156	ASN
1	EA	273	ASN
1	EA	280	GLN

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Mol	Chain	Res	Type
1	EA	294	ASN
1	EA	302	ASN
1	EA	382	GLN
1	EB	22	ASN
1	EB	25	ASN
1	EB	58	GLN
1	EB	67	ASN
1	EB	111	GLN
1	EB	128	GLN
1	EB	129	GLN
1	EB	154	GLN
1	EB	178	ASN
1	EB	196	ASN
1	EB	232	ASN
1	EB	307	GLN
1	EB	322	ASN
1	EB	328	GLN
1	EB	378	GLN
1	EB	380	ASN
1	EC	25	ASN
1	EC	154	GLN
1	EC	158	ASN
1	EC	205	ASN
1	EC	294	ASN
1	EC	313	GLN
1	EC	321	ASN
1	EC	331	ASN
1	EC	337	GLN
1	EC	373	ASN
1	ED	58	GLN
1	ED	96	ASN
1	ED	104	ASN
1	ED	264	ASN
1	ED	305	ASN
1	ED	322	ASN
1	ED	391	GLN
1	EE	22	ASN
1	EE	58	GLN
1	EE	98	GLN
1	EE	114	GLN
1	EE	128	GLN
1	EE	307	GLN

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Mol	Chain	Res	Type
1	EE	318	ASN
1	EE	322	ASN
1	EE	328	GLN
1	EE	337	GLN
1	EE	351	ASN
1	EE	391	GLN
1	EF	21	ASN
1	EF	25	ASN
1	EF	106	ASN
1	EF	111	GLN
1	EF	114	GLN
1	EF	132	ASN
1	EF	251	ASN
1	EF	267	GLN
1	EF	302	ASN
1	EF	305	ASN
1	EF	322	ASN
1	EF	351	ASN
1	EF	382	GLN
1	EF	391	GLN
1	EG	67	ASN
1	EG	96	ASN
1	EG	111	GLN
1	EG	140	ASN
1	EG	154	GLN
1	EG	178	ASN
1	EG	269	ASN
1	EG	309	GLN
1	EG	364	ASN
1	EG	378	GLN
1	EH	21	ASN
1	EH	96	ASN
1	EH	106	ASN
1	EH	154	GLN
1	EH	178	ASN
1	EH	196	ASN
1	EH	251	ASN
1	EH	264	ASN
1	EH	309	GLN
1	EH	322	ASN
1	EH	400	ASN
1	EI	25	ASN

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Mol	Chain	Res	Type
1	EI	154	GLN
1	EI	267	GLN
1	EI	279	ASN
1	EI	322	ASN
1	EI	357	ASN
1	EJ	111	GLN
1	EJ	154	GLN
1	EJ	232	ASN
1	EJ	273	ASN
1	EJ	302	ASN
1	EJ	307	GLN
1	EJ	309	GLN
1	EK	154	GLN
1	EK	156	ASN
1	EK	191	ASN
1	EK	205	ASN
1	EK	267	GLN
1	EK	295	ASN
1	EK	322	ASN
1	EK	328	GLN
1	FA	4	GLN
1	FA	58	GLN
1	FA	104	ASN
1	FA	106	ASN
1	FA	111	GLN
1	FA	114	GLN
1	FA	154	GLN
1	FA	178	ASN
1	FA	212	HIS
1	FA	267	GLN
1	FA	279	ASN
1	FA	294	ASN
1	FA	295	ASN
1	FA	307	GLN
1	FA	309	GLN
1	FA	318	ASN
1	FA	328	GLN
1	FA	393	GLN
1	FB	78	GLN
1	FB	111	GLN
1	FB	154	GLN
1	FB	205	ASN

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Mol	Chain	Res	Type
1	FB	302	ASN
1	FB	313	GLN
1	FB	321	ASN
1	FB	322	ASN
1	FB	391	GLN
1	FC	21	ASN
1	FC	128	GLN
1	FC	189	GLN
1	FC	196	ASN
1	FC	205	ASN
1	FC	267	GLN
1	FC	318	ASN
1	FC	322	ASN
1	FC	337	GLN
1	FC	364	ASN
1	FC	380	ASN
1	FC	396	ASN
1	FD	111	GLN
1	FD	128	GLN
1	FD	154	GLN
1	FD	193	HIS
1	FD	196	ASN
1	FD	212	HIS
1	FD	244	ASN
1	FD	295	ASN
1	FD	309	GLN
1	FD	321	ASN
1	FD	322	ASN
1	FE	21	ASN
1	FE	22	ASN
1	FE	111	GLN
1	FE	128	GLN
1	FE	193	HIS
1	FE	205	ASN
1	FE	279	ASN
1	FE	313	GLN
1	FE	322	ASN
1	FE	328	GLN
1	FE	331	ASN
1	FE	386	GLN
1	FF	21	ASN
1	FF	106	ASN

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Mol	Chain	Res	Type
1	FF	156	ASN
1	FF	244	ASN
1	FF	267	GLN
1	FF	328	GLN
1	FF	331	ASN
1	FF	337	GLN
1	FF	393	GLN
1	FG	25	ASN
1	FG	78	GLN
1	FG	193	HIS
1	FG	268	GLN
1	FG	273	ASN
1	FG	351	ASN
1	FG	396	ASN
1	FH	111	GLN
1	FH	196	ASN
1	FH	251	ASN
1	FH	281	ASN
1	FH	322	ASN
1	FH	337	GLN
1	FH	391	GLN
1	FI	10	ASN
1	FI	106	ASN
1	FI	158	ASN
1	FI	193	HIS
1	FI	196	ASN
1	FI	244	ASN
1	FI	251	ASN
1	FI	281	ASN
1	FI	307	GLN
1	FI	321	ASN
1	FI	322	ASN
1	FI	331	ASN
1	FI	364	ASN
1	FI	391	GLN
1	FJ	22	ASN
1	FJ	25	ASN
1	FJ	154	GLN
1	FJ	191	ASN
1	FJ	212	HIS
1	FJ	234	ASN
1	FJ	267	GLN

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Mol	Chain	Res	Type
1	FJ	268	GLN
1	FJ	274	ASN
1	FJ	279	ASN
1	FJ	302	ASN
1	FJ	305	ASN
1	FJ	321	ASN
1	FJ	322	ASN
1	FJ	328	GLN
1	FJ	357	ASN
1	FK	25	ASN
1	FK	78	GLN
1	FK	79	ASN
1	FK	98	GLN
1	FK	106	ASN
1	FK	128	GLN
1	FK	154	GLN
1	FK	156	ASN
1	FK	178	ASN
1	FK	189	GLN
1	FK	232	ASN
1	FK	267	GLN
1	FK	302	ASN
1	FK	313	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

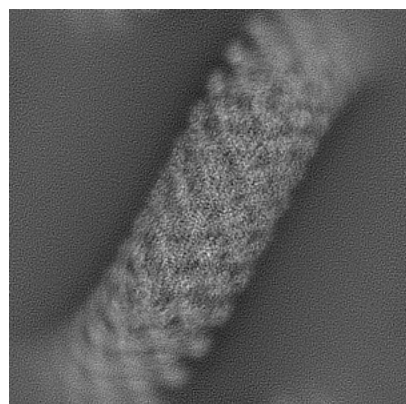
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9909. These allow visual inspection of the internal detail of the map and identification of artifacts.

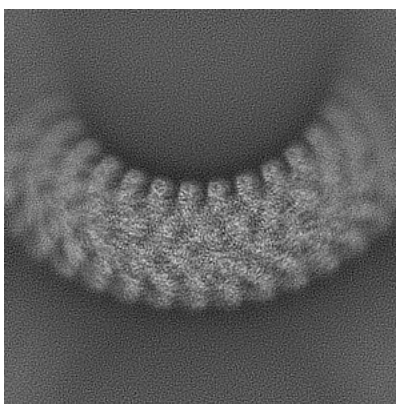
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

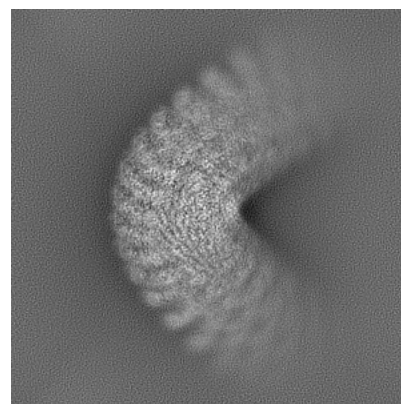
6.1.1 Primary map



X

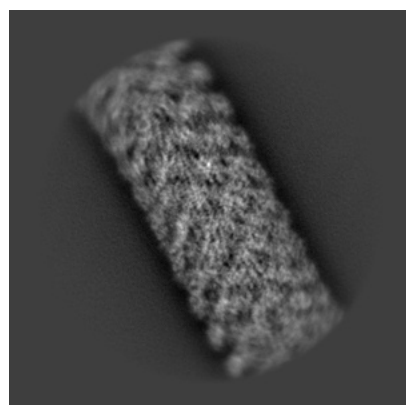


Y

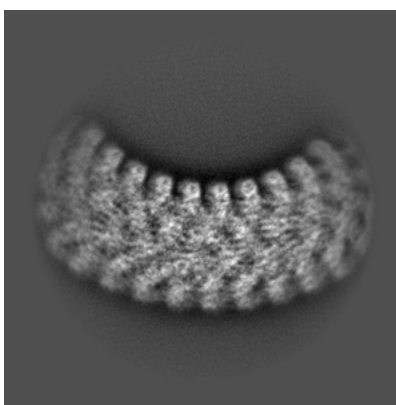


Z

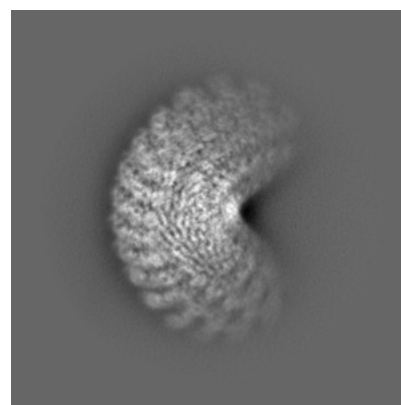
6.1.2 Raw map



X



Y

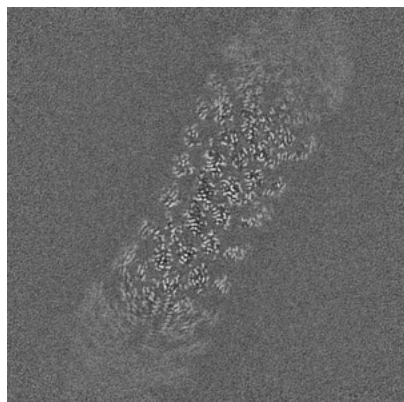


Z

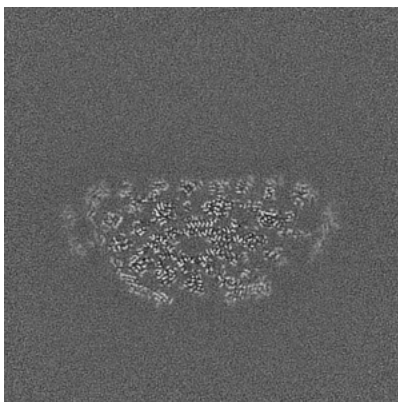
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

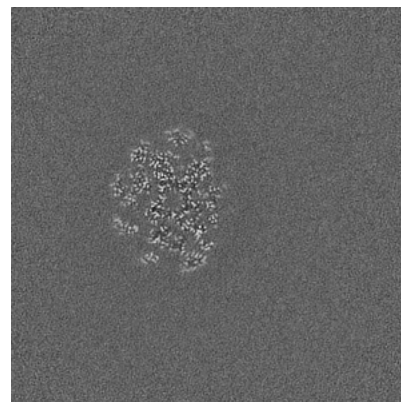
6.2.1 Primary map



X Index: 192

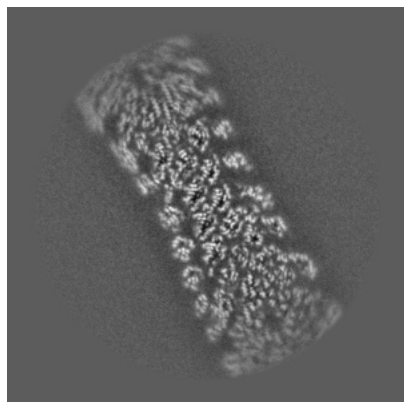


Y Index: 192

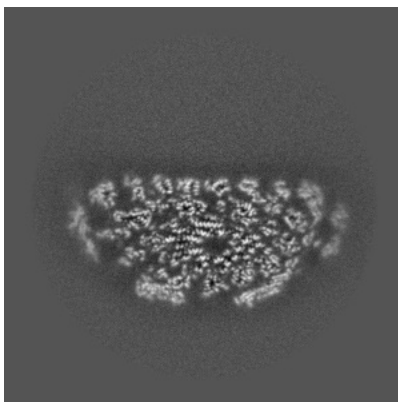


Z Index: 192

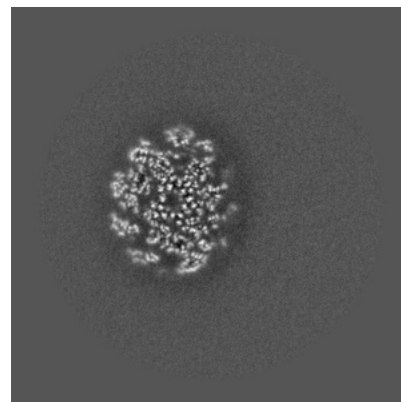
6.2.2 Raw map



X Index: 192



Y Index: 192

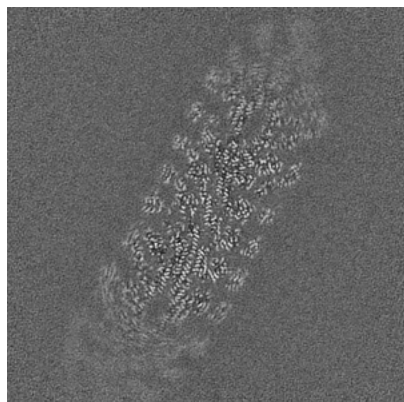


Z Index: 192

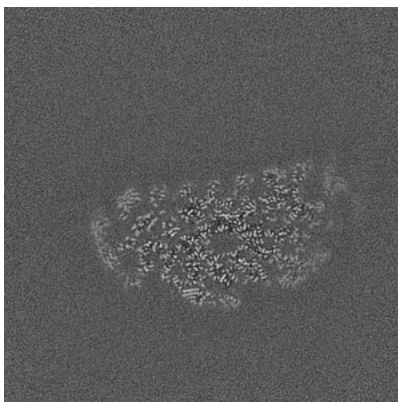
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

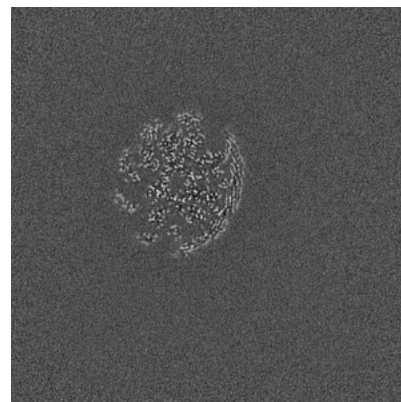
6.3.1 Primary map



X Index: 175

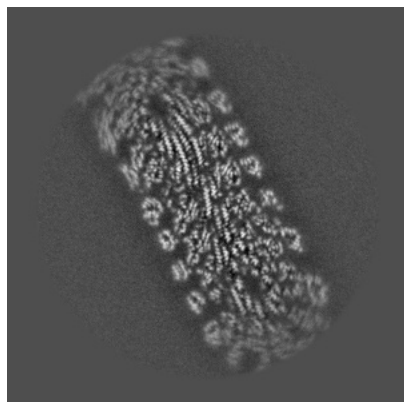


Y Index: 207

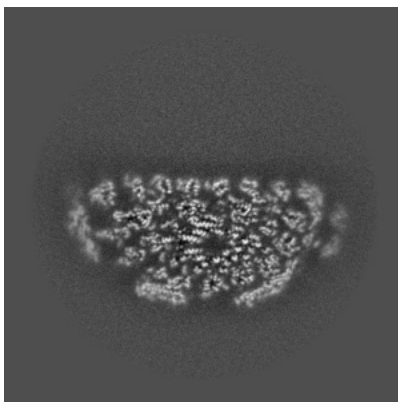


Z Index: 226

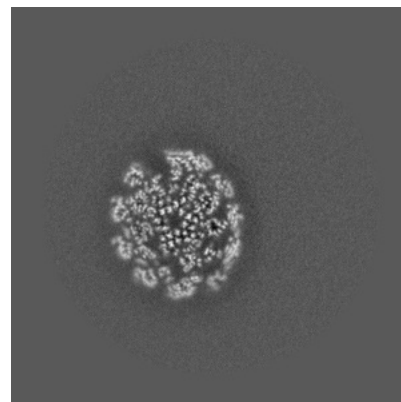
6.3.2 Raw map



X Index: 174



Y Index: 193

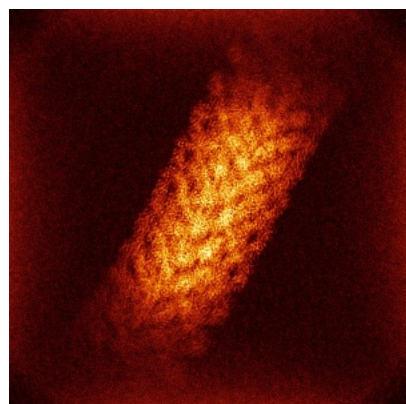


Z Index: 229

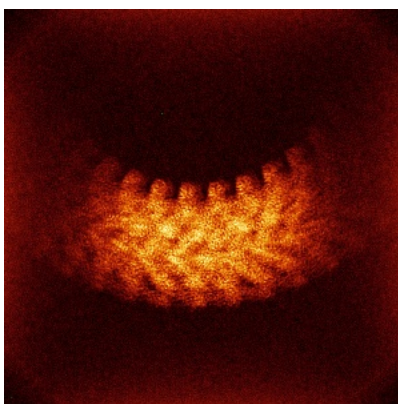
The images above show the largest variance slices of the map in three orthogonal directions.

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

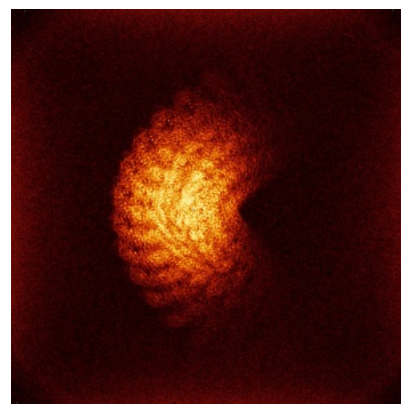
6.4.1 Primary map



X

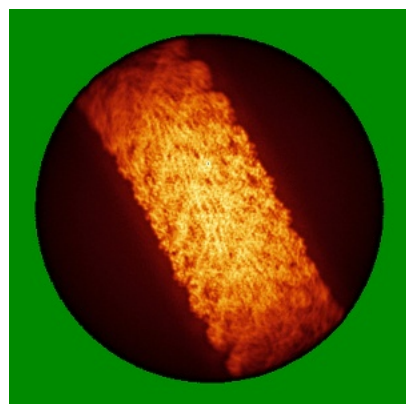


Y

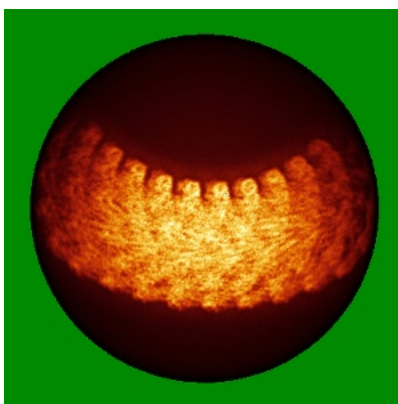


Z

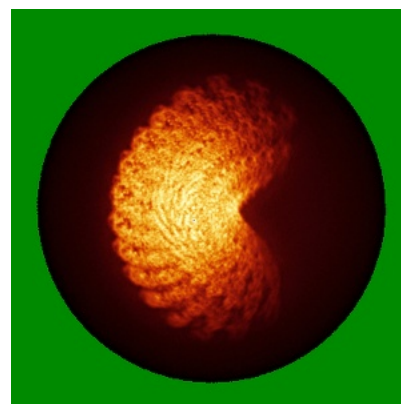
6.4.2 Raw map



X



Y

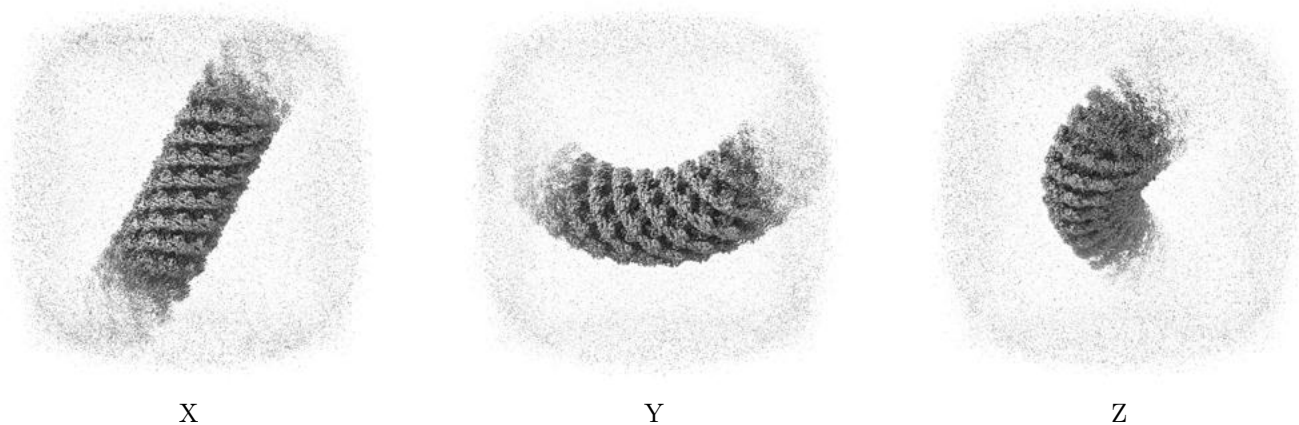


Z

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.

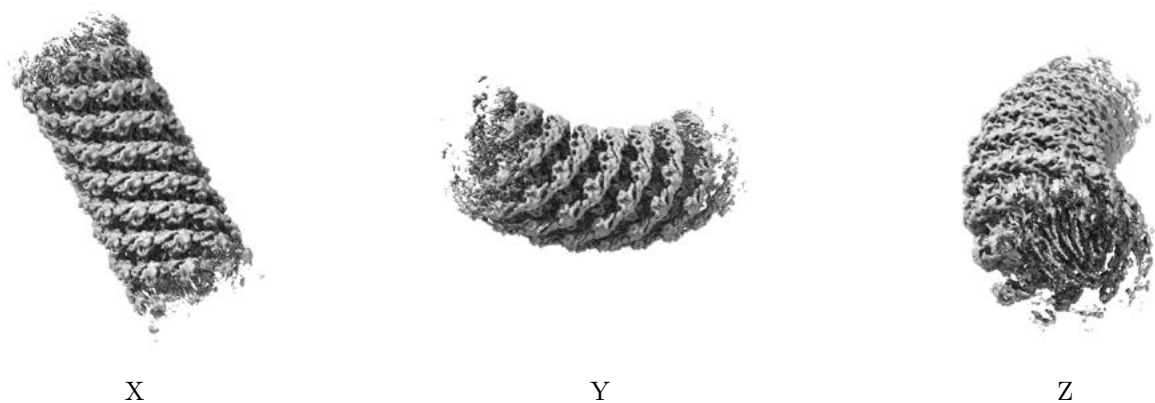
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. 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.

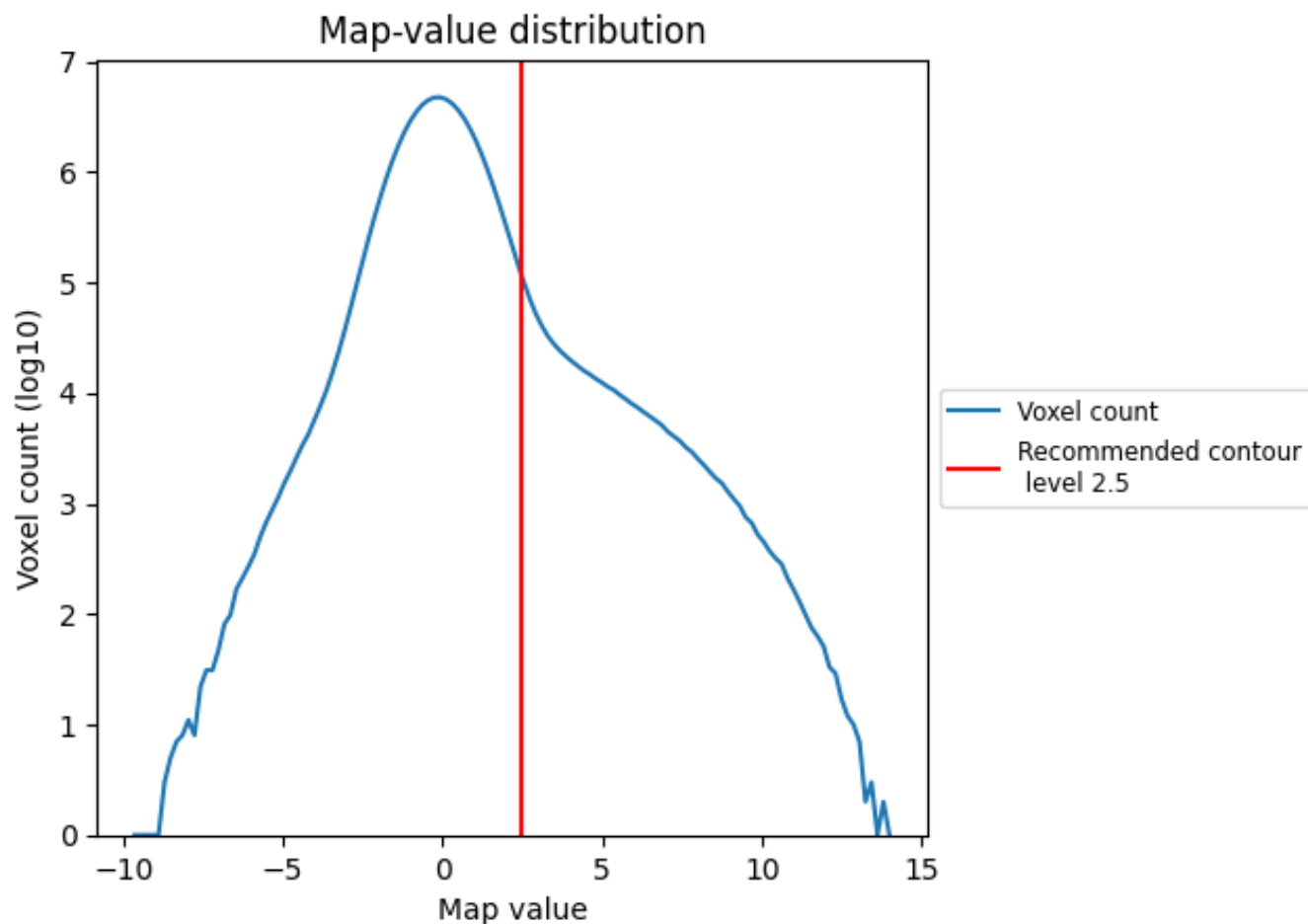
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

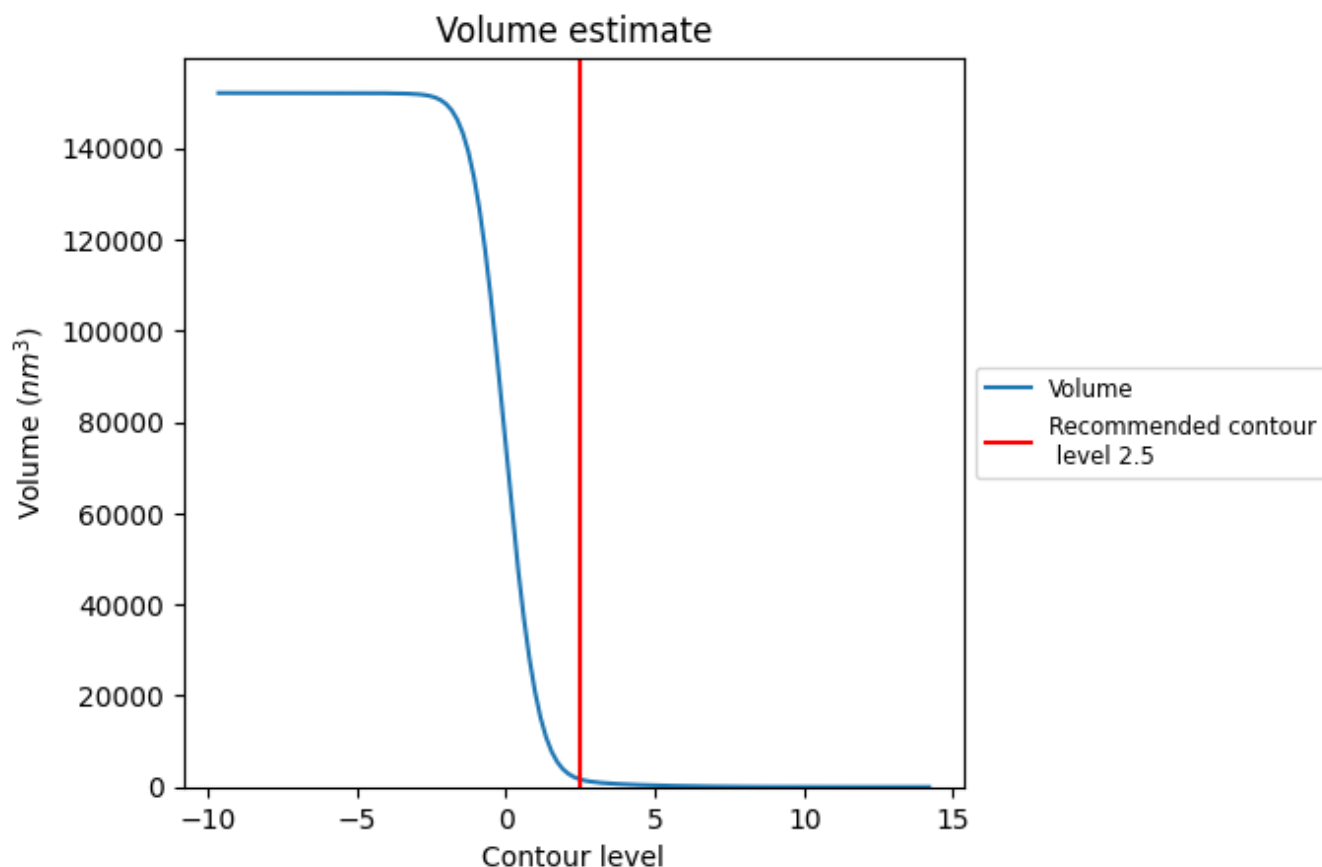
This section contains the results of statistical analysis of the map.

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.

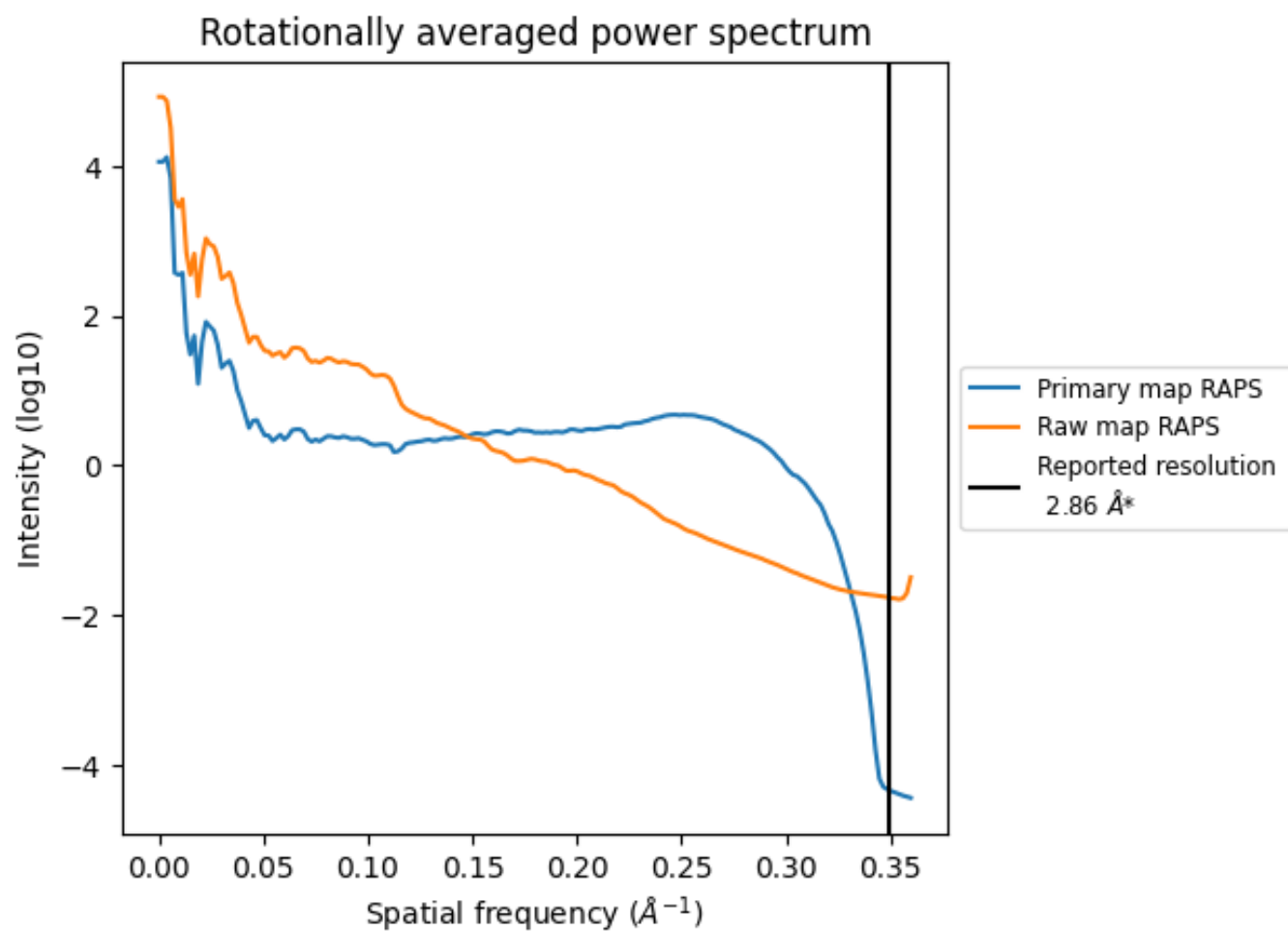
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1662 nm³; this corresponds to an approximate mass of 1501 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 ⓘ

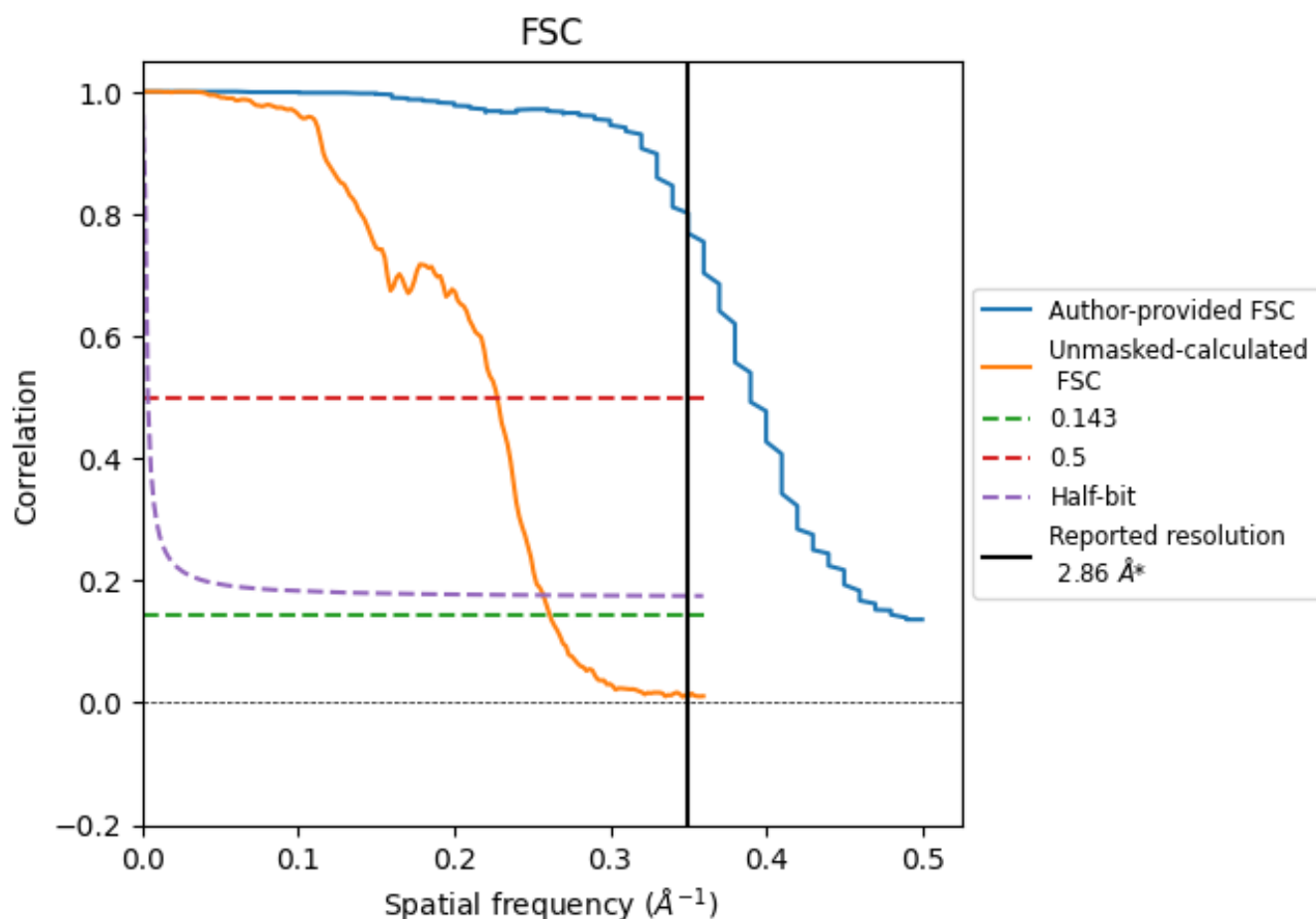


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.07	nan	-
Unmasked-calculated*	3.83	4.40	3.89

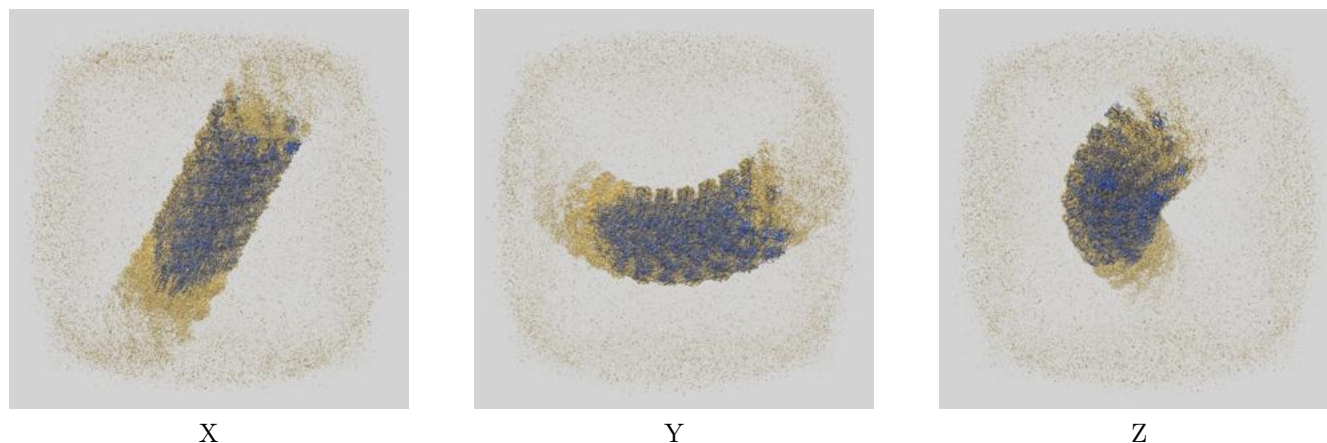
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.07 differs from the reported value 2.86 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

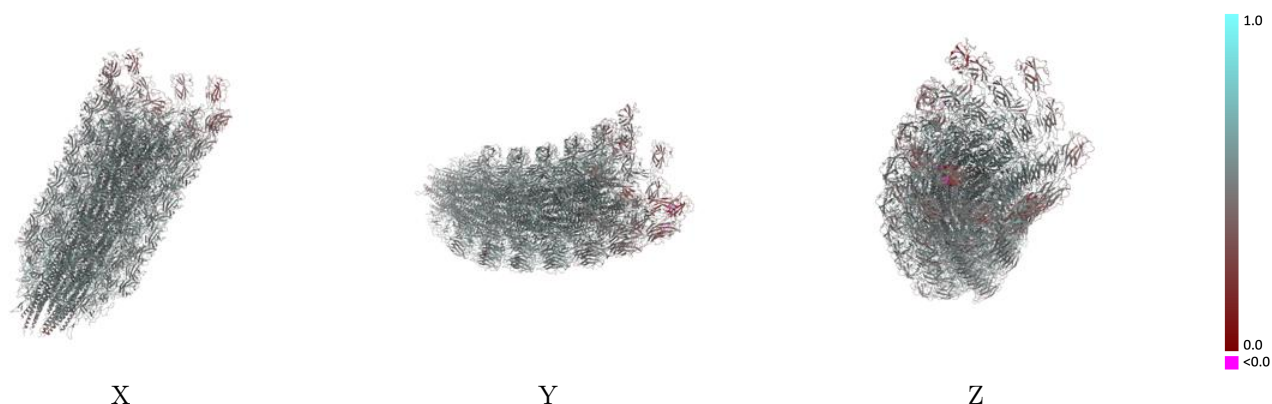
This section contains information regarding the fit between EMDB map EMD-9909 and PDB model 6K3I. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



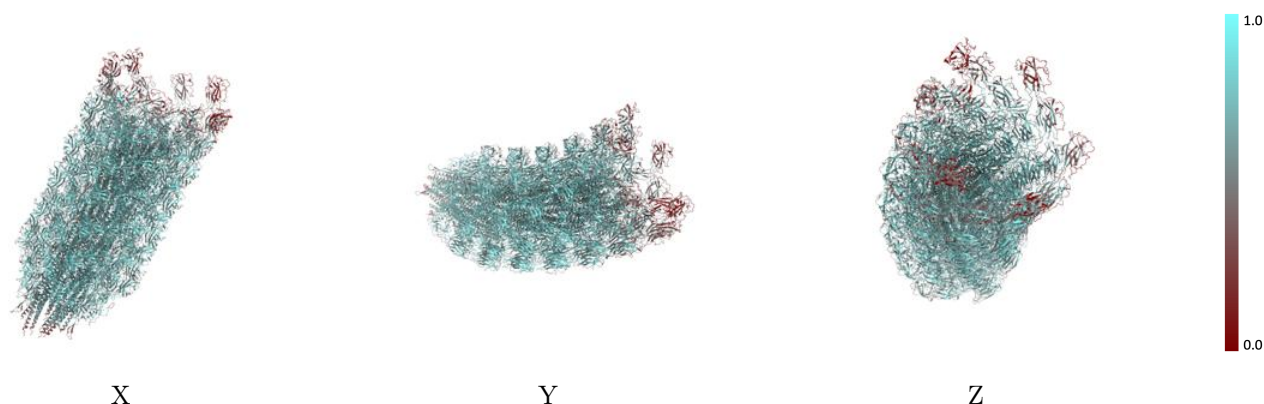
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



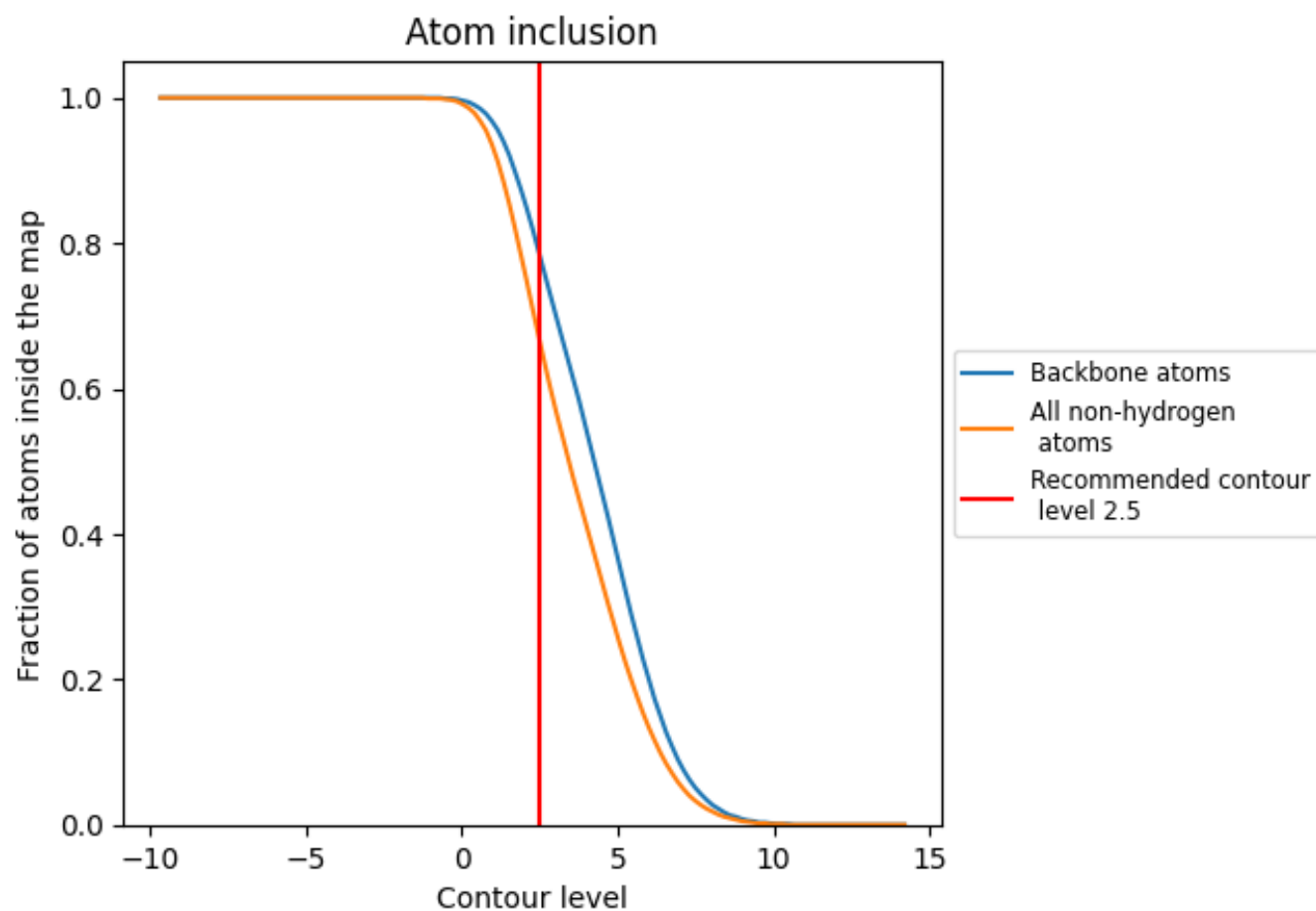
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6660	 0.5040
AA	 0.5440	 0.4610
AB	 0.6360	 0.4920
AC	 0.6470	 0.5010
AD	 0.6080	 0.4910
AE	 0.6300	 0.4910
AF	 0.6250	 0.4870
AG	 0.6640	 0.4990
AH	 0.6820	 0.5100
AI	 0.6790	 0.5040
AJ	 0.6910	 0.5110
AK	 0.6940	 0.5110
BA	 0.6820	 0.5080
BB	 0.7120	 0.5190
BC	 0.7100	 0.5190
BD	 0.7140	 0.5140
BE	 0.7210	 0.5200
BF	 0.7030	 0.5120
BG	 0.7220	 0.5180
BH	 0.7180	 0.5260
BI	 0.7210	 0.5220
BJ	 0.7310	 0.5210
BK	 0.7510	 0.5270
CA	 0.7110	 0.5150
CB	 0.7110	 0.5220
CC	 0.7130	 0.5190
CD	 0.7260	 0.5190
CE	 0.7340	 0.5240
CF	 0.7380	 0.5260
CG	 0.7030	 0.5110
CH	 0.7220	 0.5260
CI	 0.7130	 0.5230
CJ	 0.7270	 0.5240
CK	 0.7450	 0.5270
DA	 0.7010	 0.5120



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Chain	Atom inclusion	Q-score
DB	 0.7070	 0.5140
DC	 0.7080	 0.5230
DD	 0.7070	 0.5230
DE	 0.7460	 0.5250
DF	 0.7220	 0.5190
DG	 0.6730	 0.5050
DH	 0.7090	 0.5200
DI	 0.7060	 0.5190
DJ	 0.7040	 0.5130
DK	 0.7150	 0.5120
EA	 0.6510	 0.4940
EB	 0.6810	 0.5110
EC	 0.7090	 0.5200
ED	 0.7010	 0.5190
EE	 0.6870	 0.5040
EF	 0.6590	 0.4960
EG	 0.6150	 0.4830
EH	 0.6810	 0.5100
EI	 0.6790	 0.5150
EJ	 0.6650	 0.5040
EK	 0.6210	 0.4830
FA	 0.5670	 0.4720
FB	 0.5700	 0.4790
FC	 0.6470	 0.5010
FD	 0.6270	 0.4990
FE	 0.5640	 0.4690
FF	 0.5110	 0.4520
FG	 0.4400	 0.4370
FH	 0.5190	 0.4660
FI	 0.5640	 0.4760
FJ	 0.4980	 0.4550
FK	 0.4010	 0.4210