



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:48 PM UTC

PDB ID : 3JC1 / pdb_00003jc1
EMDB ID : EMD-6461
Title : Electron cryo-microscopy of the IST1-CHMP1B ESCRT-III copolymer
Authors : McCullough, J.; Clippinger, A.K.; Talledge, N.; Skowyra, M.L.; Saunders, M.G.; Naismith, T.V.; Colf, L.A.; Afonine, P.; Arthur, C.; Sundquist, W.I.; Hanson, P.I.; Frost, A.
Deposited on : 2015-11-09
Resolution : 4.00 Å(reported)
Based on initial model : 3FRR

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

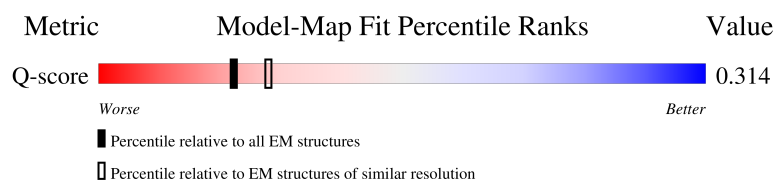
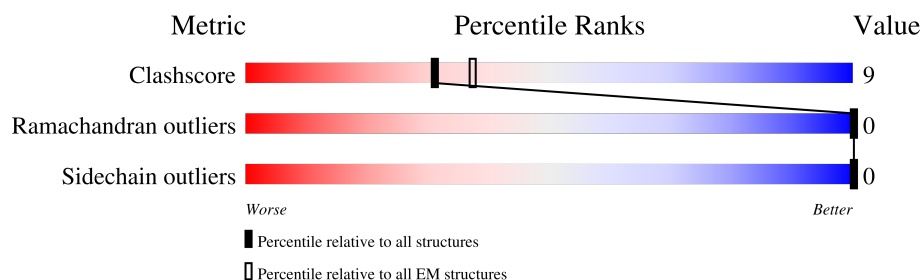
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	Aa	182	78% 76% 24%
1	Ac	182	81% 75% 25%
1	Ae	182	77% 75% 25%
1	Ag	182	77% 75% 25%

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Mol	Chain	Length	Quality of chain	
1	Ai	182	79%	24%
1	Ak	182	79%	25%
1	Am	182	81%	24%
1	Ao	182	80%	24%
1	Aq	182	78%	24%
1	As	182	75%	24%
1	Au	182	77%	23%
1	Aw	182	79%	24%
1	Ay	182	81%	23%
1	Ba	182	86%	24%
1	Bc	182	88%	24%
1	Be	182	87%	22%
1	Bg	182	78%	24%
1	Bi	182	80%	25%
1	Bk	182	84%	26%
1	Bm	182	81%	25%
1	Bo	182	80%	25%
1	Bq	182	81%	25%
1	Bs	182	79%	26%
1	Bu	182	80%	24%
1	Bw	182	79%	24%
1	By	182	74%	23%
1	Ca	182	72%	24%
1	Cc	182	72%	24%
1	Ce	182	72%	24%

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Mol	Chain	Length	Quality of chain	
1	Cg	182	75%	24%
1	Ci	182	80%	24%
1	Ck	182	80%	24%
1	Cm	182	76%	24%
1	Co	182	80%	24%
2	Ab	160	54%	26%
2	Ad	160	49%	26%
2	Af	160	42%	26%
2	Ah	160	43%	24%
2	Aj	160	46%	23%
2	Al	160	49%	23%
2	An	160	53%	24%
2	Ap	160	54%	22%
2	Ar	160	53%	24%
2	At	160	53%	24%
2	Av	160	50%	24%
2	Ax	160	52%	24%
2	Az	160	57%	22%
2	Bb	160	58%	21%
2	Bd	160	63%	21%
2	Bf	160	66%	21%
2	Bh	160	62%	26%
2	Bj	160	62%	21%
2	Bl	160	55%	20%
2	Bn	160	50%	21%

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Mol	Chain	Length	Quality of chain
2	Bp	160	44% 77% 23%
2	Br	160	46% 78% 22%
2	Bt	160	50% 76% 24%
2	Bv	160	53% 77% 23%
2	Bx	160	54% 76% 24%
2	Bz	160	49% 77% 23%
2	Cb	160	48% 76% 24%
2	Cd	160	50% 76% 24%
2	Cf	160	49% 76% 24%
2	Ch	160	50% 75% 25%
2	Cj	160	50% 76% 24%
2	Cl	160	54% 75% 25%
2	Cn	160	59% 74% 26%
2	Cp	160	66% 82% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 92106 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 Increased Sodium Tolerance 1 (IST1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Ac	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Ae	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Ag	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Ai	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Ak	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Am	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Ao	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Aq	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	As	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Au	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Aw	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Ay	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Ba	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Bc	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Be	182	Total 1466	C 934	N 256	O 269	S 7	0	0
1	Bg	182	Total 1466	C 934	N 256	O 269	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bi	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bk	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bm	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bo	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bq	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bs	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bu	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Bw	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	By	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ca	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Cc	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ce	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Cg	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ci	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Ck	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Cm	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		
1	Co	182	Total	C	N	O	S	0	0
			1466	934	256	269	7		

- Molecule 2 is a protein called Charged multivesicular body protein 1b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ad	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Af	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ah	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Aj	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Al	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	An	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ap	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ar	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	At	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Av	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ax	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Az	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bb	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bd	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bf	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bh	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bj	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bl	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bn	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bp	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Br	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bt	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bv	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bx	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Bz	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cb	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cd	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cf	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Ch	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cj	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cl	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cn	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		
2	Cp	160	Total	C	N	O	S	0	0
			1243	765	220	245	13		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	34	GLU	LYS	conflict	UNP Q7LBR1
Ad	34	GLU	LYS	conflict	UNP Q7LBR1
Af	34	GLU	LYS	conflict	UNP Q7LBR1
Ah	34	GLU	LYS	conflict	UNP Q7LBR1
Aj	34	GLU	LYS	conflict	UNP Q7LBR1
Al	34	GLU	LYS	conflict	UNP Q7LBR1
An	34	GLU	LYS	conflict	UNP Q7LBR1
Ap	34	GLU	LYS	conflict	UNP Q7LBR1
Ar	34	GLU	LYS	conflict	UNP Q7LBR1
At	34	GLU	LYS	conflict	UNP Q7LBR1
Av	34	GLU	LYS	conflict	UNP Q7LBR1
Ax	34	GLU	LYS	conflict	UNP Q7LBR1
Az	34	GLU	LYS	conflict	UNP Q7LBR1
Bb	34	GLU	LYS	conflict	UNP Q7LBR1
Bd	34	GLU	LYS	conflict	UNP Q7LBR1
Bf	34	GLU	LYS	conflict	UNP Q7LBR1
Bh	34	GLU	LYS	conflict	UNP Q7LBR1

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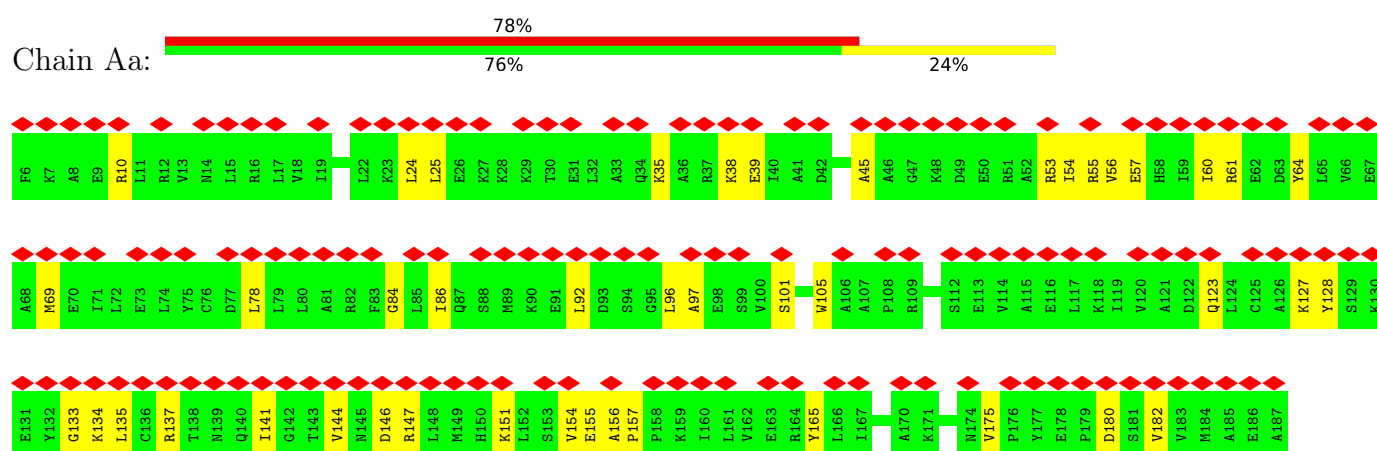
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Chain	Residue	Modelled	Actual	Comment	Reference
Bj	34	GLU	LYS	conflict	UNP Q7LBR1
Bl	34	GLU	LYS	conflict	UNP Q7LBR1
Bn	34	GLU	LYS	conflict	UNP Q7LBR1
Bp	34	GLU	LYS	conflict	UNP Q7LBR1
Br	34	GLU	LYS	conflict	UNP Q7LBR1
Bt	34	GLU	LYS	conflict	UNP Q7LBR1
Bv	34	GLU	LYS	conflict	UNP Q7LBR1
Bx	34	GLU	LYS	conflict	UNP Q7LBR1
Bz	34	GLU	LYS	conflict	UNP Q7LBR1
Cb	34	GLU	LYS	conflict	UNP Q7LBR1
Cd	34	GLU	LYS	conflict	UNP Q7LBR1
Cf	34	GLU	LYS	conflict	UNP Q7LBR1
Ch	34	GLU	LYS	conflict	UNP Q7LBR1
Cj	34	GLU	LYS	conflict	UNP Q7LBR1
Cl	34	GLU	LYS	conflict	UNP Q7LBR1
Cn	34	GLU	LYS	conflict	UNP Q7LBR1
Cp	34	GLU	LYS	conflict	UNP Q7LBR1

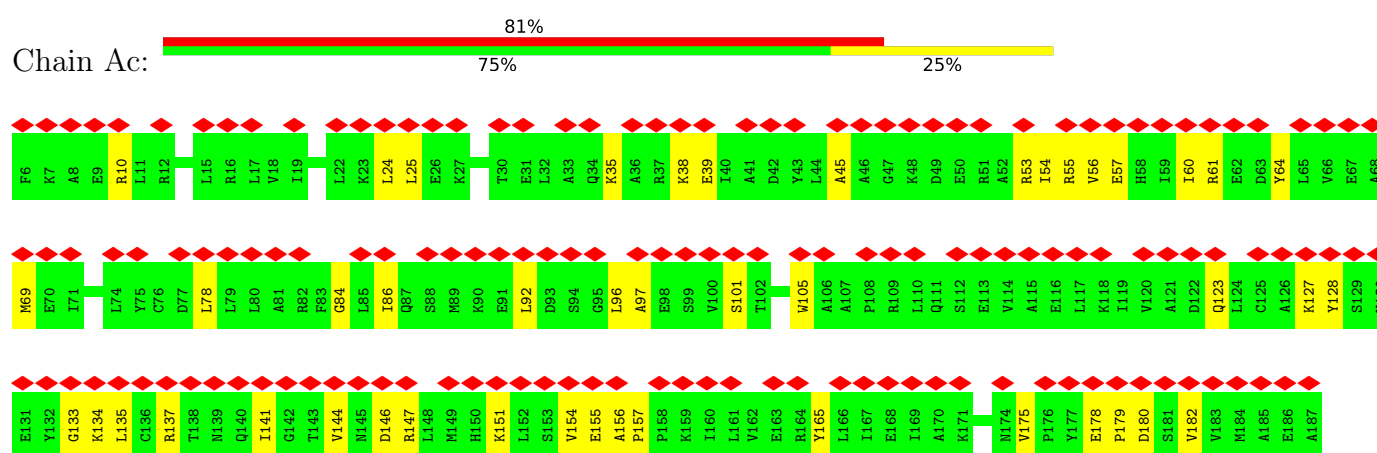
3 Residue-property plots

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

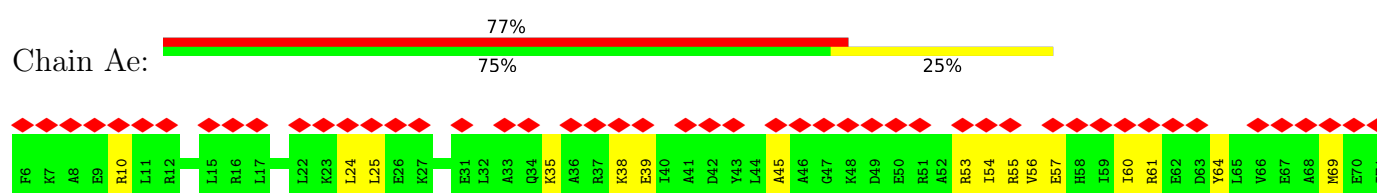
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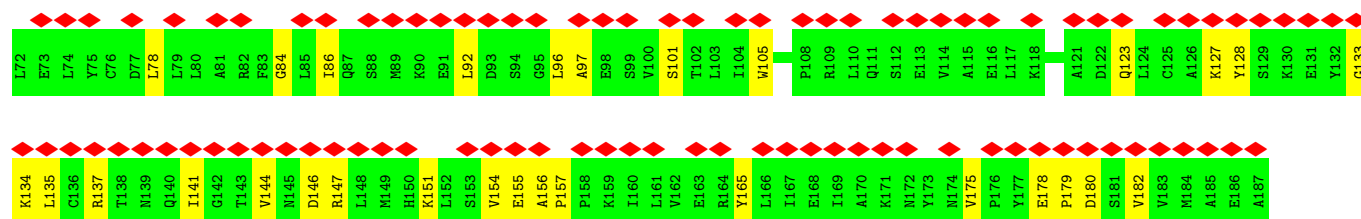


- Molecule 1: Increased Sodium Tolerance 1 (IST1)

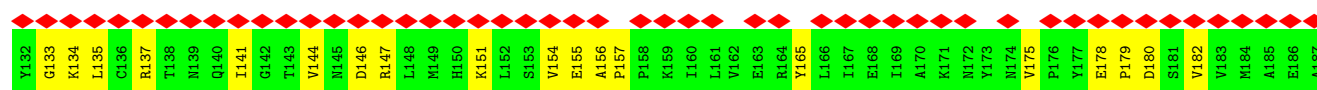
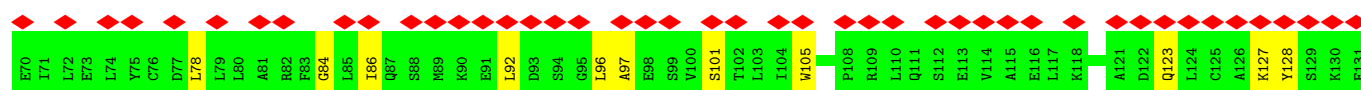
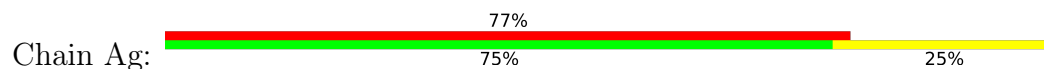


- Molecule 1: Increased Sodium Tolerance 1 (IST1)

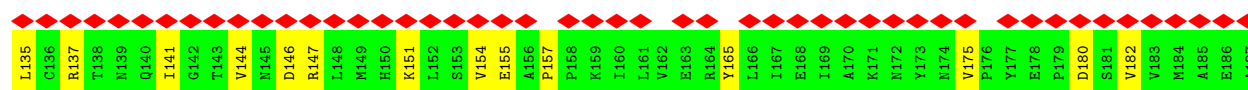
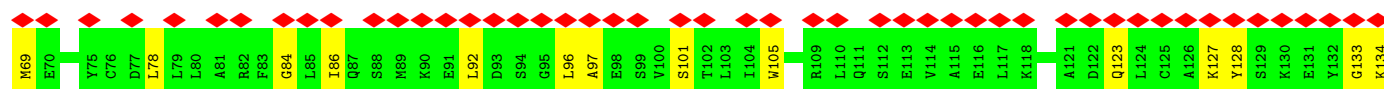
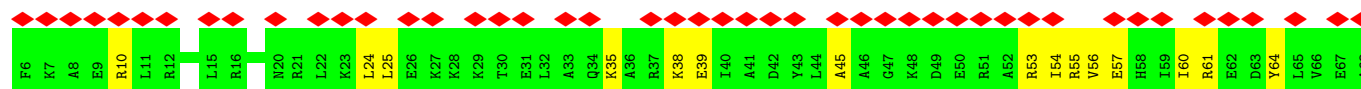
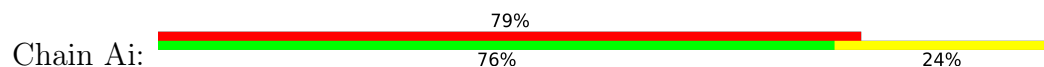




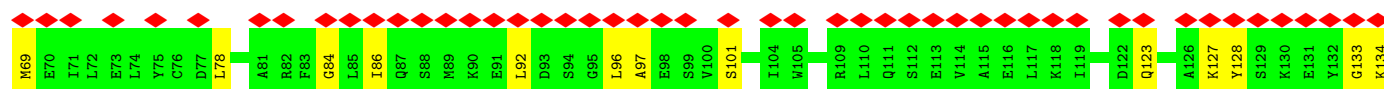
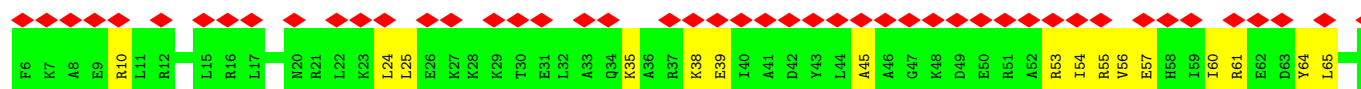
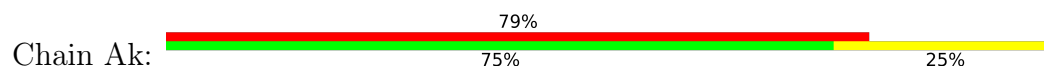
• Molecule 1: Increased Sodium Tolerance 1 (IST1)

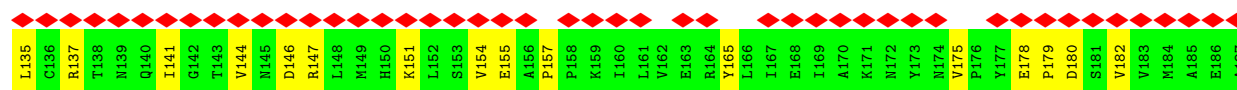


• Molecule 1: Increased Sodium Tolerance 1 (IST1)

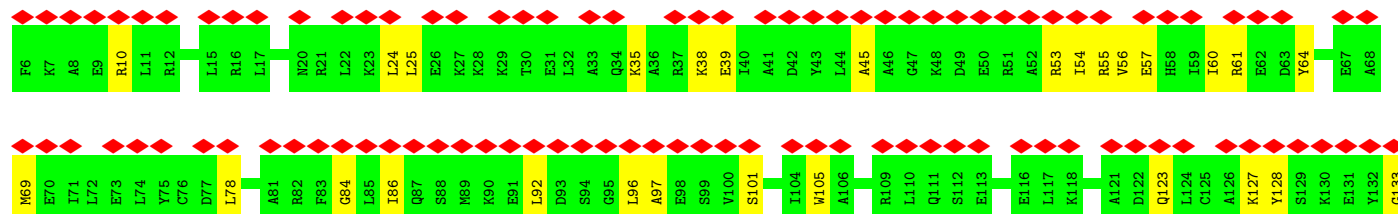
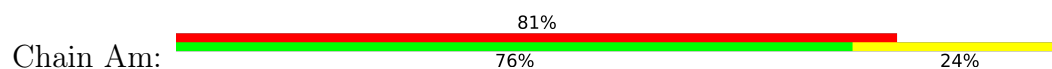


• Molecule 1: Increased Sodium Tolerance 1 (IST1)

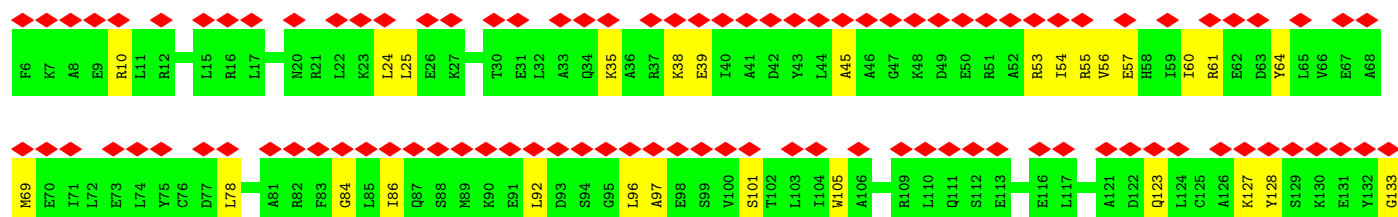
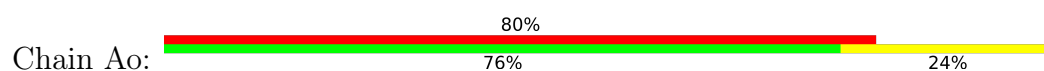




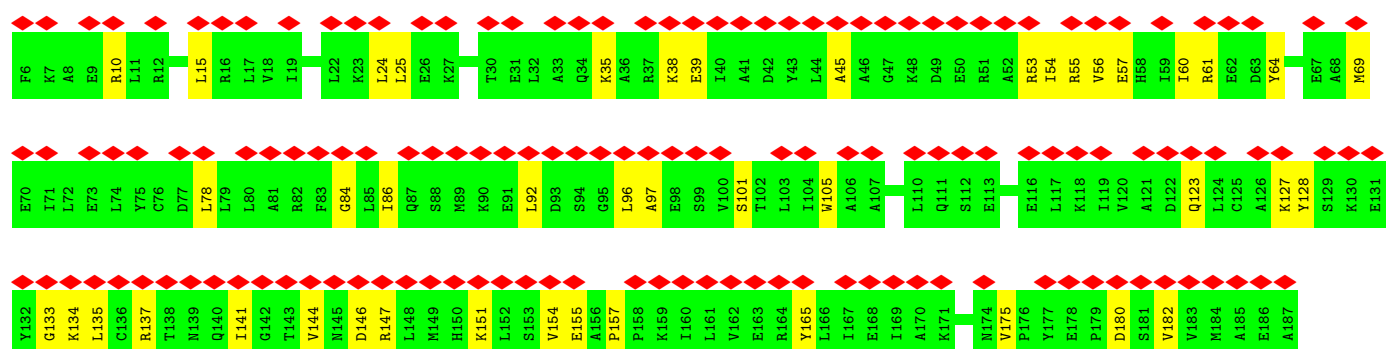
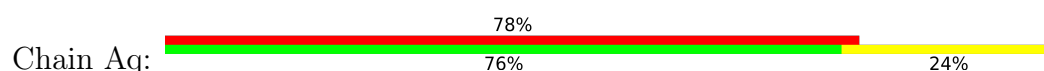
• Molecule 1: Increased Sodium Tolerance 1 (IST1)



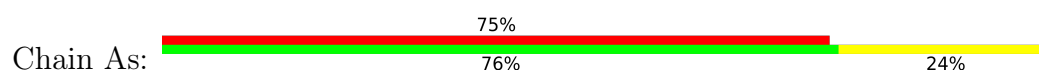
• Molecule 1: Increased Sodium Tolerance 1 (IST1)



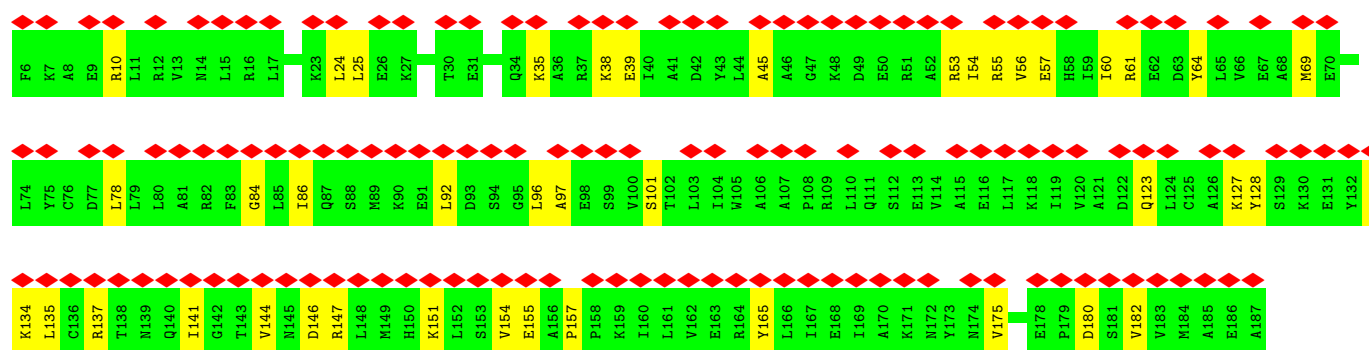
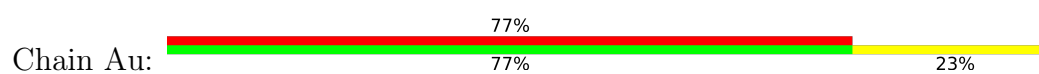
• Molecule 1: Increased Sodium Tolerance 1 (IST1)



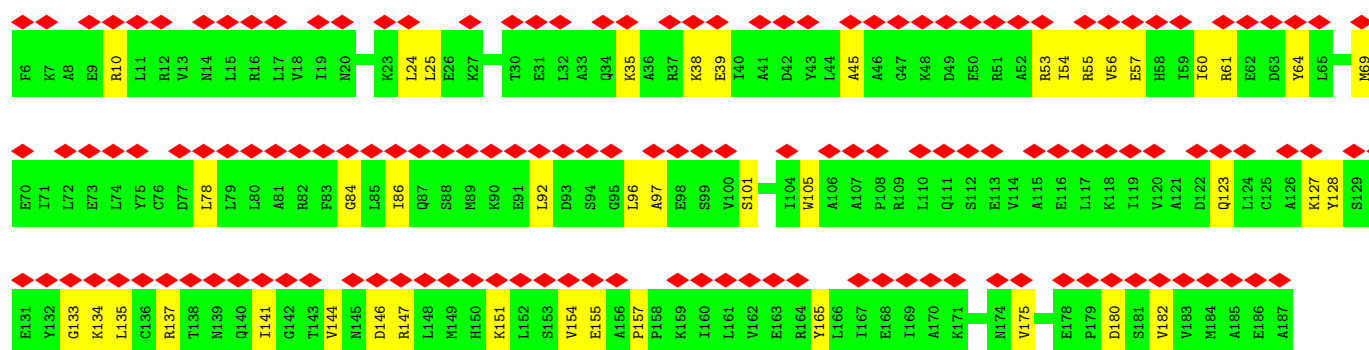
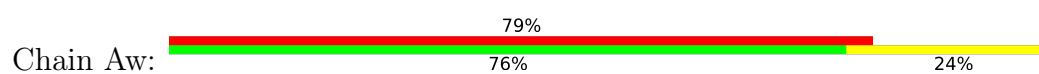
• Molecule 1: Increased Sodium Tolerance 1 (IST1)



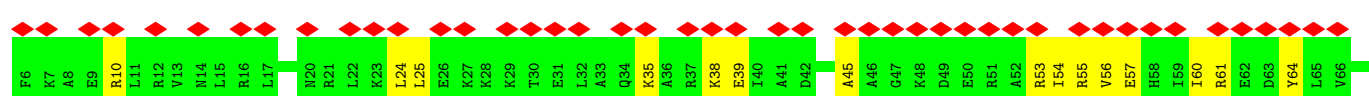
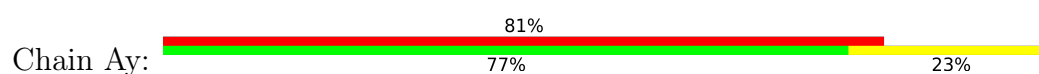
• Molecule 1: Increased Sodium Tolerance 1 (IST1)

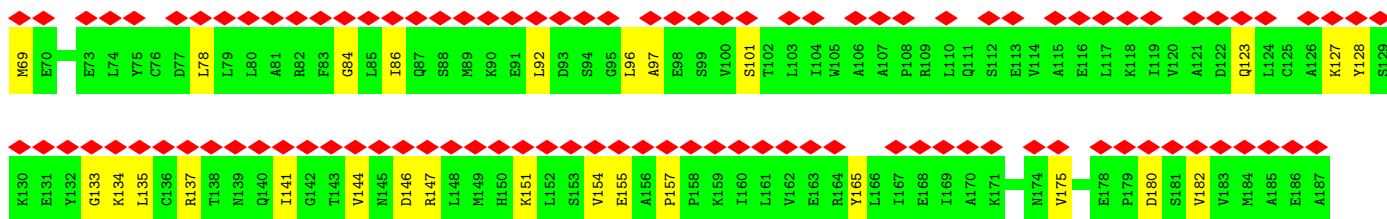


• Molecule 1: Increased Sodium Tolerance 1 (IST1)

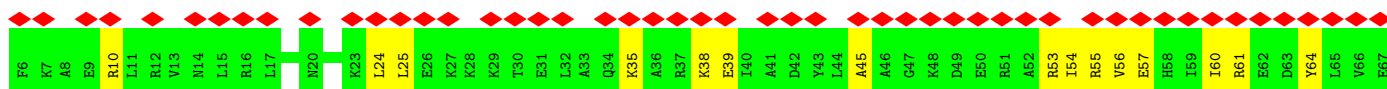
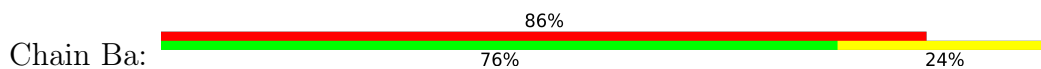


• Molecule 1: Increased Sodium Tolerance 1 (IST1)

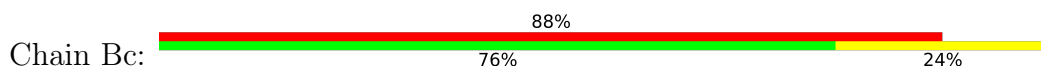




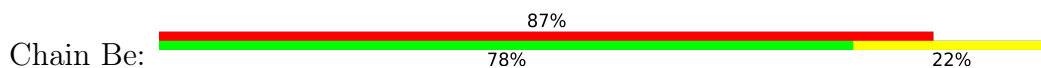
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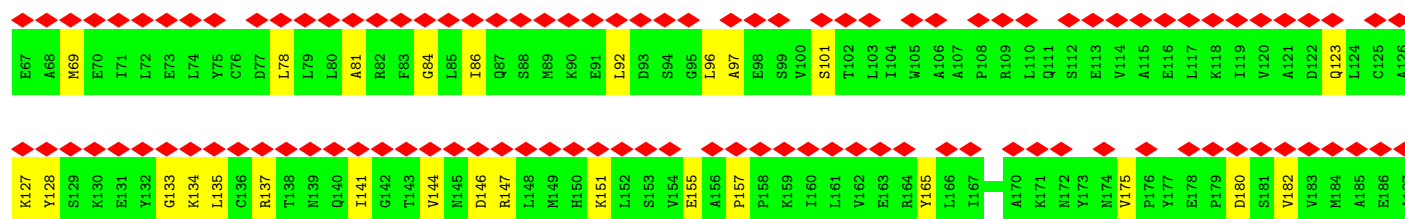


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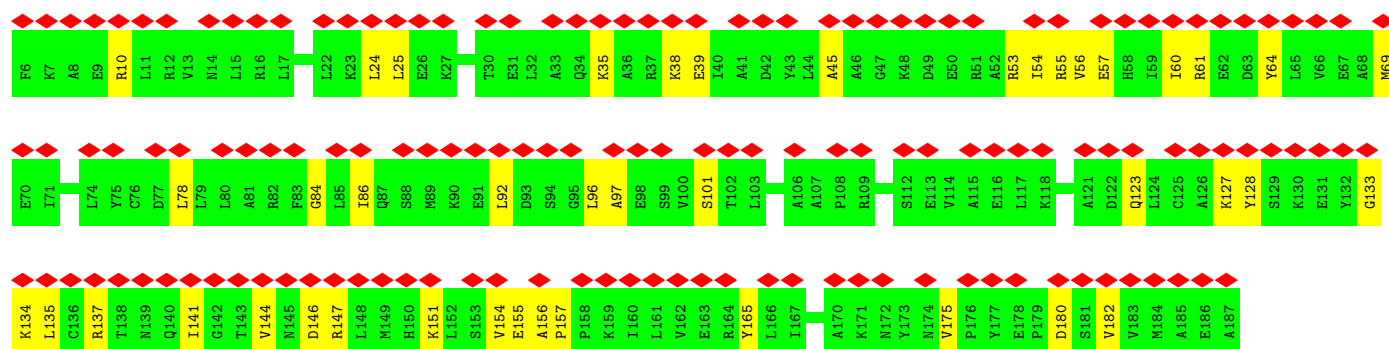
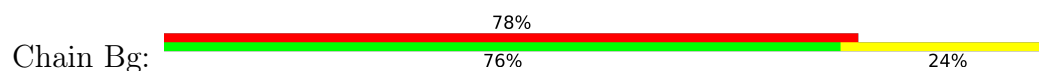


• Molecule 1: Increased Sodium Tolerance 1 (IST1)

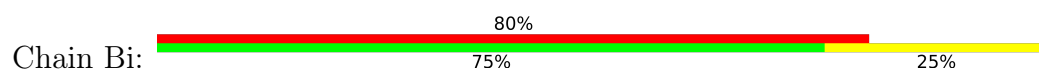




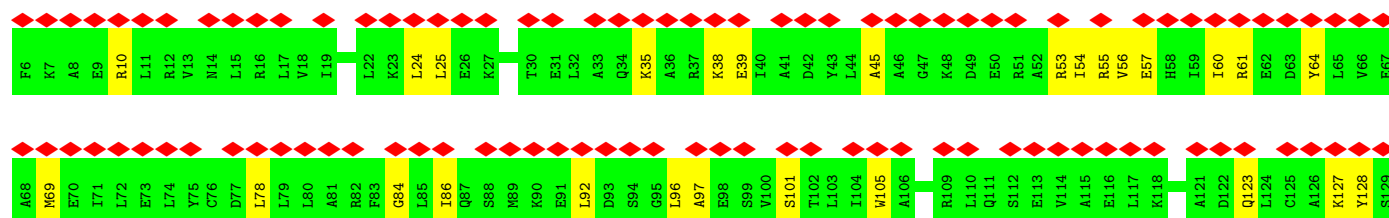
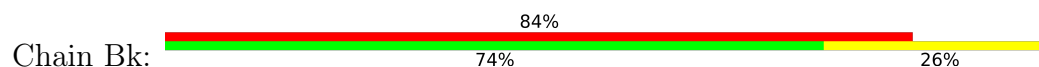
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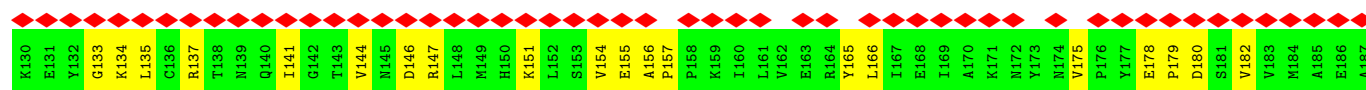


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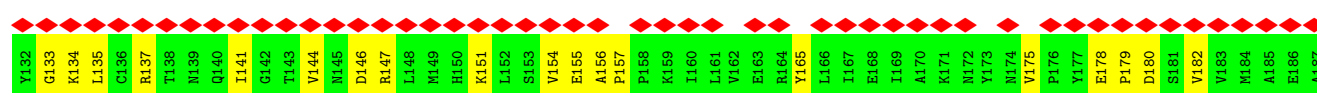
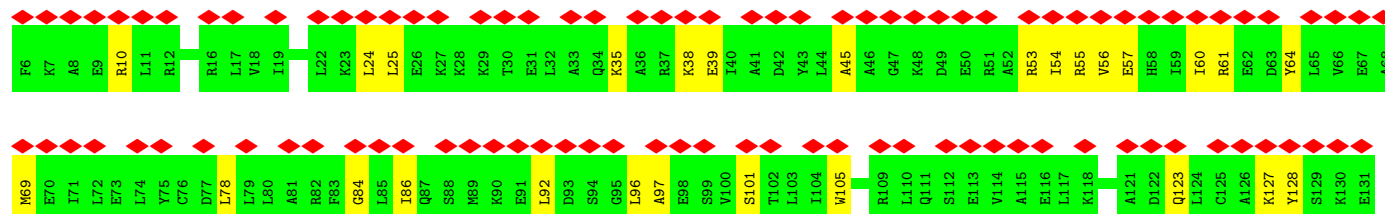
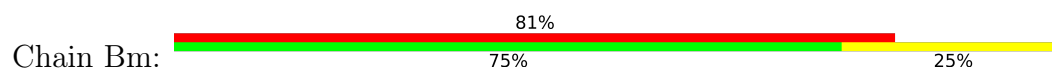


• Molecule 1: Increased Sodium Tolerance 1 (IST1)

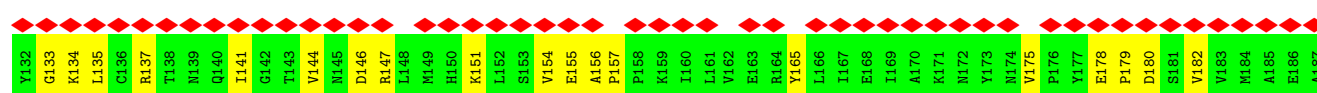
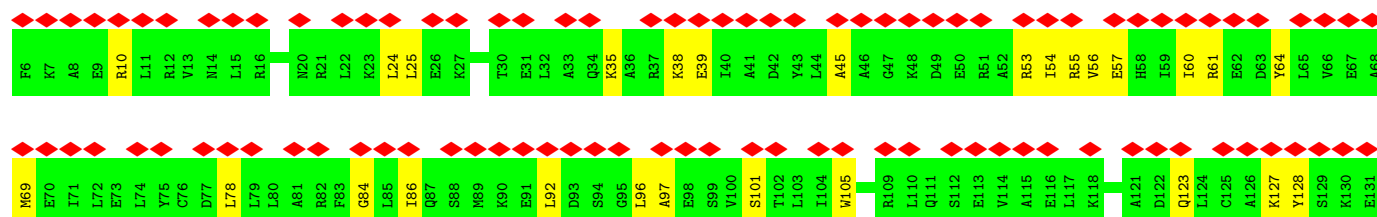
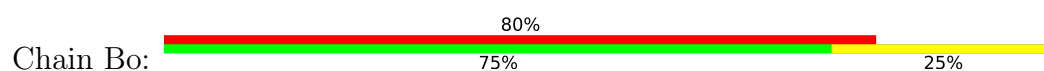




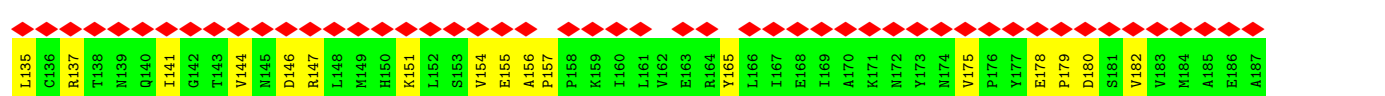
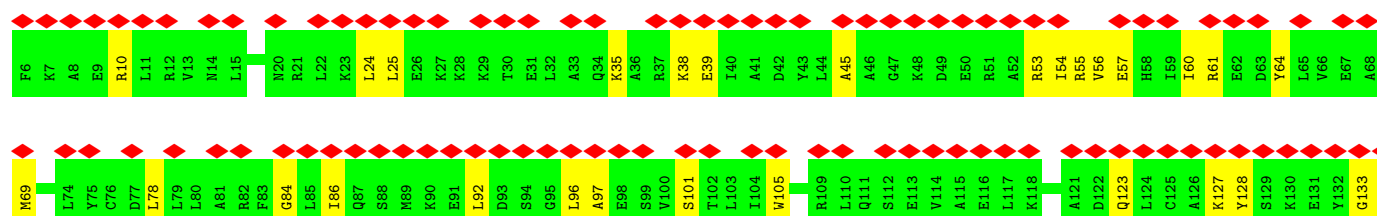
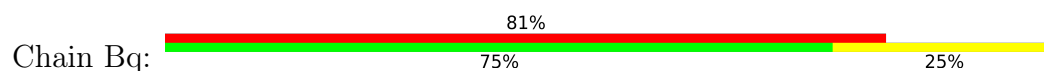
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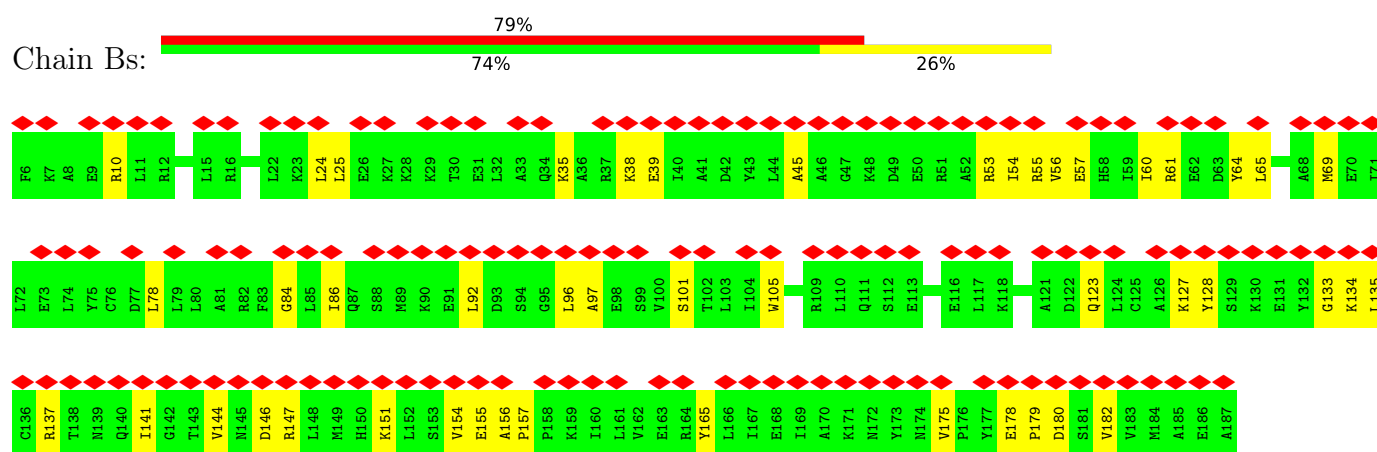
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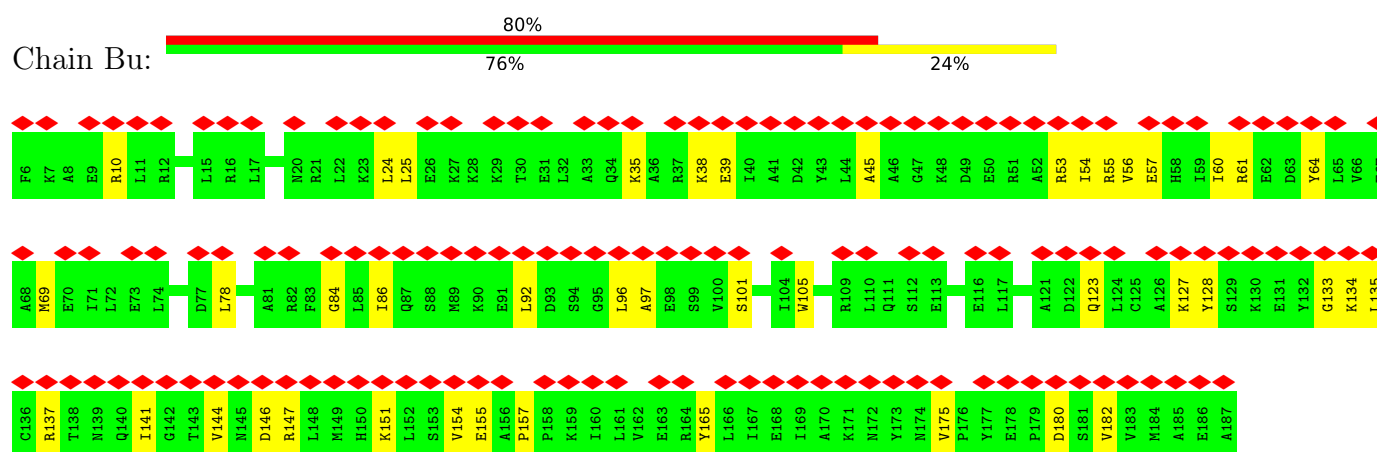
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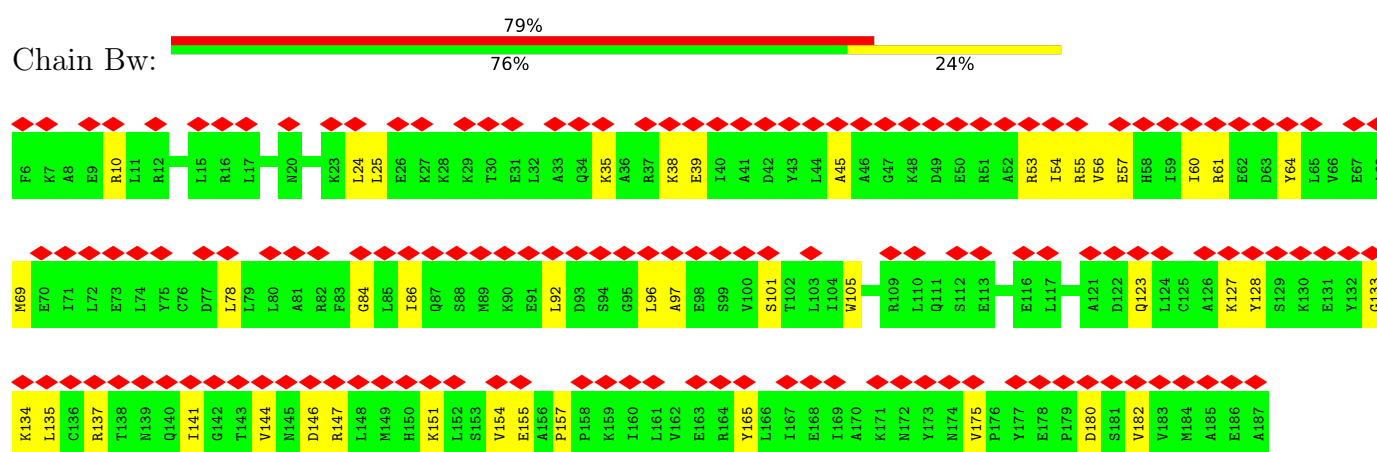
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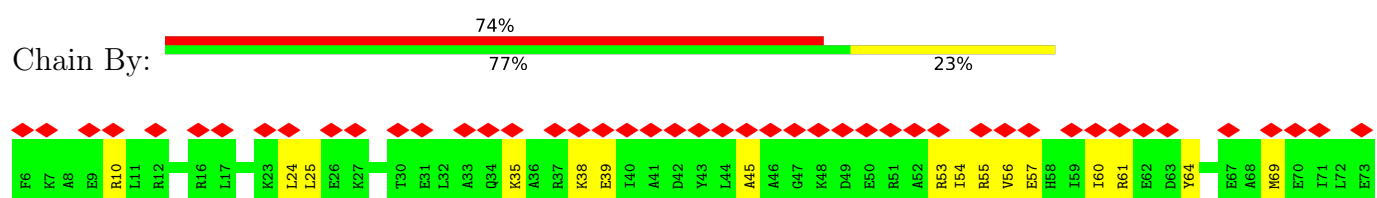
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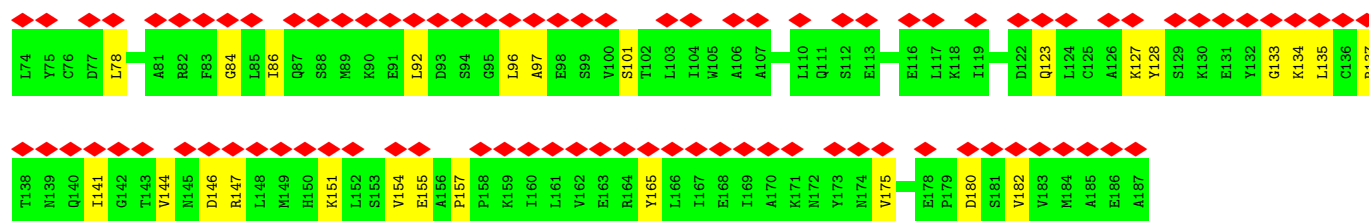


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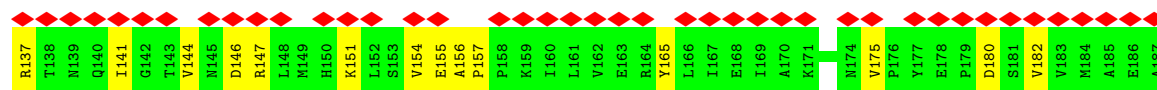
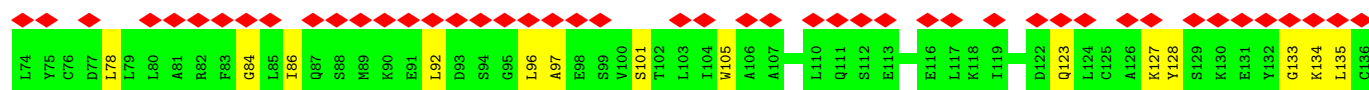
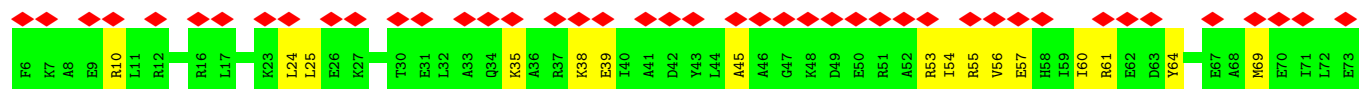
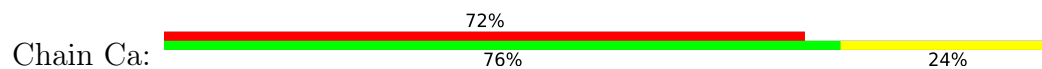


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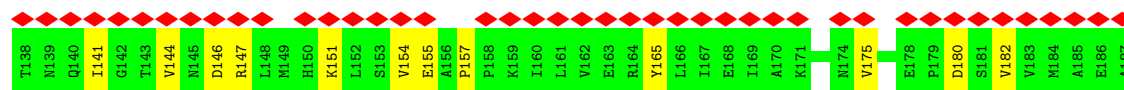
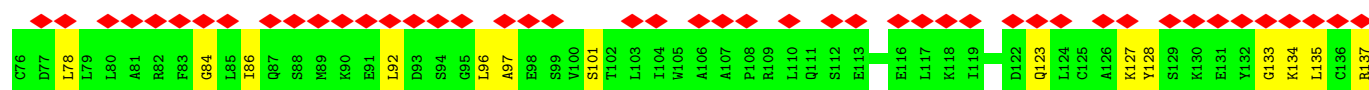
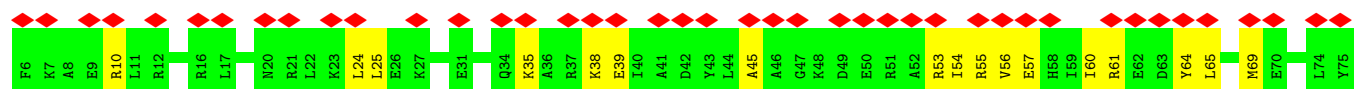
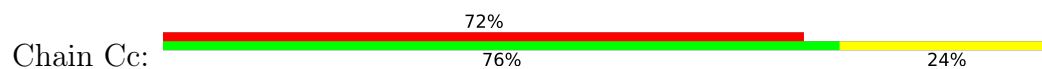




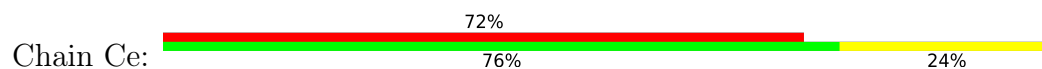
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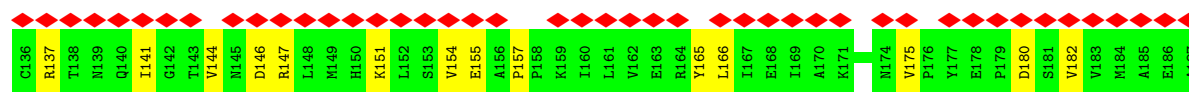


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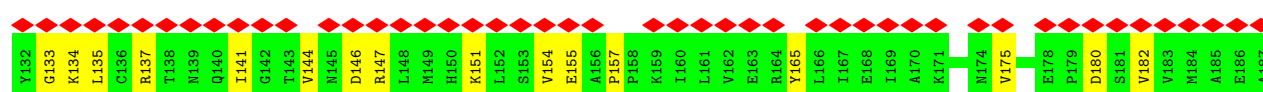
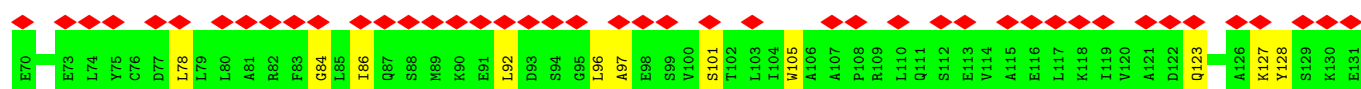
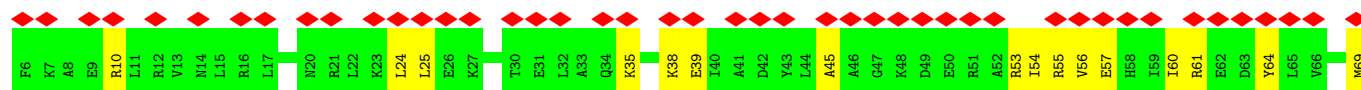
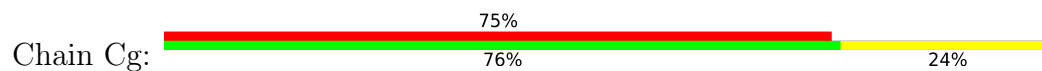


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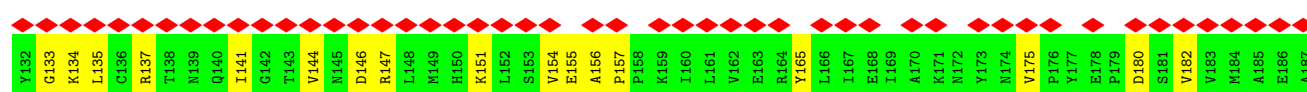
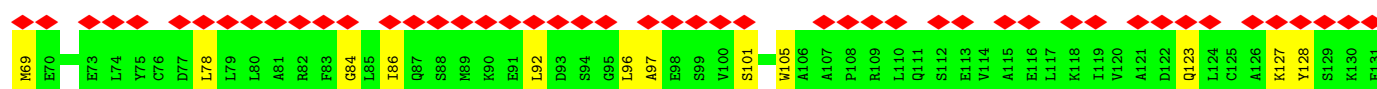
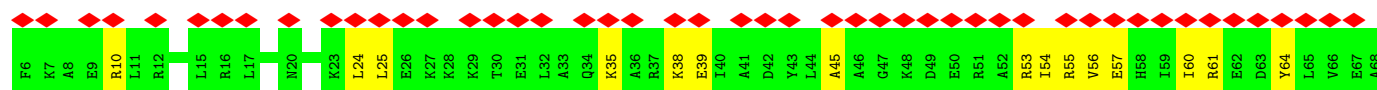
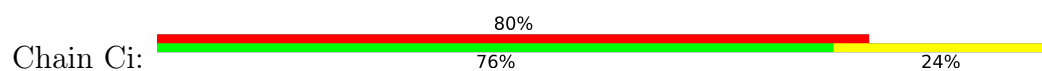




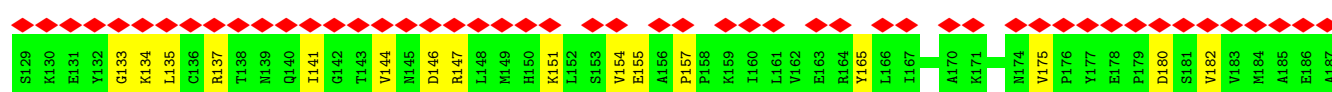
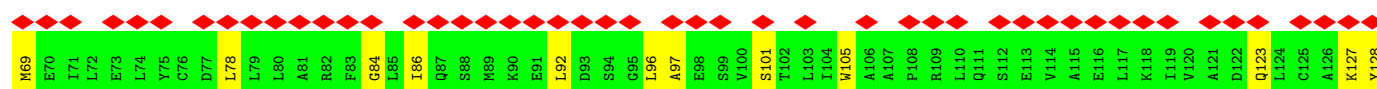
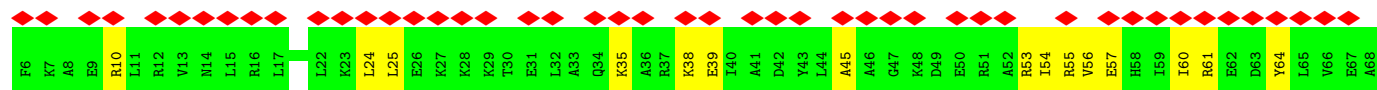
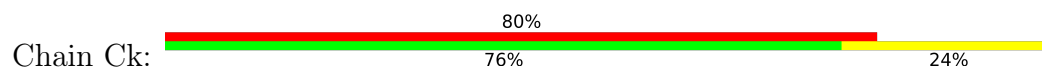
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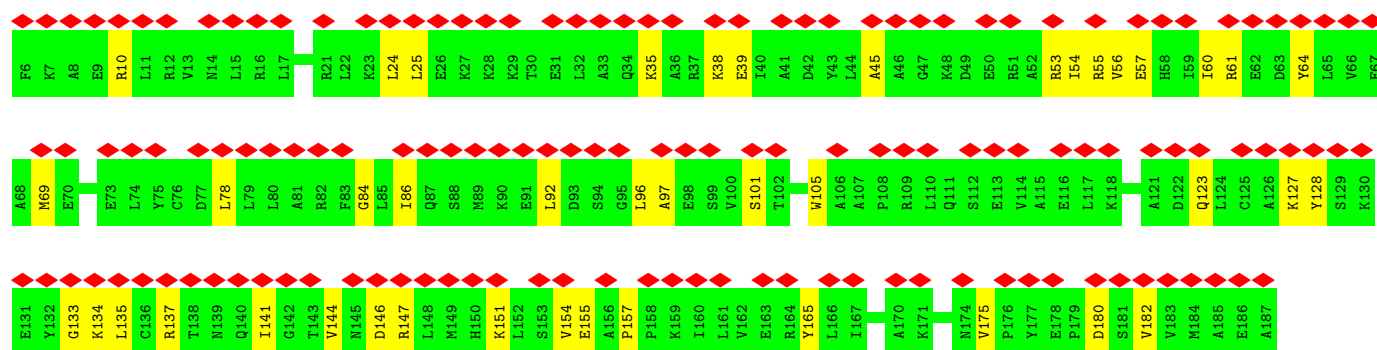
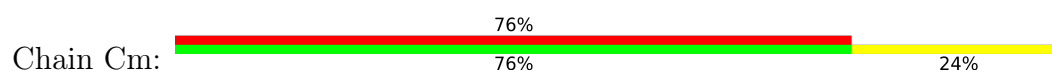
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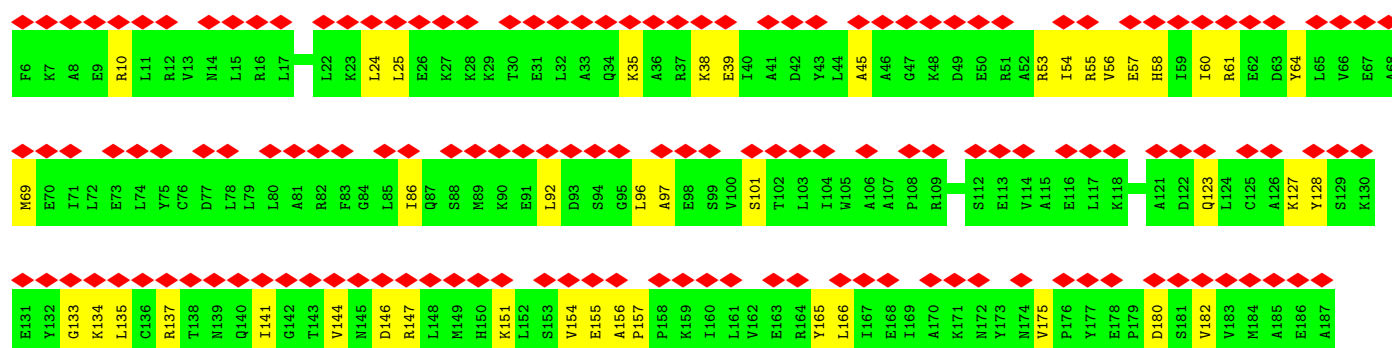
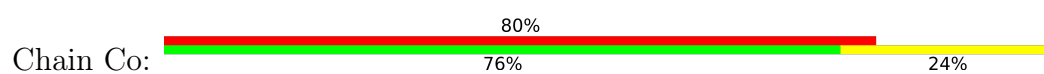
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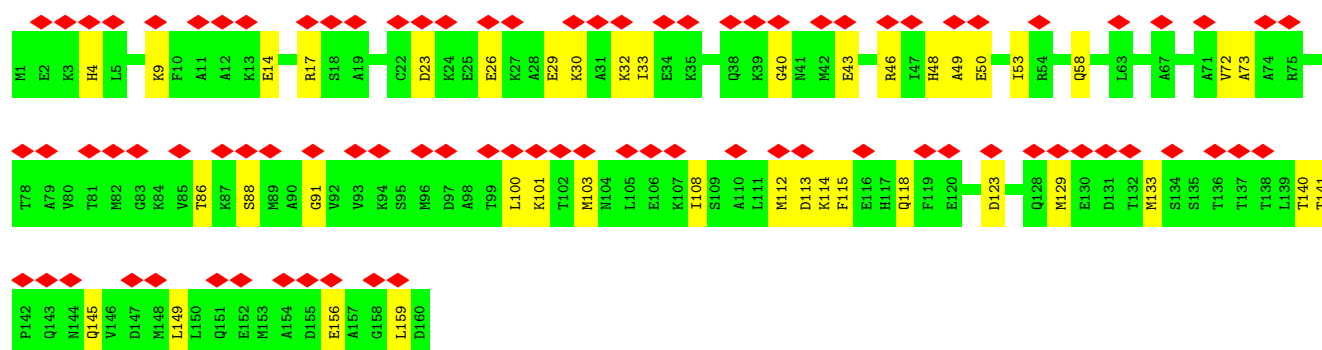
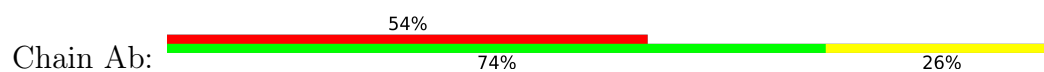
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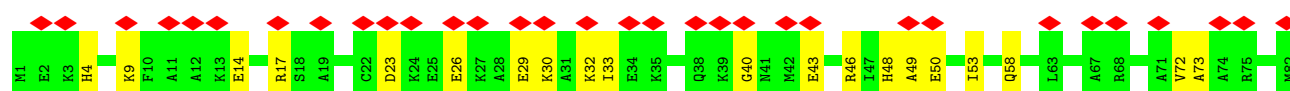
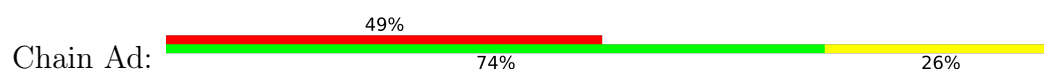
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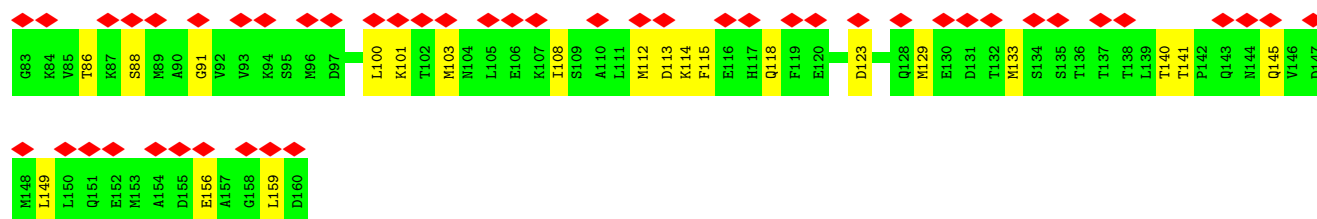


• Molecule 2: Charged multivesicular body protein 1b

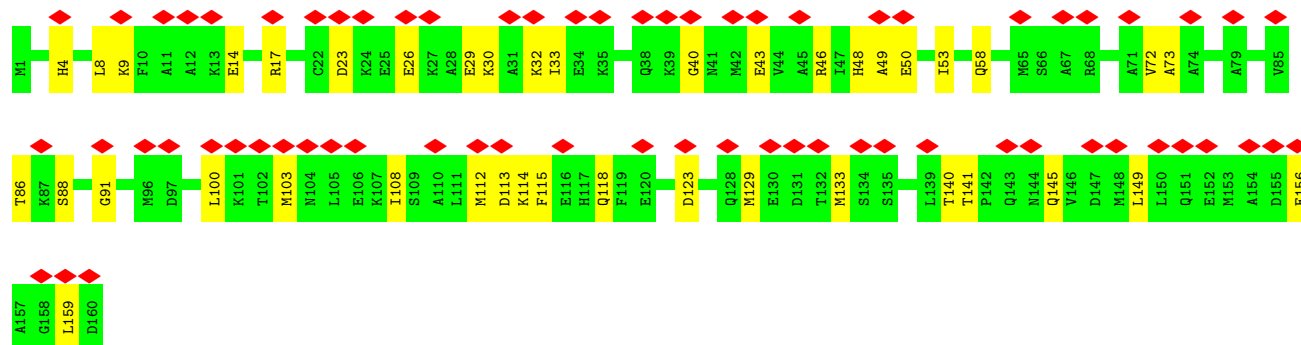
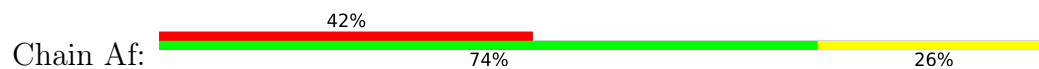


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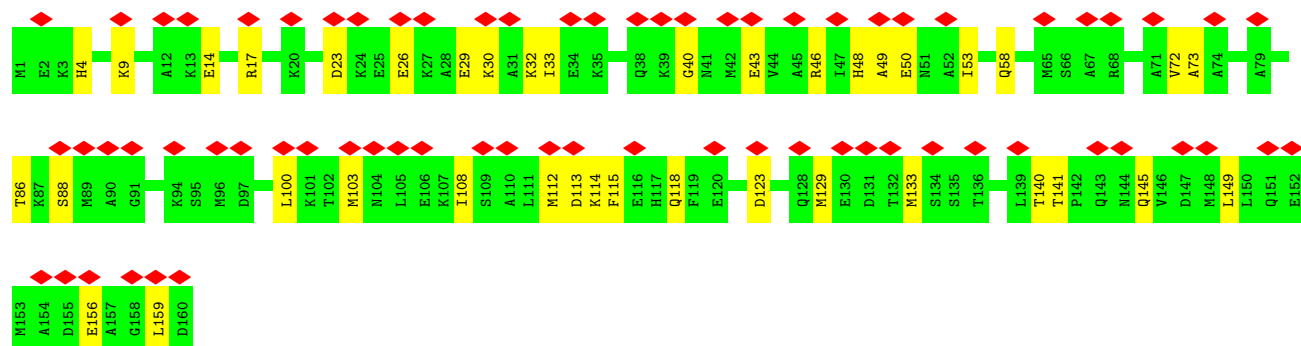
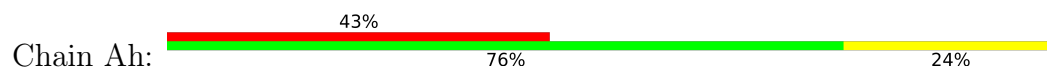




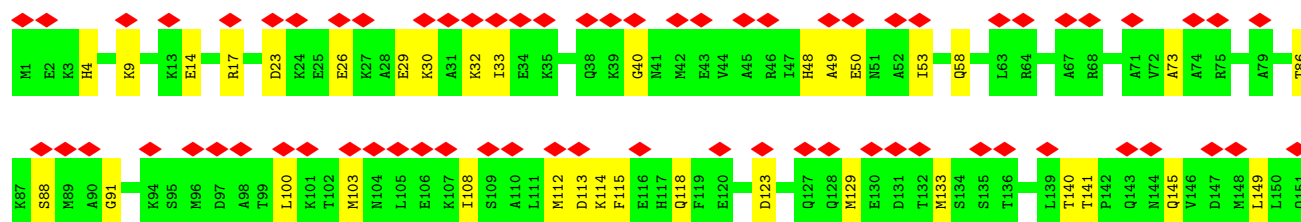
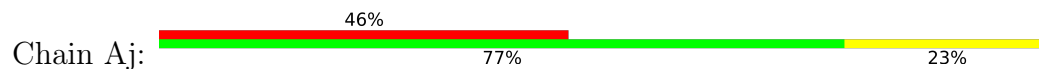
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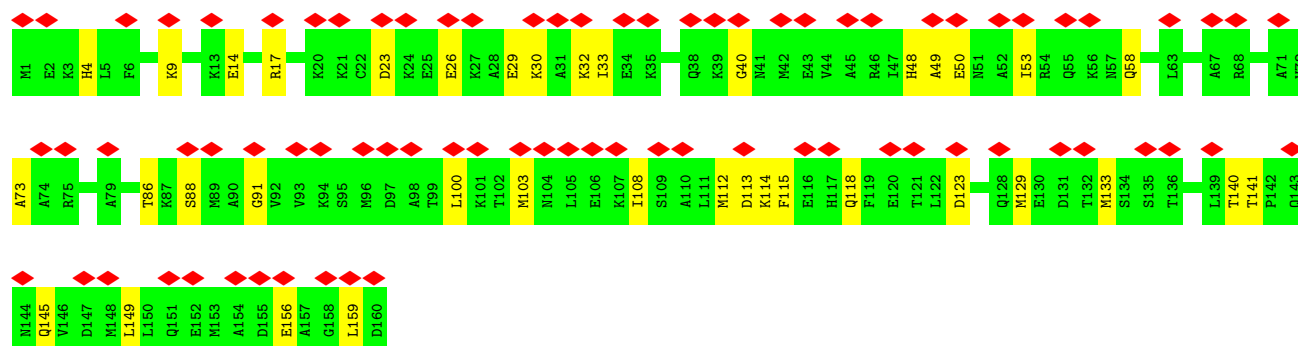
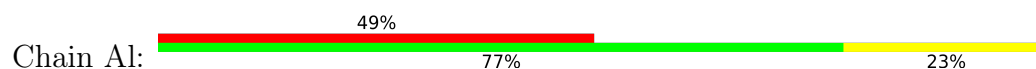


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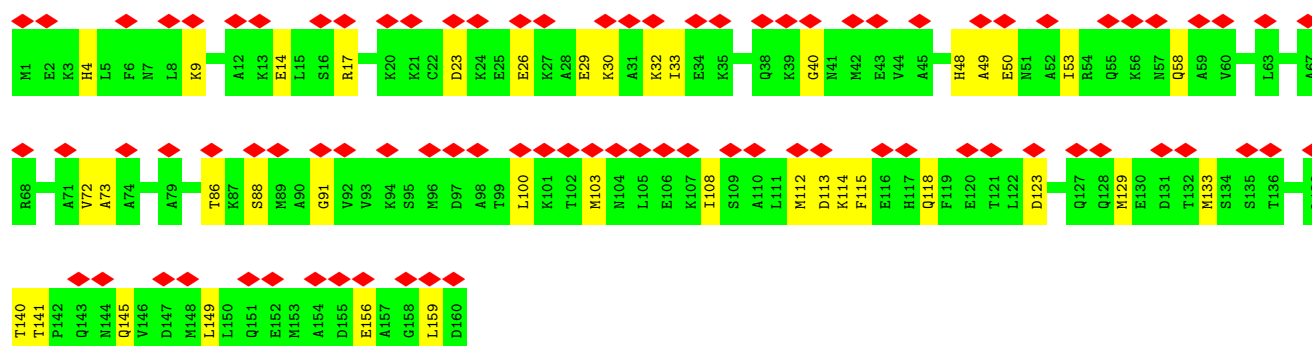
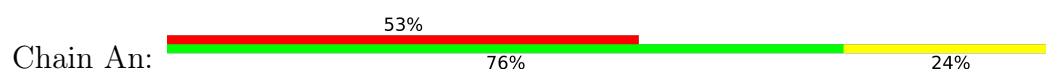




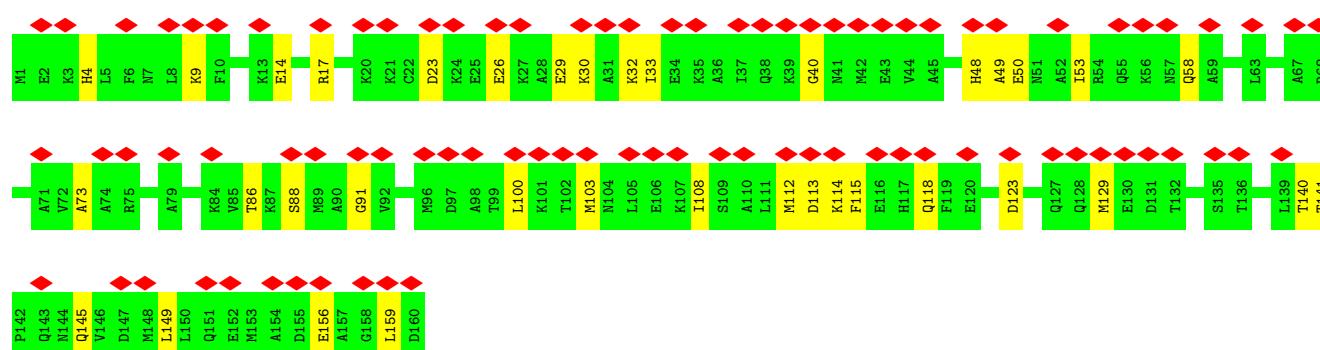
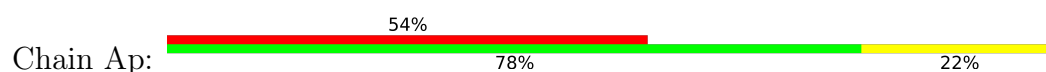
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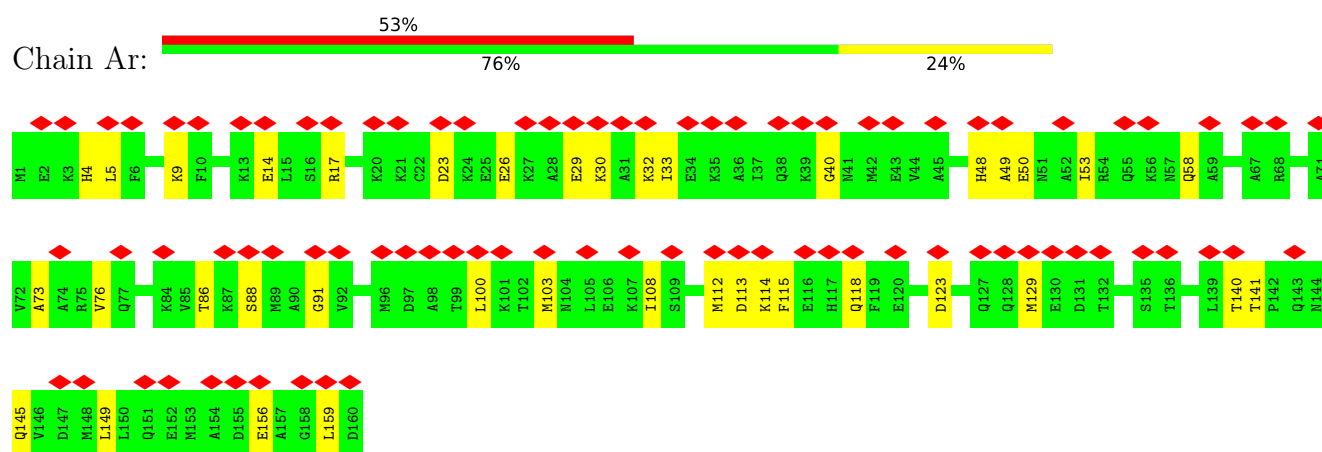
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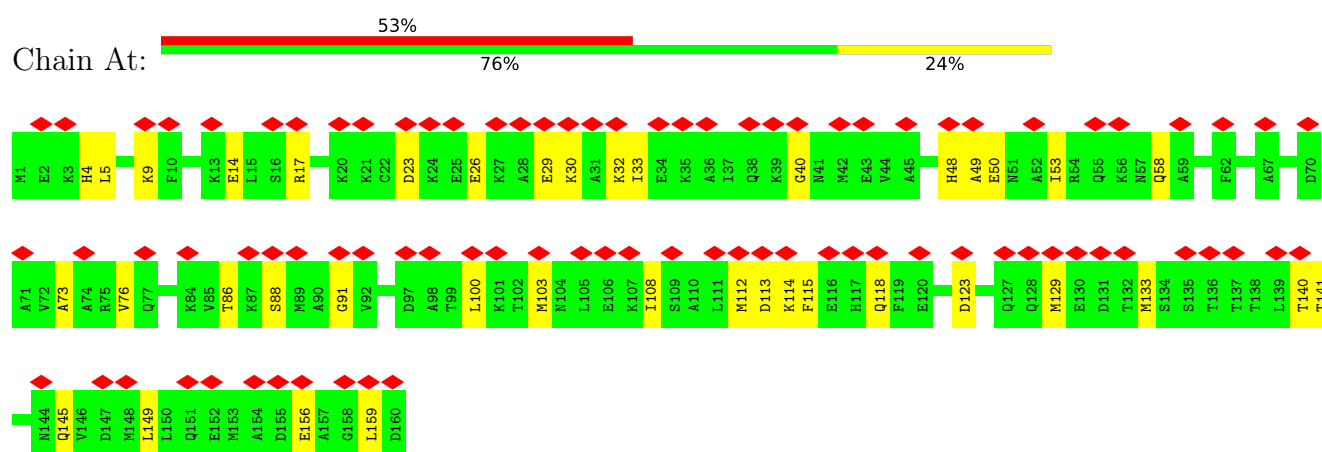
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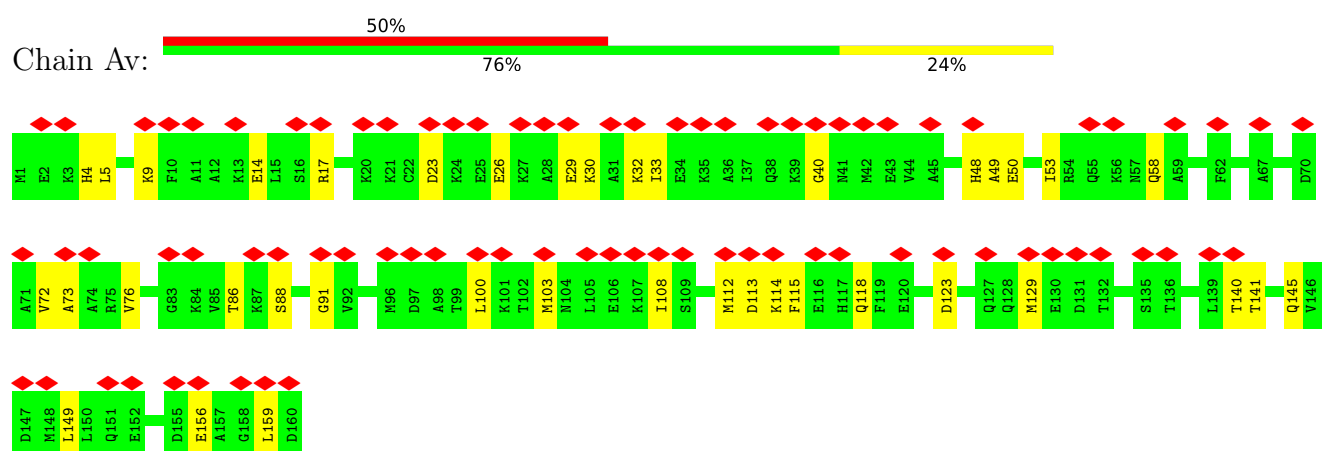
• Molecule 2: Charged multivesicular body protein 1b



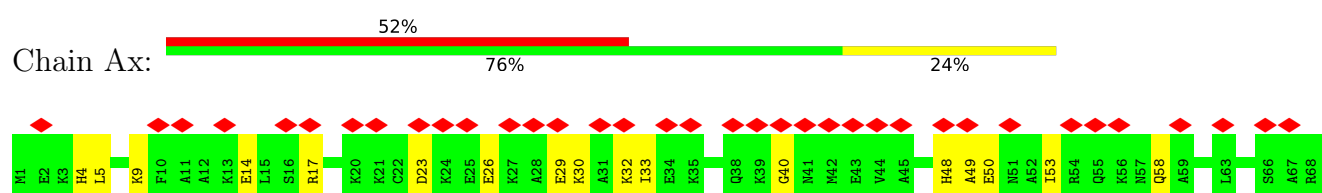
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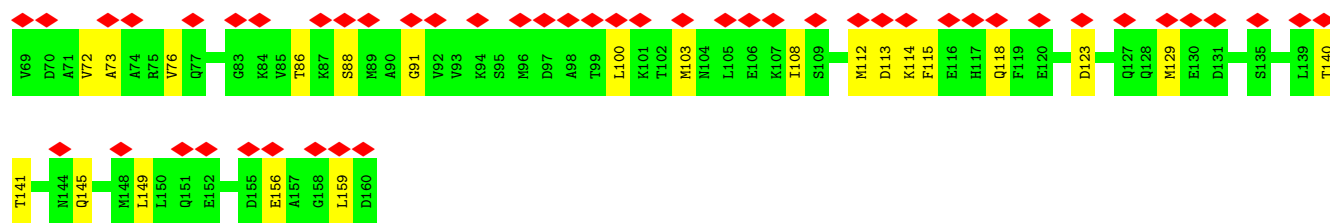


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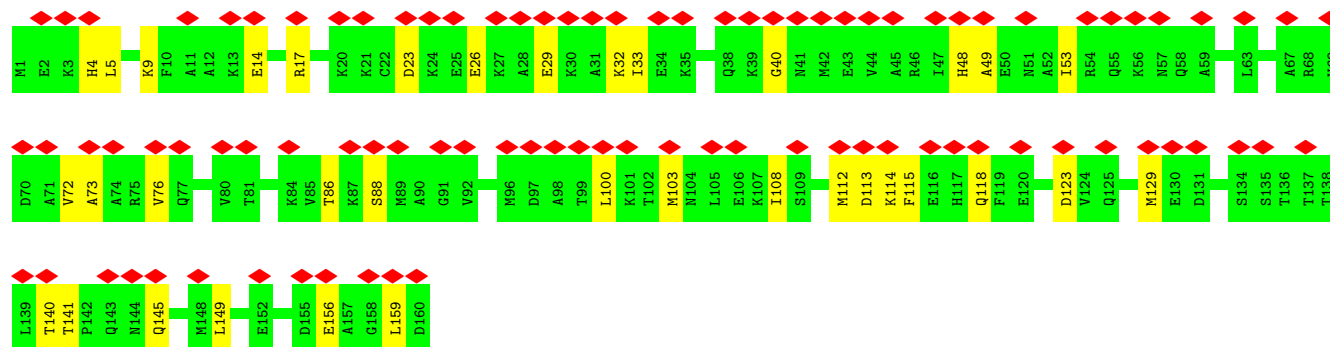
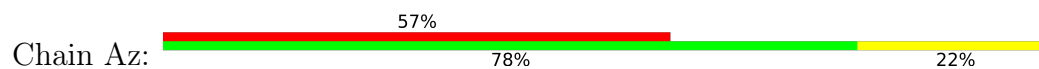


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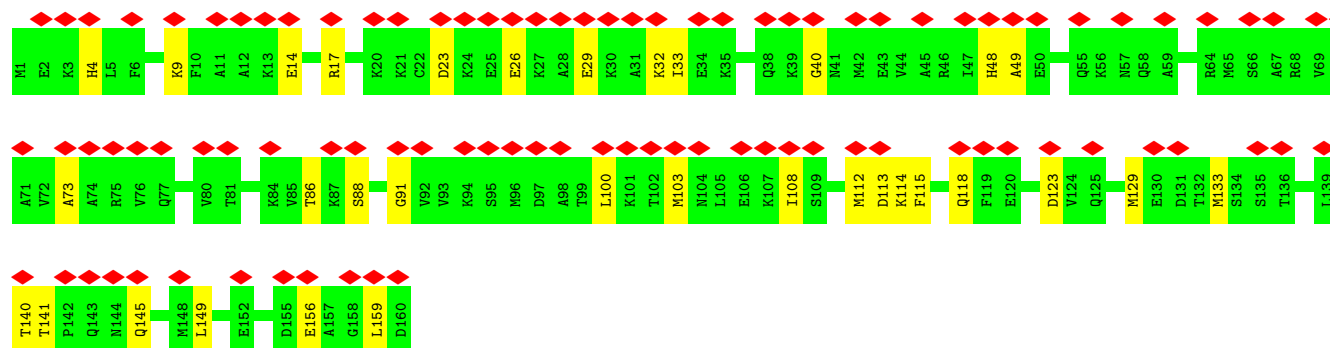
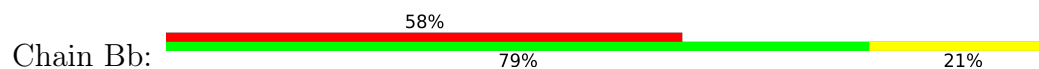




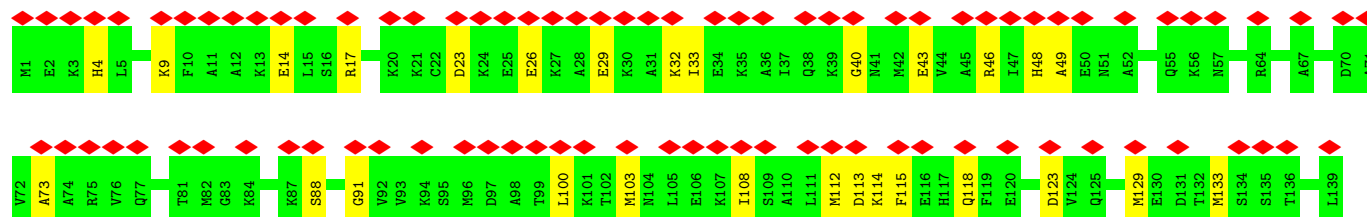
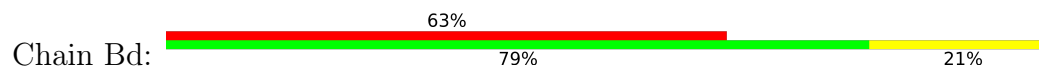
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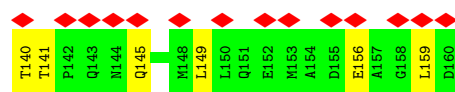


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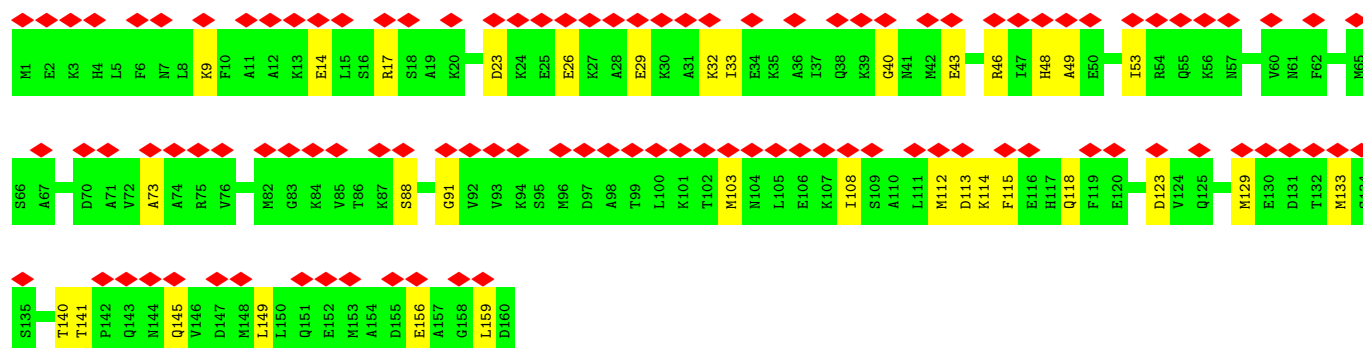
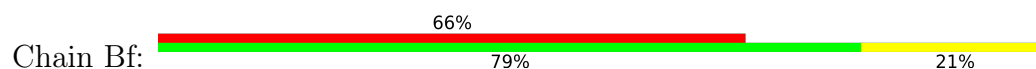


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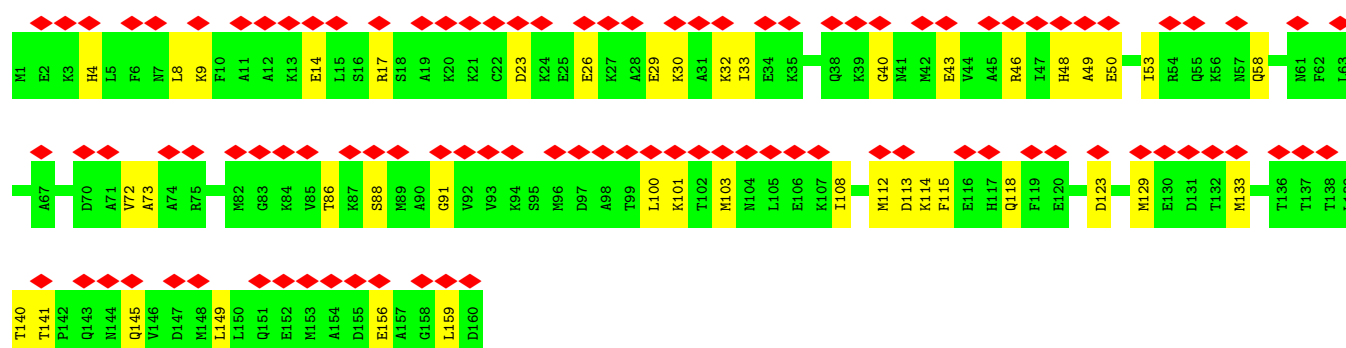
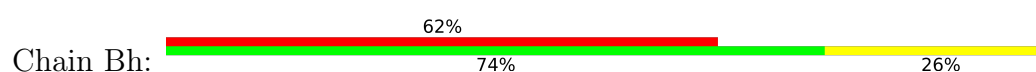




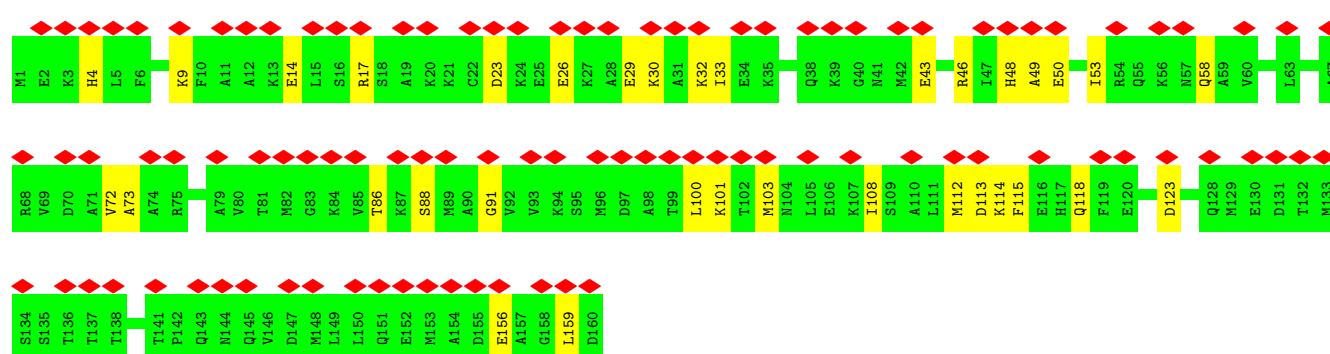
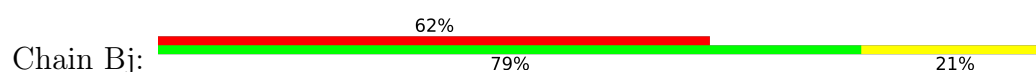
• Molecule 2: Charged multivesicular body protein 1b



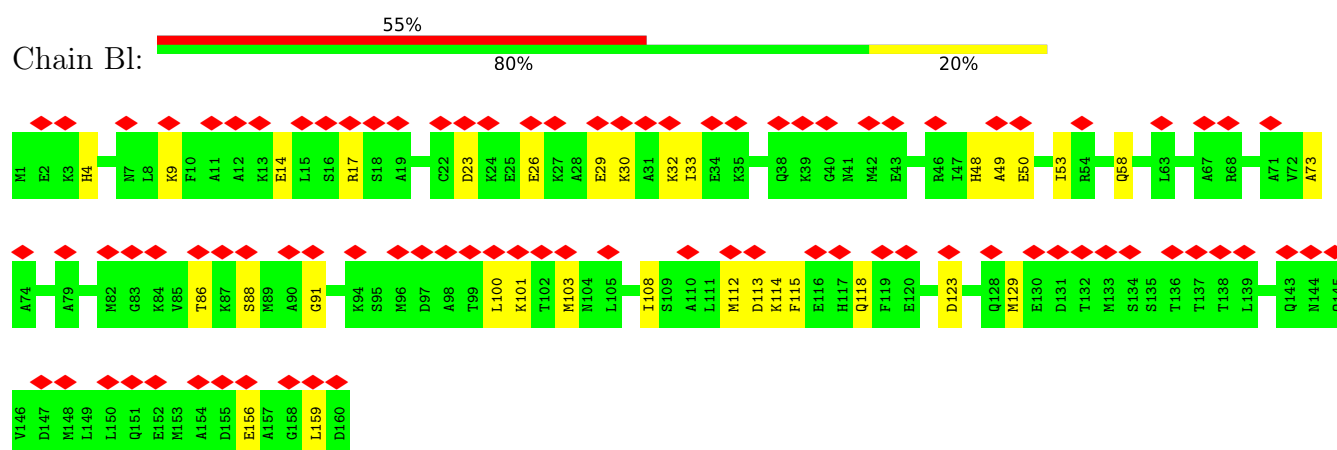
• Molecule 2: Charged multivesicular body protein 1b



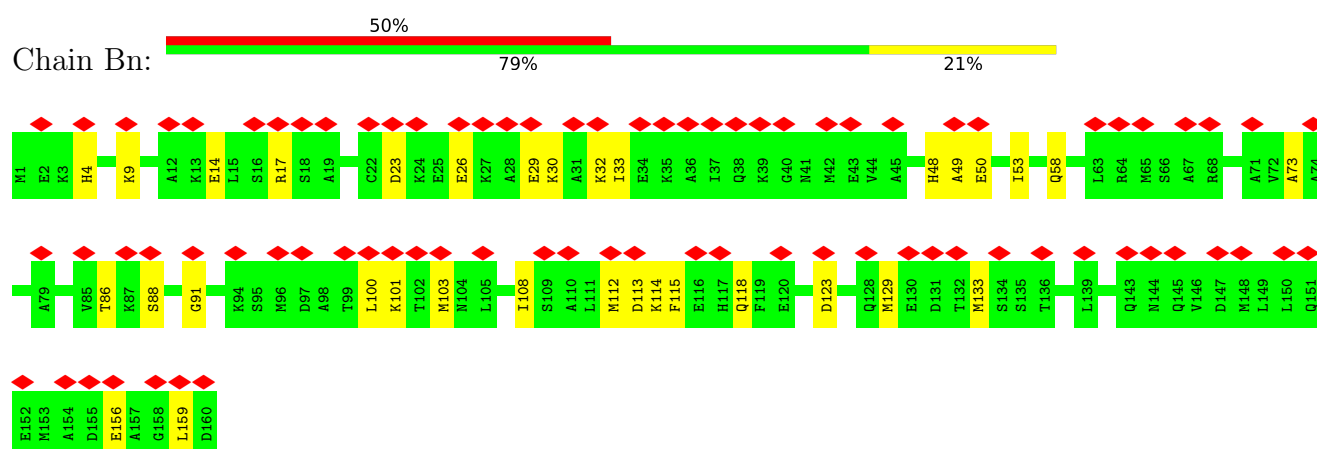
• Molecule 2: Charged multivesicular body protein 1b



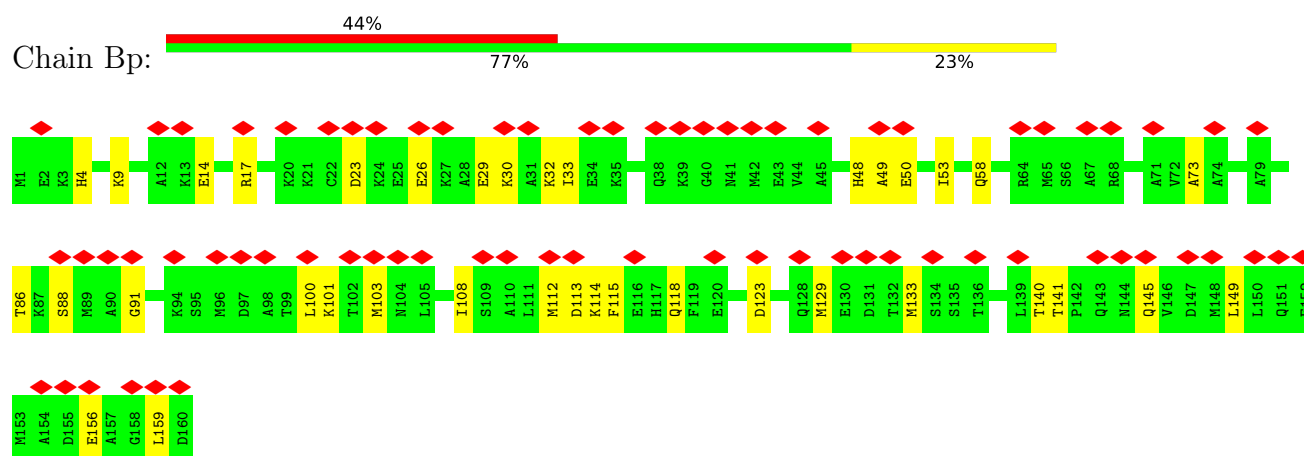
• Molecule 2: Charged multivesicular body protein 1b



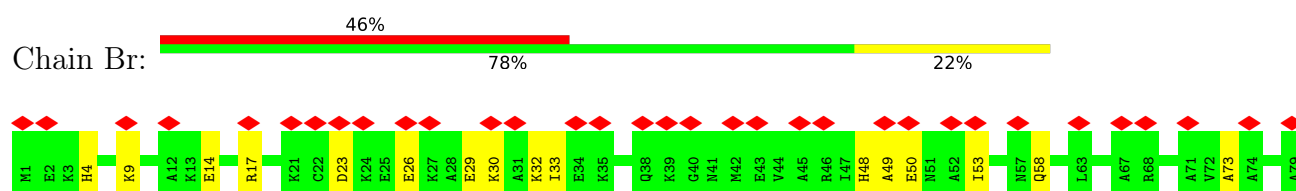
• Molecule 2: Charged multivesicular body protein 1b

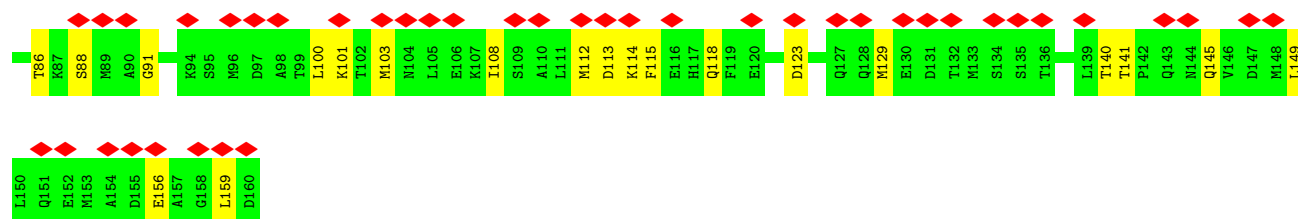


• Molecule 2: Charged multivesicular body protein 1b

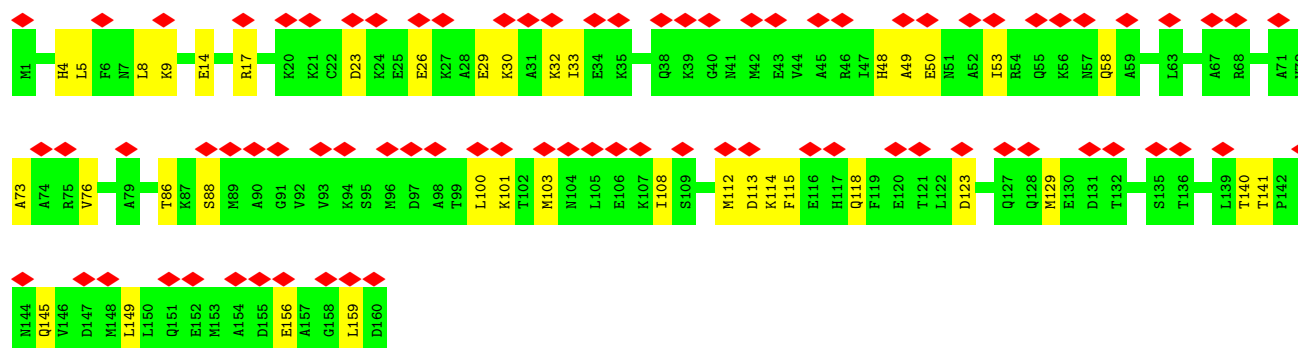
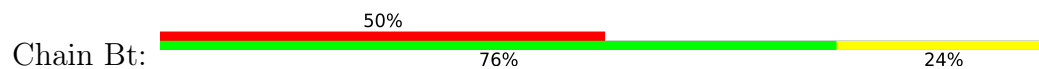


• Molecule 2: Charged multivesicular body protein 1b

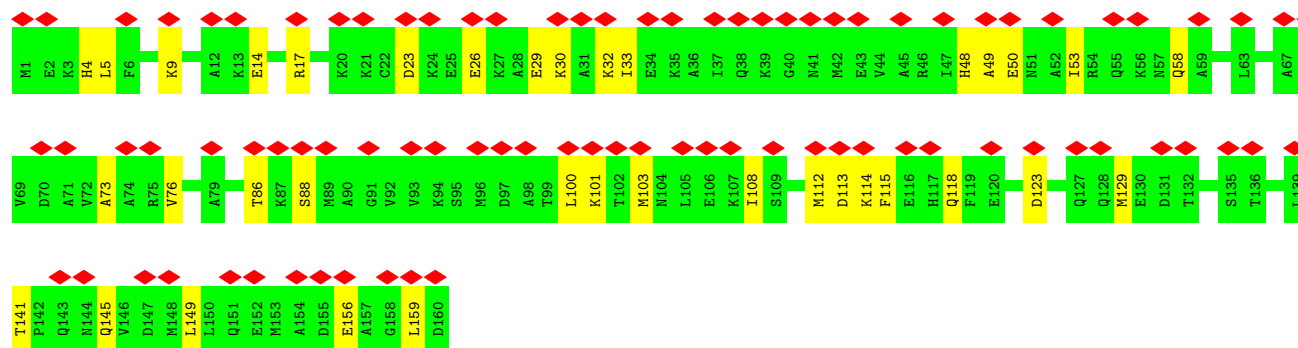
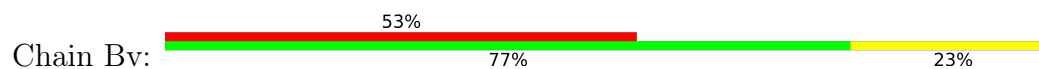




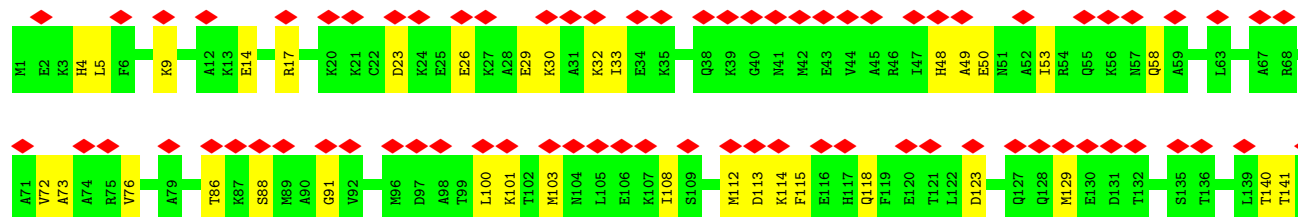
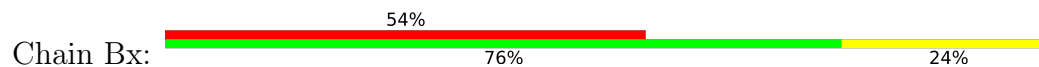
• Molecule 2: Charged multivesicular body protein 1b

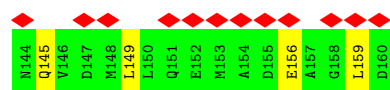


• Molecule 2: Charged multivesicular body protein 1b

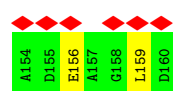
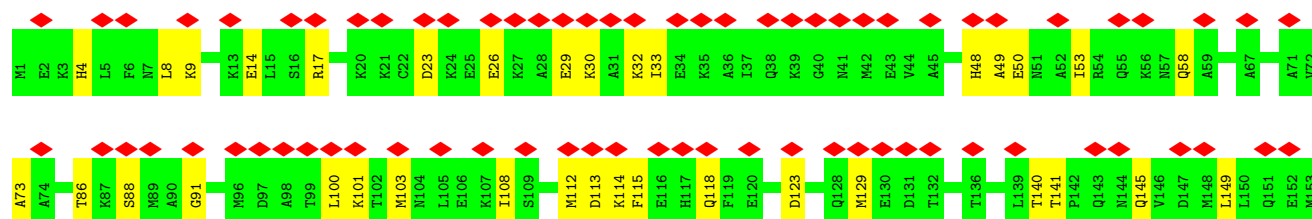
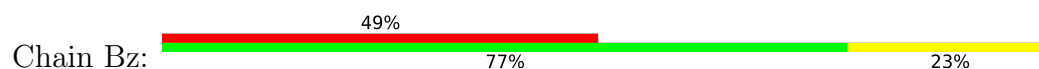


• Molecule 2: Charged multivesicular body protein 1b

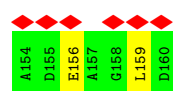
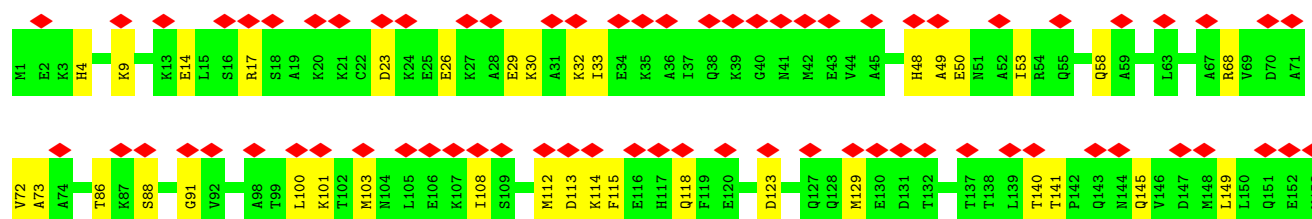
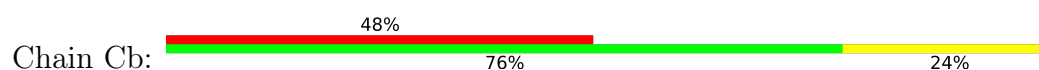




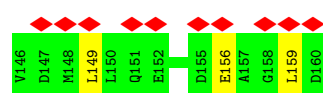
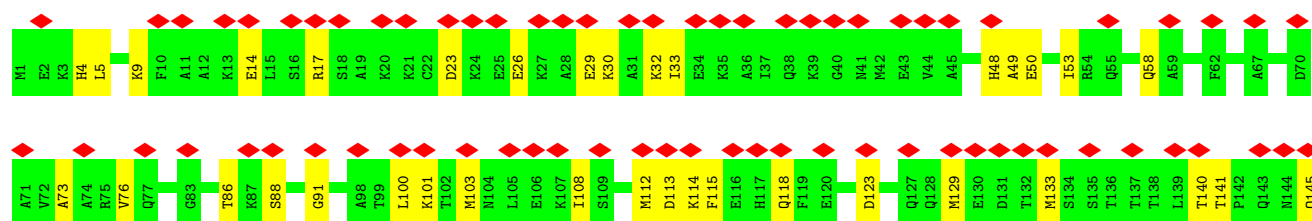
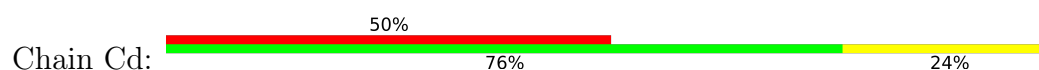
• Molecule 2: Charged multivesicular body protein 1b



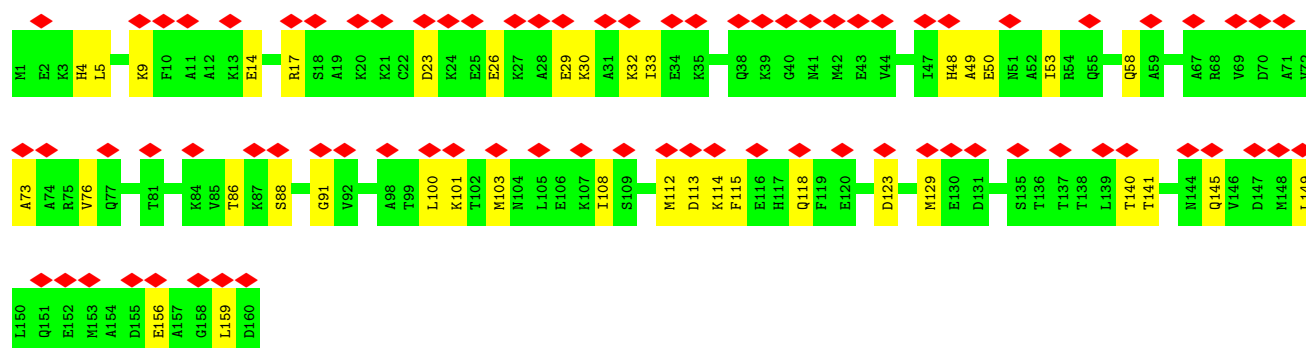
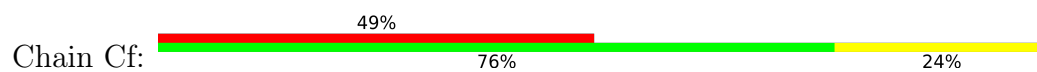
• Molecule 2: Charged multivesicular body protein 1b



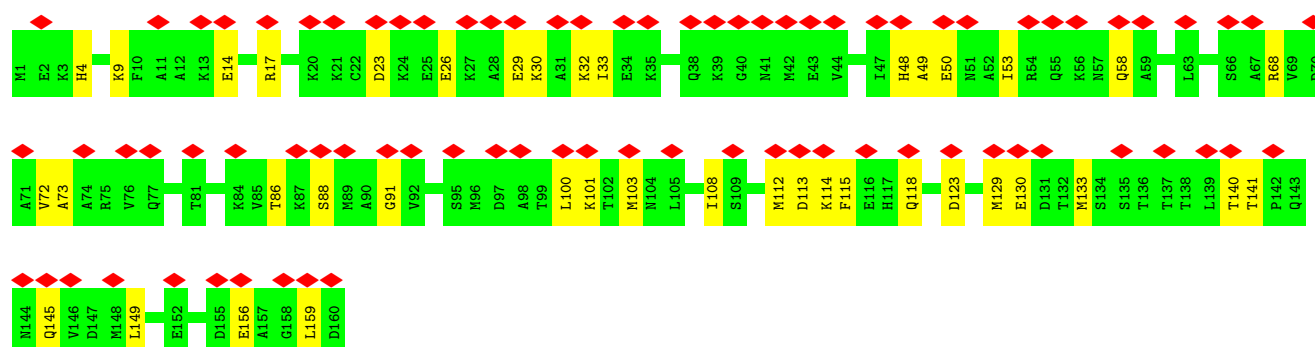
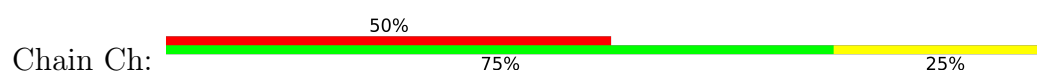
• Molecule 2: Charged multivesicular body protein 1b



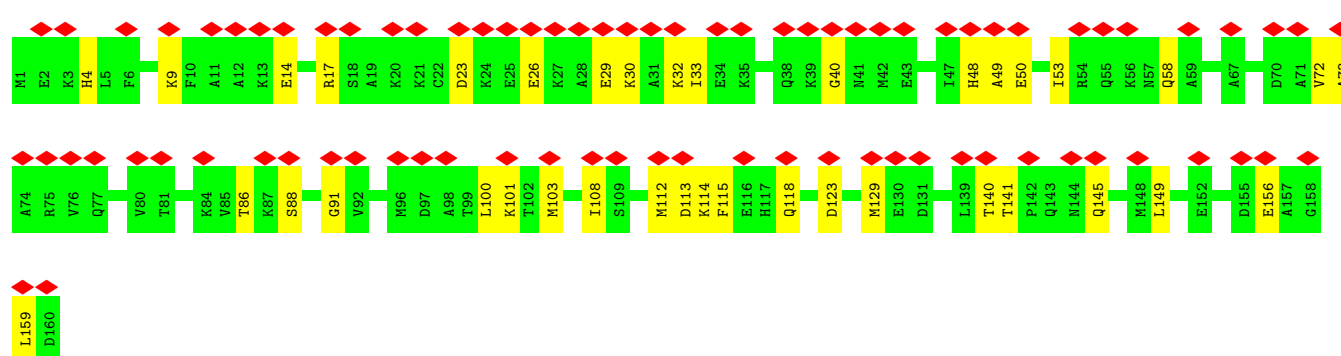
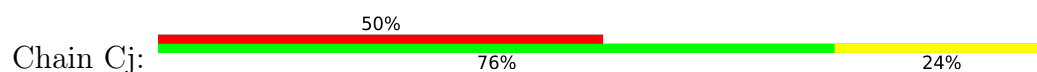
• Molecule 2: Charged multivesicular body protein 1b



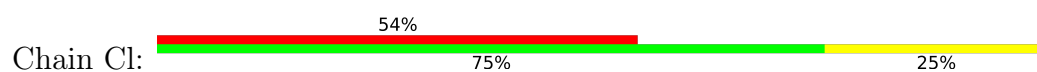
• Molecule 2: Charged multivesicular body protein 1b

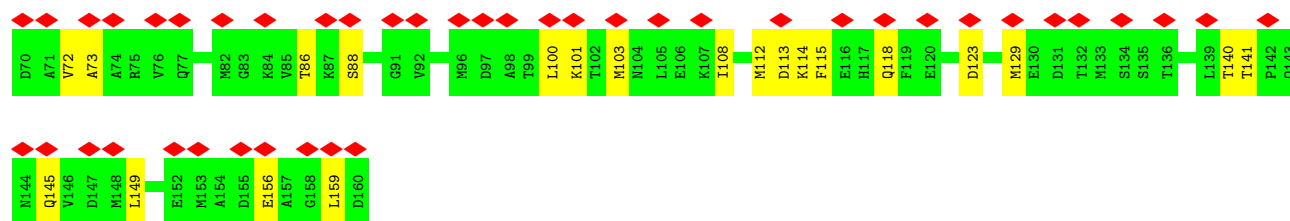


• Molecule 2: Charged multivesicular body protein 1b

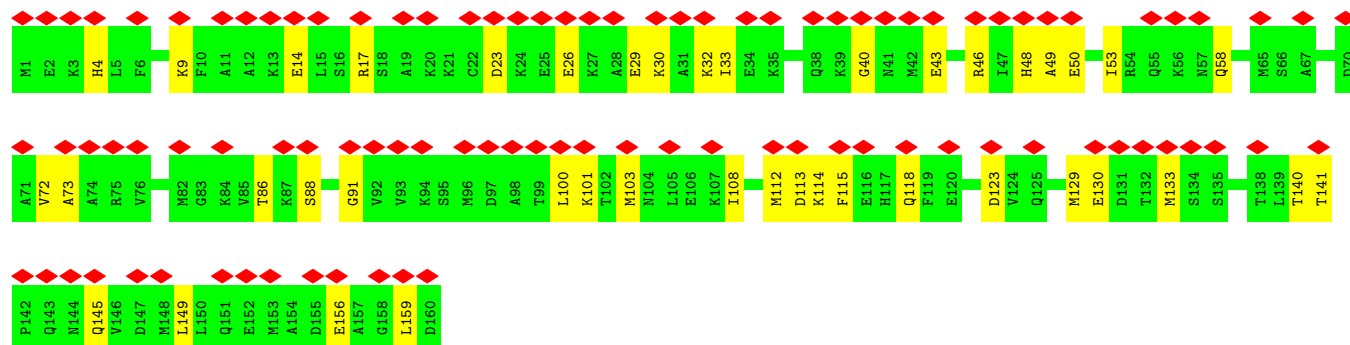
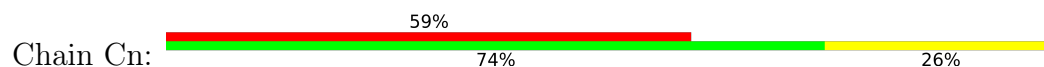


• Molecule 2: Charged multivesicular body protein 1b

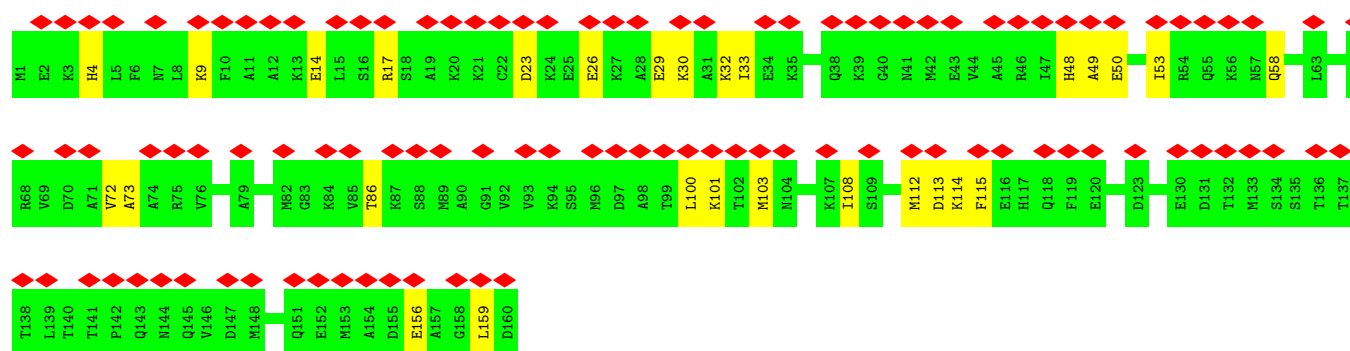
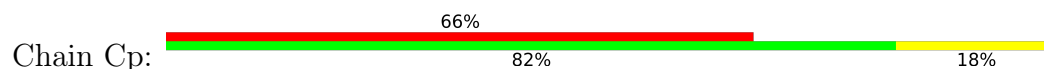




• Molecule 2: Charged multivesicular body protein 1b



• Molecule 2: Charged multivesicular body protein 1b



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=21.06°, rise=2.96 Å, axial sym=C1	Depositor
Number of segments used	188713	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TITAN KRIOS, FEI TECNAI F20, JEOL 3200FSC	Depositor
Voltage (kV)	300, 200, 300	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	600, 600, 600	Depositor
Maximum defocus (nm)	3000, 3000, 3000	Depositor
Magnification	59000, 50000, 59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	46.757	Depositor
Minimum map value	-40.775	Depositor
Average map value	0.015	Depositor
Map value standard deviation	3.645	Depositor
Recommended contour level	12	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Aa	0.48	0/1484	0.81	0/1997
1	Ac	0.48	0/1484	0.81	0/1997
1	Ae	0.48	0/1484	0.81	0/1997
1	Ag	0.48	0/1484	0.81	0/1997
1	Ai	0.48	0/1484	0.81	0/1997
1	Ak	0.48	0/1484	0.81	0/1997
1	Am	0.48	0/1484	0.81	0/1997
1	Ao	0.48	0/1484	0.81	0/1997
1	Aq	0.48	0/1484	0.81	0/1997
1	As	0.48	0/1484	0.81	0/1997
1	Au	0.48	0/1484	0.81	0/1997
1	Aw	0.48	0/1484	0.81	0/1997
1	Ay	0.48	0/1484	0.82	0/1997
1	Ba	0.48	0/1484	0.81	0/1997
1	Bc	0.48	0/1484	0.81	0/1997
1	Be	0.48	0/1484	0.81	0/1997
1	Bg	0.48	0/1484	0.81	0/1997
1	Bi	0.48	0/1484	0.81	0/1997
1	Bk	0.48	0/1484	0.81	0/1997
1	Bm	0.48	0/1484	0.81	0/1997
1	Bo	0.48	0/1484	0.81	0/1997
1	Bq	0.48	0/1484	0.81	0/1997
1	Bs	0.48	0/1484	0.81	0/1997
1	Bu	0.48	0/1484	0.81	0/1997
1	Bw	0.48	0/1484	0.81	0/1997
1	By	0.48	0/1484	0.81	0/1997
1	Ca	0.48	0/1484	0.81	0/1997
1	Cc	0.48	0/1484	0.81	0/1997
1	Ce	0.48	0/1484	0.81	0/1997
1	Cg	0.48	0/1484	0.81	0/1997
1	Ci	0.48	0/1484	0.81	0/1997
1	Ck	0.48	0/1484	0.81	0/1997
1	Cm	0.48	0/1484	0.81	0/1997
1	Co	0.48	0/1484	0.81	0/1997

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Ab	0.55	0/1251	0.85	0/1671
2	Ad	0.56	0/1251	0.85	0/1671
2	Af	0.55	0/1251	0.85	0/1671
2	Ah	0.56	0/1251	0.85	0/1671
2	Aj	0.56	0/1251	0.85	0/1671
2	Al	0.55	0/1251	0.85	0/1671
2	An	0.55	0/1251	0.85	0/1671
2	Ap	0.56	0/1251	0.85	0/1671
2	Ar	0.56	0/1251	0.85	0/1671
2	At	0.56	0/1251	0.85	0/1671
2	Av	0.56	0/1251	0.85	0/1671
2	Ax	0.55	0/1251	0.85	0/1671
2	Az	0.55	0/1251	0.85	0/1671
2	Bb	0.56	0/1251	0.85	0/1671
2	Bd	0.56	0/1251	0.85	0/1671
2	Bf	0.55	0/1251	0.85	0/1671
2	Bh	0.56	0/1251	0.85	0/1671
2	Bj	0.56	0/1251	0.85	0/1671
2	Bl	0.55	0/1251	0.85	0/1671
2	Bn	0.56	0/1251	0.85	0/1671
2	Bp	0.55	0/1251	0.85	0/1671
2	Br	0.56	0/1251	0.85	0/1671
2	Bt	0.56	0/1251	0.85	0/1671
2	Bv	0.56	0/1251	0.85	0/1671
2	Bx	0.56	0/1251	0.85	0/1671
2	Bz	0.56	0/1251	0.85	0/1671
2	Cb	0.56	0/1251	0.85	0/1671
2	Cd	0.56	0/1251	0.85	0/1671
2	Cf	0.56	0/1251	0.85	0/1671
2	Ch	0.56	0/1251	0.85	0/1671
2	Cj	0.56	0/1251	0.85	0/1671
2	Cl	0.56	0/1251	0.85	0/1671
2	Cn	0.55	0/1251	0.85	0/1671
2	Cp	0.56	0/1251	0.85	0/1671
All	All	0.51	0/92990	0.83	0/124712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	1466	0	1541	30	0
1	Ac	1466	0	1541	31	0
1	Ae	1466	0	1541	32	0
1	Ag	1466	0	1541	31	0
1	Ai	1466	0	1541	29	0
1	Ak	1466	0	1541	30	0
1	Am	1466	0	1541	29	0
1	Ao	1466	0	1541	30	0
1	Aq	1466	0	1541	30	0
1	As	1466	0	1541	31	0
1	Au	1466	0	1541	28	0
1	Aw	1466	0	1541	29	0
1	Ay	1466	0	1541	29	0
1	Ba	1466	0	1541	30	0
1	Bc	1466	0	1541	30	0
1	Be	1466	0	1541	26	0
1	Bg	1466	0	1541	30	0
1	Bi	1466	0	1541	32	0
1	Bk	1466	0	1541	32	0
1	Bm	1466	0	1541	32	0
1	Bo	1466	0	1541	31	0
1	Bq	1466	0	1541	32	0
1	Bs	1466	0	1541	32	0
1	Bu	1466	0	1541	29	0
1	Bw	1466	0	1541	30	0
1	By	1466	0	1541	28	0
1	Ca	1466	0	1541	31	0
1	Cc	1466	0	1541	29	0
1	Ce	1466	0	1541	30	0
1	Cg	1466	0	1541	30	0
1	Ci	1466	0	1541	31	0
1	Ck	1466	0	1541	29	0
1	Cm	1466	0	1541	29	0
1	Co	1466	0	1541	30	0
2	Ab	1243	0	1279	35	0
2	Ad	1243	0	1279	35	0
2	Af	1243	0	1279	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ah	1243	0	1279	33	0
2	Aj	1243	0	1279	32	0
2	Al	1243	0	1279	33	0
2	An	1243	0	1279	33	0
2	Ap	1243	0	1279	32	0
2	Ar	1243	0	1279	31	0
2	At	1243	0	1279	32	0
2	Av	1243	0	1279	34	0
2	Ax	1243	0	1279	32	0
2	Az	1243	0	1279	29	0
2	Bb	1243	0	1279	27	0
2	Bd	1243	0	1279	26	0
2	Bf	1243	0	1279	25	0
2	Bh	1243	0	1279	36	0
2	Bj	1243	0	1279	27	0
2	Bl	1243	0	1279	26	0
2	Bn	1243	0	1279	28	0
2	Bp	1243	0	1279	31	0
2	Br	1243	0	1279	29	0
2	Bt	1243	0	1279	31	0
2	Bv	1243	0	1279	30	0
2	Bx	1243	0	1279	33	0
2	Bz	1243	0	1279	34	0
2	Cb	1243	0	1279	33	0
2	Cd	1243	0	1279	33	0
2	Cf	1243	0	1279	32	0
2	Ch	1243	0	1279	36	0
2	Cj	1243	0	1279	33	0
2	Cl	1243	0	1279	35	0
2	Cn	1243	0	1279	37	0
2	Cp	1243	0	1279	21	0
All	All	92106	0	95880	1660	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 9.

All (1660) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bh:149:LEU:HD11	2:Ch:30:LYS:HE2	1.68	0.75
2:At:30:LYS:HE2	2:Bb:149:LEU:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bx:30:LYS:HE2	2:Cf:149:LEU:HD11	1.69	0.75
2:Ax:30:LYS:HE2	2:Bf:149:LEU:HD11	1.68	0.74
2:Bl:30:LYS:HE2	2:Bt:149:LEU:HD11	1.69	0.74
2:An:30:LYS:HE2	2:Av:149:LEU:HD11	1.70	0.74
2:Bz:30:LYS:HE2	2:Ch:149:LEU:HD11	1.68	0.74
2:Af:149:LEU:HD11	2:Cn:30:LYS:HE2	1.68	0.74
2:Bj:30:LYS:HE2	2:Br:149:LEU:HD11	1.68	0.74
2:Ah:30:LYS:HE2	2:Ap:149:LEU:HD11	1.70	0.74
2:Bv:30:LYS:HE2	2:Cd:149:LEU:HD11	1.70	0.73
2:Cb:30:LYS:HE2	2:Cj:149:LEU:HD11	1.70	0.73
2:Ad:149:LEU:HD11	2:Cl:30:LYS:HE2	1.69	0.73
2:Af:30:LYS:HE2	2:An:149:LEU:HD11	1.69	0.73
2:Av:30:LYS:HE2	2:Bd:149:LEU:HD11	1.69	0.73
2:Ap:30:LYS:HE2	2:Ax:149:LEU:HD11	1.70	0.73
1:Bc:133:GLY:H	1:Bc:137:ARG:HB2	1.53	0.73
2:Al:30:LYS:HE2	2:At:149:LEU:HD11	1.71	0.73
1:Bg:133:GLY:H	1:Bg:137:ARG:HB2	1.53	0.73
1:Bs:133:GLY:H	1:Bs:137:ARG:HB2	1.53	0.73
2:Cd:30:LYS:HE2	2:Cl:149:LEU:HD11	1.71	0.73
2:Ab:30:LYS:HE2	2:Aj:149:LEU:HD11	1.70	0.72
1:Be:133:GLY:H	1:Be:137:ARG:HB2	1.53	0.72
1:Bw:133:GLY:H	1:Bw:137:ARG:HB2	1.53	0.72
1:Ci:133:GLY:H	1:Ci:137:ARG:HB2	1.53	0.72
1:Am:133:GLY:H	1:Am:137:ARG:HB2	1.53	0.72
2:Ar:30:LYS:HE2	2:Az:149:LEU:HD11	1.71	0.72
2:Bn:30:LYS:HE2	2:Bv:149:LEU:HD11	1.70	0.72
1:Bu:133:GLY:H	1:Bu:137:ARG:HB2	1.53	0.72
1:Ck:133:GLY:H	1:Ck:137:ARG:HB2	1.53	0.72
1:Ak:133:GLY:H	1:Ak:137:ARG:HB2	1.53	0.72
2:Cf:30:LYS:HE2	2:Cn:149:LEU:HD11	1.70	0.72
2:Ad:30:LYS:HE2	2:Al:149:LEU:HD11	1.70	0.72
1:Ao:133:GLY:H	1:Ao:137:ARG:HB2	1.53	0.72
1:Ay:133:GLY:H	1:Ay:137:ARG:HB2	1.53	0.72
1:Co:133:GLY:H	1:Co:137:ARG:HB2	1.53	0.72
1:Ac:133:GLY:H	1:Ac:137:ARG:HB2	1.53	0.72
1:Bo:133:GLY:H	1:Bo:137:ARG:HB2	1.53	0.72
2:Bp:149:LEU:HD11	2:Cp:30:LYS:HE2	1.70	0.72
1:Cg:133:GLY:H	1:Cg:137:ARG:HB2	1.53	0.72
1:Ag:133:GLY:H	1:Ag:137:ARG:HB2	1.53	0.72
1:Ak:134:LYS:HG2	1:Ak:135:LEU:H	1.55	0.72
1:Bg:134:LYS:HG2	1:Bg:135:LEU:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:134:LYS:HG2	1:Bm:135:LEU:H	1.55	0.72
1:Bs:134:LYS:HG2	1:Bs:135:LEU:H	1.55	0.72
2:Aj:30:LYS:HE2	2:Ar:149:LEU:HD11	1.71	0.72
1:Ba:134:LYS:HG2	1:Ba:135:LEU:H	1.55	0.72
1:Bi:133:GLY:H	1:Bi:137:ARG:HB2	1.53	0.72
1:Ca:133:GLY:H	1:Ca:137:ARG:HB2	1.53	0.72
1:Ce:133:GLY:H	1:Ce:137:ARG:HB2	1.53	0.72
1:Ci:134:LYS:HG2	1:Ci:135:LEU:H	1.55	0.72
1:Cm:133:GLY:H	1:Cm:137:ARG:HB2	1.53	0.72
1:Co:134:LYS:HG2	1:Co:135:LEU:H	1.55	0.72
1:Ae:134:LYS:HG2	1:Ae:135:LEU:H	1.55	0.71
1:Ba:133:GLY:H	1:Ba:137:ARG:HB2	1.53	0.71
1:Bk:133:GLY:H	1:Bk:137:ARG:HB2	1.53	0.71
2:Bp:30:LYS:HE2	2:Bx:149:LEU:HD11	1.72	0.71
2:Ah:149:LEU:HD11	2:Bh:30:LYS:HE2	1.69	0.71
1:As:133:GLY:H	1:As:137:ARG:HB2	1.53	0.71
2:Br:30:LYS:HE2	2:Bz:149:LEU:HD11	1.72	0.71
1:Ac:134:LYS:HG2	1:Ac:135:LEU:H	1.55	0.71
1:Aq:134:LYS:HG2	1:Aq:135:LEU:H	1.55	0.71
1:As:134:LYS:HG2	1:As:135:LEU:H	1.55	0.71
1:Ay:134:LYS:HG2	1:Ay:135:LEU:H	1.55	0.71
1:Ca:134:LYS:HG2	1:Ca:135:LEU:H	1.55	0.71
2:Ab:149:LEU:HD11	2:Cj:30:LYS:HE2	1.70	0.71
1:Aq:133:GLY:H	1:Aq:137:ARG:HB2	1.54	0.71
1:Au:133:GLY:H	1:Au:137:ARG:HB2	1.53	0.71
1:Ai:134:LYS:HG2	1:Ai:135:LEU:H	1.55	0.71
1:Be:134:LYS:HG2	1:Be:135:LEU:H	1.55	0.71
1:Aw:133:GLY:H	1:Aw:137:ARG:HB2	1.53	0.71
1:Bi:134:LYS:HG2	1:Bi:135:LEU:H	1.55	0.71
1:Cc:134:LYS:HG2	1:Cc:135:LEU:H	1.55	0.71
1:Bk:134:LYS:HG2	1:Bk:135:LEU:H	1.55	0.71
1:Bq:133:GLY:H	1:Bq:137:ARG:HB2	1.53	0.71
1:Bq:134:LYS:HG2	1:Bq:135:LEU:H	1.55	0.71
1:By:134:LYS:HG2	1:By:135:LEU:H	1.55	0.71
1:Cg:134:LYS:HG2	1:Cg:135:LEU:H	1.55	0.71
1:Cm:134:LYS:HG2	1:Cm:135:LEU:H	1.55	0.71
1:Aa:133:GLY:H	1:Aa:137:ARG:HB2	1.54	0.71
1:Ae:133:GLY:H	1:Ae:137:ARG:HB2	1.53	0.71
1:Bu:134:LYS:HG2	1:Bu:135:LEU:H	1.55	0.71
1:Ck:134:LYS:HG2	1:Ck:135:LEU:H	1.55	0.71
1:Aa:134:LYS:HG2	1:Aa:135:LEU:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bo:134:LYS:HG2	1:Bo:135:LEU:H	1.55	0.70
1:Cc:133:GLY:H	1:Cc:137:ARG:HB2	1.53	0.70
1:Ai:133:GLY:H	1:Ai:137:ARG:HB2	1.53	0.70
1:Au:134:LYS:HG2	1:Au:135:LEU:H	1.55	0.70
2:Bt:30:LYS:HE2	2:Cb:149:LEU:HD11	1.72	0.70
1:By:133:GLY:H	1:By:137:ARG:HB2	1.53	0.70
1:Bm:133:GLY:H	1:Bm:137:ARG:HB2	1.53	0.70
1:Am:134:LYS:HG2	1:Am:135:LEU:H	1.55	0.70
1:Bc:134:LYS:HG2	1:Bc:135:LEU:H	1.55	0.70
1:Ao:134:LYS:HG2	1:Ao:135:LEU:H	1.55	0.70
1:Ag:134:LYS:HG2	1:Ag:135:LEU:H	1.55	0.70
1:Bw:134:LYS:HG2	1:Bw:135:LEU:H	1.55	0.69
1:Ce:134:LYS:HG2	1:Ce:135:LEU:H	1.55	0.69
1:Aw:134:LYS:HG2	1:Aw:135:LEU:H	1.55	0.69
1:Ce:133:GLY:N	1:Ce:137:ARG:HB2	2.12	0.65
1:Aw:133:GLY:N	1:Aw:137:ARG:HB2	2.13	0.64
1:Ae:133:GLY:N	1:Ae:137:ARG:HB2	2.13	0.64
1:Bi:133:GLY:N	1:Bi:137:ARG:HB2	2.13	0.64
1:Bg:133:GLY:N	1:Bg:137:ARG:HB2	2.13	0.64
1:Aq:133:GLY:N	1:Aq:137:ARG:HB2	2.13	0.64
1:Ba:133:GLY:N	1:Ba:137:ARG:HB2	2.13	0.64
1:Bo:133:GLY:N	1:Bo:137:ARG:HB2	2.13	0.64
1:By:133:GLY:N	1:By:137:ARG:HB2	2.13	0.64
1:Ca:133:GLY:N	1:Ca:137:ARG:HB2	2.13	0.64
1:Ck:133:GLY:N	1:Ck:137:ARG:HB2	2.13	0.64
1:Ak:133:GLY:N	1:Ak:137:ARG:HB2	2.13	0.64
1:Au:133:GLY:N	1:Au:137:ARG:HB2	2.13	0.64
1:Bm:133:GLY:N	1:Bm:137:ARG:HB2	2.13	0.64
1:Aa:133:GLY:N	1:Aa:137:ARG:HB2	2.13	0.64
1:Bs:133:GLY:N	1:Bs:137:ARG:HB2	2.13	0.64
1:Bu:133:GLY:N	1:Bu:137:ARG:HB2	2.13	0.64
1:Bc:133:GLY:N	1:Bc:137:ARG:HB2	2.13	0.64
1:Ci:133:GLY:N	1:Ci:137:ARG:HB2	2.13	0.64
1:Cg:133:GLY:N	1:Cg:137:ARG:HB2	2.13	0.64
1:Co:133:GLY:N	1:Co:137:ARG:HB2	2.13	0.64
1:Ag:133:GLY:N	1:Ag:137:ARG:HB2	2.13	0.64
1:Ao:133:GLY:N	1:Ao:137:ARG:HB2	2.13	0.64
2:Cl:4:HIS:HD2	2:Cn:88:SER:HA	1.63	0.64
1:Ai:133:GLY:N	1:Ai:137:ARG:HB2	2.13	0.63
1:As:133:GLY:N	1:As:137:ARG:HB2	2.13	0.63
1:Ac:133:GLY:N	1:Ac:137:ARG:HB2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:133:GLY:N	1:Am:137:ARG:HB2	2.13	0.63
1:Be:133:GLY:N	1:Be:137:ARG:HB2	2.13	0.63
1:Cc:133:GLY:N	1:Cc:137:ARG:HB2	2.13	0.63
2:Ab:88:SER:HA	2:Bh:4:HIS:HD2	1.64	0.63
1:Bk:133:GLY:N	1:Bk:137:ARG:HB2	2.13	0.63
1:Bo:61:ARG:HH12	1:Bo:155:GLU:H	1.47	0.63
1:Ac:61:ARG:HH12	1:Ac:155:GLU:H	1.47	0.63
2:Av:4:HIS:HD2	2:Ax:88:SER:HA	1.64	0.63
1:Ae:154:VAL:HG11	1:Ag:84:GLY:HA3	1.81	0.63
1:Ag:61:ARG:HH12	1:Ag:155:GLU:H	1.47	0.63
1:Ay:133:GLY:N	1:Ay:137:ARG:HB2	2.13	0.63
1:Bm:154:VAL:HG11	1:Bo:84:GLY:HA3	1.81	0.63
1:Bw:133:GLY:N	1:Bw:137:ARG:HB2	2.13	0.63
1:Cm:133:GLY:N	1:Cm:137:ARG:HB2	2.13	0.63
1:Bk:61:ARG:HH12	1:Bk:155:GLU:H	1.47	0.63
1:Bq:133:GLY:N	1:Bq:137:ARG:HB2	2.13	0.63
2:Bj:4:HIS:HD2	2:Bl:88:SER:HA	1.63	0.62
1:Bg:61:ARG:HH12	1:Bg:155:GLU:H	1.47	0.62
1:Bq:154:VAL:HG11	1:Bs:84:GLY:HA3	1.81	0.62
1:Bc:61:ARG:HH12	1:Bc:155:GLU:H	1.47	0.62
1:Bi:154:VAL:HG11	1:Bk:84:GLY:HA3	1.81	0.62
1:Ci:61:ARG:HH12	1:Ci:155:GLU:H	1.47	0.62
2:Ad:4:HIS:HD2	2:Af:88:SER:HA	1.64	0.62
2:Az:4:HIS:HD2	2:Bb:88:SER:HA	1.65	0.62
1:Ba:61:ARG:HH12	1:Ba:155:GLU:H	1.47	0.62
2:Bd:4:HIS:HD2	2:Bf:88:SER:HA	1.65	0.62
1:Cc:154:VAL:HG11	1:Ce:84:GLY:HA3	1.81	0.62
2:Ch:4:HIS:HD2	2:Cj:88:SER:HA	1.64	0.62
1:Am:61:ARG:HH12	1:Am:155:GLU:H	1.47	0.62
1:Bi:61:ARG:HH12	1:Bi:155:GLU:H	1.47	0.62
1:Bk:154:VAL:HG11	1:Bm:84:GLY:HA3	1.81	0.62
1:Bs:61:ARG:HH12	1:Bs:155:GLU:H	1.47	0.62
2:Bx:4:HIS:HD2	2:Bz:88:SER:HA	1.63	0.62
1:Cm:61:ARG:HH12	1:Cm:155:GLU:H	1.47	0.62
2:Ah:4:HIS:HD2	2:Aj:88:SER:HA	1.63	0.62
1:Ai:61:ARG:HH12	1:Ai:155:GLU:H	1.47	0.62
1:Aw:154:VAL:HG11	1:Ay:84:GLY:HA3	1.81	0.62
2:Bl:4:HIS:HD2	2:Bn:88:SER:HA	1.64	0.62
1:Co:61:ARG:HH12	1:Co:155:GLU:H	1.47	0.62
1:Bo:154:VAL:HG11	1:Bq:84:GLY:HA3	1.82	0.62
2:Bj:88:SER:HA	2:Cp:4:HIS:HD2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cb:4:HIS:HD2	2:Cd:88:SER:HA	1.64	0.62
2:Cf:4:HIS:HD2	2:Ch:88:SER:HA	1.64	0.62
2:An:4:HIS:HD2	2:Ap:88:SER:HA	1.64	0.62
2:Ap:4:HIS:HD2	2:Ar:88:SER:HA	1.63	0.62
1:Aq:61:ARG:HH12	1:Aq:155:GLU:H	1.47	0.62
1:Bu:61:ARG:HH12	1:Bu:155:GLU:H	1.47	0.62
1:Ai:154:VAL:HG11	1:Ak:84:GLY:HA3	1.81	0.61
2:At:4:HIS:HD2	2:Av:88:SER:HA	1.64	0.61
1:Au:154:VAL:HG11	1:Aw:84:GLY:HA3	1.82	0.61
1:Aw:61:ARG:HH12	1:Aw:155:GLU:H	1.47	0.61
2:Bb:4:HIS:HD2	2:Bd:88:SER:HA	1.65	0.61
1:Bg:84:GLY:HA3	1:Cm:154:VAL:HG11	1.81	0.61
1:By:61:ARG:HH12	1:By:155:GLU:H	1.47	0.61
1:Ak:61:ARG:HH12	1:Ak:155:GLU:H	1.47	0.61
1:Bs:154:VAL:HG11	1:Bu:84:GLY:HA3	1.81	0.61
1:Ca:154:VAL:HG11	1:Cc:84:GLY:HA3	1.81	0.61
2:Cd:4:HIS:HD2	2:Cf:88:SER:HA	1.65	0.61
1:Ce:61:ARG:HH12	1:Ce:155:GLU:H	1.47	0.61
1:Aa:154:VAL:HG11	1:Ac:84:GLY:HA3	1.82	0.61
1:Ac:154:VAL:HG11	1:Ae:84:GLY:HA3	1.82	0.61
2:Ar:4:HIS:HD2	2:At:88:SER:HA	1.65	0.61
1:Be:61:ARG:HH12	1:Be:155:GLU:H	1.47	0.61
2:Bn:4:HIS:HD2	2:Bp:88:SER:HA	1.63	0.61
1:Ck:61:ARG:HH12	1:Ck:155:GLU:H	1.47	0.61
1:Aa:61:ARG:HH12	1:Aa:155:GLU:H	1.47	0.61
1:Bm:61:ARG:HH12	1:Bm:155:GLU:H	1.47	0.61
1:Bq:61:ARG:HH12	1:Bq:155:GLU:H	1.47	0.61
2:Af:4:HIS:HD2	2:Ah:88:SER:HA	1.64	0.61
1:Am:154:VAL:HG11	1:Ao:84:GLY:HA3	1.81	0.61
1:As:61:ARG:HH12	1:As:155:GLU:H	1.47	0.61
2:Bz:4:HIS:HD2	2:Cb:88:SER:HA	1.65	0.61
1:Cc:61:ARG:HH12	1:Cc:155:GLU:H	1.47	0.61
1:Aa:84:GLY:HA3	1:Bg:154:VAL:HG11	1.82	0.61
1:Ak:154:VAL:HG11	1:Am:84:GLY:HA3	1.82	0.61
2:Bh:88:SER:HA	2:Cn:4:HIS:HD2	1.64	0.61
2:Bp:4:HIS:HD2	2:Br:88:SER:HA	1.65	0.61
1:Ag:154:VAL:HG11	1:Ai:84:GLY:HA3	1.82	0.61
2:Cj:4:HIS:HD2	2:Cl:88:SER:HA	1.66	0.61
2:Ab:4:HIS:HD2	2:Ad:88:SER:HA	1.65	0.61
1:Ae:61:ARG:HH12	1:Ae:155:GLU:H	1.47	0.61
1:Ce:154:VAL:HG11	1:Cg:84:GLY:HA3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ci:154:VAL:HG11	1:Ck:84:GLY:HA3	1.82	0.61
2:Aj:4:HIS:HD2	2:Al:88:SER:HA	1.64	0.61
1:Bw:154:VAL:HG11	1:By:84:GLY:HA3	1.81	0.61
1:Ao:154:VAL:HG11	1:Aq:84:GLY:HA3	1.82	0.60
2:Al:4:HIS:HD2	2:An:88:SER:HA	1.64	0.60
2:Br:4:HIS:HD2	2:Bt:88:SER:HA	1.64	0.60
2:Bt:4:HIS:HD2	2:Bv:88:SER:HA	1.65	0.60
1:Bw:61:ARG:HH12	1:Bw:155:GLU:H	1.47	0.60
1:Aq:154:VAL:HG11	1:As:84:GLY:HA3	1.82	0.60
1:As:154:VAL:HG11	1:Au:84:GLY:HA3	1.81	0.60
1:Ba:154:VAL:HG11	1:Bc:84:GLY:HA3	1.82	0.60
2:Ax:4:HIS:HD2	2:Az:88:SER:HA	1.65	0.60
1:Bu:154:VAL:HG11	1:Bw:84:GLY:HA3	1.82	0.60
1:Au:61:ARG:HH12	1:Au:155:GLU:H	1.47	0.60
1:Ca:61:ARG:HH12	1:Ca:155:GLU:H	1.47	0.60
1:Cg:61:ARG:HH12	1:Cg:155:GLU:H	1.47	0.60
1:Ck:154:VAL:HG11	1:Cm:84:GLY:HA3	1.81	0.60
1:Ay:61:ARG:HH12	1:Ay:155:GLU:H	1.47	0.60
1:By:154:VAL:HG11	1:Ca:84:GLY:HA3	1.82	0.60
1:Ca:86:ILE:O	1:Ca:127:LYS:NZ	2.29	0.60
1:Ao:61:ARG:HH12	1:Ao:155:GLU:H	1.47	0.60
1:As:86:ILE:O	1:As:127:LYS:NZ	2.29	0.59
2:Bv:4:HIS:HD2	2:Bx:88:SER:HA	1.65	0.59
1:Bc:154:VAL:HG11	1:Be:84:GLY:HA3	1.83	0.59
1:Bi:84:GLY:HA3	1:Co:154:VAL:HG11	1.84	0.59
1:Ak:86:ILE:O	1:Ak:127:LYS:NZ	2.29	0.59
1:Cg:154:VAL:HG11	1:Ci:84:GLY:HA3	1.83	0.59
2:Ax:53:ILE:HD12	2:Bf:145:GLN:HG3	1.84	0.59
1:Ay:154:VAL:HG11	1:Ba:84:GLY:HA3	1.83	0.58
1:Bu:86:ILE:O	1:Bu:127:LYS:NZ	2.29	0.58
2:Bz:53:ILE:HD12	2:Ch:145:GLN:HG3	1.84	0.58
2:Bh:145:GLN:HG3	2:Ch:53:ILE:HD12	1.84	0.58
2:Af:145:GLN:HG3	2:Cn:53:ILE:HD12	1.86	0.58
2:Bj:53:ILE:HD12	2:Br:145:GLN:HG3	1.86	0.58
2:Cp:14:GLU:OE1	2:Cp:17:ARG:NH2	2.37	0.58
2:Ah:14:GLU:OE1	2:Ah:17:ARG:NH2	2.37	0.58
2:Ap:14:GLU:OE1	2:Ap:17:ARG:NH2	2.37	0.58
2:Bp:145:GLN:HG3	2:Cp:53:ILE:HD12	1.86	0.58
2:Br:14:GLU:OE1	2:Br:17:ARG:NH2	2.37	0.58
2:Bz:14:GLU:OE1	2:Bz:17:ARG:NH2	2.37	0.58
2:Ad:14:GLU:OE1	2:Ad:17:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ah:145:GLN:HG3	2:Bh:53:ILE:HD12	1.86	0.57
2:Az:14:GLU:OE1	2:Az:17:ARG:NH2	2.37	0.57
2:Bf:14:GLU:OE1	2:Bf:17:ARG:NH2	2.37	0.57
2:Bl:53:ILE:HD12	2:Bt:145:GLN:HG3	1.86	0.57
1:Ce:86:ILE:O	1:Ce:127:LYS:NZ	2.29	0.57
1:Au:60:ILE:HG21	1:Au:157:PRO:HG2	1.86	0.57
2:Bl:14:GLU:OE1	2:Bl:17:ARG:NH2	2.37	0.57
2:Bp:14:GLU:OE1	2:Bp:17:ARG:NH2	2.37	0.57
2:Bx:14:GLU:OE1	2:Bx:17:ARG:NH2	2.37	0.57
2:Cj:14:GLU:OE1	2:Cj:17:ARG:NH2	2.37	0.57
2:Cn:14:GLU:OE1	2:Cn:17:ARG:NH2	2.37	0.57
1:Ae:60:ILE:HG21	1:Ae:157:PRO:HG2	1.86	0.57
2:Af:14:GLU:OE1	2:Af:17:ARG:NH2	2.37	0.57
1:Aq:60:ILE:HG21	1:Aq:157:PRO:HG2	1.86	0.57
2:Ar:14:GLU:OE1	2:Ar:17:ARG:NH2	2.37	0.57
1:Au:86:ILE:O	1:Au:127:LYS:NZ	2.29	0.57
2:Av:14:GLU:OE1	2:Av:17:ARG:NH2	2.37	0.57
2:Cd:14:GLU:OE1	2:Cd:17:ARG:NH2	2.37	0.57
2:Ch:14:GLU:OE1	2:Ch:17:ARG:NH2	2.37	0.57
2:An:14:GLU:OE1	2:An:17:ARG:NH2	2.37	0.57
2:Bh:14:GLU:OE1	2:Bh:17:ARG:NH2	2.37	0.57
1:By:60:ILE:HG21	1:By:157:PRO:HG2	1.86	0.57
1:Ce:60:ILE:HG21	1:Ce:157:PRO:HG2	1.86	0.57
2:Aj:14:GLU:OE1	2:Aj:17:ARG:NH2	2.37	0.57
2:Bb:14:GLU:OE1	2:Bb:17:ARG:NH2	2.37	0.57
2:Bd:14:GLU:OE1	2:Bd:17:ARG:NH2	2.37	0.57
2:Bn:53:ILE:HD12	2:Bv:145:GLN:HG3	1.86	0.57
2:Cb:14:GLU:OE1	2:Cb:17:ARG:NH2	2.37	0.57
1:Aa:60:ILE:HG21	1:Aa:157:PRO:HG2	1.86	0.57
1:Cc:60:ILE:HG21	1:Cc:157:PRO:HG2	1.86	0.57
1:Ac:60:ILE:HG21	1:Ac:157:PRO:HG2	1.86	0.57
1:Aw:60:ILE:HG21	1:Aw:157:PRO:HG2	1.86	0.57
2:Bt:14:GLU:OE1	2:Bt:17:ARG:NH2	2.37	0.57
2:Ab:14:GLU:OE1	2:Ab:17:ARG:NH2	2.37	0.57
1:Be:60:ILE:HG21	1:Be:157:PRO:HG2	1.86	0.57
1:Bi:60:ILE:HG21	1:Bi:157:PRO:HG2	1.86	0.57
2:Bx:53:ILE:HD12	2:Cf:145:GLN:HG3	1.85	0.57
1:Ca:60:ILE:HG21	1:Ca:157:PRO:HG2	1.86	0.57
2:Cf:14:GLU:OE1	2:Cf:17:ARG:NH2	2.37	0.57
2:Ax:14:GLU:OE1	2:Ax:17:ARG:NH2	2.38	0.57
1:Bg:60:ILE:HG21	1:Bg:157:PRO:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:60:ILE:HG21	1:Bk:157:PRO:HG2	1.86	0.57
1:Bm:60:ILE:HG21	1:Bm:157:PRO:HG2	1.86	0.57
2:Bn:14:GLU:OE1	2:Bn:17:ARG:NH2	2.37	0.57
1:Bu:60:ILE:HG21	1:Bu:157:PRO:HG2	1.86	0.57
1:Ag:60:ILE:HG21	1:Ag:157:PRO:HG2	1.86	0.57
2:Av:53:ILE:HD12	2:Bd:145:GLN:HG3	1.86	0.57
1:Ba:60:ILE:HG21	1:Ba:157:PRO:HG2	1.86	0.57
2:Bh:141:THR:HG21	2:Ch:50:GLU:HG2	1.87	0.57
1:Co:60:ILE:HG21	1:Co:157:PRO:HG2	1.86	0.57
2:Ah:53:ILE:HD12	2:Ap:145:GLN:HG3	1.87	0.56
1:Ai:60:ILE:HG21	1:Ai:157:PRO:HG2	1.86	0.56
1:Ao:60:ILE:HG21	1:Ao:157:PRO:HG2	1.86	0.56
2:At:14:GLU:OE1	2:At:17:ARG:NH2	2.38	0.56
2:Bj:14:GLU:OE1	2:Bj:17:ARG:NH2	2.37	0.56
2:Bv:14:GLU:OE1	2:Bv:17:ARG:NH2	2.37	0.56
2:Cf:53:ILE:HD12	2:Cn:145:GLN:HG3	1.86	0.56
1:Cm:60:ILE:HG21	1:Cm:157:PRO:HG2	1.86	0.56
2:Ad:145:GLN:HG3	2:Cl:53:ILE:HD12	1.87	0.56
1:Ak:60:ILE:HG21	1:Ak:157:PRO:HG2	1.86	0.56
2:Al:14:GLU:OE1	2:Al:17:ARG:NH2	2.37	0.56
2:Ab:113:ASP:OD1	2:Ab:114:LYS:N	2.39	0.56
1:Am:86:ILE:O	1:Am:127:LYS:NZ	2.29	0.56
1:Ao:53:ARG:O	1:Ao:56:VAL:HG12	2.06	0.56
2:Bf:113:ASP:OD1	2:Bf:114:LYS:N	2.39	0.56
2:Bh:113:ASP:OD1	2:Bh:114:LYS:N	2.39	0.56
2:Bn:113:ASP:OD1	2:Bn:114:LYS:N	2.39	0.56
1:Bo:60:ILE:HG21	1:Bo:157:PRO:HG2	1.86	0.56
2:Br:113:ASP:OD1	2:Br:114:LYS:N	2.39	0.56
2:Bt:113:ASP:OD1	2:Bt:114:LYS:N	2.39	0.56
2:Bv:113:ASP:OD1	2:Bv:114:LYS:N	2.39	0.56
2:Bx:113:ASP:OD1	2:Bx:114:LYS:N	2.39	0.56
1:Ca:53:ARG:O	1:Ca:56:VAL:HG12	2.06	0.56
1:Ci:60:ILE:HG21	1:Ci:157:PRO:HG2	1.86	0.56
1:Am:53:ARG:O	1:Am:56:VAL:HG12	2.06	0.56
1:Ay:60:ILE:HG21	1:Ay:157:PRO:HG2	1.86	0.56
2:Bl:113:ASP:OD1	2:Bl:114:LYS:N	2.39	0.56
1:Bq:60:ILE:HG21	1:Bq:157:PRO:HG2	1.86	0.56
1:Bs:60:ILE:HG21	1:Bs:157:PRO:HG2	1.86	0.56
1:Bu:53:ARG:O	1:Bu:56:VAL:HG12	2.06	0.56
1:Bw:53:ARG:O	1:Bw:56:VAL:HG12	2.06	0.56
2:Bz:113:ASP:OD1	2:Bz:114:LYS:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cl:14:GLU:OE1	2:Cl:17:ARG:NH2	2.37	0.56
2:Ad:113:ASP:OD1	2:Ad:114:LYS:N	2.39	0.56
1:Ag:53:ARG:O	1:Ag:56:VAL:HG12	2.06	0.56
1:Ai:53:ARG:O	1:Ai:56:VAL:HG12	2.06	0.56
2:Aj:113:ASP:OD1	2:Aj:114:LYS:N	2.39	0.56
1:Am:60:ILE:HG21	1:Am:157:PRO:HG2	1.86	0.56
1:Bc:60:ILE:HG21	1:Bc:157:PRO:HG2	1.86	0.56
1:Bg:53:ARG:O	1:Bg:56:VAL:HG12	2.06	0.56
2:Bj:113:ASP:OD1	2:Bj:114:LYS:N	2.39	0.56
2:Bp:113:ASP:OD1	2:Bp:114:LYS:N	2.39	0.56
1:By:53:ARG:O	1:By:56:VAL:HG12	2.06	0.56
2:Cb:113:ASP:OD1	2:Cb:114:LYS:N	2.39	0.56
1:Cc:53:ARG:O	1:Cc:56:VAL:HG12	2.06	0.56
1:Ck:60:ILE:HG21	1:Ck:157:PRO:HG2	1.86	0.56
1:Cm:53:ARG:O	1:Cm:56:VAL:HG12	2.06	0.56
2:Af:53:ILE:HD12	2:An:145:GLN:HG3	1.87	0.56
1:Ak:53:ARG:O	1:Ak:56:VAL:HG12	2.06	0.56
2:Al:113:ASP:OD1	2:Al:114:LYS:N	2.39	0.56
2:An:113:ASP:OD1	2:An:114:LYS:N	2.39	0.56
1:As:53:ARG:O	1:As:56:VAL:HG12	2.06	0.56
1:Bs:53:ARG:O	1:Bs:56:VAL:HG12	2.06	0.56
1:Co:53:ARG:O	1:Co:56:VAL:HG12	2.06	0.56
1:Ac:53:ARG:O	1:Ac:56:VAL:HG12	2.06	0.56
2:Ad:53:ILE:HD12	2:Al:145:GLN:HG3	1.88	0.56
2:Af:113:ASP:OD1	2:Af:114:LYS:N	2.39	0.56
1:Aq:53:ARG:O	1:Aq:56:VAL:HG12	2.06	0.56
2:At:53:ILE:HD12	2:Bb:145:GLN:HG3	1.86	0.56
1:Au:53:ARG:O	1:Au:56:VAL:HG12	2.06	0.56
1:Aw:53:ARG:O	1:Aw:56:VAL:HG12	2.06	0.56
1:Bo:53:ARG:O	1:Bo:56:VAL:HG12	2.06	0.56
1:Bq:53:ARG:O	1:Bq:56:VAL:HG12	2.06	0.56
2:Cd:113:ASP:OD1	2:Cd:114:LYS:N	2.39	0.56
1:Ce:53:ARG:O	1:Ce:56:VAL:HG12	2.06	0.56
2:Ch:113:ASP:OD1	2:Ch:114:LYS:N	2.39	0.56
1:Ck:53:ARG:O	1:Ck:56:VAL:HG12	2.06	0.56
1:Aa:53:ARG:O	1:Aa:56:VAL:HG12	2.06	0.56
1:Ae:53:ARG:O	1:Ae:56:VAL:HG12	2.06	0.56
2:Ah:113:ASP:OD1	2:Ah:114:LYS:N	2.39	0.56
1:Be:53:ARG:O	1:Be:56:VAL:HG12	2.06	0.56
2:Cf:113:ASP:OD1	2:Cf:114:LYS:N	2.39	0.56
1:Cg:53:ARG:O	1:Cg:56:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cg:86:ILE:O	1:Cg:127:LYS:NZ	2.29	0.56
1:Ci:53:ARG:O	1:Ci:56:VAL:HG12	2.06	0.56
2:Cp:113:ASP:OD1	2:Cp:114:LYS:N	2.39	0.56
2:Ab:145:GLN:HG3	2:Cj:53:ILE:HD12	1.88	0.56
2:Ap:113:ASP:OD1	2:Ap:114:LYS:N	2.39	0.56
1:Ay:53:ARG:O	1:Ay:56:VAL:HG12	2.06	0.56
1:Ba:53:ARG:O	1:Ba:56:VAL:HG12	2.06	0.56
1:Bc:53:ARG:O	1:Bc:56:VAL:HG12	2.06	0.56
2:Bd:113:ASP:OD1	2:Bd:114:LYS:N	2.39	0.56
1:Bm:53:ARG:O	1:Bm:56:VAL:HG12	2.06	0.56
1:Bw:60:ILE:HG21	1:Bw:157:PRO:HG2	1.86	0.56
2:Cn:113:ASP:OD1	2:Cn:114:LYS:N	2.39	0.56
2:Ab:53:ILE:HD12	2:Aj:145:GLN:HG3	1.88	0.56
1:As:60:ILE:HG21	1:As:157:PRO:HG2	1.86	0.56
1:Bi:53:ARG:O	1:Bi:56:VAL:HG12	2.06	0.56
2:Cj:113:ASP:OD1	2:Cj:114:LYS:N	2.39	0.56
2:Cl:113:ASP:OD1	2:Cl:114:LYS:N	2.39	0.56
1:Bk:53:ARG:O	1:Bk:56:VAL:HG12	2.06	0.55
2:Ap:53:ILE:HD12	2:Ax:145:GLN:HG3	1.87	0.55
2:Ar:113:ASP:OD1	2:Ar:114:LYS:N	2.39	0.55
1:Aw:86:ILE:O	1:Aw:127:LYS:NZ	2.29	0.55
2:Ax:113:ASP:OD1	2:Ax:114:LYS:N	2.39	0.55
2:Bp:53:ILE:HD12	2:Bx:145:GLN:HG3	1.88	0.55
1:Cg:60:ILE:HG21	1:Cg:157:PRO:HG2	1.86	0.55
2:Az:113:ASP:OD1	2:Az:114:LYS:N	2.39	0.55
1:Bw:86:ILE:O	1:Bw:127:LYS:NZ	2.29	0.55
2:At:113:ASP:OD1	2:At:114:LYS:N	2.39	0.55
2:Av:113:ASP:OD1	2:Av:114:LYS:N	2.39	0.55
2:An:53:ILE:HD12	2:Av:145:GLN:HG3	1.87	0.55
2:Bh:33:ILE:HD11	2:Bh:49:ALA:HA	1.89	0.55
1:Bm:24:LEU:HD13	2:Bp:123:ASP:HB3	1.88	0.55
2:Cl:33:ILE:HD11	2:Cl:49:ALA:HA	1.89	0.55
2:Ab:33:ILE:HD11	2:Ab:49:ALA:HA	1.89	0.55
2:Ad:33:ILE:HD11	2:Ad:49:ALA:HA	1.89	0.55
2:Bb:113:ASP:OD1	2:Bb:114:LYS:N	2.39	0.55
1:Ae:24:LEU:HD13	2:Ah:123:ASP:HB3	1.89	0.55
1:Bq:24:LEU:HD13	2:Bt:123:ASP:HB3	1.89	0.55
2:Bz:50:GLU:HG2	2:Ch:141:THR:HG21	1.89	0.55
2:Bb:33:ILE:HD11	2:Bb:49:ALA:HA	1.89	0.55
2:Bj:33:ILE:HD11	2:Bj:49:ALA:HA	1.89	0.55
2:Cd:53:ILE:HD12	2:Cl:145:GLN:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cj:33:ILE:HD11	2:Cj:49:ALA:HA	1.89	0.55
2:Cn:33:ILE:HD11	2:Cn:49:ALA:HA	1.89	0.55
1:Ai:24:LEU:HD13	2:Al:123:ASP:HB3	1.89	0.55
2:Bd:33:ILE:HD11	2:Bd:49:ALA:HA	1.89	0.55
2:Bf:33:ILE:HD11	2:Bf:49:ALA:HA	1.89	0.55
1:Bk:24:LEU:HD13	2:Bn:123:ASP:HB3	1.89	0.55
2:Ch:33:ILE:HD11	2:Ch:49:ALA:HA	1.89	0.55
1:Bo:86:ILE:O	1:Bo:127:LYS:NZ	2.29	0.55
2:Cp:33:ILE:HD11	2:Cp:49:ALA:HA	1.89	0.55
2:Af:33:ILE:HD11	2:Af:49:ALA:HA	1.89	0.54
2:Bn:33:ILE:HD11	2:Bn:49:ALA:HA	1.89	0.54
2:Bp:33:ILE:HD11	2:Bp:49:ALA:HA	1.89	0.54
2:Ah:33:ILE:HD11	2:Ah:49:ALA:HA	1.89	0.54
2:Av:33:ILE:HD11	2:Av:49:ALA:HA	1.89	0.54
2:Az:33:ILE:HD11	2:Az:49:ALA:HA	1.89	0.54
2:Bl:33:ILE:HD11	2:Bl:49:ALA:HA	1.89	0.54
2:Cf:33:ILE:HD11	2:Cf:49:ALA:HA	1.89	0.54
2:Ax:33:ILE:HD11	2:Ax:49:ALA:HA	1.89	0.54
2:Bv:53:ILE:HD12	2:Cd:145:GLN:HG3	1.87	0.54
2:Cb:53:ILE:HD12	2:Cj:145:GLN:HG3	1.88	0.54
1:Ci:86:ILE:O	1:Ci:127:LYS:NZ	2.29	0.54
2:Ar:53:ILE:HD12	2:Az:145:GLN:HG3	1.88	0.54
2:Bh:123:ASP:HB3	1:Cm:24:LEU:HD13	1.89	0.54
1:Bo:24:LEU:HD13	2:Br:123:ASP:HB3	1.90	0.54
2:Br:33:ILE:HD11	2:Br:49:ALA:HA	1.89	0.54
2:Aj:53:ILE:HD12	2:Ar:145:GLN:HG3	1.89	0.54
1:Am:24:LEU:HD13	2:Ap:123:ASP:HB3	1.89	0.54
2:Cd:50:GLU:HG2	2:Cl:141:THR:HG21	1.90	0.54
2:Al:53:ILE:HD12	2:At:145:GLN:HG3	1.88	0.54
2:Ax:50:GLU:HG2	2:Bf:141:THR:HG21	1.88	0.54
2:Cd:33:ILE:HD11	2:Cd:49:ALA:HA	1.89	0.54
2:Ab:123:ASP:HB3	1:Bg:24:LEU:HD13	1.90	0.54
2:Aj:33:ILE:HD11	2:Aj:49:ALA:HA	1.89	0.54
2:Bt:33:ILE:HD11	2:Bt:49:ALA:HA	1.89	0.54
2:Bx:50:GLU:HG2	2:Cf:141:THR:HG21	1.90	0.54
1:Aa:24:LEU:HD13	2:Ad:123:ASP:HB3	1.90	0.54
2:At:33:ILE:HD11	2:At:49:ALA:HA	1.89	0.54
1:Ac:24:LEU:HD13	2:Af:123:ASP:HB3	1.90	0.54
2:Av:50:GLU:HG2	2:Bd:141:THR:HG21	1.90	0.54
1:Bi:24:LEU:HD13	2:Bl:123:ASP:HB3	1.90	0.54
1:Bs:24:LEU:HD13	2:Bv:123:ASP:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cf:50:GLU:HG2	2:Cn:141:THR:HG21	1.90	0.54
1:Ag:24:LEU:HD13	2:Aj:123:ASP:HB3	1.90	0.54
1:Ay:86:ILE:O	1:Ay:127:LYS:NZ	2.29	0.54
2:Br:53:ILE:HD12	2:Bz:145:GLN:HG3	1.89	0.54
1:Ck:24:LEU:HD13	2:Cn:123:ASP:HB3	1.90	0.54
2:Bt:53:ILE:HD12	2:Cb:145:GLN:HG3	1.89	0.53
1:Bu:24:LEU:HD13	2:Bx:123:ASP:HB3	1.90	0.53
2:Bx:33:ILE:HD11	2:Bx:49:ALA:HA	1.89	0.53
1:Ak:24:LEU:HD13	2:An:123:ASP:HB3	1.90	0.53
2:Al:33:ILE:HD11	2:Al:49:ALA:HA	1.89	0.53
2:An:33:ILE:HD11	2:An:49:ALA:HA	1.89	0.53
1:Bw:24:LEU:HD13	2:Bz:123:ASP:HB3	1.89	0.53
2:Cb:33:ILE:HD11	2:Cb:49:ALA:HA	1.89	0.53
1:Ao:24:LEU:HD13	2:Ar:123:ASP:HB3	1.90	0.53
2:Bv:33:ILE:HD11	2:Bv:49:ALA:HA	1.89	0.53
2:Ar:33:ILE:HD11	2:Ar:49:ALA:HA	1.89	0.53
2:Bp:141:THR:HG21	2:Cp:50:GLU:HG2	1.89	0.53
1:As:24:LEU:HD13	2:Av:123:ASP:HB3	1.89	0.53
2:Bz:33:ILE:HD11	2:Bz:49:ALA:HA	1.89	0.53
2:Ap:33:ILE:HD11	2:Ap:49:ALA:HA	1.89	0.53
2:Ap:50:GLU:HG2	2:Ax:141:THR:HG21	1.91	0.53
1:Ao:86:ILE:O	1:Ao:127:LYS:NZ	2.29	0.53
1:Au:24:LEU:HD13	2:Ax:123:ASP:HB3	1.89	0.53
1:Ci:24:LEU:HD13	2:Cl:123:ASP:HB3	1.90	0.53
2:Bt:50:GLU:HG2	2:Cb:141:THR:HG21	1.90	0.53
2:Bv:50:GLU:HG2	2:Cd:141:THR:HG21	1.90	0.53
1:Aw:24:LEU:HD13	2:Az:123:ASP:HB3	1.89	0.53
2:Bl:50:GLU:HG2	2:Bt:141:THR:HG21	1.89	0.53
1:Ca:24:LEU:HD13	2:Cd:123:ASP:HB3	1.89	0.53
1:Ck:86:ILE:O	1:Ck:127:LYS:NZ	2.29	0.53
1:Aq:24:LEU:HD13	2:At:123:ASP:HB3	1.90	0.53
2:Ar:50:GLU:HG2	2:Az:141:THR:HG21	1.91	0.53
2:Az:86:THR:OG1	2:Bd:129:MET:HE1	2.08	0.53
2:Bn:50:GLU:HG2	2:Bv:141:THR:HG21	1.90	0.53
2:Bp:50:GLU:HG2	2:Bx:141:THR:HG21	1.89	0.53
1:By:24:LEU:HD13	2:Cb:123:ASP:HB3	1.90	0.53
1:Cc:24:LEU:HD13	2:Cf:123:ASP:HB3	1.90	0.53
2:At:50:GLU:HG2	2:Bb:141:THR:HG21	1.91	0.52
2:Bb:86:THR:OG1	2:Bf:129:MET:HE1	2.09	0.52
2:Al:40:GLY:HA3	2:Bz:101:LYS:NZ	2.25	0.52
1:By:86:ILE:O	1:By:127:LYS:NZ	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ax:86:THR:OG1	2:Bb:129:MET:HE1	2.10	0.52
1:Bm:86:ILE:O	1:Bm:127:LYS:NZ	2.29	0.52
2:Ah:141:THR:HG21	2:Bh:50:GLU:HG2	1.90	0.52
2:Bj:50:GLU:HG2	2:Br:141:THR:HG21	1.90	0.52
1:Bs:92:LEU:HD13	1:Bs:97:ALA:HA	1.92	0.52
1:Bw:92:LEU:HD13	1:Bw:97:ALA:HA	1.92	0.52
1:Cg:24:LEU:HD13	2:Cj:123:ASP:HB3	1.90	0.52
2:Af:141:THR:HG21	2:Cn:50:GLU:HG2	1.91	0.52
1:Bk:86:ILE:O	1:Bk:127:LYS:NZ	2.29	0.52
1:Am:92:LEU:HD13	1:Am:97:ALA:HA	1.92	0.52
1:Ao:92:LEU:HD13	1:Ao:97:ALA:HA	1.92	0.52
2:Bj:123:ASP:HB3	1:Co:24:LEU:HD13	1.92	0.52
1:Bu:92:LEU:HD13	1:Bu:97:ALA:HA	1.92	0.52
1:By:92:LEU:HD13	1:By:97:ALA:HA	1.92	0.52
2:Ab:141:THR:HG21	2:Cj:50:GLU:HG2	1.92	0.52
2:Ah:50:GLU:HG2	2:Ap:141:THR:HG21	1.90	0.52
1:Ak:92:LEU:HD13	1:Ak:97:ALA:HA	1.92	0.52
2:An:40:GLY:HA3	2:Cb:101:LYS:NZ	2.25	0.52
2:At:40:GLY:HA3	2:Ch:101:LYS:NZ	2.25	0.52
1:Ba:24:LEU:HD13	2:Bd:123:ASP:HB3	1.91	0.52
2:Bl:129:MET:HE1	2:Cp:86:THR:OG1	2.10	0.52
1:Bq:92:LEU:HD13	1:Bq:97:ALA:HA	1.92	0.52
2:Ab:86:THR:OG1	2:Af:129:MET:HE1	2.10	0.52
1:Ag:86:ILE:O	1:Ag:127:LYS:NZ	2.29	0.52
1:Ag:92:LEU:HD13	1:Ag:97:ALA:HA	1.92	0.52
1:As:92:LEU:HD13	1:As:97:ALA:HA	1.92	0.52
1:Bc:24:LEU:HD13	2:Bf:123:ASP:HB3	1.92	0.52
1:Ae:92:LEU:HD13	1:Ae:97:ALA:HA	1.92	0.52
1:Ai:92:LEU:HD13	1:Ai:97:ALA:HA	1.92	0.52
1:Aq:92:LEU:HD13	1:Aq:97:ALA:HA	1.92	0.52
1:Ba:86:ILE:O	1:Ba:127:LYS:NZ	2.29	0.52
1:Bo:92:LEU:HD13	1:Bo:97:ALA:HA	1.92	0.52
1:Ca:92:LEU:HD13	1:Ca:97:ALA:HA	1.92	0.52
1:Ac:92:LEU:HD13	1:Ac:97:ALA:HA	1.92	0.52
2:Ah:86:THR:OG1	2:Al:129:MET:HE1	2.10	0.52
1:Au:92:LEU:HD13	1:Au:97:ALA:HA	1.92	0.52
1:Bk:92:LEU:HD13	1:Bk:97:ALA:HA	1.92	0.52
1:Bm:92:LEU:HD13	1:Bm:97:ALA:HA	1.92	0.52
1:Cc:92:LEU:HD13	1:Cc:97:ALA:HA	1.92	0.52
2:Ch:86:THR:OG1	2:Cl:129:MET:HE1	2.09	0.52
2:Ad:129:MET:HE1	2:Bh:86:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bi:86:ILE:O	1:Bi:127:LYS:NZ	2.29	0.51
2:Cf:86:THR:OG1	2:Cj:129:MET:HE1	2.10	0.51
1:Co:86:ILE:O	1:Co:127:LYS:NZ	2.29	0.51
1:Aa:92:LEU:HD13	1:Aa:97:ALA:HA	1.92	0.51
2:Af:40:GLY:HA3	2:Bt:101:LYS:NZ	2.25	0.51
2:Ap:86:THR:OG1	2:At:129:MET:HE1	2.10	0.51
2:Ar:86:THR:OG1	2:Av:129:MET:HE1	2.11	0.51
2:Cj:86:THR:OG1	2:Cn:129:MET:HE1	2.11	0.51
2:Ah:40:GLY:HA3	2:Bv:101:LYS:NZ	2.26	0.51
2:Aj:86:THR:OG1	2:An:129:MET:HE1	2.10	0.51
1:Bi:92:LEU:HD13	1:Bi:97:ALA:HA	1.92	0.51
2:Bj:86:THR:OG1	2:Bn:129:MET:HE1	2.10	0.51
2:Bt:86:THR:OG1	2:Bx:129:MET:HE1	2.10	0.51
2:Bx:86:THR:OG1	2:Cb:129:MET:HE1	2.11	0.51
2:Al:50:GLU:HG2	2:At:141:THR:HG21	1.92	0.51
1:Ay:24:LEU:HD13	2:Bb:123:ASP:HB3	1.91	0.51
2:Bp:86:THR:OG1	2:Bt:129:MET:HE1	2.11	0.51
1:Bq:86:ILE:O	1:Bq:127:LYS:NZ	2.29	0.51
2:Cb:50:GLU:HG2	2:Cj:141:THR:HG21	1.91	0.51
1:Ce:92:LEU:HD13	1:Ce:97:ALA:HA	1.92	0.51
1:Cg:92:LEU:HD13	1:Cg:97:ALA:HA	1.92	0.51
2:Av:86:THR:OG1	2:Az:129:MET:HE1	2.11	0.51
2:Bz:86:THR:OG1	2:Cd:129:MET:HE1	2.11	0.51
1:Ce:24:LEU:HD13	2:Ch:123:ASP:HB3	1.92	0.51
2:Ad:86:THR:OG1	2:Ah:129:MET:HE1	2.10	0.51
1:Aw:92:LEU:HD13	1:Aw:97:ALA:HA	1.92	0.51
1:Co:92:LEU:HD13	1:Co:97:ALA:HA	1.92	0.51
2:Ab:40:GLY:HA3	2:Bp:101:LYS:NZ	2.26	0.51
2:Ad:40:GLY:HA3	2:Br:101:LYS:NZ	2.26	0.51
1:Bg:92:LEU:HD13	1:Bg:97:ALA:HA	1.92	0.51
1:Cm:86:ILE:O	1:Cm:127:LYS:NZ	2.29	0.51
1:Ci:92:LEU:HD13	1:Ci:97:ALA:HA	1.92	0.51
1:Ac:86:ILE:O	1:Ac:127:LYS:NZ	2.29	0.51
2:Br:50:GLU:HG2	2:Bz:141:THR:HG21	1.91	0.51
2:Br:86:THR:OG1	2:Bv:129:MET:HE1	2.11	0.51
2:Cd:86:THR:OG1	2:Ch:129:MET:HE1	2.11	0.51
1:Ck:92:LEU:HD13	1:Ck:97:ALA:HA	1.92	0.51
2:Ad:50:GLU:HG2	2:Al:141:THR:HG21	1.92	0.51
2:Af:50:GLU:HG2	2:An:141:THR:HG21	1.92	0.51
1:Aq:86:ILE:O	1:Aq:127:LYS:NZ	2.29	0.51
1:Ay:92:LEU:HD13	1:Ay:97:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bh:129:MET:HE1	2:Cl:86:THR:OG1	2.11	0.51
1:Cm:92:LEU:HD13	1:Cm:97:ALA:HA	1.92	0.51
2:Ab:129:MET:HE1	2:Cn:86:THR:OG1	2.11	0.50
1:Ae:86:ILE:O	1:Ae:127:LYS:NZ	2.29	0.50
2:Af:86:THR:OG1	2:Aj:129:MET:HE1	2.11	0.50
2:Al:86:THR:OG1	2:Ap:129:MET:HE1	2.11	0.50
1:Ba:92:LEU:HD13	1:Ba:97:ALA:HA	1.92	0.50
1:Bc:92:LEU:HD13	1:Bc:97:ALA:HA	1.92	0.50
1:Be:92:LEU:HD13	1:Be:97:ALA:HA	1.92	0.50
1:Bq:57:GLU:O	1:Bq:60:ILE:HG22	2.12	0.50
2:An:50:GLU:HG2	2:Av:141:THR:HG21	1.91	0.50
2:Ap:40:GLY:HA3	2:Cd:101:LYS:NZ	2.25	0.50
1:Ca:57:GLU:O	1:Ca:60:ILE:HG22	2.12	0.50
1:Cg:57:GLU:O	1:Cg:60:ILE:HG22	2.12	0.50
1:Aa:86:ILE:O	1:Aa:127:LYS:NZ	2.29	0.50
1:Ac:57:GLU:O	1:Ac:60:ILE:HG22	2.11	0.50
2:Ad:141:THR:HG21	2:Cl:50:GLU:HG2	1.92	0.50
2:Aj:40:GLY:HA3	2:Bx:101:LYS:NZ	2.26	0.50
2:Aj:50:GLU:HG2	2:Ar:141:THR:HG21	1.92	0.50
2:Av:40:GLY:HA3	2:Cj:101:LYS:NZ	2.26	0.50
1:Ay:57:GLU:O	1:Ay:60:ILE:HG22	2.12	0.50
1:Bg:57:GLU:O	1:Bg:60:ILE:HG22	2.12	0.50
1:Bm:57:GLU:O	1:Bm:60:ILE:HG22	2.12	0.50
2:Cj:40:GLY:HA3	2:Cp:101:LYS:NZ	2.26	0.50
1:Ai:57:GLU:O	1:Ai:60:ILE:HG22	2.12	0.50
1:As:57:GLU:O	1:As:60:ILE:HG22	2.12	0.50
1:Ba:57:GLU:O	1:Ba:60:ILE:HG22	2.12	0.50
1:Bi:57:GLU:O	1:Bi:60:ILE:HG22	2.12	0.50
2:Bl:101:LYS:NZ	2:Cn:40:GLY:HA3	2.26	0.50
2:Bv:86:THR:OG1	2:Bz:129:MET:HE1	2.11	0.50
2:Ab:50:GLU:HG2	2:Aj:141:THR:HG21	1.92	0.50
2:Ar:40:GLY:HA3	2:Cf:101:LYS:NZ	2.26	0.50
1:Bu:57:GLU:O	1:Bu:60:ILE:HG22	2.12	0.50
1:Ce:54:ILE:HG21	1:Cg:78:LEU:HA	1.93	0.50
1:Ai:35:LYS:O	1:Ai:38:LYS:HB3	2.12	0.50
1:Am:57:GLU:O	1:Am:60:ILE:HG22	2.12	0.50
1:Au:57:GLU:O	1:Au:60:ILE:HG22	2.12	0.50
1:Bc:57:GLU:O	1:Bc:60:ILE:HG22	2.12	0.50
1:Bi:54:ILE:HG21	1:Bk:78:LEU:HA	1.94	0.50
2:Bl:86:THR:OG1	2:Bp:129:MET:HE1	2.12	0.50
2:Cb:86:THR:OG1	2:Cf:129:MET:HE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:57:GLU:O	1:Ae:60:ILE:HG22	2.12	0.50
1:Ag:35:LYS:O	1:Ag:38:LYS:HB3	2.12	0.50
1:Ag:57:GLU:O	1:Ag:60:ILE:HG22	2.12	0.50
1:Ao:57:GLU:O	1:Ao:60:ILE:HG22	2.12	0.50
1:Bc:86:ILE:O	1:Bc:127:LYS:NZ	2.29	0.50
1:Bo:35:LYS:O	1:Bo:38:LYS:HB3	2.12	0.50
1:Bq:35:LYS:O	1:Bq:38:LYS:HB3	2.12	0.50
1:Ck:57:GLU:O	1:Ck:60:ILE:HG22	2.12	0.50
1:Cm:57:GLU:O	1:Cm:60:ILE:HG22	2.12	0.50
1:Co:57:GLU:O	1:Co:60:ILE:HG22	2.12	0.50
1:Aa:35:LYS:O	1:Aa:38:LYS:HB3	2.12	0.50
1:Ay:35:LYS:O	1:Ay:38:LYS:HB3	2.12	0.50
2:Bh:40:GLY:HA3	2:Bn:101:LYS:NZ	2.27	0.50
1:Bi:35:LYS:O	1:Bi:38:LYS:HB3	2.12	0.50
2:Bj:101:LYS:NZ	2:Cl:40:GLY:HA3	2.26	0.50
1:Aa:57:GLU:O	1:Aa:60:ILE:HG22	2.12	0.50
2:At:86:THR:OG1	2:Ax:129:MET:HE1	2.11	0.50
1:By:57:GLU:O	1:By:60:ILE:HG22	2.12	0.50
1:Ci:57:GLU:O	1:Ci:60:ILE:HG22	2.12	0.50
1:Ao:35:LYS:O	1:Ao:38:LYS:HB3	2.12	0.49
1:Aq:57:GLU:O	1:Aq:60:ILE:HG22	2.12	0.49
1:Aw:35:LYS:O	1:Aw:38:LYS:HB3	2.12	0.49
1:Ba:35:LYS:O	1:Ba:38:LYS:HB3	2.12	0.49
2:Bb:103:MET:HG3	2:Bb:108:ILE:HD11	1.94	0.49
1:Bg:35:LYS:O	1:Bg:38:LYS:HB3	2.12	0.49
2:Bh:140:THR:HG21	2:Ch:58:GLN:NE2	2.27	0.49
1:Cc:57:GLU:O	1:Cc:60:ILE:HG22	2.12	0.49
2:Cj:103:MET:HG3	2:Cj:108:ILE:HD11	1.95	0.49
1:Ak:57:GLU:O	1:Ak:60:ILE:HG22	2.12	0.49
1:Au:35:LYS:O	1:Au:38:LYS:HB3	2.12	0.49
2:Az:103:MET:HG3	2:Az:108:ILE:HD11	1.94	0.49
1:Bc:35:LYS:O	1:Bc:38:LYS:HB3	2.12	0.49
2:Bn:86:THR:OG1	2:Br:129:MET:HE1	2.11	0.49
1:Bw:57:GLU:O	1:Bw:60:ILE:HG22	2.12	0.49
2:Cb:103:MET:HG3	2:Cb:108:ILE:HD11	1.95	0.49
1:Ce:57:GLU:O	1:Ce:60:ILE:HG22	2.12	0.49
1:Cg:35:LYS:O	1:Cg:38:LYS:HB3	2.12	0.49
1:Ci:35:LYS:O	1:Ci:38:LYS:HB3	2.12	0.49
2:At:103:MET:HG3	2:At:108:ILE:HD11	1.95	0.49
1:Be:57:GLU:O	1:Be:60:ILE:HG22	2.12	0.49
1:Bg:86:ILE:O	1:Bg:127:LYS:NZ	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:35:LYS:O	1:Bk:38:LYS:HB3	2.12	0.49
1:Bk:57:GLU:O	1:Bk:60:ILE:HG22	2.12	0.49
1:Bs:35:LYS:O	1:Bs:38:LYS:HB3	2.12	0.49
1:Bs:57:GLU:O	1:Bs:60:ILE:HG22	2.12	0.49
1:Bw:35:LYS:O	1:Bw:38:LYS:HB3	2.12	0.49
1:Co:35:LYS:O	1:Co:38:LYS:HB3	2.12	0.49
2:An:86:THR:OG1	2:Ar:129:MET:HE1	2.11	0.49
1:As:35:LYS:O	1:As:38:LYS:HB3	2.12	0.49
1:Cc:35:LYS:O	1:Cc:38:LYS:HB3	2.12	0.49
1:Ce:35:LYS:O	1:Ce:38:LYS:HB3	2.12	0.49
1:Ck:35:LYS:O	1:Ck:38:LYS:HB3	2.12	0.49
1:Ak:35:LYS:O	1:Ak:38:LYS:HB3	2.12	0.49
2:Ar:103:MET:HG3	2:Ar:108:ILE:HD11	1.94	0.49
1:Bo:57:GLU:O	1:Bo:60:ILE:HG22	2.12	0.49
1:By:35:LYS:O	1:By:38:LYS:HB3	2.12	0.49
1:Ca:35:LYS:O	1:Ca:38:LYS:HB3	2.12	0.49
2:Ch:103:MET:HG3	2:Ch:108:ILE:HD11	1.94	0.49
2:Cl:103:MET:HG3	2:Cl:108:ILE:HD11	1.95	0.49
1:Ae:35:LYS:O	1:Ae:38:LYS:HB3	2.12	0.49
1:Ao:10:ARG:HE	1:Ao:123:GLN:NE2	2.11	0.49
1:Aw:57:GLU:O	1:Aw:60:ILE:HG22	2.12	0.49
1:Bg:45:ALA:HB2	1:Bg:175:VAL:HG11	1.95	0.49
2:Bh:103:MET:HG3	2:Bh:108:ILE:HD11	1.95	0.49
1:Bs:86:ILE:O	1:Bs:127:LYS:NZ	2.29	0.49
2:Bz:58:GLN:NE2	2:Ch:140:THR:HG21	2.27	0.49
2:Ab:103:MET:HG3	2:Ab:108:ILE:HD11	1.95	0.49
1:Ac:35:LYS:O	1:Ac:38:LYS:HB3	2.12	0.49
1:Am:35:LYS:O	1:Am:38:LYS:HB3	2.12	0.49
1:Aq:10:ARG:HE	1:Aq:123:GLN:NE2	2.11	0.49
1:Aq:35:LYS:O	1:Aq:38:LYS:HB3	2.12	0.49
1:As:45:ALA:HB2	1:As:175:VAL:HG11	1.95	0.49
1:Be:35:LYS:O	1:Be:38:LYS:HB3	2.12	0.49
2:Bj:103:MET:HG3	2:Bj:108:ILE:HD11	1.95	0.49
1:Bs:10:ARG:HE	1:Bs:123:GLN:NE2	2.11	0.49
1:Ca:45:ALA:HB2	1:Ca:175:VAL:HG11	1.95	0.49
2:Cd:103:MET:HG3	2:Cd:108:ILE:HD11	1.95	0.49
1:Ce:10:ARG:HE	1:Ce:123:GLN:NE2	2.11	0.49
1:Cm:45:ALA:HB2	1:Cm:175:VAL:HG11	1.95	0.49
1:Aq:45:ALA:HB2	1:Aq:175:VAL:HG11	1.95	0.49
1:Aq:61:ARG:HH12	1:Aq:155:GLU:N	2.11	0.49
1:Ba:61:ARG:HH12	1:Ba:155:GLU:N	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bd:103:MET:HG3	2:Bd:108:ILE:HD11	1.95	0.49
1:Bk:45:ALA:HB2	1:Bk:175:VAL:HG11	1.95	0.49
2:Bn:100:LEU:HD22	2:Bp:118:GLN:HE22	1.78	0.49
1:Bu:10:ARG:HE	1:Bu:123:GLN:NE2	2.11	0.49
2:Bv:103:MET:HG3	2:Bv:108:ILE:HD11	1.95	0.49
1:By:10:ARG:HE	1:By:123:GLN:NE2	2.11	0.49
1:Cc:10:ARG:HE	1:Cc:123:GLN:NE2	2.11	0.49
1:Cc:45:ALA:HB2	1:Cc:175:VAL:HG11	1.95	0.49
1:Ce:45:ALA:HB2	1:Ce:175:VAL:HG11	1.95	0.49
1:Cg:61:ARG:HH12	1:Cg:155:GLU:N	2.11	0.49
1:Ci:45:ALA:HB2	1:Ci:175:VAL:HG11	1.95	0.49
1:Ci:61:ARG:HH12	1:Ci:155:GLU:N	2.11	0.49
1:Ck:45:ALA:HB2	1:Ck:175:VAL:HG11	1.95	0.49
1:Aa:45:ALA:HB2	1:Aa:175:VAL:HG11	1.95	0.49
1:Ac:45:ALA:HB2	1:Ac:175:VAL:HG11	1.95	0.49
1:Ag:61:ARG:HH12	1:Ag:155:GLU:N	2.11	0.49
1:Am:10:ARG:HE	1:Am:123:GLN:NE2	2.11	0.49
2:An:103:MET:HG3	2:An:108:ILE:HD11	1.94	0.49
1:Au:45:ALA:HB2	1:Au:175:VAL:HG11	1.95	0.49
2:Av:103:MET:HG3	2:Av:108:ILE:HD11	1.94	0.49
1:Ay:45:ALA:HB2	1:Ay:175:VAL:HG11	1.95	0.49
1:Ba:45:ALA:HB2	1:Ba:175:VAL:HG11	1.95	0.49
1:Bc:45:ALA:HB2	1:Bc:175:VAL:HG11	1.95	0.49
1:Bc:54:ILE:HG21	1:Be:78:LEU:HA	1.94	0.49
1:Be:45:ALA:HB2	1:Be:175:VAL:HG11	1.95	0.49
1:Bi:45:ALA:HB2	1:Bi:175:VAL:HG11	1.95	0.49
1:Bw:61:ARG:HH12	1:Bw:155:GLU:N	2.11	0.49
1:By:45:ALA:HB2	1:By:175:VAL:HG11	1.95	0.49
2:Bz:103:MET:HG3	2:Bz:108:ILE:HD11	1.95	0.49
1:Cg:45:ALA:HB2	1:Cg:175:VAL:HG11	1.95	0.49
1:Co:45:ALA:HB2	1:Co:175:VAL:HG11	1.95	0.49
2:Cp:103:MET:HG3	2:Cp:108:ILE:HD11	1.94	0.49
1:Ai:86:ILE:O	1:Ai:127:LYS:NZ	2.29	0.49
1:Ao:45:ALA:HB2	1:Ao:175:VAL:HG11	1.95	0.49
1:As:61:ARG:HH12	1:As:155:GLU:N	2.11	0.49
1:Aw:45:ALA:HB2	1:Aw:175:VAL:HG11	1.95	0.49
2:Az:40:GLY:HA3	2:Cn:101:LYS:NZ	2.27	0.49
2:Bb:40:GLY:HA3	2:Bh:101:LYS:NZ	2.28	0.49
1:Bi:78:LEU:HA	1:Co:54:ILE:HG21	1.94	0.49
1:Bm:35:LYS:O	1:Bm:38:LYS:HB3	2.12	0.49
1:Bm:45:ALA:HB2	1:Bm:175:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bw:45:ALA:HB2	1:Bw:175:VAL:HG11	1.95	0.49
1:By:61:ARG:HH12	1:By:155:GLU:N	2.11	0.49
1:Cm:35:LYS:O	1:Cm:38:LYS:HB3	2.12	0.49
1:Am:45:ALA:HB2	1:Am:175:VAL:HG11	1.95	0.48
1:As:60:ILE:HD13	1:As:165:TYR:CE2	2.48	0.48
1:Au:10:ARG:HE	1:Au:123:GLN:NE2	2.11	0.48
1:Ay:10:ARG:HE	1:Ay:123:GLN:NE2	2.11	0.48
1:Bg:61:ARG:HH12	1:Bg:155:GLU:N	2.11	0.48
1:Bm:54:ILE:HG21	1:Bo:78:LEU:HA	1.95	0.48
1:Bo:45:ALA:HB2	1:Bo:175:VAL:HG11	1.95	0.48
1:Bs:60:ILE:HD13	1:Bs:165:TYR:CE2	2.48	0.48
1:Cg:10:ARG:HE	1:Cg:123:GLN:NE2	2.11	0.48
1:Ae:54:ILE:HG21	1:Ag:78:LEU:HA	1.95	0.48
1:Ak:60:ILE:HD13	1:Ak:165:TYR:CE2	2.49	0.48
1:Ao:61:ARG:HH12	1:Ao:155:GLU:N	2.11	0.48
2:Ax:103:MET:HG3	2:Ax:108:ILE:HD11	1.94	0.48
2:Bp:103:MET:HG3	2:Bp:108:ILE:HD11	1.94	0.48
1:Bu:35:LYS:O	1:Bu:38:LYS:HB3	2.12	0.48
1:Bw:10:ARG:HE	1:Bw:123:GLN:NE2	2.11	0.48
1:Ca:60:ILE:HD13	1:Ca:165:TYR:CE2	2.49	0.48
1:Aa:54:ILE:HG21	1:Ac:78:LEU:HA	1.95	0.48
2:Af:140:THR:HG21	2:Cn:58:GLN:NE2	2.29	0.48
1:Ai:60:ILE:HD13	1:Ai:165:TYR:CE2	2.49	0.48
1:Ak:45:ALA:HB2	1:Ak:175:VAL:HG11	1.95	0.48
2:Al:103:MET:HG3	2:Al:108:ILE:HD11	1.95	0.48
1:Aq:54:ILE:HG21	1:As:78:LEU:HA	1.95	0.48
1:Aw:54:ILE:HG21	1:Ay:78:LEU:HA	1.95	0.48
2:Ax:58:GLN:NE2	2:Bf:140:THR:HG21	2.28	0.48
1:Ay:60:ILE:HD13	1:Ay:165:TYR:CE2	2.49	0.48
1:Bm:61:ARG:HH12	1:Bm:155:GLU:N	2.11	0.48
1:Bq:45:ALA:HB2	1:Bq:175:VAL:HG11	1.95	0.48
2:Bt:103:MET:HG3	2:Bt:108:ILE:HD11	1.95	0.48
1:Ca:54:ILE:HG21	1:Cc:78:LEU:HA	1.95	0.48
1:Cc:54:ILE:HG21	1:Ce:78:LEU:HA	1.94	0.48
1:Cc:86:ILE:O	1:Cc:127:LYS:NZ	2.29	0.48
2:Ab:101:LYS:NZ	2:Bd:40:GLY:HA3	2.28	0.48
1:Ae:45:ALA:HB2	1:Ae:175:VAL:HG11	1.95	0.48
1:Ag:45:ALA:HB2	1:Ag:175:VAL:HG11	1.95	0.48
1:Ag:60:ILE:HD13	1:Ag:165:TYR:CE2	2.49	0.48
2:Ah:103:MET:HG3	2:Ah:108:ILE:HD11	1.95	0.48
1:Ai:10:ARG:HE	1:Ai:123:GLN:NE2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aq:60:ILE:HD13	1:Aq:165:TYR:CE2	2.49	0.48
1:Aw:10:ARG:HE	1:Aw:123:GLN:NE2	2.11	0.48
1:Ay:61:ARG:HH12	1:Ay:155:GLU:N	2.11	0.48
1:Ba:54:ILE:HG21	1:Bc:78:LEU:HA	1.94	0.48
2:Bl:100:LEU:HD22	2:Bn:118:GLN:HE22	1.79	0.48
1:Bm:60:ILE:HD13	1:Bm:165:TYR:CE2	2.48	0.48
1:Bq:60:ILE:HD13	1:Bq:165:TYR:CE2	2.49	0.48
1:Bu:45:ALA:HB2	1:Bu:175:VAL:HG11	1.95	0.48
1:By:54:ILE:HG21	1:Ca:78:LEU:HA	1.95	0.48
1:Ce:61:ARG:HH12	1:Ce:155:GLU:N	2.11	0.48
1:Cg:60:ILE:HD13	1:Cg:165:TYR:CE2	2.49	0.48
1:Ae:60:ILE:HD13	1:Ae:165:TYR:CE2	2.49	0.48
1:Ai:45:ALA:HB2	1:Ai:175:VAL:HG11	1.95	0.48
1:Ak:10:ARG:HE	1:Ak:123:GLN:NE2	2.11	0.48
1:As:10:ARG:HE	1:As:123:GLN:NE2	2.11	0.48
1:Aw:60:ILE:HD13	1:Aw:165:TYR:CE2	2.49	0.48
1:Ba:10:ARG:HE	1:Ba:123:GLN:NE2	2.11	0.48
1:Ba:60:ILE:HD13	1:Ba:165:TYR:CE2	2.49	0.48
1:Bc:60:ILE:HD13	1:Bc:165:TYR:CE2	2.49	0.48
2:Bf:103:MET:HG3	2:Bf:108:ILE:HD11	1.95	0.48
1:Bu:61:ARG:HH12	1:Bu:155:GLU:N	2.11	0.48
1:By:60:ILE:HD13	1:By:165:TYR:CE2	2.49	0.48
1:Ca:61:ARG:HH12	1:Ca:155:GLU:N	2.11	0.48
1:Cc:60:ILE:HD13	1:Cc:165:TYR:CE2	2.49	0.48
1:Aa:60:ILE:HD13	1:Aa:165:TYR:CE2	2.48	0.48
2:Af:103:MET:HG3	2:Af:108:ILE:HD11	1.95	0.48
1:Au:60:ILE:HD13	1:Au:165:TYR:CE2	2.49	0.48
1:Be:60:ILE:HD13	1:Be:165:TYR:CE2	2.49	0.48
1:Be:86:ILE:O	1:Be:127:LYS:NZ	2.29	0.48
1:Bq:10:ARG:HE	1:Bq:123:GLN:NE2	2.11	0.48
1:Bs:45:ALA:HB2	1:Bs:175:VAL:HG11	1.95	0.48
1:Ci:60:ILE:HD13	1:Ci:165:TYR:CE2	2.49	0.48
1:Ac:60:ILE:HD13	1:Ac:165:TYR:CE2	2.49	0.48
1:Ag:86:ILE:HD11	1:Ag:128:TYR:OH	2.14	0.48
2:Aj:100:LEU:HD22	2:Al:118:GLN:HE22	1.79	0.48
1:Am:86:ILE:HD11	1:Am:128:TYR:OH	2.14	0.48
1:As:54:ILE:HG21	1:Au:78:LEU:HA	1.95	0.48
1:As:86:ILE:HD11	1:As:128:TYR:OH	2.14	0.48
1:Bo:60:ILE:HD13	1:Bo:165:TYR:CE2	2.49	0.48
2:Br:100:LEU:HD22	2:Bt:118:GLN:HE22	1.79	0.48
1:Bu:60:ILE:HD13	1:Bu:165:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ca:86:ILE:HD11	1:Ca:128:TYR:OH	2.14	0.48
1:Ce:60:ILE:HD13	1:Ce:165:TYR:CE2	2.49	0.48
1:Cg:54:ILE:HG21	1:Ci:78:LEU:HA	1.94	0.48
1:Aa:78:LEU:HA	1:Bg:54:ILE:HG21	1.95	0.48
2:Af:100:LEU:HD22	2:Ah:118:GLN:HE22	1.79	0.48
1:Au:61:ARG:HH12	1:Au:155:GLU:N	2.11	0.48
1:Be:86:ILE:HD11	1:Be:128:TYR:OH	2.14	0.48
1:Bg:60:ILE:HD13	1:Bg:165:TYR:CE2	2.49	0.48
1:Bk:60:ILE:HD13	1:Bk:165:TYR:CE2	2.49	0.48
1:Bs:86:ILE:HD11	1:Bs:128:TYR:OH	2.14	0.48
1:Bu:86:ILE:HD11	1:Bu:128:TYR:OH	2.14	0.48
2:Cf:103:MET:HG3	2:Cf:108:ILE:HD11	1.95	0.48
1:Ci:54:ILE:HG21	1:Ck:78:LEU:HA	1.94	0.48
1:Cm:60:ILE:HD13	1:Cm:165:TYR:CE2	2.49	0.48
1:Co:60:ILE:HD13	1:Co:165:TYR:CE2	2.49	0.48
2:Ad:140:THR:HG21	2:Cl:58:GLN:NE2	2.29	0.48
1:Ae:61:ARG:HH12	1:Ae:155:GLU:N	2.11	0.48
1:Am:60:ILE:HD13	1:Am:165:TYR:CE2	2.48	0.48
2:An:100:LEU:HD22	2:Ap:118:GLN:HE22	1.79	0.48
1:Bc:86:ILE:HD11	1:Bc:128:TYR:OH	2.14	0.48
1:Be:10:ARG:HE	1:Be:123:GLN:NE2	2.11	0.48
2:Bj:58:GLN:NE2	2:Br:140:THR:HG21	2.29	0.48
1:Bk:10:ARG:HE	1:Bk:123:GLN:NE2	2.11	0.48
2:Bl:103:MET:HG3	2:Bl:108:ILE:HD11	1.94	0.48
1:Bm:86:ILE:HD11	1:Bm:128:TYR:OH	2.14	0.48
2:Bn:103:MET:HG3	2:Bn:108:ILE:HD11	1.95	0.48
1:Ca:10:ARG:HE	1:Ca:123:GLN:NE2	2.11	0.48
1:Ci:86:ILE:HD11	1:Ci:128:TYR:OH	2.14	0.48
1:Ck:60:ILE:HD13	1:Ck:165:TYR:CE2	2.49	0.48
1:Co:10:ARG:HE	1:Co:123:GLN:NE2	2.11	0.48
1:Ae:86:ILE:HD11	1:Ae:128:TYR:OH	2.14	0.48
1:Am:61:ARG:HH12	1:Am:155:GLU:N	2.11	0.48
1:Ao:60:ILE:HD13	1:Ao:165:TYR:CE2	2.49	0.48
1:Au:86:ILE:HD11	1:Au:128:TYR:OH	2.14	0.48
1:Ba:86:ILE:HD11	1:Ba:128:TYR:OH	2.14	0.48
1:Bg:86:ILE:HD11	1:Bg:128:TYR:OH	2.14	0.48
2:Bh:118:GLN:HE22	2:Cn:100:LEU:HD22	1.79	0.48
2:Bt:100:LEU:HD22	2:Bv:118:GLN:HE22	1.79	0.48
1:Bu:54:ILE:HG21	1:Bw:78:LEU:HA	1.95	0.48
2:Bx:103:MET:HG3	2:Bx:108:ILE:HD11	1.95	0.48
1:Ck:10:ARG:HE	1:Ck:123:GLN:NE2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ck:86:ILE:HD11	1:Ck:128:TYR:OH	2.14	0.48
1:Cm:61:ARG:HH12	1:Cm:155:GLU:N	2.11	0.48
2:Cn:103:MET:HG3	2:Cn:108:ILE:HD11	1.95	0.48
1:Aa:10:ARG:HE	1:Aa:123:GLN:NE2	2.11	0.47
1:Ac:10:ARG:HE	1:Ac:123:GLN:NE2	2.11	0.47
1:Ae:10:ARG:HE	1:Ae:123:GLN:NE2	2.11	0.47
2:Ah:140:THR:HG21	2:Bh:58:GLN:NE2	2.29	0.47
1:Ao:86:ILE:HD11	1:Ao:128:TYR:OH	2.14	0.47
1:Ay:86:ILE:HD11	1:Ay:128:TYR:OH	2.14	0.47
1:Bi:10:ARG:HE	1:Bi:123:GLN:NE2	2.11	0.47
2:Bl:58:GLN:NE2	2:Bt:140:THR:HG21	2.29	0.47
1:Bo:10:ARG:HE	1:Bo:123:GLN:NE2	2.11	0.47
1:Bo:86:ILE:HD11	1:Bo:128:TYR:OH	2.14	0.47
1:Cg:86:ILE:HD11	1:Cg:128:TYR:OH	2.14	0.47
1:Cm:86:ILE:HD11	1:Cm:128:TYR:OH	2.14	0.47
2:Ab:118:GLN:HE22	2:Bh:100:LEU:HD22	1.79	0.47
1:Ag:54:ILE:HG21	1:Ai:78:LEU:HA	1.95	0.47
1:Ak:86:ILE:HD11	1:Ak:128:TYR:OH	2.14	0.47
2:Ap:100:LEU:HD22	2:Ar:118:GLN:HE22	1.79	0.47
1:Bg:10:ARG:HE	1:Bg:123:GLN:NE2	2.11	0.47
1:Bg:78:LEU:HA	1:Cm:54:ILE:HG21	1.95	0.47
1:Bi:60:ILE:HD13	1:Bi:165:TYR:CE2	2.49	0.47
1:Bw:60:ILE:HD13	1:Bw:165:TYR:CE2	2.48	0.47
1:By:86:ILE:HD11	1:By:128:TYR:OH	2.14	0.47
1:Ce:86:ILE:HD11	1:Ce:128:TYR:OH	2.14	0.47
1:Ci:10:ARG:HE	1:Ci:123:GLN:NE2	2.11	0.47
2:Cl:100:LEU:HD22	2:Cn:118:GLN:HE22	1.79	0.47
1:Aa:86:ILE:HD11	1:Aa:128:TYR:OH	2.14	0.47
2:Ad:100:LEU:HD22	2:Af:118:GLN:HE22	1.80	0.47
2:Ap:103:MET:HG3	2:Ap:108:ILE:HD11	1.95	0.47
1:Aw:61:ARG:HH12	1:Aw:155:GLU:N	2.11	0.47
1:Bk:54:ILE:HG21	1:Bm:78:LEU:HA	1.95	0.47
1:Bo:54:ILE:HG21	1:Bq:78:LEU:HA	1.95	0.47
2:Bp:100:LEU:HD22	2:Br:118:GLN:HE22	1.80	0.47
1:Cc:61:ARG:HH12	1:Cc:155:GLU:N	2.11	0.47
1:Cc:86:ILE:HD11	1:Cc:128:TYR:OH	2.14	0.47
1:Cm:10:ARG:HE	1:Cm:123:GLN:NE2	2.11	0.47
1:Co:86:ILE:HD11	1:Co:128:TYR:OH	2.14	0.47
2:Ad:103:MET:HG3	2:Ad:108:ILE:HD11	1.95	0.47
2:Af:29:GLU:OE2	2:Af:48:HIS:CD2	2.68	0.47
2:Al:29:GLU:OE2	2:Al:48:HIS:CD2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:54:ILE:HG21	1:Aq:78:LEU:HA	1.95	0.47
2:Ax:40:GLY:HA3	2:Cl:101:LYS:NZ	2.28	0.47
1:Ay:54:ILE:HG21	1:Ba:78:LEU:HA	1.94	0.47
1:Bc:10:ARG:HE	1:Bc:123:GLN:NE2	2.11	0.47
2:Bf:29:GLU:OE2	2:Bf:48:HIS:CD2	2.68	0.47
1:Bm:10:ARG:HE	1:Bm:123:GLN:NE2	2.11	0.47
2:Bn:29:GLU:OE2	2:Bn:48:HIS:CD2	2.68	0.47
2:Bn:58:GLN:NE2	2:Bv:140:THR:HG21	2.29	0.47
2:Bx:58:GLN:NE2	2:Cf:140:THR:HG21	2.28	0.47
2:Ah:100:LEU:HD22	2:Aj:118:GLN:HE22	1.79	0.47
1:Au:54:ILE:HG21	1:Aw:78:LEU:HA	1.96	0.47
1:Aw:86:ILE:HD11	1:Aw:128:TYR:OH	2.14	0.47
2:Bp:140:THR:HG21	2:Cp:58:GLN:NE2	2.30	0.47
1:Bq:54:ILE:HG21	1:Bs:78:LEU:HA	1.95	0.47
2:Br:29:GLU:OE2	2:Br:48:HIS:CD2	2.68	0.47
1:Bs:54:ILE:HG21	1:Bu:78:LEU:HA	1.95	0.47
2:Ab:29:GLU:OE2	2:Ab:48:HIS:CD2	2.68	0.47
2:Ad:29:GLU:OE2	2:Ad:48:HIS:CD2	2.68	0.47
2:Ad:101:LYS:NZ	2:Bf:40:GLY:HA3	2.30	0.47
2:Af:58:GLN:NE2	2:An:140:THR:HG21	2.30	0.47
2:Ah:29:GLU:OE2	2:Ah:48:HIS:CD2	2.68	0.47
2:Ah:58:GLN:NE2	2:Ap:140:THR:HG21	2.29	0.47
2:Aj:29:GLU:OE2	2:Aj:48:HIS:CD2	2.68	0.47
1:Ak:54:ILE:HG21	1:Am:78:LEU:HA	1.96	0.47
1:Am:54:ILE:HG21	1:Ao:78:LEU:HA	1.95	0.47
2:Bd:29:GLU:OE2	2:Bd:48:HIS:CD2	2.68	0.47
1:Bi:86:ILE:HD11	1:Bi:128:TYR:OH	2.14	0.47
2:Bl:29:GLU:OE2	2:Bl:48:HIS:CD2	2.68	0.47
1:Bs:61:ARG:HH12	1:Bs:155:GLU:N	2.11	0.47
2:Bv:29:GLU:OE2	2:Bv:48:HIS:CD2	2.68	0.47
2:Bx:100:LEU:HD22	2:Bz:118:GLN:HE22	1.79	0.47
2:Ab:100:LEU:HD22	2:Ad:118:GLN:HE22	1.80	0.47
1:Ac:86:ILE:HD11	1:Ac:128:TYR:OH	2.14	0.47
1:Ai:54:ILE:HG21	1:Ak:78:LEU:HA	1.95	0.47
1:Ai:86:ILE:HD11	1:Ai:128:TYR:OH	2.14	0.47
2:Al:100:LEU:HD22	2:An:118:GLN:HE22	1.79	0.47
1:Aq:86:ILE:HD11	1:Aq:128:TYR:OH	2.14	0.47
2:Av:100:LEU:HD22	2:Ax:118:GLN:HE22	1.79	0.47
2:Bb:29:GLU:OE2	2:Bb:48:HIS:CD2	2.68	0.47
1:Be:61:ARG:HH12	1:Be:155:GLU:N	2.11	0.47
2:Bh:29:GLU:OE2	2:Bh:48:HIS:CD2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:61:ARG:HH12	1:Bk:155:GLU:N	2.11	0.47
2:Bp:29:GLU:OE2	2:Bp:48:HIS:CD2	2.68	0.47
2:Br:103:MET:HG3	2:Br:108:ILE:HD11	1.95	0.47
2:Bt:29:GLU:OE2	2:Bt:48:HIS:CD2	2.68	0.47
1:Bw:86:ILE:HD11	1:Bw:128:TYR:OH	2.14	0.47
2:Bx:29:GLU:OE2	2:Bx:48:HIS:CD2	2.68	0.47
1:Ck:54:ILE:HG21	1:Cm:78:LEU:HA	1.96	0.47
2:Cn:29:GLU:OE2	2:Cn:48:HIS:CD2	2.68	0.47
1:Ag:10:ARG:HE	1:Ag:123:GLN:NE2	2.11	0.47
2:Aj:103:MET:HG3	2:Aj:108:ILE:HD11	1.95	0.47
2:Ax:100:LEU:HD22	2:Az:118:GLN:HE22	1.79	0.47
2:Az:29:GLU:OE2	2:Az:48:HIS:CD2	2.68	0.47
1:Bk:86:ILE:HD11	1:Bk:128:TYR:OH	2.14	0.47
1:Bw:54:ILE:HG21	1:By:78:LEU:HA	1.95	0.47
2:Bz:29:GLU:OE2	2:Bz:48:HIS:CD2	2.68	0.47
2:Cp:29:GLU:OE2	2:Cp:48:HIS:CD2	2.68	0.47
2:Ap:29:GLU:OE2	2:Ap:48:HIS:CD2	2.68	0.47
2:Ar:100:LEU:HD22	2:At:118:GLN:HE22	1.80	0.47
2:Av:58:GLN:NE2	2:Bd:140:THR:HG21	2.29	0.47
1:Bq:86:ILE:HD11	1:Bq:128:TYR:OH	2.14	0.47
2:Cf:58:GLN:NE2	2:Cn:140:THR:HG21	2.29	0.47
2:An:29:GLU:OE2	2:An:48:HIS:CD2	2.68	0.47
2:At:58:GLN:NE2	2:Bb:140:THR:HG21	2.29	0.47
2:Av:29:GLU:OE2	2:Av:48:HIS:CD2	2.68	0.47
2:Bv:100:LEU:HD22	2:Bx:118:GLN:HE22	1.80	0.47
2:Bz:100:LEU:HD22	2:Cb:118:GLN:HE22	1.80	0.47
2:Cb:29:GLU:OE2	2:Cb:48:HIS:CD2	2.68	0.47
2:Cd:100:LEU:HD22	2:Cf:118:GLN:HE22	1.79	0.47
2:Ax:29:GLU:OE2	2:Ax:48:HIS:CD2	2.68	0.46
2:Bj:29:GLU:OE2	2:Bj:48:HIS:CD2	2.68	0.46
2:Cl:29:GLU:OE2	2:Cl:48:HIS:CD2	2.68	0.46
1:Aa:180:ASP:HB3	1:Aa:182:VAL:HG22	1.98	0.46
2:At:29:GLU:OE2	2:At:48:HIS:CD2	2.68	0.46
2:Cb:100:LEU:HD22	2:Cd:118:GLN:HE22	1.79	0.46
2:Cd:29:GLU:OE2	2:Cd:48:HIS:CD2	2.68	0.46
2:Ch:29:GLU:OE2	2:Ch:48:HIS:CD2	2.68	0.46
2:Ch:100:LEU:HD22	2:Cj:118:GLN:HE22	1.80	0.46
2:Ab:140:THR:HG21	2:Cj:58:GLN:NE2	2.31	0.46
2:Ar:29:GLU:OE2	2:Ar:48:HIS:CD2	2.68	0.46
1:Bi:180:ASP:HB3	1:Bi:182:VAL:HG22	1.97	0.46
1:Ac:54:ILE:HG21	1:Ae:78:LEU:HA	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ad:58:GLN:NE2	2:Al:140:THR:HG21	2.31	0.46
1:Ak:61:ARG:HH12	1:Ak:155:GLU:N	2.11	0.46
2:Cf:29:GLU:OE2	2:Cf:48:HIS:CD2	2.68	0.46
1:Ck:180:ASP:HB3	1:Ck:182:VAL:HG22	1.97	0.46
1:Ac:61:ARG:HH12	1:Ac:155:GLU:N	2.11	0.46
1:Bk:180:ASP:HB3	1:Bk:182:VAL:HG22	1.98	0.46
2:Cj:29:GLU:OE2	2:Cj:48:HIS:CD2	2.68	0.46
1:Ck:61:ARG:HH12	1:Ck:155:GLU:N	2.11	0.46
1:Ag:180:ASP:HB3	1:Ag:182:VAL:HG22	1.98	0.46
1:Bc:180:ASP:HB3	1:Bc:182:VAL:HG22	1.98	0.46
2:Bj:100:LEU:HD22	2:Bl:118:GLN:HE22	1.79	0.46
2:At:100:LEU:HD22	2:Av:118:GLN:HE22	1.79	0.46
1:Bo:180:ASP:HB3	1:Bo:182:VAL:HG22	1.98	0.46
1:Ae:180:ASP:HB3	1:Ae:182:VAL:HG22	1.97	0.46
1:Bg:180:ASP:HB3	1:Bg:182:VAL:HG22	1.97	0.46
1:Cm:180:ASP:HB3	1:Cm:182:VAL:HG22	1.98	0.46
1:Co:137:ARG:O	1:Co:141:ILE:HG23	2.16	0.46
1:Aa:101:SER:HB3	1:Aa:144:VAL:HG12	1.98	0.46
1:Ay:137:ARG:O	1:Ay:141:ILE:HG23	2.17	0.46
1:Ba:180:ASP:HB3	1:Ba:182:VAL:HG22	1.97	0.46
2:Bd:100:LEU:HD22	2:Bf:118:GLN:HE22	1.81	0.46
2:Bj:118:GLN:HE22	2:Cp:100:LEU:HD22	1.81	0.46
2:Bp:58:GLN:NE2	2:Bx:140:THR:HG21	2.31	0.46
1:Bq:61:ARG:HH12	1:Bq:155:GLU:N	2.11	0.46
2:Bv:58:GLN:NE2	2:Cd:140:THR:HG21	2.30	0.46
1:Ca:101:SER:HB3	1:Ca:144:VAL:HG12	1.99	0.46
1:Ac:180:ASP:HB3	1:Ac:182:VAL:HG22	1.98	0.45
1:Aq:101:SER:HB3	1:Aq:144:VAL:HG12	1.99	0.45
1:As:101:SER:HB3	1:As:144:VAL:HG12	1.99	0.45
1:Bg:137:ARG:O	1:Bg:141:ILE:HG23	2.17	0.45
1:Bq:180:ASP:HB3	1:Bq:182:VAL:HG22	1.97	0.45
1:Bw:137:ARG:O	1:Bw:141:ILE:HG23	2.17	0.45
1:Ag:137:ARG:O	1:Ag:141:ILE:HG23	2.17	0.45
1:Am:101:SER:HB3	1:Am:144:VAL:HG12	1.99	0.45
1:Am:137:ARG:O	1:Am:141:ILE:HG23	2.16	0.45
1:Ao:101:SER:HB3	1:Ao:144:VAL:HG12	1.99	0.45
1:Ao:137:ARG:O	1:Ao:141:ILE:HG23	2.17	0.45
1:As:137:ARG:O	1:As:141:ILE:HG23	2.17	0.45
1:Bc:101:SER:HB3	1:Bc:144:VAL:HG12	1.98	0.45
1:Be:101:SER:HB3	1:Be:144:VAL:HG12	1.99	0.45
1:Be:137:ARG:O	1:Be:141:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:101:SER:HB3	1:Bg:144:VAL:HG12	1.99	0.45
1:Bo:137:ARG:O	1:Bo:141:ILE:HG23	2.17	0.45
1:Bu:101:SER:HB3	1:Bu:144:VAL:HG12	1.99	0.45
2:Cb:58:GLN:NE2	2:Cj:140:THR:HG21	2.30	0.45
2:Cf:100:LEU:HD22	2:Ch:118:GLN:HE22	1.81	0.45
1:Cg:137:ARG:O	1:Cg:141:ILE:HG23	2.17	0.45
1:Cm:137:ARG:O	1:Cm:141:ILE:HG23	2.17	0.45
1:Ae:101:SER:HB3	1:Ae:144:VAL:HG12	1.99	0.45
1:Au:137:ARG:O	1:Au:141:ILE:HG23	2.16	0.45
1:Bk:101:SER:HB3	1:Bk:144:VAL:HG12	1.99	0.45
1:Bm:101:SER:HB3	1:Bm:144:VAL:HG12	1.99	0.45
1:Bq:137:ARG:O	1:Bq:141:ILE:HG23	2.17	0.45
1:Bw:101:SER:HB3	1:Bw:144:VAL:HG12	1.99	0.45
1:By:180:ASP:HB3	1:By:182:VAL:HG22	1.97	0.45
1:Ca:137:ARG:O	1:Ca:141:ILE:HG23	2.17	0.45
1:Cc:101:SER:HB3	1:Cc:144:VAL:HG12	1.99	0.45
1:Cc:137:ARG:O	1:Cc:141:ILE:HG23	2.17	0.45
2:Ab:58:GLN:NE2	2:Aj:140:THR:HG21	2.31	0.45
1:Ac:101:SER:HB3	1:Ac:144:VAL:HG12	1.99	0.45
1:Ae:137:ARG:O	1:Ae:141:ILE:HG23	2.17	0.45
1:Ag:101:SER:HB3	1:Ag:144:VAL:HG12	1.99	0.45
1:Ak:101:SER:HB3	1:Ak:144:VAL:HG12	1.99	0.45
2:Ap:58:GLN:NE2	2:Ax:140:THR:HG21	2.30	0.45
1:As:180:ASP:HB3	1:As:182:VAL:HG22	1.98	0.45
2:Av:23:ASP:O	2:Av:26:GLU:HB3	2.17	0.45
2:Az:100:LEU:HD22	2:Bb:118:GLN:HE22	1.81	0.45
1:Bi:101:SER:HB3	1:Bi:144:VAL:HG12	1.99	0.45
1:By:101:SER:HB3	1:By:144:VAL:HG12	1.99	0.45
1:Ce:101:SER:HB3	1:Ce:144:VAL:HG12	1.99	0.45
1:Ci:137:ARG:O	1:Ci:141:ILE:HG23	2.17	0.45
2:Ah:23:ASP:O	2:Ah:26:GLU:HB3	2.17	0.45
1:Ai:101:SER:HB3	1:Ai:144:VAL:HG12	1.99	0.45
2:Aj:23:ASP:O	2:Aj:26:GLU:HB3	2.17	0.45
1:Ak:180:ASP:HB3	1:Ak:182:VAL:HG22	1.97	0.45
2:An:58:GLN:NE2	2:Av:140:THR:HG21	2.30	0.45
2:Ap:23:ASP:O	2:Ap:26:GLU:HB3	2.17	0.45
2:Bb:100:LEU:HD22	2:Bd:118:GLN:HE22	1.80	0.45
1:Bc:61:ARG:HH12	1:Bc:155:GLU:N	2.11	0.45
1:Bo:101:SER:HB3	1:Bo:144:VAL:HG12	1.99	0.45
1:Bq:101:SER:HB3	1:Bq:144:VAL:HG12	1.99	0.45
1:Bu:137:ARG:O	1:Bu:141:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ca:180:ASP:HB3	1:Ca:182:VAL:HG22	1.97	0.45
1:Cg:180:ASP:HB3	1:Cg:182:VAL:HG22	1.98	0.45
1:Cm:101:SER:HB3	1:Cm:144:VAL:HG12	1.99	0.45
1:Co:39:GLU:OE1	1:Co:55:ARG:NH2	2.50	0.45
2:Ad:23:ASP:O	2:Ad:26:GLU:HB3	2.17	0.45
1:Ai:137:ARG:O	1:Ai:141:ILE:HG23	2.17	0.45
2:Al:58:GLN:NE2	2:At:140:THR:HG21	2.31	0.45
1:Au:101:SER:HB3	1:Au:144:VAL:HG12	1.99	0.45
1:Aw:180:ASP:HB3	1:Aw:182:VAL:HG22	1.97	0.45
2:Ax:23:ASP:O	2:Ax:26:GLU:HB3	2.17	0.45
2:Az:23:ASP:O	2:Az:26:GLU:HB3	2.17	0.45
1:Ba:137:ARG:O	1:Ba:141:ILE:HG23	2.17	0.45
1:Be:39:GLU:OE1	1:Be:55:ARG:NH2	2.50	0.45
1:Bi:61:ARG:HH12	1:Bi:155:GLU:N	2.11	0.45
1:Bu:180:ASP:HB3	1:Bu:182:VAL:HG22	1.98	0.45
1:Bw:39:GLU:OE1	1:Bw:55:ARG:NH2	2.50	0.45
1:Bw:180:ASP:HB3	1:Bw:182:VAL:HG22	1.97	0.45
1:Cc:180:ASP:HB3	1:Cc:182:VAL:HG22	1.97	0.45
2:Cd:58:GLN:NE2	2:Cl:140:THR:HG21	2.30	0.45
2:Cj:100:LEU:HD22	2:Cl:118:GLN:HE22	1.80	0.45
1:Co:101:SER:HB3	1:Co:144:VAL:HG12	1.99	0.45
1:Ac:39:GLU:OE1	1:Ac:55:ARG:NH2	2.50	0.45
2:Af:23:ASP:O	2:Af:26:GLU:HB3	2.17	0.45
1:Ai:39:GLU:OE1	1:Ai:55:ARG:NH2	2.50	0.45
1:Am:180:ASP:HB3	1:Am:182:VAL:HG22	1.98	0.45
1:Ao:39:GLU:OE1	1:Ao:55:ARG:NH2	2.50	0.45
1:Ao:180:ASP:HB3	1:Ao:182:VAL:HG22	1.98	0.45
1:Aq:180:ASP:HB3	1:Aq:182:VAL:HG22	1.98	0.45
2:Ar:23:ASP:O	2:Ar:26:GLU:HB3	2.17	0.45
2:At:23:ASP:O	2:At:26:GLU:HB3	2.17	0.45
1:Au:180:ASP:HB3	1:Au:182:VAL:HG22	1.97	0.45
1:Aw:101:SER:HB3	1:Aw:144:VAL:HG12	1.99	0.45
1:Ay:101:SER:HB3	1:Ay:144:VAL:HG12	1.99	0.45
1:Ba:101:SER:HB3	1:Ba:144:VAL:HG12	1.99	0.45
1:Be:180:ASP:HB3	1:Be:182:VAL:HG22	1.97	0.45
1:Bg:39:GLU:OE1	1:Bg:55:ARG:NH2	2.50	0.45
1:Bm:137:ARG:O	1:Bm:141:ILE:HG23	2.17	0.45
1:Bm:180:ASP:HB3	1:Bm:182:VAL:HG22	1.97	0.45
2:Br:23:ASP:O	2:Br:26:GLU:HB3	2.17	0.45
2:Bz:23:ASP:O	2:Bz:26:GLU:HB3	2.17	0.45
2:Cb:23:ASP:O	2:Cb:26:GLU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Cf:23:ASP:O	2:Cf:26:GLU:HB3	2.17	0.45
1:Cg:101:SER:HB3	1:Cg:144:VAL:HG12	1.99	0.45
1:Co:180:ASP:HB3	1:Co:182:VAL:HG22	1.98	0.45
2:Ab:23:ASP:O	2:Ab:26:GLU:HB3	2.17	0.45
1:Am:39:GLU:OE1	1:Am:55:ARG:NH2	2.50	0.45
2:An:23:ASP:O	2:An:26:GLU:HB3	2.17	0.45
2:Ar:58:GLN:NE2	2:Az:140:THR:HG21	2.31	0.45
1:Ba:39:GLU:OE1	1:Ba:55:ARG:NH2	2.50	0.45
2:Bb:23:ASP:O	2:Bb:26:GLU:HB3	2.17	0.45
2:Bf:23:ASP:O	2:Bf:26:GLU:HB3	2.17	0.45
1:Bi:137:ARG:O	1:Bi:141:ILE:HG23	2.17	0.45
1:Bk:39:GLU:OE1	1:Bk:55:ARG:NH2	2.50	0.45
2:Bl:23:ASP:O	2:Bl:26:GLU:HB3	2.17	0.45
1:Bq:39:GLU:OE1	1:Bq:55:ARG:NH2	2.50	0.45
1:Bs:101:SER:HB3	1:Bs:144:VAL:HG12	1.99	0.45
1:Ca:39:GLU:OE1	1:Ca:55:ARG:NH2	2.50	0.45
1:Ce:180:ASP:HB3	1:Ce:182:VAL:HG22	1.98	0.45
1:Ck:101:SER:HB3	1:Ck:144:VAL:HG12	1.99	0.45
1:Ai:180:ASP:HB3	1:Ai:182:VAL:HG22	1.98	0.45
2:Al:23:ASP:O	2:Al:26:GLU:HB3	2.17	0.45
1:As:39:GLU:OE1	1:As:55:ARG:NH2	2.50	0.45
1:As:146:ASP:OD1	1:As:147:ARG:N	2.50	0.45
2:At:159:LEU:HD23	2:Bz:103:MET:HE1	1.99	0.45
1:Au:39:GLU:OE1	1:Au:55:ARG:NH2	2.50	0.45
1:Ay:39:GLU:OE1	1:Ay:55:ARG:NH2	2.50	0.45
1:Bc:137:ARG:O	1:Bc:141:ILE:HG23	2.17	0.45
2:Bh:23:ASP:O	2:Bh:26:GLU:HB3	2.17	0.45
1:Bm:39:GLU:OE1	1:Bm:55:ARG:NH2	2.50	0.45
1:Bo:39:GLU:OE1	1:Bo:55:ARG:NH2	2.50	0.45
1:Bw:146:ASP:OD1	1:Bw:147:ARG:N	2.50	0.45
2:Bx:23:ASP:O	2:Bx:26:GLU:HB3	2.17	0.45
1:By:146:ASP:OD1	1:By:147:ARG:N	2.50	0.45
2:Cd:23:ASP:O	2:Cd:26:GLU:HB3	2.17	0.45
1:Ci:101:SER:HB3	1:Ci:144:VAL:HG12	1.99	0.45
1:Ci:180:ASP:HB3	1:Ci:182:VAL:HG22	1.97	0.45
2:Cj:23:ASP:O	2:Cj:26:GLU:HB3	2.17	0.45
2:Cl:23:ASP:O	2:Cl:26:GLU:HB3	2.17	0.45
1:Aq:146:ASP:OD1	1:Aq:147:ARG:N	2.50	0.45
1:Aw:39:GLU:OE1	1:Aw:55:ARG:NH2	2.50	0.45
1:Aw:137:ARG:O	1:Aw:141:ILE:HG23	2.16	0.45
2:Bd:23:ASP:O	2:Bd:26:GLU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bn:23:ASP:O	2:Bn:26:GLU:HB3	2.17	0.45
2:Bp:23:ASP:O	2:Bp:26:GLU:HB3	2.17	0.45
1:Bs:39:GLU:OE1	1:Bs:55:ARG:NH2	2.50	0.45
2:Bt:23:ASP:O	2:Bt:26:GLU:HB3	2.17	0.45
2:Bv:23:ASP:O	2:Bv:26:GLU:HB3	2.17	0.45
1:Cc:39:GLU:OE1	1:Cc:55:ARG:NH2	2.50	0.45
2:Ch:23:ASP:O	2:Ch:26:GLU:HB3	2.17	0.45
1:Ck:146:ASP:OD1	1:Ck:147:ARG:N	2.50	0.45
1:Cm:39:GLU:OE1	1:Cm:55:ARG:NH2	2.50	0.45
1:Aa:137:ARG:O	1:Aa:141:ILE:HG23	2.17	0.44
2:Aj:58:GLN:NE2	2:Ar:140:THR:HG21	2.31	0.44
1:Bc:146:ASP:OD1	1:Bc:147:ARG:N	2.51	0.44
1:Be:146:ASP:OD1	1:Be:147:ARG:N	2.50	0.44
2:Bj:101:LYS:NZ	2:Cl:39:LYS:O	2.38	0.44
1:Cg:39:GLU:OE1	1:Cg:55:ARG:NH2	2.50	0.44
1:Ci:146:ASP:OD1	1:Ci:147:ARG:N	2.51	0.44
1:Aa:61:ARG:HH12	1:Aa:155:GLU:N	2.11	0.44
1:Ac:137:ARG:O	1:Ac:141:ILE:HG23	2.17	0.44
1:Au:146:ASP:OD1	1:Au:147:ARG:N	2.50	0.44
1:Ay:86:ILE:HD13	1:Ay:96:LEU:HD12	1.99	0.44
1:Bc:39:GLU:OE1	1:Bc:55:ARG:NH2	2.50	0.44
1:Bg:64:TYR:HB3	1:Bg:151:LYS:O	2.18	0.44
2:Bj:23:ASP:O	2:Bj:26:GLU:HB3	2.17	0.44
1:Bs:180:ASP:HB3	1:Bs:182:VAL:HG22	1.97	0.44
1:Ce:39:GLU:OE1	1:Ce:55:ARG:NH2	2.50	0.44
1:Cg:146:ASP:OD1	1:Cg:147:ARG:N	2.50	0.44
1:Ci:39:GLU:OE1	1:Ci:55:ARG:NH2	2.50	0.44
1:Ck:137:ARG:O	1:Ck:141:ILE:HG23	2.17	0.44
2:Cn:23:ASP:O	2:Cn:26:GLU:HB3	2.17	0.44
1:Ae:39:GLU:OE1	1:Ae:55:ARG:NH2	2.50	0.44
1:Aq:86:ILE:HD13	1:Aq:96:LEU:HD12	2.00	0.44
1:As:86:ILE:HD13	1:As:96:LEU:HD12	1.99	0.44
1:Au:64:TYR:HB3	1:Au:151:LYS:O	2.18	0.44
1:Ay:180:ASP:HB3	1:Ay:182:VAL:HG22	1.98	0.44
2:Bd:159:LEU:HD23	2:Cj:103:MET:HE1	1.99	0.44
1:By:39:GLU:OE1	1:By:55:ARG:NH2	2.50	0.44
1:By:86:ILE:HD13	1:By:96:LEU:HD12	2.00	0.44
1:Ca:146:ASP:OD1	1:Ca:147:ARG:N	2.51	0.44
1:Cc:146:ASP:OD1	1:Cc:147:ARG:N	2.50	0.44
1:Ce:64:TYR:HB3	1:Ce:151:LYS:O	2.18	0.44
1:Ck:39:GLU:OE1	1:Ck:55:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:64:TYR:HB3	1:Ac:151:LYS:O	2.18	0.44
1:Ag:39:GLU:OE1	1:Ag:55:ARG:NH2	2.50	0.44
1:Ai:61:ARG:HH12	1:Ai:155:GLU:N	2.11	0.44
1:Ak:137:ARG:O	1:Ak:141:ILE:HG23	2.17	0.44
1:Aq:39:GLU:OE1	1:Aq:55:ARG:NH2	2.50	0.44
1:Bk:64:TYR:HB3	1:Bk:151:LYS:O	2.18	0.44
2:Bt:58:GLN:NE2	2:Cb:140:THR:HG21	2.31	0.44
1:Bu:39:GLU:OE1	1:Bu:55:ARG:NH2	2.50	0.44
1:Bu:146:ASP:OD1	1:Bu:147:ARG:N	2.50	0.44
1:Bw:64:TYR:HB3	1:Bw:151:LYS:O	2.18	0.44
1:By:137:ARG:O	1:By:141:ILE:HG23	2.17	0.44
1:Cc:64:TYR:HB3	1:Cc:151:LYS:O	2.18	0.44
1:Ce:146:ASP:OD1	1:Ce:147:ARG:N	2.51	0.44
1:Ck:64:TYR:HB3	1:Ck:151:LYS:O	2.18	0.44
1:Cm:146:ASP:OD1	1:Cm:147:ARG:N	2.50	0.44
1:Ag:64:TYR:HB3	1:Ag:151:LYS:O	2.18	0.44
1:Ao:64:TYR:HB3	1:Ao:151:LYS:O	2.18	0.44
1:As:64:TYR:HB3	1:As:151:LYS:O	2.18	0.44
2:Ax:159:LEU:HD23	2:Cd:103:MET:HE1	2.00	0.44
1:Ba:146:ASP:OD1	1:Ba:147:ARG:N	2.51	0.44
1:Bc:64:TYR:HB3	1:Bc:151:LYS:O	2.18	0.44
1:Bs:64:TYR:HB3	1:Bs:151:LYS:O	2.18	0.44
1:Bs:137:ARG:O	1:Bs:141:ILE:HG23	2.17	0.44
1:Bs:146:ASP:OD1	1:Bs:147:ARG:N	2.50	0.44
1:Ca:86:ILE:HD13	1:Ca:96:LEU:HD12	2.00	0.44
1:Ce:137:ARG:O	1:Ce:141:ILE:HG23	2.17	0.44
1:Cg:86:ILE:HD13	1:Cg:96:LEU:HD12	2.00	0.44
1:Co:64:TYR:HB3	1:Co:151:LYS:O	2.18	0.44
2:Cp:23:ASP:O	2:Cp:26:GLU:HB3	2.17	0.44
1:Ak:39:GLU:OE1	1:Ak:55:ARG:NH2	2.50	0.44
1:Ak:64:TYR:HB3	1:Ak:151:LYS:O	2.18	0.44
1:Ao:146:ASP:OD1	1:Ao:147:ARG:N	2.51	0.44
1:Aq:137:ARG:O	1:Aq:141:ILE:HG23	2.17	0.44
1:Ay:64:TYR:HB3	1:Ay:151:LYS:O	2.18	0.44
1:Bi:39:GLU:OE1	1:Bi:55:ARG:NH2	2.50	0.44
1:Bo:64:TYR:HB3	1:Bo:151:LYS:O	2.18	0.44
1:Bq:146:ASP:OD1	1:Bq:147:ARG:N	2.50	0.44
1:Ca:64:TYR:HB3	1:Ca:151:LYS:O	2.18	0.44
1:Co:61:ARG:HH12	1:Co:155:GLU:N	2.11	0.44
1:Co:146:ASP:OD1	1:Co:147:ARG:N	2.50	0.44
1:Aa:39:GLU:OE1	1:Aa:55:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:137:ARG:O	1:Bk:141:ILE:HG23	2.17	0.44
1:Cg:64:TYR:HB3	1:Cg:151:LYS:O	2.18	0.44
2:Ab:9:LYS:HD3	2:Ab:73:ALA:HB1	2.00	0.44
2:Ah:9:LYS:HD3	2:Ah:73:ALA:HB1	2.00	0.44
1:Ai:146:ASP:OD1	1:Ai:147:ARG:N	2.50	0.44
1:Ba:64:TYR:HB3	1:Ba:151:LYS:O	2.18	0.44
1:Bk:146:ASP:OD1	1:Bk:147:ARG:N	2.50	0.44
2:Bl:9:LYS:HD3	2:Bl:73:ALA:HB1	2.00	0.44
2:Cl:9:LYS:HD3	2:Cl:73:ALA:HB1	2.00	0.44
1:Cm:64:TYR:HB3	1:Cm:151:LYS:O	2.18	0.44
1:Ae:146:ASP:OD1	1:Ae:147:ARG:N	2.50	0.44
1:Ag:146:ASP:OD1	1:Ag:147:ARG:N	2.50	0.44
1:Ao:86:ILE:HD13	1:Ao:96:LEU:HD12	2.00	0.44
1:Aw:64:TYR:HB3	1:Aw:151:LYS:O	2.18	0.44
1:Aw:86:ILE:HD13	1:Aw:96:LEU:HD12	2.00	0.44
1:Aw:146:ASP:OD1	1:Aw:147:ARG:N	2.50	0.44
2:Bd:9:LYS:HD3	2:Bd:73:ALA:HB1	2.00	0.44
1:Be:64:TYR:HB3	1:Be:151:LYS:O	2.18	0.44
1:Bg:146:ASP:OD1	1:Bg:147:ARG:N	2.50	0.44
2:Bj:9:LYS:HD3	2:Bj:73:ALA:HB1	2.00	0.44
1:Bs:86:ILE:HD13	1:Bs:96:LEU:HD12	2.00	0.44
1:Bu:64:TYR:HB3	1:Bu:151:LYS:O	2.18	0.44
1:Am:146:ASP:OD1	1:Am:147:ARG:N	2.50	0.43
1:Ba:86:ILE:HD13	1:Ba:96:LEU:HD12	1.99	0.43
1:Bi:146:ASP:OD1	1:Bi:147:ARG:N	2.51	0.43
1:Bm:146:ASP:OD1	1:Bm:147:ARG:N	2.50	0.43
1:Bo:146:ASP:OD1	1:Bo:147:ARG:N	2.50	0.43
1:Ci:86:ILE:HD13	1:Ci:96:LEU:HD12	2.00	0.43
1:Ak:86:ILE:HD13	1:Ak:96:LEU:HD12	2.00	0.43
1:Ak:146:ASP:OD1	1:Ak:147:ARG:N	2.50	0.43
1:Am:64:TYR:HB3	1:Am:151:LYS:O	2.18	0.43
1:Ay:146:ASP:OD1	1:Ay:147:ARG:N	2.50	0.43
2:Bj:91:GLY:HA3	2:Cp:4:HIS:NE2	2.33	0.43
2:Bp:9:LYS:HD3	2:Bp:73:ALA:HB1	2.00	0.43
1:Bw:86:ILE:HD13	1:Bw:96:LEU:HD12	2.00	0.43
1:Ac:146:ASP:OD1	1:Ac:147:ARG:N	2.50	0.43
1:Aq:64:TYR:HB3	1:Aq:151:LYS:O	2.18	0.43
2:Az:159:LEU:HD23	2:Cf:103:MET:HE1	2.00	0.43
2:Bb:159:LEU:HD23	2:Ch:103:MET:HE1	1.99	0.43
2:Bf:159:LEU:HD23	2:Cl:103:MET:HE1	1.99	0.43
1:Bi:64:TYR:HB3	1:Bi:151:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:156:ALA:HA	1:Bk:157:PRO:HD3	1.89	0.43
1:Bq:64:TYR:HB3	1:Bq:151:LYS:O	2.18	0.43
1:Ai:86:ILE:HD13	1:Ai:96:LEU:HD12	1.99	0.43
2:Av:156:GLU:HA	2:Av:159:LEU:HD12	2.00	0.43
1:Bm:64:TYR:HB3	1:Bm:151:LYS:O	2.18	0.43
1:Cc:86:ILE:HD13	1:Cc:96:LEU:HD12	2.00	0.43
1:Ce:86:ILE:HD13	1:Ce:96:LEU:HD12	2.00	0.43
1:Ci:64:TYR:HB3	1:Ci:151:LYS:O	2.18	0.43
2:Cn:9:LYS:HD3	2:Cn:73:ALA:HB1	2.00	0.43
1:Aa:146:ASP:OD1	1:Aa:147:ARG:N	2.51	0.43
2:Ad:9:LYS:HD3	2:Ad:73:ALA:HB1	2.00	0.43
1:Bm:156:ALA:HA	1:Bm:157:PRO:HD3	1.89	0.43
1:Aa:156:ALA:HA	1:Aa:157:PRO:HD3	1.89	0.43
2:Af:9:LYS:HD3	2:Af:73:ALA:HB1	2.00	0.43
2:An:159:LEU:HD23	2:Bt:103:MET:HE1	2.01	0.43
2:Bb:9:LYS:HD3	2:Bb:73:ALA:HB1	2.00	0.43
1:Be:86:ILE:HD13	1:Be:96:LEU:HD12	2.00	0.43
1:Bi:156:ALA:HA	1:Bi:157:PRO:HD3	1.89	0.43
1:Bq:86:ILE:HD13	1:Bq:96:LEU:HD12	2.00	0.43
2:Br:9:LYS:HD3	2:Br:73:ALA:HB1	2.00	0.43
2:Cd:156:GLU:HA	2:Cd:159:LEU:HD12	2.01	0.43
1:Ci:156:ALA:HA	1:Ci:157:PRO:HD3	1.89	0.43
1:Ac:86:ILE:HD13	1:Ac:96:LEU:HD12	2.00	0.43
1:Ai:64:TYR:HB3	1:Ai:151:LYS:O	2.18	0.43
2:Ap:159:LEU:HD23	2:Bv:103:MET:HE1	2.00	0.43
2:Ar:156:GLU:HA	2:Ar:159:LEU:HD12	2.01	0.43
1:Bk:86:ILE:HD13	1:Bk:96:LEU:HD12	2.00	0.43
1:Bo:61:ARG:HH12	1:Bo:155:GLU:N	2.11	0.43
2:Bz:156:GLU:HA	2:Bz:159:LEU:HD12	2.01	0.43
2:Cf:156:GLU:HA	2:Cf:159:LEU:HD12	2.00	0.43
2:Ax:156:GLU:HA	2:Ax:159:LEU:HD12	2.00	0.43
2:Bb:156:GLU:HA	2:Bb:159:LEU:HD12	2.00	0.43
2:Bh:9:LYS:HD3	2:Bh:73:ALA:HB1	2.00	0.43
2:Bh:53:ILE:HD13	2:Bh:53:ILE:HA	1.85	0.43
1:Bi:86:ILE:HD13	1:Bi:96:LEU:HD12	2.00	0.43
2:Br:58:GLN:NE2	2:Bz:140:THR:HG21	2.32	0.43
2:Ch:4:HIS:NE2	2:Cj:91:GLY:HA3	2.33	0.43
2:Ch:9:LYS:HD3	2:Ch:73:ALA:HB1	2.00	0.43
1:Co:86:ILE:HD13	1:Co:96:LEU:HD12	2.00	0.43
1:Aa:64:TYR:HB3	1:Aa:151:LYS:O	2.18	0.43
1:Ae:64:TYR:HB3	1:Ae:151:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:86:ILE:HD13	1:Bm:96:LEU:HD12	2.00	0.43
1:Bw:134:LYS:HG2	1:Bw:135:LEU:N	2.30	0.43
1:By:64:TYR:HB3	1:By:151:LYS:O	2.18	0.43
2:Cj:156:GLU:HA	2:Cj:159:LEU:HD12	2.01	0.43
1:Aa:86:ILE:HD13	1:Aa:96:LEU:HD12	2.00	0.43
2:Ab:133:MET:HG3	2:Cl:72:VAL:HG23	2.01	0.43
1:Ae:86:ILE:HD13	1:Ae:96:LEU:HD12	2.00	0.43
2:Al:9:LYS:HD3	2:Al:73:ALA:HB1	2.00	0.43
2:Al:159:LEU:HD23	2:Br:103:MET:HE1	2.01	0.43
1:Au:86:ILE:HD13	1:Au:96:LEU:HD12	2.00	0.43
1:Bm:134:LYS:HG2	1:Bm:135:LEU:N	2.30	0.43
1:Bu:86:ILE:HD13	1:Bu:96:LEU:HD12	2.00	0.43
2:Bv:9:LYS:HD3	2:Bv:73:ALA:HB1	2.00	0.43
2:Bx:156:GLU:HA	2:Bx:159:LEU:HD12	2.00	0.43
2:Ap:156:GLU:HA	2:Ap:159:LEU:HD12	2.01	0.42
1:Bg:86:ILE:HD13	1:Bg:96:LEU:HD12	2.00	0.42
1:Bo:156:ALA:HA	1:Bo:157:PRO:HD3	1.89	0.42
2:Cf:9:LYS:HD3	2:Cf:73:ALA:HB1	2.00	0.42
1:Cm:86:ILE:HD13	1:Cm:96:LEU:HD12	2.00	0.42
2:Ab:156:GLU:HA	2:Ab:159:LEU:HD12	2.01	0.42
2:An:112:MET:O	2:An:115:PHE:HB3	2.19	0.42
2:At:112:MET:O	2:At:115:PHE:HB3	2.19	0.42
2:Av:159:LEU:HD23	2:Cb:103:MET:HE1	2.00	0.42
2:Ax:9:LYS:HD3	2:Ax:73:ALA:HB1	2.00	0.42
2:Az:156:GLU:HA	2:Az:159:LEU:HD12	2.00	0.42
1:Bg:134:LYS:HG2	1:Bg:135:LEU:N	2.30	0.42
2:Cb:112:MET:O	2:Cb:115:PHE:HB3	2.19	0.42
1:Ag:86:ILE:HD13	1:Ag:96:LEU:HD12	2.00	0.42
2:Aj:9:LYS:HD3	2:Aj:73:ALA:HB1	2.00	0.42
1:Am:86:ILE:HD13	1:Am:96:LEU:HD12	2.00	0.42
2:An:9:LYS:HD3	2:An:73:ALA:HB1	2.00	0.42
2:Az:53:ILE:HA	2:Az:53:ILE:HD13	1.85	0.42
2:Az:112:MET:O	2:Az:115:PHE:HB3	2.19	0.42
1:Bk:166:LEU:HD23	1:Bk:166:LEU:HA	1.91	0.42
2:Bn:156:GLU:HA	2:Bn:159:LEU:HD12	2.00	0.42
1:Bo:86:ILE:HD13	1:Bo:96:LEU:HD12	2.00	0.42
2:Cd:112:MET:O	2:Cd:115:PHE:HB3	2.19	0.42
1:Co:156:ALA:HA	1:Co:157:PRO:HD3	1.89	0.42
2:Ab:159:LEU:HD23	2:Cp:103:MET:HE1	2.02	0.42
1:Ao:134:LYS:HG2	1:Ao:135:LEU:N	2.31	0.42
2:At:9:LYS:HD3	2:At:73:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Av:112:MET:O	2:Av:115:PHE:HB3	2.19	0.42
2:Bf:9:LYS:HD3	2:Bf:73:ALA:HB1	2.00	0.42
2:Bj:156:GLU:HA	2:Bj:159:LEU:HD12	2.01	0.42
2:Bn:9:LYS:HD3	2:Bn:73:ALA:HB1	2.00	0.42
2:Bv:112:MET:O	2:Bv:115:PHE:HB3	2.19	0.42
2:Bx:112:MET:O	2:Bx:115:PHE:HB3	2.19	0.42
1:Ae:134:LYS:HG2	1:Ae:135:LEU:N	2.31	0.42
2:Ah:159:LEU:HD23	2:Bn:103:MET:HE1	2.02	0.42
1:Au:25:LEU:HD23	1:Au:69:MET:SD	2.60	0.42
1:Ba:156:ALA:HA	1:Ba:157:PRO:HD3	1.89	0.42
2:Bz:9:LYS:HD3	2:Bz:73:ALA:HB1	2.00	0.42
2:Cb:9:LYS:HD3	2:Cb:73:ALA:HB1	2.00	0.42
2:Ch:112:MET:O	2:Ch:115:PHE:HB3	2.19	0.42
2:Af:156:GLU:HA	2:Af:159:LEU:HD12	2.01	0.42
2:Al:156:GLU:HA	2:Al:159:LEU:HD12	2.01	0.42
2:Ar:112:MET:O	2:Ar:115:PHE:HB3	2.19	0.42
2:Ax:112:MET:O	2:Ax:115:PHE:HB3	2.20	0.42
2:Az:9:LYS:HD3	2:Az:73:ALA:HB1	2.00	0.42
1:Bc:86:ILE:HD13	1:Bc:96:LEU:HD12	2.00	0.42
1:By:25:LEU:HD23	1:By:69:MET:SD	2.60	0.42
2:Cb:32:LYS:HG3	2:Cb:48:HIS:CE1	2.55	0.42
2:Cb:68:ARG:HG3	2:Ch:130:GLU:HG3	2.02	0.42
2:Ch:156:GLU:HA	2:Ch:159:LEU:HD12	2.01	0.42
2:Cj:9:LYS:HD3	2:Cj:73:ALA:HB1	2.00	0.42
2:Cj:112:MET:O	2:Cj:115:PHE:HB3	2.19	0.42
2:Cl:156:GLU:HA	2:Cl:159:LEU:HD12	2.01	0.42
2:Cp:9:LYS:HD3	2:Cp:73:ALA:HB1	2.00	0.42
2:Ab:112:MET:O	2:Ab:115:PHE:HB3	2.19	0.42
2:Ah:32:LYS:HG3	2:Ah:48:HIS:CE1	2.55	0.42
2:Ap:100:LEU:HD22	2:Ar:118:GLN:NE2	2.35	0.42
2:Ar:9:LYS:HD3	2:Ar:73:ALA:HB1	2.00	0.42
2:Ar:159:LEU:HD23	2:Bx:103:MET:HE1	2.02	0.42
1:As:25:LEU:HD23	1:As:69:MET:SD	2.60	0.42
2:At:32:LYS:HG3	2:At:48:HIS:CE1	2.55	0.42
2:At:100:LEU:HD22	2:Av:118:GLN:NE2	2.35	0.42
2:At:156:GLU:HA	2:At:159:LEU:HD12	2.00	0.42
1:Aw:25:LEU:HD23	1:Aw:69:MET:SD	2.60	0.42
2:Az:32:LYS:HG3	2:Az:48:HIS:CE1	2.55	0.42
2:Bl:100:LEU:HD22	2:Bn:118:GLN:NE2	2.35	0.42
2:Bp:156:GLU:HA	2:Bp:159:LEU:HD12	2.01	0.42
2:Bt:156:GLU:HA	2:Bt:159:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bw:25:LEU:HD23	1:Bw:69:MET:SD	2.60	0.42
2:Cb:156:GLU:HA	2:Cb:159:LEU:HD12	2.01	0.42
2:Ab:91:GLY:HA3	2:Bh:4:HIS:NE2	2.35	0.42
2:Ap:9:LYS:HD3	2:Ap:73:ALA:HB1	2.00	0.42
2:Ap:112:MET:O	2:Ap:115:PHE:HB3	2.19	0.42
2:Bd:156:GLU:HA	2:Bd:159:LEU:HD12	2.01	0.42
2:Bh:118:GLN:NE2	2:Cn:100:LEU:HD22	2.35	0.42
1:Bi:166:LEU:HD23	1:Bi:166:LEU:HA	1.91	0.42
2:Bl:32:LYS:HG3	2:Bl:48:HIS:CE1	2.55	0.42
2:Bn:100:LEU:HD22	2:Bp:118:GLN:NE2	2.34	0.42
2:Br:32:LYS:HG3	2:Br:48:HIS:CE1	2.55	0.42
2:Bt:9:LYS:HD3	2:Bt:73:ALA:HB1	2.00	0.42
2:Bx:100:LEU:HD22	2:Bz:118:GLN:NE2	2.35	0.42
1:Ca:25:LEU:HD23	1:Ca:69:MET:SD	2.60	0.42
1:Cc:25:LEU:HD23	1:Cc:69:MET:SD	2.60	0.42
2:Cd:9:LYS:HD3	2:Cd:73:ALA:HB1	2.00	0.42
2:Cn:53:ILE:HD13	2:Cn:53:ILE:HA	1.85	0.42
2:Ab:32:LYS:HG3	2:Ab:48:HIS:CE1	2.55	0.42
2:Ad:112:MET:O	2:Ad:115:PHE:HB3	2.20	0.42
2:Ah:156:GLU:HA	2:Ah:159:LEU:HD12	2.01	0.42
2:An:32:LYS:HG3	2:An:48:HIS:CE1	2.55	0.42
2:Av:9:LYS:HD3	2:Av:73:ALA:HB1	2.00	0.42
2:Bb:112:MET:O	2:Bb:115:PHE:HB3	2.19	0.42
2:Bh:112:MET:O	2:Bh:115:PHE:HB3	2.19	0.42
2:Bj:4:HIS:NE2	2:Bl:91:GLY:HA3	2.35	0.42
2:Bn:112:MET:O	2:Bn:115:PHE:HB3	2.19	0.42
2:Bp:32:LYS:HG3	2:Bp:48:HIS:CE1	2.55	0.42
1:Bq:156:ALA:HA	1:Bq:157:PRO:HD3	1.89	0.42
2:Bv:32:LYS:HG3	2:Bv:48:HIS:CE1	2.55	0.42
2:Bx:9:LYS:HD3	2:Bx:73:ALA:HB1	2.00	0.42
2:Bx:32:LYS:HG3	2:Bx:48:HIS:CE1	2.55	0.42
1:Ce:25:LEU:HD23	1:Ce:69:MET:SD	2.60	0.42
2:Cf:112:MET:O	2:Cf:115:PHE:HB3	2.19	0.42
1:Co:166:LEU:HD23	1:Co:166:LEU:HA	1.91	0.42
2:Ad:32:LYS:HG3	2:Ad:48:HIS:CE1	2.55	0.42
2:Ah:4:HIS:NE2	2:Aj:91:GLY:HA3	2.34	0.42
2:Aj:156:GLU:HA	2:Aj:159:LEU:HD12	2.01	0.42
2:Al:112:MET:O	2:Al:115:PHE:HB3	2.20	0.42
1:Ao:25:LEU:HD23	1:Ao:69:MET:SD	2.60	0.42
2:Ap:32:LYS:HG3	2:Ap:48:HIS:CE1	2.55	0.42
1:Aq:25:LEU:HD23	1:Aq:69:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:25:LEU:HD23	1:Ay:69:MET:SD	2.60	0.42
2:Bj:112:MET:O	2:Bj:115:PHE:HB3	2.19	0.42
2:Bv:156:GLU:HA	2:Bv:159:LEU:HD12	2.01	0.42
2:Cb:72:VAL:HG23	2:Ch:133:MET:HG3	2.01	0.42
2:Ad:133:MET:HG3	2:Cn:72:VAL:HG23	2.02	0.41
2:Ad:159:LEU:HD23	2:Bj:103:MET:HE1	2.02	0.41
2:Af:112:MET:O	2:Af:115:PHE:HB3	2.20	0.41
2:Af:133:MET:HG3	2:Bh:72:VAL:HG23	2.02	0.41
2:Aj:159:LEU:HD23	2:Bp:103:MET:HE1	2.01	0.41
1:Am:25:LEU:HD23	1:Am:69:MET:SD	2.60	0.41
2:Ar:32:LYS:HG3	2:Ar:48:HIS:CE1	2.55	0.41
2:Av:100:LEU:HD22	2:Ax:118:GLN:NE2	2.35	0.41
2:Ax:32:LYS:HG3	2:Ax:48:HIS:CE1	2.55	0.41
1:Ba:25:LEU:HD23	1:Ba:69:MET:SD	2.60	0.41
2:Bd:4:HIS:NE2	2:Bf:91:GLY:HA3	2.34	0.41
1:Bi:81:ALA:HB2	1:Co:58:HIS:CE1	2.55	0.41
2:Bj:32:LYS:HG3	2:Bj:48:HIS:CE1	2.55	0.41
2:Bl:112:MET:O	2:Bl:115:PHE:HB3	2.20	0.41
2:Br:156:GLU:HA	2:Br:159:LEU:HD12	2.01	0.41
1:Bu:25:LEU:HD23	1:Bu:69:MET:SD	2.60	0.41
2:Bx:4:HIS:NE2	2:Bz:91:GLY:HA3	2.35	0.41
2:Bz:4:HIS:NE2	2:Cb:91:GLY:HA3	2.35	0.41
2:Cd:32:LYS:HG3	2:Cd:48:HIS:CE1	2.55	0.41
2:Ch:32:LYS:HG3	2:Ch:48:HIS:CE1	2.55	0.41
1:Ck:86:ILE:HD13	1:Ck:96:LEU:HD12	2.00	0.41
1:Ac:156:ALA:HA	1:Ac:157:PRO:HD3	1.89	0.41
1:Ae:156:ALA:HA	1:Ae:157:PRO:HD3	1.89	0.41
2:Aj:32:LYS:HG3	2:Aj:48:HIS:CE1	2.55	0.41
1:Ak:25:LEU:HD23	1:Ak:69:MET:SD	2.60	0.41
2:An:156:GLU:HA	2:An:159:LEU:HD12	2.00	0.41
2:Av:4:HIS:NE2	2:Ax:91:GLY:HA3	2.35	0.41
2:Br:100:LEU:HD22	2:Bt:118:GLN:NE2	2.35	0.41
1:Bs:25:LEU:HD23	1:Bs:69:MET:SD	2.60	0.41
2:Cn:149:LEU:HA	2:Cn:149:LEU:HD12	1.88	0.41
2:Cn:156:GLU:HA	2:Cn:159:LEU:HD12	2.00	0.41
2:Ad:156:GLU:HA	2:Ad:159:LEU:HD12	2.00	0.41
2:Af:159:LEU:HD23	2:Bl:103:MET:HE1	2.02	0.41
2:Ah:112:MET:O	2:Ah:115:PHE:HB3	2.19	0.41
2:Bf:112:MET:O	2:Bf:115:PHE:HB3	2.19	0.41
1:Bm:178:GLU:HA	1:Bm:179:PRO:HD2	1.95	0.41
2:Br:112:MET:O	2:Br:115:PHE:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bz:112:MET:O	2:Bz:115:PHE:HB3	2.19	0.41
2:Cj:32:LYS:HG3	2:Cj:48:HIS:CE1	2.55	0.41
2:Cp:112:MET:O	2:Cp:115:PHE:HB3	2.19	0.41
1:Ag:156:ALA:HA	1:Ag:157:PRO:HD3	1.90	0.41
2:An:100:LEU:HD22	2:Ap:118:GLN:NE2	2.35	0.41
2:Ar:4:HIS:NE2	2:At:91:GLY:HA3	2.35	0.41
2:Az:4:HIS:NE2	2:Bb:91:GLY:HA3	2.35	0.41
2:Bd:112:MET:O	2:Bd:115:PHE:HB3	2.19	0.41
2:Bf:149:LEU:HA	2:Bf:149:LEU:HD12	1.89	0.41
2:Bh:32:LYS:HG3	2:Bh:48:HIS:CE1	2.55	0.41
2:Bh:156:GLU:HA	2:Bh:159:LEU:HD12	2.01	0.41
1:Bi:25:LEU:HD23	1:Bi:69:MET:SD	2.60	0.41
1:Bk:25:LEU:HD23	1:Bk:69:MET:SD	2.60	0.41
2:Bp:112:MET:O	2:Bp:115:PHE:HB3	2.20	0.41
1:Bq:178:GLU:HA	1:Bq:179:PRO:HD2	1.95	0.41
2:Bz:32:LYS:HG3	2:Bz:48:HIS:CE1	2.55	0.41
1:Cg:25:LEU:HD23	1:Cg:69:MET:SD	2.60	0.41
2:Cn:112:MET:O	2:Cn:115:PHE:HB3	2.19	0.41
2:Af:32:LYS:HG3	2:Af:48:HIS:CE1	2.55	0.41
2:Aj:100:LEU:HD22	2:Al:118:GLN:NE2	2.35	0.41
2:Av:53:ILE:HD13	2:Av:53:ILE:HA	1.85	0.41
2:Ax:100:LEU:HD22	2:Az:118:GLN:NE2	2.35	0.41
2:Bb:32:LYS:HG3	2:Bb:48:HIS:CE1	2.55	0.41
2:Bf:156:GLU:HA	2:Bf:159:LEU:HD12	2.01	0.41
2:Bt:112:MET:O	2:Bt:115:PHE:HB3	2.19	0.41
1:Ca:156:ALA:HA	1:Ca:157:PRO:HD3	1.89	0.41
2:Cb:100:LEU:HD22	2:Cd:118:GLN:NE2	2.35	0.41
1:Ck:25:LEU:HD23	1:Ck:69:MET:SD	2.60	0.41
2:Cp:156:GLU:HA	2:Cp:159:LEU:HD12	2.01	0.41
2:Ab:118:GLN:NE2	2:Bh:100:LEU:HD22	2.35	0.41
2:Ad:4:HIS:NE2	2:Af:91:GLY:HA3	2.35	0.41
2:Ad:100:LEU:HD22	2:Af:118:GLN:NE2	2.36	0.41
2:Af:8:LEU:HD23	2:Af:8:LEU:HA	1.89	0.41
2:Al:32:LYS:HG3	2:Al:48:HIS:CE1	2.55	0.41
2:Az:72:VAL:HG23	2:Bf:133:MET:HG3	2.03	0.41
1:Be:58:HIS:CE1	1:Be:81:ALA:HB2	2.56	0.41
2:Bh:8:LEU:HD23	2:Bh:8:LEU:HA	1.89	0.41
2:Bl:156:GLU:HA	2:Bl:159:LEU:HD12	2.00	0.41
1:Bm:25:LEU:HD23	1:Bm:69:MET:SD	2.60	0.41
2:Bn:4:HIS:NE2	2:Bp:91:GLY:HA3	2.35	0.41
2:Cd:100:LEU:HD22	2:Cf:118:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ch:53:ILE:HA	2:Ch:53:ILE:HD13	1.85	0.41
2:Ch:72:VAL:HG23	2:Cn:133:MET:HG3	2.02	0.41
1:Ci:134:LYS:HG2	1:Ci:135:LEU:N	2.30	0.41
1:Ae:25:LEU:HD23	1:Ae:69:MET:SD	2.60	0.41
2:An:4:HIS:NE2	2:Ap:91:GLY:HA3	2.35	0.41
1:Bc:25:LEU:HD23	1:Bc:69:MET:SD	2.60	0.41
1:Be:25:LEU:HD23	1:Be:69:MET:SD	2.60	0.41
2:Bf:32:LYS:HG3	2:Bf:48:HIS:CE1	2.55	0.41
2:Bn:32:LYS:HG3	2:Bn:48:HIS:CE1	2.55	0.41
1:Bs:65:LEU:HD23	1:Bs:65:LEU:HA	1.94	0.41
2:Bv:4:HIS:NE2	2:Bx:91:GLY:HA3	2.36	0.41
2:Cf:4:HIS:NE2	2:Ch:91:GLY:HA3	2.35	0.41
2:Cf:32:LYS:HG3	2:Cf:48:HIS:CE1	2.55	0.41
1:Ci:25:LEU:HD23	1:Ci:69:MET:SD	2.60	0.41
2:Cl:4:HIS:NE2	2:Cn:91:GLY:HA3	2.35	0.41
2:Cl:100:LEU:HD22	2:Cn:118:GLN:NE2	2.35	0.41
1:Ae:178:GLU:HA	1:Ae:179:PRO:HD2	1.95	0.41
2:Ah:100:LEU:HD22	2:Aj:118:GLN:NE2	2.35	0.41
2:Aj:112:MET:O	2:Aj:115:PHE:HB3	2.19	0.41
1:Am:105:TRP:CD1	1:Am:141:ILE:HB	2.56	0.41
1:Aq:15:LEU:HD23	1:Aq:15:LEU:HA	1.95	0.41
2:Av:32:LYS:HG3	2:Av:48:HIS:CE1	2.55	0.41
2:Bd:32:LYS:HG3	2:Bd:48:HIS:CE1	2.55	0.41
2:Bf:53:ILE:HD13	2:Bf:53:ILE:HA	1.85	0.41
2:Bh:91:GLY:HA3	2:Cn:4:HIS:NE2	2.35	0.41
2:Bn:133:MET:HG3	2:Cp:72:VAL:HG23	2.03	0.41
2:Bt:100:LEU:HD22	2:Bv:118:GLN:NE2	2.36	0.41
1:Ca:134:LYS:HG2	1:Ca:135:LEU:N	2.30	0.41
2:Cb:4:HIS:NE2	2:Cd:91:GLY:HA3	2.36	0.41
2:Ch:68:ARG:HG3	2:Cn:130:GLU:HG3	2.02	0.41
2:Ch:100:LEU:HD22	2:Cj:118:GLN:NE2	2.36	0.41
2:Cl:32:LYS:HG3	2:Cl:48:HIS:CE1	2.55	0.41
1:Cm:25:LEU:HD23	1:Cm:69:MET:SD	2.60	0.41
1:Aa:105:TRP:CD1	1:Aa:141:ILE:HB	2.56	0.41
1:Ac:25:LEU:HD23	1:Ac:69:MET:SD	2.60	0.41
2:Ad:72:VAL:HG23	2:Aj:133:MET:HG3	2.02	0.41
2:Af:100:LEU:HD22	2:Ah:118:GLN:NE2	2.35	0.41
1:Ag:25:LEU:HD23	1:Ag:69:MET:SD	2.60	0.41
1:Ag:105:TRP:CD1	1:Ag:141:ILE:HB	2.56	0.41
2:Ap:4:HIS:NE2	2:Ar:91:GLY:HA3	2.35	0.41
1:Bi:105:TRP:CD1	1:Bi:141:ILE:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bq:25:LEU:HD23	1:Bq:69:MET:SD	2.60	0.41
1:Bq:105:TRP:CD1	1:Bq:141:ILE:HB	2.56	0.41
1:Bs:178:GLU:HA	1:Bs:179:PRO:HD2	1.95	0.41
2:Bt:32:LYS:HG3	2:Bt:48:HIS:CE1	2.55	0.41
2:Bx:149:LEU:HA	2:Bx:149:LEU:HD12	1.88	0.41
2:Cf:53:ILE:HD13	2:Cf:53:ILE:HA	1.85	0.41
1:Cg:134:LYS:HG2	1:Cg:135:LEU:N	2.31	0.41
2:Cl:112:MET:O	2:Cl:115:PHE:HB3	2.20	0.41
1:Co:25:LEU:HD23	1:Co:69:MET:SD	2.60	0.41
1:Co:134:LYS:HG2	1:Co:135:LEU:N	2.30	0.41
2:Cp:32:LYS:HG3	2:Cp:48:HIS:CE1	2.55	0.41
1:Aa:25:LEU:HD23	1:Aa:69:MET:SD	2.60	0.41
1:Ak:65:LEU:HD23	1:Ak:65:LEU:HA	1.94	0.41
2:Al:40:GLY:HA3	2:Bz:101:LYS:HZ1	1.84	0.41
2:Al:100:LEU:HD22	2:An:118:GLN:NE2	2.35	0.41
2:Ap:149:LEU:HA	2:Ap:149:LEU:HD12	1.89	0.41
1:As:105:TRP:CD1	1:As:141:ILE:HB	2.56	0.41
2:At:4:HIS:NE2	2:Av:91:GLY:HA3	2.36	0.41
2:Av:72:VAL:HG23	2:Bb:133:MET:HG3	2.03	0.41
1:Ba:134:LYS:HG2	1:Ba:135:LEU:N	2.30	0.41
1:Bc:105:TRP:CD1	1:Bc:141:ILE:HB	2.56	0.41
1:Bg:156:ALA:HA	1:Bg:157:PRO:HD3	1.89	0.41
1:Bk:105:TRP:CD1	1:Bk:141:ILE:HB	2.56	0.41
2:Bl:4:HIS:NE2	2:Bn:91:GLY:HA3	2.35	0.41
1:Bo:25:LEU:HD23	1:Bo:69:MET:SD	2.60	0.41
1:Bs:156:ALA:HA	1:Bs:157:PRO:HD3	1.89	0.41
1:Bu:105:TRP:CD1	1:Bu:141:ILE:HB	2.56	0.41
1:Ca:105:TRP:CD1	1:Ca:141:ILE:HB	2.56	0.41
1:Ck:105:TRP:CD1	1:Ck:141:ILE:HB	2.56	0.41
2:Ab:4:HIS:NE2	2:Ad:91:GLY:HA3	2.35	0.40
1:Ac:178:GLU:HA	1:Ac:179:PRO:HD2	1.95	0.40
1:Ag:178:GLU:HA	1:Ag:179:PRO:HD2	1.95	0.40
1:Ai:25:LEU:HD23	1:Ai:69:MET:SD	2.60	0.40
1:Ak:178:GLU:HA	1:Ak:179:PRO:HD2	1.95	0.40
1:Ay:134:LYS:HG2	1:Ay:135:LEU:N	2.31	0.40
1:Bg:25:LEU:HD23	1:Bg:69:MET:SD	2.60	0.40
2:Bj:72:VAL:HG23	2:Bp:133:MET:HG3	2.03	0.40
2:Bp:4:HIS:NE2	2:Br:91:GLY:HA3	2.35	0.40
1:Bw:105:TRP:CD1	1:Bw:141:ILE:HB	2.56	0.40
2:Bz:53:ILE:HA	2:Bz:53:ILE:HD13	1.85	0.40
2:Bz:100:LEU:HD22	2:Cb:118:GLN:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ch:4:HIS:CD2	2:Cj:91:GLY:HA3	2.57	0.40
1:Cm:105:TRP:CD1	1:Cm:141:ILE:HB	2.56	0.40
1:Ac:105:TRP:CD1	1:Ac:141:ILE:HB	2.56	0.40
2:Ad:43:GLU:O	2:Ad:46:ARG:HB3	2.22	0.40
2:Al:4:HIS:NE2	2:An:91:GLY:HA3	2.36	0.40
1:As:134:LYS:HG2	1:As:135:LEU:N	2.31	0.40
1:As:156:ALA:HA	1:As:157:PRO:HD3	1.89	0.40
1:Aw:105:TRP:CD1	1:Aw:141:ILE:HB	2.56	0.40
2:Bh:133:MET:HG3	2:Cj:72:VAL:HG23	2.03	0.40
2:Bj:43:GLU:O	2:Bj:46:ARG:HB3	2.22	0.40
1:Bo:105:TRP:CD1	1:Bo:141:ILE:HB	2.56	0.40
1:Bs:105:TRP:CD1	1:Bs:141:ILE:HB	2.56	0.40
1:Ce:166:LEU:HD23	1:Ce:166:LEU:HA	1.91	0.40
1:Ci:105:TRP:CD1	1:Ci:141:ILE:HB	2.56	0.40
2:Cl:53:ILE:HD13	2:Cl:53:ILE:HA	1.85	0.40
2:Cn:32:LYS:HG3	2:Cn:48:HIS:CE1	2.55	0.40
2:Ab:100:LEU:HD22	2:Ad:118:GLN:NE2	2.36	0.40
2:Af:43:GLU:O	2:Af:46:ARG:HB3	2.22	0.40
2:Aj:4:HIS:NE2	2:Al:91:GLY:HA3	2.35	0.40
2:At:5:LEU:HD13	2:At:76:VAL:HG12	2.04	0.40
2:Av:5:LEU:HD13	2:Av:76:VAL:HG12	2.04	0.40
2:Ax:5:LEU:HD13	2:Ax:76:VAL:HG12	2.04	0.40
2:Az:100:LEU:HD22	2:Bb:118:GLN:NE2	2.37	0.40
2:Bb:4:HIS:NE2	2:Bd:91:GLY:HA3	2.35	0.40
2:Bd:43:GLU:O	2:Bd:46:ARG:HB3	2.22	0.40
1:Bm:105:TRP:CD1	1:Bm:141:ILE:HB	2.56	0.40
2:Bx:72:VAL:HG23	2:Cd:133:MET:HG3	2.02	0.40
2:Bz:8:LEU:HD23	2:Bz:8:LEU:HA	1.89	0.40
2:Cn:43:GLU:O	2:Cn:46:ARG:HB3	2.22	0.40
2:Ab:43:GLU:O	2:Ab:46:ARG:HB3	2.22	0.40
2:Af:72:VAL:HG23	2:Al:133:MET:HG3	2.03	0.40
2:Ah:43:GLU:O	2:Ah:46:ARG:HB3	2.22	0.40
2:An:72:VAL:HG23	2:At:133:MET:HG3	2.02	0.40
1:Aq:105:TRP:CD1	1:Aq:141:ILE:HB	2.56	0.40
2:Ar:5:LEU:HD13	2:Ar:76:VAL:HG12	2.04	0.40
2:Bf:43:GLU:O	2:Bf:46:ARG:HB3	2.22	0.40
1:Bk:178:GLU:HA	1:Bk:179:PRO:HD2	1.95	0.40
1:Bo:178:GLU:HA	1:Bo:179:PRO:HD2	1.95	0.40
2:Bt:5:LEU:HD13	2:Bt:76:VAL:HG12	2.03	0.40
2:Bt:8:LEU:HD23	2:Bt:8:LEU:HA	1.89	0.40
2:Bv:5:LEU:HD13	2:Bv:76:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Bx:5:LEU:HD13	2:Bx:76:VAL:HG12	2.04	0.40
2:Cd:5:LEU:HD13	2:Cd:76:VAL:HG12	2.04	0.40
1:Ce:105:TRP:CD1	1:Ce:141:ILE:HB	2.56	0.40
2:Cf:5:LEU:HD13	2:Cf:76:VAL:HG12	2.04	0.40
1:Cg:105:TRP:CD1	1:Cg:141:ILE:HB	2.56	0.40
2:Cj:100:LEU:HD22	2:Cl:118:GLN:NE2	2.36	0.40
2:Ab:72:VAL:HG23	2:Ah:133:MET:HG3	2.03	0.40
1:Ae:105:TRP:CD1	1:Ae:141:ILE:HB	2.56	0.40
2:Ah:72:VAL:HG23	2:An:133:MET:HG3	2.02	0.40
1:Ai:105:TRP:CD1	1:Ai:141:ILE:HB	2.56	0.40
1:Ao:105:TRP:CD1	1:Ao:141:ILE:HB	2.56	0.40
2:Ax:72:VAL:HG23	2:Bd:133:MET:HG3	2.03	0.40
2:Az:5:LEU:HD13	2:Az:76:VAL:HG12	2.04	0.40
2:Bh:43:GLU:O	2:Bh:46:ARG:HB3	2.22	0.40
1:Bq:134:LYS:HG2	1:Bq:135:LEU:N	2.30	0.40
1:Cc:65:LEU:HD23	1:Cc:65:LEU:HA	1.94	0.40
2:Cd:4:HIS:NE2	2:Cf:91:GLY:HA3	2.36	0.40
2:Cl:43:GLU:O	2:Cl:46:ARG:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ac	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ae	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ag	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ai	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ak	180/182 (99%)	173 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Am	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ao	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Aq	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	As	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Au	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Aw	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ay	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ba	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bc	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Be	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bg	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bi	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bk	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bm	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bo	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bq	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bs	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bu	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Bw	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	By	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ca	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Cc	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ce	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Cg	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ci	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Ck	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Cm	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
1	Co	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
2	Ab	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ad	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Af	158/160 (99%)	152 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ah	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Aj	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Al	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	An	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ap	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ar	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	At	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Av	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ax	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Az	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bb	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bd	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bf	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bh	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bj	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bl	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bn	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bp	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Br	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bt	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bv	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bx	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Bz	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cb	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cd	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cf	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Ch	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cj	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cl	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cn	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
2	Cp	158/160 (99%)	152 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11492/11628 (99%)	11050 (96%)	442 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	158/158 (100%)	158 (100%)	0	100	100
1	Ac	158/158 (100%)	158 (100%)	0	100	100
1	Ae	158/158 (100%)	158 (100%)	0	100	100
1	Ag	158/158 (100%)	158 (100%)	0	100	100
1	Ai	158/158 (100%)	158 (100%)	0	100	100
1	Ak	158/158 (100%)	158 (100%)	0	100	100
1	Am	158/158 (100%)	158 (100%)	0	100	100
1	Ao	158/158 (100%)	158 (100%)	0	100	100
1	Aq	158/158 (100%)	158 (100%)	0	100	100
1	As	158/158 (100%)	158 (100%)	0	100	100
1	Au	158/158 (100%)	158 (100%)	0	100	100
1	Aw	158/158 (100%)	158 (100%)	0	100	100
1	Ay	158/158 (100%)	158 (100%)	0	100	100
1	Ba	158/158 (100%)	158 (100%)	0	100	100
1	Bc	158/158 (100%)	158 (100%)	0	100	100
1	Be	158/158 (100%)	158 (100%)	0	100	100
1	Bg	158/158 (100%)	158 (100%)	0	100	100
1	Bi	158/158 (100%)	158 (100%)	0	100	100
1	Bk	158/158 (100%)	158 (100%)	0	100	100
1	Bm	158/158 (100%)	158 (100%)	0	100	100
1	Bo	158/158 (100%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bq	158/158 (100%)	158 (100%)	0	100	100
1	Bs	158/158 (100%)	158 (100%)	0	100	100
1	Bu	158/158 (100%)	158 (100%)	0	100	100
1	Bw	158/158 (100%)	158 (100%)	0	100	100
1	By	158/158 (100%)	158 (100%)	0	100	100
1	Ca	158/158 (100%)	158 (100%)	0	100	100
1	Cc	158/158 (100%)	158 (100%)	0	100	100
1	Ce	158/158 (100%)	158 (100%)	0	100	100
1	Cg	158/158 (100%)	158 (100%)	0	100	100
1	Ci	158/158 (100%)	158 (100%)	0	100	100
1	Ck	158/158 (100%)	158 (100%)	0	100	100
1	Cm	158/158 (100%)	158 (100%)	0	100	100
1	Co	158/158 (100%)	158 (100%)	0	100	100
2	Ab	136/136 (100%)	136 (100%)	0	100	100
2	Ad	136/136 (100%)	136 (100%)	0	100	100
2	Af	136/136 (100%)	136 (100%)	0	100	100
2	Ah	136/136 (100%)	136 (100%)	0	100	100
2	Aj	136/136 (100%)	136 (100%)	0	100	100
2	Al	136/136 (100%)	136 (100%)	0	100	100
2	An	136/136 (100%)	136 (100%)	0	100	100
2	Ap	136/136 (100%)	136 (100%)	0	100	100
2	Ar	136/136 (100%)	136 (100%)	0	100	100
2	At	136/136 (100%)	136 (100%)	0	100	100
2	Av	136/136 (100%)	136 (100%)	0	100	100
2	Ax	136/136 (100%)	136 (100%)	0	100	100
2	Az	136/136 (100%)	136 (100%)	0	100	100
2	Bb	136/136 (100%)	136 (100%)	0	100	100
2	Bd	136/136 (100%)	136 (100%)	0	100	100
2	Bf	136/136 (100%)	136 (100%)	0	100	100
2	Bh	136/136 (100%)	136 (100%)	0	100	100
2	Bj	136/136 (100%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bl	136/136 (100%)	136 (100%)	0	100	100
2	Bn	136/136 (100%)	136 (100%)	0	100	100
2	Bp	136/136 (100%)	136 (100%)	0	100	100
2	Br	136/136 (100%)	136 (100%)	0	100	100
2	Bt	136/136 (100%)	136 (100%)	0	100	100
2	Bv	136/136 (100%)	136 (100%)	0	100	100
2	Bx	136/136 (100%)	136 (100%)	0	100	100
2	Bz	136/136 (100%)	136 (100%)	0	100	100
2	Cb	136/136 (100%)	136 (100%)	0	100	100
2	Cd	136/136 (100%)	136 (100%)	0	100	100
2	Cf	136/136 (100%)	136 (100%)	0	100	100
2	Ch	136/136 (100%)	136 (100%)	0	100	100
2	Cj	136/136 (100%)	136 (100%)	0	100	100
2	Cl	136/136 (100%)	136 (100%)	0	100	100
2	Cn	136/136 (100%)	136 (100%)	0	100	100
2	Cp	136/136 (100%)	136 (100%)	0	100	100
All	All	9996/9996 (100%)	9996 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (261) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	123	GLN
1	Aa	140	GLN
2	Ab	4	HIS
2	Ab	48	HIS
2	Ab	57	ASN
2	Ab	58	GLN
2	Ab	118	GLN
1	Ac	20	ASN
1	Ac	123	GLN
1	Ac	139	ASN
1	Ac	140	GLN
2	Ad	4	HIS
2	Ad	48	HIS

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Mol	Chain	Res	Type
2	Ad	57	ASN
2	Ad	58	GLN
2	Ad	118	GLN
1	Ae	20	ASN
1	Ae	123	GLN
1	Ae	140	GLN
2	Af	4	HIS
2	Af	41	ASN
2	Af	48	HIS
2	Af	57	ASN
2	Af	58	GLN
2	Af	118	GLN
1	Ag	20	ASN
1	Ag	123	GLN
1	Ag	140	GLN
2	Ah	4	HIS
2	Ah	48	HIS
2	Ah	57	ASN
2	Ah	58	GLN
2	Ah	118	GLN
1	Ai	20	ASN
1	Ai	123	GLN
1	Ai	140	GLN
2	Aj	4	HIS
2	Aj	48	HIS
2	Aj	57	ASN
2	Aj	58	GLN
2	Aj	118	GLN
1	Ak	20	ASN
1	Ak	123	GLN
1	Ak	140	GLN
2	Al	4	HIS
2	Al	48	HIS
2	Al	57	ASN
2	Al	58	GLN
2	Al	118	GLN
1	Am	20	ASN
1	Am	123	GLN
1	Am	140	GLN
2	An	4	HIS
2	An	48	HIS
2	An	57	ASN

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Mol	Chain	Res	Type
2	An	58	GLN
2	An	118	GLN
1	Ao	20	ASN
1	Ao	123	GLN
1	Ao	140	GLN
2	Ap	4	HIS
2	Ap	48	HIS
2	Ap	57	ASN
2	Ap	58	GLN
2	Ap	118	GLN
1	Aq	20	ASN
1	Aq	123	GLN
1	Aq	140	GLN
1	Aq	174	ASN
2	Ar	4	HIS
2	Ar	48	HIS
2	Ar	57	ASN
2	Ar	58	GLN
2	Ar	118	GLN
1	As	20	ASN
1	As	123	GLN
1	As	140	GLN
2	At	4	HIS
2	At	48	HIS
2	At	57	ASN
2	At	58	GLN
2	At	118	GLN
1	Au	123	GLN
1	Au	140	GLN
2	Av	4	HIS
2	Av	48	HIS
2	Av	57	ASN
2	Av	58	GLN
2	Av	118	GLN
1	Aw	20	ASN
1	Aw	123	GLN
1	Aw	140	GLN
2	Ax	4	HIS
2	Ax	48	HIS
2	Ax	57	ASN
2	Ax	58	GLN
2	Ax	118	GLN

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Mol	Chain	Res	Type
1	Ay	20	ASN
1	Ay	123	GLN
1	Ay	140	GLN
2	Az	4	HIS
2	Az	48	HIS
2	Az	57	ASN
2	Az	118	GLN
1	Ba	20	ASN
1	Ba	123	GLN
1	Ba	140	GLN
2	Bb	4	HIS
2	Bb	48	HIS
2	Bb	57	ASN
2	Bb	118	GLN
1	Bc	123	GLN
1	Bc	140	GLN
2	Bd	4	HIS
2	Bd	48	HIS
2	Bd	57	ASN
2	Bd	118	GLN
1	Be	123	GLN
1	Be	140	GLN
2	Bf	48	HIS
2	Bf	57	ASN
2	Bf	118	GLN
1	Bg	20	ASN
1	Bg	123	GLN
1	Bg	140	GLN
2	Bh	4	HIS
2	Bh	48	HIS
2	Bh	57	ASN
2	Bh	58	GLN
2	Bh	118	GLN
1	Bi	20	ASN
1	Bi	123	GLN
1	Bi	140	GLN
2	Bj	4	HIS
2	Bj	48	HIS
2	Bj	57	ASN
2	Bj	58	GLN
2	Bj	118	GLN
1	Bk	20	ASN

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Mol	Chain	Res	Type
1	Bk	123	GLN
1	Bk	140	GLN
2	Bl	4	HIS
2	Bl	48	HIS
2	Bl	57	ASN
2	Bl	58	GLN
2	Bl	118	GLN
1	Bm	20	ASN
1	Bm	123	GLN
1	Bm	140	GLN
2	Bn	4	HIS
2	Bn	48	HIS
2	Bn	57	ASN
2	Bn	58	GLN
2	Bn	118	GLN
1	Bo	20	ASN
1	Bo	123	GLN
1	Bo	140	GLN
2	Bp	4	HIS
2	Bp	48	HIS
2	Bp	57	ASN
2	Bp	58	GLN
2	Bp	118	GLN
1	Bq	20	ASN
1	Bq	123	GLN
1	Bq	140	GLN
2	Br	4	HIS
2	Br	48	HIS
2	Br	57	ASN
2	Br	58	GLN
2	Br	118	GLN
1	Bs	20	ASN
1	Bs	123	GLN
1	Bs	140	GLN
2	Bt	4	HIS
2	Bt	48	HIS
2	Bt	57	ASN
2	Bt	58	GLN
2	Bt	118	GLN
1	Bu	20	ASN
1	Bu	123	GLN
1	Bu	140	GLN

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Mol	Chain	Res	Type
2	Bv	4	HIS
2	Bv	48	HIS
2	Bv	57	ASN
2	Bv	58	GLN
2	Bv	118	GLN
1	Bw	123	GLN
1	Bw	140	GLN
2	Bx	4	HIS
2	Bx	48	HIS
2	Bx	57	ASN
2	Bx	58	GLN
2	Bx	118	GLN
1	By	123	GLN
1	By	140	GLN
2	Bz	4	HIS
2	Bz	48	HIS
2	Bz	57	ASN
2	Bz	58	GLN
2	Bz	118	GLN
1	Ca	20	ASN
1	Ca	123	GLN
1	Ca	140	GLN
2	Cb	4	HIS
2	Cb	48	HIS
2	Cb	57	ASN
2	Cb	58	GLN
2	Cb	118	GLN
1	Cc	20	ASN
1	Cc	123	GLN
1	Cc	140	GLN
2	Cd	4	HIS
2	Cd	48	HIS
2	Cd	57	ASN
2	Cd	58	GLN
2	Cd	118	GLN
1	Ce	20	ASN
1	Ce	123	GLN
1	Ce	140	GLN
2	Cf	4	HIS
2	Cf	48	HIS
2	Cf	57	ASN
2	Cf	58	GLN

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Mol	Chain	Res	Type
2	Cf	118	GLN
1	Cg	20	ASN
1	Cg	123	GLN
1	Cg	140	GLN
2	Ch	4	HIS
2	Ch	48	HIS
2	Ch	57	ASN
2	Ch	58	GLN
2	Ch	118	GLN
1	Ci	20	ASN
1	Ci	123	GLN
1	Ci	140	GLN
2	Cj	4	HIS
2	Cj	48	HIS
2	Cj	57	ASN
2	Cj	118	GLN
1	Ck	20	ASN
1	Ck	123	GLN
2	Cl	4	HIS
2	Cl	48	HIS
2	Cl	57	ASN
2	Cl	58	GLN
2	Cl	118	GLN
1	Cm	20	ASN
1	Cm	123	GLN
1	Cm	140	GLN
2	Cn	4	HIS
2	Cn	48	HIS
2	Cn	57	ASN
2	Cn	58	GLN
2	Cn	118	GLN
1	Co	20	ASN
1	Co	123	GLN
1	Co	140	GLN
2	Cp	4	HIS
2	Cp	48	HIS
2	Cp	57	ASN
2	Cp	58	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

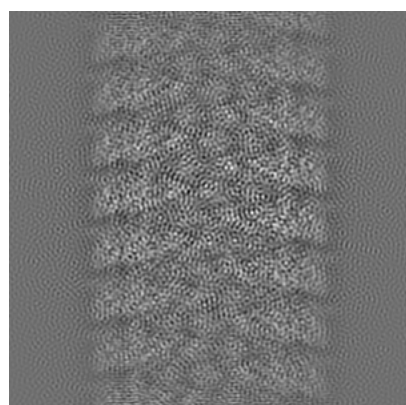
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6461. These allow visual inspection of the internal detail of the map and identification of artifacts.

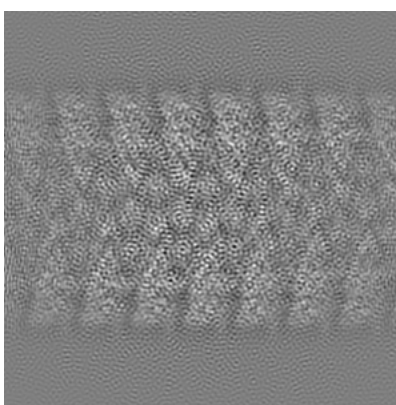
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

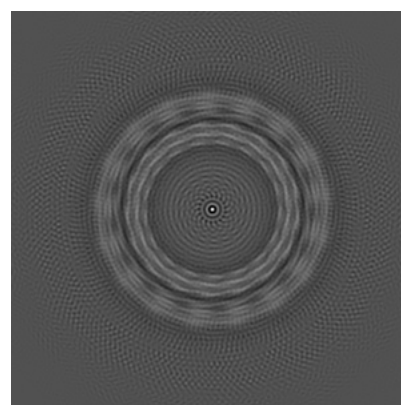
6.1.1 Primary map



X



Y

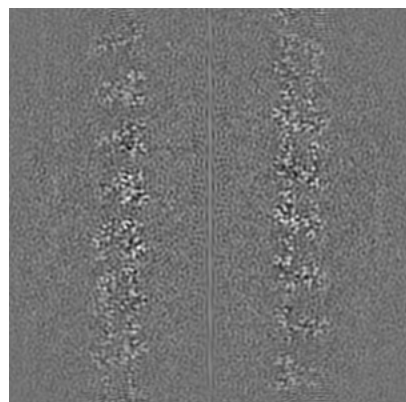


Z

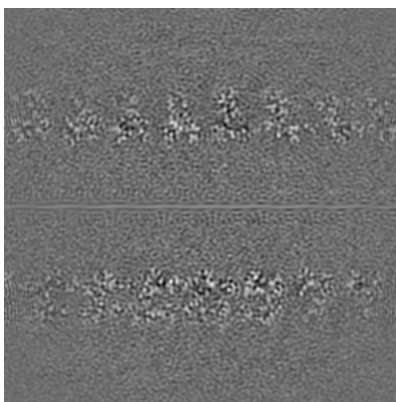
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

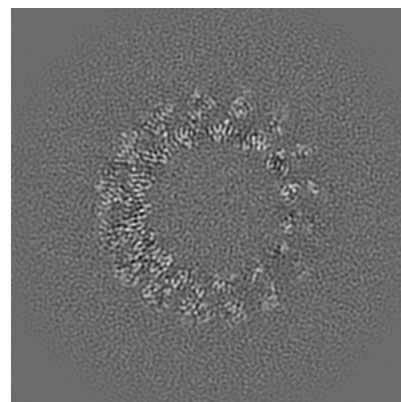
6.2.1 Primary map



X Index: 162



Y Index: 162

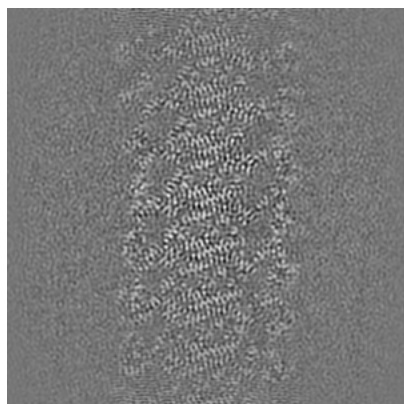


Z Index: 162

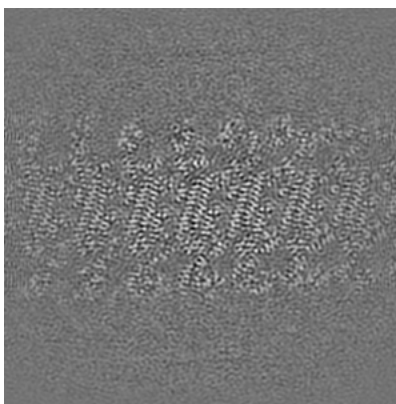
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

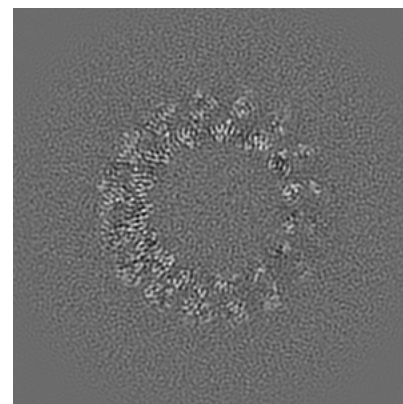
6.3.1 Primary map



X Index: 101



Y Index: 223

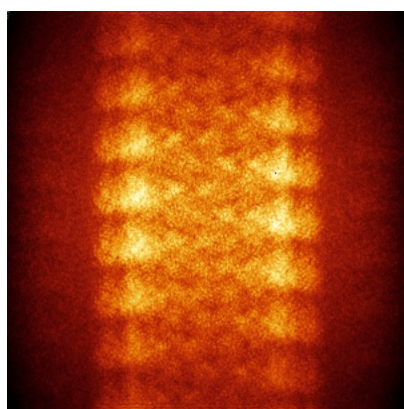


Z Index: 162

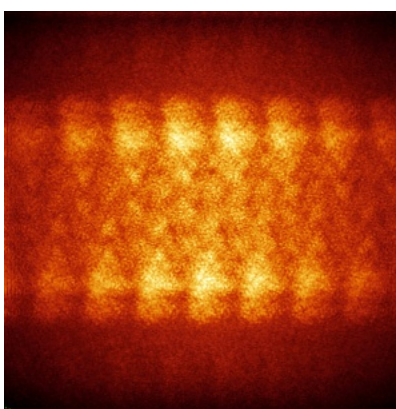
The images above show the largest variance slices of the map in three orthogonal directions.

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

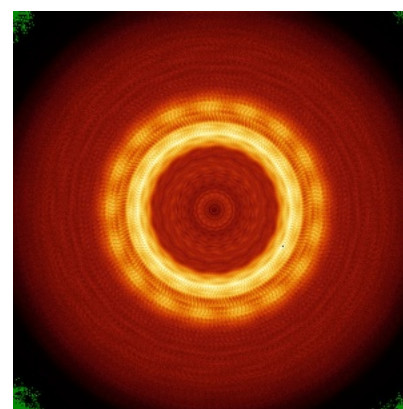
6.4.1 Primary map



X



Y

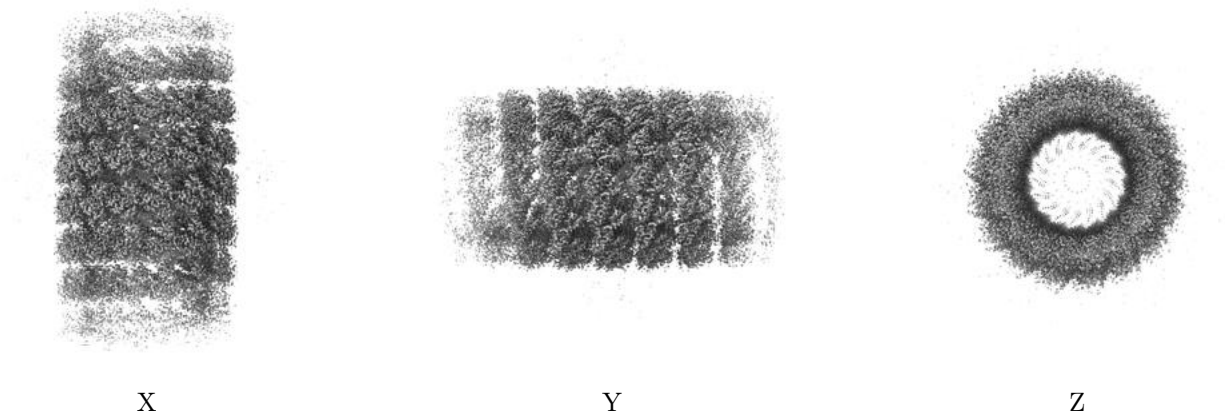


Z

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 12.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

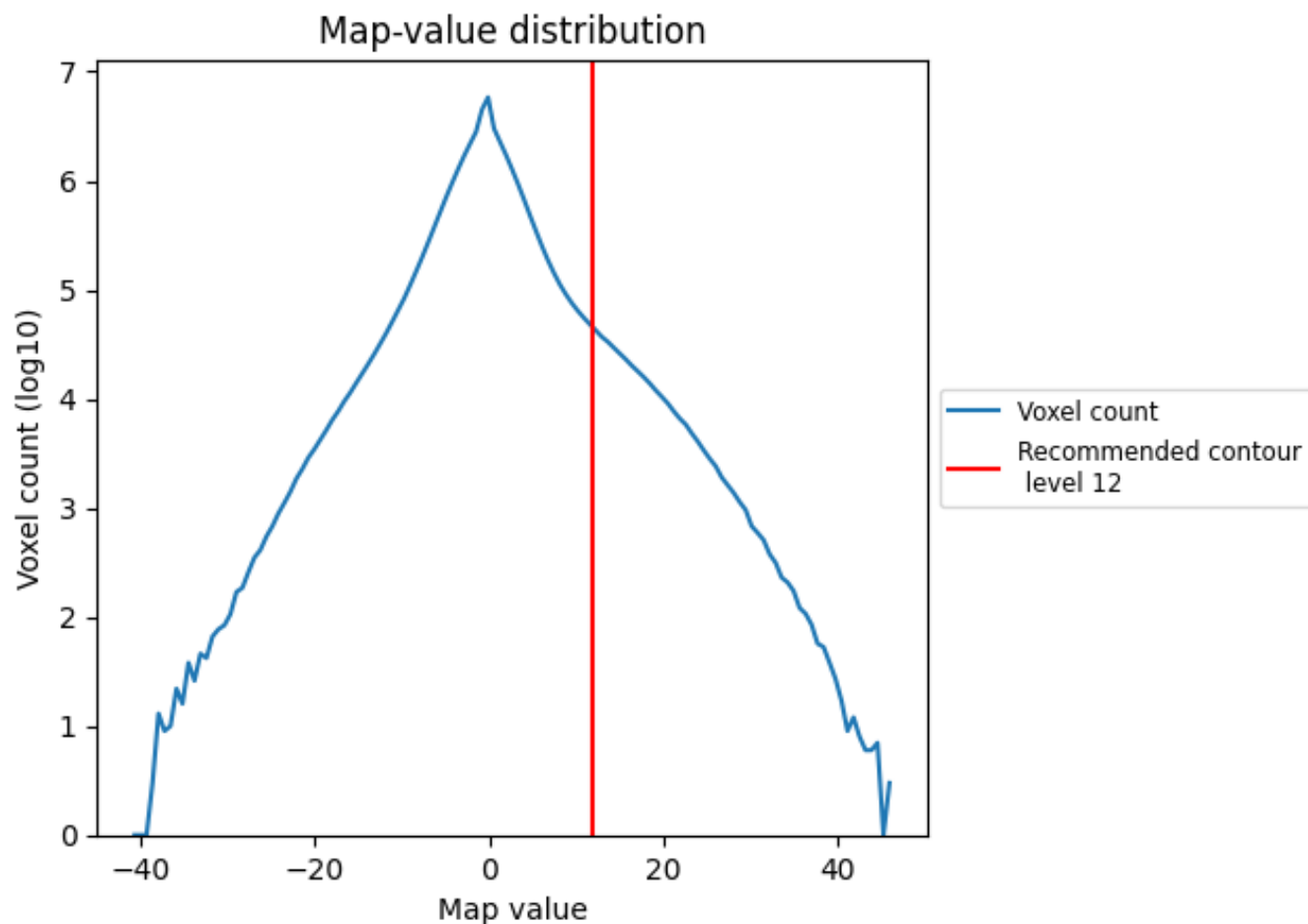
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

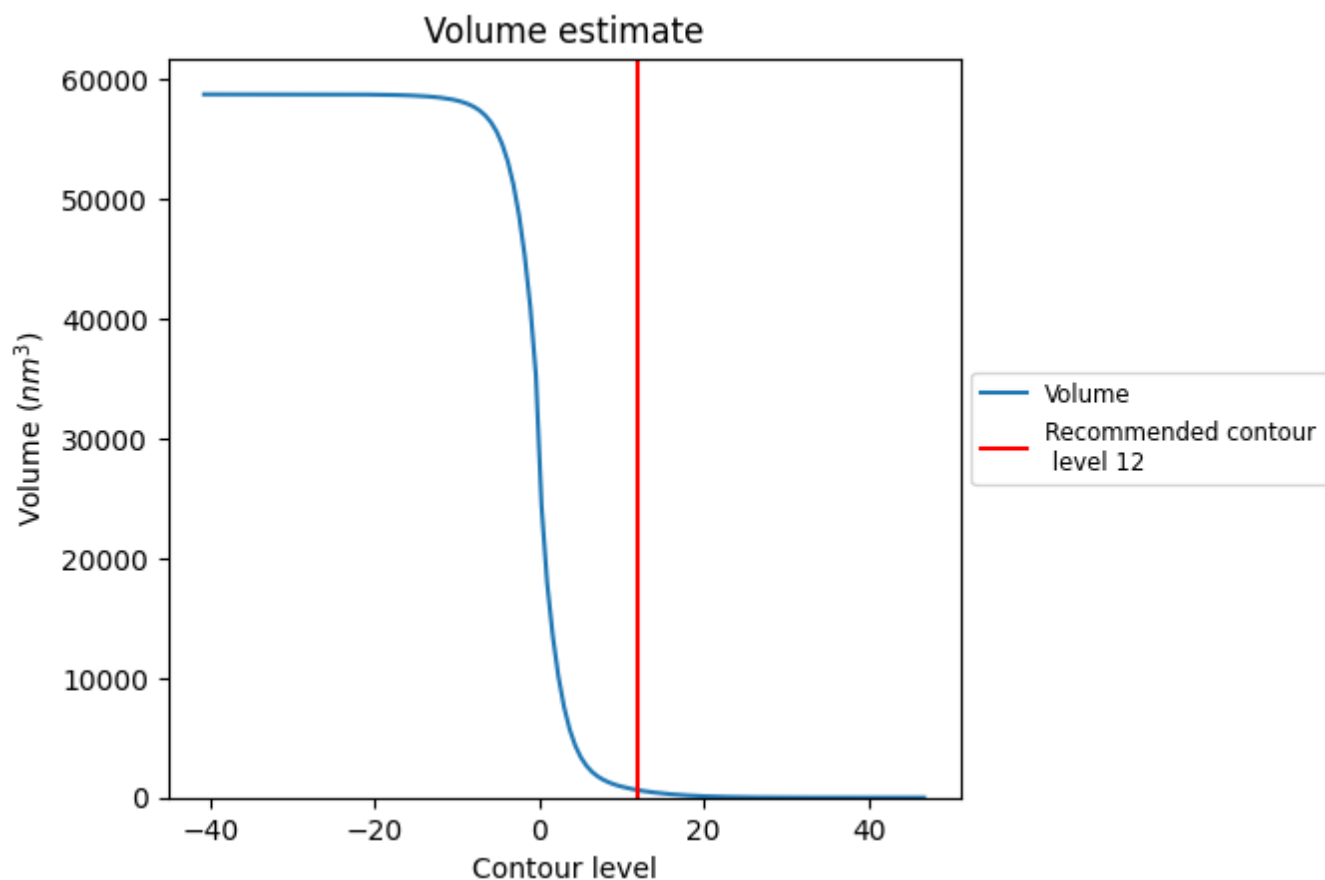
This section contains the results of statistical analysis of the map.

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.

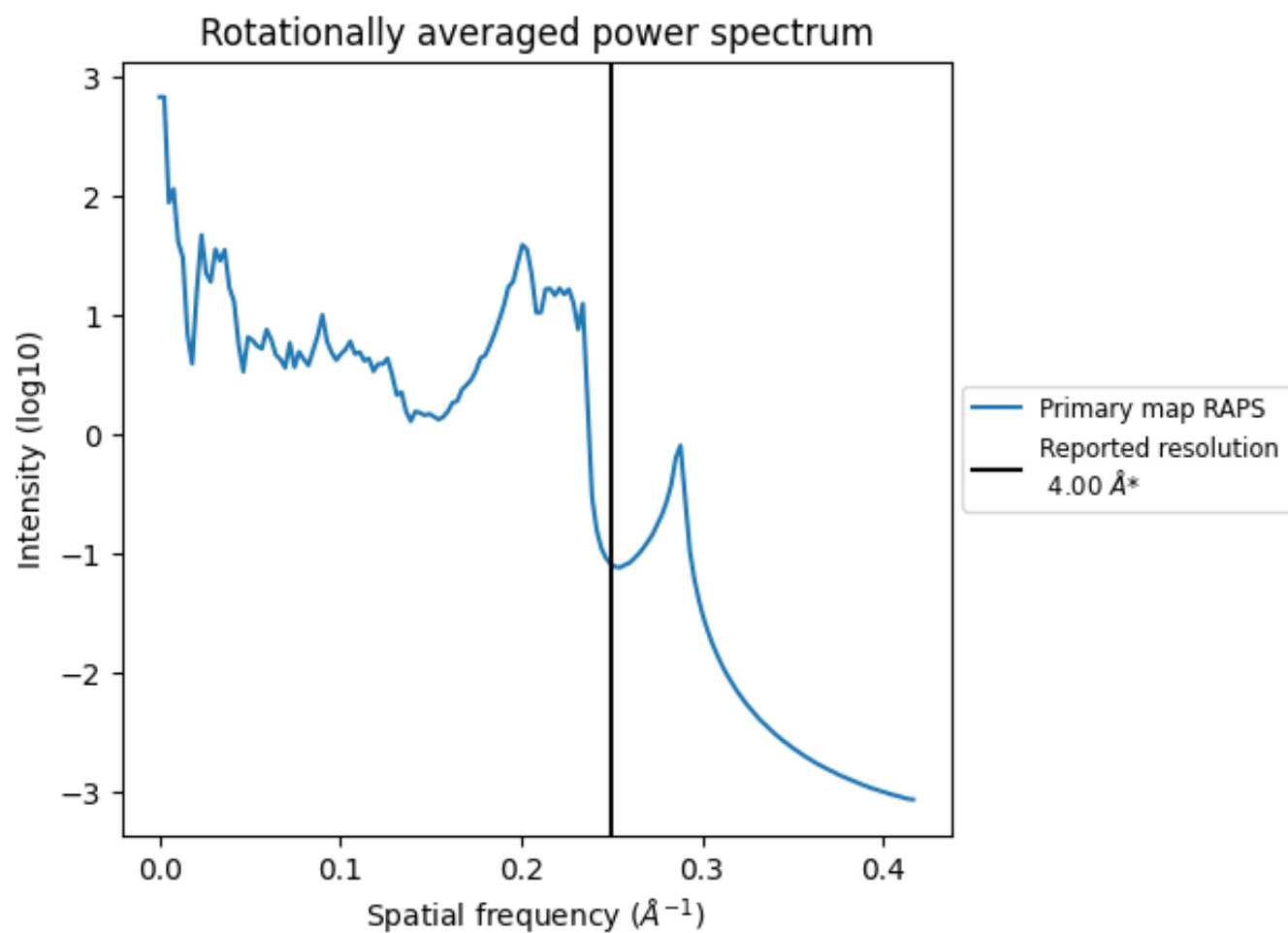
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 620 nm³; this corresponds to an approximate mass of 560 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 0.250 Å⁻¹

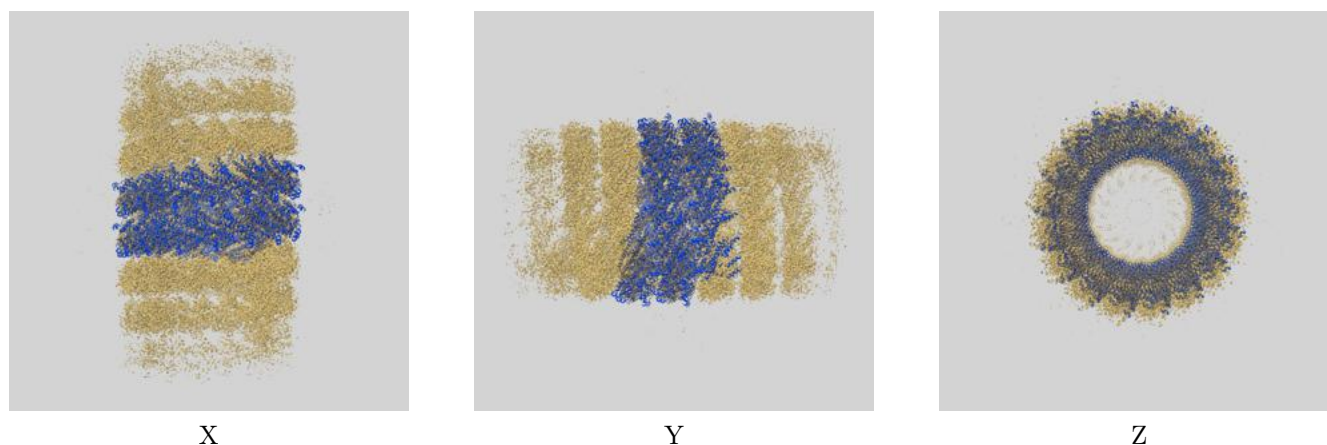
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

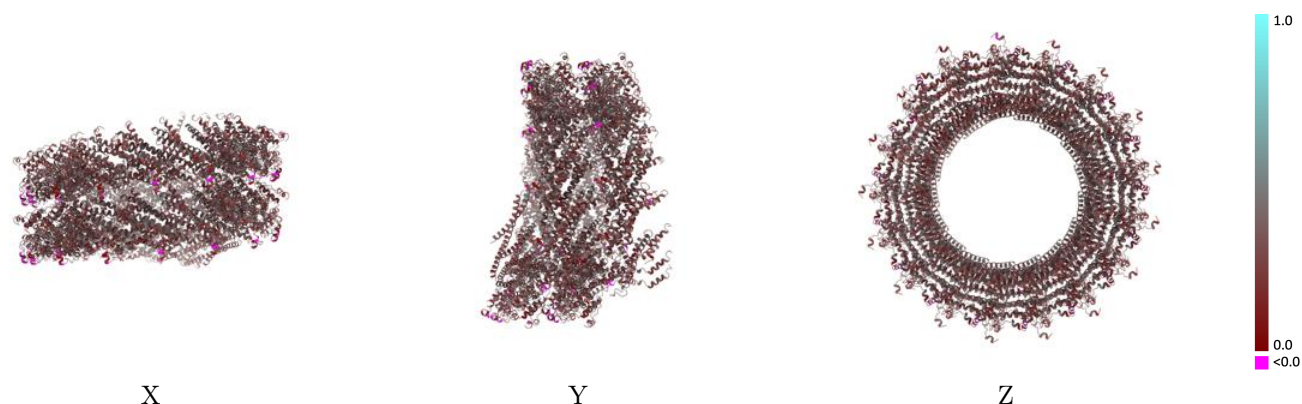
This section contains information regarding the fit between EMDB map EMD-6461 and PDB model 3JC1. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



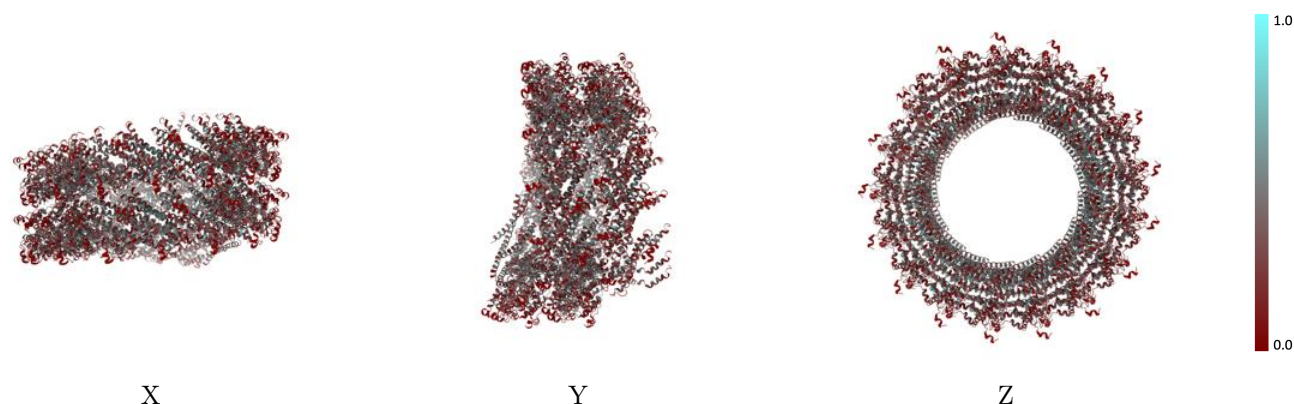
The images above show the 3D surface view of the map at the recommended contour level 12.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



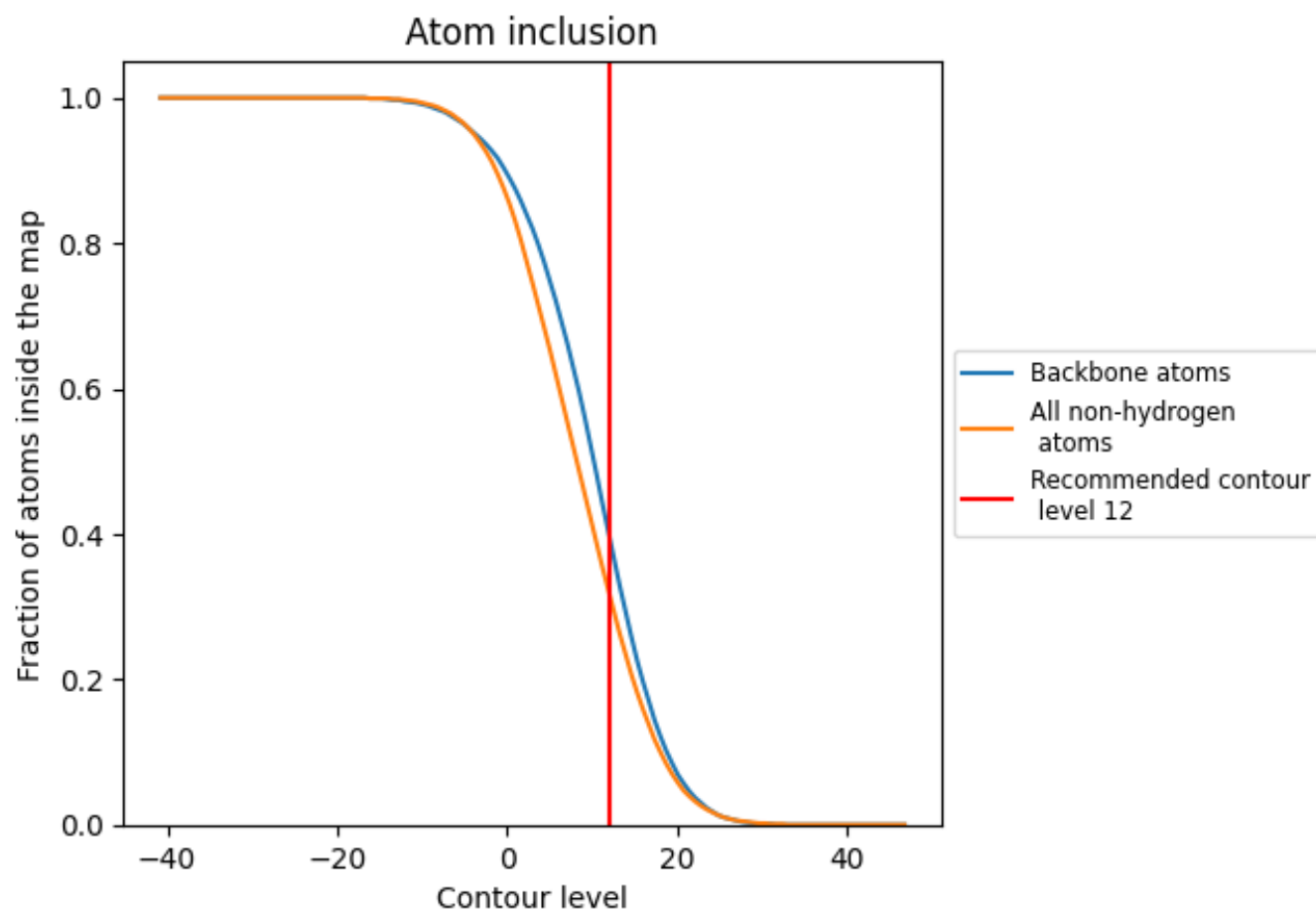
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 32% 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 (12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3190	 0.3140
Aa	 0.2550	 0.3020
Ab	 0.3880	 0.3260
Ac	 0.2580	 0.3070
Ad	 0.4090	 0.3390
Ae	 0.2680	 0.3150
Af	 0.4320	 0.3530
Ag	 0.2670	 0.3160
Ah	 0.4310	 0.3470
Ai	 0.2650	 0.3150
Aj	 0.4280	 0.3410
Ak	 0.2670	 0.3120
Al	 0.4150	 0.3290
Am	 0.2620	 0.3090
An	 0.3960	 0.3220
Ao	 0.2570	 0.3020
Ap	 0.3830	 0.3160
Aq	 0.2480	 0.3050
Ar	 0.3860	 0.3200
As	 0.2580	 0.3070
At	 0.3960	 0.3270
Au	 0.2540	 0.3110
Av	 0.3940	 0.3320
Aw	 0.2490	 0.3100
Ax	 0.3880	 0.3300
Ay	 0.2430	 0.3050
Az	 0.3700	 0.3250
Ba	 0.2240	 0.2940
Bb	 0.3600	 0.3100
Bc	 0.2130	 0.2860
Bd	 0.3410	 0.3020
Be	 0.2060	 0.2830
Bf	 0.3400	 0.3020
Bg	 0.2540	 0.2940
Bh	 0.3610	 0.3130



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Chain	Atom inclusion	Q-score
Bi	 0.2340	 0.3000
Bj	 0.3540	 0.3180
Bk	 0.2320	 0.3080
Bl	 0.3800	 0.3370
Bm	 0.2530	 0.3120
Bn	 0.4050	 0.3480
Bo	 0.2500	 0.3140
Bp	 0.4180	 0.3470
Bq	 0.2620	 0.3100
Br	 0.4220	 0.3380
Bs	 0.2610	 0.3070
Bt	 0.4040	 0.3260
Bu	 0.2510	 0.3070
Bv	 0.3980	 0.3200
Bw	 0.2620	 0.3050
Bx	 0.3940	 0.3160
By	 0.2770	 0.3100
Bz	 0.3990	 0.3230
Ca	 0.2840	 0.3110
Cb	 0.4220	 0.3300
Cc	 0.2770	 0.3150
Cd	 0.4240	 0.3350
Ce	 0.2920	 0.3120
Cf	 0.4110	 0.3330
Cg	 0.2820	 0.3060
Ch	 0.4050	 0.3260
Ci	 0.2600	 0.2990
Cj	 0.3920	 0.3120
Ck	 0.2550	 0.2880
Cl	 0.3790	 0.3020
Cm	 0.2600	 0.2880
Cn	 0.3750	 0.3030
Co	 0.2300	 0.2940
Cp	 0.3440	 0.3090