wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 02:55 AM EDT

PDB ID	:	5JJ1
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 (i) symbol.

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

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

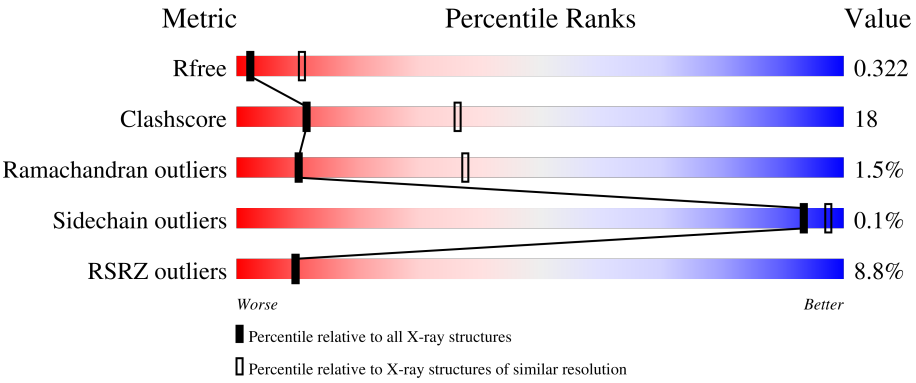
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	610	7% 62% 33%
1	B	610	6% 59% 35%
1	C	610	9% 57% 38%
1	D	610	10% 58% 35%
1	E	610	8% 60% 34%

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Mol	Chain	Length	Quality of chain
1	F	610	7% 59% 36%
1	G	610	9% 60% 34%
1	H	610	9% 57% 37%
1	I	610	7% 57% 36%
1	J	610	11% 61% 33%
1	K	610	9% 63% 32%
1	L	610	9% 64% 30%

2 Entry composition (i)

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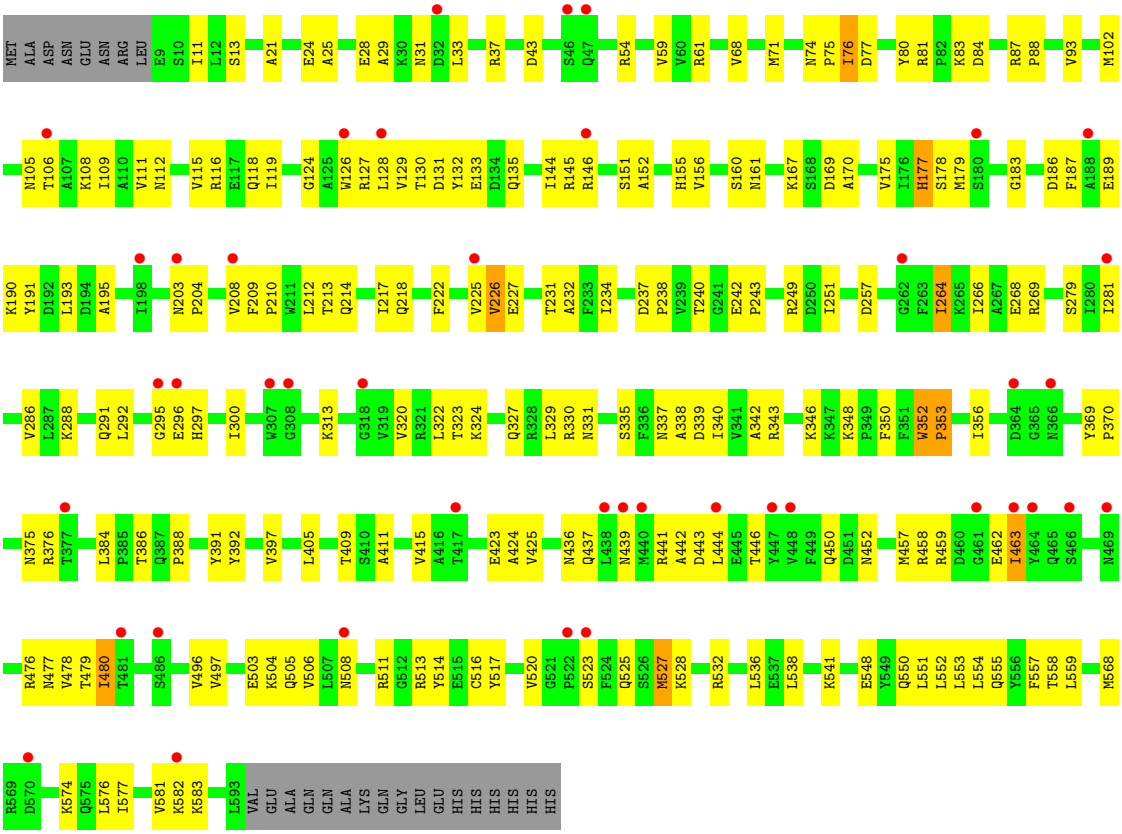
Chain	Residue	Modelled	Actual	Comment	Reference
L	604	GLU	-	expression tag	UNP P26744
L	605	HIS	-	expression tag	UNP P26744
L	606	HIS	-	expression tag	UNP P26744
L	607	HIS	-	expression tag	UNP P26744
L	608	HIS	-	expression tag	UNP P26744
L	609	HIS	-	expression tag	UNP P26744
L	610	HIS	-	expression tag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

3 Residue-property plots (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.

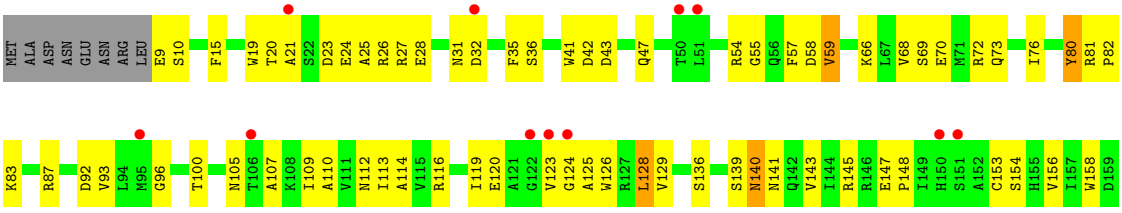
• Molecule 1: Portal protein

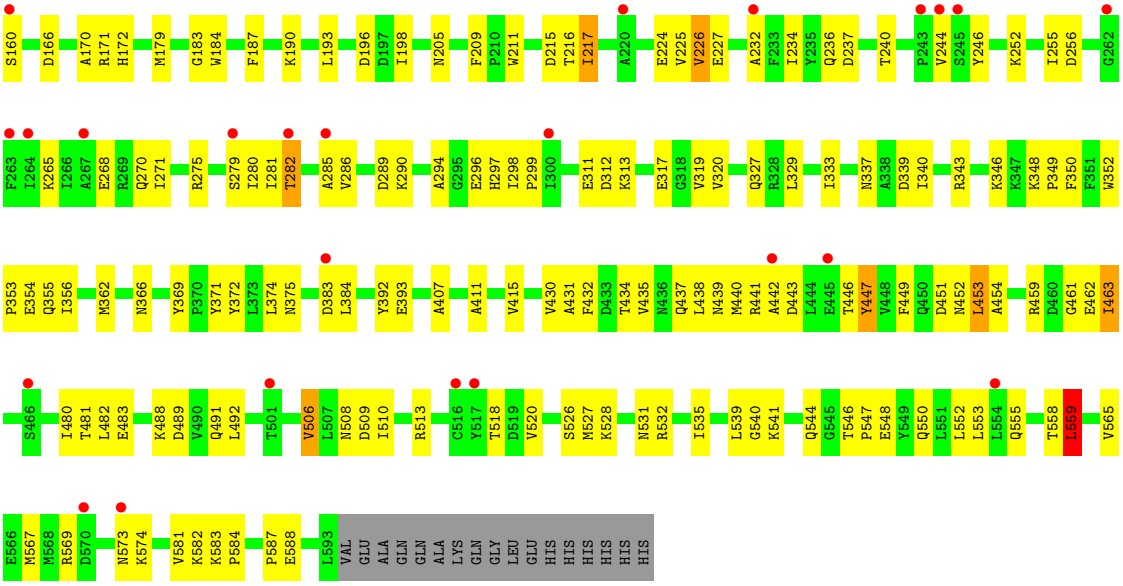
Chain A:



• Molecule 1: Portal protein

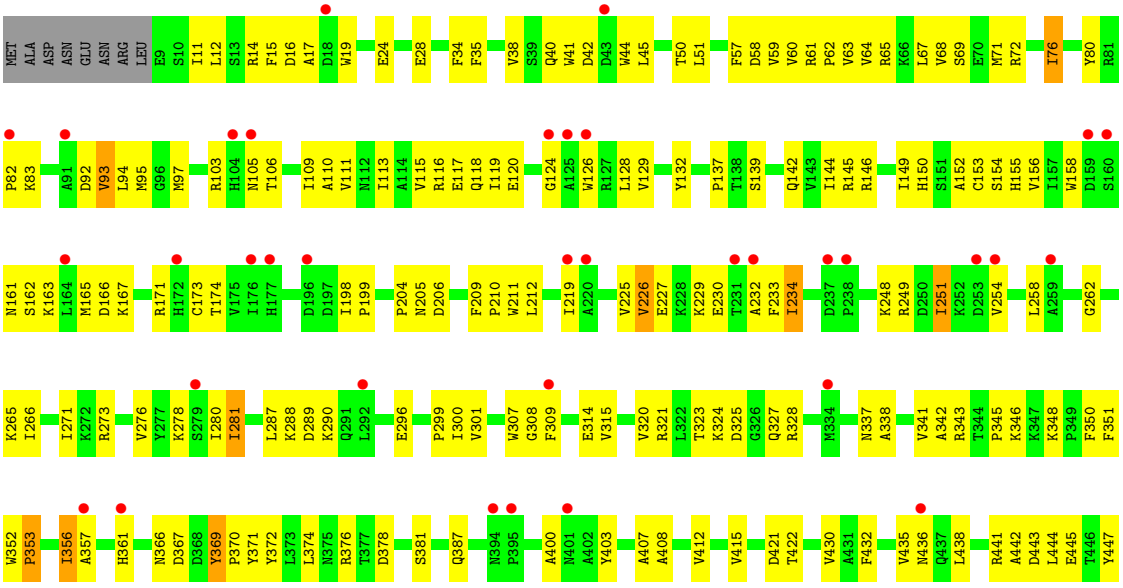
Chain B:





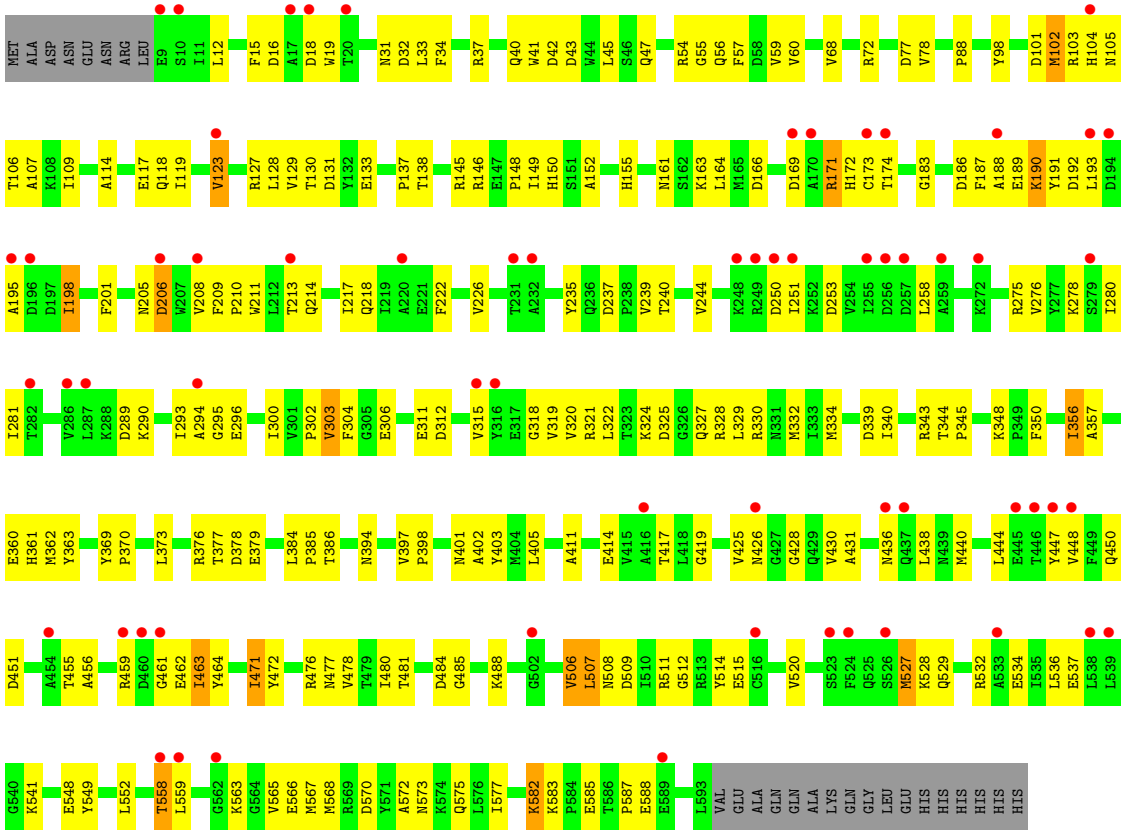
• Molecule 1: Portal protein

Chain C:



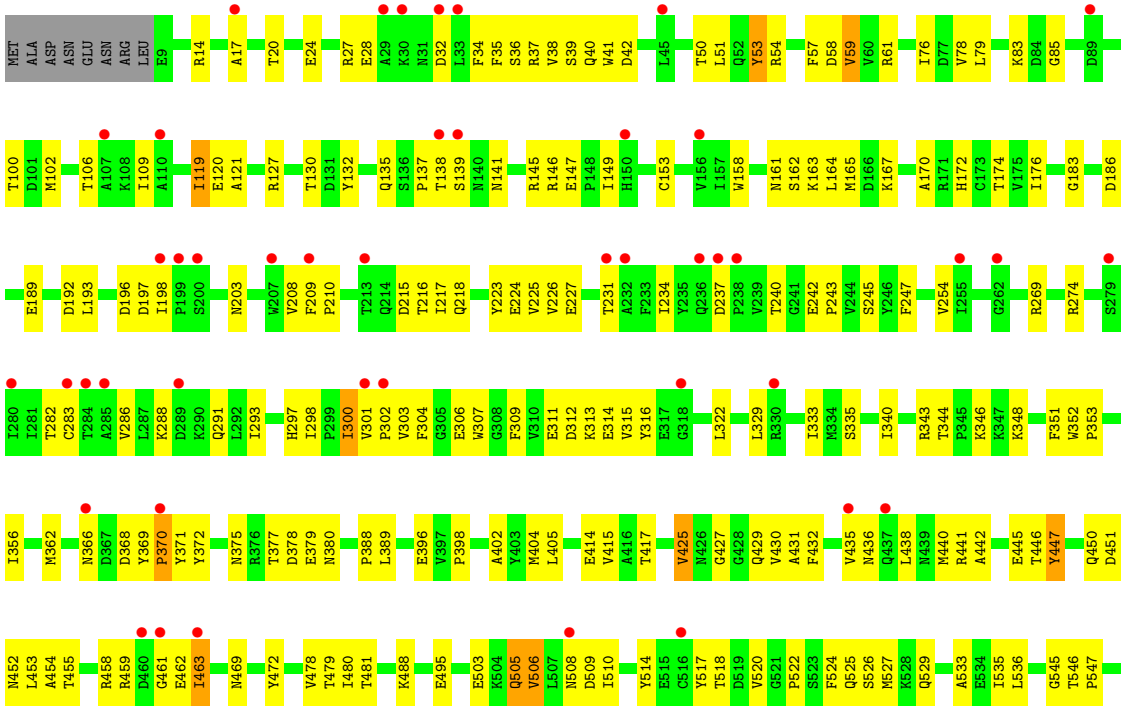
• Molecule 1: Portal protein

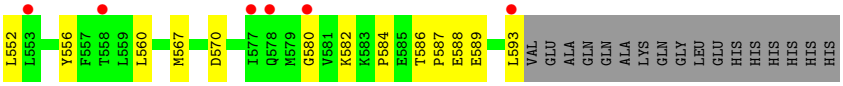
Chain D:



• Molecule 1: Portal protein

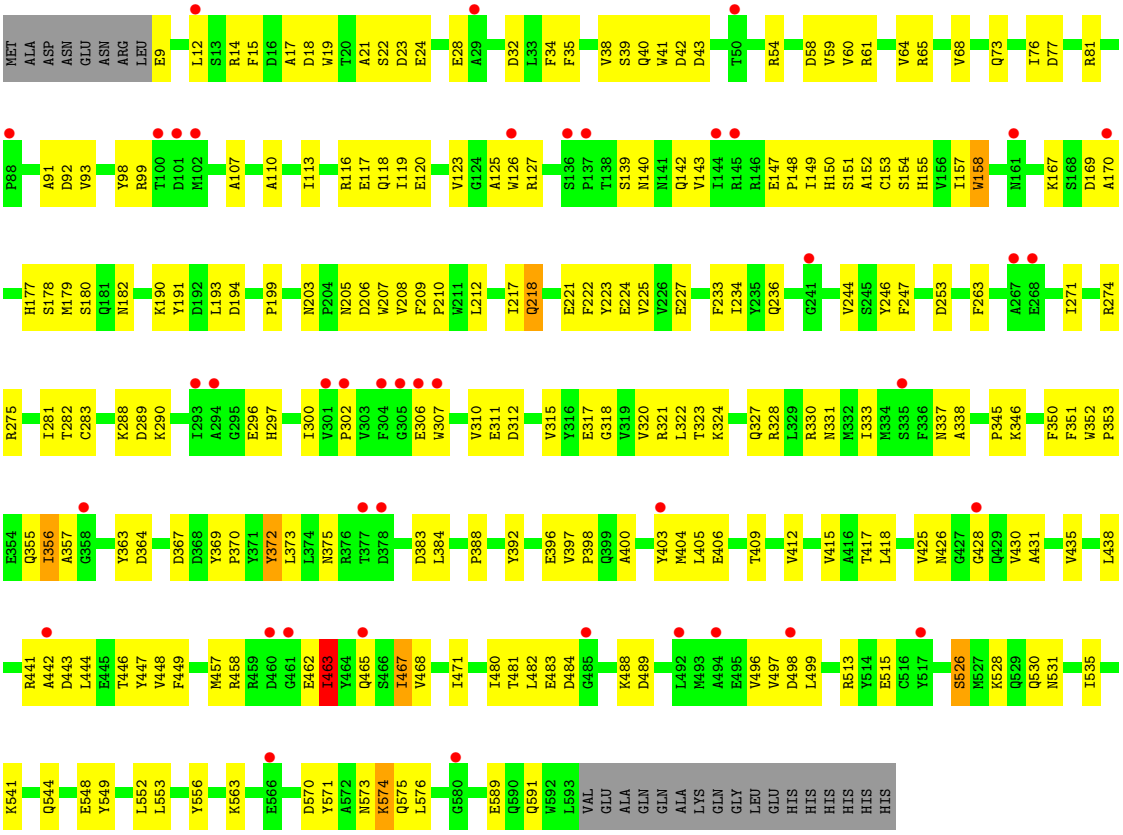
Chain E:





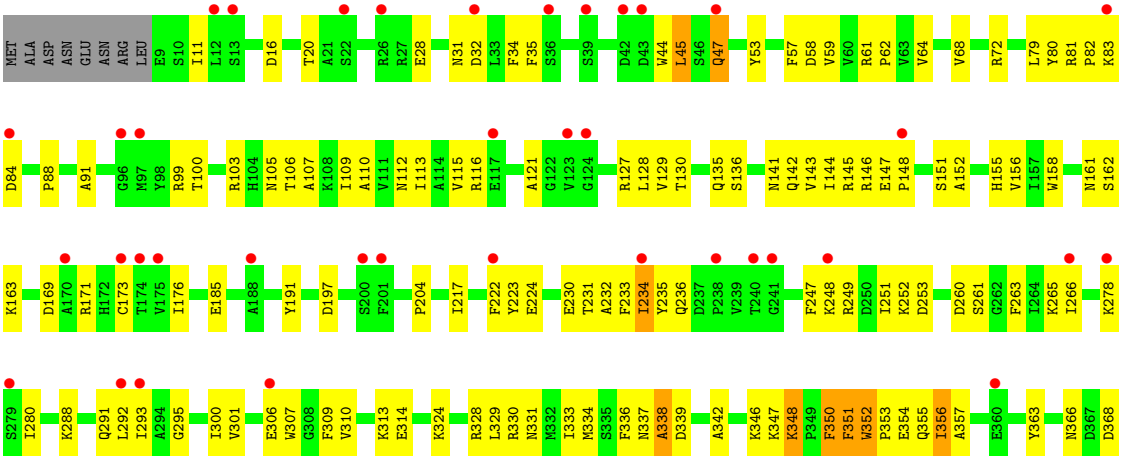
• Molecule 1: Portal protein

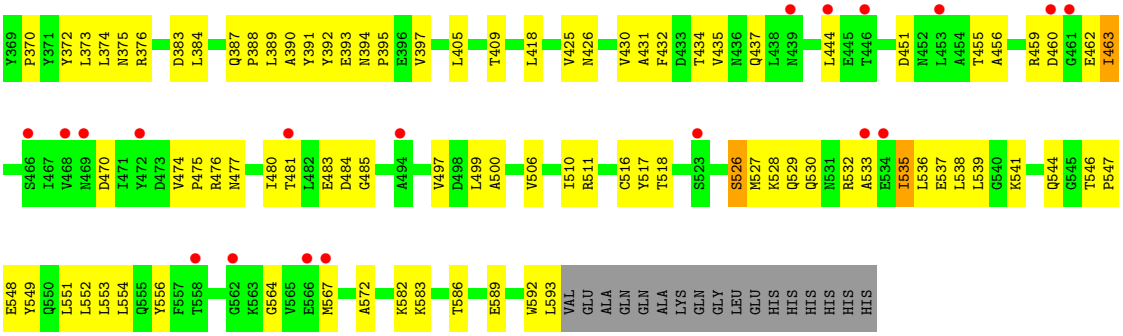
Chain F:



• Molecule 1: Portal protein

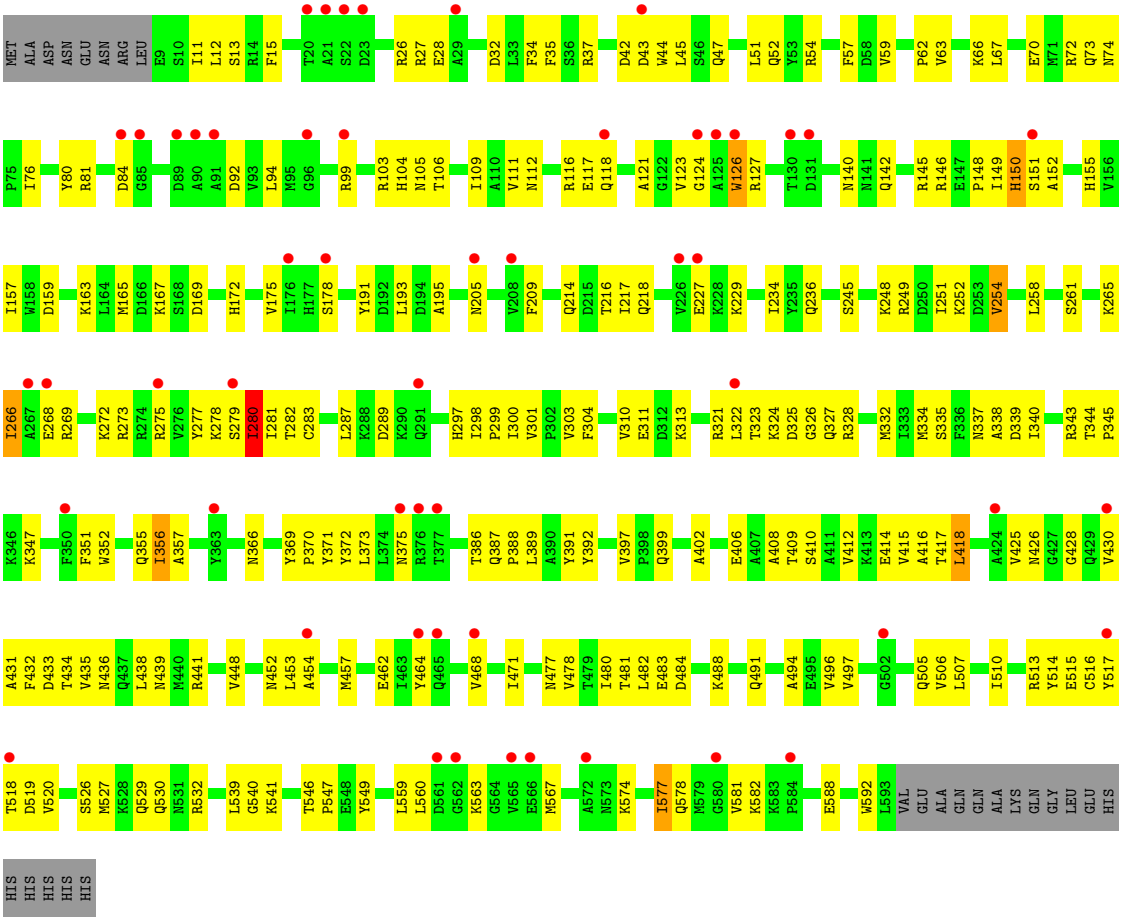
Chain G:





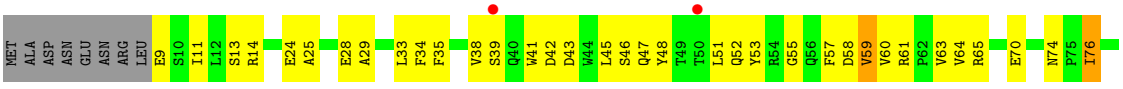
• Molecule 1: Portal protein

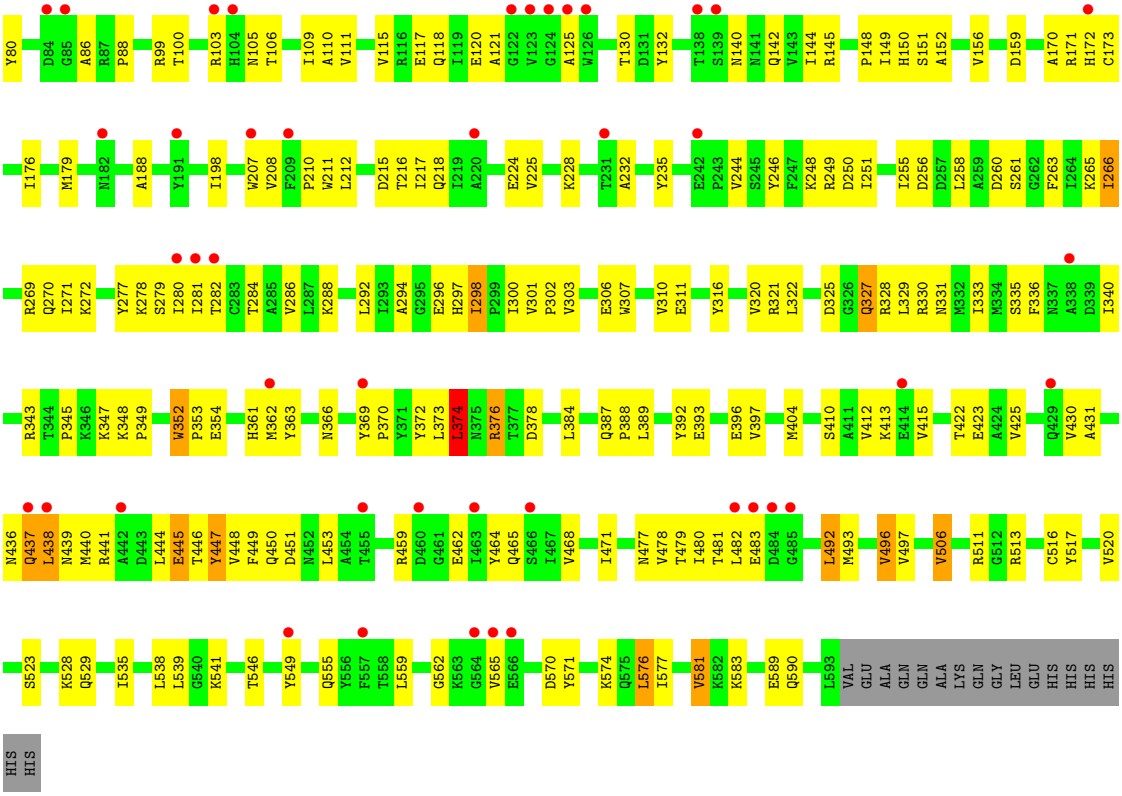
Chain H:



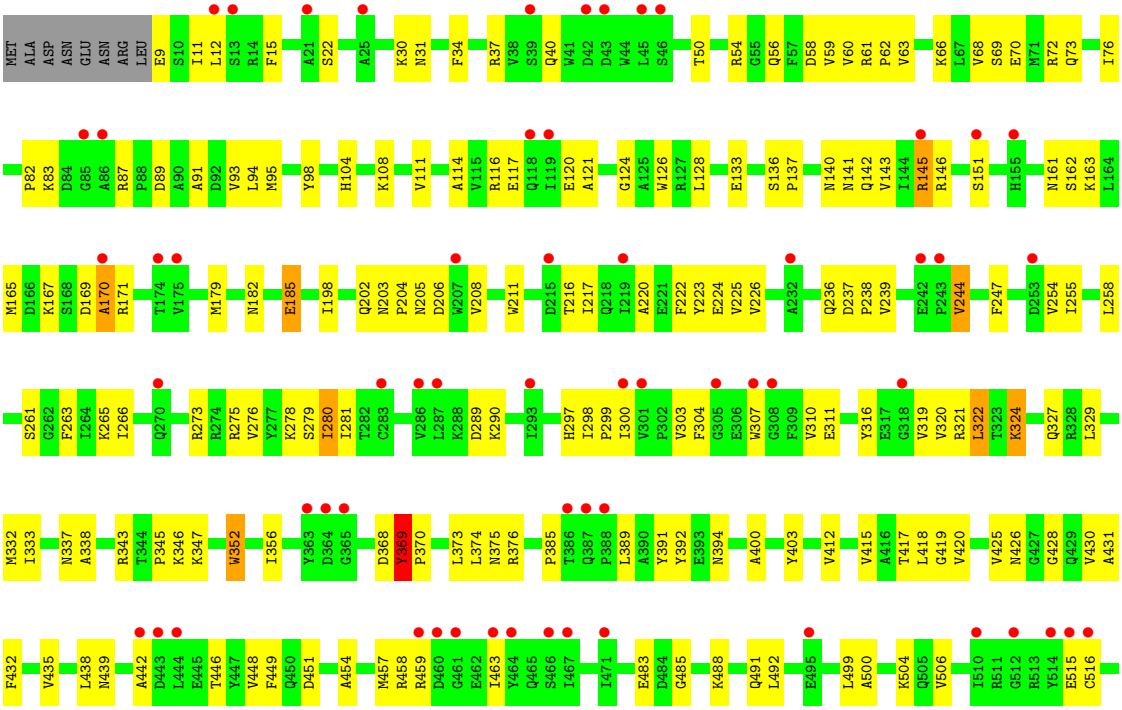
• Molecule 1: Portal protein

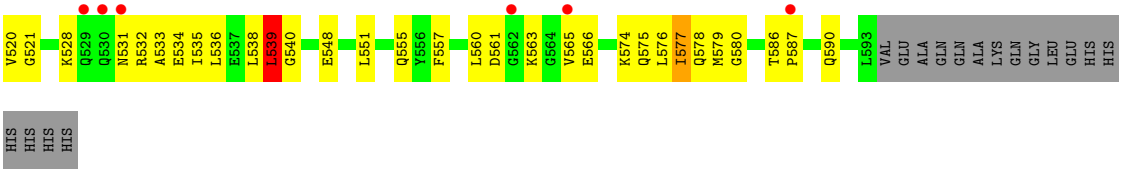
Chain I:





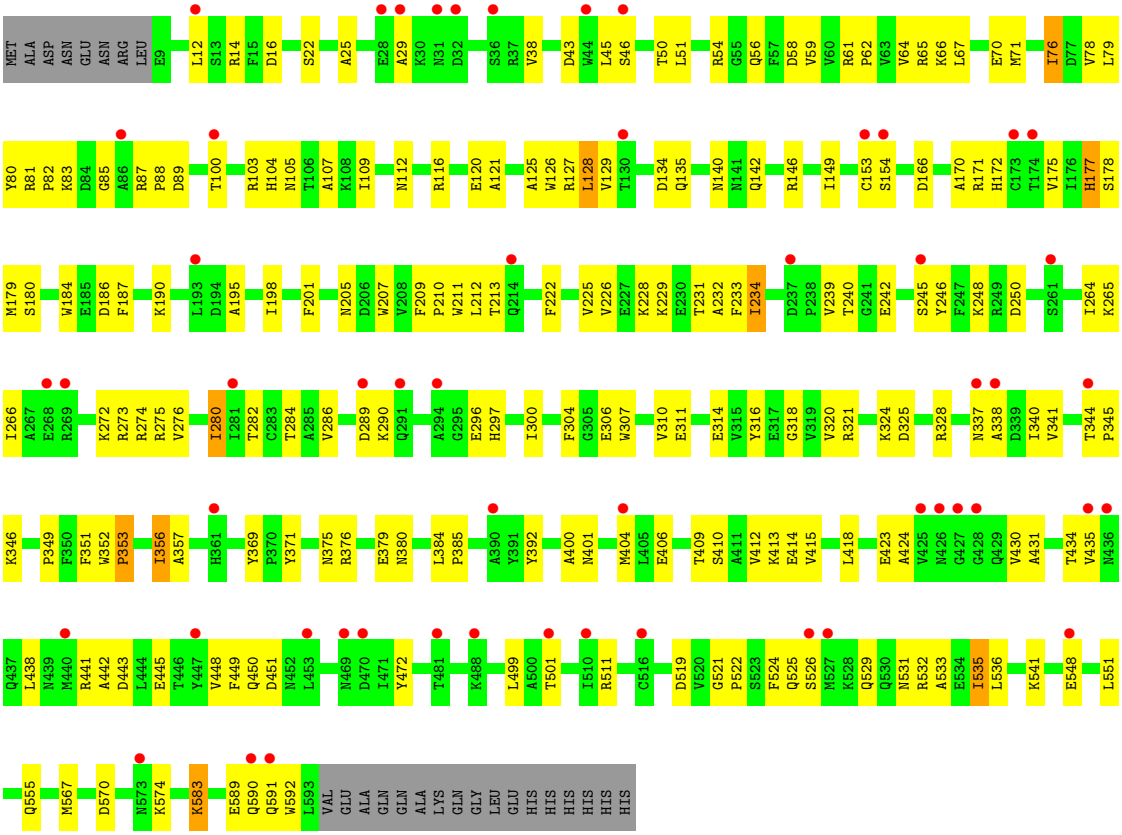
• Molecule 1: Portal protein





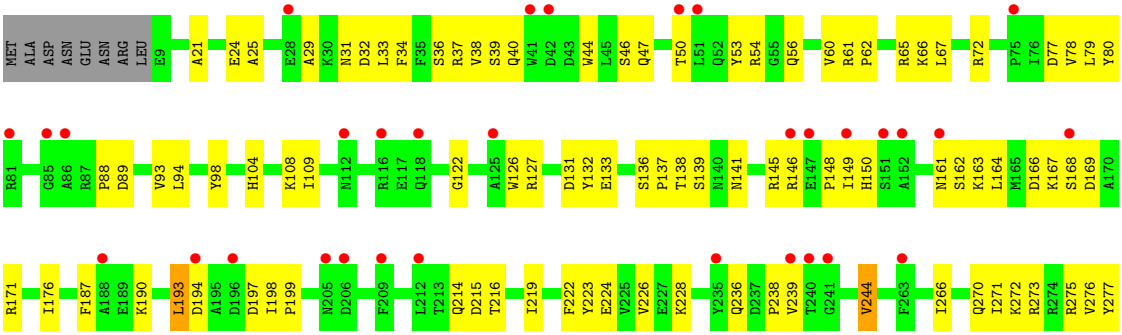
• Molecule 1: Portal protein

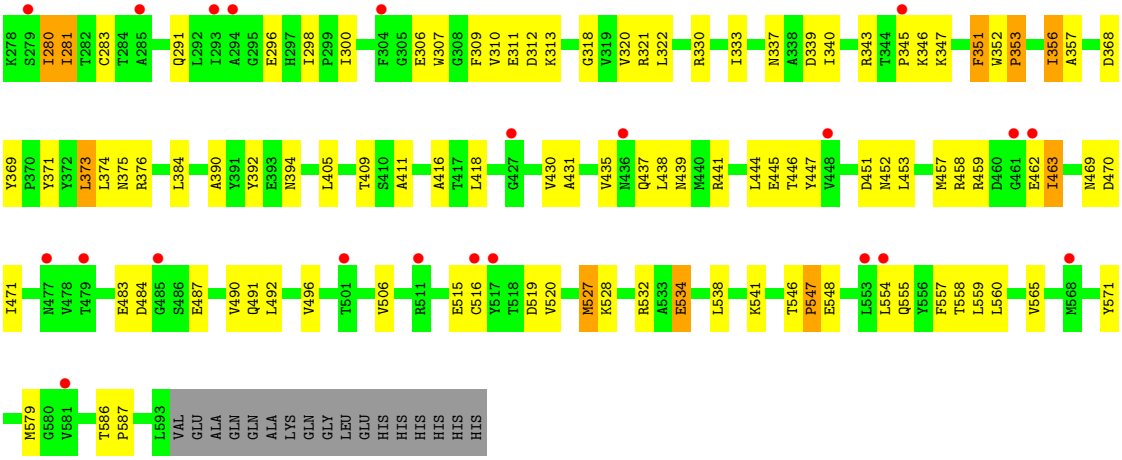
Chain K:



• Molecule 1: Portal protein

Chain L:




K278 S279 I280 I281 T282 C283 T284 A285 Q291 L292 I293 A294 G295 E296 H297 I298 P299 I300 F304 G305 E306 W307 G308 F309 V310 E311 D312 K313 G318 V319 V320 R321 L322 R330 I333 N337 A338 D339 I340 R343 T344 P345 K346 K347 F351 W352 P353 I356 A357 D368
Y369 P370 Y371 Y372 L373 L374 N375 R376 L384 A390 Y391 Y392 E393 N394 L405 T409 S410 A411 A416 T417 L418 G427 V430 A431 V435 N436 Q437 L438 N439 M440 R441 L444 E445 T446 Y447 V448 D451 N452 L453 M457 R458 R459 D460 G461 E462 I463 N469 D470
I471 N477 V478 T479 E483 D484 G485 S486 E487 V490 Q491 L492 V496 T501 V506 R511 E515 C516 Y517 T518 D519 V520 M527 K528 R532 A533 E534 L538 K541 T546 P547 E548 L553 L554 Q555 Y556 F557 T558 L559 L560 V565 M568 Y571
M579 G580 V581 T586 P587 L593 VAL GLU ALA GLN GLN ALA LYS GLN GLY LEU GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 49.54 – 3.30	Depositor EDS
% Data completeness (in resolution range)	85.0 (15.00-3.30) 85.3 (49.54-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.295 , 0.315 0.309 , 0.322	Depositor DCC
R_{free} test set	1737 reflections (0.99%)	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)	0.21 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	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	0.81	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/4826	0.58	0/6550
1	B	0.32	1/4812 (0.0%)	0.63	3/6533 (0.0%)
1	C	0.33	1/4812 (0.0%)	0.60	0/6533
1	D	0.30	0/4825	0.60	1/6550 (0.0%)
1	E	0.30	1/4822 (0.0%)	0.57	0/6546
1	F	0.28	0/4812	0.59	1/6533 (0.0%)
1	G	0.33	1/4808 (0.0%)	0.63	4/6528 (0.1%)
1	H	0.30	1/4812 (0.0%)	0.59	0/6533
1	I	0.30	1/4812 (0.0%)	0.61	3/6533 (0.0%)
1	J	0.30	1/4812 (0.0%)	0.59	1/6533 (0.0%)
1	K	0.28	0/4818	0.57	0/6541
1	L	0.28	0/4812	0.58	1/6533 (0.0%)
All	All	0.30	7/57783 (0.0%)	0.60	14/78446 (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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	LYS	C-N	9.99	1.53	1.34
1	E	203	ASN	C-N	8.28	1.50	1.34
1	H	352	TRP	C-N	8.19	1.49	1.34
1	J	203	ASN	C-N	7.31	1.48	1.34
1	I	298	ILE	C-N	5.64	1.45	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	539	LEU	CA-CB-CG	7.27	132.03	115.30
1	D	192	ASP	N-CA-CB	-7.04	97.92	110.60
1	G	470	ASP	N-CA-C	6.31	128.03	111.00
1	I	492	LEU	CA-CB-CG	6.24	129.65	115.30
1	G	348	LYS	C-N-CD	6.21	141.43	128.40

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	158	0
1	B	4710	0	4536	182	0
1	C	4710	0	4536	205	0
1	D	4723	0	4562	191	0
1	E	4720	0	4553	176	0
1	F	4710	0	4536	174	0
1	G	4706	0	4532	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	4710	0	4536	188	0
1	I	4710	0	4536	206	0
1	J	4710	0	4536	171	0
1	K	4716	0	4547	165	0
1	L	4710	0	4536	154	0
All	All	56559	0	54508	1959	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 18.

The worst 5 of 1959 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%)	13 42
1	B	583/610 (96%)	461 (79%)	112 (19%)	10 (2%)	9 35
1	C	583/610 (96%)	442 (76%)	130 (22%)	11 (2%)	8 34
1	D	583/610 (96%)	451 (77%)	123 (21%)	9 (2%)	10 38
1	E	583/610 (96%)	454 (78%)	120 (21%)	9 (2%)	10 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	583/610 (96%)	448 (77%)	129 (22%)	6 (1%)	15 46
1	G	583/610 (96%)	438 (75%)	135 (23%)	10 (2%)	9 35
1	H	583/610 (96%)	440 (76%)	134 (23%)	9 (2%)	10 38
1	I	583/610 (96%)	436 (75%)	137 (24%)	10 (2%)	9 35
1	J	583/610 (96%)	443 (76%)	132 (23%)	8 (1%)	11 38
1	K	583/610 (96%)	455 (78%)	121 (21%)	7 (1%)	13 42
1	L	583/610 (96%)	450 (77%)	125 (21%)	8 (1%)	11 38
All	All	6996/7320 (96%)	5379 (77%)	1513 (22%)	104 (2%)	10 38

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	512/536 (96%)	512 (100%)	0	100 100
1	B	508/536 (95%)	506 (100%)	2 (0%)	91 95
1	C	508/536 (95%)	508 (100%)	0	100 100
1	D	512/536 (96%)	511 (100%)	1 (0%)	93 97
1	E	511/536 (95%)	511 (100%)	0	100 100
1	F	508/536 (95%)	508 (100%)	0	100 100
1	G	507/536 (95%)	505 (100%)	2 (0%)	91 95
1	H	508/536 (95%)	508 (100%)	0	100 100
1	I	508/536 (95%)	506 (100%)	2 (0%)	91 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	508/536 (95%)	506 (100%)	2 (0%)	91 95
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%)	93 97

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	G	350	PHE
1	G	351	PHE
1	I	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	218	GLN
1	G	236	GLN
1	K	450	GLN
1	I	401	ASN
1	I	437	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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%)	0.36	42 (7%)	15	15	16, 65, 94, 113	0
1	B	585/610 (95%)	0.28	35 (5%)	21	21	19, 62, 89, 109	0
1	C	585/610 (95%)	0.36	54 (9%)	9	9	19, 61, 91, 130	0
1	D	585/610 (95%)	0.56	62 (10%)	6	6	21, 66, 97, 184	0
1	E	585/610 (95%)	0.41	51 (8%)	10	10	19, 63, 98, 205	0
1	F	585/610 (95%)	0.36	42 (7%)	15	15	22, 60, 94, 142	0
1	G	585/610 (95%)	0.40	57 (9%)	7	8	18, 59, 92, 136	0
1	H	585/610 (95%)	0.38	53 (9%)	9	9	20, 62, 93, 117	0
1	I	585/610 (95%)	0.39	45 (7%)	13	12	19, 66, 99, 192	0
1	J	585/610 (95%)	0.45	66 (11%)	5	5	21, 65, 97, 142	0
1	K	585/610 (95%)	0.39	54 (9%)	9	9	27, 67, 100, 132	0
1	L	585/610 (95%)	0.40	54 (9%)	9	9	21, 64, 102, 156	0
All	All	7020/7320 (95%)	0.39	615 (8%)	10	10	16, 63, 96, 205	0

The worst 5 of 615 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	238	PRO	11.8
1	E	232	ALA	11.4
1	D	558	THR	10.9
1	L	516	CYS	9.0
1	D	516	CYS	8.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.