



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:34 AM UTC

PDB ID : 6X62 / pdb_00006x62
EMDB ID : EMD-22068
Title : Legionella pneumophila Dot T4SS OMC
Authors : Durie, C.L.; Sheedlo, M.J.; Chung, J.M.; Byrne, B.G.; Su, M.; Knight, T.; Swanson, M.S.; Lacy, D.B.; Ohi, M.D.
Deposited on : 2020-05-27
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

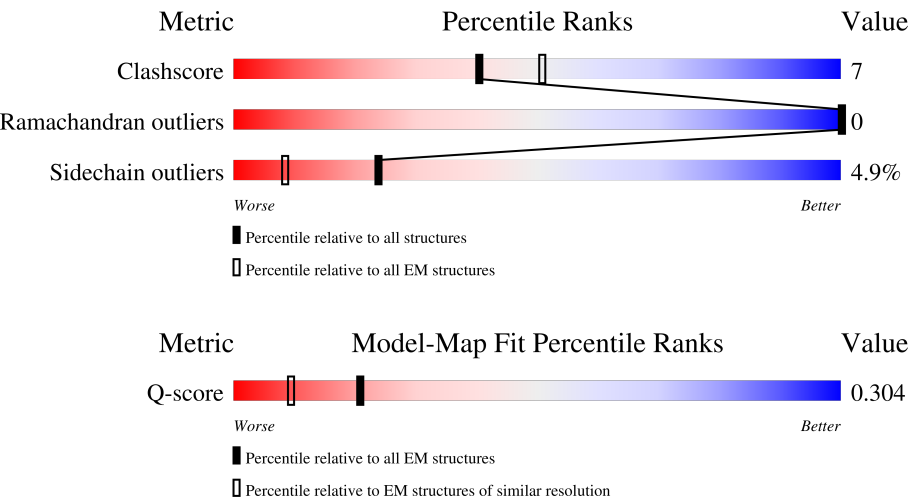
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	AC	303	5% 51%11%..34%
1	BC	303	6% 50%13%..34%
1	CC	303	7% 50%12%..34%
1	DC	303	5% 50%14%..34%

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Mol	Chain	Length	Quality of chain
1	EC	303	
1	FC	303	
1	GC	303	
1	HC	303	
1	IC	303	
1	JC	303	
1	KC	303	
1	LC	303	
1	MC	303	
2	AH	361	
2	BH	361	
2	CH	361	
2	DH	361	
2	EH	361	
2	FH	361	
2	GH	361	
2	HH	361	
2	IH	361	
2	JH	361	
2	KH	361	
2	LH	361	
2	MH	361	
3	AK	189	
3	BK	189	
3	CK	189	

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Mol	Chain	Length	Quality of chain
3	DK	189	
3	EK	189	
3	FK	189	
3	GK	189	
3	HK	189	
3	IK	189	
3	JK	189	
3	KK	189	
3	LK	189	
3	MK	189	
4	AX	579	
4	AY	579	
4	AZ	579	
4	BX	579	
4	BY	579	
4	BZ	579	
4	CX	579	
4	CY	579	
4	CZ	579	
4	DX	579	
4	DY	579	
4	DZ	579	
4	EX	579	
4	EY	579	
4	EZ	579	

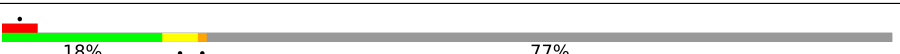
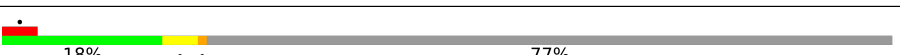
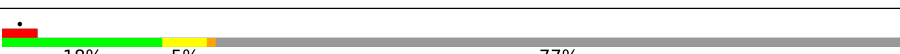
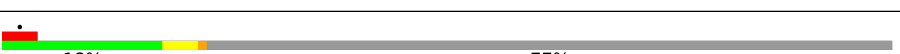
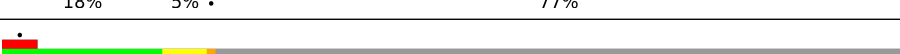
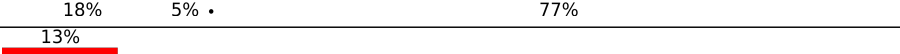
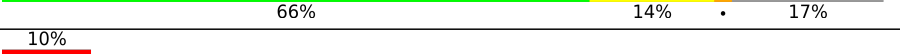
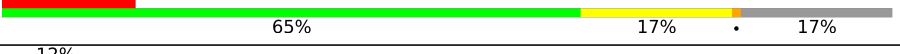
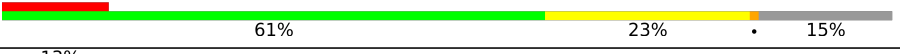
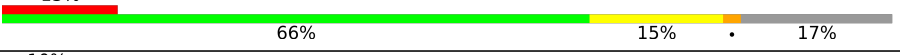
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Mol	Chain	Length	Quality of chain
4	FX	579	
4	FY	579	
4	FZ	579	
4	GX	579	
4	GY	579	
4	GZ	579	
4	HX	579	
4	HY	579	
4	HZ	579	
4	IX	579	
4	IY	579	
4	IZ	579	
4	JX	579	
4	JY	579	
4	JZ	579	
4	KX	579	
4	KY	579	
4	KZ	579	
4	LX	579	
4	LY	579	
4	LZ	579	
4	MX	579	
4	MY	579	
4	MZ	579	
4	N	579	

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Mol	Chain	Length	Quality of chain
4	O	579	
4	P	579	
4	Q	579	
4	R	579	
4	S	579	
4	T	579	
4	U	579	
4	V	579	
4	W	579	
4	X	579	
4	Y	579	
4	Z	579	
5	AD	163	
5	Ad	163	
5	BD	163	
5	Bd	163	
5	CD	163	
5	Cd	163	
5	DD	163	
5	Dd	163	
5	ED	163	
5	Ed	163	
5	FD	163	
5	Fd	163	
5	GD	163	

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Mol	Chain	Length	Quality of chain
5	Gd	163	
5	HD	163	
5	Hd	163	
5	ID	163	
5	Id	163	
5	JD	163	
5	Jd	163	
5	KD	163	
5	Kd	163	
5	LD	163	
5	Ld	163	
5	MD	163	
5	Md	163	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 109070 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 DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	EC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	FC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	GC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	HC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	IC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	JC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	KC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	LC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	MC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	BC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	CC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	DC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		

- Molecule 2 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	EH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	FH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	GH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	HH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	IH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	JH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	AH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	KH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	LH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	MH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	BH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
2	CH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		

- Molecule 3 is a protein called Inner membrane lipoprotein YiaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	EK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	FK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	GK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	HK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	IK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	JK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	KK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	LK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	MK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	AK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	BK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
3	CK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

- Molecule 4 is a protein called Type IV secretion system unknown protein fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	DY	52	Total	C	N	O		0	0
			260	156	52	52			
4	DZ	70	Total	C	N	O		0	0
			350	210	70	70			
4	EX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	EY	52	Total	C	N	O		0	0
			260	156	52	52			
4	EZ	70	Total	C	N	O		0	0
			350	210	70	70			
4	FX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	FY	52	Total	C	N	O		0	0
			260	156	52	52			
4	FZ	70	Total	C	N	O		0	0
			350	210	70	70			
4	GX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	GY	52	Total	C	N	O		0	0
			260	156	52	52			
4	GZ	70	Total	C	N	O		0	0
			350	210	70	70			
4	HX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	HY	52	Total	C	N	O		0	0
			260	156	52	52			

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	HZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	IX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	IY	52	Total	C	N	O	0	0
			260	156	52	52		
4	IZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	JX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	JY	52	Total	C	N	O	0	0
			260	156	52	52		
4	JZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	KX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	KY	52	Total	C	N	O	0	0
			260	156	52	52		
4	KZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	LX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	LY	52	Total	C	N	O	0	0
			260	156	52	52		
4	LZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	MX	228	Total	C	N	O	0	0
			1140	684	228	228		
4	MY	52	Total	C	N	O	0	0
			260	156	52	52		
4	MZ	70	Total	C	N	O	0	0
			350	210	70	70		
4	N	136	Total	C	N	O	S	0
			1108	701	201	202	4	0
4	O	136	Total	C	N	O	S	0
			1108	701	201	202	4	0
4	P	136	Total	C	N	O	S	0
			1108	701	201	202	4	0
4	Q	136	Total	C	N	O	S	0
			1108	701	201	202	4	0
4	R	136	Total	C	N	O	S	0
			1108	701	201	202	4	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	T	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	U	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	V	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	W	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	X	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	Y	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	Z	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
4	AX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	AY	52	Total	C	N	O		0	0
			260	156	52	52			
4	AZ	70	Total	C	N	O		0	0
			350	210	70	70			
4	BX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	BY	52	Total	C	N	O		0	0
			260	156	52	52			
4	BZ	70	Total	C	N	O		0	0
			350	210	70	70			
4	CX	228	Total	C	N	O		0	0
			1140	684	228	228			
4	CY	52	Total	C	N	O		0	0
			260	156	52	52			
4	CZ	70	Total	C	N	O		0	0
			350	210	70	70			

- Molecule 5 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Dd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	ED	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ed	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	FD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Fd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	GD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	AD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Gd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	HD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Hd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	ID	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Id	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	JD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Jd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	KD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Kd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	LD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Ld	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	MD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Md	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	Ad	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	BD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Bd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		

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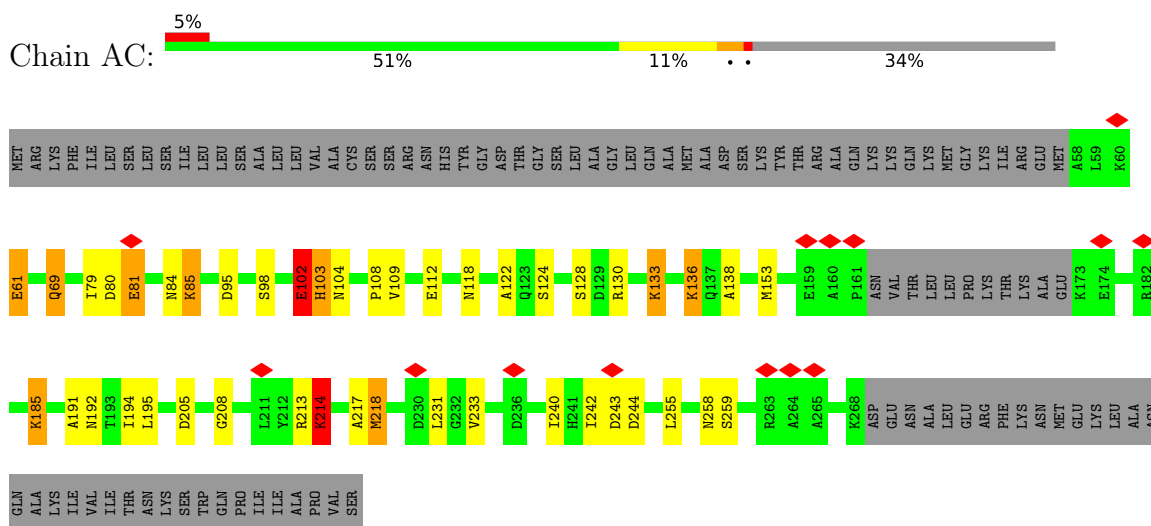
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	CD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
5	Cd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
5	DD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		

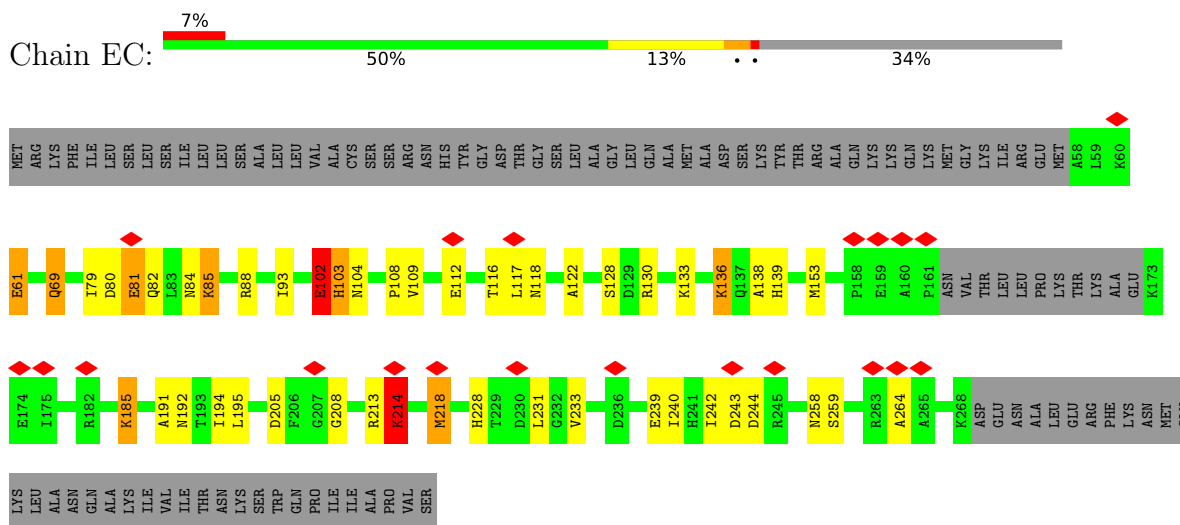
3 Residue-property plots

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.

• Molecule 1: DotC

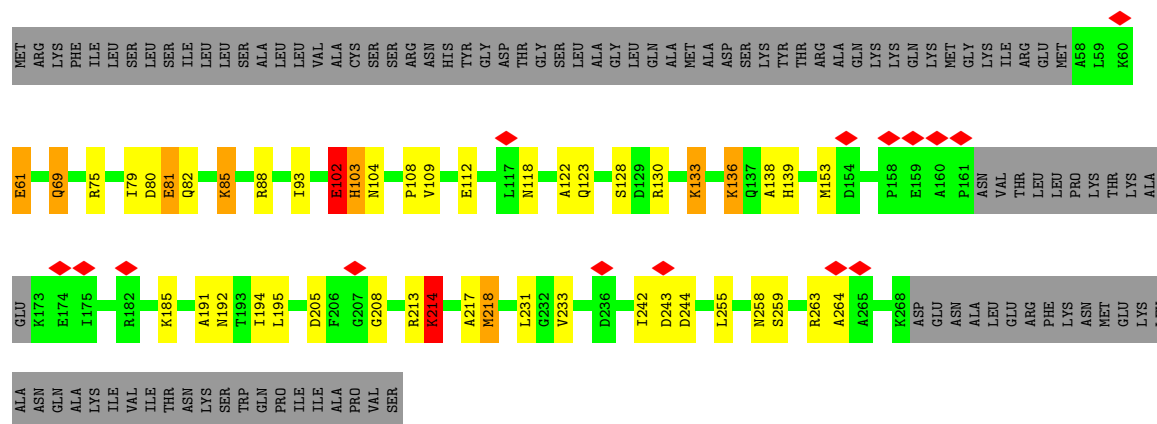


• Molecule 1: DotC

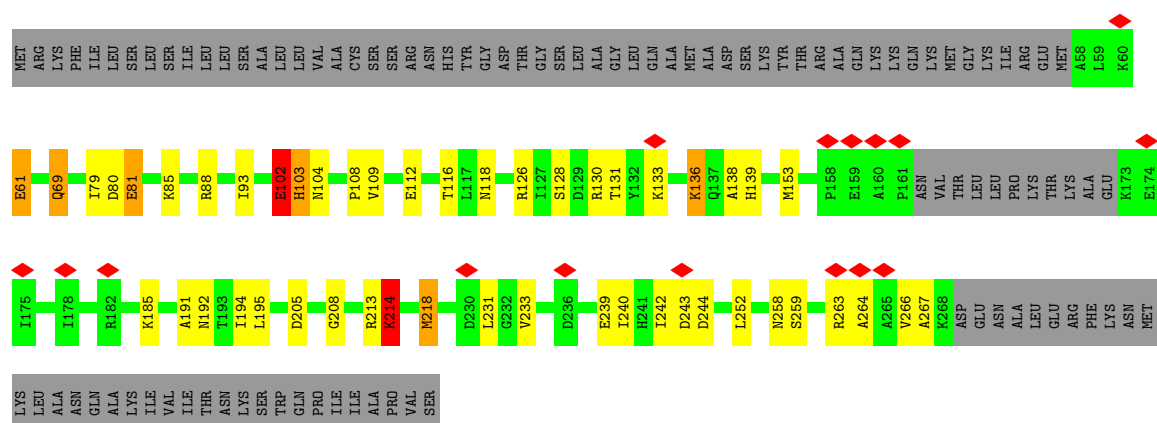


• Molecule 1: DotC

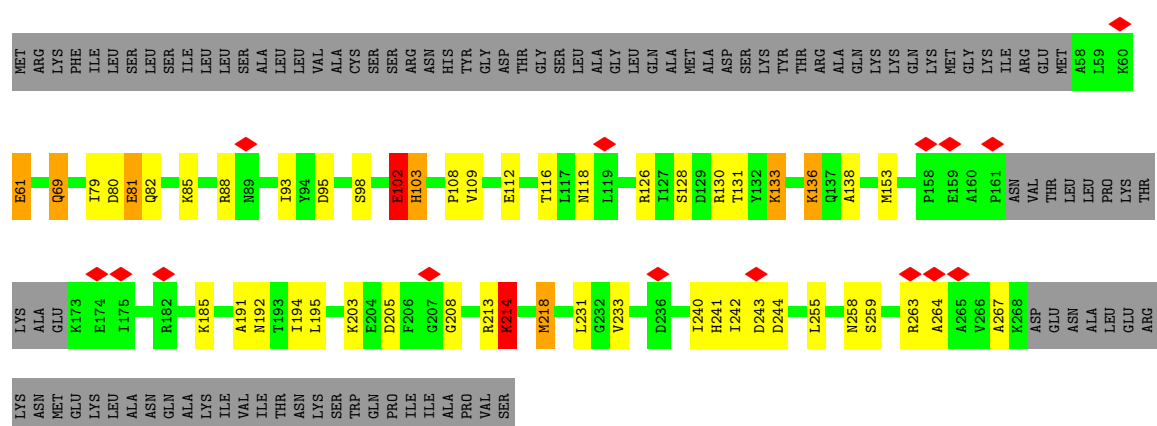




- Molecule 1: DotC



- Molecule 1: DotC

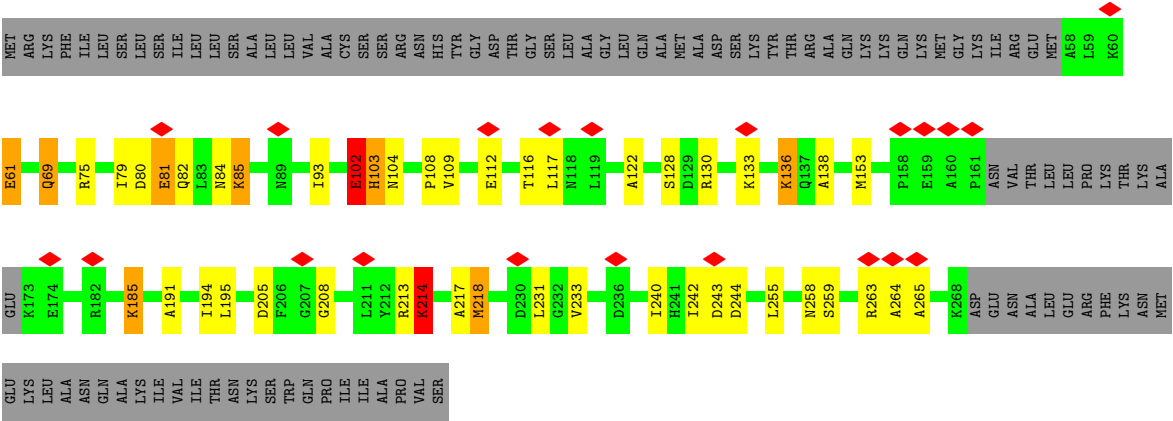


- Molecule 1: DotC

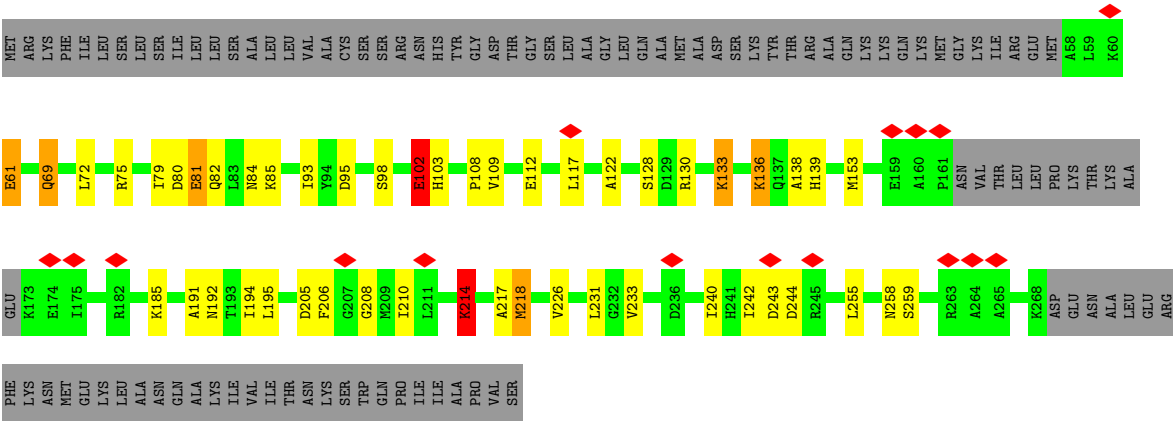




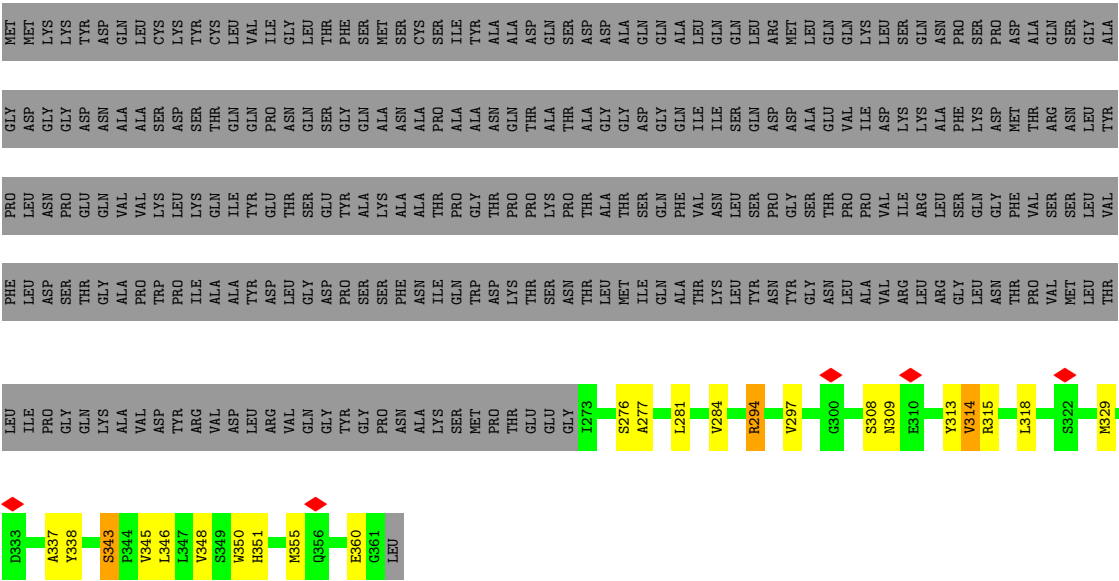




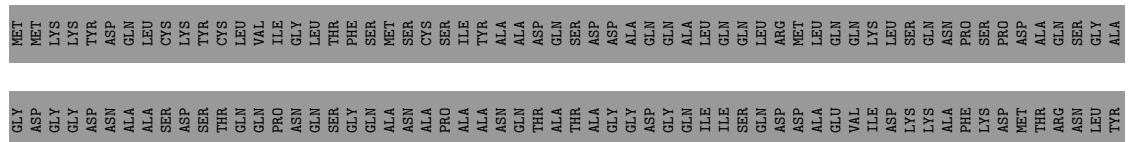
• Molecule 1: DotC



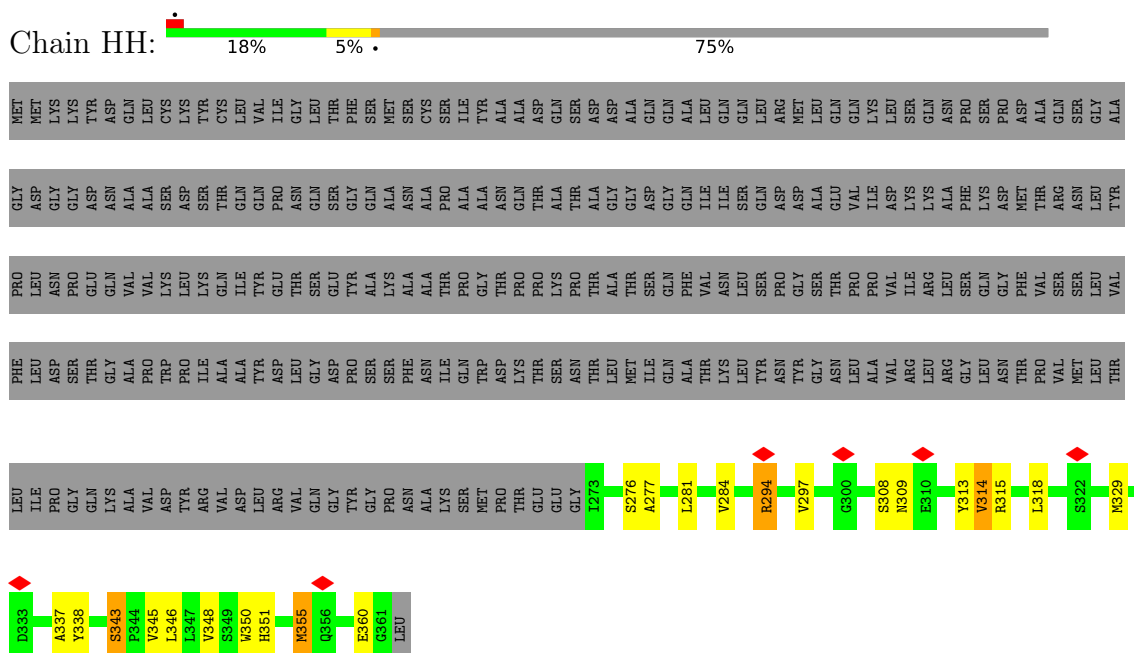
• Molecule 2: Type IV secretion protein IcmK



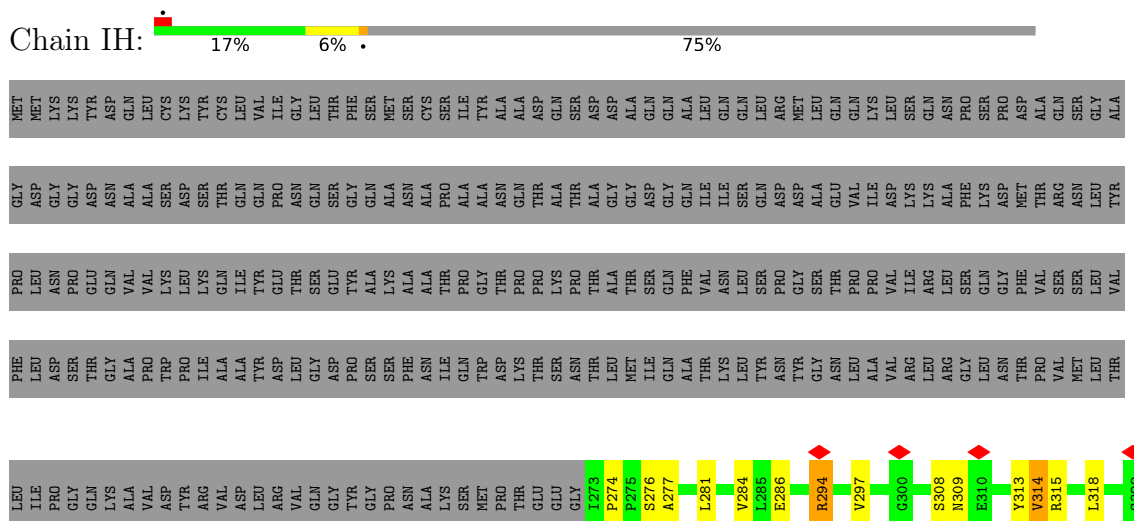
Chain EH: 19% 5% 75%

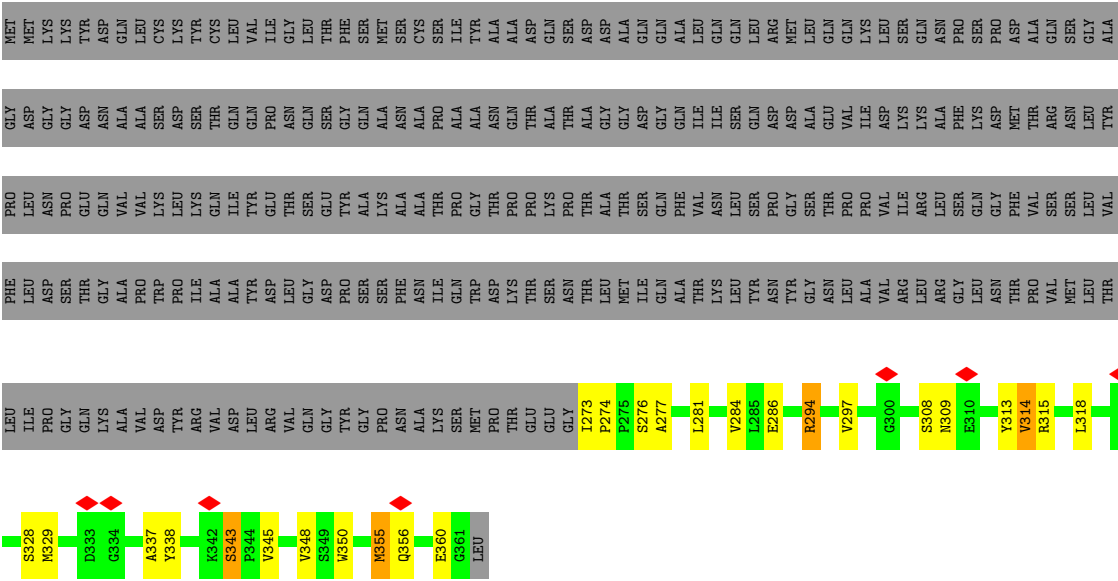


- Molecule 2: Type IV secretion protein IcmK

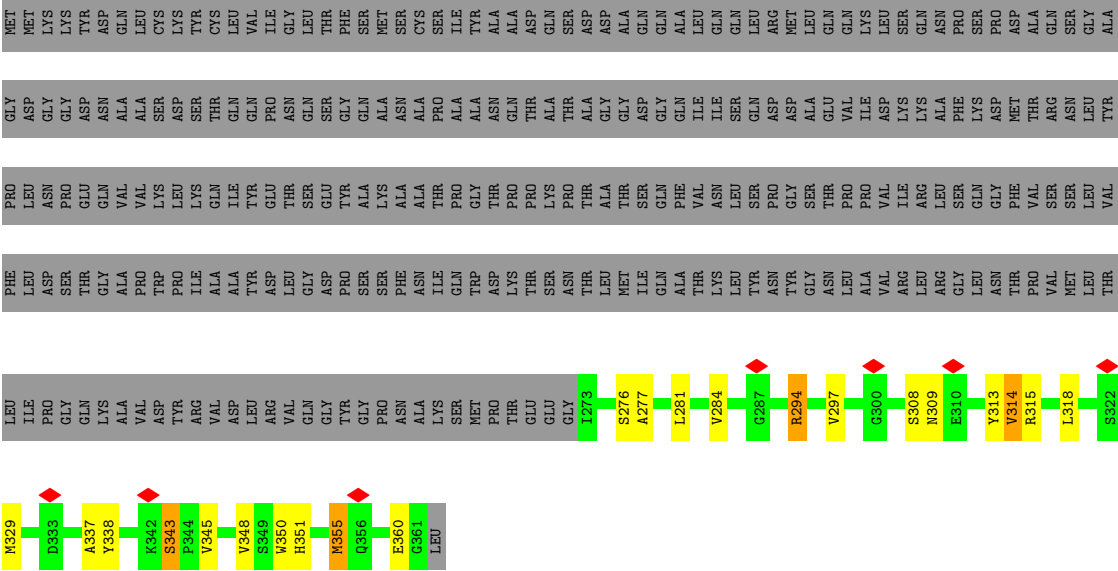


- Molecule 2: Type IV secretion protein IcmK

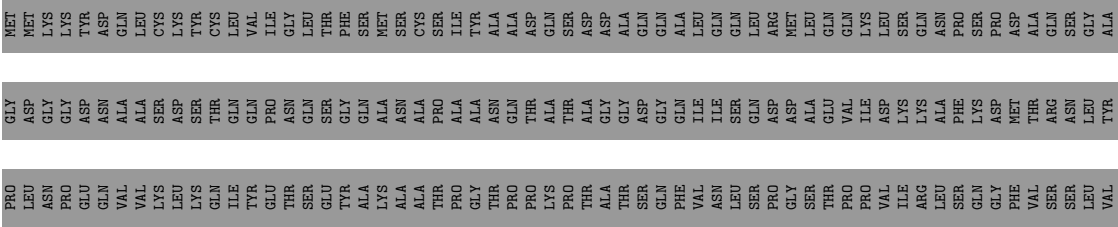




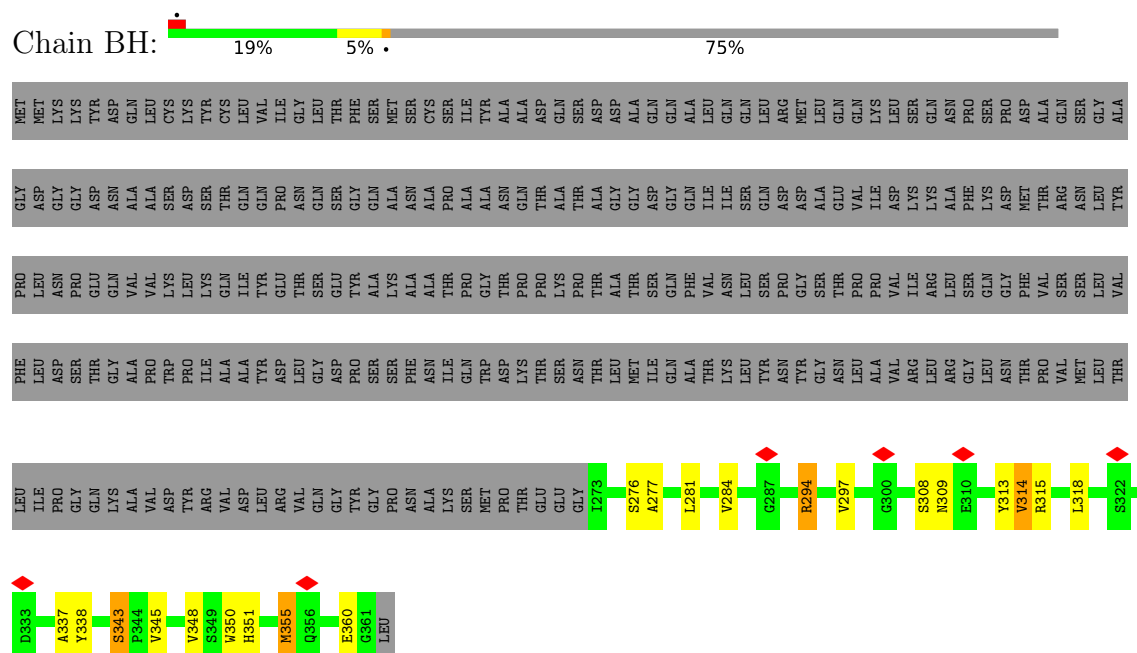
• Molecule 2: Type IV secretion protein IcmK



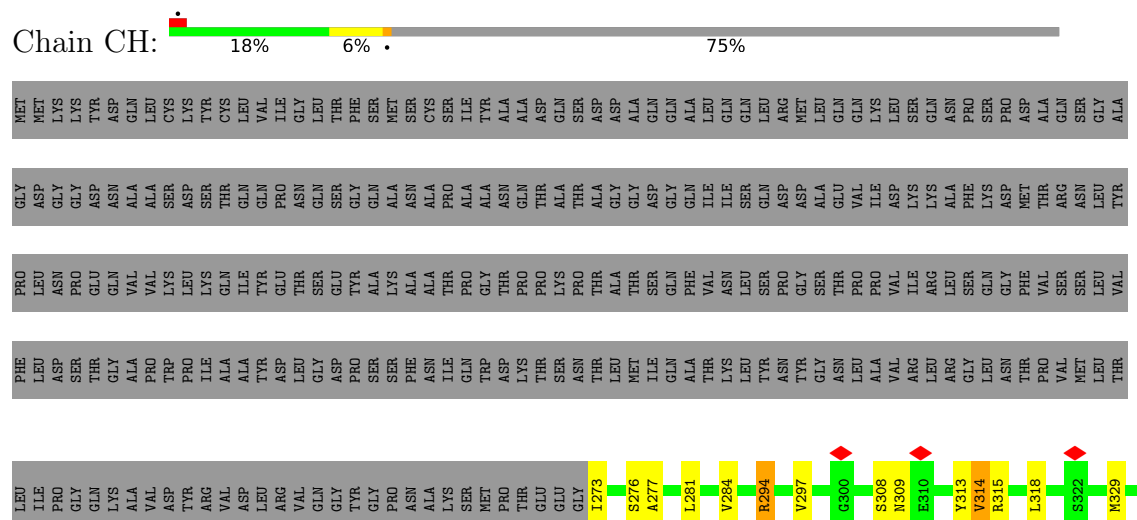
• Molecule 2: Type IV secretion protein IcmK



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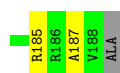
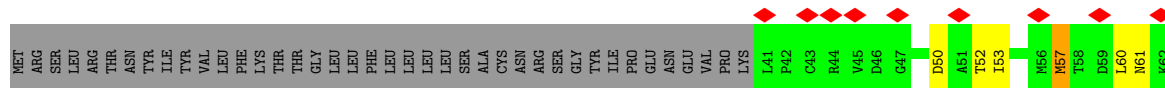


- Molecule 2: Type IV secretion protein IcmK

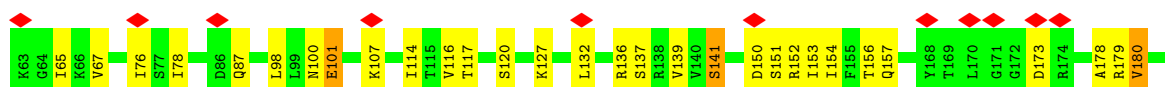
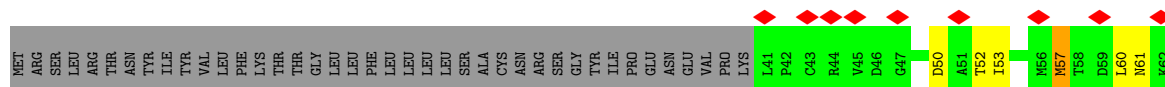




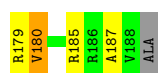
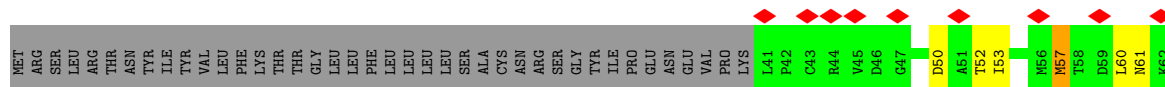
• Molecule 3: Inner membrane lipoprotein YiaD



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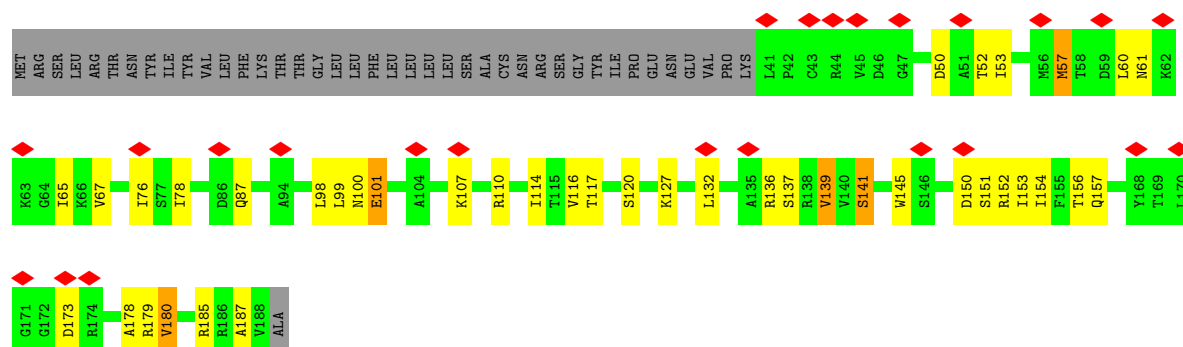


• Molecule 3: Inner membrane lipoprotein YiaD

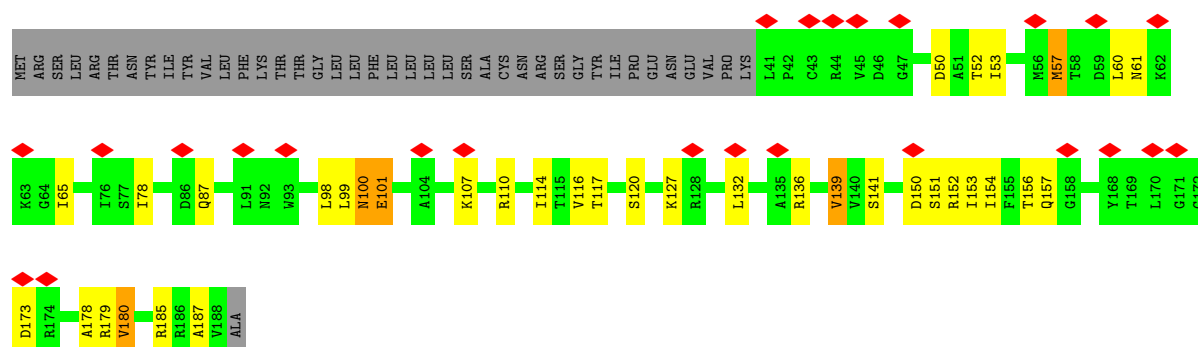


• Molecule 3: Inner membrane lipoprotein YiaD

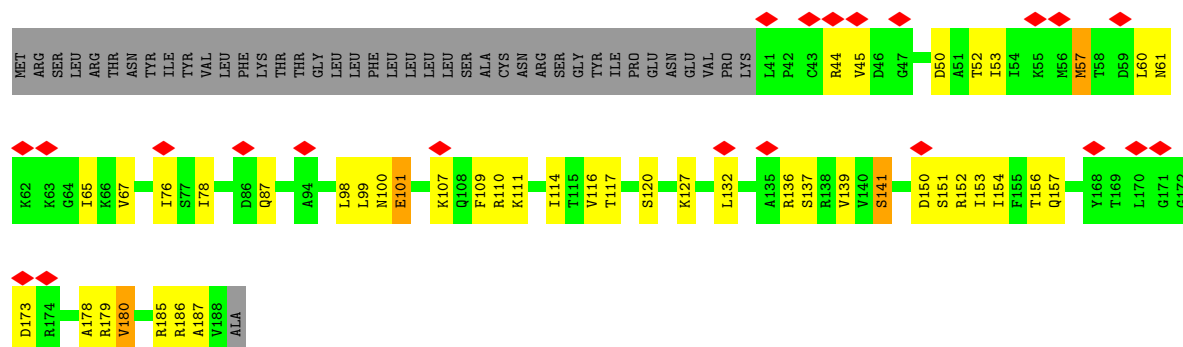




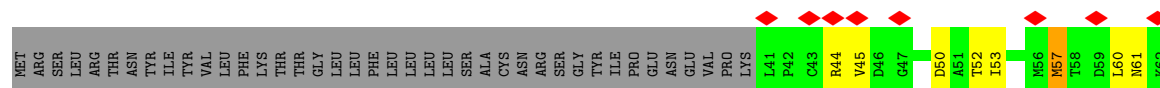
• Molecule 3: Inner membrane lipoprotein YiaD

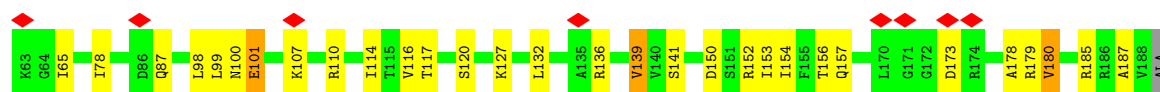


• Molecule 3: Inner membrane lipoprotein YiaD

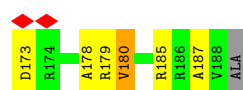
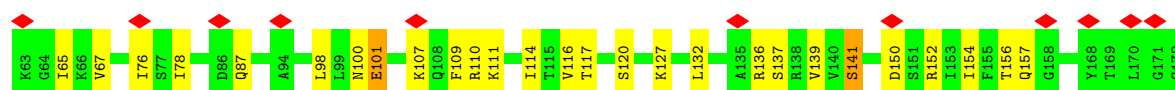
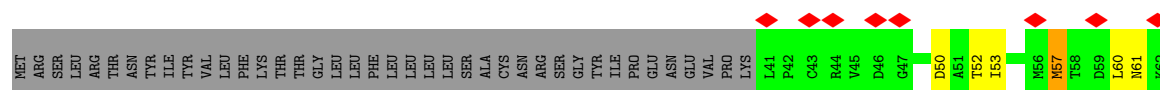


• Molecule 3: Inner membrane lipoprotein YiaD

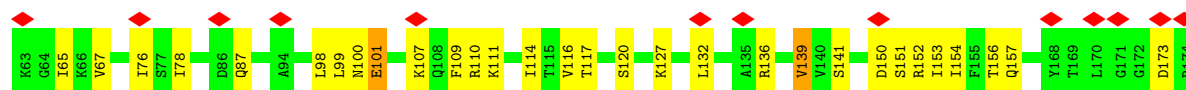
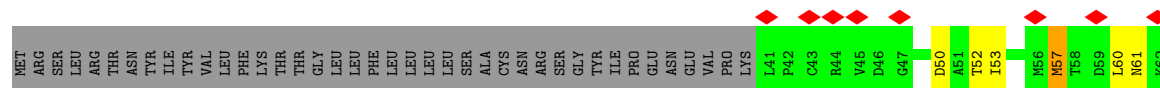




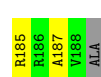
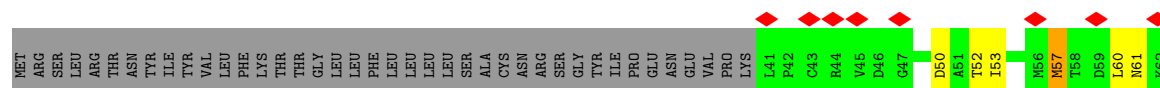
• Molecule 3: Inner membrane lipoprotein YiaD



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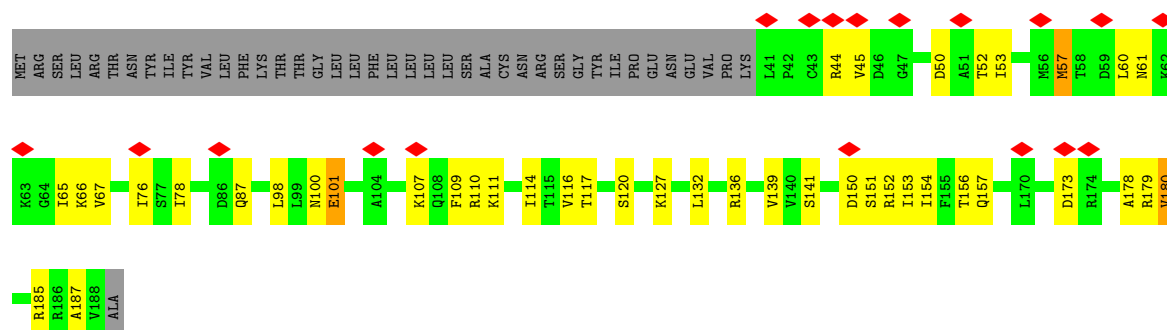


• Molecule 3: Inner membrane lipoprotein YiaD

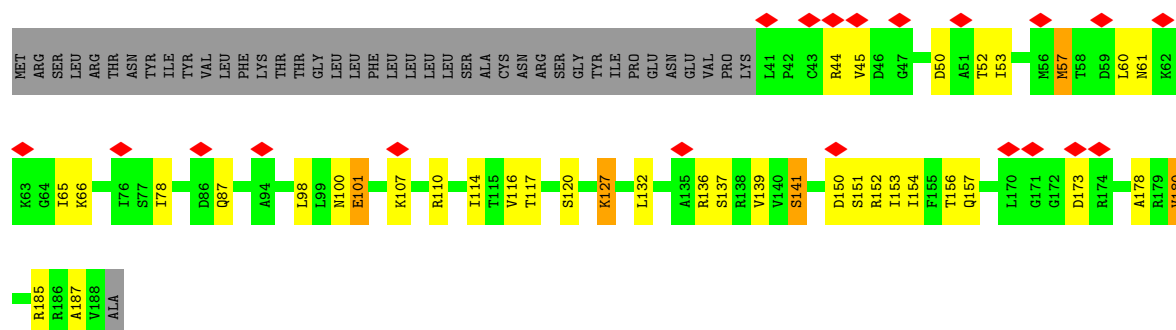


• Molecule 3: Inner membrane lipoprotein YiaD

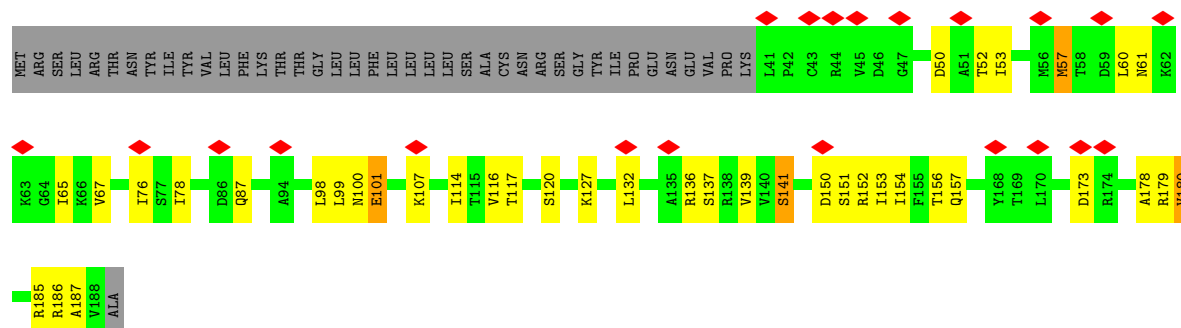




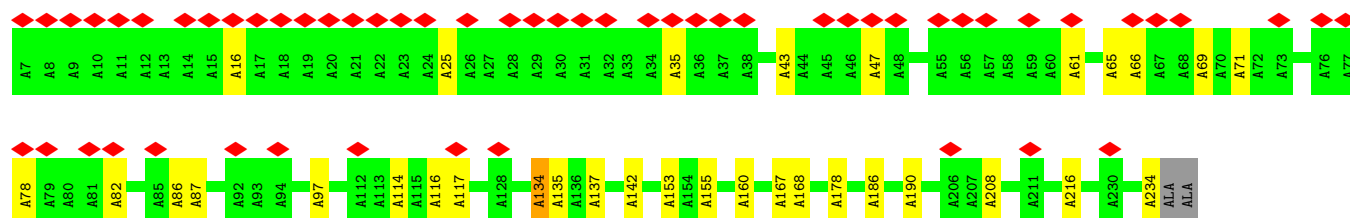
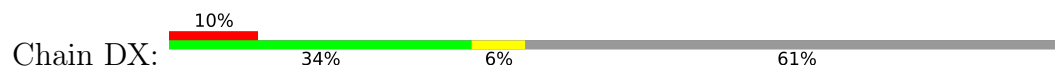
• Molecule 3: Inner membrane lipoprotein YiaD



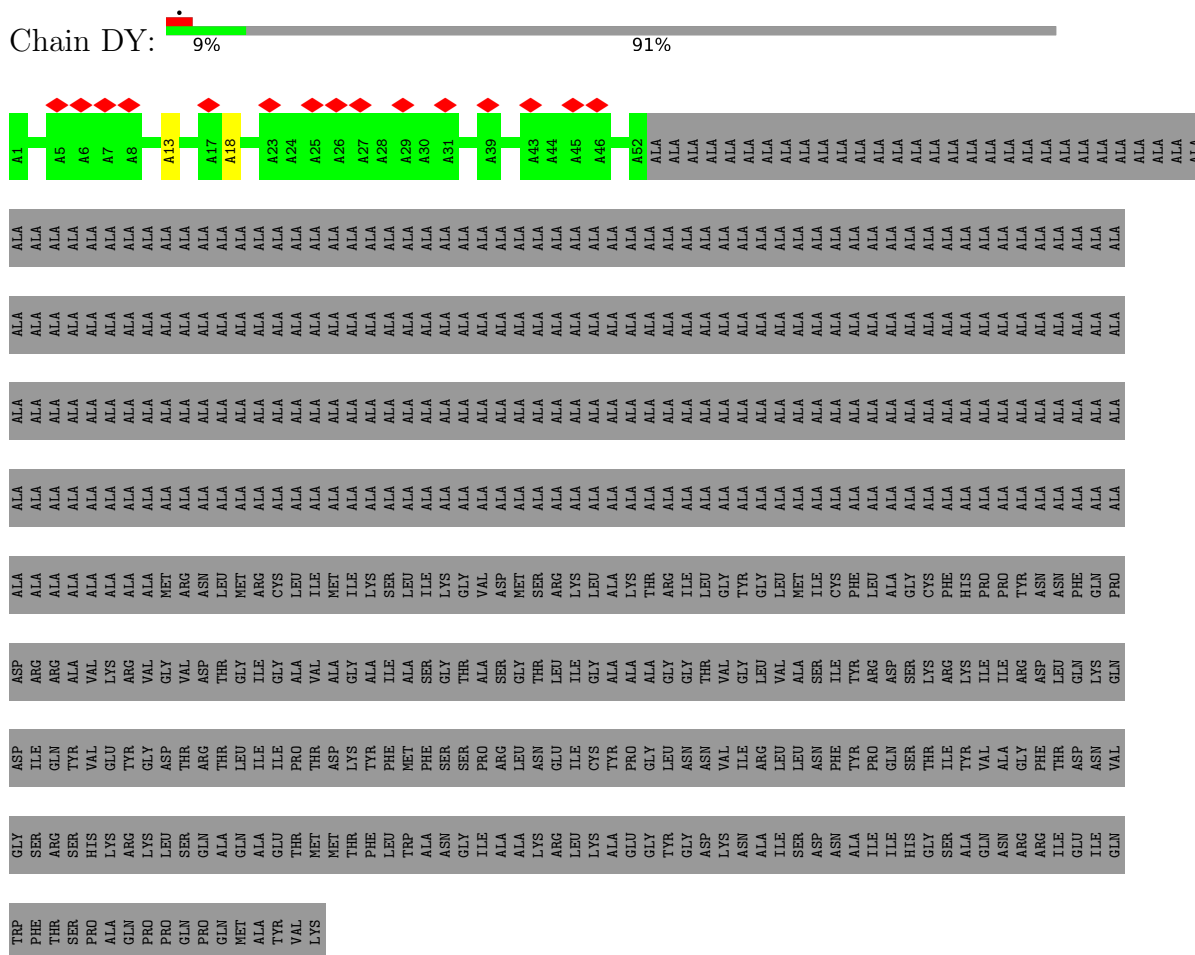
• Molecule 3: Inner membrane lipoprotein YiaD



• Molecule 4: Type IV secretion system unknown protein fragment

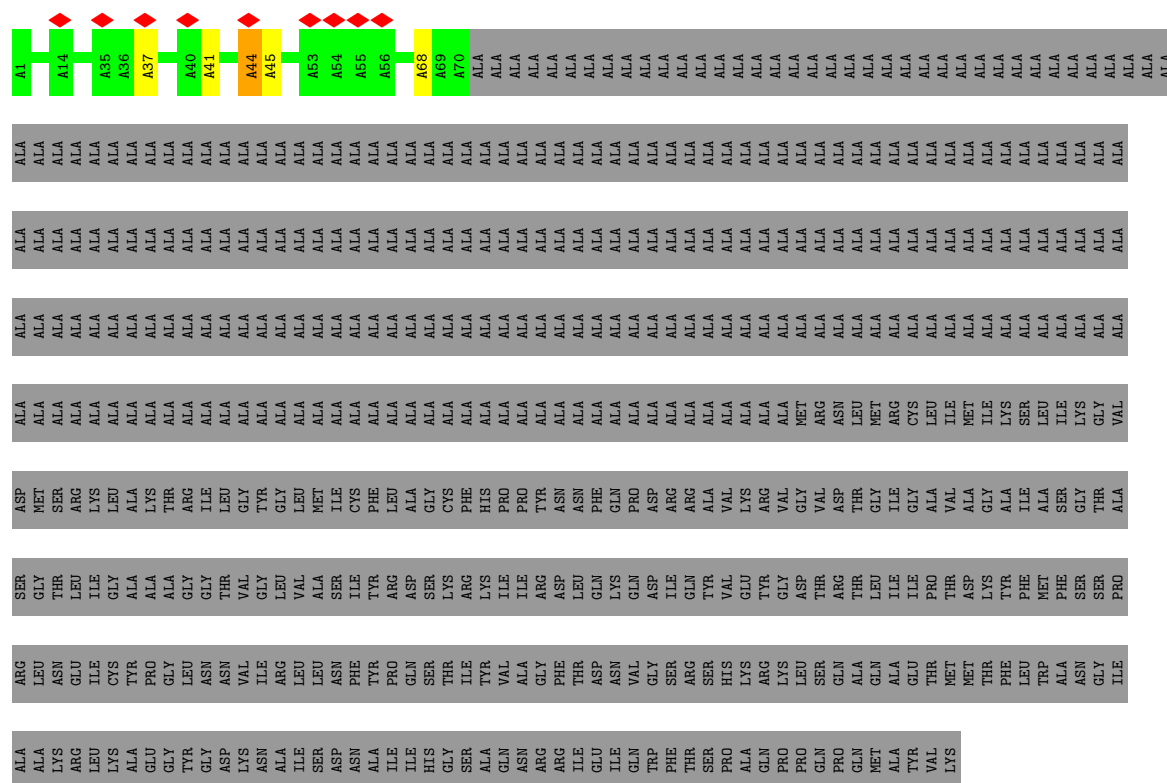


- Molecule 4: Type IV secretion system unknown protein fragment

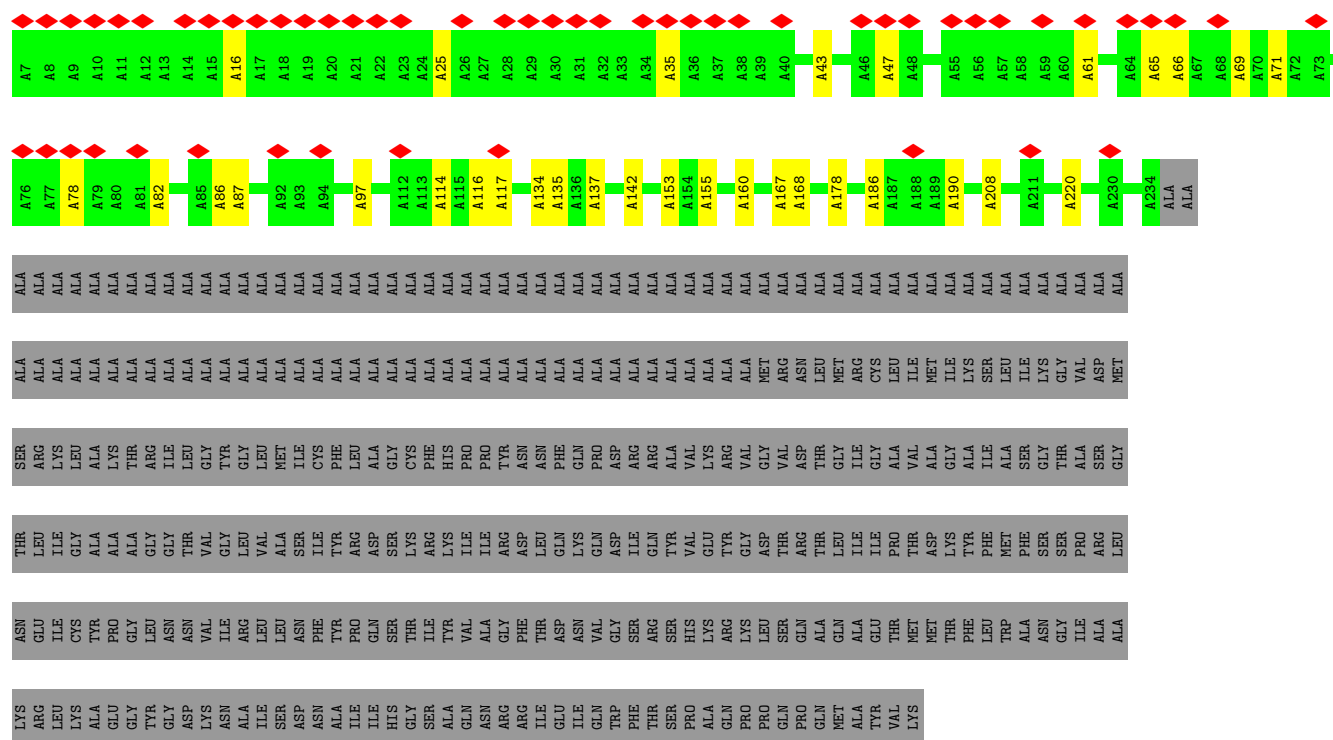
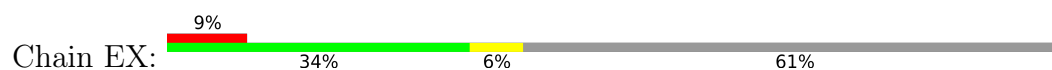


- Molecule 4: Type IV secretion system unknown protein fragment

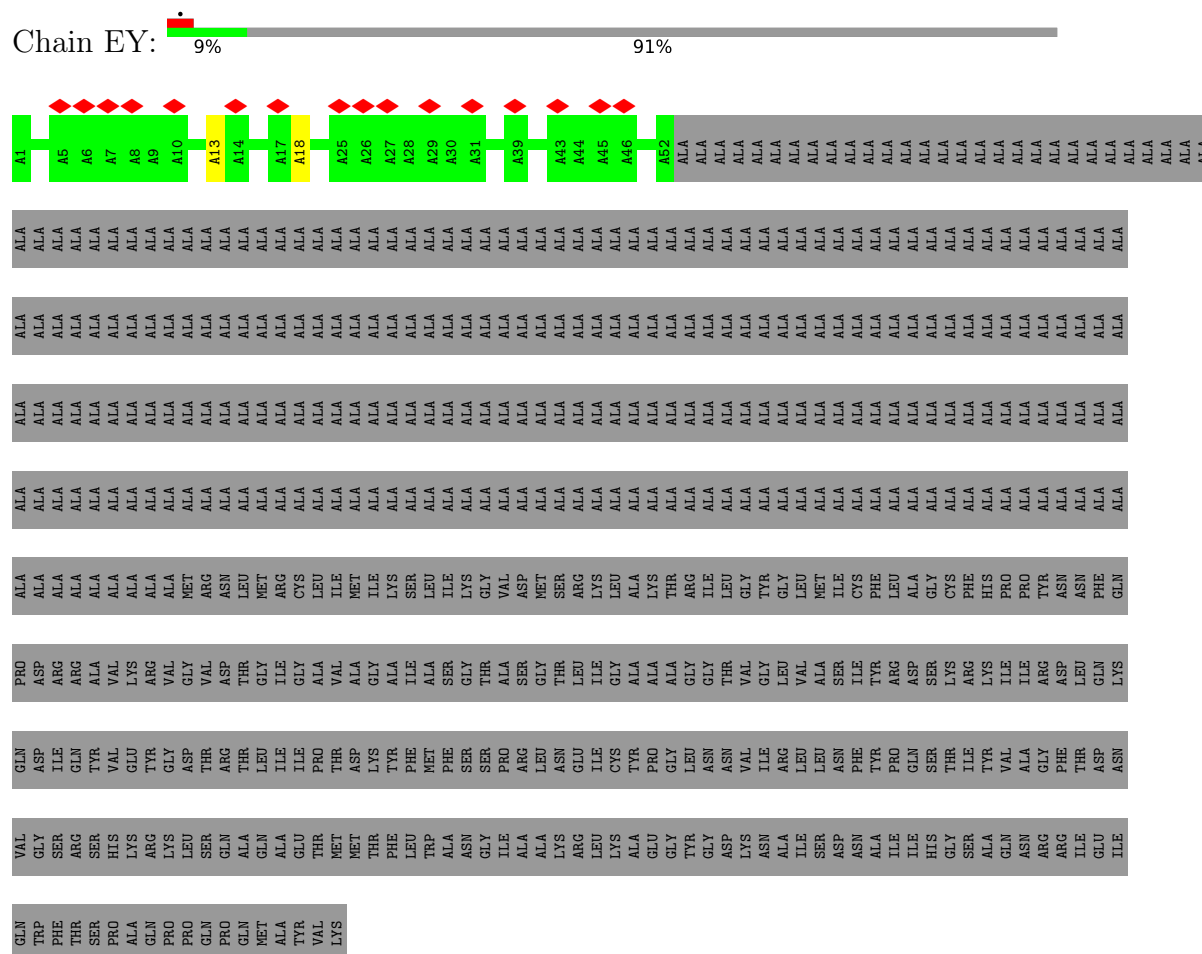




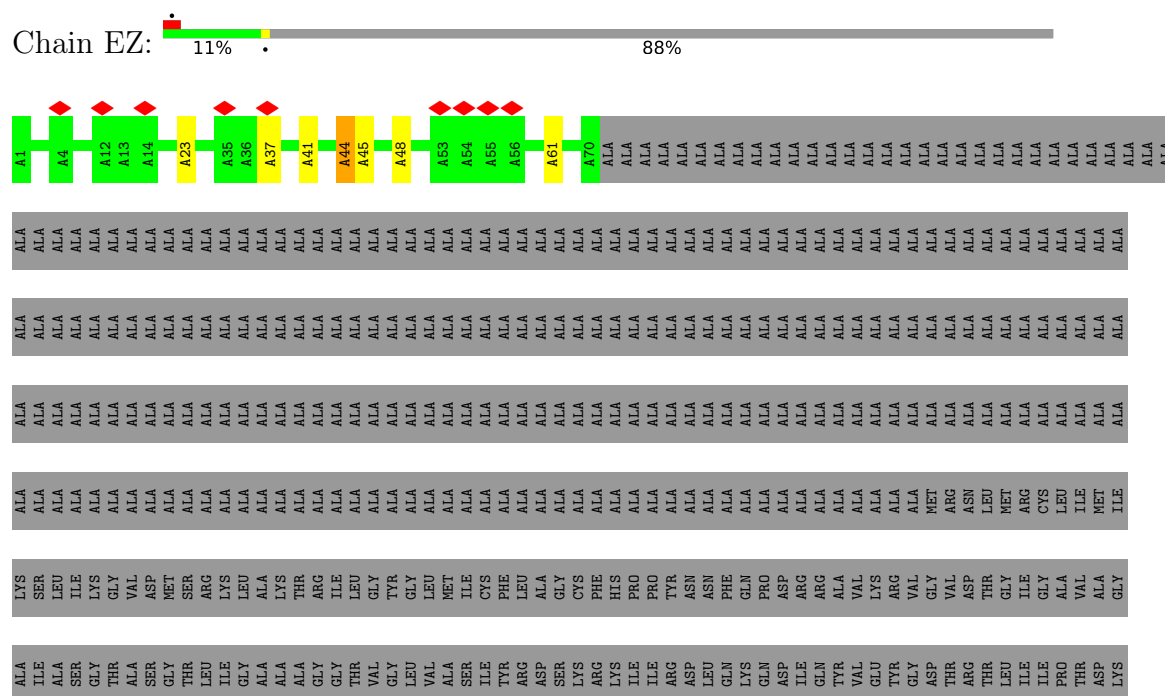
• Molecule 4: Type IV secretion system unknown protein fragment



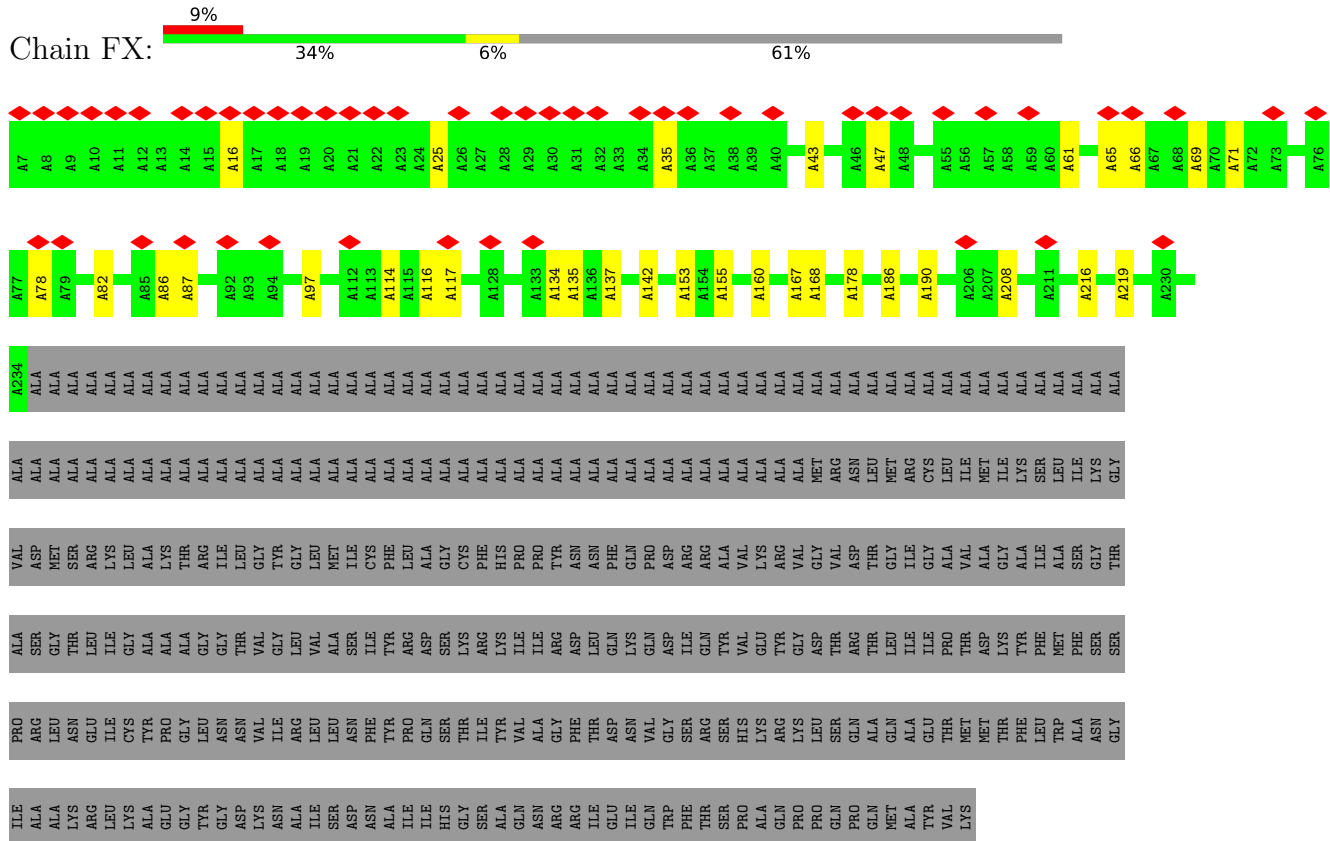
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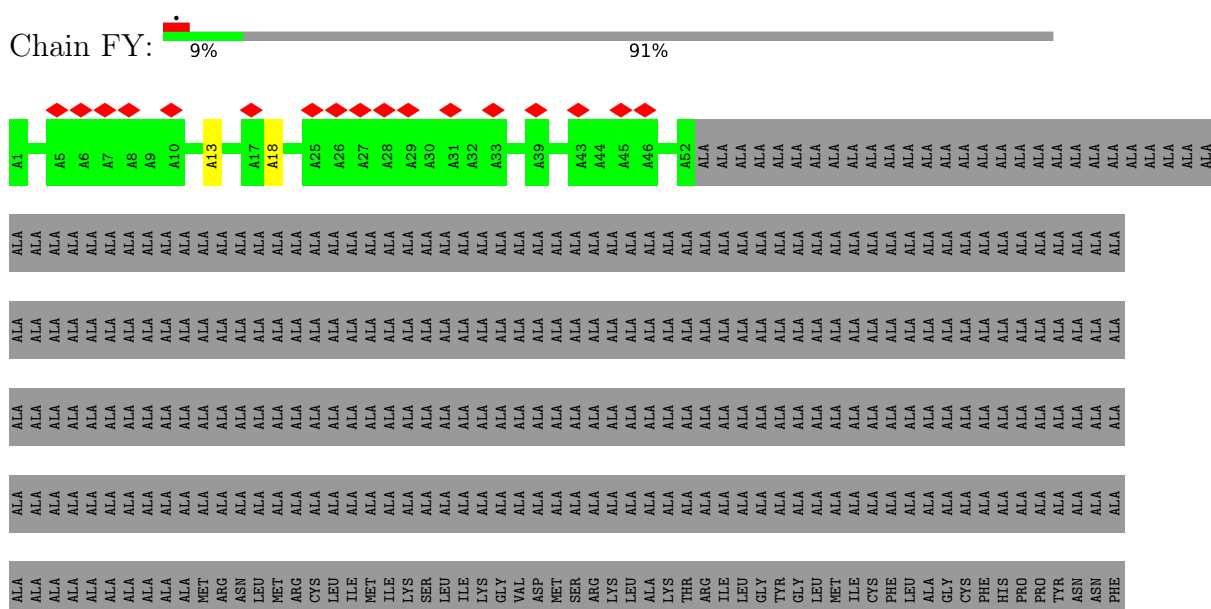
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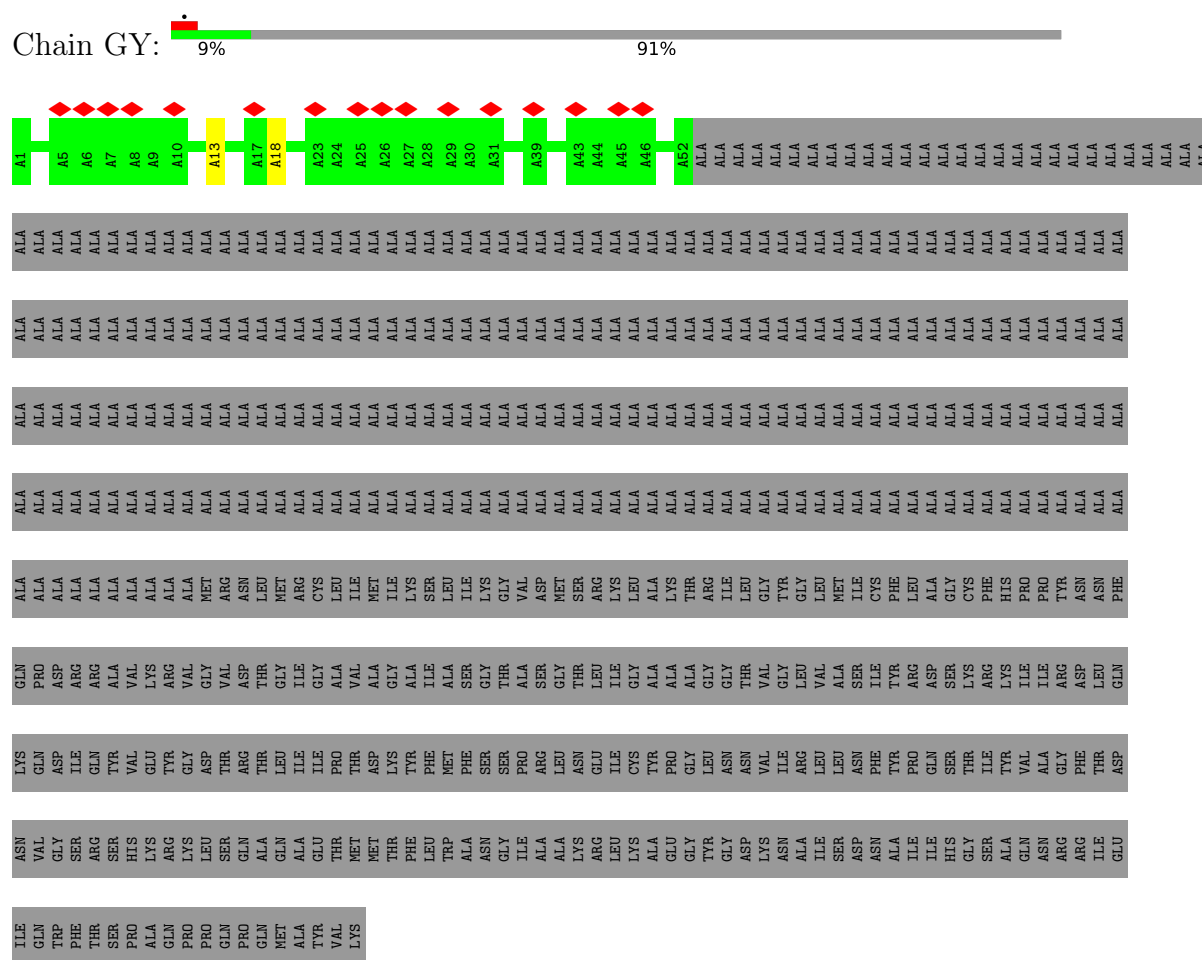


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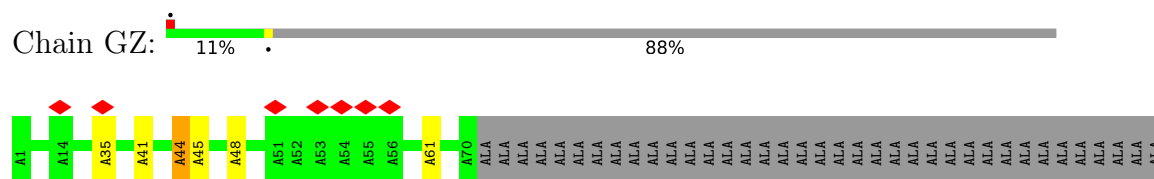




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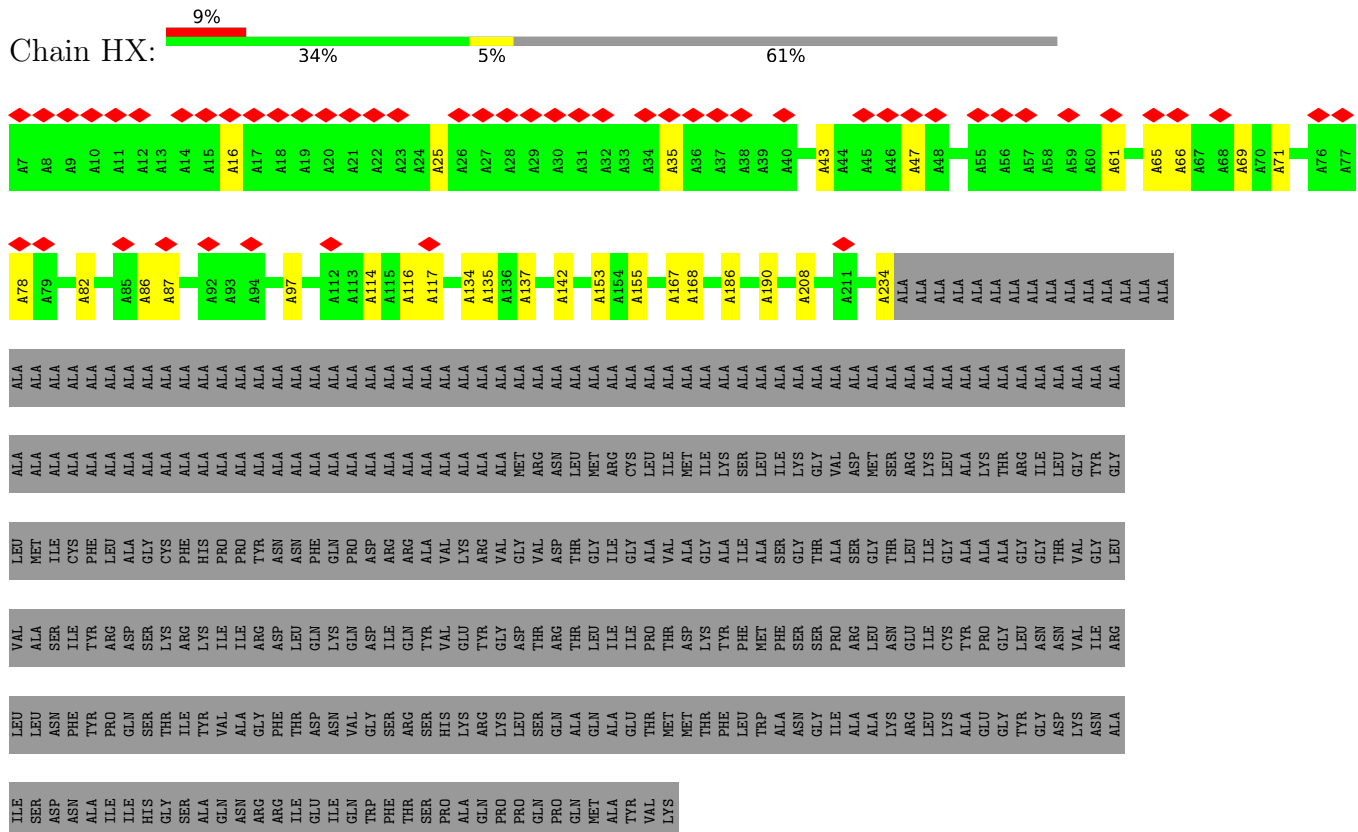


- Molecule 4: Type IV secretion system unknown protein fragment



[illegible]

- Molecule 4: Type IV secretion system unknown protein fragment



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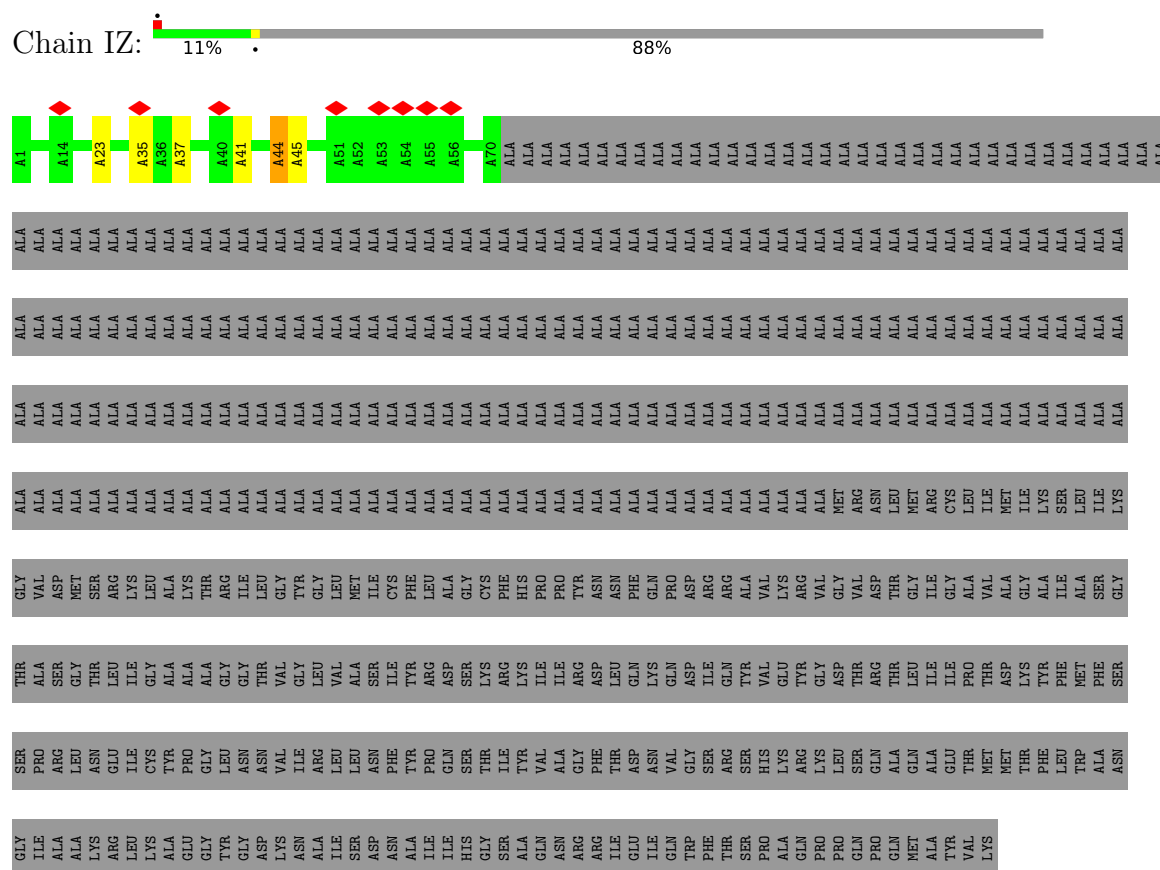




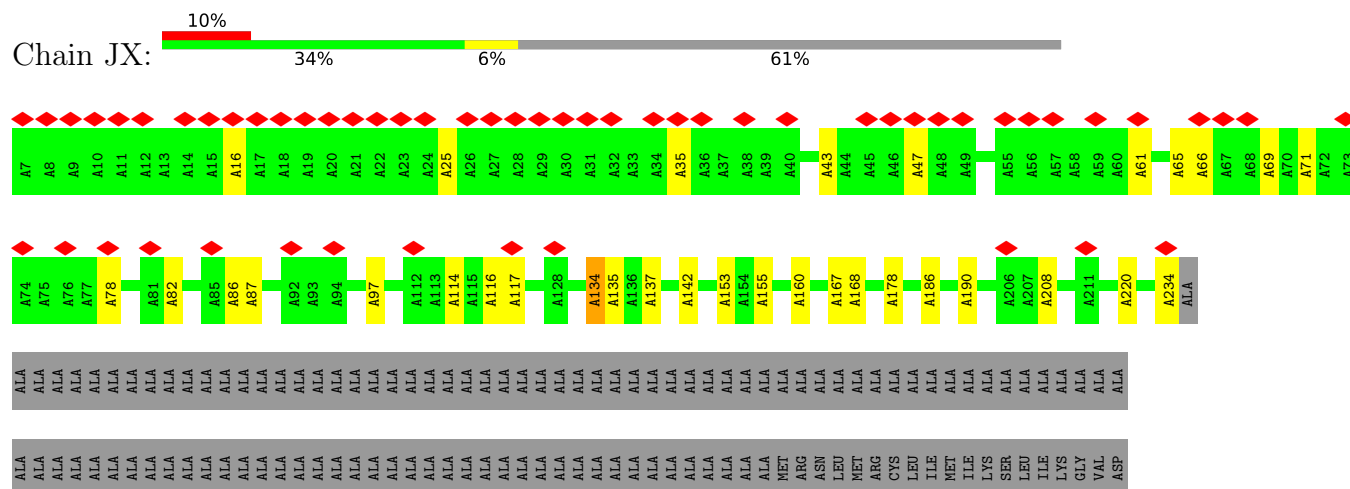
● Molecule 4: Type IV secretion system unknown protein fragment



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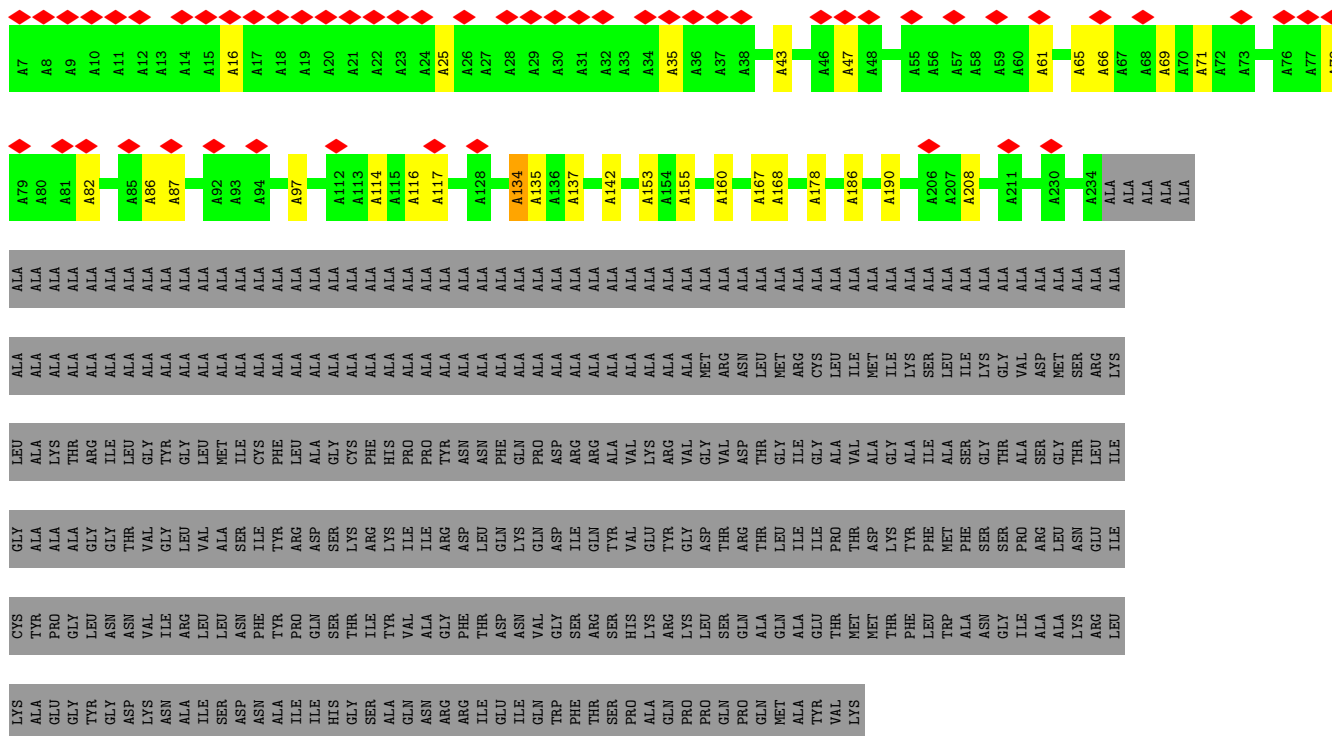
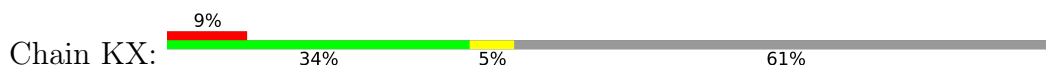


- Molecule 4: Type IV secretion system unknown protein fragment

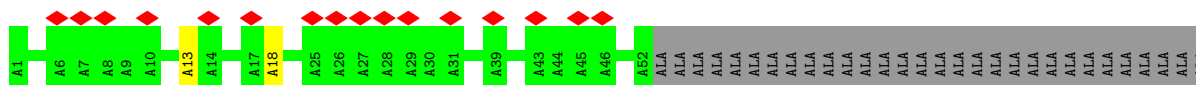


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- Molecule 4: Type IV secretion system unknown protein fragment

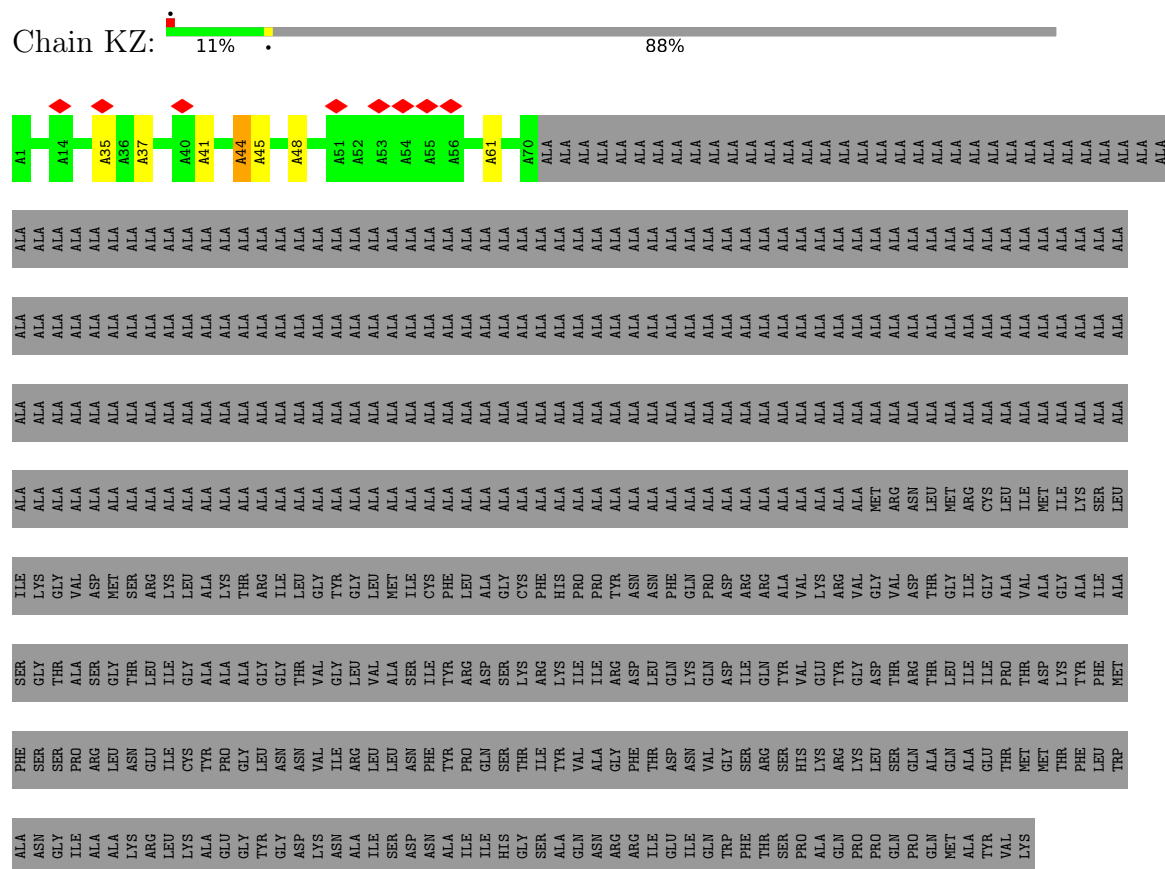


- Molecule 4: Type IV secretion system unknown protein fragment

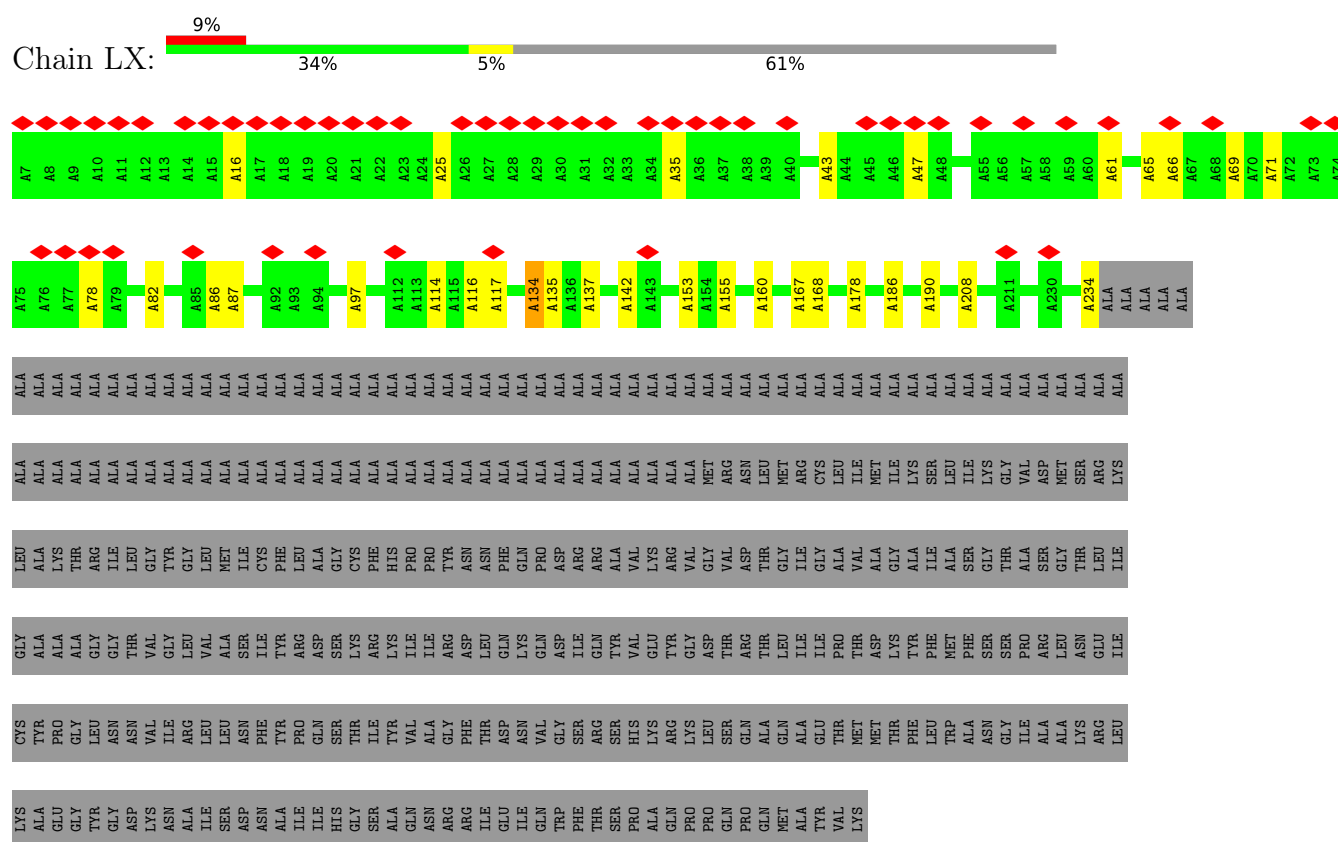


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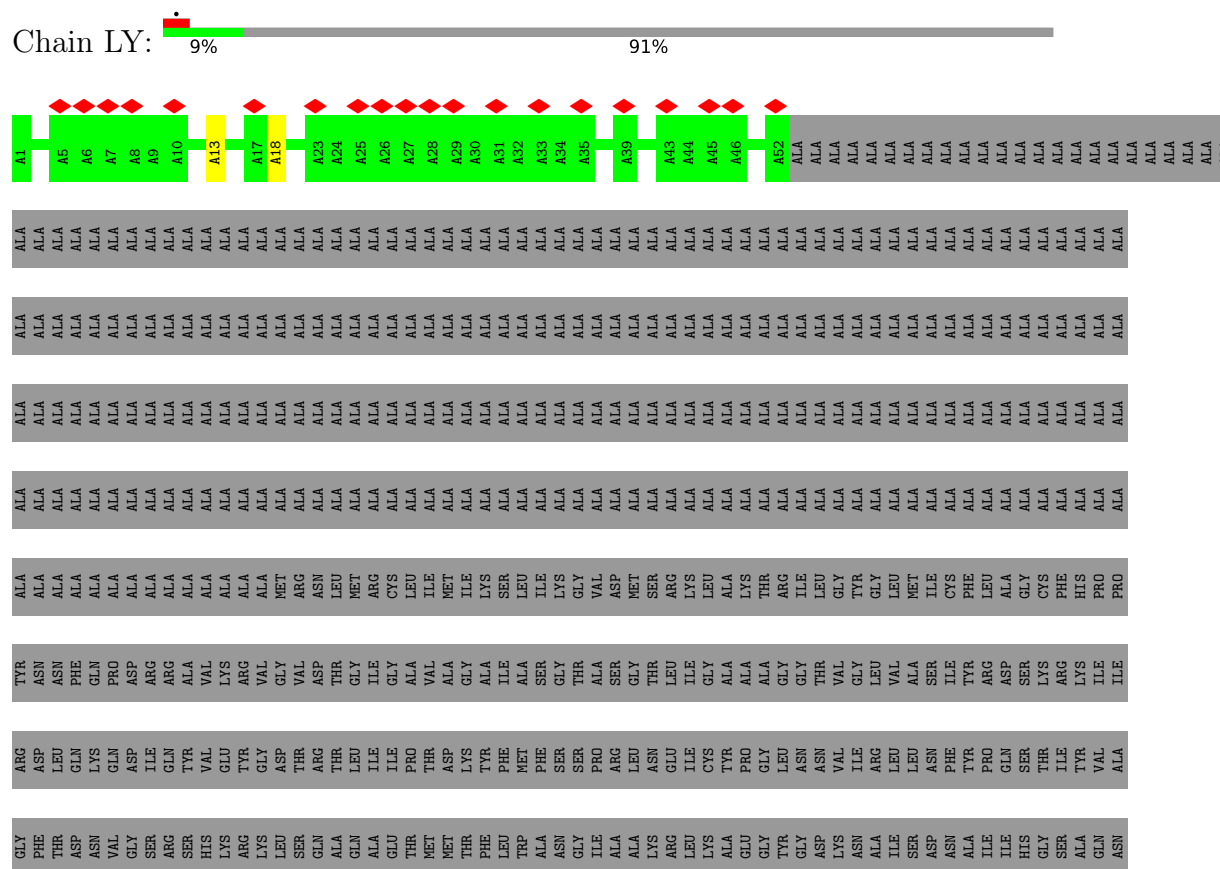
- Molecule 4: Type IV secretion system unknown protein fragment



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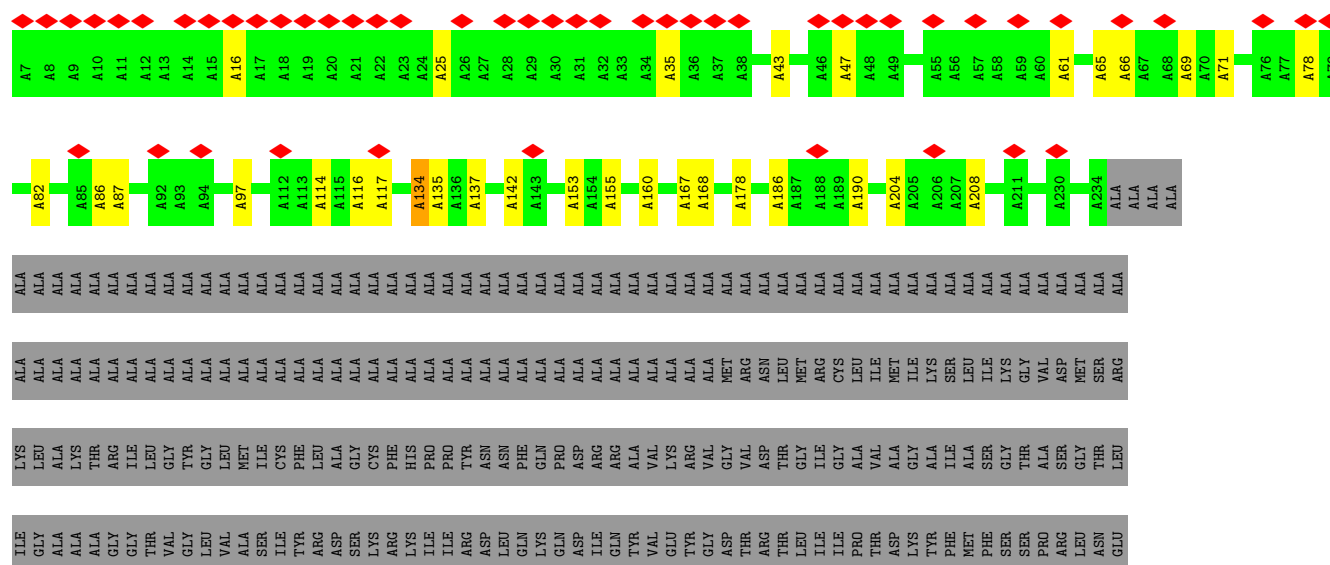
- Molecule 4: Type IV secretion system unknown protein fragment



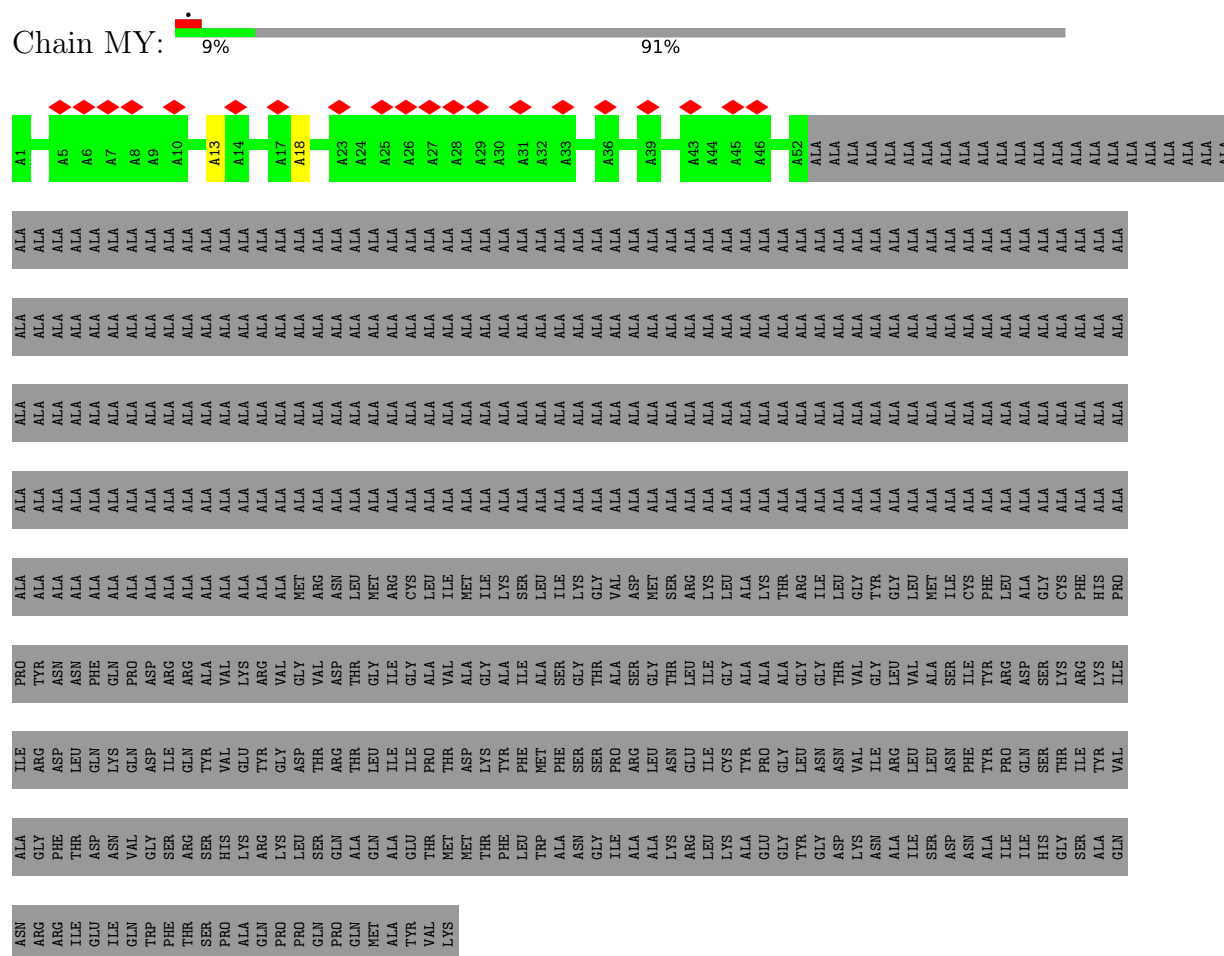
Chain LZ: 11% 88%



Chain MX:



- Molecule 4: Type IV secretion system unknown protein fragment



- Molecule 4: Type IV secretion system unknown protein fragment



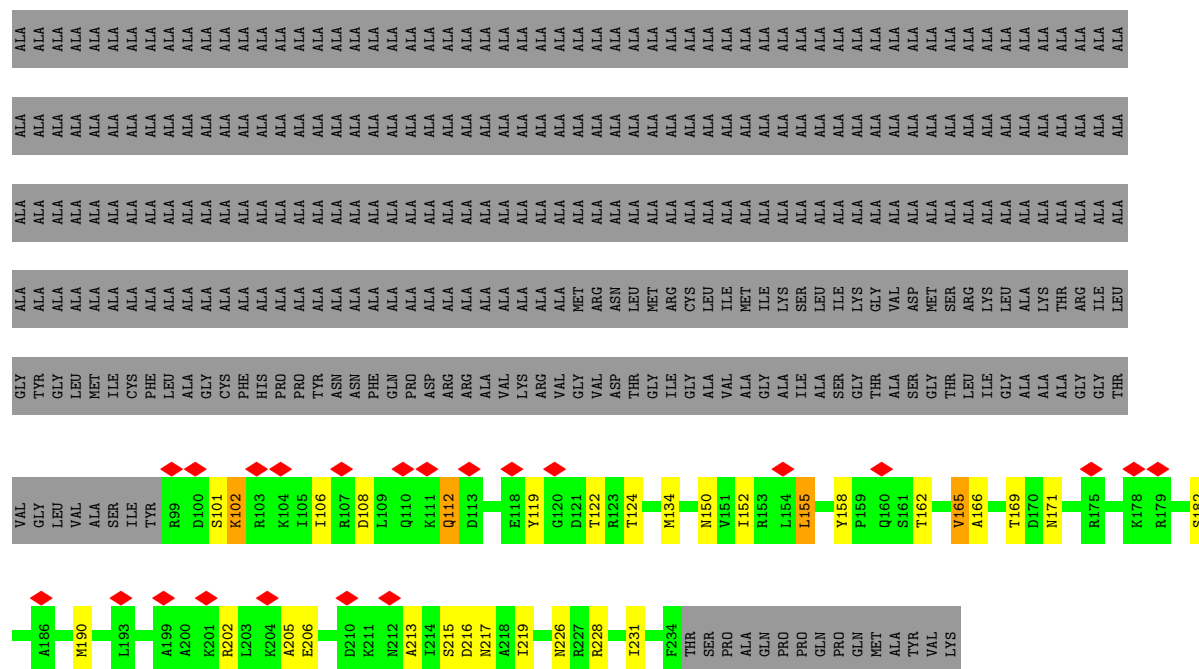
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- Molecule 4: Type IV secretion system unknown protein fragment

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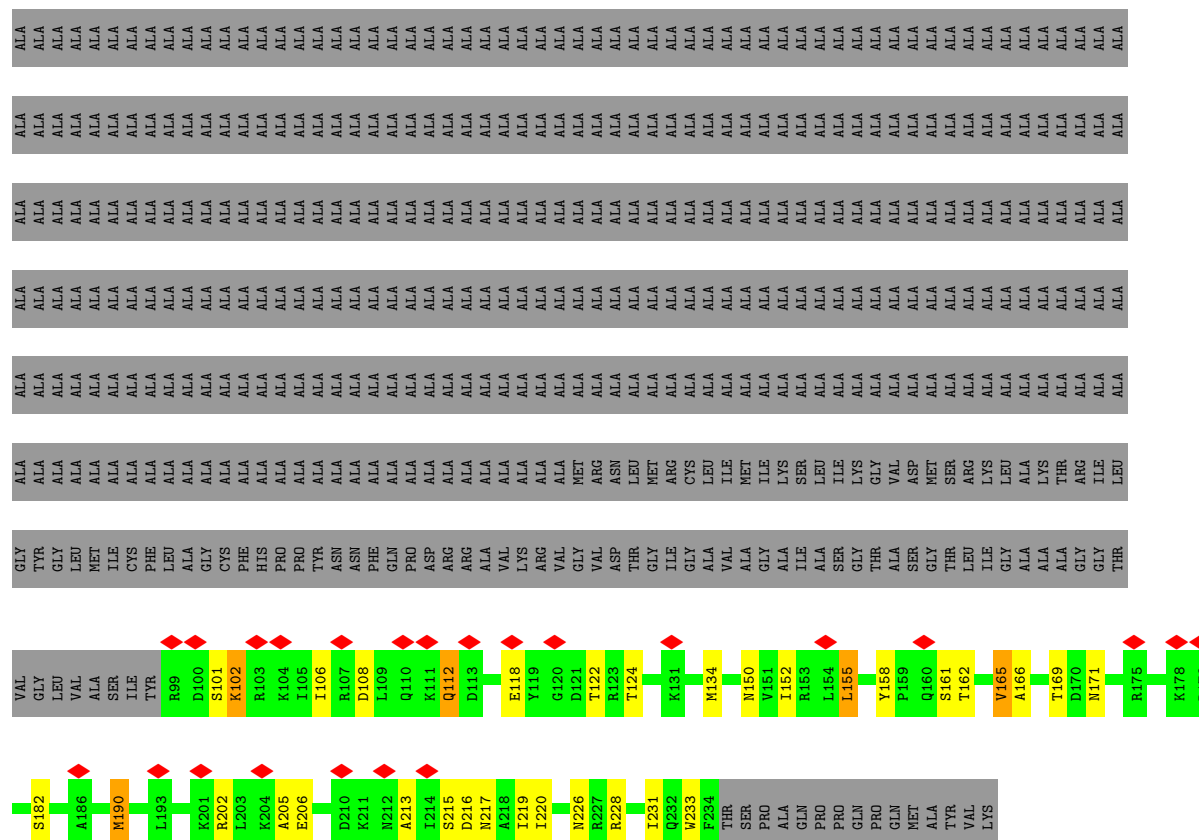
- Molecule 4: Type IV secretion system unknown protein fragment

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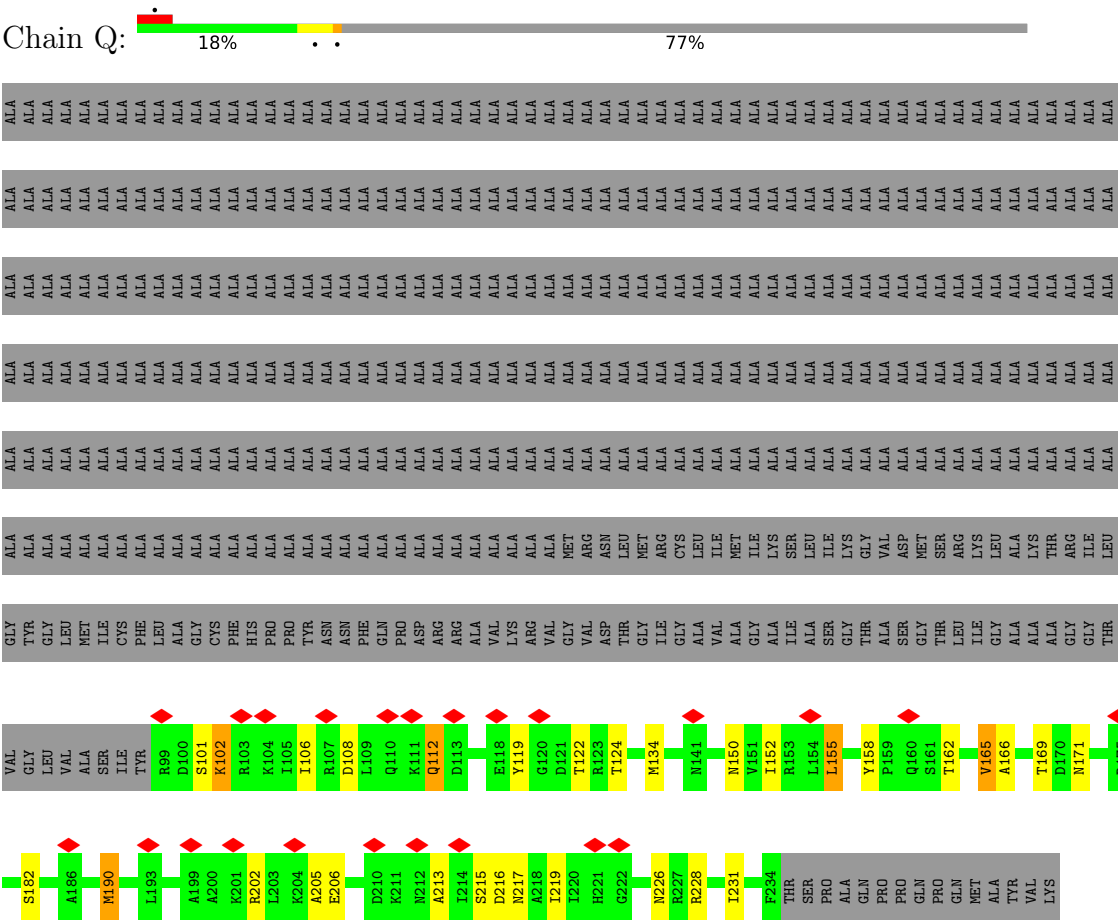


- Molecule 4: Type IV secretion system unknown protein fragment

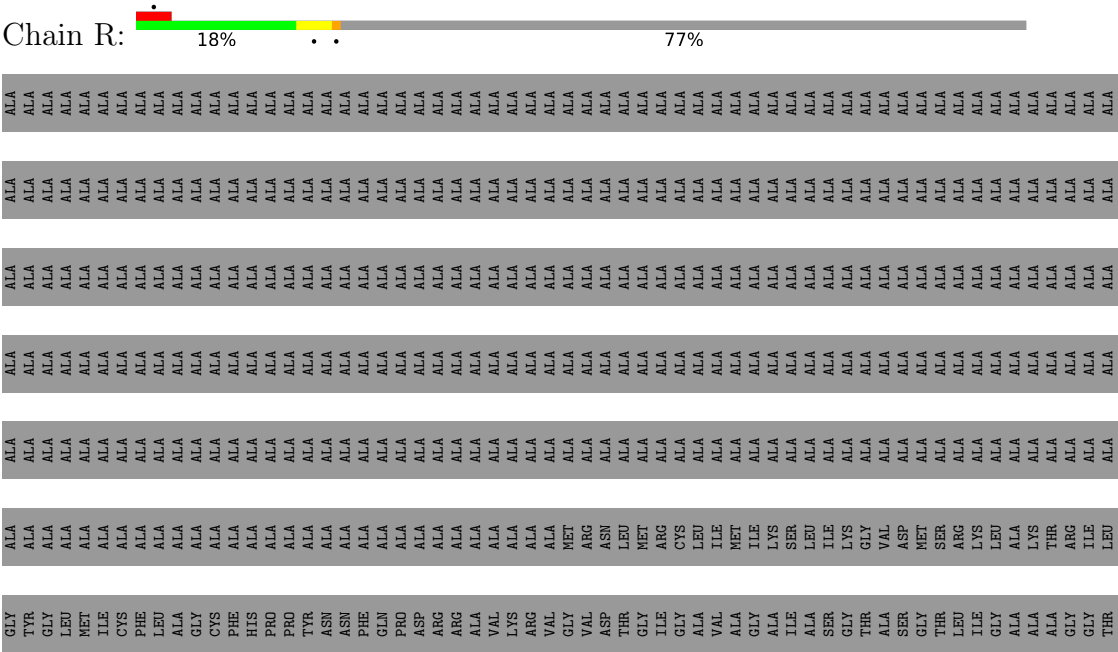
Chain P: 18% 5% 77%

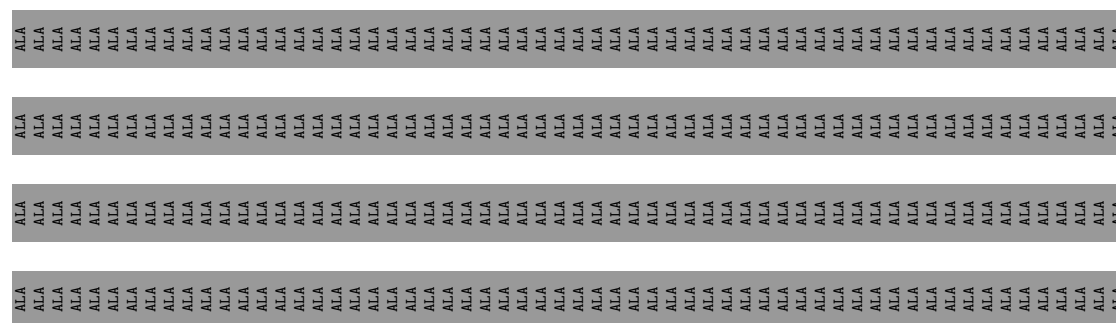


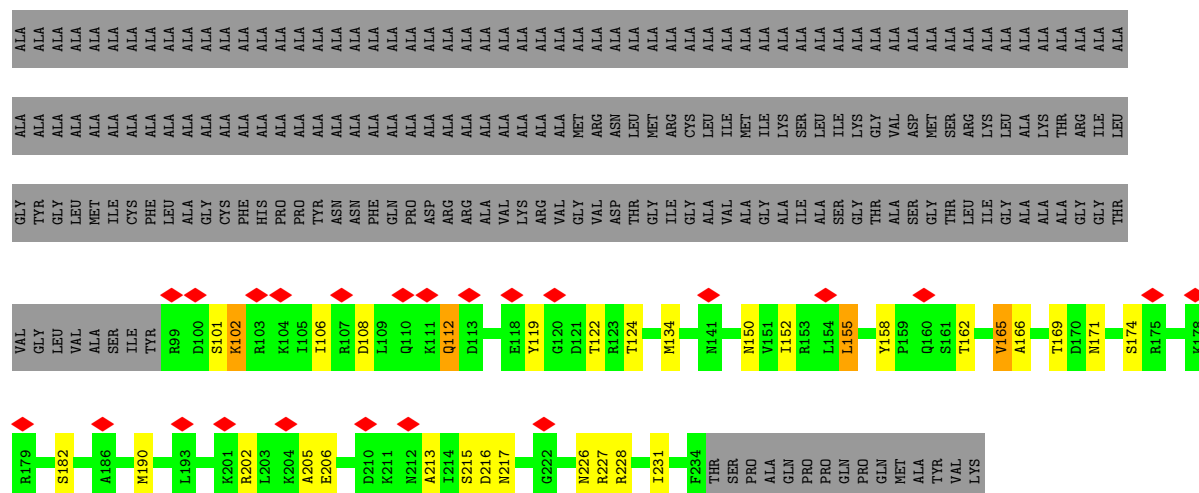
- Molecule 4: Type IV secretion system unknown protein fragment



● Molecule 4: Type IV secretion system unknown protein fragment

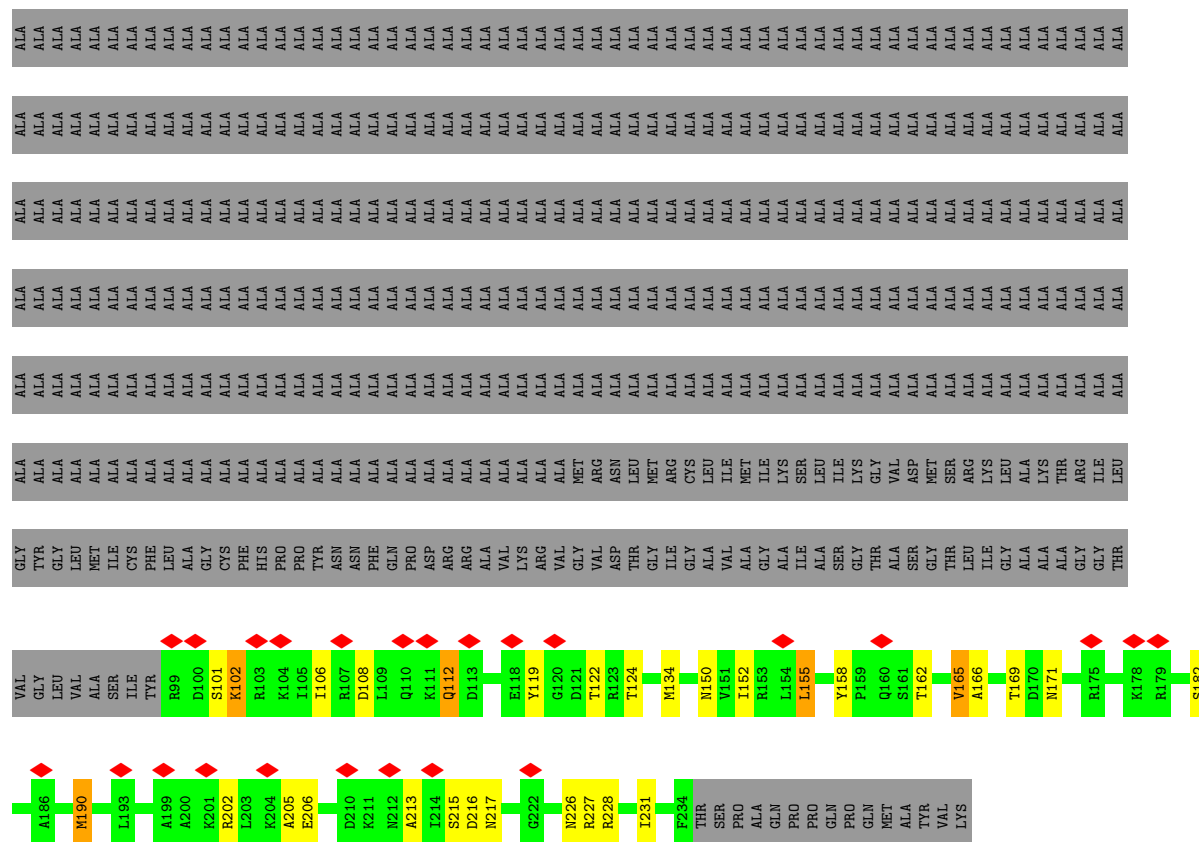






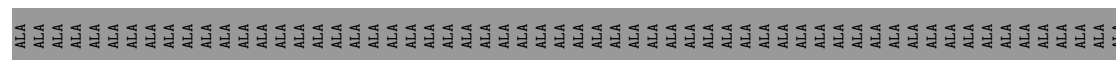
- Molecule 4: Type IV secretion system unknown protein fragment

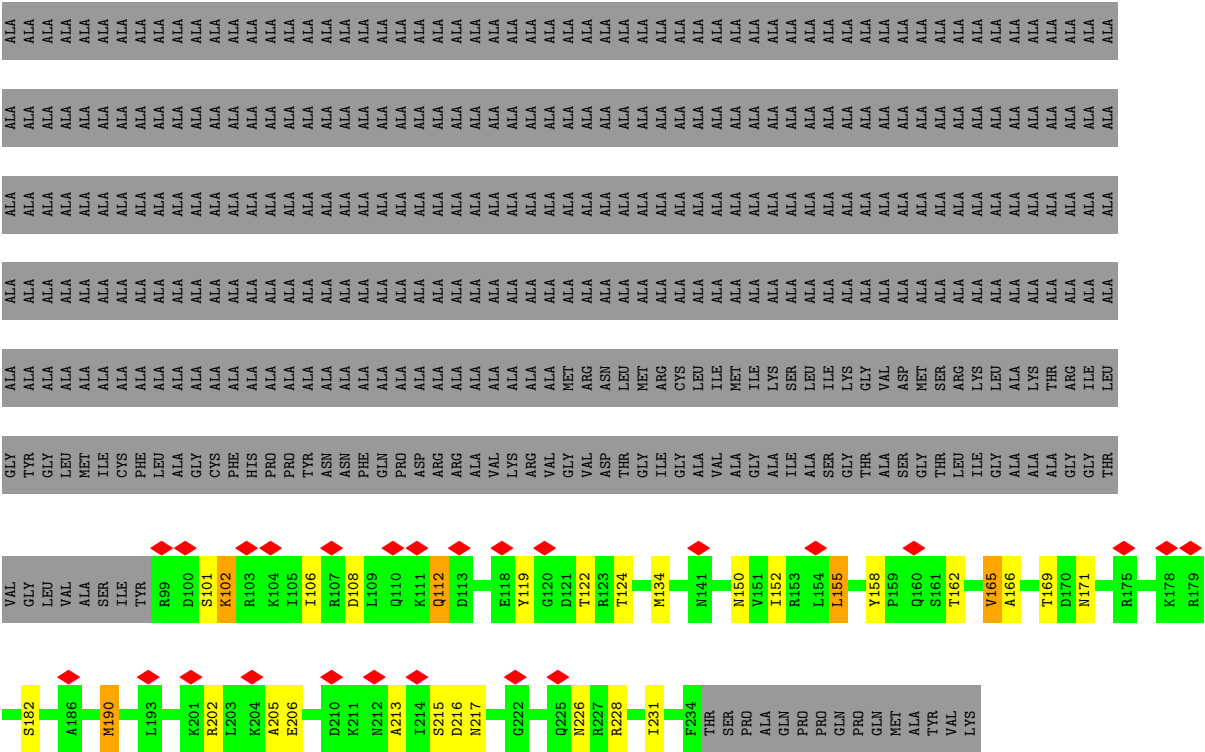
Chain U: 18% 77%



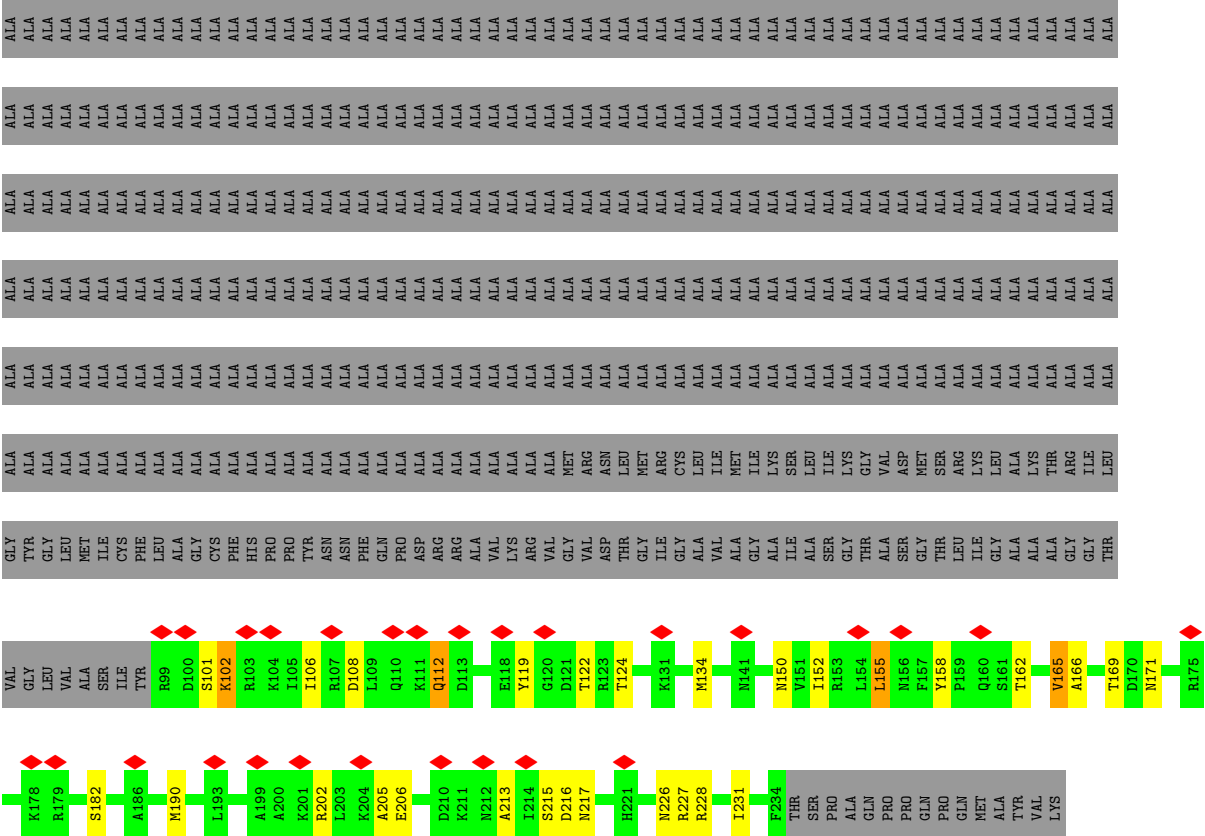
- Molecule 4: Type IV secretion system unknown protein fragment

Chain V: 18% 77%

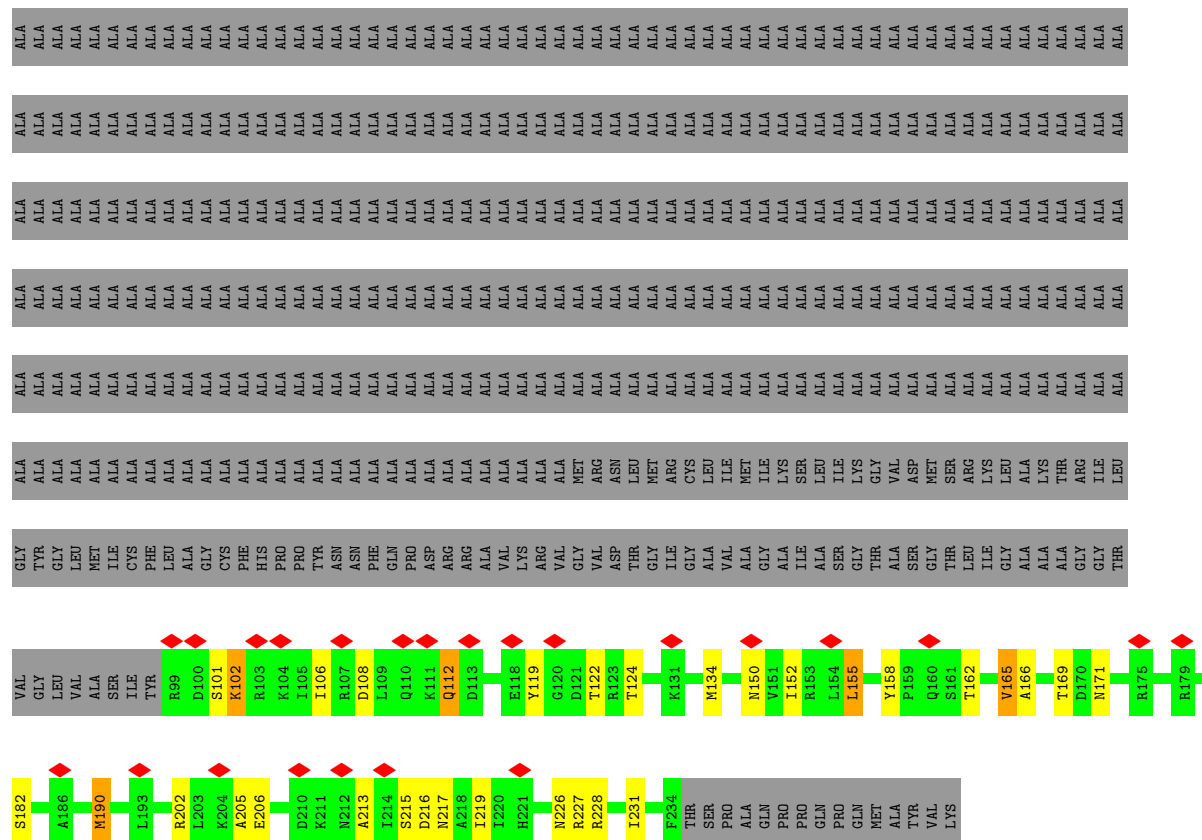




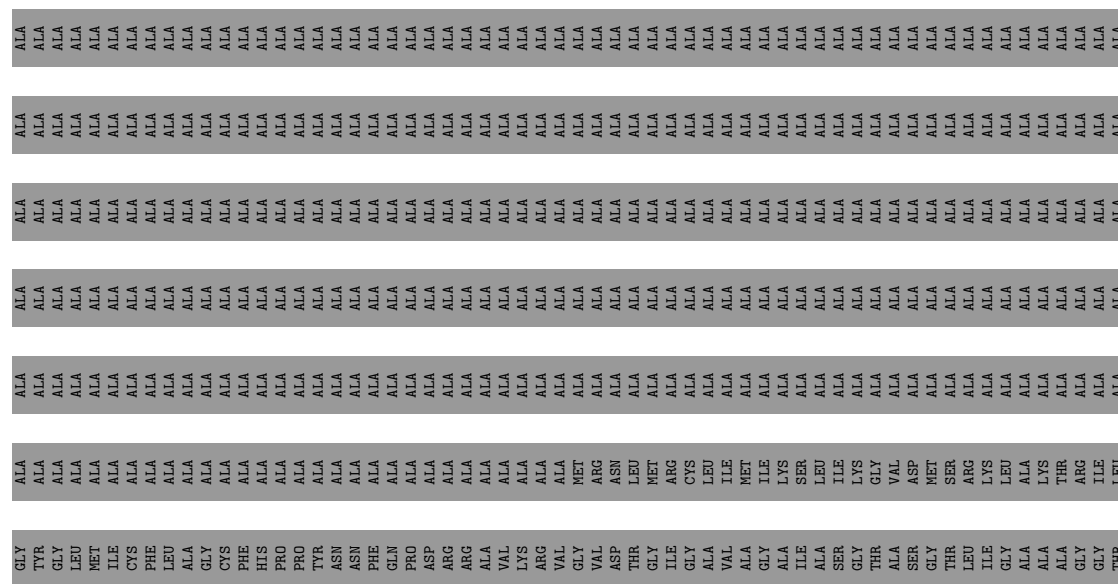
● Molecule 4: Type IV secretion system unknown protein fragment



Chain X: 18% 5% 77%

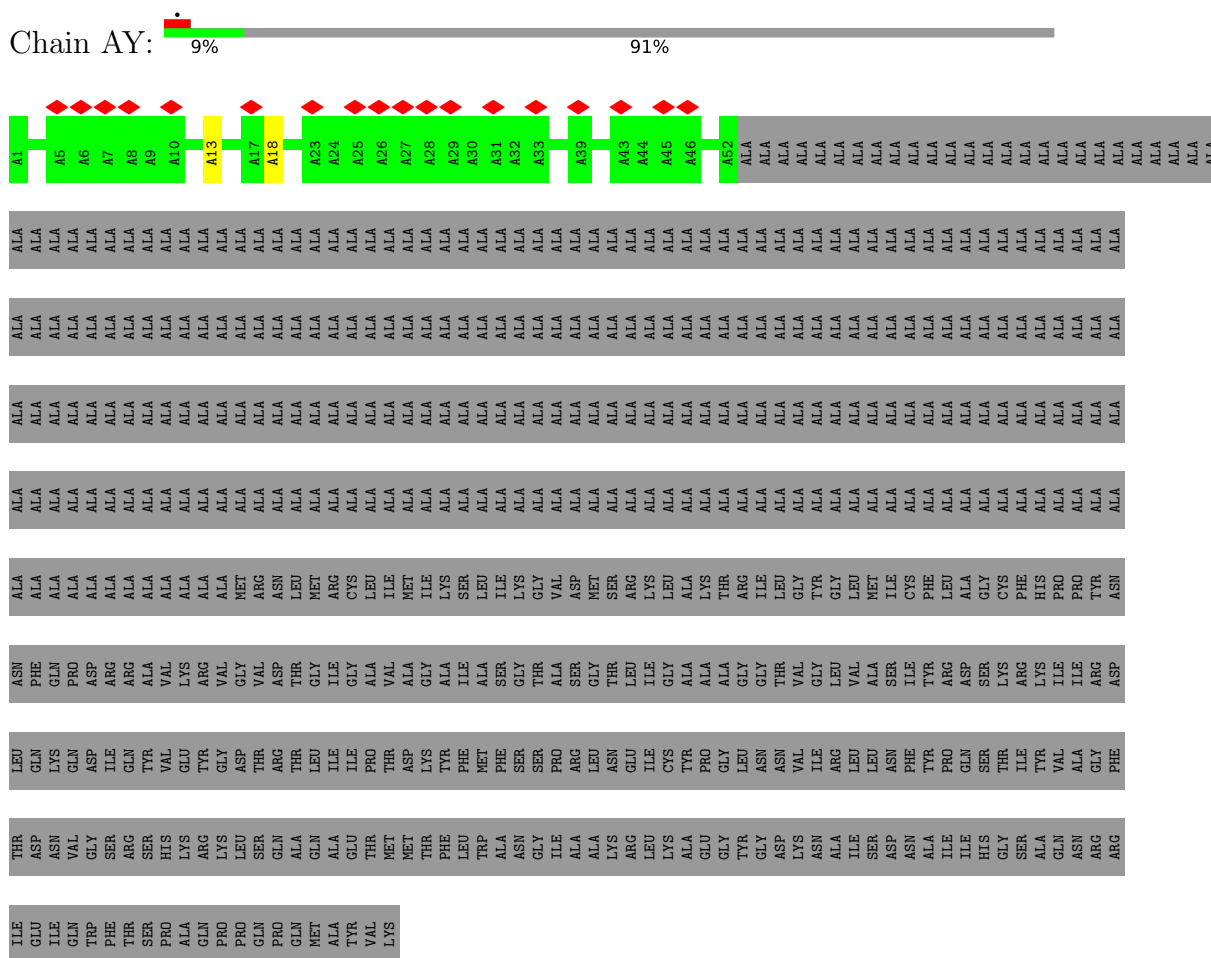


Chain Y: 18% 5% 77%

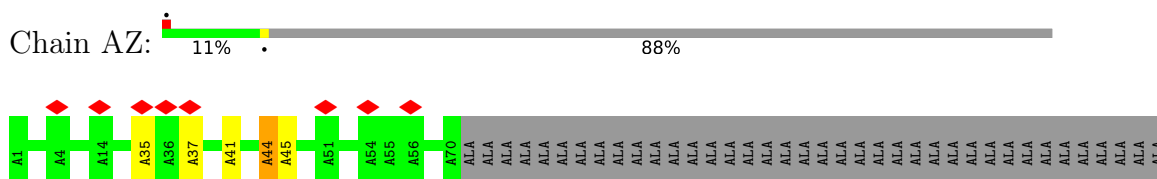


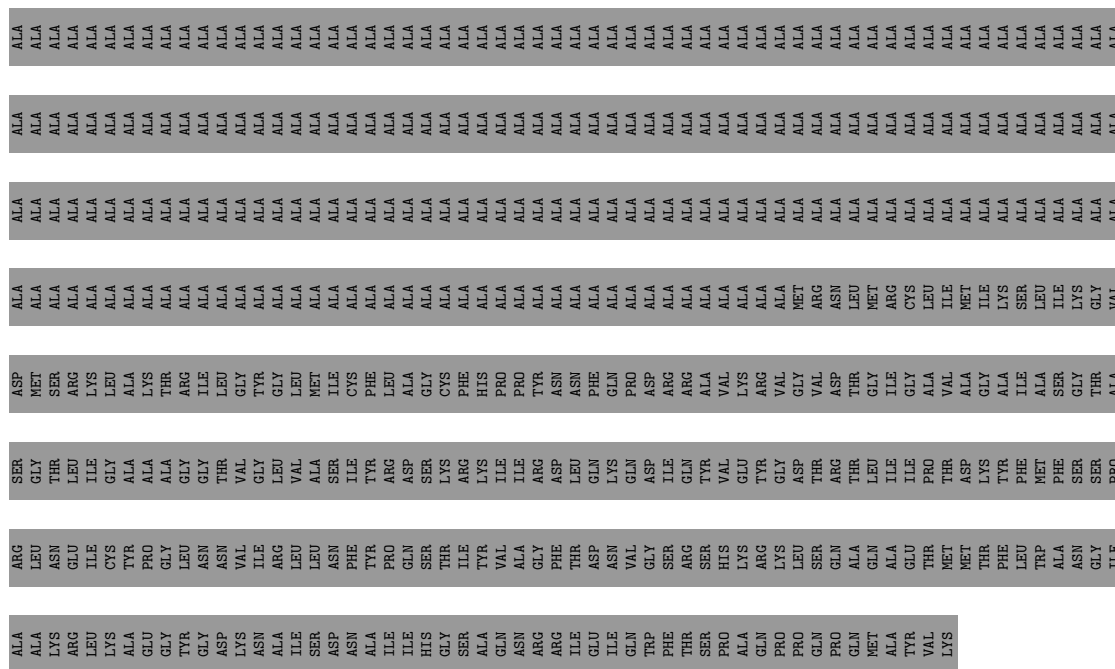


- Molecule 4: Type IV secretion system unknown protein fragment

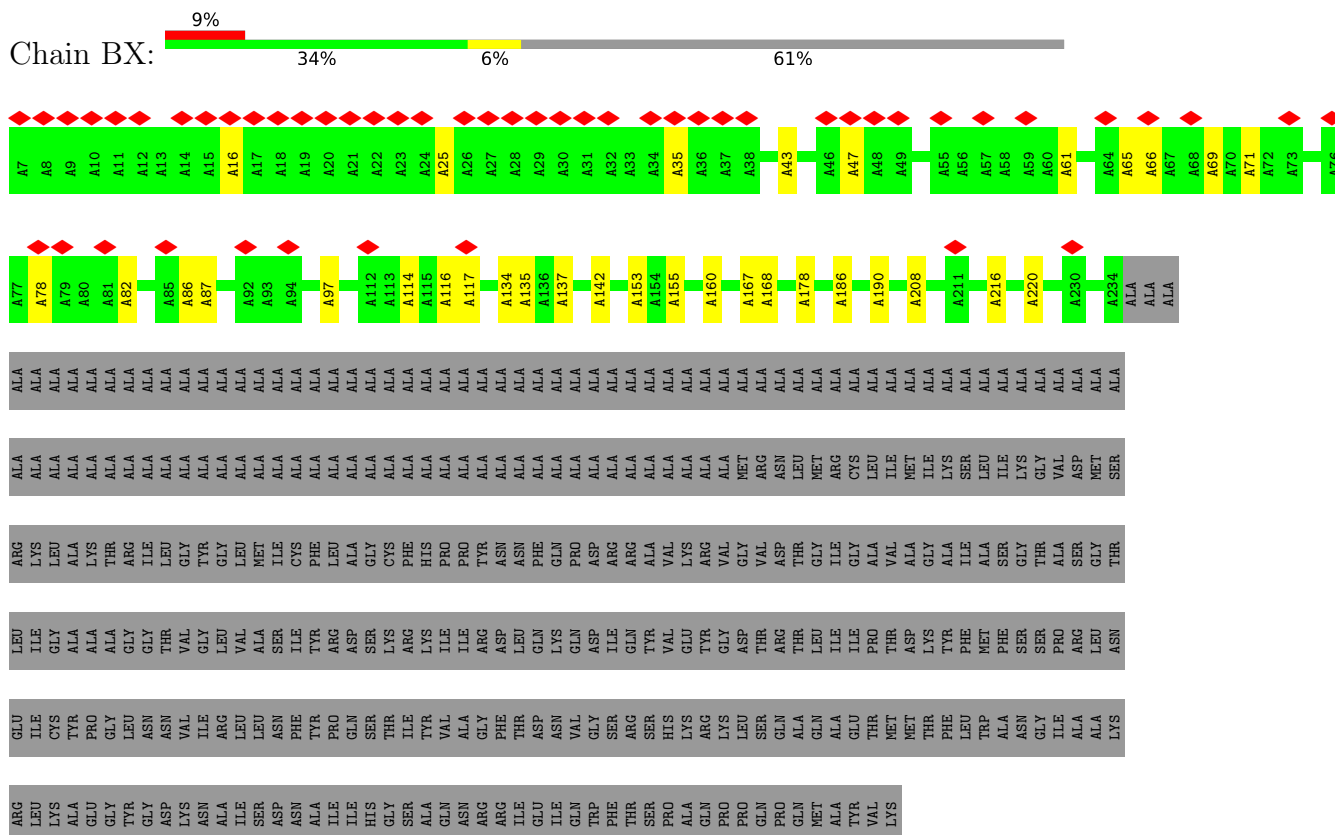


- Molecule 4: Type IV secretion system unknown protein fragment





- Molecule 4: Type IV secretion system unknown protein fragment

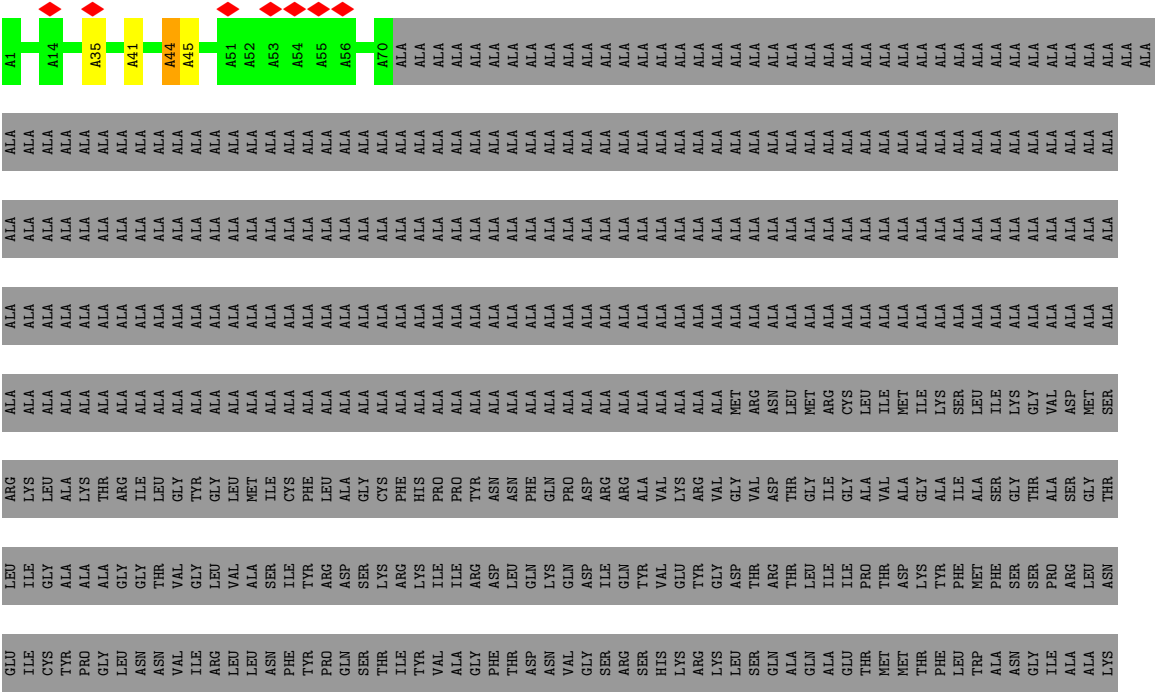


- Molecule 4: Type IV secretion system unknown protein fragment





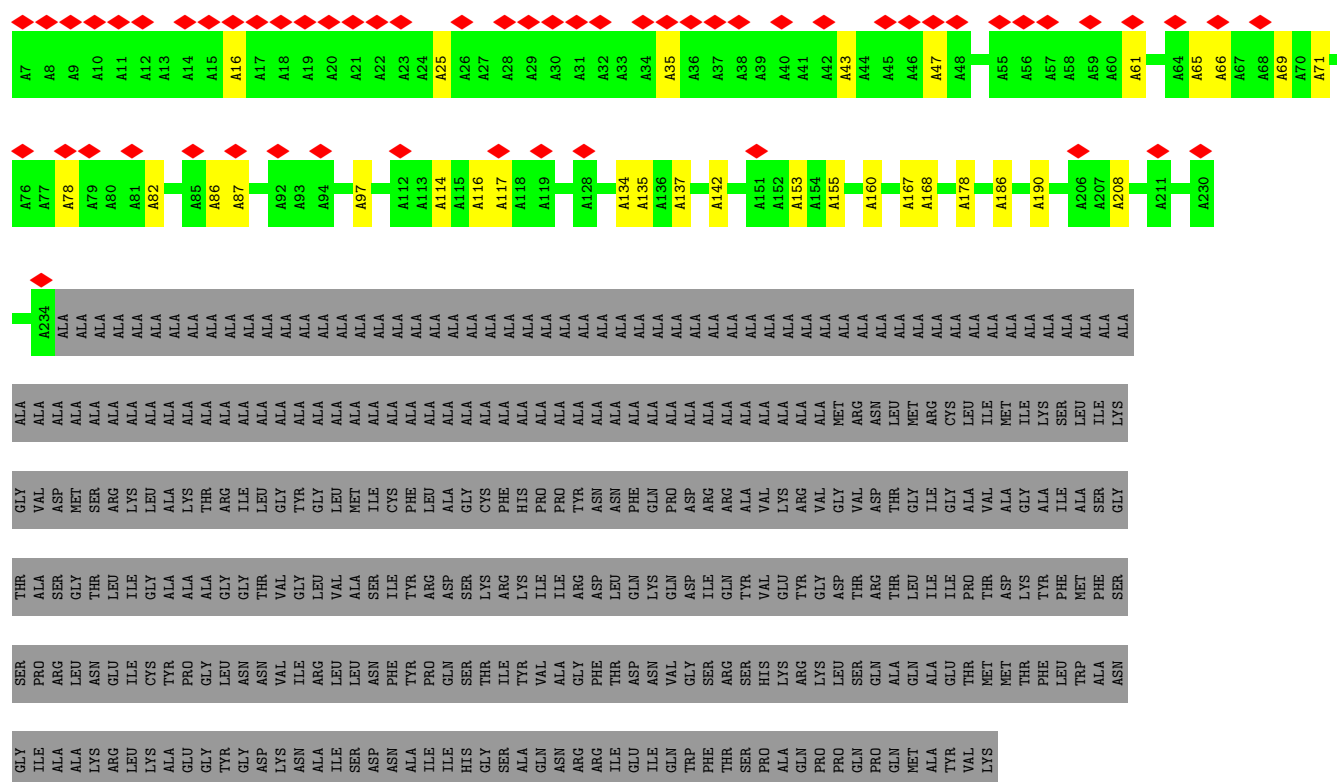
● Molecule 4: Type IV secretion system unknown protein fragment



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

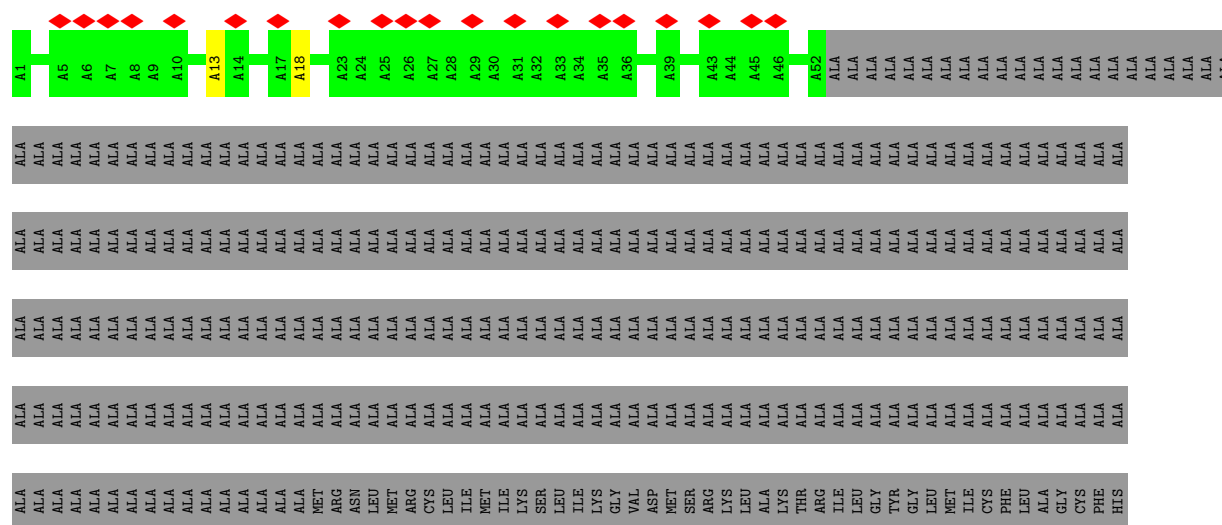
• Molecule 4: Type IV secretion system unknown protein fragment

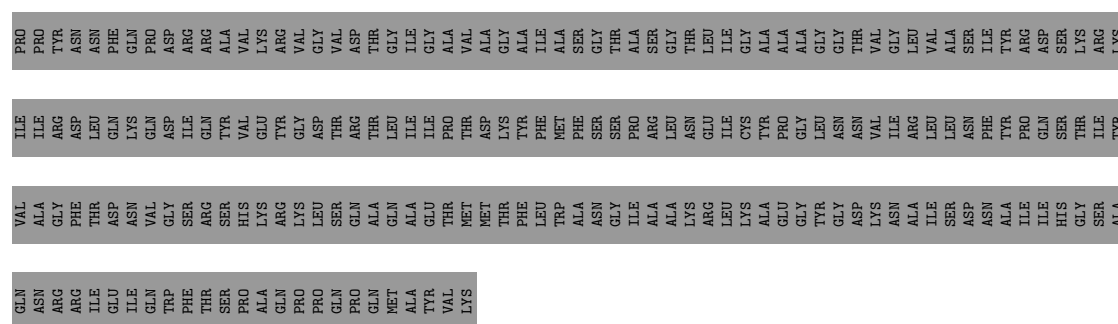
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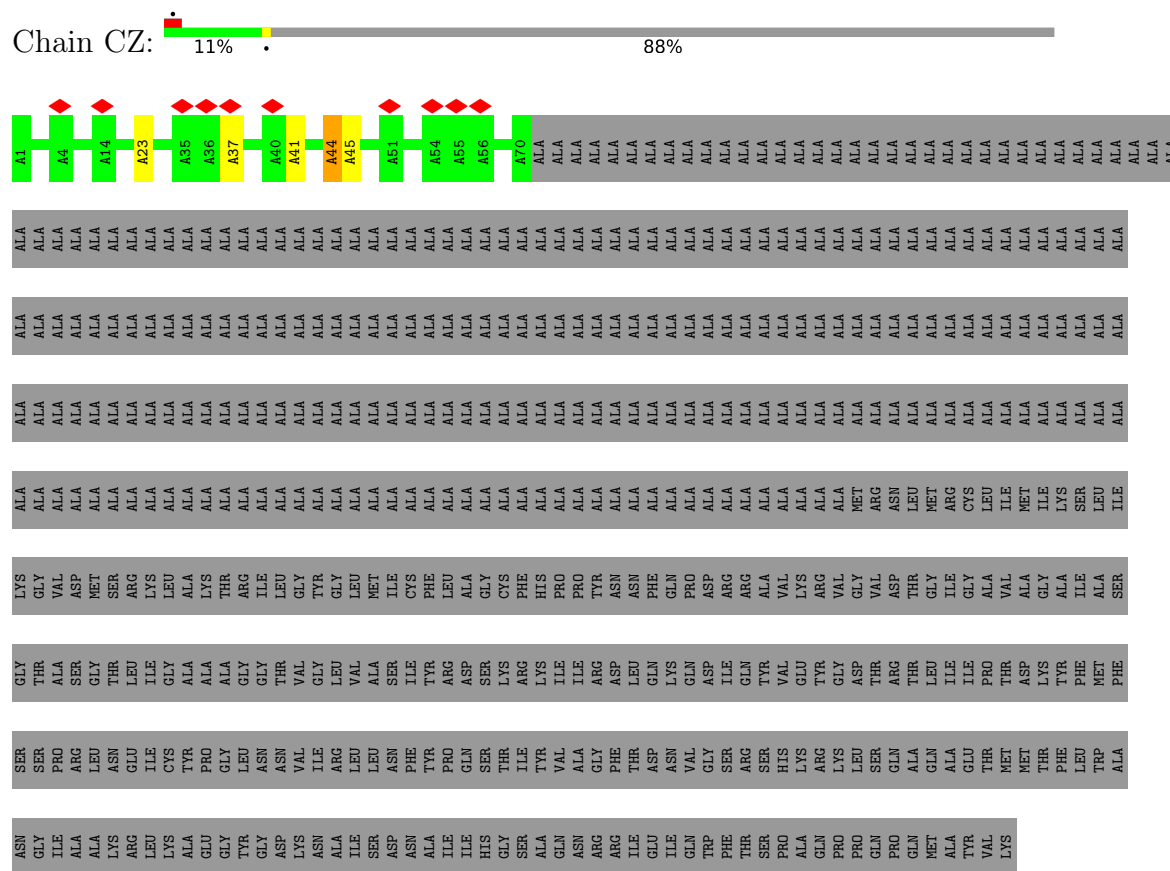
• Molecule 4: Type IV secretion system unknown protein fragment

Chain CY: 

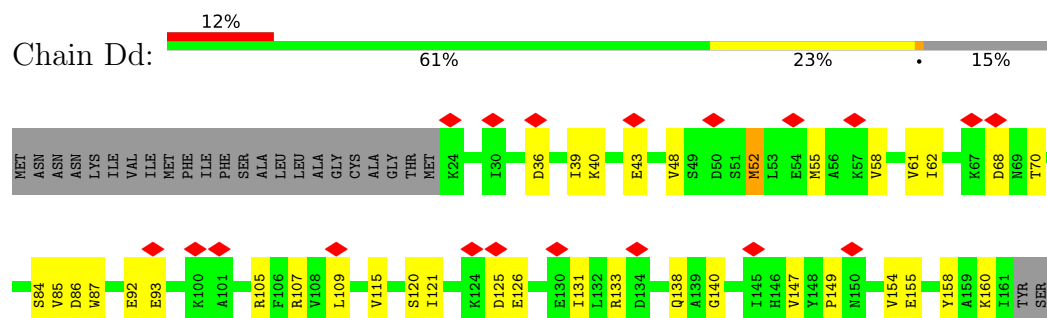




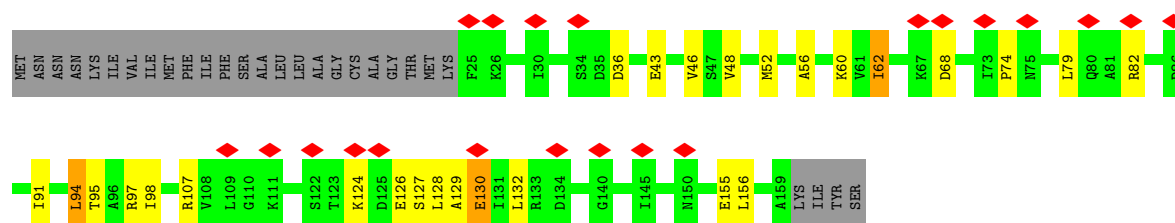
- Molecule 4: Type IV secretion system unknown protein fragment



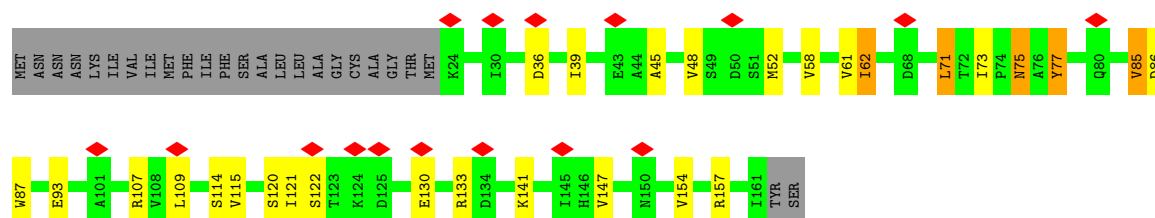
- Molecule 5: DotD



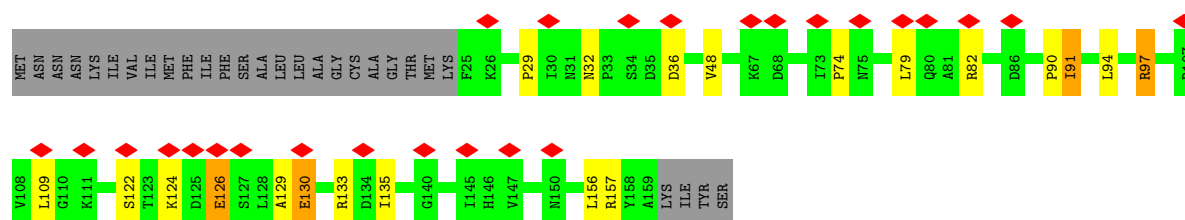
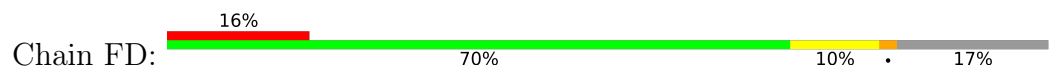
- Molecule 5: DotD



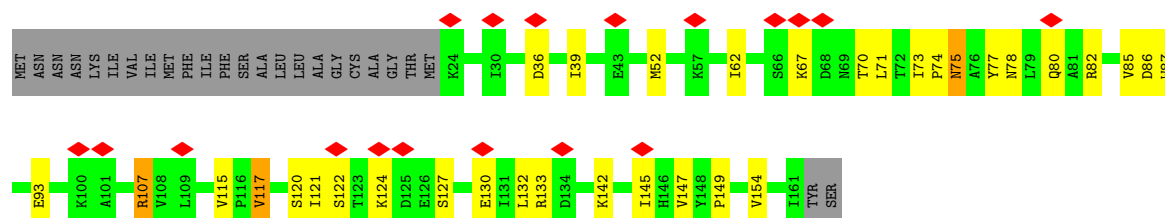
• Molecule 5: DotD



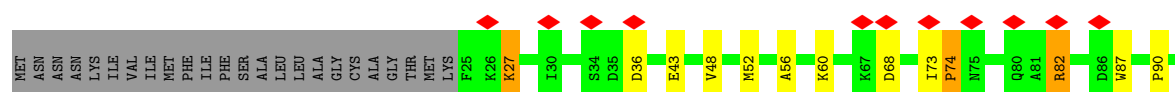
• Molecule 5: DotD

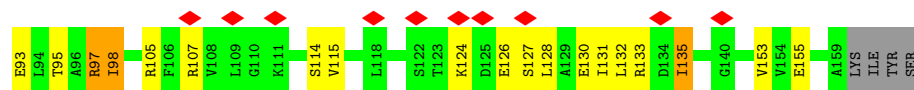


• Molecule 5: DotD

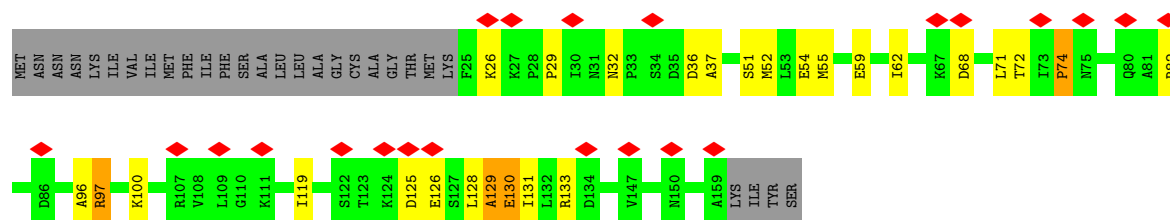


• Molecule 5: DotD

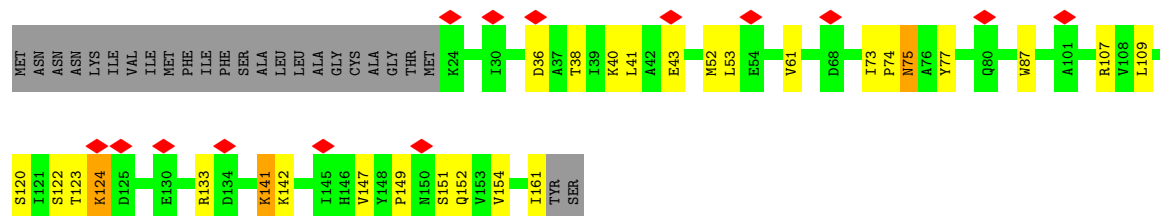




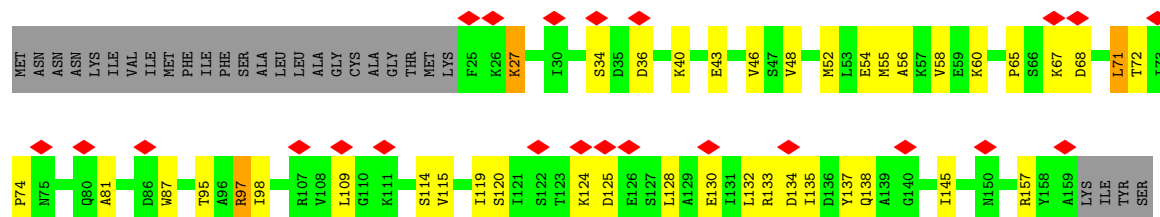
• Molecule 5: DotD



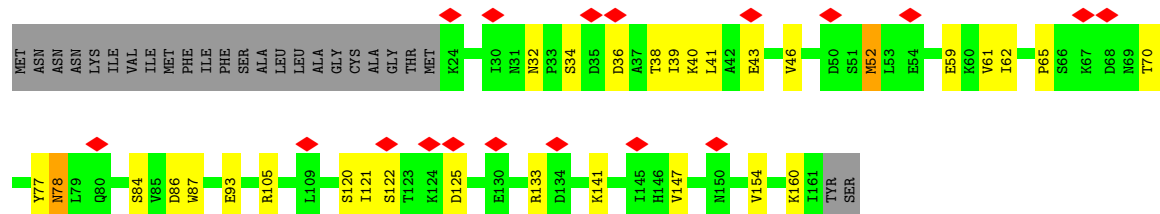
• Molecule 5: DotD



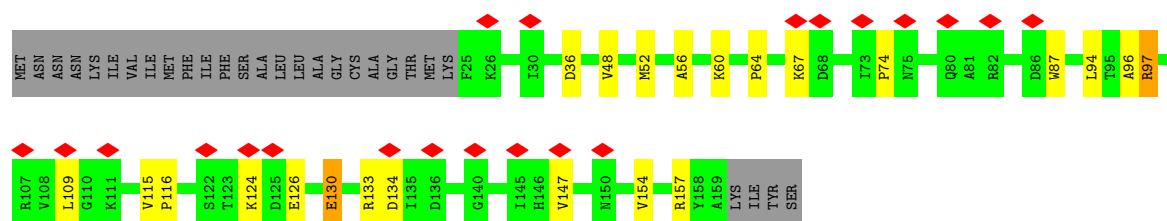
• Molecule 5: DotD



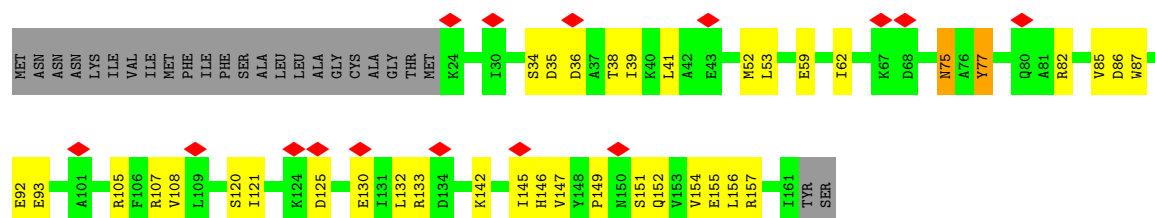
• Molecule 5: DotD



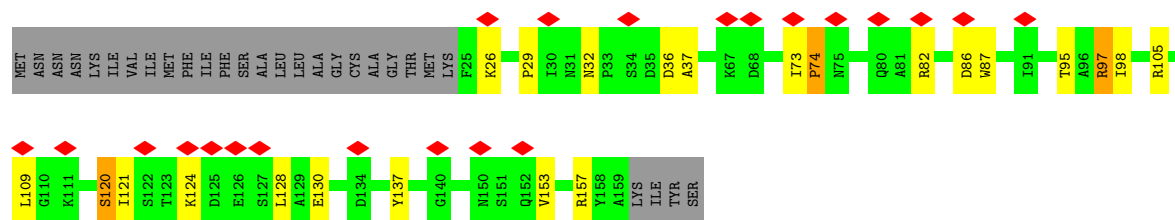
• Molecule 5: DotD



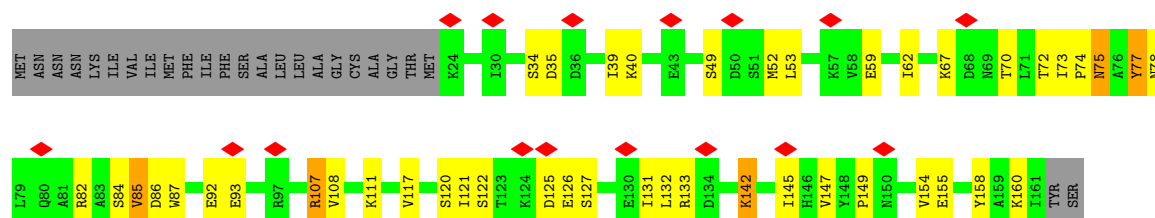
• Molecule 5: DotD



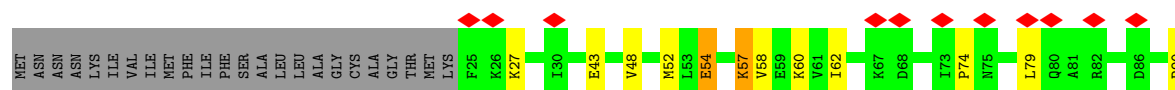
• Molecule 5: DotD

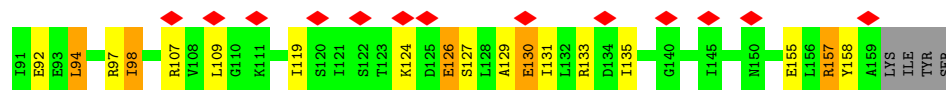


• Molecule 5: DotD

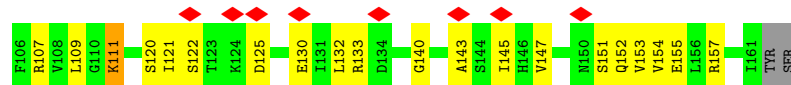
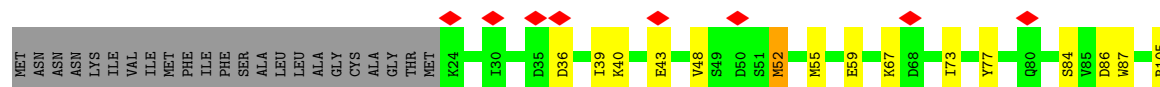


• Molecule 5: DotD

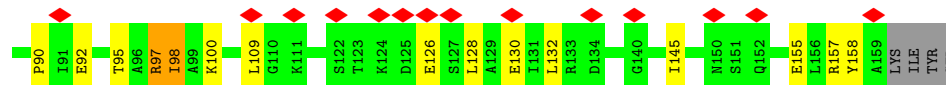
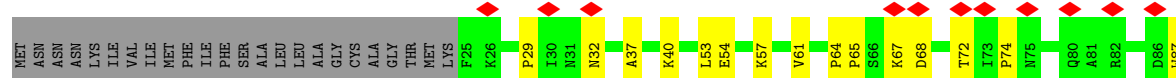




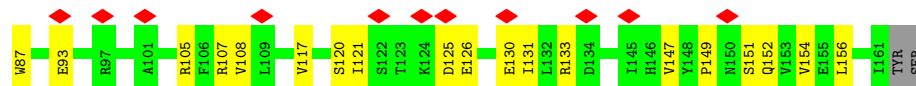
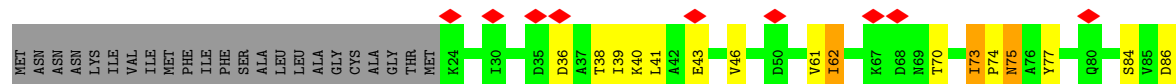
• Molecule 5: DotD



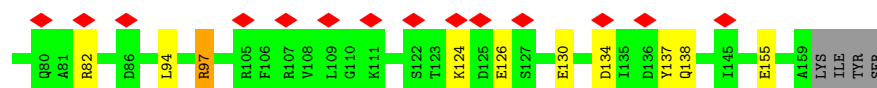
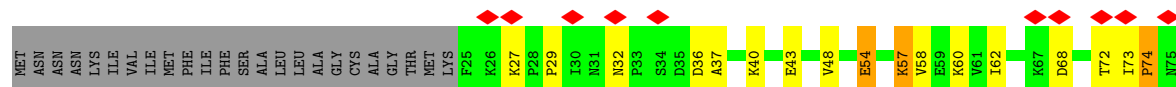
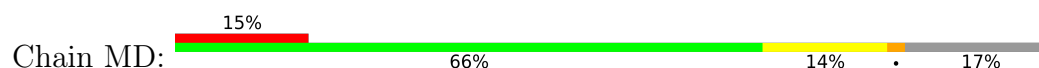
• Molecule 5: DotD



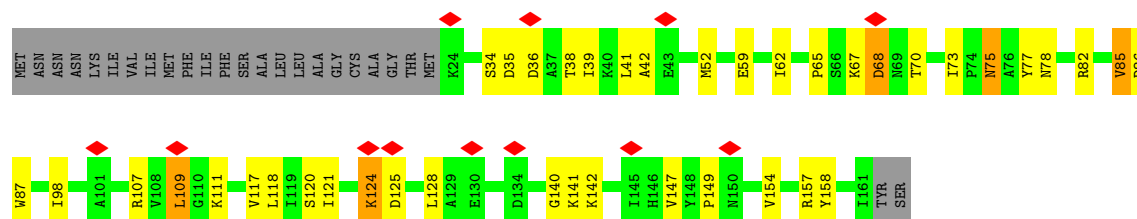
• Molecule 5: DotD



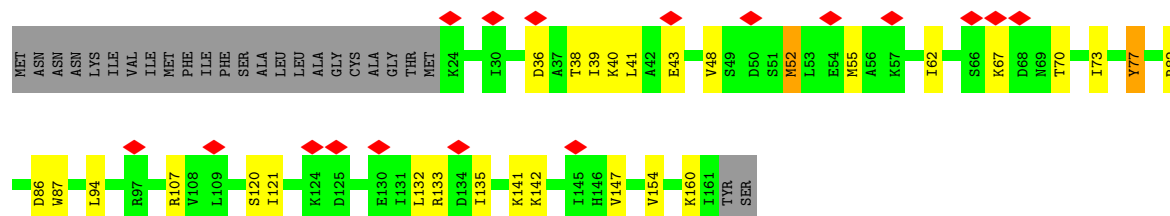
• Molecule 5: DotD



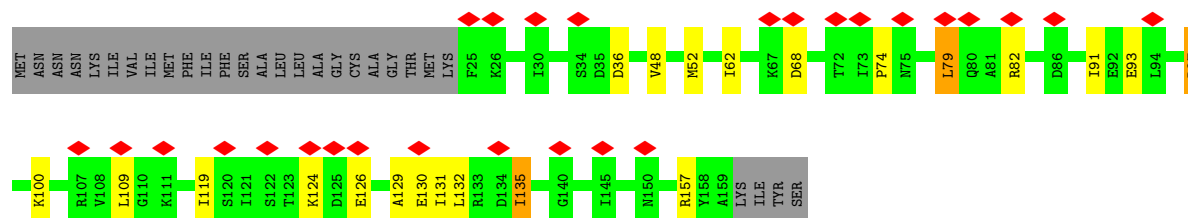
• Molecule 5: DotD



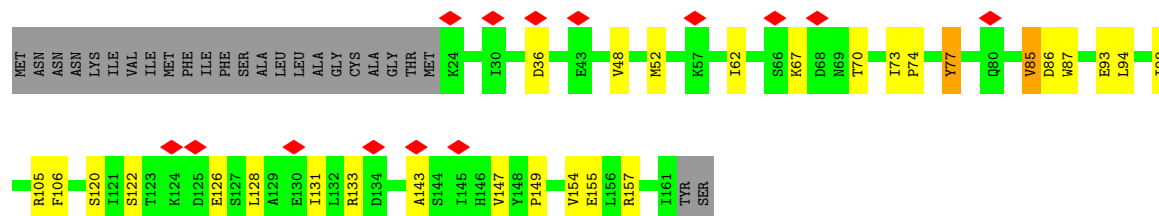
• Molecule 5: DotD



• Molecule 5: DotD

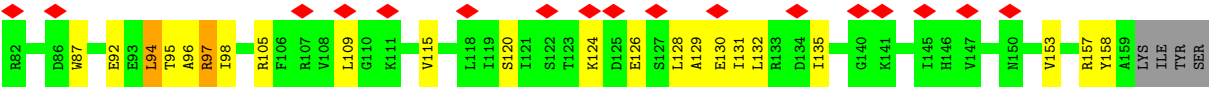


• Molecule 5: DotD



• Molecule 5: DotD

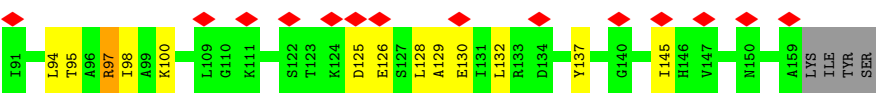
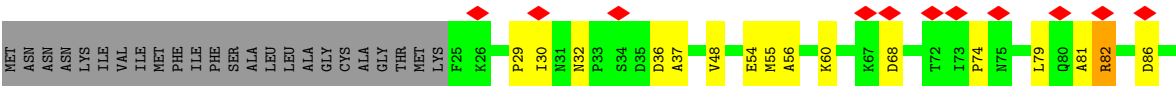




• Molecule 5: DotD



• Molecule 5: DotD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C13	Depositor
Number of particles used	12200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.136	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	836.39996, 836.39996, 836.39996	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	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	AC	0.64	0/1629	1.14	10/2214 (0.5%)
1	BC	0.64	0/1629	1.14	10/2214 (0.5%)
1	CC	0.64	0/1629	1.14	10/2214 (0.5%)
1	DC	0.64	0/1629	1.14	10/2214 (0.5%)
1	EC	0.64	0/1629	1.14	10/2214 (0.5%)
1	FC	0.64	0/1629	1.14	10/2214 (0.5%)
1	GC	0.64	0/1629	1.14	10/2214 (0.5%)
1	HC	0.64	0/1629	1.14	10/2214 (0.5%)
1	IC	0.64	0/1629	1.14	10/2214 (0.5%)
1	JC	0.64	0/1629	1.14	10/2214 (0.5%)
1	KC	0.64	0/1629	1.14	10/2214 (0.5%)
1	LC	0.64	0/1629	1.14	10/2214 (0.5%)
1	MC	0.64	0/1629	1.14	10/2214 (0.5%)
2	AH	0.66	0/695	1.13	4/947 (0.4%)
2	BH	0.66	0/695	1.13	4/947 (0.4%)
2	CH	0.66	0/695	1.13	4/947 (0.4%)
2	DH	0.66	0/695	1.13	4/947 (0.4%)
2	EH	0.66	0/695	1.13	4/947 (0.4%)
2	FH	0.66	0/695	1.13	4/947 (0.4%)
2	GH	0.66	0/695	1.13	4/947 (0.4%)
2	HH	0.66	0/695	1.13	4/947 (0.4%)
2	IH	0.66	0/695	1.13	4/947 (0.4%)
2	JH	0.66	0/695	1.13	4/947 (0.4%)
2	KH	0.66	0/695	1.13	4/947 (0.4%)
2	LH	0.66	0/695	1.13	4/947 (0.4%)
2	MH	0.66	0/695	1.13	4/947 (0.4%)
3	AK	0.62	0/1171	1.11	8/1583 (0.5%)
3	BK	0.63	0/1171	1.11	8/1583 (0.5%)
3	CK	0.62	0/1171	1.11	8/1583 (0.5%)
3	DK	0.62	0/1171	1.11	8/1583 (0.5%)
3	EK	0.63	0/1171	1.11	8/1583 (0.5%)
3	FK	0.62	0/1171	1.11	8/1583 (0.5%)
3	GK	0.63	0/1171	1.11	8/1583 (0.5%)
3	HK	0.63	0/1171	1.11	8/1583 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	IK	0.63	0/1171	1.11	8/1583 (0.5%)
3	JK	0.62	0/1171	1.11	8/1583 (0.5%)
3	KK	0.63	0/1171	1.11	8/1583 (0.5%)
3	LK	0.63	0/1171	1.11	8/1583 (0.5%)
3	MK	0.62	0/1171	1.11	8/1583 (0.5%)
4	AX	0.28	0/1139	0.67	2/1593 (0.1%)
4	AY	0.25	0/259	0.70	0/361
4	AZ	0.31	0/349	0.81	2/487 (0.4%)
4	BX	0.28	0/1139	0.65	0/1593
4	BY	0.25	0/259	0.70	0/361
4	BZ	0.31	0/349	0.82	2/487 (0.4%)
4	CX	0.28	0/1139	0.65	0/1593
4	CY	0.25	0/259	0.70	0/361
4	CZ	0.32	0/349	0.82	2/487 (0.4%)
4	DX	0.28	0/1139	0.67	2/1593 (0.1%)
4	DY	0.25	0/259	0.70	0/361
4	DZ	0.32	0/349	0.81	2/487 (0.4%)
4	EX	0.28	0/1139	0.65	0/1593
4	EY	0.25	0/259	0.70	0/361
4	EZ	0.31	0/349	0.82	2/487 (0.4%)
4	FX	0.28	0/1139	0.65	0/1593
4	FY	0.25	0/259	0.70	0/361
4	FZ	0.32	0/349	0.82	2/487 (0.4%)
4	GX	0.28	0/1139	0.65	0/1593
4	GY	0.25	0/259	0.71	0/361
4	GZ	0.31	0/349	0.81	2/487 (0.4%)
4	HX	0.28	0/1139	0.65	0/1593
4	HY	0.26	0/259	0.70	0/361
4	HZ	0.31	0/349	0.82	2/487 (0.4%)
4	IX	0.28	0/1139	0.65	0/1593
4	IY	0.25	0/259	0.71	0/361
4	IZ	0.31	0/349	0.82	2/487 (0.4%)
4	JX	0.28	0/1139	0.67	2/1593 (0.1%)
4	JY	0.25	0/259	0.70	0/361
4	JZ	0.31	0/349	0.82	2/487 (0.4%)
4	KX	0.28	0/1139	0.67	2/1593 (0.1%)
4	KY	0.25	0/259	0.71	0/361
4	KZ	0.32	0/349	0.82	2/487 (0.4%)
4	LX	0.28	0/1139	0.67	2/1593 (0.1%)
4	LY	0.26	0/259	0.71	0/361
4	LZ	0.31	0/349	0.82	2/487 (0.4%)
4	MX	0.28	0/1139	0.67	2/1593 (0.1%)
4	MY	0.26	0/259	0.70	0/361

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	MZ	0.31	0/349	0.82	2/487 (0.4%)
4	N	0.54	0/1130	1.08	3/1522 (0.2%)
4	O	0.54	0/1130	1.08	3/1522 (0.2%)
4	P	0.54	0/1130	1.08	3/1522 (0.2%)
4	Q	0.54	0/1130	1.08	3/1522 (0.2%)
4	R	0.54	0/1130	1.08	3/1522 (0.2%)
4	S	0.54	0/1130	1.08	3/1522 (0.2%)
4	T	0.54	0/1130	1.07	3/1522 (0.2%)
4	U	0.54	0/1130	1.08	3/1522 (0.2%)
4	V	0.54	0/1130	1.07	3/1522 (0.2%)
4	W	0.54	0/1130	1.07	3/1522 (0.2%)
4	X	0.54	0/1130	1.07	3/1522 (0.2%)
4	Y	0.54	0/1130	1.08	3/1522 (0.2%)
4	Z	0.54	0/1130	1.08	3/1522 (0.2%)
5	AD	0.94	5/1060 (0.5%)	1.44	23/1441 (1.6%)
5	Ad	0.84	2/1086 (0.2%)	1.20	7/1474 (0.5%)
5	BD	0.76	2/1060 (0.2%)	1.29	9/1441 (0.6%)
5	Bd	0.70	0/1086	1.14	5/1474 (0.3%)
5	CD	0.81	2/1060 (0.2%)	1.28	14/1441 (1.0%)
5	Cd	0.74	3/1086 (0.3%)	1.16	7/1474 (0.5%)
5	DD	0.93	5/1060 (0.5%)	1.40	14/1441 (1.0%)
5	Dd	0.79	0/1086	1.23	6/1474 (0.4%)
5	ED	0.75	1/1060 (0.1%)	1.24	10/1441 (0.7%)
5	Ed	0.69	1/1086 (0.1%)	1.12	5/1474 (0.3%)
5	FD	0.98	7/1060 (0.7%)	1.35	16/1441 (1.1%)
5	Fd	0.70	0/1086	1.10	6/1474 (0.4%)
5	GD	0.86	1/1060 (0.1%)	1.41	17/1441 (1.2%)
5	Gd	0.71	0/1086	1.22	7/1474 (0.5%)
5	HD	0.77	1/1060 (0.1%)	1.46	19/1441 (1.3%)
5	Hd	0.70	1/1086 (0.1%)	1.16	3/1474 (0.2%)
5	ID	0.78	0/1060	1.22	8/1441 (0.6%)
5	Id	0.70	0/1086	1.12	5/1474 (0.3%)
5	JD	0.82	3/1060 (0.3%)	1.32	10/1441 (0.7%)
5	Jd	0.82	2/1086 (0.2%)	1.28	13/1474 (0.9%)
5	KD	0.93	4/1060 (0.4%)	1.50	19/1441 (1.3%)
5	Kd	0.77	1/1086 (0.1%)	1.14	5/1474 (0.3%)
5	LD	0.86	3/1060 (0.3%)	1.26	13/1441 (0.9%)
5	Ld	0.67	0/1086	1.11	5/1474 (0.3%)
5	MD	0.93	2/1060 (0.2%)	1.56	17/1441 (1.2%)
5	Md	0.87	4/1086 (0.4%)	1.35	9/1474 (0.6%)
All	All	0.62	50/110734 (0.0%)	1.09	635/151086 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	AX	0	2
4	AZ	0	1
4	BX	0	2
4	BZ	0	1
4	CX	0	2
4	CZ	0	1
4	DX	0	2
4	DZ	0	1
4	EX	0	2
4	EZ	0	1
4	FX	0	2
4	FZ	0	1
4	GX	0	2
4	GZ	0	1
4	HX	0	2
4	HZ	0	1
4	IX	0	2
4	IZ	0	1
4	JX	0	2
4	JZ	0	1
4	KX	0	2
4	KZ	0	1
4	LX	0	2
4	LZ	0	1
4	MX	0	2
4	MZ	0	1
4	N	0	1
4	O	0	1
4	P	0	1
4	Q	0	1
4	R	0	1
4	S	0	1
4	T	0	1
4	U	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
5	AD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	BD	0	1
5	Bd	0	1
5	CD	0	2
5	DD	0	2
5	Dd	0	1
5	ED	0	3
5	Ed	0	2
5	FD	0	2
5	Fd	0	1
5	GD	0	3
5	HD	0	2
5	ID	0	3
5	Id	0	1
5	JD	0	1
5	Jd	0	1
5	KD	0	3
5	LD	0	2
5	Ld	0	1
5	MD	0	3
5	Md	0	2
All	All	0	90

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Ad	52	MET	SD-CE	-9.22	1.56	1.79
5	FD	135	ILE	CG1-CD1	-9.10	1.16	1.51
5	DD	97	ARG	CZ-NH2	-8.92	1.21	1.33
5	AD	26	LYS	CE-NZ	-8.75	1.23	1.49
5	Md	111	LYS	C-N	-8.47	1.21	1.33
5	MD	97	ARG	CZ-NH2	-8.05	1.23	1.33
5	FD	97	ARG	CZ-NH2	-8.01	1.23	1.33
5	FD	130	GLU	CB-CG	-7.97	1.28	1.52
5	Jd	111	LYS	CD-CE	-7.59	1.29	1.52
5	AD	119	ILE	CG1-CD1	-7.34	1.23	1.51
5	AD	97	ARG	CZ-NH2	-7.31	1.24	1.33
5	CD	97	ARG	CG-CD	-7.31	1.30	1.52
5	JD	26	LYS	CD-CE	-7.15	1.30	1.52
5	KD	27	LYS	CD-CE	-7.13	1.31	1.52
5	DD	97	ARG	CG-CD	-6.89	1.31	1.52
5	JD	26	LYS	CG-CD	-6.78	1.32	1.52
5	Md	109	LEU	CG-CD2	-6.62	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	KD	97	ARG	CG-CD	-6.52	1.32	1.52
5	Jd	111	LYS	CB-CG	-6.42	1.33	1.52
5	DD	97	ARG	CD-NE	-6.37	1.37	1.46
5	Md	124	LYS	CD-CE	-6.35	1.33	1.52
5	Cd	111	LYS	C-N	-6.30	1.23	1.33
5	FD	130	GLU	CG-CD	-6.18	1.36	1.52
5	JD	97	ARG	CZ-NH2	-6.10	1.25	1.33
5	KD	130	GLU	CG-CD	-5.96	1.37	1.52
5	BD	97	ARG	CG-CD	-5.85	1.34	1.52
5	LD	97	ARG	CZ-NH2	-5.79	1.25	1.33
5	GD	27	LYS	CB-CG	5.74	1.69	1.52
5	AD	26	LYS	CG-CD	-5.70	1.35	1.52
5	MD	97	ARG	CD-NE	-5.66	1.38	1.46
5	DD	97	ARG	CB-CG	-5.66	1.35	1.52
5	LD	98	ILE	CG1-CD1	-5.65	1.29	1.51
5	KD	27	LYS	CG-CD	-5.65	1.35	1.52
5	AD	52	MET	SD-CE	-5.64	1.65	1.79
5	HD	97	ARG	CZ-NH2	-5.62	1.26	1.33
5	FD	97	ARG	CD-NE	-5.61	1.38	1.46
5	CD	30	ILE	CG1-CD1	-5.59	1.29	1.51
5	Cd	62	ILE	CG1-CD1	-5.57	1.30	1.51
5	FD	97	ARG	CG-CD	-5.46	1.36	1.52
5	Hd	52	MET	CB-CG	-5.45	1.36	1.52
5	ED	62	ILE	CG1-CD1	-5.36	1.30	1.51
5	LD	97	ARG	CG-CD	-5.36	1.36	1.52
5	Ad	52	MET	CB-CG	-5.23	1.36	1.52
5	FD	126	GLU	CG-CD	-5.20	1.39	1.52
5	Cd	52	MET	CB-CG	-5.20	1.36	1.52
5	Ed	107	ARG	CG-CD	-5.14	1.37	1.52
5	DD	30	ILE	CG1-CD1	-5.08	1.31	1.51
5	Md	141	LYS	CG-CD	-5.06	1.37	1.52
5	BD	119	ILE	CG1-CD1	-5.04	1.32	1.51
5	Kd	155	GLU	CB-CG	-5.00	1.37	1.52

All (635) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	MD	57	LYS	CD-CE-NZ	-18.23	53.55	111.90
5	KD	27	LYS	CD-CE-NZ	-17.14	57.04	111.90
5	HD	27	LYS	CD-CE-NZ	16.62	165.09	111.90
5	JD	26	LYS	CD-CE-NZ	-15.91	61.00	111.90
5	DD	82	ARG	NE-CZ-NH1	-14.81	106.69	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	MD	27	LYS	CD-CE-NZ	-14.36	65.96	111.90
5	MD	97	ARG	NE-CZ-NH2	-14.11	106.50	119.20
5	DD	97	ARG	CA-CB-CG	-13.99	86.12	114.10
3	KK	101	GLU	CA-CB-CG	12.81	139.72	114.10
3	BK	101	GLU	CA-CB-CG	12.81	139.71	114.10
3	IK	101	GLU	CA-CB-CG	12.79	139.68	114.10
3	DK	101	GLU	CA-CB-CG	12.79	139.68	114.10
3	EK	101	GLU	CA-CB-CG	12.79	139.67	114.10
3	FK	101	GLU	CA-CB-CG	12.79	139.67	114.10
3	JK	101	GLU	CA-CB-CG	12.78	139.66	114.10
3	CK	101	GLU	CA-CB-CG	12.78	139.65	114.10
3	HK	101	GLU	CA-CB-CG	12.77	139.65	114.10
3	AK	101	GLU	CA-CB-CG	12.77	139.65	114.10
3	LK	101	GLU	CA-CB-CG	12.77	139.64	114.10
3	MK	101	GLU	CA-CB-CG	12.77	139.64	114.10
3	GK	101	GLU	CA-CB-CG	12.77	139.63	114.10
5	GD	135	ILE	CG1-CB-CG2	-12.65	72.73	110.70
5	AD	26	LYS	CD-CE-NZ	-12.01	73.48	111.90
5	Gd	124	LYS	CD-CE-NZ	-11.58	74.86	111.90
5	Md	124	LYS	CD-CE-NZ	-11.50	75.10	111.90
5	FD	97	ARG	CA-CB-CG	-11.36	91.39	114.10
5	HD	27	LYS	CG-CD-CE	-11.07	85.84	111.30
1	MC	61	GLU	CA-CB-CG	10.87	135.83	114.10
1	FC	61	GLU	CA-CB-CG	10.86	135.82	114.10
1	JC	61	GLU	CA-CB-CG	10.85	135.81	114.10
1	GC	61	GLU	CA-CB-CG	10.85	135.80	114.10
1	HC	61	GLU	CA-CB-CG	10.85	135.79	114.10
1	KC	61	GLU	CA-CB-CG	10.85	135.79	114.10
1	EC	61	GLU	CA-CB-CG	10.84	135.79	114.10
1	CC	61	GLU	CA-CB-CG	10.84	135.78	114.10
1	IC	61	GLU	CA-CB-CG	10.84	135.77	114.10
1	BC	61	GLU	CA-CB-CG	10.84	135.78	114.10
1	DC	61	GLU	CA-CB-CG	10.84	135.78	114.10
1	LC	61	GLU	CA-CB-CG	10.83	135.77	114.10
1	AC	61	GLU	CA-CB-CG	10.82	135.74	114.10
5	DD	82	ARG	NE-CZ-NH2	10.37	128.53	119.20
5	LD	97	ARG	CA-CB-CG	-10.25	93.60	114.10
5	JD	97	ARG	CA-CB-CG	-9.81	94.49	114.10
5	AD	52	MET	CA-CB-CG	9.69	133.49	114.10
5	MD	97	ARG	CA-CB-CG	-9.47	95.16	114.10
5	AD	130	GLU	CA-CB-CG	9.36	132.82	114.10
2	FH	294	ARG	CG-CD-NE	9.28	132.40	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	HH	294	ARG	CG-CD-NE	9.28	132.41	112.00
2	GH	294	ARG	CG-CD-NE	9.27	132.40	112.00
2	CH	294	ARG	CG-CD-NE	9.27	132.40	112.00
2	IH	294	ARG	CG-CD-NE	9.27	132.39	112.00
2	LH	294	ARG	CG-CD-NE	9.27	132.39	112.00
2	MH	294	ARG	CG-CD-NE	9.27	132.39	112.00
2	BH	294	ARG	CG-CD-NE	9.27	132.39	112.00
2	KH	294	ARG	CG-CD-NE	9.27	132.39	112.00
2	DH	294	ARG	CG-CD-NE	9.26	132.38	112.00
2	JH	294	ARG	CG-CD-NE	9.26	132.38	112.00
2	EH	294	ARG	CG-CD-NE	9.26	132.37	112.00
2	AH	294	ARG	CG-CD-NE	9.25	132.34	112.00
5	Jd	77	TYR	CA-C-N	9.11	142.18	126.32
5	Jd	77	TYR	C-N-CA	9.11	142.18	126.32
1	CC	61	GLU	CB-CG-CD	9.01	127.92	112.60
1	AC	61	GLU	CB-CG-CD	9.00	127.90	112.60
1	KC	61	GLU	CB-CG-CD	9.00	127.90	112.60
1	EC	61	GLU	CB-CG-CD	8.99	127.89	112.60
1	LC	61	GLU	CB-CG-CD	8.99	127.89	112.60
1	FC	61	GLU	CB-CG-CD	8.99	127.88	112.60
1	HC	61	GLU	CB-CG-CD	8.99	127.88	112.60
1	JC	61	GLU	CB-CG-CD	8.99	127.88	112.60
1	GC	61	GLU	CB-CG-CD	8.98	127.87	112.60
1	BC	61	GLU	CB-CG-CD	8.98	127.87	112.60
1	IC	61	GLU	CB-CG-CD	8.97	127.86	112.60
1	MC	61	GLU	CB-CG-CD	8.97	127.85	112.60
1	DC	61	GLU	CB-CG-CD	8.97	127.85	112.60
5	FD	135	ILE	CG1-CB-CG2	-8.78	84.36	110.70
1	HC	81	GLU	CA-CB-CG	8.75	131.59	114.10
1	IC	81	GLU	CA-CB-CG	8.75	131.59	114.10
1	CC	81	GLU	CA-CB-CG	8.74	131.59	114.10
1	AC	81	GLU	CA-CB-CG	8.74	131.57	114.10
1	EC	81	GLU	CA-CB-CG	8.73	131.56	114.10
1	GC	81	GLU	CA-CB-CG	8.73	131.56	114.10
1	LC	81	GLU	CA-CB-CG	8.73	131.55	114.10
1	DC	81	GLU	CA-CB-CG	8.72	131.55	114.10
1	JC	81	GLU	CA-CB-CG	8.72	131.54	114.10
1	KC	81	GLU	CA-CB-CG	8.72	131.53	114.10
1	BC	81	GLU	CA-CB-CG	8.72	131.54	114.10
1	FC	81	GLU	CA-CB-CG	8.70	131.50	114.10
1	MC	81	GLU	CA-CB-CG	8.70	131.50	114.10
5	Md	77	TYR	CA-C-N	8.65	141.66	125.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Md	77	TYR	C-N-CA	8.65	141.66	125.66
5	CD	68	ASP	CA-C-N	8.62	136.05	122.61
5	CD	68	ASP	C-N-CA	8.62	136.05	122.61
5	Md	109	LEU	CD1-CG-CD2	-8.59	91.90	110.80
5	KD	57	LYS	CB-CG-CD	8.59	131.05	111.30
5	HD	72	THR	CA-C-N	-8.57	116.42	122.59
5	HD	72	THR	C-N-CA	-8.57	116.42	122.59
5	FD	97	ARG	NE-CZ-NH2	-8.54	111.52	119.20
5	HD	52	MET	CA-CB-CG	8.22	130.55	114.10
5	HD	55	MET	CG-SD-CE	-8.22	82.81	100.90
5	FD	97	ARG	CG-CD-NE	8.22	130.07	112.00
5	Dd	160	LYS	CD-CE-NZ	-8.19	85.70	111.90
5	Ad	77	TYR	CA-C-N	8.18	140.55	126.32
5	Ad	77	TYR	C-N-CA	8.18	140.55	126.32
5	ED	97	ARG	CA-CB-CG	-8.10	97.90	114.10
5	Ld	77	TYR	CA-C-N	8.08	140.38	126.32
5	Ld	77	TYR	C-N-CA	8.08	140.38	126.32
5	GD	68	ASP	CA-C-N	8.08	135.21	122.61
5	GD	68	ASP	C-N-CA	8.08	135.21	122.61
5	Kd	77	TYR	CA-C-N	8.07	140.35	126.32
5	Kd	77	TYR	C-N-CA	8.07	140.35	126.32
5	CD	97	ARG	CA-CB-CG	-8.06	97.99	114.10
5	Hd	52	MET	CG-SD-CE	-8.04	83.21	100.90
5	BD	100	LYS	CD-CE-NZ	-8.00	86.30	111.90
5	Dd	77	TYR	CA-C-N	7.95	140.16	126.32
5	Dd	77	TYR	C-N-CA	7.95	140.16	126.32
5	BD	131	ILE	CA-CB-CG1	7.94	123.90	110.40
5	LD	97	ARG	NE-CZ-NH2	-7.92	112.07	119.20
5	DD	97	ARG	NE-CZ-NH2	-7.81	112.17	119.20
5	Ad	55	MET	CG-SD-CE	-7.67	84.04	100.90
5	Bd	77	TYR	CA-C-N	7.65	139.63	126.32
5	Bd	77	TYR	C-N-CA	7.65	139.63	126.32
5	GD	98	ILE	CG1-CB-CG2	-7.62	87.83	110.70
5	AD	130	GLU	N-CA-CB	-7.61	98.77	110.42
5	Jd	142	LYS	N-CA-C	-7.61	104.61	114.04
5	Cd	160	LYS	CD-CE-NZ	-7.56	87.71	111.90
5	Ed	77	TYR	CA-C-N	7.39	139.18	126.32
5	Ed	77	TYR	C-N-CA	7.39	139.18	126.32
5	Hd	77	TYR	CA-C-N	7.32	139.05	126.32
5	Hd	77	TYR	C-N-CA	7.32	139.05	126.32
5	Jd	107	ARG	NE-CZ-NH1	-7.31	114.19	121.50
5	DD	82	ARG	CG-CD-NE	-7.29	95.97	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Dd	52	MET	CB-CA-C	-7.25	99.45	110.90
5	ID	52	MET	CA-CB-CG	7.22	128.55	114.10
5	JD	26	LYS	CA-CB-CG	7.22	128.54	114.10
5	HD	52	MET	CG-SD-CE	7.22	116.78	100.90
3	CK	101	GLU	N-CA-CB	7.21	122.53	110.41
3	GK	101	GLU	N-CA-CB	7.21	122.52	110.41
3	DK	101	GLU	N-CA-CB	7.20	122.51	110.41
3	FK	101	GLU	N-CA-CB	7.20	122.51	110.41
5	Gd	109	LEU	CB-CG-CD1	7.20	132.29	110.70
3	IK	101	GLU	N-CA-CB	7.20	122.50	110.41
5	Ld	107	ARG	CG-CD-NE	-7.20	96.16	112.00
3	JK	101	GLU	N-CA-CB	7.20	122.50	110.41
3	LK	101	GLU	N-CA-CB	7.19	122.49	110.41
3	EK	101	GLU	N-CA-CB	7.19	122.49	110.41
3	MK	101	GLU	N-CA-CB	7.19	122.49	110.41
3	AK	101	GLU	N-CA-CB	7.19	122.49	110.41
5	JD	26	LYS	CB-CA-C	-7.19	96.73	110.24
5	HD	114	SER	CA-C-N	-7.18	117.42	122.59
5	HD	114	SER	C-N-CA	-7.18	117.42	122.59
3	HK	101	GLU	N-CA-CB	7.17	122.46	110.41
5	Jd	107	ARG	CG-CD-NE	-7.17	96.22	112.00
3	KK	101	GLU	N-CA-CB	7.17	122.45	110.41
3	BK	101	GLU	N-CA-CB	7.16	122.45	110.41
5	Cd	52	MET	CG-SD-CE	-7.13	85.21	100.90
5	HD	97	ARG	CA-CB-CG	-7.10	99.90	114.10
5	GD	27	LYS	CD-CE-NZ	-7.08	89.23	111.90
5	MD	94	LEU	CB-CG-CD2	7.08	131.95	110.70
5	Id	77	TYR	CA-C-N	7.07	137.96	126.86
5	Id	77	TYR	C-N-CA	7.07	137.96	126.86
5	ED	68	ASP	CA-C-N	7.07	135.04	121.54
5	ED	68	ASP	C-N-CA	7.07	135.04	121.54
5	DD	74	PRO	CA-C-N	7.03	133.57	122.61
5	DD	74	PRO	C-N-CA	7.03	133.57	122.61
5	Jd	111	LYS	CB-CG-CD	-7.02	95.16	111.30
5	Kd	111	LYS	CA-C-N	7.01	130.19	120.65
5	Kd	111	LYS	C-N-CA	7.01	130.19	120.65
5	DD	82	ARG	CD-NE-CZ	7.00	134.20	124.40
1	FC	258	ASN	N-CA-C	-7.00	97.83	108.67
1	EC	258	ASN	N-CA-C	-6.98	97.85	108.67
1	BC	258	ASN	N-CA-C	-6.98	97.85	108.67
1	MC	258	ASN	N-CA-C	-6.98	97.85	108.67
1	LC	258	ASN	N-CA-C	-6.98	97.86	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CC	258	ASN	N-CA-C	-6.97	97.86	108.67
1	KC	258	ASN	N-CA-C	-6.97	97.86	108.67
1	JC	258	ASN	N-CA-C	-6.97	97.87	108.67
1	DC	258	ASN	N-CA-C	-6.97	97.87	108.67
1	GC	258	ASN	N-CA-C	-6.96	97.87	108.67
1	AC	258	ASN	N-CA-C	-6.96	97.88	108.67
1	HC	258	ASN	N-CA-C	-6.96	97.89	108.67
1	IC	258	ASN	N-CA-C	-6.95	97.90	108.67
5	AD	68	ASP	CA-C-N	6.93	134.77	121.54
5	AD	68	ASP	C-N-CA	6.93	134.77	121.54
5	Ad	94	LEU	CD1-CG-CD2	-6.93	95.56	110.80
1	GC	69	GLN	CB-CG-CD	6.90	124.33	112.60
1	HC	69	GLN	CB-CG-CD	6.90	124.33	112.60
1	BC	69	GLN	CB-CG-CD	6.90	124.33	112.60
1	LC	69	GLN	CB-CG-CD	6.90	124.33	112.60
1	EC	69	GLN	CB-CG-CD	6.89	124.32	112.60
5	KD	98	ILE	CG1-CB-CG2	-6.89	90.02	110.70
1	KC	69	GLN	CB-CG-CD	6.89	124.31	112.60
1	AC	69	GLN	CB-CG-CD	6.89	124.31	112.60
5	GD	52	MET	CG-SD-CE	6.88	116.04	100.90
1	CC	69	GLN	CB-CG-CD	6.88	124.30	112.60
5	GD	97	ARG	CA-CB-CG	-6.88	100.35	114.10
1	IC	69	GLN	CB-CG-CD	6.88	124.29	112.60
1	MC	69	GLN	CB-CG-CD	6.87	124.28	112.60
1	JC	69	GLN	CB-CG-CD	6.87	124.28	112.60
1	FC	69	GLN	CB-CG-CD	6.86	124.27	112.60
5	AD	96	ALA	CA-C-N	-6.86	111.22	122.54
5	AD	96	ALA	C-N-CA	-6.86	111.22	122.54
1	DC	69	GLN	CB-CG-CD	6.86	124.26	112.60
5	ED	94	LEU	CB-CG-CD2	6.86	131.28	110.70
5	Md	111	LYS	CA-C-N	6.85	129.92	120.39
5	Md	111	LYS	C-N-CA	6.85	129.92	120.39
5	Gd	77	TYR	CA-C-N	6.79	138.22	125.66
5	Gd	77	TYR	C-N-CA	6.79	138.22	125.66
5	GD	114	SER	CA-C-N	-6.74	117.74	122.59
5	GD	114	SER	C-N-CA	-6.74	117.74	122.59
5	LD	74	PRO	CA-C-N	6.70	134.34	121.54
5	LD	74	PRO	C-N-CA	6.70	134.34	121.54
5	ED	74	PRO	CA-C-N	6.68	134.30	121.54
5	ED	74	PRO	C-N-CA	6.68	134.30	121.54
5	ID	74	PRO	CA-C-N	6.66	133.00	122.61
5	ID	74	PRO	C-N-CA	6.66	133.00	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	JD	97	ARG	CG-CD-NE	6.66	126.65	112.00
5	Cd	73	ILE	N-CA-C	-6.66	101.56	108.15
5	KD	97	ARG	CA-CB-CG	-6.64	100.82	114.10
5	CD	94	LEU	CB-CG-CD2	6.63	130.58	110.70
5	KD	126	GLU	CG-CD-OE2	-6.61	103.20	118.40
5	ID	97	ARG	NE-CZ-NH2	6.58	125.12	119.20
5	CD	97	ARG	CG-CD-NE	6.55	126.41	112.00
5	Fd	77	TYR	CA-C-N	6.52	135.19	124.31
5	Fd	77	TYR	C-N-CA	6.52	135.19	124.31
5	CD	74	PRO	CA-C-N	6.51	133.98	121.54
5	CD	74	PRO	C-N-CA	6.51	133.98	121.54
2	AH	294	ARG	CD-NE-CZ	6.49	133.49	124.40
5	Ad	55	MET	CB-CG-SD	6.49	132.18	112.70
2	DH	294	ARG	CD-NE-CZ	6.49	133.49	124.40
2	EH	294	ARG	CD-NE-CZ	6.48	133.47	124.40
5	AD	52	MET	CB-CA-C	-6.48	99.98	110.74
5	KD	74	PRO	CA-C-N	6.48	133.92	121.54
5	KD	74	PRO	C-N-CA	6.48	133.92	121.54
2	HH	294	ARG	CD-NE-CZ	6.47	133.47	124.40
2	JH	294	ARG	CD-NE-CZ	6.47	133.46	124.40
2	GH	294	ARG	CD-NE-CZ	6.47	133.46	124.40
2	KH	294	ARG	CD-NE-CZ	6.47	133.46	124.40
5	ED	126	GLU	CB-CG-CD	6.46	123.58	112.60
2	IH	294	ARG	CD-NE-CZ	6.46	133.44	124.40
2	CH	294	ARG	CD-NE-CZ	6.46	133.44	124.40
2	FH	294	ARG	CD-NE-CZ	6.45	133.43	124.40
2	LH	294	ARG	CD-NE-CZ	6.45	133.43	124.40
2	BH	294	ARG	CD-NE-CZ	6.45	133.42	124.40
5	HD	74	PRO	CA-C-N	6.44	133.84	121.54
5	HD	74	PRO	C-N-CA	6.44	133.84	121.54
2	MH	294	ARG	CD-NE-CZ	6.44	133.42	124.40
5	FD	74	PRO	CA-C-N	6.43	132.64	122.61
5	FD	74	PRO	C-N-CA	6.43	132.64	122.61
5	BD	74	PRO	CA-C-N	6.42	133.79	121.54
5	BD	74	PRO	C-N-CA	6.42	133.79	121.54
5	Id	142	LYS	N-CA-C	-6.41	106.09	114.04
5	Dd	92	GLU	CB-CA-C	-6.38	100.01	110.85
5	Jd	67	LYS	CG-CD-CE	-6.37	96.65	111.30
5	DD	82	ARG	CA-CB-CG	6.34	126.78	114.10
5	ID	97	ARG	CA-CB-CG	-6.33	101.44	114.10
5	BD	135	ILE	CG1-CB-CG2	-6.33	91.72	110.70
5	Ad	142	LYS	N-CA-C	-6.32	106.11	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FD	135	ILE	N-CA-CB	6.30	120.03	110.58
5	Jd	107	ARG	NE-CZ-NH2	6.28	124.85	119.20
5	BD	52	MET	CA-CB-CG	6.26	126.62	114.10
5	Ed	71	LEU	CD1-CG-CD2	-6.25	97.04	110.80
3	HK	101	GLU	CB-CG-CD	6.25	123.22	112.60
5	Id	53	LEU	CB-CG-CD1	-6.25	91.96	110.70
3	LK	101	GLU	CB-CG-CD	6.24	123.20	112.60
3	MK	101	GLU	CB-CG-CD	6.23	123.20	112.60
3	GK	101	GLU	CB-CG-CD	6.22	123.18	112.60
3	JK	101	GLU	CB-CG-CD	6.22	123.18	112.60
3	AK	101	GLU	CB-CG-CD	6.22	123.18	112.60
3	EK	101	GLU	CB-CG-CD	6.22	123.18	112.60
3	CK	101	GLU	CB-CG-CD	6.22	123.17	112.60
3	FK	101	GLU	CB-CG-CD	6.22	123.17	112.60
5	MD	74	PRO	CA-C-N	6.22	132.31	122.61
5	MD	74	PRO	C-N-CA	6.22	132.31	122.61
3	BK	101	GLU	CB-CG-CD	6.21	123.16	112.60
3	IK	101	GLU	CB-CG-CD	6.21	123.16	112.60
3	DK	101	GLU	CB-CG-CD	6.21	123.16	112.60
5	FD	90	PRO	CA-C-N	6.21	129.28	120.53
5	FD	90	PRO	C-N-CA	6.21	129.28	120.53
3	KK	101	GLU	CB-CG-CD	6.21	123.15	112.60
5	AD	74	PRO	CA-C-N	6.20	132.28	122.61
5	AD	74	PRO	C-N-CA	6.20	132.28	122.61
5	AD	129	ALA	CA-C-N	6.20	134.43	122.53
5	AD	129	ALA	C-N-CA	6.20	134.43	122.53
2	LH	294	ARG	NE-CZ-NH2	6.19	124.77	119.20
5	GD	74	PRO	CA-C-N	6.18	133.35	121.54
5	GD	74	PRO	C-N-CA	6.18	133.35	121.54
2	MH	294	ARG	NE-CZ-NH2	6.17	124.76	119.20
5	HD	115	VAL	CB-CA-C	6.17	117.31	110.71
2	CH	294	ARG	NE-CZ-NH2	6.17	124.75	119.20
5	MD	72	THR	CA-C-N	-6.17	116.61	123.02
5	MD	72	THR	C-N-CA	-6.17	116.61	123.02
2	JH	294	ARG	NE-CZ-NH2	6.15	124.74	119.20
2	FH	294	ARG	NE-CZ-NH2	6.14	124.72	119.20
2	HH	294	ARG	NE-CZ-NH2	6.13	124.72	119.20
2	KH	294	ARG	NE-CZ-NH2	6.13	124.72	119.20
2	BH	294	ARG	NE-CZ-NH2	6.13	124.72	119.20
5	ID	96	ALA	CA-C-N	-6.12	110.67	122.06
5	ID	96	ALA	C-N-CA	-6.12	110.67	122.06
2	EH	294	ARG	NE-CZ-NH2	6.12	124.71	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AH	294	ARG	NE-CZ-NH2	6.12	124.71	119.20
2	IH	294	ARG	NE-CZ-NH2	6.11	124.70	119.20
2	GH	294	ARG	NE-CZ-NH2	6.09	124.69	119.20
5	Jd	67	LYS	CB-CG-CD	6.09	125.31	111.30
2	DH	294	ARG	NE-CZ-NH2	6.09	124.68	119.20
5	Ed	114	SER	CA-CB-OG	-6.03	99.05	111.10
5	AD	97	ARG	CA-CB-CG	-6.02	102.06	114.10
5	MD	54	GLU	N-CA-CB	6.02	120.52	110.41
5	KD	157	ARG	N-CA-CB	6.01	119.94	110.56
5	AD	131	ILE	CA-CB-CG1	6.00	120.60	110.40
5	Fd	78	ASN	CA-CB-CG	5.99	118.59	112.60
5	KD	57	LYS	CA-CB-CG	5.98	126.07	114.10
5	HD	97	ARG	CG-CD-NE	5.97	125.13	112.00
5	AD	26	LYS	N-CA-C	5.96	119.27	109.85
5	MD	57	LYS	CG-CD-CE	5.96	125.02	111.30
5	HD	54	GLU	N-CA-CB	5.95	120.10	110.40
1	FC	81	GLU	N-CA-CB	5.94	119.79	110.46
1	MC	81	GLU	N-CA-CB	5.94	119.78	110.46
5	CD	52	MET	CA-CB-CG	5.94	125.97	114.10
1	KC	81	GLU	N-CA-CB	5.93	119.77	110.46
1	HC	81	GLU	N-CA-CB	5.93	119.77	110.46
1	BC	81	GLU	N-CA-CB	5.93	119.77	110.46
1	DC	81	GLU	N-CA-CB	5.92	119.76	110.46
5	CD	96	ALA	CA-C-N	-5.92	111.24	121.66
5	CD	96	ALA	C-N-CA	-5.92	111.24	121.66
1	JC	81	GLU	N-CA-CB	5.92	119.75	110.46
1	EC	81	GLU	N-CA-CB	5.91	119.74	110.46
1	GC	81	GLU	N-CA-CB	5.91	119.74	110.46
1	IC	81	GLU	N-CA-CB	5.91	119.74	110.46
1	LC	81	GLU	N-CA-CB	5.91	119.74	110.46
4	P	155	LEU	CA-CB-CG	5.91	136.98	116.30
4	R	155	LEU	CA-CB-CG	5.91	136.98	116.30
4	N	155	LEU	CA-CB-CG	5.91	136.97	116.30
4	X	155	LEU	CA-CB-CG	5.91	136.97	116.30
4	O	155	LEU	CA-CB-CG	5.91	136.97	116.30
4	S	155	LEU	CA-CB-CG	5.91	136.97	116.30
4	T	155	LEU	CA-CB-CG	5.90	136.96	116.30
4	Z	155	LEU	CA-CB-CG	5.90	136.97	116.30
4	U	155	LEU	CA-CB-CG	5.90	136.96	116.30
4	W	155	LEU	CA-CB-CG	5.90	136.96	116.30
1	CC	81	GLU	N-CA-CB	5.90	119.73	110.46
1	AC	81	GLU	N-CA-CB	5.90	119.72	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	155	LEU	CA-CB-CG	5.90	136.95	116.30
4	Y	155	LEU	CA-CB-CG	5.90	136.95	116.30
4	Q	155	LEU	CA-CB-CG	5.89	136.93	116.30
5	GD	90	PRO	CA-C-N	5.83	128.76	120.53
5	GD	90	PRO	C-N-CA	5.83	128.76	120.53
5	FD	82	ARG	CG-CD-NE	5.82	124.81	112.00
5	Ed	107	ARG	CB-CG-CD	-5.81	97.93	111.30
5	MD	57	LYS	CA-C-N	-5.80	112.26	121.02
5	MD	57	LYS	C-N-CA	-5.80	112.26	121.02
5	AD	126	GLU	CA-CB-CG	5.79	125.67	114.10
5	FD	97	ARG	NE-CZ-NH1	5.78	127.28	121.50
5	ED	126	GLU	N-CA-CB	5.76	120.32	111.56
5	Dd	109	LEU	CD1-CG-CD2	-5.75	98.15	110.80
5	KD	54	GLU	N-CA-CB	5.72	119.72	110.40
5	JD	82	ARG	NE-CZ-NH2	5.71	124.34	119.20
5	Jd	67	LYS	CA-CB-CG	-5.71	102.67	114.10
5	BD	79	LEU	CB-CA-C	-5.71	98.05	109.99
5	Gd	124	LYS	CG-CD-CE	5.71	124.43	111.30
5	CD	126	GLU	CA-CB-CG	5.71	125.51	114.10
5	JD	97	ARG	CB-CG-CD	5.70	124.40	111.30
5	FD	82	ARG	NE-CZ-NH2	5.70	124.33	119.20
5	Md	73	ILE	N-CA-C	-5.67	102.54	108.15
5	Kd	52	MET	CG-SD-CE	-5.66	88.44	100.90
5	FD	130	GLU	CB-CA-C	-5.64	100.37	110.70
5	MD	97	ARG	NE-CZ-NH1	5.64	127.14	121.50
5	AD	55	MET	CG-SD-CE	-5.63	88.51	100.90
5	JD	120	SER	N-CA-C	-5.63	100.51	109.23
5	ED	130	GLU	CB-CG-CD	-5.62	103.05	112.60
5	Ld	73	ILE	N-CA-C	-5.61	102.60	108.15
5	Cd	142	LYS	N-CA-C	-5.61	107.09	114.04
5	LD	72	THR	CA-C-N	-5.60	117.19	123.02
5	LD	72	THR	C-N-CA	-5.60	117.19	123.02
5	Fd	117	VAL	CB-CA-C	5.60	117.28	111.23
1	HC	214	LYS	CG-CD-CE	5.57	124.11	111.30
1	AC	214	LYS	CG-CD-CE	5.57	124.10	111.30
1	KC	214	LYS	CG-CD-CE	5.57	124.10	111.30
1	DC	214	LYS	CG-CD-CE	5.57	124.10	111.30
1	EC	214	LYS	CG-CD-CE	5.56	124.09	111.30
1	CC	214	LYS	CG-CD-CE	5.56	124.09	111.30
1	FC	214	LYS	CG-CD-CE	5.56	124.08	111.30
1	BC	214	LYS	CG-CD-CE	5.56	124.08	111.30
5	ED	52	MET	CA-CB-CG	5.56	125.21	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	IC	214	LYS	CG-CD-CE	5.55	124.07	111.30
1	JC	214	LYS	CG-CD-CE	5.55	124.08	111.30
1	GC	214	LYS	CG-CD-CE	5.55	124.07	111.30
5	JD	74	PRO	CA-C-N	5.55	132.13	121.54
5	JD	74	PRO	C-N-CA	5.55	132.13	121.54
1	MC	214	LYS	CG-CD-CE	5.54	124.05	111.30
1	LC	214	LYS	CG-CD-CE	5.54	124.05	111.30
5	Jd	52	MET	CB-CA-C	-5.54	102.18	110.88
5	GD	115	VAL	CB-CA-C	5.54	116.63	110.71
5	Fd	107	ARG	NE-CZ-NH2	5.53	124.18	119.20
5	KD	57	LYS	CD-CE-NZ	5.50	129.52	111.90
5	Ld	117	VAL	CB-CA-C	5.49	117.16	111.23
5	Ad	141	LYS	CA-CB-CG	5.49	125.07	114.10
5	GD	82	ARG	NE-CZ-NH2	5.47	124.12	119.20
4	FZ	44	ALA	CA-C-N	5.46	131.97	121.54
4	FZ	44	ALA	C-N-CA	5.46	131.97	121.54
4	EZ	44	ALA	CA-C-N	5.46	131.96	121.54
4	EZ	44	ALA	C-N-CA	5.46	131.96	121.54
4	IZ	44	ALA	CA-C-N	5.45	131.95	121.54
4	IZ	44	ALA	C-N-CA	5.45	131.95	121.54
4	MZ	44	ALA	CA-C-N	5.45	131.95	121.54
4	MZ	44	ALA	C-N-CA	5.45	131.95	121.54
4	V	112	GLN	CA-C-N	5.45	130.10	122.36
4	V	112	GLN	C-N-CA	5.45	130.10	122.36
4	LZ	44	ALA	CA-C-N	5.45	131.94	121.54
4	LZ	44	ALA	C-N-CA	5.45	131.94	121.54
4	R	112	GLN	CA-C-N	5.45	130.09	122.36
4	R	112	GLN	C-N-CA	5.45	130.09	122.36
4	DZ	44	ALA	CA-C-N	5.44	131.93	121.54
4	DZ	44	ALA	C-N-CA	5.44	131.93	121.54
3	BK	127	LYS	CA-CB-CG	5.44	124.98	114.10
3	AK	127	LYS	CA-CB-CG	5.44	124.98	114.10
5	Md	109	LEU	CB-CA-C	5.44	118.56	110.62
4	X	112	GLN	CA-C-N	5.44	130.08	122.36
4	X	112	GLN	C-N-CA	5.44	130.08	122.36
4	KZ	44	ALA	CA-C-N	5.44	131.93	121.54
4	KZ	44	ALA	C-N-CA	5.44	131.93	121.54
4	HZ	44	ALA	CA-C-N	5.43	131.92	121.54
4	HZ	44	ALA	C-N-CA	5.43	131.92	121.54
4	CZ	44	ALA	CA-C-N	5.43	131.92	121.54
4	CZ	44	ALA	C-N-CA	5.43	131.92	121.54
4	GZ	44	ALA	CA-C-N	5.43	131.92	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GZ	44	ALA	C-N-CA	5.43	131.92	121.54
4	U	112	GLN	CA-C-N	5.43	130.07	122.36
4	U	112	GLN	C-N-CA	5.43	130.07	122.36
3	MK	127	LYS	CA-CB-CG	5.43	124.96	114.10
4	O	112	GLN	CA-C-N	5.43	130.07	122.36
4	O	112	GLN	C-N-CA	5.43	130.07	122.36
4	P	112	GLN	CA-C-N	5.43	130.07	122.36
4	P	112	GLN	C-N-CA	5.43	130.07	122.36
3	CK	127	LYS	CA-CB-CG	5.43	124.96	114.10
3	EK	127	LYS	CA-CB-CG	5.43	124.95	114.10
4	N	112	GLN	CA-C-N	5.43	130.06	122.36
4	N	112	GLN	C-N-CA	5.43	130.06	122.36
4	AZ	44	ALA	CA-C-N	5.43	131.91	121.54
4	AZ	44	ALA	C-N-CA	5.43	131.91	121.54
4	BZ	44	ALA	CA-C-N	5.42	131.90	121.54
4	BZ	44	ALA	C-N-CA	5.42	131.90	121.54
3	HK	127	LYS	CA-CB-CG	5.42	124.94	114.10
3	GK	127	LYS	CA-CB-CG	5.42	124.94	114.10
3	HK	100	ASN	CA-C-N	-5.42	111.01	121.58
3	HK	100	ASN	C-N-CA	-5.42	111.01	121.58
3	JK	127	LYS	CA-CB-CG	5.42	124.94	114.10
4	Q	112	GLN	CA-C-N	5.42	130.06	122.36
4	Q	112	GLN	C-N-CA	5.42	130.06	122.36
3	FK	127	LYS	CA-CB-CG	5.42	124.93	114.10
4	JZ	44	ALA	CA-C-N	5.41	131.88	121.54
4	JZ	44	ALA	C-N-CA	5.41	131.88	121.54
4	Z	112	GLN	CA-C-N	5.41	130.05	122.36
4	Z	112	GLN	C-N-CA	5.41	130.05	122.36
3	LK	100	ASN	CA-C-N	-5.41	111.03	121.58
3	LK	100	ASN	C-N-CA	-5.41	111.03	121.58
3	AK	100	ASN	CA-C-N	-5.41	111.03	121.58
3	AK	100	ASN	C-N-CA	-5.41	111.03	121.58
5	KD	52	MET	CA-CB-CG	5.41	124.92	114.10
3	IK	127	LYS	CA-CB-CG	5.41	124.92	114.10
3	DK	127	LYS	CA-CB-CG	5.41	124.92	114.10
3	GK	100	ASN	CA-C-N	-5.41	111.04	121.58
3	GK	100	ASN	C-N-CA	-5.41	111.04	121.58
3	JK	100	ASN	CA-C-N	-5.41	111.04	121.58
3	JK	100	ASN	C-N-CA	-5.41	111.04	121.58
4	W	112	GLN	CA-C-N	5.41	130.04	122.36
4	W	112	GLN	C-N-CA	5.41	130.04	122.36
3	EK	100	ASN	CA-C-N	-5.40	111.04	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EK	100	ASN	C-N-CA	-5.40	111.04	121.58
3	LK	127	LYS	CA-CB-CG	5.40	124.91	114.10
3	DK	100	ASN	CA-C-N	-5.40	111.05	121.58
3	DK	100	ASN	C-N-CA	-5.40	111.05	121.58
3	IK	100	ASN	CA-C-N	-5.40	111.05	121.58
3	IK	100	ASN	C-N-CA	-5.40	111.05	121.58
3	KK	127	LYS	CA-CB-CG	5.40	124.90	114.10
4	T	112	GLN	CA-C-N	5.40	130.03	122.36
4	T	112	GLN	C-N-CA	5.40	130.03	122.36
3	MK	100	ASN	CA-C-N	-5.40	111.06	121.58
3	MK	100	ASN	C-N-CA	-5.40	111.06	121.58
3	BK	100	ASN	CA-C-N	-5.40	111.05	121.58
3	BK	100	ASN	C-N-CA	-5.40	111.05	121.58
4	S	112	GLN	CA-C-N	5.39	130.02	122.36
4	S	112	GLN	C-N-CA	5.39	130.02	122.36
4	Y	112	GLN	CA-C-N	5.39	130.02	122.36
4	Y	112	GLN	C-N-CA	5.39	130.02	122.36
5	DD	54	GLU	N-CA-CB	5.39	119.18	110.40
5	GD	93	GLU	CA-CB-CG	-5.38	103.33	114.10
3	KK	100	ASN	CA-C-N	-5.38	111.08	121.58
3	KK	100	ASN	C-N-CA	-5.38	111.08	121.58
3	FK	100	ASN	CA-C-N	-5.38	111.08	121.58
3	FK	100	ASN	C-N-CA	-5.38	111.08	121.58
3	CK	100	ASN	CA-C-N	-5.38	111.09	121.58
3	CK	100	ASN	C-N-CA	-5.38	111.09	121.58
5	DD	100	LYS	CA-CB-CG	5.38	124.86	114.10
5	Jd	78	ASN	CA-CB-CG	5.34	117.94	112.60
5	DD	68	ASP	CA-C-N	5.33	131.71	121.54
5	DD	68	ASP	C-N-CA	5.33	131.71	121.54
5	Gd	142	LYS	N-CA-C	-5.32	107.33	113.88
5	Jd	92	GLU	CB-CA-C	-5.32	102.50	110.90
5	CD	97	ARG	CD-NE-CZ	-5.31	116.97	124.40
5	KD	94	LEU	CB-CG-CD2	5.30	126.62	110.70
5	MD	68	ASP	CA-C-N	5.29	131.64	121.54
5	MD	68	ASP	C-N-CA	5.29	131.64	121.54
5	KD	157	ARG	CB-CA-C	-5.27	101.11	109.80
5	AD	130	GLU	CB-CA-C	5.26	118.24	109.56
5	MD	82	ARG	NE-CZ-NH2	5.26	123.93	119.20
5	Md	78	ASN	CA-CB-CG	5.26	117.86	112.60
5	Bd	155	GLU	CA-CB-CG	5.25	124.61	114.10
5	LD	53	LEU	CA-C-N	-5.25	112.29	122.06
5	LD	53	LEU	C-N-CA	-5.25	112.29	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FD	133	ARG	CA-C-N	-5.25	112.89	122.38
5	FD	133	ARG	C-N-CA	-5.25	112.89	122.38
5	Fd	107	ARG	NE-CZ-NH1	-5.24	116.26	121.50
5	Gd	141	LYS	CA-CB-CG	5.23	124.56	114.10
5	ID	97	ARG	CG-CD-NE	5.23	123.50	112.00
5	Bd	86	ASP	CB-CG-OD1	5.22	130.41	118.40
5	KD	131	ILE	CG1-CB-CG2	-5.21	95.05	110.70
1	CC	80	ASP	CA-C-N	-5.21	112.37	122.06
1	CC	80	ASP	C-N-CA	-5.21	112.37	122.06
1	GC	80	ASP	CA-C-N	-5.21	112.37	122.06
1	GC	80	ASP	C-N-CA	-5.21	112.37	122.06
1	LC	80	ASP	CA-C-N	-5.21	112.37	122.06
1	LC	80	ASP	C-N-CA	-5.21	112.37	122.06
1	AC	80	ASP	CA-C-N	-5.21	112.38	122.06
1	AC	80	ASP	C-N-CA	-5.21	112.38	122.06
1	MC	80	ASP	CA-C-N	-5.20	112.38	122.06
1	MC	80	ASP	C-N-CA	-5.20	112.38	122.06
1	KC	80	ASP	CA-C-N	-5.20	112.39	122.06
1	KC	80	ASP	C-N-CA	-5.20	112.39	122.06
1	EC	80	ASP	CA-C-N	-5.20	112.40	122.06
1	EC	80	ASP	C-N-CA	-5.20	112.40	122.06
1	JC	80	ASP	CA-C-N	-5.20	112.39	122.06
1	JC	80	ASP	C-N-CA	-5.20	112.39	122.06
5	KD	157	ARG	CB-CG-CD	-5.19	99.36	111.30
1	BC	80	ASP	CA-C-N	-5.19	112.40	122.06
1	BC	80	ASP	C-N-CA	-5.19	112.40	122.06
1	HC	80	ASP	CA-C-N	-5.19	112.41	122.06
1	HC	80	ASP	C-N-CA	-5.19	112.41	122.06
5	Id	92	GLU	CB-CA-C	-5.19	102.71	110.90
5	BD	68	ASP	CA-C-N	5.18	131.44	121.54
5	BD	68	ASP	C-N-CA	5.18	131.44	121.54
1	DC	80	ASP	CA-C-N	-5.18	112.42	122.06
1	DC	80	ASP	C-N-CA	-5.18	112.42	122.06
1	IC	80	ASP	CA-C-N	-5.18	112.43	122.06
1	IC	80	ASP	C-N-CA	-5.18	112.43	122.06
1	FC	80	ASP	CA-C-N	-5.16	112.46	122.06
1	FC	80	ASP	C-N-CA	-5.16	112.46	122.06
5	HD	71	LEU	CD1-CG-CD2	-5.16	99.45	110.80
5	FD	91	ILE	N-CA-CB	-5.14	104.04	110.47
5	AD	72	THR	CA-C-N	-5.13	118.90	122.59
5	AD	72	THR	C-N-CA	-5.13	118.90	122.59
5	HD	68	ASP	CA-C-N	5.13	131.33	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	HD	68	ASP	C-N-CA	5.13	131.33	121.54
4	MX	134	ALA	CA-C-N	5.13	131.33	121.54
4	MX	134	ALA	C-N-CA	5.13	131.33	121.54
4	LX	134	ALA	CA-C-N	5.12	131.31	121.54
4	LX	134	ALA	C-N-CA	5.12	131.31	121.54
4	KX	134	ALA	CA-C-N	5.11	131.30	121.54
4	KX	134	ALA	C-N-CA	5.11	131.30	121.54
4	JX	134	ALA	CA-C-N	5.11	131.30	121.54
4	JX	134	ALA	C-N-CA	5.11	131.30	121.54
5	CD	54	GLU	N-CA-CB	5.11	118.99	110.41
5	CD	115	VAL	CB-CA-C	5.11	116.41	110.89
5	DD	94	LEU	CB-CG-CD2	5.11	126.02	110.70
5	Cd	77	TYR	CA-C-N	5.10	135.47	126.45
5	Cd	77	TYR	C-N-CA	5.10	135.47	126.45
4	DX	134	ALA	CA-C-N	5.10	131.27	121.54
4	DX	134	ALA	C-N-CA	5.10	131.27	121.54
5	LD	90	PRO	CA-C-N	5.09	128.52	120.47
5	LD	90	PRO	C-N-CA	5.09	128.52	120.47
4	AX	134	ALA	CA-C-N	5.09	131.26	121.54
4	AX	134	ALA	C-N-CA	5.09	131.26	121.54
5	Bd	86	ASP	CA-CB-CG	5.09	117.69	112.60
5	KD	90	PRO	CA-C-N	5.08	128.96	120.62
5	KD	90	PRO	C-N-CA	5.08	128.96	120.62
3	HK	187	ALA	CA-C-N	5.08	130.85	121.70
3	HK	187	ALA	C-N-CA	5.08	130.85	121.70
3	BK	187	ALA	CA-C-N	5.07	130.82	121.70
3	BK	187	ALA	C-N-CA	5.07	130.82	121.70
5	AD	54	GLU	N-CA-CB	5.07	118.66	110.40
5	GD	82	ARG	CG-CD-NE	5.06	123.13	112.00
3	IK	187	ALA	CA-C-N	5.05	130.79	121.70
3	IK	187	ALA	C-N-CA	5.05	130.79	121.70
3	JK	187	ALA	CA-C-N	5.05	130.79	121.70
3	JK	187	ALA	C-N-CA	5.05	130.79	121.70
3	KK	187	ALA	CA-C-N	5.05	130.79	121.70
3	KK	187	ALA	C-N-CA	5.05	130.79	121.70
3	DK	187	ALA	CA-C-N	5.05	130.78	121.70
3	DK	187	ALA	C-N-CA	5.05	130.78	121.70
5	KD	52	MET	CB-CA-C	-5.05	102.41	110.79
1	HC	102	GLU	CA-CB-CG	5.04	124.18	114.10
3	EK	187	ALA	CA-C-N	5.04	130.77	121.70
3	EK	187	ALA	C-N-CA	5.04	130.77	121.70
1	GC	102	GLU	CA-CB-CG	5.04	124.17	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	MK	187	ALA	CA-C-N	5.04	130.76	121.70
3	MK	187	ALA	C-N-CA	5.04	130.76	121.70
2	JH	355	MET	CG-SD-CE	-5.03	89.83	100.90
2	LH	355	MET	CG-SD-CE	-5.03	89.83	100.90
1	BC	102	GLU	CA-CB-CG	5.03	124.16	114.10
3	AK	187	ALA	CA-C-N	5.03	130.75	121.70
3	AK	187	ALA	C-N-CA	5.03	130.75	121.70
3	CK	187	ALA	CA-C-N	5.03	130.75	121.70
3	CK	187	ALA	C-N-CA	5.03	130.75	121.70
2	GH	355	MET	CG-SD-CE	-5.03	89.84	100.90
5	HD	97	ARG	CB-CG-CD	5.03	122.86	111.30
1	EC	102	GLU	CA-CB-CG	5.02	124.15	114.10
2	DH	355	MET	CG-SD-CE	-5.02	89.85	100.90
3	FK	187	ALA	CA-C-N	5.02	130.74	121.70
3	FK	187	ALA	C-N-CA	5.02	130.74	121.70
3	GK	187	ALA	CA-C-N	5.02	130.74	121.70
3	GK	187	ALA	C-N-CA	5.02	130.74	121.70
5	AD	128	LEU	CD1-CG-CD2	-5.02	99.75	110.80
2	BH	355	MET	CG-SD-CE	-5.02	89.85	100.90
1	FC	102	GLU	CA-CB-CG	5.02	124.14	114.10
1	JC	102	GLU	CA-CB-CG	5.02	124.14	114.10
2	HH	355	MET	CG-SD-CE	-5.02	89.86	100.90
2	IH	355	MET	CG-SD-CE	-5.02	89.86	100.90
2	KH	355	MET	CG-SD-CE	-5.02	89.86	100.90
2	CH	355	MET	CG-SD-CE	-5.02	89.86	100.90
2	AH	355	MET	CG-SD-CE	-5.02	89.86	100.90
1	LC	102	GLU	CA-CB-CG	5.02	124.14	114.10
3	LK	187	ALA	CA-C-N	5.02	130.73	121.70
3	LK	187	ALA	C-N-CA	5.02	130.73	121.70
1	DC	102	GLU	CA-CB-CG	5.02	124.14	114.10
1	KC	102	GLU	CA-CB-CG	5.02	124.13	114.10
1	CC	102	GLU	CA-CB-CG	5.01	124.13	114.10
1	MC	102	GLU	CA-CB-CG	5.01	124.13	114.10
5	Cd	78	ASN	CA-CB-CG	5.01	117.61	112.60
2	EH	355	MET	CG-SD-CE	-5.01	89.89	100.90
5	LD	100	LYS	CB-CG-CD	-5.01	99.78	111.30
2	MH	355	MET	CG-SD-CE	-5.01	89.89	100.90
2	FH	355	MET	CG-SD-CE	-5.00	89.89	100.90
1	AC	102	GLU	CA-CB-CG	5.00	124.11	114.10
1	IC	102	GLU	CA-CB-CG	5.00	124.10	114.10
5	LD	68	ASP	CA-C-N	5.00	131.09	121.54
5	LD	68	ASP	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (90) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AD	51	SER	Peptide
4	AX	142	ALA	Peptide
4	AX	153	ALA	Peptide
4	AZ	45	ALA	Peptide
5	BD	124	LYS	Peptide
4	BX	142	ALA	Peptide
4	BX	153	ALA	Peptide
4	BZ	45	ALA	Peptide
5	Bd	85	VAL	Peptide
5	CD	124	LYS	Peptide
5	CD	51	SER	Peptide
4	CX	142	ALA	Peptide
4	CX	153	ALA	Peptide
4	CZ	45	ALA	Peptide
5	DD	126	GLU	Sidechain
5	DD	81	ALA	Peptide
4	DX	142	ALA	Peptide
4	DX	153	ALA	Peptide
4	DZ	45	ALA	Peptide
5	Dd	85	VAL	Peptide
5	ED	124	LYS	Peptide
5	ED	127	SER	Peptide
5	ED	130	GLU	Sidechain
4	EX	142	ALA	Peptide
4	EX	153	ALA	Peptide
4	EZ	45	ALA	Peptide
5	Ed	62	ILE	Peptide
5	Ed	85	VAL	Peptide
5	FD	124	LYS	Peptide
5	FD	126	GLU	Sidechain
4	FX	142	ALA	Peptide
4	FX	153	ALA	Peptide
4	FZ	45	ALA	Peptide
5	Fd	85	VAL	Peptide
5	GD	124	LYS	Peptide
5	GD	126	GLU	Sidechain
5	GD	133	ARG	Sidechain
4	GX	142	ALA	Peptide
4	GX	153	ALA	Peptide
4	GZ	45	ALA	Peptide

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Mol	Chain	Res	Type	Group
5	HD	124	LYS	Peptide
5	HD	125	ASP	Peptide
4	HX	142	ALA	Peptide
4	HX	153	ALA	Peptide
4	HZ	45	ALA	Peptide
5	ID	124	LYS	Peptide
5	ID	126	GLU	Sidechain
5	ID	130	GLU	Peptide
4	IX	142	ALA	Peptide
4	IX	153	ALA	Peptide
4	IZ	45	ALA	Peptide
5	Id	85	VAL	Peptide
5	JD	124	LYS	Peptide
4	JX	142	ALA	Peptide
4	JX	153	ALA	Peptide
4	JZ	45	ALA	Peptide
5	Jd	85	VAL	Peptide
5	KD	124	LYS	Peptide
5	KD	126	GLU	Sidechain
5	KD	127	SER	Peptide
4	KX	142	ALA	Peptide
4	KX	153	ALA	Peptide
4	KZ	45	ALA	Peptide
5	LD	126	GLU	Sidechain
5	LD	61	VAL	Peptide
4	LX	142	ALA	Peptide
4	LX	153	ALA	Peptide
4	LZ	45	ALA	Peptide
5	Ld	62	ILE	Peptide
5	MD	124	LYS	Peptide
5	MD	126	GLU	Sidechain
5	MD	155	GLU	Sidechain
4	MX	142	ALA	Peptide
4	MX	153	ALA	Peptide
4	MZ	45	ALA	Peptide
5	Md	68	ASP	Peptide
5	Md	85	VAL	Peptide
4	N	134	MET	Peptide
4	O	134	MET	Peptide
4	P	134	MET	Peptide
4	Q	134	MET	Peptide
4	R	134	MET	Peptide

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Mol	Chain	Res	Type	Group
4	S	134	MET	Peptide
4	T	134	MET	Peptide
4	U	134	MET	Peptide
4	V	134	MET	Peptide
4	W	134	MET	Peptide
4	X	134	MET	Peptide
4	Y	134	MET	Peptide
4	Z	134	MET	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	1596	0	1602	26	0
1	BC	1596	0	1602	29	0
1	CC	1596	0	1602	32	0
1	DC	1596	0	1602	29	0
1	EC	1596	0	1602	32	0
1	FC	1596	0	1602	30	0
1	GC	1596	0	1602	32	0
1	HC	1596	0	1602	35	0
1	IC	1596	0	1602	36	0
1	JC	1596	0	1602	29	0
1	KC	1596	0	1602	29	0
1	LC	1596	0	1602	27	0
1	MC	1596	0	1602	23	0
2	AH	678	0	689	11	0
2	BH	678	0	689	12	0
2	CH	678	0	689	13	0
2	DH	678	0	689	12	0
2	EH	678	0	689	11	0
2	FH	678	0	689	13	0
2	GH	678	0	689	11	0
2	HH	678	0	689	15	0
2	IH	678	0	689	18	0
2	JH	678	0	689	17	0
2	KH	678	0	689	18	0
2	LH	678	0	689	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	MH	678	0	689	14	0
3	AK	1152	0	1192	22	0
3	BK	1152	0	1192	21	0
3	CK	1152	0	1192	21	0
3	DK	1152	0	1192	20	0
3	EK	1152	0	1192	20	0
3	FK	1152	0	1192	21	0
3	GK	1152	0	1192	22	0
3	HK	1152	0	1192	20	0
3	IK	1152	0	1192	23	0
3	JK	1152	0	1192	20	0
3	KK	1152	0	1192	19	0
3	LK	1152	0	1192	21	0
3	MK	1152	0	1192	21	0
4	AX	1140	0	1139	16	0
4	AY	260	0	262	1	0
4	AZ	350	0	352	3	0
4	BX	1140	0	1139	17	0
4	BY	260	0	262	1	0
4	BZ	350	0	352	3	0
4	CX	1140	0	1139	15	0
4	CY	260	0	262	1	0
4	CZ	350	0	352	3	0
4	DX	1140	0	1139	17	0
4	DY	260	0	262	1	0
4	DZ	350	0	352	3	0
4	EX	1140	0	1139	16	0
4	EY	260	0	262	1	0
4	EZ	350	0	352	4	0
4	FX	1140	0	1139	17	0
4	FY	260	0	262	1	0
4	FZ	350	0	352	3	0
4	GX	1140	0	1139	16	0
4	GY	260	0	262	1	0
4	GZ	350	0	352	4	0
4	HX	1140	0	1139	15	0
4	HY	260	0	262	1	0
4	HZ	350	0	352	3	0
4	IX	1140	0	1139	16	0
4	IY	260	0	262	1	0
4	IZ	350	0	352	5	0
4	JX	1140	0	1139	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	JY	260	0	262	1	0
4	JZ	350	0	352	5	0
4	KX	1140	0	1139	15	0
4	KY	260	0	262	1	0
4	KZ	350	0	352	5	0
4	LX	1140	0	1139	16	0
4	LY	260	0	262	1	0
4	LZ	350	0	352	3	0
4	MX	1140	0	1139	16	0
4	MY	260	0	262	1	0
4	MZ	350	0	352	3	0
4	N	1108	0	1107	18	0
4	O	1108	0	1107	15	0
4	P	1108	0	1107	18	0
4	Q	1108	0	1107	16	0
4	R	1108	0	1107	15	0
4	S	1108	0	1107	15	0
4	T	1108	0	1107	16	0
4	U	1108	0	1107	16	0
4	V	1108	0	1107	15	0
4	W	1108	0	1107	15	0
4	X	1108	0	1107	18	0
4	Y	1108	0	1107	18	0
4	Z	1108	0	1107	19	0
5	AD	1040	0	1063	11	0
5	Ad	1066	0	1103	19	0
5	BD	1040	0	1066	11	0
5	Bd	1066	0	1103	20	0
5	CD	1040	0	1066	22	0
5	Cd	1066	0	1103	21	0
5	DD	1040	0	1066	18	0
5	Dd	1066	0	1103	25	0
5	ED	1040	0	1066	16	0
5	Ed	1066	0	1103	21	0
5	FD	1040	0	1066	12	0
5	Fd	1066	0	1103	23	0
5	GD	1040	0	1066	19	0
5	Gd	1066	0	1103	20	0
5	HD	1040	0	1066	29	0
5	Hd	1066	0	1103	23	0
5	ID	1040	0	1066	17	0
5	Id	1066	0	1103	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	JD	1040	0	1064	16	0
5	Jd	1066	0	1103	29	0
5	KD	1040	0	1064	18	0
5	Kd	1066	0	1103	26	0
5	LD	1040	0	1066	16	0
5	Ld	1066	0	1103	22	0
5	MD	1040	0	1062	18	0
5	Md	1066	0	1101	28	0
All	All	109070	0	110643	1531	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 7.

All (1531) 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:AC:128:SER:HA	1:BC:243:ASP:O	1.79	0.83
2:KH:355:MET:HE1	4:KZ:35:ALA:HA	1.64	0.80
1:FC:128:SER:HA	1:GC:243:ASP:O	1.82	0.80
4:P:124:THR:HA	4:P:231:ILE:O	1.84	0.78
4:O:124:THR:HA	4:O:231:ILE:O	1.84	0.78
4:Q:124:THR:HA	4:Q:231:ILE:O	1.84	0.78
4:T:124:THR:HA	4:T:231:ILE:O	1.84	0.78
4:N:124:THR:HA	4:N:231:ILE:O	1.84	0.78
4:Z:124:THR:HA	4:Z:231:ILE:O	1.84	0.78
4:S:124:THR:HA	4:S:231:ILE:O	1.84	0.78
4:V:124:THR:HA	4:V:231:ILE:O	1.84	0.78
4:Y:124:THR:HA	4:Y:231:ILE:O	1.84	0.78
4:X:124:THR:HA	4:X:231:ILE:O	1.84	0.78
4:R:124:THR:HA	4:R:231:ILE:O	1.84	0.77
4:W:124:THR:HA	4:W:231:ILE:O	1.84	0.77
1:EC:243:ASP:O	1:DC:128:SER:HA	1.84	0.77
4:U:124:THR:HA	4:U:231:ILE:O	1.84	0.76
2:JH:355:MET:HE1	4:JZ:35:ALA:HA	1.69	0.73
5:GD:131:ILE:O	5:GD:135:ILE:HB	1.89	0.72
5:LD:98:ILE:HD11	5:LD:128:LEU:HB2	1.72	0.71
2:IH:355:MET:HE1	4:IZ:35:ALA:HA	1.73	0.69
1:HC:263:ARG:HE	5:ID:97:ARG:HH12	1.39	0.68
5:Jd:87:TRP:O	5:Jd:120:SER:HA	1.94	0.67
5:GD:48:VAL:HG23	5:Gd:52:MET:HG3	1.75	0.66
5:CD:54:GLU:HA	5:CD:57:LYS:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:264:ALA:O	5:ID:97:ARG:NH2	2.25	0.66
2:HH:355:MET:HE1	4:HZ:35:ALA:HA	1.76	0.66
1:FC:255:LEU:HD13	1:GC:240:ILE:HG12	1.78	0.66
1:HC:88:ARG:HH21	5:Hd:122:SER:HB2	1.62	0.65
5:Dd:55:MET:HE2	1:DC:210:ILE:HG23	1.79	0.64
1:BC:128:SER:HA	1:CC:243:ASP:O	1.98	0.64
5:AD:97:ARG:NH2	1:MC:264:ALA:O	2.30	0.64
5:Fd:87:TRP:O	5:Fd:120:SER:HA	1.97	0.64
5:Hd:87:TRP:O	5:Hd:120:SER:HA	1.97	0.64
3:JK:110:ARG:HH12	4:JZ:35:ALA:HB2	1.61	0.63
1:EC:88:ARG:HH21	5:Ed:122:SER:HB2	1.63	0.63
1:KC:192:ASN:ND2	5:Kd:36:ASP:OD2	2.30	0.63
5:Ad:48:VAL:O	5:Ad:52:MET:HB2	1.98	0.63
1:JC:130:ARG:O	1:KC:241:HIS:HA	1.98	0.63
5:MD:58:VAL:HG21	5:Md:59:GLU:HB3	1.80	0.63
5:Md:87:TRP:O	5:Md:120:SER:HA	1.98	0.63
5:CD:130:GLU:OE2	5:Cd:107:ARG:NH2	2.32	0.63
5:DD:98:ILE:HD11	5:DD:128:LEU:HB2	1.79	0.62
5:Id:87:TRP:O	5:Id:120:SER:HA	1.99	0.62
1:EC:192:ASN:ND2	5:Ed:36:ASP:OD2	2.32	0.62
3:HK:110:ARG:HH12	4:HZ:35:ALA:HB2	1.64	0.62
4:LX:135:ALA:HA	4:LX:155:ALA:H	1.65	0.62
5:Ld:87:TRP:O	5:Ld:120:SER:HA	1.99	0.62
4:GX:135:ALA:HA	4:GX:155:ALA:H	1.65	0.62
4:KX:135:ALA:HA	4:KX:155:ALA:H	1.65	0.62
4:IX:135:ALA:HA	4:IX:155:ALA:H	1.65	0.62
4:JX:135:ALA:HA	4:JX:155:ALA:H	1.65	0.62
4:MX:135:ALA:HA	4:MX:155:ALA:H	1.65	0.62
4:HX:135:ALA:HA	4:HX:155:ALA:H	1.65	0.62
1:LC:128:SER:HA	1:MC:243:ASP:O	1.99	0.62
4:CX:135:ALA:HA	4:CX:155:ALA:H	1.65	0.62
4:FX:135:ALA:HA	4:FX:155:ALA:H	1.65	0.62
1:IC:192:ASN:ND2	5:Id:36:ASP:OD2	2.33	0.62
4:BX:135:ALA:HA	4:BX:155:ALA:H	1.65	0.62
1:FC:192:ASN:ND2	5:Fd:36:ASP:OD2	2.34	0.61
4:AX:135:ALA:HA	4:AX:155:ALA:H	1.65	0.61
1:AC:243:ASP:O	1:MC:128:SER:HA	2.00	0.61
3:EK:185:ARG:NH2	4:Q:213:ALA:O	2.34	0.61
1:LC:192:ASN:ND2	5:Ld:36:ASP:OD2	2.34	0.61
4:DX:135:ALA:HA	4:DX:155:ALA:H	1.65	0.61
1:FC:264:ALA:O	5:GD:97:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:EX:135:ALA:HA	4:EX:155:ALA:H	1.65	0.60
1:EC:128:SER:HA	1:FC:243:ASP:O	2.01	0.60
1:GC:266:VAL:HG21	5:HD:98:ILE:HG22	1.82	0.60
1:KC:264:ALA:O	5:LD:97:ARG:NH1	2.34	0.60
1:IC:130:ARG:O	1:JC:241:HIS:HA	2.00	0.60
5:HD:43:GLU:OE1	4:U:227:ARG:NH1	2.34	0.60
5:JD:137:TYR:O	5:Jd:160:LYS:NZ	2.35	0.60
5:BD:82:ARG:HH11	5:BD:126:GLU:HA	1.67	0.60
5:KD:92:GLU:OE2	5:KD:158:TYR:OH	2.19	0.60
1:FC:133:LYS:HD2	1:GC:239:GLU:HG3	1.82	0.60
5:HD:87:TRP:O	5:HD:120:SER:HA	2.01	0.60
1:CC:264:ALA:H	5:DD:97:ARG:HH22	1.50	0.59
5:ED:48:VAL:HG23	5:Ed:52:MET:HG2	1.84	0.59
1:JC:116:THR:HG22	2:KH:329:MET:HG2	1.84	0.59
5:Dd:36:ASP:OD2	1:DC:192:ASN:ND2	2.35	0.59
5:Md:98:ILE:HG23	5:Md:128:LEU:HD22	1.84	0.59
1:BC:264:ALA:O	5:CD:97:ARG:NH2	2.29	0.59
1:HC:192:ASN:ND2	5:Hd:36:ASP:OD2	2.35	0.59
5:HD:56:ALA:O	5:HD:60:LYS:HB2	2.02	0.59
1:BC:263:ARG:HE	5:CD:97:ARG:HH12	1.49	0.59
1:CC:128:SER:HA	1:DC:243:ASP:O	2.02	0.59
1:HC:128:SER:HA	1:IC:243:ASP:O	2.03	0.59
3:IK:110:ARG:HH12	4:IZ:35:ALA:HB2	1.66	0.59
3:EK:87:GLN:NE2	3:EK:173:ASP:OD1	2.36	0.59
3:KK:87:GLN:NE2	3:KK:173:ASP:OD1	2.36	0.58
5:MD:58:VAL:HG12	5:Md:65:PRO:HG3	1.83	0.58
3:DK:87:GLN:NE2	3:DK:173:ASP:OD1	2.36	0.58
1:LC:264:ALA:N	5:MD:97:ARG:HH22	2.01	0.58
3:BK:87:GLN:NE2	3:BK:173:ASP:OD1	2.36	0.58
5:Ad:132:LEU:HA	5:Ad:135:ILE:HD12	1.85	0.58
5:Bd:74:PRO:HG2	5:Bd:149:PRO:HG3	1.86	0.58
1:GC:192:ASN:ND2	5:Gd:36:ASP:OD2	2.36	0.58
3:IK:87:GLN:NE2	3:IK:173:ASP:OD1	2.36	0.58
3:GK:87:GLN:NE2	3:GK:173:ASP:OD1	2.36	0.58
4:IX:220:ALA:HB2	5:Id:77:TYR:H	1.69	0.58
5:Jd:107:ARG:NH1	5:Jd:155:GLU:OE1	2.36	0.58
4:BX:25:ALA:H	4:BX:43:ALA:HB3	1.68	0.58
5:DD:95:THR:HA	5:DD:98:ILE:HG22	1.84	0.58
5:Dd:87:TRP:O	5:Dd:120:SER:HA	2.04	0.58
3:FK:110:ARG:HH12	4:FZ:35:ALA:HB2	1.67	0.58
3:HK:87:GLN:NE2	3:HK:173:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CD:56:ALA:O	5:CD:60:LYS:HB2	2.03	0.58
3:CK:87:GLN:NE2	3:CK:173:ASP:OD1	2.36	0.58
4:CX:25:ALA:H	4:CX:43:ALA:HB3	1.68	0.58
3:AK:87:GLN:NE2	3:AK:173:ASP:OD1	2.36	0.58
4:DX:25:ALA:H	4:DX:43:ALA:HB3	1.68	0.58
1:KC:93:ILE:HA	5:KD:48:VAL:HG11	1.86	0.58
2:LH:355:MET:HE1	4:LZ:35:ALA:HA	1.86	0.58
3:LK:87:GLN:NE2	3:LK:173:ASP:OD1	2.36	0.58
5:Ld:130:GLU:OE2	5:Ld:133:ARG:NH2	2.36	0.58
3:MK:87:GLN:NE2	3:MK:173:ASP:OD1	2.36	0.58
4:AX:25:ALA:H	4:AX:43:ALA:HB3	1.68	0.58
3:FK:87:GLN:NE2	3:FK:173:ASP:OD1	2.36	0.58
4:IX:25:ALA:H	4:IX:43:ALA:HB3	1.68	0.58
5:LD:132:LEU:HD12	5:LD:145:ILE:HG21	1.86	0.58
4:EX:25:ALA:H	4:EX:43:ALA:HB3	1.68	0.57
5:JD:109:LEU:O	5:JD:157:ARG:HA	2.04	0.57
4:JX:25:ALA:H	4:JX:43:ALA:HB3	1.68	0.57
5:MD:43:GLU:OE1	4:Z:227:ARG:NH1	2.37	0.57
4:P:217:ASN:OD1	4:P:226:ASN:ND2	2.37	0.57
4:W:217:ASN:OD1	4:W:226:ASN:ND2	2.37	0.57
4:X:217:ASN:OD1	4:X:226:ASN:ND2	2.37	0.57
4:IX:97:ALA:HA	4:IX:116:ALA:O	2.05	0.57
5:JD:130:GLU:OE2	5:Jd:107:ARG:NH2	2.37	0.57
3:JK:87:GLN:NE2	3:JK:173:ASP:OD1	2.36	0.57
5:Ld:126:GLU:HG2	5:Ld:131:ILE:HG13	1.86	0.57
4:N:217:ASN:OD1	4:N:226:ASN:ND2	2.37	0.57
4:O:217:ASN:OD1	4:O:226:ASN:ND2	2.37	0.57
4:Q:217:ASN:OD1	4:Q:226:ASN:ND2	2.37	0.57
4:V:217:ASN:OD1	4:V:226:ASN:ND2	2.37	0.57
4:Y:217:ASN:OD1	4:Y:226:ASN:ND2	2.37	0.57
4:Z:217:ASN:OD1	4:Z:226:ASN:ND2	2.37	0.57
5:HD:132:LEU:HD12	5:HD:145:ILE:HG21	1.86	0.57
1:CC:122:ALA:HB1	1:DC:139:HIS:HB2	1.86	0.57
4:DX:97:ALA:HA	4:DX:116:ALA:O	2.05	0.57
5:HD:134:ASP:OD1	5:HD:138:GLN:NE2	2.37	0.57
4:CX:97:ALA:HA	4:CX:116:ALA:O	2.05	0.57
5:Cd:132:LEU:HB3	5:Cd:145:ILE:HG21	1.87	0.57
4:FX:97:ALA:HA	4:FX:116:ALA:O	2.05	0.57
5:JD:87:TRP:O	5:JD:120:SER:HA	2.04	0.57
4:KX:97:ALA:HA	4:KX:116:ALA:O	2.05	0.57
4:LX:97:ALA:HA	4:LX:116:ALA:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MX:25:ALA:H	4:MX:43:ALA:HB3	1.68	0.57
4:U:217:ASN:OD1	4:U:226:ASN:ND2	2.37	0.57
5:Cd:74:PRO:HG2	5:Cd:149:PRO:HG3	1.85	0.57
3:KK:110:ARG:HH12	4:KZ:35:ALA:HB2	1.69	0.57
4:BX:97:ALA:HA	4:BX:116:ALA:O	2.05	0.57
1:GC:263:ARG:O	5:HD:87:TRP:NE1	2.37	0.57
4:KX:25:ALA:H	4:KX:43:ALA:HB3	1.68	0.57
4:S:217:ASN:OD1	4:S:226:ASN:ND2	2.37	0.57
1:EC:136:LYS:NZ	1:EC:205:ASP:OD2	2.38	0.57
1:EC:240:ILE:HG12	1:DC:255:LEU:HD13	1.87	0.57
4:EX:97:ALA:HA	4:EX:116:ALA:O	2.05	0.57
4:FX:25:ALA:H	4:FX:43:ALA:HB3	1.68	0.57
1:HC:126:ARG:NH2	2:IH:274:PRO:O	2.38	0.57
3:IK:117:THR:HA	3:IK:157:GLN:O	2.05	0.57
1:KC:136:LYS:NZ	1:KC:205:ASP:OD2	2.38	0.57
1:LC:136:LYS:NZ	1:LC:205:ASP:OD2	2.38	0.57
4:R:217:ASN:OD1	4:R:226:ASN:ND2	2.37	0.57
1:DC:136:LYS:NZ	1:DC:205:ASP:OD2	2.38	0.57
3:DK:117:THR:HA	3:DK:157:GLN:O	2.05	0.56
4:DZ:37:ALA:O	1:DC:84:ASN:ND2	2.38	0.56
4:HX:97:ALA:HA	4:HX:116:ALA:O	2.05	0.56
1:JC:126:ARG:HD2	2:KH:276:SER:HA	1.87	0.56
4:LX:25:ALA:H	4:LX:43:ALA:HB3	1.68	0.56
3:EK:117:THR:HA	3:EK:157:GLN:O	2.05	0.56
4:GX:97:ALA:HA	4:GX:116:ALA:O	2.05	0.56
5:Ed:130:GLU:OE1	5:Ed:133:ARG:NH2	2.38	0.56
3:FK:117:THR:HA	3:FK:157:GLN:O	2.05	0.56
3:GK:117:THR:HA	3:GK:157:GLN:O	2.05	0.56
1:HC:116:THR:HG22	2:IH:329:MET:HG2	1.87	0.56
1:HC:136:LYS:NZ	1:HC:205:ASP:OD2	2.38	0.56
3:HK:117:THR:HA	3:HK:157:GLN:O	2.05	0.56
4:HX:25:ALA:H	4:HX:43:ALA:HB3	1.68	0.56
5:Jd:126:GLU:HG2	5:Jd:131:ILE:HG13	1.87	0.56
3:AK:117:THR:HA	3:AK:157:GLN:O	2.05	0.56
4:Q:108:ASP:OD1	4:Q:150:ASN:ND2	2.39	0.56
4:T:217:ASN:OD1	4:T:226:ASN:ND2	2.37	0.56
3:BK:117:THR:HA	3:BK:157:GLN:O	2.05	0.56
5:CD:94:LEU:HD22	5:CD:135:ILE:HD11	1.87	0.56
5:DD:56:ALA:O	5:DD:60:LYS:HB2	2.06	0.56
3:DK:185:ARG:NH2	4:P:213:ALA:O	2.37	0.56
1:HC:126:ARG:HD2	2:IH:276:SER:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:JX:97:ALA:HA	4:JX:116:ALA:O	2.05	0.56
3:MK:117:THR:HA	3:MK:157:GLN:O	2.05	0.56
4:O:108:ASP:OD1	4:O:150:ASN:ND2	2.39	0.56
4:S:108:ASP:OD1	4:S:150:ASN:ND2	2.39	0.56
1:CC:136:LYS:NZ	1:CC:205:ASP:OD2	2.38	0.56
3:CK:117:THR:HA	3:CK:157:GLN:O	2.05	0.56
4:GX:25:ALA:H	4:GX:43:ALA:HB3	1.68	0.56
5:Gd:87:TRP:O	5:Gd:120:SER:HA	2.05	0.56
5:KD:79:LEU:HB3	5:KD:129:ALA:HB2	1.87	0.56
5:Kd:87:TRP:O	5:Kd:120:SER:HA	2.06	0.56
4:W:108:ASP:OD1	4:W:150:ASN:ND2	2.39	0.56
4:AX:97:ALA:HA	4:AX:116:ALA:O	2.05	0.56
4:DY:13:ALA:HB3	4:DY:18:ALA:HB3	1.88	0.56
5:ID:130:GLU:OE2	5:Id:107:ARG:NH2	2.38	0.56
1:FC:93:ILE:HA	5:FD:48:VAL:HG11	1.87	0.56
1:GC:136:LYS:NZ	1:GC:205:ASP:OD2	2.38	0.56
1:IC:136:LYS:NZ	1:IC:205:ASP:OD2	2.38	0.56
3:JK:117:THR:HA	3:JK:157:GLN:O	2.05	0.56
3:LK:117:THR:HA	3:LK:157:GLN:O	2.05	0.56
3:EK:120:SER:HA	3:EK:178:ALA:HA	1.88	0.56
1:FC:136:LYS:NZ	1:FC:205:ASP:OD2	2.38	0.56
4:FY:13:ALA:HB3	4:FY:18:ALA:HB3	1.88	0.56
3:AK:120:SER:HA	3:AK:178:ALA:HA	1.88	0.56
4:P:108:ASP:OD1	4:P:150:ASN:ND2	2.39	0.56
1:BC:136:LYS:NZ	1:BC:205:ASP:OD2	2.38	0.56
5:Dd:36:ASP:OD1	1:DC:75:ARG:NH1	2.39	0.56
4:EY:13:ALA:HB3	4:EY:18:ALA:HB3	1.88	0.56
5:LD:130:GLU:OE2	5:Ld:105:ARG:NH2	2.34	0.56
3:LK:120:SER:HA	3:LK:178:ALA:HA	1.88	0.56
4:MX:97:ALA:HA	4:MX:116:ALA:O	2.05	0.56
4:Y:108:ASP:OD1	4:Y:150:ASN:ND2	2.39	0.56
4:BY:13:ALA:HB3	4:BY:18:ALA:HB3	1.88	0.56
3:CK:120:SER:HA	3:CK:178:ALA:HA	1.88	0.56
4:CY:13:ALA:HB3	4:CY:18:ALA:HB3	1.88	0.56
1:JC:136:LYS:NZ	1:JC:205:ASP:OD2	2.38	0.56
1:MC:93:ILE:HA	5:MD:48:VAL:HG11	1.88	0.56
4:AY:13:ALA:HB3	4:AY:18:ALA:HB3	1.88	0.56
5:GD:130:GLU:OE1	5:Gd:107:ARG:NH2	2.39	0.55
3:KK:117:THR:HA	3:KK:157:GLN:O	2.05	0.55
4:U:108:ASP:OD1	4:U:150:ASN:ND2	2.39	0.55
4:V:108:ASP:OD1	4:V:150:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DD:29:PRO:HB2	5:DD:32:ASN:HB2	1.89	0.55
3:DK:120:SER:HA	3:DK:178:ALA:HA	1.88	0.55
5:ED:98:ILE:HD11	5:ED:128:LEU:HB2	1.88	0.55
3:KK:185:ARG:NH2	4:W:213:ALA:O	2.39	0.55
3:MK:120:SER:HA	3:MK:178:ALA:HA	1.88	0.55
4:Z:108:ASP:OD1	4:Z:150:ASN:ND2	2.39	0.55
5:GD:43:GLU:OE2	4:T:227:ARG:NH1	2.40	0.55
3:KK:120:SER:HA	3:KK:178:ALA:HA	1.88	0.55
4:MY:13:ALA:HB3	4:MY:18:ALA:HB3	1.88	0.55
5:Cd:87:TRP:O	5:Cd:120:SER:HA	2.07	0.55
1:AC:136:LYS:NZ	1:AC:205:ASP:OD2	2.38	0.55
1:FC:108:PRO:HD3	1:FC:138:ALA:HB2	1.89	0.55
3:FK:120:SER:HA	3:FK:178:ALA:HA	1.88	0.55
1:GC:108:PRO:HD3	1:GC:138:ALA:HB2	1.89	0.55
3:JK:120:SER:HA	3:JK:178:ALA:HA	1.88	0.55
5:MD:62:ILE:O	5:Md:67:LYS:NZ	2.38	0.55
4:R:108:ASP:OD1	4:R:150:ASN:ND2	2.39	0.55
5:Bd:126:GLU:HG2	5:Bd:131:ILE:HG13	1.88	0.55
3:GK:120:SER:HA	3:GK:178:ALA:HA	1.88	0.55
3:HK:120:SER:HA	3:HK:178:ALA:HA	1.88	0.55
3:IK:120:SER:HA	3:IK:178:ALA:HA	1.88	0.55
4:X:108:ASP:OD1	4:X:150:ASN:ND2	2.39	0.55
3:BK:120:SER:HA	3:BK:178:ALA:HA	1.88	0.55
1:CC:112:GLU:OE2	1:CC:130:ARG:NH1	2.40	0.55
1:AC:112:GLU:OE2	1:AC:130:ARG:NH1	2.40	0.55
3:DK:50:ASP:HA	3:DK:53:ILE:HD12	1.89	0.55
4:HY:13:ALA:HB3	4:HY:18:ALA:HB3	1.88	0.55
1:JC:112:GLU:OE2	1:JC:130:ARG:NH1	2.40	0.55
1:KC:112:GLU:OE2	1:KC:130:ARG:NH1	2.40	0.55
5:KD:43:GLU:OE2	4:X:227:ARG:NH1	2.39	0.55
4:T:108:ASP:OD1	4:T:150:ASN:ND2	2.39	0.55
1:BC:112:GLU:OE2	1:BC:130:ARG:NH1	2.40	0.55
3:BK:50:ASP:HA	3:BK:53:ILE:HD12	1.89	0.55
5:Cd:70:THR:HA	5:Cd:133:ARG:HE	1.72	0.55
1:DC:112:GLU:OE2	1:DC:130:ARG:NH1	2.40	0.55
1:EC:112:GLU:OE2	1:EC:130:ARG:NH1	2.40	0.55
4:GY:13:ALA:HB3	4:GY:18:ALA:HB3	1.88	0.55
1:IC:112:GLU:OE2	1:IC:130:ARG:NH1	2.40	0.55
3:KK:50:ASP:HA	3:KK:53:ILE:HD12	1.89	0.55
4:LY:13:ALA:HB3	4:LY:18:ALA:HB3	1.88	0.55
3:MK:50:ASP:HA	3:MK:53:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:166:ALA:HA	4:N:206:GLU:O	2.07	0.55
5:FD:79:LEU:HB3	5:FD:129:ALA:HB2	1.89	0.55
4:IY:13:ALA:HB3	4:IY:18:ALA:HB3	1.88	0.55
3:AK:50:ASP:HA	3:AK:53:ILE:HD12	1.89	0.55
4:Y:166:ALA:HA	4:Y:206:GLU:O	2.07	0.55
3:CK:50:ASP:HA	3:CK:53:ILE:HD12	1.89	0.55
3:LK:50:ASP:HA	3:LK:53:ILE:HD12	1.89	0.55
1:MC:112:GLU:OE2	1:MC:130:ARG:NH1	2.40	0.55
1:CC:103:HIS:CE1	5:Cd:161:ILE:HG21	2.42	0.55
1:CC:255:LEU:HD13	1:DC:240:ILE:HG12	1.88	0.55
5:Dd:40:LYS:HA	5:Dd:43:GLU:HG2	1.89	0.55
1:EC:108:PRO:HD3	1:EC:138:ALA:HB2	1.89	0.55
5:AD:71:LEU:O	5:AD:133:ARG:NH2	2.40	0.55
1:HC:108:PRO:HD3	1:HC:138:ALA:HB2	1.89	0.55
1:LC:108:PRO:HD3	1:LC:138:ALA:HB2	1.89	0.55
5:MD:54:GLU:HA	5:MD:57:LYS:HG2	1.88	0.55
4:N:108:ASP:OD1	4:N:150:ASN:ND2	2.39	0.55
3:FK:50:ASP:HA	3:FK:53:ILE:HD12	1.89	0.54
1:HC:112:GLU:OE2	1:HC:130:ARG:NH1	2.40	0.54
5:Id:86:ASP:HA	5:Id:121:ILE:O	2.06	0.54
1:KC:108:PRO:HD3	1:KC:138:ALA:HB2	1.89	0.54
1:LC:75:ARG:NH1	5:Ld:36:ASP:OD1	2.39	0.54
3:DK:127:LYS:NZ	4:DX:216:ALA:O	2.31	0.54
1:EC:264:ALA:H	5:FD:97:ARG:HH22	1.54	0.54
3:EK:50:ASP:HA	3:EK:53:ILE:HD12	1.89	0.54
1:GC:103:HIS:CE1	5:Gd:161:ILE:HG21	2.43	0.54
1:GC:112:GLU:OE2	1:GC:130:ARG:NH1	2.40	0.54
3:JK:50:ASP:HA	3:JK:53:ILE:HD12	1.89	0.54
1:KC:88:ARG:HH21	5:Kd:122:SER:HB2	1.71	0.54
4:U:166:ALA:HA	4:U:206:GLU:O	2.07	0.54
5:DD:132:LEU:HD12	5:DD:145:ILE:HG21	1.89	0.54
1:FC:112:GLU:OE2	1:FC:130:ARG:NH1	2.40	0.54
5:Hd:147:VAL:HG22	5:Hd:154:VAL:HG22	1.89	0.54
1:LC:112:GLU:OE2	1:LC:130:ARG:NH1	2.40	0.54
5:Ld:73:ILE:O	5:Ld:133:ARG:NH1	2.41	0.54
1:MC:108:PRO:HD3	1:MC:138:ALA:HB2	1.89	0.54
1:MC:136:LYS:NZ	1:MC:205:ASP:OD2	2.38	0.54
4:P:166:ALA:HA	4:P:206:GLU:O	2.07	0.54
2:DH:351:HIS:ND1	5:Dd:93:GLU:OE2	2.40	0.54
3:GK:50:ASP:HA	3:GK:53:ILE:HD12	1.89	0.54
1:IC:75:ARG:NH1	5:Id:36:ASP:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JC:126:ARG:NH2	2:KH:274:PRO:O	2.41	0.54
1:MC:192:ASN:ND2	5:Md:36:ASP:OD2	2.41	0.54
5:Ad:87:TRP:O	5:Ad:120:SER:HA	2.08	0.54
5:CD:29:PRO:HB2	5:CD:32:ASN:HB2	1.89	0.54
1:IC:108:PRO:HD3	1:IC:138:ALA:HB2	1.89	0.54
4:JY:13:ALA:HB3	4:JY:18:ALA:HB3	1.88	0.54
4:V:166:ALA:HA	4:V:206:GLU:O	2.07	0.54
1:DC:93:ILE:HA	5:DD:48:VAL:HG11	1.89	0.54
3:JK:132:LEU:O	3:JK:136:ARG:HB2	2.08	0.54
4:KY:13:ALA:HB3	4:KY:18:ALA:HB3	1.88	0.54
3:MK:132:LEU:O	3:MK:136:ARG:HB2	2.08	0.54
4:T:166:ALA:HA	4:T:206:GLU:O	2.07	0.54
4:W:166:ALA:HA	4:W:206:GLU:O	2.07	0.54
5:BD:62:ILE:O	5:Bd:67:LYS:NZ	2.41	0.54
5:Dd:74:PRO:HG2	5:Dd:149:PRO:HG3	1.89	0.54
3:EK:132:LEU:O	3:EK:136:ARG:HB2	2.08	0.54
1:GC:231:LEU:HB2	1:GC:244:ASP:HB3	1.90	0.54
3:HK:50:ASP:HA	3:HK:53:ILE:HD12	1.89	0.54
1:IC:131:THR:HA	1:JC:240:ILE:O	2.08	0.54
3:CK:132:LEU:O	3:CK:136:ARG:HB2	2.08	0.54
1:AC:108:PRO:HD3	1:AC:138:ALA:HB2	1.89	0.54
1:FC:231:LEU:HB2	1:FC:244:ASP:HB3	1.90	0.54
3:IK:50:ASP:HA	3:IK:53:ILE:HD12	1.89	0.54
1:JC:108:PRO:HD3	1:JC:138:ALA:HB2	1.89	0.54
3:KK:132:LEU:O	3:KK:136:ARG:HB2	2.08	0.54
4:Q:166:ALA:HA	4:Q:206:GLU:O	2.07	0.54
5:Ad:147:VAL:HG22	5:Ad:154:VAL:HG22	1.90	0.54
1:DC:108:PRO:HD3	1:DC:138:ALA:HB2	1.89	0.54
1:HC:231:LEU:HB2	1:HC:244:ASP:HB3	1.90	0.54
5:ID:94:LEU:O	5:ID:97:ARG:N	2.40	0.54
5:MD:134:ASP:OD1	5:MD:138:GLN:NE2	2.40	0.54
4:Q:101:SER:OG	4:Q:102:LYS:N	2.41	0.54
4:Z:101:SER:OG	4:Z:102:LYS:N	2.41	0.54
3:BK:132:LEU:O	3:BK:136:ARG:HB2	2.08	0.54
3:FK:132:LEU:O	3:FK:136:ARG:HB2	2.08	0.54
1:GC:128:SER:HA	1:HC:243:ASP:O	2.07	0.54
1:IC:231:LEU:HB2	1:IC:244:ASP:HB3	1.90	0.54
4:O:101:SER:OG	4:O:102:LYS:N	2.41	0.54
4:R:166:ALA:HA	4:R:206:GLU:O	2.07	0.54
1:BC:93:ILE:HA	5:BD:48:VAL:HG11	1.89	0.54
1:EC:231:LEU:HB2	1:EC:244:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AD:62:ILE:O	5:Ad:67:LYS:NZ	2.40	0.53
2:HH:351:HIS:ND1	5:Hd:93:GLU:OE2	2.41	0.53
3:IK:132:LEU:O	3:IK:136:ARG:HB2	2.08	0.53
3:LK:185:ARG:NH2	4:X:213:ALA:O	2.42	0.53
5:Md:109:LEU:HD22	5:Md:157:ARG:HG2	1.90	0.53
4:O:213:ALA:O	3:CK:185:ARG:NH2	2.40	0.53
4:R:101:SER:OG	4:R:102:LYS:N	2.41	0.53
4:X:101:SER:OG	4:X:102:LYS:N	2.41	0.53
2:BH:284:VAL:HG23	2:BH:337:ALA:HB1	1.90	0.53
2:CH:284:VAL:HG23	2:CH:337:ALA:HB1	1.90	0.53
3:GK:65:ILE:HG13	3:GK:98:LEU:HD11	1.91	0.53
1:IC:116:THR:HG22	2:JH:329:MET:HG2	1.91	0.53
3:LK:132:LEU:O	3:LK:136:ARG:HB2	2.08	0.53
4:T:101:SER:OG	4:T:102:LYS:N	2.41	0.53
4:Z:166:ALA:HA	4:Z:206:GLU:O	2.07	0.53
1:BC:192:ASN:ND2	5:Bd:36:ASP:OD2	2.40	0.53
2:DH:284:VAL:HG23	2:DH:337:ALA:HB1	1.90	0.53
3:FK:65:ILE:HG13	3:FK:98:LEU:HD11	1.91	0.53
5:GD:56:ALA:O	5:GD:60:LYS:HB2	2.08	0.53
3:HK:65:ILE:HG13	3:HK:98:LEU:HD11	1.91	0.53
1:IC:264:ALA:H	5:JD:97:ARG:HH22	1.57	0.53
4:W:101:SER:OG	4:W:102:LYS:N	2.41	0.53
4:X:166:ALA:HA	4:X:206:GLU:O	2.07	0.53
1:BC:108:PRO:HD3	1:BC:138:ALA:HB2	1.89	0.53
5:Bd:98:ILE:HG23	5:Bd:128:LEU:HD22	1.90	0.53
3:EK:65:ILE:HG13	3:EK:98:LEU:HD11	1.91	0.53
2:HH:284:VAL:HG23	2:HH:337:ALA:HB1	1.90	0.53
3:IK:65:ILE:HG13	3:IK:98:LEU:HD11	1.91	0.53
2:LH:351:HIS:ND1	5:Ld:93:GLU:OE2	2.42	0.53
4:S:166:ALA:HA	4:S:206:GLU:O	2.07	0.53
2:EH:284:VAL:HG23	2:EH:337:ALA:HB1	1.90	0.53
5:Ed:87:TRP:O	5:Ed:120:SER:HA	2.08	0.53
5:FD:29:PRO:HB2	5:FD:32:ASN:HB2	1.91	0.53
2:IH:284:VAL:HG23	2:IH:337:ALA:HB1	1.90	0.53
1:JC:231:LEU:HB2	1:JC:244:ASP:HB3	1.90	0.53
3:LK:110:ARG:HH12	4:LZ:35:ALA:HB2	1.73	0.53
3:AK:132:LEU:O	3:AK:136:ARG:HB2	2.08	0.53
3:HK:132:LEU:O	3:HK:136:ARG:HB2	2.08	0.53
2:AH:284:VAL:HG23	2:AH:337:ALA:HB1	1.90	0.53
3:AK:65:ILE:HG13	3:AK:98:LEU:HD11	1.91	0.53
4:P:101:SER:OG	4:P:102:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:101:SER:OG	4:U:102:LYS:N	2.41	0.53
1:CC:108:PRO:HD3	1:CC:138:ALA:HB2	1.89	0.53
1:DC:231:LEU:HB2	1:DC:244:ASP:HB3	1.90	0.53
1:AC:192:ASN:ND2	5:Ad:36:ASP:OD2	2.42	0.53
1:EC:130:ARG:NH2	5:FD:122:SER:OG	2.41	0.53
5:KD:119:ILE:HG21	5:KD:135:ILE:HG23	1.90	0.53
2:MH:284:VAL:HG23	2:MH:337:ALA:HB1	1.90	0.53
3:MK:65:ILE:HG13	3:MK:98:LEU:HD11	1.91	0.53
1:IC:93:ILE:HA	5:ID:48:VAL:HG11	1.90	0.53
5:JD:29:PRO:HB2	5:JD:32:ASN:HB2	1.89	0.53
5:Kd:48:VAL:O	5:Kd:52:MET:HB2	2.09	0.53
1:LC:264:ALA:H	5:MD:97:ARG:HH22	1.56	0.53
1:MC:231:LEU:HB2	1:MC:244:ASP:HB3	1.90	0.53
5:MD:130:GLU:OE1	5:Md:107:ARG:NH2	2.41	0.53
5:Bd:70:THR:HA	5:Bd:133:ARG:HE	1.74	0.53
3:DK:132:LEU:O	3:DK:136:ARG:HB2	2.08	0.53
3:HK:185:ARG:NH2	4:T:213:ALA:O	2.42	0.53
5:Md:147:VAL:HG22	5:Md:154:VAL:HG22	1.90	0.53
4:N:101:SER:OG	4:N:102:LYS:N	2.41	0.53
4:O:166:ALA:HA	4:O:206:GLU:O	2.07	0.53
4:S:101:SER:OG	4:S:102:LYS:N	2.41	0.53
4:Y:101:SER:OG	4:Y:102:LYS:N	2.41	0.53
3:BK:65:ILE:HG13	3:BK:98:LEU:HD11	1.91	0.53
1:AC:231:LEU:HB2	1:AC:244:ASP:HB3	1.90	0.52
3:DK:65:ILE:HG13	3:DK:98:LEU:HD11	1.91	0.52
2:GH:284:VAL:HG23	2:GH:337:ALA:HB1	1.90	0.52
3:GK:132:LEU:O	3:GK:136:ARG:HB2	2.08	0.52
3:LK:65:ILE:HG13	3:LK:98:LEU:HD11	1.91	0.52
5:Ld:147:VAL:HG22	5:Ld:154:VAL:HG22	1.90	0.52
1:CC:93:ILE:HA	5:CD:48:VAL:HG11	1.90	0.52
5:Id:147:VAL:HG22	5:Id:154:VAL:HG22	1.91	0.52
1:KC:128:SER:HA	1:LC:243:ASP:O	2.09	0.52
1:LC:231:LEU:HB2	1:LC:244:ASP:HB3	1.90	0.52
1:BC:231:LEU:HB2	1:BC:244:ASP:HB3	1.90	0.52
1:KC:231:LEU:HB2	1:KC:244:ASP:HB3	1.90	0.52
1:CC:231:LEU:HB2	1:CC:244:ASP:HB3	1.90	0.52
2:GH:355:MET:HE1	4:GZ:35:ALA:HA	1.90	0.52
3:JK:65:ILE:HG13	3:JK:98:LEU:HD11	1.91	0.52
5:MD:29:PRO:HB2	5:MD:32:ASN:HB2	1.89	0.52
2:FH:284:VAL:HG23	2:FH:337:ALA:HB1	1.90	0.52
5:Fd:70:THR:HA	5:Fd:133:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IC:126:ARG:HD2	2:JH:276:SER:HA	1.92	0.52
2:JH:284:VAL:HG23	2:JH:337:ALA:HB1	1.90	0.52
2:LH:284:VAL:HG23	2:LH:337:ALA:HB1	1.90	0.52
5:Md:38:THR:HA	5:Md:41:LEU:HB2	1.91	0.52
5:ED:82:ARG:HA	5:ED:82:ARG:HH21	1.74	0.52
3:KK:65:ILE:HG13	3:KK:98:LEU:HD11	1.91	0.52
5:LD:29:PRO:HB2	5:LD:32:ASN:HB2	1.90	0.52
4:V:101:SER:OG	4:V:102:LYS:N	2.41	0.52
1:GC:130:ARG:O	1:HC:241:HIS:HA	2.10	0.52
2:AH:277:ALA:HA	1:MC:118:ASN:HB2	1.92	0.52
2:KH:284:VAL:HG23	2:KH:337:ALA:HB1	1.90	0.52
3:CK:65:ILE:HG13	3:CK:98:LEU:HD11	1.91	0.52
2:FH:355:MET:HE1	4:FZ:35:ALA:HA	1.92	0.52
3:FK:185:ARG:NH2	4:R:213:ALA:O	2.43	0.52
3:JK:185:ARG:NH2	4:V:213:ALA:O	2.43	0.52
5:ED:79:LEU:HB3	5:ED:129:ALA:HB2	1.91	0.52
1:GC:118:ASN:HB2	2:HH:277:ALA:HA	1.92	0.52
1:BC:88:ARG:HH21	5:Bd:122:SER:HB2	1.75	0.52
5:CD:98:ILE:HD11	5:CD:128:LEU:HB2	1.91	0.52
5:ED:60:LYS:HZ2	5:Ed:141:LYS:H	1.58	0.51
5:Fd:147:VAL:HG22	5:Fd:154:VAL:HG22	1.92	0.51
1:GC:93:ILE:HA	5:GD:48:VAL:HG11	1.91	0.51
3:GK:110:ARG:HH12	4:GZ:35:ALA:HB2	1.75	0.51
5:Bd:87:TRP:O	5:Bd:120:SER:HA	2.10	0.51
5:Dd:70:THR:HA	5:Dd:133:ARG:HE	1.75	0.51
5:Ed:61:VAL:HG13	5:Ed:62:ILE:HG23	1.92	0.51
1:CC:130:ARG:NH2	5:DD:86:ASP:OD1	2.42	0.51
2:EH:308:SER:OG	2:EH:309:ASN:N	2.44	0.51
2:IH:308:SER:OG	2:IH:309:ASN:N	2.44	0.51
1:JC:131:THR:HA	1:KC:240:ILE:O	2.10	0.51
1:KC:130:ARG:O	1:LC:241:HIS:HA	2.10	0.51
5:Bd:147:VAL:HG22	5:Bd:154:VAL:HG22	1.92	0.51
2:GH:308:SER:OG	2:GH:309:ASN:N	2.44	0.51
3:JK:153:ILE:HG23	5:Jd:85:VAL:HG22	1.93	0.51
2:AH:308:SER:OG	2:AH:309:ASN:N	2.44	0.51
3:MK:110:ARG:HH12	4:MZ:35:ALA:HB2	1.75	0.51
1:AC:255:LEU:HD13	1:BC:240:ILE:HG12	1.92	0.51
2:DH:308:SER:OG	2:DH:309:ASN:N	2.44	0.51
5:FD:91:ILE:HG12	5:FD:156:LEU:HD11	1.93	0.51
5:Jd:73:ILE:O	5:Jd:133:ARG:NH1	2.42	0.51
1:AC:133:LYS:HD2	1:BC:239:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IH:351:HIS:ND1	5:Id:93:GLU:OE2	2.44	0.51
3:IK:150:ASP:O	3:IK:152:ARG:NH2	2.44	0.51
2:KH:308:SER:OG	2:KH:309:ASN:N	2.44	0.51
5:Ed:86:ASP:HA	5:Ed:121:ILE:O	2.11	0.51
5:Id:132:LEU:HB3	5:Id:145:ILE:HG21	1.93	0.51
2:CH:308:SER:OG	2:CH:309:ASN:N	2.44	0.51
5:ED:95:THR:HA	5:ED:98:ILE:HG22	1.93	0.51
1:HC:130:ARG:O	1:IC:241:HIS:HA	2.11	0.51
3:MK:150:ASP:O	3:MK:152:ARG:NH2	2.44	0.51
5:Ed:147:VAL:HG22	5:Ed:154:VAL:HG22	1.92	0.50
1:FC:217:ALA:HB1	5:Fd:62:ILE:HG21	1.93	0.50
3:JK:150:ASP:O	3:JK:152:ARG:NH2	2.44	0.50
2:AH:276:SER:OG	2:AH:277:ALA:N	2.45	0.50
3:LK:150:ASP:O	3:LK:152:ARG:NH2	2.44	0.50
5:FD:48:VAL:HG23	5:Fd:52:MET:HG3	1.93	0.50
5:JD:98:ILE:HD11	5:JD:128:LEU:HB2	1.93	0.50
2:LH:308:SER:OG	2:LH:309:ASN:N	2.44	0.50
1:CC:84:ASN:ND2	4:CZ:37:ALA:O	2.44	0.50
5:Cd:40:LYS:HA	5:Cd:43:GLU:HG2	1.93	0.50
3:DK:150:ASP:O	3:DK:152:ARG:NH2	2.44	0.50
3:GK:150:ASP:O	3:GK:152:ARG:NH2	2.44	0.50
2:MH:276:SER:OG	2:MH:277:ALA:N	2.45	0.50
5:CD:105:ARG:HB2	5:CD:153:VAL:HG22	1.92	0.50
3:CK:150:ASP:O	3:CK:152:ARG:NH2	2.44	0.50
5:ED:62:ILE:HD11	5:Ed:71:LEU:HD21	1.93	0.50
3:FK:150:ASP:O	3:FK:152:ARG:NH2	2.44	0.50
5:Id:82:ARG:NH2	5:Id:125:ASP:O	2.44	0.50
2:JH:308:SER:OG	2:JH:309:ASN:N	2.44	0.50
5:Ad:40:LYS:HA	5:Ad:43:GLU:HG2	1.93	0.50
5:CD:87:TRP:O	5:CD:120:SER:HA	2.11	0.50
3:EK:150:ASP:O	3:EK:152:ARG:NH2	2.44	0.50
2:HH:314:VAL:HG23	2:HH:338:TYR:HB2	1.94	0.50
2:IH:314:VAL:HG23	2:IH:338:TYR:HB2	1.94	0.50
2:LH:314:VAL:HG23	2:LH:338:TYR:HB2	1.94	0.50
2:MH:355:MET:HE1	4:MZ:35:ALA:HA	1.93	0.50
5:BD:48:VAL:HG23	5:Bd:52:MET:HG2	1.92	0.50
1:EC:239:GLU:HG3	1:DC:133:LYS:HD2	1.93	0.50
5:Ed:109:LEU:HD12	5:Ed:157:ARG:HG2	1.93	0.50
1:HC:93:ILE:HA	5:HD:48:VAL:HG11	1.93	0.50
3:HK:150:ASP:O	3:HK:152:ARG:NH2	2.44	0.50
2:KH:314:VAL:HG23	2:KH:338:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:KK:150:ASP:O	3:KK:152:ARG:NH2	2.44	0.50
5:Md:86:ASP:HA	5:Md:121:ILE:O	2.10	0.50
3:BK:150:ASP:O	3:BK:152:ARG:NH2	2.44	0.50
2:GH:314:VAL:HG23	2:GH:338:TYR:HB2	1.94	0.50
1:HC:267:ALA:HA	5:Hd:61:VAL:HG21	1.94	0.50
1:KC:118:ASN:HB2	2:LH:277:ALA:HA	1.94	0.50
2:LH:276:SER:OG	2:LH:277:ALA:N	2.45	0.50
3:AK:150:ASP:O	3:AK:152:ARG:NH2	2.44	0.50
2:EH:314:VAL:HG23	2:EH:338:TYR:HB2	1.94	0.50
2:AH:314:VAL:HG23	2:AH:338:TYR:HB2	1.94	0.50
5:Ld:70:THR:HA	5:Ld:133:ARG:HE	1.76	0.50
2:MH:308:SER:OG	2:MH:309:ASN:N	2.44	0.50
2:MH:314:VAL:HG23	2:MH:338:TYR:HB2	1.94	0.50
4:W:169:THR:HG23	4:W:182:SER:HB3	1.94	0.50
2:FH:314:VAL:HG23	2:FH:338:TYR:HB2	1.94	0.50
1:GC:264:ALA:H	5:HD:97:ARG:NH2	2.10	0.50
5:Gd:147:VAL:HG22	5:Gd:154:VAL:HG22	1.93	0.50
2:JH:314:VAL:HG23	2:JH:338:TYR:HB2	1.94	0.50
4:P:215:SER:OG	4:P:216:ASP:N	2.45	0.50
4:U:169:THR:HG23	4:U:182:SER:HB3	1.94	0.50
2:BH:308:SER:OG	2:BH:309:ASN:N	2.44	0.50
5:Dd:86:ASP:HA	5:Dd:121:ILE:O	2.11	0.49
5:Dd:105:ARG:NH2	5:DD:130:GLU:OE2	2.44	0.49
5:FD:130:GLU:OE1	5:Fd:107:ARG:NH2	2.34	0.49
3:CK:114:ILE:HB	3:CK:154:ILE:HG12	1.94	0.49
2:EH:351:HIS:ND1	5:Ed:93:GLU:OE1	2.45	0.49
5:HD:119:ILE:HD11	5:HD:135:ILE:HA	1.94	0.49
2:HH:308:SER:OG	2:HH:309:ASN:N	2.44	0.49
2:JH:351:HIS:ND1	5:Jd:93:GLU:OE1	2.45	0.49
3:KK:114:ILE:HB	3:KK:154:ILE:HG12	1.95	0.49
3:LK:114:ILE:HB	3:LK:154:ILE:HG12	1.95	0.49
3:MK:114:ILE:HB	3:MK:154:ILE:HG12	1.94	0.49
4:O:215:SER:OG	4:O:216:ASP:N	2.45	0.49
4:X:169:THR:HG23	4:X:182:SER:HB3	1.94	0.49
4:X:215:SER:OG	4:X:216:ASP:N	2.45	0.49
3:BK:127:LYS:NZ	4:BX:216:ALA:O	2.40	0.49
5:Hd:78:ASN:C	5:Hd:78:ASN:HD22	2.21	0.49
5:ID:56:ALA:O	5:ID:60:LYS:HB2	2.12	0.49
5:Kd:151:SER:OG	5:Kd:152:GLN:N	2.45	0.49
1:LC:255:LEU:HD13	1:MC:240:ILE:HG12	1.94	0.49
5:LD:54:GLU:HA	5:LD:57:LYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AK:114:ILE:HB	3:AK:154:ILE:HG12	1.95	0.49
4:V:169:THR:HG23	4:V:182:SER:HB3	1.94	0.49
4:Y:169:THR:HG23	4:Y:182:SER:HB3	1.94	0.49
5:Cd:117:VAL:HG13	5:Cd:142:LYS:HE3	1.94	0.49
5:Dd:158:TYR:O	5:DD:137:TYR:OH	2.27	0.49
2:FH:308:SER:OG	2:FH:309:ASN:N	2.44	0.49
1:IC:132:TYR:O	1:JC:239:GLU:HA	2.12	0.49
5:JD:95:THR:HA	5:JD:98:ILE:HG22	1.94	0.49
4:Q:215:SER:OG	4:Q:216:ASP:N	2.45	0.49
4:W:215:SER:OG	4:W:216:ASP:N	2.45	0.49
2:BH:314:VAL:HG23	2:BH:338:TYR:HB2	1.94	0.49
3:BK:114:ILE:HB	3:BK:154:ILE:HG12	1.94	0.49
5:CD:52:MET:HE3	5:Cd:52:MET:HE1	1.94	0.49
5:CD:92:GLU:OE2	5:CD:158:TYR:OH	2.30	0.49
2:CH:314:VAL:HG23	2:CH:338:TYR:HB2	1.94	0.49
2:DH:314:VAL:HG23	2:DH:338:TYR:HB2	1.94	0.49
3:DK:114:ILE:HB	3:DK:154:ILE:HG12	1.95	0.49
5:GD:36:ASP:OD1	5:GD:36:ASP:N	2.46	0.49
3:KK:114:ILE:O	3:KK:154:ILE:HA	2.13	0.49
1:LC:118:ASN:HB2	2:MH:277:ALA:HA	1.95	0.49
5:Ld:84:SER:HB2	5:Ld:125:ASP:H	1.78	0.49
3:BK:114:ILE:O	3:BK:154:ILE:HA	2.13	0.49
1:IC:109:VAL:HG13	1:IC:208:GLY:HA3	1.95	0.49
5:LD:37:ALA:HB2	5:Ld:39:ILE:HD13	1.93	0.49
4:N:213:ALA:O	3:BK:185:ARG:NH2	2.45	0.49
4:S:215:SER:OG	4:S:216:ASP:N	2.45	0.49
4:T:169:THR:HG23	4:T:182:SER:HB3	1.94	0.49
3:BK:136:ARG:NH2	3:BK:173:ASP:OD2	2.45	0.49
3:EK:114:ILE:HB	3:EK:154:ILE:HG12	1.95	0.49
2:FH:351:HIS:ND1	5:Fd:93:GLU:OE1	2.46	0.49
1:HC:109:VAL:HG13	1:HC:208:GLY:HA3	1.95	0.49
3:IK:114:ILE:HB	3:IK:154:ILE:HG12	1.95	0.49
5:Id:151:SER:OG	5:Id:152:GLN:N	2.45	0.49
1:JC:132:TYR:O	1:KC:239:GLU:HA	2.12	0.49
3:JK:114:ILE:O	3:JK:154:ILE:HA	2.13	0.49
3:JK:114:ILE:HB	3:JK:154:ILE:HG12	1.95	0.49
2:KH:356:GLN:HG3	4:KZ:37:ALA:HA	1.95	0.49
3:LK:114:ILE:O	3:LK:154:ILE:HA	2.13	0.49
2:MH:321:LEU:HD22	5:Md:118:LEU:HD21	1.94	0.49
3:AK:114:ILE:O	3:AK:154:ILE:HA	2.13	0.49
3:AK:185:ARG:NH2	4:Z:213:ALA:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:169:THR:HG23	4:S:182:SER:HB3	1.94	0.49
5:DD:82:ARG:NH1	5:DD:125:ASP:OD1	2.46	0.49
5:Hd:38:THR:HA	5:Hd:41:LEU:HB2	1.95	0.49
1:IC:126:ARG:NH2	2:JH:274:PRO:O	2.46	0.49
5:Ld:86:ASP:HA	5:Ld:121:ILE:O	2.13	0.49
4:N:215:SER:OG	4:N:216:ASP:N	2.45	0.49
4:Y:215:SER:OG	4:Y:216:ASP:N	2.45	0.49
4:Z:169:THR:HG23	4:Z:182:SER:HB3	1.94	0.49
2:BH:276:SER:OG	2:BH:277:ALA:N	2.45	0.49
3:BK:110:ARG:HH12	4:BZ:35:ALA:HB2	1.78	0.49
3:DK:66:LYS:NZ	4:P:118:GLU:O	2.32	0.49
3:EK:114:ILE:O	3:EK:154:ILE:HA	2.13	0.49
3:GK:114:ILE:O	3:GK:154:ILE:HA	2.13	0.49
3:GK:114:ILE:HB	3:GK:154:ILE:HG12	1.95	0.49
3:GK:136:ARG:NH2	3:GK:173:ASP:OD2	2.45	0.49
3:GK:185:ARG:NH2	4:S:213:ALA:O	2.46	0.49
1:IC:128:SER:HA	1:JC:243:ASP:O	2.13	0.49
1:GC:116:THR:HG22	2:HH:329:MET:HG2	1.95	0.49
5:Id:38:THR:HA	5:Id:41:LEU:HB2	1.95	0.49
5:KD:109:LEU:O	5:KD:157:ARG:HA	2.13	0.49
4:N:169:THR:HG23	4:N:182:SER:HB3	1.94	0.49
4:R:215:SER:OG	4:R:216:ASP:N	2.45	0.49
4:V:215:SER:OG	4:V:216:ASP:N	2.45	0.49
5:CD:129:ALA:HA	5:CD:132:LEU:HD12	1.94	0.49
5:Fd:117:VAL:HG23	5:Fd:142:LYS:HE3	1.94	0.48
5:GD:98:ILE:HD11	5:GD:128:LEU:HB3	1.95	0.48
5:Hd:40:LYS:HA	5:Hd:43:GLU:HG2	1.95	0.48
1:JC:109:VAL:HG13	1:JC:208:GLY:HA3	1.95	0.48
5:Jd:86:ASP:HA	5:Jd:121:ILE:O	2.13	0.48
2:CH:276:SER:OG	2:CH:277:ALA:N	2.45	0.48
3:HK:114:ILE:HB	3:HK:154:ILE:HG12	1.95	0.48
3:HK:136:ARG:NH2	3:HK:173:ASP:OD2	2.45	0.48
5:Id:75:ASN:C	5:Id:75:ASN:HD22	2.21	0.48
5:Jd:74:PRO:HG2	5:Jd:149:PRO:HG3	1.93	0.48
5:Jd:132:LEU:HB3	5:Jd:145:ILE:HG21	1.95	0.48
5:LD:40:LYS:HE3	5:Ld:46:VAL:HG11	1.95	0.48
5:LD:155:GLU:OE2	5:LD:157:ARG:NH1	2.46	0.48
5:MD:37:ALA:HB2	5:Md:39:ILE:HD13	1.95	0.48
3:MK:179:ARG:NH2	4:Y:119:TYR:OH	2.46	0.48
4:MX:114:ALA:HA	4:MX:134:ALA:HB3	1.96	0.48
1:BC:264:ALA:H	5:CD:97:ARG:NH2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:263:ARG:O	5:GD:87:TRP:NE1	2.46	0.48
3:FK:114:ILE:HB	3:FK:154:ILE:HG12	1.95	0.48
4:FX:114:ALA:HA	4:FX:134:ALA:HB3	1.96	0.48
5:Hd:84:SER:HB2	5:Hd:125:ASP:H	1.77	0.48
5:KD:54:GLU:HA	5:KD:57:LYS:HG2	1.95	0.48
4:U:215:SER:OG	4:U:216:ASP:N	2.45	0.48
4:Z:215:SER:OG	4:Z:216:ASP:N	2.45	0.48
5:BD:109:LEU:O	5:BD:157:ARG:HA	2.12	0.48
4:EX:114:ALA:HA	4:EX:134:ALA:HB3	1.95	0.48
4:IX:114:ALA:HA	4:IX:134:ALA:HB3	1.95	0.48
5:Id:34:SER:OG	5:Id:35:ASP:N	2.45	0.48
2:JH:313:TYR:HA	2:JH:338:TYR:O	2.14	0.48
2:LH:313:TYR:HA	2:LH:338:TYR:O	2.14	0.48
3:MK:114:ILE:O	3:MK:154:ILE:HA	2.12	0.48
3:MK:185:ARG:NH2	4:Y:213:ALA:O	2.47	0.48
4:R:169:THR:HG23	4:R:182:SER:HB3	1.94	0.48
4:AX:220:ALA:HB2	5:Ad:77:TYR:H	1.79	0.48
3:CK:114:ILE:O	3:CK:154:ILE:HA	2.13	0.48
1:GC:109:VAL:HG13	1:GC:208:GLY:HA3	1.95	0.48
2:HH:276:SER:OG	2:HH:277:ALA:N	2.45	0.48
2:KH:276:SER:OG	2:KH:277:ALA:N	2.45	0.48
3:LK:136:ARG:NH2	3:LK:173:ASP:OD2	2.45	0.48
4:O:169:THR:HG23	4:O:182:SER:HB3	1.94	0.48
4:T:215:SER:OG	4:T:216:ASP:N	2.45	0.48
4:CX:114:ALA:HA	4:CX:134:ALA:HB3	1.96	0.48
2:GH:313:TYR:HA	2:GH:338:TYR:O	2.14	0.48
5:AD:130:GLU:OE1	5:Ad:107:ARG:NH2	2.47	0.48
4:GX:47:ALA:O	4:GX:66:ALA:HA	2.14	0.48
4:LX:47:ALA:O	4:LX:66:ALA:HA	2.14	0.48
4:LX:114:ALA:HA	4:LX:134:ALA:HB3	1.95	0.48
4:Q:169:THR:HG23	4:Q:182:SER:HB3	1.94	0.48
2:EH:313:TYR:HA	2:EH:338:TYR:O	2.14	0.48
3:FK:114:ILE:O	3:FK:154:ILE:HA	2.13	0.48
2:HH:313:TYR:HA	2:HH:338:TYR:O	2.14	0.48
4:HX:114:ALA:HA	4:HX:134:ALA:HB3	1.96	0.48
2:IH:313:TYR:HA	2:IH:338:TYR:O	2.14	0.48
3:IK:114:ILE:O	3:IK:154:ILE:HA	2.13	0.48
1:JC:116:THR:HA	2:KH:328:SER:O	2.14	0.48
5:Jd:147:VAL:HG22	5:Jd:154:VAL:HG22	1.96	0.48
5:MD:36:ASP:OD1	5:MD:36:ASP:N	2.46	0.48
1:DC:103:HIS:CE1	1:DC:226:VAL:HG21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:ED:129:ALA:HA	5:ED:132:LEU:HD12	1.96	0.48
4:FX:47:ALA:O	4:FX:66:ALA:HA	2.14	0.48
5:Fd:67:LYS:HD2	5:Fd:71:LEU:HD21	1.96	0.48
1:HC:133:LYS:HD2	1:IC:239:GLU:HG3	1.95	0.48
4:P:169:THR:HG23	4:P:182:SER:HB3	1.94	0.48
4:P:220:ILE:HG13	5:Cd:39:ILE:HG23	1.95	0.48
5:BD:130:GLU:OE1	5:Bd:105:ARG:NH2	2.46	0.48
4:BX:114:ALA:HA	4:BX:134:ALA:HB3	1.95	0.48
1:CC:109:VAL:HG13	1:CC:208:GLY:HA3	1.95	0.48
4:DX:69:ALA:HA	4:DX:86:ALA:HB3	1.96	0.48
2:EH:276:SER:OG	2:EH:277:ALA:N	2.45	0.48
1:FC:75:ARG:NH1	5:Fd:36:ASP:OD1	2.47	0.48
3:HK:114:ILE:O	3:HK:154:ILE:HA	2.13	0.48
5:ID:147:VAL:HG22	5:ID:154:VAL:HG12	1.95	0.48
4:JX:114:ALA:HA	4:JX:134:ALA:HB3	1.96	0.48
5:KD:60:LYS:HD3	5:Kd:140:GLY:HA2	1.94	0.48
5:LD:64:PRO:HG2	5:LD:67:LYS:HB2	1.96	0.48
3:MK:145:TRP:CG	5:Md:124:LYS:HZ1	2.32	0.48
3:AK:179:ARG:NH2	4:Z:119:TYR:OH	2.47	0.48
5:CD:95:THR:HA	5:CD:98:ILE:HG22	1.96	0.48
4:CX:47:ALA:O	4:CX:66:ALA:HA	2.14	0.48
1:DC:109:VAL:HG13	1:DC:208:GLY:HA3	1.95	0.48
4:DX:16:ALA:HA	4:DX:35:ALA:H	1.79	0.48
5:Dd:140:GLY:HA2	5:DD:60:LYS:HZ3	1.78	0.48
4:EX:16:ALA:HA	4:EX:35:ALA:H	1.79	0.48
5:Fd:73:ILE:O	5:Fd:133:ARG:NH1	2.47	0.48
5:Hd:86:ASP:HA	5:Hd:121:ILE:O	2.14	0.48
4:IX:47:ALA:O	4:IX:66:ALA:HA	2.14	0.48
4:JX:47:ALA:O	4:JX:66:ALA:HA	2.14	0.48
2:KH:313:TYR:HA	2:KH:338:TYR:O	2.14	0.48
1:LC:109:VAL:HG13	1:LC:208:GLY:HA3	1.95	0.48
1:MC:109:VAL:HG13	1:MC:208:GLY:HA3	1.95	0.48
4:AX:114:ALA:HA	4:AX:134:ALA:HB3	1.95	0.48
2:DH:276:SER:OG	2:DH:277:ALA:N	2.45	0.47
5:ED:91:ILE:HG12	5:ED:156:LEU:HD11	1.95	0.47
1:GC:131:THR:HA	1:HC:240:ILE:O	2.14	0.47
5:HD:58:VAL:HG12	5:Hd:65:PRO:HG3	1.95	0.47
5:Hd:59:GLU:HA	5:Hd:62:ILE:HG22	1.96	0.47
5:ID:130:GLU:OE1	5:Id:105:ARG:NH2	2.46	0.47
5:Jd:59:GLU:HA	5:Jd:62:ILE:HG22	1.95	0.47
1:KC:109:VAL:HG13	1:KC:208:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MX:47:ALA:O	4:MX:66:ALA:HA	2.14	0.47
2:BH:313:TYR:HA	2:BH:338:TYR:O	2.14	0.47
4:BX:47:ALA:O	4:BX:66:ALA:HA	2.14	0.47
1:AC:109:VAL:HG13	1:AC:208:GLY:HA3	1.95	0.47
4:FX:69:ALA:HA	4:FX:86:ALA:HB3	1.96	0.47
5:AD:37:ALA:HB2	5:Ad:39:ILE:HD13	1.95	0.47
4:HX:47:ALA:O	4:HX:66:ALA:HA	2.14	0.47
4:JX:71:ALA:HA	4:JX:87:ALA:HA	1.96	0.47
2:MH:313:TYR:HA	2:MH:338:TYR:O	2.14	0.47
4:AX:69:ALA:HA	4:AX:86:ALA:HB3	1.96	0.47
5:Cd:73:ILE:O	5:Cd:133:ARG:NH1	2.48	0.47
3:DK:114:ILE:O	3:DK:154:ILE:HA	2.13	0.47
5:Dd:115:VAL:HG13	1:CC:117:LEU:HD13	1.97	0.47
4:FX:71:ALA:HA	4:FX:87:ALA:HA	1.97	0.47
4:HX:71:ALA:HA	4:HX:87:ALA:HA	1.97	0.47
5:ID:87:TRP:CZ3	5:ID:94:LEU:HB2	2.49	0.47
3:IK:136:ARG:NH2	3:IK:173:ASP:OD2	2.45	0.47
4:KX:71:ALA:HA	4:KX:87:ALA:HA	1.97	0.47
4:BX:69:ALA:HA	4:BX:86:ALA:HB3	1.96	0.47
2:CH:313:TYR:HA	2:CH:338:TYR:O	2.14	0.47
4:CX:69:ALA:HA	4:CX:86:ALA:HB3	1.96	0.47
4:EX:69:ALA:HA	4:EX:86:ALA:HB3	1.97	0.47
5:Ed:36:ASP:HA	5:Ed:39:ILE:HB	1.97	0.47
3:FK:179:ARG:NH2	4:R:119:TYR:OH	2.47	0.47
5:HD:109:LEU:HD23	5:HD:157:ARG:HE	1.79	0.47
4:IX:71:ALA:HA	4:IX:87:ALA:HA	1.97	0.47
2:JH:276:SER:OG	2:JH:277:ALA:N	2.45	0.47
2:AH:313:TYR:HA	2:AH:338:TYR:O	2.14	0.47
4:KX:47:ALA:O	4:KX:66:ALA:HA	2.14	0.47
1:BC:109:VAL:HG13	1:BC:208:GLY:HA3	1.95	0.47
3:CK:136:ARG:NH2	3:CK:173:ASP:OD2	2.45	0.47
2:FH:313:TYR:HA	2:FH:338:TYR:O	2.14	0.47
4:GX:71:ALA:HA	4:GX:87:ALA:HA	1.97	0.47
3:IK:185:ARG:NH2	4:U:213:ALA:O	2.48	0.47
4:JX:16:ALA:HA	4:JX:35:ALA:H	1.79	0.47
1:KC:131:THR:HA	1:LC:240:ILE:O	2.14	0.47
5:Ld:61:VAL:HG13	5:Ld:62:ILE:HG23	1.96	0.47
2:DH:313:TYR:HA	2:DH:338:TYR:O	2.14	0.47
4:DX:71:ALA:HA	4:DX:87:ALA:HA	1.97	0.47
1:EC:84:ASN:ND2	4:EZ:37:ALA:O	2.47	0.47
1:EC:109:VAL:HG13	1:EC:208:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:122:ALA:HB1	1:FC:139:HIS:HB2	1.96	0.47
4:EX:71:ALA:HA	4:EX:87:ALA:HA	1.97	0.47
5:Ed:48:VAL:O	5:Ed:52:MET:HB2	2.14	0.47
1:GC:88:ARG:HH21	5:Gd:122:SER:HB2	1.80	0.47
4:GX:114:ALA:HA	4:GX:134:ALA:HB3	1.95	0.47
5:Ld:151:SER:OG	5:Ld:152:GLN:N	2.47	0.47
4:MX:69:ALA:HA	4:MX:86:ALA:HB3	1.96	0.47
5:Cd:38:THR:HA	5:Cd:41:LEU:HB2	1.97	0.47
4:DX:47:ALA:O	4:DX:66:ALA:HA	2.14	0.47
4:DX:114:ALA:HA	4:DX:134:ALA:HB3	1.96	0.47
5:Dd:126:GLU:HB2	5:Dd:131:ILE:HG23	1.95	0.47
1:EC:93:ILE:HA	5:ED:48:VAL:HG11	1.96	0.47
1:EC:116:THR:HG22	2:FH:329:MET:HG2	1.97	0.47
1:FC:109:VAL:HG13	1:FC:208:GLY:HA3	1.95	0.47
1:FC:264:ALA:H	5:GD:97:ARG:HH12	1.61	0.47
4:FX:16:ALA:HA	4:FX:35:ALA:H	1.79	0.47
4:IX:16:ALA:HA	4:IX:35:ALA:H	1.79	0.47
5:Kd:130:GLU:OE1	5:Kd:133:ARG:NH2	2.47	0.47
4:LX:69:ALA:HA	4:LX:86:ALA:HB3	1.96	0.47
4:LX:71:ALA:HA	4:LX:87:ALA:HA	1.97	0.47
5:Ld:74:PRO:HG2	5:Ld:149:PRO:HG3	1.97	0.47
4:MX:71:ALA:HA	4:MX:87:ALA:HA	1.97	0.47
5:AD:36:ASP:OD1	5:AD:36:ASP:N	2.48	0.47
4:GX:69:ALA:HA	4:GX:86:ALA:HB3	1.96	0.47
4:HX:69:ALA:HA	4:HX:86:ALA:HB3	1.97	0.47
4:KX:16:ALA:HA	4:KX:35:ALA:H	1.79	0.47
4:LX:16:ALA:HA	4:LX:35:ALA:H	1.79	0.47
4:MX:16:ALA:HA	4:MX:35:ALA:H	1.79	0.47
4:O:119:TYR:OH	3:CK:179:ARG:NH2	2.48	0.47
4:AX:47:ALA:O	4:AX:66:ALA:HA	2.14	0.47
4:BX:16:ALA:HA	4:BX:35:ALA:H	1.79	0.47
4:CX:16:ALA:HA	4:CX:35:ALA:H	1.79	0.47
1:AC:217:ALA:HB1	5:Ad:62:ILE:HG21	1.97	0.47
2:GH:276:SER:OG	2:GH:277:ALA:N	2.45	0.47
4:KX:114:ALA:HA	4:KX:134:ALA:HB3	1.96	0.47
5:Kd:147:VAL:HG22	5:Kd:154:VAL:HG22	1.95	0.47
4:AX:16:ALA:HA	4:AX:35:ALA:H	1.79	0.47
4:EX:47:ALA:O	4:EX:66:ALA:HA	2.14	0.47
5:Fd:86:ASP:HA	5:Fd:121:ILE:O	2.14	0.47
4:BX:71:ALA:HA	4:BX:87:ALA:HA	1.97	0.47
4:CX:71:ALA:HA	4:CX:87:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:GX:16:ALA:HA	4:GX:35:ALA:H	1.79	0.46
1:BC:217:ALA:HB1	5:Bd:62:ILE:HG21	1.97	0.46
5:Bd:48:VAL:O	5:Bd:52:MET:HB2	2.15	0.46
4:CX:61:ALA:HA	4:CX:78:ALA:HB3	1.98	0.46
4:EX:61:ALA:HA	4:EX:78:ALA:HB3	1.98	0.46
5:Gd:75:ASN:C	5:Gd:75:ASN:HD22	2.24	0.46
1:HC:131:THR:HA	1:IC:240:ILE:O	2.15	0.46
4:JX:69:ALA:HA	4:JX:86:ALA:HB3	1.96	0.46
4:GX:61:ALA:HA	4:GX:78:ALA:HB3	1.98	0.46
1:HC:255:LEU:HD13	1:IC:240:ILE:HG12	1.97	0.46
4:HX:16:ALA:HA	4:HX:35:ALA:H	1.79	0.46
4:IX:69:ALA:HA	4:IX:86:ALA:HB3	1.96	0.46
2:JH:356:GLN:HG3	4:JZ:37:ALA:HA	1.97	0.46
4:JX:65:ALA:HA	4:JX:82:ALA:O	2.16	0.46
4:AX:71:ALA:HA	4:AX:87:ALA:HA	1.97	0.46
4:DX:61:ALA:HA	4:DX:78:ALA:HB3	1.98	0.46
5:Dd:48:VAL:O	5:Dd:52:MET:HB2	2.14	0.46
4:FX:61:ALA:HA	4:FX:78:ALA:HB3	1.98	0.46
3:HK:139:VAL:HG22	4:HX:234:ALA:HB1	1.98	0.46
5:KD:107:ARG:HB2	5:KD:155:GLU:HG2	1.97	0.46
4:KX:65:ALA:HA	4:KX:82:ALA:O	2.16	0.46
5:Ld:38:THR:HA	5:Ld:41:LEU:HB2	1.96	0.46
4:V:171:ASN:HB3	4:V:217:ASN:HD22	1.81	0.46
1:AC:84:ASN:ND2	4:AZ:37:ALA:O	2.48	0.46
5:Dd:39:ILE:HD13	5:DD:37:ALA:HB2	1.98	0.46
4:FX:65:ALA:HA	4:FX:82:ALA:O	2.16	0.46
5:Fd:74:PRO:HG2	5:Fd:149:PRO:HG3	1.96	0.46
1:HC:118:ASN:HB2	2:IH:277:ALA:HA	1.97	0.46
4:HX:65:ALA:HA	4:HX:82:ALA:O	2.16	0.46
1:JC:118:ASN:HB2	2:KH:277:ALA:HA	1.97	0.46
5:JD:36:ASP:N	5:JD:36:ASP:OD1	2.48	0.46
4:KX:69:ALA:HA	4:KX:86:ALA:HB3	1.96	0.46
5:Kd:107:ARG:HD3	5:Kd:153:VAL:HG21	1.98	0.46
5:Ld:40:LYS:HA	5:Ld:43:GLU:HG2	1.97	0.46
5:MD:137:TYR:OH	5:Md:158:TYR:O	2.26	0.46
5:Md:117:VAL:HG23	5:Md:142:LYS:HE3	1.98	0.46
4:T:171:ASN:HB3	4:T:217:ASN:HD22	1.81	0.46
4:AX:61:ALA:HA	4:AX:78:ALA:HB3	1.98	0.46
4:BX:61:ALA:HA	4:BX:78:ALA:HB3	1.98	0.46
4:GX:65:ALA:HA	4:GX:82:ALA:O	2.16	0.46
1:JC:203:LYS:NZ	2:KH:286:GLU:OE1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:MX:65:ALA:HA	4:MX:82:ALA:O	2.16	0.46
5:Md:147:VAL:HG12	5:Md:149:PRO:HG3	1.97	0.46
4:Q:171:ASN:HB3	4:Q:217:ASN:HD22	1.81	0.46
1:BC:263:ARG:O	5:CD:87:TRP:NE1	2.49	0.46
3:DK:136:ARG:NH2	3:DK:173:ASP:OD2	2.45	0.46
5:Fd:75:ASN:C	5:Fd:75:ASN:HD22	2.23	0.46
1:GC:126:ARG:HD2	2:HH:276:SER:HA	1.98	0.46
5:Gd:123:THR:OG1	5:Gd:124:LYS:N	2.47	0.46
4:HX:61:ALA:HA	4:HX:78:ALA:HB3	1.98	0.46
3:IK:179:ARG:NH2	4:U:119:TYR:OH	2.49	0.46
4:IX:61:ALA:HA	4:IX:78:ALA:HB3	1.98	0.46
5:JD:86:ASP:HA	5:JD:121:ILE:O	2.15	0.46
5:Jd:75:ASN:HD22	5:Jd:75:ASN:C	2.23	0.46
4:MX:61:ALA:HA	4:MX:78:ALA:HB3	1.98	0.46
4:N:171:ASN:HB3	4:N:217:ASN:HD22	1.81	0.46
4:BX:65:ALA:HA	4:BX:82:ALA:O	2.16	0.46
5:Cd:151:SER:OG	5:Cd:152:GLN:N	2.49	0.46
5:Fd:132:LEU:HB3	5:Fd:145:ILE:HG21	1.97	0.46
5:AD:82:ARG:NH2	5:AD:125:ASP:OD1	2.41	0.46
5:Kd:111:LYS:HD3	5:Kd:111:LYS:HA	1.80	0.46
4:LX:65:ALA:HA	4:LX:82:ALA:O	2.16	0.46
3:MK:136:ARG:NH2	3:MK:173:ASP:OD2	2.45	0.46
4:Z:171:ASN:HB3	4:Z:217:ASN:HD22	1.81	0.46
4:AX:65:ALA:HA	4:AX:82:ALA:O	2.16	0.46
1:CC:264:ALA:O	5:DD:97:ARG:NH1	2.42	0.46
5:ED:56:ALA:O	5:ED:60:LYS:HB2	2.16	0.46
4:X:171:ASN:HB3	4:X:217:ASN:HD22	1.81	0.46
2:BH:355:MET:HE1	4:BZ:35:ALA:HA	1.98	0.46
5:CD:48:VAL:HG23	5:Cd:52:MET:HG3	1.98	0.46
5:Dd:147:VAL:HG22	5:Dd:154:VAL:HG22	1.96	0.46
1:EC:118:ASN:HB2	2:FH:277:ALA:HA	1.98	0.46
2:FH:276:SER:OG	2:FH:277:ALA:N	2.45	0.46
1:GC:264:ALA:H	5:HD:97:ARG:HH22	1.63	0.46
1:KC:116:THR:HG22	2:LH:329:MET:HG2	1.98	0.46
4:U:152:ILE:HA	4:U:155:LEU:HD23	1.98	0.46
4:U:190:MET:HE2	4:U:190:MET:HB3	1.90	0.46
1:HC:116:THR:HA	2:IH:328:SER:O	2.16	0.45
1:IC:118:ASN:HB2	2:JH:277:ALA:HA	1.98	0.45
5:ID:64:PRO:HG2	5:ID:67:LYS:HB2	1.97	0.45
2:IH:276:SER:OG	2:IH:277:ALA:N	2.45	0.45
4:IX:65:ALA:HA	4:IX:82:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:JX:61:ALA:HA	4:JX:78:ALA:HB3	1.98	0.45
5:Jd:34:SER:OG	5:Jd:35:ASP:N	2.48	0.45
5:Jd:84:SER:HB3	5:Jd:125:ASP:H	1.81	0.45
4:N:152:ILE:HA	4:N:155:LEU:HD23	1.98	0.45
4:Y:171:ASN:HB3	4:Y:217:ASN:HD22	1.81	0.45
4:Z:152:ILE:HA	4:Z:155:LEU:HD23	1.98	0.45
4:CX:65:ALA:HA	4:CX:82:ALA:O	2.16	0.45
4:EX:65:ALA:HA	4:EX:82:ALA:O	2.16	0.45
5:HD:43:GLU:HA	5:HD:46:VAL:HG12	1.98	0.45
1:JC:217:ALA:HB1	5:Jd:62:ILE:HG21	1.97	0.45
4:Q:158:TYR:O	4:Q:202:ARG:NH2	2.50	0.45
4:R:171:ASN:HB3	4:R:217:ASN:HD22	1.81	0.45
4:W:171:ASN:HB3	4:W:217:ASN:HD22	1.81	0.45
1:AC:118:ASN:HB2	2:BH:277:ALA:HA	1.99	0.45
3:JK:136:ARG:NH2	3:JK:173:ASP:OD2	2.45	0.45
3:KK:109:PHE:O	3:KK:111:LYS:NZ	2.42	0.45
1:LC:85:LYS:HB2	1:LC:85:LYS:HE2	1.85	0.45
5:Md:52:MET:HE2	5:Md:52:MET:HB2	1.82	0.45
4:O:152:ILE:HA	4:O:155:LEU:HD23	1.98	0.45
4:R:152:ILE:HA	4:R:155:LEU:HD23	1.98	0.45
4:T:152:ILE:HA	4:T:155:LEU:HD23	1.98	0.45
4:U:158:TYR:O	4:U:202:ARG:NH2	2.50	0.45
5:Dd:84:SER:HB2	5:Dd:125:ASP:H	1.81	0.45
1:EC:139:HIS:HB2	1:DC:122:ALA:HB1	1.98	0.45
1:IC:264:ALA:H	5:JD:97:ARG:NH2	2.14	0.45
5:Id:36:ASP:HA	5:Id:39:ILE:HB	1.97	0.45
5:LD:109:LEU:O	5:LD:157:ARG:HA	2.16	0.45
4:R:158:TYR:O	4:R:202:ARG:NH2	2.50	0.45
4:X:152:ILE:HA	4:X:155:LEU:HD23	1.98	0.45
4:X:158:TYR:O	4:X:202:ARG:NH2	2.50	0.45
4:Y:152:ILE:HA	4:Y:155:LEU:HD23	1.98	0.45
4:Z:158:TYR:O	4:Z:202:ARG:NH2	2.50	0.45
1:CC:217:ALA:HB1	5:Cd:62:ILE:HG21	1.99	0.45
5:Dd:107:ARG:NH1	5:Dd:155:GLU:OE1	2.50	0.45
3:EK:153:ILE:HG23	5:Ed:85:VAL:HG22	1.99	0.45
4:LX:61:ALA:HA	4:LX:78:ALA:HB3	1.98	0.45
4:Q:152:ILE:HA	4:Q:155:LEU:HD23	1.98	0.45
5:BD:79:LEU:HB3	5:BD:129:ALA:HB2	1.97	0.45
3:BK:57:MET:O	3:BK:61:ASN:ND2	2.50	0.45
5:Bd:106:PHE:HA	5:Bd:154:VAL:O	2.16	0.45
5:Cd:147:VAL:HG22	5:Cd:154:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DZ:68:ALA:HA	1:DC:72:LEU:HD21	1.98	0.45
5:Ed:73:ILE:O	5:Ed:133:ARG:NH1	2.44	0.45
5:Fd:36:ASP:HA	5:Fd:39:ILE:HB	1.98	0.45
5:HD:137:TYR:O	5:Hd:160:LYS:NZ	2.48	0.45
4:KX:61:ALA:HA	4:KX:78:ALA:HB3	1.98	0.45
4:O:158:TYR:O	4:O:202:ARG:NH2	2.50	0.45
4:T:158:TYR:O	4:T:202:ARG:NH2	2.50	0.45
4:W:158:TYR:O	4:W:202:ARG:NH2	2.50	0.45
3:BK:153:ILE:HG23	5:Bd:85:VAL:HG22	1.98	0.45
5:AD:74:PRO:HD2	5:AD:129:ALA:HB1	1.98	0.45
5:HD:130:GLU:OE2	5:Hd:105:ARG:NH2	2.49	0.45
3:HK:57:MET:O	3:HK:61:ASN:ND2	2.50	0.45
3:JK:57:MET:O	3:JK:61:ASN:ND2	2.50	0.45
1:KC:263:ARG:O	5:LD:87:TRP:NE1	2.50	0.45
4:P:171:ASN:HB3	4:P:217:ASN:HD22	1.81	0.45
5:Fd:130:GLU:OE2	5:Fd:133:ARG:NH2	2.49	0.45
5:GD:95:THR:HA	5:GD:98:ILE:HG22	1.99	0.45
4:KX:190:ALA:HA	4:KX:208:ALA:HB3	1.99	0.45
5:Ld:75:ASN:C	5:Ld:75:ASN:HD22	2.24	0.45
4:O:171:ASN:HB3	4:O:217:ASN:HD22	1.81	0.45
4:S:171:ASN:HB3	4:S:217:ASN:HD22	1.81	0.45
4:V:152:ILE:HA	4:V:155:LEU:HD23	1.98	0.45
5:HD:40:LYS:HE3	5:Hd:46:VAL:HG21	1.98	0.45
3:LK:179:ARG:NH2	4:X:119:TYR:OH	2.50	0.45
5:Md:75:ASN:C	5:Md:75:ASN:HD22	2.24	0.45
3:FK:127:LYS:NZ	4:FX:216:ALA:O	2.40	0.45
5:Hd:36:ASP:HA	5:Hd:39:ILE:HB	1.98	0.45
1:KC:264:ALA:H	5:LD:97:ARG:HH22	1.64	0.45
4:LX:190:ALA:HA	4:LX:208:ALA:HB3	1.99	0.45
5:Md:82:ARG:NH2	5:Md:125:ASP:O	2.50	0.45
4:N:118:GLU:O	3:BK:66:LYS:NZ	2.34	0.45
4:P:152:ILE:HA	4:P:155:LEU:HD23	1.98	0.45
4:U:171:ASN:HB3	4:U:217:ASN:HD22	1.81	0.45
4:W:152:ILE:HA	4:W:155:LEU:HD23	1.98	0.45
4:Y:190:MET:HE2	4:Y:190:MET:HB3	1.90	0.45
5:Ad:73:ILE:O	5:Ad:133:ARG:NH1	2.45	0.45
5:HD:60:LYS:HZ2	5:Hd:141:LYS:H	1.65	0.44
4:JX:190:ALA:HA	4:JX:208:ALA:HB3	1.99	0.44
3:LK:57:MET:O	3:LK:61:ASN:ND2	2.50	0.44
1:GC:153:MET:HE1	1:GC:191:ALA:HB1	2.00	0.44
4:MX:190:ALA:HA	4:MX:208:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:158:TYR:O	4:N:202:ARG:NH2	2.50	0.44
4:V:158:TYR:O	4:V:202:ARG:NH2	2.50	0.44
4:V:226:ASN:O	4:V:228:ARG:NH1	2.51	0.44
3:EK:57:MET:O	3:EK:61:ASN:ND2	2.50	0.44
3:EK:136:ARG:NH2	3:EK:173:ASP:OD2	2.45	0.44
5:HD:67:LYS:HB2	5:HD:67:LYS:HE3	1.86	0.44
2:KH:318:LEU:HD13	2:KH:348:VAL:HG21	2.00	0.44
2:LH:318:LEU:HD13	2:LH:348:VAL:HG21	2.00	0.44
1:MC:217:ALA:HB1	5:Md:62:ILE:HG21	1.99	0.44
4:S:152:ILE:HA	4:S:155:LEU:HD23	1.98	0.44
4:S:226:ASN:O	4:S:228:ARG:NH1	2.51	0.44
4:Y:158:TYR:O	4:Y:202:ARG:NH2	2.50	0.44
1:DC:153:MET:HE1	1:DC:191:ALA:HB1	2.00	0.44
4:DX:65:ALA:HA	4:DX:82:ALA:O	2.16	0.44
1:FC:88:ARG:HH21	5:Fd:122:SER:HB2	1.81	0.44
5:GD:105:ARG:HB3	5:GD:153:VAL:HG23	1.99	0.44
1:HC:264:ALA:H	5:ID:97:ARG:NH2	2.14	0.44
3:IK:186:ARG:NH1	4:IZ:23:ALA:O	2.48	0.44
4:IX:168:ALA:HA	4:IX:186:ALA:HB3	2.00	0.44
4:IX:190:ALA:HA	4:IX:208:ALA:HB3	1.99	0.44
5:KD:94:LEU:O	5:KD:98:ILE:HB	2.18	0.44
4:KX:168:ALA:HA	4:KX:186:ALA:HB3	2.00	0.44
4:P:158:TYR:O	4:P:202:ARG:NH2	2.50	0.44
4:T:226:ASN:O	4:T:228:ARG:NH1	2.51	0.44
5:CD:128:LEU:HA	5:CD:131:ILE:HG12	1.98	0.44
5:Cd:75:ASN:HD22	5:Cd:75:ASN:C	2.25	0.44
1:FC:85:LYS:HB2	1:FC:85:LYS:HE2	1.85	0.44
2:HH:281:LEU:HA	2:HH:284:VAL:HG22	2.00	0.44
1:JC:153:MET:HE1	1:JC:191:ALA:HB1	2.00	0.44
5:JD:37:ALA:HB2	5:Jd:39:ILE:HD13	1.99	0.44
5:Jd:40:LYS:HE3	5:Jd:40:LYS:HB3	1.81	0.44
4:LX:168:ALA:HA	4:LX:186:ALA:HB3	2.00	0.44
2:MH:318:LEU:HD13	2:MH:348:VAL:HG21	2.00	0.44
4:S:158:TYR:O	4:S:202:ARG:NH2	2.50	0.44
3:FK:57:MET:O	3:FK:61:ASN:ND2	2.50	0.44
3:GK:179:ARG:NH2	4:S:119:TYR:OH	2.51	0.44
4:GX:168:ALA:HA	4:GX:186:ALA:HB3	2.00	0.44
3:JK:179:ARG:NH2	4:V:119:TYR:OH	2.51	0.44
4:JX:168:ALA:HA	4:JX:186:ALA:HB3	2.00	0.44
4:MX:168:ALA:HA	4:MX:186:ALA:HB3	2.00	0.44
4:Q:226:ASN:O	4:Q:228:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:85:LYS:HB2	1:CC:85:LYS:HE2	1.85	0.44
1:AC:153:MET:HE1	1:AC:191:ALA:HB1	2.00	0.44
3:DK:57:MET:O	3:DK:61:ASN:ND2	2.50	0.44
1:EC:153:MET:HE1	1:EC:191:ALA:HB1	2.00	0.44
5:GD:60:LYS:HZ2	5:Gd:141:LYS:H	1.65	0.44
4:HX:190:ALA:HA	4:HX:208:ALA:HB3	1.99	0.44
2:JH:281:LEU:HA	2:JH:284:VAL:HG22	2.00	0.44
4:MX:204:ALA:HB3	4:Z:191:THR:HG21	2.00	0.44
4:W:165:VAL:HG12	4:W:205:ALA:HA	2.00	0.44
4:AX:168:ALA:HA	4:AX:186:ALA:HB3	2.00	0.44
4:AX:190:ALA:HA	4:AX:208:ALA:HB3	1.99	0.44
5:CD:109:LEU:HD22	5:CD:157:ARG:HG3	2.00	0.44
5:Dd:68:ASP:OD2	5:Dd:70:THR:OG1	2.31	0.44
3:FK:145:TRP:CG	5:Fd:124:LYS:HZ1	2.36	0.44
3:GK:57:MET:O	3:GK:61:ASN:ND2	2.50	0.44
5:AD:29:PRO:HB2	5:AD:32:ASN:HB2	1.99	0.44
4:HX:168:ALA:HA	4:HX:186:ALA:HB3	2.00	0.44
1:IC:153:MET:HE1	1:IC:191:ALA:HB1	2.00	0.44
2:JH:318:LEU:HD13	2:JH:348:VAL:HG21	2.00	0.44
4:U:165:VAL:HG12	4:U:205:ALA:HA	2.00	0.44
4:W:226:ASN:O	4:W:228:ARG:NH1	2.51	0.44
5:BD:36:ASP:OD1	5:BD:36:ASP:N	2.50	0.44
4:EX:117:ALA:H	4:EX:137:ALA:HA	1.83	0.44
4:FX:219:ALA:HB1	5:Fd:80:GLN:HG3	2.00	0.44
4:GX:117:ALA:H	4:GX:137:ALA:HA	1.83	0.44
4:HX:117:ALA:H	4:HX:137:ALA:HA	1.83	0.44
2:AH:318:LEU:HD13	2:AH:348:VAL:HG21	2.00	0.44
5:Jd:108:VAL:HB	5:Jd:158:TYR:HE2	1.83	0.44
3:KK:136:ARG:NH2	3:KK:173:ASP:OD2	2.45	0.44
5:Kd:40:LYS:HA	5:Kd:43:GLU:HG2	2.00	0.44
3:AK:57:MET:O	3:AK:61:ASN:ND2	2.50	0.44
4:X:226:ASN:O	4:X:228:ARG:NH1	2.51	0.44
4:Y:226:ASN:O	4:Y:228:ARG:NH1	2.51	0.44
1:BC:153:MET:HE1	1:BC:191:ALA:HB1	2.00	0.44
3:CK:156:THR:HG23	5:Cd:82:ARG:HB2	2.00	0.44
2:EH:318:LEU:HD13	2:EH:348:VAL:HG21	2.00	0.43
1:FC:153:MET:HE1	1:FC:191:ALA:HB1	2.00	0.43
4:FX:168:ALA:HA	4:FX:186:ALA:HB3	2.00	0.43
5:HD:95:THR:HA	5:HD:98:ILE:HG12	2.00	0.43
1:IC:263:ARG:O	5:JD:87:TRP:NE1	2.51	0.43
5:Jd:49:SER:O	5:Jd:53:LEU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:118:ASN:HB2	2:CH:277:ALA:HA	2.00	0.43
4:EX:167:ALA:O	4:EX:186:ALA:HB3	2.18	0.43
5:Ed:75:ASN:HD22	5:Ed:75:ASN:C	2.24	0.43
2:FH:281:LEU:HA	2:FH:284:VAL:HG22	2.00	0.43
2:FH:318:LEU:HD13	2:FH:348:VAL:HG21	2.00	0.43
5:HD:34:SER:O	5:Hd:32:ASN:ND2	2.43	0.43
5:HD:36:ASP:OD1	5:Hd:34:SER:OG	2.35	0.43
5:Id:59:GLU:HA	5:Id:62:ILE:HG22	1.99	0.43
4:KX:117:ALA:H	4:KX:137:ALA:HA	1.83	0.43
1:LC:116:THR:HG22	2:MH:329:MET:HG2	1.99	0.43
4:Q:219:ILE:HD12	4:Q:219:ILE:HA	1.91	0.43
4:X:190:MET:HE2	4:X:190:MET:HB3	1.90	0.43
4:BX:168:ALA:HA	4:BX:186:ALA:HB3	2.00	0.43
5:Bd:73:ILE:O	5:Bd:133:ARG:NH1	2.50	0.43
2:DH:318:LEU:HD22	2:DH:350:TRP:HA	2.01	0.43
2:DH:318:LEU:HD13	2:DH:348:VAL:HG21	2.00	0.43
4:DX:117:ALA:H	4:DX:137:ALA:HA	1.83	0.43
4:EX:168:ALA:HA	4:EX:186:ALA:HB3	2.00	0.43
4:FX:117:ALA:H	4:FX:137:ALA:HA	1.84	0.43
2:GH:318:LEU:HD13	2:GH:348:VAL:HG21	2.00	0.43
1:HC:153:MET:HE1	1:HC:191:ALA:HB1	2.00	0.43
1:IC:85:LYS:HB2	1:IC:85:LYS:HE2	1.85	0.43
5:Id:147:VAL:HG12	5:Id:149:PRO:HG3	2.00	0.43
5:Jd:117:VAL:HG23	5:Jd:142:LYS:HE2	1.99	0.43
5:Kd:109:LEU:HD12	5:Kd:157:ARG:HG2	2.00	0.43
2:LH:281:LEU:HA	2:LH:284:VAL:HG22	2.00	0.43
5:Ld:108:VAL:HA	5:Ld:156:LEU:O	2.19	0.43
4:MX:117:ALA:H	4:MX:137:ALA:HA	1.83	0.43
4:P:190:MET:HE2	4:P:190:MET:HB3	1.90	0.43
4:S:165:VAL:HG12	4:S:205:ALA:HA	2.00	0.43
4:U:226:ASN:O	4:U:228:ARG:NH1	2.51	0.43
5:CD:36:ASP:OD1	5:CD:36:ASP:N	2.52	0.43
4:DX:167:ALA:O	4:DX:186:ALA:HB3	2.18	0.43
5:FD:94:LEU:O	5:FD:97:ARG:N	2.50	0.43
4:FX:167:ALA:O	4:FX:186:ALA:HB3	2.18	0.43
1:GC:267:ALA:HA	5:Gd:61:VAL:HG21	2.00	0.43
1:JC:102:GLU:OE1	1:JC:103:HIS:N	2.52	0.43
1:KC:153:MET:HE1	1:KC:191:ALA:HB1	2.00	0.43
5:KD:130:GLU:OE1	5:Kd:107:ARG:HD2	2.19	0.43
4:LX:117:ALA:H	4:LX:137:ALA:HA	1.83	0.43
1:MC:153:MET:HE1	1:MC:191:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:190:MET:HE2	4:N:190:MET:HB3	1.90	0.43
4:R:226:ASN:O	4:R:228:ARG:NH1	2.51	0.43
5:BD:91:ILE:HG13	5:BD:135:ILE:HD11	2.00	0.43
1:CC:153:MET:HE1	1:CC:191:ALA:HB1	2.00	0.43
2:CH:318:LEU:HD22	2:CH:350:TRP:HA	2.01	0.43
4:CX:168:ALA:HA	4:CX:186:ALA:HB3	2.00	0.43
1:DC:102:GLU:OE1	1:DC:103:HIS:N	2.52	0.43
1:AC:102:GLU:OE1	1:AC:103:HIS:N	2.52	0.43
4:DX:190:ALA:HA	4:DX:208:ALA:HB3	1.99	0.43
1:EC:213:ARG:HA	1:EC:213:ARG:HD2	1.89	0.43
3:FK:109:PHE:O	3:FK:111:LYS:NZ	2.42	0.43
1:GC:102:GLU:OE1	1:GC:103:HIS:N	2.52	0.43
4:GX:167:ALA:O	4:GX:186:ALA:HB3	2.18	0.43
4:GX:190:ALA:HA	4:GX:208:ALA:HB3	1.99	0.43
2:AH:318:LEU:HD22	2:AH:350:TRP:HA	2.01	0.43
5:Jd:72:THR:HG23	5:Jd:73:ILE:HG13	1.99	0.43
1:KC:102:GLU:OE1	1:KC:103:HIS:N	2.52	0.43
2:LH:318:LEU:HD22	2:LH:350:TRP:HA	2.01	0.43
4:Y:165:VAL:HG12	4:Y:205:ALA:HA	2.00	0.43
2:BH:318:LEU:HD22	2:BH:350:TRP:HA	2.01	0.43
4:CX:190:ALA:HA	4:CX:208:ALA:HB3	1.99	0.43
1:EC:102:GLU:OE1	1:EC:103:HIS:N	2.52	0.43
2:FH:318:LEU:HD22	2:FH:350:TRP:HA	2.01	0.43
5:Gd:40:LYS:HA	5:Gd:43:GLU:HG2	2.00	0.43
1:HC:102:GLU:OE1	1:HC:103:HIS:N	2.52	0.43
4:JX:117:ALA:H	4:JX:137:ALA:HA	1.83	0.43
2:MH:318:LEU:HD22	2:MH:350:TRP:HA	2.01	0.43
3:AK:109:PHE:O	3:AK:111:LYS:NZ	2.42	0.43
4:AX:117:ALA:H	4:AX:137:ALA:HA	1.83	0.43
2:BH:318:LEU:HD13	2:BH:348:VAL:HG21	2.00	0.43
4:CX:167:ALA:O	4:CX:186:ALA:HB3	2.18	0.43
4:DX:168:ALA:HA	4:DX:186:ALA:HB3	2.00	0.43
1:FC:123:GLN:OE1	1:GC:252:LEU:HD21	2.19	0.43
5:FD:109:LEU:O	5:FD:157:ARG:HA	2.19	0.43
3:FK:116:VAL:O	3:FK:156:THR:HA	2.19	0.43
3:GK:116:VAL:O	3:GK:156:THR:HA	2.19	0.43
4:HX:167:ALA:O	4:HX:186:ALA:HB3	2.18	0.43
2:IH:318:LEU:HD13	2:IH:348:VAL:HG21	2.00	0.43
3:IK:57:MET:O	3:IK:61:ASN:ND2	2.50	0.43
4:IX:117:ALA:H	4:IX:137:ALA:HA	1.83	0.43
4:KX:167:ALA:O	4:KX:186:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LX:167:ALA:O	4:LX:186:ALA:HB3	2.18	0.43
1:MC:102:GLU:OE1	1:MC:103:HIS:N	2.52	0.43
3:AK:136:ARG:NH2	3:AK:173:ASP:OD2	2.45	0.43
4:N:226:ASN:O	4:N:228:ARG:NH1	2.51	0.43
4:O:226:ASN:O	4:O:228:ARG:NH1	2.51	0.43
4:P:226:ASN:O	4:P:228:ARG:NH1	2.51	0.43
4:BX:190:ALA:HA	4:BX:208:ALA:HB3	1.99	0.43
1:CC:213:ARG:HA	1:CC:213:ARG:HD2	1.89	0.43
2:CH:318:LEU:HD13	2:CH:348:VAL:HG21	2.00	0.43
5:DD:55:MET:HE2	5:DD:55:MET:HB2	1.74	0.43
5:Dd:62:ILE:HG21	1:DC:217:ALA:HB1	2.01	0.43
1:EC:185:LYS:HZ2	1:EC:185:LYS:HG2	1.64	0.43
2:EH:318:LEU:HD22	2:EH:350:TRP:HA	2.01	0.43
1:FC:102:GLU:OE1	1:FC:103:HIS:N	2.52	0.43
3:GK:145:TRP:CG	5:Gd:124:LYS:HZ1	2.36	0.43
1:HC:203:LYS:NZ	2:IH:286:GLU:OE1	2.45	0.43
1:JC:213:ARG:HA	1:JC:213:ARG:HD2	1.88	0.43
4:JX:167:ALA:O	4:JX:186:ALA:HB3	2.18	0.43
1:CC:102:GLU:OE1	1:CC:103:HIS:N	2.52	0.43
3:CK:99:LEU:HD23	3:CK:99:LEU:HA	1.90	0.43
4:CX:117:ALA:H	4:CX:137:ALA:HA	1.83	0.43
5:ED:43:GLU:HA	5:ED:46:VAL:HG12	2.01	0.43
3:EK:116:VAL:O	3:EK:156:THR:HA	2.19	0.43
4:FX:190:ALA:HA	4:FX:208:ALA:HB3	1.99	0.43
2:HH:318:LEU:HD13	2:HH:348:VAL:HG21	2.00	0.43
5:ID:36:ASP:OD1	5:ID:36:ASP:N	2.52	0.43
2:AH:281:LEU:HA	2:AH:284:VAL:HG22	2.00	0.43
2:KH:318:LEU:HD22	2:KH:350:TRP:HA	2.01	0.43
5:Kd:36:ASP:HA	5:Kd:39:ILE:HB	2.00	0.43
3:LK:78:ILE:HB	3:LK:180:VAL:HG22	2.01	0.43
5:MD:40:LYS:HB3	5:Md:42:ALA:HB1	2.01	0.43
3:MK:78:ILE:HB	3:MK:180:VAL:HG22	2.01	0.43
3:MK:116:VAL:O	3:MK:156:THR:HA	2.19	0.43
4:Q:190:MET:HE2	4:Q:190:MET:HB3	1.90	0.43
5:Dd:52:MET:HE1	1:DC:206:PHE:HE2	1.83	0.43
4:EX:190:ALA:HA	4:EX:208:ALA:HB3	1.99	0.43
4:EX:220:ALA:HB2	5:Ed:77:TYR:H	1.84	0.43
3:FK:136:ARG:NH2	3:FK:173:ASP:OD2	2.45	0.43
5:Fd:82:ARG:HA	5:Fd:127:SER:HA	2.00	0.43
1:IC:102:GLU:OE1	1:IC:103:HIS:N	2.52	0.43
5:ID:109:LEU:HD22	5:ID:157:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:IX:167:ALA:O	4:IX:186:ALA:HB3	2.18	0.43
5:JD:73:ILE:HA	5:JD:74:PRO:HD3	1.81	0.43
2:JH:318:LEU:HD22	2:JH:350:TRP:HA	2.01	0.43
3:JK:116:VAL:O	3:JK:156:THR:HA	2.19	0.43
2:KH:281:LEU:HA	2:KH:284:VAL:HG22	2.00	0.43
3:KK:116:VAL:O	3:KK:156:THR:HA	2.19	0.43
3:MK:153:ILE:HG23	5:Md:85:VAL:HG22	2.00	0.43
3:AK:116:VAL:O	3:AK:156:THR:HA	2.19	0.43
3:AK:156:THR:HG23	5:Ad:82:ARG:HB2	2.01	0.43
4:N:165:VAL:HG12	4:N:205:ALA:HA	2.00	0.43
5:Ad:70:THR:HA	5:Ad:133:ARG:HE	1.83	0.43
2:BH:351:HIS:ND1	5:Bd:93:GLU:OE2	2.52	0.43
4:BX:117:ALA:H	4:BX:137:ALA:HA	1.83	0.43
4:BX:167:ALA:O	4:BX:186:ALA:HB3	2.18	0.43
2:DH:281:LEU:HA	2:DH:284:VAL:HG22	2.00	0.42
2:DH:329:MET:HG2	1:CC:116:THR:HG22	2.01	0.42
1:EC:85:LYS:HB2	1:EC:85:LYS:HE2	1.85	0.42
2:HH:318:LEU:HD22	2:HH:350:TRP:HA	2.01	0.42
2:IH:281:LEU:HA	2:IH:284:VAL:HG22	2.00	0.42
3:JK:99:LEU:HD23	3:JK:99:LEU:HA	1.90	0.42
5:Kd:143:ALA:HA	5:Kd:157:ARG:O	2.17	0.42
4:MX:167:ALA:O	4:MX:186:ALA:HB3	2.18	0.42
3:AK:78:ILE:HB	3:AK:180:VAL:HG22	2.01	0.42
3:DK:116:VAL:O	3:DK:156:THR:HA	2.19	0.42
5:ED:94:LEU:HD23	5:ED:98:ILE:HB	2.00	0.42
2:GH:318:LEU:HD22	2:GH:350:TRP:HA	2.01	0.42
3:HK:116:VAL:O	3:HK:156:THR:HA	2.19	0.42
5:ID:133:ARG:HH11	5:Id:157:ARG:HH11	1.67	0.42
5:Id:130:GLU:OE1	5:Id:133:ARG:NH2	2.47	0.42
4:JX:220:ALA:HB2	5:Jd:77:TYR:H	1.84	0.42
2:AH:329:MET:HG2	1:MC:116:THR:HG22	2.01	0.42
1:KC:213:ARG:HA	1:KC:213:ARG:HD2	1.89	0.42
5:KD:130:GLU:HA	5:KD:133:ARG:HB3	2.01	0.42
1:BC:102:GLU:OE1	1:BC:103:HIS:N	2.52	0.42
1:FC:233:VAL:HG12	1:FC:242:ILE:HA	2.02	0.42
3:GK:78:ILE:HB	3:GK:180:VAL:HG22	2.01	0.42
3:GK:139:VAL:HG22	4:GX:234:ALA:HB1	2.01	0.42
3:HK:78:ILE:HB	3:HK:180:VAL:HG22	2.01	0.42
5:Id:146:HIS:HB2	5:Id:155:GLU:HG2	2.00	0.42
3:JK:78:ILE:HB	3:JK:180:VAL:HG22	2.01	0.42
3:JK:139:VAL:HG22	4:JX:234:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:KK:78:ILE:HB	3:KK:180:VAL:HG22	2.01	0.42
1:LC:153:MET:HE1	1:LC:191:ALA:HB1	2.00	0.42
3:LK:99:LEU:HD23	3:LK:99:LEU:HA	1.90	0.42
4:Q:165:VAL:HG12	4:Q:205:ALA:HA	2.00	0.42
3:BK:116:VAL:O	3:BK:156:THR:HA	2.19	0.42
3:CK:186:ARG:NH1	4:CZ:23:ALA:O	2.50	0.42
1:EC:264:ALA:H	5:FD:97:ARG:NH2	2.16	0.42
5:ED:60:LYS:HA	5:ED:60:LYS:HD2	1.91	0.42
3:FK:78:ILE:HB	3:FK:180:VAL:HG22	2.01	0.42
4:GZ:41:ALA:HB3	4:GZ:44:ALA:HB2	2.02	0.42
5:Gd:151:SER:OG	5:Gd:152:GLN:N	2.53	0.42
3:HK:99:LEU:HD23	3:HK:99:LEU:HA	1.90	0.42
2:IH:356:GLN:HG3	4:IZ:37:ALA:HA	2.00	0.42
3:IK:78:ILE:HB	3:IK:180:VAL:HG22	2.01	0.42
4:JZ:41:ALA:HB3	4:JZ:44:ALA:HB2	2.02	0.42
4:KZ:41:ALA:HB3	4:KZ:44:ALA:HB2	2.02	0.42
5:Kd:86:ASP:HA	5:Kd:121:ILE:O	2.19	0.42
1:LC:102:GLU:OE1	1:LC:103:HIS:N	2.52	0.42
4:P:219:ILE:HD12	4:P:219:ILE:HA	1.90	0.42
4:Z:165:VAL:HG12	4:Z:205:ALA:HA	2.00	0.42
3:BK:78:ILE:HB	3:BK:180:VAL:HG22	2.01	0.42
1:CC:265:ALA:HB3	5:DD:86:ASP:H	1.84	0.42
3:DK:137:SER:O	3:DK:141:SER:OG	2.38	0.42
1:GC:233:VAL:HG12	1:GC:242:ILE:HA	2.02	0.42
5:GD:27:LYS:HE2	5:GD:27:LYS:HB2	1.68	0.42
4:HZ:41:ALA:HB3	4:HZ:44:ALA:HB2	2.02	0.42
3:IK:99:LEU:HD23	3:IK:99:LEU:HA	1.90	0.42
4:IZ:41:ALA:HB3	4:IZ:44:ALA:HB2	2.02	0.42
5:Kd:40:LYS:HB3	5:Kd:40:LYS:HE2	1.79	0.42
3:AK:110:ARG:HH12	4:AZ:35:ALA:HB2	1.85	0.42
4:O:165:VAL:HG12	4:O:205:ALA:HA	2.00	0.42
4:R:165:VAL:HG12	4:R:205:ALA:HA	2.00	0.42
4:Z:226:ASN:O	4:Z:228:ARG:NH1	2.51	0.42
5:Ad:160:LYS:HD3	5:Ad:160:LYS:HA	1.85	0.42
1:BC:116:THR:HG22	2:CH:329:MET:HG2	2.02	0.42
1:CC:263:ARG:HG3	5:Cd:62:ILE:HD11	2.01	0.42
1:EC:233:VAL:HG12	1:EC:242:ILE:HA	2.01	0.42
5:HD:81:ALA:HB3	5:HD:128:LEU:HD12	2.02	0.42
1:IC:75:ARG:HA	1:IC:75:ARG:HD2	1.95	0.42
1:IC:213:ARG:HA	1:IC:213:ARG:HD2	1.89	0.42
5:ID:48:VAL:HG23	5:Id:52:MET:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IH:318:LEU:HD22	2:IH:350:TRP:HA	2.01	0.42
5:JD:105:ARG:HB3	5:JD:153:VAL:HG23	2.01	0.42
5:LD:92:GLU:OE2	5:LD:158:TYR:OH	2.30	0.42
3:LK:116:VAL:O	3:LK:156:THR:HA	2.19	0.42
4:V:165:VAL:HG12	4:V:205:ALA:HA	2.00	0.42
4:X:165:VAL:HG12	4:X:205:ALA:HA	2.00	0.42
4:AX:167:ALA:O	4:AX:186:ALA:HB3	2.18	0.42
2:CH:281:LEU:HA	2:CH:284:VAL:HG22	2.00	0.42
1:DC:233:VAL:HG12	1:DC:242:ILE:HA	2.02	0.42
3:EK:78:ILE:HB	3:EK:180:VAL:HG22	2.01	0.42
2:GH:281:LEU:HA	2:GH:284:VAL:HG22	2.00	0.42
5:Gd:74:PRO:HG2	5:Gd:149:PRO:HG3	2.02	0.42
1:HC:233:VAL:HG12	1:HC:242:ILE:HA	2.02	0.42
5:HD:71:LEU:O	5:HD:133:ARG:NE	2.53	0.42
5:Jd:70:THR:HA	5:Jd:133:ARG:HE	1.84	0.42
3:KK:57:MET:O	3:KK:61:ASN:ND2	2.50	0.42
5:Kd:55:MET:HE3	5:Kd:55:MET:HB3	1.87	0.42
5:MD:60:LYS:HD3	5:Md:140:GLY:HA2	2.02	0.42
5:Bd:87:TRP:CD2	5:Bd:94:LEU:HD13	2.55	0.42
5:Cd:106:PHE:HA	5:Cd:154:VAL:O	2.20	0.42
3:DK:151:SER:OG	3:DK:153:ILE:O	2.38	0.42
3:EK:151:SER:OG	3:EK:153:ILE:O	2.38	0.42
4:FZ:41:ALA:HB3	4:FZ:44:ALA:HB2	2.02	0.42
1:LC:95:ASP:OD2	1:LC:98:SER:OG	2.32	0.42
5:MD:48:VAL:HG23	5:Md:52:MET:HE3	2.01	0.42
4:T:165:VAL:HG12	4:T:205:ALA:HA	2.00	0.42
3:BK:151:SER:OG	3:BK:153:ILE:O	2.38	0.42
3:CK:116:VAL:O	3:CK:156:THR:HA	2.19	0.42
1:AC:122:ALA:HB1	1:BC:139:HIS:HB2	2.02	0.42
5:Dd:73:ILE:O	5:Dd:133:ARG:NH1	2.48	0.42
3:FK:151:SER:OG	3:FK:153:ILE:O	2.38	0.42
3:IK:109:PHE:O	3:IK:111:LYS:NZ	2.42	0.42
3:IK:116:VAL:O	3:IK:156:THR:HA	2.19	0.42
1:KC:95:ASP:OD2	1:KC:98:SER:OG	2.32	0.42
4:LZ:41:ALA:HB3	4:LZ:44:ALA:HB2	2.02	0.42
4:P:165:VAL:HG12	4:P:205:ALA:HA	2.00	0.42
3:BK:137:SER:O	3:BK:141:SER:OG	2.38	0.42
3:CK:57:MET:O	3:CK:61:ASN:ND2	2.50	0.42
3:CK:78:ILE:HB	3:CK:180:VAL:HG22	2.01	0.42
3:CK:151:SER:OG	3:CK:153:ILE:O	2.38	0.42
5:GD:73:ILE:HA	5:GD:74:PRO:HD3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Gd:53:LEU:HD21	4:T:174:SER:HA	2.01	0.42
1:IC:233:VAL:HG12	1:IC:242:ILE:HA	2.02	0.42
3:KK:179:ARG:NH2	4:W:119:TYR:OH	2.53	0.42
5:Kd:132:LEU:HB3	5:Kd:145:ILE:HG21	2.02	0.42
1:LC:213:ARG:HA	1:LC:213:ARG:HD2	1.88	0.42
4:P:161:SER:HG	4:P:233:TRP:CD1	2.38	0.42
4:R:190:MET:HE2	4:R:190:MET:HB3	1.90	0.42
5:BD:93:GLU:O	5:BD:97:ARG:HG3	2.19	0.42
3:DK:78:ILE:HB	3:DK:180:VAL:HG22	2.01	0.41
2:EH:281:LEU:HA	2:EH:284:VAL:HG22	2.00	0.41
5:FD:36:ASP:N	5:FD:36:ASP:OD1	2.49	0.41
2:GH:343:SER:OG	2:GH:345:VAL:O	2.38	0.41
3:GK:99:LEU:HD23	3:GK:99:LEU:HA	1.90	0.41
3:GK:151:SER:OG	3:GK:153:ILE:O	2.38	0.41
5:AD:97:ARG:HA	5:AD:100:LYS:HG2	2.02	0.41
5:HD:27:LYS:HB2	5:HD:27:LYS:HE3	1.79	0.41
5:HD:65:PRO:HD3	5:Hd:71:LEU:HD13	2.01	0.41
2:HH:343:SER:OG	2:HH:345:VAL:O	2.38	0.41
5:Id:108:VAL:HG12	5:Id:156:LEU:HB3	2.03	0.41
1:JC:95:ASP:OD2	1:JC:98:SER:OG	2.32	0.41
1:JC:126:ARG:HG3	1:KC:246:VAL:HG22	2.01	0.41
1:JC:233:VAL:HG12	1:JC:242:ILE:HA	2.01	0.41
5:MD:73:ILE:HA	5:MD:74:PRO:HD3	1.82	0.41
3:AK:151:SER:OG	3:AK:153:ILE:O	2.38	0.41
4:O:219:ILE:HD12	4:O:219:ILE:HA	1.91	0.41
5:Ad:38:THR:HA	5:Ad:41:LEU:HB2	2.01	0.41
1:BC:255:LEU:HD13	1:CC:240:ILE:HG12	2.02	0.41
2:BH:281:LEU:HA	2:BH:284:VAL:HG22	2.00	0.41
2:CH:346:LEU:HD23	2:CH:346:LEU:HA	1.93	0.41
1:DC:79:ILE:HD12	1:DC:195:LEU:HD13	2.02	0.41
1:AC:240:ILE:HG12	1:MC:255:LEU:HD13	2.02	0.41
2:DH:346:LEU:HD23	2:DH:346:LEU:HA	1.93	0.41
5:Gd:38:THR:HA	5:Gd:41:LEU:HB2	2.02	0.41
5:Gd:40:LYS:HB3	5:Gd:40:LYS:HE2	1.74	0.41
5:Gd:52:MET:HE3	5:Gd:52:MET:HB3	1.77	0.41
2:HH:346:LEU:HD23	2:HH:346:LEU:HA	1.93	0.41
2:AH:343:SER:OG	2:AH:345:VAL:O	2.38	0.41
5:Jd:82:ARG:NE	5:Jd:125:ASP:OD2	2.43	0.41
4:MZ:41:ALA:HB3	4:MZ:44:ALA:HB2	2.02	0.41
5:Md:59:GLU:HA	5:Md:62:ILE:HG22	2.01	0.41
4:Z:190:MET:HE2	4:Z:190:MET:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CH:343:SER:OG	2:CH:345:VAL:O	2.38	0.41
5:DD:36:ASP:OD1	5:DD:36:ASP:N	2.50	0.41
1:AC:124:SER:HA	1:BC:247:LEU:O	2.20	0.41
3:DK:139:VAL:HG22	4:DX:234:ALA:HB1	2.02	0.41
1:EC:79:ILE:HD12	1:EC:195:LEU:HD13	2.03	0.41
4:EZ:41:ALA:HB3	4:EZ:44:ALA:HB2	2.02	0.41
1:FC:118:ASN:HB2	2:GH:277:ALA:HA	2.00	0.41
3:GK:67:VAL:HG22	3:GK:76:ILE:HG22	2.03	0.41
1:HC:95:ASP:OD2	1:HC:98:SER:OG	2.32	0.41
1:HC:213:ARG:HA	1:HC:213:ARG:HD2	1.89	0.41
3:HK:179:ARG:NH2	4:T:119:TYR:OH	2.54	0.41
2:IH:343:SER:OG	2:IH:345:VAL:O	2.38	0.41
3:IK:67:VAL:HG22	3:IK:76:ILE:HG22	2.03	0.41
1:KC:79:ILE:HD12	1:KC:195:LEU:HD13	2.03	0.41
5:Kd:73:ILE:O	5:Kd:133:ARG:NH1	2.44	0.41
5:LD:95:THR:HA	5:LD:98:ILE:HG22	2.01	0.41
2:LH:343:SER:OG	2:LH:345:VAL:O	2.38	0.41
2:MH:343:SER:OG	2:MH:345:VAL:O	2.38	0.41
5:Ad:86:ASP:HA	5:Ad:121:ILE:O	2.21	0.41
2:BH:343:SER:OG	2:BH:345:VAL:O	2.38	0.41
1:CC:79:ILE:HD12	1:CC:195:LEU:HD13	2.03	0.41
1:CC:233:VAL:HG12	1:CC:242:ILE:HA	2.01	0.41
2:DH:343:SER:OG	2:DH:345:VAL:O	2.39	0.41
1:EC:214:LYS:O	1:EC:218:MET:HB2	2.21	0.41
2:EH:343:SER:OG	2:EH:345:VAL:O	2.38	0.41
3:EK:67:VAL:HG22	3:EK:76:ILE:HG22	2.03	0.41
5:Ed:115:VAL:HG13	1:DC:117:LEU:HD13	2.03	0.41
1:FC:79:ILE:HD12	1:FC:195:LEU:HD13	2.02	0.41
2:FH:343:SER:OG	2:FH:345:VAL:O	2.39	0.41
3:GK:137:SER:O	3:GK:141:SER:OG	2.38	0.41
2:JH:343:SER:OG	2:JH:345:VAL:O	2.38	0.41
5:KD:58:VAL:HG11	5:Kd:59:GLU:HB3	2.01	0.41
1:MC:214:LYS:O	1:MC:218:MET:HB2	2.21	0.41
3:MK:151:SER:OG	3:MK:153:ILE:O	2.38	0.41
1:AC:214:LYS:O	1:AC:218:MET:HB2	2.21	0.41
1:FC:214:LYS:O	1:FC:218:MET:HB2	2.21	0.41
5:Hd:70:THR:HA	5:Hd:133:ARG:HE	1.86	0.41
5:KD:48:VAL:HG23	5:Kd:52:MET:HG2	2.03	0.41
2:MH:281:LEU:HA	2:MH:284:VAL:HG22	2.00	0.41
3:CK:67:VAL:HG22	3:CK:76:ILE:HG22	2.03	0.41
1:AC:231:LEU:HB2	1:AC:244:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:122:ALA:HB1	1:GC:139:HIS:HB2	2.03	0.41
1:FC:231:LEU:HB2	1:FC:244:ASP:O	2.21	0.41
5:HD:36:ASP:OD1	5:HD:36:ASP:N	2.52	0.41
5:HD:48:VAL:HG23	5:Hd:52:MET:HG2	2.01	0.41
3:HK:151:SER:OG	3:HK:153:ILE:O	2.38	0.41
1:JC:79:ILE:HD12	1:JC:195:LEU:HD13	2.03	0.41
1:JC:214:LYS:O	1:JC:218:MET:HB2	2.21	0.41
5:KD:107:ARG:O	5:KD:155:GLU:HA	2.21	0.41
2:KH:343:SER:OG	2:KH:345:VAL:O	2.39	0.41
1:LC:79:ILE:HD12	1:LC:195:LEU:HD13	2.03	0.41
5:Ld:39:ILE:HD12	4:Y:220:ILE:HG13	2.03	0.41
3:MK:99:LEU:HD23	3:MK:99:LEU:HA	1.90	0.41
4:N:161:SER:HG	4:N:233:TRP:CD1	2.38	0.41
4:S:190:MET:HE2	4:S:190:MET:HB3	1.90	0.41
4:V:190:MET:HE2	4:V:190:MET:HB3	1.90	0.41
4:AX:160:ALA:HB3	4:AX:178:ALA:O	2.21	0.41
1:BC:233:VAL:HG12	1:BC:242:ILE:HA	2.02	0.41
5:Dd:120:SER:H	5:Dd:138:GLN:NE2	2.18	0.41
4:EX:160:ALA:HB3	4:EX:178:ALA:O	2.21	0.41
1:IC:79:ILE:HD12	1:IC:195:LEU:HD13	2.03	0.41
1:IC:231:LEU:HB2	1:IC:244:ASP:O	2.21	0.41
4:JX:160:ALA:HB3	4:JX:178:ALA:O	2.21	0.41
1:KC:79:ILE:HA	1:KC:82:GLN:HB3	2.03	0.41
1:LC:214:LYS:O	1:LC:218:MET:HB2	2.21	0.41
4:N:219:ILE:HD12	4:N:219:ILE:HA	1.91	0.41
1:BC:231:LEU:HB2	1:BC:244:ASP:O	2.21	0.41
4:BX:160:ALA:HB3	4:BX:178:ALA:O	2.21	0.41
1:DC:214:LYS:O	1:DC:218:MET:HB2	2.21	0.41
1:FC:213:ARG:HA	1:FC:213:ARG:HD2	1.89	0.41
4:FX:160:ALA:HB3	4:FX:178:ALA:O	2.21	0.41
1:GC:79:ILE:HD12	1:GC:195:LEU:HD13	2.03	0.41
1:HC:231:LEU:HB2	1:HC:244:ASP:O	2.21	0.41
1:IC:95:ASP:OD2	1:IC:98:SER:OG	2.32	0.41
5:ID:130:GLU:O	5:ID:134:ASP:HB2	2.20	0.41
1:JC:79:ILE:HA	1:JC:82:GLN:HB3	2.03	0.41
1:KC:231:LEU:HB2	1:KC:244:ASP:O	2.21	0.41
2:KH:273:ILE:HD13	2:KH:273:ILE:HA	1.97	0.41
4:KX:160:ALA:HB3	4:KX:178:ALA:O	2.21	0.41
1:MC:233:VAL:HG12	1:MC:242:ILE:HA	2.01	0.41
5:Md:34:SER:OG	5:Md:35:ASP:N	2.54	0.41
4:Z:219:ILE:HD12	4:Z:219:ILE:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ad:40:LYS:HB3	5:Ad:40:LYS:HE2	1.89	0.41
1:BC:79:ILE:HD12	1:BC:195:LEU:HD13	2.03	0.41
1:BC:214:LYS:O	1:BC:218:MET:HB2	2.21	0.41
1:CC:185:LYS:HZ2	1:CC:185:LYS:HG2	1.63	0.41
1:AC:233:VAL:HG12	1:AC:242:ILE:HA	2.02	0.41
4:DX:160:ALA:HB3	4:DX:178:ALA:O	2.21	0.41
4:DZ:41:ALA:HB3	4:DZ:44:ALA:HB2	2.02	0.41
1:EC:79:ILE:HA	1:EC:82:GLN:HB3	2.02	0.41
1:EC:117:LEU:HD13	5:Fd:115:VAL:HG13	2.02	0.41
3:EK:137:SER:O	3:EK:141:SER:OG	2.38	0.41
3:EK:179:ARG:NH2	4:Q:119:TYR:OH	2.54	0.41
5:Ed:45:ALA:HA	5:Ed:48:VAL:HG12	2.03	0.41
1:GC:214:LYS:O	1:GC:218:MET:HB2	2.21	0.41
5:GD:107:ARG:O	5:GD:155:GLU:HA	2.21	0.41
1:HC:79:ILE:HD12	1:HC:195:LEU:HD13	2.03	0.41
1:IC:79:ILE:HA	1:IC:82:GLN:HB3	2.03	0.41
1:IC:214:LYS:O	1:IC:218:MET:HB2	2.21	0.41
5:JD:137:TYR:OH	5:Jd:158:TYR:O	2.38	0.41
1:KC:214:LYS:O	1:KC:218:MET:HB2	2.21	0.41
1:KC:233:VAL:HG12	1:KC:242:ILE:HA	2.01	0.41
5:KD:60:LYS:NZ	5:Kd:143:ALA:O	2.53	0.41
1:LC:231:LEU:HB2	1:LC:244:ASP:O	2.21	0.41
1:LC:233:VAL:HG12	1:LC:242:ILE:HA	2.01	0.41
3:LK:151:SER:OG	3:LK:153:ILE:O	2.38	0.41
1:MC:231:LEU:HB2	1:MC:244:ASP:O	2.21	0.41
3:AK:66:LYS:NZ	4:Z:118:GLU:O	2.41	0.41
3:AK:67:VAL:HG22	3:AK:76:ILE:HG22	2.03	0.41
4:AZ:41:ALA:HB3	4:AZ:44:ALA:HB2	2.02	0.41
4:BZ:41:ALA:HB3	4:BZ:44:ALA:HB2	2.02	0.41
5:Bd:143:ALA:HA	5:Bd:157:ARG:O	2.20	0.41
1:CC:75:ARG:HA	1:CC:75:ARG:HD2	1.94	0.41
1:DC:79:ILE:HA	1:DC:82:GLN:HB3	2.03	0.41
1:DC:95:ASP:OD2	1:DC:98:SER:OG	2.32	0.41
1:EC:228:HIS:O	1:EC:228:HIS:ND1	2.53	0.41
5:Ed:58:VAL:HA	5:Ed:61:VAL:HG12	2.03	0.41
1:GC:213:ARG:HA	1:GC:213:ARG:HD2	1.88	0.41
4:GZ:48:ALA:O	4:GZ:61:ALA:N	2.51	0.41
4:JZ:48:ALA:O	4:JZ:61:ALA:N	2.50	0.41
5:KD:62:ILE:HB	5:Kd:67:LYS:HE2	2.03	0.41
3:KK:137:SER:O	3:KK:141:SER:OG	2.38	0.41
3:LK:109:PHE:O	3:LK:111:LYS:NZ	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LX:160:ALA:HB3	4:LX:178:ALA:O	2.21	0.41
4:MX:160:ALA:HB3	4:MX:178:ALA:O	2.21	0.41
4:X:227:ARG:HH11	4:X:227:ARG:HD3	1.76	0.41
4:Y:219:ILE:HD12	4:Y:219:ILE:HA	1.91	0.41
5:BD:132:LEU:HA	5:BD:135:ILE:HG22	2.01	0.41
4:CZ:41:ALA:HB3	4:CZ:44:ALA:HB2	2.02	0.41
1:AC:213:ARG:NH2	5:AD:59:GLU:OE1	2.53	0.40
5:Dd:58:VAL:HA	5:Dd:61:VAL:HG12	2.03	0.40
1:EC:231:LEU:HB2	1:EC:244:ASP:O	2.21	0.40
2:EH:346:LEU:HD23	2:EH:346:LEU:HA	1.93	0.40
4:EZ:48:ALA:O	4:EZ:61:ALA:N	2.50	0.40
5:GD:132:LEU:HD23	5:GD:132:LEU:HA	1.87	0.40
5:Gd:73:ILE:O	5:Gd:133:ARG:NH1	2.52	0.40
1:HC:79:ILE:HA	1:HC:82:GLN:HB3	2.03	0.40
4:IX:160:ALA:HB3	4:IX:178:ALA:O	2.21	0.40
3:KK:67:VAL:HG22	3:KK:76:ILE:HG22	2.03	0.40
4:KZ:48:ALA:O	4:KZ:61:ALA:N	2.51	0.40
3:LK:139:VAL:HG22	4:LX:234:ALA:HB1	2.03	0.40
1:MC:79:ILE:HA	1:MC:82:GLN:HB3	2.03	0.40
3:MK:57:MET:O	3:MK:61:ASN:ND2	2.50	0.40
5:Md:68:ASP:OD2	5:Md:70:THR:N	2.54	0.40
3:AK:44:ARG:HE	3:AK:45:VAL:HG13	1.86	0.40
1:BC:79:ILE:HA	1:BC:82:GLN:HB3	2.03	0.40
1:CC:79:ILE:HA	1:CC:82:GLN:HB3	2.03	0.40
1:CC:214:LYS:O	1:CC:218:MET:HB2	2.21	0.40
4:CX:160:ALA:HB3	4:CX:178:ALA:O	2.21	0.40
5:DD:79:LEU:HB3	5:DD:129:ALA:HB2	2.03	0.40
3:DK:67:VAL:HG22	3:DK:76:ILE:HG22	2.03	0.40
3:EK:186:ARG:NH1	4:EZ:23:ALA:O	2.53	0.40
3:IK:151:SER:OG	3:IK:153:ILE:O	2.38	0.40
5:Jd:82:ARG:HA	5:Jd:127:SER:HA	2.02	0.40
1:LC:79:ILE:HA	1:LC:82:GLN:HB3	2.03	0.40
1:LC:133:LYS:HD2	1:MC:239:GLU:HG3	2.02	0.40
1:MC:79:ILE:HD12	1:MC:195:LEU:HD13	2.03	0.40
3:BK:44:ARG:HE	3:BK:45:VAL:HG13	1.87	0.40
1:CC:231:LEU:HB2	1:CC:244:ASP:O	2.21	0.40
5:ED:36:ASP:N	5:ED:36:ASP:OD1	2.51	0.40
5:ED:107:ARG:O	5:ED:155:GLU:HA	2.22	0.40
4:GX:160:ALA:HB3	4:GX:178:ALA:O	2.21	0.40
5:ID:115:VAL:HA	5:ID:116:PRO:HD3	1.93	0.40
2:MH:346:LEU:HD23	2:MH:346:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:MK:137:SER:O	3:MK:141:SER:OG	2.38	0.40
4:N:220:ILE:HG13	5:Ad:39:ILE:HG23	2.03	0.40
4:X:219:ILE:HD12	4:X:219:ILE:HA	1.91	0.40
5:Cd:45:ALA:HA	5:Cd:48:VAL:HG12	2.03	0.40
1:AC:95:ASP:OD2	1:AC:98:SER:OG	2.32	0.40
1:AC:185:LYS:HZ2	1:AC:185:LYS:HG2	1.64	0.40
1:FC:79:ILE:HA	1:FC:82:GLN:HB3	2.03	0.40
3:FK:67:VAL:HG22	3:FK:76:ILE:HG22	2.03	0.40
1:GC:231:LEU:HB2	1:GC:244:ASP:O	2.21	0.40
5:GD:82:ARG:HE	5:GD:127:SER:HB3	1.87	0.40
5:HD:27:LYS:HZ2	3:HK:100:ASN:CG	2.25	0.40
1:IC:116:THR:HA	2:JH:328:SER:O	2.21	0.40
3:IK:137:SER:O	3:IK:141:SER:OG	2.38	0.40
1:JC:88:ARG:HH21	5:Jd:122:SER:HB2	1.86	0.40
5:KD:130:GLU:OE2	5:Kd:105:ARG:NH2	2.54	0.40
5:Kd:84:SER:HB2	5:Kd:125:ASP:H	1.86	0.40
5:LD:64:PRO:HA	5:LD:65:PRO:HD3	1.93	0.40
3:LK:67:VAL:HG22	3:LK:76:ILE:HG22	2.03	0.40
4:Y:227:ARG:HH11	4:Y:227:ARG:HD3	1.76	0.40
2:CH:273:ILE:HD13	2:CH:273:ILE:HA	1.97	0.40
1:AC:79:ILE:HD12	1:AC:195:LEU:HD13	2.03	0.40
1:AC:85:LYS:HB2	1:AC:85:LYS:HE2	1.85	0.40
1:HC:214:LYS:O	1:HC:218:MET:HB2	2.21	0.40
3:IK:44:ARG:HE	3:IK:45:VAL:HG13	1.86	0.40
5:Id:52:MET:HE3	5:Id:52:MET:HB3	1.89	0.40
3:JK:44:ARG:HE	3:JK:45:VAL:HG13	1.86	0.40
4:W:227:ARG:HH11	4:W:227:ARG:HD3	1.76	0.40
4:BX:220:ALA:HB2	5:Bd:77:TYR:H	1.87	0.40
5:CD:64:PRO:HA	5:CD:65:PRO:HD3	1.97	0.40
3:CK:137:SER:O	3:CK:141:SER:OG	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	BC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	CC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	DC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	EC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	FC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	GC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	HC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	IC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	JC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	KC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	LC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
1	MC	196/303 (65%)	186 (95%)	10 (5%)	0	100	100
2	AH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	BH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	CH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
2	DH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	EH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	FH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	GH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	HH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	IH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	JH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	KH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
2	LH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
2	MH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
3	AK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	BK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	CK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	DK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	FK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	GK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	HK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	IK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	JK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	KK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	LK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
3	MK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
4	AX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	AY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	AZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	BX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	BY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	BZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	CX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	CY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	CZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	DX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	DY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	DZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	EX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	EY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	EZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	FX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	FY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	FZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	GX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	GY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	GZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	HX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	HY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	HZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	IX	226/579 (39%)	200 (88%)	26 (12%)	0	100	100
4	IY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	IZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	JX	226/579 (39%)	200 (88%)	26 (12%)	0	100	100
4	JY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	JZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	KX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	KY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	KZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	LX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	LY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	LZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	MX	226/579 (39%)	201 (89%)	25 (11%)	0	100	100
4	MY	50/579 (9%)	40 (80%)	10 (20%)	0	100	100
4	MZ	68/579 (12%)	60 (88%)	8 (12%)	0	100	100
4	N	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	O	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	P	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	Q	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	R	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	S	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	T	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	U	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	V	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	W	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	X	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	Y	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
4	Z	134/579 (23%)	123 (92%)	11 (8%)	0	100	100
5	AD	133/163 (82%)	120 (90%)	13 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ad	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
5	BD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
5	Bd	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
5	CD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
5	Cd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	DD	133/163 (82%)	124 (93%)	9 (7%)	0	100	100
5	Dd	136/163 (83%)	128 (94%)	8 (6%)	0	100	100
5	ED	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
5	Ed	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	FD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
5	Fd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	GD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
5	Gd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
5	HD	133/163 (82%)	123 (92%)	10 (8%)	0	100	100
5	Hd	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
5	ID	133/163 (82%)	122 (92%)	11 (8%)	0	100	100
5	Id	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	JD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
5	Jd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
5	KD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
5	Kd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
5	LD	133/163 (82%)	124 (93%)	9 (7%)	0	100	100
5	Ld	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
5	MD	133/163 (82%)	124 (93%)	9 (7%)	0	100	100
5	Md	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
All	All	15288/45435 (34%)	13993 (92%)	1295 (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	AC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	BC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	CC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	DC	169/257 (66%)	157 (93%)	12 (7%)	13	38
1	EC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	FC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	GC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	HC	169/257 (66%)	156 (92%)	13 (8%)	12	37
1	IC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	JC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	KC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	LC	169/257 (66%)	155 (92%)	14 (8%)	10	34
1	MC	169/257 (66%)	155 (92%)	14 (8%)	10	34
2	AH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	BH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	CH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	DH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	EH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	FH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	GH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	HH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	IH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	JH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	KH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	LH	75/300 (25%)	69 (92%)	6 (8%)	11	35
2	MH	75/300 (25%)	69 (92%)	6 (8%)	11	35
3	AK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	BK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	CK	126/163 (77%)	118 (94%)	8 (6%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	EK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	FK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	GK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	HK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	IK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	JK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	KK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	LK	126/163 (77%)	118 (94%)	8 (6%)	16	42
3	MK	126/163 (77%)	118 (94%)	8 (6%)	16	42
4	N	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	O	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	P	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	Q	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	R	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	S	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	T	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	U	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	V	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	W	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	X	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	Y	118/203 (58%)	111 (94%)	7 (6%)	18	44
4	Z	118/203 (58%)	111 (94%)	7 (6%)	18	44
5	AD	116/139 (84%)	116 (100%)	0	100	100
5	Ad	119/139 (86%)	119 (100%)	0	100	100
5	BD	116/139 (84%)	116 (100%)	0	100	100
5	Bd	119/139 (86%)	119 (100%)	0	100	100
5	CD	116/139 (84%)	116 (100%)	0	100	100
5	Cd	119/139 (86%)	118 (99%)	1 (1%)	73	77
5	DD	116/139 (84%)	116 (100%)	0	100	100
5	Dd	119/139 (86%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	ED	116/139 (84%)	116 (100%)	0	100	100
5	Ed	119/139 (86%)	118 (99%)	1 (1%)	73	77
5	FD	116/139 (84%)	116 (100%)	0	100	100
5	Fd	119/139 (86%)	118 (99%)	1 (1%)	73	77
5	GD	116/139 (84%)	116 (100%)	0	100	100
5	Gd	119/139 (86%)	118 (99%)	1 (1%)	73	77
5	HD	116/139 (84%)	116 (100%)	0	100	100
5	Hd	119/139 (86%)	118 (99%)	1 (1%)	73	77
5	ID	116/139 (84%)	116 (100%)	0	100	100
5	Id	119/139 (86%)	118 (99%)	1 (1%)	73	77
5	JD	116/139 (84%)	116 (100%)	0	100	100
5	Jd	119/139 (86%)	118 (99%)	1 (1%)	73	77
5	KD	116/139 (84%)	116 (100%)	0	100	100
5	Kd	119/139 (86%)	119 (100%)	0	100	100
5	LD	116/139 (84%)	116 (100%)	0	100	100
5	Ld	119/139 (86%)	118 (99%)	1 (1%)	73	77
5	MD	116/139 (84%)	116 (100%)	0	100	100
5	Md	119/139 (86%)	118 (99%)	1 (1%)	73	77
All	All	9399/15613 (60%)	8938 (95%)	461 (5%)	24	48

All (461) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AC	61	GLU
1	AC	69	GLN
1	AC	81	GLU
1	AC	85	LYS
1	AC	102	GLU
1	AC	103	HIS
1	AC	104	ASN
1	AC	133	LYS
1	AC	136	LYS
1	AC	185	LYS
1	AC	194	ILE
1	AC	214	LYS
1	AC	218	MET

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Mol	Chain	Res	Type
1	AC	259	SER
2	DH	294	ARG
2	DH	297	VAL
2	DH	314	VAL
2	DH	315	ARG
2	DH	343	SER
2	DH	360	GLU
3	DK	52	THR
3	DK	57	MET
3	DK	60	LEU
3	DK	101	GLU
3	DK	107	LYS
3	DK	139	VAL
3	DK	141	SER
3	DK	180	VAL
1	EC	61	GLU
1	EC	69	GLN
1	EC	81	GLU
1	EC	85	LYS
1	EC	102	GLU
1	EC	103	HIS
1	EC	104	ASN
1	EC	133	LYS
1	EC	136	LYS
1	EC	185	LYS
1	EC	194	ILE
1	EC	214	LYS
1	EC	218	MET
1	EC	259	SER
2	EH	294	ARG
2	EH	297	VAL
2	EH	314	VAL
2	EH	315	ARG
2	EH	343	SER
2	EH	360	GLU
3	EK	52	THR
3	EK	57	MET
3	EK	60	LEU
3	EK	101	GLU
3	EK	107	LYS
3	EK	139	VAL
3	EK	141	SER

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Mol	Chain	Res	Type
3	EK	180	VAL
5	Ed	75	ASN
1	FC	61	GLU
1	FC	69	GLN
1	FC	81	GLU
1	FC	85	LYS
1	FC	102	GLU
1	FC	103	HIS
1	FC	104	ASN
1	FC	133	LYS
1	FC	136	LYS
1	FC	185	LYS
1	FC	194	ILE
1	FC	214	LYS
1	FC	218	MET
1	FC	259	SER
2	FH	294	ARG
2	FH	297	VAL
2	FH	314	VAL
2	FH	315	ARG
2	FH	343	SER
2	FH	360	GLU
3	FK	52	THR
3	FK	57	MET
3	FK	60	LEU
3	FK	101	GLU
3	FK	107	LYS
3	FK	139	VAL
3	FK	141	SER
3	FK	180	VAL
5	Fd	75	ASN
1	GC	61	GLU
1	GC	69	GLN
1	GC	81	GLU
1	GC	85	LYS
1	GC	102	GLU
1	GC	103	HIS
1	GC	104	ASN
1	GC	133	LYS
1	GC	136	LYS
1	GC	185	LYS
1	GC	194	ILE

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Mol	Chain	Res	Type
1	GC	214	LYS
1	GC	218	MET
1	GC	259	SER
2	GH	294	ARG
2	GH	297	VAL
2	GH	314	VAL
2	GH	315	ARG
2	GH	343	SER
2	GH	360	GLU
3	GK	52	THR
3	GK	57	MET
3	GK	60	LEU
3	GK	101	GLU
3	GK	107	LYS
3	GK	139	VAL
3	GK	141	SER
3	GK	180	VAL
5	Gd	75	ASN
1	HC	61	GLU
1	HC	69	GLN
1	HC	81	GLU
1	HC	85	LYS
1	HC	102	GLU
1	HC	103	HIS
1	HC	133	LYS
1	HC	136	LYS
1	HC	185	LYS
1	HC	194	ILE
1	HC	214	LYS
1	HC	218	MET
1	HC	259	SER
2	HH	294	ARG
2	HH	297	VAL
2	HH	314	VAL
2	HH	315	ARG
2	HH	343	SER
2	HH	360	GLU
3	HK	52	THR
3	HK	57	MET
3	HK	60	LEU
3	HK	101	GLU
3	HK	107	LYS

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Mol	Chain	Res	Type
3	HK	139	VAL
3	HK	141	SER
3	HK	180	VAL
5	Hd	78	ASN
1	IC	61	GLU
1	IC	69	GLN
1	IC	81	GLU
1	IC	85	LYS
1	IC	102	GLU
1	IC	103	HIS
1	IC	104	ASN
1	IC	133	LYS
1	IC	136	LYS
1	IC	185	LYS
1	IC	194	ILE
1	IC	214	LYS
1	IC	218	MET
1	IC	259	SER
2	IH	294	ARG
2	IH	297	VAL
2	IH	314	VAL
2	IH	315	ARG
2	IH	343	SER
2	IH	360	GLU
3	IK	52	THR
3	IK	57	MET
3	IK	60	LEU
3	IK	101	GLU
3	IK	107	LYS
3	IK	139	VAL
3	IK	141	SER
3	IK	180	VAL
5	Id	75	ASN
1	JC	61	GLU
1	JC	69	GLN
1	JC	81	GLU
1	JC	85	LYS
1	JC	102	GLU
1	JC	103	HIS
1	JC	104	ASN
1	JC	133	LYS
1	JC	136	LYS

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Mol	Chain	Res	Type
1	JC	185	LYS
1	JC	194	ILE
1	JC	214	LYS
1	JC	218	MET
1	JC	259	SER
2	JH	294	ARG
2	JH	297	VAL
2	JH	314	VAL
2	JH	315	ARG
2	JH	343	SER
2	JH	360	GLU
3	JK	52	THR
3	JK	57	MET
3	JK	60	LEU
3	JK	101	GLU
3	JK	107	LYS
3	JK	139	VAL
3	JK	141	SER
3	JK	180	VAL
2	AH	294	ARG
2	AH	297	VAL
2	AH	314	VAL
2	AH	315	ARG
2	AH	343	SER
2	AH	360	GLU
5	Jd	75	ASN
1	KC	61	GLU
1	KC	69	GLN
1	KC	81	GLU
1	KC	85	LYS
1	KC	102	GLU
1	KC	103	HIS
1	KC	104	ASN
1	KC	133	LYS
1	KC	136	LYS
1	KC	185	LYS
1	KC	194	ILE
1	KC	214	LYS
1	KC	218	MET
1	KC	259	SER
2	KH	294	ARG
2	KH	297	VAL

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Mol	Chain	Res	Type
2	KH	314	VAL
2	KH	315	ARG
2	KH	343	SER
2	KH	360	GLU
3	KK	52	THR
3	KK	57	MET
3	KK	60	LEU
3	KK	101	GLU
3	KK	107	LYS
3	KK	139	VAL
3	KK	141	SER
3	KK	180	VAL
1	LC	61	GLU
1	LC	69	GLN
1	LC	81	GLU
1	LC	85	LYS
1	LC	102	GLU
1	LC	103	HIS
1	LC	104	ASN
1	LC	133	LYS
1	LC	136	LYS
1	LC	185	LYS
1	LC	194	ILE
1	LC	214	LYS
1	LC	218	MET
1	LC	259	SER
2	LH	294	ARG
2	LH	297	VAL
2	LH	314	VAL
2	LH	315	ARG
2	LH	343	SER
2	LH	360	GLU
3	LK	52	THR
3	LK	57	MET
3	LK	60	LEU
3	LK	101	GLU
3	LK	107	LYS
3	LK	139	VAL
3	LK	141	SER
3	LK	180	VAL
5	Ld	75	ASN
1	MC	61	GLU

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Mol	Chain	Res	Type
1	MC	69	GLN
1	MC	81	GLU
1	MC	85	LYS
1	MC	102	GLU
1	MC	103	HIS
1	MC	104	ASN
1	MC	133	LYS
1	MC	136	LYS
1	MC	185	LYS
1	MC	194	ILE
1	MC	214	LYS
1	MC	218	MET
1	MC	259	SER
2	MH	294	ARG
2	MH	297	VAL
2	MH	314	VAL
2	MH	315	ARG
2	MH	343	SER
2	MH	360	GLU
3	MK	52	THR
3	MK	57	MET
3	MK	60	LEU
3	MK	101	GLU
3	MK	107	LYS
3	MK	139	VAL
3	MK	141	SER
3	MK	180	VAL
5	Md	75	ASN
3	AK	52	THR
3	AK	57	MET
3	AK	60	LEU
3	AK	101	GLU
3	AK	107	LYS
3	AK	139	VAL
3	AK	141	SER
3	AK	180	VAL
4	N	102	LYS
4	N	106	ILE
4	N	112	GLN
4	N	122	THR
4	N	162	THR
4	N	165	VAL

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Mol	Chain	Res	Type
4	N	190	MET
4	O	102	LYS
4	O	106	ILE
4	O	112	GLN
4	O	122	THR
4	O	162	THR
4	O	165	VAL
4	O	190	MET
4	P	102	LYS
4	P	106	ILE
4	P	112	GLN
4	P	122	THR
4	P	162	THR
4	P	165	VAL
4	P	190	MET
4	Q	102	LYS
4	Q	106	ILE
4	Q	112	GLN
4	Q	122	THR
4	Q	162	THR
4	Q	165	VAL
4	Q	190	MET
4	R	102	LYS
4	R	106	ILE
4	R	112	GLN
4	R	122	THR
4	R	162	THR
4	R	165	VAL
4	R	190	MET
4	S	102	LYS
4	S	106	ILE
4	S	112	GLN
4	S	122	THR
4	S	162	THR
4	S	165	VAL
4	S	190	MET
4	T	102	LYS
4	T	106	ILE
4	T	112	GLN
4	T	122	THR
4	T	162	THR
4	T	165	VAL

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Mol	Chain	Res	Type
4	T	190	MET
4	U	102	LYS
4	U	106	ILE
4	U	112	GLN
4	U	122	THR
4	U	162	THR
4	U	165	VAL
4	U	190	MET
4	V	102	LYS
4	V	106	ILE
4	V	112	GLN
4	V	122	THR
4	V	162	THR
4	V	165	VAL
4	V	190	MET
4	W	102	LYS
4	W	106	ILE
4	W	112	GLN
4	W	122	THR
4	W	162	THR
4	W	165	VAL
4	W	190	MET
4	X	102	LYS
4	X	106	ILE
4	X	112	GLN
4	X	122	THR
4	X	162	THR
4	X	165	VAL
4	X	190	MET
4	Y	102	LYS
4	Y	106	ILE
4	Y	112	GLN
4	Y	122	THR
4	Y	162	THR
4	Y	165	VAL
4	Y	190	MET
4	Z	102	LYS
4	Z	106	ILE
4	Z	112	GLN
4	Z	122	THR
4	Z	162	THR
4	Z	165	VAL

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Mol	Chain	Res	Type
4	Z	190	MET
1	BC	61	GLU
1	BC	69	GLN
1	BC	81	GLU
1	BC	85	LYS
1	BC	102	GLU
1	BC	103	HIS
1	BC	104	ASN
1	BC	133	LYS
1	BC	136	LYS
1	BC	185	LYS
1	BC	194	ILE
1	BC	214	LYS
1	BC	218	MET
1	BC	259	SER
2	BH	294	ARG
2	BH	297	VAL
2	BH	314	VAL
2	BH	315	ARG
2	BH	343	SER
2	BH	360	GLU
3	BK	52	THR
3	BK	57	MET
3	BK	60	LEU
3	BK	101	GLU
3	BK	107	LYS
3	BK	139	VAL
3	BK	141	SER
3	BK	180	VAL
1	CC	61	GLU
1	CC	69	GLN
1	CC	81	GLU
1	CC	85	LYS
1	CC	102	GLU
1	CC	103	HIS
1	CC	104	ASN
1	CC	133	LYS
1	CC	136	LYS
1	CC	185	LYS
1	CC	194	ILE
1	CC	214	LYS
1	CC	218	MET

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Mol	Chain	Res	Type
1	CC	259	SER
2	CH	294	ARG
2	CH	297	VAL
2	CH	314	VAL
2	CH	315	ARG
2	CH	343	SER
2	CH	360	GLU
3	CK	52	THR
3	CK	57	MET
3	CK	60	LEU
3	CK	101	GLU
3	CK	107	LYS
3	CK	139	VAL
3	CK	141	SER
3	CK	180	VAL
5	Cd	75	ASN
1	DC	61	GLU
1	DC	69	GLN
1	DC	81	GLU
1	DC	85	LYS
1	DC	102	GLU
1	DC	133	LYS
1	DC	136	LYS
1	DC	185	LYS
1	DC	194	ILE
1	DC	214	LYS
1	DC	218	MET
1	DC	259	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
5	Dd	75	ASN
1	EC	97	ASN
1	EC	123	GLN
1	EC	139	HIS
5	Ed	75	ASN
1	FC	115	ASN
1	FC	139	HIS
1	FC	192	ASN
1	FC	241	HIS
5	Fd	75	ASN

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Mol	Chain	Res	Type
1	GC	97	ASN
1	GC	103	HIS
1	GC	139	HIS
1	GC	241	HIS
5	GD	80	GLN
3	GK	87	GLN
5	AD	80	GLN
5	Gd	75	ASN
1	HC	139	HIS
1	HC	192	ASN
5	Hd	31	ASN
5	Hd	75	ASN
5	Hd	78	ASN
1	IC	115	ASN
1	IC	139	HIS
1	IC	241	HIS
1	JC	97	ASN
1	JC	123	GLN
1	JC	139	HIS
5	Jd	75	ASN
1	KC	97	ASN
1	KC	139	HIS
1	KC	192	ASN
5	KD	31	ASN
5	Kd	80	GLN
1	LC	139	HIS
5	LD	80	GLN
3	LK	87	GLN
5	Ld	75	ASN
1	MC	139	HIS
5	MD	138	GLN
3	MK	87	GLN
5	Md	32	ASN
5	Md	75	ASN
4	N	141	ASN
4	N	156	ASN
4	N	183	GLN
4	O	141	ASN
4	O	150	ASN
4	O	156	ASN
4	O	183	GLN
4	P	141	ASN

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Mol	Chain	Res	Type
4	P	149	ASN
4	P	150	ASN
4	P	156	ASN
4	P	183	GLN
4	Q	141	ASN
4	Q	149	ASN
4	Q	150	ASN
4	Q	156	ASN
4	Q	183	GLN
4	R	141	ASN
4	R	149	ASN
4	R	156	ASN
4	R	183	GLN
4	S	141	ASN
4	S	150	ASN
4	S	156	ASN
4	S	183	GLN
4	T	141	ASN
4	T	150	ASN
4	T	156	ASN
4	T	183	GLN
4	U	156	ASN
4	U	183	GLN
4	V	149	ASN
4	V	150	ASN
4	V	156	ASN
4	V	183	GLN
4	W	141	ASN
4	W	150	ASN
4	W	156	ASN
4	W	183	GLN
4	X	141	ASN
4	X	149	ASN
4	X	150	ASN
4	X	156	ASN
4	X	183	GLN
4	Y	141	ASN
4	Y	149	ASN
4	Y	150	ASN
4	Y	156	ASN
4	Y	183	GLN
4	Z	141	ASN

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Mol	Chain	Res	Type
4	Z	149	ASN
4	Z	156	ASN
4	Z	183	GLN
1	CC	97	ASN
1	CC	123	GLN
1	CC	139	HIS
5	CD	69	ASN
5	Cd	75	ASN
1	DC	97	ASN
1	DC	104	ASN
1	DC	115	ASN
1	DC	139	HIS

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.

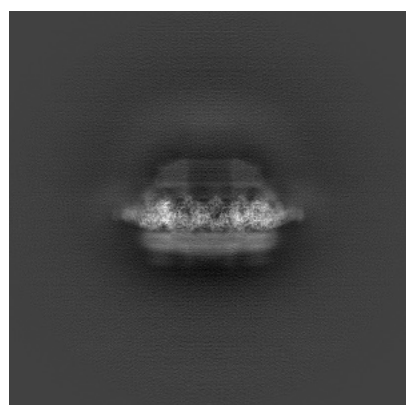
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22068. These allow visual inspection of the internal detail of the map and identification of artifacts.

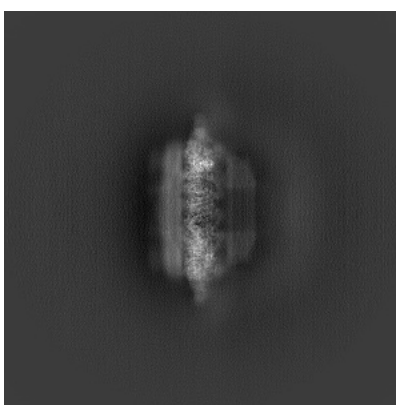
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

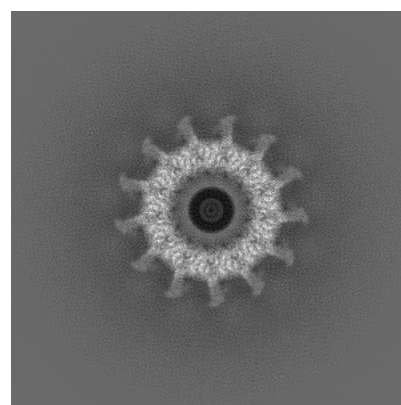
6.1.1 Primary map



X



Y

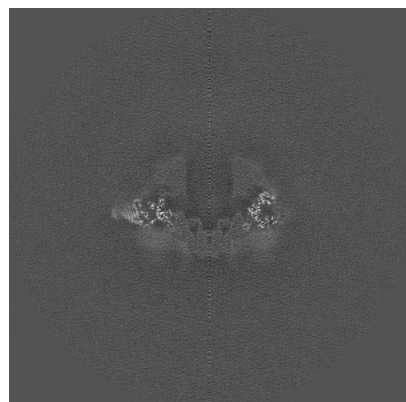


Z

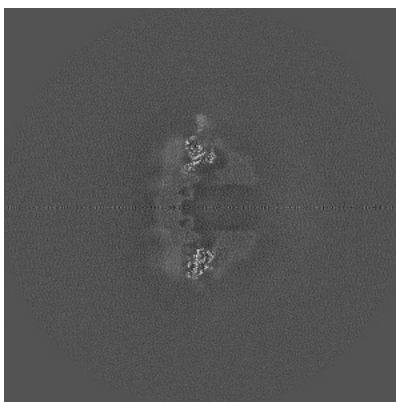
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

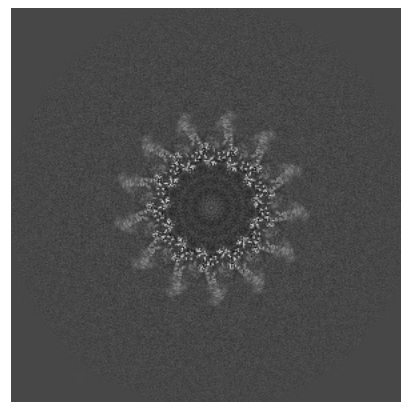
6.2.1 Primary map



X Index: 255



Y Index: 255

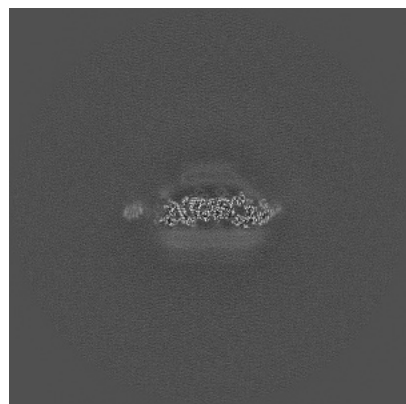


Z Index: 255

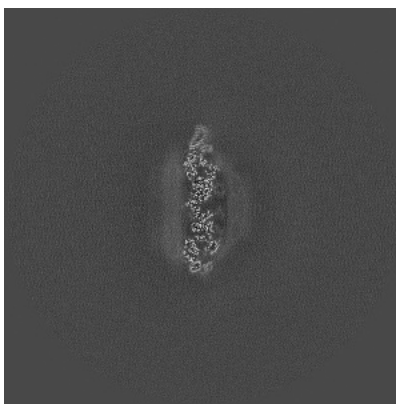
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

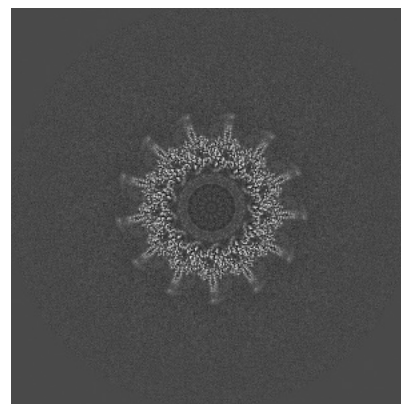
6.3.1 Primary map



X Index: 314



Y Index: 200

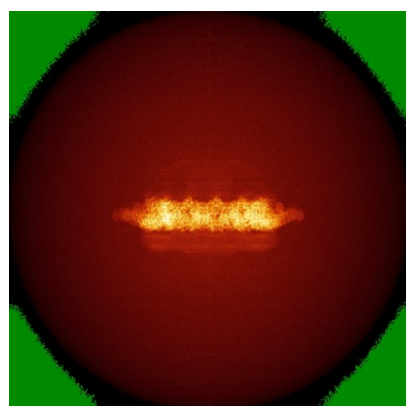


Z Index: 242

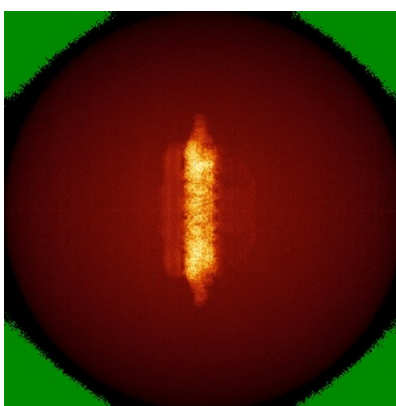
The images above show the largest variance slices of the map in three orthogonal directions.

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

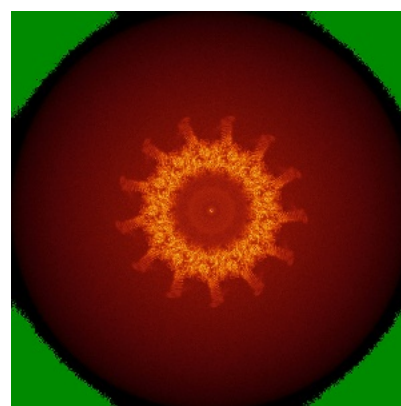
6.4.1 Primary map



X



Y

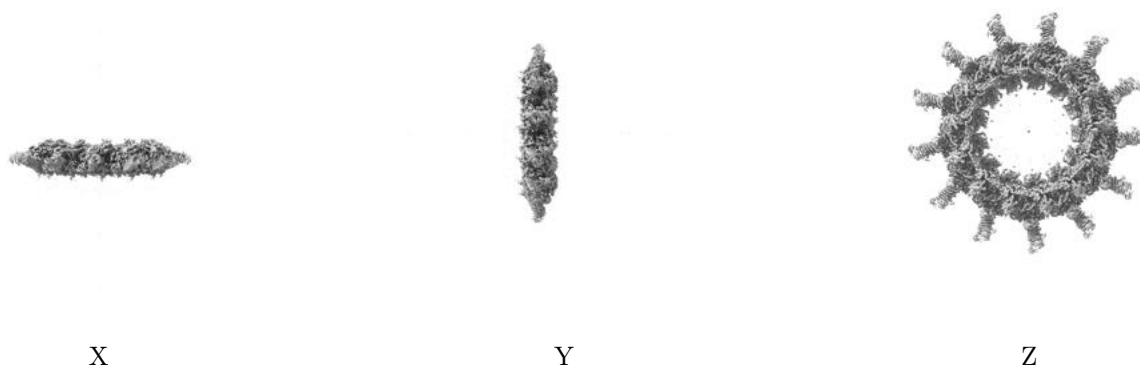


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

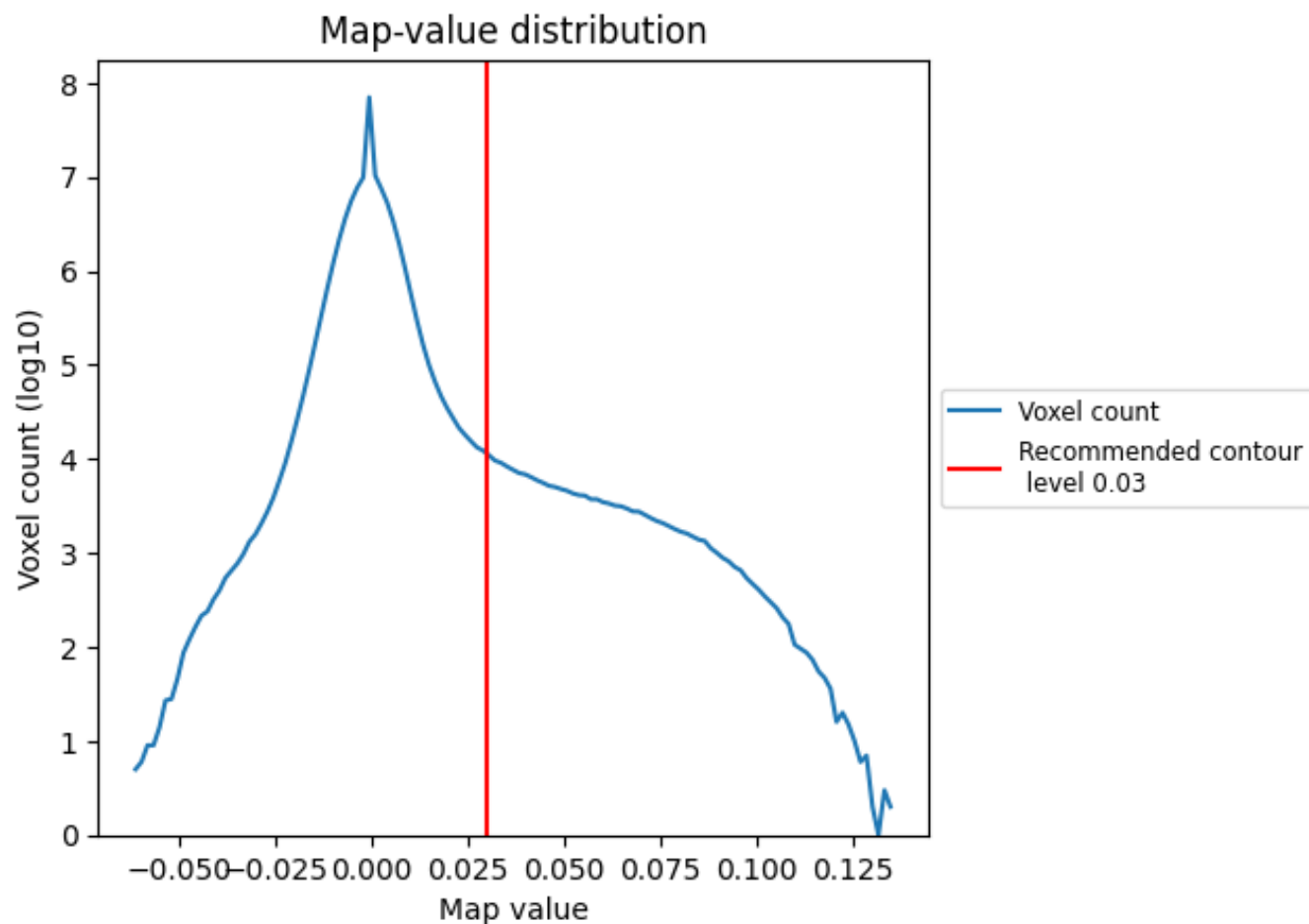
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

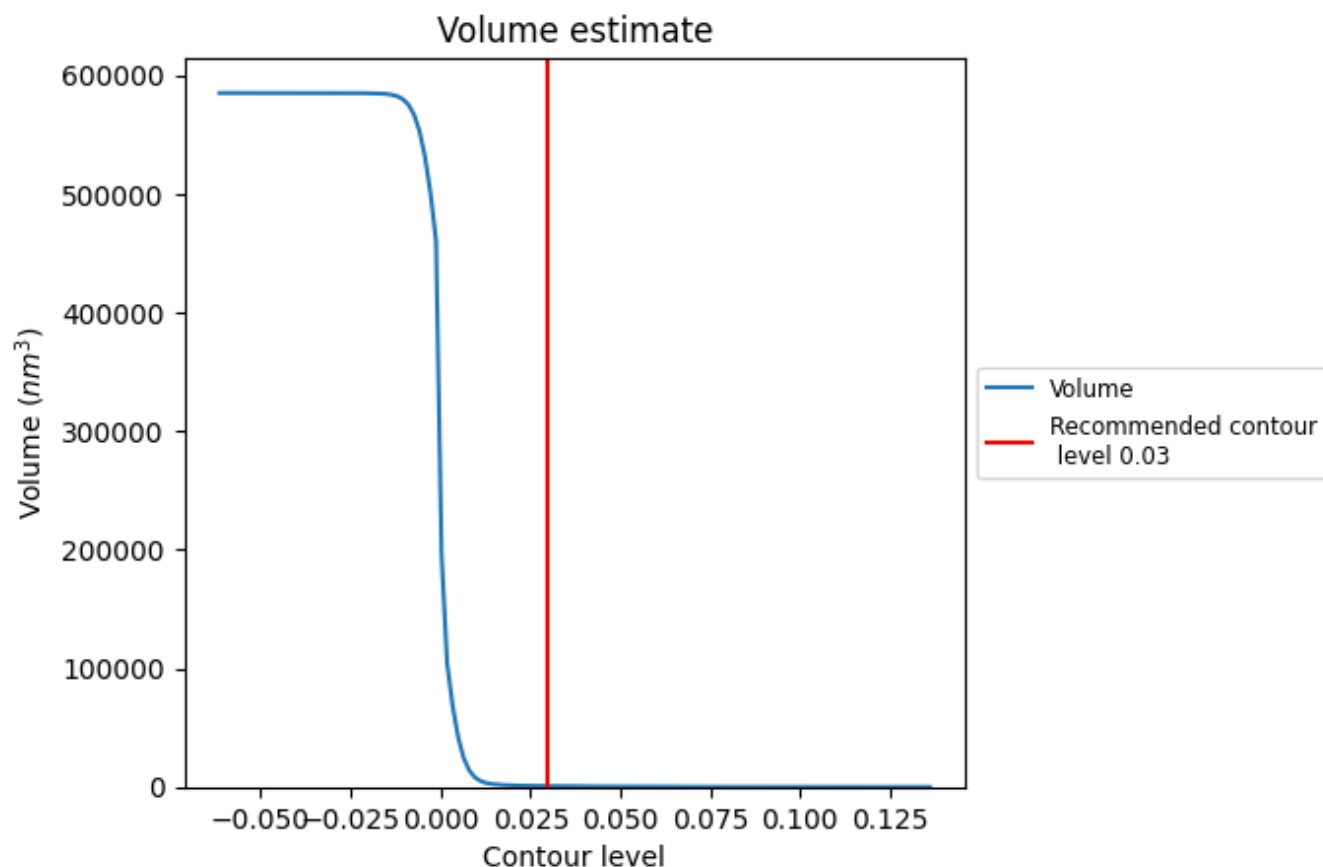
This section contains the results of statistical analysis of the map.

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.

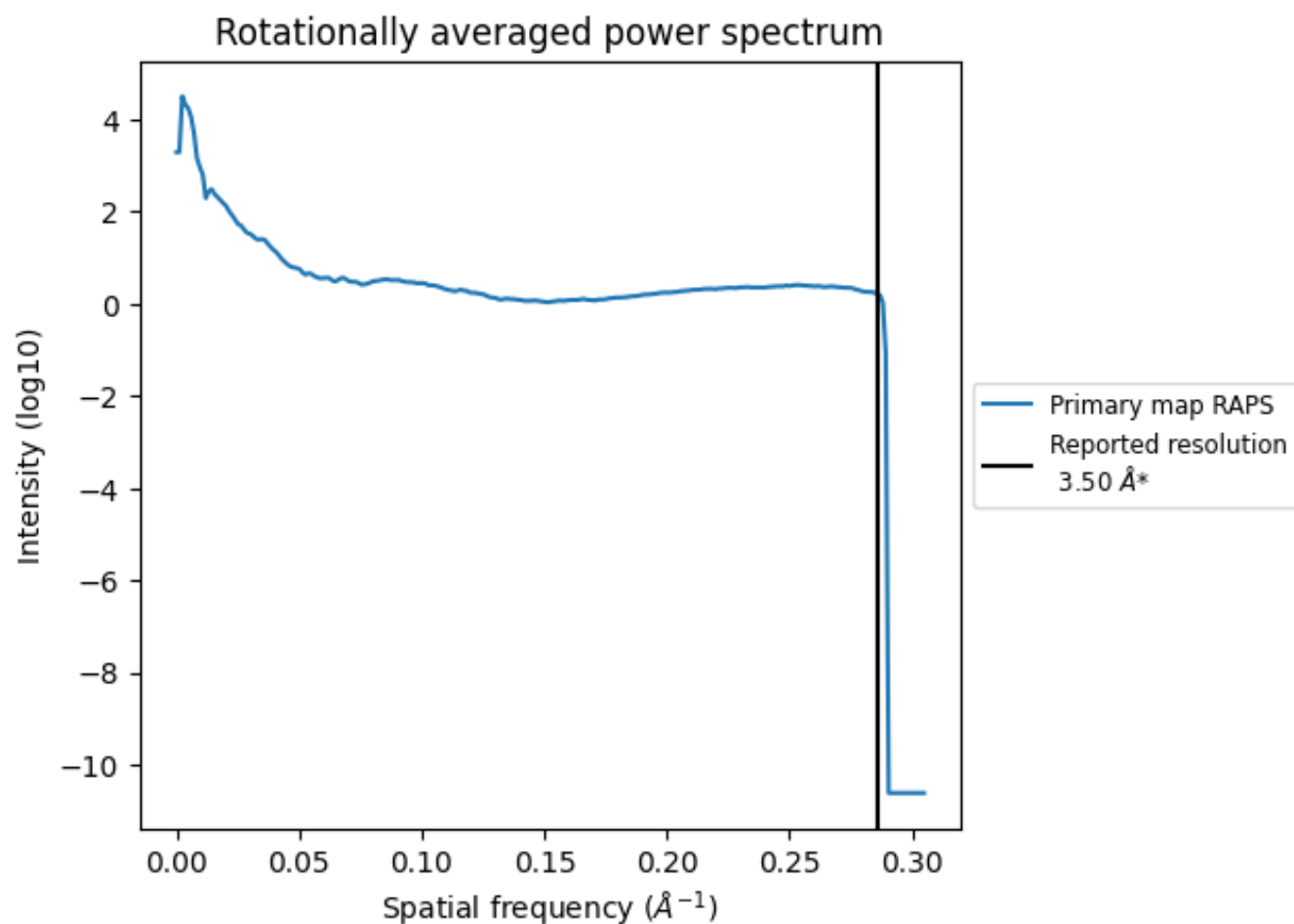
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 751 nm³; this corresponds to an approximate mass of 679 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 ⓘ

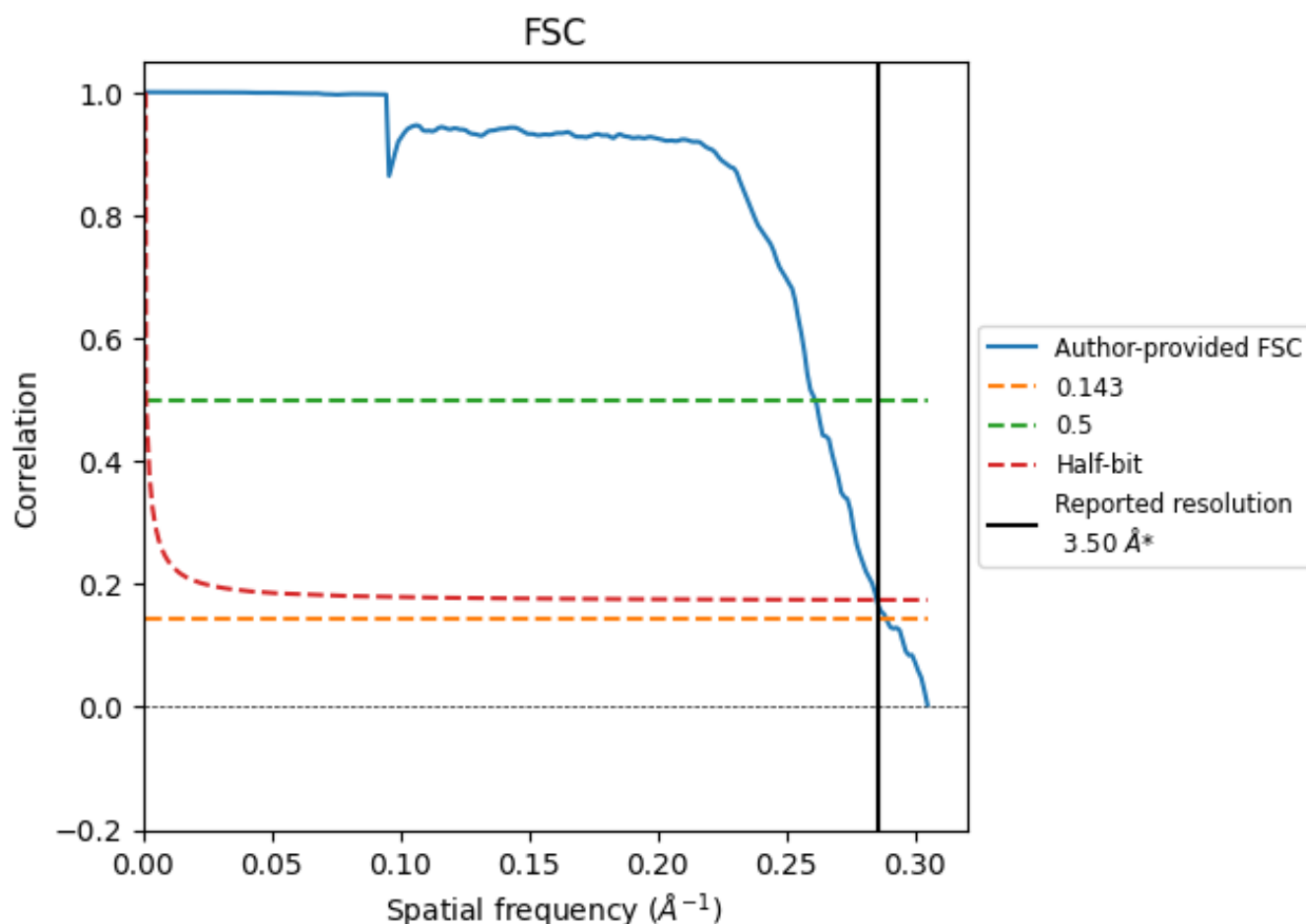


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

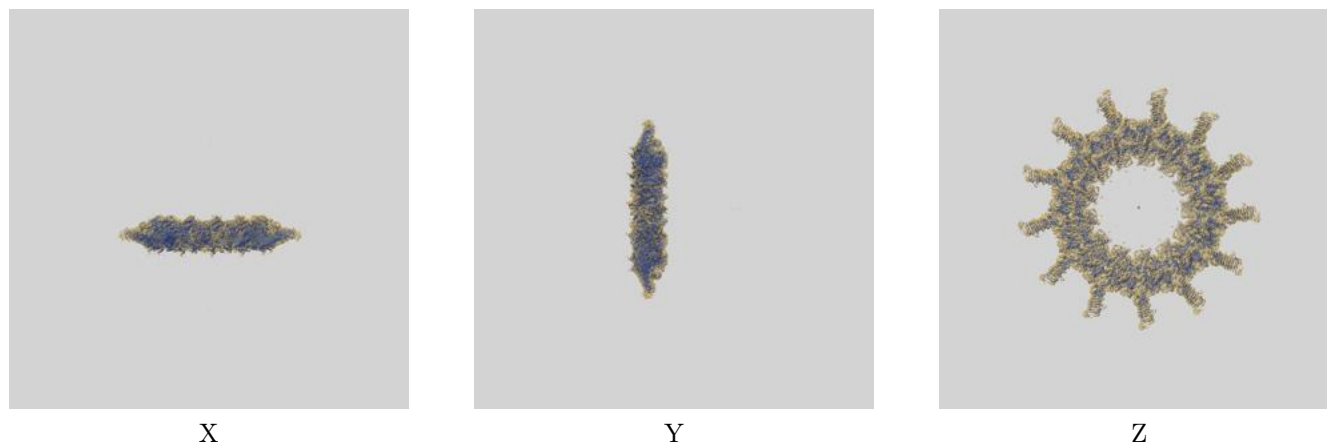
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	3.83	3.51
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

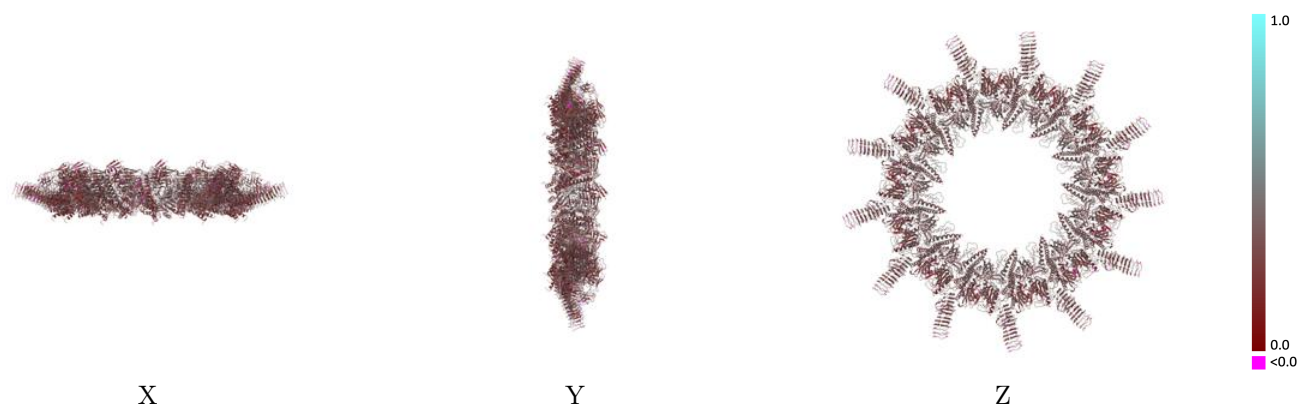
This section contains information regarding the fit between EMDB map EMD-22068 and PDB model 6X62. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)

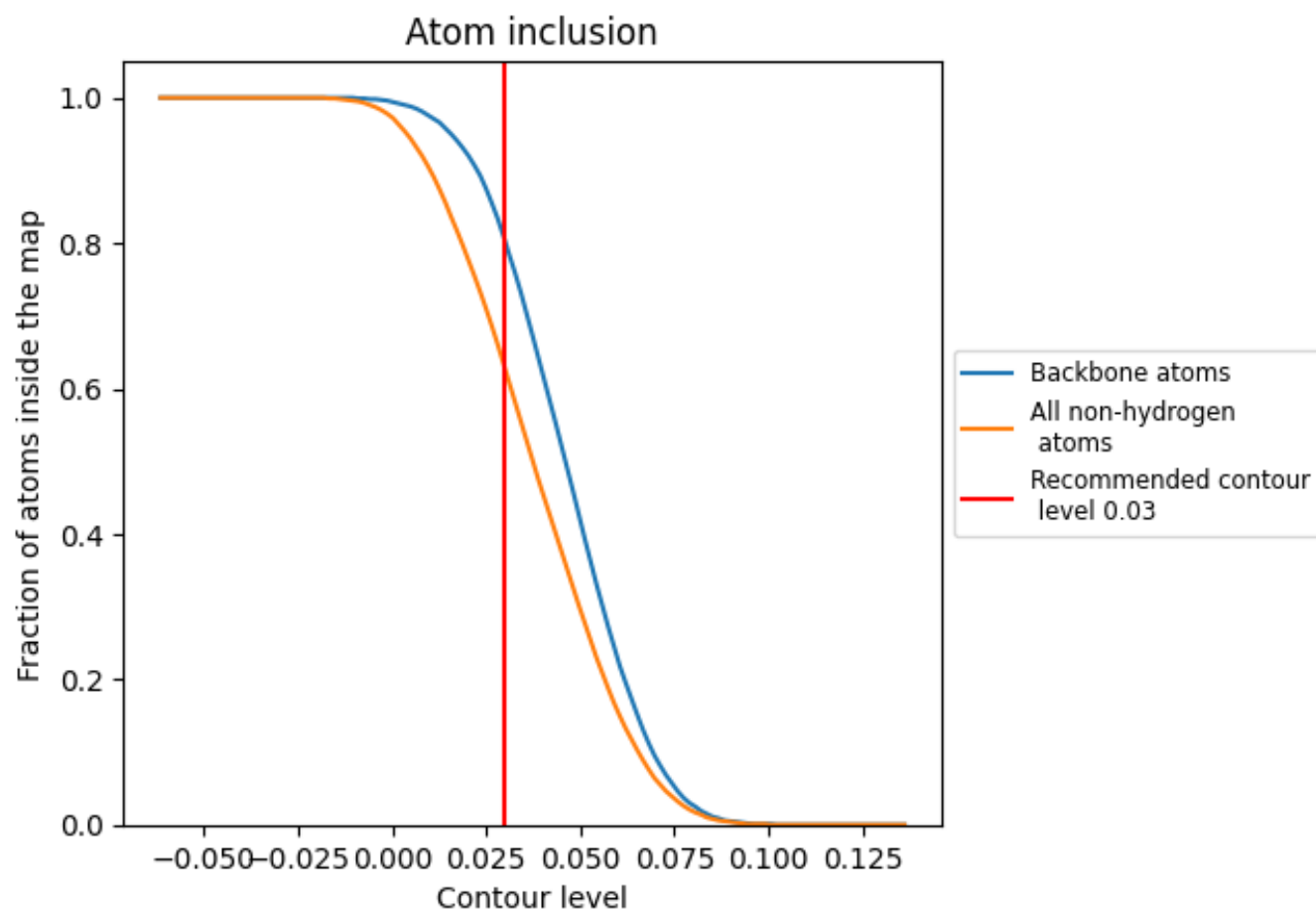


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6280	 0.3040
AC	 0.6600	 0.3360
AD	 0.5790	 0.2700
AH	 0.6480	 0.3360
AK	 0.6230	 0.2930
AX	 0.6260	 0.3080
AY	 0.5730	 0.2800
AZ	 0.7460	 0.3520
Ad	 0.6150	 0.3220
BC	 0.6450	 0.3210
BD	 0.5790	 0.2660
BH	 0.6560	 0.3380
BK	 0.6220	 0.2960
BX	 0.6370	 0.3040
BY	 0.6230	 0.3010
BZ	 0.7630	 0.3610
Bd	 0.6160	 0.3190
CC	 0.6480	 0.3160
CD	 0.5690	 0.2640
CH	 0.6630	 0.3390
CK	 0.6130	 0.2910
CX	 0.6250	 0.2930
CY	 0.6000	 0.3040
CZ	 0.7540	 0.3580
Cd	 0.6090	 0.3080
DC	 0.6550	 0.3370
DD	 0.5820	 0.2750
DH	 0.6690	 0.3450
DK	 0.6260	 0.2950
DX	 0.6360	 0.3080
DY	 0.6310	 0.3240
DZ	 0.7430	 0.3500
Dd	 0.6120	 0.3100
EC	 0.6510	 0.3200
ED	 0.5900	 0.2690



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Chain	Atom inclusion	Q-score
EH	 0.6630	 0.3490
EK	 0.6190	 0.2880
EX	 0.6320	 0.3000
EY	 0.6150	 0.2940
EZ	 0.7430	 0.3590
Ed	 0.6200	 0.3140
FC	 0.6640	 0.3370
FD	 0.5760	 0.2730
FH	 0.6620	 0.3420
FK	 0.6210	 0.2890
FX	 0.6440	 0.3040
FY	 0.6120	 0.2990
FZ	 0.7460	 0.3630
Fd	 0.6090	 0.3120
GC	 0.6570	 0.3310
GD	 0.5830	 0.2740
GH	 0.6530	 0.3360
GK	 0.6050	 0.2840
GX	 0.6320	 0.3030
GY	 0.6150	 0.3110
GZ	 0.7430	 0.3640
Gd	 0.6240	 0.3210
HC	 0.6520	 0.3330
HD	 0.5840	 0.2740
HH	 0.6500	 0.3340
HK	 0.6080	 0.2890
HX	 0.6320	 0.3050
HY	 0.5920	 0.2880
HZ	 0.7510	 0.3680
Hd	 0.6090	 0.3120
IC	 0.6520	 0.3250
ID	 0.5850	 0.2630
IH	 0.6540	 0.3340
IK	 0.6140	 0.2900
IX	 0.6370	 0.2930
IY	 0.6080	 0.2840
IZ	 0.7430	 0.3570
Id	 0.6140	 0.3070
JC	 0.6490	 0.3190
JD	 0.5880	 0.2730
JH	 0.6510	 0.3450
JK	 0.6220	 0.3000

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Chain	Atom inclusion	Q-score
JX	 0.6310	 0.2940
JY	 0.6000	 0.3000
JZ	 0.7510	 0.3650
Jd	 0.6120	 0.3110
KC	 0.6510	 0.3270
KD	 0.5680	 0.2710
KH	 0.6540	 0.3400
KK	 0.6210	 0.2970
KX	 0.6260	 0.3010
KY	 0.6000	 0.2900
KZ	 0.7570	 0.3600
Kd	 0.6080	 0.3120
LC	 0.6450	 0.3270
LD	 0.5860	 0.2700
LH	 0.6530	 0.3320
LK	 0.6160	 0.2920
LX	 0.6370	 0.2960
LY	 0.6120	 0.2840
LZ	 0.7630	 0.3620
Ld	 0.6070	 0.3170
MC	 0.6550	 0.3310
MD	 0.5690	 0.2640
MH	 0.6570	 0.3310
MK	 0.6210	 0.2910
MX	 0.6390	 0.2960
MY	 0.5890	 0.2740
MZ	 0.7430	 0.3680
Md	 0.6290	 0.3140
N	 0.6120	 0.2790
O	 0.6130	 0.2750
P	 0.6110	 0.2770
Q	 0.6090	 0.2740
R	 0.6030	 0.2780
S	 0.6090	 0.2800
T	 0.6110	 0.2790
U	 0.6050	 0.2760
V	 0.6000	 0.2690
W	 0.5990	 0.2700
X	 0.6040	 0.2740
Y	 0.6130	 0.2750
Z	 0.6010	 0.2760