



## Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 02:17 AM EST

PDB ID : 5UZ9  
EMDB ID : EMD-8624  
Title : Cryo EM structure of anti-CRISPRs, AcrF1 and AcrF2, bound to type I-F crRNA-guided CRISPR surveillance complex  
Authors : Chowdhury, S.; Carter, J.; Rollins, M.F.; Jackson, R.N.; Hoffmann, C.; Nosaka, L.; Bondy-Denomy, J.; Maxwell, K.L.; Davidson, A.R.; Fischer, E.R.; Lander, G.C.; Wiedenheft, B.  
Deposited on : 2017-02-25  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

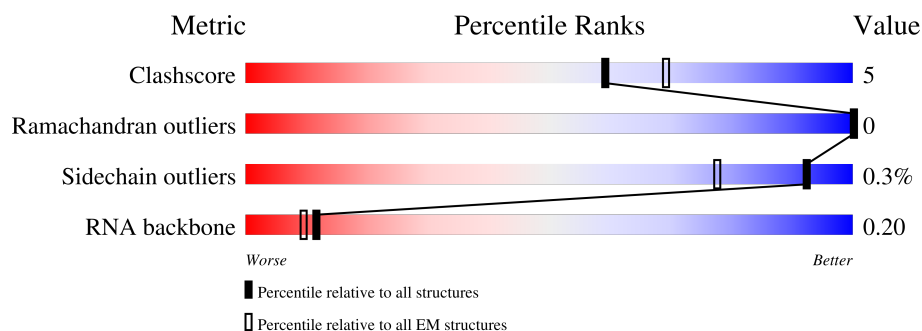
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1-A	434	<div> <div>51%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	2-A	434	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	3-A	434	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	4-A	434	<div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	5-A	434	<div> <div>84%</div> <div>14%</div> <div>.</div> </div>
2	1-B	327	<div> <div>14%</div> <div>76%</div> <div>17%</div> <div>7%</div> </div>
2	2-B	327	<div> <div>74%</div> <div>19%</div> <div>7%</div> </div>









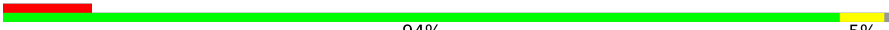


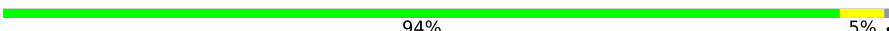




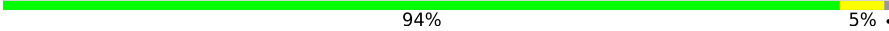








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Mol	Chain	Length	Quality of chain
2	3-B	327	
2	4-B	327	
2	5-B	327	
3	1-C	341	
3	1-D	341	
3	1-E	341	
3	1-F	341	
3	1-G	341	
3	1-H	341	
3	2-C	341	
3	2-D	341	
3	2-E	341	
3	2-F	341	
3	2-G	341	
3	2-H	341	
3	3-C	341	
3	3-D	341	
3	3-E	341	
3	3-F	341	
3	3-G	341	
3	3-H	341	
3	4-C	341	
3	4-D	341	
3	4-E	341	
3	4-F	341	

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Mol	Chain	Length	Quality of chain
3	4-G	341	 86% 11% .
3	4-H	341	 84% 13% .
3	5-C	341	 75% 11% 14%
3	5-D	341	 84% 13% ..
3	5-E	341	 84% 13% ..
3	5-F	341	 85% 12% ..
3	5-G	341	 84% 13% ..
3	5-H	341	 85% 12% ..
4	1-I	77	 10% 94% 5% .
4	1-J	77	 9% 92% 6% .
4	2-I	77	 91% 8% .
4	2-J	77	 94% 5% .
4	3-I	77	 91% 8% .
4	3-J	77	 90% 9% .
4	4-I	77	 91% 8% .
4	4-J	77	 90% 9% .
4	5-I	77	 94% 5% .
4	5-J	77	 94% 5% .
5	1-K	96	 51% 81% 10% 8%
5	2-K	96	 79% 12% 8%
5	3-K	96	 80% 11% 8%
5	4-K	96	 82% 9% 8%
5	5-K	96	 79% 12% 8%
6	1-L	189	 90% 99% .
6	2-L	189	 99% .

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Mol	Chain	Length	Quality of chain
6	3-L	189	 98% .
6	4-L	189	 99% .
6	5-L	189	 99% .
7	1-M	60	 32% 37% 45% 18%
7	2-M	60	 43% 45% 12%
7	3-M	60	 33% 48% 18%
7	4-M	60	 30% 53% 17%
7	5-M	60	 37% 37% 25% .

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 121825 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 CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	424	Total	C	N	O	S	0	0
			3011	1879	574	555	3		
1	2-A	424	Total	C	N	O	S	0	0
			3011	1879	574	555	3		
1	3-A	424	Total	C	N	O	S	0	0
			3011	1879	574	555	3		
1	4-A	424	Total	C	N	O	S	0	0
			3011	1879	574	555	3		
1	5-A	424	Total	C	N	O	S	0	0
			3011	1879	574	555	3		

- Molecule 2 is a protein called CRISPR-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-B	305	Total	C	N	O	S	0	0
			2374	1504	440	425	5		
2	2-B	305	Total	C	N	O	S	0	0
			2374	1504	440	425	5		
2	3-B	305	Total	C	N	O	S	0	0
			2374	1504	440	425	5		
2	4-B	305	Total	C	N	O	S	0	0
			2374	1504	440	425	5		
2	5-B	305	Total	C	N	O	S	0	0
			2374	1504	440	425	5		

- Molecule 3 is a protein called CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-C	293	Total	C	N	O	S	0	0
			2272	1430	409	431	2		
3	2-C	293	Total	C	N	O	S	0	0
			2272	1430	409	431	2		
3	3-C	293	Total	C	N	O	S	0	0
			2272	1430	409	431	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	4-C	293	Total	C	N	O	S	0	0
			2272	1430	409	431	2		
3	5-C	293	Total	C	N	O	S	0	0
			2272	1430	409	431	2		
3	1-D	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	2-D	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	3-D	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	4-D	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	5-D	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	1-E	334	Total	C	N	O	S	0	0
			2561	1611	466	482	2		
3	2-E	334	Total	C	N	O	S	0	0
			2561	1611	466	482	2		
3	3-E	334	Total	C	N	O	S	0	0
			2561	1611	466	482	2		
3	4-E	334	Total	C	N	O	S	0	0
			2561	1611	466	482	2		
3	5-E	334	Total	C	N	O	S	0	0
			2561	1611	466	482	2		
3	1-F	335	Total	C	N	O	S	0	0
			2566	1614	467	483	2		
3	2-F	335	Total	C	N	O	S	0	0
			2566	1614	467	483	2		
3	3-F	335	Total	C	N	O	S	0	0
			2566	1614	467	483	2		
3	4-F	335	Total	C	N	O	S	0	0
			2566	1614	467	483	2		
3	5-F	335	Total	C	N	O	S	0	0
			2566	1614	467	483	2		
3	1-G	333	Total	C	N	O	S	0	0
			2557	1608	466	481	2		
3	2-G	333	Total	C	N	O	S	0	0
			2557	1608	466	481	2		
3	3-G	333	Total	C	N	O	S	0	0
			2557	1608	466	481	2		
3	4-G	333	Total	C	N	O	S	0	0
			2557	1608	466	481	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	5-G	333	Total	C	N	O	S	0	0
			2557	1608	466	481	2		
3	1-H	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	2-H	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	3-H	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	4-H	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		
3	5-H	333	Total	C	N	O	S	0	0
			2554	1603	466	483	2		

- Molecule 4 is a protein called Anti-CRISPR protein Acr30-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-I	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	2-I	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	3-I	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	4-I	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	5-I	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	1-J	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	2-J	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	3-J	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	4-J	76	Total	C	N	O	S	0	0
			604	378	108	116	2		
4	5-J	76	Total	C	N	O	S	0	0
			604	378	108	116	2		

- Molecule 5 is a protein called Anti-CRISPR protein 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1-K	88	Total	C	N	O	S	0	0
			680	417	112	149	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	2-K	88	Total	C	N	O	S	0	0
			680	417	112	149	2		
5	3-K	88	Total	C	N	O	S	0	0
			680	417	112	149	2		
5	4-K	88	Total	C	N	O	S	0	0
			680	417	112	149	2		
5	5-K	88	Total	C	N	O	S	0	0
			680	417	112	149	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	MET	-	expression tag	UNP Q6TM72
K	2	HIS	-	expression tag	UNP Q6TM72
K	3	HIS	-	expression tag	UNP Q6TM72
K	4	HIS	-	expression tag	UNP Q6TM72
K	5	HIS	-	expression tag	UNP Q6TM72
K	6	HIS	-	expression tag	UNP Q6TM72
K	7	HIS	-	expression tag	UNP Q6TM72

- Molecule 6 is a protein called CRISPR-associated endonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	1-L	189	Total	C	N	O	1	0
			757	379	189	189		
6	2-L	189	Total	C	N	O	1	0
			757	379	189	189		
6	3-L	189	Total	C	N	O	1	0
			757	379	189	189		
6	4-L	189	Total	C	N	O	1	0
			757	379	189	189		
6	5-L	189	Total	C	N	O	1	0
			757	379	189	189		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	PHE	-	expression tag	UNP Q02MM2
L	0	THR	-	expression tag	UNP Q02MM2
L	22	CYS	SER	see remark 999	UNP Q02MM2

- Molecule 7 is a RNA chain called CRISPR RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1-M	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		
7	2-M	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		
7	3-M	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		
7	4-M	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		
7	5-M	60	Total	C	N	O	P	0	0
			1271	569	223	420	59		

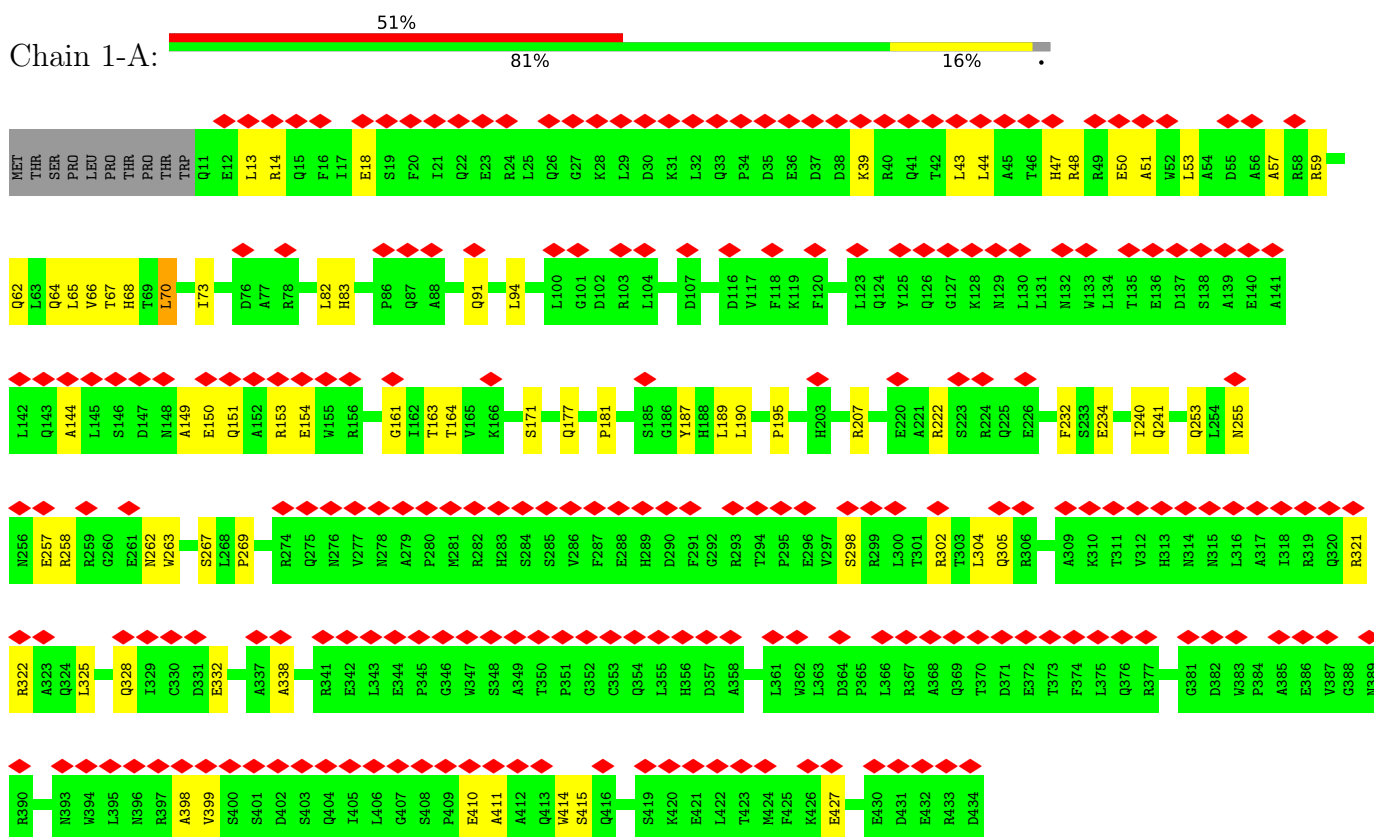
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	53	A	G	see remark 999	GB 115583796

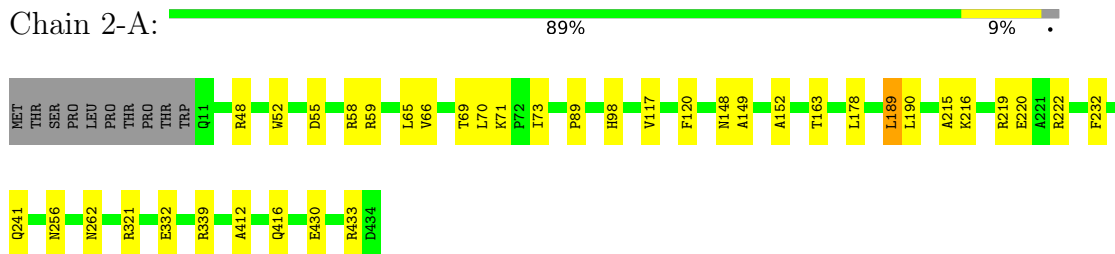
### 3 Residue-property plots

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


#### • Molecule 1: CRISPR-associated protein Csy1

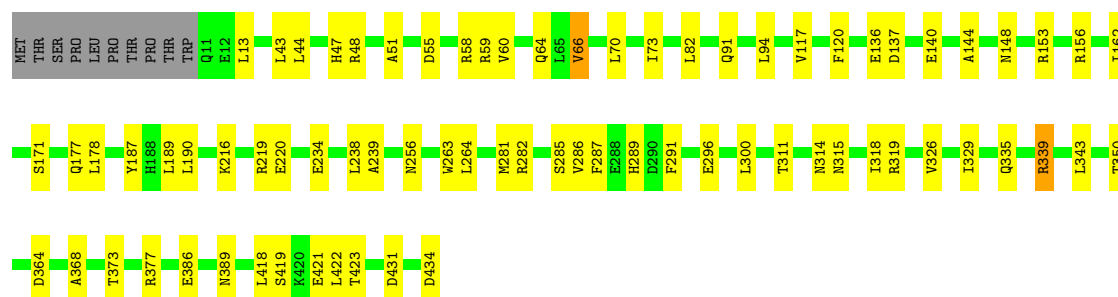


#### • Molecule 1: CRISPR-associated protein Csy1




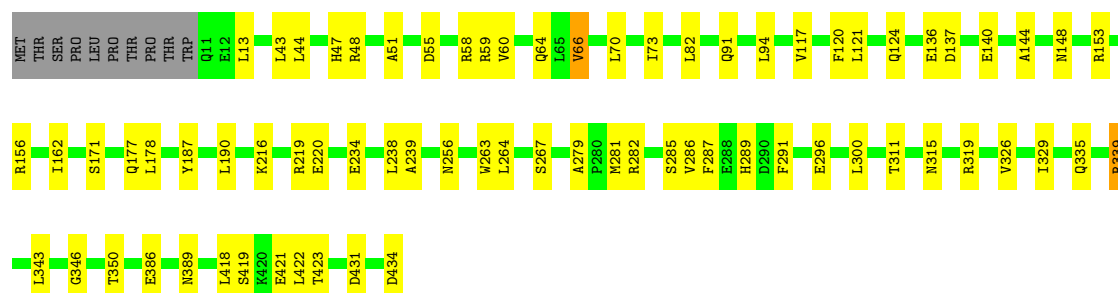
#### • Molecule 1: CRISPR-associated protein Csy1

Chain 3-A:  80% 17% .




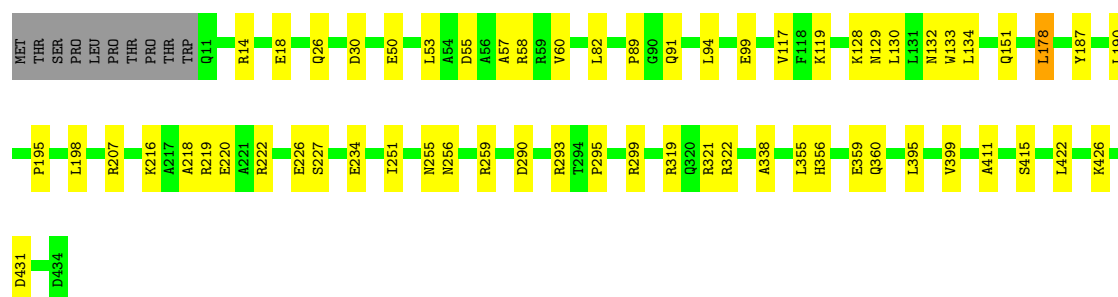
• Molecule 1: CRISPR-associated protein Csy1

Chain 4-A:  81% 16% .




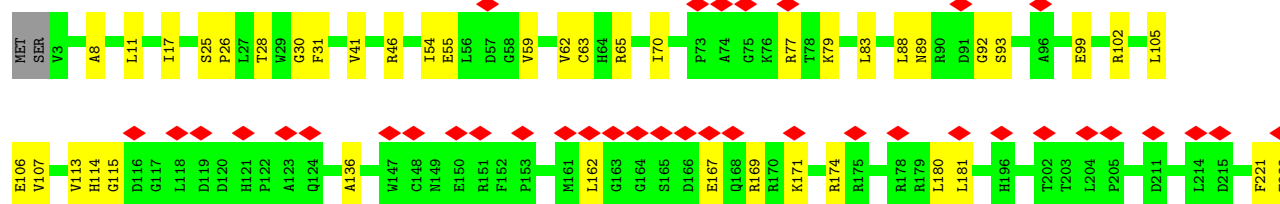
• Molecule 1: CRISPR-associated protein Csy1

Chain 5-A:  84% 14% .

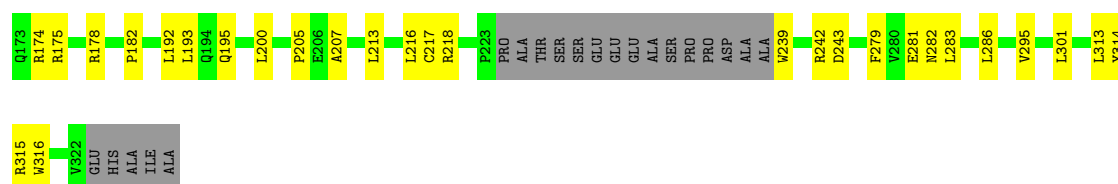


• Molecule 2: CRISPR-associated protein Csy2

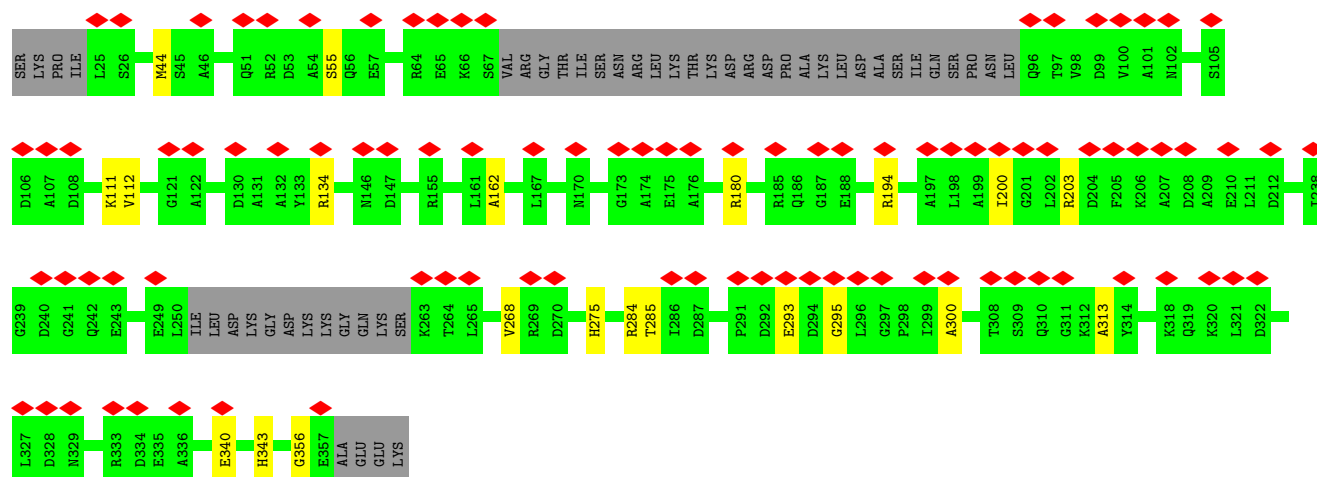
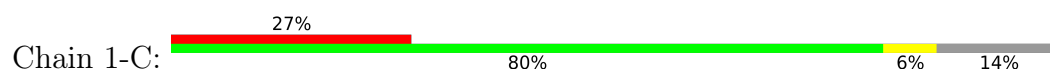
Chain 1-B:  14% 76% 17% 7% .



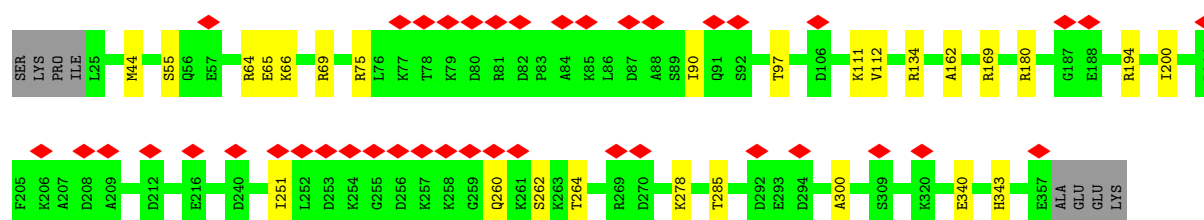
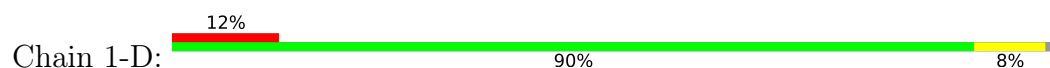




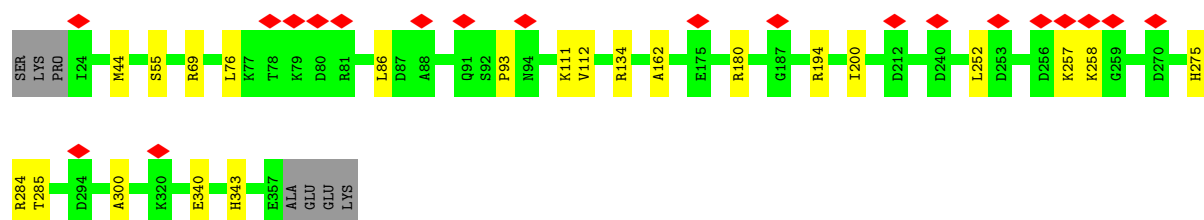
• Molecule 3: CRISPR-associated protein Csy3



• Molecule 3: CRISPR-associated protein Csy3

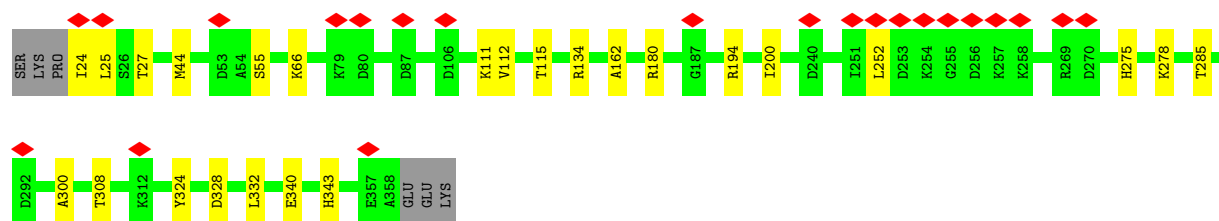


• Molecule 3: CRISPR-associated protein Csy3

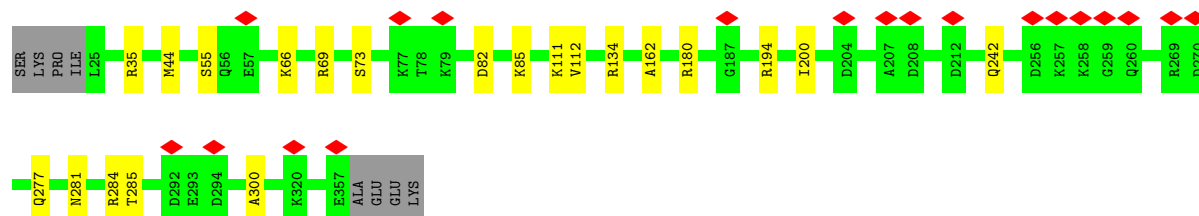


• Molecule 3: CRISPR-associated protein Csy3

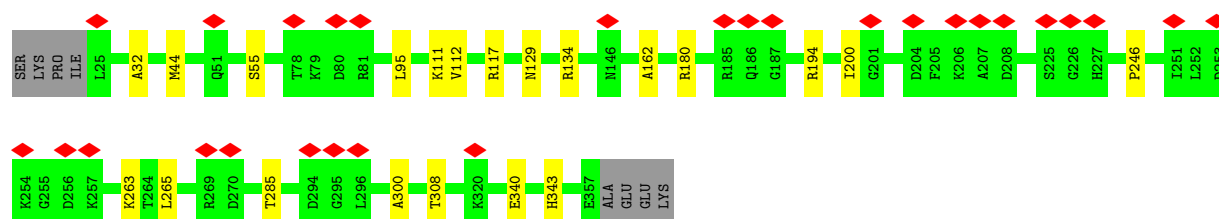




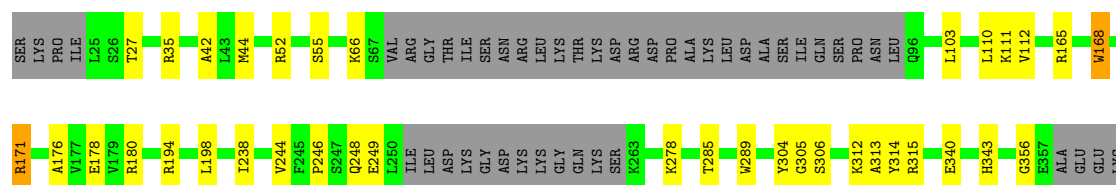
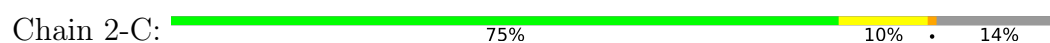
• Molecule 3: CRISPR-associated protein Csy3



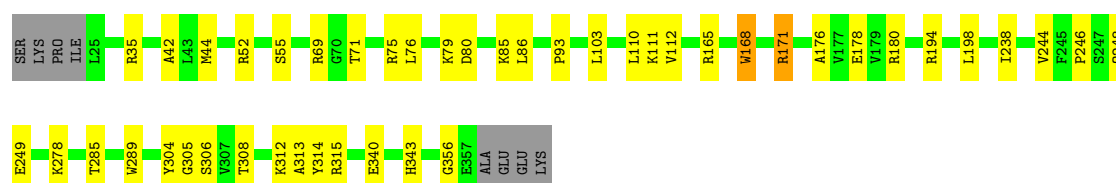
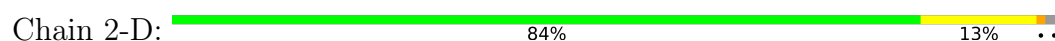
• Molecule 3: CRISPR-associated protein Csy3



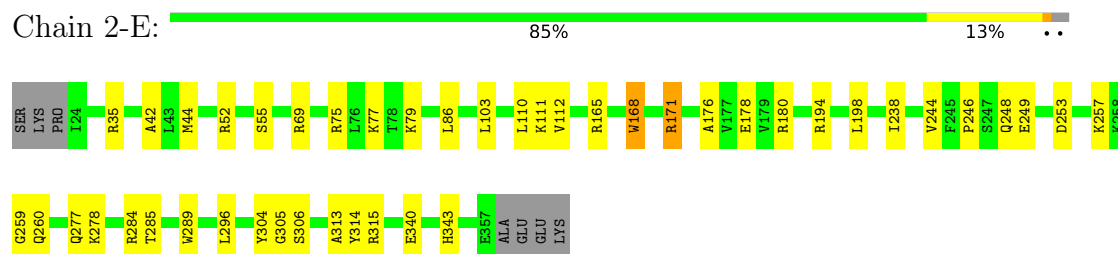
• Molecule 3: CRISPR-associated protein Csy3



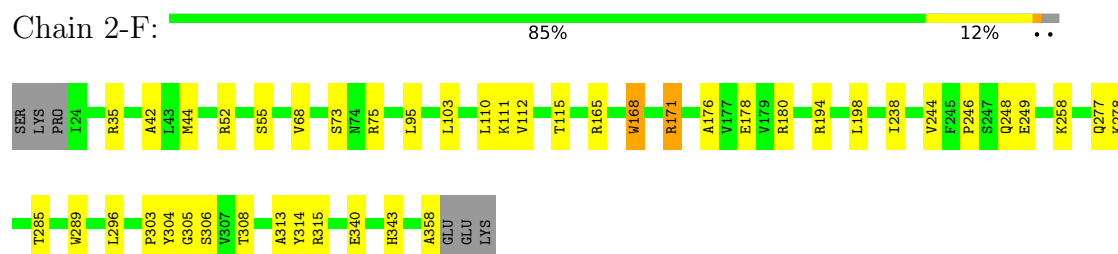
• Molecule 3: CRISPR-associated protein Csy3



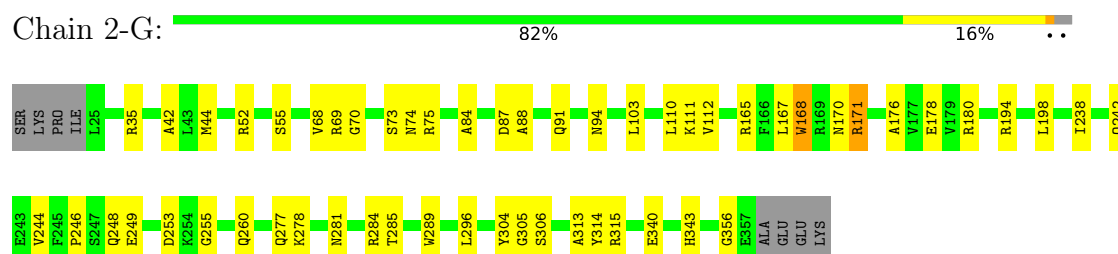
- Molecule 3: CRISPR-associated protein Csy3



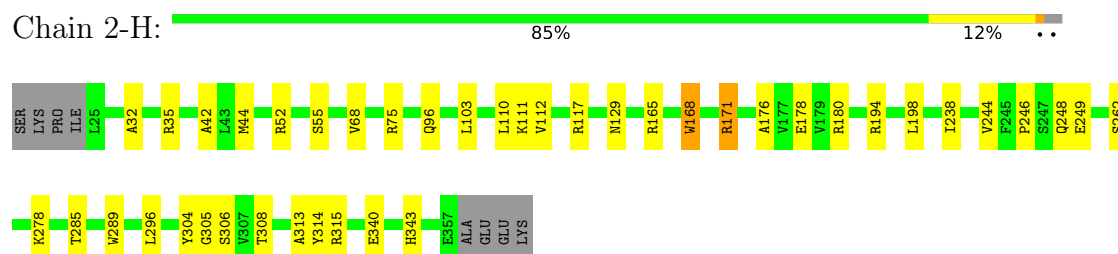
- Molecule 3: CRISPR-associated protein Csy3



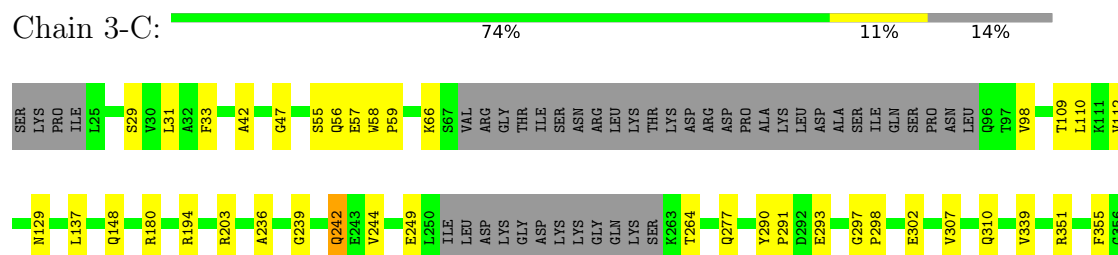
- Molecule 3: CRISPR-associated protein Csy3



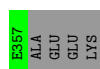
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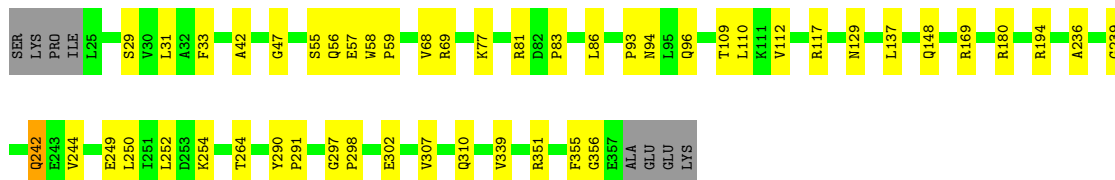






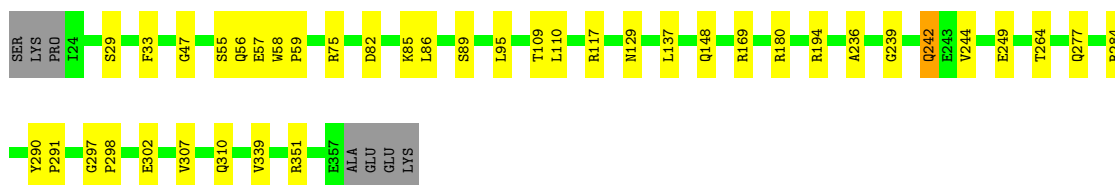
• Molecule 3: CRISPR-associated protein Csy3

Chain 3-D:  83% 14% .



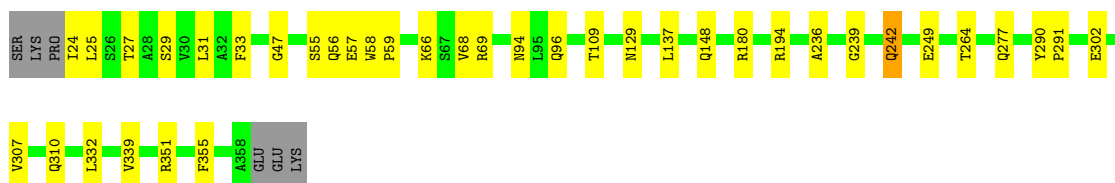
• Molecule 3: CRISPR-associated protein Csy3

Chain 3-E:  86% 11% .




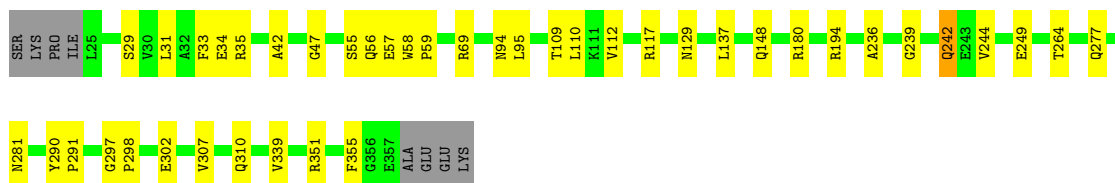
• Molecule 3: CRISPR-associated protein Csy3

Chain 3-F:  87% 11% .




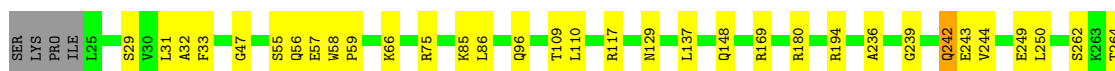
• Molecule 3: CRISPR-associated protein Csy3

Chain 3-G:  85% 12% .



• Molecule 3: CRISPR-associated protein Csy3

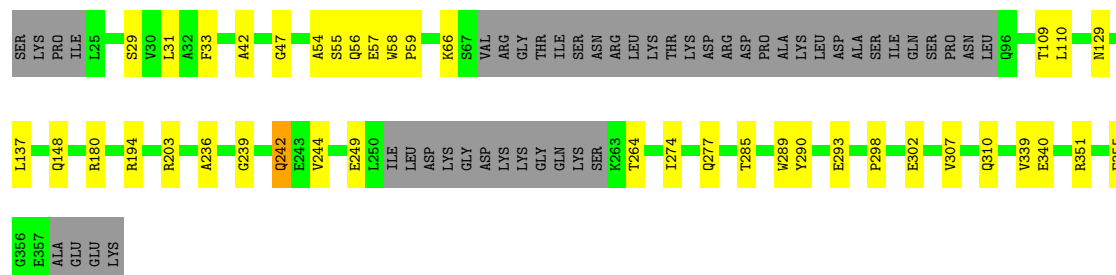
Chain 3-H:  85% 12% .





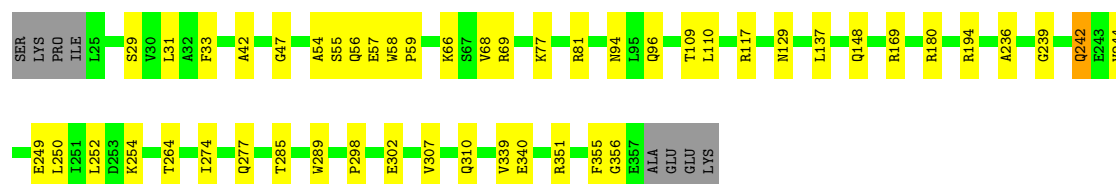
• Molecule 3: CRISPR-associated protein Csy3

Chain 4-C: 74% 11% 14%



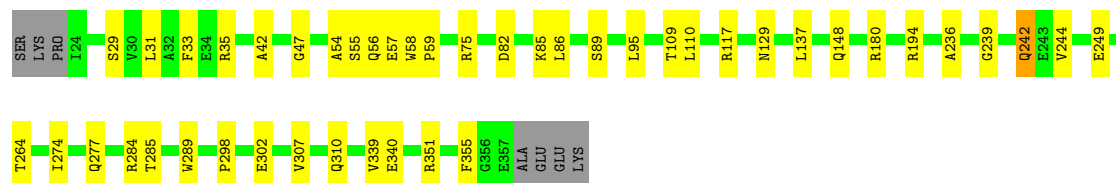
• Molecule 3: CRISPR-associated protein Csy3

Chain 4-D: 83% 14% .



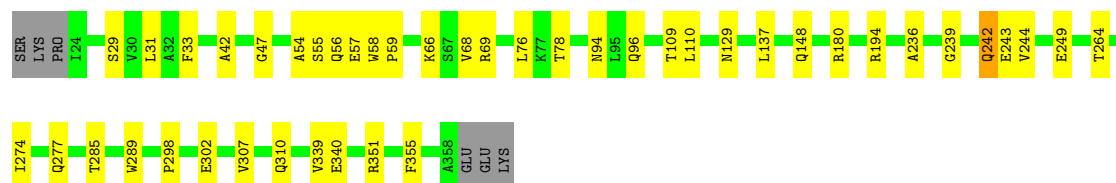
• Molecule 3: CRISPR-associated protein Csy3

Chain 4-E: 85% 13% .



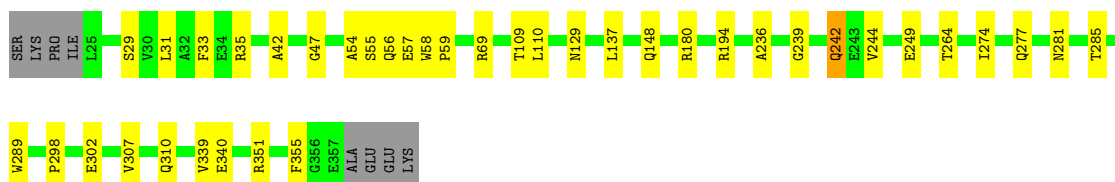
• Molecule 3: CRISPR-associated protein Csy3

Chain 4-F: 85% 13% .



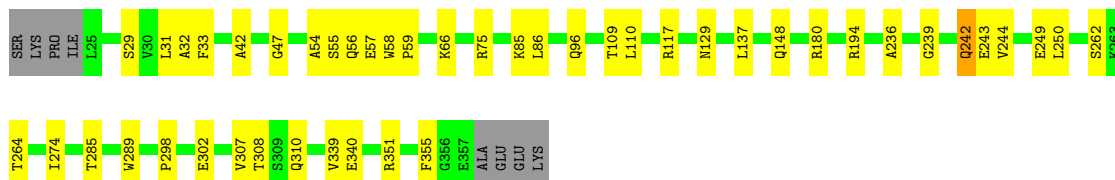
• Molecule 3: CRISPR-associated protein Csy3

Chain 4-G: 86% 11% .



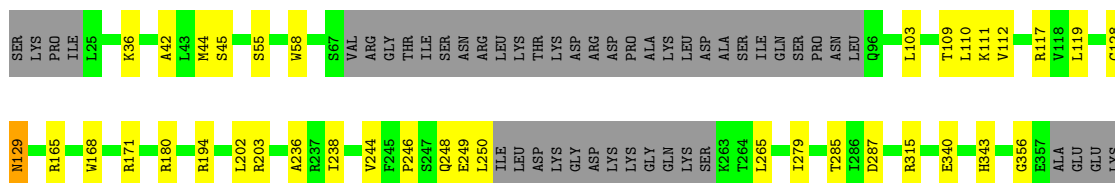
• Molecule 3: CRISPR-associated protein Csy3

Chain 4-H: 84% 13% •



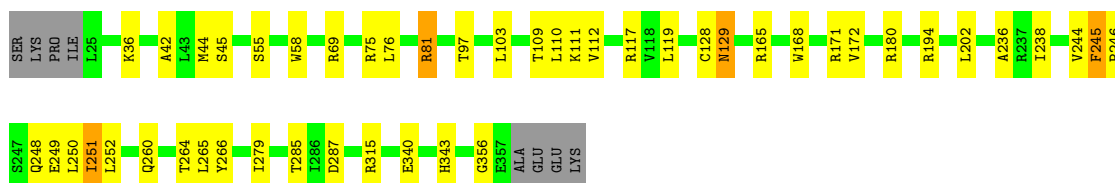
• Molecule 3: CRISPR-associated protein Csy3

Chain 5-C: 75% 11% 14%



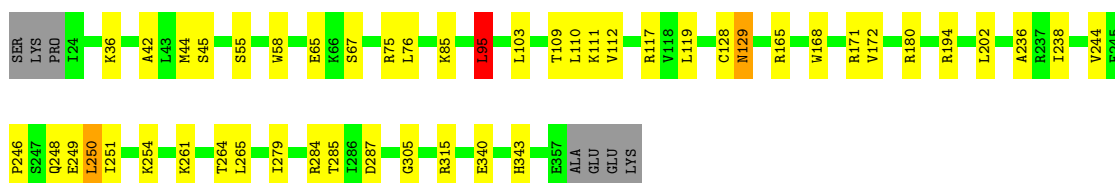
• Molecule 3: CRISPR-associated protein Csy3

Chain 5-D: 84% 13% ••



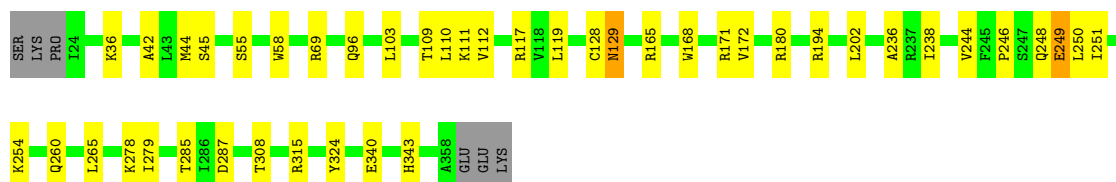
• Molecule 3: CRISPR-associated protein Csy3

Chain 5-E: 84% 13% ••



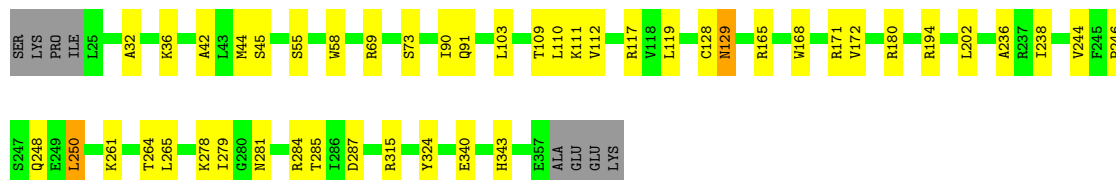
• Molecule 3: CRISPR-associated protein Csy3

Chain 5-F: 85% 12% ••



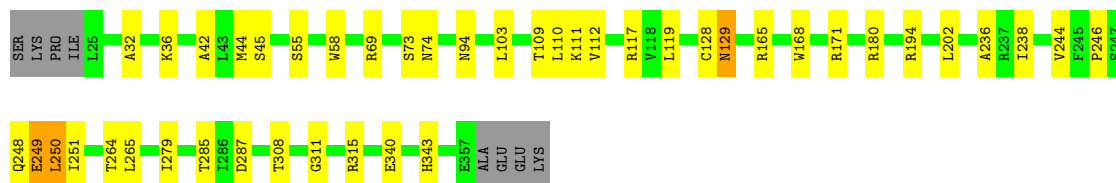
- Molecule 3: CRISPR-associated protein Csy3

Chain 5-G: 84% 13% ..



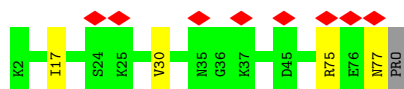
- Molecule 3: CRISPR-associated protein Csy3

Chain 5-H: 85% 12% ..



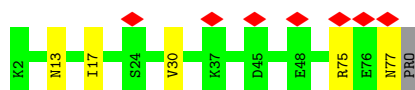
- Molecule 4: Anti-CRISPR protein Acr30-35

Chain 1-I: 10% 94% 5% •



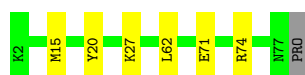
- Molecule 4: Anti-CRISPR protein Acr30-35

Chain 1-J: 9% 92% 6% •



- Molecule 4: Anti-CRISPR protein Acr30-35

Chain 2-I: 91% 8% •



- Molecule 4: Anti-CRISPR protein Acr30-35

Chain 2-J:  94% 5%



• Molecule 4: Anti-CRISPR protein Acr30-35

Chain 3-I:  91% 8%



• Molecule 4: Anti-CRISPR protein Acr30-35

Chain 3-J:  90% 9%



• Molecule 4: Anti-CRISPR protein Acr30-35

Chain 4-I:  91% 8%



• Molecule 4: Anti-CRISPR protein Acr30-35

Chain 4-J:  90% 9%



• Molecule 4: Anti-CRISPR protein Acr30-35

Chain 5-I:  94% 5%

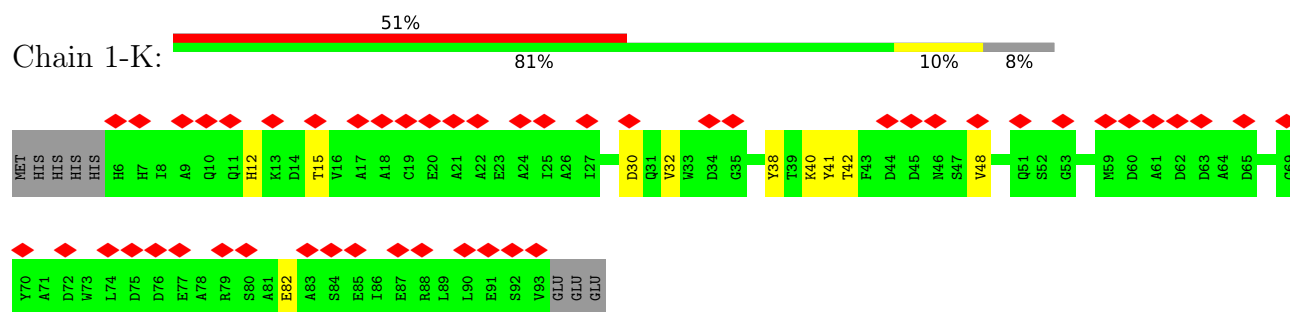


• Molecule 4: Anti-CRISPR protein Acr30-35

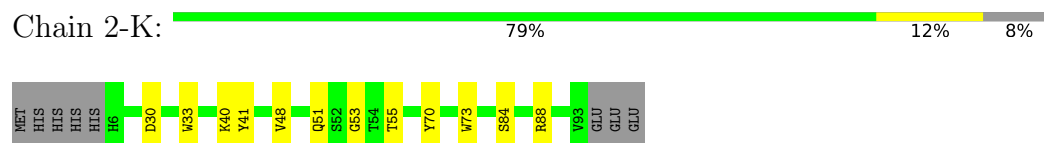
Chain 5-J:  94% 5%



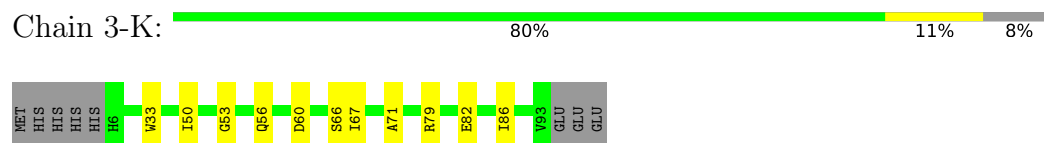
• Molecule 5: Anti-CRISPR protein 30



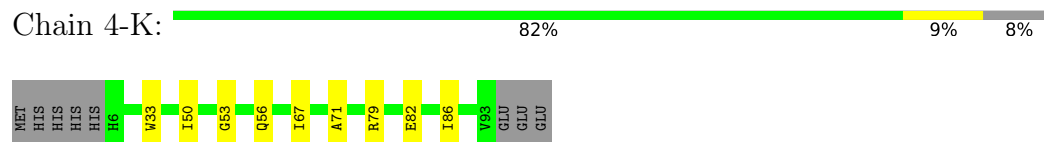
- Molecule 5: Anti-CRISPR protein 30



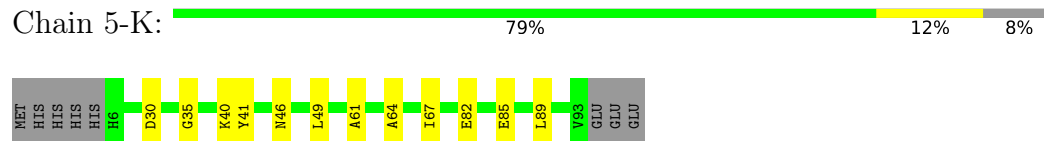
- Molecule 5: Anti-CRISPR protein 30



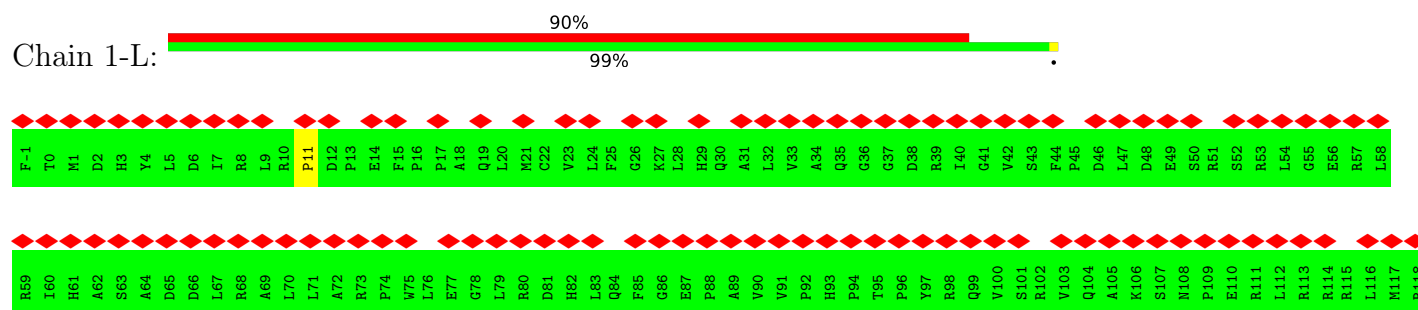
- Molecule 5: Anti-CRISPR protein 30

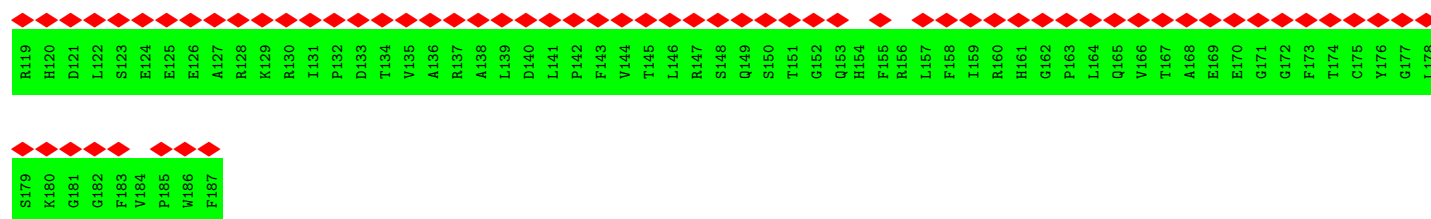


- Molecule 5: Anti-CRISPR protein 30



- Molecule 6: CRISPR-associated endonuclease Cas6/Csy4





- Molecule 6: CRISPR-associated endonuclease Cas6/Csy4

Chain 2-L: 99%



- Molecule 6: CRISPR-associated endonuclease Cas6/Csy4

Chain 3-L: 98%



- Molecule 6: CRISPR-associated endonuclease Cas6/Csy4

Chain 4-L: 99%



- Molecule 6: CRISPR-associated endonuclease Cas6/Csy4

Chain 5-L: 99%



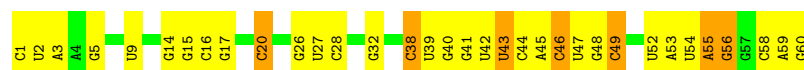
- Molecule 7: CRISPR RNA (60-MER)

Chain 1-M: 32%

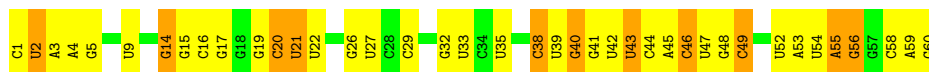


- Molecule 7: CRISPR RNA (60-MER)

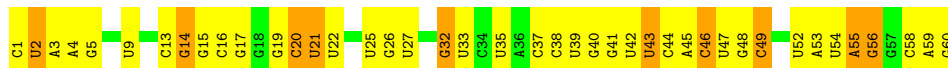
Chain 2-M: 43%



## ● Molecule 7: CRISPR RNA (60-MER)

Chain 3-M:  33% 48% 18%

## ● Molecule 7: CRISPR RNA (60-MER)

Chain 4-M:  30% 53% 17%

## ● Molecule 7: CRISPR RNA (60-MER)

Chain 5-M:  37% 37% 25%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51212	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Particles were ctf-corrected during 2D and 3D processing.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0274	Depositor
Map size (Å)	216.29999, 216.29999, 216.29999	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1-A	0.29	0/3070	0.50	2/4186 (0.0%)
1	2-A	0.29	0/3070	0.50	1/4186 (0.0%)
1	3-A	0.29	0/3070	0.49	0/4186
1	4-A	0.28	0/3070	0.49	0/4186
1	5-A	0.31	0/3070	0.53	1/4186 (0.0%)
2	1-B	0.35	0/2431	0.58	0/3310
2	2-B	0.37	1/2431 (0.0%)	0.57	0/3310
2	3-B	0.34	0/2431	0.60	3/3310 (0.1%)
2	4-B	0.32	0/2431	0.61	3/3310 (0.1%)
2	5-B	0.40	1/2431 (0.0%)	0.62	0/3310
3	1-C	0.34	0/2315	0.53	0/3143
3	1-D	0.33	0/2601	0.53	0/3532
3	1-E	0.34	0/2608	0.55	1/3540 (0.0%)
3	1-F	0.34	0/2613	0.54	1/3547 (0.0%)
3	1-G	0.34	0/2604	0.54	0/3533
3	1-H	0.34	0/2601	0.54	0/3532
3	2-C	0.37	0/2315	0.54	0/3143
3	2-D	0.36	0/2601	0.54	0/3532
3	2-E	0.36	0/2608	0.56	1/3540 (0.0%)
3	2-F	0.36	0/2613	0.56	1/3547 (0.0%)
3	2-G	0.37	0/2604	0.56	1/3533 (0.0%)
3	2-H	0.37	0/2601	0.55	1/3532 (0.0%)
3	3-C	0.36	0/2315	0.55	0/3143
3	3-D	0.35	0/2601	0.56	0/3532
3	3-E	0.35	0/2608	0.55	0/3540
3	3-F	0.36	0/2613	0.56	0/3547
3	3-G	0.36	0/2604	0.55	0/3533
3	3-H	0.36	0/2601	0.55	0/3532
3	4-C	0.34	0/2315	0.53	0/3143
3	4-D	0.33	0/2601	0.54	0/3532
3	4-E	0.34	0/2608	0.54	0/3540
3	4-F	0.35	0/2613	0.55	0/3547
3	4-G	0.34	0/2604	0.54	0/3533
3	4-H	0.34	0/2601	0.54	0/3532

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	5-C	0.42	0/2315	0.55	0/3143
3	5-D	0.40	0/2601	0.56	0/3532
3	5-E	0.41	0/2608	0.57	1/3540 (0.0%)
3	5-F	0.41	0/2613	0.57	0/3547
3	5-G	0.41	0/2604	0.57	0/3533
3	5-H	0.42	0/2601	0.57	0/3532
4	1-I	0.32	0/614	0.49	0/824
4	1-J	0.32	0/614	0.49	0/824
4	2-I	0.34	0/614	0.51	0/824
4	2-J	0.34	0/614	0.51	0/824
4	3-I	0.35	0/614	0.51	0/824
4	3-J	0.35	0/614	0.51	0/824
4	4-I	0.33	0/614	0.50	0/824
4	4-J	0.33	0/614	0.50	0/824
4	5-I	0.37	0/614	0.49	0/824
4	5-J	0.38	0/614	0.49	0/824
5	1-K	0.27	0/691	0.52	0/938
5	2-K	0.27	0/691	0.48	0/938
5	3-K	0.26	0/691	0.51	0/938
5	4-K	0.26	0/691	0.50	0/938
5	5-K	0.27	0/691	0.51	0/938
6	1-L	0.24	0/759	0.48	0/947
6	2-L	0.24	0/759	0.47	0/947
6	3-L	0.24	0/759	0.49	0/947
6	4-L	0.24	0/759	0.48	0/947
6	5-L	0.24	0/759	0.48	0/947
7	1-M	0.57	0/1419	1.14	16/2210 (0.7%)
7	2-M	0.61	0/1419	1.13	12/2210 (0.5%)
7	3-M	0.60	0/1419	1.16	17/2210 (0.8%)
7	4-M	0.55	0/1419	1.14	15/2210 (0.7%)
7	5-M	0.71	0/1419	1.20	15/2210 (0.7%)
All	All	0.37	2/124700 (0.0%)	0.60	92/170330 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-A	0	1
1	3-A	0	1
1	4-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	5-A	0	2
2	5-B	0	2
3	2-C	0	2
3	2-D	0	2
3	2-E	0	2
3	2-F	0	2
3	2-G	0	3
3	2-H	0	2
3	3-C	0	3
3	3-D	0	3
3	3-E	0	3
3	3-F	0	3
3	3-G	0	5
3	3-H	0	4
3	4-C	0	4
3	4-D	0	4
3	4-E	0	4
3	4-F	0	4
3	4-G	0	4
3	4-H	0	5
3	5-C	0	2
3	5-D	0	1
3	5-E	0	4
3	5-F	0	2
3	5-G	0	2
3	5-H	0	3
All	All	0	80

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-B	316	TRP	CB-CG	-5.42	1.40	1.50
2	2-B	316	TRP	CB-CG	-5.17	1.41	1.50

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5-M	1	C	O4'-C1'-N1	11.50	117.40	108.20
7	4-M	1	C	O4'-C1'-N1	11.00	117.00	108.20
7	3-M	1	C	O4'-C1'-N1	10.90	116.92	108.20
7	1-M	1	C	O4'-C1'-N1	8.62	115.09	108.20
2	4-B	262	TYR	C-N-CA	8.17	142.12	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5-M	40	G	N3-C4-C5	-8.10	124.55	128.60
7	5-M	40	G	N3-C4-N9	8.07	130.84	126.00
7	1-M	40	G	N3-C4-N9	7.83	130.70	126.00
1	5-A	178	LEU	CA-CB-CG	7.73	133.07	115.30
7	5-M	40	G	C4-N9-C1'	7.66	136.45	126.50
7	2-M	40	G	N3-C4-N9	7.63	130.58	126.00
7	2-M	40	G	N3-C4-C5	-7.61	124.80	128.60
7	2-M	1	C	O4'-C1'-N1	7.57	114.26	108.20
7	1-M	40	G	N3-C4-C5	-7.55	124.82	128.60
2	3-B	262	TYR	C-N-CA	7.55	140.58	121.70
7	1-M	40	G	C4-N9-C1'	7.54	136.30	126.50
7	2-M	40	G	C4-N9-C1'	7.46	136.20	126.50
7	4-M	40	G	N3-C4-N9	7.13	130.28	126.00
3	1-E	252	LEU	CA-CB-CG	7.06	131.54	115.30
7	3-M	21	U	C2-N1-C1'	7.00	126.10	117.70
7	3-M	40	G	N3-C4-N9	7.00	130.20	126.00
7	5-M	1	C	C2-N1-C1'	6.99	126.49	118.80
7	5-M	46	C	N3-C2-O2	-6.96	117.03	121.90
7	5-M	46	C	N1-C2-O2	6.88	123.03	118.90
7	4-M	1	C	C2-N1-C1'	6.86	126.34	118.80
7	3-M	1	C	C2-N1-C1'	6.82	126.30	118.80
7	4-M	40	G	N3-C4-C5	-6.82	125.19	128.60
7	1-M	46	C	N1-C2-O2	6.75	122.95	118.90
7	3-M	1	C	N1-C2-O2	6.71	122.93	118.90
7	3-M	40	G	N3-C4-C5	-6.63	125.28	128.60
7	4-M	1	C	N1-C2-O2	6.63	122.88	118.90
7	1-M	40	G	C8-N9-C1'	-6.63	118.39	127.00
7	5-M	40	G	C8-N9-C1'	-6.61	118.40	127.00
7	1-M	46	C	N3-C2-O2	-6.59	117.29	121.90
7	3-M	40	G	C4-N9-C1'	6.58	135.05	126.50
7	5-M	1	C	C6-N1-C2	-6.56	117.68	120.30
7	4-M	40	G	C4-N9-C1'	6.51	134.96	126.50
7	2-M	40	G	C8-N9-C1'	-6.48	118.58	127.00
7	2-M	46	C	N1-C2-O2	6.45	122.77	118.90
7	1-M	1	C	N1-C2-O2	6.43	122.76	118.90
7	2-M	46	C	N3-C2-O2	-6.40	117.42	121.90
7	3-M	46	C	N3-C2-O2	-6.34	117.46	121.90
7	3-M	46	C	N1-C2-O2	6.26	122.66	118.90
7	5-M	1	C	N3-C2-O2	-6.23	117.54	121.90
7	3-M	21	U	C5-C6-N1	6.18	125.79	122.70
7	5-M	40	G	C2-N3-C4	6.09	114.94	111.90
7	4-M	46	C	N1-C2-O2	6.03	122.52	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1-M	1	C	C2-N1-C1'	6.02	125.43	118.80
7	4-M	46	C	N3-C2-O2	-5.99	117.71	121.90
7	2-M	1	C	N1-C2-O2	5.94	122.47	118.90
1	1-A	189	LEU	CA-CB-CG	5.91	128.89	115.30
1	1-A	70	LEU	CA-CB-CG	5.90	128.86	115.30
7	3-M	40	G	C8-N9-C1'	-5.79	119.48	127.00
7	2-M	1	C	C2-N1-C1'	5.78	125.16	118.80
7	4-M	21	U	N1-C2-O2	5.78	126.85	122.80
2	3-B	301	LEU	CA-CB-CG	5.73	128.48	115.30
7	3-M	21	U	N1-C2-O2	5.69	126.78	122.80
7	4-M	21	U	N3-C2-O2	-5.68	118.22	122.20
7	1-M	46	C	C6-N1-C2	-5.68	118.03	120.30
7	4-M	40	G	C8-N9-C1'	-5.67	119.62	127.00
2	3-B	277	LEU	CA-CB-CG	5.65	128.29	115.30
2	4-B	301	LEU	CA-CB-CG	5.63	128.24	115.30
7	2-M	40	G	C2-N3-C4	5.60	114.70	111.90
2	4-B	277	LEU	CA-CB-CG	5.58	128.13	115.30
1	2-A	189	LEU	CA-CB-CG	5.57	128.11	115.30
7	4-M	21	U	C2-N1-C1'	5.54	124.35	117.70
7	5-M	46	C	C6-N1-C2	-5.52	118.09	120.30
7	5-M	39	U	C5-C6-N1	-5.42	119.99	122.70
7	4-M	40	G	C2-N3-C4	5.36	114.58	111.90
7	3-M	40	G	C2-N3-C4	5.27	114.54	111.90
3	5-E	95	LEU	CA-CB-CG	5.27	127.41	115.30
7	1-M	40	G	C2-N3-C4	5.25	114.52	111.90
7	1-M	46	C	C2-N1-C1'	5.24	124.57	118.80
3	1-F	252	LEU	CA-CB-CG	5.21	127.28	115.30
7	3-M	1	C	N3-C2-O2	-5.18	118.28	121.90
7	3-M	21	U	N3-C2-O2	-5.18	118.58	122.20
7	1-M	1	C	N3-C2-O2	-5.17	118.28	121.90
7	5-M	43	U	C2-N1-C1'	5.13	123.86	117.70
7	3-M	46	C	C6-N1-C2	-5.12	118.25	120.30
7	4-M	43	U	C2-N1-C1'	5.12	123.84	117.70
7	3-M	43	U	C2-N1-C1'	5.09	123.81	117.70
7	1-M	21	U	N3-C2-O2	-5.08	118.64	122.20
7	4-M	1	C	N3-C2-O2	-5.07	118.35	121.90
7	2-M	43	U	C2-N1-C1'	5.07	123.78	117.70
7	1-M	21	U	C2-N1-C1'	5.06	123.77	117.70
7	5-M	60	G	N3-C4-N9	-5.05	122.97	126.00
7	2-M	46	C	C6-N1-C2	-5.04	118.28	120.30
7	1-M	43	U	C2-N1-C1'	5.04	123.75	117.70
3	2-H	296	LEU	CA-CB-CG	5.03	126.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-G	296	LEU	CA-CB-CG	5.01	126.81	115.30
3	2-E	296	LEU	CA-CB-CG	5.00	126.81	115.30
3	2-F	296	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-A	66	VAL	Peptide
3	2-C	168	TRP	Peptide
3	2-C	249	GLU	Peptide
3	2-D	168	TRP	Peptide
3	2-D	249	GLU	Peptide
3	2-E	168	TRP	Peptide
3	2-E	249	GLU	Peptide
3	2-F	168	TRP	Peptide
3	2-F	249	GLU	Peptide
3	2-G	168	TRP	Peptide
3	2-G	249	GLU	Peptide
3	2-G	74	ASN	Peptide
3	2-H	168	TRP	Peptide
3	2-H	249	GLU	Peptide
1	3-A	66	VAL	Peptide
3	3-C	242	GLN	Peptide
3	3-C	55	SER	Peptide
3	3-C	58	TRP	Peptide
3	3-D	242	GLN	Peptide
3	3-D	55	SER	Peptide
3	3-D	58	TRP	Peptide
3	3-E	242	GLN	Peptide
3	3-E	55	SER	Peptide
3	3-E	58	TRP	Peptide
3	3-F	242	GLN	Peptide
3	3-F	55	SER	Peptide
3	3-F	58	TRP	Peptide
3	3-G	242	GLN	Peptide
3	3-G	55	SER	Peptide
3	3-G	58	TRP	Peptide
3	3-G	94	ASN	Peptide
3	3-G	95	LEU	Peptide
3	3-H	242	GLN	Peptide
3	3-H	250	LEU	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
3	3-H	55	SER	Peptide
3	3-H	58	TRP	Peptide
1	4-A	66	VAL	Peptide
3	4-C	242	GLN	Peptide
3	4-C	54	ALA	Peptide
3	4-C	55	SER	Peptide
3	4-C	58	TRP	Peptide
3	4-D	242	GLN	Peptide
3	4-D	54	ALA	Peptide
3	4-D	55	SER	Peptide
3	4-D	58	TRP	Peptide
3	4-E	242	GLN	Peptide
3	4-E	54	ALA	Peptide
3	4-E	55	SER	Peptide
3	4-E	58	TRP	Peptide
3	4-F	242	GLN	Peptide
3	4-F	54	ALA	Peptide
3	4-F	55	SER	Peptide
3	4-F	58	TRP	Peptide
3	4-G	242	GLN	Peptide
3	4-G	54	ALA	Peptide
3	4-G	55	SER	Peptide
3	4-G	58	TRP	Peptide
3	4-H	242	GLN	Peptide
3	4-H	250	LEU	Peptide
3	4-H	54	ALA	Peptide
3	4-H	55	SER	Peptide
3	4-H	58	TRP	Peptide
1	5-A	178	LEU	Peptide
1	5-A	226	GLU	Peptide
2	5-B	281	GLU	Peptide
2	5-B	86	ASN	Peptide
3	5-C	171	ARG	Peptide
3	5-C	249	GLU	Peptide
3	5-D	171	ARG	Peptide
3	5-E	171	ARG	Peptide
3	5-E	249	GLU	Peptide
3	5-E	250	LEU	Peptide
3	5-E	95	LEU	Peptide
3	5-F	171	ARG	Peptide
3	5-F	249	GLU	Peptide
3	5-G	171	ARG	Peptide

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Mol	Chain	Res	Type	Group
3	5-G	250	LEU	Peptide
3	5-H	171	ARG	Peptide
3	5-H	249	GLU	Peptide
3	5-H	250	LEU	Peptide

## 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	1-A	3011	0	2651	48	0
1	2-A	3011	0	2651	25	0
1	3-A	3011	0	2651	51	0
1	4-A	3011	0	2651	51	0
1	5-A	3011	0	2651	43	0
2	1-B	2374	0	2345	40	0
2	2-B	2374	0	2345	40	0
2	3-B	2374	0	2345	38	0
2	4-B	2374	0	2345	37	0
2	5-B	2374	0	2345	42	0
3	1-C	2272	0	2232	14	0
3	1-D	2554	0	2522	17	0
3	1-E	2561	0	2542	12	0
3	1-F	2566	0	2547	18	0
3	1-G	2557	0	2542	15	0
3	1-H	2554	0	2522	15	0
3	2-C	2272	0	2232	21	0
3	2-D	2554	0	2522	27	0
3	2-E	2561	0	2542	27	0
3	2-F	2566	0	2547	28	0
3	2-G	2557	0	2542	34	0
3	2-H	2554	0	2522	26	0
3	3-C	2272	0	2232	22	0
3	3-D	2554	0	2522	26	0
3	3-E	2561	0	2542	24	0
3	3-F	2566	0	2547	24	0
3	3-G	2557	0	2542	23	0
3	3-H	2554	0	2522	26	0
3	4-C	2272	0	2232	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4-D	2554	0	2522	27	0
3	4-E	2561	0	2542	26	0
3	4-F	2566	0	2547	23	0
3	4-G	2557	0	2542	22	0
3	4-H	2554	0	2522	27	0
3	5-C	2272	0	2232	25	0
3	5-D	2554	0	2522	56	0
3	5-E	2561	0	2542	40	0
3	5-F	2566	0	2547	32	0
3	5-G	2557	0	2542	32	0
3	5-H	2554	0	2522	29	0
4	1-I	604	0	590	3	0
4	1-J	604	0	590	3	0
4	2-I	604	0	590	4	0
4	2-J	604	0	590	3	0
4	3-I	604	0	590	3	0
4	3-J	604	0	590	6	0
4	4-I	604	0	590	3	0
4	4-J	604	0	590	6	0
4	5-I	604	0	590	4	0
4	5-J	604	0	590	3	0
5	1-K	680	0	617	6	0
5	2-K	680	0	617	8	0
5	3-K	680	0	617	7	0
5	4-K	680	0	617	7	0
5	5-K	680	0	617	7	0
6	1-L	757	0	205	1	0
6	2-L	757	0	205	1	0
6	3-L	757	0	205	3	0
6	4-L	757	0	205	2	0
6	5-L	757	0	205	1	0
7	1-M	1271	0	644	13	0
7	2-M	1271	0	644	11	0
7	3-M	1271	0	644	15	0
7	4-M	1271	0	644	16	0
7	5-M	1271	0	644	27	0
All	All	121825	0	112745	1111	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 5.

All (1111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:249:GLU:HB2	7:M:33:U:C6	1.39	1.58
3:D:249:GLU:CB	7:M:33:U:C6	2.07	1.37
3:D:246:PRO:CG	3:D:265:LEU:HD22	1.80	1.10
3:D:246:PRO:HG3	3:D:265:LEU:HD13	1.35	1.09
3:D:246:PRO:HG2	3:D:265:LEU:CD2	1.84	1.07
3:D:249:GLU:HG2	7:M:34:C:OP2	1.63	0.99
3:D:249:GLU:CB	7:M:33:U:C5	2.45	0.99
3:D:249:GLU:CB	7:M:33:U:H6	1.58	0.98
3:F:25:LEU:O	3:F:332:LEU:HD22	1.67	0.94
3:D:246:PRO:HG2	3:D:265:LEU:HD22	0.94	0.89
3:D:249:GLU:HB3	7:M:33:U:C6	2.05	0.89
3:D:249:GLU:HB3	7:M:33:U:C5	2.09	0.87
3:H:246:PRO:HG2	3:H:265:LEU:HD13	1.54	0.86
3:D:250:LEU:CD1	3:E:95:LEU:HG	2.08	0.83
3:F:27:THR:HG23	3:F:332:LEU:HD11	1.59	0.83
5:K:84:SER:O	5:K:88:ARG:HB2	1.81	0.81
3:D:249:GLU:HB2	7:M:33:U:H6	0.66	0.76
3:F:25:LEU:HG	3:F:332:LEU:HD22	1.70	0.73
3:F:25:LEU:HG	3:F:332:LEU:CD2	2.18	0.73
2:B:88:LEU:HG	3:H:308:THR:HG22	1.71	0.71
3:G:87:ASP:O	3:G:91:GLN:HB2	1.91	0.71
1:A:296:GLU:O	1:A:300:LEU:HB2	1.90	0.71
2:B:131:GLN:HB2	2:B:156:ASN:HD21	1.57	0.69
3:D:250:LEU:HD22	3:E:67:SER:HB2	1.75	0.69
1:A:296:GLU:O	1:A:300:LEU:HB2	1.93	0.68
3:F:25:LEU:O	3:F:332:LEU:CD2	2.41	0.68
1:A:207:ARG:HH12	1:A:257:GLU:HB2	1.58	0.68
3:E:57:GLU:HB3	3:E:59:PRO:HD2	1.76	0.68
2:B:159:LEU:HD21	2:B:172:ASN:HB3	1.75	0.68
3:D:57:GLU:HB3	3:D:59:PRO:HD2	1.76	0.68
3:G:57:GLU:HB3	3:G:59:PRO:HD2	1.76	0.68
2:B:135:GLY:O	3:H:117:ARG:NH1	2.27	0.68
3:E:57:GLU:HB3	3:E:59:PRO:HD2	1.77	0.67
3:C:57:GLU:HB3	3:C:59:PRO:HD2	1.76	0.67
3:F:57:GLU:HB3	3:F:59:PRO:HD2	1.76	0.67
3:H:57:GLU:HB3	3:H:59:PRO:HD2	1.76	0.67
3:F:277:GLN:HE22	3:G:68:VAL:HG22	1.59	0.67
3:C:57:GLU:HB3	3:C:59:PRO:HD2	1.77	0.67
3:D:249:GLU:CG	7:M:34:C:OP2	2.39	0.67
3:H:246:PRO:CG	3:H:265:LEU:HD13	2.24	0.67
3:H:57:GLU:HB3	3:H:59:PRO:HD2	1.77	0.67
3:F:57:GLU:HB3	3:F:59:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:GLY:O	3:H:117:ARG:NH1	2.28	0.66
2:B:200:LEU:HD11	2:B:205:PRO:HA	1.77	0.66
2:B:167:GLU:O	2:B:171:LYS:HB2	1.95	0.66
3:C:203:ARG:NH2	6:L:11:PRO:O	2.28	0.66
1:A:364:ASP:O	1:A:368:ALA:HB3	1.96	0.66
3:G:90:ILE:HG13	3:G:91:GLN:HG3	1.77	0.66
3:G:57:GLU:HB3	3:G:59:PRO:HD2	1.77	0.66
5:K:46:ASN:HB3	5:K:61:ALA:HB3	1.78	0.66
3:D:248:GLN:HB2	3:D:266:TYR:HB2	1.76	0.65
3:D:250:LEU:HD11	3:E:95:LEU:HG	1.77	0.65
3:E:284:ARG:NH2	7:M:26:G:OP2	2.29	0.65
3:D:57:GLU:HB3	3:D:59:PRO:HD2	1.77	0.65
2:B:167:GLU:O	2:B:171:LYS:HB2	1.96	0.65
1:A:48:ARG:O	1:A:52:TRP:HB3	1.97	0.65
3:E:277:GLN:HE22	3:F:66:LYS:HE3	1.61	0.65
2:B:17:ILE:HD12	2:B:105:LEU:HD23	1.79	0.64
3:D:239:GLY:HA3	3:D:242:GLN:HE21	1.63	0.64
1:A:255:ASN:HB2	1:A:257:GLU:HG2	1.80	0.64
3:C:356:GLY:H	3:D:75:ARG:HH21	1.46	0.64
3:F:239:GLY:HA3	3:F:242:GLN:HE21	1.63	0.64
3:H:239:GLY:HA3	3:H:242:GLN:HE21	1.63	0.64
1:A:91:GLN:HB2	2:B:315:ARG:HH11	1.62	0.64
3:F:25:LEU:O	3:F:332:LEU:HD22	1.98	0.64
3:E:284:ARG:NH2	7:M:26:G:OP2	2.31	0.64
3:F:250:LEU:HA	7:M:21:U:H3	1.63	0.64
2:B:89:ASN:HB3	2:B:92:GLY:H	1.62	0.63
3:E:239:GLY:HA3	3:E:242:GLN:HE21	1.63	0.63
2:B:135:GLY:O	3:H:117:ARG:NH1	2.31	0.63
2:B:122:PRO:O	2:B:125:GLU:HB3	1.97	0.63
3:G:239:GLY:HA3	3:G:242:GLN:HE21	1.63	0.63
1:A:219:ARG:NH2	1:A:234:GLU:OE1	2.32	0.63
3:H:239:GLY:HA3	3:H:242:GLN:HE21	1.64	0.63
3:C:239:GLY:HA3	3:C:242:GLN:HE21	1.63	0.63
3:G:277:GLN:HE22	3:H:66:LYS:HE3	1.63	0.63
3:C:66:LYS:NZ	6:L:149:GLN:O	2.32	0.62
3:E:239:GLY:HA3	3:E:242:GLN:HE21	1.64	0.62
3:F:239:GLY:HA3	3:F:242:GLN:HE21	1.64	0.62
2:B:55:GLU:HB3	2:B:114:HIS:HB2	1.82	0.62
3:E:284:ARG:NH2	7:M:26:G:OP2	2.32	0.62
1:A:219:ARG:NH2	1:A:234:GLU:OE1	2.33	0.62
1:A:117:VAL:O	1:A:120:PHE:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:ARG:NH2	6:L:11:PRO:O	2.33	0.62
3:C:239:GLY:HA3	3:C:242:GLN:HE21	1.64	0.62
3:C:285:THR:HG22	3:C:298:PRO:HB2	1.82	0.62
3:G:239:GLY:HA3	3:G:242:GLN:HE21	1.64	0.62
3:D:65:GLU:OE2	3:D:260:GLN:NE2	2.32	0.62
1:A:117:VAL:O	1:A:120:PHE:HB3	1.99	0.62
3:E:284:ARG:NH2	7:M:26:G:OP2	2.33	0.62
1:A:216:LYS:O	1:A:220:GLU:HB2	2.00	0.62
3:H:251:ILE:HD12	3:H:264:THR:HG21	1.82	0.62
3:F:24:ILE:HG13	3:F:25:LEU:HD13	1.82	0.62
3:E:284:ARG:NH2	7:M:26:G:OP2	2.33	0.61
3:E:285:THR:HG22	3:E:298:PRO:HB2	1.82	0.61
3:H:285:THR:HG22	3:H:298:PRO:HB2	1.82	0.61
1:A:216:LYS:O	1:A:220:GLU:HB2	2.01	0.61
3:D:239:GLY:HA3	3:D:242:GLN:HE21	1.64	0.61
5:K:30:ASP:HB2	5:K:40:LYS:HB2	1.81	0.61
3:H:117:ARG:HE	3:H:119:LEU:HD21	1.66	0.61
3:F:180:ARG:HG2	3:F:194:ARG:HG2	1.83	0.61
3:D:285:THR:HG22	3:D:298:PRO:HB2	1.82	0.61
3:F:117:ARG:HE	3:F:119:LEU:HD21	1.66	0.61
3:D:117:ARG:HE	3:D:119:LEU:HD21	1.66	0.60
3:E:117:ARG:HE	3:E:119:LEU:HD21	1.66	0.60
5:K:70:TYR:HA	5:K:73:TRP:HD1	1.66	0.60
3:C:66:LYS:NZ	6:L:149:GLN:O	2.32	0.60
3:F:285:THR:HG22	3:F:298:PRO:HB2	1.82	0.60
3:D:248:GLN:HB3	3:D:266:TYR:N	2.16	0.60
3:G:180:ARG:HG2	3:G:194:ARG:HG2	1.83	0.60
1:A:287:PHE:O	1:A:291:PHE:HB2	2.01	0.60
1:A:418:LEU:O	1:A:422:LEU:HB2	2.02	0.60
2:B:70:ILE:HD12	2:B:79:LYS:HD3	1.83	0.60
1:A:253:GLN:O	1:A:258:ARG:NH2	2.35	0.60
2:B:221:PHE:HA	2:B:239:TRP:HA	1.84	0.60
5:K:30:ASP:HB3	5:K:40:LYS:HB2	1.83	0.60
2:B:17:ILE:HB	2:B:105:LEU:HB2	1.84	0.60
3:E:180:ARG:HG2	3:E:194:ARG:HG2	1.82	0.60
3:G:117:ARG:HE	3:G:119:LEU:HD21	1.66	0.60
2:B:193:LEU:HG	2:B:286:LEU:HD22	1.83	0.60
3:G:44:MET:HG2	3:G:112:VAL:HG22	1.84	0.60
3:G:285:THR:HG22	3:G:298:PRO:HB2	1.82	0.60
3:C:180:ARG:HG2	3:C:194:ARG:HG2	1.82	0.60
2:B:17:ILE:HD13	2:B:139:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLU:O	1:A:156:ARG:NH1	2.34	0.59
3:F:44:MET:HG2	3:F:112:VAL:HG22	1.84	0.59
3:H:44:MET:HG2	3:H:112:VAL:HG22	1.84	0.59
3:D:180:ARG:HG2	3:D:194:ARG:HG2	1.83	0.59
3:D:250:LEU:HD13	3:E:95:LEU:HG	1.83	0.59
3:C:117:ARG:HE	3:C:119:LEU:HD21	1.66	0.59
3:H:263:LYS:O	3:H:263:LYS:HG2	2.02	0.59
1:A:59:ARG:NH1	5:K:53:GLY:O	2.36	0.59
2:B:17:ILE:HB	2:B:105:LEU:HB2	1.85	0.59
3:D:94:ASN:HB3	3:D:96:GLN:HE21	1.68	0.59
3:C:287:ASP:OD2	3:C:315:ARG:NH1	2.36	0.59
3:E:287:ASP:OD2	3:E:315:ARG:NH1	2.36	0.59
7:M:54:U:OP2	7:M:55:A:N6	2.36	0.59
7:M:54:U:OP2	7:M:55:A:N6	2.36	0.59
3:H:287:ASP:OD2	3:H:315:ARG:NH1	2.36	0.59
7:M:54:U:OP2	7:M:55:A:N6	2.36	0.59
3:E:248:GLN:HE22	3:E:278:LYS:HD3	1.68	0.59
1:A:14:ARG:O	1:A:18:GLU:HB2	2.02	0.59
7:M:54:U:OP2	7:M:55:A:N6	2.36	0.59
3:H:180:ARG:HG2	3:H:194:ARG:HG2	1.83	0.59
1:A:241:GLN:HB3	1:A:262:ASN:HB3	1.84	0.58
1:A:47:HIS:HA	1:A:51:ALA:HB3	1.84	0.58
1:A:68:HIS:HD1	1:A:195:PRO:HA	1.69	0.58
3:G:287:ASP:OD2	3:G:315:ARG:NH1	2.36	0.58
1:A:321:ARG:O	1:A:325:LEU:HB2	2.03	0.58
3:F:287:ASP:OD2	3:F:315:ARG:NH1	2.36	0.58
3:D:246:PRO:HG3	3:D:265:LEU:CD1	2.20	0.58
3:C:44:MET:HG2	3:C:112:VAL:HG22	1.84	0.58
3:E:44:MET:HG2	3:E:112:VAL:HG22	1.84	0.58
3:D:248:GLN:HE22	3:D:278:LYS:HD3	1.68	0.58
3:D:44:MET:HG2	3:D:112:VAL:HG22	1.84	0.58
1:A:287:PHE:O	1:A:291:PHE:HB2	2.03	0.58
7:M:54:U:OP2	7:M:55:A:N6	2.37	0.58
3:E:65:GLU:OE2	3:E:261:LYS:NZ	2.37	0.58
3:D:169:ARG:NH1	7:M:35:U:OP1	2.37	0.58
3:C:248:GLN:HE22	3:C:278:LYS:HD3	1.68	0.58
3:F:95:LEU:HD13	4:I:62:LEU:HD11	1.86	0.58
1:A:171:SER:OG	1:A:177:GLN:NE2	2.37	0.58
1:A:234:GLU:HB3	2:B:217:CYS:HB2	1.86	0.58
3:D:287:ASP:OD2	3:D:315:ARG:NH1	2.36	0.58
1:A:59:ARG:NH1	5:K:53:GLY:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ALA:O	1:A:415:SER:HB2	2.03	0.57
3:F:248:GLN:HE22	3:F:278:LYS:HD3	1.68	0.57
2:B:270:ALA:O	3:H:129:ASN:ND2	2.32	0.57
3:C:55:SER:O	3:C:111:LYS:NZ	2.38	0.57
2:B:88:LEU:HG	3:H:308:THR:HG22	1.86	0.57
3:H:148:GLN:HE22	3:H:339:VAL:HG13	1.70	0.57
3:C:249:GLU:HB2	3:C:264:THR:HG23	1.87	0.57
1:A:136:GLU:O	1:A:156:ARG:NH1	2.36	0.57
1:A:321:ARG:NH2	2:B:243:ASP:O	2.37	0.57
2:B:149:ASN:HA	2:B:153:PRO:HA	1.87	0.57
3:H:248:GLN:HE22	3:H:278:LYS:HD3	1.68	0.57
1:A:222:ARG:NH2	4:I:77:ASN:OD1	2.37	0.57
1:A:171:SER:OG	1:A:177:GLN:NE2	2.37	0.57
3:F:277:GLN:HB3	7:M:20:C:H5''	1.86	0.57
3:G:55:SER:O	3:G:111:LYS:NZ	2.38	0.57
3:G:148:GLN:HE22	3:G:339:VAL:HG13	1.70	0.56
3:H:85:LYS:NZ	4:J:20:TYR:OH	2.38	0.56
3:D:245:PHE:CD1	3:D:245:PHE:N	2.73	0.56
3:D:356:GLY:H	3:E:75:ARG:HE	1.52	0.56
3:G:55:SER:O	3:G:111:LYS:NZ	2.38	0.56
2:B:88:LEU:HG	3:H:308:THR:HG22	1.87	0.56
3:F:278:LYS:NZ	7:M:20:C:O2	2.38	0.56
3:G:248:GLN:HE22	3:G:278:LYS:HD3	1.68	0.56
3:C:148:GLN:HE22	3:C:339:VAL:HG13	1.70	0.56
3:D:148:GLN:HE22	3:D:339:VAL:HG13	1.70	0.56
3:E:148:GLN:HE22	3:E:339:VAL:HG13	1.70	0.56
3:G:277:GLN:HE22	3:H:66:LYS:HE3	1.71	0.56
3:D:55:SER:O	3:D:111:LYS:NZ	2.38	0.56
3:E:55:SER:O	3:E:111:LYS:NZ	2.38	0.56
1:A:65:LEU:HD23	1:A:163:THR:HG22	1.86	0.56
3:H:33:PHE:O	7:M:5:G:O2'	2.22	0.56
3:D:250:LEU:HD13	3:E:95:LEU:CD1	2.35	0.56
3:D:55:SER:O	3:D:111:LYS:NZ	2.38	0.56
2:B:83:LEU:HD11	2:B:99:GLU:HG2	1.88	0.56
3:E:55:SER:O	3:E:111:LYS:NZ	2.38	0.56
3:F:249:GLU:HB2	3:F:264:THR:HG23	1.87	0.56
3:F:55:SER:O	3:F:111:LYS:NZ	2.38	0.56
1:A:298:SER:OG	1:A:302:ARG:NH1	2.38	0.56
3:F:148:GLN:HE22	3:F:339:VAL:HG13	1.70	0.56
3:G:249:GLU:HB2	3:G:264:THR:HG23	1.87	0.56
3:E:257:LYS:HG2	3:E:258:LYS:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:55:SER:O	3:H:111:LYS:NZ	2.38	0.56
1:A:148:ASN:O	1:A:153:ARG:NH1	2.38	0.56
2:B:218:ARG:HD3	2:B:242:ARG:HE	1.70	0.56
3:G:284:ARG:NH2	7:M:14:G:OP2	2.39	0.56
3:E:82:ASP:O	3:E:86:LEU:HB2	2.05	0.56
5:K:32:VAL:HB	5:K:38:TYR:HB2	1.86	0.56
2:B:122:PRO:HA	2:B:125:GLU:HB3	1.87	0.56
2:B:55:GLU:HB3	2:B:114:HIS:HB2	1.87	0.55
3:C:293:GLU:HG2	3:C:295:GLY:H	1.72	0.55
2:B:54:ILE:HA	2:B:115:GLY:HA3	1.86	0.55
1:A:148:ASN:O	1:A:153:ARG:NH1	2.39	0.55
3:E:277:GLN:HE22	3:F:66:LYS:HE3	1.70	0.55
5:K:79:ARG:HA	5:K:82:GLU:HB3	1.88	0.55
1:A:321:ARG:NH1	2:B:243:ASP:OD2	2.40	0.55
3:E:69:ARG:HH21	3:E:93:PRO:HG3	1.72	0.55
3:F:55:SER:O	3:F:111:LYS:NZ	2.38	0.55
3:H:176:ALA:HA	3:H:198:LEU:HD11	1.89	0.55
3:C:36:LYS:HG3	3:C:119:LEU:HB2	1.89	0.55
3:C:55:SER:O	3:C:111:LYS:NZ	2.38	0.55
3:F:260:GLN:OE1	4:I:13:ASN:ND2	2.39	0.55
1:A:256:ASN:HD22	5:K:33:TRP:HB2	1.70	0.55
1:A:137:ASP:HA	1:A:156:ARG:HH12	1.70	0.55
3:D:36:LYS:HG3	3:D:119:LEU:HB2	1.89	0.55
2:B:197:LEU:HD21	2:B:209:THR:HA	1.89	0.55
2:B:122:PRO:HA	2:B:125:GLU:HB3	1.87	0.55
3:D:249:GLU:HB2	3:D:264:THR:HG23	1.87	0.55
3:H:249:GLU:HB2	3:H:264:THR:HG23	1.87	0.55
2:B:270:ALA:O	3:H:129:ASN:ND2	2.34	0.55
3:F:148:GLN:HE22	3:F:339:VAL:HG13	1.72	0.55
3:H:36:LYS:HG3	3:H:119:LEU:HB2	1.89	0.55
1:A:412:ALA:O	1:A:416:GLN:HB2	2.07	0.55
1:A:431:ASP:O	2:B:178:ARG:NH1	2.40	0.55
1:A:55:ASP:OD1	1:A:58:ARG:NH2	2.40	0.55
2:B:54:ILE:HA	2:B:115:GLY:HA3	1.87	0.55
3:E:148:GLN:HE22	3:E:339:VAL:HG13	1.72	0.55
1:A:94:LEU:HD13	2:B:283:LEU:HD13	1.87	0.55
3:C:284:ARG:NH2	7:M:38:C:OP2	2.40	0.55
3:E:176:ALA:HA	3:E:198:LEU:HD11	1.89	0.55
3:E:249:GLU:HB2	3:E:264:THR:HG23	1.87	0.55
2:B:10:LEU:HB3	2:B:111:LEU:HB2	1.89	0.55
3:D:169:ARG:NH1	7:M:35:U:OP1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:250:LEU:HG	3:D:250:LEU:O	2.05	0.55
3:F:36:LYS:HG3	3:F:119:LEU:HB2	1.89	0.55
3:H:33:PHE:O	7:M:5:G:O2'	2.24	0.54
2:B:295:VAL:HG21	2:B:301:LEU:HD23	1.87	0.54
3:H:55:SER:O	3:H:111:LYS:NZ	2.38	0.54
3:G:52:ARG:NH1	3:G:178:GLU:OE1	2.41	0.54
3:H:32:ALA:HB1	7:M:5:G:H1'	1.88	0.54
2:B:20:ALA:HB3	2:B:141:GLY:HA3	1.89	0.54
3:F:52:ARG:NH1	3:F:178:GLU:OE1	2.40	0.54
3:H:32:ALA:HB1	7:M:5:G:H1'	1.88	0.54
1:A:431:ASP:O	2:B:178:ARG:NH1	2.40	0.54
3:D:148:GLN:HE22	3:D:339:VAL:HG13	1.72	0.54
1:A:227:SER:H	2:B:239:TRP:HH2	1.55	0.54
3:C:52:ARG:NH1	3:C:178:GLU:OE1	2.40	0.54
3:F:176:ALA:HA	3:F:198:LEU:HD11	1.89	0.54
3:F:277:GLN:HB3	7:M:20:C:H5''	1.89	0.54
3:G:148:GLN:HE22	3:G:339:VAL:HG13	1.72	0.54
3:H:148:GLN:HE22	3:H:339:VAL:HG13	1.72	0.54
3:D:285:THR:HA	3:D:300:ALA:HA	1.90	0.54
1:A:94:LEU:HD11	2:B:315:ARG:HD3	1.88	0.54
3:E:29:SER:OG	3:E:129:ASN:ND2	2.41	0.54
3:H:85:LYS:NZ	4:J:20:TYR:OH	2.41	0.54
1:A:128:LYS:O	1:A:132:ASN:CB	2.56	0.54
3:E:52:ARG:NH1	3:E:178:GLU:OE1	2.40	0.54
3:G:356:GLY:O	3:H:75:ARG:NE	2.41	0.54
2:B:119:ASP:HB3	2:B:122:PRO:HD2	1.90	0.54
3:D:109:THR:HA	3:D:236:ALA:O	2.08	0.54
3:F:29:SER:OG	3:F:129:ASN:ND2	2.41	0.54
3:E:36:LYS:HG3	3:E:119:LEU:HB2	1.89	0.54
3:H:128:CYS:SG	3:H:129:ASN:N	2.81	0.54
1:A:427:GLU:HG3	2:B:174:ARG:HH12	1.72	0.54
3:C:285:THR:HA	3:C:300:ALA:HA	1.90	0.54
3:C:356:GLY:O	3:D:75:ARG:NH1	2.30	0.54
3:C:29:SER:OG	3:C:129:ASN:ND2	2.41	0.54
5:K:64:ALA:HA	5:K:67:ILE:HD12	1.90	0.54
3:F:285:THR:HA	3:F:300:ALA:HA	1.90	0.54
5:K:40:LYS:NZ	5:K:82:GLU:OE1	2.40	0.54
3:C:290:TYR:HB3	3:C:293:GLU:HB2	1.89	0.54
3:F:68:VAL:HG13	3:F:96:GLN:HB2	1.90	0.54
3:F:109:THR:HA	3:F:236:ALA:O	2.08	0.54
3:G:109:THR:HA	3:G:236:ALA:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:CYS:SG	3:C:129:ASN:N	2.81	0.54
3:E:254:LYS:O	4:I:67:ASN:ND2	2.39	0.54
3:G:285:THR:HA	3:G:300:ALA:HA	1.90	0.54
3:E:253:ASP:HA	3:E:260:GLN:HE22	1.73	0.54
3:F:289:TRP:O	3:F:315:ARG:NH2	2.41	0.54
3:H:289:TRP:O	3:H:315:ARG:NH2	2.41	0.54
3:H:69:ARG:HA	3:H:94:ASN:O	2.08	0.54
2:B:37:PHE:O	2:B:40:PHE:HB3	2.08	0.54
3:G:176:ALA:HA	3:G:198:LEU:HD11	1.89	0.54
1:A:418:LEU:O	1:A:422:LEU:HB2	2.08	0.54
3:E:35:ARG:NH2	3:F:243:GLU:OE1	2.41	0.54
1:A:59:ARG:NH1	5:K:53:GLY:O	2.41	0.53
1:A:430:GLU:OE2	1:A:433:ARG:NH2	2.40	0.53
3:G:289:TRP:O	3:G:315:ARG:NH2	2.41	0.53
3:C:29:SER:OG	3:C:129:ASN:ND2	2.42	0.53
3:E:29:SER:OG	3:E:129:ASN:ND2	2.41	0.53
2:B:88:LEU:HG	3:H:308:THR:HG22	1.88	0.53
3:E:180:ARG:HG2	3:E:194:ARG:HG2	1.91	0.53
5:K:12:HIS:HB3	5:K:15:THR:HB	1.89	0.53
3:C:176:ALA:HA	3:C:198:LEU:HD11	1.89	0.53
3:E:289:TRP:O	3:E:315:ARG:NH2	2.41	0.53
3:D:252:LEU:HD23	3:D:254:LYS:H	1.74	0.53
3:E:82:ASP:O	3:E:86:LEU:HB2	2.07	0.53
2:B:24:SER:OG	2:B:28:THR:OG1	2.25	0.53
3:G:281:ASN:HB2	7:M:14:G:H5'	1.89	0.53
3:F:358:ALA:O	3:G:75:ARG:NH2	2.37	0.53
3:H:52:ARG:NH1	3:H:178:GLU:OE1	2.40	0.53
3:H:109:THR:HA	3:H:236:ALA:O	2.08	0.53
3:D:128:CYS:SG	3:D:129:ASN:N	2.81	0.53
3:C:180:ARG:HG2	3:C:194:ARG:HG2	1.90	0.53
3:D:180:ARG:HG2	3:D:194:ARG:HG2	1.91	0.53
3:D:180:ARG:HG2	3:D:194:ARG:HG2	1.91	0.53
3:C:148:GLN:HE22	3:C:339:VAL:HG13	1.72	0.53
1:A:328:GLN:O	1:A:332:GLU:HB2	2.08	0.53
3:C:109:THR:HA	3:C:236:ALA:O	2.08	0.53
3:G:29:SER:OG	3:G:129:ASN:ND2	2.41	0.53
2:B:138:ARG:HH21	2:B:142:GLY:H	1.54	0.53
3:F:119:LEU:HD22	3:G:172:VAL:HG12	1.90	0.53
3:C:180:ARG:HG2	3:C:194:ARG:HG2	1.91	0.53
2:B:11:LEU:HD11	2:B:180:LEU:HD21	1.89	0.53
1:A:207:ARG:NH1	4:J:77:ASN:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:285:THR:HA	3:E:300:ALA:HA	1.90	0.53
3:H:180:ARG:HG2	3:H:194:ARG:HG2	1.90	0.53
3:C:180:ARG:HG2	3:C:194:ARG:HG2	1.91	0.53
3:D:52:ARG:NH1	3:D:178:GLU:OE1	2.41	0.53
3:G:278:LYS:NZ	7:M:14:G:N3	2.57	0.53
3:C:180:ARG:HG2	3:C:194:ARG:HG2	1.91	0.53
3:D:180:ARG:HG2	3:D:194:ARG:HG2	1.91	0.53
1:A:267:SER:HB3	2:B:30:GLY:H	1.73	0.53
3:D:29:SER:OG	3:D:129:ASN:ND2	2.41	0.53
3:G:35:ARG:NH2	3:H:243:GLU:OE1	2.41	0.53
3:H:44:MET:HG2	3:H:112:VAL:HG22	1.91	0.53
1:A:69:THR:HG22	1:A:71:LYS:H	1.74	0.53
3:H:29:SER:OG	3:H:129:ASN:ND2	2.41	0.53
3:G:36:LYS:HG3	3:G:119:LEU:HB2	1.89	0.53
3:G:44:MET:HG2	3:G:112:VAL:HG22	1.91	0.53
3:F:180:ARG:HG2	3:F:194:ARG:HG2	1.90	0.53
3:G:180:ARG:HG2	3:G:194:ARG:HG2	1.90	0.53
3:D:176:ALA:HA	3:D:198:LEU:HD11	1.89	0.53
3:H:180:ARG:HG2	3:H:194:ARG:HG2	1.91	0.53
3:E:109:THR:HA	3:E:236:ALA:O	2.08	0.53
3:G:277:GLN:HB3	7:M:14:G:H5"	1.89	0.53
1:A:355:LEU:O	1:A:359:GLU:CB	2.56	0.53
1:A:82:LEU:HD13	2:B:258:LEU:HD11	1.91	0.52
3:D:180:ARG:HG2	3:D:194:ARG:HG2	1.90	0.52
3:H:285:THR:HA	3:H:300:ALA:HA	1.90	0.52
2:B:37:PHE:HB3	2:B:59:VAL:HG11	1.90	0.52
2:B:169:ARG:O	2:B:173:GLN:HB2	2.09	0.52
3:H:180:ARG:HG2	3:H:194:ARG:HG2	1.91	0.52
3:G:117:ARG:NH1	3:H:238:ILE:O	2.40	0.52
3:G:128:CYS:SG	3:G:129:ASN:N	2.81	0.52
2:B:167:GLU:O	2:B:171:LYS:HB2	2.09	0.52
1:A:91:GLN:OE1	2:B:315:ARG:NH1	2.41	0.52
1:A:140:GLU:O	1:A:144:ALA:HB2	2.09	0.52
3:C:33:PHE:O	7:M:35:U:O2'	2.26	0.52
3:F:29:SER:OG	3:F:129:ASN:ND2	2.42	0.52
2:B:261:LEU:HD11	2:B:276:PRO:HB2	1.89	0.52
3:C:289:TRP:O	3:C:315:ARG:NH2	2.41	0.52
3:D:289:TRP:O	3:D:315:ARG:NH2	2.41	0.52
3:F:180:ARG:HG2	3:F:194:ARG:HG2	1.91	0.52
3:D:29:SER:OG	3:D:129:ASN:ND2	2.42	0.52
3:D:94:ASN:HB3	3:D:96:GLN:HE21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:82:ASP:O	3:E:86:LEU:CB	2.58	0.52
3:G:29:SER:OG	3:G:129:ASN:ND2	2.42	0.52
3:E:249:GLU:HB2	3:E:264:THR:HG23	1.92	0.52
3:H:249:GLU:HB2	3:H:264:THR:HG23	1.92	0.52
1:A:99:GLU:OE2	2:B:207:ALA:N	2.41	0.52
2:B:24:SER:HG	2:B:28:THR:HG1	1.54	0.52
3:D:250:LEU:CD1	3:E:95:LEU:CG	2.84	0.52
3:E:44:MET:HG2	3:E:112:VAL:HG22	1.91	0.52
3:H:29:SER:OG	3:H:129:ASN:ND2	2.42	0.52
3:C:33:PHE:O	7:M:35:U:O2'	2.26	0.52
3:F:180:ARG:HG2	3:F:194:ARG:HG2	1.91	0.52
3:H:180:ARG:HG2	3:H:194:ARG:HG2	1.91	0.52
1:A:50:GLU:O	1:A:151:GLN:NE2	2.42	0.52
1:A:60:VAL:HG22	1:A:117:VAL:HG11	1.91	0.52
1:A:149:ALA:O	1:A:153:ARG:HB2	2.10	0.52
3:F:180:ARG:HG2	3:F:194:ARG:HG2	1.91	0.52
3:D:252:LEU:HD23	3:D:254:LYS:H	1.74	0.52
3:F:249:GLU:HB2	3:F:264:THR:HG23	1.92	0.52
3:D:44:MET:HG2	3:D:112:VAL:HG22	1.91	0.52
3:C:66:LYS:NZ	6:L:149:GLN:O	2.43	0.52
3:E:180:ARG:HG2	3:E:194:ARG:HG2	1.91	0.52
2:B:172:ASN:OD1	2:B:175:ARG:NH2	2.39	0.52
1:A:222:ARG:HD2	1:A:232:PHE:HZ	1.73	0.52
1:A:373:THR:O	1:A:377:ARG:CB	2.58	0.52
2:B:88:LEU:HG	3:H:308:THR:HG22	1.91	0.52
1:A:53:LEU:O	1:A:57:ALA:HB2	2.10	0.52
3:D:250:LEU:HD13	3:E:95:LEU:CG	2.40	0.52
2:B:189:ARG:NH1	2:B:288:GLU:OE2	2.43	0.52
3:E:180:ARG:HG2	3:E:194:ARG:HG2	1.91	0.52
1:A:55:ASP:OD1	1:A:58:ARG:NH2	2.43	0.52
3:E:82:ASP:O	3:E:86:LEU:CB	2.58	0.52
3:C:44:MET:HG2	3:C:112:VAL:HG22	1.91	0.52
3:E:128:CYS:SG	3:E:129:ASN:N	2.81	0.52
3:F:128:CYS:SG	3:F:129:ASN:N	2.81	0.52
3:C:203:ARG:NH2	6:L:11:PRO:O	2.43	0.52
3:G:277:GLN:NE2	7:M:15:G:OP2	2.38	0.52
2:B:19:ASN:HA	2:B:142:GLY:HA3	1.91	0.52
3:E:180:ARG:HG2	3:E:194:ARG:HG2	1.91	0.52
3:G:180:ARG:HG2	3:G:194:ARG:HG2	1.91	0.52
2:B:20:ALA:HB3	2:B:103:ALA:HB3	1.90	0.52
3:C:249:GLU:HB2	3:C:264:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:180:ARG:HG2	3:G:194:ARG:HG2	1.91	0.52
3:G:180:ARG:HG2	3:G:194:ARG:HG2	1.91	0.51
2:B:34:PRO:HB2	2:B:316:TRP:HZ2	1.74	0.51
3:G:69:ARG:O	7:M:19:G:O2'	2.27	0.51
1:A:269:PRO:HD3	2:B:31:PHE:HB2	1.92	0.51
5:K:41:TYR:O	5:K:48:VAL:HA	2.10	0.51
2:B:11:LEU:HD11	2:B:180:LEU:HD21	1.91	0.51
3:H:75:ARG:HD2	3:H:86:LEU:HB3	1.92	0.51
5:K:50:ILE:O	5:K:56:GLN:HA	2.10	0.51
1:A:119:LYS:NZ	5:K:35:GLY:O	2.42	0.51
3:D:169:ARG:NH1	7:M:35:U:OP1	2.43	0.51
3:G:249:GLU:HB2	3:G:264:THR:HG23	1.92	0.51
3:C:250:LEU:HA	7:M:39:U:H5	1.74	0.51
3:D:69:ARG:HD2	7:M:39:U:H1'	1.91	0.51
3:F:44:MET:HG2	3:F:112:VAL:HG22	1.91	0.51
1:A:55:ASP:OD1	1:A:58:ARG:NH2	2.43	0.51
3:C:277:GLN:HE22	3:D:66:LYS:HE3	1.76	0.51
1:A:259:ARG:HH22	4:J:75:ARG:HG3	1.75	0.51
3:G:277:GLN:HB3	7:M:14:G:H5''	1.92	0.51
3:C:55:SER:O	3:C:111:LYS:NZ	2.44	0.51
3:D:249:GLU:HB2	3:D:264:THR:HG23	1.92	0.51
3:H:55:SER:O	3:H:111:LYS:NZ	2.44	0.51
3:D:77:LYS:O	3:D:81:ARG:NE	2.44	0.51
3:H:262:SER:OG	4:J:13:ASN:ND2	2.40	0.51
3:F:165:ARG:NH1	3:F:285:THR:OG1	2.42	0.51
3:G:278:LYS:NZ	7:M:16:C:OP1	2.35	0.51
1:A:322:ARG:HB3	1:A:414:TRP:HZ3	1.76	0.51
3:F:324:TYR:OH	3:G:73:SER:O	2.29	0.51
1:A:178:LEU:HD22	7:M:2:U:H5''	1.92	0.51
1:A:256:ASN:HD22	5:K:33:TRP:HB2	1.76	0.51
1:A:251:ILE:HB	1:A:255:ASN:HD22	1.76	0.51
1:A:356:HIS:O	1:A:360:GLN:CB	2.59	0.51
3:C:203:ARG:NH2	6:L:11:PRO:O	2.44	0.51
3:E:261:LYS:HD2	3:E:264:THR:HG22	1.92	0.51
2:B:20:ALA:HB3	2:B:103:ALA:HB3	1.93	0.50
3:C:165:ARG:HA	3:C:168:TRP:HB2	1.93	0.50
3:E:165:ARG:HA	3:E:168:TRP:HB2	1.93	0.50
4:J:71:GLU:OE2	4:J:74:ARG:NH2	2.38	0.50
1:A:285:SER:O	1:A:289:HIS:CB	2.59	0.50
1:A:285:SER:O	1:A:289:HIS:CB	2.60	0.50
2:B:125:GLU:OE2	2:B:128:ARG:NH2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:165:ARG:HA	3:D:168:TRP:HB2	1.93	0.50
3:H:165:ARG:HA	3:H:168:TRP:HB2	1.93	0.50
3:E:257:LYS:HG2	3:E:259:GLY:H	1.76	0.50
1:A:70:LEU:HD12	1:A:73:ILE:HD12	1.93	0.50
5:K:50:ILE:O	5:K:56:GLN:HA	2.11	0.50
3:D:250:LEU:HG	3:D:252:LEU:HD23	1.92	0.50
3:F:165:ARG:HA	3:F:168:TRP:HB2	1.93	0.50
2:B:247:TRP:HD1	2:B:289:TRP:HB2	1.76	0.50
1:A:215:ALA:O	1:A:219:ARG:HB3	2.11	0.50
1:A:43:LEU:O	1:A:47:HIS:CB	2.59	0.50
5:K:79:ARG:HA	5:K:82:GLU:HB3	1.93	0.50
3:H:262:SER:OG	4:J:13:ASN:ND2	2.37	0.50
5:K:41:TYR:O	5:K:48:VAL:HA	2.11	0.50
2:B:185:ALA:HB1	2:B:301:LEU:HD11	1.94	0.50
3:D:356:GLY:H	3:E:75:ARG:HH21	1.59	0.50
1:A:44:LEU:O	1:A:48:ARG:CB	2.60	0.50
3:G:277:GLN:HE22	3:H:68:VAL:HG12	1.77	0.50
4:I:71:GLU:OE2	4:I:74:ARG:NH2	2.38	0.50
1:A:70:LEU:HD12	1:A:73:ILE:HD12	1.94	0.50
3:D:305:GLY:O	3:D:314:TYR:HB2	2.12	0.50
3:E:55:SER:O	3:E:111:LYS:NZ	2.44	0.50
1:A:239:ALA:HB3	1:A:264:LEU:HB2	1.93	0.50
2:B:55:GLU:HB3	2:B:114:HIS:HB2	1.94	0.50
3:E:305:GLY:O	3:E:314:TYR:HB2	2.12	0.50
3:F:68:VAL:HG13	3:F:96:GLN:HB2	1.94	0.50
2:B:278:ARG:HH22	2:B:312:GLY:HA2	1.77	0.50
4:J:20:TYR:HB2	4:J:27:LYS:HB3	1.93	0.50
3:D:312:LYS:HD3	3:E:86:LEU:HD11	1.94	0.49
3:G:55:SER:O	3:G:111:LYS:NZ	2.44	0.49
2:B:278:ARG:HH22	2:B:312:GLY:HA2	1.76	0.49
3:G:69:ARG:O	7:M:19:G:O2'	2.29	0.49
3:G:165:ARG:HA	3:G:168:TRP:HB2	1.93	0.49
1:A:410:GLU:O	1:A:414:TRP:HB2	2.11	0.49
1:A:117:VAL:O	1:A:120:PHE:HB3	2.12	0.49
1:A:178:LEU:HD22	7:M:2:U:H5''	1.93	0.49
2:B:10:LEU:HB3	2:B:111:LEU:HB2	1.95	0.49
1:A:55:ASP:OD1	1:A:58:ARG:NH1	2.43	0.49
3:C:165:ARG:NH1	3:C:285:THR:OG1	2.42	0.49
3:D:76:LEU:HB2	3:D:81:ARG:HE	1.77	0.49
3:C:305:GLY:O	3:C:314:TYR:HB2	2.12	0.49
3:H:305:GLY:O	3:H:314:TYR:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLN:HG3	2:B:156:ASN:HD21	1.76	0.49
2:B:10:LEU:HD23	2:B:111:LEU:HD12	1.93	0.49
2:B:17:ILE:HB	2:B:105:LEU:HB2	1.94	0.49
4:J:17:ILE:HG12	4:J:30:VAL:HG22	1.94	0.49
1:A:48:ARG:O	1:A:52:TRP:CB	2.60	0.49
3:G:87:ASP:O	3:G:91:GLN:CB	2.60	0.49
1:A:434:ASP:OXT	2:B:178:ARG:NH1	2.45	0.49
1:A:319:ARG:HA	1:A:322:ARG:HE	1.77	0.49
1:A:178:LEU:HD12	7:M:2:U:H5''	1.94	0.49
3:E:304:TYR:HE2	3:F:73:SER:HB3	1.76	0.49
3:G:305:GLY:O	3:G:314:TYR:HB2	2.12	0.49
1:A:43:LEU:O	1:A:47:HIS:CB	2.61	0.49
2:B:34:PRO:HB2	2:B:316:TRP:HZ2	1.77	0.49
1:A:44:LEU:O	1:A:48:ARG:CB	2.60	0.49
3:D:77:LYS:O	3:D:81:ARG:NE	2.45	0.49
1:A:431:ASP:OD2	2:B:174:ARG:NH1	2.41	0.49
3:G:32:ALA:HB1	7:M:11:C:H1'	1.93	0.49
4:I:17:ILE:HG12	4:I:30:VAL:HG22	1.94	0.49
3:D:308:THR:HG21	3:E:69:ARG:HH12	1.78	0.49
2:B:119:ASP:HB3	2:B:122:PRO:HD2	1.94	0.49
1:A:287:PHE:O	1:A:291:PHE:CB	2.60	0.49
3:H:32:ALA:HB1	7:M:5:G:H1'	1.95	0.49
4:I:20:TYR:HB2	4:I:27:LYS:HB3	1.93	0.49
3:F:115:THR:OG1	3:G:242:GLN:NE2	2.45	0.49
2:B:21:ASN:ND2	7:M:4:A:OP1	2.46	0.49
1:A:82:LEU:HD11	2:B:279:PHE:HD2	1.77	0.49
1:A:216:LYS:O	1:A:220:GLU:CB	2.61	0.49
1:A:70:LEU:HD22	1:A:73:ILE:HD12	1.95	0.49
3:F:115:THR:OG1	3:G:242:GLN:NE2	2.43	0.49
2:B:185:ALA:HB1	2:B:301:LEU:HD11	1.95	0.49
2:B:54:ILE:HA	2:B:115:GLY:HA3	1.95	0.49
2:B:54:ILE:HA	2:B:115:GLY:HA3	1.95	0.49
3:D:356:GLY:H	3:E:75:ARG:HH21	1.59	0.49
3:E:76:LEU:HD21	3:E:85:LYS:HG2	1.94	0.49
3:F:308:THR:HG21	3:G:69:ARG:HH12	1.77	0.49
3:F:305:GLY:O	3:F:314:TYR:HB2	2.12	0.48
1:A:26:GLN:O	1:A:30:ASP:CB	2.61	0.48
1:A:67:THR:HG23	1:A:68:HIS:CD2	2.49	0.48
2:B:64:HIS:ND1	2:B:182:PRO:O	2.43	0.48
3:F:55:SER:O	3:F:111:LYS:NZ	2.44	0.48
3:H:165:ARG:NH1	3:H:285:THR:OG1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:HD13	1:A:263:TRP:HB3	1.94	0.48
1:A:70:LEU:HD12	1:A:73:ILE:HD12	1.96	0.48
5:K:84:SER:O	5:K:88:ARG:CB	2.58	0.48
2:B:55:GLU:HB3	2:B:114:HIS:HB2	1.95	0.48
3:F:308:THR:HG21	3:G:69:ARG:HH12	1.78	0.48
1:A:296:GLU:O	1:A:300:LEU:CB	2.61	0.48
4:I:20:TYR:HB2	4:I:27:LYS:HB3	1.95	0.48
3:E:119:LEU:HD22	3:F:172:VAL:HG12	1.96	0.48
4:I:17:ILE:HG12	4:I:30:VAL:HG22	1.96	0.48
3:G:281:ASN:HB2	7:M:14:G:H5'	1.96	0.48
1:A:190:LEU:HD13	2:B:280:VAL:HG11	1.95	0.48
3:C:275:HIS:HD2	3:D:66:LYS:HD2	1.79	0.48
3:D:278:LYS:NZ	7:M:34:C:OP1	2.38	0.48
3:D:55:SER:O	3:D:111:LYS:NZ	2.44	0.48
1:A:216:LYS:O	1:A:220:GLU:CB	2.61	0.48
2:B:247:TRP:HD1	2:B:289:TRP:HB2	1.78	0.48
1:A:411:ALA:O	1:A:415:SER:CB	2.61	0.48
2:B:131:GLN:HG3	2:B:156:ASN:HD21	1.78	0.48
3:D:246:PRO:CG	3:D:265:LEU:HD13	2.24	0.48
3:F:324:TYR:OH	3:G:73:SER:O	2.32	0.48
3:G:129:ASN:ND2	3:H:311:GLY:HA3	2.29	0.48
3:H:262:SER:HG	4:J:13:ASN:HD21	1.55	0.48
1:A:256:ASN:HD22	5:K:33:TRP:HB2	1.79	0.48
4:J:20:TYR:HB2	4:J:27:LYS:HB3	1.95	0.48
3:E:277:GLN:HE22	3:F:68:VAL:HG22	1.79	0.48
1:A:137:ASP:HA	1:A:156:ARG:HH12	1.79	0.48
1:A:129:ASN:O	1:A:133:TRP:CB	2.62	0.48
1:A:395:LEU:O	1:A:399:VAL:N	2.47	0.48
3:C:356:GLY:H	3:D:75:ARG:HE	1.62	0.48
3:F:246:PRO:HG2	3:F:265:LEU:HD22	1.96	0.48
1:A:234:GLU:OE2	2:B:77:ARG:NH1	2.44	0.48
3:H:95:LEU:O	4:J:13:ASN:N	2.45	0.48
1:A:216:LYS:O	1:A:220:GLU:HB2	2.14	0.48
2:B:27:LEU:HD12	2:B:284:PHE:HE2	1.79	0.48
3:E:246:PRO:HG2	3:E:265:LEU:HD22	1.96	0.48
4:J:17:ILE:HG12	4:J:30:VAL:HG22	1.96	0.48
2:B:72:GLN:HG3	2:B:74:ALA:H	1.79	0.47
1:A:121:LEU:O	1:A:124:GLN:HB3	2.14	0.47
3:E:250:LEU:HA	7:M:27:U:H5	1.79	0.47
3:F:69:ARG:HB3	7:M:26:G:H3'	1.96	0.47
1:A:13:LEU:HB3	1:A:144:ALA:HB1	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:O	1:A:154:GLU:CB	2.62	0.47
2:B:247:TRP:HD1	2:B:289:TRP:HB2	1.79	0.47
3:G:246:PRO:HG2	3:G:265:LEU:HD22	1.96	0.47
3:D:97:THR:O	3:D:262:SER:OG	2.26	0.47
3:E:76:LEU:HD11	3:E:86:LEU:HD21	1.96	0.47
1:A:148:ASN:O	1:A:152:ALA:N	2.45	0.47
2:B:148:CYS:O	2:B:152:PHE:N	2.47	0.47
1:A:287:PHE:O	1:A:291:PHE:CB	2.62	0.47
1:A:59:ARG:HH21	1:A:62:GLN:HE22	1.62	0.47
3:D:251:ILE:HD11	3:D:264:THR:H	1.79	0.47
1:A:177:GLN:O	2:B:271:ARG:NH1	2.47	0.47
3:G:117:ARG:HG3	3:H:242:GLN:HE22	1.79	0.47
1:A:279:ALA:HB3	1:A:346:GLY:HA3	1.97	0.47
3:C:119:LEU:HD22	3:D:172:VAL:HG12	1.95	0.47
1:A:39:LYS:O	1:A:43:LEU:CB	2.62	0.47
1:A:411:ALA:HA	1:A:414:TRP:HB3	1.97	0.47
3:H:32:ALA:HB1	7:M:5:G:H1'	1.96	0.47
1:A:53:LEU:O	1:A:57:ALA:CB	2.62	0.47
3:D:97:THR:OG1	3:D:260:GLN:O	2.25	0.47
2:B:25:SER:HG	2:B:28:THR:HG1	1.63	0.47
3:E:278:LYS:NZ	7:M:26:G:N3	2.63	0.47
3:G:255:GLY:HA2	3:G:260:GLN:HB2	1.97	0.47
3:G:35:ARG:NH2	3:H:243:GLU:OE1	2.47	0.47
1:A:177:GLN:O	2:B:271:ARG:NH1	2.47	0.47
1:A:216:LYS:O	1:A:220:GLU:CB	2.62	0.47
2:B:21:ASN:ND2	7:M:4:A:OP1	2.46	0.47
1:A:422:LEU:O	1:A:426:LYS:HB2	2.14	0.47
3:E:251:ILE:HD12	3:E:264:THR:HG21	1.95	0.47
3:G:55:SER:HA	3:G:58:TRP:HE1	1.80	0.47
3:H:109:THR:HA	3:H:236:ALA:O	2.15	0.47
3:H:246:PRO:HG2	3:H:265:LEU:HD22	1.96	0.47
1:A:171:SER:OG	1:A:177:GLN:NE2	2.48	0.47
1:A:315:ASN:O	1:A:319:ARG:CB	2.62	0.47
1:A:339:ARG:O	1:A:343:LEU:CB	2.63	0.47
3:D:117:ARG:HG3	3:E:242:GLN:HE22	1.79	0.47
3:F:24:ILE:HG13	3:F:24:ILE:O	2.14	0.47
1:A:296:GLU:O	1:A:300:LEU:CB	2.61	0.47
5:K:82:GLU:HB2	5:K:85:GLU:HB2	1.97	0.47
2:B:185:ALA:HB1	2:B:301:LEU:HD11	1.96	0.47
1:A:267:SER:N	2:B:29:TRP:O	2.33	0.47
3:E:109:THR:HA	3:E:236:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:SER:HA	3:C:58:TRP:HE1	1.80	0.47
3:H:96:GLN:NE2	4:J:13:ASN:OD1	2.39	0.46
4:I:42:ARG:NH2	4:I:71:GLU:O	2.48	0.46
4:J:42:ARG:NH2	4:J:71:GLU:O	2.48	0.46
1:A:315:ASN:O	1:A:319:ARG:CB	2.63	0.46
2:B:72:GLN:HG2	2:B:78:THR:HB	1.97	0.46
3:E:55:SER:HA	3:E:58:TRP:HE1	1.80	0.46
3:F:278:LYS:NZ	7:M:20:C:O2	2.47	0.46
3:E:103:LEU:HD11	3:E:238:ILE:HD11	1.98	0.46
1:A:60:VAL:HG22	1:A:162:ILE:HB	1.97	0.46
2:B:167:GLU:O	2:B:171:LYS:CB	2.61	0.46
3:G:109:THR:HA	3:G:236:ALA:O	2.16	0.46
3:H:109:THR:HA	3:H:236:ALA:O	2.16	0.46
3:G:35:ARG:HB3	7:M:12:A:H5"	1.97	0.46
3:F:109:THR:HA	3:F:236:ALA:O	2.16	0.46
3:F:69:ARG:HA	3:F:94:ASN:O	2.16	0.46
3:D:55:SER:HA	3:D:58:TRP:HE1	1.80	0.46
3:D:277:GLN:HB3	7:M:32:G:H5"	1.96	0.46
3:D:76:LEU:HD13	3:D:81:ARG:HG3	1.98	0.46
1:A:91:GLN:HG3	1:A:94:LEU:HD12	1.98	0.46
2:B:10:LEU:HB3	2:B:111:LEU:HB2	1.98	0.46
3:H:103:LEU:HD11	3:H:238:ILE:HD11	1.98	0.46
2:B:295:VAL:HG21	2:B:301:LEU:HD22	1.98	0.46
3:C:109:THR:HA	3:C:236:ALA:O	2.16	0.46
1:A:282:ARG:O	1:A:286:VAL:N	2.48	0.46
3:F:109:THR:HA	3:F:236:ALA:O	2.15	0.46
2:B:62:VAL:HG21	2:B:180:LEU:HD22	1.96	0.46
3:D:109:THR:HA	3:D:236:ALA:O	2.15	0.46
2:B:167:GLU:O	2:B:171:LYS:CB	2.64	0.46
2:B:222:GLU:OE2	2:B:240:GLN:NE2	2.44	0.46
3:E:275:HIS:HD2	3:F:66:LYS:HD2	1.80	0.46
1:A:311:THR:O	1:A:315:ASN:N	2.49	0.46
3:D:109:THR:HA	3:D:236:ALA:O	2.16	0.46
2:B:27:LEU:HD12	2:B:284:PHE:HE2	1.81	0.46
3:C:246:PRO:HG2	3:C:265:LEU:HD22	1.96	0.46
1:A:410:GLU:O	1:A:414:TRP:CB	2.64	0.46
2:B:162:LEU:O	2:B:169:ARG:NH2	2.45	0.46
3:D:69:ARG:HD3	7:M:39:U:H1'	1.96	0.46
3:C:103:LEU:HD11	3:C:238:ILE:HD11	1.98	0.46
1:A:434:ASP:OXT	2:B:178:ARG:NH1	2.48	0.46
3:G:42:ALA:HB2	3:G:274:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:HD22	2:B:216:LEU:HD13	1.96	0.46
3:G:324:TYR:OH	3:H:73:SER:O	2.34	0.46
3:G:281:ASN:HB2	7:M:14:G:H5'	1.98	0.46
1:A:332:GLU:OE2	1:A:339:ARG:NH2	2.47	0.46
3:G:103:LEU:HD11	3:G:238:ILE:HD11	1.98	0.46
1:A:82:LEU:HD22	2:B:279:PHE:HD2	1.81	0.46
3:G:281:ASN:HB2	7:M:14:G:H5'	1.98	0.46
1:A:82:LEU:HD22	2:B:279:PHE:HD2	1.80	0.46
3:F:302:GLU:OE1	3:F:351:ARG:NH2	2.49	0.46
3:G:302:GLU:OE1	3:G:351:ARG:NH2	2.49	0.46
3:H:302:GLU:OE1	3:H:351:ARG:NH2	2.49	0.46
3:C:109:THR:HA	3:C:236:ALA:O	2.15	0.46
3:G:109:THR:HA	3:G:236:ALA:O	2.15	0.46
3:F:278:LYS:NZ	7:M:22:U:OP1	2.37	0.46
1:A:190:LEU:HD21	2:B:314:TYR:HE2	1.81	0.46
2:B:72:GLN:HG2	2:B:78:THR:HB	1.98	0.46
3:F:33:PHE:HZ	3:F:137:LEU:HD21	1.81	0.46
2:B:62:VAL:HG21	2:B:180:LEU:HD22	1.98	0.46
2:B:167:GLU:O	2:B:171:LYS:CB	2.62	0.46
3:H:42:ALA:HB2	3:H:274:ILE:HG12	1.98	0.46
2:B:162:LEU:O	2:B:169:ARG:NH2	2.45	0.46
3:D:246:PRO:CG	3:D:265:LEU:CD2	2.67	0.46
1:A:44:LEU:O	1:A:48:ARG:CB	2.65	0.45
2:B:131:GLN:HG3	2:B:156:ASN:HD21	1.80	0.45
3:H:302:GLU:OE1	3:H:351:ARG:NH2	2.49	0.45
3:C:302:GLU:OE1	3:C:351:ARG:NH2	2.49	0.45
3:F:42:ALA:HB2	3:F:274:ILE:HG12	1.98	0.45
1:A:219:ARG:NH2	1:A:234:GLU:OE1	2.40	0.45
3:F:55:SER:HA	3:F:58:TRP:HE1	1.80	0.45
1:A:304:LEU:HG	1:A:399:VAL:HG21	1.99	0.45
2:B:15:LEU:O	2:B:106:GLU:HA	2.16	0.45
3:E:109:THR:HA	3:E:236:ALA:O	2.16	0.45
3:E:117:ARG:HG3	3:F:242:GLN:HE22	1.82	0.45
3:F:302:GLU:OE1	3:F:351:ARG:NH2	2.49	0.45
3:F:110:LEU:HD13	3:F:244:VAL:HG11	1.99	0.45
3:C:313:ALA:HB2	3:D:90:ILE:HD11	1.98	0.45
3:C:302:GLU:OE1	3:C:351:ARG:NH2	2.49	0.45
2:B:295:VAL:HG21	2:B:301:LEU:HD22	1.99	0.45
3:E:42:ALA:HB2	3:E:274:ILE:HG12	1.98	0.45
3:E:302:GLU:OE1	3:E:351:ARG:NH2	2.49	0.45
3:E:340:GLU:HA	3:E:343:HIS:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:55:SER:HA	3:H:58:TRP:HE1	1.80	0.45
3:F:168:TRP:CD1	3:F:171:ARG:HB3	2.52	0.45
1:A:13:LEU:HD23	1:A:144:ALA:HA	1.98	0.45
1:A:311:THR:O	1:A:315:ASN:N	2.49	0.45
3:C:110:LEU:HD13	3:C:244:VAL:HG11	1.98	0.45
2:B:65:ARG:HB2	2:B:106:GLU:HB3	1.98	0.45
3:D:356:GLY:O	3:E:75:ARG:NE	2.50	0.45
3:H:168:TRP:CD1	3:H:171:ARG:HB3	2.52	0.45
3:E:33:PHE:HZ	3:E:137:LEU:HD21	1.81	0.45
3:E:302:GLU:OE1	3:E:351:ARG:NH2	2.49	0.45
3:C:42:ALA:HB2	3:C:274:ILE:HG12	1.98	0.45
3:C:165:ARG:NH2	3:C:202:LEU:O	2.50	0.45
3:D:110:LEU:HD13	3:D:244:VAL:HG11	1.98	0.45
3:D:165:ARG:NH2	3:D:202:LEU:O	2.50	0.45
3:G:165:ARG:NH1	3:G:285:THR:OG1	2.42	0.45
3:H:248:GLN:HE21	3:H:250:LEU:HB3	1.82	0.45
2:B:41:VAL:HG21	2:B:59:VAL:HB	1.98	0.45
1:A:189:LEU:HD21	2:B:271:ARG:HB2	1.98	0.45
2:B:162:LEU:O	2:B:169:ARG:NH2	2.49	0.45
3:D:168:TRP:CD1	3:D:171:ARG:HB3	2.52	0.45
1:A:282:ARG:O	1:A:286:VAL:N	2.50	0.45
3:G:47:GLY:HA3	3:G:56:GLN:HB3	1.99	0.45
3:H:47:GLY:HA3	3:H:56:GLN:HB3	1.99	0.45
3:H:33:PHE:HZ	3:H:137:LEU:HD21	1.82	0.45
1:A:130:LEU:O	1:A:134:LEU:CB	2.65	0.45
3:D:340:GLU:HA	3:D:343:HIS:HD2	1.82	0.45
5:K:30:ASP:HB2	5:K:40:LYS:HB2	1.99	0.45
3:F:103:LEU:HD11	3:F:238:ILE:HD11	1.98	0.45
3:F:27:THR:HG23	3:F:332:LEU:HD11	1.97	0.45
3:F:76:LEU:HB3	3:F:78:THR:HG23	1.99	0.45
3:H:165:ARG:NH2	3:H:202:LEU:O	2.50	0.45
2:B:136:ALA:HA	3:H:117:ARG:NH1	2.32	0.45
2:B:248:LEU:HD23	2:B:288:GLU:HB3	1.98	0.45
3:C:304:TYR:O	3:C:306:SER:N	2.50	0.45
3:F:73:SER:OG	3:F:75:ARG:NE	2.50	0.45
3:C:33:PHE:HZ	3:C:137:LEU:HD21	1.81	0.45
3:G:297:GLY:HA3	3:G:298:PRO:HD3	1.85	0.45
3:G:302:GLU:OE1	3:G:351:ARG:NH2	2.49	0.45
3:H:33:PHE:HZ	3:H:137:LEU:HD21	1.81	0.45
3:D:33:PHE:HZ	3:D:137:LEU:HD21	1.82	0.45
3:D:302:GLU:OE1	3:D:351:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:O	1:A:299:ARG:HB2	2.16	0.45
3:F:249:GLU:HG3	7:M:22:U:H6	1.82	0.45
3:H:32:ALA:HB1	7:M:5:G:H1'	1.99	0.45
3:D:103:LEU:HD11	3:D:238:ILE:HD11	1.98	0.45
3:D:304:TYR:O	3:D:306:SER:N	2.50	0.45
3:E:168:TRP:CD1	3:E:171:ARG:HB3	2.52	0.45
3:H:68:VAL:HG22	3:H:96:GLN:HB2	1.99	0.45
3:D:302:GLU:OE1	3:D:351:ARG:NH2	2.49	0.45
3:G:33:PHE:HZ	3:G:137:LEU:HD21	1.81	0.45
3:G:47:GLY:HA3	3:G:56:GLN:HB3	1.99	0.45
3:H:289:TRP:CD1	3:H:340:GLU:HG3	2.52	0.45
1:A:218:ALA:O	1:A:222:ARG:HB2	2.17	0.45
3:D:165:ARG:NH1	3:D:285:THR:OG1	2.42	0.45
3:E:165:ARG:NH2	3:E:202:LEU:O	2.50	0.45
3:G:248:GLN:HE21	3:G:250:LEU:HB3	1.82	0.45
3:H:103:LEU:HD11	3:H:238:ILE:HD11	1.99	0.45
1:A:338:ALA:HB2	2:B:181:LEU:HG	1.99	0.45
3:G:284:ARG:NH2	7:M:14:G:OP2	2.50	0.45
1:A:149:ALA:HA	1:A:152:ALA:HB3	1.99	0.45
2:B:169:ARG:O	2:B:173:GLN:CB	2.65	0.45
1:A:47:HIS:HA	1:A:51:ALA:HB3	1.99	0.45
1:A:281:MET:HG3	1:A:350:THR:H	1.82	0.45
3:H:47:GLY:HA3	3:H:56:GLN:HB3	1.99	0.45
3:D:103:LEU:HD11	3:D:238:ILE:HD11	1.99	0.45
2:B:124:GLN:O	2:B:128:ARG:CB	2.65	0.44
3:F:304:TYR:O	3:F:306:SER:N	2.50	0.44
3:D:297:GLY:HA3	3:D:298:PRO:HD3	1.85	0.44
3:D:42:ALA:HB2	3:D:274:ILE:HG12	1.98	0.44
3:D:69:ARG:O	7:M:37:C:O2'	2.35	0.44
3:F:289:TRP:CD1	3:F:340:GLU:HG3	2.52	0.44
1:A:216:LYS:O	1:A:220:GLU:HB3	2.16	0.44
2:B:131:GLN:HE22	2:B:155:PRO:HA	1.81	0.44
3:F:340:GLU:HA	3:F:343:HIS:HD2	1.82	0.44
3:G:103:LEU:HD11	3:G:238:ILE:HD11	1.99	0.44
1:A:215:ALA:O	1:A:219:ARG:CB	2.65	0.44
3:H:304:TYR:O	3:H:306:SER:N	2.50	0.44
3:D:33:PHE:HZ	3:D:137:LEU:HD21	1.81	0.44
3:D:47:GLY:HA3	3:D:56:GLN:HB3	1.99	0.44
3:G:289:TRP:CD1	3:G:340:GLU:HG3	2.52	0.44
3:C:340:GLU:HA	3:C:343:HIS:HD2	1.82	0.44
3:F:248:GLN:HE21	3:F:250:LEU:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:246:PRO:O	3:C:248:GLN:N	2.51	0.44
3:H:246:PRO:O	3:H:248:GLN:N	2.51	0.44
3:E:307:VAL:HG12	3:E:310:GLN:H	1.83	0.44
2:B:192:LEU:O	2:B:195:GLN:HB3	2.18	0.44
3:G:165:ARG:NH2	3:G:202:LEU:O	2.50	0.44
1:A:411:ALA:O	1:A:415:SER:CB	2.65	0.44
2:B:11:LEU:HD11	2:B:180:LEU:HD21	1.99	0.44
2:B:124:GLN:HE21	2:B:128:ARG:HD3	1.82	0.44
1:A:64:GLN:HG2	1:A:66:VAL:HG13	1.99	0.44
2:B:34:PRO:HB3	2:B:252:PRO:HD2	2.00	0.44
3:C:33:PHE:HZ	3:C:137:LEU:HD21	1.82	0.44
3:E:110:LEU:HD13	3:E:244:VAL:HG11	1.98	0.44
2:B:89:ASN:HB3	2:B:93:SER:H	1.82	0.44
2:B:125:GLU:O	2:B:129:GLN:HB2	2.16	0.44
3:D:246:PRO:O	3:D:248:GLN:N	2.51	0.44
3:F:69:ARG:HA	3:F:94:ASN:O	2.17	0.44
1:A:64:GLN:HG2	1:A:66:VAL:HG13	2.00	0.44
1:A:326:VAL:HA	1:A:329:ILE:HG22	1.98	0.44
3:E:289:TRP:CD1	3:E:340:GLU:HG3	2.52	0.44
3:F:33:PHE:HZ	3:F:137:LEU:HD21	1.82	0.44
3:E:248:GLN:HE21	3:E:250:LEU:HB3	1.82	0.44
3:C:306:SER:HA	3:C:313:ALA:HA	2.00	0.44
3:H:340:GLU:HA	3:H:343:HIS:HD2	1.83	0.44
1:A:326:VAL:HA	1:A:329:ILE:HG22	1.99	0.44
1:A:419:SER:O	1:A:423:THR:CB	2.66	0.44
1:A:91:GLN:HG3	1:A:94:LEU:HD12	1.99	0.44
1:A:190:LEU:HD21	2:B:314:TYR:HE2	1.82	0.44
3:C:289:TRP:CD1	3:C:340:GLU:HG3	2.52	0.44
3:C:307:VAL:HG12	3:C:310:GLN:H	1.83	0.44
3:D:47:GLY:HA3	3:D:56:GLN:HB3	1.99	0.44
1:A:91:GLN:OE1	2:B:315:ARG:NH1	2.51	0.44
3:F:42:ALA:HB2	3:F:279:ILE:HD11	2.00	0.44
3:F:165:ARG:NH2	3:F:202:LEU:O	2.50	0.44
1:A:64:GLN:HG2	1:A:66:VAL:HG13	1.99	0.44
1:A:67:THR:HG22	1:A:83:HIS:HA	1.98	0.44
1:A:190:LEU:HD11	2:B:314:TYR:HE2	1.82	0.44
3:C:268:VAL:HG12	3:D:64:ARG:HH12	1.83	0.44
3:C:168:TRP:CD1	3:C:171:ARG:HB3	2.52	0.44
3:F:110:LEU:HD13	3:F:244:VAL:HG11	2.00	0.44
3:G:168:TRP:CD1	3:G:171:ARG:HB3	2.52	0.44
3:C:307:VAL:HG12	3:C:310:GLN:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:VAL:HG13	3:D:96:GLN:HB2	1.99	0.44
3:G:307:VAL:HG12	3:G:310:GLN:H	1.83	0.44
2:B:244:LYS:HE2	2:B:248:LEU:H	1.82	0.44
3:E:33:PHE:HZ	3:E:137:LEU:HD21	1.82	0.44
3:C:248:GLN:HE21	3:C:250:LEU:HB3	1.82	0.44
3:H:340:GLU:HA	3:H:343:HIS:HD2	1.82	0.44
2:B:248:LEU:HB3	2:B:286:LEU:HD11	1.98	0.44
3:E:110:LEU:HD13	3:E:244:VAL:HG11	2.00	0.44
3:G:246:PRO:O	3:G:248:GLN:N	2.51	0.44
3:F:47:GLY:HA3	3:F:56:GLN:HB3	1.99	0.44
3:D:42:ALA:HB2	3:D:279:ILE:HD11	2.00	0.44
3:E:103:LEU:HD11	3:E:238:ILE:HD11	1.99	0.44
3:E:165:ARG:NH1	3:E:285:THR:OG1	2.42	0.44
3:G:110:LEU:HD13	3:G:244:VAL:HG11	1.98	0.44
1:A:241:GLN:HB3	1:A:262:ASN:O	2.18	0.44
2:B:257:ALA:HB2	2:B:280:VAL:HG12	1.99	0.44
2:B:124:GLN:O	2:B:128:ARG:HB3	2.17	0.44
3:G:110:LEU:HD13	3:G:244:VAL:HG11	2.00	0.44
3:G:304:TYR:O	3:G:306:SER:N	2.50	0.44
3:C:98:VAL:HG21	6:L:152:GLY:H	1.82	0.44
3:E:85:LYS:O	3:E:89:SER:HB3	2.18	0.44
3:E:307:VAL:HG12	3:E:310:GLN:H	1.83	0.44
3:F:47:GLY:HA3	3:F:56:GLN:HB3	1.99	0.44
1:A:53:LEU:O	1:A:57:ALA:CB	2.65	0.44
1:A:187:TYR:OH	2:B:46:ARG:NH1	2.47	0.44
1:A:338:ALA:HB1	2:B:182:PRO:HD3	1.99	0.44
3:H:249:GLU:HB2	7:M:9:U:C6	2.53	0.44
2:B:70:ILE:HD12	2:B:79:LYS:HD3	2.01	0.43
3:C:340:GLU:HA	3:C:343:HIS:HD2	1.83	0.43
3:E:304:TYR:O	3:E:306:SER:N	2.50	0.43
3:H:306:SER:HA	3:H:313:ALA:HA	2.00	0.43
3:E:47:GLY:HA3	3:E:56:GLN:HB3	1.99	0.43
3:D:289:TRP:CD1	3:D:340:GLU:HG3	2.52	0.43
2:B:123:ALA:O	2:B:126:ILE:HB	2.17	0.43
3:G:340:GLU:HA	3:G:343:HIS:HD2	1.82	0.43
3:D:83:PRO:HA	3:D:86:LEU:HB2	1.99	0.43
3:H:96:GLN:NE2	4:J:13:ASN:OD1	2.41	0.43
1:A:195:PRO:HB2	1:A:198:LEU:HB3	2.00	0.43
3:H:42:ALA:HB2	3:H:279:ILE:HD11	2.00	0.43
2:B:63:CYS:H	2:B:107:VAL:HG23	1.83	0.43
3:D:69:ARG:NH2	7:M:38:C:O2'	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:297:GLY:HA3	3:E:298:PRO:HD3	1.85	0.43
1:A:94:LEU:HD11	2:B:315:ARG:HD3	1.99	0.43
3:C:290:TYR:HE2	3:C:293:GLU:HB2	1.84	0.43
3:G:33:PHE:HZ	3:G:137:LEU:HD21	1.82	0.43
5:K:67:ILE:O	5:K:71:ALA:HB2	2.17	0.43
3:F:103:LEU:HD11	3:F:238:ILE:HD11	1.99	0.43
2:B:27:LEU:HD12	2:B:284:PHE:HE2	1.84	0.43
3:D:79:LYS:NZ	3:D:80:ASP:OD1	2.48	0.43
5:K:82:GLU:HG3	5:K:86:ILE:HG13	2.00	0.43
3:G:307:VAL:HG12	3:G:310:GLN:H	1.83	0.43
2:B:88:LEU:HD11	3:H:308:THR:HA	1.99	0.43
4:J:75:ARG:HD2	4:J:77:ASN:H	1.83	0.43
3:G:306:SER:HA	3:G:313:ALA:HA	2.00	0.43
1:A:419:SER:O	1:A:423:THR:OG1	2.26	0.43
3:C:47:GLY:HA3	3:C:56:GLN:HB3	1.99	0.43
1:A:222:ARG:HG3	2:B:239:TRP:CE2	2.53	0.43
3:C:42:ALA:HB2	3:C:279:ILE:HD11	2.00	0.43
5:K:41:TYR:HB2	5:K:49:LEU:HB3	2.01	0.43
1:A:181:PRO:HG2	2:B:305:HIS:HE1	1.84	0.43
3:F:246:PRO:O	3:F:248:GLN:N	2.51	0.43
3:F:258:LYS:HZ2	4:I:15:MET:HG3	1.82	0.43
3:H:110:LEU:HD13	3:H:244:VAL:HG11	2.00	0.43
5:K:60:ASP:O	5:K:66:SER:OG	2.33	0.43
5:K:67:ILE:O	5:K:71:ALA:HB2	2.18	0.43
1:A:140:GLU:O	1:A:144:ALA:HB2	2.19	0.43
3:E:47:GLY:HA3	3:E:56:GLN:HB3	1.99	0.43
3:E:117:ARG:HG3	3:F:242:GLN:HE22	1.84	0.43
1:A:89:PRO:HB3	2:B:313:LEU:HD21	2.00	0.43
2:B:175:ARG:HG3	2:B:178:ARG:HH22	1.84	0.43
3:E:42:ALA:HB2	3:E:279:ILE:HD11	2.00	0.43
3:H:110:LEU:HD13	3:H:244:VAL:HG11	1.98	0.43
3:E:42:ALA:HB1	3:E:112:VAL:HG13	2.01	0.43
3:F:42:ALA:HB1	3:F:112:VAL:HG13	2.01	0.43
3:F:306:SER:HA	3:F:313:ALA:HA	2.00	0.43
3:F:340:GLU:HA	3:F:343:HIS:HD2	1.83	0.43
1:A:386:GLU:O	1:A:389:ASN:HB2	2.18	0.43
3:F:307:VAL:HG12	3:F:310:GLN:H	1.83	0.43
3:G:284:ARG:NH2	7:M:14:G:OP2	2.52	0.43
2:B:282:ASN:OD1	7:M:3:A:N6	2.52	0.43
1:A:150:GLU:O	1:A:154:GLU:HB3	2.17	0.43
2:B:62:VAL:HG21	2:B:180:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:ALA:HB1	3:D:200:ILE:HD13	2.01	0.43
2:B:55:GLU:HB3	2:B:114:HIS:HB2	1.99	0.43
3:D:340:GLU:HA	3:D:343:HIS:HD2	1.83	0.43
3:E:306:SER:HA	3:E:313:ALA:HA	2.00	0.43
3:C:277:GLN:HB3	7:M:38:C:H5"	2.01	0.43
1:A:187:TYR:OH	2:B:46:ARG:NH1	2.49	0.43
1:A:339:ARG:O	1:A:343:LEU:CB	2.66	0.43
2:B:215:ASP:OD1	2:B:244:LYS:NZ	2.38	0.43
3:F:31:LEU:HB2	3:F:355:PHE:HB2	2.01	0.43
3:G:110:LEU:HD13	3:G:244:VAL:HG11	2.01	0.43
3:H:307:VAL:HG12	3:H:310:GLN:H	1.83	0.43
3:C:103:LEU:HD11	3:C:238:ILE:HD11	1.99	0.43
3:C:340:GLU:HA	3:C:343:HIS:HD2	1.84	0.43
3:G:162:ALA:HB1	3:G:200:ILE:HD13	2.01	0.43
3:H:340:GLU:HA	3:H:343:HIS:HD2	1.84	0.43
3:D:306:SER:HA	3:D:313:ALA:HA	2.00	0.43
1:A:91:GLN:OE1	2:B:315:ARG:NH1	2.49	0.43
3:D:307:VAL:HG12	3:D:310:GLN:H	1.83	0.43
3:F:307:VAL:HG12	3:F:310:GLN:H	1.83	0.43
3:G:31:LEU:HB2	3:G:355:PHE:HB2	2.01	0.43
1:A:65:LEU:HB3	1:A:163:THR:HA	2.01	0.42
3:E:110:LEU:HD13	3:E:244:VAL:HG11	2.01	0.42
3:H:110:LEU:HD13	3:H:244:VAL:HG11	2.01	0.42
2:B:125:GLU:OE2	2:B:129:GLN:NE2	2.47	0.42
3:D:249:GLU:HA	3:D:249:GLU:OE1	2.19	0.42
3:G:42:ALA:HB2	3:G:279:ILE:HD11	2.00	0.42
1:A:219:ARG:HA	1:A:222:ARG:HG2	2.00	0.42
3:E:246:PRO:O	3:E:248:GLN:N	2.51	0.42
3:C:290:TYR:CD1	3:C:291:PRO:HD2	2.55	0.42
3:C:47:GLY:HA3	3:C:56:GLN:HB3	1.99	0.42
3:C:110:LEU:HD13	3:C:244:VAL:HG11	2.01	0.42
3:D:250:LEU:HD22	3:E:95:LEU:HB3	2.01	0.42
3:G:324:TYR:OH	3:H:74:ASN:O	2.37	0.42
3:F:308:THR:HG21	3:G:69:ARG:HH12	1.83	0.42
1:A:89:PRO:HD2	1:A:98:HIS:CD2	2.54	0.42
3:C:110:LEU:HD13	3:C:244:VAL:HG11	2.00	0.42
3:G:340:GLU:HA	3:G:343:HIS:HD2	1.83	0.42
3:E:169:ARG:NH1	7:M:29:C:OP1	2.50	0.42
3:F:96:GLN:HG2	4:I:13:ASN:OD1	2.19	0.42
4:I:75:ARG:HD2	4:I:77:ASN:H	1.84	0.42
2:B:136:ALA:HA	3:H:117:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:340:GLU:HA	3:E:343:HIS:HD2	1.83	0.42
3:F:290:TYR:CD1	3:F:291:PRO:HD2	2.55	0.42
3:H:307:VAL:HG12	3:H:310:GLN:H	1.83	0.42
3:C:31:LEU:HB2	3:C:355:PHE:HB2	2.01	0.42
1:A:68:HIS:ND1	1:A:195:PRO:HA	2.35	0.42
1:A:161:GLY:HA2	1:A:164:THR:HG22	2.00	0.42
2:B:10:LEU:HD23	2:B:111:LEU:HD12	2.02	0.42
3:F:31:LEU:HB2	3:F:355:PHE:HB2	2.02	0.42
3:H:290:TYR:CD1	3:H:291:PRO:HD2	2.55	0.42
3:E:340:GLU:HA	3:E:343:HIS:HD2	1.84	0.42
3:H:162:ALA:HB1	3:H:200:ILE:HD13	2.01	0.42
3:D:110:LEU:HD13	3:D:244:VAL:HG11	2.00	0.42
3:D:165:ARG:NH1	3:D:285:THR:OG1	2.53	0.42
2:B:125:GLU:OE2	2:B:128:ARG:NH2	2.53	0.42
3:G:34:GLU:OE2	3:H:169:ARG:NE	2.52	0.42
7:M:49:C:H2'	7:M:56:G:H22	1.85	0.42
1:A:419:SER:O	1:A:423:THR:CB	2.68	0.42
3:D:31:LEU:HB2	3:D:355:PHE:HB2	2.01	0.42
3:D:117:ARG:HG3	3:E:242:GLN:HE22	1.85	0.42
4:I:42:ARG:NH2	4:I:71:GLU:O	2.53	0.42
2:B:17:ILE:HB	2:B:105:LEU:HB3	2.01	0.42
1:A:190:LEU:HD21	2:B:314:TYR:HE2	1.85	0.42
3:C:27:THR:HG21	3:D:75:ARG:HH12	1.85	0.42
3:C:44:MET:HG2	3:C:112:VAL:HG22	2.02	0.42
3:C:31:LEU:HB2	3:C:355:PHE:HB2	2.02	0.42
3:D:31:LEU:HB2	3:D:355:PHE:HB2	2.02	0.42
3:D:69:ARG:HD2	3:D:93:PRO:HD2	2.02	0.42
3:D:290:TYR:CD1	3:D:291:PRO:HD2	2.55	0.42
3:D:307:VAL:HG12	3:D:310:GLN:H	1.83	0.42
3:G:290:TYR:CD1	3:G:291:PRO:HD2	2.55	0.42
4:J:42:ARG:NH2	4:J:71:GLU:O	2.53	0.42
3:C:250:LEU:HA	7:M:39:U:C5	2.55	0.42
3:D:340:GLU:HA	3:D:343:HIS:HD2	1.84	0.42
3:F:275:HIS:HD2	3:G:66:LYS:HD2	1.84	0.42
3:D:44:MET:HG2	3:D:112:VAL:HG22	2.02	0.42
3:E:44:MET:HG2	3:E:112:VAL:HG22	2.02	0.42
3:G:167:LEU:O	3:G:170:ASN:N	2.46	0.42
3:H:42:ALA:HB1	3:H:112:VAL:HG13	2.01	0.42
3:G:31:LEU:HB2	3:G:355:PHE:HB2	2.02	0.42
2:B:65:ARG:HB3	2:B:106:GLU:HB3	2.01	0.42
3:D:119:LEU:HD22	3:E:172:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:49:C:H2'	7:M:56:G:H22	1.85	0.42
1:A:305:GLN:NE2	1:A:398:ALA:O	2.52	0.42
3:E:162:ALA:HB1	3:E:200:ILE:HD13	2.01	0.42
3:C:42:ALA:HB1	3:C:112:VAL:HG13	2.01	0.42
3:G:84:ALA:O	3:G:88:ALA:HB2	2.19	0.42
3:D:250:LEU:HD22	3:E:95:LEU:HB3	2.02	0.42
2:B:34:PRO:HB3	2:B:252:PRO:HD2	2.02	0.42
4:J:29:ARG:NH2	4:J:31:GLU:OE2	2.53	0.42
2:B:32:PRO:HG3	2:B:105:LEU:HD11	2.02	0.42
3:C:162:ALA:HB1	3:C:200:ILE:HD13	2.01	0.42
5:K:42:THR:HG22	5:K:48:VAL:HG22	2.02	0.42
7:M:49:C:H2'	7:M:56:G:H22	1.85	0.42
2:B:290:LEU:HB2	2:B:294:ARG:NH1	2.35	0.42
3:F:44:MET:HG2	3:F:112:VAL:HG22	2.02	0.42
3:G:165:ARG:NH1	3:G:285:THR:OG1	2.53	0.42
3:E:290:TYR:CD1	3:E:291:PRO:HD2	2.55	0.42
3:F:25:LEU:O	3:F:332:LEU:CD2	2.67	0.42
3:D:44:MET:HA	3:D:111:LYS:O	2.21	0.41
1:A:187:TYR:OH	2:B:46:ARG:NH1	2.51	0.41
1:A:238:LEU:HD13	1:A:263:TRP:HB3	2.01	0.41
1:A:326:VAL:HG23	1:A:421:GLU:HG3	2.02	0.41
3:D:110:LEU:HD13	3:D:244:VAL:HG11	2.01	0.41
3:F:340:GLU:HA	3:F:343:HIS:HD2	1.84	0.41
3:C:165:ARG:NH1	3:C:285:THR:OG1	2.53	0.41
3:E:165:ARG:NH1	3:E:285:THR:OG1	2.53	0.41
3:C:110:LEU:HD13	3:C:244:VAL:HG11	2.02	0.41
3:E:110:LEU:HD13	3:E:244:VAL:HG11	2.02	0.41
1:A:60:VAL:HG22	1:A:162:ILE:HB	2.02	0.41
3:H:31:LEU:HB2	3:H:355:PHE:HB2	2.01	0.41
3:E:45:SER:O	3:E:111:LYS:HB3	2.20	0.41
3:F:303:PRO:HG2	3:G:73:SER:HB2	2.02	0.41
3:G:253:ASP:HB3	4:J:63:GLY:HA3	2.02	0.41
4:J:29:ARG:NH2	4:J:31:GLU:OE2	2.53	0.41
1:A:419:SER:O	1:A:423:THR:OG1	2.27	0.41
4:I:29:ARG:NH2	4:I:31:GLU:OE2	2.53	0.41
1:A:14:ARG:NH2	1:A:18:GLU:OE2	2.53	0.41
3:F:165:ARG:HH11	3:F:285:THR:HG1	1.65	0.41
2:B:26:PRO:HD2	2:B:282:ASN:HD21	1.84	0.41
3:D:42:ALA:HB1	3:D:112:VAL:HG13	2.01	0.41
3:F:165:ARG:NH1	3:F:285:THR:OG1	2.53	0.41
3:G:42:ALA:HB1	3:G:112:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:44:MET:HG2	3:H:112:VAL:HG22	2.02	0.41
3:H:165:ARG:NH1	3:H:285:THR:OG1	2.53	0.41
1:A:290:ASP:HB2	1:A:293:ARG:HH21	1.84	0.41
3:D:45:SER:O	3:D:111:LYS:HB3	2.20	0.41
2:B:62:VAL:HG21	2:B:180:LEU:HD22	2.01	0.41
2:B:88:LEU:HD13	2:B:92:GLY:HA2	2.02	0.41
3:G:110:LEU:HD13	3:G:244:VAL:HG11	2.02	0.41
3:G:82:ASP:H	3:G:85:LYS:HD2	1.84	0.41
3:D:76:LEU:HD13	3:D:85:LYS:HE3	2.01	0.41
3:E:77:LYS:HG2	3:E:79:LYS:H	1.85	0.41
2:B:83:LEU:HD11	2:B:99:GLU:HG2	2.02	0.41
3:F:110:LEU:HD13	3:F:244:VAL:HG11	2.01	0.41
3:G:281:ASN:HB2	7:M:14:G:H5'	2.01	0.41
3:F:45:SER:O	3:F:111:LYS:HB3	2.20	0.41
2:B:278:ARG:NH2	2:B:314:TYR:OH	2.53	0.41
2:B:305:HIS:HB3	2:B:316:TRP:CD1	2.55	0.41
3:F:27:THR:HG21	3:F:328:ASP:OD1	2.20	0.41
2:B:24:SER:HG	2:B:28:THR:HG1	1.65	0.41
3:C:312:LYS:HD3	3:D:86:LEU:HD11	2.01	0.41
1:A:47:HIS:HA	1:A:51:ALA:HB3	2.02	0.41
3:D:110:LEU:HD13	3:D:244:VAL:HG11	2.02	0.41
3:H:45:SER:O	3:H:111:LYS:HB3	2.20	0.41
1:A:187:TYR:OH	2:B:46:ARG:NH1	2.53	0.41
3:F:44:MET:HA	3:F:111:LYS:O	2.21	0.41
3:G:70:GLY:HA3	3:G:94:ASN:HB2	2.02	0.41
5:K:51:GLN:HA	5:K:55:THR:O	2.21	0.41
2:B:8:ALA:HB3	2:B:113:VAL:HB	2.03	0.41
3:E:44:MET:HA	3:E:111:LYS:O	2.21	0.41
3:D:71:THR:HA	3:D:93:PRO:HB3	2.02	0.41
2:B:215:ASP:OD1	2:B:244:LYS:NZ	2.38	0.41
3:C:297:GLY:HA3	3:C:298:PRO:HD3	1.85	0.41
3:H:31:LEU:HB2	3:H:355:PHE:HB2	2.02	0.41
3:H:110:LEU:HD13	3:H:244:VAL:HG11	2.02	0.41
4:I:29:ARG:NH2	4:I:31:GLU:OE2	2.54	0.41
1:A:386:GLU:O	1:A:389:ASN:HB2	2.21	0.41
2:B:45:GLN:OE1	2:B:56:LEU:N	2.44	0.41
3:D:68:VAL:HG13	3:D:96:GLN:HB2	2.02	0.41
3:E:85:LYS:O	3:E:89:SER:HB3	2.21	0.41
1:A:190:LEU:HD21	2:B:314:TYR:HE2	1.86	0.41
3:D:251:ILE:HB	3:D:264:THR:CG2	2.49	0.41
3:E:42:ALA:HB1	3:E:112:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:42:ALA:HB1	3:F:112:VAL:HG13	2.03	0.41
3:G:261:LYS:HD2	3:G:264:THR:HG22	2.01	0.41
5:K:67:ILE:HD13	5:K:89:LEU:HG	2.03	0.41
1:A:50:GLU:OE2	1:A:151:GLN:NE2	2.54	0.41
3:F:162:ALA:HB1	3:F:200:ILE:HD13	2.01	0.41
3:H:44:MET:HA	3:H:111:LYS:O	2.21	0.41
3:G:44:MET:HG2	3:G:112:VAL:HG22	2.02	0.41
4:I:20:TYR:HB2	4:I:27:LYS:HB2	2.03	0.41
1:A:239:ALA:HB3	1:A:264:LEU:HB2	2.02	0.41
1:A:281:MET:HG3	1:A:350:THR:H	1.86	0.41
1:A:314:ASN:O	1:A:318:ILE:CB	2.69	0.41
3:H:75:ARG:HD2	3:H:86:LEU:HB3	2.03	0.41
1:A:238:LEU:HD13	1:A:263:TRP:HB3	2.02	0.41
2:B:88:LEU:HD11	3:H:308:THR:HA	2.03	0.41
3:C:45:SER:O	3:C:111:LYS:HB3	2.20	0.41
2:B:102:ARG:HD3	2:B:102:ARG:HA	1.92	0.40
3:G:44:MET:HA	3:G:111:LYS:O	2.21	0.40
2:B:303:TRP:HB3	2:B:318:THR:HG22	2.02	0.40
1:A:326:VAL:HG23	1:A:421:GLU:HG3	2.02	0.40
3:E:31:LEU:HB2	3:E:355:PHE:HB2	2.01	0.40
3:F:251:ILE:HG23	3:F:254:LYS:HB2	2.04	0.40
3:G:45:SER:O	3:G:111:LYS:HB3	2.20	0.40
1:A:232:PHE:HD2	2:B:219:ILE:HB	1.86	0.40
1:A:13:LEU:HD23	1:A:144:ALA:HA	2.03	0.40
1:A:335:GLN:O	1:A:339:ARG:HD3	2.21	0.40
2:B:71:SER:HB3	2:B:80:VAL:HG23	2.03	0.40
5:K:82:GLU:HG3	5:K:86:ILE:HG13	2.03	0.40
3:C:44:MET:HA	3:C:111:LYS:O	2.21	0.40
2:B:244:LYS:HE2	2:B:248:LEU:H	1.86	0.40
3:G:42:ALA:HB1	3:G:112:VAL:HG13	2.04	0.40
1:A:335:GLN:O	1:A:339:ARG:HD3	2.21	0.40
3:G:277:GLN:HG2	7:M:13:C:H2'	2.02	0.40
7:M:49:C:H2'	7:M:56:G:H22	1.85	0.40
1:A:57:ALA:HA	1:A:60:VAL:HG23	2.03	0.40
3:D:250:LEU:CD1	3:E:95:LEU:CD1	2.99	0.40
2:B:185:ALA:O	2:B:289:TRP:HA	2.22	0.40
7:M:49:C:H2'	7:M:56:G:H22	1.87	0.40
1:A:189:LEU:HB2	2:B:277:LEU:HB3	2.03	0.40
3:C:42:ALA:HB1	3:C:112:VAL:HG13	2.04	0.40
3:D:42:ALA:HB1	3:D:112:VAL:HG13	2.04	0.40
5:K:67:ILE:O	5:K:71:ALA:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:ALA:HB1	3:C:112:VAL:HG13	2.03	0.40
3:E:165:ARG:HH11	3:E:285:THR:HG1	1.67	0.40
3:E:305:GLY:N	3:E:315:ARG:HB2	2.37	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	1-A	422/434 (97%)	380 (90%)	42 (10%)	0	100	100
1	2-A	422/434 (97%)	387 (92%)	35 (8%)	0	100	100
1	3-A	422/434 (97%)	389 (92%)	33 (8%)	0	100	100
1	4-A	422/434 (97%)	389 (92%)	33 (8%)	0	100	100
1	5-A	422/434 (97%)	385 (91%)	37 (9%)	0	100	100
2	1-B	301/327 (92%)	265 (88%)	36 (12%)	0	100	100
2	2-B	301/327 (92%)	264 (88%)	37 (12%)	0	100	100
2	3-B	301/327 (92%)	262 (87%)	39 (13%)	0	100	100
2	4-B	301/327 (92%)	265 (88%)	36 (12%)	0	100	100
2	5-B	301/327 (92%)	249 (83%)	52 (17%)	0	100	100
3	1-C	287/341 (84%)	263 (92%)	24 (8%)	0	100	100
3	1-D	331/341 (97%)	300 (91%)	31 (9%)	0	100	100
3	1-E	332/341 (97%)	301 (91%)	31 (9%)	0	100	100
3	1-F	333/341 (98%)	306 (92%)	27 (8%)	0	100	100
3	1-G	331/341 (97%)	305 (92%)	26 (8%)	0	100	100
3	1-H	331/341 (97%)	305 (92%)	26 (8%)	0	100	100
3	2-C	287/341 (84%)	265 (92%)	22 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2-D	331/341 (97%)	305 (92%)	26 (8%)	0	100	100
3	2-E	332/341 (97%)	306 (92%)	26 (8%)	0	100	100
3	2-F	333/341 (98%)	300 (90%)	33 (10%)	0	100	100
3	2-G	331/341 (97%)	300 (91%)	31 (9%)	0	100	100
3	2-H	331/341 (97%)	304 (92%)	27 (8%)	0	100	100
3	3-C	287/341 (84%)	262 (91%)	25 (9%)	0	100	100
3	3-D	331/341 (97%)	296 (89%)	35 (11%)	0	100	100
3	3-E	332/341 (97%)	300 (90%)	32 (10%)	0	100	100
3	3-F	333/341 (98%)	303 (91%)	30 (9%)	0	100	100
3	3-G	331/341 (97%)	295 (89%)	36 (11%)	0	100	100
3	3-H	331/341 (97%)	300 (91%)	31 (9%)	0	100	100
3	4-C	287/341 (84%)	260 (91%)	27 (9%)	0	100	100
3	4-D	331/341 (97%)	293 (88%)	38 (12%)	0	100	100
3	4-E	332/341 (97%)	297 (90%)	35 (10%)	0	100	100
3	4-F	333/341 (98%)	300 (90%)	33 (10%)	0	100	100
3	4-G	331/341 (97%)	294 (89%)	37 (11%)	0	100	100
3	4-H	331/341 (97%)	298 (90%)	33 (10%)	0	100	100
3	5-C	287/341 (84%)	271 (94%)	16 (6%)	0	100	100
3	5-D	331/341 (97%)	311 (94%)	20 (6%)	0	100	100
3	5-E	332/341 (97%)	308 (93%)	24 (7%)	0	100	100
3	5-F	333/341 (98%)	309 (93%)	24 (7%)	0	100	100
3	5-G	331/341 (97%)	310 (94%)	21 (6%)	0	100	100
3	5-H	331/341 (97%)	309 (93%)	22 (7%)	0	100	100
4	1-I	74/77 (96%)	71 (96%)	3 (4%)	0	100	100
4	1-J	74/77 (96%)	71 (96%)	3 (4%)	0	100	100
4	2-I	74/77 (96%)	71 (96%)	3 (4%)	0	100	100
4	2-J	74/77 (96%)	71 (96%)	3 (4%)	0	100	100
4	3-I	74/77 (96%)	69 (93%)	5 (7%)	0	100	100
4	3-J	74/77 (96%)	69 (93%)	5 (7%)	0	100	100
4	4-I	74/77 (96%)	68 (92%)	6 (8%)	0	100	100
4	4-J	74/77 (96%)	68 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	5-I	74/77 (96%)	72 (97%)	2 (3%)	0	100	100
4	5-J	74/77 (96%)	72 (97%)	2 (3%)	0	100	100
5	1-K	86/96 (90%)	77 (90%)	9 (10%)	0	100	100
5	2-K	86/96 (90%)	80 (93%)	6 (7%)	0	100	100
5	3-K	86/96 (90%)	80 (93%)	6 (7%)	0	100	100
5	4-K	86/96 (90%)	80 (93%)	6 (7%)	0	100	100
5	5-K	86/96 (90%)	78 (91%)	8 (9%)	0	100	100
6	1-L	188/189 (100%)	174 (93%)	14 (7%)	0	100	100
6	2-L	188/189 (100%)	175 (93%)	13 (7%)	0	100	100
6	3-L	188/189 (100%)	173 (92%)	15 (8%)	0	100	100
6	4-L	188/189 (100%)	167 (89%)	21 (11%)	0	100	100
6	5-L	188/189 (100%)	171 (91%)	17 (9%)	0	100	100
All	All	15450/16230 (95%)	14068 (91%)	1382 (9%)	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	1-A	248/365 (68%)	248 (100%)	0	100	100
1	2-A	248/365 (68%)	248 (100%)	0	100	100
1	3-A	248/365 (68%)	247 (100%)	1 (0%)	91	95
1	4-A	248/365 (68%)	247 (100%)	1 (0%)	91	95
1	5-A	248/365 (68%)	247 (100%)	1 (0%)	91	95
2	1-B	245/270 (91%)	245 (100%)	0	100	100
2	2-B	245/270 (91%)	244 (100%)	1 (0%)	91	95
2	3-B	245/270 (91%)	245 (100%)	0	100	100
2	4-B	245/270 (91%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5-B	245/270 (91%)	245 (100%)	0	100	100
3	1-C	230/272 (85%)	229 (100%)	1 (0%)	91	95
3	1-D	258/272 (95%)	257 (100%)	1 (0%)	91	95
3	1-E	259/272 (95%)	258 (100%)	1 (0%)	91	95
3	1-F	259/272 (95%)	258 (100%)	1 (0%)	91	95
3	1-G	259/272 (95%)	258 (100%)	1 (0%)	91	95
3	1-H	258/272 (95%)	257 (100%)	1 (0%)	91	95
3	2-C	230/272 (85%)	228 (99%)	2 (1%)	78	90
3	2-D	258/272 (95%)	256 (99%)	2 (1%)	81	91
3	2-E	259/272 (95%)	257 (99%)	2 (1%)	81	91
3	2-F	259/272 (95%)	257 (99%)	2 (1%)	81	91
3	2-G	259/272 (95%)	257 (99%)	2 (1%)	81	91
3	2-H	258/272 (95%)	256 (99%)	2 (1%)	81	91
3	3-C	230/272 (85%)	230 (100%)	0	100	100
3	3-D	258/272 (95%)	258 (100%)	0	100	100
3	3-E	259/272 (95%)	259 (100%)	0	100	100
3	3-F	259/272 (95%)	259 (100%)	0	100	100
3	3-G	259/272 (95%)	259 (100%)	0	100	100
3	3-H	258/272 (95%)	258 (100%)	0	100	100
3	4-C	230/272 (85%)	230 (100%)	0	100	100
3	4-D	258/272 (95%)	258 (100%)	0	100	100
3	4-E	259/272 (95%)	259 (100%)	0	100	100
3	4-F	259/272 (95%)	259 (100%)	0	100	100
3	4-G	259/272 (95%)	259 (100%)	0	100	100
3	4-H	258/272 (95%)	258 (100%)	0	100	100
3	5-C	230/272 (85%)	229 (100%)	1 (0%)	91	95
3	5-D	258/272 (95%)	254 (98%)	4 (2%)	62	81
3	5-E	259/272 (95%)	258 (100%)	1 (0%)	91	95
3	5-F	259/272 (95%)	258 (100%)	1 (0%)	91	95
3	5-G	259/272 (95%)	258 (100%)	1 (0%)	91	95
3	5-H	258/272 (95%)	257 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1-I	64/65 (98%)	64 (100%)	0	100	100
4	1-J	64/65 (98%)	64 (100%)	0	100	100
4	2-I	64/65 (98%)	64 (100%)	0	100	100
4	2-J	64/65 (98%)	64 (100%)	0	100	100
4	3-I	64/65 (98%)	64 (100%)	0	100	100
4	3-J	64/65 (98%)	64 (100%)	0	100	100
4	4-I	64/65 (98%)	64 (100%)	0	100	100
4	4-J	64/65 (98%)	64 (100%)	0	100	100
4	5-I	64/65 (98%)	64 (100%)	0	100	100
4	5-J	64/65 (98%)	64 (100%)	0	100	100
5	1-K	69/77 (90%)	69 (100%)	0	100	100
5	2-K	69/77 (90%)	69 (100%)	0	100	100
5	3-K	69/77 (90%)	69 (100%)	0	100	100
5	4-K	69/77 (90%)	69 (100%)	0	100	100
5	5-K	69/77 (90%)	69 (100%)	0	100	100
All	All	11065/12370 (90%)	11034 (100%)	31 (0%)	92	97

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1-C	134	ARG
3	1-D	134	ARG
3	1-E	134	ARG
3	1-F	134	ARG
3	1-G	134	ARG
3	1-H	134	ARG
2	2-B	90	ARG
3	2-C	35	ARG
3	2-C	171	ARG
3	2-D	35	ARG
3	2-D	171	ARG
3	2-E	35	ARG
3	2-E	171	ARG
3	2-F	35	ARG
3	2-F	171	ARG
3	2-G	35	ARG
3	2-G	171	ARG

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Mol	Chain	Res	Type
3	2-H	35	ARG
3	2-H	171	ARG
1	3-A	339	ARG
1	4-A	339	ARG
1	5-A	256	ASN
3	5-C	129	ASN
3	5-D	81	ARG
3	5-D	129	ASN
3	5-D	245	PHE
3	5-D	251	ILE
3	5-E	129	ASN
3	5-F	129	ASN
3	5-G	129	ASN
3	5-H	129	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	62	GLN
3	1-D	242	GLN
3	1-G	242	GLN
1	2-A	200	HIS
1	2-A	256	ASN
1	2-A	389	ASN
2	2-B	64	HIS
2	2-B	114	HIS
2	2-B	124	GLN
2	2-B	156	ASN
2	2-B	282	ASN
3	2-C	248	GLN
3	2-D	242	GLN
3	2-D	248	GLN
3	2-E	248	GLN
3	2-F	248	GLN
3	2-F	277	GLN
3	2-G	242	GLN
3	2-G	248	GLN
3	2-H	248	GLN
5	2-K	51	GLN
1	3-A	177	GLN
1	3-A	200	HIS
1	3-A	256	ASN

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Mol	Chain	Res	Type
2	3-B	156	ASN
3	3-C	129	ASN
3	3-C	148	GLN
3	3-C	242	GLN
3	3-D	129	ASN
3	3-D	148	GLN
3	3-D	242	GLN
3	3-E	129	ASN
3	3-E	148	GLN
3	3-E	242	GLN
3	3-F	129	ASN
3	3-F	148	GLN
3	3-F	242	GLN
3	3-G	129	ASN
3	3-G	148	GLN
3	3-G	242	GLN
3	3-G	277	GLN
3	3-H	129	ASN
3	3-H	148	GLN
3	3-H	242	GLN
3	3-H	275	HIS
1	4-A	177	GLN
1	4-A	200	HIS
1	4-A	256	ASN
2	4-B	156	ASN
3	4-C	129	ASN
3	4-C	148	GLN
3	4-C	242	GLN
3	4-D	129	ASN
3	4-D	148	GLN
3	4-D	242	GLN
3	4-E	129	ASN
3	4-E	148	GLN
3	4-E	242	GLN
3	4-E	277	GLN
3	4-F	129	ASN
3	4-F	148	GLN
3	4-F	242	GLN
3	4-G	129	ASN
3	4-G	148	GLN
3	4-G	242	GLN
3	4-H	129	ASN

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Mol	Chain	Res	Type
3	4-H	148	GLN
3	4-H	242	GLN
3	4-H	275	HIS
2	5-B	131	GLN
3	5-C	248	GLN
3	5-C	343	HIS
3	5-D	343	HIS
3	5-E	248	GLN
3	5-E	343	HIS
3	5-F	242	GLN
3	5-F	248	GLN
3	5-F	343	HIS
3	5-G	248	GLN
3	5-G	343	HIS
3	5-H	129	ASN
3	5-H	248	GLN
3	5-H	343	HIS
4	5-I	13	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	1-M	59/60 (98%)	30 (50%)	0
7	2-M	59/60 (98%)	27 (45%)	0
7	3-M	59/60 (98%)	32 (54%)	0
7	4-M	59/60 (98%)	32 (54%)	0
7	5-M	59/60 (98%)	31 (52%)	0
All	All	295/300 (98%)	152 (51%)	0

All (152) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	1-M	3	A
7	1-M	9	U
7	1-M	14	G
7	1-M	15	G
7	1-M	16	C
7	1-M	17	G
7	1-M	20	C
7	1-M	21	U
7	1-M	22	U

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Mol	Chain	Res	Type
7	1-M	27	U
7	1-M	32	G
7	1-M	33	U
7	1-M	38	C
7	1-M	39	U
7	1-M	41	G
7	1-M	42	U
7	1-M	43	U
7	1-M	44	C
7	1-M	45	A
7	1-M	46	C
7	1-M	47	U
7	1-M	48	G
7	1-M	49	C
7	1-M	52	U
7	1-M	53	A
7	1-M	55	A
7	1-M	56	G
7	1-M	58	C
7	1-M	59	A
7	1-M	60	G
7	2-M	3	A
7	2-M	9	U
7	2-M	15	G
7	2-M	16	C
7	2-M	17	G
7	2-M	20	C
7	2-M	27	U
7	2-M	28	C
7	2-M	32	G
7	2-M	38	C
7	2-M	39	U
7	2-M	41	G
7	2-M	42	U
7	2-M	43	U
7	2-M	44	C
7	2-M	45	A
7	2-M	46	C
7	2-M	47	U
7	2-M	48	G
7	2-M	49	C
7	2-M	52	U

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Mol	Chain	Res	Type
7	2-M	53	A
7	2-M	55	A
7	2-M	56	G
7	2-M	58	C
7	2-M	59	A
7	2-M	60	G
7	3-M	2	U
7	3-M	3	A
7	3-M	9	U
7	3-M	14	G
7	3-M	15	G
7	3-M	16	C
7	3-M	17	G
7	3-M	20	C
7	3-M	21	U
7	3-M	22	U
7	3-M	27	U
7	3-M	32	G
7	3-M	33	U
7	3-M	38	C
7	3-M	39	U
7	3-M	40	G
7	3-M	41	G
7	3-M	42	U
7	3-M	43	U
7	3-M	44	C
7	3-M	45	A
7	3-M	46	C
7	3-M	47	U
7	3-M	48	G
7	3-M	49	C
7	3-M	52	U
7	3-M	53	A
7	3-M	55	A
7	3-M	56	G
7	3-M	58	C
7	3-M	59	A
7	3-M	60	G
7	4-M	2	U
7	4-M	3	A
7	4-M	9	U
7	4-M	14	G

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Mol	Chain	Res	Type
7	4-M	15	G
7	4-M	16	C
7	4-M	17	G
7	4-M	20	C
7	4-M	21	U
7	4-M	22	U
7	4-M	25	U
7	4-M	27	U
7	4-M	32	G
7	4-M	33	U
7	4-M	38	C
7	4-M	39	U
7	4-M	41	G
7	4-M	42	U
7	4-M	43	U
7	4-M	44	C
7	4-M	45	A
7	4-M	46	C
7	4-M	47	U
7	4-M	48	G
7	4-M	49	C
7	4-M	52	U
7	4-M	53	A
7	4-M	55	A
7	4-M	56	G
7	4-M	58	C
7	4-M	59	A
7	4-M	60	G
7	5-M	2	U
7	5-M	3	A
7	5-M	9	U
7	5-M	14	G
7	5-M	15	G
7	5-M	16	C
7	5-M	17	G
7	5-M	20	C
7	5-M	21	U
7	5-M	22	U
7	5-M	27	U
7	5-M	32	G
7	5-M	33	U
7	5-M	38	C

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Mol	Chain	Res	Type
7	5-M	39	U
7	5-M	41	G
7	5-M	42	U
7	5-M	43	U
7	5-M	44	C
7	5-M	45	A
7	5-M	46	C
7	5-M	47	U
7	5-M	48	G
7	5-M	49	C
7	5-M	52	U
7	5-M	53	A
7	5-M	55	A
7	5-M	56	G
7	5-M	58	C
7	5-M	59	A
7	5-M	60	G

There are no RNA pucker outliers to report.

## 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 monosaccharides 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.

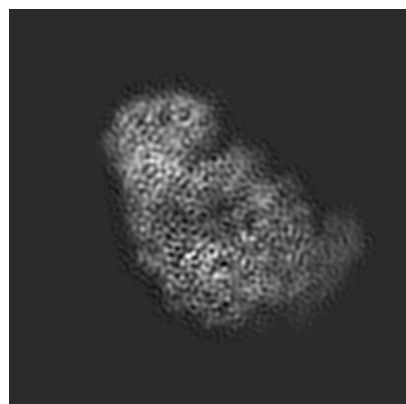
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8624. These allow visual inspection of the internal detail of the map and identification of artifacts.

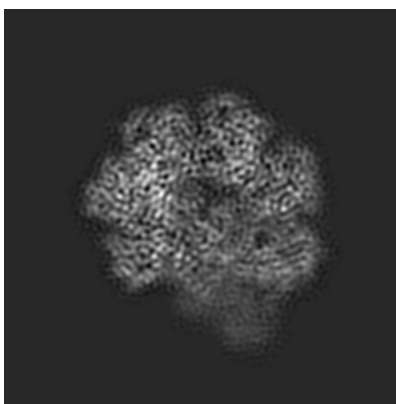
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

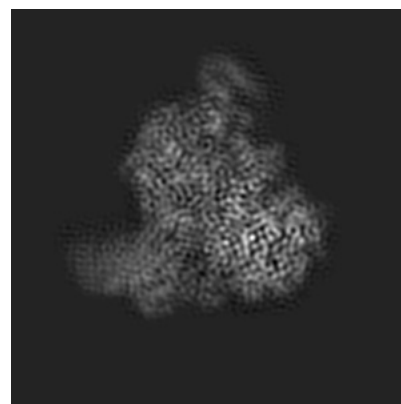
#### 6.1.1 Primary map



X

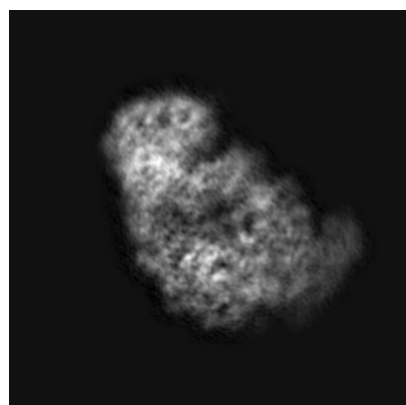


Y

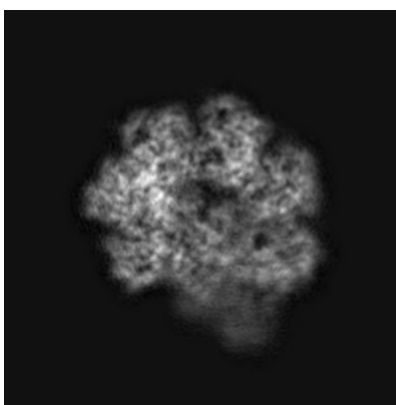


Z

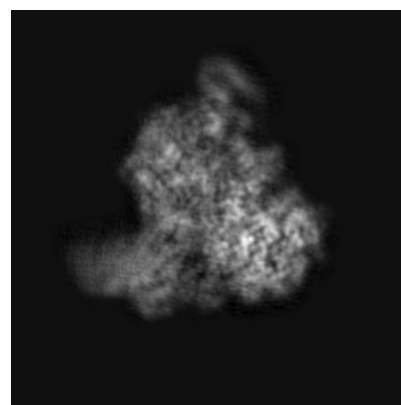
#### 6.1.2 Raw map



X



Y

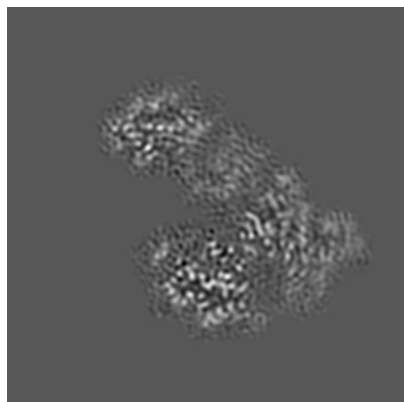


Z

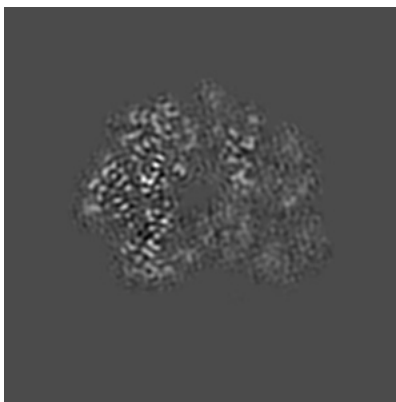
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

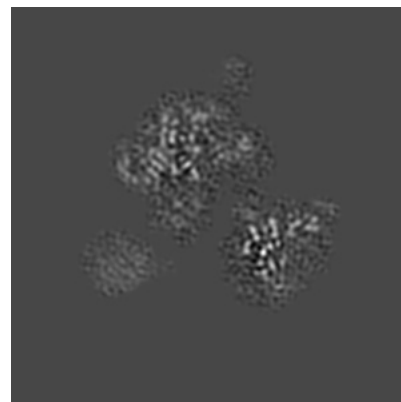
### 6.2.1 Primary map



X Index: 105

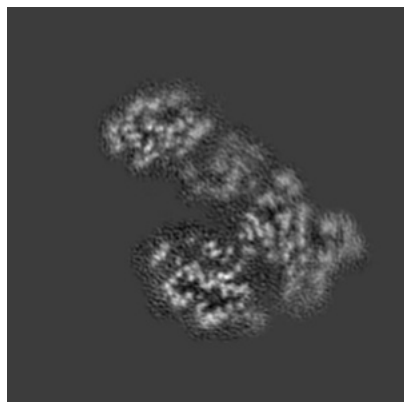


Y Index: 105

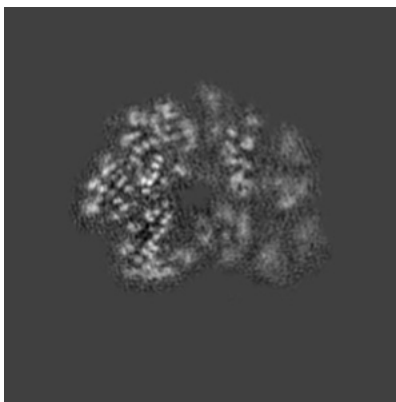


Z Index: 105

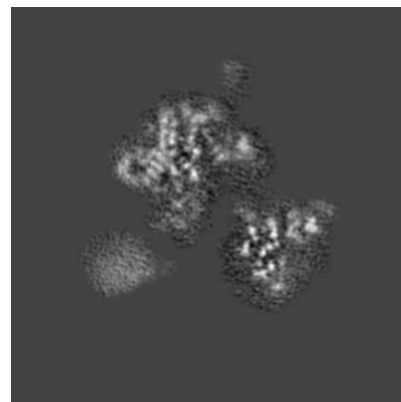
### 6.2.2 Raw map



X Index: 105



Y Index: 105

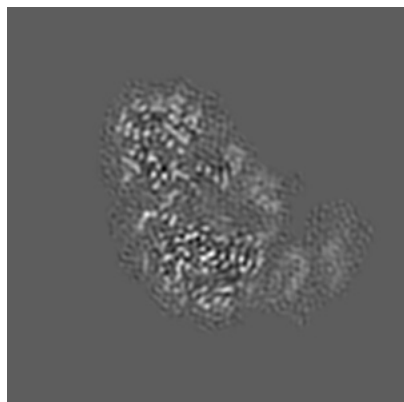


Z Index: 105

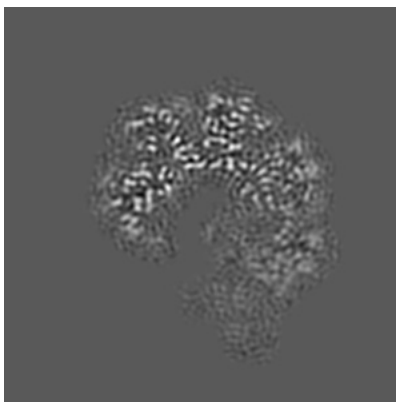
The images above show central slices of the map in three orthogonal directions.

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

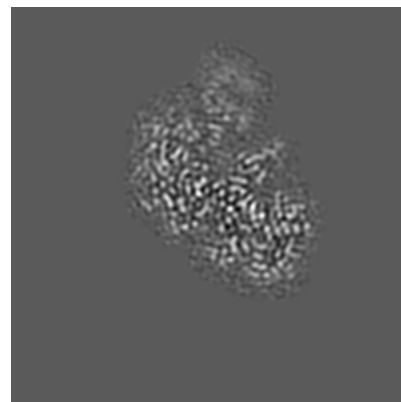
### 6.3.1 Primary map



X Index: 122

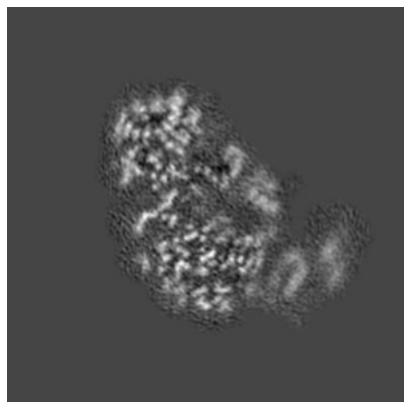


Y Index: 90

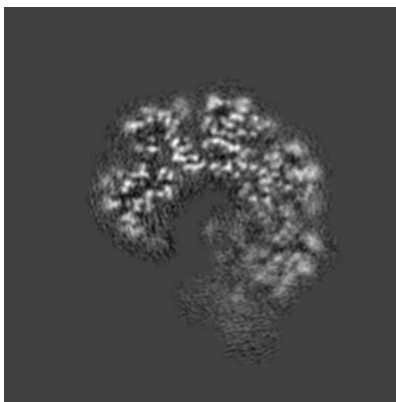


Z Index: 79

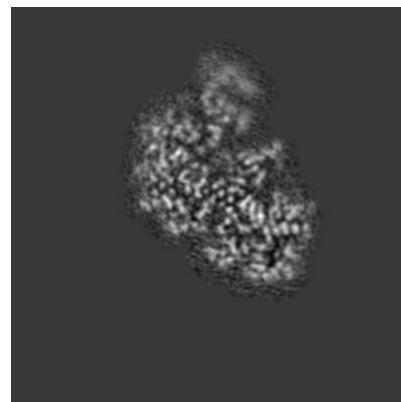
### 6.3.2 Raw map



X Index: 122



Y Index: 89



Z Index: 79

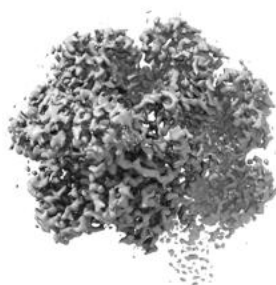
The images above show the largest variance slices of the map in three orthogonal directions.

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

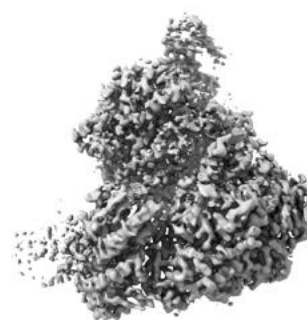
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0274. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

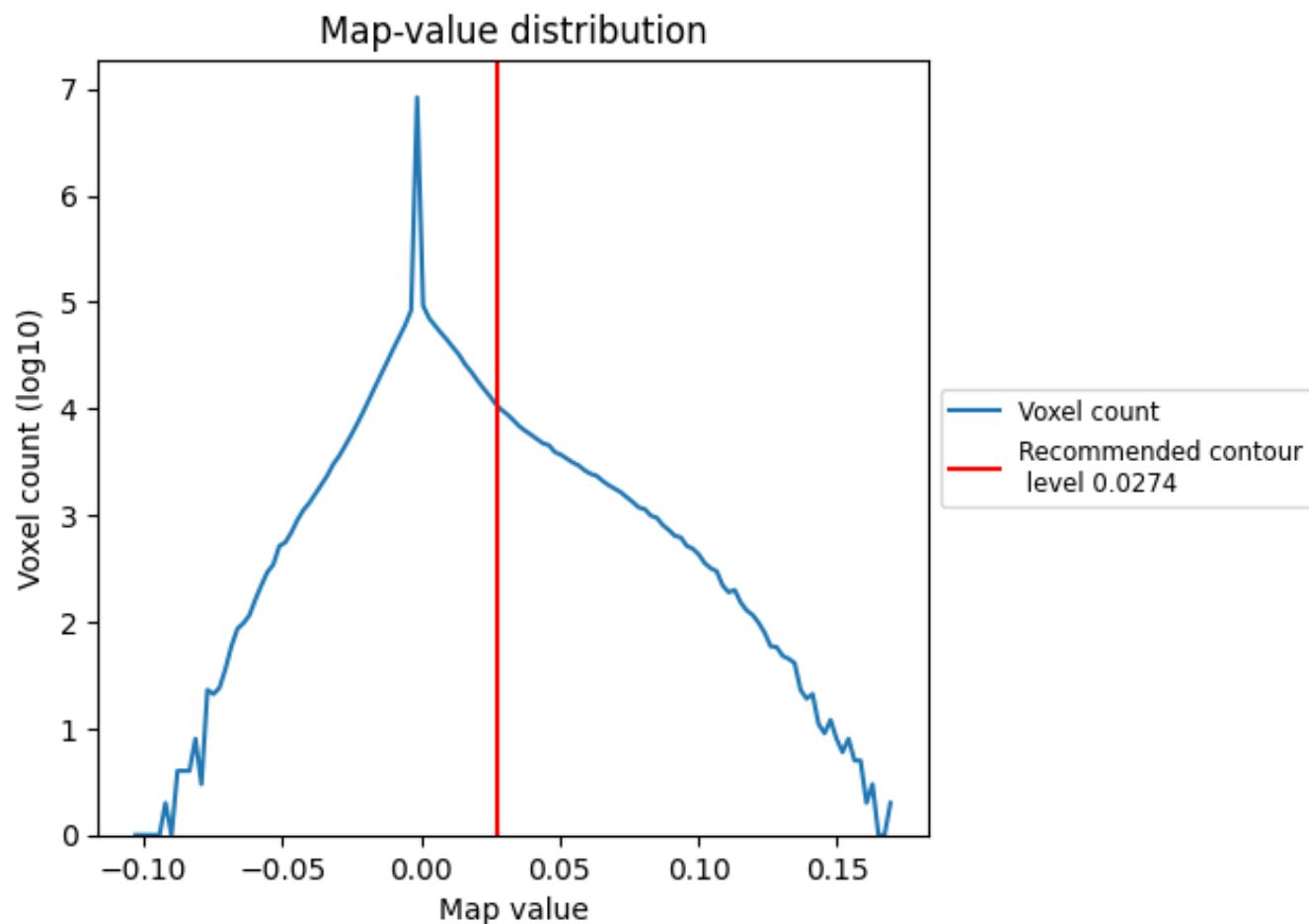
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

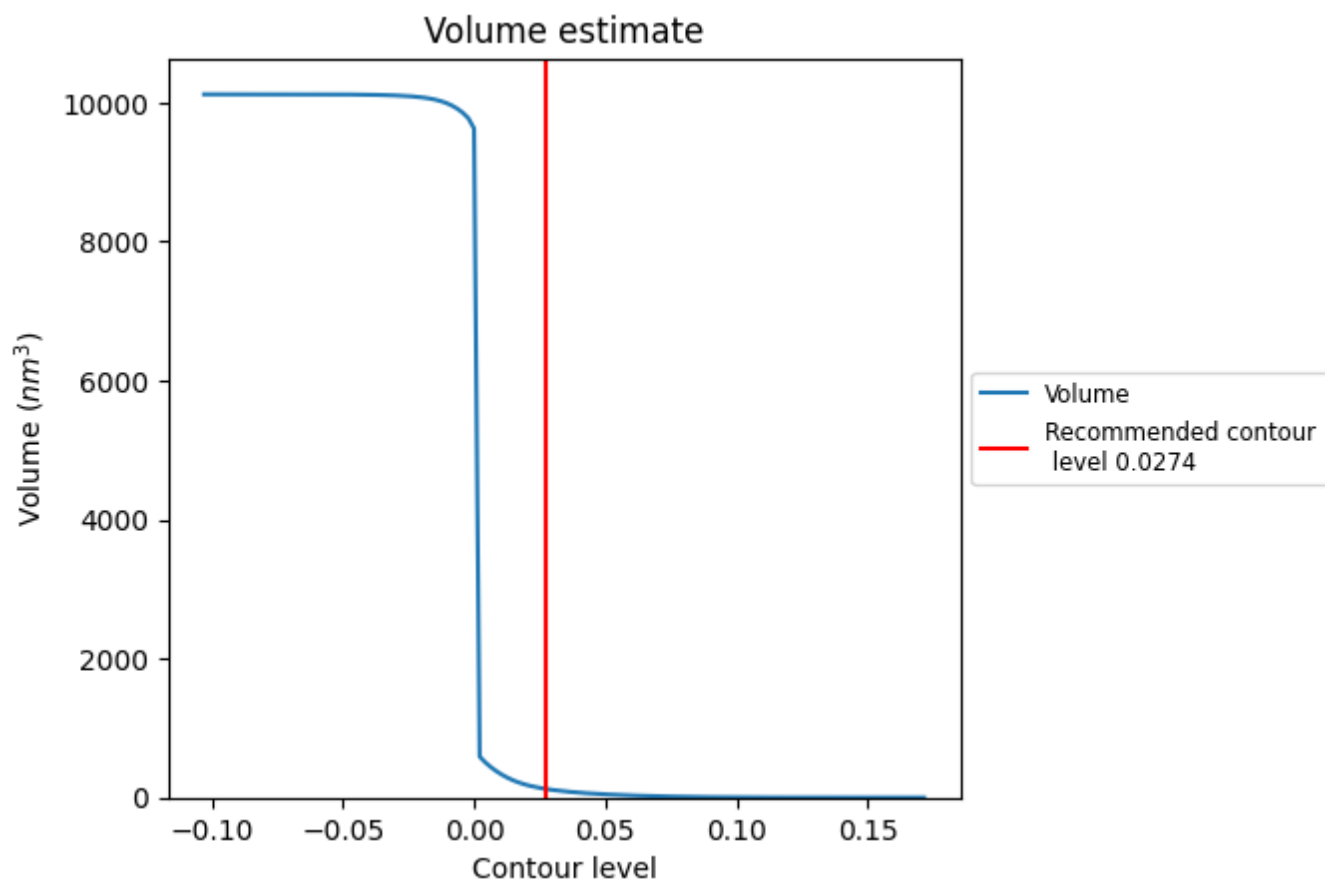
This section contains the results of statistical analysis of the map.

### 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.

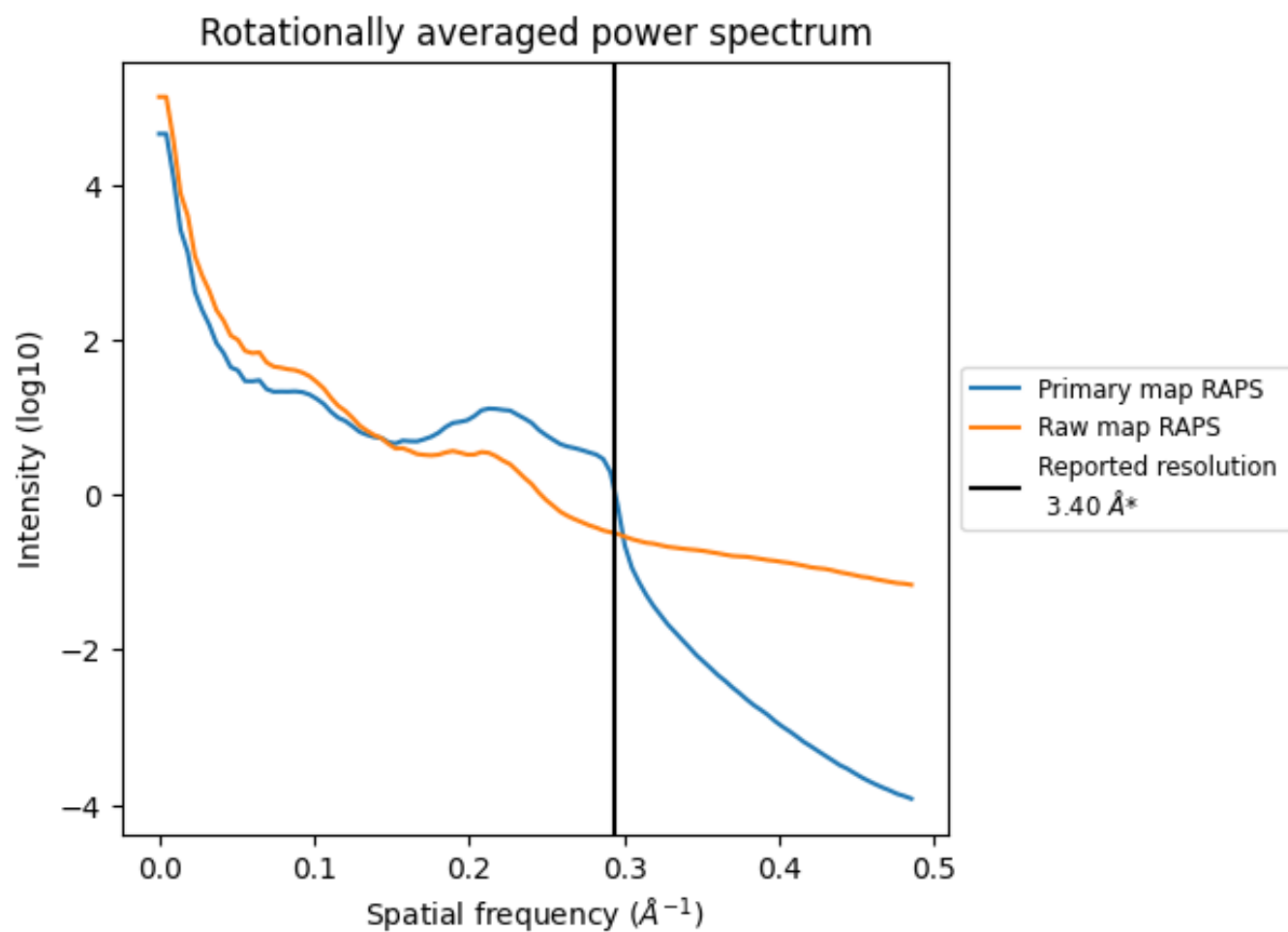
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 123 nm<sup>3</sup>; this corresponds to an approximate mass of 111 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 ⓘ



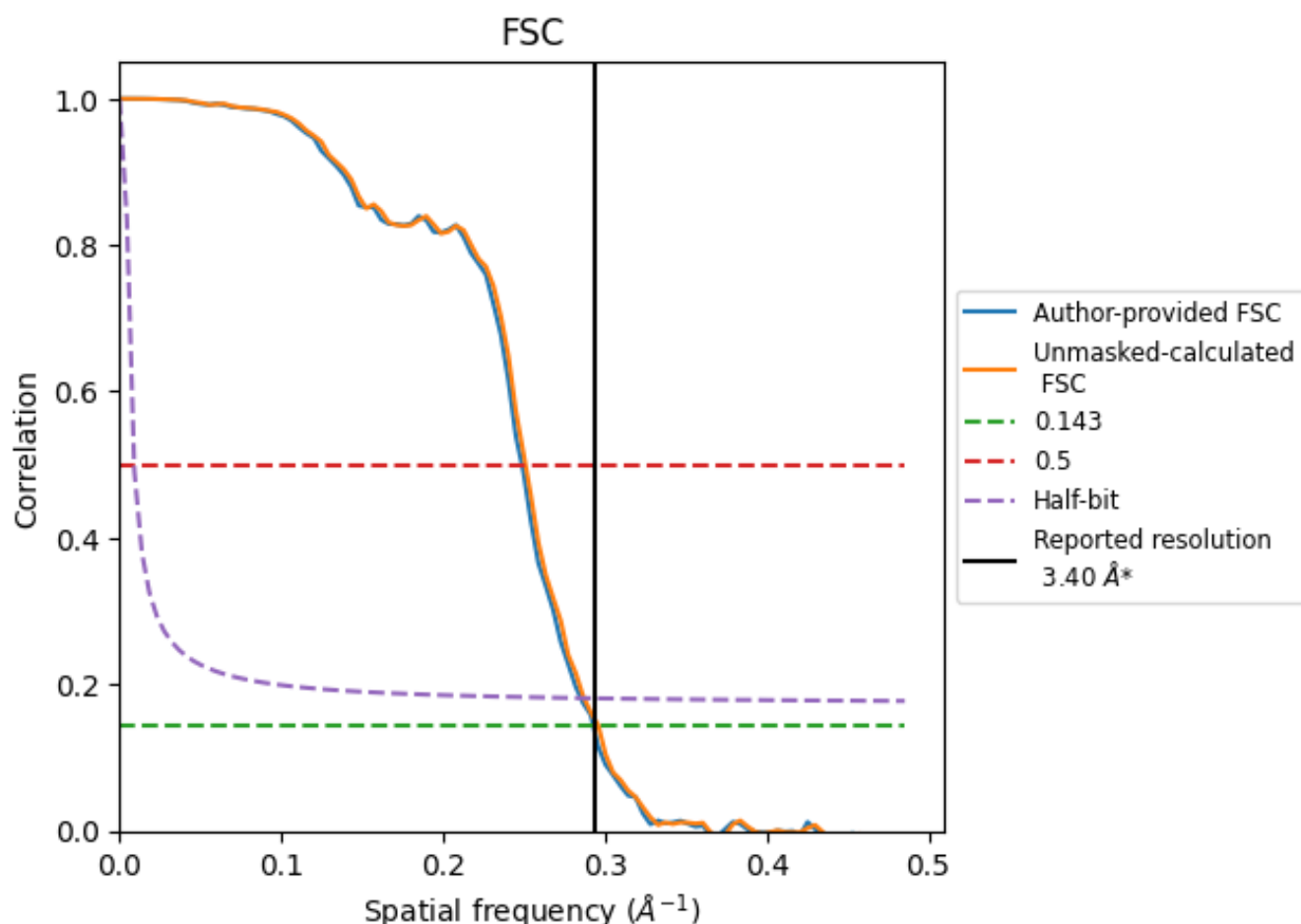
\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

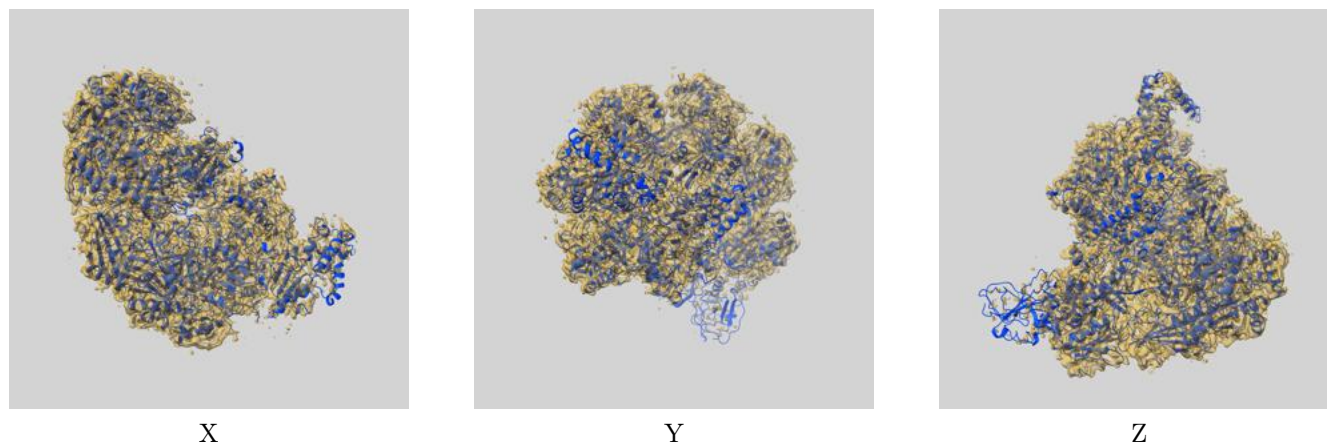
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	4.02	3.51
Unmasked-calculated*	3.38	3.99	3.48

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

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

This section contains information regarding the fit between EMDB map EMD-8624 and PDB model 5UZ9. Per-residue inclusion information can be found in section 3 on page 11.

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

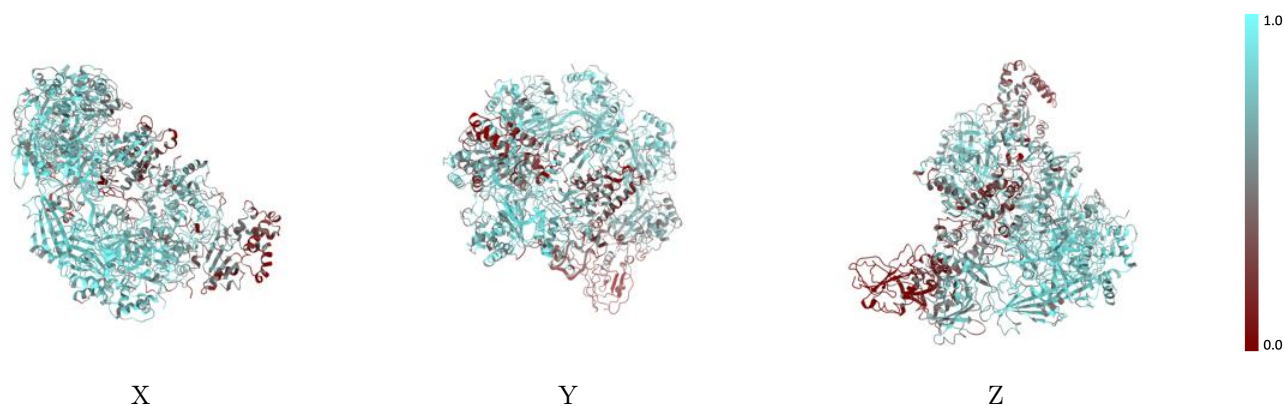


The images above show the 3D surface view of the map at the recommended contour level 0.0274 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

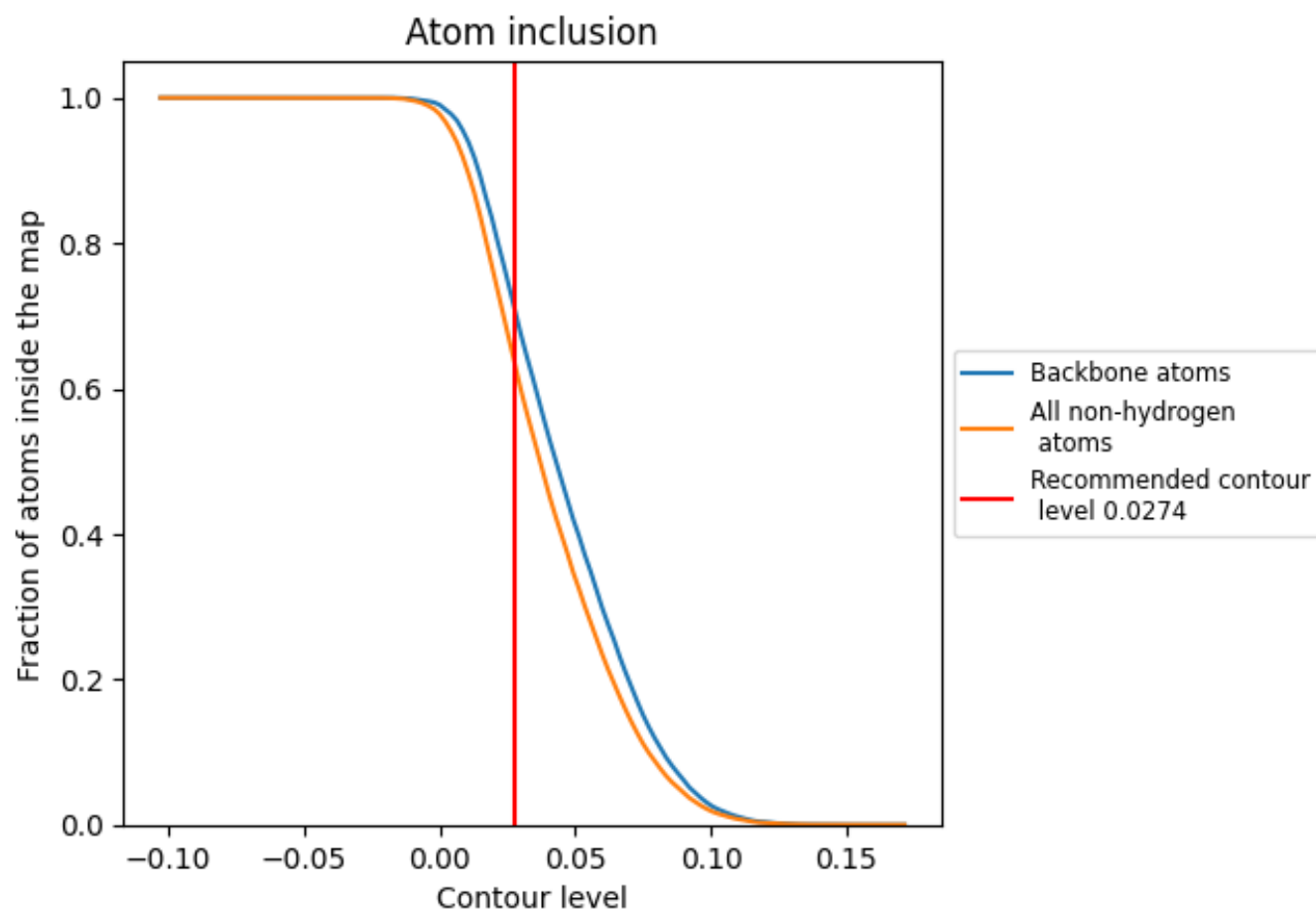
This section was not generated.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0274).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0274) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	<div></div> 0.6387
A	<div></div> 0.4427
B	<div></div> 0.6509
C	<div></div> 0.5264
D	<div></div> 0.7007
E	<div></div> 0.7662
F	<div></div> 0.7679
G	<div></div> 0.7602
H	<div></div> 0.7260
I	<div></div> 0.6978
J	<div></div> 0.7250
K	<div></div> 0.3940
L	<div></div> 0.0833
M	<div></div> 0.6231

1.0

0.0

<0.0