



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:12 AM UTC

PDB ID : 7QIJ / pdb_00007qij
Title : Complex of the Yersinia enterocolitica Type III secretion export gate YscV
with substrate:chaperone complex YscX:YscY
Authors : Gilzer, D.; Niemann, H.H.
Deposited on : 2021-12-15
Resolution : 4.10 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

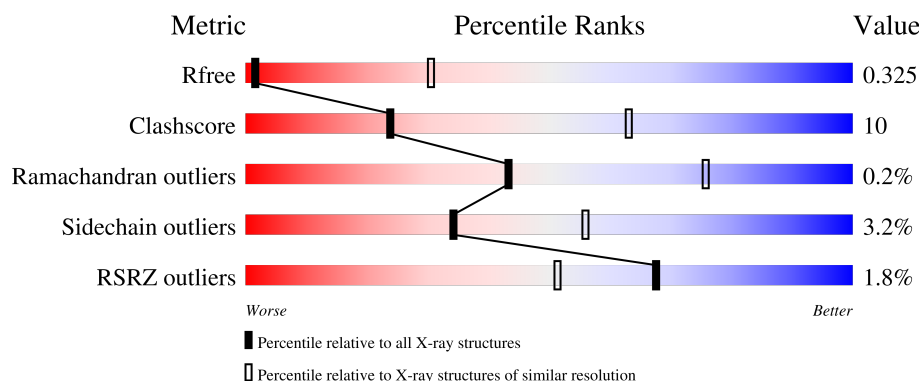
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	AA	350	3% 65% 27% 8%
1	BA	350	% 69% 24% 5%
1	CA	350	2% 66% 30% ..
1	DA	350	% 66% 26% 7%
1	EA	350	3% 68% 25% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FA	350	
1	GA	350	
1	HA	350	
1	IA	350	
1	JA	350	
1	KA	350	
1	LA	350	
1	MA	350	
1	NA	350	
1	OA	350	
1	PA	350	
1	QA	350	
1	RA	350	
2	AB	95	
2	BB	95	
2	CB	95	
2	DB	95	
2	EB	95	
2	FB	95	
2	GB	95	
2	HB	95	
2	IB	95	
2	JB	95	
2	KB	95	
2	LB	95	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	MB	95	
2	NB	95	
2	OB	95	
2	PB	95	
2	QB	95	
2	RB	95	
3	AC	122	
3	BC	122	
3	CC	122	
3	DC	122	
3	EC	122	
3	FC	122	
3	GC	122	
3	HC	122	
3	IC	122	
3	JC	122	
3	KC	122	
3	LC	122	
3	MC	122	
3	NC	122	
3	OC	122	
3	PC	122	
3	QC	122	
3	RC	122	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 73488 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 Low calcium response locus protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	323	Total	C	N	O	S	0	0	0
			2628	1676	448	495	9			
1	BA	331	Total	C	N	O	S	0	0	0
			2688	1712	458	509	9			
1	CA	343	Total	C	N	O	S	0	0	0
			2792	1779	474	530	9			
1	DA	326	Total	C	N	O	S	0	0	0
			2661	1695	451	506	9			
1	EA	329	Total	C	N	O	S	0	0	0
			2684	1710	456	509	9			
1	FA	337	Total	C	N	O	S	0	0	0
			2736	1740	466	521	9			
1	GA	341	Total	C	N	O	S	0	0	0
			2772	1766	469	528	9			
1	HA	335	Total	C	N	O	S	0	0	0
			2727	1741	460	517	9			
1	IA	336	Total	C	N	O	S	0	0	0
			2731	1738	465	519	9			
1	JA	330	Total	C	N	O	S	0	0	0
			2689	1713	457	510	9			
1	KA	335	Total	C	N	O	S	0	0	0
			2736	1746	464	517	9			
1	LA	336	Total	C	N	O	S	0	0	0
			2734	1743	462	520	9			
1	MA	322	Total	C	N	O	S	0	0	0
			2632	1683	448	493	8			
1	NA	331	Total	C	N	O	S	0	0	0
			2698	1720	456	513	9			
1	OA	331	Total	C	N	O	S	0	0	0
			2694	1718	458	509	9			
1	PA	330	Total	C	N	O	S	0	0	0
			2688	1713	457	509	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	334	Total	C	N	O	S	0	0	0
			2713	1728	462	514	9			
1	RA	344	Total	C	N	O	S	0	0	0
			2798	1782	474	533	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	355	MET	-	initiating methionine	UNP P0C2V3
AA	621	ARG	GLY	variant	UNP P0C2V3
BA	355	MET	-	initiating methionine	UNP P0C2V3
BA	621	ARG	GLY	variant	UNP P0C2V3
CA	355	MET	-	initiating methionine	UNP P0C2V3
CA	621	ARG	GLY	variant	UNP P0C2V3
DA	355	MET	-	initiating methionine	UNP P0C2V3
DA	621	ARG	GLY	variant	UNP P0C2V3
EA	355	MET	-	initiating methionine	UNP P0C2V3
EA	621	ARG	GLY	variant	UNP P0C2V3
FA	355	MET	-	initiating methionine	UNP P0C2V3
FA	621	ARG	GLY	variant	UNP P0C2V3
GA	355	MET	-	initiating methionine	UNP P0C2V3
GA	621	ARG	GLY	variant	UNP P0C2V3
HA	355	MET	-	initiating methionine	UNP P0C2V3
HA	621	ARG	GLY	variant	UNP P0C2V3
IA	355	MET	-	initiating methionine	UNP P0C2V3
IA	621	ARG	GLY	variant	UNP P0C2V3
JA	355	MET	-	initiating methionine	UNP P0C2V3
JA	621	ARG	GLY	variant	UNP P0C2V3
KA	355	MET	-	initiating methionine	UNP P0C2V3
KA	621	ARG	GLY	variant	UNP P0C2V3
LA	355	MET	-	initiating methionine	UNP P0C2V3
LA	621	ARG	GLY	variant	UNP P0C2V3
MA	355	MET	-	initiating methionine	UNP P0C2V3
MA	621	ARG	GLY	variant	UNP P0C2V3
NA	355	MET	-	initiating methionine	UNP P0C2V3
NA	621	ARG	GLY	variant	UNP P0C2V3
OA	355	MET	-	initiating methionine	UNP P0C2V3
OA	621	ARG	GLY	variant	UNP P0C2V3
PA	355	MET	-	initiating methionine	UNP P0C2V3
PA	621	ARG	GLY	variant	UNP P0C2V3
QA	355	MET	-	initiating methionine	UNP P0C2V3
QA	621	ARG	GLY	variant	UNP P0C2V3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
RA	355	MET	-	initiating methionine	UNP P0C2V3
RA	621	ARG	GLY	variant	UNP P0C2V3

- Molecule 2 is a protein called Yop proteins translocation protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CB	68	Total	C	N	O	S	0	0	0
			546	338	102	105	1			
2	JB	69	Total	C	N	O	S	0	0	0
			554	346	98	109	1			
2	KB	77	Total	C	N	O	S	0	0	0
			624	390	114	119	1			
2	RB	70	Total	C	N	O	S	0	0	0
			559	347	102	109	1			
2	GB	73	Total	C	N	O	S	0	0	0
			596	371	110	114	1			
2	LB	70	Total	C	N	O	S	0	1	0
			569	356	99	113	1			
2	NB	61	Total	C	N	O	S	0	0	0
			487	302	87	97	1			
2	OB	70	Total	C	N	O	S	0	0	0
			562	349	104	108	1			
2	PB	65	Total	C	N	O	S	0	0	0
			521	322	95	103	1			
2	EB	60	Total	C	N	O	S	0	0	0
			482	299	86	96	1			
2	FB	71	Total	C	N	O	S	3	1	0
			572	357	101	113	1			
2	HB	65	Total	C	N	O	S	1	0	0
			524	324	97	102	1			
2	IB	63	Total	C	N	O	S	0	0	0
			503	312	90	100	1			
2	AB	70	Total	C	N	O	S	0	0	0
			562	349	104	108	1			
2	BB	65	Total	C	N	O	S	0	0	0
			524	324	97	102	1			
2	DB	61	Total	C	N	O	S	0	0	0
			493	306	88	98	1			
2	MB	64	Total	C	N	O	S	0	0	0
			513	320	95	97	1			
2	QB	66	Total	C	N	O	S	0	0	0
			532	331	97	103	1			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CB	28	GLY	-	expression tag	UNP P0C2N4
CB	29	ALA	-	expression tag	UNP P0C2N4
CB	30	MET	-	expression tag	UNP P0C2N4
CB	31	GLY	-	expression tag	UNP P0C2N4
JB	28	GLY	-	expression tag	UNP P0C2N4
JB	29	ALA	-	expression tag	UNP P0C2N4
JB	30	MET	-	expression tag	UNP P0C2N4
JB	31	GLY	-	expression tag	UNP P0C2N4
KB	28	GLY	-	expression tag	UNP P0C2N4
KB	29	ALA	-	expression tag	UNP P0C2N4
KB	30	MET	-	expression tag	UNP P0C2N4
KB	31	GLY	-	expression tag	UNP P0C2N4
RB	28	GLY	-	expression tag	UNP P0C2N4
RB	29	ALA	-	expression tag	UNP P0C2N4
RB	30	MET	-	expression tag	UNP P0C2N4
RB	31	GLY	-	expression tag	UNP P0C2N4
GB	28	GLY	-	expression tag	UNP P0C2N4
GB	29	ALA	-	expression tag	UNP P0C2N4
GB	30	MET	-	expression tag	UNP P0C2N4
GB	31	GLY	-	expression tag	UNP P0C2N4
LB	28	GLY	-	expression tag	UNP P0C2N4
LB	29	ALA	-	expression tag	UNP P0C2N4
LB	30	MET	-	expression tag	UNP P0C2N4
LB	31	GLY	-	expression tag	UNP P0C2N4
NB	28	GLY	-	expression tag	UNP P0C2N4
NB	29	ALA	-	expression tag	UNP P0C2N4
NB	30	MET	-	expression tag	UNP P0C2N4
NB	31	GLY	-	expression tag	UNP P0C2N4
OB	28	GLY	-	expression tag	UNP P0C2N4
OB	29	ALA	-	expression tag	UNP P0C2N4
OB	30	MET	-	expression tag	UNP P0C2N4
OB	31	GLY	-	expression tag	UNP P0C2N4
PB	28	GLY	-	expression tag	UNP P0C2N4
PB	29	ALA	-	expression tag	UNP P0C2N4
PB	30	MET	-	expression tag	UNP P0C2N4
PB	31	GLY	-	expression tag	UNP P0C2N4
EB	28	GLY	-	expression tag	UNP P0C2N4
EB	29	ALA	-	expression tag	UNP P0C2N4
EB	30	MET	-	expression tag	UNP P0C2N4
EB	31	GLY	-	expression tag	UNP P0C2N4
FB	28	GLY	-	expression tag	UNP P0C2N4
FB	29	ALA	-	expression tag	UNP P0C2N4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FB	30	MET	-	expression tag	UNP P0C2N4
FB	31	GLY	-	expression tag	UNP P0C2N4
HB	28	GLY	-	expression tag	UNP P0C2N4
HB	29	ALA	-	expression tag	UNP P0C2N4
HB	30	MET	-	expression tag	UNP P0C2N4
HB	31	GLY	-	expression tag	UNP P0C2N4
IB	28	GLY	-	expression tag	UNP P0C2N4
IB	29	ALA	-	expression tag	UNP P0C2N4
IB	30	MET	-	expression tag	UNP P0C2N4
IB	31	GLY	-	expression tag	UNP P0C2N4
AB	28	GLY	-	expression tag	UNP P0C2N4
AB	29	ALA	-	expression tag	UNP P0C2N4
AB	30	MET	-	expression tag	UNP P0C2N4
AB	31	GLY	-	expression tag	UNP P0C2N4
BB	28	GLY	-	expression tag	UNP P0C2N4
BB	29	ALA	-	expression tag	UNP P0C2N4
BB	30	MET	-	expression tag	UNP P0C2N4
BB	31	GLY	-	expression tag	UNP P0C2N4
DB	28	GLY	-	expression tag	UNP P0C2N4
DB	29	ALA	-	expression tag	UNP P0C2N4
DB	30	MET	-	expression tag	UNP P0C2N4
DB	31	GLY	-	expression tag	UNP P0C2N4
MB	28	GLY	-	expression tag	UNP P0C2N4
MB	29	ALA	-	expression tag	UNP P0C2N4
MB	30	MET	-	expression tag	UNP P0C2N4
MB	31	GLY	-	expression tag	UNP P0C2N4
QB	28	GLY	-	expression tag	UNP P0C2N4
QB	29	ALA	-	expression tag	UNP P0C2N4
QB	30	MET	-	expression tag	UNP P0C2N4
QB	31	GLY	-	expression tag	UNP P0C2N4

- Molecule 3 is a protein called Chaperone protein YscY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CC	108	Total	C	N	O	S	0	0	0
			879	549	169	157	4			
3	JC	109	Total	C	N	O	S	2	0	0
			883	548	170	161	4			
3	KC	112	Total	C	N	O	S	0	0	0
			904	562	174	164	4			
3	RC	108	Total	C	N	O	S	0	1	0
			878	549	168	156	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	GC	108	Total	C	N	O	S	3	1	0
			878	549	168	156	5			
3	LC	105	Total	C	N	O	S	0	0	0
			851	533	162	152	4			
3	NC	102	Total	C	N	O	S	0	0	0
			826	515	159	148	4			
3	OC	108	Total	C	N	O	S	0	0	0
			875	543	169	159	4			
3	PC	109	Total	C	N	O	S	0	0	0
			883	551	170	158	4			
3	EC	98	Total	C	N	O	S	0	0	0
			800	499	155	142	4			
3	FC	106	Total	C	N	O	S	0	0	0
			858	536	165	153	4			
3	HC	102	Total	C	N	O	S	0	1	0
			830	519	160	147	4			
3	IC	89	Total	C	N	O	S	0	0	0
			732	460	142	126	4			
3	AC	93	Total	C	N	O	S	0	0	0
			754	473	142	136	3			
3	BC	95	Total	C	N	O	S	0	0	0
			771	482	144	141	4			
3	DC	101	Total	C	N	O	S	0	0	0
			817	513	156	144	4			
3	MC	96	Total	C	N	O	S	0	0	0
			784	489	153	138	4			
3	QC	93	Total	C	N	O	S	0	0	0
			761	477	147	133	4			

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	-7	MET	-	initiating methionine	UNP P0C2N2
CC	-6	GLY	-	expression tag	UNP P0C2N2
CC	-5	HIS	-	expression tag	UNP P0C2N2
CC	-4	HIS	-	expression tag	UNP P0C2N2
CC	-3	HIS	-	expression tag	UNP P0C2N2
CC	-2	HIS	-	expression tag	UNP P0C2N2
CC	-1	HIS	-	expression tag	UNP P0C2N2
CC	0	HIS	-	expression tag	UNP P0C2N2
CC	1	GLY	-	expression tag	UNP P0C2N2
JC	-7	MET	-	initiating methionine	UNP P0C2N2
JC	-6	GLY	-	expression tag	UNP P0C2N2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JC	-5	HIS	-	expression tag	UNP P0C2N2
JC	-4	HIS	-	expression tag	UNP P0C2N2
JC	-3	HIS	-	expression tag	UNP P0C2N2
JC	-2	HIS	-	expression tag	UNP P0C2N2
JC	-1	HIS	-	expression tag	UNP P0C2N2
JC	0	HIS	-	expression tag	UNP P0C2N2
JC	1	GLY	-	expression tag	UNP P0C2N2
KC	-7	MET	-	initiating methionine	UNP P0C2N2
KC	-6	GLY	-	expression tag	UNP P0C2N2
KC	-5	HIS	-	expression tag	UNP P0C2N2
KC	-4	HIS	-	expression tag	UNP P0C2N2
KC	-3	HIS	-	expression tag	UNP P0C2N2
KC	-2	HIS	-	expression tag	UNP P0C2N2
KC	-1	HIS	-	expression tag	UNP P0C2N2
KC	0	HIS	-	expression tag	UNP P0C2N2
KC	1	GLY	-	expression tag	UNP P0C2N2
RC	-7	MET	-	initiating methionine	UNP P0C2N2
RC	-6	GLY	-	expression tag	UNP P0C2N2
RC	-5	HIS	-	expression tag	UNP P0C2N2
RC	-4	HIS	-	expression tag	UNP P0C2N2
RC	-3	HIS	-	expression tag	UNP P0C2N2
RC	-2	HIS	-	expression tag	UNP P0C2N2
RC	-1	HIS	-	expression tag	UNP P0C2N2
RC	0	HIS	-	expression tag	UNP P0C2N2
RC	1	GLY	-	expression tag	UNP P0C2N2
GC	-7	MET	-	initiating methionine	UNP P0C2N2
GC	-6	GLY	-	expression tag	UNP P0C2N2
GC	-5	HIS	-	expression tag	UNP P0C2N2
GC	-4	HIS	-	expression tag	UNP P0C2N2
GC	-3	HIS	-	expression tag	UNP P0C2N2
GC	-2	HIS	-	expression tag	UNP P0C2N2
GC	-1	HIS	-	expression tag	UNP P0C2N2
GC	0	HIS	-	expression tag	UNP P0C2N2
GC	1	GLY	-	expression tag	UNP P0C2N2
LC	-7	MET	-	initiating methionine	UNP P0C2N2
LC	-6	GLY	-	expression tag	UNP P0C2N2
LC	-5	HIS	-	expression tag	UNP P0C2N2
LC	-4	HIS	-	expression tag	UNP P0C2N2
LC	-3	HIS	-	expression tag	UNP P0C2N2
LC	-2	HIS	-	expression tag	UNP P0C2N2
LC	-1	HIS	-	expression tag	UNP P0C2N2
LC	0	HIS	-	expression tag	UNP P0C2N2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
LC	1	GLY	-	expression tag	UNP P0C2N2
NC	-7	MET	-	initiating methionine	UNP P0C2N2
NC	-6	GLY	-	expression tag	UNP P0C2N2
NC	-5	HIS	-	expression tag	UNP P0C2N2
NC	-4	HIS	-	expression tag	UNP P0C2N2
NC	-3	HIS	-	expression tag	UNP P0C2N2
NC	-2	HIS	-	expression tag	UNP P0C2N2
NC	-1	HIS	-	expression tag	UNP P0C2N2
NC	0	HIS	-	expression tag	UNP P0C2N2
NC	1	GLY	-	expression tag	UNP P0C2N2
OC	-7	MET	-	initiating methionine	UNP P0C2N2
OC	-6	GLY	-	expression tag	UNP P0C2N2
OC	-5	HIS	-	expression tag	UNP P0C2N2
OC	-4	HIS	-	expression tag	UNP P0C2N2
OC	-3	HIS	-	expression tag	UNP P0C2N2
OC	-2	HIS	-	expression tag	UNP P0C2N2
OC	-1	HIS	-	expression tag	UNP P0C2N2
OC	0	HIS	-	expression tag	UNP P0C2N2
OC	1	GLY	-	expression tag	UNP P0C2N2
PC	-7	MET	-	initiating methionine	UNP P0C2N2
PC	-6	GLY	-	expression tag	UNP P0C2N2
PC	-5	HIS	-	expression tag	UNP P0C2N2
PC	-4	HIS	-	expression tag	UNP P0C2N2
PC	-3	HIS	-	expression tag	UNP P0C2N2
PC	-2	HIS	-	expression tag	UNP P0C2N2
PC	-1	HIS	-	expression tag	UNP P0C2N2
PC	0	HIS	-	expression tag	UNP P0C2N2
PC	1	GLY	-	expression tag	UNP P0C2N2
EC	-7	MET	-	initiating methionine	UNP P0C2N2
EC	-6	GLY	-	expression tag	UNP P0C2N2
EC	-5	HIS	-	expression tag	UNP P0C2N2
EC	-4	HIS	-	expression tag	UNP P0C2N2
EC	-3	HIS	-	expression tag	UNP P0C2N2
EC	-2	HIS	-	expression tag	UNP P0C2N2
EC	-1	HIS	-	expression tag	UNP P0C2N2
EC	0	HIS	-	expression tag	UNP P0C2N2
EC	1	GLY	-	expression tag	UNP P0C2N2
FC	-7	MET	-	initiating methionine	UNP P0C2N2
FC	-6	GLY	-	expression tag	UNP P0C2N2
FC	-5	HIS	-	expression tag	UNP P0C2N2
FC	-4	HIS	-	expression tag	UNP P0C2N2
FC	-3	HIS	-	expression tag	UNP P0C2N2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FC	-2	HIS	-	expression tag	UNP P0C2N2
FC	-1	HIS	-	expression tag	UNP P0C2N2
FC	0	HIS	-	expression tag	UNP P0C2N2
FC	1	GLY	-	expression tag	UNP P0C2N2
HC	-7	MET	-	initiating methionine	UNP P0C2N2
HC	-6	GLY	-	expression tag	UNP P0C2N2
HC	-5	HIS	-	expression tag	UNP P0C2N2
HC	-4	HIS	-	expression tag	UNP P0C2N2
HC	-3	HIS	-	expression tag	UNP P0C2N2
HC	-2	HIS	-	expression tag	UNP P0C2N2
HC	-1	HIS	-	expression tag	UNP P0C2N2
HC	0	HIS	-	expression tag	UNP P0C2N2
HC	1	GLY	-	expression tag	UNP P0C2N2
IC	-7	MET	-	initiating methionine	UNP P0C2N2
IC	-6	GLY	-	expression tag	UNP P0C2N2
IC	-5	HIS	-	expression tag	UNP P0C2N2
IC	-4	HIS	-	expression tag	UNP P0C2N2
IC	-3	HIS	-	expression tag	UNP P0C2N2
IC	-2	HIS	-	expression tag	UNP P0C2N2
IC	-1	HIS	-	expression tag	UNP P0C2N2
IC	0	HIS	-	expression tag	UNP P0C2N2
IC	1	GLY	-	expression tag	UNP P0C2N2
AC	-7	MET	-	initiating methionine	UNP P0C2N2
AC	-6	GLY	-	expression tag	UNP P0C2N2
AC	-5	HIS	-	expression tag	UNP P0C2N2
AC	-4	HIS	-	expression tag	UNP P0C2N2
AC	-3	HIS	-	expression tag	UNP P0C2N2
AC	-2	HIS	-	expression tag	UNP P0C2N2
AC	-1	HIS	-	expression tag	UNP P0C2N2
AC	0	HIS	-	expression tag	UNP P0C2N2
AC	1	GLY	-	expression tag	UNP P0C2N2
BC	-7	MET	-	initiating methionine	UNP P0C2N2
BC	-6	GLY	-	expression tag	UNP P0C2N2
BC	-5	HIS	-	expression tag	UNP P0C2N2
BC	-4	HIS	-	expression tag	UNP P0C2N2
BC	-3	HIS	-	expression tag	UNP P0C2N2
BC	-2	HIS	-	expression tag	UNP P0C2N2
BC	-1	HIS	-	expression tag	UNP P0C2N2
BC	0	HIS	-	expression tag	UNP P0C2N2
BC	1	GLY	-	expression tag	UNP P0C2N2
DC	-7	MET	-	initiating methionine	UNP P0C2N2
DC	-6	GLY	-	expression tag	UNP P0C2N2

Continued on next page...

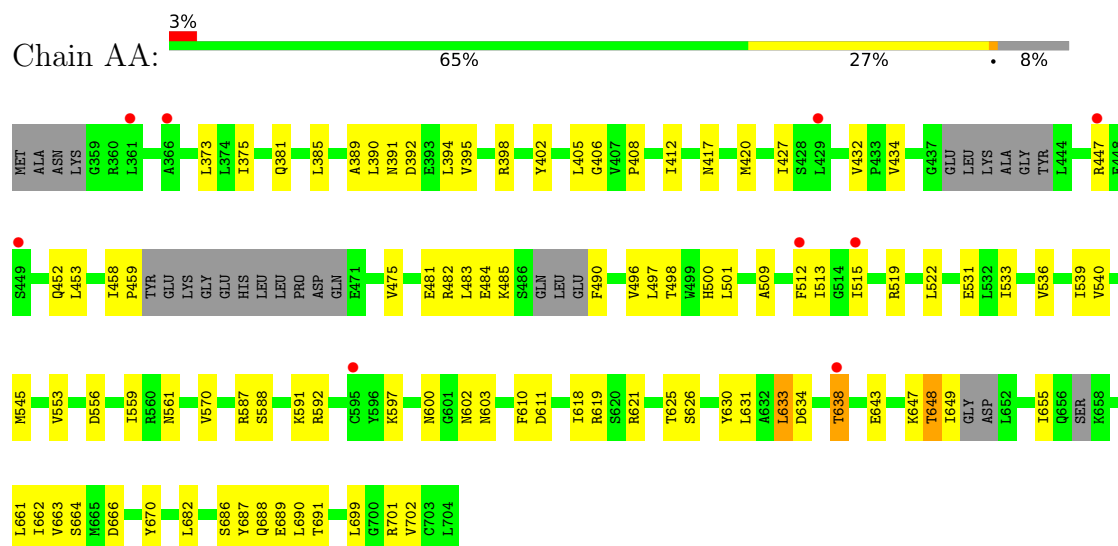
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DC	-5	HIS	-	expression tag	UNP P0C2N2
DC	-4	HIS	-	expression tag	UNP P0C2N2
DC	-3	HIS	-	expression tag	UNP P0C2N2
DC	-2	HIS	-	expression tag	UNP P0C2N2
DC	-1	HIS	-	expression tag	UNP P0C2N2
DC	0	HIS	-	expression tag	UNP P0C2N2
DC	1	GLY	-	expression tag	UNP P0C2N2
MC	-7	MET	-	initiating methionine	UNP P0C2N2
MC	-6	GLY	-	expression tag	UNP P0C2N2
MC	-5	HIS	-	expression tag	UNP P0C2N2
MC	-4	HIS	-	expression tag	UNP P0C2N2
MC	-3	HIS	-	expression tag	UNP P0C2N2
MC	-2	HIS	-	expression tag	UNP P0C2N2
MC	-1	HIS	-	expression tag	UNP P0C2N2
MC	0	HIS	-	expression tag	UNP P0C2N2
MC	1	GLY	-	expression tag	UNP P0C2N2
QC	-7	MET	-	initiating methionine	UNP P0C2N2
QC	-6	GLY	-	expression tag	UNP P0C2N2
QC	-5	HIS	-	expression tag	UNP P0C2N2
QC	-4	HIS	-	expression tag	UNP P0C2N2
QC	-3	HIS	-	expression tag	UNP P0C2N2
QC	-2	HIS	-	expression tag	UNP P0C2N2
QC	-1	HIS	-	expression tag	UNP P0C2N2
QC	0	HIS	-	expression tag	UNP P0C2N2
QC	1	GLY	-	expression tag	UNP P0C2N2

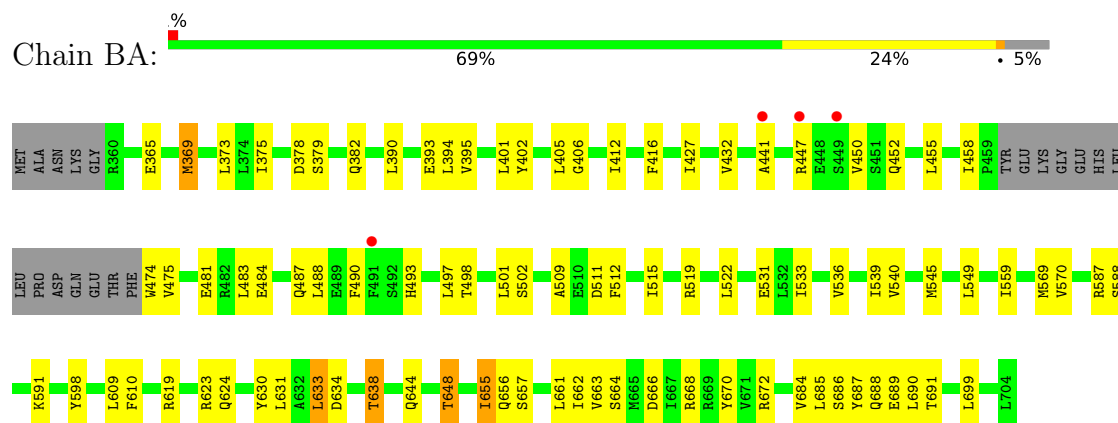
3 Residue-property plots [i](#)

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

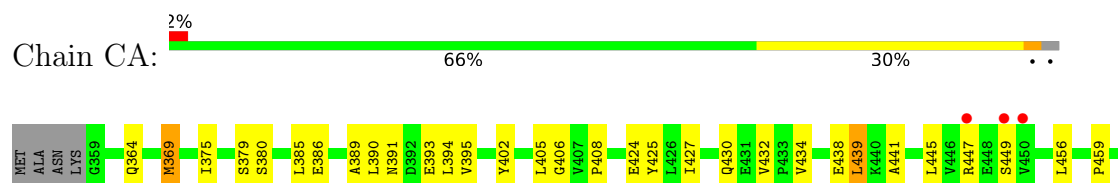
- Molecule 1: Low calcium response locus protein D

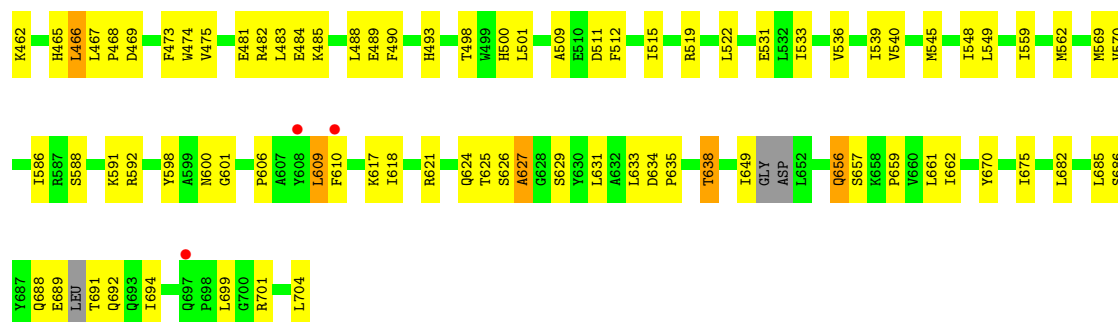


- Molecule 1: Low calcium response locus protein D

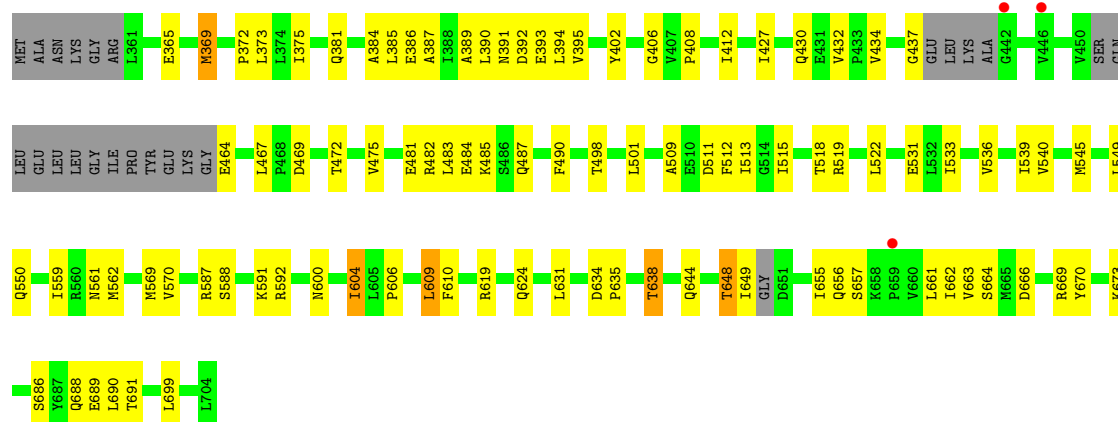


- Molecule 1: Low calcium response locus protein D

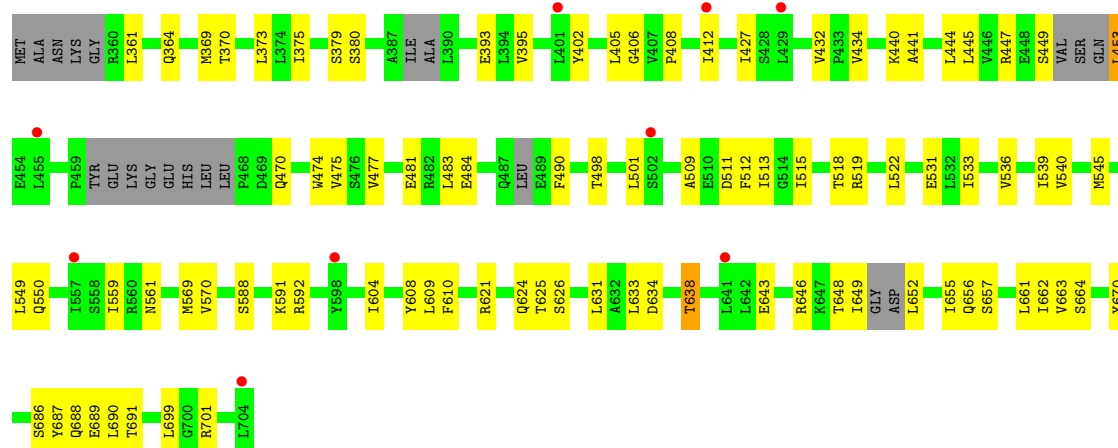




• Molecule 1: Low calcium response locus protein D

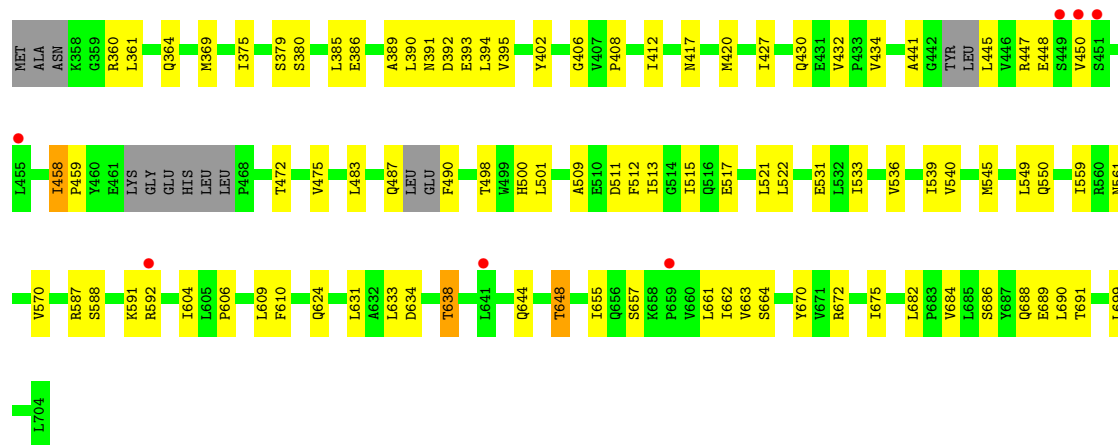


• Molecule 1: Low calcium response locus protein D

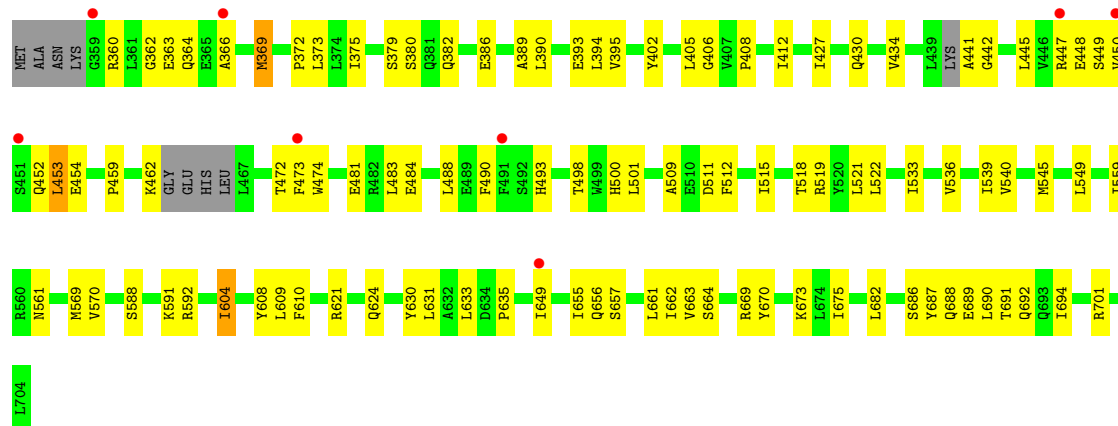


• Molecule 1: Low calcium response locus protein D

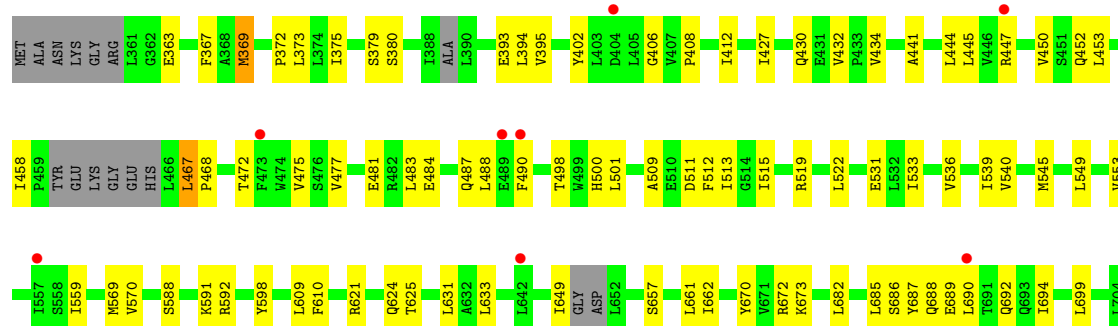
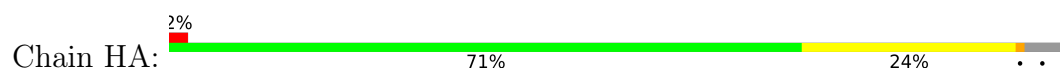




• Molecule 1: Low calcium response locus protein D

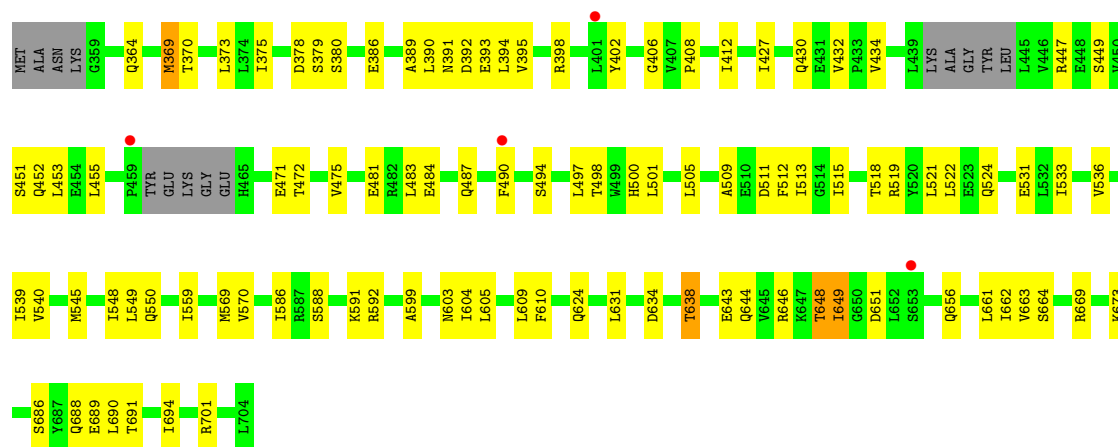


• Molecule 1: Low calcium response locus protein D

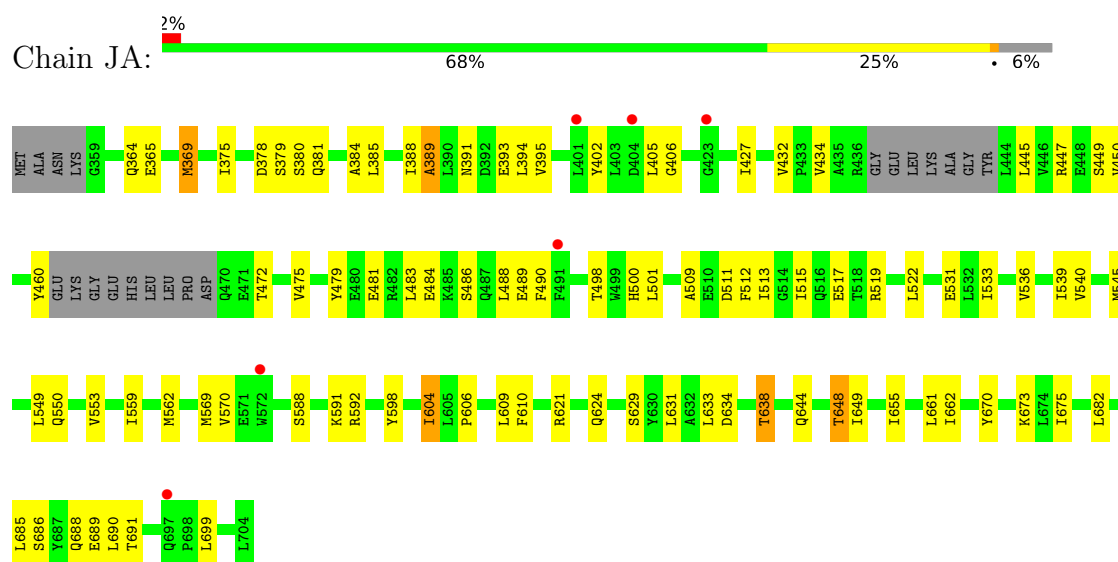


• Molecule 1: Low calcium response locus protein D

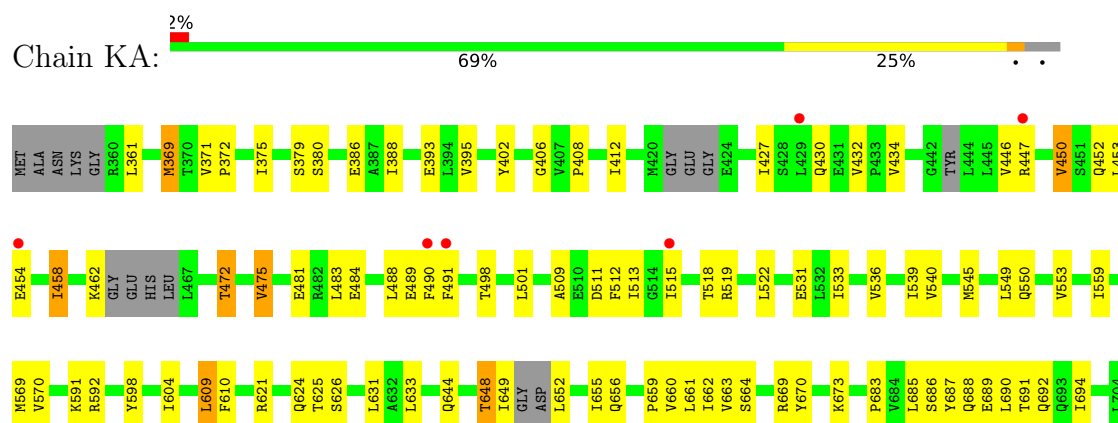




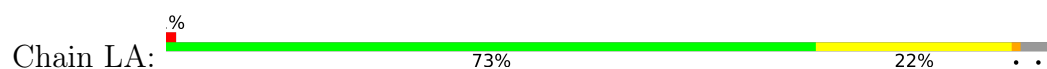
- Molecule 1: Low calcium response locus protein D

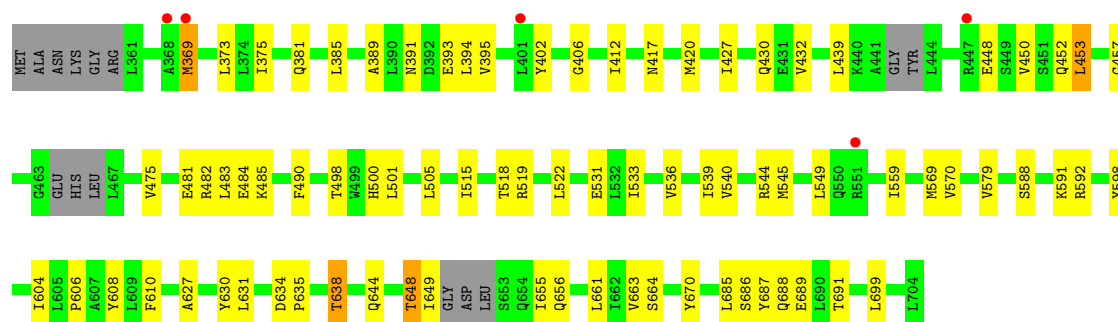


- Molecule 1: Low calcium response locus protein D

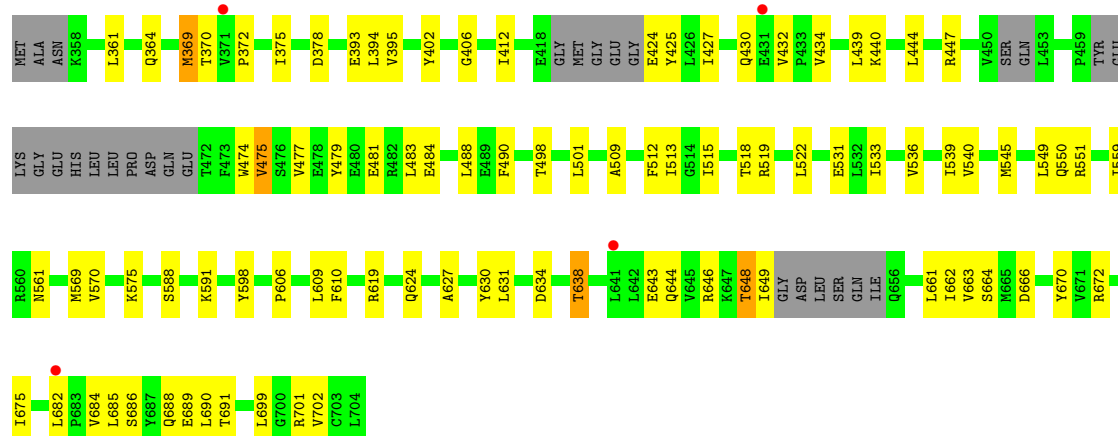


- Molecule 1: Low calcium response locus protein D

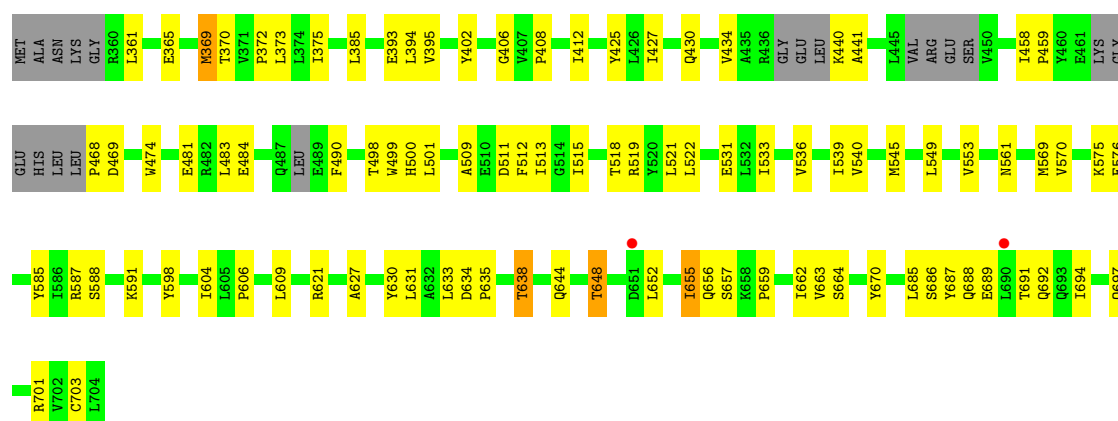




● Molecule 1: Low calcium response locus protein D

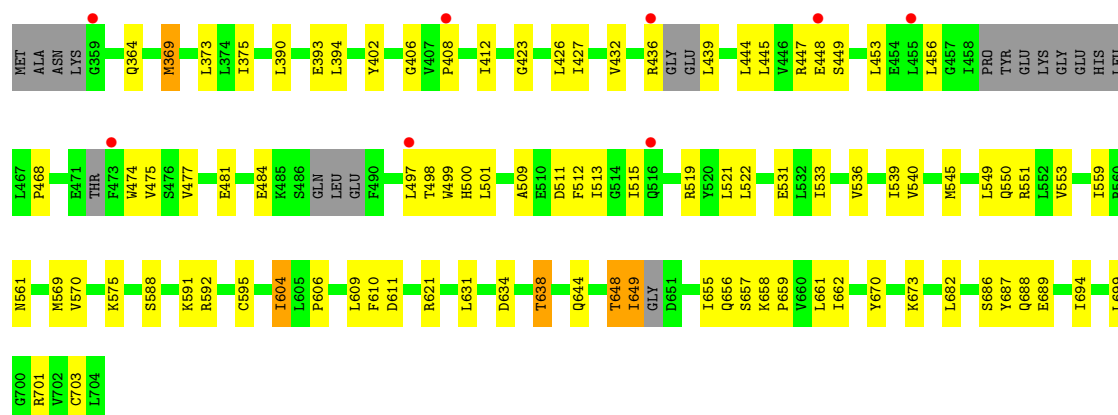


● Molecule 1: Low calcium response locus protein D



● Molecule 1: Low calcium response locus protein D

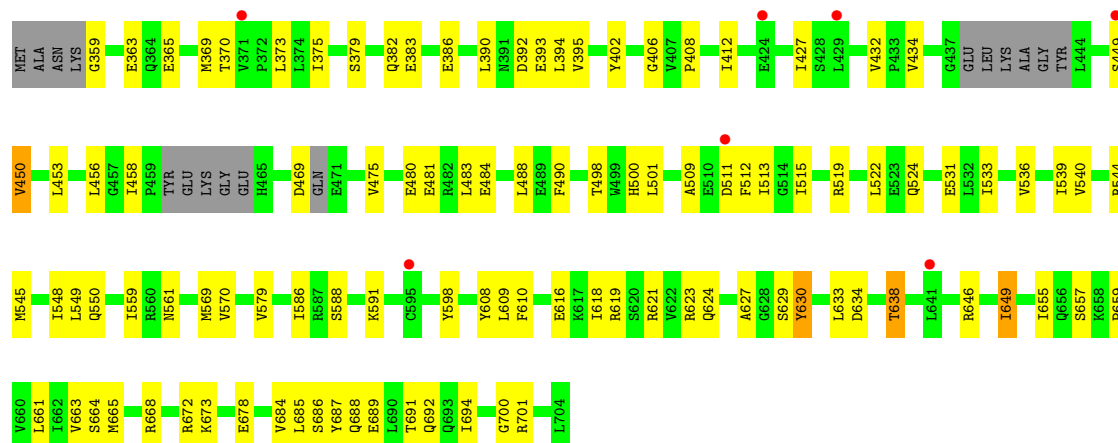




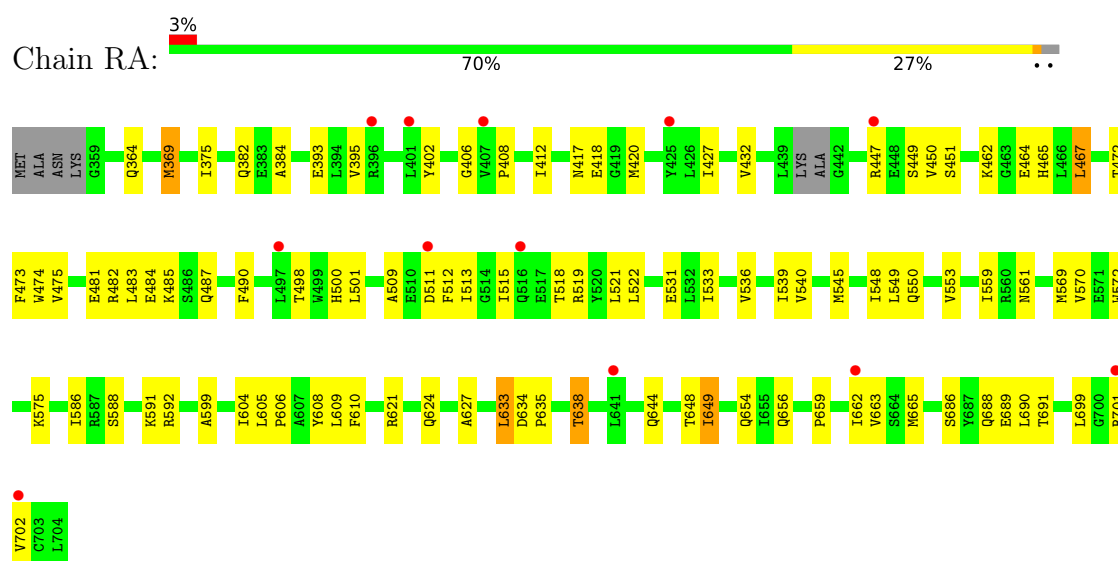
- Molecule 1: Low calcium response locus protein D



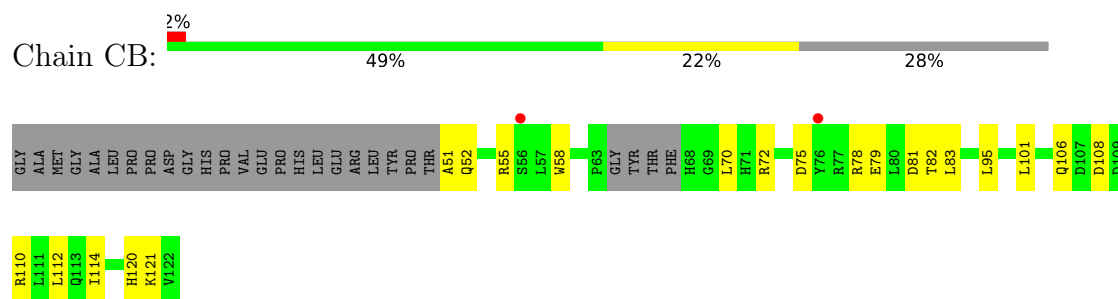
- Molecule 1: Low calcium response locus protein D



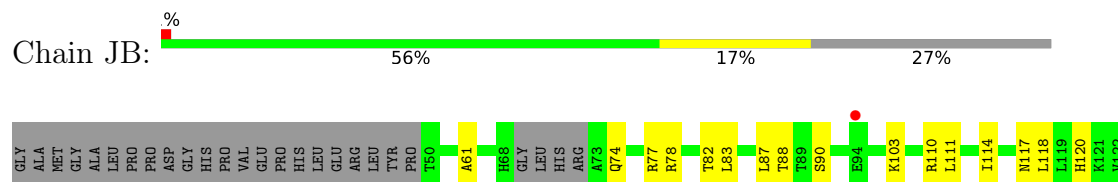
- Molecule 1: Low calcium response locus protein D



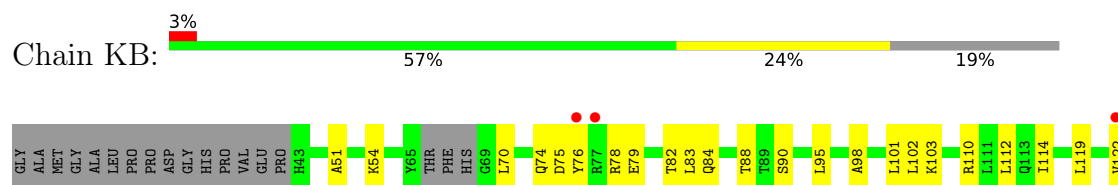
- Molecule 2: Yop proteins translocation protein X



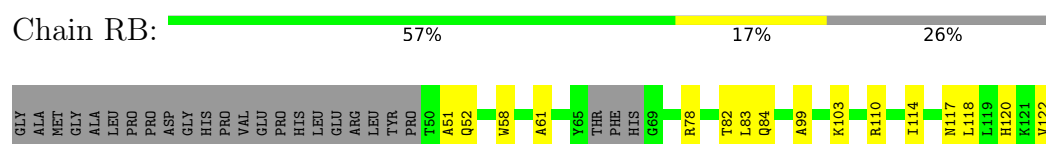
- Molecule 2: Yop proteins translocation protein X



- Molecule 2: Yop proteins translocation protein X

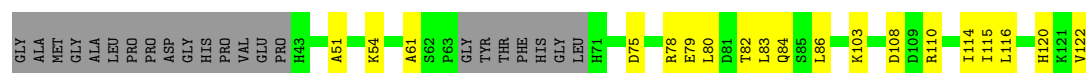


- Molecule 2: Yop proteins translocation protein X

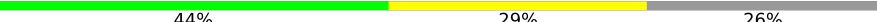


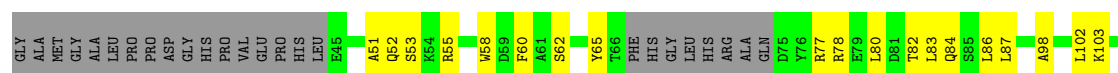
- Molecule 2: Yop proteins translocation protein X

Chain GB:  57% 20% 23%

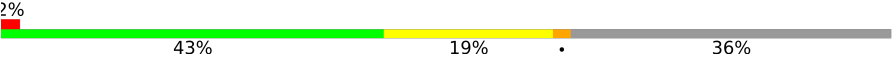


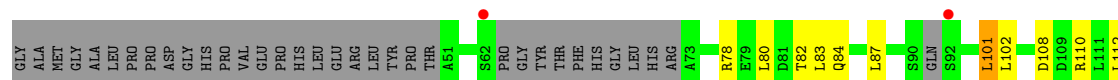
• Molecule 2: Yop proteins translocation protein X

Chain LB:  44% 29% 26%

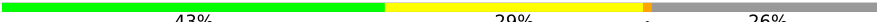


• Molecule 2: Yop proteins translocation protein X

Chain NB:  2% 43% 19% 36%



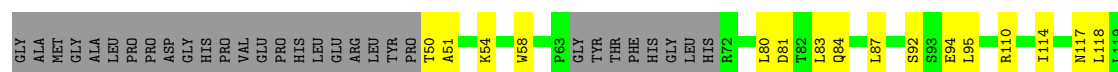
• Molecule 2: Yop proteins translocation protein X

Chain OB:  43% 29% 26%

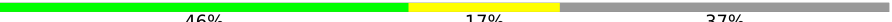


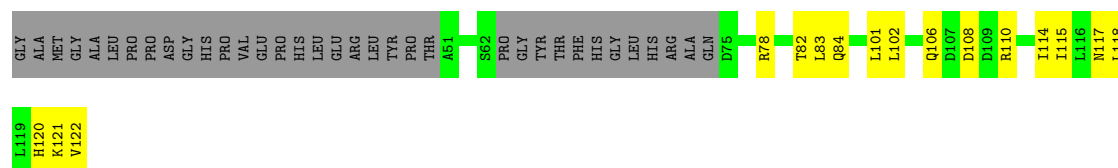
• Molecule 2: Yop proteins translocation protein X

Chain PB:  48% 20% 32%

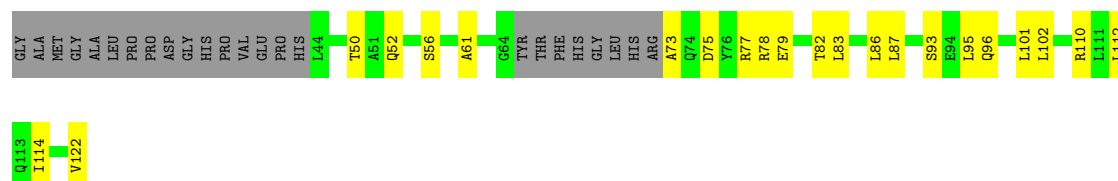


• Molecule 2: Yop proteins translocation protein X

Chain EB:  46% 17% 37%



- Molecule 2: Yop proteins translocation protein X



- Molecule 2: Yop proteins translocation protein X



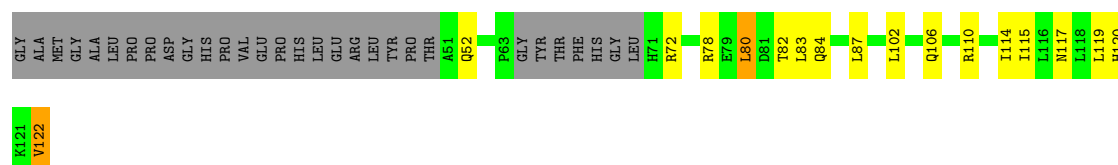
- Molecule 2: Yop proteins translocation protein X



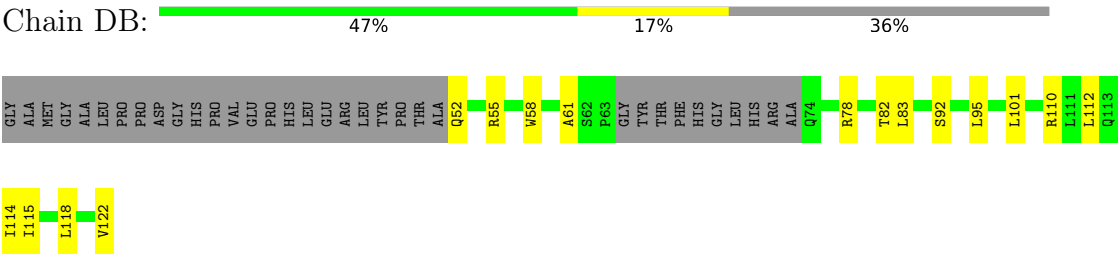
- Molecule 2: Yop proteins translocation protein X



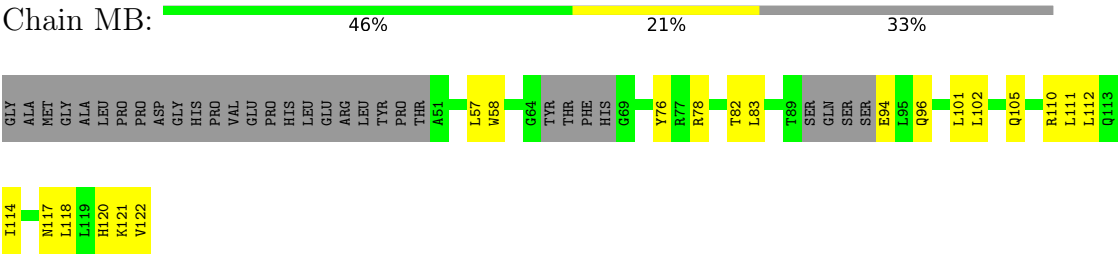
- Molecule 2: Yop proteins translocation protein X



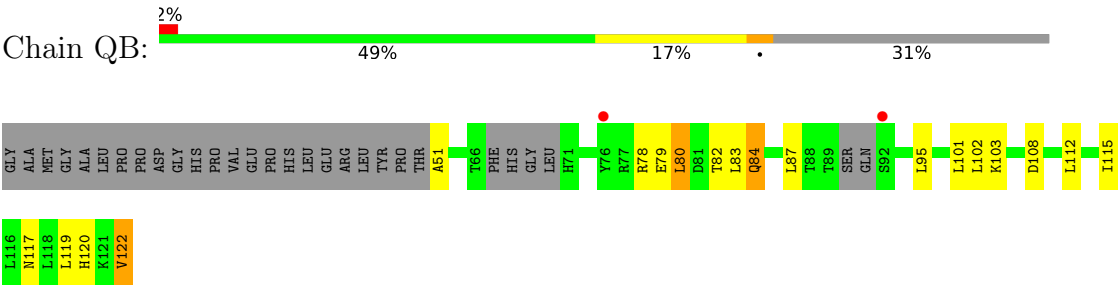
• Molecule 2: Yop proteins translocation protein X



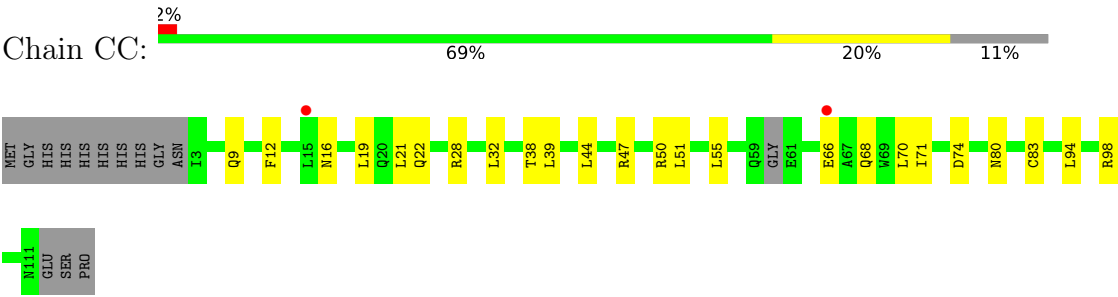
• Molecule 2: Yop proteins translocation protein X



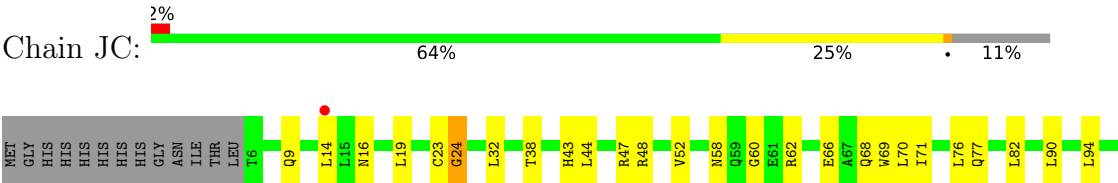
• Molecule 2: Yop proteins translocation protein X



• Molecule 3: Chaperone protein YscY

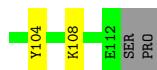


• Molecule 3: Chaperone protein YscY

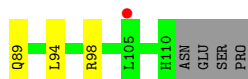




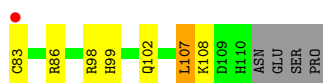
• Molecule 3: Chaperone protein YscY



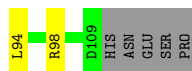
• Molecule 3: Chaperone protein YscY



• Molecule 3: Chaperone protein YscY



• Molecule 3: Chaperone protein YscY

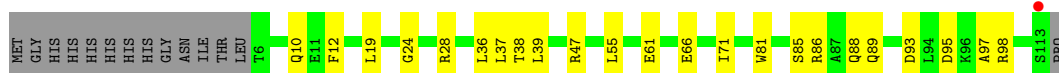
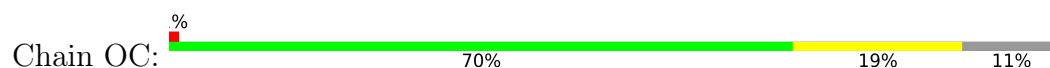


• Molecule 3: Chaperone protein YscY

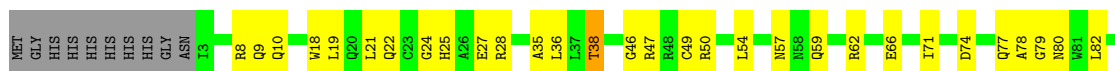




- Molecule 3: Chaperone protein YscY



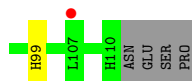
- Molecule 3: Chaperone protein YscY



- Molecule 3: Chaperone protein YscY



- Molecule 3: Chaperone protein YscY

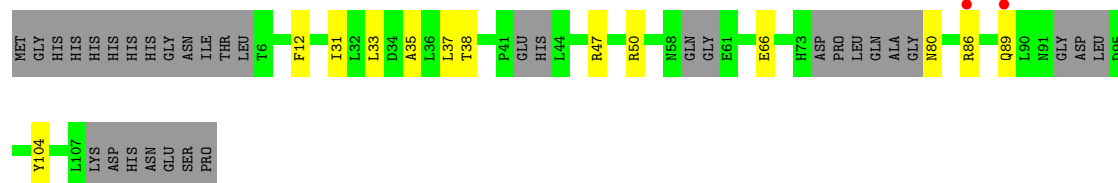


- Molecule 3: Chaperone protein YscY

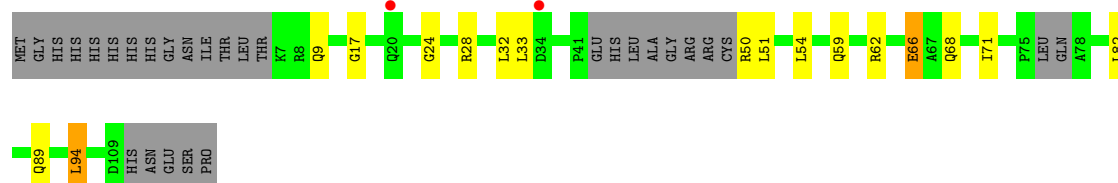




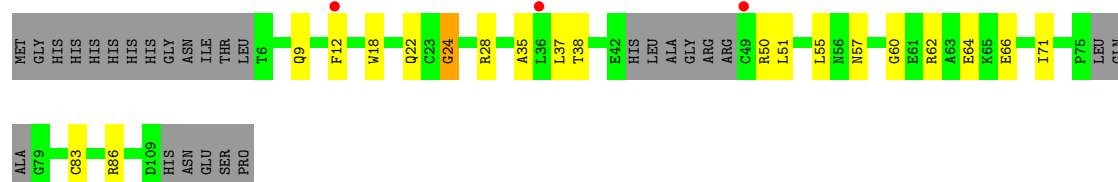
• Molecule 3: Chaperone protein YscY



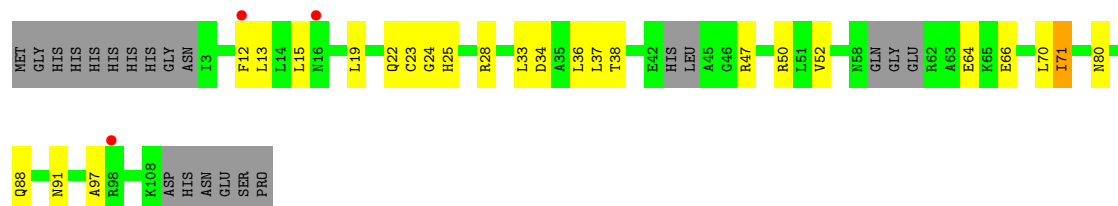
• Molecule 3: Chaperone protein YscY



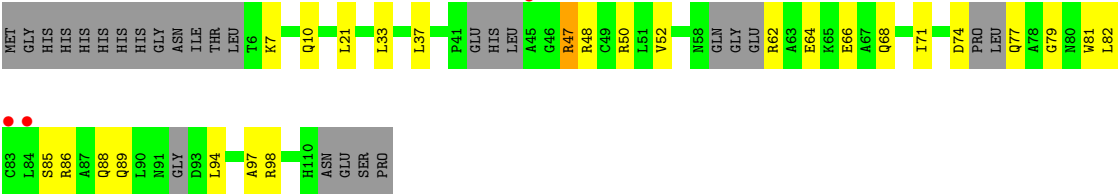
• Molecule 3: Chaperone protein YscY



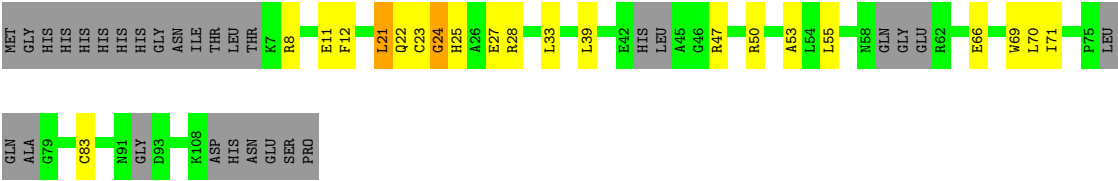
• Molecule 3: Chaperone protein YscY



• Molecule 3: Chaperone protein YscY



● Molecule 3: Chaperone protein YscY



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	143.46Å 324.92Å 369.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 4.10 49.83 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.83-4.10) 90.9 (49.83-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.305 , 0.325 0.306 , 0.325	Depositor DCC
R_{free} test set	6770 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	153.2	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 152.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	73488	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	AA	0.10	0/2667	0.30	0/3597
1	BA	0.10	0/2731	0.29	0/3689
1	CA	0.11	0/2838	0.33	0/3832
1	DA	0.11	0/2704	0.33	0/3652
1	EA	0.10	0/2725	0.29	0/3674
1	FA	0.11	0/2779	0.33	0/3749
1	GA	0.11	0/2817	0.34	0/3805
1	HA	0.11	0/2770	0.31	0/3741
1	IA	0.10	0/2775	0.32	0/3749
1	JA	0.11	0/2732	0.32	0/3690
1	KA	0.11	0/2778	0.32	0/3749
1	LA	0.11	0/2777	0.32	0/3749
1	MA	0.10	0/2673	0.33	0/3607
1	NA	0.10	0/2741	0.30	0/3699
1	OA	0.10	0/2734	0.31	0/3687
1	PA	0.11	0/2730	0.32	0/3687
1	QA	0.10	0/2756	0.31	0/3722
1	RA	0.11	0/2845	0.34	0/3844
2	AB	0.14	0/569	0.50	0/765
2	BB	0.17	0/529	0.53	0/711
2	CB	0.19	0/552	0.56	0/742
2	DB	0.15	0/497	0.51	0/668
2	EB	0.17	0/485	0.52	0/651
2	FB	0.19	0/581	0.61	0/783
2	GB	0.16	0/604	0.51	0/814
2	HB	0.15	0/529	0.49	0/711
2	IB	0.19	0/507	0.61	0/682
2	JB	0.16	0/561	0.52	0/756
2	KB	0.17	0/633	0.53	0/853
2	LB	0.19	0/579	0.66	0/781
2	MB	0.14	0/517	0.43	0/693
2	NB	0.20	0/489	0.55	1/655 (0.2%)
2	OB	0.18	0/569	0.56	0/765
2	PB	0.16	0/525	0.59	0/706

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	QB	0.17	0/537	0.49	0/721
2	RB	0.17	0/565	0.51	0/760
3	AC	0.10	0/766	0.33	0/1033
3	BC	0.10	0/783	0.28	0/1056
3	CC	0.12	0/894	0.34	0/1208
3	DC	0.11	0/829	0.35	0/1118
3	EC	0.11	0/812	0.31	0/1092
3	FC	0.12	0/873	0.34	0/1179
3	GC	0.14	0/897	0.36	0/1213
3	HC	0.12	0/844	0.35	0/1139
3	IC	0.11	0/741	0.31	0/995
3	JC	0.13	0/900	0.35	0/1216
3	KC	0.16	0/920	0.44	0/1244
3	LC	0.13	0/865	0.38	0/1168
3	MC	0.11	0/794	0.31	0/1066
3	NC	0.12	0/841	0.35	0/1137
3	OC	0.11	0/891	0.30	0/1204
3	PC	0.12	0/899	0.36	0/1216
3	QC	0.10	0/771	0.26	0/1035
3	RC	0.12	0/897	0.36	0/1213
All	All	0.12	0/74617	0.36	1/100671 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	NB	119	LEU	N-CA-C	5.03	116.84	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2628	0	2660	61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	2688	0	2723	59	0
1	CA	2792	0	2814	76	0
1	DA	2661	0	2673	70	0
1	EA	2684	0	2705	55	0
1	FA	2736	0	2757	57	0
1	GA	2772	0	2792	70	0
1	HA	2727	0	2759	53	0
1	IA	2731	0	2754	67	0
1	JA	2689	0	2714	59	0
1	KA	2736	0	2772	65	0
1	LA	2734	0	2761	61	0
1	MA	2632	0	2673	61	0
1	NA	2698	0	2713	65	0
1	OA	2694	0	2723	65	0
1	PA	2688	0	2719	65	0
1	QA	2713	0	2739	76	0
1	RA	2798	0	2815	71	0
2	AB	562	0	560	11	0
2	BB	524	0	527	14	0
2	CB	546	0	548	18	0
2	DB	493	0	497	12	0
2	EB	482	0	487	14	0
2	FB	572	0	579	20	0
2	GB	596	0	598	10	0
2	HB	524	0	527	13	0
2	IB	503	0	507	13	0
2	JB	554	0	549	10	0
2	KB	624	0	624	20	0
2	LB	569	0	571	23	0
2	MB	513	0	520	13	0
2	NB	487	0	491	14	0
2	OB	562	0	560	22	0
2	PB	521	0	527	15	0
2	QB	532	0	532	15	0
2	RB	559	0	560	15	0
3	AC	754	0	744	11	0
3	BC	771	0	757	17	0
3	CC	879	0	873	18	0
3	DC	817	0	823	17	0
3	EC	800	0	790	17	0
3	FC	858	0	851	22	0
3	GC	878	0	876	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	HC	830	0	827	14	0
3	IC	732	0	734	10	0
3	JC	883	0	866	21	0
3	KC	904	0	895	25	0
3	LC	851	0	850	22	0
3	MC	784	0	776	19	0
3	NC	826	0	815	20	0
3	OC	875	0	859	16	0
3	PC	883	0	877	27	0
3	QC	761	0	758	16	0
3	RC	878	0	876	18	0
All	All	73488	0	73877	1494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1494 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:QA:687:TYR:HB3	2:QB:119:LEU:HD11	1.44	0.96
2:EB:84:GLN:HE22	2:EB:106:GLN:HB2	1.30	0.94
1:AA:687:TYR:HB3	2:AB:119:LEU:HD11	1.53	0.90
2:BB:87:LEU:HD12	2:BB:102:LEU:HD12	1.59	0.84
1:LA:627:ALA:HB2	1:MA:575:LYS:HD3	1.60	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AA	311/350 (89%)	283 (91%)	27 (9%)	1 (0%)	36 70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	327/350 (93%)	302 (92%)	25 (8%)	0	100	100
1	CA	337/350 (96%)	294 (87%)	41 (12%)	2 (1%)	21	58
1	DA	318/350 (91%)	288 (91%)	30 (9%)	0	100	100
1	EA	317/350 (91%)	289 (91%)	28 (9%)	0	100	100
1	FA	329/350 (94%)	299 (91%)	30 (9%)	0	100	100
1	GA	335/350 (96%)	298 (89%)	37 (11%)	0	100	100
1	HA	327/350 (93%)	294 (90%)	33 (10%)	0	100	100
1	IA	330/350 (94%)	296 (90%)	32 (10%)	2 (1%)	21	58
1	JA	324/350 (93%)	289 (89%)	34 (10%)	1 (0%)	36	70
1	KA	325/350 (93%)	296 (91%)	27 (8%)	2 (1%)	21	58
1	LA	328/350 (94%)	298 (91%)	30 (9%)	0	100	100
1	MA	312/350 (89%)	276 (88%)	36 (12%)	0	100	100
1	NA	321/350 (92%)	290 (90%)	31 (10%)	0	100	100
1	OA	319/350 (91%)	284 (89%)	35 (11%)	0	100	100
1	PA	322/350 (92%)	284 (88%)	37 (12%)	1 (0%)	36	70
1	QA	326/350 (93%)	292 (90%)	33 (10%)	1 (0%)	36	70
1	RA	340/350 (97%)	299 (88%)	40 (12%)	1 (0%)	36	70
2	AB	66/95 (70%)	61 (92%)	5 (8%)	0	100	100
2	BB	61/95 (64%)	57 (93%)	4 (7%)	0	100	100
2	CB	64/95 (67%)	59 (92%)	4 (6%)	1 (2%)	7	37
2	DB	57/95 (60%)	55 (96%)	2 (4%)	0	100	100
2	EB	56/95 (59%)	54 (96%)	2 (4%)	0	100	100
2	FB	68/95 (72%)	64 (94%)	4 (6%)	0	100	100
2	GB	69/95 (73%)	66 (96%)	3 (4%)	0	100	100
2	HB	61/95 (64%)	54 (88%)	7 (12%)	0	100	100
2	IB	59/95 (62%)	57 (97%)	2 (3%)	0	100	100
2	JB	65/95 (68%)	62 (95%)	3 (5%)	0	100	100
2	KB	73/95 (77%)	67 (92%)	6 (8%)	0	100	100
2	LB	67/95 (70%)	55 (82%)	11 (16%)	1 (2%)	8	39
2	MB	58/95 (61%)	54 (93%)	4 (7%)	0	100	100
2	NB	55/95 (58%)	53 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	OB	66/95 (70%)	63 (96%)	3 (4%)	0	100	100
2	PB	61/95 (64%)	54 (88%)	7 (12%)	0	100	100
2	QB	60/95 (63%)	58 (97%)	2 (3%)	0	100	100
2	RB	66/95 (70%)	63 (96%)	3 (4%)	0	100	100
3	AC	87/122 (71%)	80 (92%)	7 (8%)	0	100	100
3	BC	89/122 (73%)	84 (94%)	4 (4%)	1 (1%)	11	44
3	CC	104/122 (85%)	100 (96%)	4 (4%)	0	100	100
3	DC	95/122 (78%)	89 (94%)	5 (5%)	1 (1%)	11	44
3	EC	90/122 (74%)	84 (93%)	6 (7%)	0	100	100
3	FC	102/122 (84%)	93 (91%)	9 (9%)	0	100	100
3	GC	107/122 (88%)	97 (91%)	10 (9%)	0	100	100
3	HC	98/122 (80%)	90 (92%)	7 (7%)	1 (1%)	12	46
3	IC	79/122 (65%)	74 (94%)	5 (6%)	0	100	100
3	JC	107/122 (88%)	99 (92%)	7 (6%)	1 (1%)	14	49
3	KC	110/122 (90%)	105 (96%)	5 (4%)	0	100	100
3	LC	101/122 (83%)	95 (94%)	6 (6%)	0	100	100
3	MC	86/122 (70%)	82 (95%)	4 (5%)	0	100	100
3	NC	100/122 (82%)	93 (93%)	7 (7%)	0	100	100
3	OC	106/122 (87%)	98 (92%)	8 (8%)	0	100	100
3	PC	107/122 (88%)	99 (92%)	8 (8%)	0	100	100
3	QC	83/122 (68%)	78 (94%)	4 (5%)	1 (1%)	10	42
3	RC	107/122 (88%)	100 (94%)	6 (6%)	1 (1%)	14	49
All	All	8738/10206 (86%)	7947 (91%)	772 (9%)	19 (0%)	43	76

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CA	469	ASP
1	CA	627	ALA
1	PA	391	ASN
2	CB	120	HIS
2	LB	77	ARG

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	AA	290/312 (93%)	282 (97%)	8 (3%)	38	59
1	BA	296/312 (95%)	285 (96%)	11 (4%)	30	52
1	CA	307/312 (98%)	293 (95%)	14 (5%)	24	47
1	DA	294/312 (94%)	282 (96%)	12 (4%)	27	50
1	EA	296/312 (95%)	284 (96%)	12 (4%)	27	50
1	FA	301/312 (96%)	290 (96%)	11 (4%)	30	52
1	GA	305/312 (98%)	295 (97%)	10 (3%)	33	55
1	HA	302/312 (97%)	291 (96%)	11 (4%)	31	53
1	IA	302/312 (97%)	292 (97%)	10 (3%)	33	55
1	JA	297/312 (95%)	284 (96%)	13 (4%)	25	48
1	KA	303/312 (97%)	288 (95%)	15 (5%)	22	45
1	LA	302/312 (97%)	291 (96%)	11 (4%)	31	53
1	MA	290/312 (93%)	281 (97%)	9 (3%)	35	56
1	NA	297/312 (95%)	287 (97%)	10 (3%)	32	55
1	OA	297/312 (95%)	288 (97%)	9 (3%)	36	57
1	PA	298/312 (96%)	286 (96%)	12 (4%)	28	50
1	QA	300/312 (96%)	288 (96%)	12 (4%)	28	50
1	RA	308/312 (99%)	297 (96%)	11 (4%)	31	53
2	AB	61/81 (75%)	60 (98%)	1 (2%)	55	69
2	BB	58/81 (72%)	56 (97%)	2 (3%)	32	55
2	CB	60/81 (74%)	60 (100%)	0	100	100
2	DB	56/81 (69%)	55 (98%)	1 (2%)	51	67
2	EB	54/81 (67%)	54 (100%)	0	100	100
2	FB	64/81 (79%)	62 (97%)	2 (3%)	35	56
2	GB	66/81 (82%)	62 (94%)	4 (6%)	17	41
2	HB	58/81 (72%)	58 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	IB	56/81 (69%)	55 (98%)	1 (2%)	51	67
2	JB	61/81 (75%)	61 (100%)	0	100	100
2	KB	68/81 (84%)	67 (98%)	1 (2%)	57	70
2	LB	64/81 (79%)	64 (100%)	0	100	100
2	MB	55/81 (68%)	53 (96%)	2 (4%)	31	53
2	NB	54/81 (67%)	52 (96%)	2 (4%)	30	52
2	OB	61/81 (75%)	60 (98%)	1 (2%)	55	69
2	PB	58/81 (72%)	58 (100%)	0	100	100
2	QB	58/81 (72%)	55 (95%)	3 (5%)	21	45
2	RB	61/81 (75%)	61 (100%)	0	100	100
3	AC	78/103 (76%)	75 (96%)	3 (4%)	29	51
3	BC	81/103 (79%)	80 (99%)	1 (1%)	63	73
3	CC	92/103 (89%)	91 (99%)	1 (1%)	65	74
3	DC	85/103 (82%)	82 (96%)	3 (4%)	32	54
3	EC	83/103 (81%)	81 (98%)	2 (2%)	43	63
3	FC	89/103 (86%)	88 (99%)	1 (1%)	65	74
3	GC	92/103 (89%)	87 (95%)	5 (5%)	20	44
3	HC	86/103 (84%)	83 (96%)	3 (4%)	32	54
3	IC	76/103 (74%)	76 (100%)	0	100	100
3	JC	92/103 (89%)	89 (97%)	3 (3%)	33	55
3	KC	94/103 (91%)	91 (97%)	3 (3%)	34	56
3	LC	89/103 (86%)	87 (98%)	2 (2%)	45	64
3	MC	81/103 (79%)	79 (98%)	2 (2%)	42	62
3	NC	85/103 (82%)	84 (99%)	1 (1%)	63	73
3	OC	91/103 (88%)	89 (98%)	2 (2%)	45	64
3	PC	92/103 (89%)	89 (97%)	3 (3%)	33	55
3	QC	79/103 (77%)	77 (98%)	2 (2%)	42	62
3	RC	92/103 (89%)	91 (99%)	1 (1%)	65	74
All	All	8015/8928 (90%)	7756 (97%)	259 (3%)	34	56

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	EC	71	ILE
2	IB	105	GLN
1	IA	649	ILE
1	IA	604	ILE
2	BB	80	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
3	RC	56	ASN
3	PC	56	ASN
3	QC	56	ASN
3	GC	57	ASN
2	OB	96	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	AA	323/350 (92%)	0.29	9 (2%)	55	41	150, 183, 241, 261	0
1	BA	331/350 (94%)	0.25	4 (1%)	76	60	150, 181, 241, 253	0
1	CA	343/350 (98%)	0.30	6 (1%)	69	52	143, 175, 228, 240	0
1	DA	326/350 (93%)	0.28	3 (0%)	81	65	144, 179, 238, 249	0
1	EA	329/350 (94%)	0.40	9 (2%)	56	42	145, 181, 253, 269	0
1	FA	337/350 (96%)	0.28	7 (2%)	63	48	143, 175, 233, 245	0
1	GA	341/350 (97%)	0.29	8 (2%)	61	46	142, 169, 216, 228	0
1	HA	335/350 (95%)	0.32	8 (2%)	59	45	145, 178, 239, 254	0
1	IA	336/350 (96%)	0.24	4 (1%)	76	60	142, 180, 264, 272	0
1	JA	330/350 (94%)	0.34	6 (1%)	67	51	137, 165, 207, 214	0
1	KA	335/350 (95%)	0.31	6 (1%)	67	51	137, 162, 211, 223	0
1	LA	336/350 (96%)	0.31	5 (1%)	72	54	140, 170, 227, 239	0
1	MA	322/350 (92%)	0.26	4 (1%)	76	60	150, 179, 242, 255	0
1	NA	331/350 (94%)	0.29	2 (0%)	85	72	155, 185, 245, 255	0
1	OA	331/350 (94%)	0.29	8 (2%)	59	45	148, 176, 240, 252	0
1	PA	330/350 (94%)	0.34	5 (1%)	72	54	142, 172, 216, 238	0
1	QA	334/350 (95%)	0.28	7 (2%)	63	48	139, 171, 245, 255	0
1	RA	344/350 (98%)	0.35	12 (3%)	47	35	138, 163, 207, 223	0
2	AB	70/95 (73%)	0.31	0	100	100	186, 247, 257, 263	0
2	BB	65/95 (68%)	0.23	0	100	100	179, 232, 248, 257	0
2	CB	68/95 (71%)	0.21	2 (2%)	53	40	161, 189, 221, 230	0
2	DB	61/95 (64%)	0.10	0	100	100	173, 234, 251, 256	0
2	EB	60/95 (63%)	0.23	0	100	100	184, 242, 259, 262	0
2	FB	71/95 (74%)	0.28	0	100	100	165, 226, 250, 255	1 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	GB	73/95 (76%)	0.23	0 100 100	163, 192, 211, 216	0
2	HB	65/95 (68%)	0.27	1 (1%) 72 54	182, 214, 243, 246	1 (1%)
2	IB	63/95 (66%)	0.17	0 100 100	181, 236, 248, 251	0
2	JB	69/95 (72%)	0.15	1 (1%) 73 56	156, 189, 216, 229	0
2	KB	77/95 (81%)	0.35	3 (3%) 43 34	166, 187, 209, 212	0
2	LB	70/95 (73%)	0.27	0 100 100	147, 203, 219, 222	1 (1%)
2	MB	64/95 (67%)	0.25	0 100 100	187, 238, 249, 251	0
2	NB	61/95 (64%)	0.30	2 (3%) 49 37	183, 242, 260, 263	0
2	OB	70/95 (73%)	0.32	0 100 100	187, 215, 237, 243	0
2	PB	65/95 (68%)	0.24	0 100 100	173, 220, 236, 241	0
2	QB	66/95 (69%)	0.28	2 (3%) 52 39	172, 245, 259, 264	0
2	RB	70/95 (73%)	0.31	0 100 100	164, 194, 216, 225	0
3	AC	93/122 (76%)	0.36	2 (2%) 62 47	224, 248, 257, 259	0
3	BC	95/122 (77%)	0.33	3 (3%) 50 38	215, 238, 258, 264	0
3	CC	108/122 (88%)	0.36	2 (1%) 66 50	166, 188, 206, 215	0
3	DC	101/122 (82%)	0.35	3 (2%) 52 39	203, 237, 258, 261	0
3	EC	98/122 (80%)	0.28	1 (1%) 79 62	229, 252, 264, 269	0
3	FC	106/122 (86%)	0.48	3 (2%) 55 41	219, 233, 248, 260	0
3	GC	108/122 (88%)	0.23	5 (4%) 37 30	116, 181, 207, 228	1 (0%)
3	HC	102/122 (83%)	0.02	0 100 100	185, 213, 230, 238	0
3	IC	89/122 (72%)	0.46	2 (2%) 62 47	216, 248, 269, 274	0
3	JC	109/122 (89%)	0.34	2 (1%) 67 51	163, 187, 237, 244	1 (0%)
3	KC	112/122 (91%)	0.27	2 (1%) 67 51	152, 177, 213, 245	0
3	LC	105/122 (86%)	0.42	3 (2%) 53 40	173, 205, 230, 234	0
3	MC	96/122 (78%)	0.45	3 (3%) 51 38	217, 249, 264, 268	0
3	NC	102/122 (83%)	0.18	0 100 100	228, 252, 259, 264	0
3	OC	108/122 (88%)	0.21	1 (0%) 81 65	194, 217, 230, 249	0
3	PC	109/122 (89%)	0.28	2 (1%) 67 51	187, 216, 229, 238	0
3	QC	93/122 (76%)	0.40	0 100 100	221, 249, 259, 268	0
3	RC	108/122 (88%)	0.38	5 (4%) 37 30	125, 187, 199, 219	1 (0%)
All	All	9044/10206 (88%)	0.30	163 (1%) 67 51	116, 188, 251, 274	6 (0%)

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	PA	448	GLU	5.2
1	DA	659	PRO	4.9
1	CA	449	SER	4.3
1	CA	697	GLN	4.3
2	KB	122	VAL	4.2

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.