



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 09:18 PM UTC

PDB ID : 5JJ1 / pdb_00005jj1
Title : Structure of the Immature Procapsid Conformation of P22 Portal Protein
Authors : Lokareddy, R.K.; Cingolani, G.
Deposited on : 2016-04-22
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

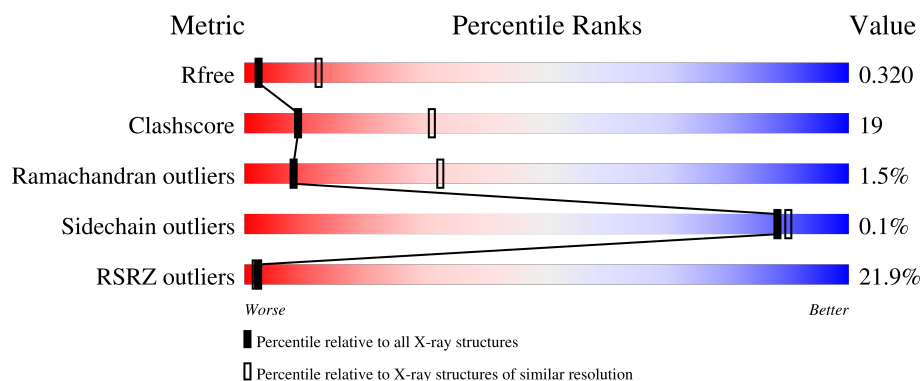
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	A	610	24% 61% 33% ..
1	B	610	16% 57% 36% ..
1	C	610	20% 56% 39% ..
1	D	610	25% 57% 35% ..
1	E	610	21% 58% 36% ..

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Mol	Chain	Length	Quality of chain
1	F	610	21%58%37%
1	G	610	18%57%37%
1	H	610	24%55%39%
1	I	610	20%55%38%
1	J	610	20%60%34%
1	K	610	22%61%34%
1	L	610	20%63%31%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 56559 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
1	A	585	Total	C	N	O	S	0	0	0
			4724	2976	806	921	21			
1	B	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	C	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	D	585	Total	C	N	O	S	0	0	0
			4723	2977	805	920	21			
1	E	585	Total	C	N	O	S	0	0	0
			4720	2974	805	920	21			
1	F	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	G	585	Total	C	N	O	S	0	0	0
			4706	2966	804	915	21			
1	H	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	I	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	J	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	K	585	Total	C	N	O	S	0	0	0
			4716	2971	805	919	21			
1	L	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	LEU	-	expression tag	UNP P26744
A	604	GLU	-	expression tag	UNP P26744
A	605	HIS	-	expression tag	UNP P26744
A	606	HIS	-	expression tag	UNP P26744
A	607	HIS	-	expression tag	UNP P26744

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP P26744
A	609	HIS	-	expression tag	UNP P26744
A	610	HIS	-	expression tag	UNP P26744
B	603	LEU	-	expression tag	UNP P26744
B	604	GLU	-	expression tag	UNP P26744
B	605	HIS	-	expression tag	UNP P26744
B	606	HIS	-	expression tag	UNP P26744
B	607	HIS	-	expression tag	UNP P26744
B	608	HIS	-	expression tag	UNP P26744
B	609	HIS	-	expression tag	UNP P26744
B	610	HIS	-	expression tag	UNP P26744
C	603	LEU	-	expression tag	UNP P26744
C	604	GLU	-	expression tag	UNP P26744
C	605	HIS	-	expression tag	UNP P26744
C	606	HIS	-	expression tag	UNP P26744
C	607	HIS	-	expression tag	UNP P26744
C	608	HIS	-	expression tag	UNP P26744
C	609	HIS	-	expression tag	UNP P26744
C	610	HIS	-	expression tag	UNP P26744
D	603	LEU	-	expression tag	UNP P26744
D	604	GLU	-	expression tag	UNP P26744
D	605	HIS	-	expression tag	UNP P26744
D	606	HIS	-	expression tag	UNP P26744
D	607	HIS	-	expression tag	UNP P26744
D	608	HIS	-	expression tag	UNP P26744
D	609	HIS	-	expression tag	UNP P26744
D	610	HIS	-	expression tag	UNP P26744
E	603	LEU	-	expression tag	UNP P26744
E	604	GLU	-	expression tag	UNP P26744
E	605	HIS	-	expression tag	UNP P26744
E	606	HIS	-	expression tag	UNP P26744
E	607	HIS	-	expression tag	UNP P26744
E	608	HIS	-	expression tag	UNP P26744
E	609	HIS	-	expression tag	UNP P26744
E	610	HIS	-	expression tag	UNP P26744
F	603	LEU	-	expression tag	UNP P26744
F	604	GLU	-	expression tag	UNP P26744
F	605	HIS	-	expression tag	UNP P26744
F	606	HIS	-	expression tag	UNP P26744
F	607	HIS	-	expression tag	UNP P26744
F	608	HIS	-	expression tag	UNP P26744
F	609	HIS	-	expression tag	UNP P26744

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Chain	Residue	Modelled	Actual	Comment	Reference
F	610	HIS	-	expression tag	UNP P26744
G	603	LEU	-	expression tag	UNP P26744
G	604	GLU	-	expression tag	UNP P26744
G	605	HIS	-	expression tag	UNP P26744
G	606	HIS	-	expression tag	UNP P26744
G	607	HIS	-	expression tag	UNP P26744
G	608	HIS	-	expression tag	UNP P26744
G	609	HIS	-	expression tag	UNP P26744
G	610	HIS	-	expression tag	UNP P26744
H	603	LEU	-	expression tag	UNP P26744
H	604	GLU	-	expression tag	UNP P26744
H	605	HIS	-	expression tag	UNP P26744
H	606	HIS	-	expression tag	UNP P26744
H	607	HIS	-	expression tag	UNP P26744
H	608	HIS	-	expression tag	UNP P26744
H	609	HIS	-	expression tag	UNP P26744
H	610	HIS	-	expression tag	UNP P26744
I	603	LEU	-	expression tag	UNP P26744
I	604	GLU	-	expression tag	UNP P26744
I	605	HIS	-	expression tag	UNP P26744
I	606	HIS	-	expression tag	UNP P26744
I	607	HIS	-	expression tag	UNP P26744
I	608	HIS	-	expression tag	UNP P26744
I	609	HIS	-	expression tag	UNP P26744
I	610	HIS	-	expression tag	UNP P26744
J	603	LEU	-	expression tag	UNP P26744
J	604	GLU	-	expression tag	UNP P26744
J	605	HIS	-	expression tag	UNP P26744
J	606	HIS	-	expression tag	UNP P26744
J	607	HIS	-	expression tag	UNP P26744
J	608	HIS	-	expression tag	UNP P26744
J	609	HIS	-	expression tag	UNP P26744
J	610	HIS	-	expression tag	UNP P26744
K	603	LEU	-	expression tag	UNP P26744
K	604	GLU	-	expression tag	UNP P26744
K	605	HIS	-	expression tag	UNP P26744
K	606	HIS	-	expression tag	UNP P26744
K	607	HIS	-	expression tag	UNP P26744
K	608	HIS	-	expression tag	UNP P26744
K	609	HIS	-	expression tag	UNP P26744
K	610	HIS	-	expression tag	UNP P26744
L	603	LEU	-	expression tag	UNP P26744

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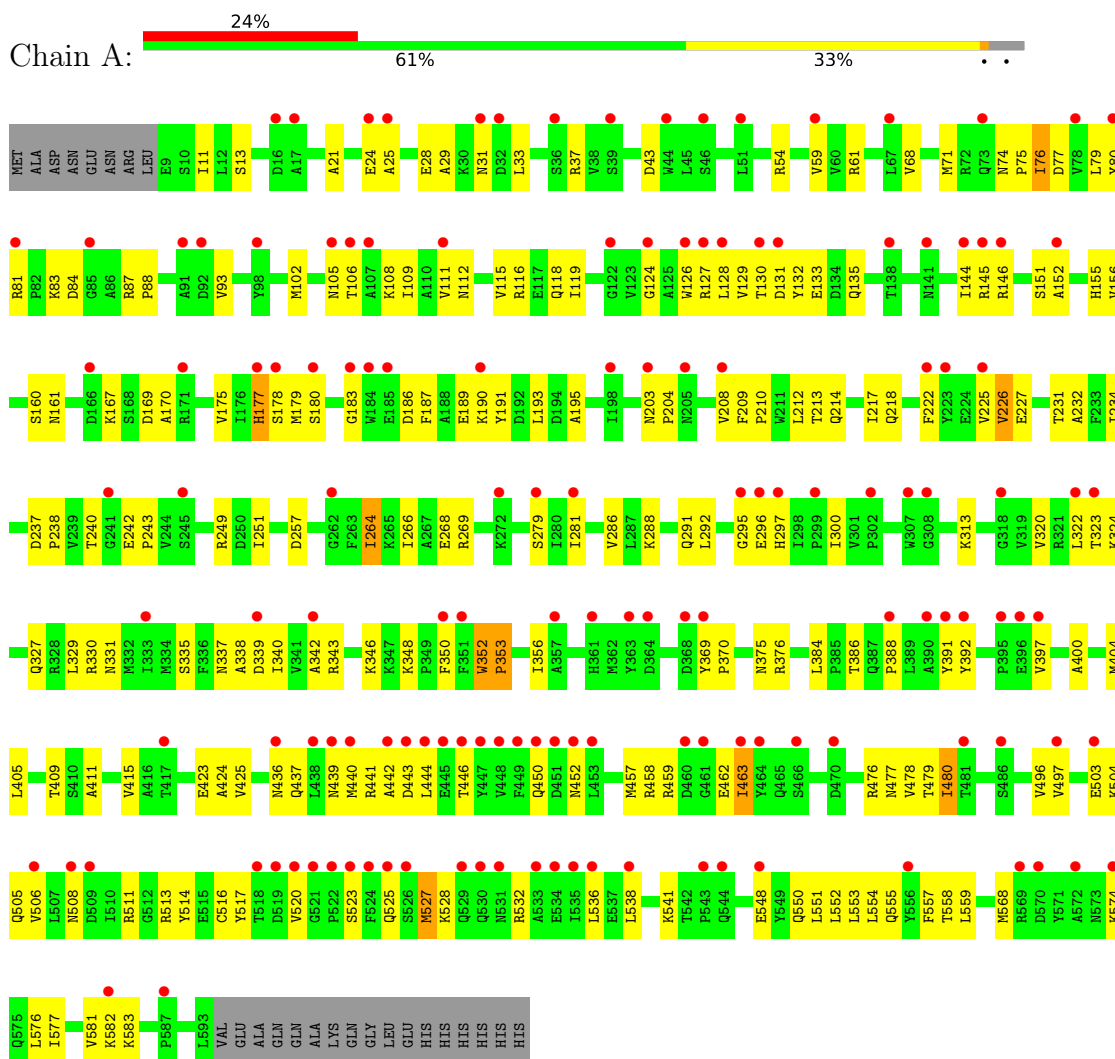
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Chain	Residue	Modelled	Actual	Comment	Reference
L	604	GLU	-	expression tag	UNP P26744
L	605	HIS	-	expression tag	UNP P26744
L	606	HIS	-	expression tag	UNP P26744
L	607	HIS	-	expression tag	UNP P26744
L	608	HIS	-	expression tag	UNP P26744
L	609	HIS	-	expression tag	UNP P26744
L	610	HIS	-	expression tag	UNP P26744

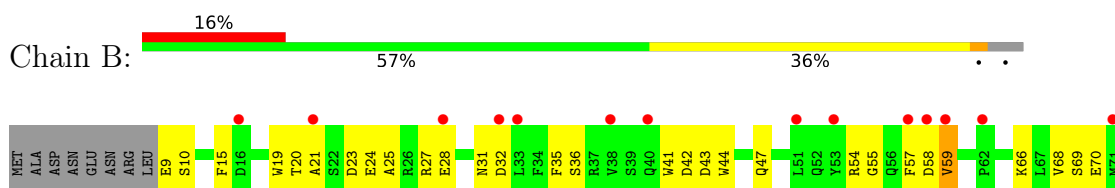
3 Residue-property plots

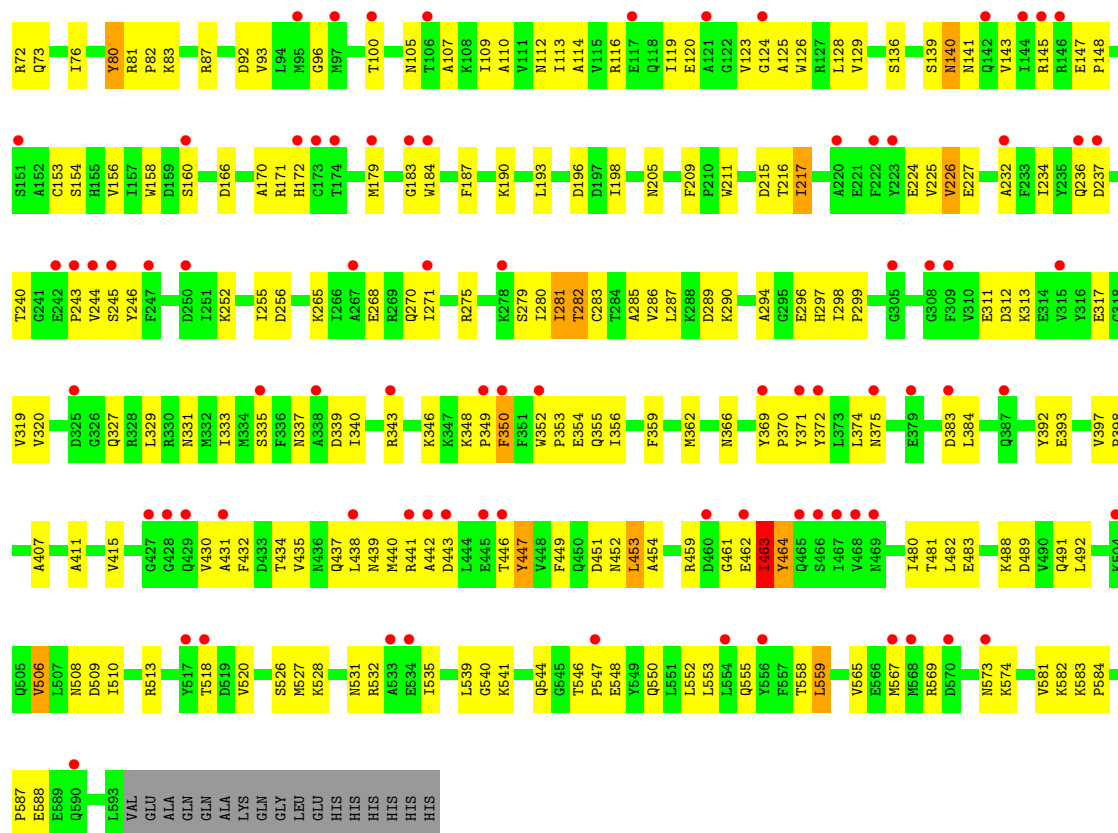
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

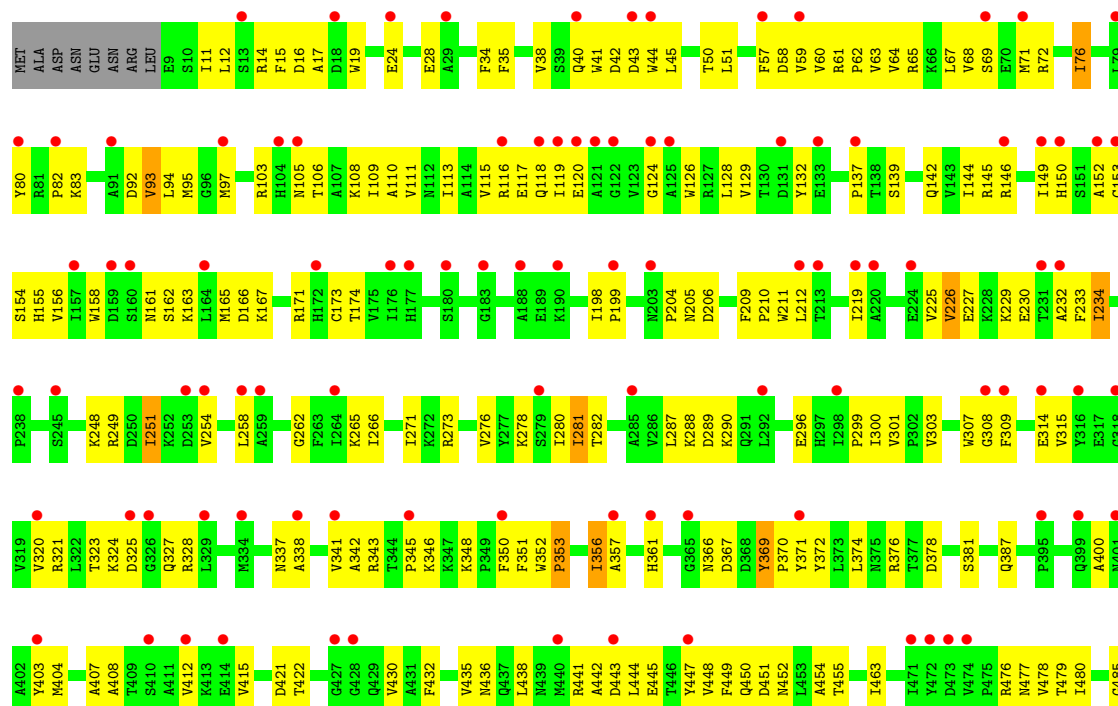


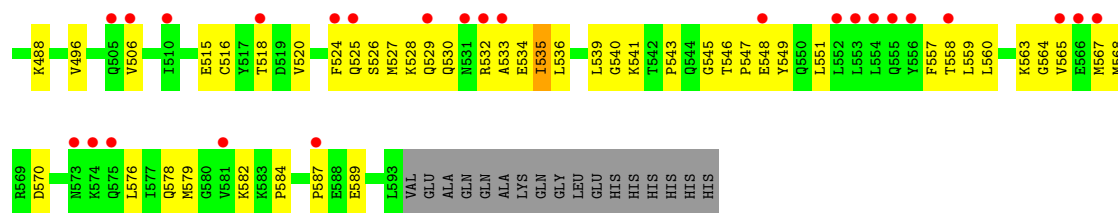
• Molecule 1: Portal protein



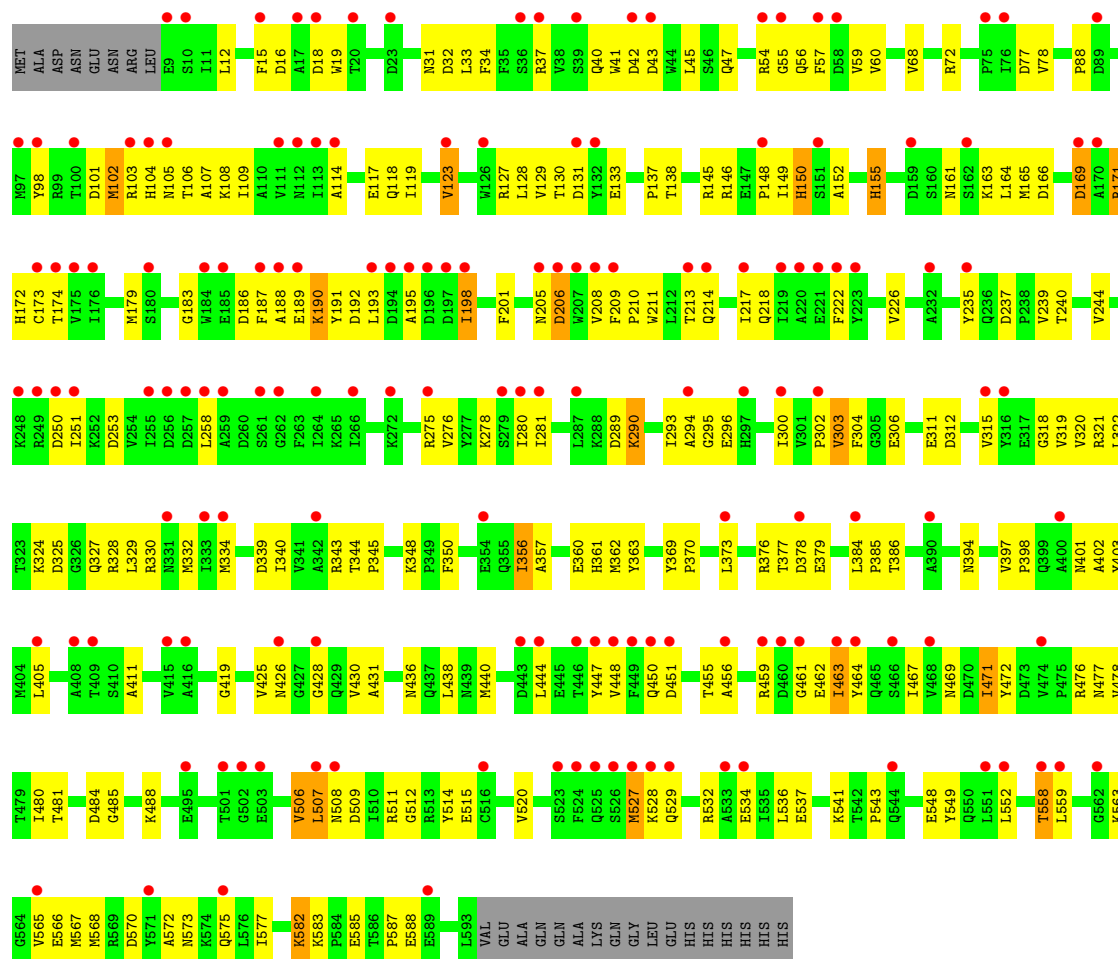


● Molecule 1: Portal protein

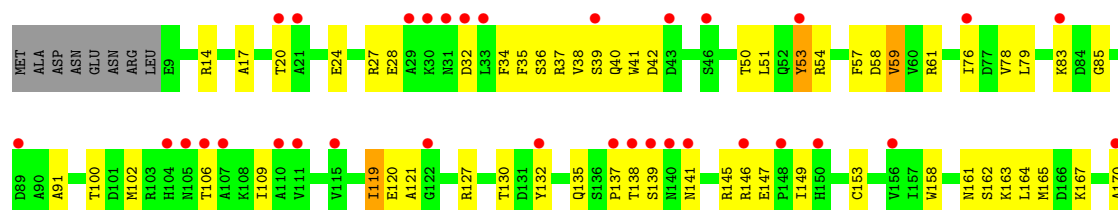


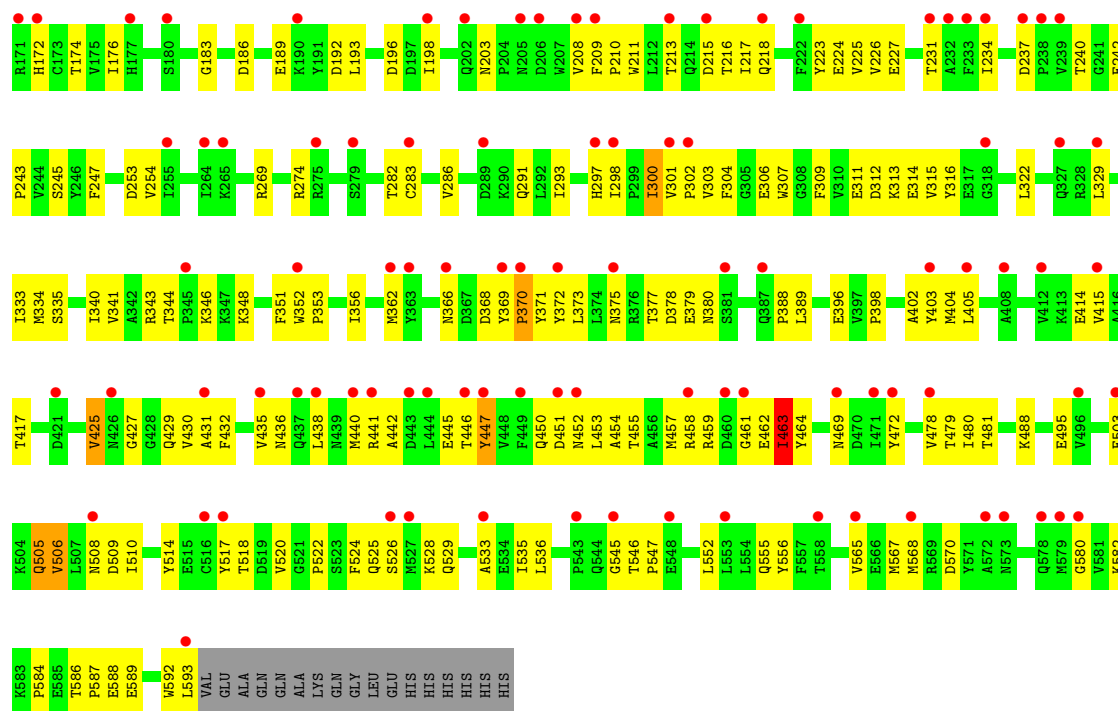


• Molecule 1: Portal protein

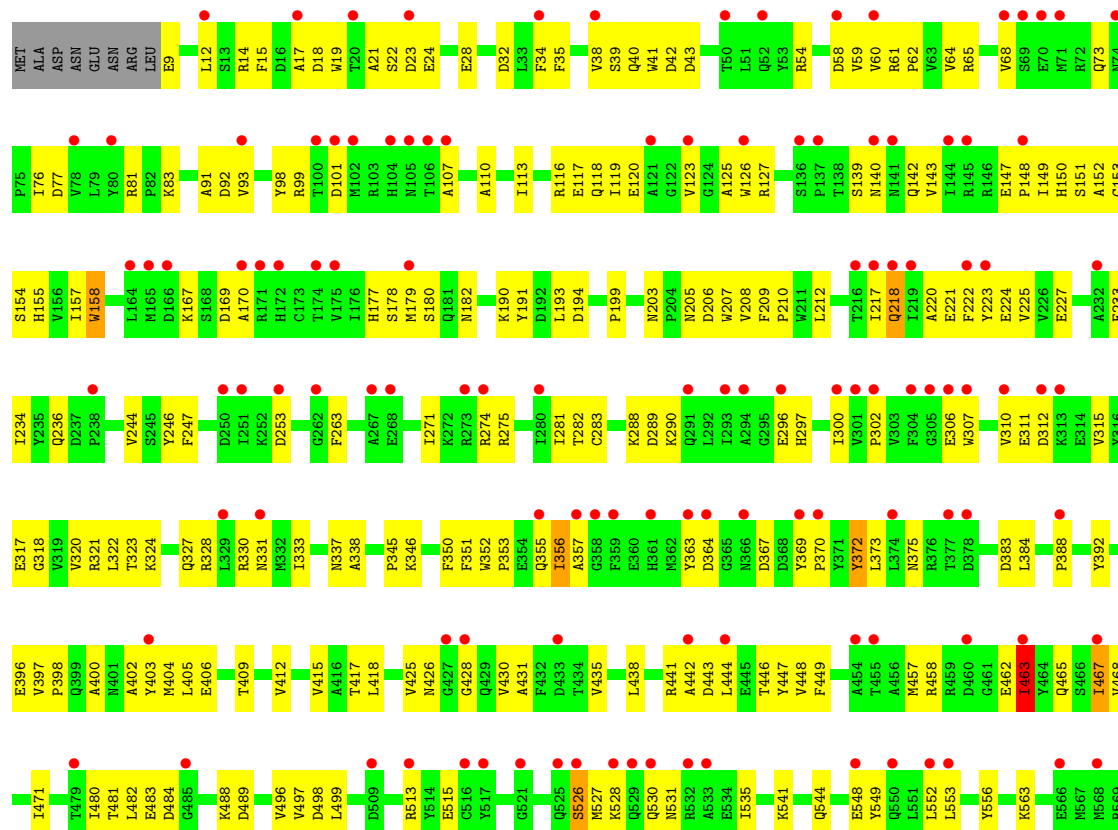


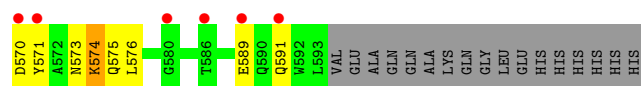
• Molecule 1: Portal protein



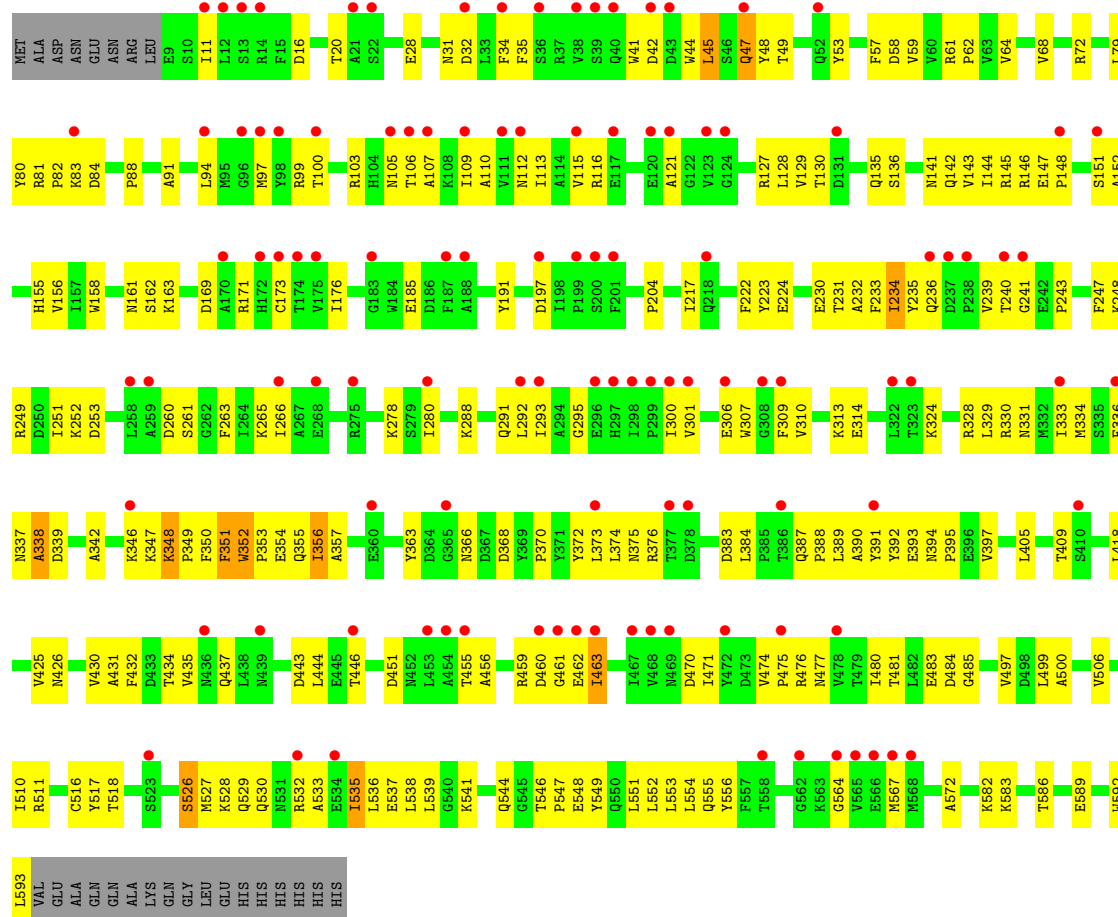


● Molecule 1: Portal protein

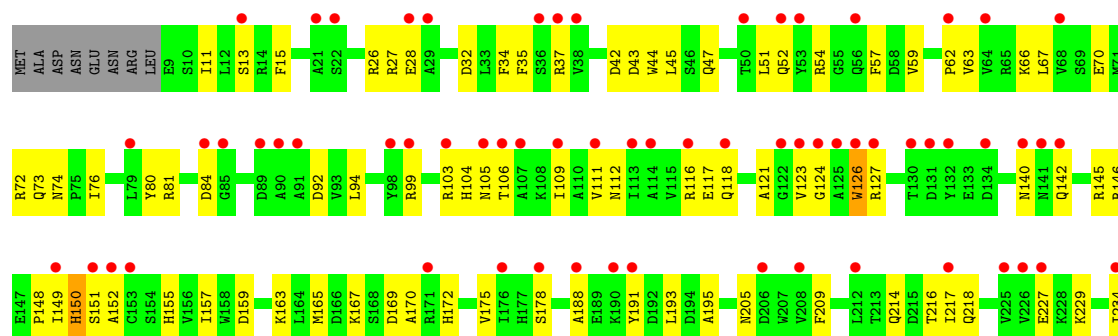


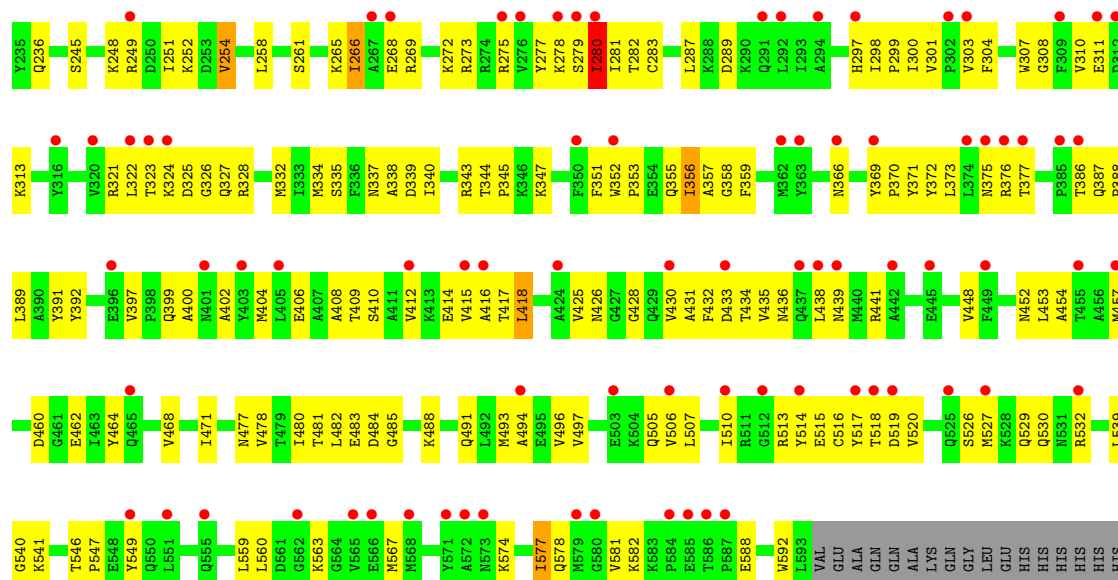


• Molecule 1: Portal protein

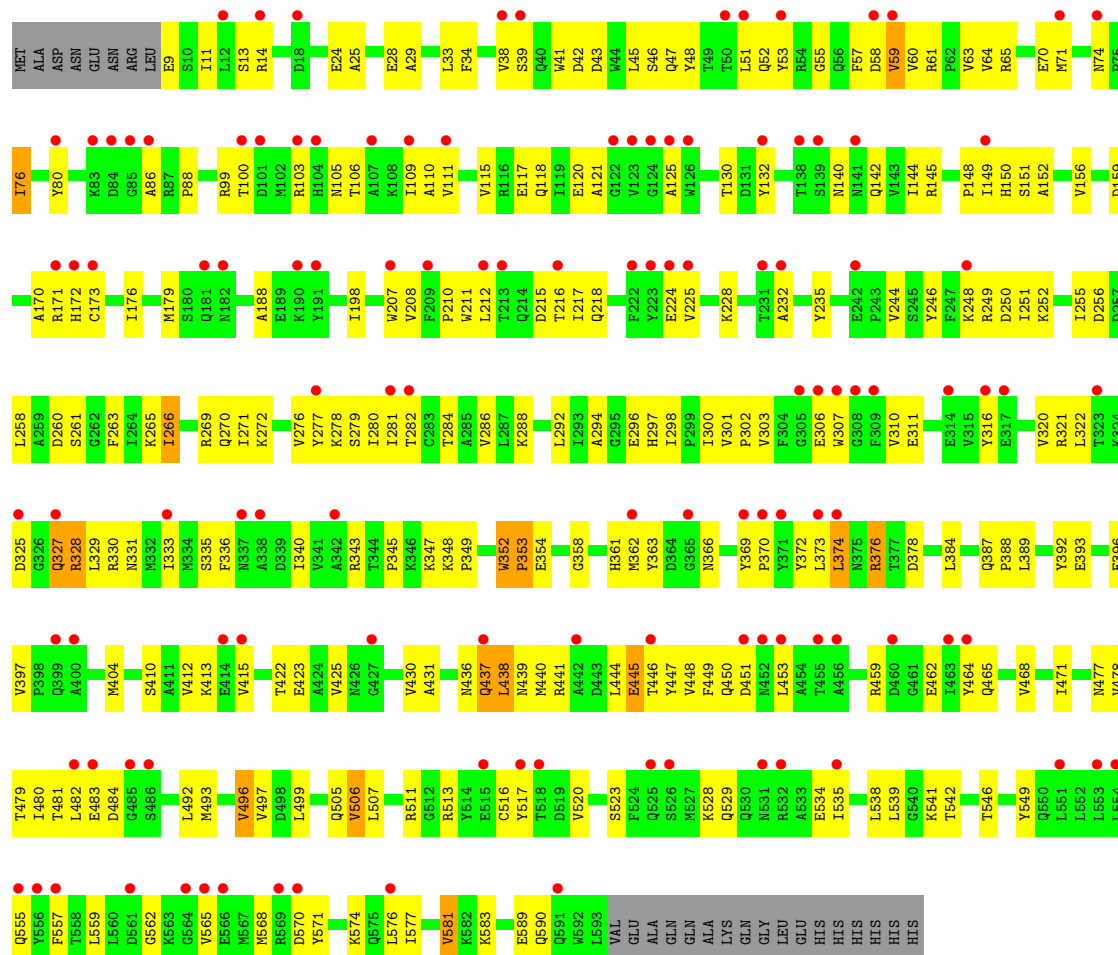


• Molecule 1: Portal protein

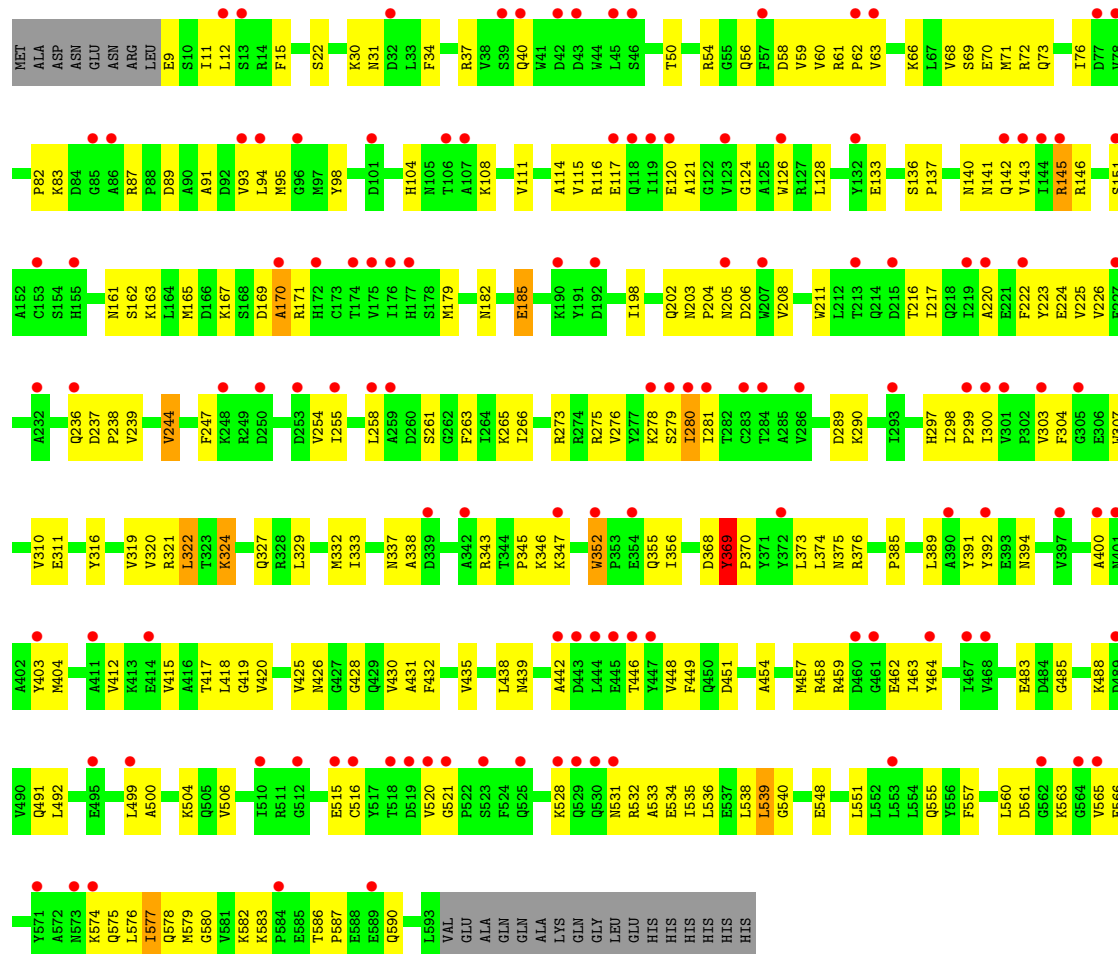




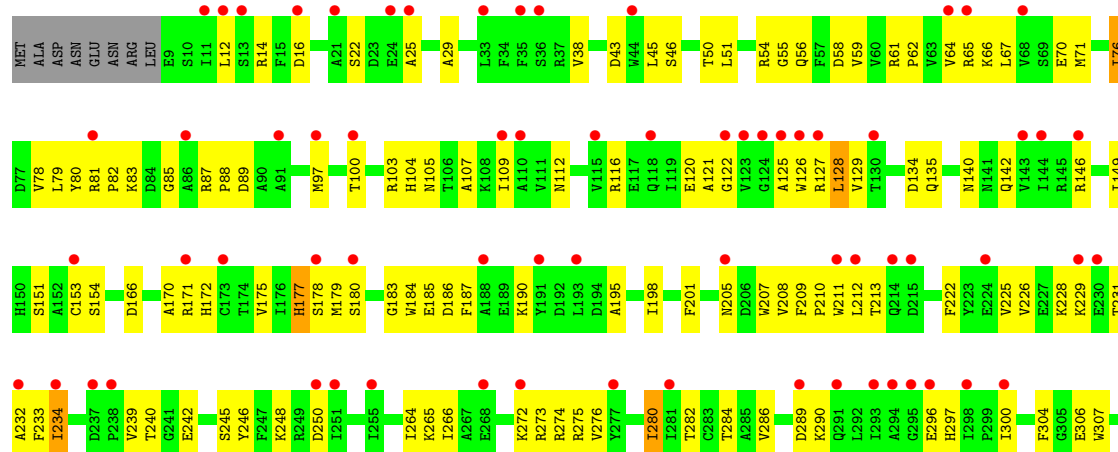
• Molecule 1: Portal protein

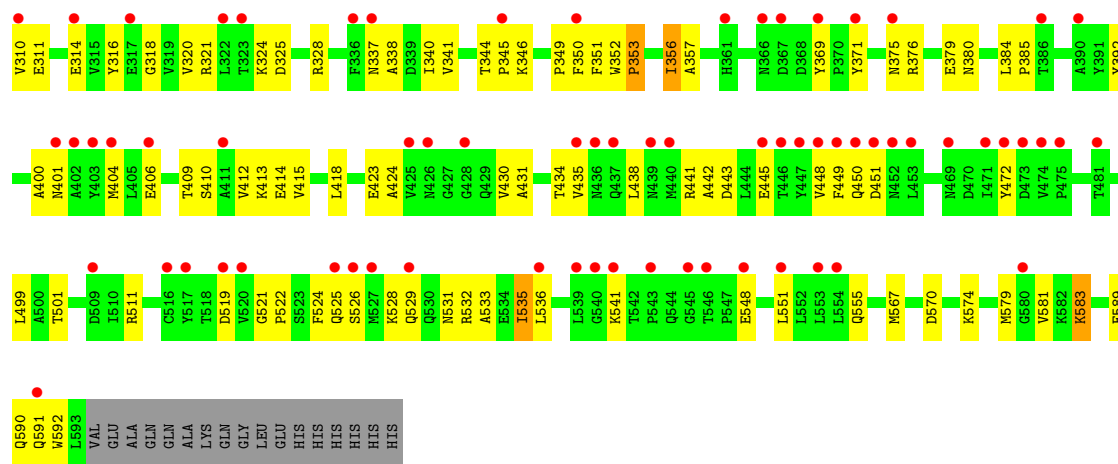


• Molecule 1: Portal protein

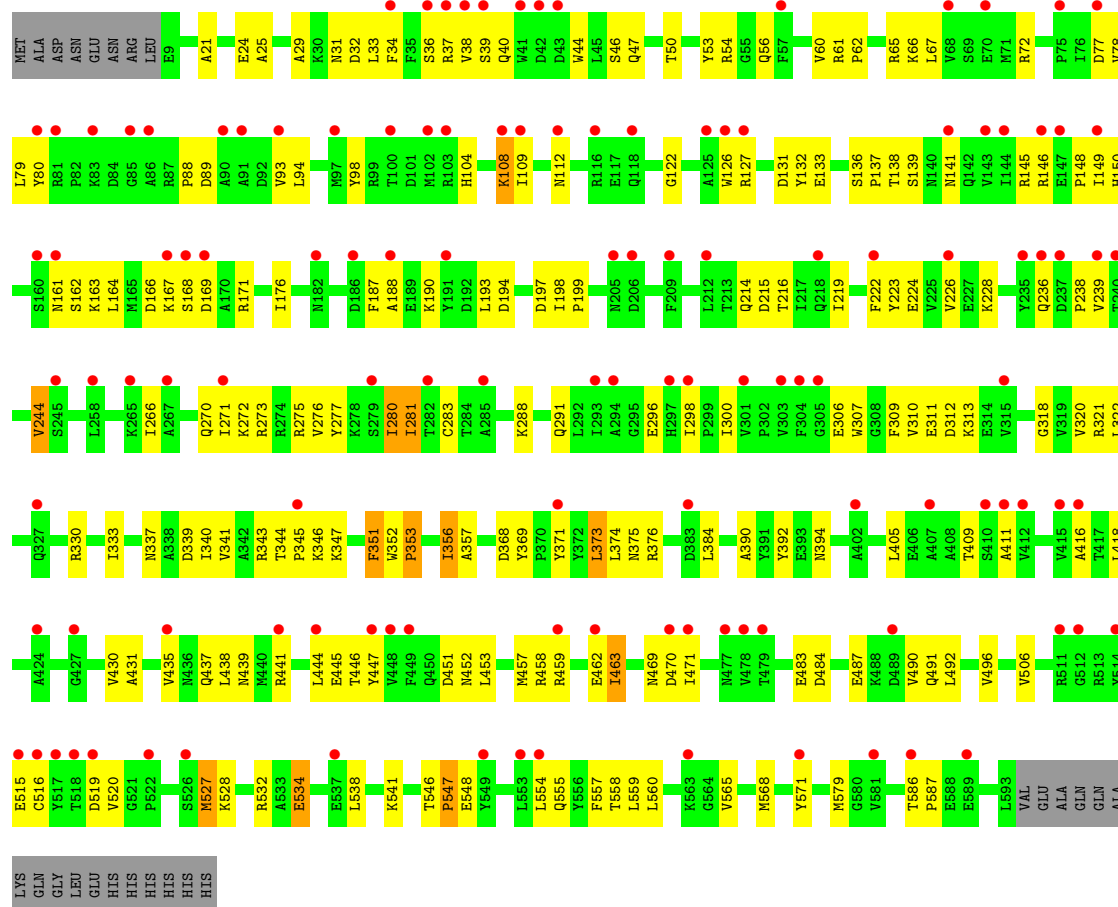


• Molecule 1: Portal protein





• Molecule 1: Portal protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	316.81Å 316.81Å 138.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30 15.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	85.0 (15.00-3.30) 84.1 (15.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.295 , 0.315 0.310 , 0.320	Depositor DCC
R_{free} test set	1737 reflections (0.84%)	wwPDB-VP
Wilson B-factor (Å ²)	91.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-l	Xtriage
Reported twinning fraction	0.502 for H, K, L 0.498 for -H, K, -L	Depositor
Outliers	15 of 175831 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	56559	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.61% 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	A	0.20	0/4826	0.58	0/6550
1	B	0.26	1/4812 (0.0%)	0.65	6/6533 (0.1%)
1	C	0.25	1/4812 (0.0%)	0.61	0/6533
1	D	0.23	0/4825	0.63	5/6550 (0.1%)
1	E	0.22	1/4822 (0.0%)	0.57	0/6546
1	F	0.21	0/4812	0.59	3/6533 (0.0%)
1	G	0.30	1/4808 (0.0%)	0.68	11/6528 (0.2%)
1	H	0.22	1/4812 (0.0%)	0.57	0/6533
1	I	0.24	0/4812	0.63	4/6533 (0.1%)
1	J	0.25	1/4812 (0.0%)	0.60	0/6533
1	K	0.20	0/4818	0.60	3/6541 (0.0%)
1	L	0.20	0/4812	0.59	1/6533 (0.0%)
All	All	0.23	6/57783 (0.0%)	0.61	33/78446 (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	5
1	B	0	6
1	C	0	8
1	D	0	11
1	E	0	9
1	F	0	10
1	G	0	7
1	H	0	8
1	I	0	8
1	J	0	10
1	K	0	7
1	L	0	7
All	All	0	96

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	LYS	C-N	8.29	1.53	1.33
1	E	203	ASN	C-N	6.90	1.50	1.33
1	H	352	TRP	C-N	6.83	1.49	1.33
1	J	203	ASN	C-N	6.11	1.48	1.33
1	B	80	TYR	C-N	5.85	1.45	1.33

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	470	ASP	N-CA-C	12.72	128.03	111.75
1	G	240	THR	N-CA-C	10.54	122.52	111.14
1	G	471	ILE	N-CA-C	-9.04	105.12	113.71
1	I	484	ASP	N-CA-C	8.84	121.72	111.11
1	D	150	HIS	N-CA-C	8.20	121.03	111.02

There are no chirality outliers.

5 of 96 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	SER	Peptide
1	A	177	HIS	Peptide
1	A	264	ILE	Peptide
1	A	352	TRP	Peptide
1	A	527	MET	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4724	0	4562	162	0
1	B	4710	0	4536	189	0
1	C	4710	0	4536	218	0
1	D	4723	0	4562	201	0
1	E	4720	0	4553	190	0
1	F	4710	0	4536	184	0
1	G	4706	0	4532	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	4710	0	4536	200	0
1	I	4710	0	4536	214	0
1	J	4710	0	4536	180	0
1	K	4716	0	4547	177	0
1	L	4710	0	4536	158	0
All	All	56559	0	54508	2061	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 19.

The worst 5 of 2061 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:I:297:HIS:HB3	1:I:450:GLN:OE1	1.30	1.26
1:I:447:TYR:OH	1:I:513:ARG:CD	1.88	1.21
1:I:447:TYR:OH	1:I:513:ARG:HD2	0.93	1.08
1:B:282:THR:OG1	1:B:285:ALA:O	1.85	0.95
1:I:297:HIS:CB	1:I:450:GLN:OE1	2.16	0.93

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	A	583/610 (96%)	461 (79%)	115 (20%)	7 (1%)	10	37
1	B	583/610 (96%)	461 (79%)	112 (19%)	10 (2%)	7	30
1	C	583/610 (96%)	442 (76%)	130 (22%)	11 (2%)	6	28
1	D	583/610 (96%)	451 (77%)	123 (21%)	9 (2%)	8	32
1	E	583/610 (96%)	454 (78%)	120 (21%)	9 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	583/610 (96%)	448 (77%)	129 (22%)	6 (1%)	12	40
1	G	583/610 (96%)	438 (75%)	135 (23%)	10 (2%)	7	30
1	H	583/610 (96%)	440 (76%)	134 (23%)	9 (2%)	8	32
1	I	583/610 (96%)	436 (75%)	137 (24%)	10 (2%)	7	30
1	J	583/610 (96%)	443 (76%)	132 (23%)	8 (1%)	9	33
1	K	583/610 (96%)	455 (78%)	121 (21%)	7 (1%)	10	37
1	L	583/610 (96%)	450 (77%)	125 (21%)	8 (1%)	9	33
All	All	6996/7320 (96%)	5379 (77%)	1513 (22%)	104 (2%)	8	32

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	VAL
1	B	226	VAL
1	B	244	VAL
1	B	282	THR
1	C	281	ILE

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	512/536 (96%)	512 (100%)	0	100	100
1	B	508/536 (95%)	506 (100%)	2 (0%)	84	84
1	C	508/536 (95%)	508 (100%)	0	100	100
1	D	512/536 (96%)	511 (100%)	1 (0%)	87	88
1	E	511/536 (95%)	510 (100%)	1 (0%)	87	88
1	F	508/536 (95%)	508 (100%)	0	100	100
1	G	507/536 (95%)	506 (100%)	1 (0%)	87	88
1	H	508/536 (95%)	508 (100%)	0	100	100
1	I	508/536 (95%)	506 (100%)	2 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	508/536 (95%)	506 (100%)	2 (0%)	84	84
1	K	510/536 (95%)	510 (100%)	0	100	100
1	L	508/536 (95%)	508 (100%)	0	100	100
All	All	6108/6432 (95%)	6099 (100%)	9 (0%)	88	90

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	324	LYS
1	J	539	LEU
1	E	463	ILE
1	G	351	PHE
1	I	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	218	GLN
1	G	437	GLN
1	L	331	ASN
1	F	439	ASN
1	G	155	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/610 (95%)	1.31	145 (24%) 2 1	16, 65, 94, 113	0
1	B	585/610 (95%)	1.15	96 (16%) 4 4	19, 62, 89, 109	0
1	C	585/610 (95%)	1.21	124 (21%) 2 2	19, 61, 91, 130	0
1	D	585/610 (95%)	1.43	155 (26%) 1 1	21, 66, 97, 184	0
1	E	585/610 (95%)	1.32	128 (21%) 2 2	19, 63, 98, 205	0
1	F	585/610 (95%)	1.24	128 (21%) 2 2	22, 60, 94, 142	0
1	G	585/610 (95%)	1.18	111 (18%) 3 3	18, 59, 92, 136	0
1	H	585/610 (95%)	1.30	145 (24%) 2 1	20, 62, 93, 117	0
1	I	585/610 (95%)	1.25	121 (20%) 2 2	19, 66, 99, 192	0
1	J	585/610 (95%)	1.29	124 (21%) 2 2	21, 65, 97, 142	0
1	K	585/610 (95%)	1.29	137 (23%) 2 2	27, 67, 100, 132	0
1	L	585/610 (95%)	1.29	123 (21%) 2 2	21, 64, 102, 156	0
All	All	7020/7320 (95%)	1.27	1537 (21%) 2 2	16, 63, 96, 205	0

The worst 5 of 1537 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	232	ALA	22.8
1	C	574	LYS	16.2
1	H	572	ALA	14.7
1	D	220	ALA	13.2
1	L	516	CYS	12.6

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.