



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 08:47 PM UTC

PDB ID : 4V43 / pdb_00004v43
Title : Structural and mechanistic basis for allostery in the bacterial chaperonin GroEL
Authors : Wang, J.
Deposited on : 2002-01-02
Resolution : 3.52 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

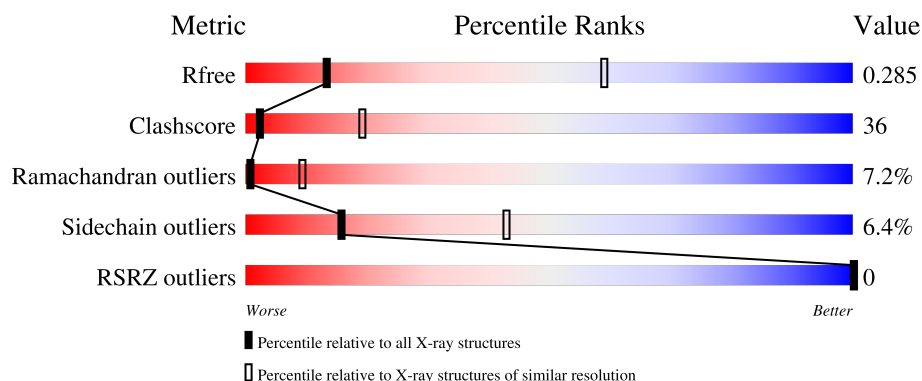
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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.



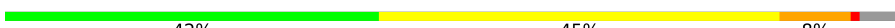
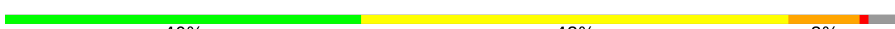
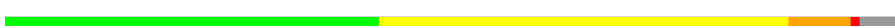
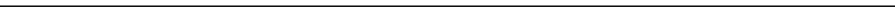
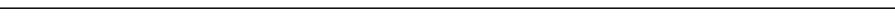
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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 $\leq 5\%$. 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	1	547	41% 46% 8% ...
1	2	547	41% 46% 8% ...
1	A	547	41% 46% 8% ...
1	B	547	42% 45% 8% ...
1	C	547	42% 45% 8% ...

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Mol	Chain	Length	Quality of chain
1	D	547	 41% 46% 8% . .
1	E	547	 43% 45% 7% . .
1	F	547	 42% 45% 8% . .
1	G	547	 42% 45% 8% . .
1	H	547	 40% 48% 8% . .
1	I	547	 42% 46% 7% . .
1	J	547	 44% 43% 8% . .
1	K	547	 42% 46% 8% . .
1	L	547	 41% 46% 8% . .
1	M	547	 41% 45% 9% . .
1	N	547	 41% 46% 8% . .
1	O	547	 42% 45% 9% . .
1	P	547	 42% 46% 8% . .
1	Q	547	 41% 47% 8% . .
1	R	547	 43% 45% 8% . .
1	S	547	 42% 46% 7% . .
1	T	547	 42% 44% 9% . .
1	U	547	 41% 45% 9% . .
1	V	547	 41% 46% 8% . .
1	W	547	 40% 46% 8% . .
1	X	547	 42% 45% 8% . .
1	Y	547	 43% 45% 7% . .
1	Z	547	 41% 46% 8% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 107996 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 GROEL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	B	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	C	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	D	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	E	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	F	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	G	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	H	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	I	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	J	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	K	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	L	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	M	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	N	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	O	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	P	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	R	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	S	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	T	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	U	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	V	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	W	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	X	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	Y	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	Z	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	1	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			
1	2	525	Total	C	N	O	S	0	0	0
			3857	2400	667	770	20			

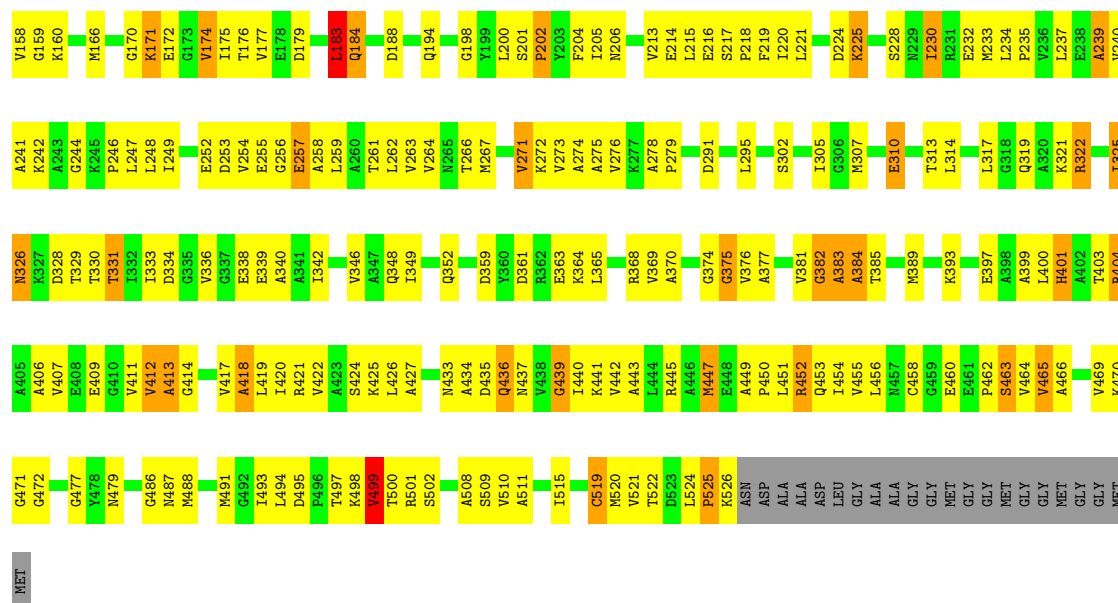
There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
A	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
B	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
B	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
C	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
C	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
D	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
D	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
E	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
E	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
F	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
F	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
G	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
G	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
H	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5

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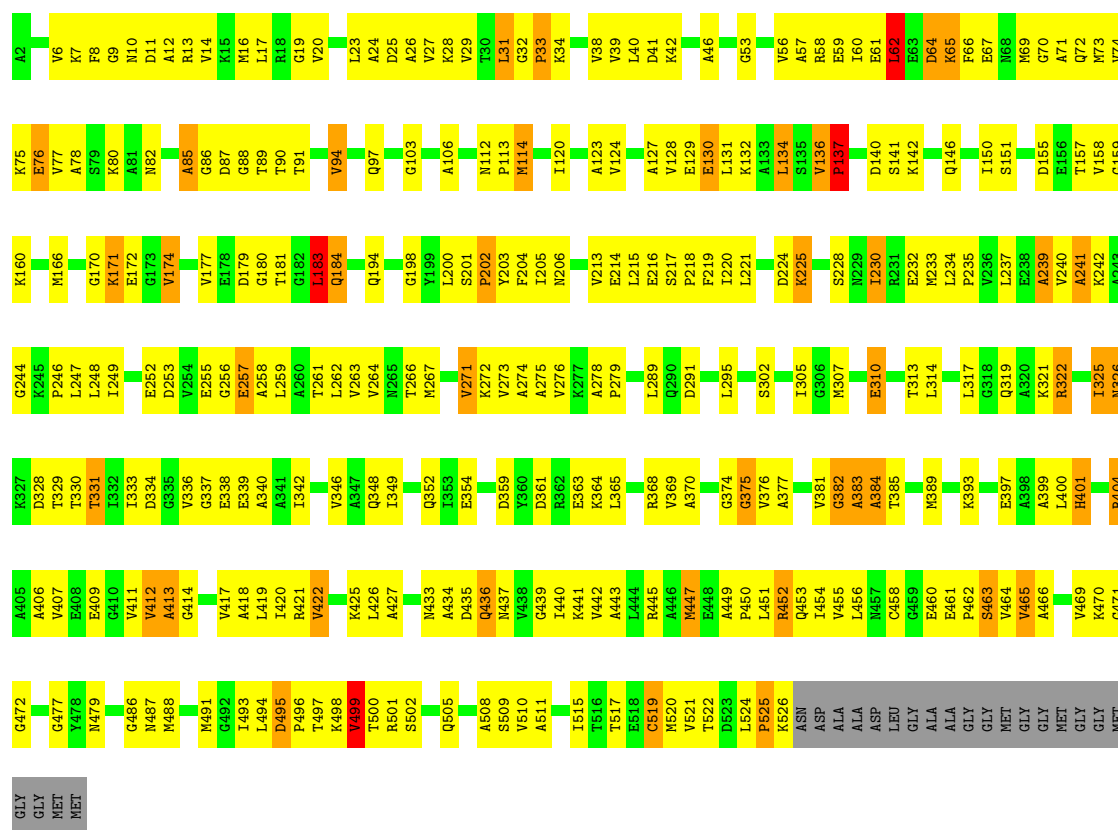
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Chain	Residue	Modelled	Actual	Comment	Reference
H	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
I	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
I	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
J	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
J	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
K	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
K	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
L	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
L	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
M	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
M	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
N	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
N	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
O	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
O	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
P	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
P	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
Q	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
Q	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
R	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
R	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
S	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
S	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
T	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
T	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
U	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
U	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
V	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
V	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
W	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
W	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
X	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
X	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
Y	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
Y	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
Z	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
Z	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
1	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
1	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5
2	398	ALA	ASP	SEE REMARK 999	UNP P0A6F5
2	434	ALA	GLU	SEE REMARK 999	UNP P0A6F5



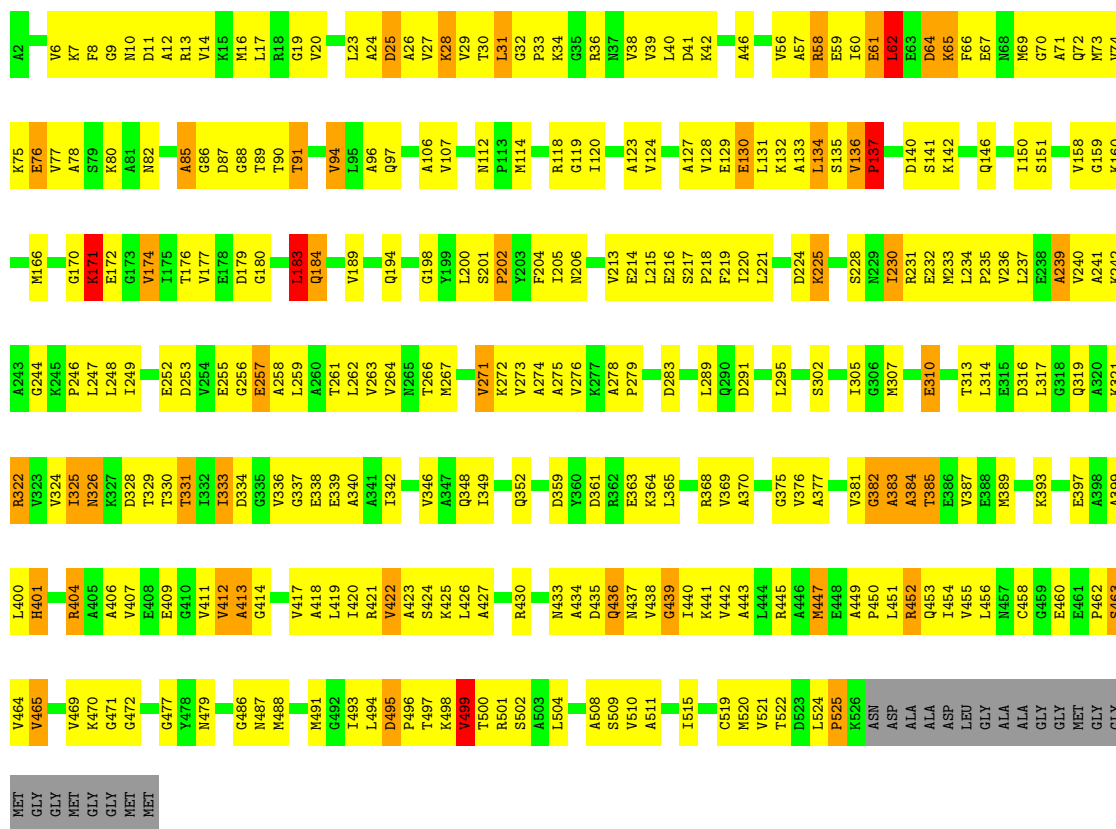
• Molecule 1: GROEL PROTEIN

Chain C: 42% 45% 8% . .

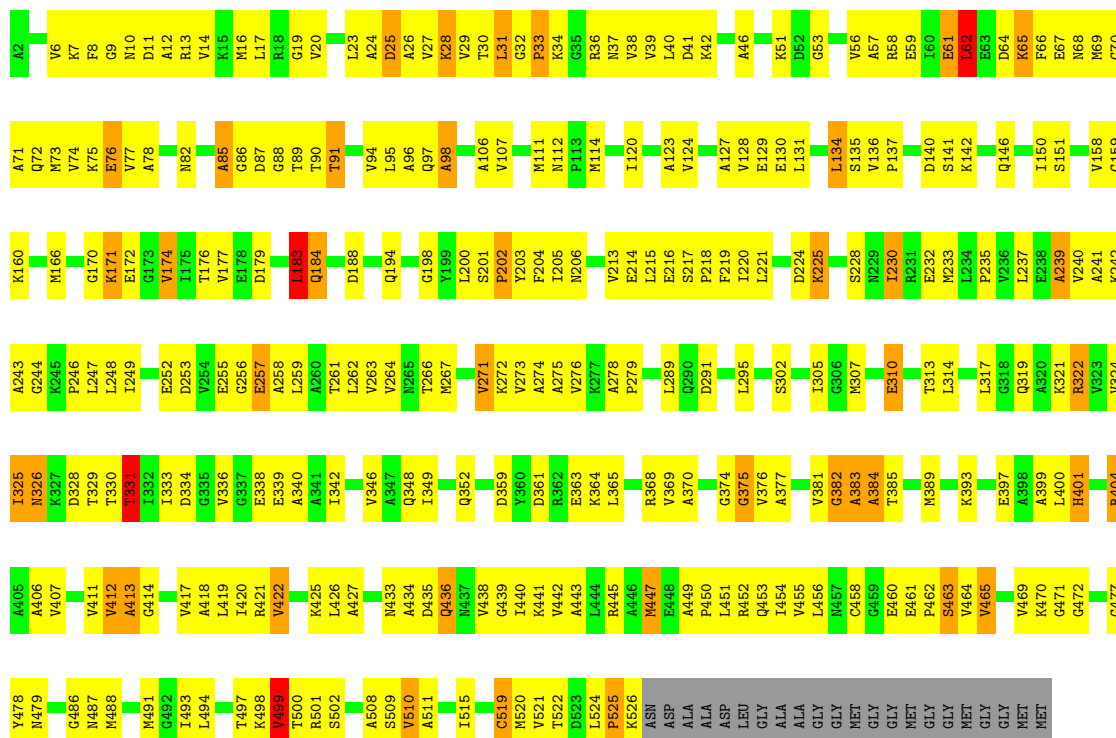


• Molecule 1: GROEL PROTEIN

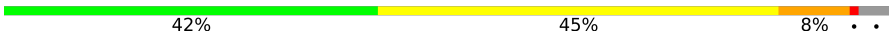
Chain D: 41% 46% 8% . .

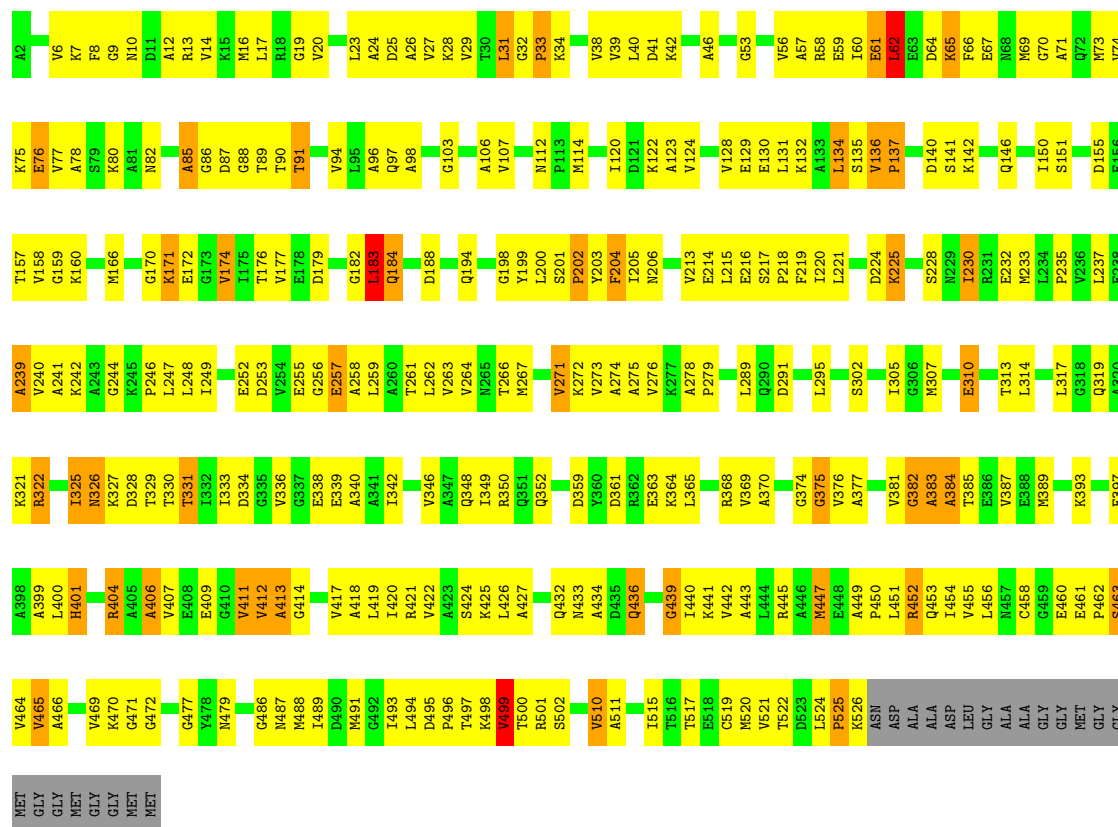


Chain E:

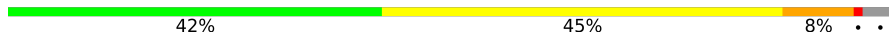


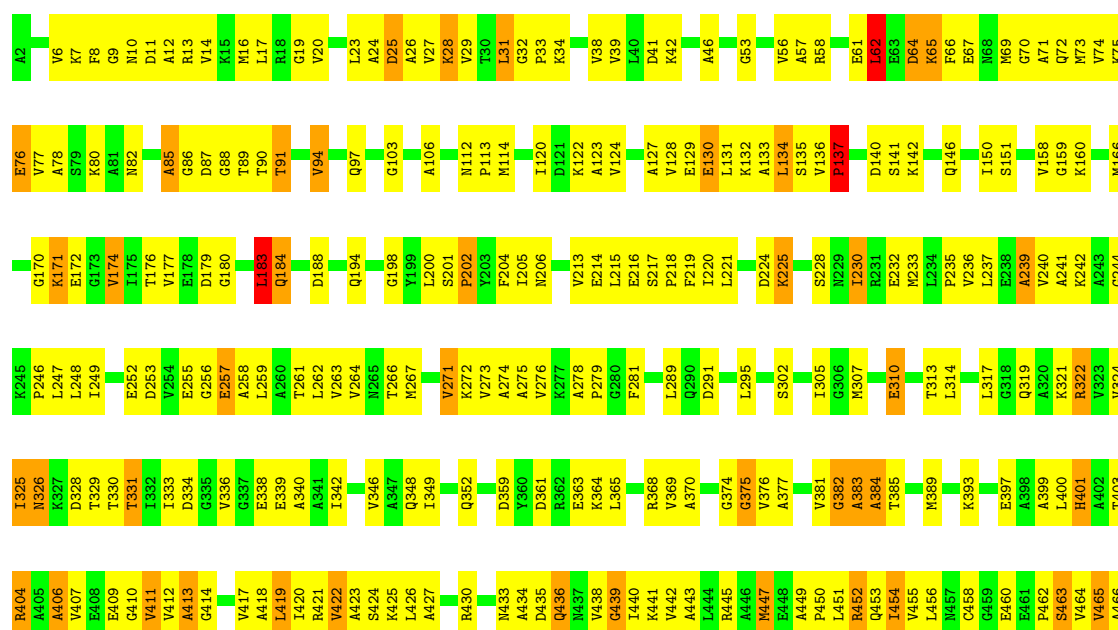
• Molecule 1: GROEL PROTEIN

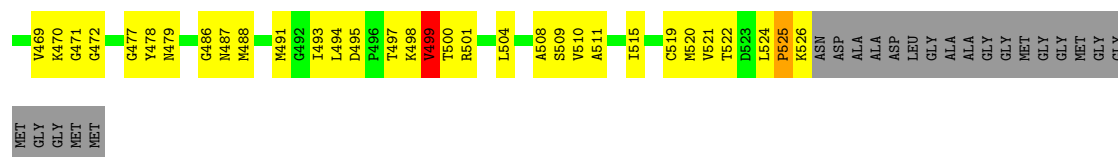
Chain F: 



• Molecule 1: GROEL PROTEIN

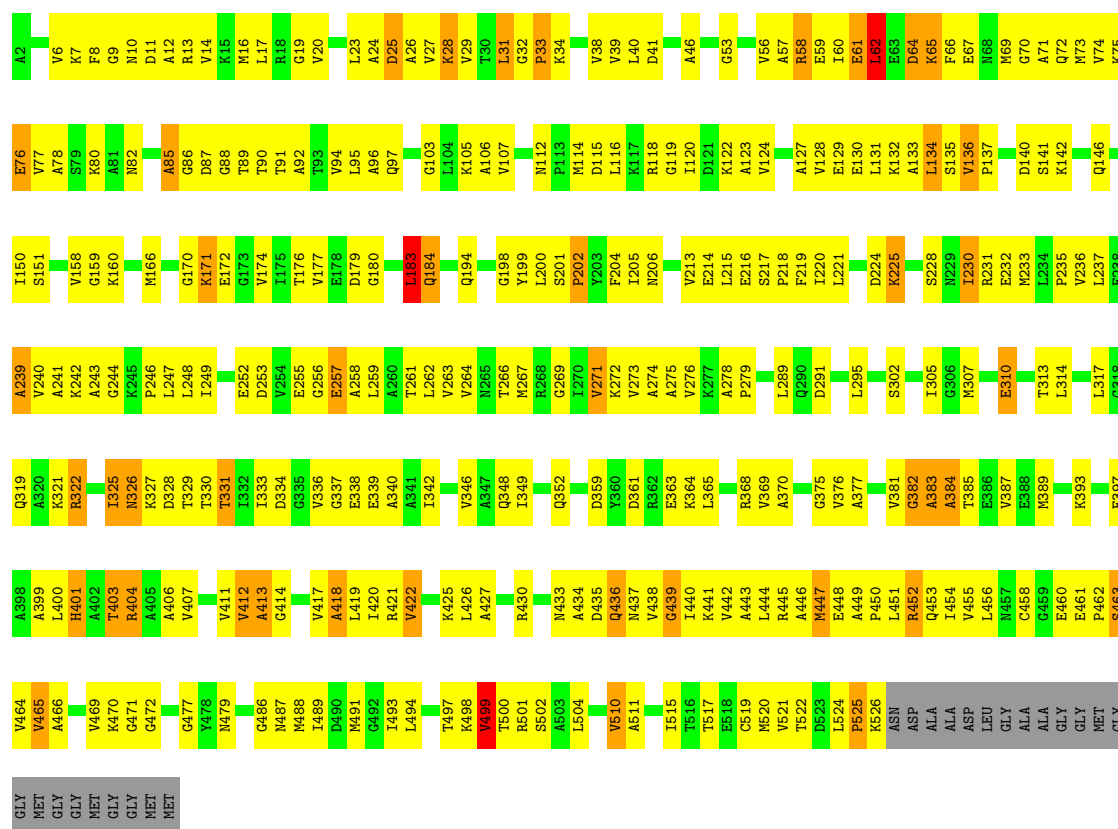
Chain G: 





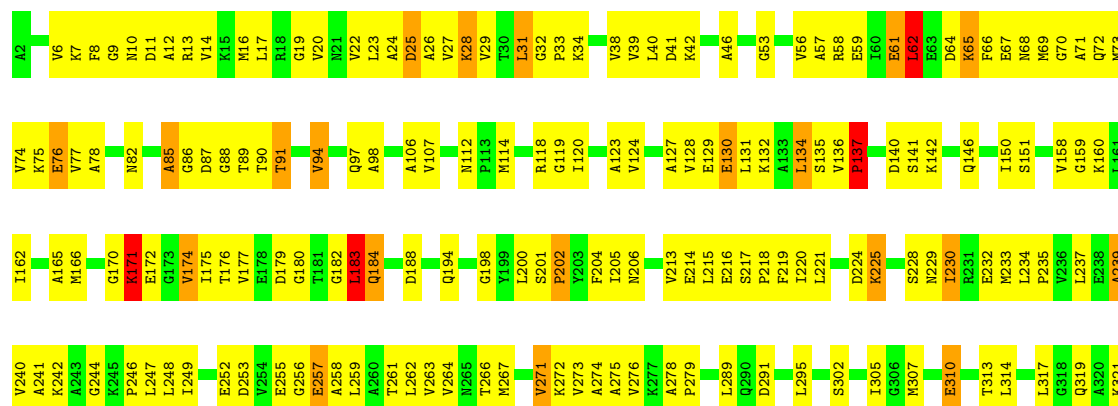
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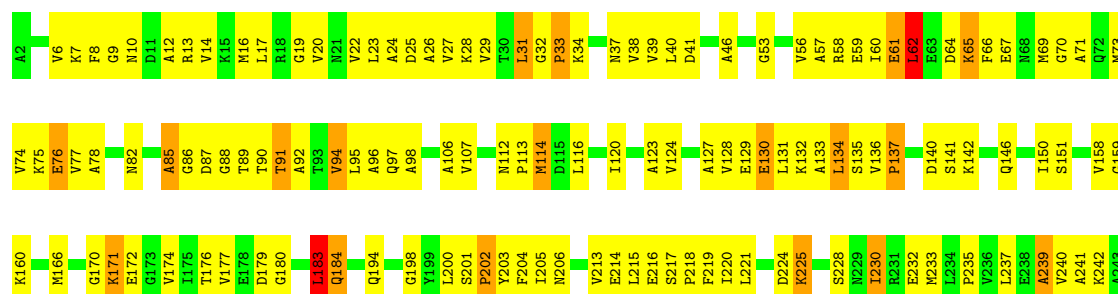
Chain H: 40% 48% 8% . .

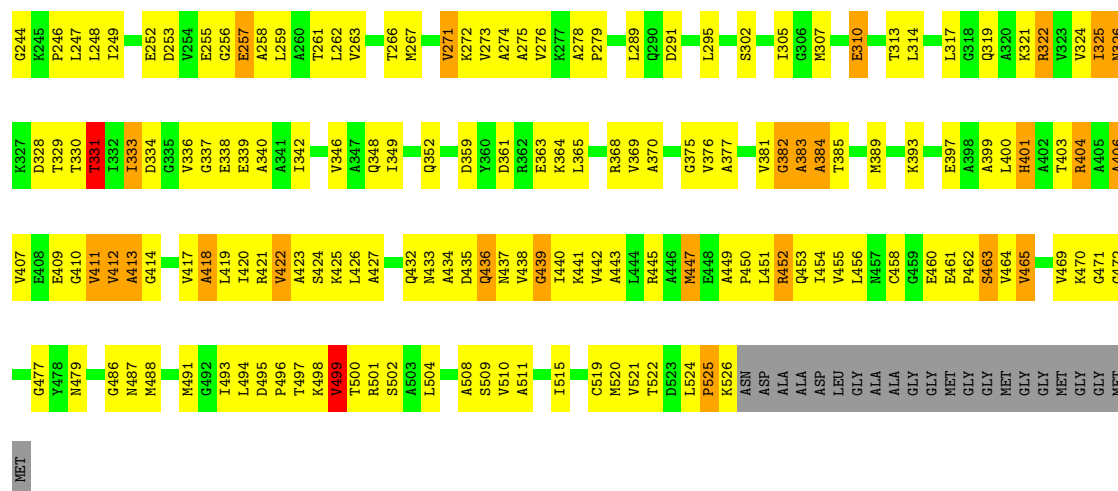


• Molecule 1: GROEL PROTEIN

Chain I: 42% 46% 7% . .

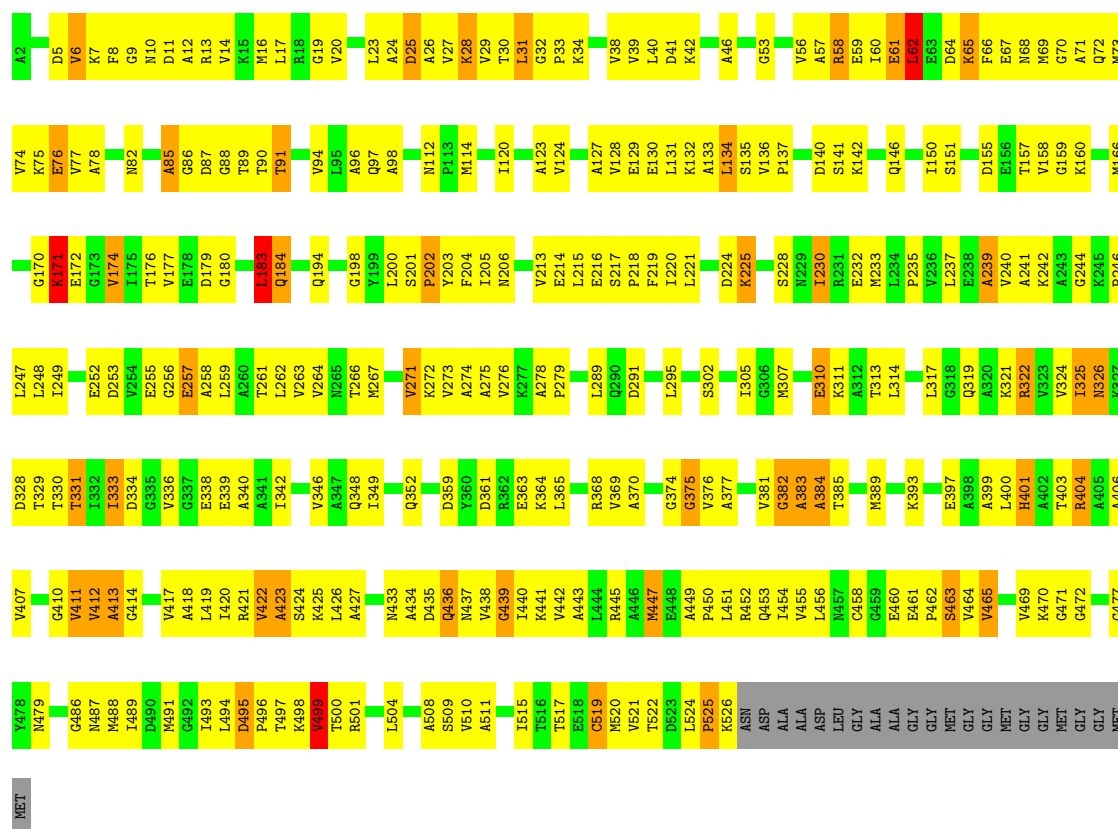






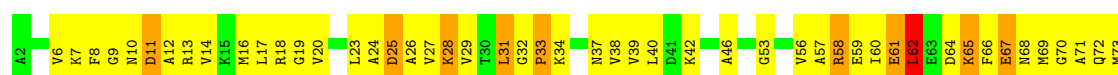
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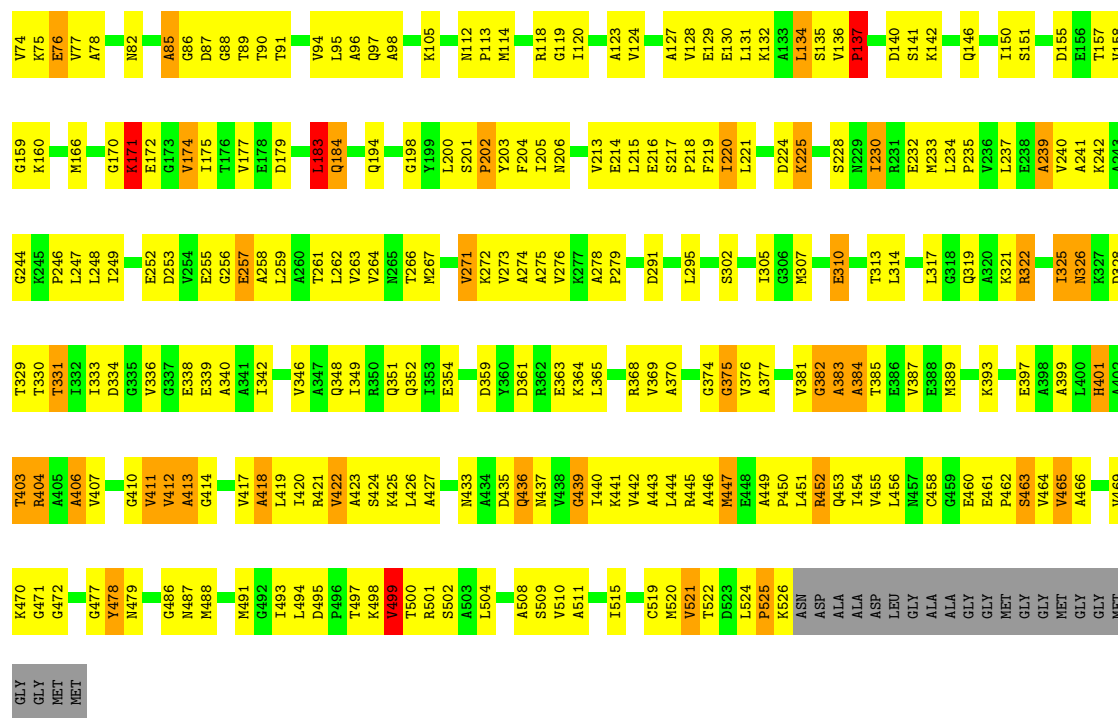
Chain L: 41% 46% 8% . .



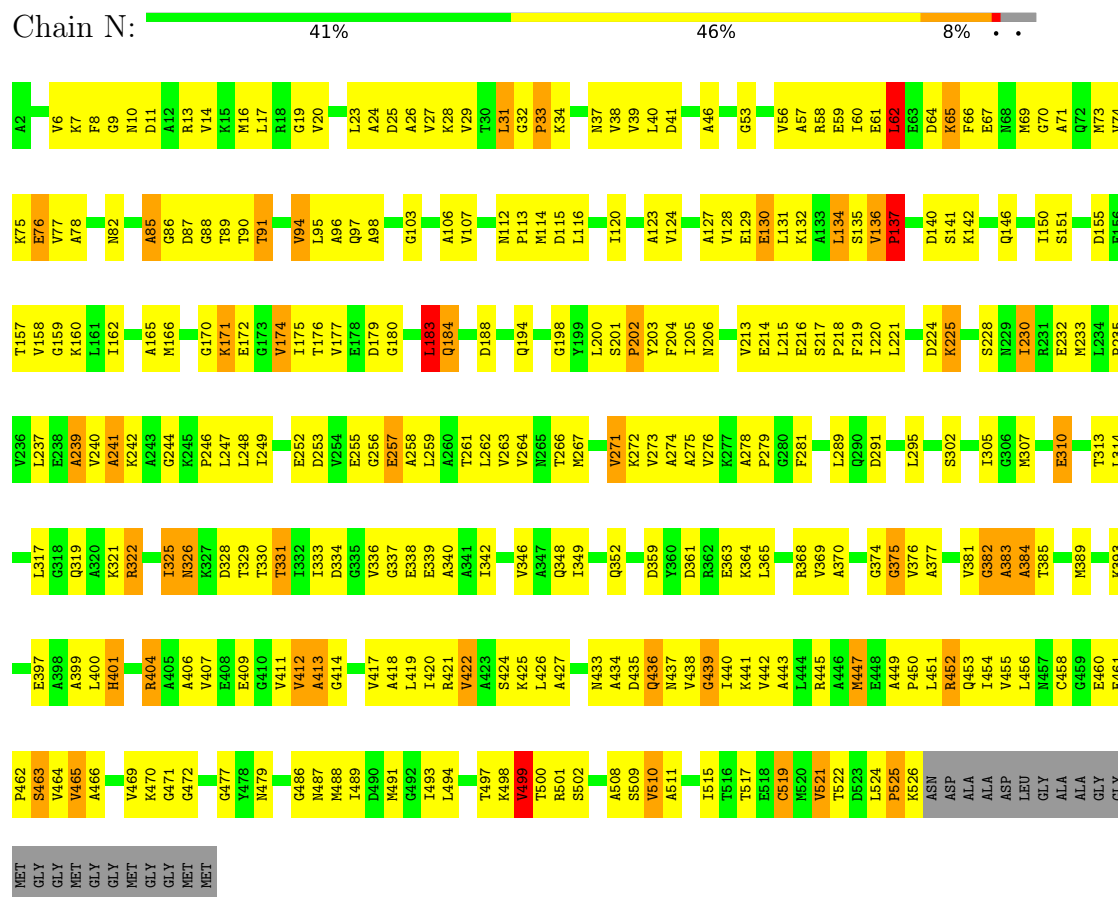
• Molecule 1: GROEL PROTEIN

Chain M: 41% 45% 9% . .

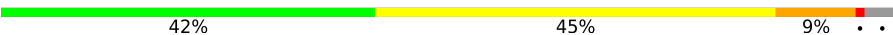


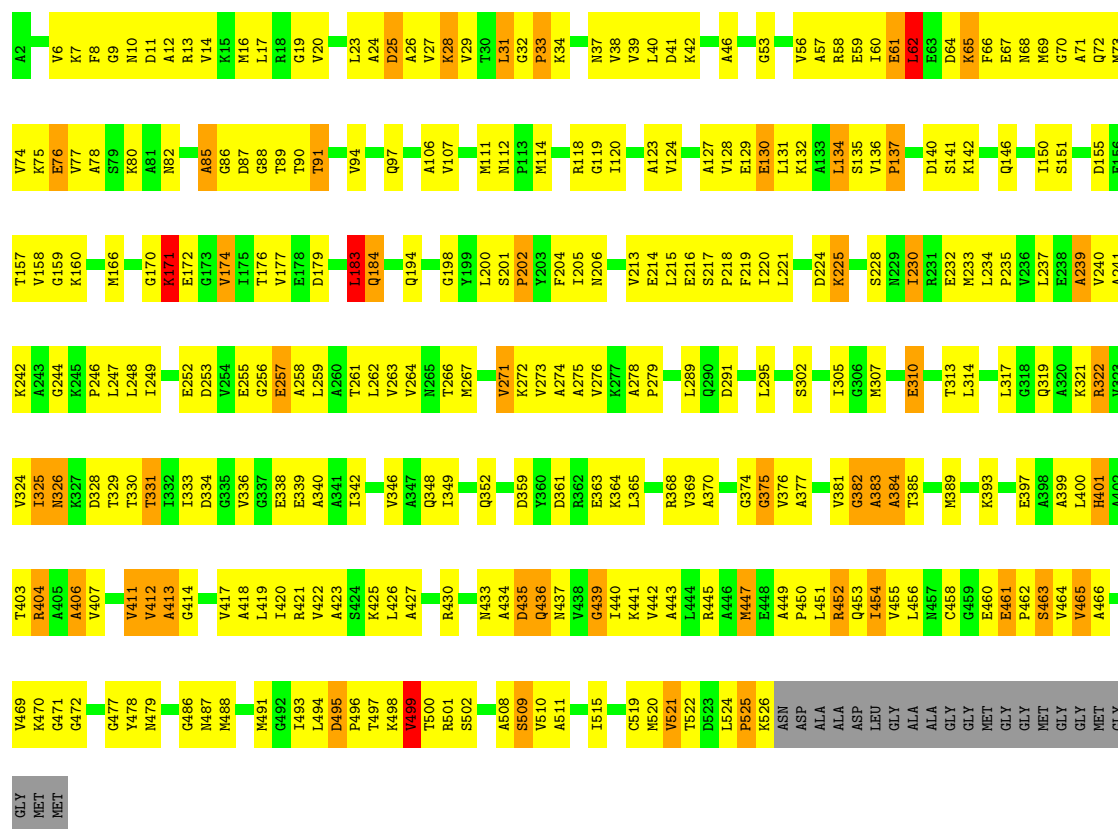


• Molecule 1: GROEL PROTEIN

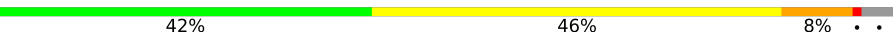


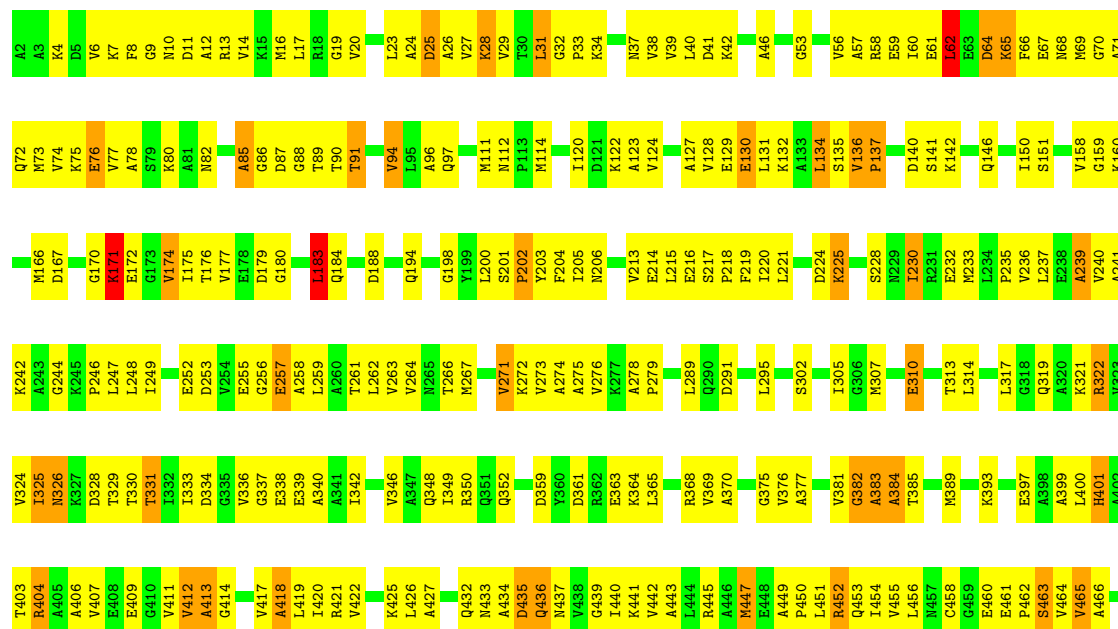
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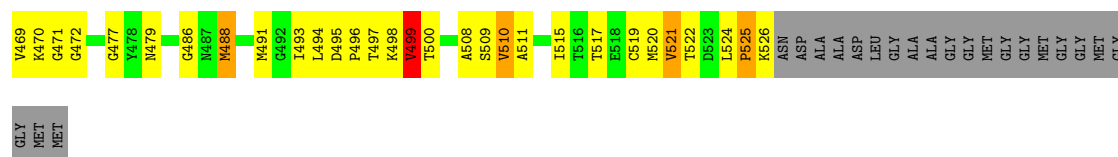
Chain O:  42% 45% 9% . .



• Molecule 1: GROEL PROTEIN

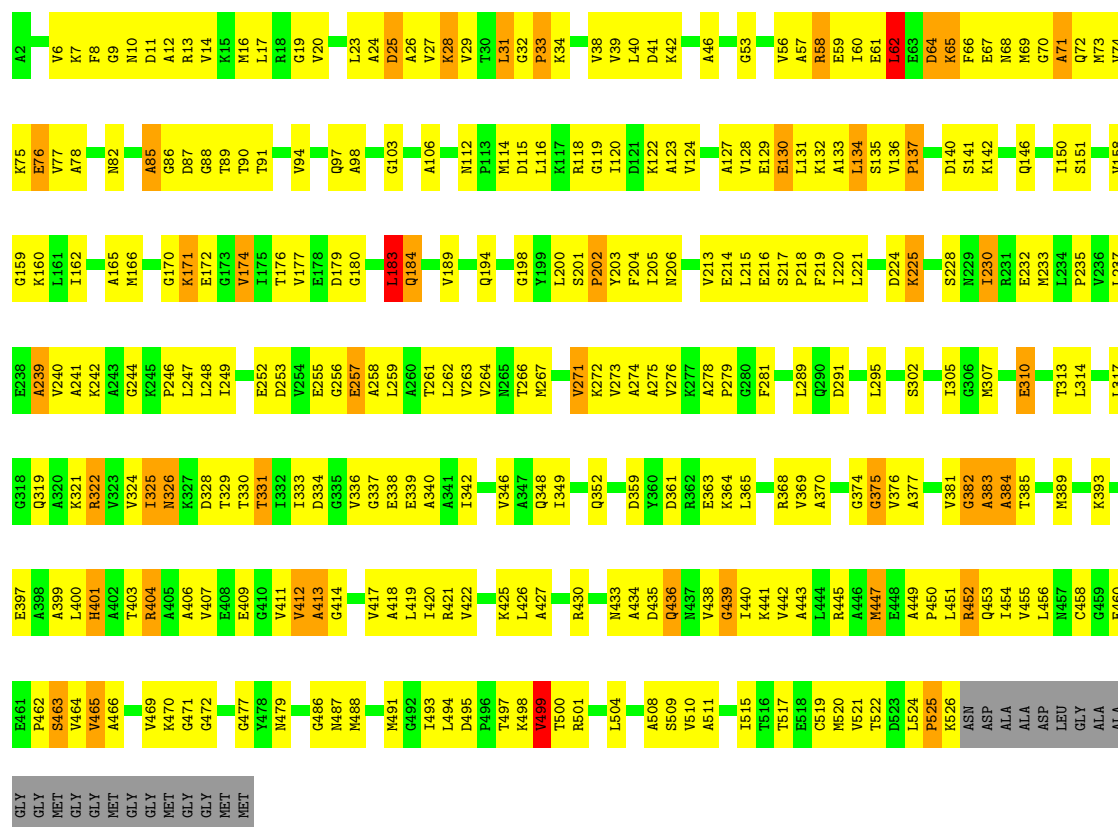
Chain P:  42% 46% 8% . .





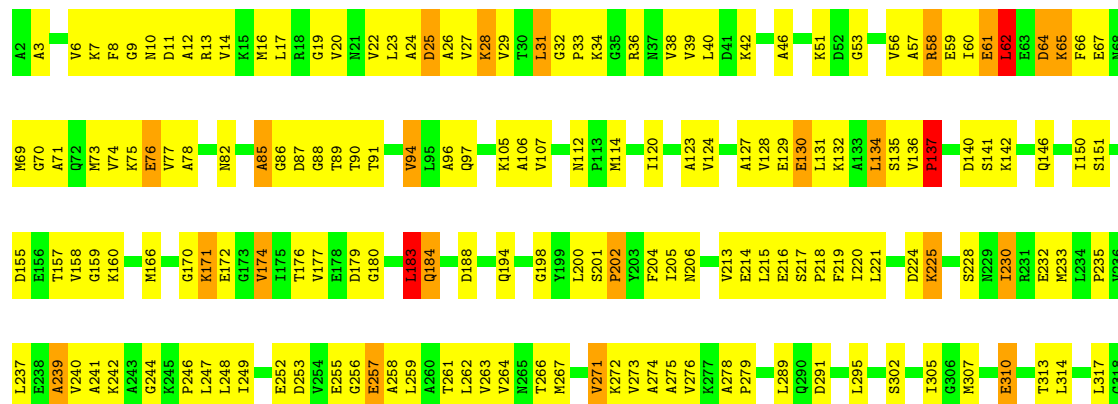
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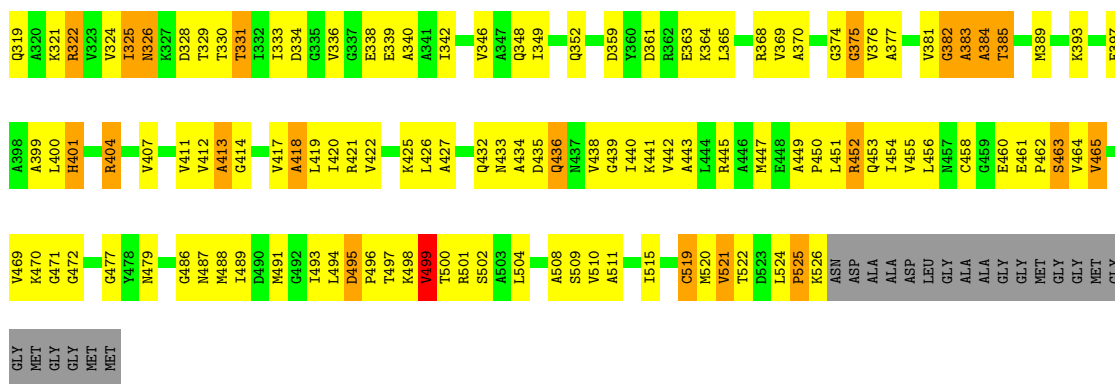
Chain Q: 41% 47% 8% . .



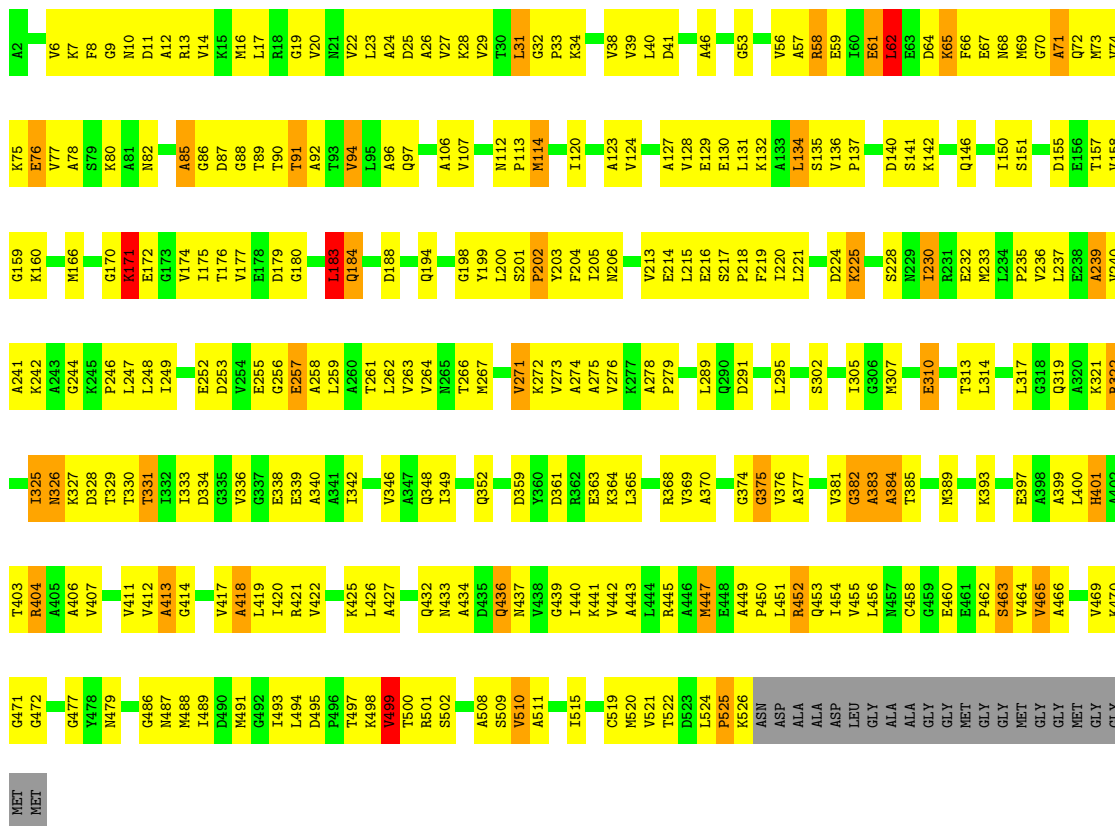
• Molecule 1: GROEL PROTEIN

Chain R: 43% 45% 8% . .

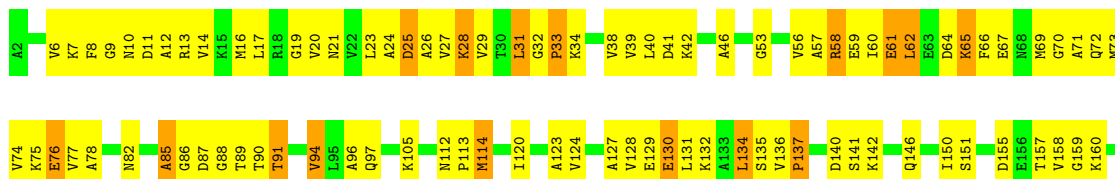


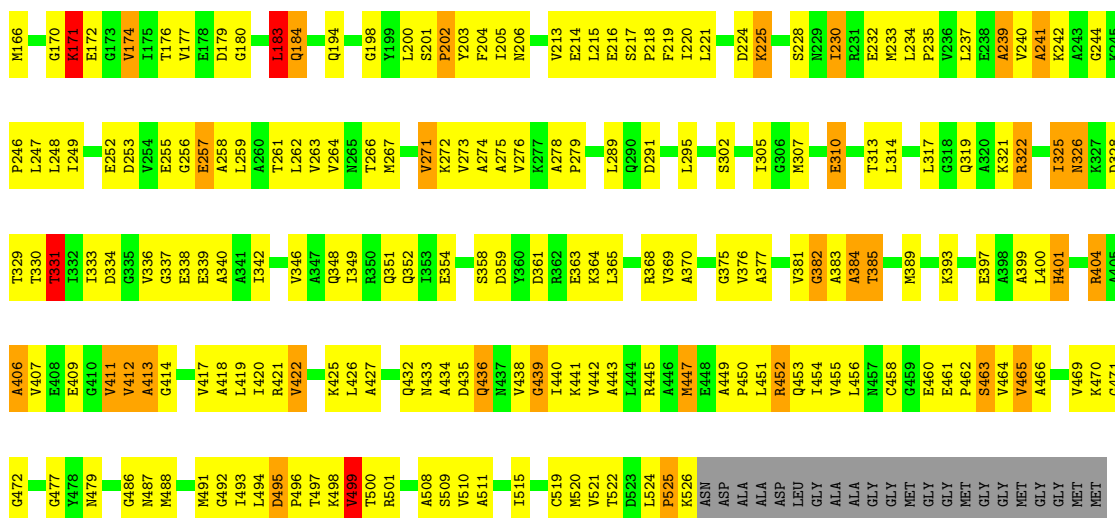


- Molecule 1: GROEL PROTEIN



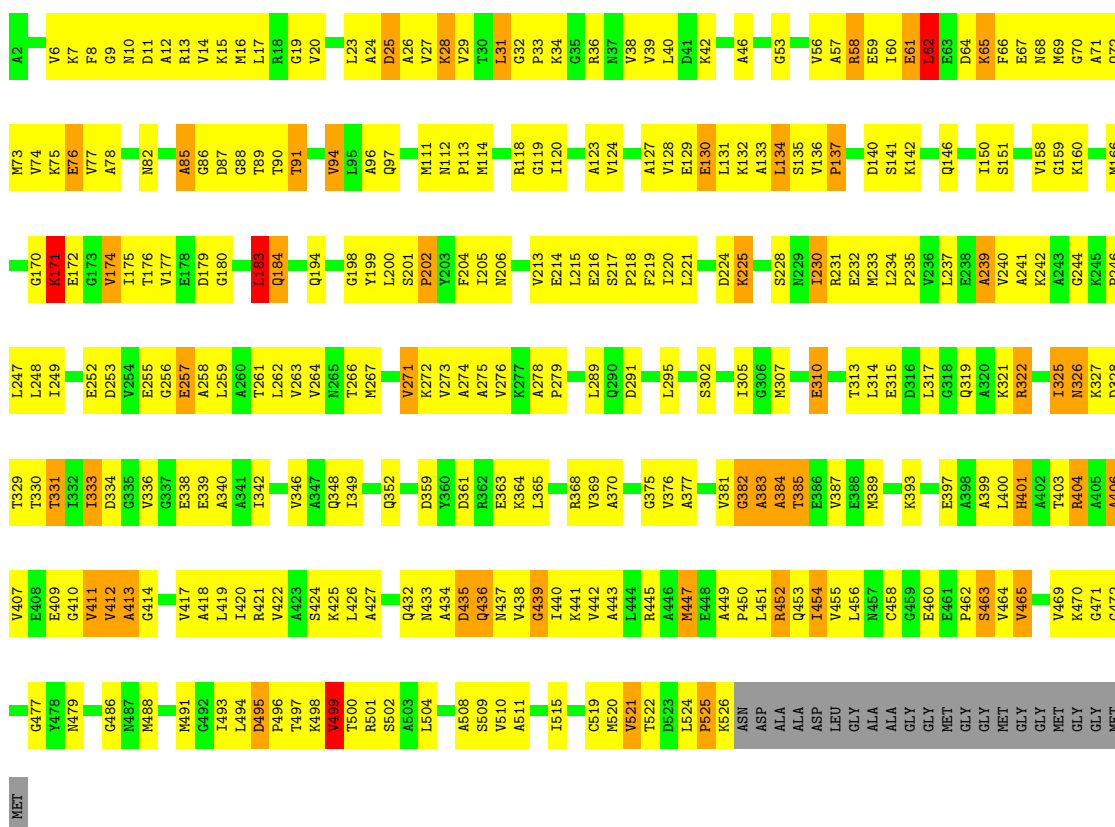
- Molecule 1: GROEL PROTEIN





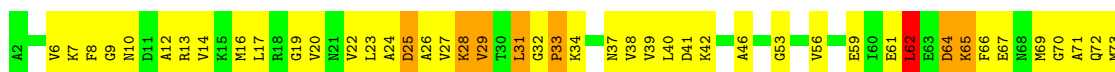
• Molecule 1: GROEL PROTEIN

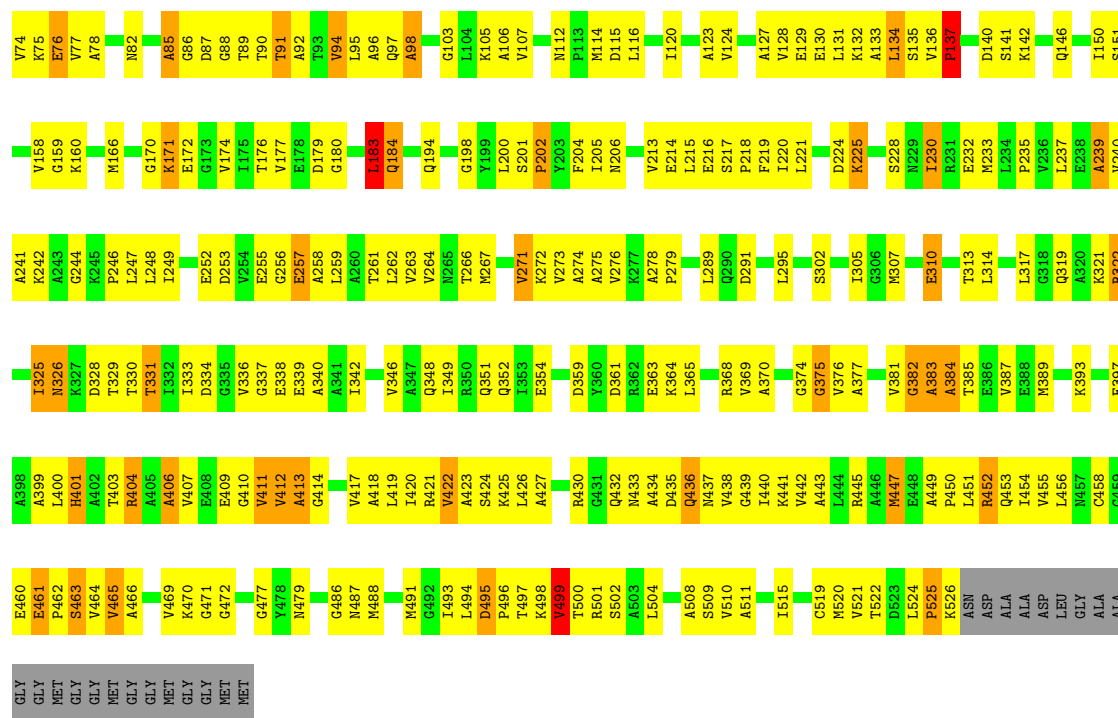
Chain U: 41% 45% 9% . .



• Molecule 1: GROEL PROTEIN

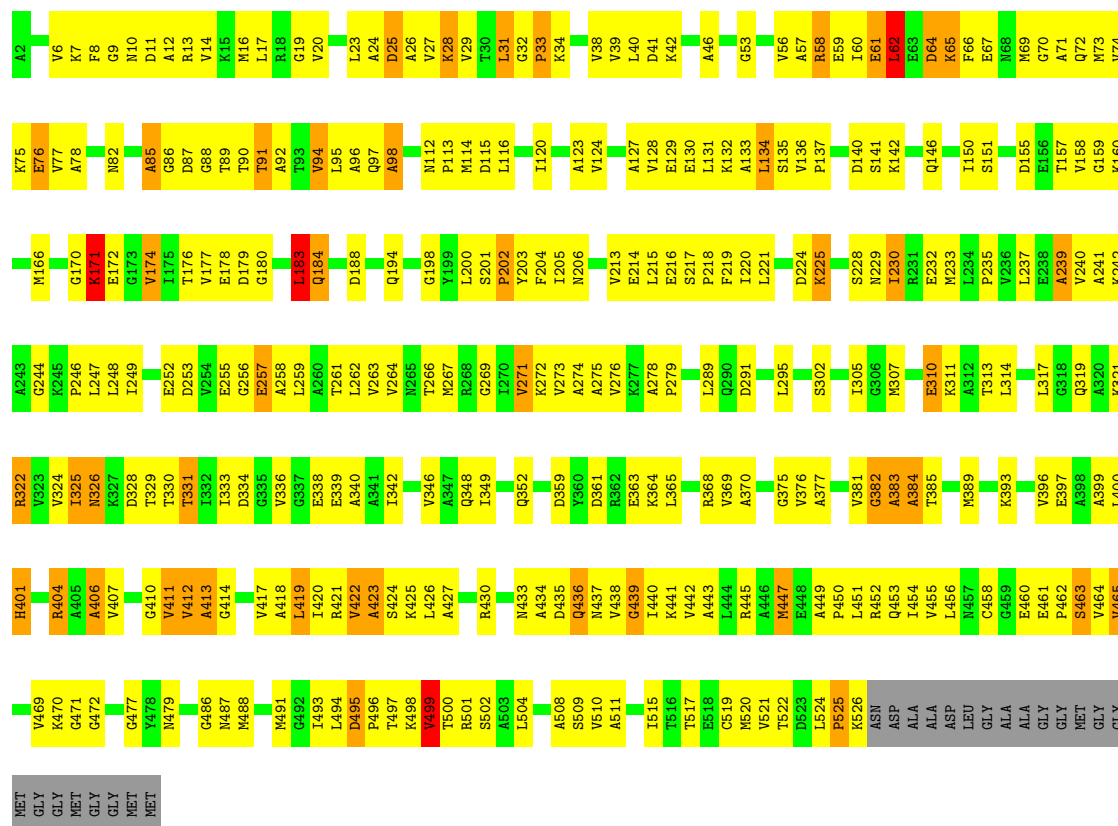
Chain V: 41% 46% 8% . .



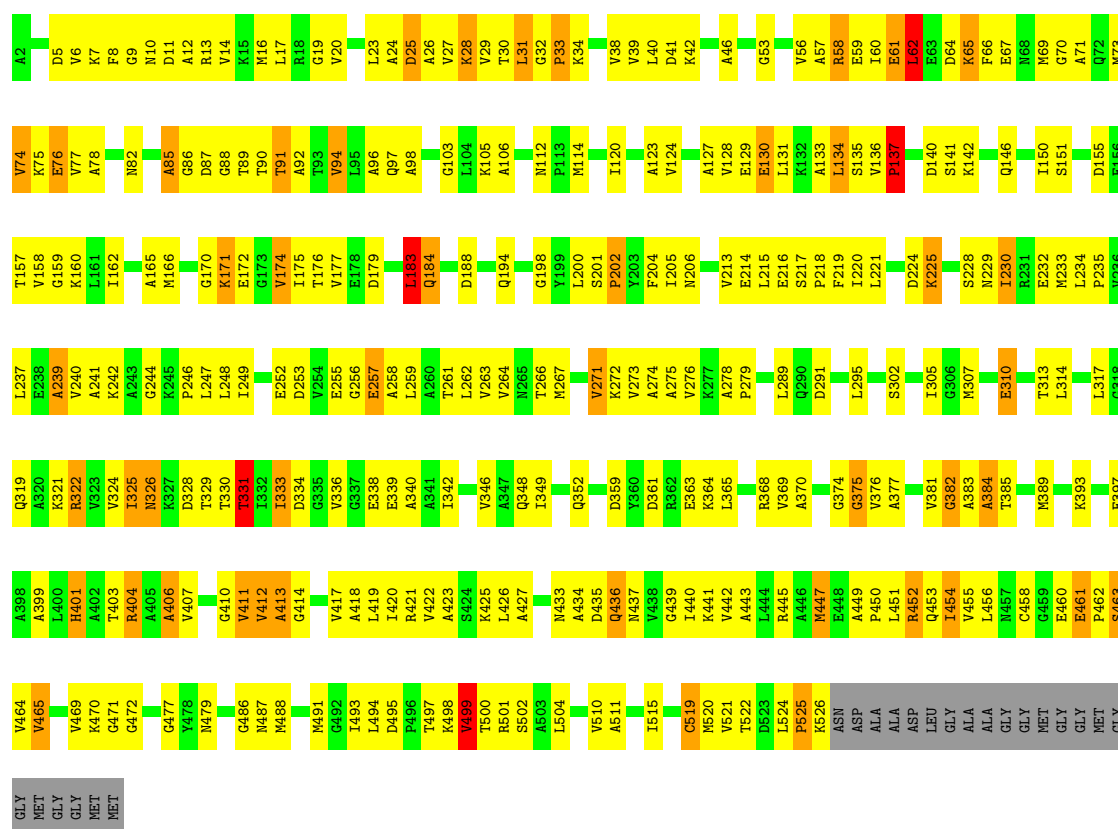
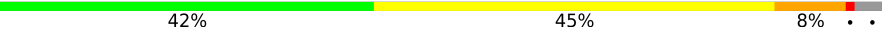


Molecule 1: GROEL PROTEIN

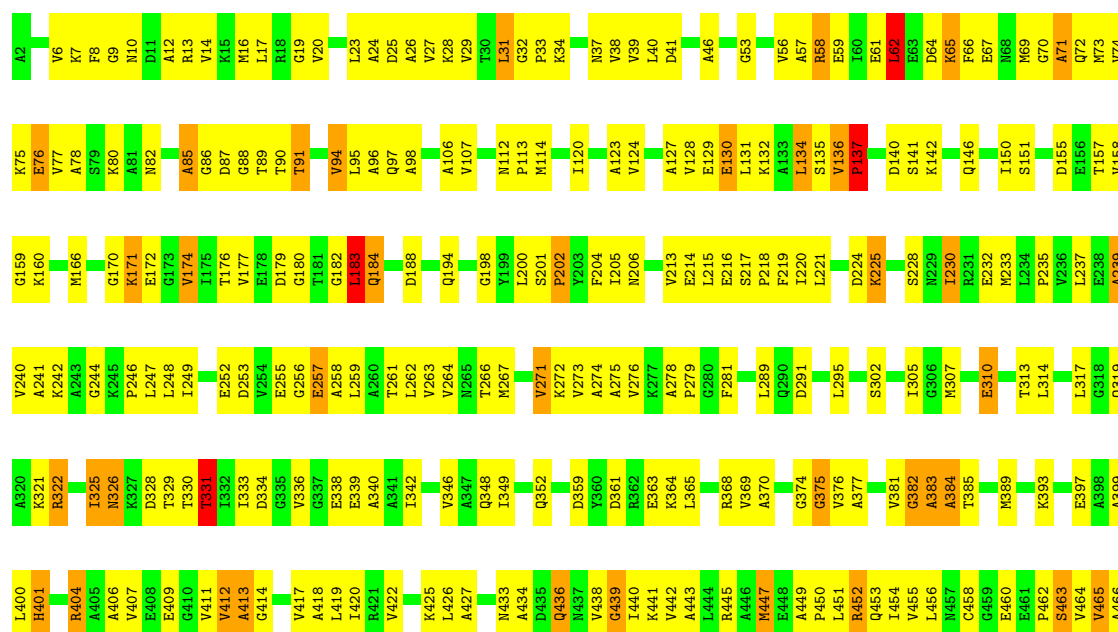
Chain W: 40% 46% 8% . .

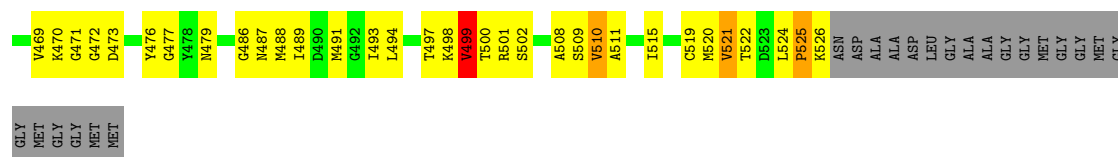


Molecule 1: GROEL PROTEIN

Chain X: 

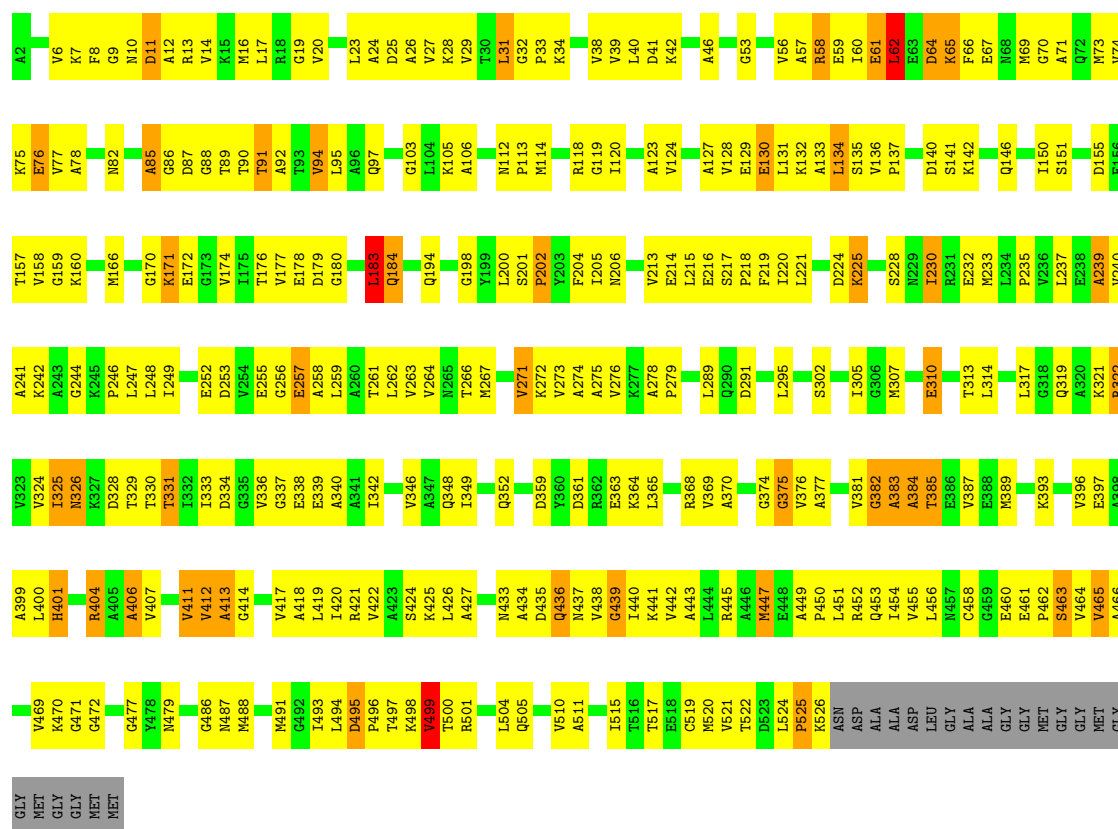
• Molecule 1: GROEL PROTEIN

Chain Y: 



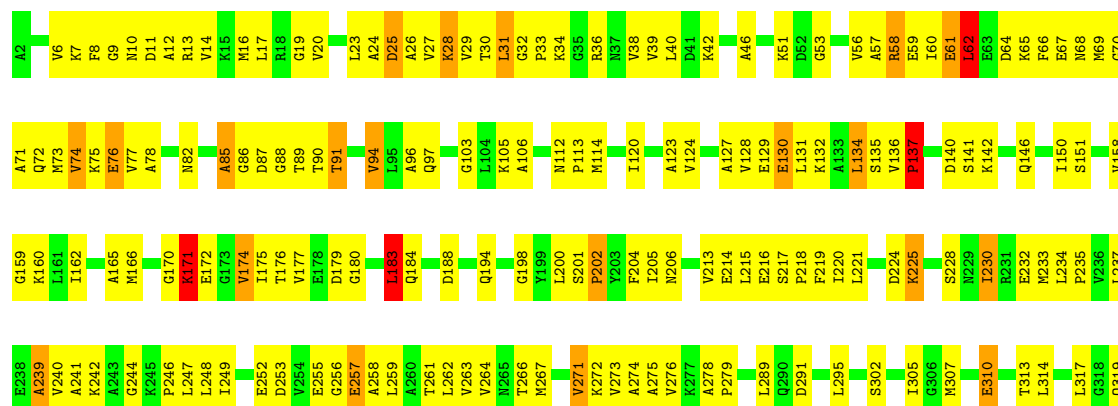
• Molecule 1: GROEL PROTEIN

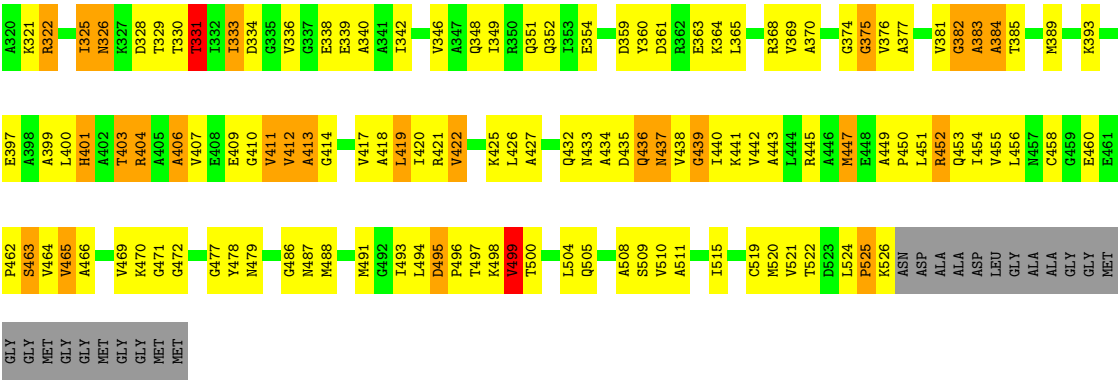
Chain Z: 41% 46% 8% . .



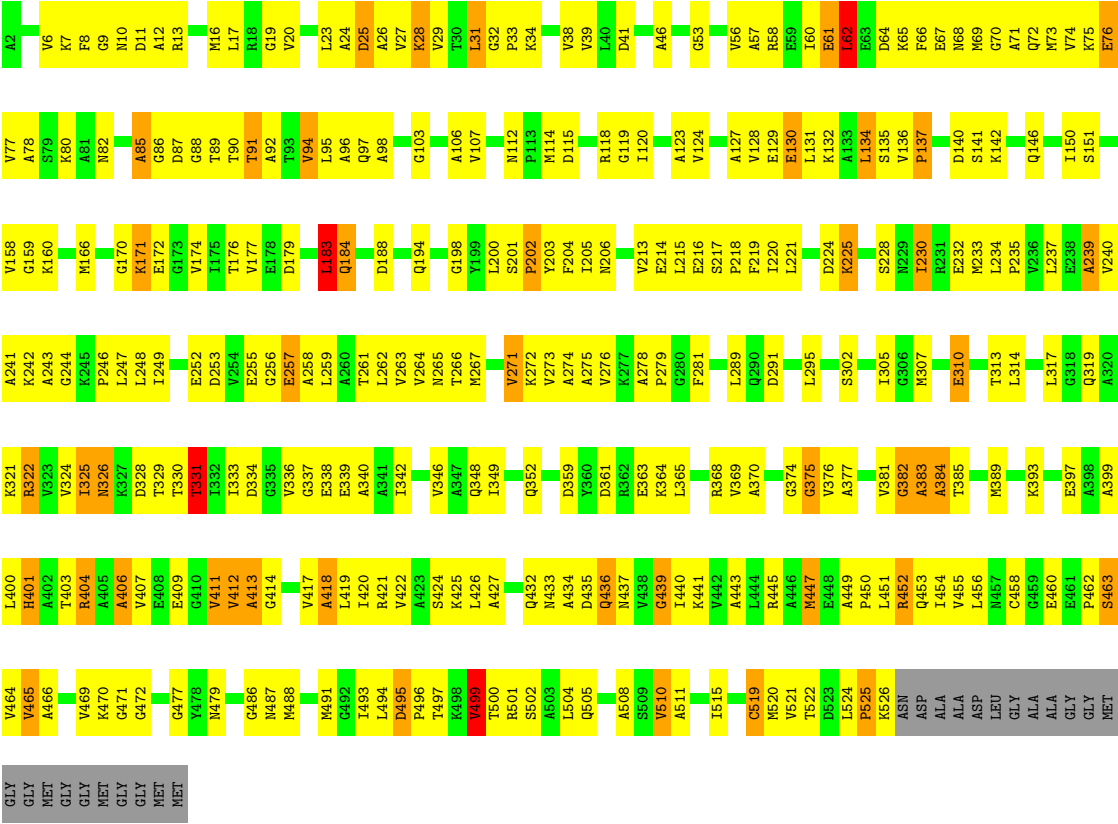
• Molecule 1: GROEL PROTEIN

Chain 1: 41% 46% 8% . .





● Molecule 1: GROEL PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.67Å 264.24Å 294.80Å 90.00° 92.39° 90.00°	Depositor
Resolution (Å)	20.00 – 3.52 20.00 – 3.52	Depositor EDS
% Data completeness (in resolution range)	76.5 (20.00-3.52) 76.7 (20.00-3.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.56Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.291 , 0.298 0.280 , 0.285	Depositor DCC
R_{free} test set	9897 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	107996	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.66	0/3885	1.03	18/5245 (0.3%)
1	2	0.62	0/3885	1.01	17/5245 (0.3%)
1	A	0.60	0/3885	1.00	19/5245 (0.4%)
1	B	0.60	0/3885	1.00	16/5245 (0.3%)
1	C	0.62	1/3885 (0.0%)	1.01	19/5245 (0.4%)
1	D	0.60	0/3885	1.00	19/5245 (0.4%)
1	E	0.61	0/3885	1.00	14/5245 (0.3%)
1	F	0.61	0/3885	1.01	22/5245 (0.4%)
1	G	0.60	0/3885	1.00	16/5245 (0.3%)
1	H	0.60	0/3885	1.01	20/5245 (0.4%)
1	I	0.65	0/3885	1.03	18/5245 (0.3%)
1	J	0.61	0/3885	1.00	19/5245 (0.4%)
1	K	0.64	1/3885 (0.0%)	1.02	17/5245 (0.3%)
1	L	0.62	0/3885	1.01	19/5245 (0.4%)
1	M	0.68	0/3885	1.02	18/5245 (0.3%)
1	N	0.66	0/3885	1.02	20/5245 (0.4%)
1	O	0.61	0/3885	1.01	18/5245 (0.3%)
1	P	0.61	1/3885 (0.0%)	1.01	21/5245 (0.4%)
1	Q	0.61	0/3885	1.00	17/5245 (0.3%)
1	R	0.59	0/3885	1.00	15/5245 (0.3%)
1	S	0.60	1/3885 (0.0%)	0.99	13/5245 (0.2%)
1	T	0.60	1/3885 (0.0%)	1.00	17/5245 (0.3%)
1	U	0.60	0/3885	1.00	18/5245 (0.3%)
1	V	0.63	0/3885	1.02	20/5245 (0.4%)
1	W	0.61	0/3885	1.02	18/5245 (0.3%)
1	X	0.68	0/3885	1.02	20/5245 (0.4%)
1	Y	0.64	0/3885	1.01	16/5245 (0.3%)
1	Z	0.60	0/3885	1.00	19/5245 (0.4%)
All	All	0.62	5/108780 (0.0%)	1.01	503/146860 (0.3%)

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	Y	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	114	MET	SD-CE	5.71	1.93	1.79
1	P	488	MET	SD-CE	-5.51	1.65	1.79
1	S	114	MET	SD-CE	5.38	1.93	1.79
1	C	114	MET	SD-CE	5.32	1.92	1.79
1	T	114	MET	SD-CE	5.14	1.92	1.79

The worst 5 of 503 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	436	GLN	N-CA-C	-7.77	104.41	114.04
1	V	241	ALA	N-CA-C	-7.71	102.51	112.23
1	Q	241	ALA	N-CA-C	-7.61	102.64	112.23
1	K	241	ALA	N-CA-C	-7.59	102.67	112.23
1	R	241	ALA	N-CA-C	-7.57	102.70	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	476	TYR	Sidechain

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	1	3857	0	3989	293	0
1	2	3857	0	3989	289	0
1	A	3857	0	3989	293	0
1	B	3857	0	3989	284	0
1	C	3857	0	3989	282	1
1	D	3857	0	3989	292	2
1	E	3857	0	3989	271	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3857	0	3989	274	1
1	G	3857	0	3989	291	0
1	H	3857	0	3989	292	0
1	I	3857	0	3989	277	0
1	J	3857	0	3989	277	0
1	K	3857	0	3989	290	0
1	L	3857	0	3989	290	0
1	M	3857	0	3989	292	0
1	N	3857	0	3989	297	0
1	O	3857	0	3989	286	0
1	P	3857	0	3989	285	2
1	Q	3857	0	3989	286	0
1	R	3857	0	3989	277	0
1	S	3857	0	3989	277	0
1	T	3857	0	3989	284	2
1	U	3857	0	3989	292	0
1	V	3857	0	3989	292	0
1	W	3857	0	3989	296	2
1	X	3857	0	3989	287	0
1	Y	3857	0	3989	290	0
1	Z	3857	0	3989	288	0
All	All	107996	0	111692	7814	5

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 36.

The worst 5 of 7814 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:E:230:ILE:HD12	1:E:261:THR:HG21	1.32	1.10
1:W:230:ILE:HD12	1:W:261:THR:HG21	1.33	1.10
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.33	1.10
1:P:230:ILE:HD12	1:P:261:THR:HG21	1.33	1.10
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.32	1.10

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:THR:N	1:W:311:LYS:NZ[1_556]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLU:OE1	1:F:350:ARG:NH1[1_455]	2.10	0.10
1:P:167:ASP:OD2	1:T:358:SER:OG[1_455]	2.15	0.05
1:P:350:ARG:NH1	1:T:354:GLU:OE1[1_455]	2.17	0.03
1:D:316:ASP:OD2	1:W:311:LYS:CE[1_556]	2.18	0.02

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	1	523/547 (96%)	393 (75%)	93 (18%)	37 (7%)	1	10
1	2	523/547 (96%)	397 (76%)	90 (17%)	36 (7%)	1	10
1	A	523/547 (96%)	397 (76%)	87 (17%)	39 (8%)	1	9
1	B	523/547 (96%)	398 (76%)	91 (17%)	34 (6%)	1	11
1	C	523/547 (96%)	400 (76%)	87 (17%)	36 (7%)	1	10
1	D	523/547 (96%)	394 (75%)	88 (17%)	41 (8%)	1	8
1	E	523/547 (96%)	393 (75%)	94 (18%)	36 (7%)	1	10
1	F	523/547 (96%)	397 (76%)	91 (17%)	35 (7%)	1	11
1	G	523/547 (96%)	399 (76%)	88 (17%)	36 (7%)	1	10
1	H	523/547 (96%)	393 (75%)	90 (17%)	40 (8%)	1	8
1	I	523/547 (96%)	391 (75%)	95 (18%)	37 (7%)	1	10
1	J	523/547 (96%)	398 (76%)	88 (17%)	37 (7%)	1	10
1	K	523/547 (96%)	396 (76%)	89 (17%)	38 (7%)	1	9
1	L	523/547 (96%)	399 (76%)	84 (16%)	40 (8%)	1	8
1	M	523/547 (96%)	397 (76%)	87 (17%)	39 (8%)	1	9
1	N	523/547 (96%)	399 (76%)	88 (17%)	36 (7%)	1	10
1	O	523/547 (96%)	394 (75%)	92 (18%)	37 (7%)	1	10
1	P	523/547 (96%)	392 (75%)	94 (18%)	37 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	523/547 (96%)	395 (76%)	91 (17%)	37 (7%)	1	10
1	R	523/547 (96%)	395 (76%)	88 (17%)	40 (8%)	1	8
1	S	523/547 (96%)	400 (76%)	84 (16%)	39 (8%)	1	9
1	T	523/547 (96%)	401 (77%)	84 (16%)	38 (7%)	1	9
1	U	523/547 (96%)	394 (75%)	91 (17%)	38 (7%)	1	9
1	V	523/547 (96%)	392 (75%)	94 (18%)	37 (7%)	1	10
1	W	523/547 (96%)	396 (76%)	87 (17%)	40 (8%)	1	8
1	X	523/547 (96%)	400 (76%)	87 (17%)	36 (7%)	1	10
1	Y	523/547 (96%)	400 (76%)	87 (17%)	36 (7%)	1	10
1	Z	523/547 (96%)	391 (75%)	94 (18%)	38 (7%)	1	9
All	All	14644/15316 (96%)	11091 (76%)	2503 (17%)	1050 (7%)	1	9

5 of 1050 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PRO
1	A	202	PRO
1	A	256	GLY
1	A	334	ASP
1	A	384	ALA

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 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	1	403/412 (98%)	374 (93%)	29 (7%)	13	39
1	2	403/412 (98%)	378 (94%)	25 (6%)	16	44
1	A	403/412 (98%)	377 (94%)	26 (6%)	15	42
1	B	403/412 (98%)	378 (94%)	25 (6%)	16	44
1	C	403/412 (98%)	378 (94%)	25 (6%)	16	44
1	D	403/412 (98%)	378 (94%)	25 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	403/412 (98%)	377 (94%)	26 (6%)	15	42
1	F	403/412 (98%)	379 (94%)	24 (6%)	17	44
1	G	403/412 (98%)	377 (94%)	26 (6%)	15	42
1	H	403/412 (98%)	380 (94%)	23 (6%)	18	46
1	I	403/412 (98%)	374 (93%)	29 (7%)	13	39
1	J	403/412 (98%)	379 (94%)	24 (6%)	17	44
1	K	403/412 (98%)	377 (94%)	26 (6%)	15	42
1	L	403/412 (98%)	380 (94%)	23 (6%)	18	46
1	M	403/412 (98%)	375 (93%)	28 (7%)	14	40
1	N	403/412 (98%)	377 (94%)	26 (6%)	15	42
1	O	403/412 (98%)	379 (94%)	24 (6%)	17	44
1	P	403/412 (98%)	378 (94%)	25 (6%)	16	44
1	Q	403/412 (98%)	380 (94%)	23 (6%)	18	46
1	R	403/412 (98%)	378 (94%)	25 (6%)	16	44
1	S	403/412 (98%)	378 (94%)	25 (6%)	16	44
1	T	403/412 (98%)	376 (93%)	27 (7%)	15	41
1	U	403/412 (98%)	378 (94%)	25 (6%)	16	44
1	V	403/412 (98%)	376 (93%)	27 (7%)	15	41
1	W	403/412 (98%)	377 (94%)	26 (6%)	15	42
1	X	403/412 (98%)	374 (93%)	29 (7%)	13	39
1	Y	403/412 (98%)	377 (94%)	26 (6%)	15	42
1	Z	403/412 (98%)	378 (94%)	25 (6%)	16	44
All	All	11284/11536 (98%)	10567 (94%)	717 (6%)	16	43

5 of 717 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	183	LEU
1	W	401	HIS
1	S	495	ASP
1	S	174	VAL
1	U	403	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 377 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	97	GLN
1	V	146	GLN
1	R	351	GLN
1	T	206	ASN
1	W	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1	525/547 (95%)	-1.59	0 100 100	14, 53, 105, 117	0
1	2	525/547 (95%)	-1.54	0 100 100	17, 68, 135, 147	0
1	A	525/547 (95%)	-1.50	0 100 100	17, 76, 156, 168	0
1	B	525/547 (95%)	-1.51	0 100 100	21, 69, 146, 158	0
1	C	525/547 (95%)	-1.54	0 100 100	17, 67, 130, 142	0
1	D	525/547 (95%)	-1.53	0 100 100	21, 80, 143, 155	0
1	E	525/547 (95%)	-1.46	0 100 100	20, 79, 169, 181	0
1	F	525/547 (95%)	-1.51	0 100 100	18, 71, 148, 160	0
1	G	525/547 (95%)	-1.48	0 100 100	17, 77, 168, 180	0
1	H	525/547 (95%)	-1.53	0 100 100	15, 71, 157, 169	0
1	I	525/547 (95%)	-1.61	0 100 100	13, 52, 107, 119	0
1	J	525/547 (95%)	-1.51	0 100 100	15, 72, 143, 155	0
1	K	525/547 (95%)	-1.53	0 100 100	12, 58, 146, 158	0
1	L	525/547 (95%)	-1.51	0 100 100	16, 74, 160, 171	0
1	M	525/547 (95%)	-1.58	0 100 100	12, 50, 109, 121	0
1	N	525/547 (95%)	-1.54	0 100 100	14, 58, 133, 145	0
1	O	525/547 (95%)	-1.49	0 100 100	20, 80, 164, 176	0
1	P	525/547 (95%)	-1.52	0 100 100	19, 68, 149, 161	0
1	Q	525/547 (95%)	-1.48	0 100 100	16, 82, 162, 174	0
1	R	525/547 (95%)	-1.45	0 100 100	20, 73, 174, 186	0
1	S	525/547 (95%)	-1.52	0 100 100	21, 75, 155, 167	0
1	T	525/547 (95%)	-1.55	0 100 100	18, 71, 141, 153	0
1	U	525/547 (95%)	-1.49	0 100 100	21, 78, 159, 171	0
1	V	525/547 (95%)	-1.53	0 100 100	15, 68, 148, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
1	W	525/547 (95%)	-1.51	0	100100	16, 73, 153, 165	0
1	X	525/547 (95%)	-1.59	0	100100	11, 50, 112, 124	0
1	Y	525/547 (95%)	-1.55	0	100100	11, 60, 142, 154	0
1	Z	525/547 (95%)	-1.50	0	100100	18, 67, 161, 173	0
All	All	14700/15316 (95%)	-1.52	0	100100	11, 67, 155, 186	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.