Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 01:32 PM EDT

PDB ID	:	4V4K
Title	:	Bacteriophage P22 Portal Protein bound to middle Tail Factor GP4. This file contain the second biological assembly
Authors	:	Olia, A.S.; Cingolani, G.
Deposited on	:	2010-04-19
Resolution	:	3.25 Å(reported)

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

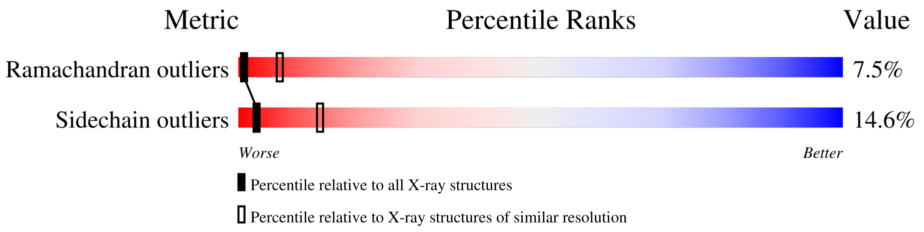
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.25 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))
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)

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%

Mol	Chain	Length	Quality of chain
1	A	602	 76% 18% • 5%
1	B	602	 76% 18% • 5%
1	C	602	 76% 18% • 5%
1	D	602	 76% 18% • 5%
1	E	602	 76% 18% • 5%
1	F	602	 76% 18% • 5%
1	G	602	 76% 18% • 5%
1	H	602	 76% 18% • 5%
1	I	602	 76% 18% • 5%
1	J	602	 76% 18% • 5%

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Mol	Chain	Length	Quality of chain
1	K	602	 76% 18% • 5%
1	L	602	 76% 18% • 5%
1	M	602	 77% 17% • 5%
1	N	602	 76% 18% • 5%
1	O	602	 77% 17% • 5%
1	P	602	 77% 17% • 5%
1	Q	602	 76% 17% • 5%
1	R	602	 76% 17% • 5%
1	S	602	 76% 18% • 5%
1	T	602	 77% 17% • 5%
1	U	602	 77% 17% • 5%
1	V	602	 77% 17% • 5%
1	W	602	 76% 17% • 5%
1	X	602	 76% 17% • 5%
2	Y	166	 73% 12% • • 12%
2	Z	166	 73% 12% • • 12%
2	a	166	 73% 13% • • 12%
2	b	166	 73% 13% • • 12%
2	c	166	 72% 13% • • 12%
2	d	166	 73% 12% • • 12%
2	e	166	 73% 12% • • 12%
2	f	166	 73% 13% • • 12%
2	g	166	 72% 13% • • 12%
2	h	166	 73% 12% • • 12%
2	i	166	 73% 12% • • 12%

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Mol	Chain	Length	Quality of chain
2	j	166	 73% 13% •• 12%
2	k	166	 75% 11% • 13%
2	l	166	 74% 12% • 13%
2	m	166	 75% 11% • 13%
2	n	166	 74% 12% • 13%
2	o	166	 73% 13% • 13%
2	p	166	 73% 13% • 13%
2	q	166	 75% 11% • 13%
2	r	166	 74% 12% • 13%
2	s	166	 74% 12% • 13%
2	t	166	 74% 12% • 13%
2	u	166	 74% 12% • 13%
2	v	166	 74% 12% • 13%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 135120 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 PORTAL PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	M	569	4564	2871	786	887	4	16	0	0	0
1	N	569	4564	2871	786	887	4	16	0	0	0
1	O	569	4564	2871	786	887	4	16	0	0	0
1	P	569	4564	2871	786	887	4	16	0	0	0
1	Q	569	4564	2871	786	887	4	16	0	0	0
1	R	569	4564	2871	786	887	4	16	0	0	0
1	S	569	4564	2871	786	887	4	16	0	0	0
1	T	569	4564	2871	786	887	4	16	0	0	0
1	U	569	4564	2871	786	887	4	16	0	0	0
1	V	569	4564	2871	786	887	4	16	0	0	0
1	W	569	4564	2871	786	887	4	16	0	0	0
1	X	569	4564	2871	786	887	4	16	0	0	0
1	A	569	4553	2865	783	885	4	16	0	0	0
1	B	569	4553	2865	783	885	4	16	0	0	0
1	C	569	4553	2865	783	885	4	16	0	0	0
1	D	569	4553	2865	783	885	4	16	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	E	569	Total C N O S Se 4553 2865 783 885 4 16	0	0	0
1	F	569	Total C N O S Se 4553 2865 783 885 4 16	0	0	0
1	G	569	Total C N O S Se 4553 2865 783 885 4 16	0	0	0
1	H	569	Total C N O S Se 4553 2865 783 885 4 16	0	0	0
1	I	569	Total C N O S Se 4553 2865 783 885 4 16	0	0	0
1	J	569	Total C N O S Se 4553 2865 783 885 4 16	0	0	0
1	K	569	Total C N O S Se 4553 2865 783 885 4 16	0	0	0
1	L	569	Total C N O S Se 4553 2865 783 885 4 16	0	0	0

- Molecule 2 is a protein called PACKAGED DNA STABILIZATION PROTEIN GP4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	k	145	Total C N O S 1052 654 182 211 5	0	0	0
2	l	145	Total C N O S 1052 654 182 211 5	0	0	0
2	m	145	Total C N O S 1052 654 182 211 5	0	0	0
2	n	145	Total C N O S 1052 654 182 211 5	0	0	0
2	o	145	Total C N O S 1052 654 182 211 5	0	0	0
2	p	145	Total C N O S 1052 654 182 211 5	0	0	0
2	q	145	Total C N O S 1052 654 182 211 5	0	0	0
2	r	145	Total C N O S 1052 654 182 211 5	0	0	0
2	s	145	Total C N O S 1052 654 182 211 5	0	0	0
2	t	145	Total C N O S 1052 654 182 211 5	0	0	0
2	u	145	Total C N O S 1052 654 182 211 5	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	v	145	Total C N O S 1052 654 182 211 5	0	0	0
2	Y	146	Total C N O S 1048 652 179 212 5	0	0	0
2	Z	146	Total C N O S 1048 652 179 212 5	0	0	0
2	a	146	Total C N O S 1048 652 179 212 5	0	0	0
2	b	146	Total C N O S 1048 652 179 212 5	0	0	0
2	c	146	Total C N O S 1048 652 179 212 5	0	0	0
2	d	146	Total C N O S 1048 652 179 212 5	0	0	0
2	e	146	Total C N O S 1048 652 179 212 5	0	0	0
2	f	146	Total C N O S 1048 652 179 212 5	0	0	0
2	g	146	Total C N O S 1048 652 179 212 5	0	0	0
2	h	146	Total C N O S 1048 652 179 212 5	0	0	0
2	i	146	Total C N O S 1048 652 179 212 5	0	0	0
2	j	146	Total C N O S 1048 652 179 212 5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	141	PRO	ALA	engineered mutation	UNP P26746
l	141	PRO	ALA	engineered mutation	UNP P26746
m	141	PRO	ALA	engineered mutation	UNP P26746
n	141	PRO	ALA	engineered mutation	UNP P26746
o	141	PRO	ALA	engineered mutation	UNP P26746
p	141	PRO	ALA	engineered mutation	UNP P26746
q	141	PRO	ALA	engineered mutation	UNP P26746
r	141	PRO	ALA	engineered mutation	UNP P26746
s	141	PRO	ALA	engineered mutation	UNP P26746
t	141	PRO	ALA	engineered mutation	UNP P26746
u	141	PRO	ALA	engineered mutation	UNP P26746
v	141	PRO	ALA	engineered mutation	UNP P26746
Y	150	PRO	ALA	engineered mutation	UNP P26746

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	150	PRO	ALA	engineered mutation	UNP P26746
a	150	PRO	ALA	engineered mutation	UNP P26746
b	150	PRO	ALA	engineered mutation	UNP P26746
c	150	PRO	ALA	engineered mutation	UNP P26746
d	150	PRO	ALA	engineered mutation	UNP P26746
e	150	PRO	ALA	engineered mutation	UNP P26746
f	150	PRO	ALA	engineered mutation	UNP P26746
g	150	PRO	ALA	engineered mutation	UNP P26746
h	150	PRO	ALA	engineered mutation	UNP P26746
i	150	PRO	ALA	engineered mutation	UNP P26746
j	150	PRO	ALA	engineered mutation	UNP P26746

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	21	Total O 21 21	0	0
3	N	21	Total O 21 21	0	0
3	O	21	Total O 21 21	0	0
3	P	21	Total O 21 21	0	0
3	Q	21	Total O 21 21	0	0
3	R	21	Total O 21 21	0	0
3	S	21	Total O 21 21	0	0
3	T	21	Total O 21 21	0	0
3	U	21	Total O 21 21	0	0
3	V	21	Total O 21 21	0	0
3	W	21	Total O 21 21	0	0
3	X	21	Total O 21 21	0	0
3	A	22	Total O 22 22	0	0
3	B	22	Total O 22 22	0	0

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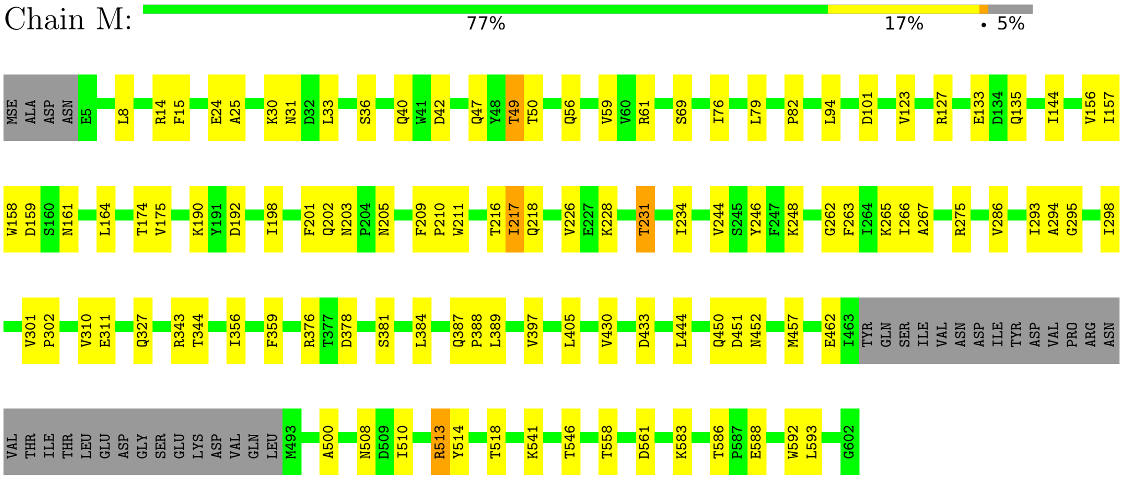
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	22	Total O 22 22	0	0
3	D	22	Total O 22 22	0	0
3	E	22	Total O 22 22	0	0
3	F	22	Total O 22 22	0	0
3	G	22	Total O 22 22	0	0
3	H	22	Total O 22 22	0	0
3	I	22	Total O 22 22	0	0
3	J	22	Total O 22 22	0	0
3	K	22	Total O 22 22	0	0
3	L	22	Total O 22 22	0	0

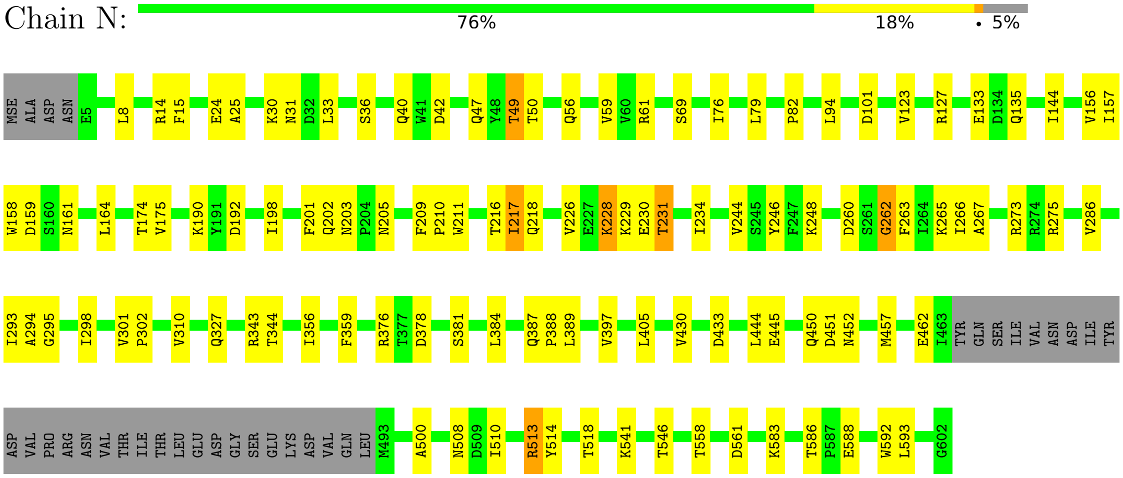
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

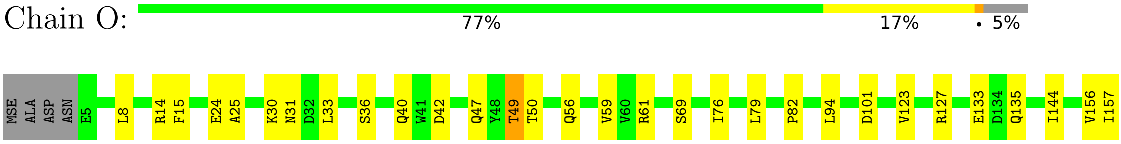
- Molecule 1: PORTAL PROTEIN

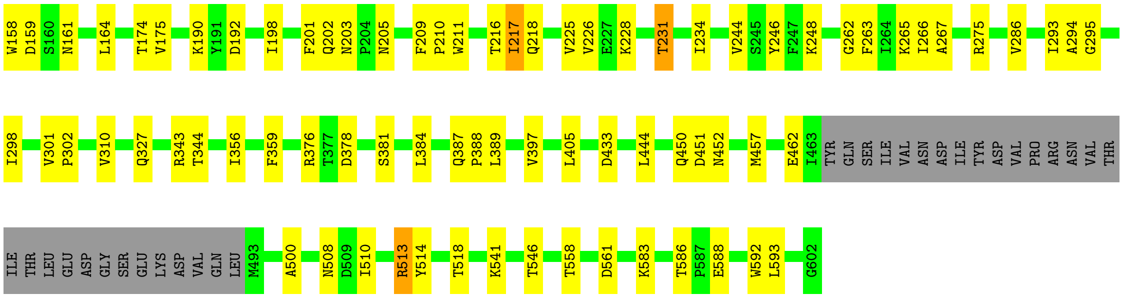


- Molecule 1: PORTAL PROTEIN



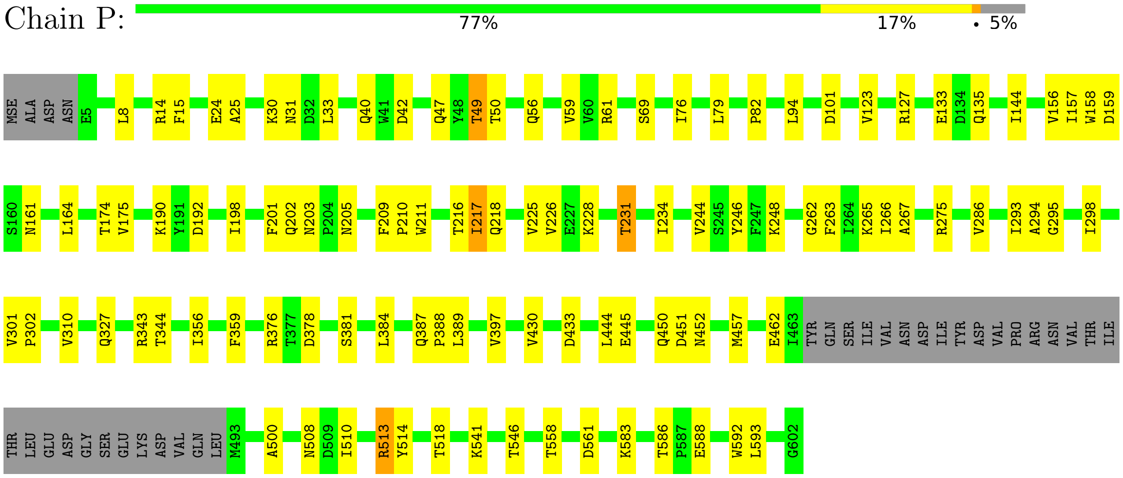
- Molecule 1: PORTAL PROTEIN





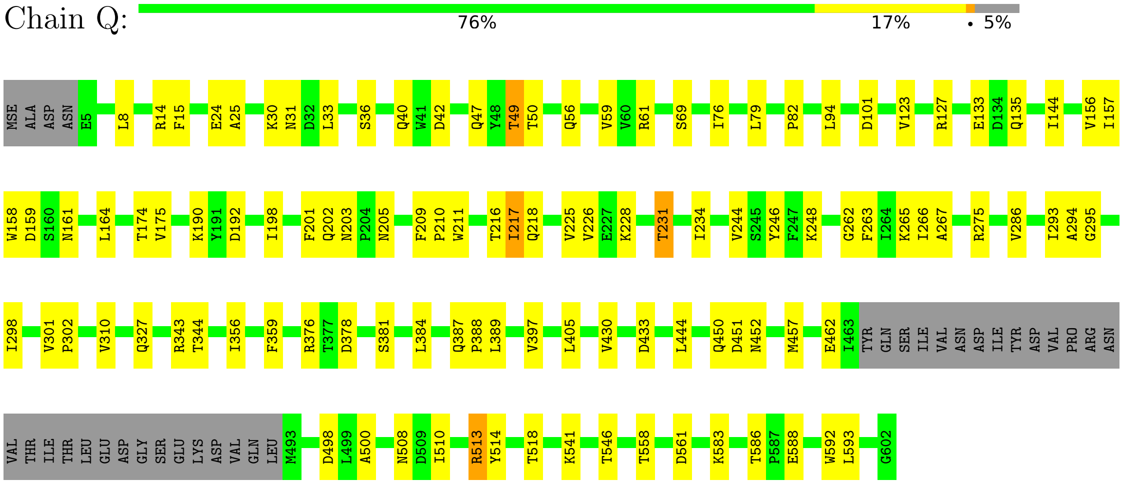
- Molecule 1: PORTAL PROTEIN

Chain P:



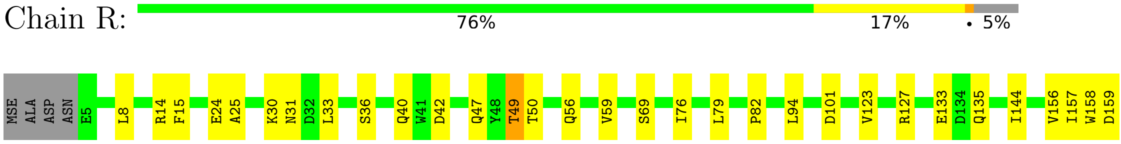
- Molecule 1: PORTAL PROTEIN

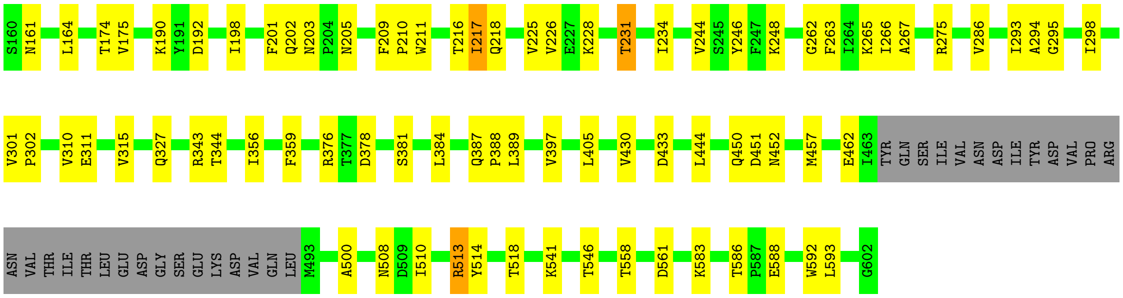
Chain Q:



- Molecule 1: PORTAL PROTEIN

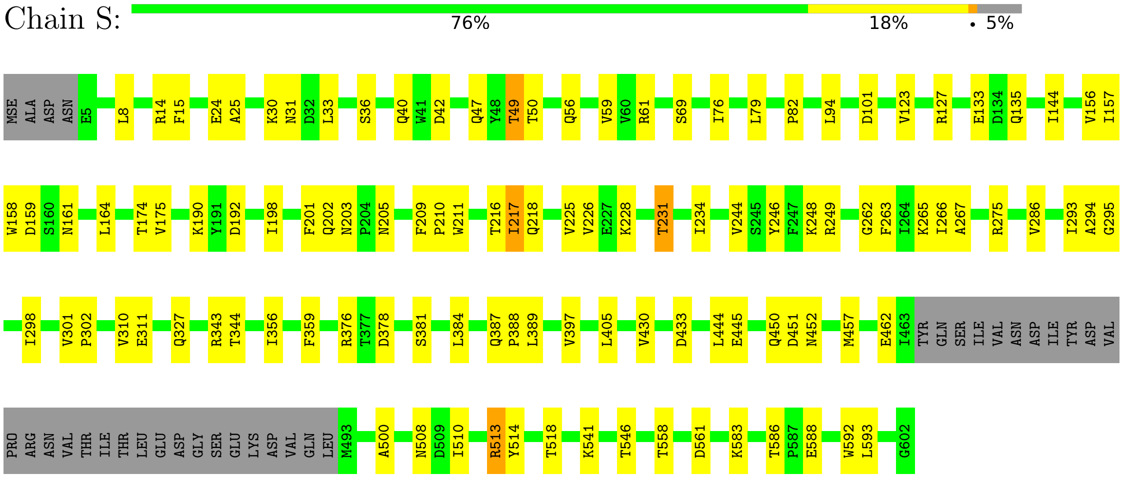
Chain R:





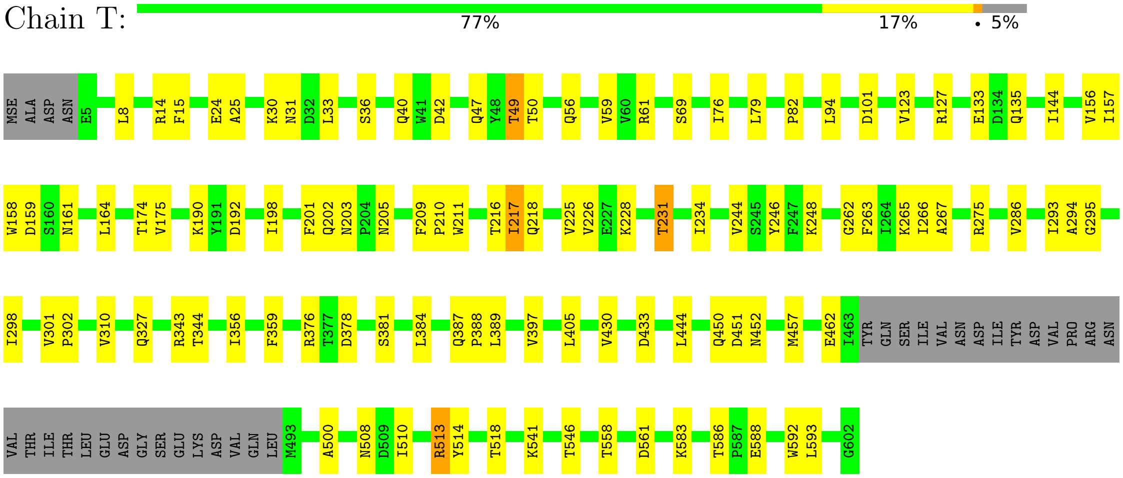
- Molecule 1: PORTAL PROTEIN

Chain S:



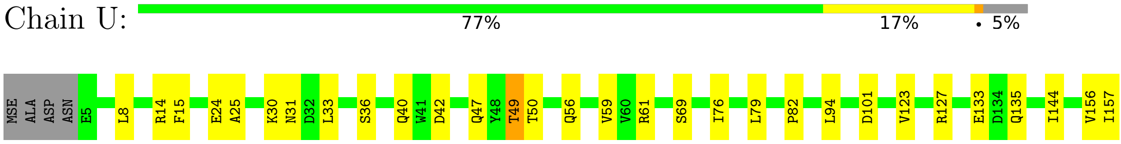
- Molecule 1: PORTAL PROTEIN

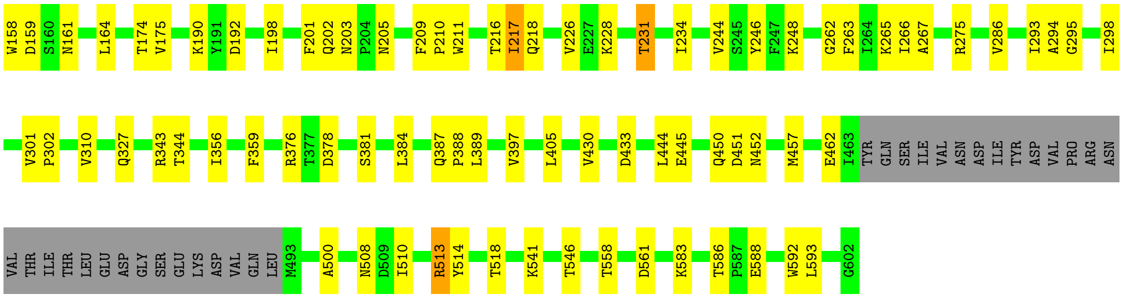
Chain T:



- Molecule 1: PORTAL PROTEIN

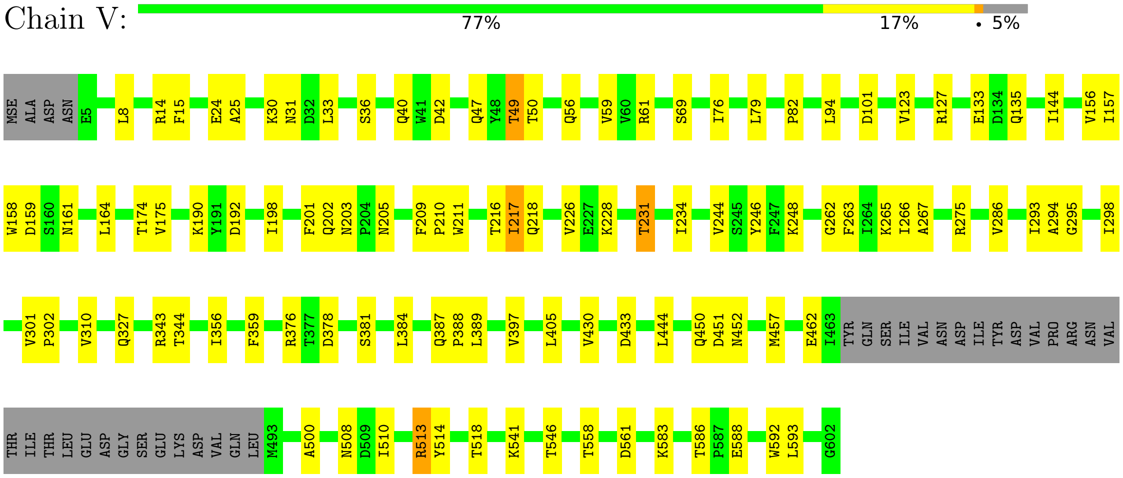
Chain U:





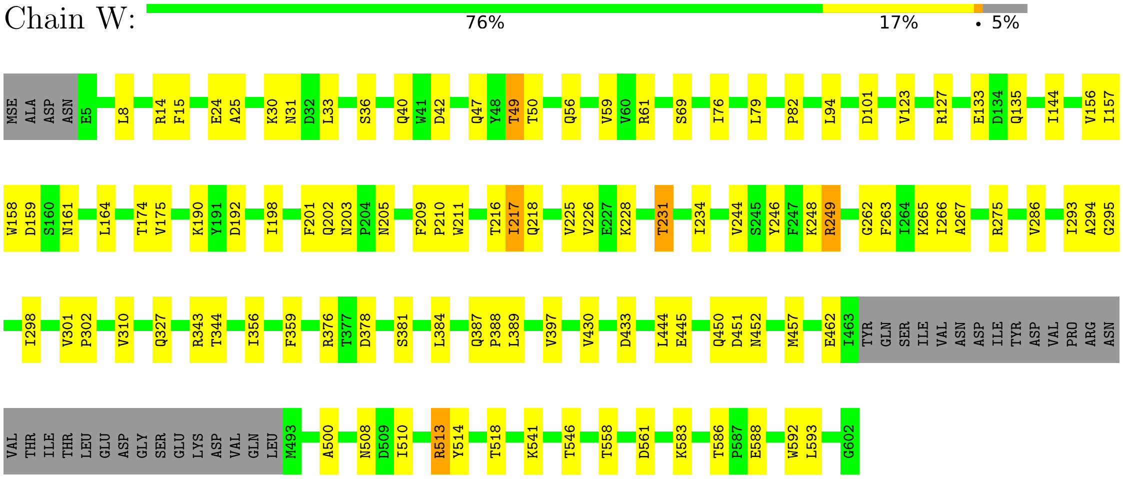
- Molecule 1: PORTAL PROTEIN

Chain V:



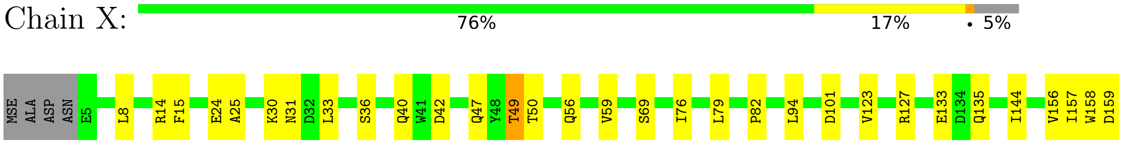
- Molecule 1: PORTAL PROTEIN

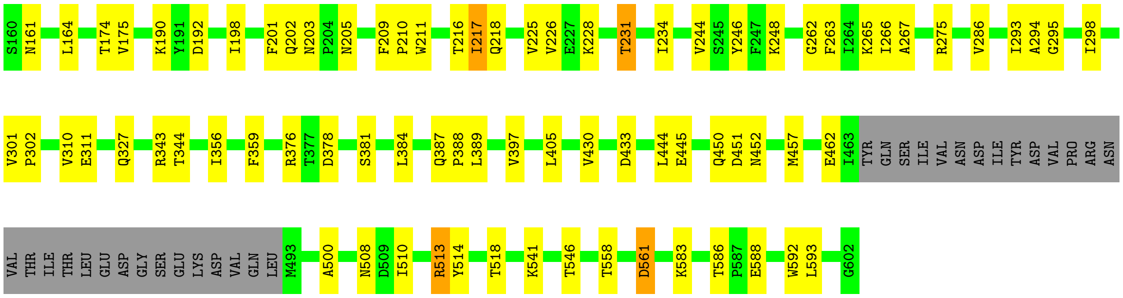
Chain W:



- Molecule 1: PORTAL PROTEIN

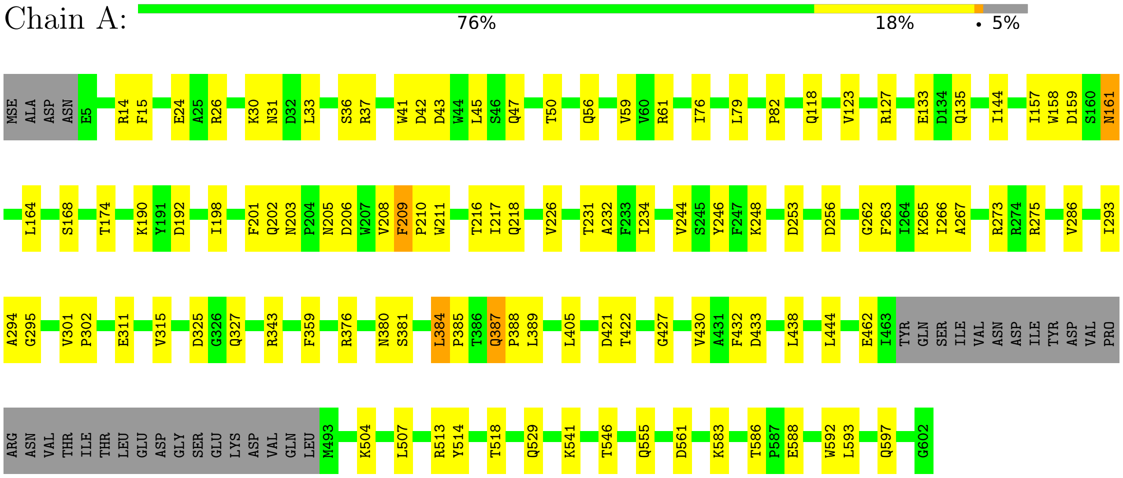
Chain X:





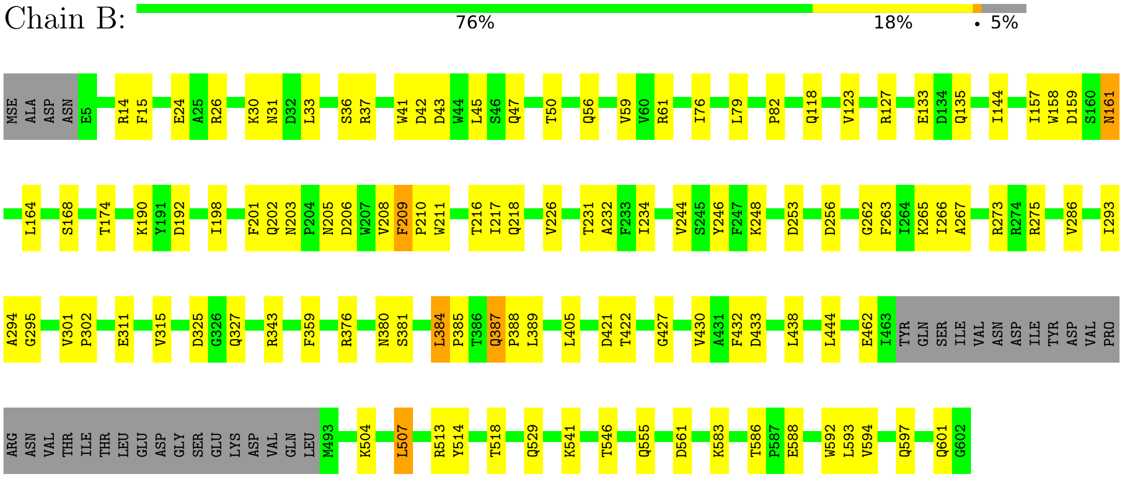
- Molecule 1: PORTAL PROTEIN

Chain A:



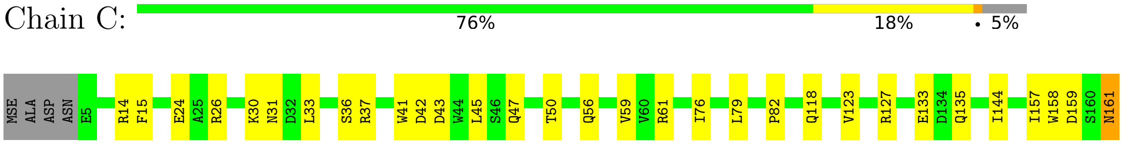
- Molecule 1: PORTAL PROTEIN

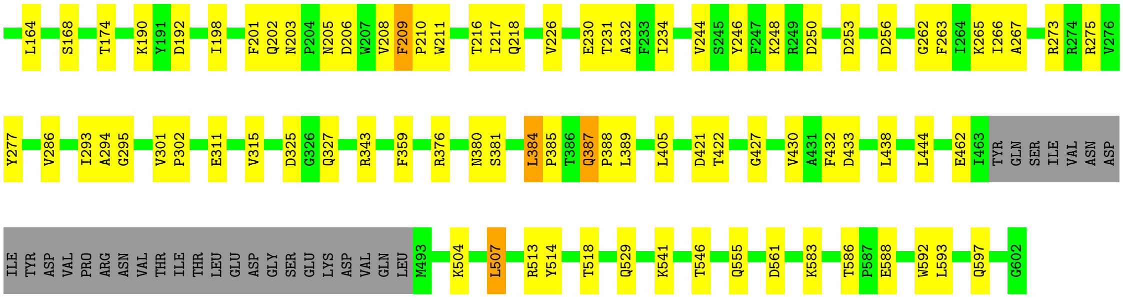
Chain B:



- Molecule 1: PORTAL PROTEIN

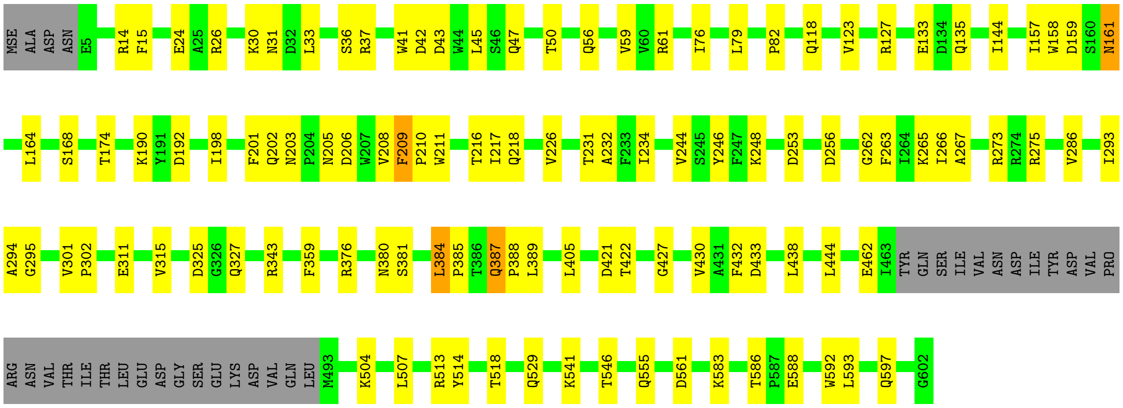
Chain C:





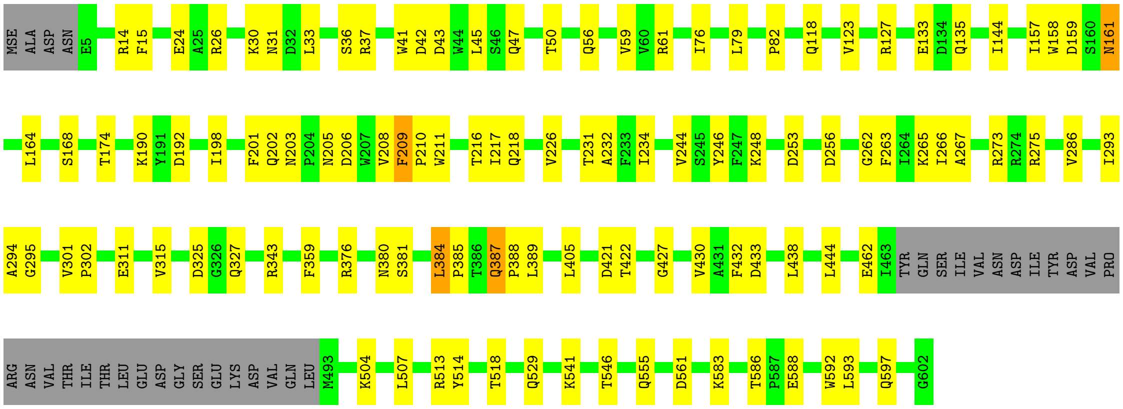
- Molecule 1: PORTAL PROTEIN

Chain D:



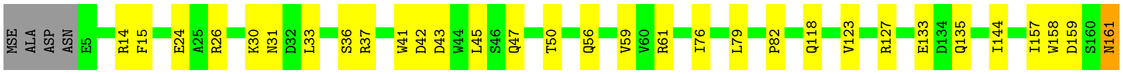
- Molecule 1: PORTAL PROTEIN

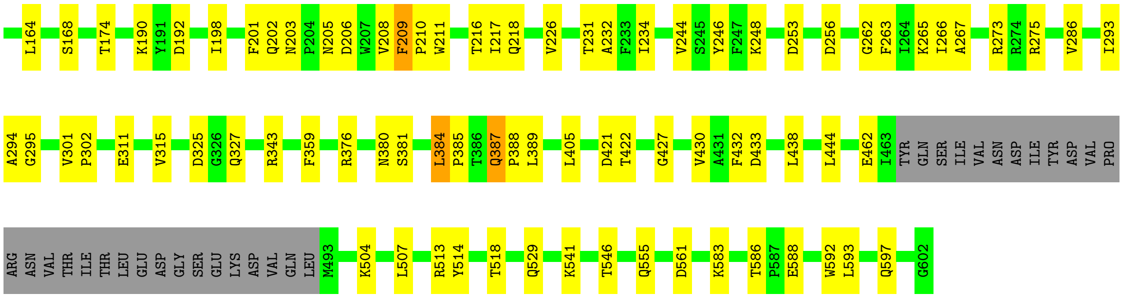
Chain E:



- Molecule 1: PORTAL PROTEIN

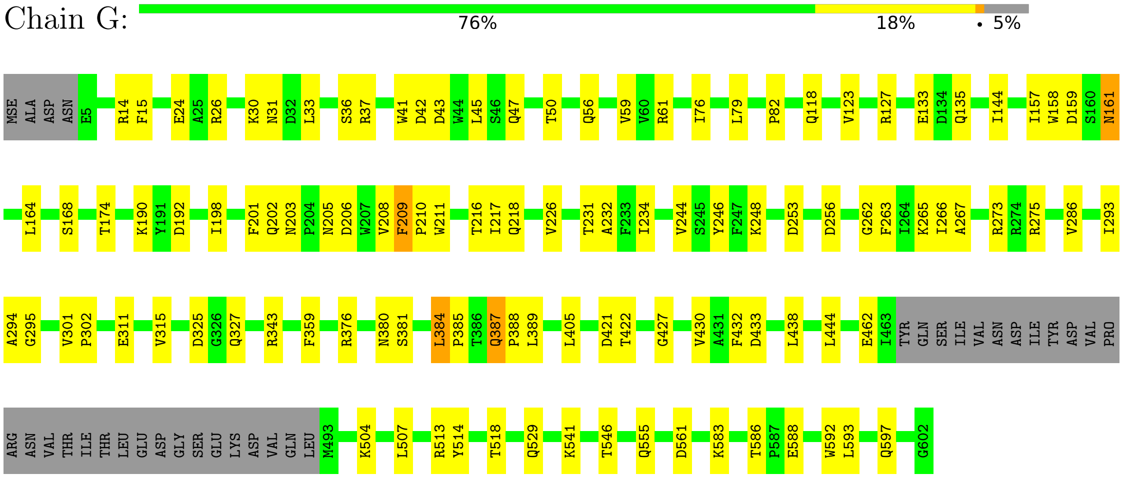
Chain F:





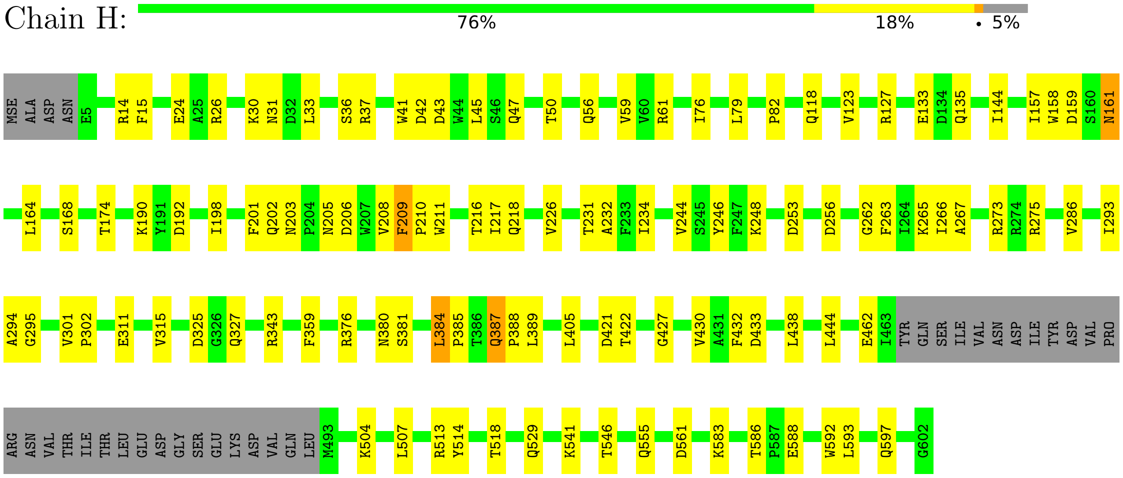
- Molecule 1: PORTAL PROTEIN

Chain G:



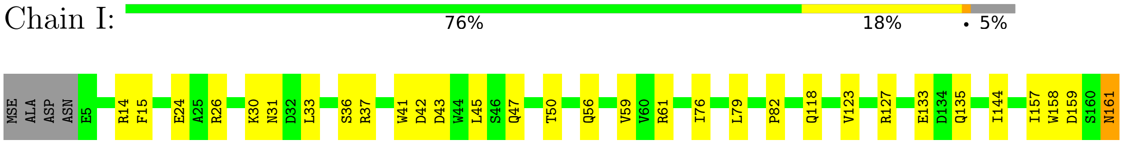
- Molecule 1: PORTAL PROTEIN

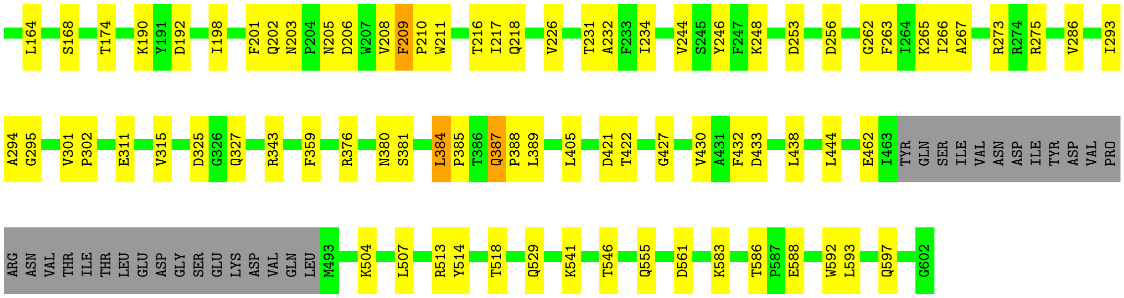
Chain H:



- Molecule 1: PORTAL PROTEIN

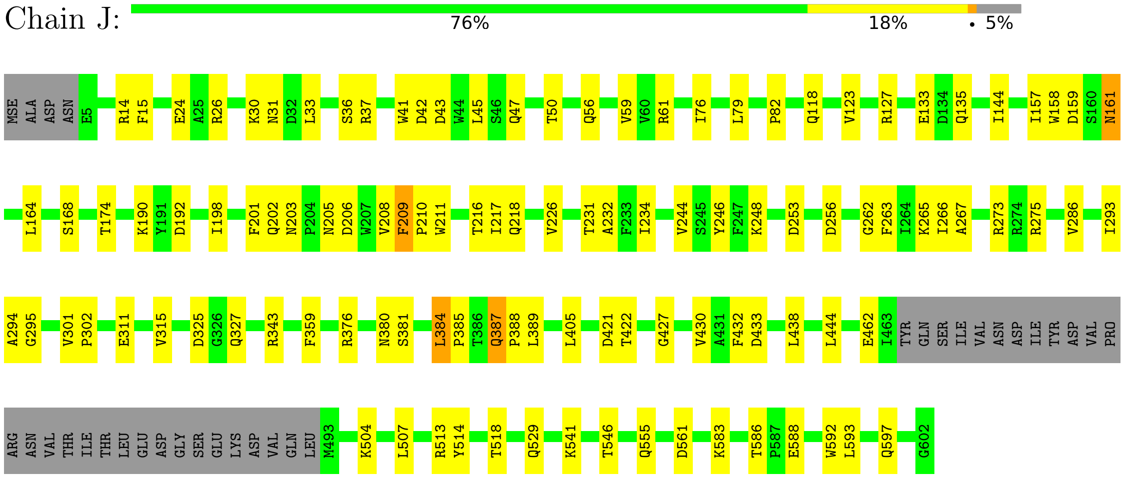
Chain I:





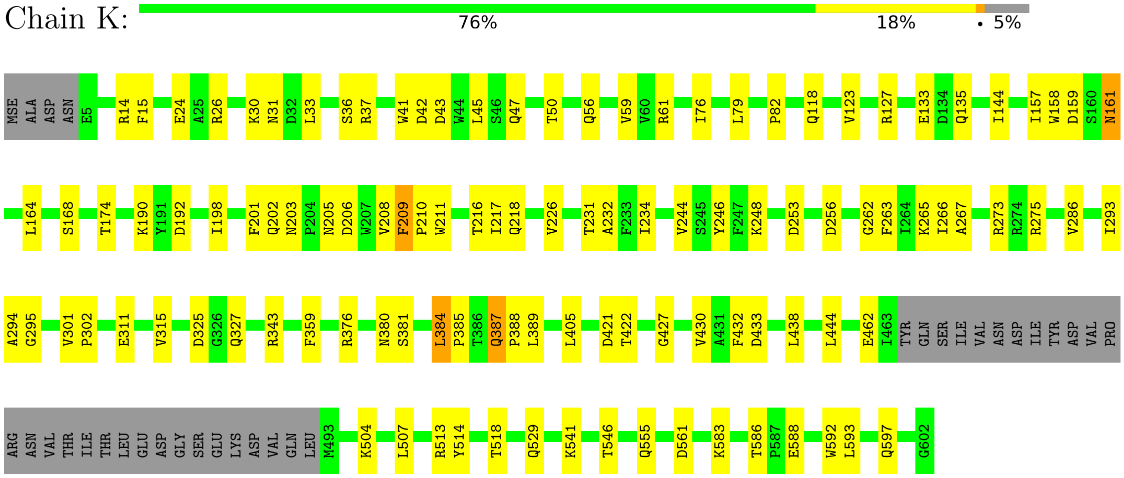
- Molecule 1: PORTAL PROTEIN

Chain J:



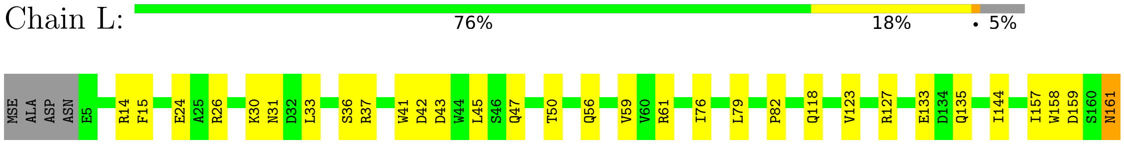
- Molecule 1: PORTAL PROTEIN

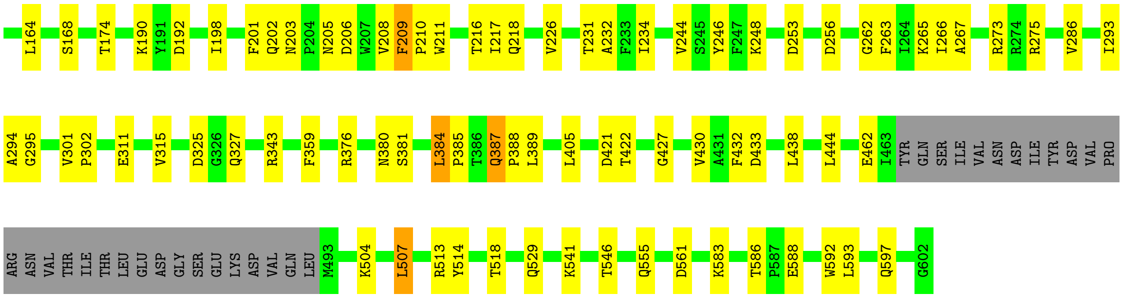
Chain K:



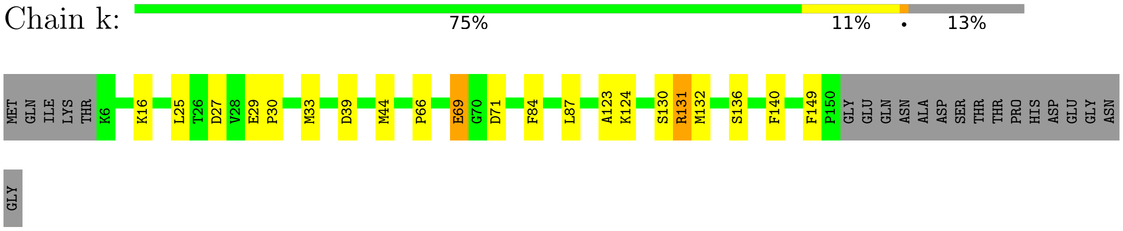
- Molecule 1: PORTAL PROTEIN

Chain L:

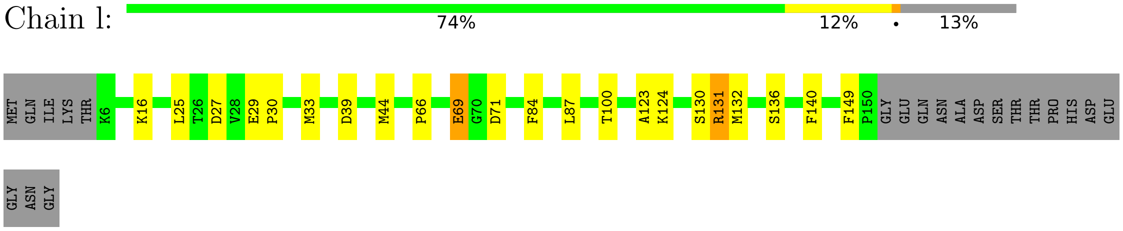




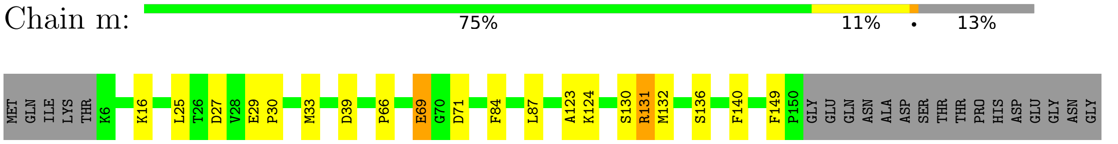
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



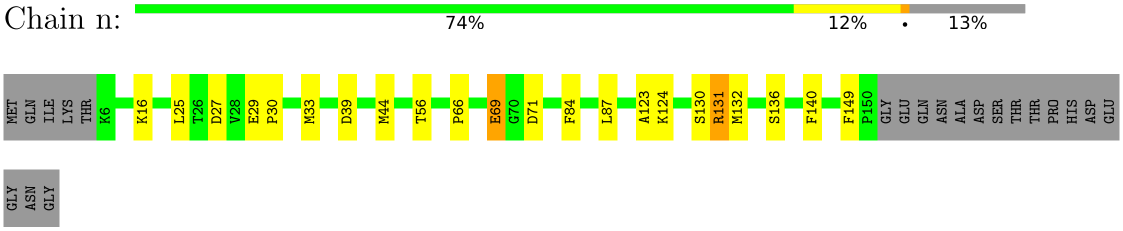
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



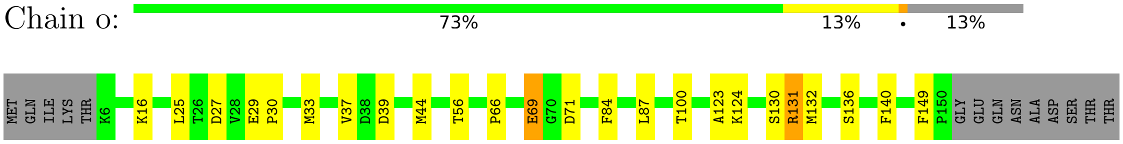
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

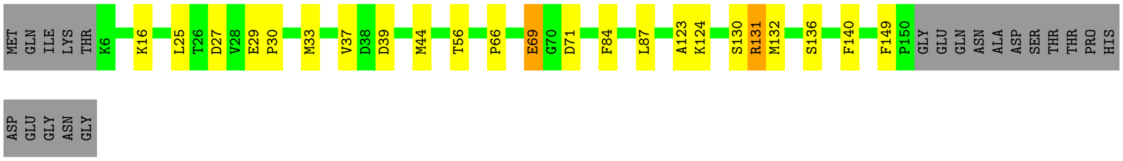


- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4



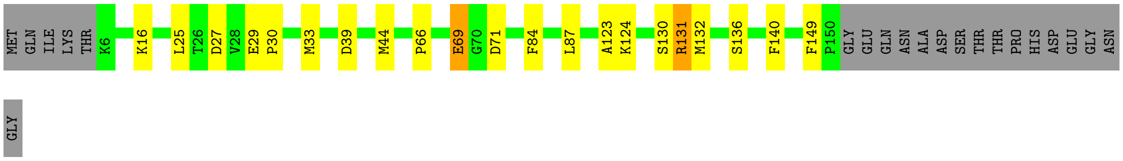
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain p:



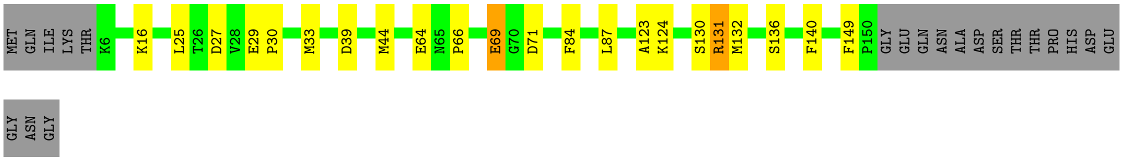
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain q:



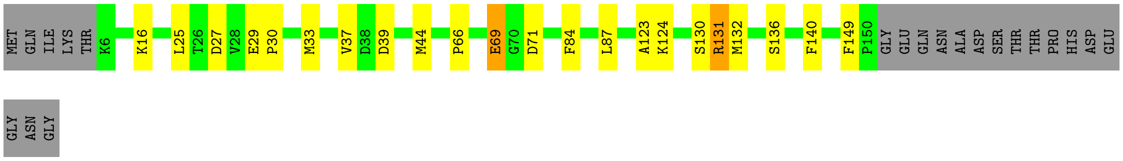
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain r:



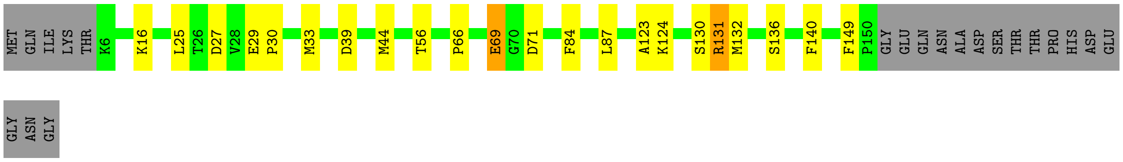
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain s:



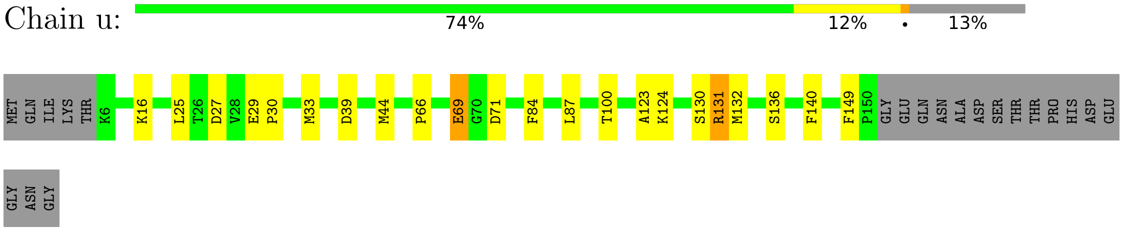
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain t:



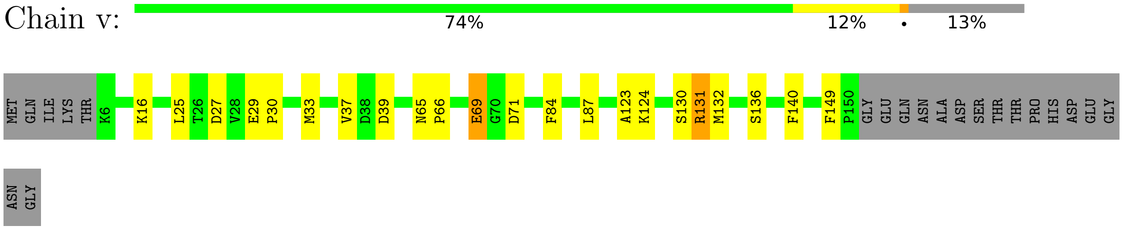
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain u:



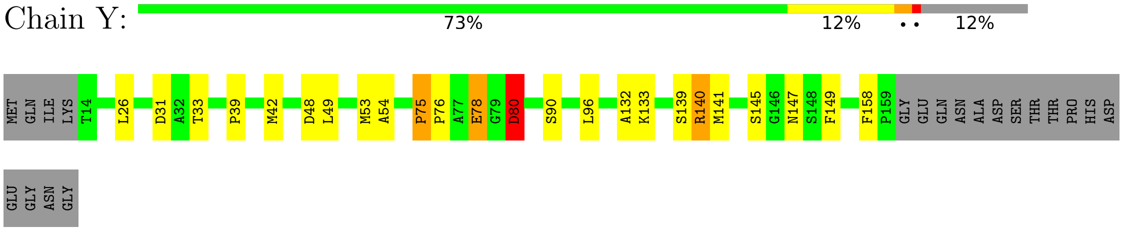
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain v:



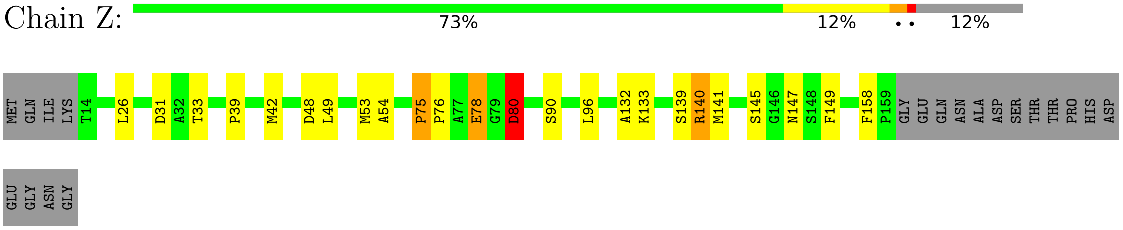
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain Y:



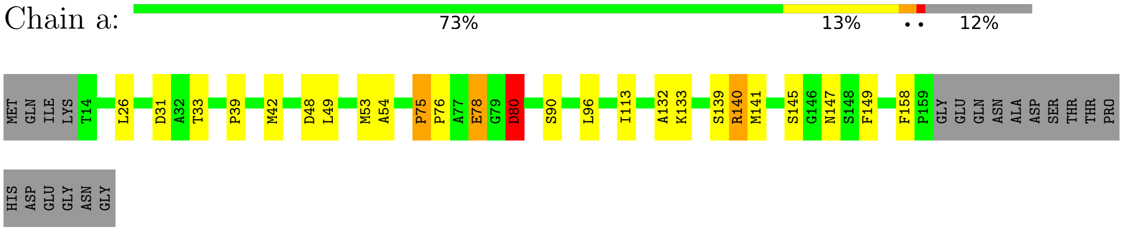
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain Z:



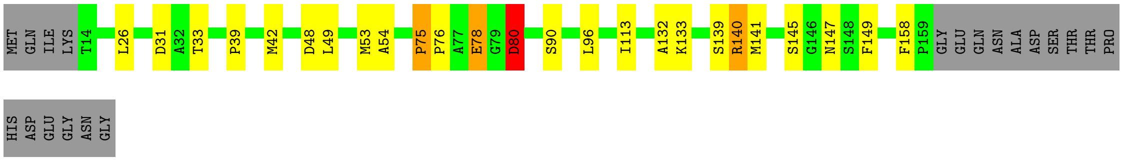
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain a:



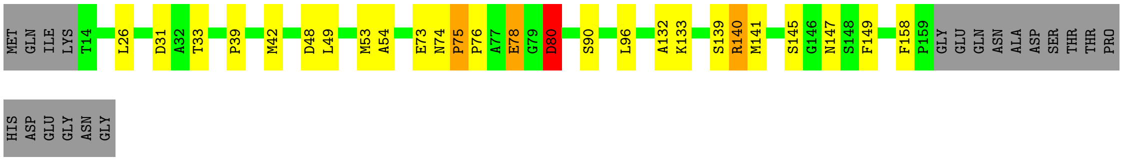
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain b:



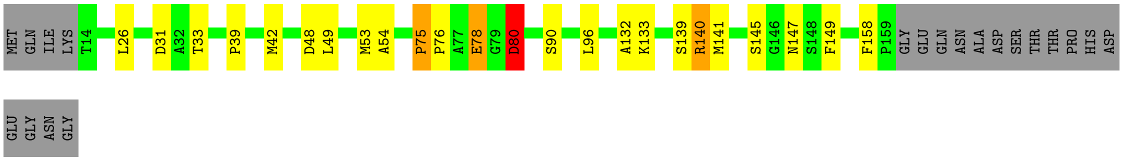
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain c:



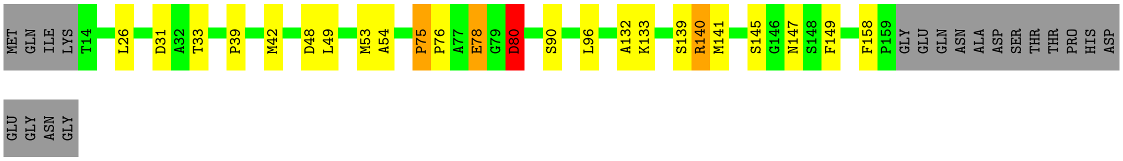
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain d:



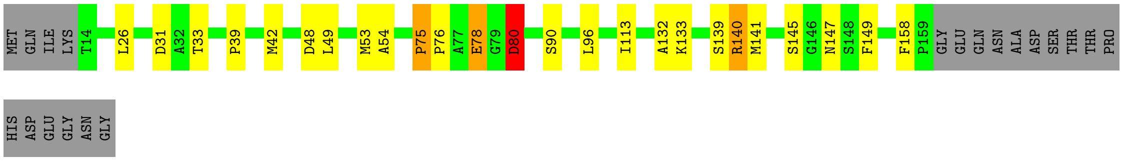
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain e:



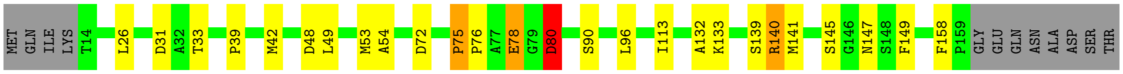
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain f:



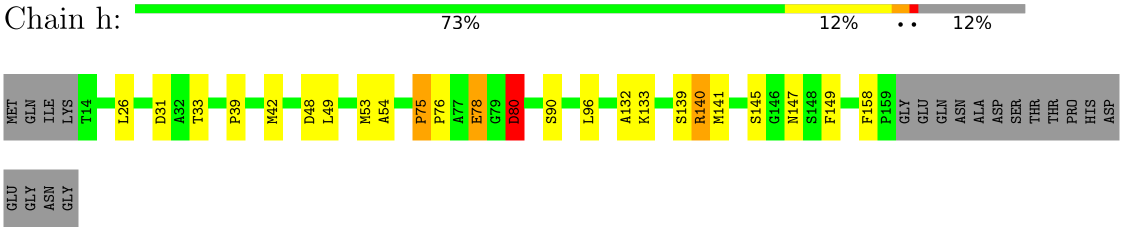
• Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain g:



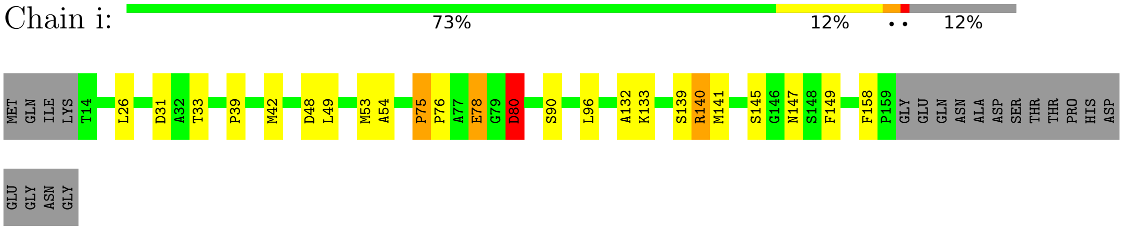
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain h:



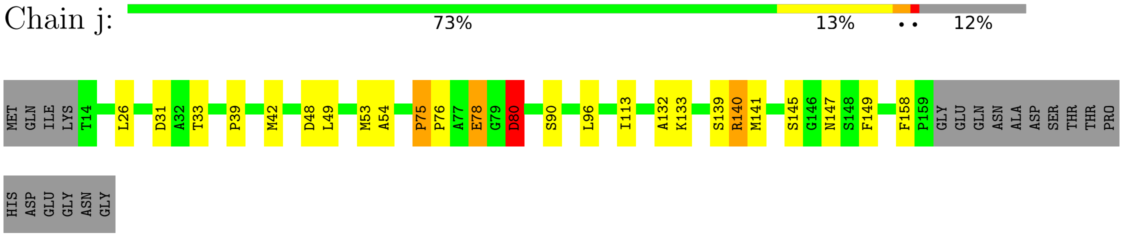
- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain i:



- Molecule 2: PACKAGED DNA STABILIZATION PROTEIN GP4

Chain j:



4 Data and refinement statistics

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	170.17Å 253.28Å 282.73Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	19.99 – 3.25 78.75 – 3.23	Depositor EDS
% Data completeness (in resolution range)	59.7 (19.99-3.25) 91.6 (78.75-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.26Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.222 , 0.236 0.318 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	65.0	Xtriage
Anisotropy	1.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 107.8	EDS
L-test for twinning[2]	$< \vert L \vert > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	135120	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 ⓘ

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	A	0.35	0/4635	0.54	0/6265
1	B	0.35	0/4635	0.54	0/6265
1	C	0.35	0/4635	0.54	0/6265
1	D	0.35	0/4635	0.54	0/6265
1	E	0.35	0/4635	0.54	0/6265
1	F	0.35	0/4635	0.54	0/6265
1	G	0.35	0/4635	0.54	0/6265
1	H	0.35	0/4635	0.54	0/6265
1	I	0.35	0/4635	0.54	0/6265
1	J	0.35	0/4635	0.54	0/6265
1	K	0.35	0/4635	0.54	0/6265
1	L	0.35	0/4635	0.54	0/6265
1	M	0.31	0/4646	0.51	0/6278
1	N	0.32	0/4646	0.51	0/6278
1	O	0.32	0/4646	0.50	0/6278
1	P	0.32	0/4646	0.51	0/6278
1	Q	0.32	0/4646	0.51	0/6278
1	R	0.32	0/4646	0.51	0/6278
1	S	0.31	0/4646	0.51	0/6278
1	T	0.31	0/4646	0.50	0/6278
1	U	0.31	0/4646	0.51	0/6278
1	V	0.32	0/4646	0.51	0/6278
1	W	0.31	0/4646	0.55	2/6278 (0.0%)
1	X	0.31	0/4646	0.50	0/6278
2	Y	0.37	0/1067	0.84	4/1452 (0.3%)
2	Z	0.37	0/1067	0.85	4/1452 (0.3%)
2	a	0.37	0/1067	0.84	4/1452 (0.3%)
2	b	0.37	0/1067	0.84	4/1452 (0.3%)
2	c	0.37	0/1067	0.84	4/1452 (0.3%)
2	d	0.37	0/1067	0.84	4/1452 (0.3%)
2	e	0.37	0/1067	0.84	4/1452 (0.3%)
2	f	0.37	0/1067	0.84	4/1452 (0.3%)
2	g	0.37	0/1067	0.84	4/1452 (0.3%)
2	h	0.37	0/1067	0.84	4/1452 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	i	0.37	0/1067	0.85	4/1452 (0.3%)
2	j	0.37	0/1067	0.84	4/1452 (0.3%)
2	k	0.32	0/1071	0.52	0/1455
2	l	0.33	0/1071	0.52	0/1455
2	m	0.33	0/1071	0.51	0/1455
2	n	0.33	0/1071	0.51	0/1455
2	o	0.33	0/1071	0.51	0/1455
2	p	0.33	0/1071	0.51	0/1455
2	q	0.32	0/1071	0.51	0/1455
2	r	0.36	0/1071	0.51	0/1455
2	s	0.32	0/1071	0.52	0/1455
2	t	0.32	0/1071	0.51	0/1455
2	u	0.31	0/1071	0.51	0/1455
2	v	0.32	0/1071	0.51	0/1455
All	All	0.34	0/137028	0.56	50/185400 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1
1	V	0	1
1	W	0	1
1	X	0	1
All	All	0	24

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	80	ASP	N-CA-CB	17.19	141.54	110.60
2	d	80	ASP	N-CA-CB	17.18	141.52	110.60
2	Z	80	ASP	N-CA-CB	17.17	141.51	110.60
2	Y	80	ASP	N-CA-CB	17.17	141.50	110.60
2	e	80	ASP	N-CA-CB	17.17	141.50	110.60
2	a	80	ASP	N-CA-CB	17.17	141.50	110.60
2	j	80	ASP	N-CA-CB	17.17	141.50	110.60
2	b	80	ASP	N-CA-CB	17.16	141.48	110.60
2	f	80	ASP	N-CA-CB	17.16	141.48	110.60
2	g	80	ASP	N-CA-CB	17.16	141.48	110.60
2	c	80	ASP	N-CA-CB	17.15	141.48	110.60
2	h	80	ASP	N-CA-CB	17.14	141.45	110.60
1	W	249	ARG	NE-CZ-NH2	-15.09	112.75	120.30
2	a	75	PRO	C-N-CD	-9.11	100.57	120.60
2	c	75	PRO	C-N-CD	-9.09	100.60	120.60
2	Z	75	PRO	C-N-CD	-9.09	100.61	120.60
2	f	75	PRO	C-N-CD	-9.08	100.62	120.60
2	i	75	PRO	C-N-CD	-9.08	100.62	120.60
2	Y	75	PRO	C-N-CD	-9.08	100.62	120.60
2	e	75	PRO	C-N-CD	-9.08	100.62	120.60
2	g	75	PRO	C-N-CD	-9.08	100.62	120.60
2	j	75	PRO	C-N-CD	-9.08	100.63	120.60
2	b	75	PRO	C-N-CD	-9.07	100.64	120.60
2	d	75	PRO	C-N-CD	-9.07	100.64	120.60
2	h	75	PRO	C-N-CD	-9.07	100.65	120.60
2	f	80	ASP	N-CA-C	-8.92	86.93	111.00
2	g	80	ASP	N-CA-C	-8.91	86.93	111.00
2	i	80	ASP	N-CA-C	-8.91	86.94	111.00
2	Z	80	ASP	N-CA-C	-8.91	86.95	111.00
2	Y	80	ASP	N-CA-C	-8.90	86.96	111.00
2	e	80	ASP	N-CA-C	-8.90	86.97	111.00
2	c	80	ASP	N-CA-C	-8.90	86.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	80	ASP	N-CA-C	-8.90	86.98	111.00
2	b	80	ASP	N-CA-C	-8.89	86.98	111.00
2	j	80	ASP	N-CA-C	-8.89	86.99	111.00
2	h	80	ASP	N-CA-C	-8.89	87.00	111.00
2	a	80	ASP	N-CA-C	-8.89	87.00	111.00
1	W	249	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	a	31	ASP	CB-CG-OD2	5.22	123.00	118.30
2	i	31	ASP	CB-CG-OD2	5.22	123.00	118.30
2	Z	31	ASP	CB-CG-OD2	5.21	122.99	118.30
2	c	31	ASP	CB-CG-OD2	5.21	122.99	118.30
2	j	31	ASP	CB-CG-OD2	5.20	122.98	118.30
2	d	31	ASP	CB-CG-OD2	5.20	122.98	118.30
2	Y	31	ASP	CB-CG-OD2	5.18	122.97	118.30
2	g	31	ASP	CB-CG-OD2	5.18	122.97	118.30
2	b	31	ASP	CB-CG-OD2	5.18	122.96	118.30
2	f	31	ASP	CB-CG-OD2	5.17	122.95	118.30
2	e	31	ASP	CB-CG-OD2	5.15	122.94	118.30
2	h	31	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	THR	Peptide
1	B	231	THR	Peptide
1	C	231	THR	Peptide
1	D	231	THR	Peptide
1	E	231	THR	Peptide
1	F	231	THR	Peptide
1	G	231	THR	Peptide
1	H	231	THR	Peptide
1	I	231	THR	Peptide
1	J	231	THR	Peptide
1	K	231	THR	Peptide
1	L	231	THR	Peptide
1	M	231	THR	Peptide
1	N	231	THR	Peptide
1	O	231	THR	Peptide
1	P	231	THR	Peptide
1	Q	231	THR	Peptide
1	R	231	THR	Peptide
1	S	231	THR	Peptide

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Mol	Chain	Res	Type	Group
1	T	231	THR	Peptide
1	U	231	THR	Peptide
1	V	231	THR	Peptide
1	W	231	THR	Peptide
1	X	231	THR	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 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	A	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	B	565/602 (94%)	434 (77%)	87 (15%)	44 (8%)	1 6
1	C	565/602 (94%)	434 (77%)	87 (15%)	44 (8%)	1 6
1	D	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	E	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	F	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	G	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	H	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	I	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	J	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	K	565/602 (94%)	434 (77%)	88 (16%)	43 (8%)	1 6
1	L	565/602 (94%)	434 (77%)	87 (15%)	44 (8%)	1 6
1	M	565/602 (94%)	446 (79%)	81 (14%)	38 (7%)	1 8
1	N	565/602 (94%)	447 (79%)	79 (14%)	39 (7%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	565/602 (94%)	447 (79%)	80 (14%)	38 (7%)	1	8
1	P	565/602 (94%)	448 (79%)	79 (14%)	38 (7%)	1	8
1	Q	565/602 (94%)	447 (79%)	79 (14%)	39 (7%)	1	8
1	R	565/602 (94%)	448 (79%)	79 (14%)	38 (7%)	1	8
1	S	565/602 (94%)	443 (78%)	83 (15%)	39 (7%)	1	8
1	T	565/602 (94%)	446 (79%)	81 (14%)	38 (7%)	1	8
1	U	565/602 (94%)	447 (79%)	79 (14%)	39 (7%)	1	8
1	V	565/602 (94%)	445 (79%)	82 (14%)	38 (7%)	1	8
1	W	565/602 (94%)	448 (79%)	78 (14%)	39 (7%)	1	8
1	X	565/602 (94%)	448 (79%)	78 (14%)	39 (7%)	1	8
2	Y	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	Z	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	a	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	b	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	c	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	d	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	e	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	f	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	g	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	h	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	i	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	j	144/166 (87%)	115 (80%)	16 (11%)	13 (9%)	1	4
2	k	143/166 (86%)	115 (80%)	17 (12%)	11 (8%)	1	6
2	l	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	6
2	m	143/166 (86%)	115 (80%)	18 (13%)	10 (7%)	1	7
2	n	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	6
2	o	143/166 (86%)	115 (80%)	17 (12%)	11 (8%)	1	6
2	p	143/166 (86%)	115 (80%)	17 (12%)	11 (8%)	1	6
2	q	143/166 (86%)	113 (79%)	19 (13%)	11 (8%)	1	6
2	r	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	6
2	s	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	t	143/166 (86%)	113 (79%)	19 (13%)	11 (8%)	1 6
2	u	143/166 (86%)	114 (80%)	18 (13%)	11 (8%)	1 6
2	v	143/166 (86%)	114 (80%)	19 (13%)	10 (7%)	1 7
All	All	17004/18432 (92%)	13318 (78%)	2419 (14%)	1267 (8%)	1 7

All (1267) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	82	PRO
1	M	263	PHE
1	M	294	ALA
1	M	462	GLU
1	M	514	TYR
1	M	561	ASP
1	M	586	THR
1	M	588	GLU
1	N	82	PRO
1	N	263	PHE
1	N	294	ALA
1	N	462	GLU
1	N	514	TYR
1	N	561	ASP
1	N	586	THR
1	N	588	GLU
1	O	82	PRO
1	O	263	PHE
1	O	294	ALA
1	O	462	GLU
1	O	514	TYR
1	O	561	ASP
1	O	586	THR
1	O	588	GLU
1	P	82	PRO
1	P	263	PHE
1	P	294	ALA
1	P	462	GLU
1	P	514	TYR
1	P	561	ASP
1	P	586	THR
1	P	588	GLU
1	Q	82	PRO

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Mol	Chain	Res	Type
1	Q	263	PHE
1	Q	294	ALA
1	Q	462	GLU
1	Q	514	TYR
1	Q	561	ASP
1	Q	586	THR
1	Q	588	GLU
1	R	82	PRO
1	R	263	PHE
1	R	294	ALA
1	R	462	GLU
1	R	514	TYR
1	R	561	ASP
1	R	586	THR
1	R	588	GLU
1	S	82	PRO
1	S	263	PHE
1	S	294	ALA
1	S	462	GLU
1	S	514	TYR
1	S	561	ASP
1	S	586	THR
1	S	588	GLU
1	T	82	PRO
1	T	263	PHE
1	T	294	ALA
1	T	462	GLU
1	T	514	TYR
1	T	561	ASP
1	T	586	THR
1	T	588	GLU
1	U	82	PRO
1	U	263	PHE
1	U	294	ALA
1	U	462	GLU
1	U	514	TYR
1	U	561	ASP
1	U	586	THR
1	U	588	GLU
1	V	82	PRO
1	V	263	PHE
1	V	294	ALA

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Mol	Chain	Res	Type
1	V	462	GLU
1	V	514	TYR
1	V	561	ASP
1	V	586	THR
1	V	588	GLU
1	W	82	PRO
1	W	263	PHE
1	W	294	ALA
1	W	462	GLU
1	W	514	TYR
1	W	561	ASP
1	W	586	THR
1	W	588	GLU
1	X	82	PRO
1	X	263	PHE
1	X	294	ALA
1	X	462	GLU
1	X	514	TYR
1	X	561	ASP
1	X	586	THR
1	X	588	GLU
2	k	25	LEU
2	k	30	PRO
2	k	123	ALA
2	l	25	LEU
2	l	30	PRO
2	l	123	ALA
2	m	25	LEU
2	m	30	PRO
2	m	123	ALA
2	n	25	LEU
2	n	30	PRO
2	n	123	ALA
2	o	25	LEU
2	o	30	PRO
2	o	123	ALA
2	p	25	LEU
2	p	30	PRO
2	p	123	ALA
2	q	25	LEU
2	q	30	PRO
2	q	123	ALA

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Mol	Chain	Res	Type
2	r	25	LEU
2	r	30	PRO
2	r	123	ALA
2	s	25	LEU
2	s	30	PRO
2	s	123	ALA
2	t	25	LEU
2	t	30	PRO
2	t	123	ALA
2	u	25	LEU
2	u	30	PRO
2	u	123	ALA
2	v	25	LEU
2	v	30	PRO
2	v	123	ALA
1	A	41	TRP
1	A	50	THR
1	A	59	VAL
1	A	82	PRO
1	A	159	ASP
1	A	208	VAL
1	A	256	ASP
1	A	263	PHE
1	A	294	ALA
1	A	387	GLN
1	A	462	GLU
1	A	504	LYS
1	A	514	TYR
1	A	561	ASP
1	A	586	THR
1	B	41	TRP
1	B	50	THR
1	B	59	VAL
1	B	82	PRO
1	B	159	ASP
1	B	208	VAL
1	B	256	ASP
1	B	263	PHE
1	B	294	ALA
1	B	387	GLN
1	B	462	GLU
1	B	504	LYS

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Mol	Chain	Res	Type
1	B	514	TYR
1	B	561	ASP
1	B	586	THR
1	C	41	TRP
1	C	50	THR
1	C	59	VAL
1	C	82	PRO
1	C	159	ASP
1	C	208	VAL
1	C	256	ASP
1	C	263	PHE
1	C	294	ALA
1	C	387	GLN
1	C	462	GLU
1	C	504	LYS
1	C	514	TYR
1	C	561	ASP
1	C	586	THR
1	D	41	TRP
1	D	50	THR
1	D	59	VAL
1	D	82	PRO
1	D	159	ASP
1	D	208	VAL
1	D	256	ASP
1	D	263	PHE
1	D	294	ALA
1	D	387	GLN
1	D	462	GLU
1	D	504	LYS
1	D	514	TYR
1	D	561	ASP
1	D	586	THR
1	E	41	TRP
1	E	50	THR
1	E	59	VAL
1	E	82	PRO
1	E	159	ASP
1	E	208	VAL
1	E	256	ASP
1	E	263	PHE
1	E	294	ALA

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Mol	Chain	Res	Type
1	E	387	GLN
1	E	462	GLU
1	E	504	LYS
1	E	514	TYR
1	E	561	ASP
1	E	586	THR
1	F	41	TRP
1	F	50	THR
1	F	59	VAL
1	F	82	PRO
1	F	159	ASP
1	F	208	VAL
1	F	256	ASP
1	F	263	PHE
1	F	294	ALA
1	F	387	GLN
1	F	462	GLU
1	F	504	LYS
1	F	514	TYR
1	F	561	ASP
1	F	586	THR
1	G	41	TRP
1	G	50	THR
1	G	59	VAL
1	G	82	PRO
1	G	159	ASP
1	G	208	VAL
1	G	256	ASP
1	G	263	PHE
1	G	294	ALA
1	G	387	GLN
1	G	462	GLU
1	G	504	LYS
1	G	514	TYR
1	G	561	ASP
1	G	586	THR
1	H	41	TRP
1	H	50	THR
1	H	59	VAL
1	H	82	PRO
1	H	159	ASP
1	H	208	VAL

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Mol	Chain	Res	Type
1	H	256	ASP
1	H	263	PHE
1	H	294	ALA
1	H	387	GLN
1	H	462	GLU
1	H	504	LYS
1	H	514	TYR
1	H	561	ASP
1	H	586	THR
1	I	41	TRP
1	I	50	THR
1	I	59	VAL
1	I	82	PRO
1	I	159	ASP
1	I	208	VAL
1	I	256	ASP
1	I	263	PHE
1	I	294	ALA
1	I	387	GLN
1	I	462	GLU
1	I	504	LYS
1	I	514	TYR
1	I	561	ASP
1	I	586	THR
1	J	41	TRP
1	J	50	THR
1	J	59	VAL
1	J	82	PRO
1	J	159	ASP
1	J	208	VAL
1	J	256	ASP
1	J	263	PHE
1	J	294	ALA
1	J	387	GLN
1	J	462	GLU
1	J	504	LYS
1	J	514	TYR
1	J	561	ASP
1	J	586	THR
1	K	41	TRP
1	K	50	THR
1	K	59	VAL

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Mol	Chain	Res	Type
1	K	82	PRO
1	K	208	VAL
1	K	256	ASP
1	K	263	PHE
1	K	294	ALA
1	K	387	GLN
1	K	462	GLU
1	K	504	LYS
1	K	514	TYR
1	K	561	ASP
1	K	586	THR
1	L	41	TRP
1	L	50	THR
1	L	59	VAL
1	L	82	PRO
1	L	159	ASP
1	L	208	VAL
1	L	256	ASP
1	L	263	PHE
1	L	294	ALA
1	L	387	GLN
1	L	462	GLU
1	L	504	LYS
1	L	514	TYR
1	L	561	ASP
1	L	586	THR
2	Y	33	THR
2	Y	39	PRO
2	Y	75	PRO
2	Y	76	PRO
2	Y	133	LYS
2	Z	33	THR
2	Z	39	PRO
2	Z	75	PRO
2	Z	76	PRO
2	Z	133	LYS
2	a	33	THR
2	a	39	PRO
2	a	75	PRO
2	a	76	PRO
2	a	133	LYS
2	b	33	THR

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Mol	Chain	Res	Type
2	b	39	PRO
2	b	75	PRO
2	b	76	PRO
2	b	133	LYS
2	c	33	THR
2	c	39	PRO
2	c	75	PRO
2	c	76	PRO
2	c	133	LYS
2	d	33	THR
2	d	39	PRO
2	d	75	PRO
2	d	76	PRO
2	d	133	LYS
2	e	33	THR
2	e	39	PRO
2	e	75	PRO
2	e	76	PRO
2	e	133	LYS
2	f	33	THR
2	f	39	PRO
2	f	75	PRO
2	f	76	PRO
2	f	133	LYS
2	g	33	THR
2	g	39	PRO
2	g	75	PRO
2	g	76	PRO
2	g	133	LYS
2	h	33	THR
2	h	39	PRO
2	h	75	PRO
2	h	76	PRO
2	h	133	LYS
2	i	33	THR
2	i	39	PRO
2	i	75	PRO
2	i	76	PRO
2	i	133	LYS
2	j	33	THR
2	j	39	PRO
2	j	75	PRO

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Mol	Chain	Res	Type
2	j	76	PRO
2	j	133	LYS
1	M	25	ALA
1	M	159	ASP
1	M	205	ASN
1	M	267	ALA
1	M	500	ALA
1	N	25	ALA
1	N	159	ASP
1	N	205	ASN
1	N	267	ALA
1	N	295	GLY
1	N	500	ALA
1	N	513	ARG
1	O	25	ALA
1	O	76	ILE
1	O	159	ASP
1	O	205	ASN
1	O	267	ALA
1	O	295	GLY
1	O	500	ALA
1	O	513	ARG
1	P	25	ALA
1	P	49	THR
1	P	159	ASP
1	P	205	ASN
1	P	267	ALA
1	P	500	ALA
1	P	513	ARG
1	Q	25	ALA
1	Q	159	ASP
1	Q	205	ASN
1	Q	267	ALA
1	Q	500	ALA
1	R	25	ALA
1	R	159	ASP
1	R	205	ASN
1	R	267	ALA
1	R	295	GLY
1	R	500	ALA
1	S	25	ALA
1	S	49	THR

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Mol	Chain	Res	Type
1	S	159	ASP
1	S	205	ASN
1	S	267	ALA
1	S	295	GLY
1	S	500	ALA
1	S	513	ARG
1	T	25	ALA
1	T	159	ASP
1	T	205	ASN
1	T	267	ALA
1	T	500	ALA
1	T	513	ARG
1	U	25	ALA
1	U	159	ASP
1	U	205	ASN
1	U	267	ALA
1	U	295	GLY
1	U	500	ALA
1	U	513	ARG
1	V	25	ALA
1	V	159	ASP
1	V	205	ASN
1	V	267	ALA
1	V	295	GLY
1	V	500	ALA
1	W	25	ALA
1	W	159	ASP
1	W	205	ASN
1	W	267	ALA
1	W	295	GLY
1	W	500	ALA
1	X	25	ALA
1	X	76	ILE
1	X	159	ASP
1	X	205	ASN
1	X	267	ALA
1	X	295	GLY
1	X	500	ALA
2	k	66	PRO
2	k	69	GLU
2	k	124	LYS
2	k	149	PHE

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Mol	Chain	Res	Type
2	l	66	PRO
2	l	69	GLU
2	l	124	LYS
2	l	131	ARG
2	l	149	PHE
2	m	66	PRO
2	m	124	LYS
2	m	149	PHE
2	n	66	PRO
2	n	124	LYS
2	n	131	ARG
2	n	149	PHE
2	o	66	PRO
2	o	124	LYS
2	o	149	PHE
2	p	66	PRO
2	p	124	LYS
2	p	149	PHE
2	q	66	PRO
2	q	69	GLU
2	q	124	LYS
2	q	149	PHE
2	r	66	PRO
2	r	69	GLU
2	r	124	LYS
2	r	131	ARG
2	r	149	PHE
2	s	66	PRO
2	s	124	LYS
2	s	149	PHE
2	t	66	PRO
2	t	124	LYS
2	t	149	PHE
2	u	66	PRO
2	u	69	GLU
2	u	124	LYS
2	u	149	PHE
2	v	66	PRO
2	v	69	GLU
2	v	124	LYS
2	v	149	PHE
1	A	267	ALA

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Mol	Chain	Res	Type
1	A	381	SER
1	A	388	PRO
1	A	588	GLU
1	B	267	ALA
1	B	381	SER
1	B	388	PRO
1	B	588	GLU
1	C	267	ALA
1	C	381	SER
1	C	388	PRO
1	C	588	GLU
1	D	267	ALA
1	D	381	SER
1	D	388	PRO
1	D	588	GLU
1	E	267	ALA
1	E	381	SER
1	E	388	PRO
1	E	588	GLU
1	F	267	ALA
1	F	381	SER
1	F	388	PRO
1	F	588	GLU
1	G	267	ALA
1	G	381	SER
1	G	388	PRO
1	G	588	GLU
1	H	267	ALA
1	H	381	SER
1	H	388	PRO
1	H	588	GLU
1	I	267	ALA
1	I	381	SER
1	I	388	PRO
1	I	588	GLU
1	J	267	ALA
1	J	381	SER
1	J	388	PRO
1	J	588	GLU
1	K	159	ASP
1	K	267	ALA
1	K	381	SER

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Mol	Chain	Res	Type
1	K	388	PRO
1	K	588	GLU
1	L	267	ALA
1	L	381	SER
1	L	388	PRO
1	L	588	GLU
2	Y	80	ASP
2	Y	132	ALA
2	Y	140	ARG
2	Y	158	PHE
2	Z	80	ASP
2	Z	132	ALA
2	Z	140	ARG
2	Z	158	PHE
2	a	80	ASP
2	a	132	ALA
2	a	140	ARG
2	a	158	PHE
2	b	80	ASP
2	b	132	ALA
2	b	140	ARG
2	b	158	PHE
2	c	80	ASP
2	c	132	ALA
2	c	140	ARG
2	c	158	PHE
2	d	80	ASP
2	d	132	ALA
2	d	140	ARG
2	d	158	PHE
2	e	80	ASP
2	e	132	ALA
2	e	140	ARG
2	e	158	PHE
2	f	80	ASP
2	f	132	ALA
2	f	140	ARG
2	f	158	PHE
2	g	80	ASP
2	g	132	ALA
2	g	140	ARG
2	g	158	PHE

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Mol	Chain	Res	Type
2	h	80	ASP
2	h	132	ALA
2	h	140	ARG
2	h	158	PHE
2	i	80	ASP
2	i	132	ALA
2	i	140	ARG
2	i	158	PHE
2	j	80	ASP
2	j	132	ALA
2	j	140	ARG
2	j	158	PHE
1	M	8	LEU
1	M	49	THR
1	M	76	ILE
1	M	210	PRO
1	M	216	THR
1	M	295	GLY
1	M	302	PRO
1	M	381	SER
1	M	388	PRO
1	M	452	ASN
1	M	513	ARG
1	N	8	LEU
1	N	49	THR
1	N	76	ILE
1	N	210	PRO
1	N	216	THR
1	N	302	PRO
1	N	388	PRO
1	N	457	MSE
1	O	8	LEU
1	O	49	THR
1	O	210	PRO
1	O	216	THR
1	O	302	PRO
1	O	381	SER
1	O	388	PRO
1	O	452	ASN
1	O	457	MSE
1	P	8	LEU
1	P	76	ILE

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Mol	Chain	Res	Type
1	P	210	PRO
1	P	216	THR
1	P	295	GLY
1	P	302	PRO
1	P	381	SER
1	P	388	PRO
1	P	452	ASN
1	P	457	MSE
1	Q	8	LEU
1	Q	49	THR
1	Q	76	ILE
1	Q	210	PRO
1	Q	216	THR
1	Q	295	GLY
1	Q	302	PRO
1	Q	381	SER
1	Q	388	PRO
1	Q	457	MSE
1	Q	513	ARG
1	R	8	LEU
1	R	49	THR
1	R	76	ILE
1	R	210	PRO
1	R	216	THR
1	R	302	PRO
1	R	388	PRO
1	R	457	MSE
1	R	513	ARG
1	S	8	LEU
1	S	76	ILE
1	S	210	PRO
1	S	216	THR
1	S	302	PRO
1	S	381	SER
1	S	388	PRO
1	S	452	ASN
1	S	457	MSE
1	T	8	LEU
1	T	49	THR
1	T	76	ILE
1	T	210	PRO
1	T	216	THR

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Mol	Chain	Res	Type
1	T	295	GLY
1	T	302	PRO
1	T	381	SER
1	T	388	PRO
1	T	452	ASN
1	U	8	LEU
1	U	49	THR
1	U	76	ILE
1	U	210	PRO
1	U	216	THR
1	U	302	PRO
1	U	388	PRO
1	U	452	ASN
1	V	8	LEU
1	V	36	SER
1	V	49	THR
1	V	76	ILE
1	V	210	PRO
1	V	216	THR
1	V	302	PRO
1	V	388	PRO
1	V	513	ARG
1	W	8	LEU
1	W	49	THR
1	W	76	ILE
1	W	210	PRO
1	W	216	THR
1	W	302	PRO
1	W	388	PRO
1	W	452	ASN
1	W	457	MSE
1	W	513	ARG
1	X	8	LEU
1	X	49	THR
1	X	210	PRO
1	X	216	THR
1	X	302	PRO
1	X	381	SER
1	X	388	PRO
1	X	457	MSE
1	X	513	ARG
2	k	131	ARG

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Mol	Chain	Res	Type
2	m	69	GLU
2	m	131	ARG
2	n	69	GLU
2	o	69	GLU
2	o	131	ARG
2	p	69	GLU
2	p	131	ARG
2	q	131	ARG
2	s	69	GLU
2	s	131	ARG
2	t	69	GLU
2	t	131	ARG
2	u	131	ARG
2	v	131	ARG
1	A	26	ARG
1	A	36	SER
1	A	205	ASN
1	A	262	GLY
1	B	26	ARG
1	B	36	SER
1	B	205	ASN
1	B	262	GLY
1	C	26	ARG
1	C	36	SER
1	C	205	ASN
1	C	262	GLY
1	D	26	ARG
1	D	36	SER
1	D	205	ASN
1	D	262	GLY
1	E	26	ARG
1	E	36	SER
1	E	205	ASN
1	E	262	GLY
1	F	26	ARG
1	F	36	SER
1	F	205	ASN
1	F	262	GLY
1	G	26	ARG
1	G	36	SER
1	G	205	ASN
1	G	262	GLY

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Mol	Chain	Res	Type
1	H	26	ARG
1	H	36	SER
1	H	205	ASN
1	H	262	GLY
1	I	26	ARG
1	I	36	SER
1	I	205	ASN
1	I	262	GLY
1	J	26	ARG
1	J	36	SER
1	J	205	ASN
1	J	262	GLY
1	K	26	ARG
1	K	36	SER
1	K	205	ASN
1	K	262	GLY
1	L	26	ARG
1	L	36	SER
1	L	205	ASN
1	L	262	GLY
2	Y	54	ALA
2	Y	78	GLU
2	Z	54	ALA
2	Z	78	GLU
2	a	54	ALA
2	a	78	GLU
2	b	54	ALA
2	b	78	GLU
2	c	54	ALA
2	c	78	GLU
2	d	54	ALA
2	d	78	GLU
2	e	54	ALA
2	e	78	GLU
2	f	54	ALA
2	f	78	GLU
2	g	54	ALA
2	g	78	GLU
2	h	54	ALA
2	h	78	GLU
2	i	54	ALA
2	i	78	GLU

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Mol	Chain	Res	Type
2	j	54	ALA
2	j	78	GLU
1	M	192	ASP
1	M	198	ILE
1	M	244	VAL
1	M	457	MSE
1	M	583	LYS
1	N	36	SER
1	N	192	ASP
1	N	198	ILE
1	N	244	VAL
1	N	381	SER
1	N	452	ASN
1	N	583	LYS
1	O	36	SER
1	O	192	ASP
1	O	198	ILE
1	O	244	VAL
1	O	508	ASN
1	O	583	LYS
1	P	192	ASP
1	P	198	ILE
1	P	244	VAL
1	P	583	LYS
1	Q	36	SER
1	Q	192	ASP
1	Q	198	ILE
1	Q	244	VAL
1	Q	452	ASN
1	Q	583	LYS
1	R	36	SER
1	R	198	ILE
1	R	244	VAL
1	R	381	SER
1	R	452	ASN
1	R	583	LYS
1	S	36	SER
1	S	192	ASP
1	S	198	ILE
1	S	244	VAL
1	S	450	GLN
1	S	583	LYS

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Mol	Chain	Res	Type
1	T	192	ASP
1	T	198	ILE
1	T	244	VAL
1	T	457	MSE
1	T	583	LYS
1	U	36	SER
1	U	192	ASP
1	U	198	ILE
1	U	244	VAL
1	U	381	SER
1	U	457	MSE
1	U	583	LYS
1	V	192	ASP
1	V	198	ILE
1	V	244	VAL
1	V	381	SER
1	V	452	ASN
1	V	457	MSE
1	V	583	LYS
1	W	36	SER
1	W	192	ASP
1	W	198	ILE
1	W	244	VAL
1	W	381	SER
1	W	583	LYS
1	X	36	SER
1	X	192	ASP
1	X	198	ILE
1	X	244	VAL
1	X	452	ASN
1	X	583	LYS
2	k	132	MET
2	l	132	MET
2	m	132	MET
2	n	132	MET
2	o	132	MET
2	p	132	MET
2	q	132	MET
2	r	132	MET
2	s	132	MET
2	t	132	MET
2	u	132	MET

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Mol	Chain	Res	Type
2	v	132	MET
1	A	161	ASN
1	A	198	ILE
1	A	209	PHE
1	A	216	THR
1	A	244	VAL
1	A	253	ASP
1	A	380	ASN
1	A	583	LYS
1	B	161	ASN
1	B	198	ILE
1	B	209	PHE
1	B	216	THR
1	B	244	VAL
1	B	253	ASP
1	B	380	ASN
1	B	583	LYS
1	C	161	ASN
1	C	198	ILE
1	C	209	PHE
1	C	216	THR
1	C	244	VAL
1	C	253	ASP
1	C	380	ASN
1	C	583	LYS
1	D	161	ASN
1	D	198	ILE
1	D	209	PHE
1	D	216	THR
1	D	244	VAL
1	D	253	ASP
1	D	380	ASN
1	D	583	LYS
1	E	161	ASN
1	E	198	ILE
1	E	209	PHE
1	E	216	THR
1	E	244	VAL
1	E	253	ASP
1	E	380	ASN
1	E	583	LYS
1	F	161	ASN

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Mol	Chain	Res	Type
1	F	198	ILE
1	F	209	PHE
1	F	216	THR
1	F	244	VAL
1	F	253	ASP
1	F	380	ASN
1	F	583	LYS
1	G	161	ASN
1	G	198	ILE
1	G	209	PHE
1	G	216	THR
1	G	244	VAL
1	G	253	ASP
1	G	380	ASN
1	G	583	LYS
1	H	161	ASN
1	H	198	ILE
1	H	209	PHE
1	H	216	THR
1	H	244	VAL
1	H	253	ASP
1	H	380	ASN
1	H	583	LYS
1	I	161	ASN
1	I	198	ILE
1	I	209	PHE
1	I	216	THR
1	I	244	VAL
1	I	253	ASP
1	I	380	ASN
1	I	583	LYS
1	J	161	ASN
1	J	198	ILE
1	J	209	PHE
1	J	216	THR
1	J	244	VAL
1	J	253	ASP
1	J	380	ASN
1	J	583	LYS
1	K	161	ASN
1	K	198	ILE
1	K	209	PHE

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Mol	Chain	Res	Type
1	K	216	THR
1	K	244	VAL
1	K	253	ASP
1	K	380	ASN
1	K	583	LYS
1	L	161	ASN
1	L	198	ILE
1	L	209	PHE
1	L	216	THR
1	L	244	VAL
1	L	253	ASP
1	L	380	ASN
1	L	583	LYS
2	Y	141	MET
2	Y	149	PHE
2	Z	141	MET
2	Z	149	PHE
2	a	141	MET
2	a	149	PHE
2	b	141	MET
2	b	149	PHE
2	c	141	MET
2	c	149	PHE
2	d	141	MET
2	d	149	PHE
2	e	141	MET
2	e	149	PHE
2	f	141	MET
2	f	149	PHE
2	g	141	MET
2	g	149	PHE
2	h	141	MET
2	h	149	PHE
2	i	141	MET
2	i	149	PHE
2	j	141	MET
2	j	149	PHE
1	M	36	SER
1	M	344	THR
1	M	450	GLN
1	M	508	ASN
1	N	262	GLY

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Mol	Chain	Res	Type
1	N	344	THR
1	N	508	ASN
1	O	217	ILE
1	O	344	THR
1	P	445	GLU
1	P	450	GLN
1	P	508	ASN
1	Q	262	GLY
1	Q	450	GLN
1	Q	508	ASN
1	R	192	ASP
1	R	217	ILE
1	R	450	GLN
1	R	508	ASN
1	S	445	GLU
1	S	508	ASN
1	T	36	SER
1	T	217	ILE
1	T	262	GLY
1	T	450	GLN
1	T	508	ASN
1	U	262	GLY
1	U	344	THR
1	U	445	GLU
1	U	450	GLN
1	U	508	ASN
1	V	344	THR
1	V	450	GLN
1	V	508	ASN
1	W	217	ILE
1	W	344	THR
1	W	450	GLN
1	W	508	ASN
1	X	344	THR
1	X	445	GLU
1	X	508	ASN
2	k	44	MET
2	l	44	MET
2	n	44	MET
2	p	44	MET
2	q	44	MET
2	r	44	MET

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Mol	Chain	Res	Type
1	A	76	ILE
1	A	192	ASP
1	A	206	ASP
1	A	232	ALA
1	A	295	GLY
1	A	302	PRO
1	B	76	ILE
1	B	192	ASP
1	B	206	ASP
1	B	232	ALA
1	B	295	GLY
1	B	302	PRO
1	C	76	ILE
1	C	192	ASP
1	C	206	ASP
1	C	232	ALA
1	C	295	GLY
1	C	302	PRO
1	D	76	ILE
1	D	192	ASP
1	D	232	ALA
1	D	295	GLY
1	D	302	PRO
1	E	76	ILE
1	E	192	ASP
1	E	206	ASP
1	E	232	ALA
1	E	295	GLY
1	E	302	PRO
1	F	76	ILE
1	F	192	ASP
1	F	206	ASP
1	F	232	ALA
1	F	295	GLY
1	F	302	PRO
1	G	76	ILE
1	G	192	ASP
1	G	206	ASP
1	G	232	ALA
1	G	295	GLY
1	G	302	PRO
1	H	76	ILE

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Mol	Chain	Res	Type
1	H	192	ASP
1	H	206	ASP
1	H	232	ALA
1	H	295	GLY
1	H	302	PRO
1	I	76	ILE
1	I	192	ASP
1	I	232	ALA
1	I	295	GLY
1	I	302	PRO
1	J	76	ILE
1	J	192	ASP
1	J	206	ASP
1	J	232	ALA
1	J	295	GLY
1	J	302	PRO
1	K	76	ILE
1	K	192	ASP
1	K	206	ASP
1	K	232	ALA
1	K	295	GLY
1	K	302	PRO
1	L	76	ILE
1	L	192	ASP
1	L	206	ASP
1	L	232	ALA
1	L	295	GLY
1	L	302	PRO
1	M	203	ASN
1	M	217	ILE
1	M	262	GLY
1	M	397	VAL
1	N	203	ASN
1	N	217	ILE
1	N	445	GLU
1	N	450	GLN
1	O	203	ASN
1	O	262	GLY
1	O	397	VAL
1	O	450	GLN
1	P	203	ASN
1	P	262	GLY

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Mol	Chain	Res	Type
1	P	344	THR
1	Q	203	ASN
1	Q	217	ILE
1	Q	344	THR
1	Q	397	VAL
1	Q	498	ASP
1	R	203	ASN
1	R	262	GLY
1	R	344	THR
1	R	397	VAL
1	S	203	ASN
1	S	217	ILE
1	S	262	GLY
1	T	203	ASN
1	T	344	THR
1	U	203	ASN
1	U	217	ILE
1	V	203	ASN
1	V	217	ILE
1	V	262	GLY
1	W	203	ASN
1	W	262	GLY
1	W	445	GLU
1	X	203	ASN
1	X	217	ILE
1	X	262	GLY
1	X	397	VAL
1	X	450	GLN
2	o	44	MET
2	s	44	MET
2	t	44	MET
2	u	44	MET
1	A	311	GLU
1	A	384	LEU
1	B	311	GLU
1	B	384	LEU
1	B	507	LEU
1	C	311	GLU
1	C	384	LEU
1	C	507	LEU
1	D	206	ASP
1	D	311	GLU

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Mol	Chain	Res	Type
1	D	384	LEU
1	E	311	GLU
1	E	384	LEU
1	F	311	GLU
1	F	384	LEU
1	G	311	GLU
1	G	384	LEU
1	H	311	GLU
1	H	384	LEU
1	I	206	ASP
1	I	311	GLU
1	I	384	LEU
1	J	311	GLU
1	J	384	LEU
1	K	311	GLU
1	K	384	LEU
1	L	311	GLU
1	L	384	LEU
1	L	507	LEU
1	N	397	VAL
1	P	217	ILE
1	S	344	THR
1	S	397	VAL
1	T	397	VAL
1	V	397	VAL
1	W	397	VAL
2	k	140	PHE
2	l	140	PHE
2	m	140	PHE
2	n	140	PHE
2	s	140	PHE
2	t	140	PHE
2	v	140	PHE
1	A	203	ASN
1	B	203	ASN
1	C	203	ASN
1	D	203	ASN
1	E	203	ASN
1	F	203	ASN
1	G	203	ASN
1	H	203	ASN
1	I	203	ASN

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Mol	Chain	Res	Type
1	J	203	ASN
1	K	203	ASN
1	L	203	ASN
1	P	397	VAL
2	o	140	PHE
2	p	140	PHE
2	q	140	PHE
2	r	140	PHE
2	u	140	PHE
1	A	385	PRO
1	A	427	GLY
1	B	385	PRO
1	B	427	GLY
1	C	385	PRO
1	C	427	GLY
1	D	385	PRO
1	D	427	GLY
1	E	385	PRO
1	E	427	GLY
1	F	385	PRO
1	F	427	GLY
1	G	385	PRO
1	G	427	GLY
1	H	385	PRO
1	H	427	GLY
1	I	385	PRO
1	I	427	GLY
1	J	385	PRO
1	J	427	GLY
1	K	385	PRO
1	K	427	GLY
1	L	385	PRO
1	L	427	GLY
1	U	397	VAL
1	M	310	VAL
1	N	310	VAL
1	O	310	VAL
1	P	310	VAL
1	Q	310	VAL
1	R	310	VAL
1	S	310	VAL
1	T	310	VAL

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Mol	Chain	Res	Type
1	U	310	VAL
1	V	310	VAL
1	W	310	VAL
1	X	310	VAL
1	A	210	PRO
1	B	210	PRO
1	C	210	PRO
1	D	210	PRO
1	E	210	PRO
1	F	210	PRO
1	G	210	PRO
1	H	210	PRO
1	I	210	PRO
1	J	210	PRO
1	K	210	PRO
1	L	210	PRO

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	A	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	B	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	C	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	D	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	E	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	F	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	G	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	H	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	I	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	J	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	K	483/510 (95%)	412 (85%)	71 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	483/510 (95%)	412 (85%)	71 (15%)	3	13
1	M	485/510 (95%)	412 (85%)	73 (15%)	3	12
1	N	485/510 (95%)	412 (85%)	73 (15%)	3	12
1	O	485/510 (95%)	413 (85%)	72 (15%)	3	13
1	P	485/510 (95%)	413 (85%)	72 (15%)	3	13
1	Q	485/510 (95%)	412 (85%)	73 (15%)	3	12
1	R	485/510 (95%)	411 (85%)	74 (15%)	2	12
1	S	485/510 (95%)	411 (85%)	74 (15%)	2	12
1	T	485/510 (95%)	412 (85%)	73 (15%)	3	12
1	U	485/510 (95%)	413 (85%)	72 (15%)	3	13
1	V	485/510 (95%)	413 (85%)	72 (15%)	3	13
1	W	485/510 (95%)	413 (85%)	72 (15%)	3	13
1	X	485/510 (95%)	411 (85%)	74 (15%)	2	12
2	Y	98/132 (74%)	85 (87%)	13 (13%)	4	16
2	Z	98/132 (74%)	85 (87%)	13 (13%)	4	16
2	a	98/132 (74%)	84 (86%)	14 (14%)	3	14
2	b	98/132 (74%)	84 (86%)	14 (14%)	3	14
2	c	98/132 (74%)	85 (87%)	13 (13%)	4	16
2	d	98/132 (74%)	85 (87%)	13 (13%)	4	16
2	e	98/132 (74%)	85 (87%)	13 (13%)	4	16
2	f	98/132 (74%)	84 (86%)	14 (14%)	3	14
2	g	98/132 (74%)	84 (86%)	14 (14%)	3	14
2	h	98/132 (74%)	85 (87%)	13 (13%)	4	16
2	i	98/132 (74%)	85 (87%)	13 (13%)	4	16
2	j	98/132 (74%)	84 (86%)	14 (14%)	3	14
2	k	100/132 (76%)	88 (88%)	12 (12%)	5	20
2	l	100/132 (76%)	87 (87%)	13 (13%)	4	17
2	m	100/132 (76%)	88 (88%)	12 (12%)	5	20
2	n	100/132 (76%)	87 (87%)	13 (13%)	4	17
2	o	100/132 (76%)	85 (85%)	15 (15%)	3	12
2	p	100/132 (76%)	86 (86%)	14 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	q	100/132 (76%)	88 (88%)	12 (12%)	5	20
2	r	100/132 (76%)	88 (88%)	12 (12%)	5	20
2	s	100/132 (76%)	87 (87%)	13 (13%)	4	17
2	t	100/132 (76%)	87 (87%)	13 (13%)	4	17
2	u	100/132 (76%)	87 (87%)	13 (13%)	4	17
2	v	100/132 (76%)	87 (87%)	13 (13%)	4	17
All	All	13992/15408 (91%)	11950 (85%)	2042 (15%)	3	13

All (2042) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	14	ARG
1	M	15	PHE
1	M	24	GLU
1	M	30	LYS
1	M	31	ASN
1	M	33	LEU
1	M	40	GLN
1	M	42	ASP
1	M	47	GLN
1	M	49	THR
1	M	50	THR
1	M	56	GLN
1	M	59	VAL
1	M	61	ARG
1	M	69	SER
1	M	79	LEU
1	M	94	LEU
1	M	101	ASP
1	M	123	VAL
1	M	127	ARG
1	M	133	GLU
1	M	135	GLN
1	M	144	ILE
1	M	156	VAL
1	M	157	ILE
1	M	158	TRP
1	M	161	ASN
1	M	164	LEU
1	M	174	THR

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Mol	Chain	Res	Type
1	M	175	VAL
1	M	190	LYS
1	M	201	PHE
1	M	202	GLN
1	M	209	PHE
1	M	211	TRP
1	M	217	ILE
1	M	218	GLN
1	M	226	VAL
1	M	228	LYS
1	M	231	THR
1	M	234	ILE
1	M	246	TYR
1	M	248	LYS
1	M	265	LYS
1	M	266	ILE
1	M	275	ARG
1	M	286	VAL
1	M	293	ILE
1	M	298	ILE
1	M	301	VAL
1	M	311	GLU
1	M	327	GLN
1	M	343	ARG
1	M	356	ILE
1	M	359	PHE
1	M	376	ARG
1	M	378	ASP
1	M	384	LEU
1	M	387	GLN
1	M	389	LEU
1	M	405	LEU
1	M	430	VAL
1	M	433	ASP
1	M	444	LEU
1	M	451	ASP
1	M	510	ILE
1	M	513	ARG
1	M	518	THR
1	M	541	LYS
1	M	546	THR
1	M	558	THR

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Mol	Chain	Res	Type
1	M	592	TRP
1	M	593	LEU
1	N	14	ARG
1	N	15	PHE
1	N	24	GLU
1	N	30	LYS
1	N	31	ASN
1	N	33	LEU
1	N	40	GLN
1	N	42	ASP
1	N	47	GLN
1	N	49	THR
1	N	50	THR
1	N	56	GLN
1	N	59	VAL
1	N	61	ARG
1	N	69	SER
1	N	79	LEU
1	N	94	LEU
1	N	101	ASP
1	N	123	VAL
1	N	127	ARG
1	N	133	GLU
1	N	135	GLN
1	N	144	ILE
1	N	156	VAL
1	N	157	ILE
1	N	158	TRP
1	N	161	ASN
1	N	164	LEU
1	N	174	THR
1	N	175	VAL
1	N	190	LYS
1	N	201	PHE
1	N	202	GLN
1	N	209	PHE
1	N	211	TRP
1	N	217	ILE
1	N	218	GLN
1	N	226	VAL
1	N	228	LYS
1	N	231	THR

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Mol	Chain	Res	Type
1	N	234	ILE
1	N	246	TYR
1	N	248	LYS
1	N	265	LYS
1	N	266	ILE
1	N	273	ARG
1	N	275	ARG
1	N	286	VAL
1	N	293	ILE
1	N	298	ILE
1	N	301	VAL
1	N	327	GLN
1	N	343	ARG
1	N	356	ILE
1	N	359	PHE
1	N	376	ARG
1	N	378	ASP
1	N	384	LEU
1	N	387	GLN
1	N	389	LEU
1	N	405	LEU
1	N	430	VAL
1	N	433	ASP
1	N	444	LEU
1	N	451	ASP
1	N	510	ILE
1	N	513	ARG
1	N	518	THR
1	N	541	LYS
1	N	546	THR
1	N	558	THR
1	N	592	TRP
1	N	593	LEU
1	O	14	ARG
1	O	15	PHE
1	O	24	GLU
1	O	30	LYS
1	O	31	ASN
1	O	33	LEU
1	O	40	GLN
1	O	42	ASP
1	O	47	GLN

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Mol	Chain	Res	Type
1	O	49	THR
1	O	50	THR
1	O	56	GLN
1	O	59	VAL
1	O	61	ARG
1	O	69	SER
1	O	79	LEU
1	O	94	LEU
1	O	101	ASP
1	O	123	VAL
1	O	127	ARG
1	O	133	GLU
1	O	135	GLN
1	O	144	ILE
1	O	156	VAL
1	O	157	ILE
1	O	158	TRP
1	O	161	ASN
1	O	164	LEU
1	O	174	THR
1	O	175	VAL
1	O	190	LYS
1	O	201	PHE
1	O	202	GLN
1	O	209	PHE
1	O	211	TRP
1	O	217	ILE
1	O	218	GLN
1	O	225	VAL
1	O	226	VAL
1	O	228	LYS
1	O	231	THR
1	O	234	ILE
1	O	246	TYR
1	O	248	LYS
1	O	265	LYS
1	O	266	ILE
1	O	275	ARG
1	O	286	VAL
1	O	293	ILE
1	O	298	ILE
1	O	301	VAL

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Mol	Chain	Res	Type
1	O	327	GLN
1	O	343	ARG
1	O	356	ILE
1	O	359	PHE
1	O	376	ARG
1	O	378	ASP
1	O	384	LEU
1	O	387	GLN
1	O	389	LEU
1	O	405	LEU
1	O	433	ASP
1	O	444	LEU
1	O	451	ASP
1	O	510	ILE
1	O	513	ARG
1	O	518	THR
1	O	541	LYS
1	O	546	THR
1	O	558	THR
1	O	592	TRP
1	O	593	LEU
1	P	14	ARG
1	P	15	PHE
1	P	24	GLU
1	P	30	LYS
1	P	31	ASN
1	P	33	LEU
1	P	40	GLN
1	P	42	ASP
1	P	47	GLN
1	P	49	THR
1	P	50	THR
1	P	56	GLN
1	P	59	VAL
1	P	61	ARG
1	P	69	SER
1	P	79	LEU
1	P	94	LEU
1	P	101	ASP
1	P	123	VAL
1	P	127	ARG
1	P	133	GLU

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Mol	Chain	Res	Type
1	P	135	GLN
1	P	144	ILE
1	P	156	VAL
1	P	157	ILE
1	P	158	TRP
1	P	161	ASN
1	P	164	LEU
1	P	174	THR
1	P	175	VAL
1	P	190	LYS
1	P	201	PHE
1	P	202	GLN
1	P	209	PHE
1	P	211	TRP
1	P	217	ILE
1	P	218	GLN
1	P	225	VAL
1	P	226	VAL
1	P	228	LYS
1	P	231	THR
1	P	234	ILE
1	P	246	TYR
1	P	248	LYS
1	P	265	LYS
1	P	266	ILE
1	P	275	ARG
1	P	286	VAL
1	P	293	ILE
1	P	298	ILE
1	P	301	VAL
1	P	327	GLN
1	P	343	ARG
1	P	356	ILE
1	P	359	PHE
1	P	376	ARG
1	P	378	ASP
1	P	384	LEU
1	P	387	GLN
1	P	389	LEU
1	P	430	VAL
1	P	433	ASP
1	P	444	LEU

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Mol	Chain	Res	Type
1	P	451	ASP
1	P	510	ILE
1	P	513	ARG
1	P	518	THR
1	P	541	LYS
1	P	546	THR
1	P	558	THR
1	P	592	TRP
1	P	593	LEU
1	Q	14	ARG
1	Q	15	PHE
1	Q	24	GLU
1	Q	30	LYS
1	Q	31	ASN
1	Q	33	LEU
1	Q	40	GLN
1	Q	42	ASP
1	Q	47	GLN
1	Q	49	THR
1	Q	50	THR
1	Q	56	GLN
1	Q	59	VAL
1	Q	61	ARG
1	Q	69	SER
1	Q	79	LEU
1	Q	94	LEU
1	Q	101	ASP
1	Q	123	VAL
1	Q	127	ARG
1	Q	133	GLU
1	Q	135	GLN
1	Q	144	ILE
1	Q	156	VAL
1	Q	157	ILE
1	Q	158	TRP
1	Q	161	ASN
1	Q	164	LEU
1	Q	174	THR
1	Q	175	VAL
1	Q	190	LYS
1	Q	201	PHE
1	Q	202	GLN

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Mol	Chain	Res	Type
1	Q	209	PHE
1	Q	211	TRP
1	Q	217	ILE
1	Q	218	GLN
1	Q	225	VAL
1	Q	226	VAL
1	Q	228	LYS
1	Q	231	THR
1	Q	234	ILE
1	Q	246	TYR
1	Q	248	LYS
1	Q	265	LYS
1	Q	266	ILE
1	Q	275	ARG
1	Q	286	VAL
1	Q	293	ILE
1	Q	298	ILE
1	Q	301	VAL
1	Q	327	GLN
1	Q	343	ARG
1	Q	356	ILE
1	Q	359	PHE
1	Q	376	ARG
1	Q	378	ASP
1	Q	384	LEU
1	Q	387	GLN
1	Q	389	LEU
1	Q	405	LEU
1	Q	430	VAL
1	Q	433	ASP
1	Q	444	LEU
1	Q	451	ASP
1	Q	510	ILE
1	Q	513	ARG
1	Q	518	THR
1	Q	541	LYS
1	Q	546	THR
1	Q	558	THR
1	Q	592	TRP
1	Q	593	LEU
1	R	14	ARG
1	R	15	PHE

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Mol	Chain	Res	Type
1	R	24	GLU
1	R	30	LYS
1	R	31	ASN
1	R	33	LEU
1	R	40	GLN
1	R	42	ASP
1	R	47	GLN
1	R	49	THR
1	R	50	THR
1	R	56	GLN
1	R	59	VAL
1	R	69	SER
1	R	79	LEU
1	R	94	LEU
1	R	101	ASP
1	R	123	VAL
1	R	127	ARG
1	R	133	GLU
1	R	135	GLN
1	R	144	ILE
1	R	156	VAL
1	R	157	ILE
1	R	158	TRP
1	R	161	ASN
1	R	164	LEU
1	R	174	THR
1	R	175	VAL
1	R	190	LYS
1	R	201	PHE
1	R	202	GLN
1	R	209	PHE
1	R	211	TRP
1	R	217	ILE
1	R	218	GLN
1	R	225	VAL
1	R	226	VAL
1	R	228	LYS
1	R	231	THR
1	R	234	ILE
1	R	246	TYR
1	R	248	LYS
1	R	265	LYS

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Mol	Chain	Res	Type
1	R	266	ILE
1	R	275	ARG
1	R	286	VAL
1	R	293	ILE
1	R	298	ILE
1	R	301	VAL
1	R	311	GLU
1	R	315	VAL
1	R	327	GLN
1	R	343	ARG
1	R	356	ILE
1	R	359	PHE
1	R	376	ARG
1	R	378	ASP
1	R	384	LEU
1	R	387	GLN
1	R	389	LEU
1	R	405	LEU
1	R	430	VAL
1	R	433	ASP
1	R	444	LEU
1	R	451	ASP
1	R	510	ILE
1	R	513	ARG
1	R	518	THR
1	R	541	LYS
1	R	546	THR
1	R	558	THR
1	R	592	TRP
1	R	593	LEU
1	S	14	ARG
1	S	15	PHE
1	S	24	GLU
1	S	30	LYS
1	S	31	ASN
1	S	33	LEU
1	S	40	GLN
1	S	42	ASP
1	S	47	GLN
1	S	49	THR
1	S	50	THR
1	S	56	GLN

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Mol	Chain	Res	Type
1	S	59	VAL
1	S	61	ARG
1	S	69	SER
1	S	79	LEU
1	S	94	LEU
1	S	101	ASP
1	S	123	VAL
1	S	127	ARG
1	S	133	GLU
1	S	135	GLN
1	S	144	ILE
1	S	156	VAL
1	S	157	ILE
1	S	158	TRP
1	S	161	ASN
1	S	164	LEU
1	S	174	THR
1	S	175	VAL
1	S	190	LYS
1	S	201	PHE
1	S	202	GLN
1	S	209	PHE
1	S	211	TRP
1	S	217	ILE
1	S	218	GLN
1	S	225	VAL
1	S	226	VAL
1	S	228	LYS
1	S	231	THR
1	S	234	ILE
1	S	246	TYR
1	S	248	LYS
1	S	265	LYS
1	S	266	ILE
1	S	275	ARG
1	S	286	VAL
1	S	293	ILE
1	S	298	ILE
1	S	301	VAL
1	S	311	GLU
1	S	327	GLN
1	S	343	ARG

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Mol	Chain	Res	Type
1	S	356	ILE
1	S	359	PHE
1	S	376	ARG
1	S	378	ASP
1	S	384	LEU
1	S	387	GLN
1	S	389	LEU
1	S	405	LEU
1	S	430	VAL
1	S	433	ASP
1	S	444	LEU
1	S	451	ASP
1	S	510	ILE
1	S	513	ARG
1	S	518	THR
1	S	541	LYS
1	S	546	THR
1	S	558	THR
1	S	592	TRP
1	S	593	LEU
1	T	14	ARG
1	T	15	PHE
1	T	24	GLU
1	T	30	LYS
1	T	31	ASN
1	T	33	LEU
1	T	40	GLN
1	T	42	ASP
1	T	47	GLN
1	T	49	THR
1	T	50	THR
1	T	56	GLN
1	T	59	VAL
1	T	61	ARG
1	T	69	SER
1	T	79	LEU
1	T	94	LEU
1	T	101	ASP
1	T	123	VAL
1	T	127	ARG
1	T	133	GLU
1	T	135	GLN

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Mol	Chain	Res	Type
1	T	144	ILE
1	T	156	VAL
1	T	157	ILE
1	T	158	TRP
1	T	161	ASN
1	T	164	LEU
1	T	174	THR
1	T	175	VAL
1	T	190	LYS
1	T	201	PHE
1	T	202	GLN
1	T	209	PHE
1	T	211	TRP
1	T	217	ILE
1	T	218	GLN
1	T	225	VAL
1	T	226	VAL
1	T	228	LYS
1	T	231	THR
1	T	234	ILE
1	T	246	TYR
1	T	248	LYS
1	T	265	LYS
1	T	266	ILE
1	T	275	ARG
1	T	286	VAL
1	T	293	ILE
1	T	298	ILE
1	T	301	VAL
1	T	327	GLN
1	T	343	ARG
1	T	356	ILE
1	T	359	PHE
1	T	376	ARG
1	T	378	ASP
1	T	384	LEU
1	T	387	GLN
1	T	389	LEU
1	T	405	LEU
1	T	430	VAL
1	T	433	ASP
1	T	444	LEU

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Mol	Chain	Res	Type
1	T	451	ASP
1	T	510	ILE
1	T	513	ARG
1	T	518	THR
1	T	541	LYS
1	T	546	THR
1	T	558	THR
1	T	592	TRP
1	T	593	LEU
1	U	14	ARG
1	U	15	PHE
1	U	24	GLU
1	U	30	LYS
1	U	31	ASN
1	U	33	LEU
1	U	40	GLN
1	U	42	ASP
1	U	47	GLN
1	U	49	THR
1	U	50	THR
1	U	56	GLN
1	U	59	VAL
1	U	61	ARG
1	U	69	SER
1	U	79	LEU
1	U	94	LEU
1	U	101	ASP
1	U	123	VAL
1	U	127	ARG
1	U	133	GLU
1	U	135	GLN
1	U	144	ILE
1	U	156	VAL
1	U	157	ILE
1	U	158	TRP
1	U	161	ASN
1	U	164	LEU
1	U	174	THR
1	U	175	VAL
1	U	190	LYS
1	U	201	PHE
1	U	202	GLN

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Mol	Chain	Res	Type
1	U	209	PHE
1	U	211	TRP
1	U	217	ILE
1	U	218	GLN
1	U	226	VAL
1	U	228	LYS
1	U	231	THR
1	U	234	ILE
1	U	246	TYR
1	U	248	LYS
1	U	265	LYS
1	U	266	ILE
1	U	275	ARG
1	U	286	VAL
1	U	293	ILE
1	U	298	ILE
1	U	301	VAL
1	U	327	GLN
1	U	343	ARG
1	U	356	ILE
1	U	359	PHE
1	U	376	ARG
1	U	378	ASP
1	U	384	LEU
1	U	387	GLN
1	U	389	LEU
1	U	405	LEU
1	U	430	VAL
1	U	433	ASP
1	U	444	LEU
1	U	451	ASP
1	U	510	ILE
1	U	513	ARG
1	U	518	THR
1	U	541	LYS
1	U	546	THR
1	U	558	THR
1	U	592	TRP
1	U	593	LEU
1	V	14	ARG
1	V	15	PHE
1	V	24	GLU

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Mol	Chain	Res	Type
1	V	30	LYS
1	V	31	ASN
1	V	33	LEU
1	V	40	GLN
1	V	42	ASP
1	V	47	GLN
1	V	49	THR
1	V	50	THR
1	V	56	GLN
1	V	59	VAL
1	V	61	ARG
1	V	69	SER
1	V	79	LEU
1	V	94	LEU
1	V	101	ASP
1	V	123	VAL
1	V	127	ARG
1	V	133	GLU
1	V	135	GLN
1	V	144	ILE
1	V	156	VAL
1	V	157	ILE
1	V	158	TRP
1	V	161	ASN
1	V	164	LEU
1	V	174	THR
1	V	175	VAL
1	V	190	LYS
1	V	201	PHE
1	V	202	GLN
1	V	209	PHE
1	V	211	TRP
1	V	217	ILE
1	V	218	GLN
1	V	226	VAL
1	V	228	LYS
1	V	231	THR
1	V	234	ILE
1	V	246	TYR
1	V	248	LYS
1	V	265	LYS
1	V	266	ILE

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Mol	Chain	Res	Type
1	V	275	ARG
1	V	286	VAL
1	V	293	ILE
1	V	298	ILE
1	V	301	VAL
1	V	327	GLN
1	V	343	ARG
1	V	356	ILE
1	V	359	PHE
1	V	376	ARG
1	V	378	ASP
1	V	384	LEU
1	V	387	GLN
1	V	389	LEU
1	V	405	LEU
1	V	430	VAL
1	V	433	ASP
1	V	444	LEU
1	V	451	ASP
1	V	510	ILE
1	V	513	ARG
1	V	518	THR
1	V	541	LYS
1	V	546	THR
1	V	558	THR
1	V	592	TRP
1	V	593	LEU
1	W	14	ARG
1	W	15	PHE
1	W	24	GLU
1	W	30	LYS
1	W	31	ASN
1	W	33	LEU
1	W	40	GLN
1	W	42	ASP
1	W	47	GLN
1	W	49	THR
1	W	50	THR
1	W	56	GLN
1	W	59	VAL
1	W	61	ARG
1	W	69	SER

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Mol	Chain	Res	Type
1	W	79	LEU
1	W	94	LEU
1	W	101	ASP
1	W	123	VAL
1	W	127	ARG
1	W	133	GLU
1	W	135	GLN
1	W	144	ILE
1	W	156	VAL
1	W	157	ILE
1	W	158	TRP
1	W	161	ASN
1	W	164	LEU
1	W	174	THR
1	W	175	VAL
1	W	190	LYS
1	W	201	PHE
1	W	202	GLN
1	W	209	PHE
1	W	211	TRP
1	W	217	ILE
1	W	218	GLN
1	W	225	VAL
1	W	226	VAL
1	W	228	LYS
1	W	231	THR
1	W	234	ILE
1	W	246	TYR
1	W	248	LYS
1	W	265	LYS
1	W	266	ILE
1	W	275	ARG
1	W	286	VAL
1	W	293	ILE
1	W	298	ILE
1	W	301	VAL
1	W	327	GLN
1	W	343	ARG
1	W	356	ILE
1	W	359	PHE
1	W	376	ARG
1	W	378	ASP

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Mol	Chain	Res	Type
1	W	384	LEU
1	W	387	GLN
1	W	389	LEU
1	W	430	VAL
1	W	433	ASP
1	W	444	LEU
1	W	451	ASP
1	W	510	ILE
1	W	513	ARG
1	W	518	THR
1	W	541	LYS
1	W	546	THR
1	W	558	THR
1	W	592	TRP
1	W	593	LEU
1	X	14	ARG
1	X	15	PHE
1	X	24	GLU
1	X	30	LYS
1	X	31	ASN
1	X	33	LEU
1	X	40	GLN
1	X	42	ASP
1	X	47	GLN
1	X	49	THR
1	X	50	THR
1	X	56	GLN
1	X	59	VAL
1	X	69	SER
1	X	79	LEU
1	X	94	LEU
1	X	101	ASP
1	X	123	VAL
1	X	127	ARG
1	X	133	GLU
1	X	135	GLN
1	X	144	ILE
1	X	156	VAL
1	X	157	ILE
1	X	158	TRP
1	X	161	ASN
1	X	164	LEU

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Mol	Chain	Res	Type
1	X	174	THR
1	X	175	VAL
1	X	190	LYS
1	X	201	PHE
1	X	202	GLN
1	X	209	PHE
1	X	211	TRP
1	X	217	ILE
1	X	218	GLN
1	X	225	VAL
1	X	226	VAL
1	X	228	LYS
1	X	231	THR
1	X	234	ILE
1	X	246	TYR
1	X	248	LYS
1	X	265	LYS
1	X	266	ILE
1	X	275	ARG
1	X	286	VAL
1	X	293	ILE
1	X	298	ILE
1	X	301	VAL
1	X	311	GLU
1	X	327	GLN
1	X	343	ARG
1	X	356	ILE
1	X	359	PHE
1	X	376	ARG
1	X	378	ASP
1	X	384	LEU
1	X	387	GLN
1	X	389	LEU
1	X	405	LEU
1	X	430	VAL
1	X	433	ASP
1	X	444	LEU
1	X	451	ASP
1	X	510	ILE
1	X	513	ARG
1	X	518	THR
1	X	541	LYS

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Mol	Chain	Res	Type
1	X	546	THR
1	X	558	THR
1	X	561	ASP
1	X	592	TRP
1	X	593	LEU
2	k	16	LYS
2	k	27	ASP
2	k	29	GLU
2	k	33	MET
2	k	39	ASP
2	k	69	GLU
2	k	71	ASP
2	k	84	PHE
2	k	87	LEU
2	k	130	SER
2	k	131	ARG
2	k	136	SER
2	l	16	LYS
2	l	27	ASP
2	l	29	GLU
2	l	33	MET
2	l	39	ASP
2	l	69	GLU
2	l	71	ASP
2	l	84	PHE
2	l	87	LEU
2	l	100	THR
2	l	130	SER
2	l	131	ARG
2	l	136	SER
2	m	16	LYS
2	m	27	ASP
2	m	29	GLU
2	m	33	MET
2	m	39	ASP
2	m	69	GLU
2	m	71	ASP
2	m	84	PHE
2	m	87	LEU
2	m	130	SER
2	m	131	ARG
2	m	136	SER

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Mol	Chain	Res	Type
2	n	16	LYS
2	n	27	ASP
2	n	29	GLU
2	n	33	MET
2	n	39	ASP
2	n	56	THR
2	n	69	GLU
2	n	71	ASP
2	n	84	PHE
2	n	87	LEU
2	n	130	SER
2	n	131	ARG
2	n	136	SER
2	o	16	LYS
2	o	27	ASP
2	o	29	GLU
2	o	33	MET
2	o	37	VAL
2	o	39	ASP
2	o	56	THR
2	o	69	GLU
2	o	71	ASP
2	o	84	PHE
2	o	87	LEU
2	o	100	THR
2	o	130	SER
2	o	131	ARG
2	o	136	SER
2	p	16	LYS
2	p	27	ASP
2	p	29	GLU
2	p	33	MET
2	p	37	VAL
2	p	39	ASP
2	p	56	THR
2	p	69	GLU
2	p	71	ASP
2	p	84	PHE
2	p	87	LEU
2	p	130	SER
2	p	131	ARG
2	p	136	SER

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Mol	Chain	Res	Type
2	q	16	LYS
2	q	27	ASP
2	q	29	GLU
2	q	33	MET
2	q	39	ASP
2	q	69	GLU
2	q	71	ASP
2	q	84	PHE
2	q	87	LEU
2	q	130	SER
2	q	131	ARG
2	q	136	SER
2	r	16	LYS
2	r	27	ASP
2	r	29	GLU
2	r	33	MET
2	r	39	ASP
2	r	69	GLU
2	r	71	ASP
2	r	84	PHE
2	r	87	LEU
2	r	130	SER
2	r	131	ARG
2	r	136	SER
2	s	16	LYS
2	s	27	ASP
2	s	29	GLU
2	s	33	MET
2	s	37	VAL
2	s	39	ASP
2	s	69	GLU
2	s	71	ASP
2	s	84	PHE
2	s	87	LEU
2	s	130	SER
2	s	131	ARG
2	s	136	SER
2	t	16	LYS
2	t	27	ASP
2	t	29	GLU
2	t	33	MET
2	t	39	ASP

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Mol	Chain	Res	Type
2	t	56	THR
2	t	69	GLU
2	t	71	ASP
2	t	84	PHE
2	t	87	LEU
2	t	130	SER
2	t	131	ARG
2	t	136	SER
2	u	16	LYS
2	u	27	ASP
2	u	29	GLU
2	u	33	MET
2	u	39	ASP
2	u	69	GLU
2	u	71	ASP
2	u	84	PHE
2	u	87	LEU
2	u	100	THR
2	u	130	SER
2	u	131	ARG
2	u	136	SER
2	v	16	LYS
2	v	27	ASP
2	v	29	GLU
2	v	33	MET
2	v	37	VAL
2	v	39	ASP
2	v	69	GLU
2	v	71	ASP
2	v	84	PHE
2	v	87	LEU
2	v	130	SER
2	v	131	ARG
2	v	136	SER
1	A	14	ARG
1	A	15	PHE
1	A	24	GLU
1	A	30	LYS
1	A	31	ASN
1	A	33	LEU
1	A	37	ARG
1	A	42	ASP

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Mol	Chain	Res	Type
1	A	43	ASP
1	A	45	LEU
1	A	47	GLN
1	A	56	GLN
1	A	61	ARG
1	A	79	LEU
1	A	118	GLN
1	A	123	VAL
1	A	127	ARG
1	A	133	GLU
1	A	135	GLN
1	A	144	ILE
1	A	157	ILE
1	A	158	TRP
1	A	161	ASN
1	A	164	LEU
1	A	168	SER
1	A	174	THR
1	A	190	LYS
1	A	201	PHE
1	A	202	GLN
1	A	209	PHE
1	A	211	TRP
1	A	217	ILE
1	A	218	GLN
1	A	226	VAL
1	A	234	ILE
1	A	246	TYR
1	A	248	LYS
1	A	265	LYS
1	A	266	ILE
1	A	273	ARG
1	A	275	ARG
1	A	286	VAL
1	A	293	ILE
1	A	301	VAL
1	A	315	VAL
1	A	325	ASP
1	A	327	GLN
1	A	343	ARG
1	A	359	PHE
1	A	376	ARG

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Mol	Chain	Res	Type
1	A	384	LEU
1	A	387	GLN
1	A	389	LEU
1	A	405	LEU
1	A	421	ASP
1	A	422	THR
1	A	430	VAL
1	A	432	PHE
1	A	433	ASP
1	A	438	LEU
1	A	444	LEU
1	A	507	LEU
1	A	513	ARG
1	A	518	THR
1	A	529	GLN
1	A	541	LYS
1	A	546	THR
1	A	555	GLN
1	A	592	TRP
1	A	593	LEU
1	A	597	GLN
1	B	14	ARG
1	B	15	PHE
1	B	24	GLU
1	B	30	LYS
1	B	31	ASN
1	B	33	LEU
1	B	37	ARG
1	B	42	ASP
1	B	43	ASP
1	B	45	LEU
1	B	47	GLN
1	B	56	GLN
1	B	61	ARG
1	B	79	LEU
1	B	118	GLN
1	B	123	VAL
1	B	127	ARG
1	B	133	GLU
1	B	135	GLN
1	B	144	ILE
1	B	157	ILE

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Mol	Chain	Res	Type
1	B	158	TRP
1	B	161	ASN
1	B	164	LEU
1	B	168	SER
1	B	174	THR
1	B	190	LYS
1	B	201	PHE
1	B	202	GLN
1	B	209	PHE
1	B	211	TRP
1	B	217	ILE
1	B	218	GLN
1	B	226	VAL
1	B	234	ILE
1	B	246	TYR
1	B	248	LYS
1	B	265	LYS
1	B	266	ILE
1	B	273	ARG
1	B	275	ARG
1	B	286	VAL
1	B	293	ILE
1	B	301	VAL
1	B	315	VAL
1	B	325	ASP
1	B	327	GLN
1	B	343	ARG
1	B	359	PHE
1	B	376	ARG
1	B	384	LEU
1	B	387	GLN
1	B	389	LEU
1	B	405	LEU
1	B	421	ASP
1	B	422	THR
1	B	430	VAL
1	B	432	PHE
1	B	433	ASP
1	B	438	LEU
1	B	444	LEU
1	B	507	LEU
1	B	513	ARG

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Mol	Chain	Res	Type
1	B	518	THR
1	B	529	GLN
1	B	541	LYS
1	B	546	THR
1	B	555	GLN
1	B	592	TRP
1	B	593	LEU
1	B	597	GLN
1	C	14	ARG
1	C	15	PHE
1	C	24	GLU
1	C	30	LYS
1	C	31	ASN
1	C	33	LEU
1	C	37	ARG
1	C	42	ASP
1	C	43	ASP
1	C	45	LEU
1	C	47	GLN
1	C	56	GLN
1	C	61	ARG
1	C	79	LEU
1	C	118	GLN
1	C	123	VAL
1	C	127	ARG
1	C	133	GLU
1	C	135	GLN
1	C	144	ILE
1	C	157	ILE
1	C	158	TRP
1	C	161	ASN
1	C	164	LEU
1	C	168	SER
1	C	174	THR
1	C	190	LYS
1	C	201	PHE
1	C	202	GLN
1	C	209	PHE
1	C	211	TRP
1	C	217	ILE
1	C	218	GLN
1	C	226	VAL

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Mol	Chain	Res	Type
1	C	234	ILE
1	C	246	TYR
1	C	248	LYS
1	C	265	LYS
1	C	266	ILE
1	C	273	ARG
1	C	275	ARG
1	C	286	VAL
1	C	293	ILE
1	C	301	VAL
1	C	315	VAL
1	C	325	ASP
1	C	327	GLN
1	C	343	ARG
1	C	359	PHE
1	C	376	ARG
1	C	384	LEU
1	C	387	GLN
1	C	389	LEU
1	C	405	LEU
1	C	421	ASP
1	C	422	THR
1	C	430	VAL
1	C	432	PHE
1	C	433	ASP
1	C	438	LEU
1	C	444	LEU
1	C	507	LEU
1	C	513	ARG
1	C	518	THR
1	C	529	GLN
1	C	541	LYS
1	C	546	THR
1	C	555	GLN
1	C	592	TRP
1	C	593	LEU
1	C	597	GLN
1	D	14	ARG
1	D	15	PHE
1	D	24	GLU
1	D	30	LYS
1	D	31	ASN

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Mol	Chain	Res	Type
1	D	33	LEU
1	D	37	ARG
1	D	42	ASP
1	D	43	ASP
1	D	45	LEU
1	D	47	GLN
1	D	56	GLN
1	D	61	ARG
1	D	79	LEU
1	D	118	GLN
1	D	123	VAL
1	D	127	ARG
1	D	133	GLU
1	D	135	GLN
1	D	144	ILE
1	D	157	ILE
1	D	158	TRP
1	D	161	ASN
1	D	164	LEU
1	D	168	SER
1	D	174	THR
1	D	190	LYS
1	D	201	PHE
1	D	202	GLN
1	D	209	PHE
1	D	211	TRP
1	D	217	ILE
1	D	218	GLN
1	D	226	VAL
1	D	234	ILE
1	D	246	TYR
1	D	248	LYS
1	D	265	LYS
1	D	266	ILE
1	D	273	ARG
1	D	275	ARG
1	D	286	VAL
1	D	293	ILE
1	D	301	VAL
1	D	315	VAL
1	D	325	ASP
1	D	327	GLN

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Mol	Chain	Res	Type
1	D	343	ARG
1	D	359	PHE
1	D	376	ARG
1	D	384	LEU
1	D	387	GLN
1	D	389	LEU
1	D	405	LEU
1	D	421	ASP
1	D	422	THR
1	D	430	VAL
1	D	432	PHE
1	D	433	ASP
1	D	438	LEU
1	D	444	LEU
1	D	507	LEU
1	D	513	ARG
1	D	518	THR
1	D	529	GLN
1	D	541	LYS
1	D	546	THR
1	D	555	GLN
1	D	592	TRP
1	D	593	LEU
1	D	597	GLN
1	E	14	ARG
1	E	15	PHE
1	E	24	GLU
1	E	30	LYS
1	E	31	ASN
1	E	33	LEU
1	E	37	ARG
1	E	42	ASP
1	E	43	ASP
1	E	45	LEU
1	E	47	GLN
1	E	56	GLN
1	E	61	ARG
1	E	79	LEU
1	E	118	GLN
1	E	123	VAL
1	E	127	ARG
1	E	133	GLU

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Mol	Chain	Res	Type
1	E	135	GLN
1	E	144	ILE
1	E	157	ILE
1	E	158	TRP
1	E	161	ASN
1	E	164	LEU
1	E	168	SER
1	E	174	THR
1	E	190	LYS
1	E	201	PHE
1	E	202	GLN
1	E	209	PHE
1	E	211	TRP
1	E	217	ILE
1	E	218	GLN
1	E	226	VAL
1	E	234	ILE
1	E	246	TYR
1	E	248	LYS
1	E	265	LYS
1	E	266	ILE
1	E	273	ARG
1	E	275	ARG
1	E	286	VAL
1	E	293	ILE
1	E	301	VAL
1	E	315	VAL
1	E	325	ASP
1	E	327	GLN
1	E	343	ARG
1	E	359	PHE
1	E	376	ARG
1	E	384	LEU
1	E	387	GLN
1	E	389	LEU
1	E	405	LEU
1	E	421	ASP
1	E	422	THR
1	E	430	VAL
1	E	432	PHE
1	E	433	ASP
1	E	438	LEU

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Mol	Chain	Res	Type
1	E	444	LEU
1	E	507	LEU
1	E	513	ARG
1	E	518	THR
1	E	529	GLN
1	E	541	LYS
1	E	546	THR
1	E	555	GLN
1	E	592	TRP
1	E	593	LEU
1	E	597	GLN
1	F	14	ARG
1	F	15	PHE
1	F	24	GLU
1	F	30	LYS
1	F	31	ASN
1	F	33	LEU
1	F	37	ARG
1	F	42	ASP
1	F	43	ASP
1	F	45	LEU
1	F	47	GLN
1	F	56	GLN
1	F	61	ARG
1	F	79	LEU
1	F	118	GLN
1	F	123	VAL
1	F	127	ARG
1	F	133	GLU
1	F	135	GLN
1	F	144	ILE
1	F	157	ILE
1	F	158	TRP
1	F	161	ASN
1	F	164	LEU
1	F	168	SER
1	F	174	THR
1	F	190	LYS
1	F	201	PHE
1	F	202	GLN
1	F	209	PHE
1	F	211	TRP

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Mol	Chain	Res	Type
1	F	217	ILE
1	F	218	GLN
1	F	226	VAL
1	F	234	ILE
1	F	246	TYR
1	F	248	LYS
1	F	265	LYS
1	F	266	ILE
1	F	273	ARG
1	F	275	ARG
1	F	286	VAL
1	F	293	ILE
1	F	301	VAL
1	F	315	VAL
1	F	325	ASP
1	F	327	GLN
1	F	343	ARG
1	F	359	PHE
1	F	376	ARG
1	F	384	LEU
1	F	387	GLN
1	F	389	LEU
1	F	405	LEU
1	F	421	ASP
1	F	422	THR
1	F	430	VAL
1	F	432	PHE
1	F	433	ASP
1	F	438	LEU
1	F	444	LEU
1	F	507	LEU
1	F	513	ARG
1	F	518	THR
1	F	529	GLN
1	F	541	LYS
1	F	546	THR
1	F	555	GLN
1	F	592	TRP
1	F	593	LEU
1	F	597	GLN
1	G	14	ARG
1	G	15	PHE

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Mol	Chain	Res	Type
1	G	24	GLU
1	G	30	LYS
1	G	31	ASN
1	G	33	LEU
1	G	37	ARG
1	G	42	ASP
1	G	43	ASP
1	G	45	LEU
1	G	47	GLN
1	G	56	GLN
1	G	61	ARG
1	G	79	LEU
1	G	118	GLN
1	G	123	VAL
1	G	127	ARG
1	G	133	GLU
1	G	135	GLN
1	G	144	ILE
1	G	157	ILE
1	G	158	TRP
1	G	161	ASN
1	G	164	LEU
1	G	168	SER
1	G	174	THR
1	G	190	LYS
1	G	201	PHE
1	G	202	GLN
1	G	209	PHE
1	G	211	TRP
1	G	217	ILE
1	G	218	GLN
1	G	226	VAL
1	G	234	ILE
1	G	246	TYR
1	G	248	LYS
1	G	265	LYS
1	G	266	ILE
1	G	273	ARG
1	G	275	ARG
1	G	286	VAL
1	G	293	ILE
1	G	301	VAL

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Mol	Chain	Res	Type
1	G	315	VAL
1	G	325	ASP
1	G	327	GLN
1	G	343	ARG
1	G	359	PHE
1	G	376	ARG
1	G	384	LEU
1	G	387	GLN
1	G	389	LEU
1	G	405	LEU
1	G	421	ASP
1	G	422	THR
1	G	430	VAL
1	G	432	PHE
1	G	433	ASP
1	G	438	LEU
1	G	444	LEU
1	G	507	LEU
1	G	513	ARG
1	G	518	THR
1	G	529	GLN
1	G	541	LYS
1	G	546	THR
1	G	555	GLN
1	G	592	TRP
1	G	593	LEU
1	G	597	GLN
1	H	14	ARG
1	H	15	PHE
1	H	24	GLU
1	H	30	LYS
1	H	31	ASN
1	H	33	LEU
1	H	37	ARG
1	H	42	ASP
1	H	43	ASP
1	H	45	LEU
1	H	47	GLN
1	H	56	GLN
1	H	61	ARG
1	H	79	LEU
1	H	118	GLN

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Mol	Chain	Res	Type
1	H	123	VAL
1	H	127	ARG
1	H	133	GLU
1	H	135	GLN
1	H	144	ILE
1	H	157	ILE
1	H	158	TRP
1	H	161	ASN
1	H	164	LEU
1	H	168	SER
1	H	174	THR
1	H	190	LYS
1	H	201	PHE
1	H	202	GLN
1	H	209	PHE
1	H	211	TRP
1	H	217	ILE
1	H	218	GLN
1	H	226	VAL
1	H	234	ILE
1	H	246	TYR
1	H	248	LYS
1	H	265	LYS
1	H	266	ILE
1	H	273	ARG
1	H	275	ARG
1	H	286	VAL
1	H	293	ILE
1	H	301	VAL
1	H	315	VAL
1	H	325	ASP
1	H	327	GLN
1	H	343	ARG
1	H	359	PHE
1	H	376	ARG
1	H	384	LEU
1	H	387	GLN
1	H	389	LEU
1	H	405	LEU
1	H	421	ASP
1	H	422	THR
1	H	430	VAL

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Mol	Chain	Res	Type
1	H	432	PHE
1	H	433	ASP
1	H	438	LEU
1	H	444	LEU
1	H	507	LEU
1	H	513	ARG
1	H	518	THR
1	H	529	GLN
1	H	541	LYS
1	H	546	THR
1	H	555	GLN
1	H	592	TRP
1	H	593	LEU
1	H	597	GLN
1	I	14	ARG
1	I	15	PHE
1	I	24	GLU
1	I	30	LYS
1	I	31	ASN
1	I	33	LEU
1	I	37	ARG
1	I	42	ASP
1	I	43	ASP
1	I	45	LEU
1	I	47	GLN
1	I	56	GLN
1	I	61	ARG
1	I	79	LEU
1	I	118	GLN
1	I	123	VAL
1	I	127	ARG
1	I	133	GLU
1	I	135	GLN
1	I	144	ILE
1	I	157	ILE
1	I	158	TRP
1	I	161	ASN
1	I	164	LEU
1	I	168	SER
1	I	174	THR
1	I	190	LYS
1	I	201	PHE

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Mol	Chain	Res	Type
1	I	202	GLN
1	I	209	PHE
1	I	211	TRP
1	I	217	ILE
1	I	218	GLN
1	I	226	VAL
1	I	234	ILE
1	I	246	TYR
1	I	248	LYS
1	I	265	LYS
1	I	266	ILE
1	I	273	ARG
1	I	275	ARG
1	I	286	VAL
1	I	293	ILE
1	I	301	VAL
1	I	315	VAL
1	I	325	ASP
1	I	327	GLN
1	I	343	ARG
1	I	359	PHE
1	I	376	ARG
1	I	384	LEU
1	I	387	GLN
1	I	389	LEU
1	I	405	LEU
1	I	421	ASP
1	I	422	THR
1	I	430	VAL
1	I	432	PHE
1	I	433	ASP
1	I	438	LEU
1	I	444	LEU
1	I	507	LEU
1	I	513	ARG
1	I	518	THR
1	I	529	GLN
1	I	541	LYS
1	I	546	THR
1	I	555	GLN
1	I	592	TRP
1	I	593	LEU

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Mol	Chain	Res	Type
1	I	597	GLN
1	J	14	ARG
1	J	15	PHE
1	J	24	GLU
1	J	30	LYS
1	J	31	ASN
1	J	33	LEU
1	J	37	ARG
1	J	42	ASP
1	J	43	ASP
1	J	45	LEU
1	J	47	GLN
1	J	56	GLN
1	J	61	ARG
1	J	79	LEU
1	J	118	GLN
1	J	123	VAL
1	J	127	ARG
1	J	133	GLU
1	J	135	GLN
1	J	144	ILE
1	J	157	ILE
1	J	158	TRP
1	J	161	ASN
1	J	164	LEU
1	J	168	SER
1	J	174	THR
1	J	190	LYS
1	J	201	PHE
1	J	202	GLN
1	J	209	PHE
1	J	211	TRP
1	J	217	ILE
1	J	218	GLN
1	J	226	VAL
1	J	234	ILE
1	J	246	TYR
1	J	248	LYS
1	J	265	LYS
1	J	266	ILE
1	J	273	ARG
1	J	275	ARG

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Mol	Chain	Res	Type
1	J	286	VAL
1	J	293	ILE
1	J	301	VAL
1	J	315	VAL
1	J	325	ASP
1	J	327	GLN
1	J	343	ARG
1	J	359	PHE
1	J	376	ARG
1	J	384	LEU
1	J	387	GLN
1	J	389	LEU
1	J	405	LEU
1	J	421	ASP
1	J	422	THR
1	J	430	VAL
1	J	432	PHE
1	J	433	ASP
1	J	438	LEU
1	J	444	LEU
1	J	507	LEU
1	J	513	ARG
1	J	518	THR
1	J	529	GLN
1	J	541	LYS
1	J	546	THR
1	J	555	GLN
1	J	592	TRP
1	J	593	LEU
1	J	597	GLN
1	K	14	ARG
1	K	15	PHE
1	K	24	GLU
1	K	30	LYS
1	K	31	ASN
1	K	33	LEU
1	K	37	ARG
1	K	42	ASP
1	K	43	ASP
1	K	45	LEU
1	K	47	GLN
1	K	56	GLN

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Mol	Chain	Res	Type
1	K	61	ARG
1	K	79	LEU
1	K	118	GLN
1	K	123	VAL
1	K	127	ARG
1	K	133	GLU
1	K	135	GLN
1	K	144	ILE
1	K	157	ILE
1	K	158	TRP
1	K	161	ASN
1	K	164	LEU
1	K	168	SER
1	K	174	THR
1	K	190	LYS
1	K	201	PHE
1	K	202	GLN
1	K	209	PHE
1	K	211	TRP
1	K	217	ILE
1	K	218	GLN
1	K	226	VAL
1	K	234	ILE
1	K	246	TYR
1	K	248	LYS
1	K	265	LYS
1	K	266	ILE
1	K	273	ARG
1	K	275	ARG
1	K	286	VAL
1	K	293	ILE
1	K	301	VAL
1	K	315	VAL
1	K	325	ASP
1	K	327	GLN
1	K	343	ARG
1	K	359	PHE
1	K	376	ARG
1	K	384	LEU
1	K	387	GLN
1	K	389	LEU
1	K	405	LEU

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Mol	Chain	Res	Type
1	K	421	ASP
1	K	422	THR
1	K	430	VAL
1	K	432	PHE
1	K	433	ASP
1	K	438	LEU
1	K	444	LEU
1	K	507	LEU
1	K	513	ARG
1	K	518	THR
1	K	529	GLN
1	K	541	LYS
1	K	546	THR
1	K	555	GLN
1	K	592	TRP
1	K	593	LEU
1	K	597	GLN
1	L	14	ARG
1	L	15	PHE
1	L	24	GLU
1	L	30	LYS
1	L	31	ASN
1	L	33	LEU
1	L	37	ARG
1	L	42	ASP
1	L	43	ASP
1	L	45	LEU
1	L	47	GLN
1	L	56	GLN
1	L	61	ARG
1	L	79	LEU
1	L	118	GLN
1	L	123	VAL
1	L	127	ARG
1	L	133	GLU
1	L	135	GLN
1	L	144	ILE
1	L	157	ILE
1	L	158	TRP
1	L	161	ASN
1	L	164	LEU
1	L	168	SER

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Mol	Chain	Res	Type
1	L	174	THR
1	L	190	LYS
1	L	201	PHE
1	L	202	GLN
1	L	209	PHE
1	L	211	TRP
1	L	217	ILE
1	L	218	GLN
1	L	226	VAL
1	L	234	ILE
1	L	246	TYR
1	L	248	LYS
1	L	265	LYS
1	L	266	ILE
1	L	273	ARG
1	L	275	ARG
1	L	286	VAL
1	L	293	ILE
1	L	301	VAL
1	L	315	VAL
1	L	325	ASP
1	L	327	GLN
1	L	343	ARG
1	L	359	PHE
1	L	376	ARG
1	L	384	LEU
1	L	387	GLN
1	L	389	LEU
1	L	405	LEU
1	L	421	ASP
1	L	422	THR
1	L	430	VAL
1	L	432	PHE
1	L	433	ASP
1	L	438	LEU
1	L	444	LEU
1	L	507	LEU
1	L	513	ARG
1	L	518	THR
1	L	529	GLN
1	L	541	LYS
1	L	546	THR

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Mol	Chain	Res	Type
1	L	555	GLN
1	L	592	TRP
1	L	593	LEU
1	L	597	GLN
2	Y	26	LEU
2	Y	42	MET
2	Y	48	ASP
2	Y	49	LEU
2	Y	53	MET
2	Y	78	GLU
2	Y	80	ASP
2	Y	90	SER
2	Y	96	LEU
2	Y	139	SER
2	Y	140	ARG
2	Y	145	SER
2	Y	147	ASN
2	Z	26	LEU
2	Z	42	MET
2	Z	48	ASP
2	Z	49	LEU
2	Z	53	MET
2	Z	78	GLU
2	Z	80	ASP
2	Z	90	SER
2	Z	96	LEU
2	Z	139	SER
2	Z	140	ARG
2	Z	145	SER
2	Z	147	ASN
2	a	26	LEU
2	a	42	MET
2	a	48	ASP
2	a	49	LEU
2	a	53	MET
2	a	78	GLU
2	a	80	ASP
2	a	90	SER
2	a	96	LEU
2	a	113	ILE
2	a	139	SER
2	a	140	ARG

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Mol	Chain	Res	Type
2	a	145	SER
2	a	147	ASN
2	b	26	LEU
2	b	42	MET
2	b	48	ASP
2	b	49	LEU
2	b	53	MET
2	b	78	GLU
2	b	80	ASP
2	b	90	SER
2	b	96	LEU
2	b	113	ILE
2	b	139	SER
2	b	140	ARG
2	b	145	SER
2	b	147	ASN
2	c	26	LEU
2	c	42	MET
2	c	48	ASP
2	c	49	LEU
2	c	53	MET
2	c	78	GLU
2	c	80	ASP
2	c	90	SER
2	c	96	LEU
2	c	139	SER
2	c	140	ARG
2	c	145	SER
2	c	147	ASN
2	d	26	LEU
2	d	42	MET
2	d	48	ASP
2	d	49	LEU
2	d	53	MET
2	d	78	GLU
2	d	80	ASP
2	d	90	SER
2	d	96	LEU
2	d	139	SER
2	d	140	ARG
2	d	145	SER
2	d	147	ASN

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Mol	Chain	Res	Type
2	e	26	LEU
2	e	42	MET
2	e	48	ASP
2	e	49	LEU
2	e	53	MET
2	e	78	GLU
2	e	80	ASP
2	e	90	SER
2	e	96	LEU
2	e	139	SER
2	e	140	ARG
2	e	145	SER
2	e	147	ASN
2	f	26	LEU
2	f	42	MET
2	f	48	ASP
2	f	49	LEU
2	f	53	MET
2	f	78	GLU
2	f	80	ASP
2	f	90	SER
2	f	96	LEU
2	f	113	ILE
2	f	139	SER
2	f	140	ARG
2	f	145	SER
2	f	147	ASN
2	g	26	LEU
2	g	42	MET
2	g	48	ASP
2	g	49	LEU
2	g	53	MET
2	g	78	GLU
2	g	80	ASP
2	g	90	SER
2	g	96	LEU
2	g	113	ILE
2	g	139	SER
2	g	140	ARG
2	g	145	SER
2	g	147	ASN
2	h	26	LEU

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Mol	Chain	Res	Type
2	h	42	MET
2	h	48	ASP
2	h	49	LEU
2	h	53	MET
2	h	78	GLU
2	h	80	ASP
2	h	90	SER
2	h	96	LEU
2	h	139	SER
2	h	140	ARG
2	h	145	SER
2	h	147	ASN
2	i	26	LEU
2	i	42	MET
2	i	48	ASP
2	i	49	LEU
2	i	53	MET
2	i	78	GLU
2	i	80	ASP
2	i	90	SER
2	i	96	LEU
2	i	139	SER
2	i	140	ARG
2	i	145	SER
2	i	147	ASN
2	j	26	LEU
2	j	42	MET
2	j	48	ASP
2	j	49	LEU
2	j	53	MET
2	j	78	GLU
2	j	80	ASP
2	j	90	SER
2	j	96	LEU
2	j	113	ILE
2	j	139	SER
2	j	140	ARG
2	j	145	SER
2	j	147	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (319) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	31	ASN
1	M	40	GLN
1	M	508	ASN
1	M	575	GLN
1	N	31	ASN
1	N	142	GLN
1	N	508	ASN
1	N	575	GLN
1	O	31	ASN
1	O	40	GLN
1	O	135	GLN
1	O	142	GLN
1	O	450	GLN
1	O	575	GLN
1	P	31	ASN
1	P	40	GLN
1	P	575	GLN
1	Q	31	ASN
1	Q	40	GLN
1	Q	508	ASN
1	Q	575	GLN
1	R	31	ASN
1	R	508	ASN
1	R	575	GLN
1	S	31	ASN
1	S	40	GLN
1	S	135	GLN
1	S	508	ASN
1	S	575	GLN
1	T	40	GLN
1	T	450	GLN
1	T	508	ASN
1	T	575	GLN
1	U	31	ASN
1	U	40	GLN
1	U	135	GLN
1	U	142	GLN
1	U	450	GLN
1	U	508	ASN
1	U	575	GLN
1	V	31	ASN
1	V	40	GLN
1	V	508	ASN

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Mol	Chain	Res	Type
1	V	575	GLN
1	W	31	ASN
1	W	40	GLN
1	W	508	ASN
1	W	575	GLN
1	X	31	ASN
1	X	40	GLN
1	X	142	GLN
1	X	508	ASN
1	X	575	GLN
1	A	31	ASN
1	A	56	GLN
1	A	73	GLN
1	A	112	ASN
1	A	118	GLN
1	A	135	GLN
1	A	161	ASN
1	A	177	HIS
1	A	182	ASN
1	A	202	GLN
1	A	214	GLN
1	A	218	GLN
1	A	236	GLN
1	A	291	GLN
1	A	297	HIS
1	A	327	GLN
1	A	337	ASN
1	A	439	ASN
1	A	529	GLN
1	A	530	GLN
1	A	555	GLN
1	A	597	GLN
1	B	31	ASN
1	B	56	GLN
1	B	73	GLN
1	B	112	ASN
1	B	118	GLN
1	B	135	GLN
1	B	161	ASN
1	B	177	HIS
1	B	182	ASN
1	B	202	GLN

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Mol	Chain	Res	Type
1	B	214	GLN
1	B	218	GLN
1	B	236	GLN
1	B	291	GLN
1	B	297	HIS
1	B	337	ASN
1	B	439	ASN
1	B	529	GLN
1	B	530	GLN
1	B	555	GLN
1	B	597	GLN
1	C	31	ASN
1	C	56	GLN
1	C	73	GLN
1	C	112	ASN
1	C	118	GLN
1	C	135	GLN
1	C	161	ASN
1	C	177	HIS
1	C	182	ASN
1	C	202	GLN
1	C	214	GLN
1	C	218	GLN
1	C	236	GLN
1	C	291	GLN
1	C	297	HIS
1	C	337	ASN
1	C	439	ASN
1	C	529	GLN
1	C	530	GLN
1	C	555	GLN
1	C	597	GLN
1	D	31	ASN
1	D	56	GLN
1	D	73	GLN
1	D	112	ASN
1	D	118	GLN
1	D	135	GLN
1	D	161	ASN
1	D	177	HIS
1	D	182	ASN
1	D	202	GLN

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Mol	Chain	Res	Type
1	D	214	GLN
1	D	218	GLN
1	D	236	GLN
1	D	291	GLN
1	D	297	HIS
1	D	337	ASN
1	D	439	ASN
1	D	529	GLN
1	D	530	GLN
1	D	555	GLN
1	D	597	GLN
1	E	31	ASN
1	E	56	GLN
1	E	73	GLN
1	E	112	ASN
1	E	118	GLN
1	E	135	GLN
1	E	161	ASN
1	E	177	HIS
1	E	182	ASN
1	E	202	GLN
1	E	214	GLN
1	E	218	GLN
1	E	236	GLN
1	E	291	GLN
1	E	297	HIS
1	E	337	ASN
1	E	439	ASN
1	E	529	GLN
1	E	530	GLN
1	E	555	GLN
1	E	597	GLN
1	F	31	ASN
1	F	56	GLN
1	F	73	GLN
1	F	112	ASN
1	F	118	GLN
1	F	135	GLN
1	F	161	ASN
1	F	177	HIS
1	F	182	ASN
1	F	202	GLN

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Mol	Chain	Res	Type
1	F	214	GLN
1	F	218	GLN
1	F	236	GLN
1	F	291	GLN
1	F	297	HIS
1	F	327	GLN
1	F	337	ASN
1	F	439	ASN
1	F	529	GLN
1	F	530	GLN
1	F	555	GLN
1	F	597	GLN
1	G	31	ASN
1	G	73	GLN
1	G	112	ASN
1	G	118	GLN
1	G	135	GLN
1	G	161	ASN
1	G	177	HIS
1	G	182	ASN
1	G	202	GLN
1	G	214	GLN
1	G	218	GLN
1	G	236	GLN
1	G	291	GLN
1	G	297	HIS
1	G	337	ASN
1	G	439	ASN
1	G	529	GLN
1	G	530	GLN
1	G	555	GLN
1	G	597	GLN
1	H	31	ASN
1	H	73	GLN
1	H	112	ASN
1	H	118	GLN
1	H	135	GLN
1	H	161	ASN
1	H	177	HIS
1	H	182	ASN
1	H	202	GLN
1	H	214	GLN

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Mol	Chain	Res	Type
1	H	218	GLN
1	H	236	GLN
1	H	291	GLN
1	H	297	HIS
1	H	337	ASN
1	H	439	ASN
1	H	529	GLN
1	H	530	GLN
1	H	555	GLN
1	H	597	GLN
1	I	31	ASN
1	I	56	GLN
1	I	73	GLN
1	I	112	ASN
1	I	118	GLN
1	I	135	GLN
1	I	161	ASN
1	I	177	HIS
1	I	182	ASN
1	I	202	GLN
1	I	214	GLN
1	I	218	GLN
1	I	236	GLN
1	I	291	GLN
1	I	297	HIS
1	I	337	ASN
1	I	439	ASN
1	I	529	GLN
1	I	530	GLN
1	I	555	GLN
1	I	597	GLN
1	J	31	ASN
1	J	73	GLN
1	J	112	ASN
1	J	118	GLN
1	J	135	GLN
1	J	161	ASN
1	J	177	HIS
1	J	182	ASN
1	J	202	GLN
1	J	214	GLN
1	J	218	GLN

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Mol	Chain	Res	Type
1	J	236	GLN
1	J	291	GLN
1	J	297	HIS
1	J	337	ASN
1	J	439	ASN
1	J	529	GLN
1	J	530	GLN
1	J	555	GLN
1	J	597	GLN
1	K	31	ASN
1	K	56	GLN
1	K	73	GLN
1	K	112	ASN
1	K	118	GLN
1	K	135	GLN
1	K	161	ASN
1	K	177	HIS
1	K	182	ASN
1	K	202	GLN
1	K	214	GLN
1	K	218	GLN
1	K	236	GLN
1	K	291	GLN
1	K	297	HIS
1	K	327	GLN
1	K	337	ASN
1	K	439	ASN
1	K	529	GLN
1	K	530	GLN
1	K	555	GLN
1	K	597	GLN
1	L	31	ASN
1	L	56	GLN
1	L	73	GLN
1	L	112	ASN
1	L	118	GLN
1	L	135	GLN
1	L	161	ASN
1	L	177	HIS
1	L	182	ASN
1	L	202	GLN
1	L	214	GLN

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Mol	Chain	Res	Type
1	L	218	GLN
1	L	236	GLN
1	L	291	GLN
1	L	297	HIS
1	L	337	ASN
1	L	439	ASN
1	L	529	GLN
1	L	530	GLN
1	L	555	GLN
1	L	597	GLN
2	Y	94	HIS
2	Z	94	HIS
2	a	94	HIS
2	b	94	HIS
2	c	40	GLN
2	c	94	HIS
2	d	40	GLN
2	d	94	HIS
2	e	94	HIS
2	f	94	HIS
2	g	94	HIS
2	h	94	HIS
2	i	94	HIS
2	j	94	HIS

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.