



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:51 PM BST

PDB ID : 5FKI
EMDB ID: : EMD-3197
Title : Pseudorabies virus (PrV) nuclear egress complex proteins fitted as a hexameric lattice into a sub-tomogram average derived from focused- ion beam milled lamellae electron cryo-microscopic data
Authors : Hagen, C.; Dent, K.C.; Zeev Ben Mordehai, T.; Vasishtan, D.; Antonin, W.; Mettenleiter, T.C.; Gruenewald, K.
Deposited on : 2015-10-16
Resolution : 35.00 Å(reported)
Based on PDB ID : 5E8C

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

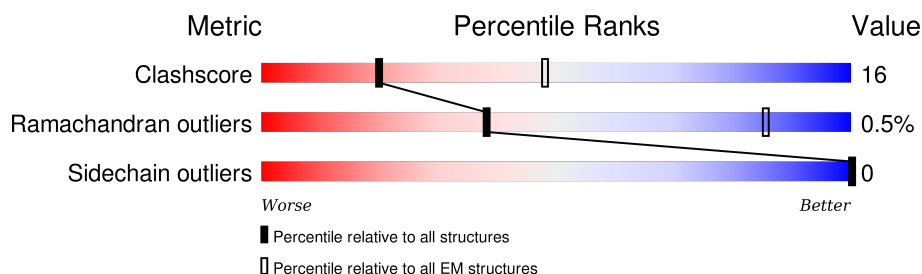
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 35.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















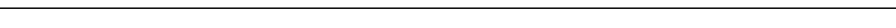











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	10	253	84% 13% .
1	12	253	84% 13% .
1	14	253	81% 15% .
1	16	253	82% 15% .
1	18	253	82% 15% .
1	1A	253	82% 15% .
1	1C	253	82% 15% .
1	1E	253	82% 15% .
1	1G	253	82% 15% .














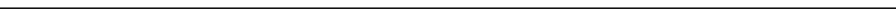











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Mol	Chain	Length	Quality of chain
1	1I	253	 82% 15% .
1	1K	253	 82% 15% .
1	1M	253	 82% 15% .
1	1O	253	 84% 13% .
1	1Q	253	 84% 13% .
1	1S	253	 81% 15% .
1	1U	253	 82% 15% .
1	1W	253	 82% 15% .
1	1Y	253	 82% 15% .
1	20	253	 84% 13% .
1	22	253	 84% 13% .
1	24	253	 81% 15% .
1	26	253	 82% 15% .
1	28	253	 82% 15% .
1	2A	253	 82% 15% .
1	2C	253	 84% 13% .
1	2E	253	 84% 13% .
1	2G	253	 82% 15% .
1	2I	253	 82% 15% .
1	2K	253	 82% 15% .
1	2M	253	 82% 15% .
1	2O	253	 84% 13% .
1	2Q	253	 84% 13% .
1	2S	253	 81% 15% .
1	2U	253	 82% 15% .


























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Mol	Chain	Length	Quality of chain
1	2W	253	 82% 15% .
1	2Y	253	 82% 15% .
1	3A	253	 82% 15% .
1	3C	253	 84% 13% .
1	3E	253	 85% 12% .
1	3G	253	 81% 15% .
1	3I	253	 82% 15% .
1	3K	253	 82% 15% .
2	11	179	 84% 10% 6%
2	13	179	 83% 11% 6%
2	15	179	 83% 11% 6%
2	17	179	 83% 11% 6%
2	19	179	 83% 11% 6%
2	1B	179	 83% 11% 6%
2	1D	179	 84% 10% 6%
2	1F	179	 83% 11% 6%
2	1H	179	 83% 11% 6%
2	1J	179	 83% 11% 6%
2	1L	179	 83% 11% 6%
2	1N	179	 83% 11% 6%
2	1P	179	 84% 9% 6%
2	1R	179	 83% 11% 6%
2	1T	179	 83% 11% 6%
2	1V	179	 83% 11% 6%
2	1X	179	 83% 11% 6%

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Mol	Chain	Length	Quality of chain
2	1Z	179	 83%11%6%
2	2I	179	 84%10%6%
2	2J	179	 84%10%6%
2	2K	179	 83%11%6%
2	2L	179	 84%10%6%
2	2M	179	 83%11%6%
2	2N	179	 84%10%6%
2	2O	179	 84%10%6%
2	2P	179	 84%10%6%
2	2Q	179	 83%11%6%
2	2R	179	 83%11%6%
2	2S	179	 83%11%6%
2	2T	179	 83%11%6%
2	2U	179	 84%10%6%
2	2V	179	 83%11%6%
2	2W	179	 83%11%6%
2	2X	179	 83%11%6%
2	2Y	179	 83%11%6%
2	2Z	179	 83%11%6%
2	3A	179	 84%10%6%
2	3B	179	 83%11%6%
2	3C	179	 83%11%6%
2	3D	179	 83%11%6%
2	3E	179	 83%11%6%
2	3F	179	 83%11%6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 108108 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 UL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1C	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1E	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1G	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1I	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1K	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1M	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1O	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1Q	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1S	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1U	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1W	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	1Y	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	10	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	12	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	14	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	16	245	Total 1523	C 976	N 270	O 271	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	18	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2A	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2C	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2E	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2G	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2I	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2K	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2M	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2O	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2Q	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2S	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2U	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2W	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	2Y	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	20	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	22	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	24	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	26	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	28	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	3A	245	Total 1523	C 976	N 270	O 271	S 6	0	0
1	3C	245	Total 1523	C 976	N 270	O 271	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3E	245	Total	C	N	O	S	0	0
			1523	976	270	271	6		
1	3G	245	Total	C	N	O	S	0	0
			1523	976	270	271	6		
1	3I	245	Total	C	N	O	S	0	0
			1523	976	270	271	6		
1	3K	245	Total	C	N	O	S	0	0
			1523	976	270	271	6		

There are 294 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	19	ALA	-	expression tag	UNP G3G955
1A	20	ILE	-	expression tag	UNP G3G955
1A	21	ALA	-	expression tag	UNP G3G955
1A	22	ASP	-	expression tag	UNP G3G955
1A	23	VAL	-	expression tag	UNP G3G955
1A	24	GLY	-	expression tag	UNP G3G955
1A	25	THR	-	expression tag	UNP G3G955
1C	19	ALA	-	expression tag	UNP G3G955
1C	20	ILE	-	expression tag	UNP G3G955
1C	21	ALA	-	expression tag	UNP G3G955
1C	22	ASP	-	expression tag	UNP G3G955
1C	23	VAL	-	expression tag	UNP G3G955
1C	24	GLY	-	expression tag	UNP G3G955
1C	25	THR	-	expression tag	UNP G3G955
1E	19	ALA	-	expression tag	UNP G3G955
1E	20	ILE	-	expression tag	UNP G3G955
1E	21	ALA	-	expression tag	UNP G3G955
1E	22	ASP	-	expression tag	UNP G3G955
1E	23	VAL	-	expression tag	UNP G3G955
1E	24	GLY	-	expression tag	UNP G3G955
1E	25	THR	-	expression tag	UNP G3G955
1G	19	ALA	-	expression tag	UNP G3G955
1G	20	ILE	-	expression tag	UNP G3G955
1G	21	ALA	-	expression tag	UNP G3G955
1G	22	ASP	-	expression tag	UNP G3G955
1G	23	VAL	-	expression tag	UNP G3G955
1G	24	GLY	-	expression tag	UNP G3G955
1G	25	THR	-	expression tag	UNP G3G955
1I	19	ALA	-	expression tag	UNP G3G955
1I	20	ILE	-	expression tag	UNP G3G955
1I	21	ALA	-	expression tag	UNP G3G955

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Chain	Residue	Modelled	Actual	Comment	Reference
1I	22	ASP	-	expression tag	UNP G3G955
1I	23	VAL	-	expression tag	UNP G3G955
1I	24	GLY	-	expression tag	UNP G3G955
1I	25	THR	-	expression tag	UNP G3G955
1K	19	ALA	-	expression tag	UNP G3G955
1K	20	ILE	-	expression tag	UNP G3G955
1K	21	ALA	-	expression tag	UNP G3G955
1K	22	ASP	-	expression tag	UNP G3G955
1K	23	VAL	-	expression tag	UNP G3G955
1K	24	GLY	-	expression tag	UNP G3G955
1K	25	THR	-	expression tag	UNP G3G955
1M	19	ALA	-	expression tag	UNP G3G955
1M	20	ILE	-	expression tag	UNP G3G955
1M	21	ALA	-	expression tag	UNP G3G955
1M	22	ASP	-	expression tag	UNP G3G955
1M	23	VAL	-	expression tag	UNP G3G955
1M	24	GLY	-	expression tag	UNP G3G955
1M	25	THR	-	expression tag	UNP G3G955
1O	19	ALA	-	expression tag	UNP G3G955
1O	20	ILE	-	expression tag	UNP G3G955
1O	21	ALA	-	expression tag	UNP G3G955
1O	22	ASP	-	expression tag	UNP G3G955
1O	23	VAL	-	expression tag	UNP G3G955
1O	24	GLY	-	expression tag	UNP G3G955
1O	25	THR	-	expression tag	UNP G3G955
1Q	19	ALA	-	expression tag	UNP G3G955
1Q	20	ILE	-	expression tag	UNP G3G955
1Q	21	ALA	-	expression tag	UNP G3G955
1Q	22	ASP	-	expression tag	UNP G3G955
1Q	23	VAL	-	expression tag	UNP G3G955
1Q	24	GLY	-	expression tag	UNP G3G955
1Q	25	THR	-	expression tag	UNP G3G955
1S	19	ALA	-	expression tag	UNP G3G955
1S	20	ILE	-	expression tag	UNP G3G955
1S	21	ALA	-	expression tag	UNP G3G955
1S	22	ASP	-	expression tag	UNP G3G955
1S	23	VAL	-	expression tag	UNP G3G955
1S	24	GLY	-	expression tag	UNP G3G955
1S	25	THR	-	expression tag	UNP G3G955
1U	19	ALA	-	expression tag	UNP G3G955
1U	20	ILE	-	expression tag	UNP G3G955
1U	21	ALA	-	expression tag	UNP G3G955

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Chain	Residue	Modelled	Actual	Comment	Reference
1U	22	ASP	-	expression tag	UNP G3G955
1U	23	VAL	-	expression tag	UNP G3G955
1U	24	GLY	-	expression tag	UNP G3G955
1U	25	THR	-	expression tag	UNP G3G955
1W	19	ALA	-	expression tag	UNP G3G955
1W	20	ILE	-	expression tag	UNP G3G955
1W	21	ALA	-	expression tag	UNP G3G955
1W	22	ASP	-	expression tag	UNP G3G955
1W	23	VAL	-	expression tag	UNP G3G955
1W	24	GLY	-	expression tag	UNP G3G955
1W	25	THR	-	expression tag	UNP G3G955
1Y	19	ALA	-	expression tag	UNP G3G955
1Y	20	ILE	-	expression tag	UNP G3G955
1Y	21	ALA	-	expression tag	UNP G3G955
1Y	22	ASP	-	expression tag	UNP G3G955
1Y	23	VAL	-	expression tag	UNP G3G955
1Y	24	GLY	-	expression tag	UNP G3G955
1Y	25	THR	-	expression tag	UNP G3G955
10	19	ALA	-	expression tag	UNP G3G955
10	20	ILE	-	expression tag	UNP G3G955
10	21	ALA	-	expression tag	UNP G3G955
10	22	ASP	-	expression tag	UNP G3G955
10	23	VAL	-	expression tag	UNP G3G955
10	24	GLY	-	expression tag	UNP G3G955
10	25	THR	-	expression tag	UNP G3G955
12	19	ALA	-	expression tag	UNP G3G955
12	20	ILE	-	expression tag	UNP G3G955
12	21	ALA	-	expression tag	UNP G3G955
12	22	ASP	-	expression tag	UNP G3G955
12	23	VAL	-	expression tag	UNP G3G955
12	24	GLY	-	expression tag	UNP G3G955
12	25	THR	-	expression tag	UNP G3G955
14	19	ALA	-	expression tag	UNP G3G955
14	20	ILE	-	expression tag	UNP G3G955
14	21	ALA	-	expression tag	UNP G3G955
14	22	ASP	-	expression tag	UNP G3G955
14	23	VAL	-	expression tag	UNP G3G955
14	24	GLY	-	expression tag	UNP G3G955
14	25	THR	-	expression tag	UNP G3G955
16	19	ALA	-	expression tag	UNP G3G955
16	20	ILE	-	expression tag	UNP G3G955
16	21	ALA	-	expression tag	UNP G3G955

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Chain	Residue	Modelled	Actual	Comment	Reference
16	22	ASP	-	expression tag	UNP G3G955
16	23	VAL	-	expression tag	UNP G3G955
16	24	GLY	-	expression tag	UNP G3G955
16	25	THR	-	expression tag	UNP G3G955
18	19	ALA	-	expression tag	UNP G3G955
18	20	ILE	-	expression tag	UNP G3G955
18	21	ALA	-	expression tag	UNP G3G955
18	22	ASP	-	expression tag	UNP G3G955
18	23	VAL	-	expression tag	UNP G3G955
18	24	GLY	-	expression tag	UNP G3G955
18	25	THR	-	expression tag	UNP G3G955
2A	19	ALA	-	expression tag	UNP G3G955
2A	20	ILE	-	expression tag	UNP G3G955
2A	21	ALA	-	expression tag	UNP G3G955
2A	22	ASP	-	expression tag	UNP G3G955
2A	23	VAL	-	expression tag	UNP G3G955
2A	24	GLY	-	expression tag	UNP G3G955
2A	25	THR	-	expression tag	UNP G3G955
2C	19	ALA	-	expression tag	UNP G3G955
2C	20	ILE	-	expression tag	UNP G3G955
2C	21	ALA	-	expression tag	UNP G3G955
2C	22	ASP	-	expression tag	UNP G3G955
2C	23	VAL	-	expression tag	UNP G3G955
2C	24	GLY	-	expression tag	UNP G3G955
2C	25	THR	-	expression tag	UNP G3G955
2E	19	ALA	-	expression tag	UNP G3G955
2E	20	ILE	-	expression tag	UNP G3G955
2E	21	ALA	-	expression tag	UNP G3G955
2E	22	ASP	-	expression tag	UNP G3G955
2E	23	VAL	-	expression tag	UNP G3G955
2E	24	GLY	-	expression tag	UNP G3G955
2E	25	THR	-	expression tag	UNP G3G955
2G	19	ALA	-	expression tag	UNP G3G955
2G	20	ILE	-	expression tag	UNP G3G955
2G	21	ALA	-	expression tag	UNP G3G955
2G	22	ASP	-	expression tag	UNP G3G955
2G	23	VAL	-	expression tag	UNP G3G955
2G	24	GLY	-	expression tag	UNP G3G955
2G	25	THR	-	expression tag	UNP G3G955
2I	19	ALA	-	expression tag	UNP G3G955
2I	20	ILE	-	expression tag	UNP G3G955
2I	21	ALA	-	expression tag	UNP G3G955

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Chain	Residue	Modelled	Actual	Comment	Reference
2I	22	ASP	-	expression tag	UNP G3G955
2I	23	VAL	-	expression tag	UNP G3G955
2I	24	GLY	-	expression tag	UNP G3G955
2I	25	THR	-	expression tag	UNP G3G955
2K	19	ALA	-	expression tag	UNP G3G955
2K	20	ILE	-	expression tag	UNP G3G955
2K	21	ALA	-	expression tag	UNP G3G955
2K	22	ASP	-	expression tag	UNP G3G955
2K	23	VAL	-	expression tag	UNP G3G955
2K	24	GLY	-	expression tag	UNP G3G955
2K	25	THR	-	expression tag	UNP G3G955
2M	19	ALA	-	expression tag	UNP G3G955
2M	20	ILE	-	expression tag	UNP G3G955
2M	21	ALA	-	expression tag	UNP G3G955
2M	22	ASP	-	expression tag	UNP G3G955
2M	23	VAL	-	expression tag	UNP G3G955
2M	24	GLY	-	expression tag	UNP G3G955
2M	25	THR	-	expression tag	UNP G3G955
2O	19	ALA	-	expression tag	UNP G3G955
2O	20	ILE	-	expression tag	UNP G3G955
2O	21	ALA	-	expression tag	UNP G3G955
2O	22	ASP	-	expression tag	UNP G3G955
2O	23	VAL	-	expression tag	UNP G3G955
2O	24	GLY	-	expression tag	UNP G3G955
2O	25	THR	-	expression tag	UNP G3G955
2Q	19	ALA	-	expression tag	UNP G3G955
2Q	20	ILE	-	expression tag	UNP G3G955
2Q	21	ALA	-	expression tag	UNP G3G955
2Q	22	ASP	-	expression tag	UNP G3G955
2Q	23	VAL	-	expression tag	UNP G3G955
2Q	24	GLY	-	expression tag	UNP G3G955
2Q	25	THR	-	expression tag	UNP G3G955
2S	19	ALA	-	expression tag	UNP G3G955
2S	20	ILE	-	expression tag	UNP G3G955
2S	21	ALA	-	expression tag	UNP G3G955
2S	22	ASP	-	expression tag	UNP G3G955
2S	23	VAL	-	expression tag	UNP G3G955
2S	24	GLY	-	expression tag	UNP G3G955
2S	25	THR	-	expression tag	UNP G3G955
2U	19	ALA	-	expression tag	UNP G3G955
2U	20	ILE	-	expression tag	UNP G3G955
2U	21	ALA	-	expression tag	UNP G3G955

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Chain	Residue	Modelled	Actual	Comment	Reference
2U	22	ASP	-	expression tag	UNP G3G955
2U	23	VAL	-	expression tag	UNP G3G955
2U	24	GLY	-	expression tag	UNP G3G955
2U	25	THR	-	expression tag	UNP G3G955
2W	19	ALA	-	expression tag	UNP G3G955
2W	20	ILE	-	expression tag	UNP G3G955
2W	21	ALA	-	expression tag	UNP G3G955
2W	22	ASP	-	expression tag	UNP G3G955
2W	23	VAL	-	expression tag	UNP G3G955
2W	24	GLY	-	expression tag	UNP G3G955
2W	25	THR	-	expression tag	UNP G3G955
2Y	19	ALA	-	expression tag	UNP G3G955
2Y	20	ILE	-	expression tag	UNP G3G955
2Y	21	ALA	-	expression tag	UNP G3G955
2Y	22	ASP	-	expression tag	UNP G3G955
2Y	23	VAL	-	expression tag	UNP G3G955
2Y	24	GLY	-	expression tag	UNP G3G955
2Y	25	THR	-	expression tag	UNP G3G955
20	19	ALA	-	expression tag	UNP G3G955
20	20	ILE	-	expression tag	UNP G3G955
20	21	ALA	-	expression tag	UNP G3G955
20	22	ASP	-	expression tag	UNP G3G955
20	23	VAL	-	expression tag	UNP G3G955
20	24	GLY	-	expression tag	UNP G3G955
20	25	THR	-	expression tag	UNP G3G955
22	19	ALA	-	expression tag	UNP G3G955
22	20	ILE	-	expression tag	UNP G3G955
22	21	ALA	-	expression tag	UNP G3G955
22	22	ASP	-	expression tag	UNP G3G955
22	23	VAL	-	expression tag	UNP G3G955
22	24	GLY	-	expression tag	UNP G3G955
22	25	THR	-	expression tag	UNP G3G955
24	19	ALA	-	expression tag	UNP G3G955
24	20	ILE	-	expression tag	UNP G3G955
24	21	ALA	-	expression tag	UNP G3G955
24	22	ASP	-	expression tag	UNP G3G955
24	23	VAL	-	expression tag	UNP G3G955
24	24	GLY	-	expression tag	UNP G3G955
24	25	THR	-	expression tag	UNP G3G955
26	19	ALA	-	expression tag	UNP G3G955
26	20	ILE	-	expression tag	UNP G3G955
26	21	ALA	-	expression tag	UNP G3G955

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Chain	Residue	Modelled	Actual	Comment	Reference
26	22	ASP	-	expression tag	UNP G3G955
26	23	VAL	-	expression tag	UNP G3G955
26	24	GLY	-	expression tag	UNP G3G955
26	25	THR	-	expression tag	UNP G3G955
28	19	ALA	-	expression tag	UNP G3G955
28	20	ILE	-	expression tag	UNP G3G955
28	21	ALA	-	expression tag	UNP G3G955
28	22	ASP	-	expression tag	UNP G3G955
28	23	VAL	-	expression tag	UNP G3G955
28	24	GLY	-	expression tag	UNP G3G955
28	25	THR	-	expression tag	UNP G3G955
3A	19	ALA	-	expression tag	UNP G3G955
3A	20	ILE	-	expression tag	UNP G3G955
3A	21	ALA	-	expression tag	UNP G3G955
3A	22	ASP	-	expression tag	UNP G3G955
3A	23	VAL	-	expression tag	UNP G3G955
3A	24	GLY	-	expression tag	UNP G3G955
3A	25	THR	-	expression tag	UNP G3G955
3C	19	ALA	-	expression tag	UNP G3G955
3C	20	ILE	-	expression tag	UNP G3G955
3C	21	ALA	-	expression tag	UNP G3G955
3C	22	ASP	-	expression tag	UNP G3G955
3C	23	VAL	-	expression tag	UNP G3G955
3C	24	GLY	-	expression tag	UNP G3G955
3C	25	THR	-	expression tag	UNP G3G955
3E	19	ALA	-	expression tag	UNP G3G955
3E	20	ILE	-	expression tag	UNP G3G955
3E	21	ALA	-	expression tag	UNP G3G955
3E	22	ASP	-	expression tag	UNP G3G955
3E	23	VAL	-	expression tag	UNP G3G955
3E	24	GLY	-	expression tag	UNP G3G955
3E	25	THR	-	expression tag	UNP G3G955
3G	19	ALA	-	expression tag	UNP G3G955
3G	20	ILE	-	expression tag	UNP G3G955
3G	21	ALA	-	expression tag	UNP G3G955
3G	22	ASP	-	expression tag	UNP G3G955
3G	23	VAL	-	expression tag	UNP G3G955
3G	24	GLY	-	expression tag	UNP G3G955
3G	25	THR	-	expression tag	UNP G3G955
3I	19	ALA	-	expression tag	UNP G3G955
3I	20	ILE	-	expression tag	UNP G3G955
3I	21	ALA	-	expression tag	UNP G3G955

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Chain	Residue	Modelled	Actual	Comment	Reference
3I	22	ASP	-	expression tag	UNP G3G955
3I	23	VAL	-	expression tag	UNP G3G955
3I	24	GLY	-	expression tag	UNP G3G955
3I	25	THR	-	expression tag	UNP G3G955
3K	19	ALA	-	expression tag	UNP G3G955
3K	20	ILE	-	expression tag	UNP G3G955
3K	21	ALA	-	expression tag	UNP G3G955
3K	22	ASP	-	expression tag	UNP G3G955
3K	23	VAL	-	expression tag	UNP G3G955
3K	24	GLY	-	expression tag	UNP G3G955
3K	25	THR	-	expression tag	UNP G3G955

- Molecule 2 is a protein called UL34 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1D	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1F	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1H	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1J	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1L	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1N	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1P	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1R	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1T	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1V	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1X	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	1Z	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	11	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	13	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	15	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	17	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	19	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2B	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2D	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2F	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2H	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2J	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2L	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2N	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2P	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2R	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2T	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2V	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2X	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	2Z	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	21	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	23	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	25	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	27	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	29	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	3B	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	3D	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	3F	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	3H	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	3J	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		
2	3L	168	Total	C	N	O	S	0	0
			1049	674	187	183	5		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1B	1	MSE	-	initiating methionine	UNP G3G8R3
1B	172	MSE	LEU	conflict	UNP G3G8R3
1D	1	MSE	-	initiating methionine	UNP G3G8R3
1D	172	MSE	LEU	conflict	UNP G3G8R3
1F	1	MSE	-	initiating methionine	UNP G3G8R3
1F	172	MSE	LEU	conflict	UNP G3G8R3
1H	1	MSE	-	initiating methionine	UNP G3G8R3
1H	172	MSE	LEU	conflict	UNP G3G8R3
1J	1	MSE	-	initiating methionine	UNP G3G8R3
1J	172	MSE	LEU	conflict	UNP G3G8R3
1L	1	MSE	-	initiating methionine	UNP G3G8R3
1L	172	MSE	LEU	conflict	UNP G3G8R3
1N	1	MSE	-	initiating methionine	UNP G3G8R3
1N	172	MSE	LEU	conflict	UNP G3G8R3
1P	1	MSE	-	initiating methionine	UNP G3G8R3
1P	172	MSE	LEU	conflict	UNP G3G8R3
1R	1	MSE	-	initiating methionine	UNP G3G8R3
1R	172	MSE	LEU	conflict	UNP G3G8R3
1T	1	MSE	-	initiating methionine	UNP G3G8R3
1T	172	MSE	LEU	conflict	UNP G3G8R3
1V	1	MSE	-	initiating methionine	UNP G3G8R3
1V	172	MSE	LEU	conflict	UNP G3G8R3
1X	1	MSE	-	initiating methionine	UNP G3G8R3
1X	172	MSE	LEU	conflict	UNP G3G8R3
1Z	1	MSE	-	initiating methionine	UNP G3G8R3

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Chain	Residue	Modelled	Actual	Comment	Reference
1Z	172	MSE	LEU	conflict	UNP G3G8R3
11	1	MSE	-	initiating methionine	UNP G3G8R3
11	172	MSE	LEU	conflict	UNP G3G8R3
13	1	MSE	-	initiating methionine	UNP G3G8R3
13	172	MSE	LEU	conflict	UNP G3G8R3
15	1	MSE	-	initiating methionine	UNP G3G8R3
15	172	MSE	LEU	conflict	UNP G3G8R3
17	1	MSE	-	initiating methionine	UNP G3G8R3
17	172	MSE	LEU	conflict	UNP G3G8R3
19	1	MSE	-	initiating methionine	UNP G3G8R3
19	172	MSE	LEU	conflict	UNP G3G8R3
2B	1	MSE	-	initiating methionine	UNP G3G8R3
2B	172	MSE	LEU	conflict	UNP G3G8R3
2D	1	MSE	-	initiating methionine	UNP G3G8R3
2D	172	MSE	LEU	conflict	UNP G3G8R3
2F	1	MSE	-	initiating methionine	UNP G3G8R3
2F	172	MSE	LEU	conflict	UNP G3G8R3
2H	1	MSE	-	initiating methionine	UNP G3G8R3
2H	172	MSE	LEU	conflict	UNP G3G8R3
2J	1	MSE	-	initiating methionine	UNP G3G8R3
2J	172	MSE	LEU	conflict	UNP G3G8R3
2L	1	MSE	-	initiating methionine	UNP G3G8R3
2L	172	MSE	LEU	conflict	UNP G3G8R3
2N	1	MSE	-	initiating methionine	UNP G3G8R3
2N	172	MSE	LEU	conflict	UNP G3G8R3
2P	1	MSE	-	initiating methionine	UNP G3G8R3
2P	172	MSE	LEU	conflict	UNP G3G8R3
2R	1	MSE	-	initiating methionine	UNP G3G8R3
2R	172	MSE	LEU	conflict	UNP G3G8R3
2T	1	MSE	-	initiating methionine	UNP G3G8R3
2T	172	MSE	LEU	conflict	UNP G3G8R3
2V	1	MSE	-	initiating methionine	UNP G3G8R3
2V	172	MSE	LEU	conflict	UNP G3G8R3
2X	1	MSE	-	initiating methionine	UNP G3G8R3
2X	172	MSE	LEU	conflict	UNP G3G8R3
2Z	1	MSE	-	initiating methionine	UNP G3G8R3
2Z	172	MSE	LEU	conflict	UNP G3G8R3
21	1	MSE	-	initiating methionine	UNP G3G8R3
21	172	MSE	LEU	conflict	UNP G3G8R3
23	1	MSE	-	initiating methionine	UNP G3G8R3
23	172	MSE	LEU	conflict	UNP G3G8R3
25	1	MSE	-	initiating methionine	UNP G3G8R3

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Chain	Residue	Modelled	Actual	Comment	Reference
25	172	MSE	LEU	conflict	UNP G3G8R3
27	1	MSE	-	initiating methionine	UNP G3G8R3
27	172	MSE	LEU	conflict	UNP G3G8R3
29	1	MSE	-	initiating methionine	UNP G3G8R3
29	172	MSE	LEU	conflict	UNP G3G8R3
3B	1	MSE	-	initiating methionine	UNP G3G8R3
3B	172	MSE	LEU	conflict	UNP G3G8R3
3D	1	MSE	-	initiating methionine	UNP G3G8R3
3D	172	MSE	LEU	conflict	UNP G3G8R3
3F	1	MSE	-	initiating methionine	UNP G3G8R3
3F	172	MSE	LEU	conflict	UNP G3G8R3
3H	1	MSE	-	initiating methionine	UNP G3G8R3
3H	172	MSE	LEU	conflict	UNP G3G8R3
3J	1	MSE	-	initiating methionine	UNP G3G8R3
3J	172	MSE	LEU	conflict	UNP G3G8R3
3L	1	MSE	-	initiating methionine	UNP G3G8R3
3L	172	MSE	LEU	conflict	UNP G3G8R3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
3	2E	1	Total Zn 1 1	0
3	20	1	Total Zn 1 1	0
3	18	1	Total Zn 1 1	0
3	2W	1	Total Zn 1 1	0
3	1Y	1	Total Zn 1 1	0
3	2I	1	Total Zn 1 1	0
3	24	1	Total Zn 1 1	0
3	1E	1	Total Zn 1 1	0
3	2M	1	Total Zn 1 1	0
3	3I	1	Total Zn 1 1	0
3	3G	1	Total Zn 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
3	16	1	Total 1	Zn 1	0
3	28	1	Total 1	Zn 1	0
3	1W	1	Total 1	Zn 1	0
3	1A	1	Total 1	Zn 1	0
3	12	1	Total 1	Zn 1	0
3	1S	1	Total 1	Zn 1	0
3	2C	1	Total 1	Zn 1	0
3	1M	1	Total 1	Zn 1	0
3	2G	1	Total 1	Zn 1	0
3	1I	1	Total 1	Zn 1	0
3	3A	1	Total 1	Zn 1	0
3	22	1	Total 1	Zn 1	0
3	2Q	1	Total 1	Zn 1	0
3	2K	1	Total 1	Zn 1	0
3	26	1	Total 1	Zn 1	0
3	2U	1	Total 1	Zn 1	0
3	1G	1	Total 1	Zn 1	0
3	2O	1	Total 1	Zn 1	0
3	3K	1	Total 1	Zn 1	0
3	2Y	1	Total 1	Zn 1	0
3	1C	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
3	3C	1	Total 1	Zn 1	0
3	14	1	Total 1	Zn 1	0
3	1U	1	Total 1	Zn 1	0
3	1O	1	Total 1	Zn 1	0
3	10	1	Total 1	Zn 1	0
3	1Q	1	Total 1	Zn 1	0
3	2A	1	Total 1	Zn 1	0
3	1K	1	Total 1	Zn 1	0
3	3E	1	Total 1	Zn 1	0
3	2S	1	Total 1	Zn 1	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
4	2E	1	Total 1	Cl 1	0
4	20	1	Total 1	Cl 1	0
4	18	1	Total 1	Cl 1	0
4	2W	1	Total 1	Cl 1	0
4	1Y	1	Total 1	Cl 1	0
4	2I	1	Total 1	Cl 1	0
4	24	1	Total 1	Cl 1	0
4	1E	1	Total 1	Cl 1	0
4	2M	1	Total 1	Cl 1	0

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Mol	Chain	Residues	Atoms		AltConf
4	3I	1	Total 1	Cl 1	0
4	3G	1	Total 1	Cl 1	0
4	16	1	Total 1	Cl 1	0
4	28	1	Total 1	Cl 1	0
4	1W	1	Total 1	Cl 1	0
4	1A	1	Total 1	Cl 1	0
4	12	1	Total 1	Cl 1	0
4	1S	1	Total 1	Cl 1	0
4	2C	1	Total 1	Cl 1	0
4	1M	1	Total 1	Cl 1	0
4	2G	1	Total 1	Cl 1	0
4	1I	1	Total 1	Cl 1	0
4	3A	1	Total 1	Cl 1	0
4	22	1	Total 1	Cl 1	0
4	2Q	1	Total 1	Cl 1	0
4	2K	1	Total 1	Cl 1	0
4	26	1	Total 1	Cl 1	0
4	2U	1	Total 1	Cl 1	0
4	1G	1	Total 1	Cl 1	0
4	2O	1	Total 1	Cl 1	0
4	3K	1	Total 1	Cl 1	0

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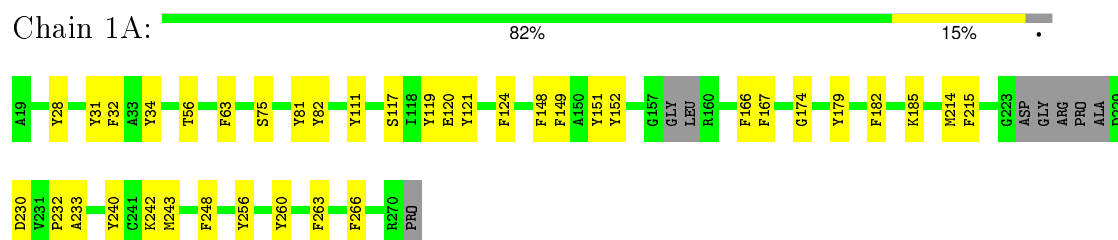
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Mol	Chain	Residues	Atoms		AltConf
4	2Y	1	Total 1	Cl 1	0
4	1C	1	Total 1	Cl 1	0
4	3C	1	Total 1	Cl 1	0
4	14	1	Total 1	Cl 1	0
4	1U	1	Total 1	Cl 1	0
4	1O	1	Total 1	Cl 1	0
4	10	1	Total 1	Cl 1	0
4	1Q	1	Total 1	Cl 1	0
4	2A	1	Total 1	Cl 1	0
4	1K	1	Total 1	Cl 1	0
4	3E	1	Total 1	Cl 1	0
4	2S	1	Total 1	Cl 1	0

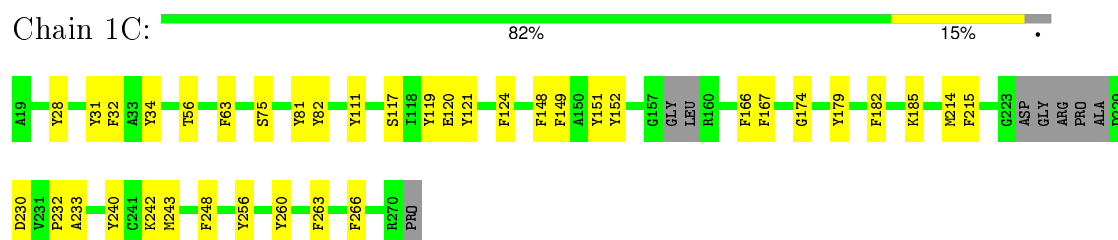
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

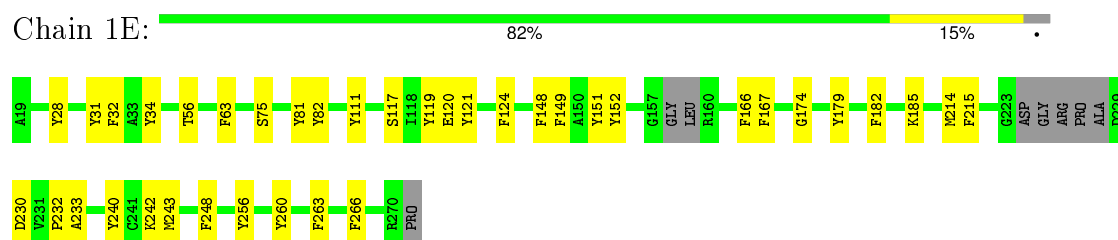
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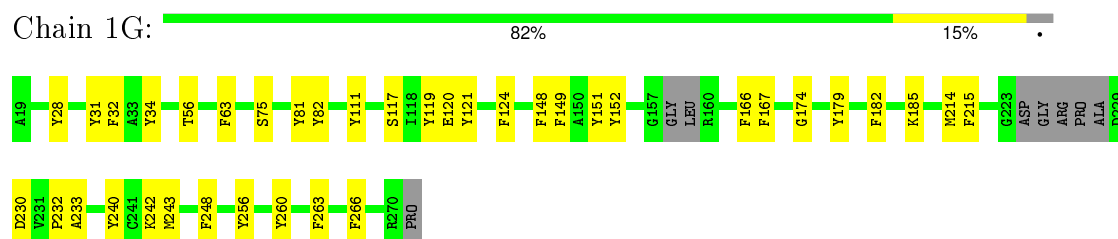
- Molecule 1: UL31



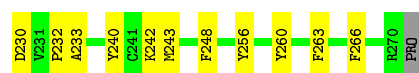
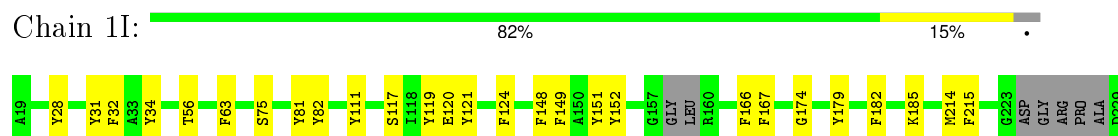
- Molecule 1: UL31



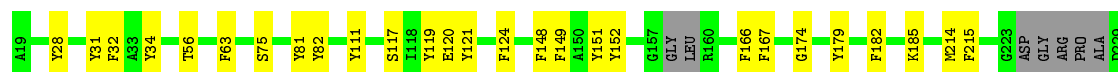
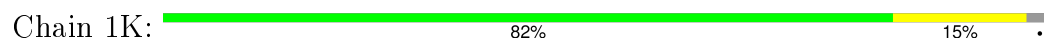
- Molecule 1: UL31



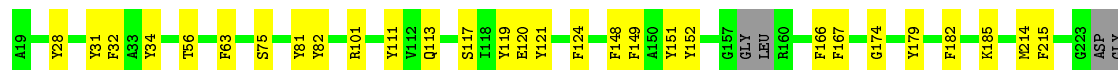
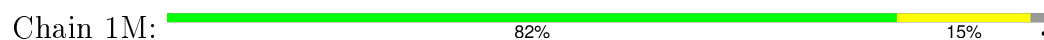
- Molecule 1: UL31



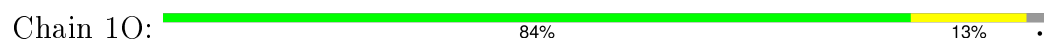
• Molecule 1: UL31



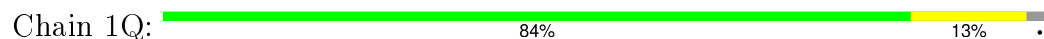
• Molecule 1: UL31



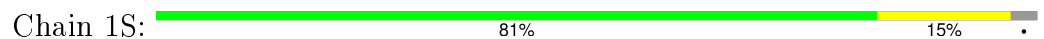
• Molecule 1: UL31

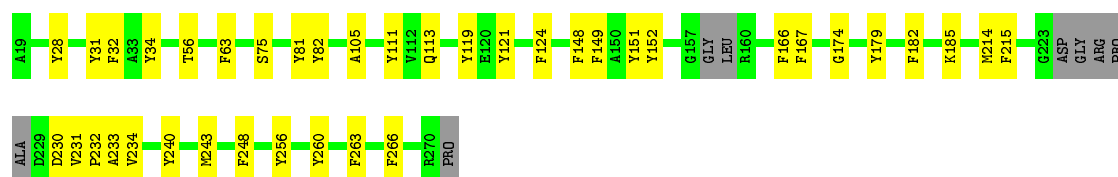


• Molecule 1: UL31



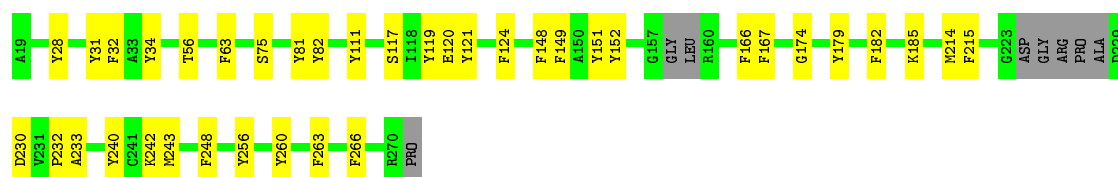
• Molecule 1: UL31





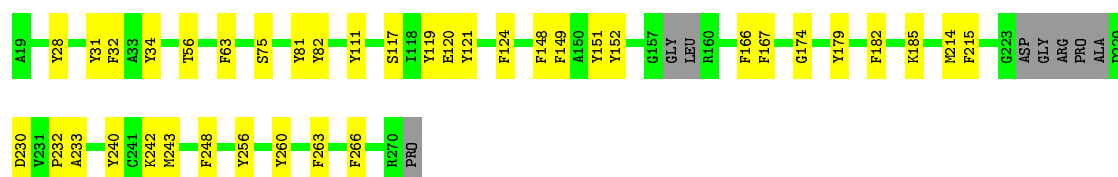
- Molecule 1: UL31

Chain 1U: 82% 15%



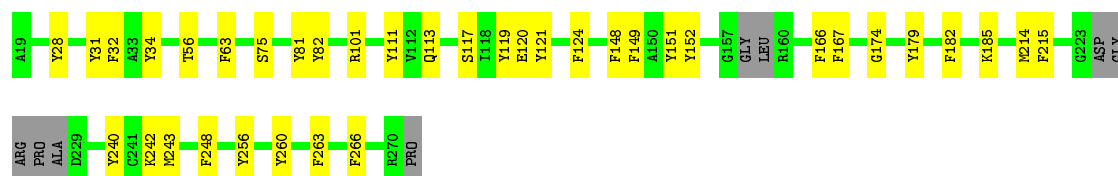
- Molecule 1: UL31

Chain 1W: 82% 15%



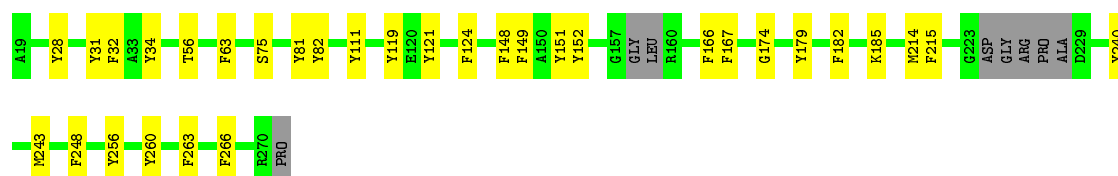
- Molecule 1: UL31

Chain 1Y: 82% 15%



- Molecule 1: UL31

Chain 10: 84% 13%



- Molecule 1: UL31

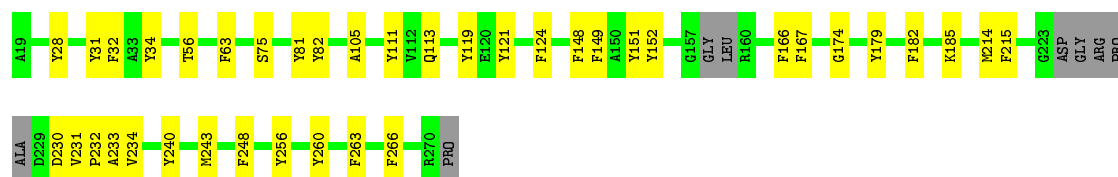
Chain 12: 84% 13%





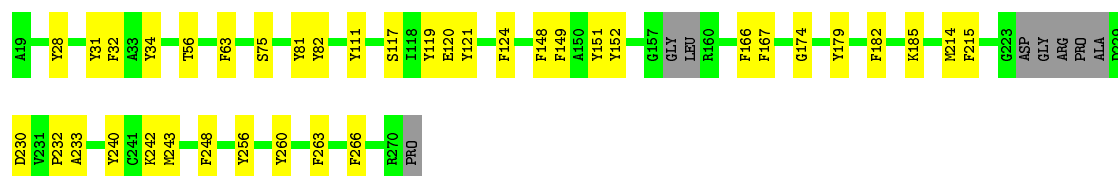
• Molecule 1: UL31

Chain 14: 81% 15%



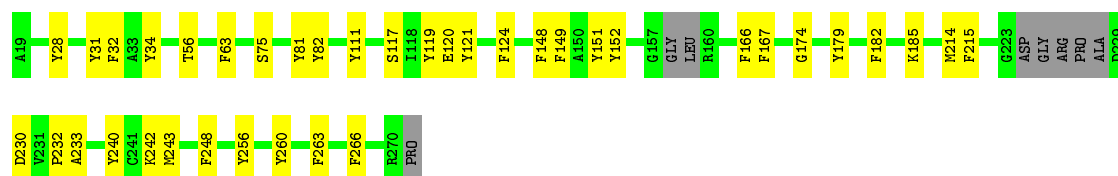
• Molecule 1: UL31

Chain 16: 82% 15%



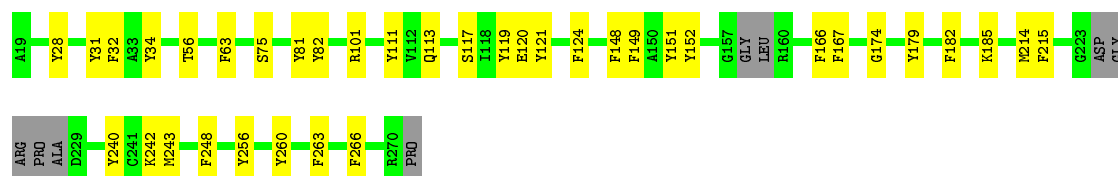
• Molecule 1: UL31

Chain 18: 82% 15%



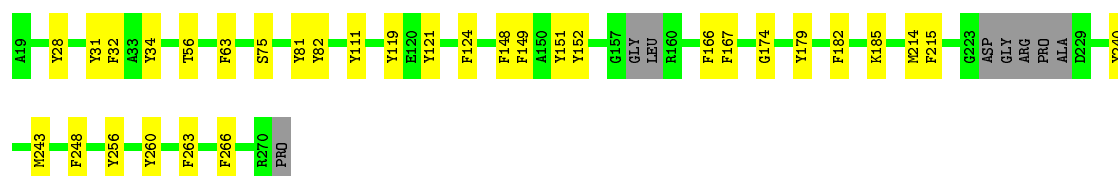
• Molecule 1: UL31

Chain 2A: 82% 15%

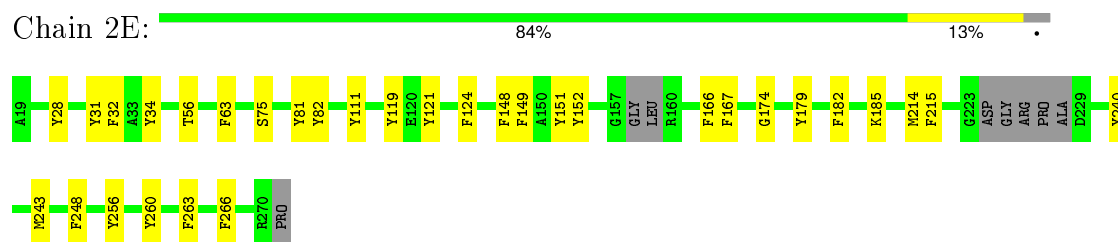


• Molecule 1: UL31

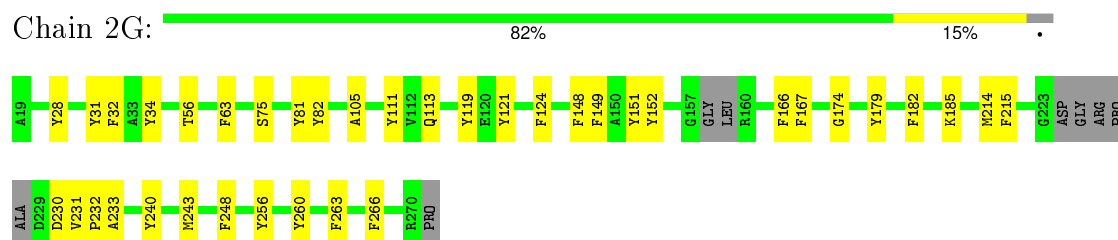
Chain 2C: 84% 13%



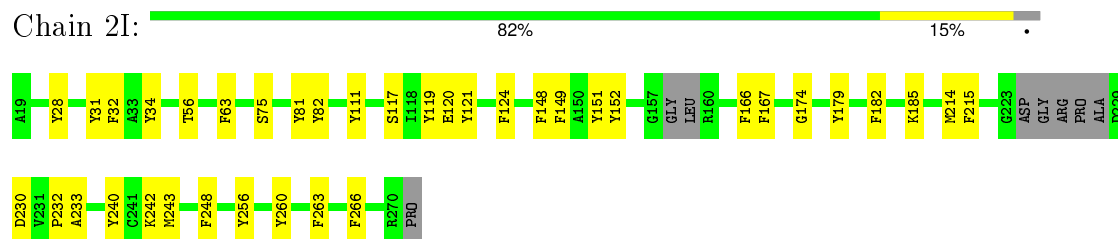
- Molecule 1: UL31



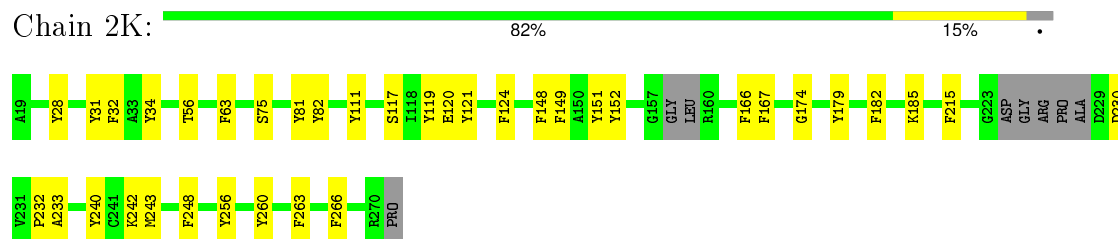
- Molecule 1: UL31



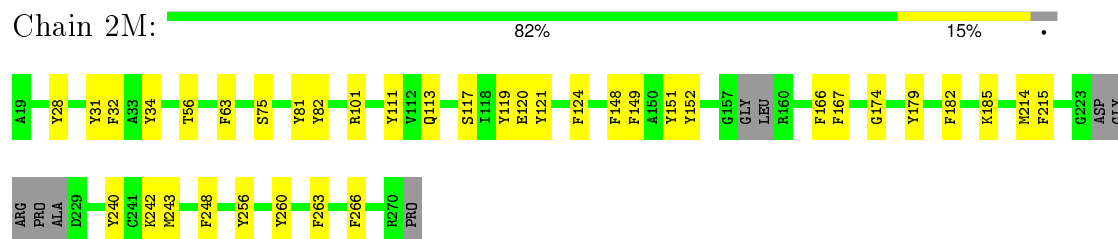
- Molecule 1: UL31



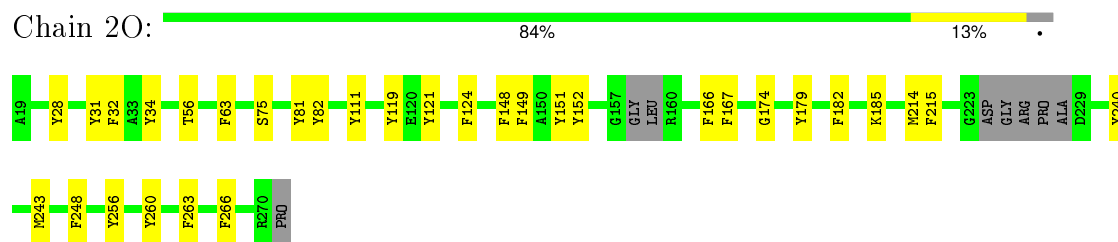
- Molecule 1: UL31



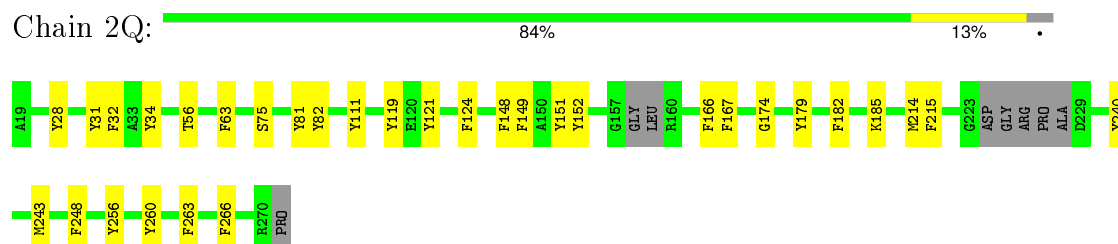
- Molecule 1: UL31



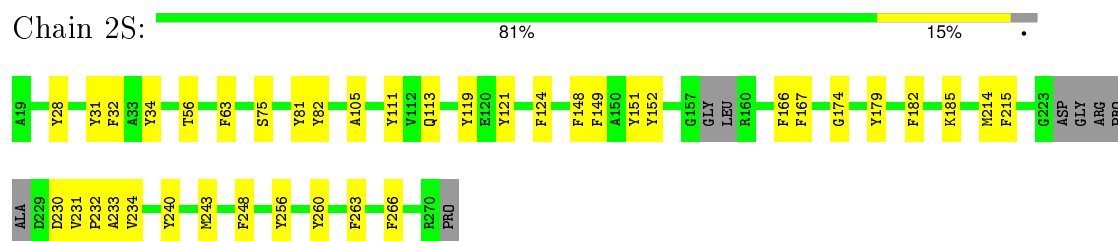
- Molecule 1: UL31



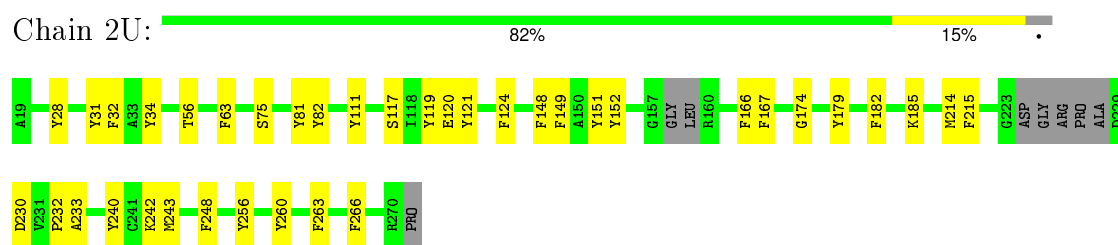
• Molecule 1: UL31



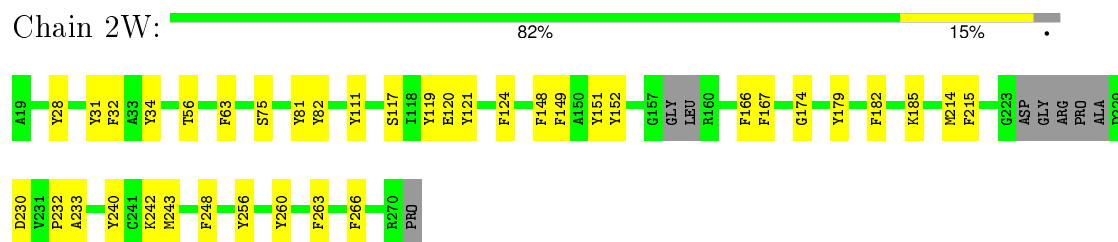
• Molecule 1: UL31



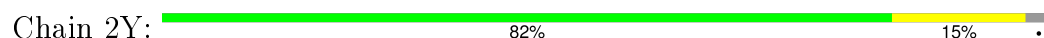
• Molecule 1: UL31

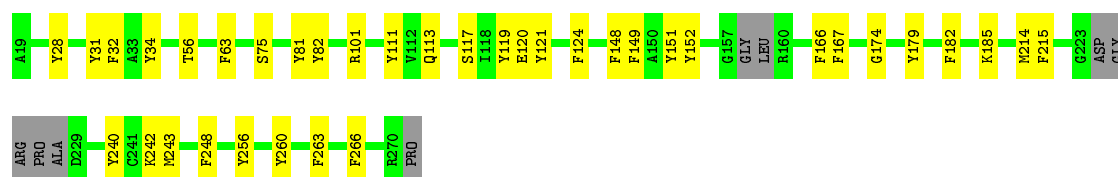


• Molecule 1: UL31



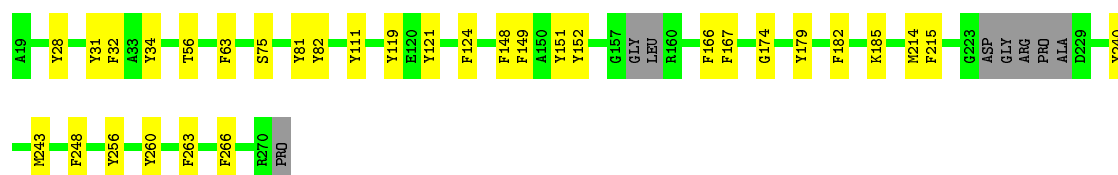
• Molecule 1: UL31





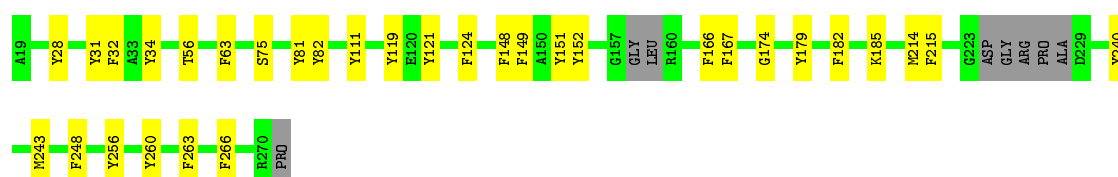
- Molecule 1: UL31

Chain 20: 84% 13%



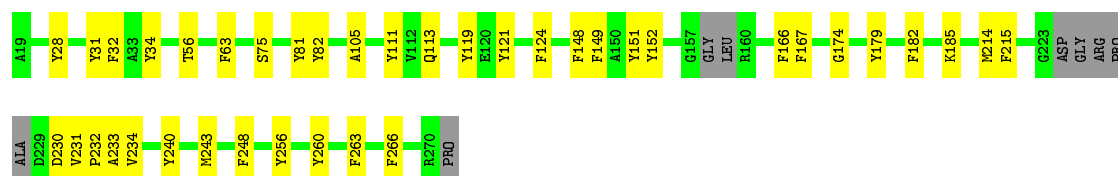
- Molecule 1: UL31

Chain 22: 84% 13%



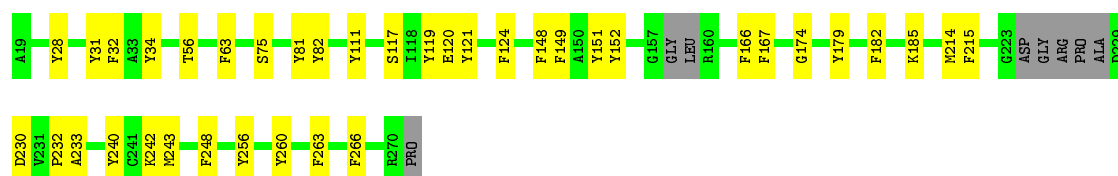
- Molecule 1: UL31

Chain 24: 81% 15%



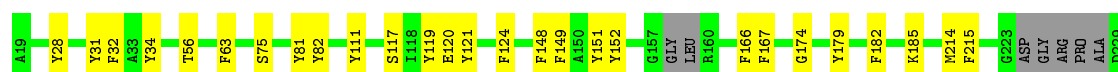
- Molecule 1: UL31

Chain 26: 82% 15%



- Molecule 1: UL31

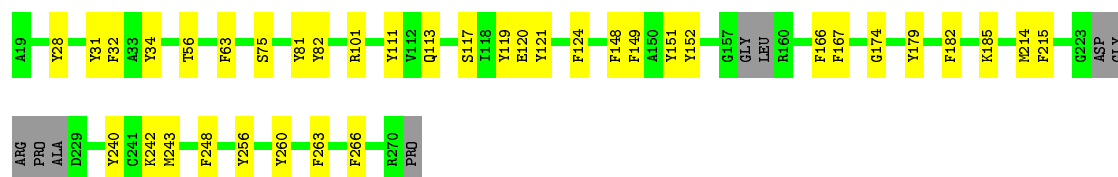
Chain 28: 82% 15%





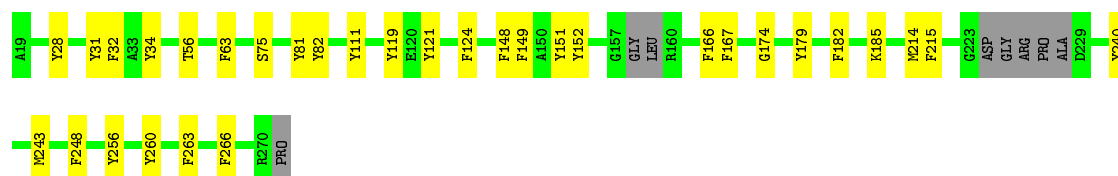
- Molecule 1: UL31

Chain 3A: 82% 15% •



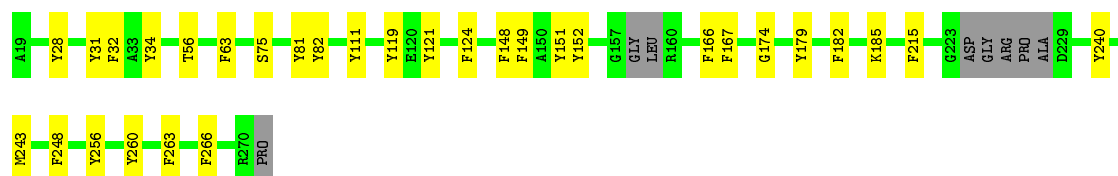
- Molecule 1: UL31

Chain 3C: 84% 13% •



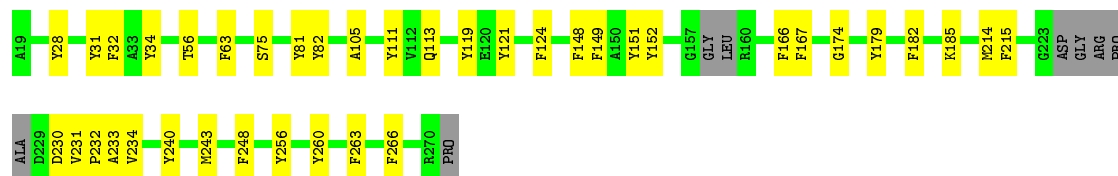
- Molecule 1: UL31

Chain 3E: 85% 12% •



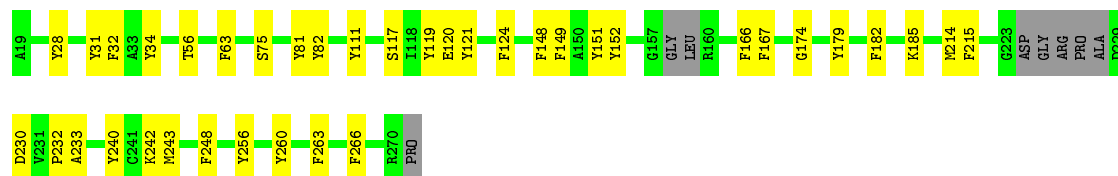
- Molecule 1: UL31

Chain 3G: 81% 15% •

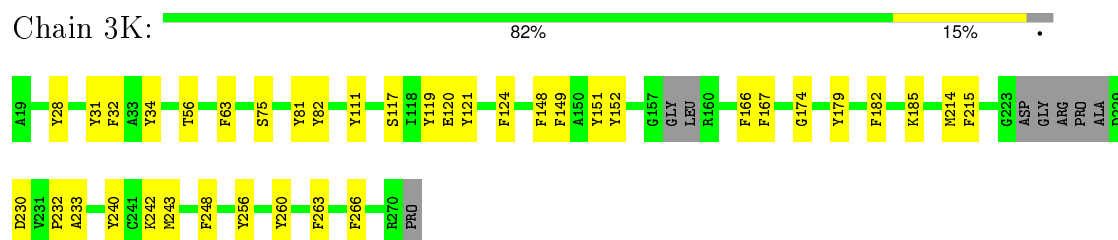


- Molecule 1: UL31

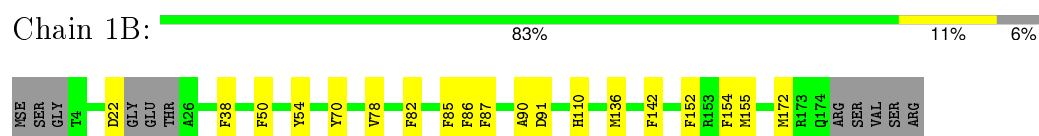
Chain 3I: 82% 15% •



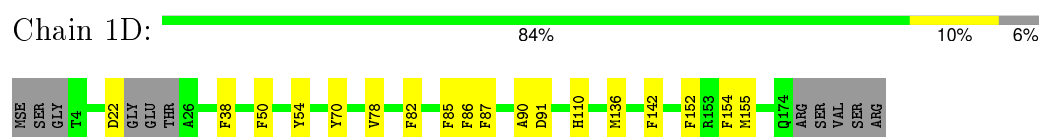
- Molecule 1: UL31



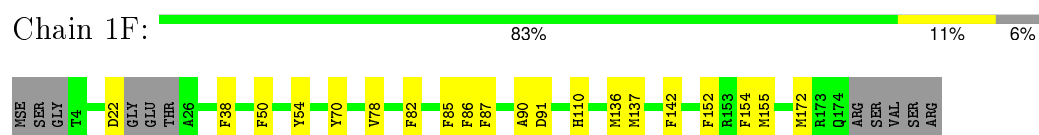
- Molecule 2: UL34 protein



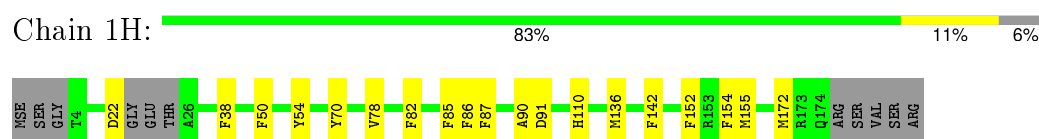
- Molecule 2: UL34 protein



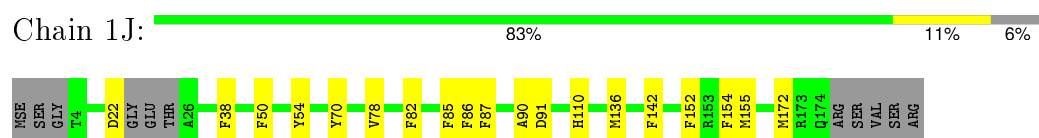
- Molecule 2: UL34 protein



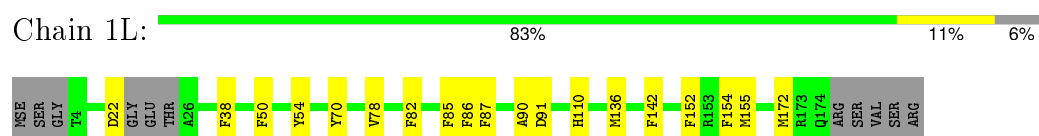
- Molecule 2: UL34 protein




- Molecule 2: UL34 protein




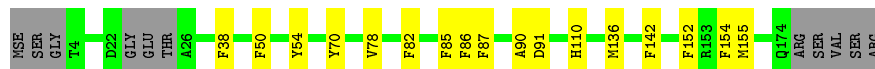
- Molecule 2: UL34 protein




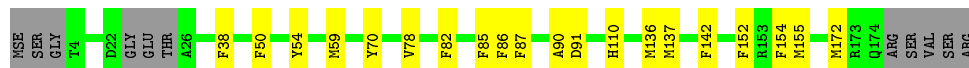
• Molecule 2: UL34 protein

Chain 1N:  83% 11% 6%


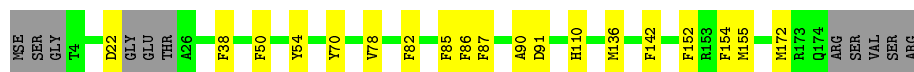
• Molecule 2: UL34 protein

Chain 1P:  84% 9% 6%


• Molecule 2: UL34 protein

Chain 1R:  83% 11% 6%


• Molecule 2: UL34 protein

Chain 1T:  83% 11% 6%


• Molecule 2: UL34 protein

Chain 1V:  83% 11% 6%


• Molecule 2: UL34 protein

Chain 1X:  83% 11% 6%

• Molecule 2: UL34 protein


Chain 1Z:  83% 11% 6%

• Molecule 2: UL34 protein

Chain 11:  84% 10% 6%




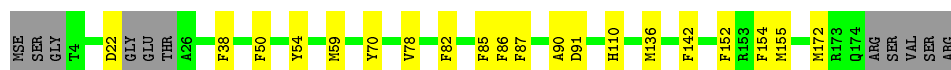
- Molecule 2: UL34 protein

Chain 13:  83% 11% 6%




- Molecule 2: UL34 protein

Chain 15:  83% 11% 6%




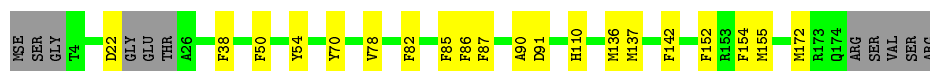
- Molecule 2: UL34 protein

Chain 17:  83% 11% 6%




- Molecule 2: UL34 protein

Chain 19:  83% 11% 6%




- Molecule 2: UL34 protein

Chain 2B:  84% 10% 6%




- Molecule 2: UL34 protein

Chain 2D:  84% 10% 6%



- Molecule 2: UL34 protein

Chain 2F:  84% 10% 6%



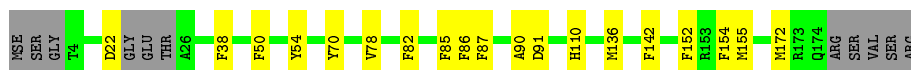
- Molecule 2: UL34 protein

Chain 2H: 83% 11% 6%



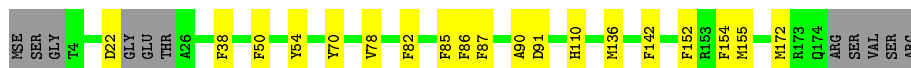
- Molecule 2: UL34 protein

Chain 2J: 83% 11% 6%



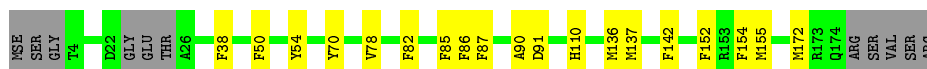
- Molecule 2: UL34 protein

Chain 2L: 83% 11% 6%



- Molecule 2: UL34 protein

Chain 2N: 83% 11% 6%



- Molecule 2: UL34 protein

Chain 2P: 84% 10% 6%



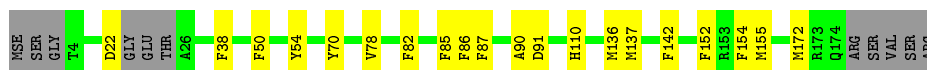
- Molecule 2: UL34 protein

Chain 2R: 83% 11% 6%




- Molecule 2: UL34 protein


Chain 2T: 83% 11% 6%




• Molecule 2: UL34 protein

Chain 2V:  83% 11% 6%


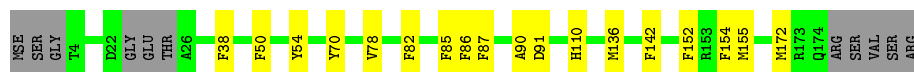
• Molecule 2: UL34 protein

Chain 2X:  83% 11% 6%


• Molecule 2: UL34 protein

Chain 2Z:  83% 11% 6%


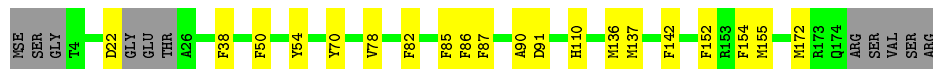
• Molecule 2: UL34 protein

Chain 21:  84% 10% 6%


• Molecule 2: UL34 protein

Chain 23:  84% 10% 6%


• Molecule 2: UL34 protein

Chain 25:  83% 11% 6%

• Molecule 2: UL34 protein


Chain 27:  84% 10% 6%

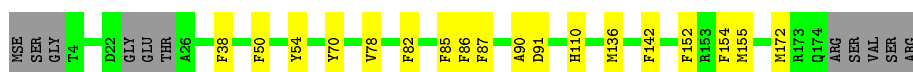
• Molecule 2: UL34 protein

Chain 29: 




- Molecule 2: UL34 protein

Chain 3B: 




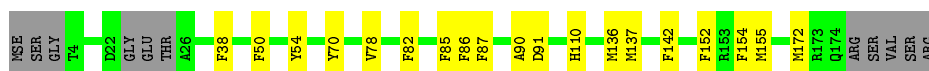
- Molecule 2: UL34 protein

Chain 3D: 




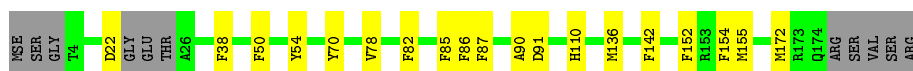
- Molecule 2: UL34 protein

Chain 3F: 




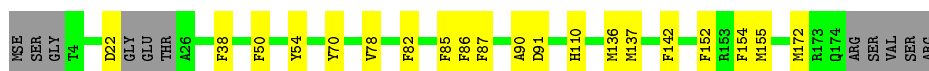
- Molecule 2: UL34 protein

Chain 3H: 




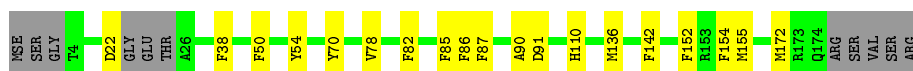
- Molecule 2: UL34 protein

Chain 3J: 



- Molecule 2: UL34 protein

Chain 3L: 



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	114	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	22500	Depositor
Image detector	GATAN MULTISCAN	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL

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 >2	RMSZ	# Z >2
1	10	0.37	0/1498	0.51	0/1971
1	12	0.37	0/1498	0.51	0/1971
1	14	0.37	0/1498	0.51	0/1971
1	16	0.36	0/1498	0.51	0/1971
1	18	0.36	0/1498	0.51	0/1971
1	1A	0.37	0/1498	0.51	0/1971
1	1C	0.37	0/1498	0.51	0/1971
1	1E	0.37	0/1498	0.51	0/1971
1	1G	0.37	0/1498	0.51	0/1971
1	1I	0.37	0/1498	0.51	0/1971
1	1K	0.37	0/1498	0.51	0/1971
1	1M	0.36	0/1498	0.51	0/1971
1	1O	0.37	0/1498	0.51	0/1971
1	1Q	0.36	0/1498	0.51	0/1971
1	1S	0.36	0/1498	0.51	0/1971
1	1U	0.37	0/1498	0.51	0/1971
1	1W	0.37	0/1498	0.51	0/1971
1	1Y	0.36	0/1498	0.51	0/1971
1	20	0.37	0/1498	0.51	0/1971
1	22	0.37	0/1498	0.51	0/1971
1	24	0.37	0/1498	0.51	0/1971
1	26	0.37	0/1498	0.51	0/1971
1	28	0.37	0/1498	0.51	0/1971
1	2A	0.36	0/1498	0.51	0/1971
1	2C	0.36	0/1498	0.51	0/1971
1	2E	0.37	0/1498	0.51	0/1971
1	2G	0.37	0/1498	0.51	0/1971
1	2I	0.37	0/1498	0.51	0/1971
1	2K	0.37	0/1498	0.51	0/1971
1	2M	0.37	0/1498	0.51	0/1971
1	2O	0.37	0/1498	0.51	0/1971
1	2Q	0.37	0/1498	0.51	0/1971

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	2S	0.36	0/1498	0.51	0/1971
1	2U	0.37	0/1498	0.51	0/1971
1	2W	0.37	0/1498	0.51	0/1971
1	2Y	0.37	0/1498	0.51	0/1971
1	3A	0.37	0/1498	0.51	0/1971
1	3C	0.36	0/1498	0.51	0/1971
1	3E	0.37	0/1498	0.51	0/1971
1	3G	0.37	0/1498	0.51	0/1971
1	3I	0.37	0/1498	0.51	0/1971
1	3K	0.37	0/1498	0.51	0/1971
2	11	0.35	0/1033	0.53	0/1361
2	13	0.35	0/1033	0.54	0/1361
2	15	0.35	0/1033	0.53	0/1361
2	17	0.35	0/1033	0.54	0/1361
2	19	0.35	0/1033	0.53	0/1361
2	1B	0.35	0/1033	0.53	0/1361
2	1D	0.35	0/1033	0.53	0/1361
2	1F	0.35	0/1033	0.54	0/1361
2	1H	0.35	0/1033	0.53	0/1361
2	1J	0.35	0/1033	0.53	0/1361
2	1L	0.35	0/1033	0.53	0/1361
2	1N	0.35	0/1033	0.54	0/1361
2	1P	0.35	0/1033	0.53	0/1361
2	1R	0.35	0/1033	0.53	0/1361
2	1T	0.35	0/1033	0.54	0/1361
2	1V	0.35	0/1033	0.53	0/1361
2	1X	0.35	0/1033	0.53	0/1361
2	1Z	0.35	0/1033	0.53	0/1361
2	21	0.35	0/1033	0.53	0/1361
2	23	0.35	0/1033	0.54	0/1361
2	25	0.35	0/1033	0.53	0/1361
2	27	0.35	0/1033	0.53	0/1361
2	29	0.35	0/1033	0.53	0/1361
2	2B	0.35	0/1033	0.53	0/1361
2	2D	0.35	0/1033	0.54	0/1361
2	2F	0.35	0/1033	0.53	0/1361
2	2H	0.35	0/1033	0.53	0/1361
2	2J	0.35	0/1033	0.53	0/1361
2	2L	0.35	0/1033	0.53	0/1361
2	2N	0.35	0/1033	0.53	0/1361
2	2P	0.35	0/1033	0.53	0/1361
2	2R	0.35	0/1033	0.54	0/1361
2	2T	0.35	0/1033	0.53	0/1361

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	2V	0.35	0/1033	0.53	0/1361
2	2X	0.35	0/1033	0.53	0/1361
2	2Z	0.35	0/1033	0.53	0/1361
2	3B	0.35	0/1033	0.54	0/1361
2	3D	0.35	0/1033	0.53	0/1361
2	3F	0.35	0/1033	0.53	0/1361
2	3H	0.35	0/1033	0.53	0/1361
2	3J	0.35	0/1033	0.53	0/1361
2	3L	0.35	0/1033	0.53	0/1361
All	All	0.36	0/106302	0.52	0/139944

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10	1523	0	1159	40	0
1	12	1523	0	1159	40	0
1	14	1523	0	1158	98	0
1	16	1523	0	1159	89	0
1	18	1523	0	1159	88	0
1	1A	1523	0	1159	85	0
1	1C	1523	0	1159	87	0
1	1E	1523	0	1159	85	0
1	1G	1523	0	1159	86	0
1	1I	1523	0	1159	85	0
1	1K	1523	0	1159	85	0
1	1M	1523	0	1159	94	0
1	1O	1523	0	1159	40	0
1	1Q	1523	0	1159	40	0
1	1S	1523	0	1158	96	0
1	1U	1523	0	1159	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1W	1523	0	1159	87	0
1	1Y	1523	0	1159	96	0
1	20	1523	0	1159	40	0
1	22	1523	0	1159	40	0
1	24	1523	0	1158	94	0
1	26	1523	0	1159	87	0
1	28	1523	0	1159	87	0
1	2A	1523	0	1159	98	0
1	2C	1523	0	1159	40	0
1	2E	1523	0	1159	40	0
1	2G	1523	0	1158	95	0
1	2I	1523	0	1159	86	0
1	2K	1523	0	1159	86	0
1	2M	1523	0	1159	95	0
1	2O	1523	0	1159	40	0
1	2Q	1523	0	1159	40	0
1	2S	1523	0	1158	97	0
1	2U	1523	0	1159	86	0
1	2W	1523	0	1159	87	0
1	2Y	1523	0	1159	97	0
1	3A	1523	0	1159	94	0
1	3C	1523	0	1159	40	0
1	3E	1523	0	1159	39	0
1	3G	1523	0	1158	94	0
1	3I	1523	0	1159	88	0
1	3K	1523	0	1159	88	0
2	11	1049	0	799	26	0
2	13	1049	0	799	27	0
2	15	1049	0	799	31	0
2	17	1049	0	799	29	0
2	19	1049	0	799	31	0
2	1B	1049	0	799	30	0
2	1D	1049	0	799	27	0
2	1F	1049	0	799	30	0
2	1H	1049	0	799	29	0
2	1J	1049	0	799	29	0
2	1L	1049	0	799	29	0
2	1N	1049	0	799	27	0
2	1P	1049	0	799	25	0
2	1R	1049	0	799	28	0
2	1T	1049	0	799	30	0
2	1V	1049	0	799	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1X	1049	0	799	31	0
2	1Z	1049	0	799	27	0
2	21	1049	0	799	26	0
2	23	1049	0	799	26	0
2	25	1049	0	799	31	0
2	27	1049	0	799	28	0
2	29	1049	0	799	31	0
2	2B	1049	0	799	26	0
2	2D	1049	0	799	26	0
2	2F	1049	0	799	26	0
2	2H	1049	0	799	31	0
2	2J	1049	0	799	29	0
2	2L	1049	0	799	30	0
2	2N	1049	0	799	27	0
2	2P	1049	0	799	26	0
2	2R	1049	0	799	27	0
2	2T	1049	0	799	31	0
2	2V	1049	0	799	29	0
2	2X	1049	0	799	31	0
2	2Z	1049	0	799	27	0
2	3B	1049	0	799	26	0
2	3D	1049	0	799	27	0
2	3F	1049	0	799	27	0
2	3H	1049	0	799	30	0
2	3J	1049	0	799	31	0
2	3L	1049	0	799	30	0
3	10	1	0	0	0	0
3	12	1	0	0	0	0
3	14	1	0	0	0	0
3	16	1	0	0	0	0
3	18	1	0	0	0	0
3	1A	1	0	0	0	0
3	1C	1	0	0	0	0
3	1E	1	0	0	0	0
3	1G	1	0	0	0	0
3	1I	1	0	0	0	0
3	1K	1	0	0	0	0
3	1M	1	0	0	0	0
3	1O	1	0	0	0	0
3	1Q	1	0	0	0	0
3	1S	1	0	0	0	0
3	1U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1W	1	0	0	0	0
3	1Y	1	0	0	0	0
3	20	1	0	0	0	0
3	22	1	0	0	0	0
3	24	1	0	0	0	0
3	26	1	0	0	0	0
3	28	1	0	0	0	0
3	2A	1	0	0	0	0
3	2C	1	0	0	0	0
3	2E	1	0	0	0	0
3	2G	1	0	0	0	0
3	2I	1	0	0	0	0
3	2K	1	0	0	0	0
3	2M	1	0	0	0	0
3	2O	1	0	0	0	0
3	2Q	1	0	0	0	0
3	2S	1	0	0	0	0
3	2U	1	0	0	0	0
3	2W	1	0	0	0	0
3	2Y	1	0	0	0	0
3	3A	1	0	0	0	0
3	3C	1	0	0	0	0
3	3E	1	0	0	0	0
3	3G	1	0	0	0	0
3	3I	1	0	0	0	0
3	3K	1	0	0	0	0
4	10	1	0	0	0	0
4	12	1	0	0	0	0
4	14	1	0	0	0	0
4	16	1	0	0	0	0
4	18	1	0	0	0	0
4	1A	1	0	0	0	0
4	1C	1	0	0	0	0
4	1E	1	0	0	0	0
4	1G	1	0	0	0	0
4	1I	1	0	0	0	0
4	1K	1	0	0	0	0
4	1M	1	0	0	0	0
4	1O	1	0	0	0	0
4	1Q	1	0	0	0	0
4	1S	1	0	0	0	0
4	1U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1W	1	0	0	0	0
4	1Y	1	0	0	0	0
4	20	1	0	0	0	0
4	22	1	0	0	0	0
4	24	1	0	0	0	0
4	26	1	0	0	0	0
4	28	1	0	0	0	0
4	2A	1	0	0	0	0
4	2C	1	0	0	0	0
4	2E	1	0	0	0	0
4	2G	1	0	0	0	0
4	2I	1	0	0	0	0
4	2K	1	0	0	0	0
4	2M	1	0	0	0	0
4	2O	1	0	0	0	0
4	2Q	1	0	0	0	0
4	2S	1	0	0	0	0
4	2U	1	0	0	0	0
4	2W	1	0	0	0	0
4	2Y	1	0	0	0	0
4	3A	1	0	0	0	0
4	3C	1	0	0	0	0
4	3E	1	0	0	0	0
4	3G	1	0	0	0	0
4	3I	1	0	0	0	0
4	3K	1	0	0	0	0
All	All	108108	0	82230	3080	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 16.

The worst 5 of 3080 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2H:22:ASP:HB2	2:2X:22:ASP:C	1.26	1.50
2:25:22:ASP:C	2:3L:22:ASP:HB2	1.30	1.50
2:1X:22:ASP:HB2	2:3H:22:ASP:C	1.30	1.49
2:2H:22:ASP:C	2:2X:22:ASP:HB2	1.30	1.49
2:2T:22:ASP:HB2	2:29:22:ASP:C	1.26	1.48

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	10	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	12	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	14	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	16	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	18	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1A	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1C	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1E	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1G	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1I	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1K	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1M	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1O	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1Q	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1S	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1U	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1W	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	1Y	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	20	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	22	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	24	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	26	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	28	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2A	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2C	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2E	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2G	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2I	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2K	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2M	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2O	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2Q	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2S	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2U	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2W	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	2Y	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	3A	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	3C	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	3E	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	3G	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	3I	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
1	3K	239/253 (94%)	230 (96%)	8 (3%)	1 (0%)	39	80
2	11	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	13	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	15	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	17	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	19	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1B	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1D	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1F	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1H	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1J	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1L	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1N	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1P	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1R	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1T	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1V	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1X	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	1Z	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2I	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2J	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2K	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2L	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2M	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2N	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2O	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2P	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2Q	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2R	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2S	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2T	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2U	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2V	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2W	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2X	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2Y	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	2Z	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3A	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3B	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3C	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3D	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3E	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3F	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3G	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3H	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3I	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3J	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3K	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
2	3L	164/179 (92%)	158 (96%)	5 (3%)	1 (1%)	30	74
All	All	16926/18144 (93%)	16296 (96%)	546 (3%)	84 (0%)	38	77

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	174	GLY
1	1C	174	GLY
1	1E	174	GLY
1	1G	174	GLY
1	1I	174	GLY

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	10	57/199 (29%)	57 (100%)	0	100	100
1	12	57/199 (29%)	57 (100%)	0	100	100
1	14	57/199 (29%)	57 (100%)	0	100	100
1	16	57/199 (29%)	57 (100%)	0	100	100
1	18	57/199 (29%)	57 (100%)	0	100	100
1	1A	57/199 (29%)	57 (100%)	0	100	100
1	1C	57/199 (29%)	57 (100%)	0	100	100
1	1E	57/199 (29%)	57 (100%)	0	100	100
1	1G	57/199 (29%)	57 (100%)	0	100	100
1	1I	57/199 (29%)	57 (100%)	0	100	100
1	1K	57/199 (29%)	57 (100%)	0	100	100
1	1M	57/199 (29%)	57 (100%)	0	100	100
1	1O	57/199 (29%)	57 (100%)	0	100	100
1	1Q	57/199 (29%)	57 (100%)	0	100	100
1	1S	57/199 (29%)	57 (100%)	0	100	100
1	1U	57/199 (29%)	57 (100%)	0	100	100
1	1W	57/199 (29%)	57 (100%)	0	100	100
1	1Y	57/199 (29%)	57 (100%)	0	100	100
1	20	57/199 (29%)	57 (100%)	0	100	100
1	22	57/199 (29%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	24	57/199 (29%)	57 (100%)	0	100	100
1	26	57/199 (29%)	57 (100%)	0	100	100
1	28	57/199 (29%)	57 (100%)	0	100	100
1	2A	57/199 (29%)	57 (100%)	0	100	100
1	2C	57/199 (29%)	57 (100%)	0	100	100
1	2E	57/199 (29%)	57 (100%)	0	100	100
1	2G	57/199 (29%)	57 (100%)	0	100	100
1	2I	57/199 (29%)	57 (100%)	0	100	100
1	2K	57/199 (29%)	57 (100%)	0	100	100
1	2M	57/199 (29%)	57 (100%)	0	100	100
1	2O	57/199 (29%)	57 (100%)	0	100	100
1	2Q	57/199 (29%)	57 (100%)	0	100	100
1	2S	57/199 (29%)	57 (100%)	0	100	100
1	2U	57/199 (29%)	57 (100%)	0	100	100
1	2W	57/199 (29%)	57 (100%)	0	100	100
1	2Y	57/199 (29%)	57 (100%)	0	100	100
1	3A	57/199 (29%)	57 (100%)	0	100	100
1	3C	57/199 (29%)	57 (100%)	0	100	100
1	3E	57/199 (29%)	57 (100%)	0	100	100
1	3G	57/199 (29%)	57 (100%)	0	100	100
1	3I	57/199 (29%)	57 (100%)	0	100	100
1	3K	57/199 (29%)	57 (100%)	0	100	100
2	11	48/146 (33%)	48 (100%)	0	100	100
2	13	48/146 (33%)	48 (100%)	0	100	100
2	15	48/146 (33%)	48 (100%)	0	100	100
2	17	48/146 (33%)	48 (100%)	0	100	100
2	19	48/146 (33%)	48 (100%)	0	100	100
2	1B	48/146 (33%)	48 (100%)	0	100	100
2	1D	48/146 (33%)	48 (100%)	0	100	100
2	1F	48/146 (33%)	48 (100%)	0	100	100
2	1H	48/146 (33%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1J	48/146 (33%)	48 (100%)	0	100	100
2	1L	48/146 (33%)	48 (100%)	0	100	100
2	1N	48/146 (33%)	48 (100%)	0	100	100
2	1P	48/146 (33%)	48 (100%)	0	100	100
2	1R	48/146 (33%)	48 (100%)	0	100	100
2	1T	48/146 (33%)	48 (100%)	0	100	100
2	1V	48/146 (33%)	48 (100%)	0	100	100
2	1X	48/146 (33%)	48 (100%)	0	100	100
2	1Z	48/146 (33%)	48 (100%)	0	100	100
2	2I	48/146 (33%)	48 (100%)	0	100	100
2	2J	48/146 (33%)	48 (100%)	0	100	100
2	2K	48/146 (33%)	48 (100%)	0	100	100
2	2L	48/146 (33%)	48 (100%)	0	100	100
2	2M	48/146 (33%)	48 (100%)	0	100	100
2	2N	48/146 (33%)	48 (100%)	0	100	100
2	2O	48/146 (33%)	48 (100%)	0	100	100
2	2P	48/146 (33%)	48 (100%)	0	100	100
2	2Q	48/146 (33%)	48 (100%)	0	100	100
2	2R	48/146 (33%)	48 (100%)	0	100	100
2	2S	48/146 (33%)	48 (100%)	0	100	100
2	2T	48/146 (33%)	48 (100%)	0	100	100
2	2V	48/146 (33%)	48 (100%)	0	100	100
2	2X	48/146 (33%)	48 (100%)	0	100	100
2	2Z	48/146 (33%)	48 (100%)	0	100	100
2	3B	48/146 (33%)	48 (100%)	0	100	100
2	3D	48/146 (33%)	48 (100%)	0	100	100
2	3F	48/146 (33%)	48 (100%)	0	100	100
2	3H	48/146 (33%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3J	48/146 (33%)	48 (100%)	0	100	100
2	3L	48/146 (33%)	48 (100%)	0	100	100
All	All	4410/14490 (30%)	4410 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 84 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.