wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 09:34 pm GMT

PDB ID	:	4V5T
Title	:	X-ray structure of the Grapevine Fanleaf virus
Authors	:	Schellenberger, P.; Sauter, C.; Lorber, B.; Bron, P.; Trapani, S.; Bergdoll, M.; Marmonier, A.; Schmitt-Keichinger, C.; Lemaire, O.; Demangeat, G.; Ritzenthaler, C.
Deposited on	:	2011-02-01
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

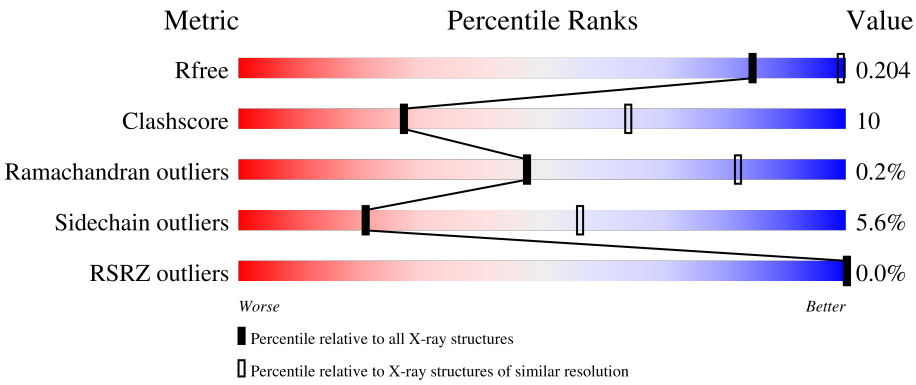
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	504	79% 19% •
1	AB	504	82% 16% •
1	AC	504	81% 17% •
1	AD	504	80% 17% •
1	AE	504	83% 16% •

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Mol	Chain	Length	Quality of chain
1	AF	504	81% 17% •
1	AG	504	80% 16% •
1	AH	504	81% 16% •
1	AI	504	81% 16% •
1	AJ	504	82% 16% •
1	AK	504	80% 18% •
1	AL	504	81% 17% •
1	AM	504	82% 16% •
1	AN	504	79% 19% •
1	AO	504	80% 18% •
1	AP	504	81% 17% •
1	AQ	504	82% 16% •
1	AR	504	81% 16% •
1	AS	504	81% 16% •
1	AT	504	80% 18% •
1	BA	504	81% 17% •
1	BB	504	81% 16% •
1	BC	504	80% 17% •
1	BD	504	83% 15% •
1	BE	504	82% 16% •
1	BF	504	79% 18% •
1	BG	504	80% 18% •
1	BH	504	80% 18% •
1	BI	504	80% 18% •
1	BJ	504	81% 17% •

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Mol	Chain	Length	Quality of chain
1	BK	504	82% 16% •
1	BL	504	81% 16% •
1	BM	504	81% 17% •
1	BN	504	81% 16% •
1	BO	504	80% 17% •
1	BP	504	81% 16% •
1	BQ	504	81% 17% •
1	BR	504	81% 16% •
1	BS	504	80% 18% •
1	BT	504	80% 18% •
1	CA	504	82% 15% •
1	CB	504	81% 17% •
1	CC	504	82% 15% •
1	CD	504	81% 17% •
1	CE	504	79% 19% •
1	CF	504	80% 17% •
1	CG	504	82% 16% •
1	CH	504	80% 17% •
1	CI	504	80% 17% •
1	CJ	504	81% 17% •
1	CK	504	81% 17% •
1	CL	504	82% 16% •
1	CM	504	79% 19% •
1	CN	504	82% 16% •
1	CO	504	80% 18% •

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Mol	Chain	Length	Quality of chain
1	CP	504	81% 16% •
1	CQ	504	82% 16% •
1	CR	504	81% 17% •
1	CS	504	81% 17% •
1	CT	504	82% 16% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 237060 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	504	3951	2555	653	721	22	0	0	0
1	AB	504	3951	2555	653	721	22	0	0	0
1	AC	504	3951	2555	653	721	22	0	0	0
1	AD	504	3951	2555	653	721	22	0	0	0
1	AE	504	3951	2555	653	721	22	0	0	0
1	AF	504	3951	2555	653	721	22	0	0	0
1	AG	504	3951	2555	653	721	22	0	0	0
1	AH	504	3951	2555	653	721	22	0	0	0
1	AI	504	3951	2555	653	721	22	0	0	0
1	AJ	504	3951	2555	653	721	22	0	0	0
1	AK	504	3951	2555	653	721	22	0	0	0
1	AL	504	3951	2555	653	721	22	0	0	0
1	AM	504	3951	2555	653	721	22	0	0	0
1	AN	504	3951	2555	653	721	22	0	0	0
1	AO	504	3951	2555	653	721	22	0	0	0
1	AP	504	3951	2555	653	721	22	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AQ	504	3951	2555	653	721	22	0	0	0
1	AR	504	3951	2555	653	721	22	0	0	0
1	AS	504	3951	2555	653	721	22	0	0	0
1	AT	504	3951	2555	653	721	22	0	0	0
1	BA	504	3951	2555	653	721	22	0	0	0
1	BB	504	3951	2555	653	721	22	0	0	0
1	BC	504	3951	2555	653	721	22	0	0	0
1	BD	504	3951	2555	653	721	22	0	0	0
1	BE	504	3951	2555	653	721	22	0	0	0
1	BF	504	3951	2555	653	721	22	0	0	0
1	BG	504	3951	2555	653	721	22	0	0	0
1	BH	504	3951	2555	653	721	22	0	0	0
1	BI	504	3951	2555	653	721	22	0	0	0
1	BJ	504	3951	2555	653	721	22	0	0	0
1	BK	504	3951	2555	653	721	22	0	0	0
1	BL	504	3951	2555	653	721	22	0	0	0
1	BM	504	3951	2555	653	721	22	0	0	0
1	BN	504	3951	2555	653	721	22	0	0	0
1	BO	504	3951	2555	653	721	22	0	0	0
1	BP	504	3951	2555	653	721	22	0	0	0
1	BQ	504	3951	2555	653	721	22	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BR	504	3951	2555	653	721	22	0	0	0
1	BS	504	3951	2555	653	721	22	0	0	0
1	BT	504	3951	2555	653	721	22	0	0	0
1	CA	504	3951	2555	653	721	22	0	0	0
1	CB	504	3951	2555	653	721	22	0	0	0
1	CC	504	3951	2555	653	721	22	0	0	0
1	CD	504	3951	2555	653	721	22	0	0	0
1	CE	504	3951	2555	653	721	22	0	0	0
1	CF	504	3951	2555	653	721	22	0	0	0
1	CG	504	3951	2555	653	721	22	0	0	0
1	CH	504	3951	2555	653	721	22	0	0	0
1	CI	504	3951	2555	653	721	22	0	0	0
1	CJ	504	3951	2555	653	721	22	0	0	0
1	CK	504	3951	2555	653	721	22	0	0	0
1	CL	504	3951	2555	653	721	22	0	0	0
1	CM	504	3951	2555	653	721	22	0	0	0
1	CN	504	3951	2555	653	721	22	0	0	0
1	CO	504	3951	2555	653	721	22	0	0	0
1	CP	504	3951	2555	653	721	22	0	0	0
1	CQ	504	3951	2555	653	721	22	0	0	0
1	CR	504	3951	2555	653	721	22	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	CS	504	3951	2555	653	721	22	0	0	0
			Total	C	N	O	S			
1	CT	504	3951	2555	653	721	22	0	0	0

3 Residue-property plots (i)

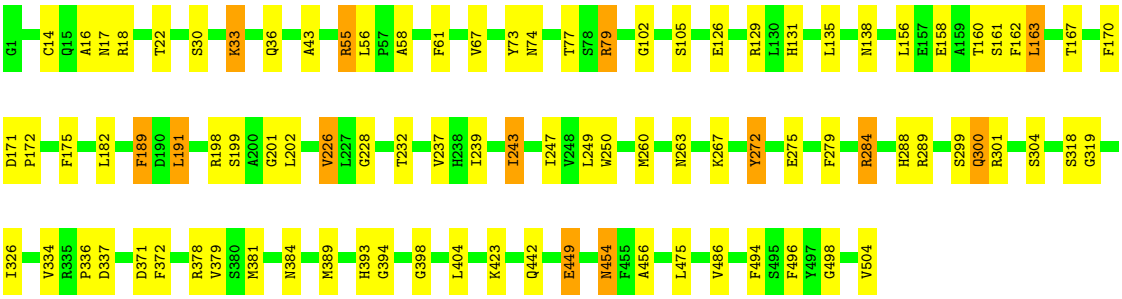
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: COAT PROTEIN

Chain AA: 79% 19% •

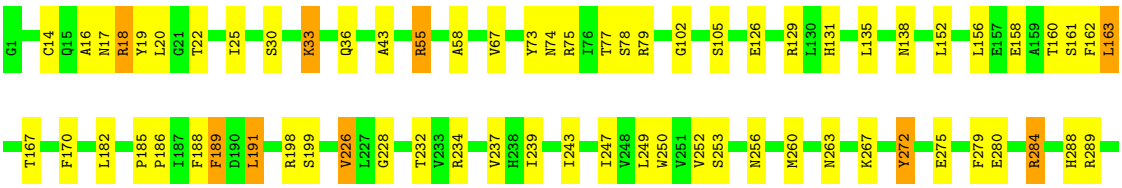
• Molecule 1: COAT PROTEIN

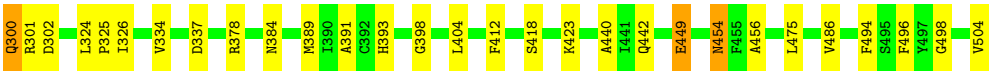
Chain AB: 82% 16% •



• Molecule 1: COAT PROTEIN

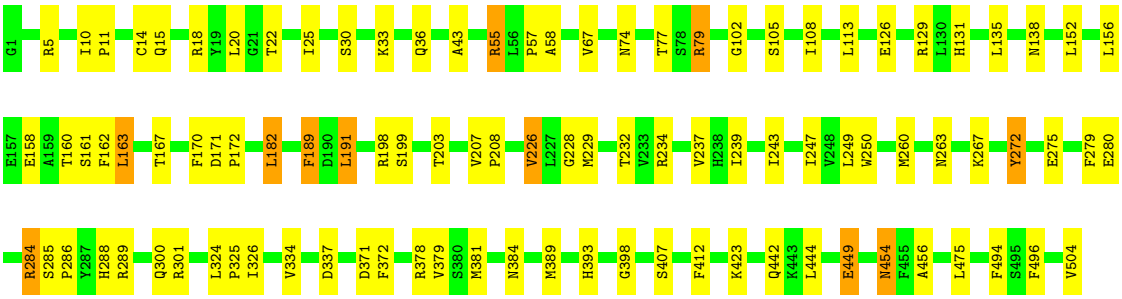
Chain AC: 81% 17% •





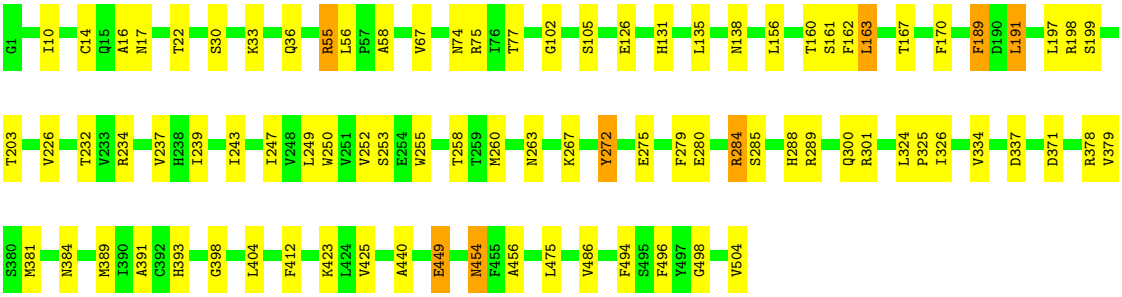
• Molecule 1: COAT PROTEIN

Chain AD:



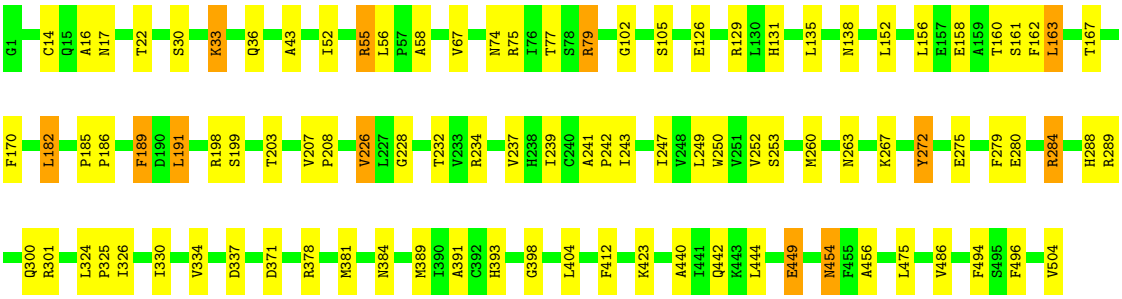
• Molecule 1: COAT PROTEIN

Chain AE:



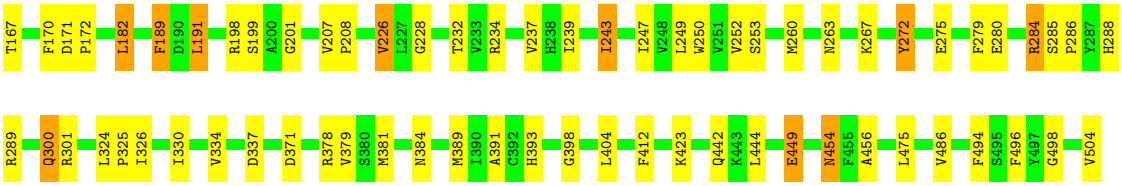
• Molecule 1: COAT PROTEIN

Chain AF:



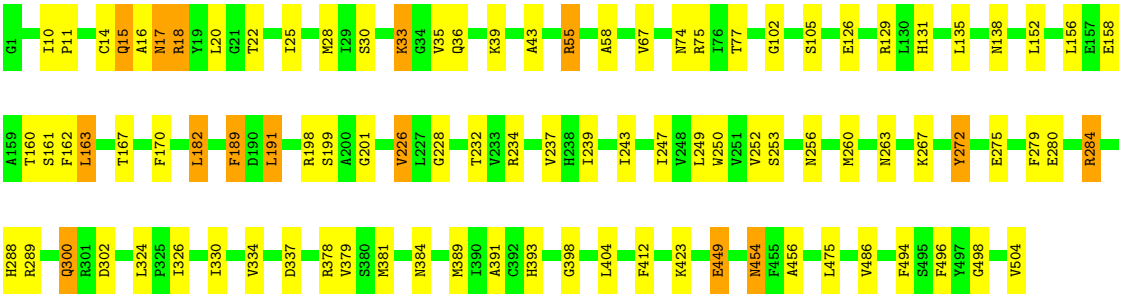
• Molecule 1: COAT PROTEIN

Chain AG:



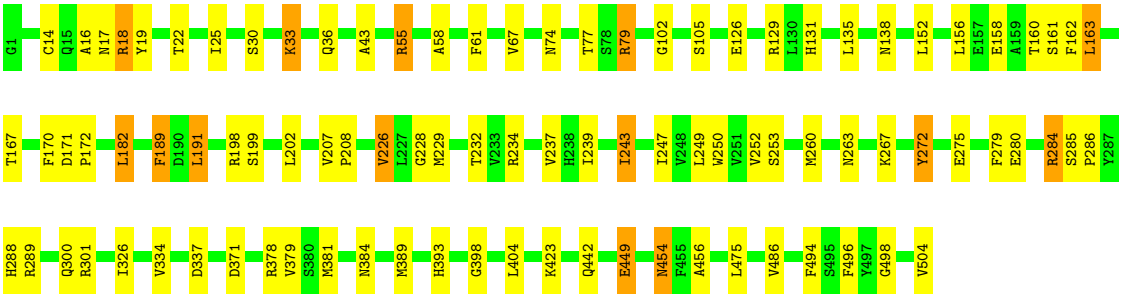
- Molecule 1: COAT PROTEIN

Chain AH:



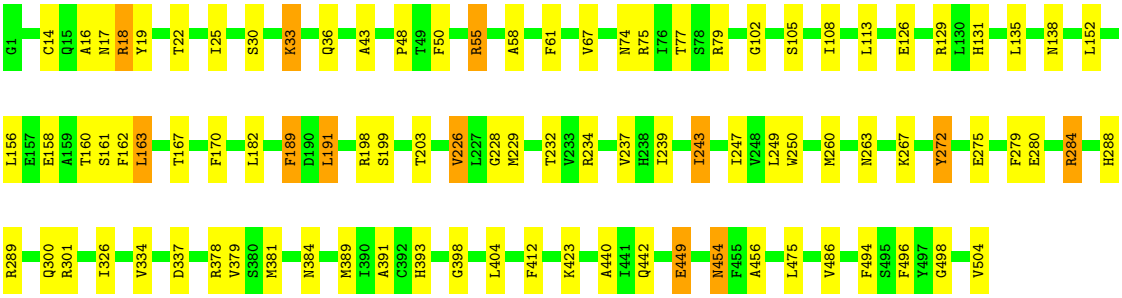
- Molecule 1: COAT PROTEIN

Chain AI:



- Molecule 1: COAT PROTEIN

Chain AJ:

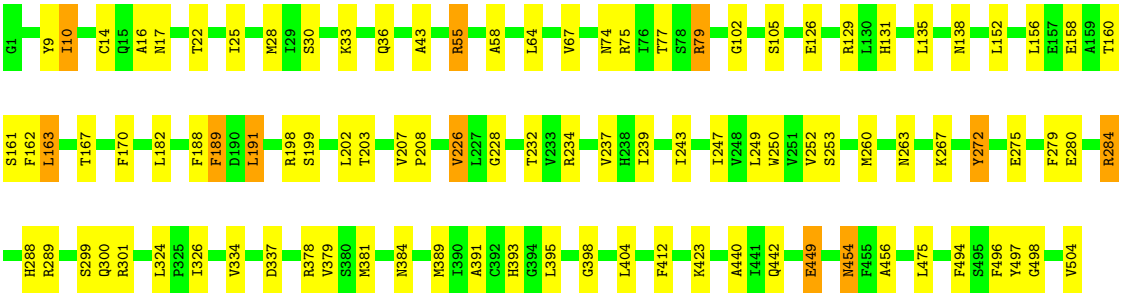


- Molecule 1: COAT PROTEIN

Chain AK:

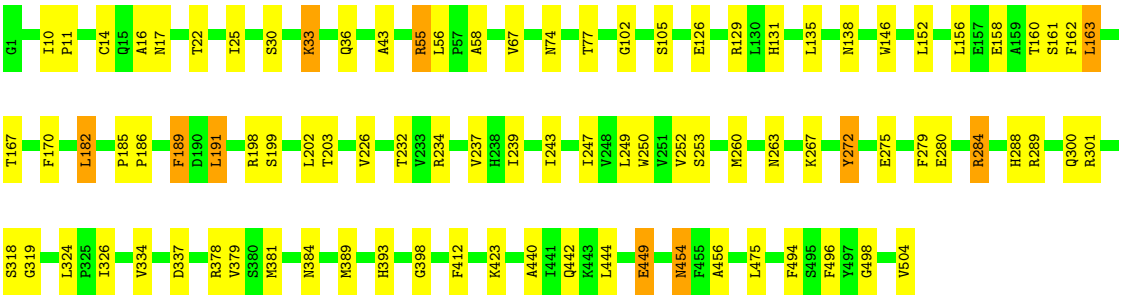
- Molecule 1: COAT PROTEIN

Chain AL: 81% 17% •



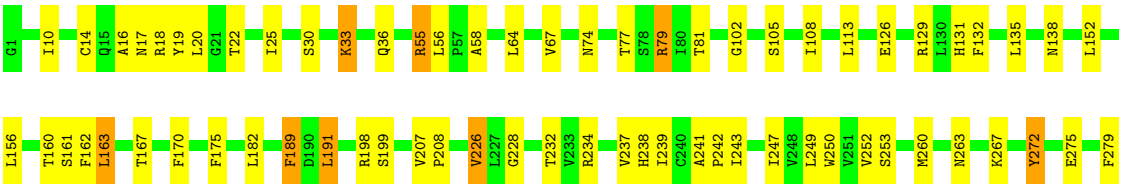
- Molecule 1: COAT PROTEIN

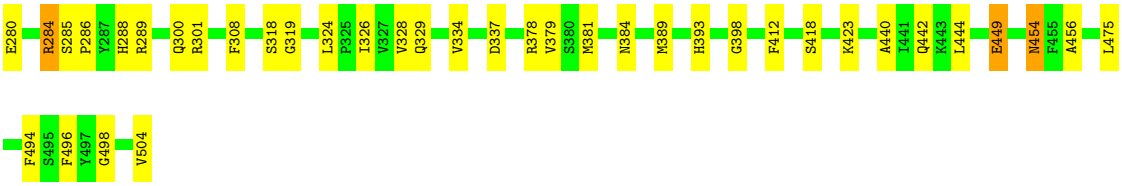
Chain AM: 82% 16% •



- Molecule 1: COAT PROTEIN

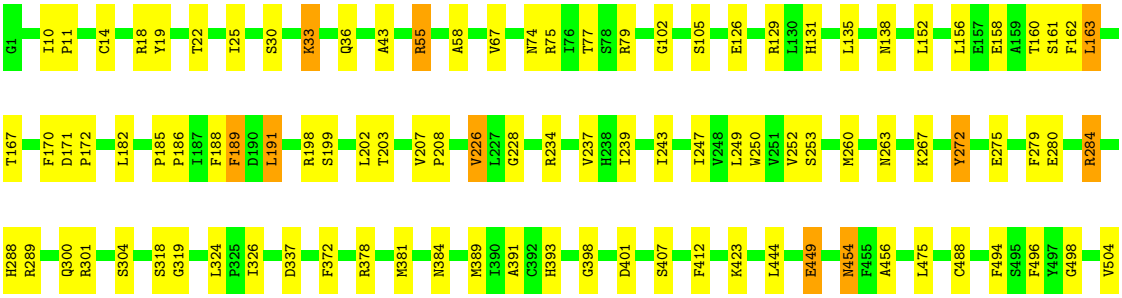
Chain AN: 79% 19% •





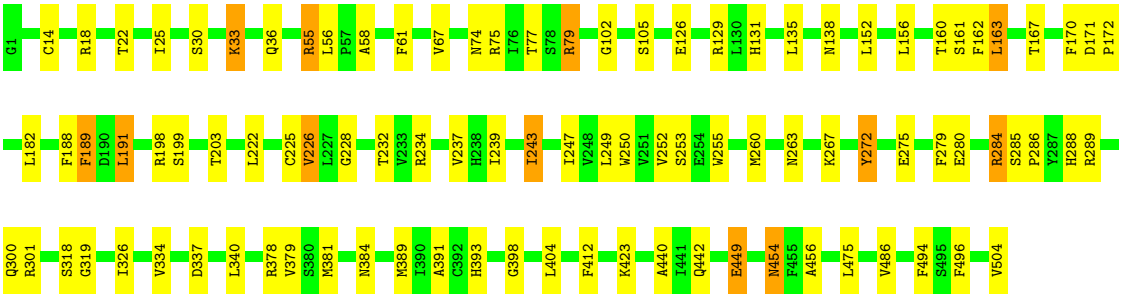
• Molecule 1: COAT PROTEIN

Chain AO: 80% 18% •



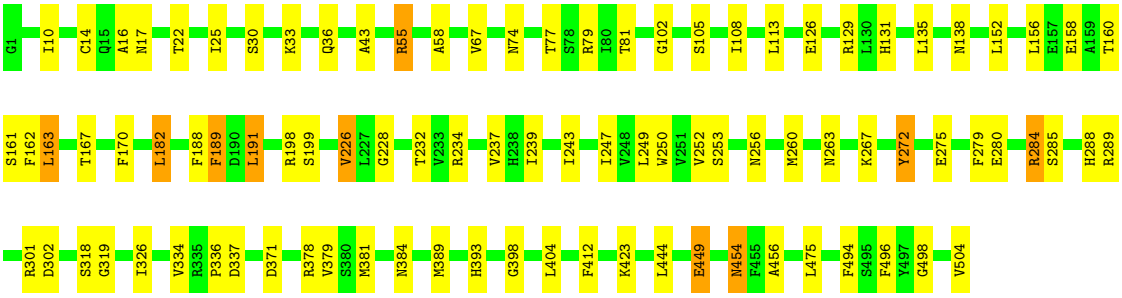
• Molecule 1: COAT PROTEIN

Chain AP: 81% 17% •



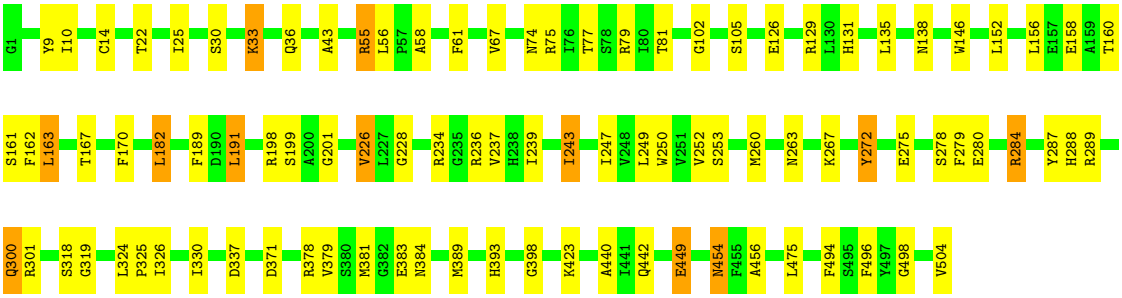
• Molecule 1: COAT PROTEIN

Chain AQ: 82% 16% •



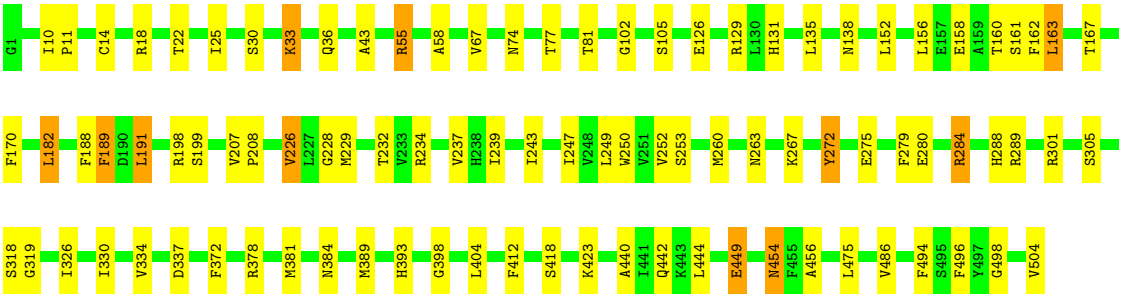
• Molecule 1: COAT PROTEIN

Chain AR: 81% 16% •



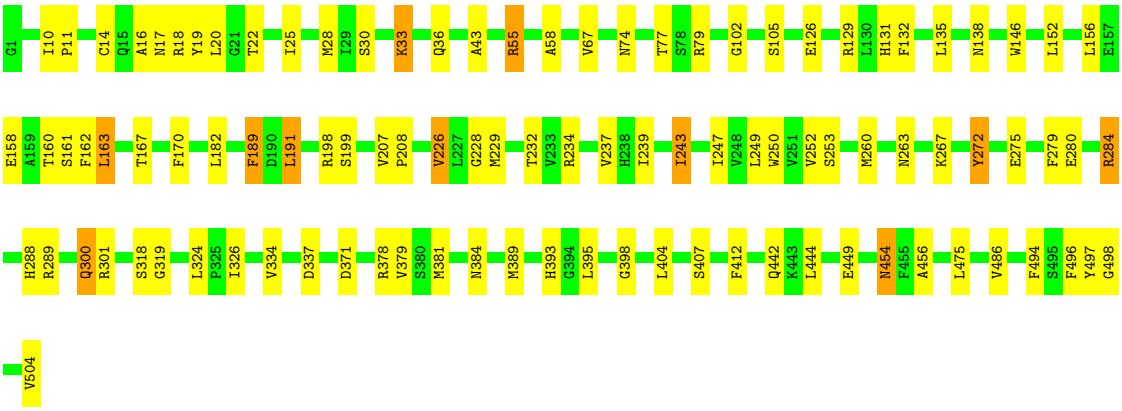
- Molecule 1: COAT PROTEIN

Chain AS:



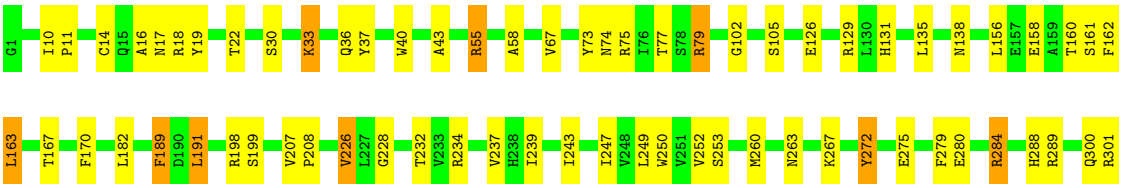
- Molecule 1: COAT PROTEIN

Chain AT:



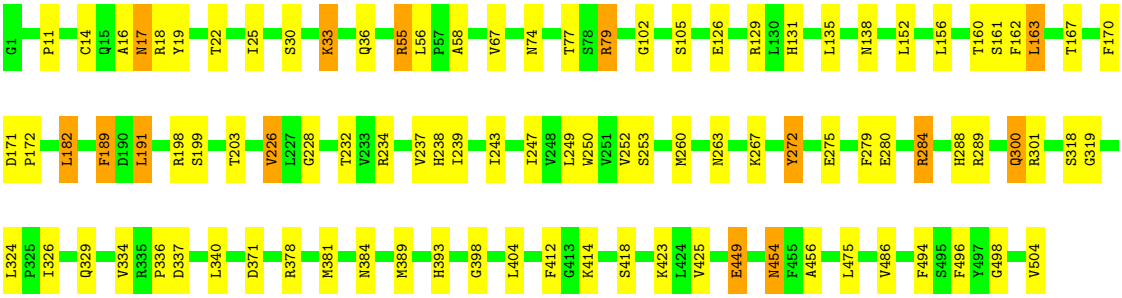
- Molecule 1: COAT PROTEIN

Chain BA:



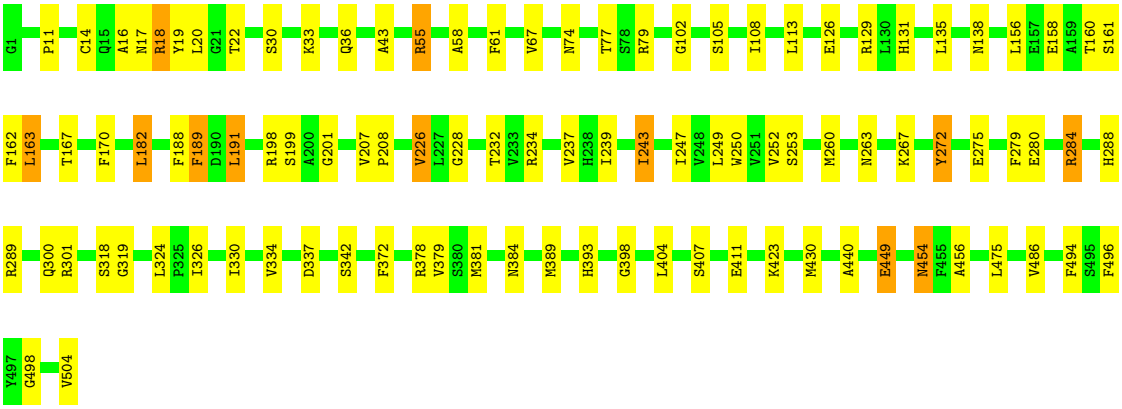
• Molecule 1: COAT PROTEIN

Chain BB:



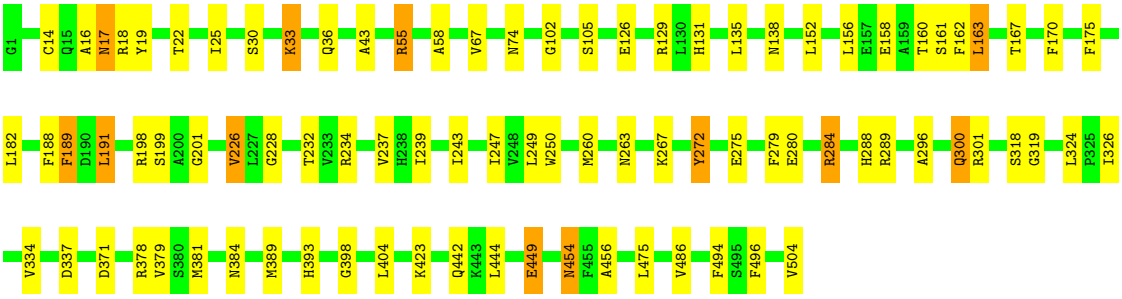
• Molecule 1: COAT PROTEIN

Chain BC:



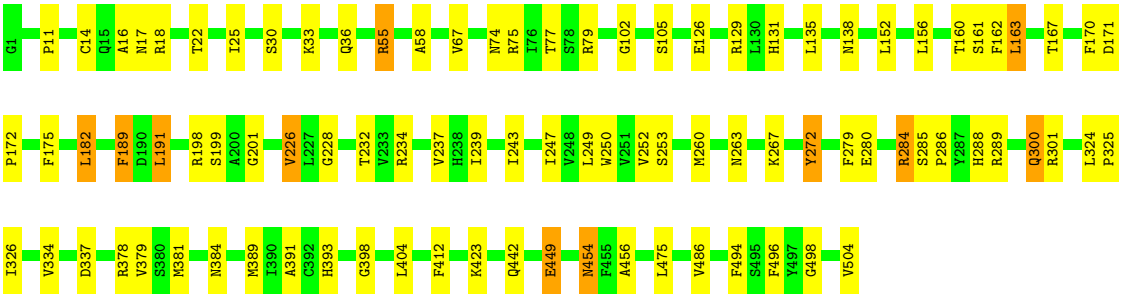
• Molecule 1: COAT PROTEIN

Chain BD:



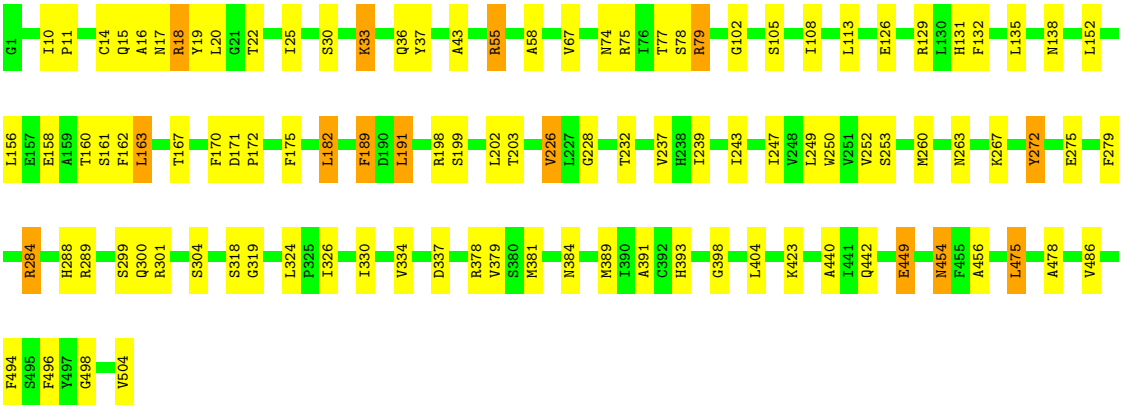
• Molecule 1: COAT PROTEIN

Chain BE:



- Molecule 1: COAT PROTEIN

Chain BF: 79% 18%

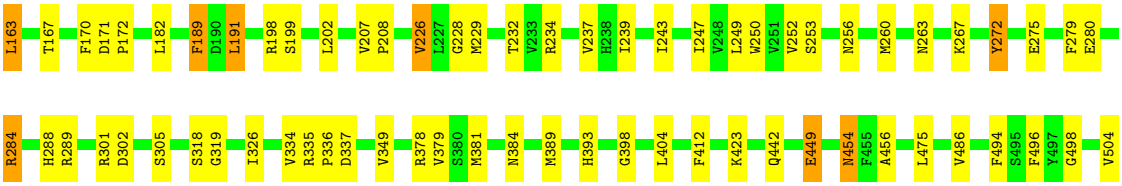


- Molecule 1: COAT PROTEIN

Chain BG: 80% 18%

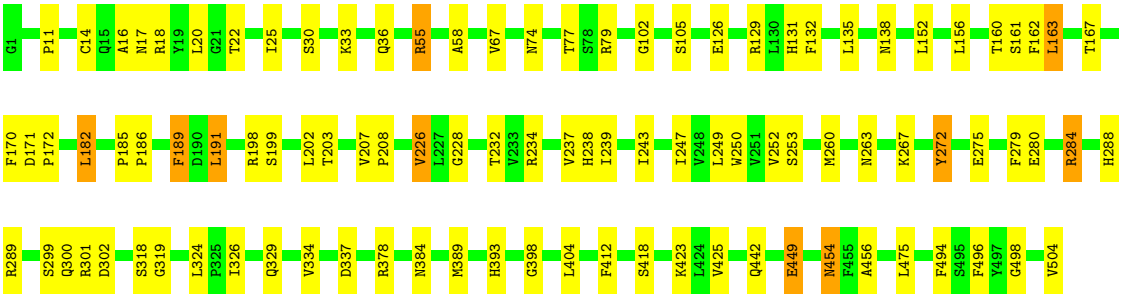
- Molecule 1: COAT PROTEIN

Chain BH: 80% 18%



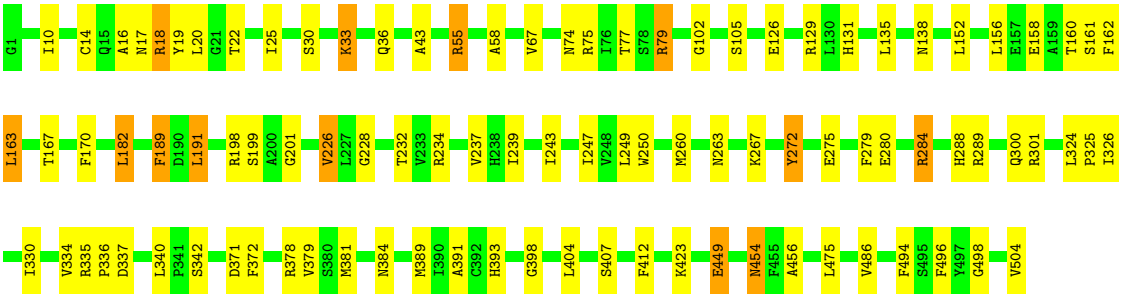
- Molecule 1: COAT PROTEIN

Chain BI:



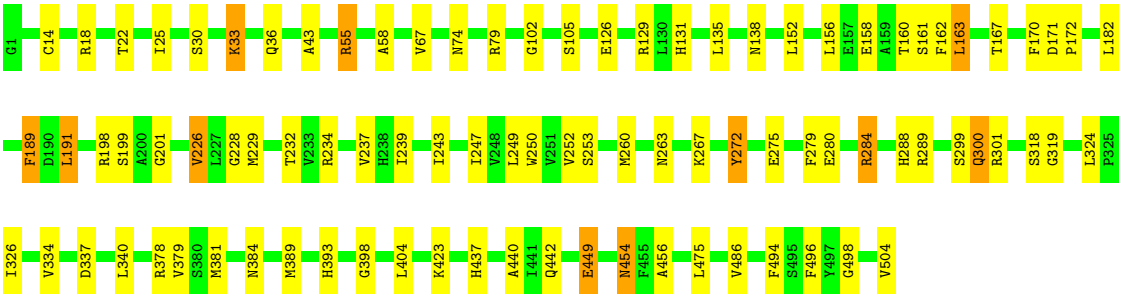
- Molecule 1: COAT PROTEIN

Chain BJ:



- Molecule 1: COAT PROTEIN

Chain BK:



- Molecule 1: COAT PROTEIN

Chain BL:

G1 Y9 C14 Q15 A16 N17 T22 I25 S30 K33 Q36 I52 R55 A58 V67 N74 T77 S78 R79 G102 S105 E126 R129 L130 H131 L135 N138 D145 L152 L156 T160 S161 F162 L163 T167

F170 D171 P172 L182 F189 D190 L191 R198 S199 A200 G201 V226 L227 G228 M229 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 M260 Y272 E275 F279 E280 R284 H288 R289 S299 Q300 R301 S318 G319 L324

P325 I326 Q329 V334 D337 D371 R378 V379 S380 M381 N384 M389 H393 G398 L404 Q405 F412 S418 K423 A440 I441 Q442 K443 L444 E449 N454 F455 A456 L475 V486 F494 S495 F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain BM: 81% 17% •

G1 P11 C14 Q15 A16 N17 R18 Y19 L20 G21 T22 I25 S30 K33 Q36 A43 R55 L56 P57 A58 V67 N74 R75 I76 T77 S78 R79 G102 S105 E126 R129 L130 H131 L135 N138 L152 L156 E157 E158 A159 T160 S161

F162 L163 T167 F170 D171 P172 L182 F189 D190 L191 R198 S199 T203 V226 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 E254 W255 M260 N263 K267 Y272 E275 F279 E280 R284 S285 H288 R289

Q300 R301 S318 G319 I326 V334 D337 R378 V379 S380 M381 N384 M389 I390 A391 C392 H393 G398 L404 S407 F412 K423 Q442 K443 L444 E449 N454 F455 A456 L475 V486 F494 S495 F496 V504

- Molecule 1: COAT PROTEIN

Chain BN: 81% 16% •

G1 C14 Q15 A16 N17 R18 Y19 T22 I25 M28 I29 S30 K33 Q36 A43 R55 A58 L64 V67 N74 T77 G102 S105 I108 L113 E126 R129 L130 H131 L135 N138 L152 L156 E157 E158 A159 T160

S161 F162 L163 T167 F170 D171 P172 L182 F189 D190 L191 R198 S199 T203 V207 P208 V226 M229 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 W255 M260 N263 K267 Y272 E275 F279 E280 R284 S285

H288 R289 Q300 R301 I326 I330 V334 D337 D371 R378 M381 N384 M389 H393 G398 L404 F412 K423 A440 E449 N454 F455 A456 L475 V486 F494 S495 F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain BO: 80% 17% •

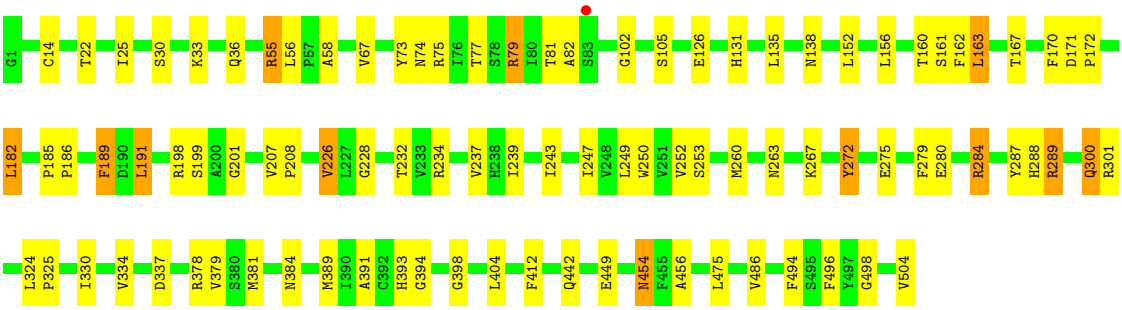
G1 I10 P11 C14 Q15 A16 N17 R18 T22 I25 S30 K33 Q36 M47 R55 A58 F61 V67 Y73 N74 R75 I76 T77 G102 S105 A117 E126 S127 P128 R129 L130 H131 L135 N138 L152 L156 T160 S161

F162 L163 T167 F170 D171 P172 F175 L182 P185 P186 F189 D190 L191 R198 S199 V226 L227 G228 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 M260 N263 K267 Y272 E275 F279 E280 R284 H288 R289

R301 L324 P325 I326 I330 P336 D337 D371 R378 V379 S380 M381 G382 E383 N384 M389 I390 A391 C392 H393 G394 G398 D401 L404 K423 L444 E449 N454 F455 A456 L475 V486 L487 C488 F494 S495 F496 Y497 G498 V504

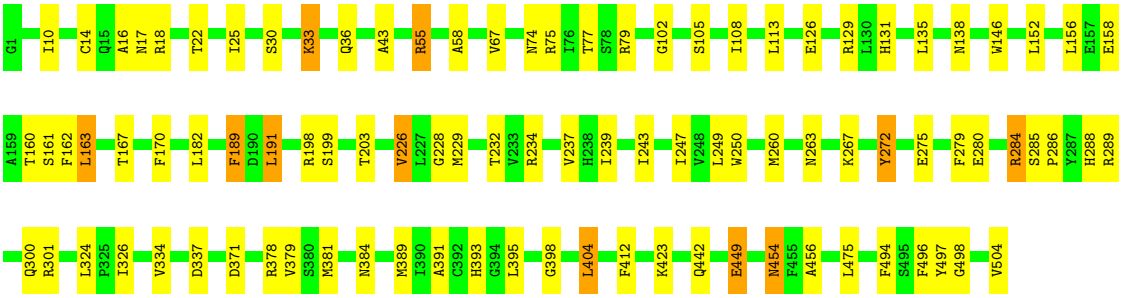
- Molecule 1: COAT PROTEIN

Chain BP: 81% 16%



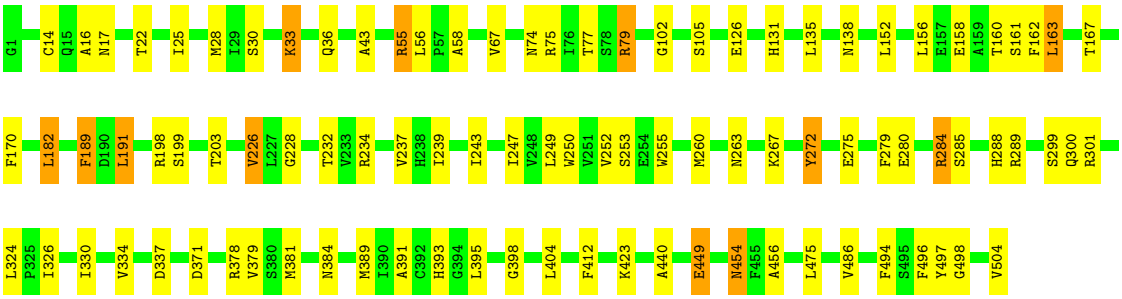
- Molecule 1: COAT PROTEIN

Chain BQ: 81% 17%



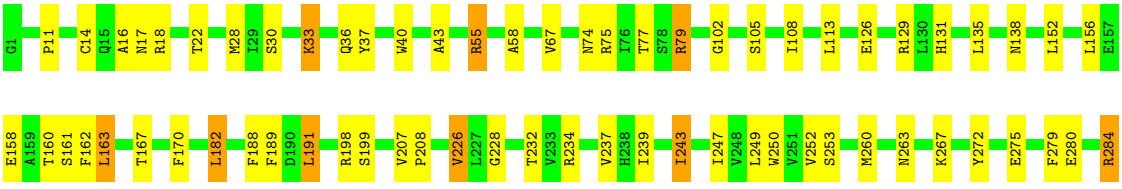
- Molecule 1: COAT PROTEIN

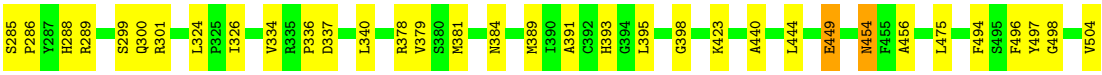
Chain BR: 81% 16%



- Molecule 1: COAT PROTEIN

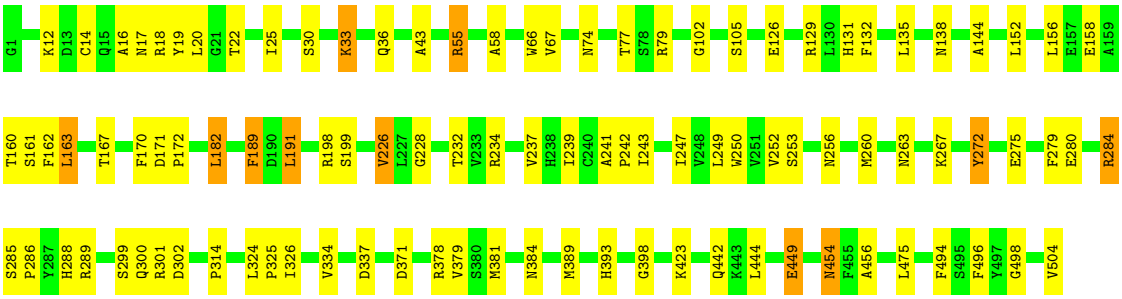
Chain BS: 80% 18%





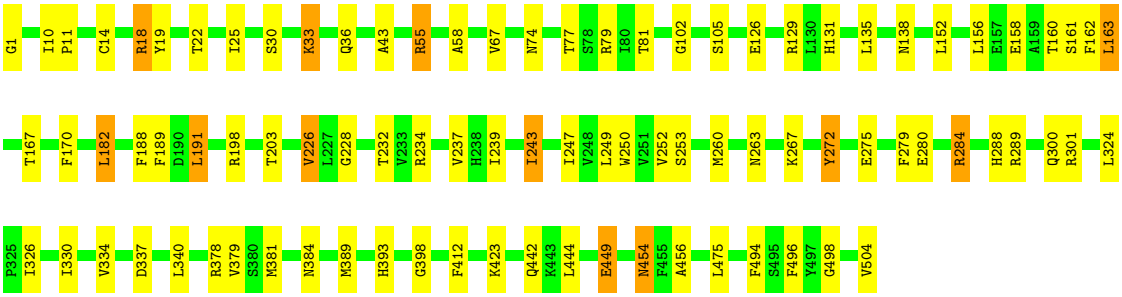
• Molecule 1: COAT PROTEIN

Chain BT:



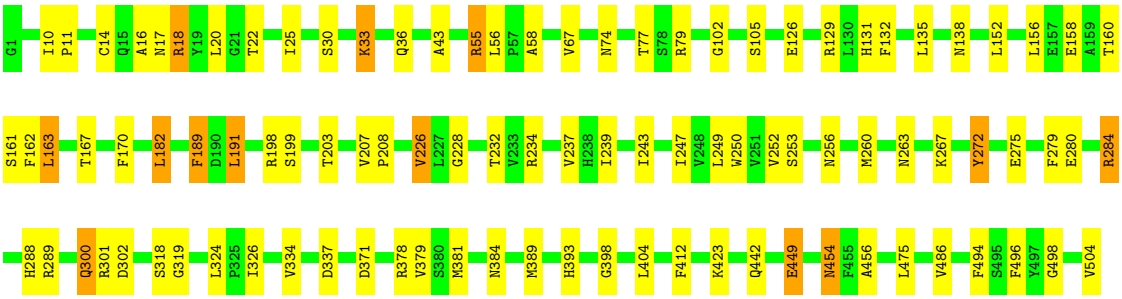
• Molecule 1: COAT PROTEIN

Chain CA:



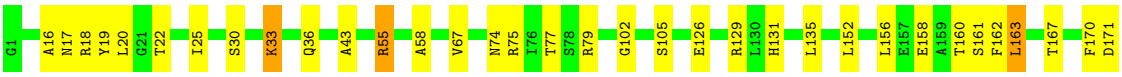
• Molecule 1: COAT PROTEIN

Chain CB:



• Molecule 1: COAT PROTEIN

Chain CC:



P172 L182 F188 F189 D190 L191 R198 S199 V226 L227 G228 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 M260 N263 K267 Y272 E275 F279 E280 R284 H288 R289 Q300 R301 I326 V334 D337

R378 V379 S380 M381 N384 M389 I390 A391 C392 H393 G398 L404 F412 K423 Q442 E449 N454 F455 A456 L475 V486 F494 S495 F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain CD: 81% 17%

G1 C14 Q15 A16 N17 L20 G21 T22 I25 S30 K33 Q36 A43 P48 T49 F50 R55 A58 V67 N74 T77 S78 R79 G102 S105 E126 S127 P128 R129 L130 H131 F132 L135 N138 L152 L156 E157 E158 A159 T160

S161 F162 L163 T167 F170 D171 P172 F175 L182 F188 F189 D190 L191 R198 S199 L202 T203 V226 L227 G228 M229 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 M260 N263 K267 Y272 E275 F279 E280

R284 H288 R289 Q300 R301 L324 P325 I326 V334 D337 D371 R378 V379 S380 M381 N384 M389 H393 G398 L404 F412 K423 A440 I441 Q442 E449 N454 F455 A456 L475 V486 F494 S495 F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain CE: 79% 19%

G1 C14 Q15 A16 N17 R18 Y19 L20 G21 T22 I25 S30 K33 Q36 A43 R55 A58 F61 V67 N74 R75 I76 T77 S78 R79 G102 S105 E126 S127 P128 R129 L130 H131 F132 L135 N138 L152 L156 E157 E158 A159 T160

S161 F162 L163 T167 F170 D171 P172 L182 F189 D190 L191 L197 R198 S199 T203 V207 P208 V226 L227 G228 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 N256 M260 N263 K267 Y272 E275 F279

E280 R284 H288 R289 Q300 R301 D302 Y309 S318 G319 I326 V334 R335 P336 D337 L340 D371 R378 M381 N384 M389 I390 A391 C392 H393 G398 L404 F412 K423 A440 I441 Q442 K443 L444 E449 N454 F455 A456 L475

V486 F494 S495 F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain CF: 80% 17%

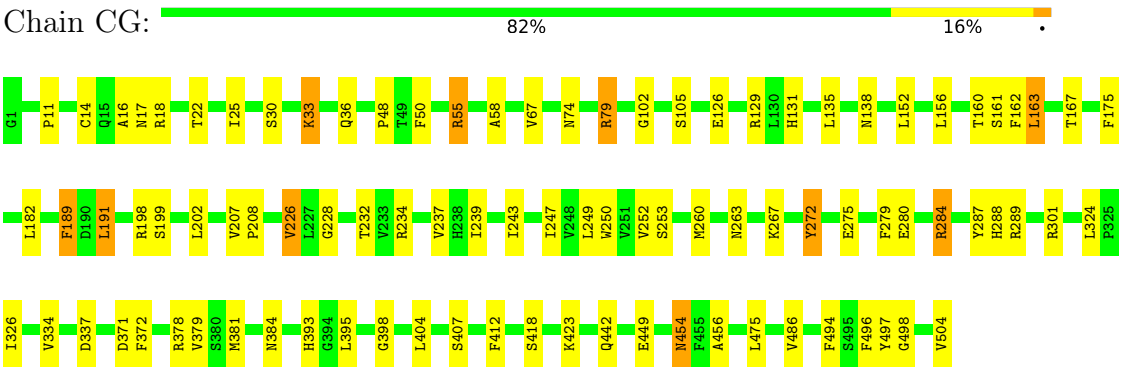
G1 C14 Q15 A16 N17 R18 Y19 L20 G21 T22 I25 S30 K33 Q36 A43 P48 T49 F50 R55 A58 V67 N74 R79 G102 S105 E126 R129 L130 H131 F132 L135 N138 L152 L156 E157 E158 A159 T160 S161 F162

L163 T167 F170 L182 F189 D190 L191 R198 S199 V207 P208 V226 L227 G228 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 M260 N263 K267 Y272 E275 F279 E280 R284 H288 R289 Q300 R301

S318 G319 L324 P325 I326 Q329 V334 D337 D371 R378 V379 S380 M381 N384 M389 H393 G398 L404 F412 S418 K423 Q442 E449 N454 F455 A456 L475 A478 V486 F494 S495 F496 Y497 G498 V504

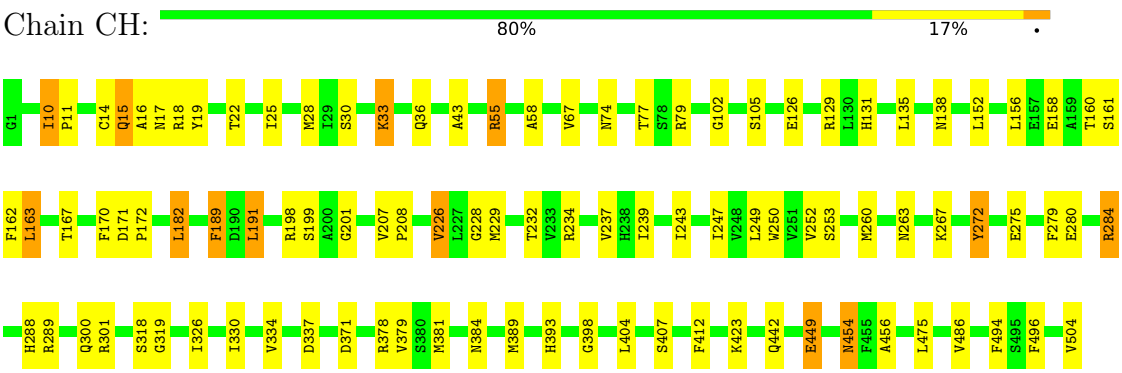
- Molecule 1: COAT PROTEIN

Chain CG:



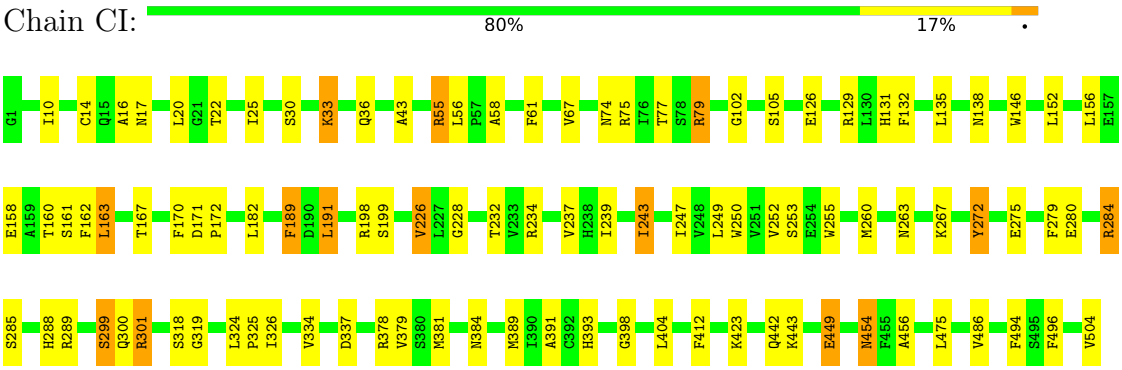
- Molecule 1: COAT PROTEIN

Chain CH:



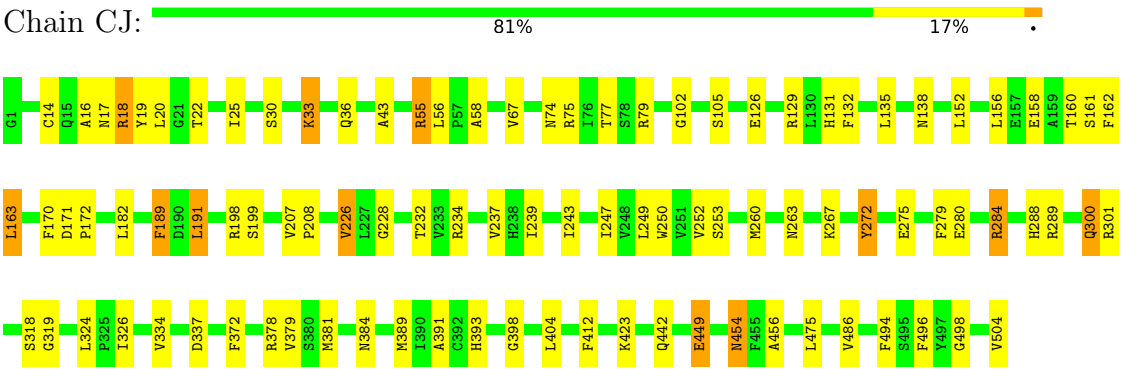
- Molecule 1: COAT PROTEIN

Chain CI:



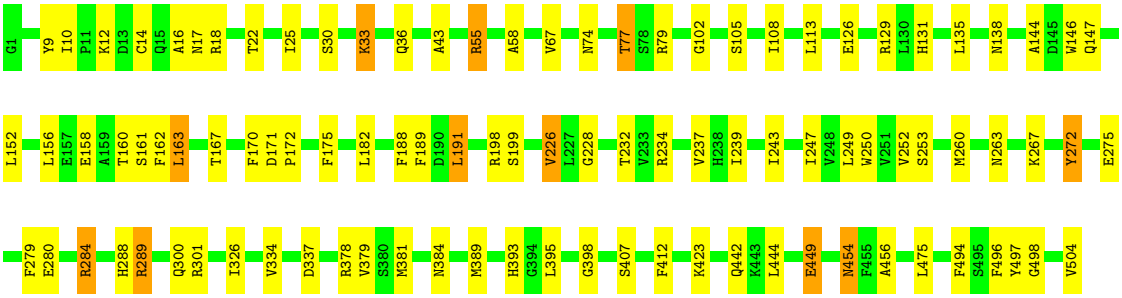
- Molecule 1: COAT PROTEIN

Chain CJ:



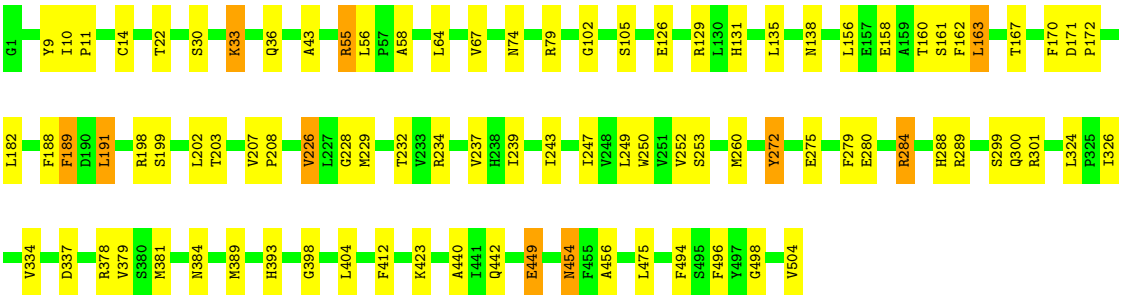
- Molecule 1: COAT PROTEIN

Chain CK: 81% 17%



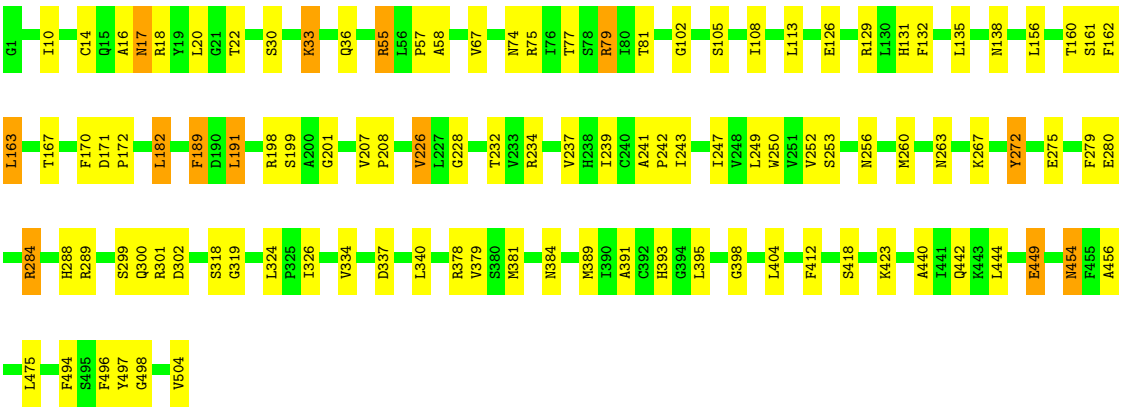
- Molecule 1: COAT PROTEIN

Chain CL: 82% 16%



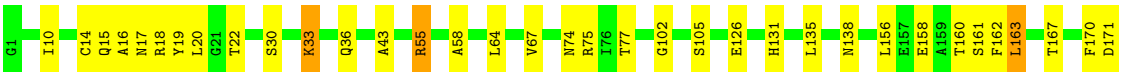
- Molecule 1: COAT PROTEIN

Chain CM: 79% 19%



- Molecule 1: COAT PROTEIN

Chain CN: 82% 16%



P172 L182 F189 D190 L191 R198 S199 V226 L227 G228 M229 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 M260 N263 K267 Y272 E275 F279 E280 R284 H288 R289 R301 S318 G319 I326 V334 R335 P336 D337

L340 R378 V379 S380 M381 N384 M389 I390 A391 C392 H393 G398 L404 S407 F412 K423 L444 E449 N454 F455 A456 L475 V486 F494 S495 F496 V504

- Molecule 1: COAT PROTEIN

Chain CO: 80% 18% •

G1 Y9 C14 Q15 A16 N17 R18 Y19 T22 I25 S30 K33 Q36 A43 R55 L56 P57 A58 V67 N74 R75 T76 T77 S78 R79 I80 T81 G102 S105 I108 L113 E126 H131 L135 N138 Q147 L152 L156

E157 E158 A159 T160 S161 F162 L163 T167 F170 F175 L182 F188 F189 D190 L191 R198 S199 T203 V207 P208 V226 L227 G228 T232 V233 R234 V237 H238 I239 C240 A241 P242 I243 I247 V248 L249 W250 V251 V252 S253 E254 W255 M260 N263 K267

Y272 E275 F279 E280 R284 S285 H288 R289 Q300 R301 L324 P325 I326 V334 D337 R378 V379 S380 M381 N384 M389 I390 A391 C392 H393 G398 L404 S418 K423 A440 I441 Q442 E449 N454 F455 A456 L475 F494 S495

F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain CP: 81% 16% •

G1 I10 C14 R18 T22 I25 M28 I29 S30 K33 Q36 A43 R55 A58 V67 N74 T77 S78 R79 G102 S105 E126 R129 L130 H131 L135 N138 L152 L156 E157 E158 A159 T160 S161 F162 L163 T167

F170 D171 P172 L182 F188 F189 D190 L191 R198 S199 V226 L227 G228 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 E254 W255 N256 M260 N263 K267 Y272 E275 F279 E280 R284 S285 P286 Y287 H288 R289

Q300 R301 D302 S318 G319 L324 P325 I326 V334 D337 R378 V379 S380 M381 N384 M389 H393 G398 L404 K423 A440 I441 Q442 E449 N454 F455 A456 L475 V486 F494 S495 F496 Y497 G498 V504

- Molecule 1: COAT PROTEIN

Chain CQ: 82% 16% •

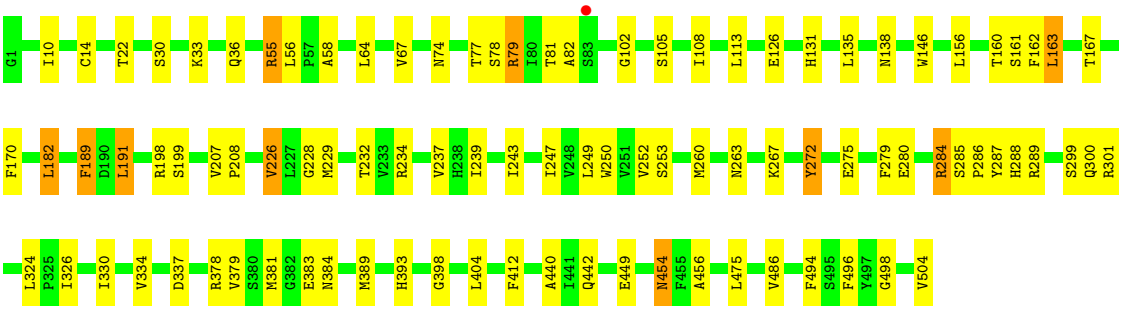
G1 C14 Q15 A16 N17 R18 T22 I25 S30 K33 Q36 A43 R55 A58 V67 N74 R75 R79 G102 S105 E126 R129 L130 H131 L135 N138 L152 L156 E157 E158 A159 T160 S161 F162 L163 T167 F170 D171

P172 F175 L182 F189 D190 L191 R198 S199 T203 V226 M229 T232 V233 R234 V237 H238 I239 I243 I247 V248 L249 W250 V251 V252 S253 M260 Y272 E275 F279 E280 R284 H288 R289 Q300 R301 S318 G319 I326 I330

V334 R335 P336 D337 R378 N384 M389 I390 A391 C392 H393 G394 L395 G398 L404 F412 K423 Q442 K443 L444 E449 N454 F455 A456 L475 V486 F494 S495 F496 Y497 G498 V504

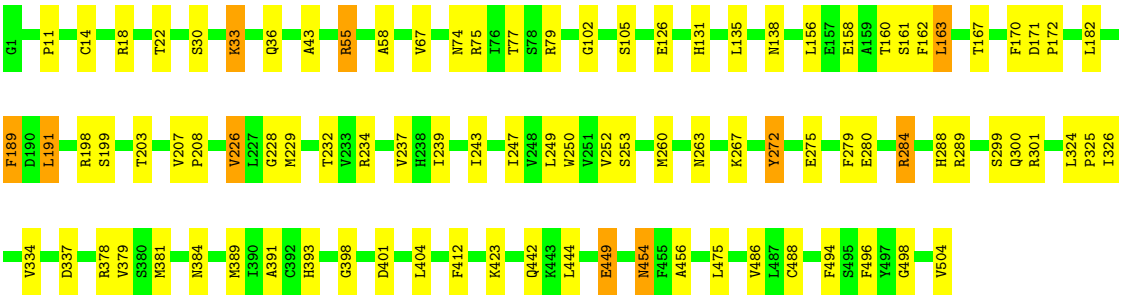
- Molecule 1: COAT PROTEIN

Chain CR:



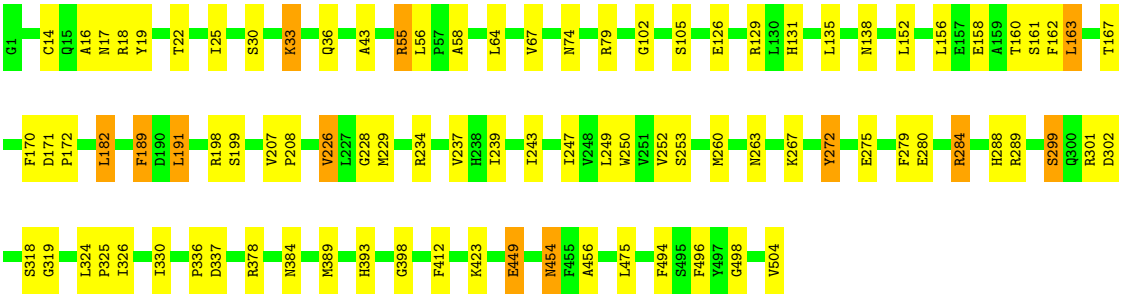
- Molecule 1: COAT PROTEIN

Chain CS:



- Molecule 1: COAT PROTEIN

Chain CT:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	279.40Å 279.60Å 293.30Å 102.40° 116.40° 108.20°	Depositor
Resolution (Å)	135.43 – 3.00 135.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.3 (135.43-3.00) 96.3 (135.43-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.207 0.187 , 0.204	Depositor DCC
R_{free} test set	66376 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-h-k-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	237060	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	AA	0.50	0/4058	0.61	2/5517 (0.0%)
1	AB	0.50	2/4058 (0.0%)	0.62	1/5517 (0.0%)
1	AC	0.49	2/4058 (0.0%)	0.62	0/5517
1	AD	0.50	2/4058 (0.0%)	0.62	0/5517
1	AE	0.53	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	AF	0.49	1/4058 (0.0%)	0.62	1/5517 (0.0%)
1	AG	0.49	1/4058 (0.0%)	0.61	0/5517
1	AH	0.51	2/4058 (0.0%)	0.62	0/5517
1	AI	0.50	2/4058 (0.0%)	0.62	0/5517
1	AJ	0.49	1/4058 (0.0%)	0.62	0/5517
1	AK	0.48	2/4058 (0.0%)	0.61	0/5517
1	AL	0.53	2/4058 (0.0%)	0.64	0/5517
1	AM	0.51	2/4058 (0.0%)	0.62	1/5517 (0.0%)
1	AN	0.50	1/4058 (0.0%)	0.63	1/5517 (0.0%)
1	AO	0.52	2/4058 (0.0%)	0.63	0/5517
1	AP	0.51	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	AQ	0.50	1/4058 (0.0%)	0.61	0/5517
1	AR	0.52	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	AS	0.51	1/4058 (0.0%)	0.62	0/5517
1	AT	0.49	1/4058 (0.0%)	0.61	0/5517
1	BA	0.49	1/4058 (0.0%)	0.63	0/5517
1	BB	0.52	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	BC	0.49	1/4058 (0.0%)	0.62	0/5517
1	BD	0.48	2/4058 (0.0%)	0.62	0/5517
1	BE	0.50	2/4058 (0.0%)	0.63	0/5517
1	BF	0.51	2/4058 (0.0%)	0.62	0/5517
1	BG	0.50	2/4058 (0.0%)	0.62	1/5517 (0.0%)
1	BH	0.49	2/4058 (0.0%)	0.62	0/5517
1	BI	0.51	1/4058 (0.0%)	0.63	0/5517
1	BJ	0.49	1/4058 (0.0%)	0.62	0/5517
1	BK	0.49	2/4058 (0.0%)	0.61	0/5517
1	BL	0.52	3/4058 (0.1%)	0.62	0/5517
1	BM	0.53	3/4058 (0.1%)	0.64	1/5517 (0.0%)
1	BN	0.51	2/4058 (0.0%)	0.63	0/5517

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	BO	0.51	3/4058 (0.1%)	0.63	0/5517
1	BP	0.53	2/4058 (0.0%)	0.65	1/5517 (0.0%)
1	BQ	0.51	2/4058 (0.0%)	0.62	0/5517
1	BR	0.51	2/4058 (0.0%)	0.62	1/5517 (0.0%)
1	BS	0.50	0/4058	0.62	0/5517
1	BT	0.48	1/4058 (0.0%)	0.62	0/5517
1	CA	0.51	1/4058 (0.0%)	0.62	0/5517
1	CB	0.51	2/4058 (0.0%)	0.62	1/5517 (0.0%)
1	CC	0.49	1/4058 (0.0%)	0.62	0/5517
1	CD	0.50	2/4058 (0.0%)	0.62	0/5517
1	CE	0.50	1/4058 (0.0%)	0.62	0/5517
1	CF	0.48	1/4058 (0.0%)	0.62	0/5517
1	CG	0.51	1/4058 (0.0%)	0.63	0/5517
1	CH	0.49	1/4058 (0.0%)	0.62	0/5517
1	CI	0.50	1/4058 (0.0%)	0.62	1/5517 (0.0%)
1	CJ	0.50	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	CK	0.48	0/4058	0.62	0/5517
1	CL	0.52	1/4058 (0.0%)	0.63	1/5517 (0.0%)
1	CM	0.51	1/4058 (0.0%)	0.62	0/5517
1	CN	0.51	1/4058 (0.0%)	0.63	0/5517
1	CO	0.51	2/4058 (0.0%)	0.63	0/5517
1	CP	0.52	2/4058 (0.0%)	0.62	0/5517
1	CQ	0.50	2/4058 (0.0%)	0.62	0/5517
1	CR	0.53	3/4058 (0.1%)	0.64	1/5517 (0.0%)
1	CS	0.52	2/4058 (0.0%)	0.63	0/5517
1	CT	0.50	1/4058 (0.0%)	0.62	1/5517 (0.0%)
All	All	0.50	95/243480 (0.0%)	0.62	20/331020 (0.0%)

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	AA	0	2
1	AB	0	2
1	AC	0	2
1	AD	0	1
1	AE	0	1
1	AF	0	2
1	AG	0	2
1	AH	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	AI	0	2
1	AJ	0	2
1	AK	0	1
1	AL	0	1
1	AM	0	2
1	AN	0	2
1	AO	0	2
1	AP	0	2
1	AQ	0	1
1	AR	0	2
1	AS	0	2
1	AT	0	2
1	BA	0	2
1	BB	0	2
1	BC	0	1
1	BD	0	2
1	BE	0	1
1	BF	0	2
1	BG	0	2
1	BH	0	1
1	BI	0	1
1	BJ	0	2
1	BK	0	2
1	BL	0	2
1	BM	0	1
1	BN	0	2
1	BO	0	2
1	BP	0	1
1	BQ	0	2
1	BR	0	2
1	BS	0	2
1	BT	0	2
1	CA	0	2
1	CB	0	2
1	CC	0	2
1	CD	0	2
1	CE	0	2
1	CF	0	2
1	CG	0	2
1	CH	0	2
1	CI	0	2
1	CJ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	CK	0	2
1	CL	0	2
1	CM	0	2
1	CN	0	2
1	CO	0	1
1	CP	0	2
1	CQ	0	2
1	CR	0	1
1	CS	0	2
1	CT	0	2
All	All	0	107

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BM	189	PHE	CE1-CZ	-6.84	1.24	1.37
1	AL	189	PHE	CE1-CZ	-6.45	1.25	1.37
1	CJ	189	PHE	CE1-CZ	-6.29	1.25	1.37
1	BL	189	PHE	CE1-CZ	-6.29	1.25	1.37
1	BN	189	PHE	CE1-CZ	-6.23	1.25	1.37

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	284	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	CJ	56	LEU	CA-CB-CG	5.46	127.86	115.30
1	AF	56	LEU	CA-CB-CG	5.34	127.57	115.30
1	CT	56	LEU	CA-CB-CG	5.29	127.46	115.30
1	AR	56	LEU	CA-CB-CG	5.25	127.36	115.30

There are no chirality outliers.

5 of 107 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	33	LYS	Peptide
1	AA	55	ARG	Peptide
1	AB	33	LYS	Peptide
1	AB	55	ARG	Peptide
1	AC	33	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3951	0	3909	91	0
1	AB	3951	0	3909	89	0
1	AC	3951	0	3909	87	0
1	AD	3951	0	3909	93	0
1	AE	3951	0	3909	86	0
1	AF	3951	0	3909	92	0
1	AG	3951	0	3909	91	0
1	AH	3951	0	3909	90	0
1	AI	3951	0	3909	88	0
1	AJ	3951	0	3909	86	0
1	AK	3951	0	3909	88	0
1	AL	3951	0	3909	87	0
1	AM	3951	0	3909	83	0
1	AN	3951	0	3909	104	0
1	AO	3951	0	3909	91	0
1	AP	3951	0	3909	87	0
1	AQ	3951	0	3909	85	0
1	AR	3951	0	3909	88	0
1	AS	3951	0	3909	89	0
1	AT	3951	0	3909	91	0
1	BA	3951	0	3909	93	0
1	BB	3951	0	3909	97	0
1	BC	3951	0	3909	85	0
1	BD	3951	0	3909	78	0
1	BE	3951	0	3909	86	0
1	BF	3951	0	3909	92	0
1	BG	3951	0	3909	92	0
1	BH	3951	0	3909	97	0
1	BI	3951	0	3909	89	0
1	BJ	3951	0	3909	93	0
1	BK	3951	0	3909	81	0
1	BL	3951	0	3909	89	0
1	BM	3951	0	3909	89	0
1	BN	3951	0	3909	80	0
1	BO	3951	0	3909	93	0
1	BP	3951	0	3909	93	0
1	BQ	3951	0	3909	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	3951	0	3909	90	0
1	BS	3951	0	3909	87	0
1	BT	3951	0	3909	87	0
1	CA	3951	0	3909	81	0
1	CB	3951	0	3909	87	0
1	CC	3951	0	3909	84	0
1	CD	3951	0	3909	89	0
1	CE	3951	0	3909	97	0
1	CF	3951	0	3909	94	0
1	CG	3951	0	3909	92	0
1	CH	3951	0	3909	91	0
1	CI	3951	0	3909	92	0
1	CJ	3951	0	3909	94	0
1	CK	3951	0	3909	84	0
1	CL	3951	0	3909	81	0
1	CM	3951	0	3909	93	0
1	CN	3951	0	3909	81	0
1	CO	3951	0	3909	96	0
1	CP	3951	0	3909	85	0
1	CQ	3951	0	3909	85	0
1	CR	3951	0	3909	86	0
1	CS	3951	0	3909	86	0
1	CT	3951	0	3909	76	0
All	All	237060	0	234540	4775	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 10.

The worst 5 of 4775 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CF:79:ARG:HH11	1:CF:79:ARG:HG3	1.18	1.07
1:CC:250:TRP:CZ3	1:CC:272:TYR:HE1	1.77	1.02
1:BO:250:TRP:CZ3	1:BO:272:TYR:HE1	1.83	0.97
1:BS:79:ARG:HG3	1:BS:79:ARG:HH11	1.31	0.96
1:BJ:250:TRP:CZ3	1:BJ:272:TYR:HE1	1.85	0.94

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	502/504 (100%)	478 (95%)	23 (5%)	1 (0%)	47	82
1	AB	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	AC	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	34	72
1	AD	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AE	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	AF	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AG	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	34	72
1	AH	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	34	72
1	AI	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	AJ	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	AK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	AL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	AM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	AN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	AO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	AP	502/504 (100%)	483 (96%)	19 (4%)	0	100	100
1	AQ	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	AR	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	82
1	AS	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	AT	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	47	82
1	BA	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	BB	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	34	72
1	BC	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	BD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	BE	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BF	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	34	72
1	BG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	BH	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	82
1	BI	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	47	82
1	BJ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	BK	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	82
1	BL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	BM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	BN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	BO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	BP	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	34	72
1	BQ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	BR	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	BS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	BT	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	CA	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	CB	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	CC	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	CD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	CE	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	82
1	CF	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	CG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82
1	CH	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	CI	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CJ	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	47	82
1	CK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	82
1	CL	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	CM	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	34	72
1	CN	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CO	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	CP	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CQ	502/504 (100%)	482 (96%)	18 (4%)	2 (0%)	34	72
1	CR	502/504 (100%)	478 (95%)	22 (4%)	2 (0%)	34	72
1	CS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	82
1	CT	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	47	82
All	All	30120/30240 (100%)	28870 (96%)	1187 (4%)	63 (0%)	47	82

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BP	82	ALA
1	CR	82	ALA
1	BM	17	ASN
1	AC	78	SER
1	BB	17	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	AB	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	AC	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	AD	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	AE	430/430 (100%)	409 (95%)	21 (5%)	25	61
1	AF	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	AG	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	AH	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	AI	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	AJ	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	AK	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	AL	430/430 (100%)	404 (94%)	26 (6%)	19	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AM	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	AN	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	AO	430/430 (100%)	408 (95%)	22 (5%)	24	60
1	AP	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	AQ	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	AR	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	AS	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	AT	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	BA	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	BB	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	BC	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	BD	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	BE	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	BF	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	BG	430/430 (100%)	408 (95%)	22 (5%)	24	60
1	BH	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	BI	430/430 (100%)	408 (95%)	22 (5%)	24	60
1	BJ	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	BK	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	BL	430/430 (100%)	403 (94%)	27 (6%)	18	51
1	BM	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	BN	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	BO	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	BP	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	BQ	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	BR	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	BS	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	BT	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	CA	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	CB	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	CC	430/430 (100%)	407 (95%)	23 (5%)	22	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	CE	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	CF	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	CG	430/430 (100%)	408 (95%)	22 (5%)	24	60
1	CH	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	CI	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	CJ	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	CK	430/430 (100%)	406 (94%)	24 (6%)	21	56
1	CL	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	CM	430/430 (100%)	403 (94%)	27 (6%)	18	51
1	CN	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	CO	430/430 (100%)	408 (95%)	22 (5%)	24	60
1	CP	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	CQ	430/430 (100%)	404 (94%)	26 (6%)	19	53
1	CR	430/430 (100%)	405 (94%)	25 (6%)	20	55
1	CS	430/430 (100%)	407 (95%)	23 (5%)	22	58
1	CT	430/430 (100%)	405 (94%)	25 (6%)	20	55
All	All	25800/25800 (100%)	24352 (94%)	1448 (6%)	21	56

5 of 1448 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BS	182	LEU
1	CH	272	TYR
1	BT	243	ILE
1	BS	167	THR
1	CD	160	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 662 such sidechains are listed below:

Mol	Chain	Res	Type
1	CB	300	GLN
1	CM	74	ASN
1	CD	74	ASN
1	CB	288	HIS

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Mol	Chain	Res	Type
1	CH	74	ASN

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 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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	504/504 (100%)	-0.59	0	100	100	23, 33, 53, 78	0
1	AB	504/504 (100%)	-0.62	0	100	100	22, 34, 54, 78	0
1	AC	504/504 (100%)	-0.58	0	100	100	23, 34, 54, 78	0
1	AD	504/504 (100%)	-0.59	0	100	100	22, 33, 52, 78	0
1	AE	504/504 (100%)	-0.53	0	100	100	17, 31, 52, 77	0
1	AF	504/504 (100%)	-0.63	0	100	100	24, 34, 54, 80	0
1	AG	504/504 (100%)	-0.62	0	100	100	23, 34, 55, 80	0
1	AH	504/504 (100%)	-0.62	0	100	100	24, 35, 56, 79	0
1	AI	504/504 (100%)	-0.61	0	100	100	23, 34, 55, 80	0
1	AJ	504/504 (100%)	-0.57	0	100	100	22, 34, 54, 80	0
1	AK	504/504 (100%)	-0.61	0	100	100	23, 34, 54, 79	0
1	AL	504/504 (100%)	-0.57	0	100	100	23, 33, 54, 77	0
1	AM	504/504 (100%)	-0.58	0	100	100	21, 32, 52, 77	0
1	AN	504/504 (100%)	-0.55	0	100	100	22, 33, 54, 78	0
1	AO	504/504 (100%)	-0.53	0	100	100	21, 33, 54, 80	0
1	AP	504/504 (100%)	-0.55	0	100	100	19, 32, 53, 79	0
1	AQ	504/504 (100%)	-0.61	0	100	100	23, 33, 54, 77	0
1	AR	504/504 (100%)	-0.57	0	100	100	21, 32, 52, 77	0
1	AS	504/504 (100%)	-0.59	0	100	100	23, 33, 54, 80	0
1	AT	504/504 (100%)	-0.55	0	100	100	22, 33, 54, 77	0
1	BA	504/504 (100%)	-0.59	0	100	100	23, 33, 54, 79	0
1	BB	504/504 (100%)	-0.59	0	100	100	23, 34, 55, 77	0
1	BC	504/504 (100%)	-0.60	0	100	100	23, 34, 54, 78	0
1	BD	504/504 (100%)	-0.57	0	100	100	23, 34, 54, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	BE	504/504 (100%)	-0.58	0	100	100	23, 33, 54, 77	0
1	BF	504/504 (100%)	-0.54	0	100	100	22, 35, 56, 80	0
1	BG	504/504 (100%)	-0.62	0	100	100	22, 34, 54, 79	0
1	BH	504/504 (100%)	-0.61	0	100	100	21, 33, 54, 75	0
1	BI	504/504 (100%)	-0.53	0	100	100	22, 32, 54, 78	0
1	BJ	504/504 (100%)	-0.60	0	100	100	22, 34, 54, 79	0
1	BK	504/504 (100%)	-0.61	0	100	100	22, 33, 53, 77	0
1	BL	504/504 (100%)	-0.57	0	100	100	21, 32, 52, 75	0
1	BM	504/504 (100%)	-0.51	0	100	100	21, 32, 52, 77	0
1	BN	504/504 (100%)	-0.57	0	100	100	20, 33, 53, 76	0
1	BO	504/504 (100%)	-0.58	0	100	100	22, 33, 53, 80	0
1	BP	504/504 (100%)	-0.50	1 (0%)	95	87	21, 32, 53, 76	0
1	BQ	504/504 (100%)	-0.57	0	100	100	22, 33, 54, 80	0
1	BR	504/504 (100%)	-0.60	0	100	100	22, 33, 54, 79	0
1	BS	504/504 (100%)	-0.57	0	100	100	22, 33, 54, 80	0
1	BT	504/504 (100%)	-0.61	0	100	100	22, 34, 53, 77	0
1	CA	504/504 (100%)	-0.61	0	100	100	23, 35, 56, 80	0
1	CB	504/504 (100%)	-0.64	0	100	100	23, 34, 54, 77	0
1	CC	504/504 (100%)	-0.61	0	100	100	23, 34, 54, 81	0
1	CD	504/504 (100%)	-0.60	0	100	100	23, 34, 54, 79	0
1	CE	504/504 (100%)	-0.61	0	100	100	23, 33, 54, 78	0
1	CF	504/504 (100%)	-0.61	0	100	100	23, 34, 55, 80	0
1	CG	504/504 (100%)	-0.58	0	100	100	24, 34, 55, 81	0
1	CH	504/504 (100%)	-0.60	0	100	100	24, 34, 55, 79	0
1	CI	504/504 (100%)	-0.59	0	100	100	23, 33, 53, 79	0
1	CJ	504/504 (100%)	-0.57	0	100	100	24, 33, 54, 79	0
1	CK	504/504 (100%)	-0.54	0	100	100	21, 34, 54, 79	0
1	CL	504/504 (100%)	-0.61	0	100	100	22, 33, 54, 77	0
1	CM	504/504 (100%)	-0.57	0	100	100	22, 32, 53, 79	0
1	CN	504/504 (100%)	-0.57	0	100	100	22, 32, 54, 79	0
1	CO	504/504 (100%)	-0.56	0	100	100	23, 32, 54, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	CP	504/504 (100%)	-0.55	0 100 100	21, 31, 53, 78	0
1	CQ	504/504 (100%)	-0.56	0 100 100	21, 32, 53, 79	0
1	CR	504/504 (100%)	-0.47	1 (0%) 95 87	17, 31, 53, 75	0
1	CS	504/504 (100%)	-0.58	0 100 100	22, 32, 53, 78	0
1	CT	504/504 (100%)	-0.60	0 100 100	21, 32, 52, 77	0
All	All	30240/30240 (100%)	-0.58	2 (0%) 100 100	17, 33, 54, 81	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CR	83	SER	2.5
1	BP	83	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.