wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 08:49 AM EDT

PDB ID	:	4V5I
Title	:	Structure of the Phage P2 Baseplate in its Activated Conformation with Ca
Authors	:	Sciara, G.; Bebeacua, C.; Bron, P.; Tremblay, D.; Ortiz-Lombardia, M.; Lichiere, J.; van Heel, M.; Campanacci, V.; Moineau, S.; Cambillau, C.
Deposited on	:	2010-02-05
Resolution	:	5.46 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 (1)) were used in the production of this report:

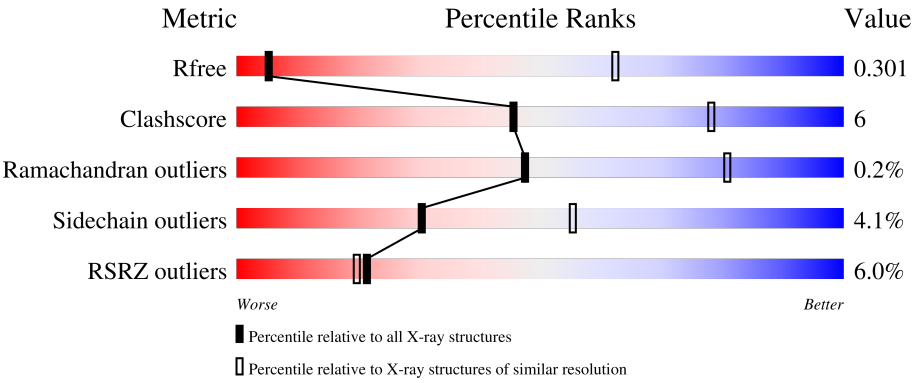
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 5.46 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	1018 (7.08-3.82)
Clashscore	141614	1005 (7.02-3.90)
Ramachandran outliers	138981	1013 (7.10-3.82)
Sidechain outliers	138945	1190 (7.12-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)

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	A0	372	11% 84% 14% ·
1	AY	372	10% 86% 12% ·
1	AZ	372	10% 83% 16% ·
1	B0	372	8% 85% 14% ·
1	BY	372	4% 86% 12% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	BZ	372	8% 85% 14%
2	AA	263	2% 89% 11%
2	AB	263	6% 92% 8%
2	AC	263	5% 92% 8%
2	AD	263	6% 87% 13%
2	AE	263	3% 90% 10%
2	AF	263	6% 90% 10%
2	AG	263	9% 89% 10%
2	AH	263	3% 92% 7%
2	AI	263	8% 92% 8%
2	AJ	263	5% 91% 9%
2	AK	263	4% 89% 11%
2	AL	263	8% 92% 8%
2	AM	263	8% 90% 10%
2	AN	263	5% 85% 15%
2	AO	263	5% 91% 9%
2	AP	263	7% 87% 12%
2	AQ	263	10% 90% 10%
2	AR	263	6% 89% 11%
2	BA	263	4% 89% 11%
2	BB	263	5% 91% 9%
2	BC	263	5% 92% 8%
2	BD	263	6% 88% 12%
2	BE	263	4% 90% 10%
2	BF	263	8% 90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	BG	263	8% 89% 10%
2	BH	263	8% 92% 7%
2	BI	263	4% 92% 8%
2	BJ	263	3% 91% 9%
2	BK	263	8% 91% 9%
2	BL	263	8% 92% 8%
2	BM	263	9% 88% 11%
2	BN	263	6% 87% 13%
2	BO	263	6% 91% 9%
2	BP	263	12% 88% 11%
2	BQ	263	8% 89% 10%
2	BR	263	10% 89% 11%
3	AS	298	5% 74% 22%
3	AT	298	5% 72% 24%
3	AU	298	2% 73% 23%
3	AV	298	5% 76% 20%
3	AW	298	3% 79% 19%
3	AX	298	4% 74% 23%
3	BS	298	4% 76% 21%
3	BT	298	3% 73% 23%
3	BU	298	3% 73% 24%
3	BV	298	5% 77% 19%
3	BW	298	2% 80% 17%
3	BX	298	4% 75% 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 119484 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 ORF16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	AY	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	AZ	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	B0	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	BY	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	BZ	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			

- Molecule 2 is a protein called PUTATIVE RECEPTOR BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AB	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AC	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AD	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AE	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AF	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AG	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AH	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AI	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AJ	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AK	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AL	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AM	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AN	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AO	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AP	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AQ	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	AR	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BA	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BB	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BC	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BD	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BE	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BF	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BG	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BH	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BI	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BJ	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BK	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BL	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BM	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BN	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BO	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BP	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BQ	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	BR	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

- Molecule 3 is a protein called ORF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AS	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AT	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AU	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AV	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AW	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	AX	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BS	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BT	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BU	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BV	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BW	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	BX	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

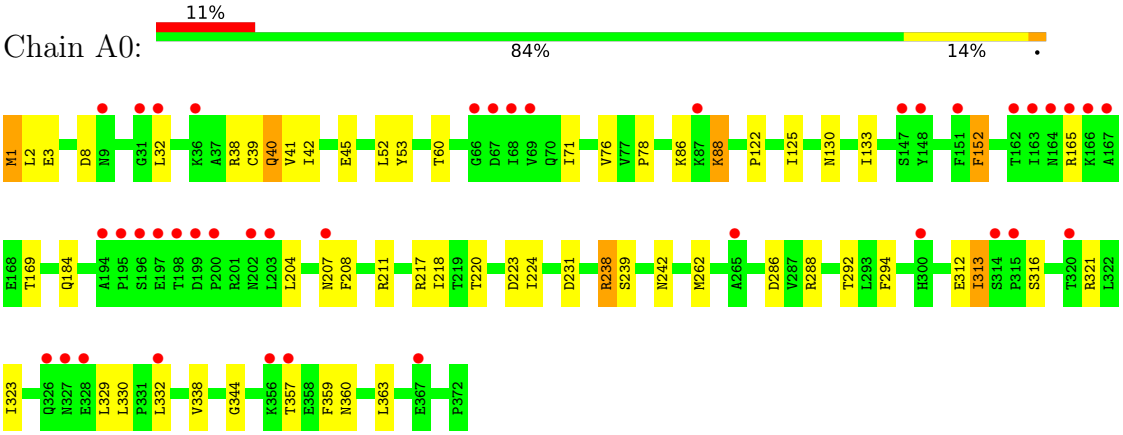
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AS	1	Total Ca 1 1	0	0
4	AT	1	Total Ca 1 1	0	0
4	AU	1	Total Ca 1 1	0	0
4	AV	1	Total Ca 1 1	0	0
4	AW	1	Total Ca 1 1	0	0
4	AX	1	Total Ca 1 1	0	0
4	BS	1	Total Ca 1 1	0	0
4	BT	1	Total Ca 1 1	0	0
4	BU	1	Total Ca 1 1	0	0
4	BV	1	Total Ca 1 1	0	0
4	BW	1	Total Ca 1 1	0	0
4	BX	1	Total Ca 1 1	0	0

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.

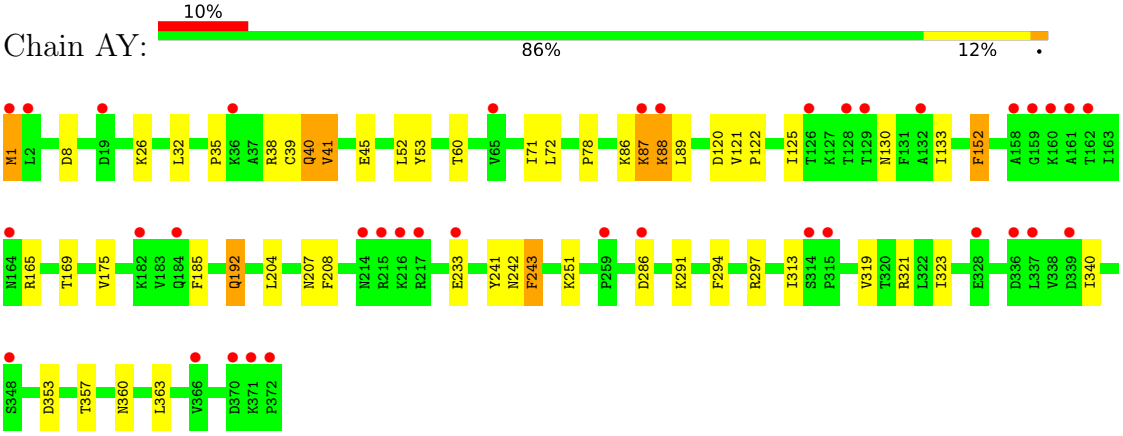
• Molecule 1: ORF16

Chain A0:



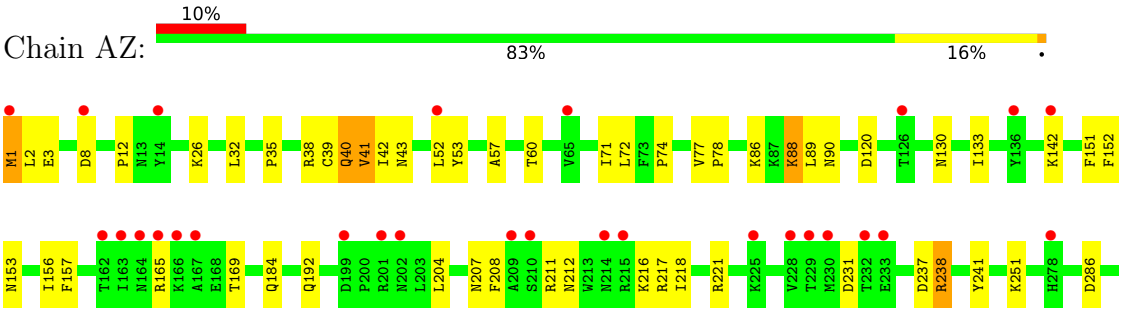
• Molecule 1: ORF16

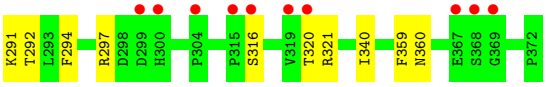
Chain AY:



• Molecule 1: ORF16

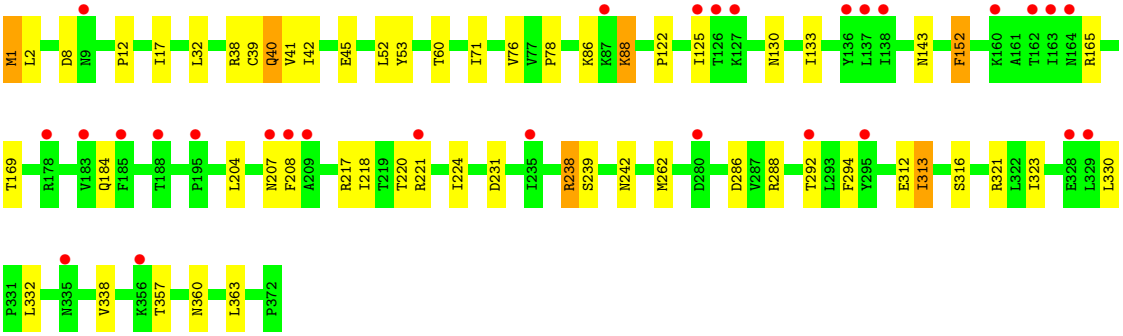
Chain AZ:





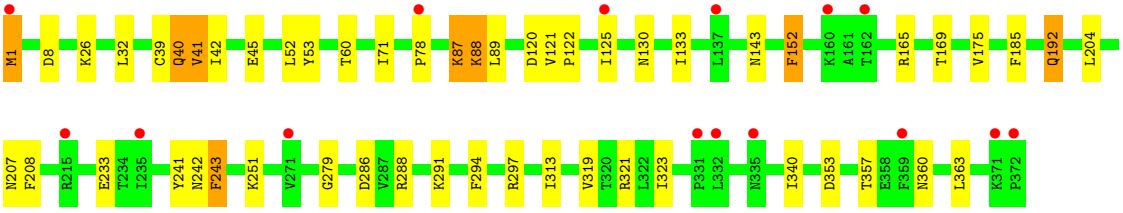
• Molecule 1: ORF16

Chain B0:



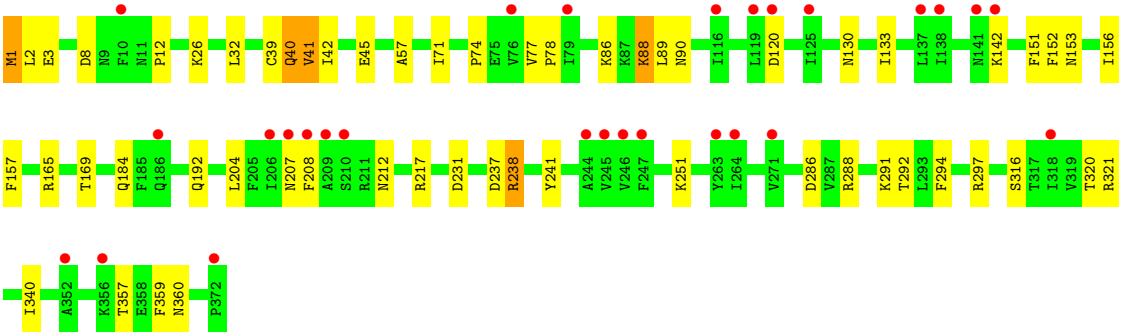
• Molecule 1: ORF16

Chain BY:



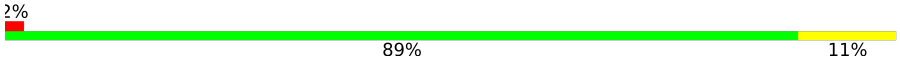
• Molecule 1: ORF16

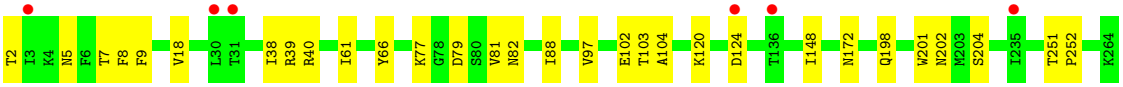
Chain BZ:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

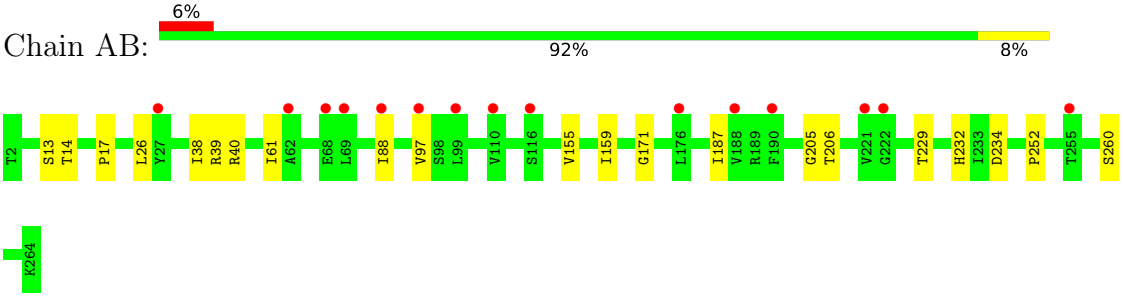
Chain AA:





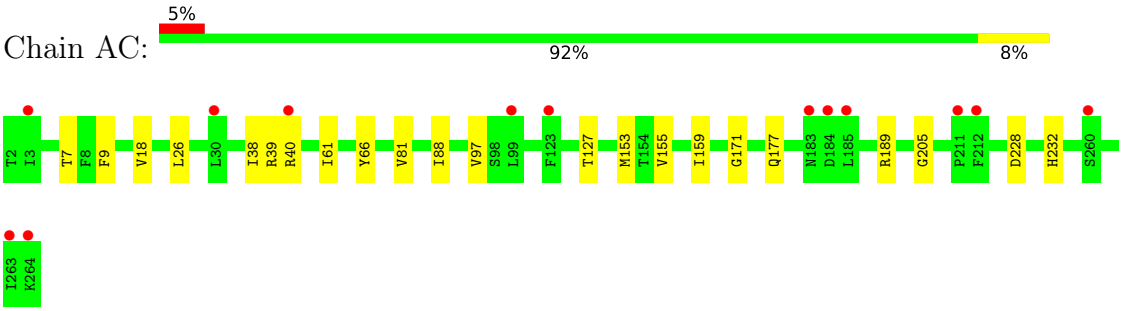
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AB:



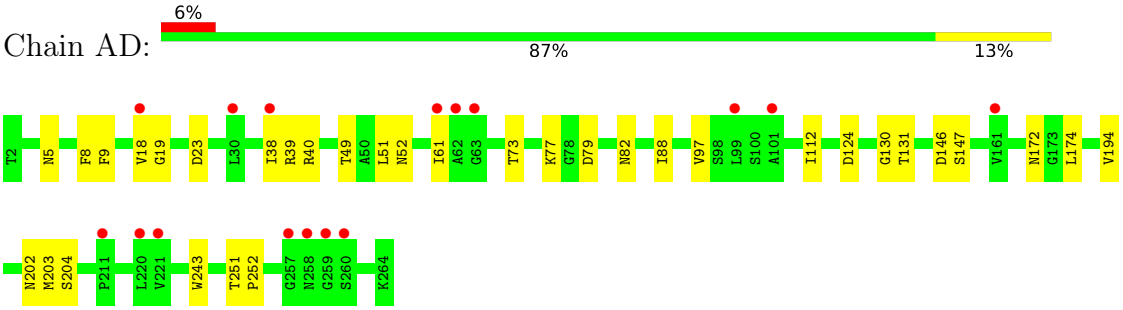
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AC:



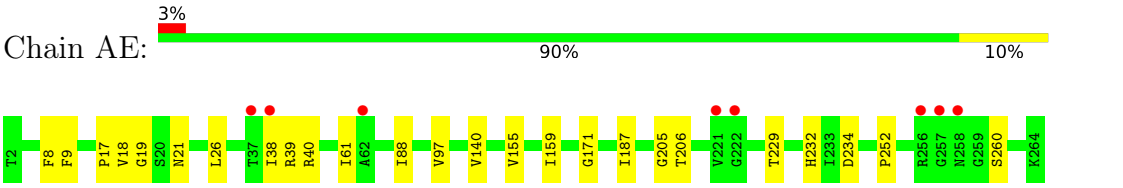
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AD:



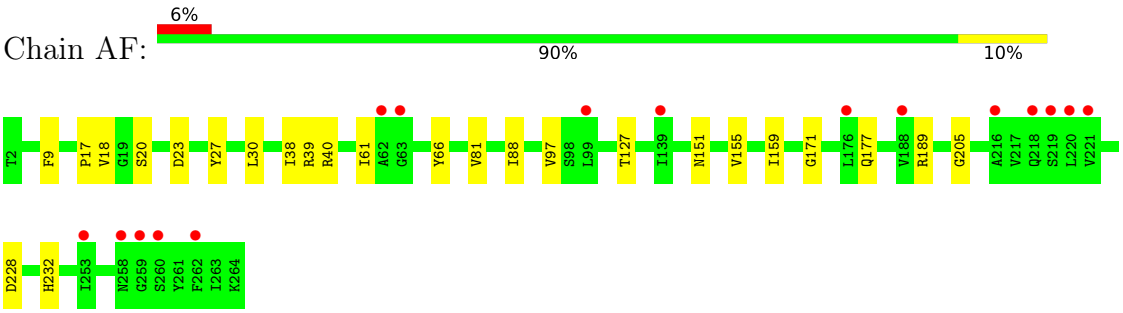
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AE:



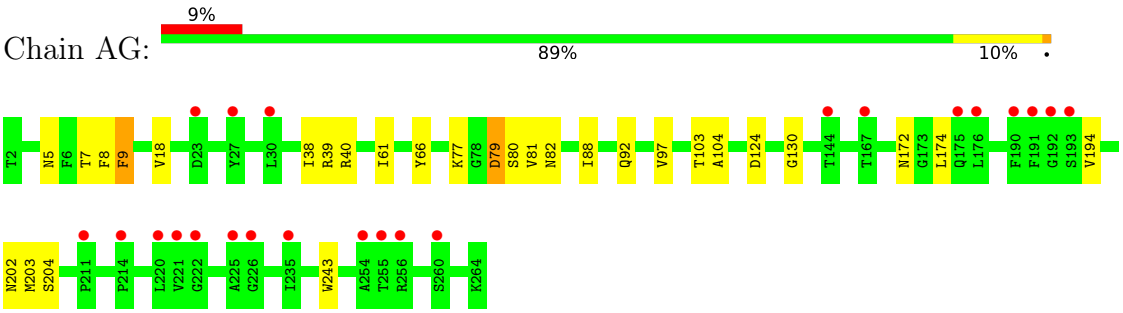
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AF:



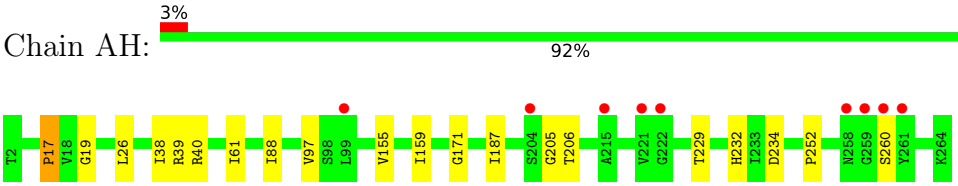
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AG:



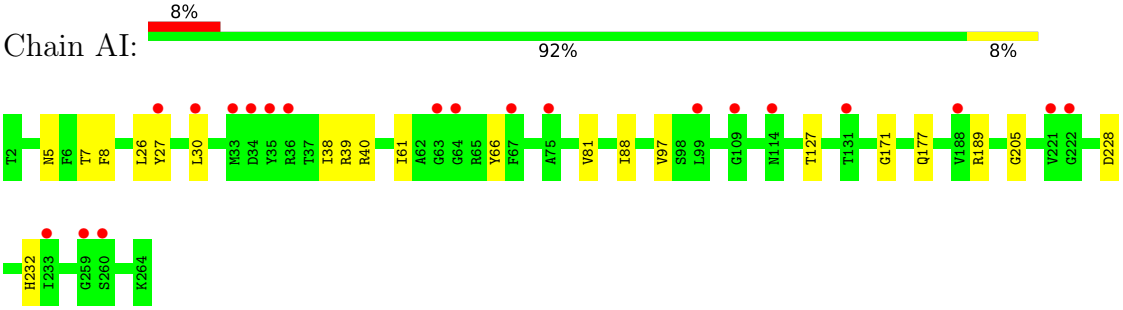
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AH:



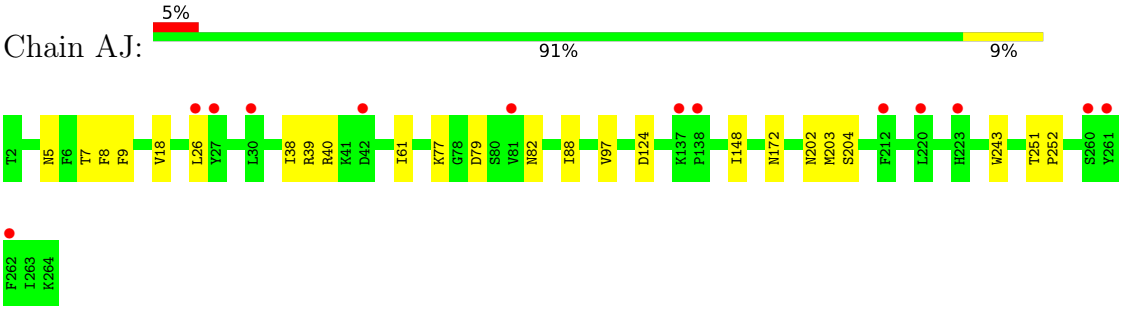
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AI:



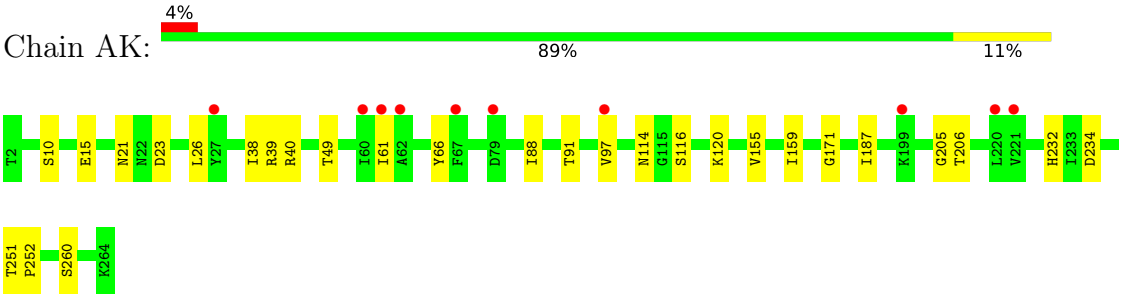
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AJ:



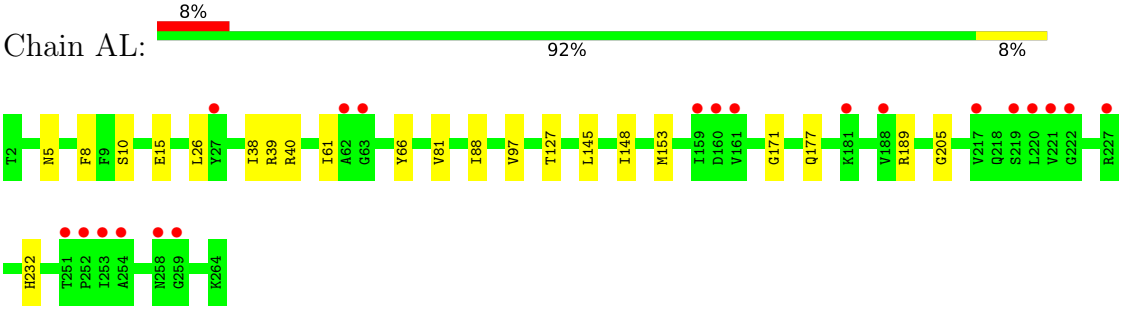
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AK:



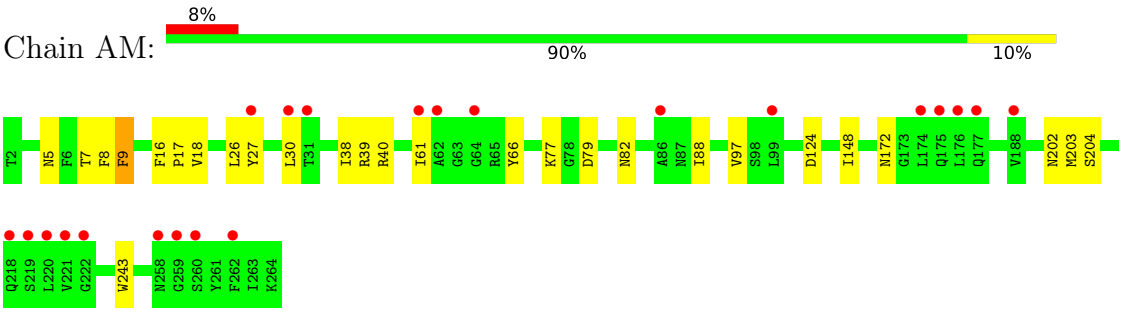
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AL:



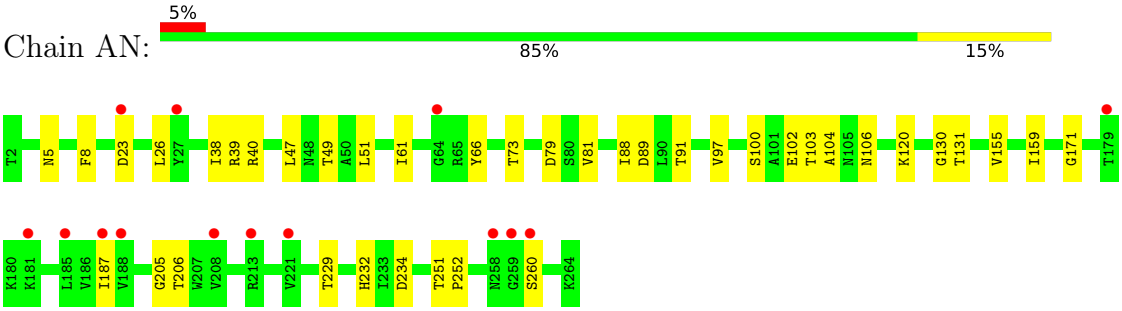
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AM:



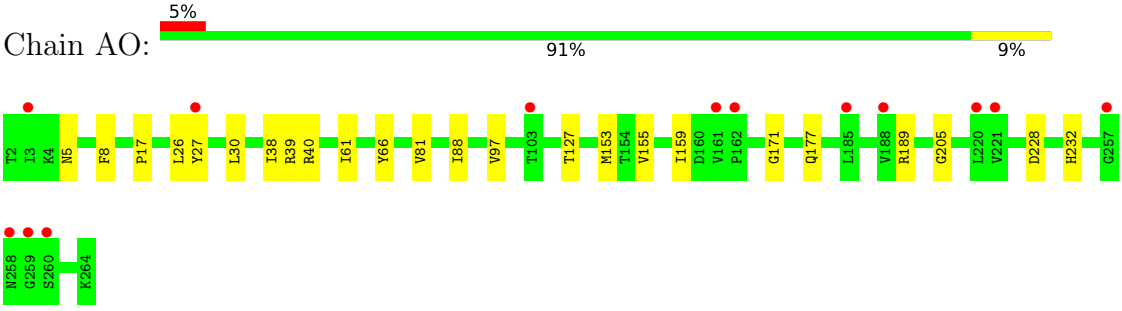
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain AN:



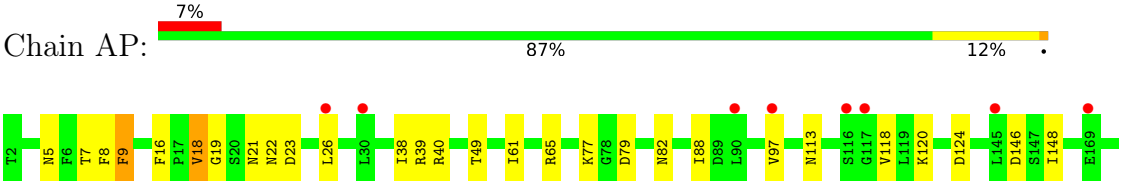
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

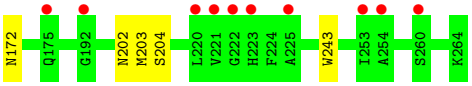
Chain AO:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

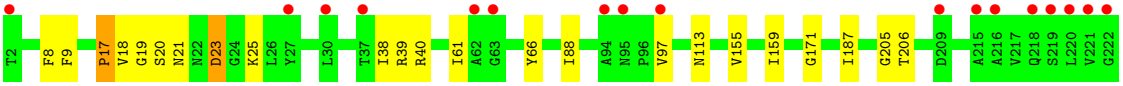
Chain AP:

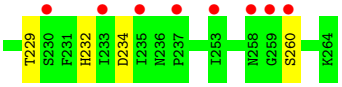




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

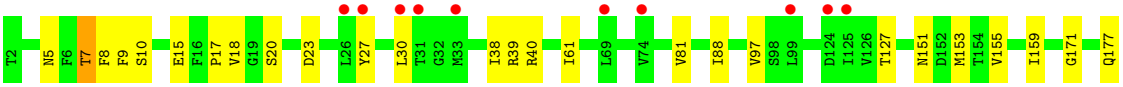
Chain AQ:

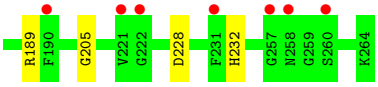




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

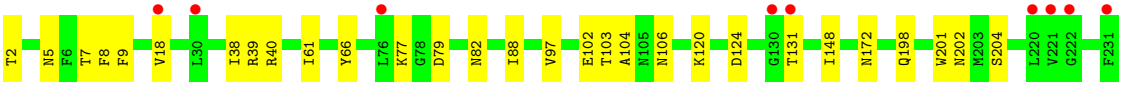
Chain AR:





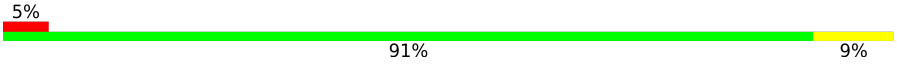
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

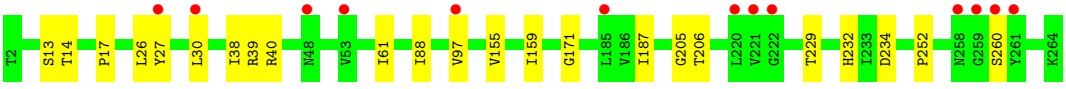
Chain BA:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

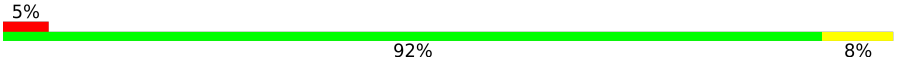
Chain BB:

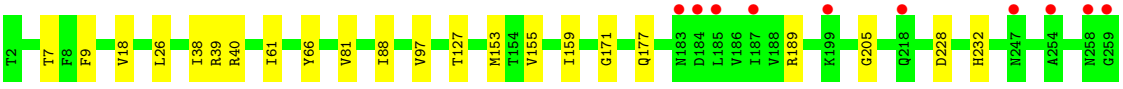




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

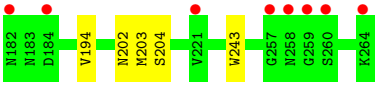
Chain BC:





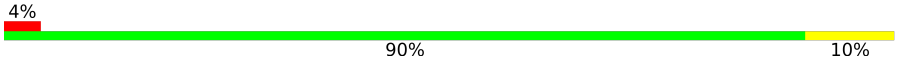
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

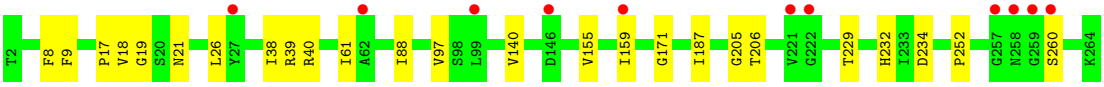
Chain BD:



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

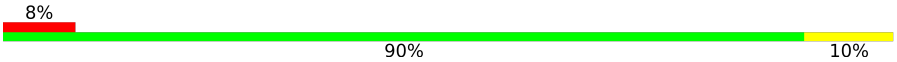
Chain BE:

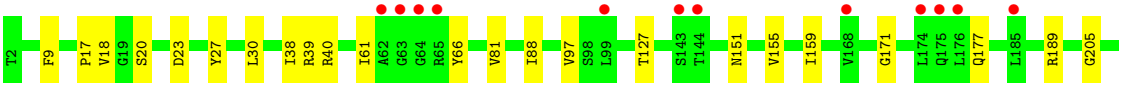


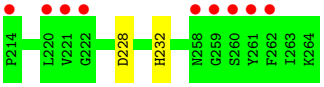


• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BF:

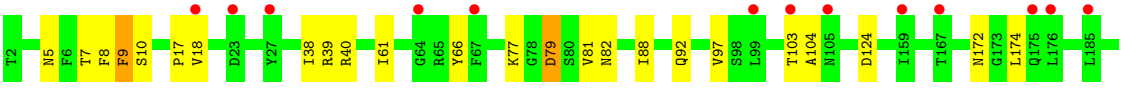


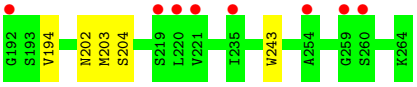




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

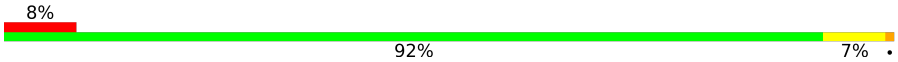
Chain BG:

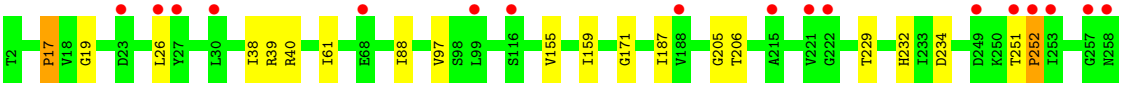




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

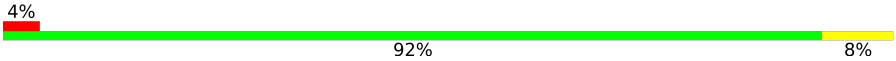
Chain BH:

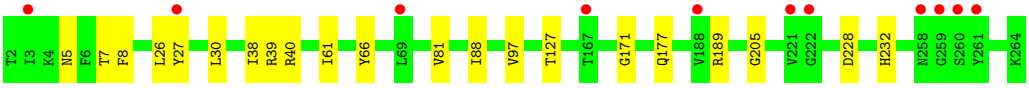




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

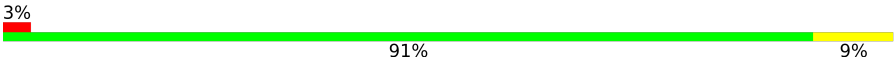
Chain BI:

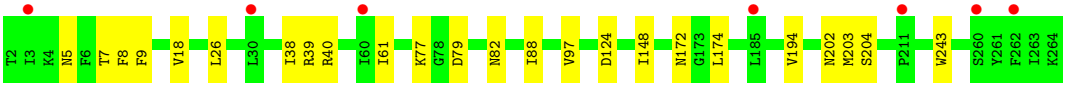




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

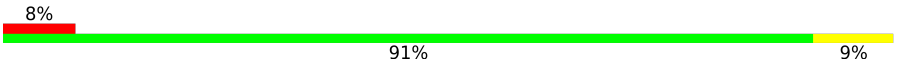
Chain BJ:

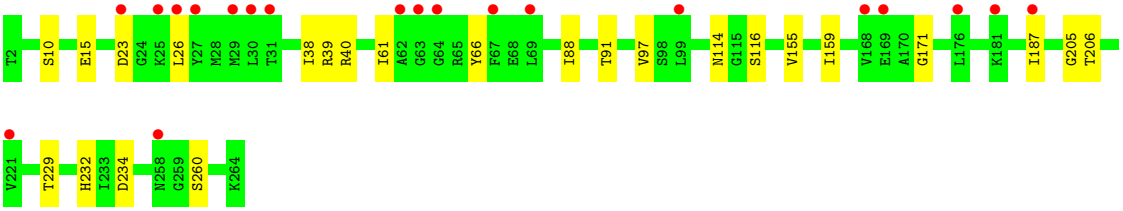




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

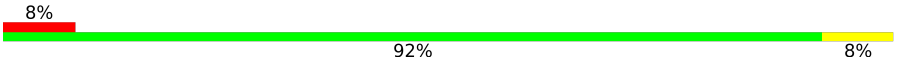
Chain BK:

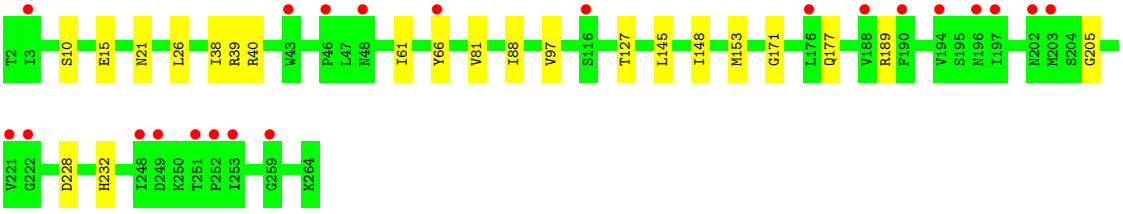




• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BL:



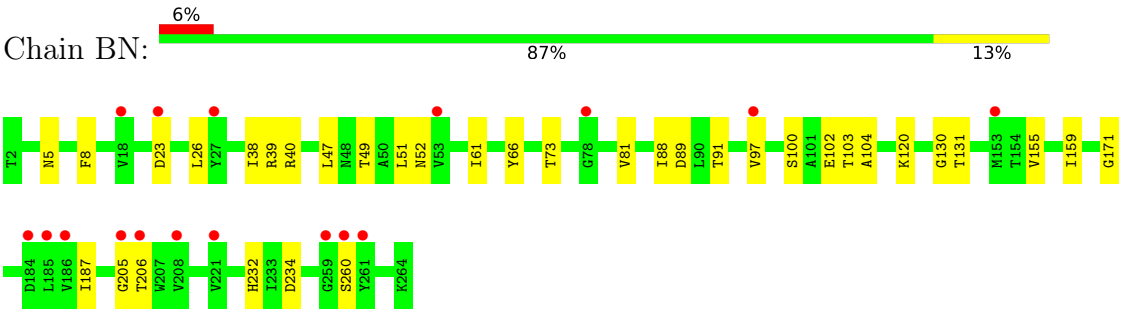


• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BM:

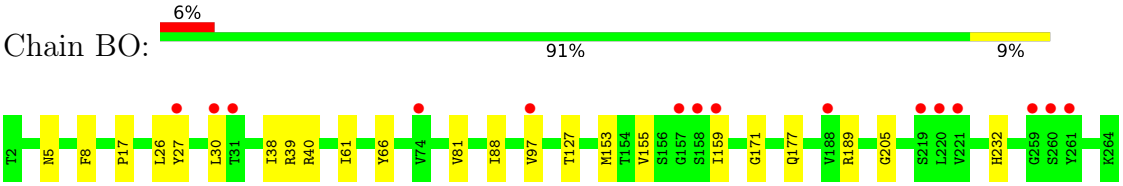
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BN:



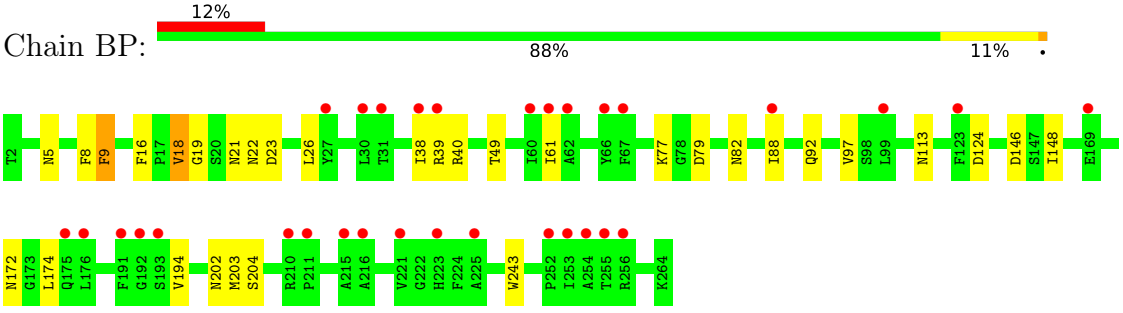
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BO:



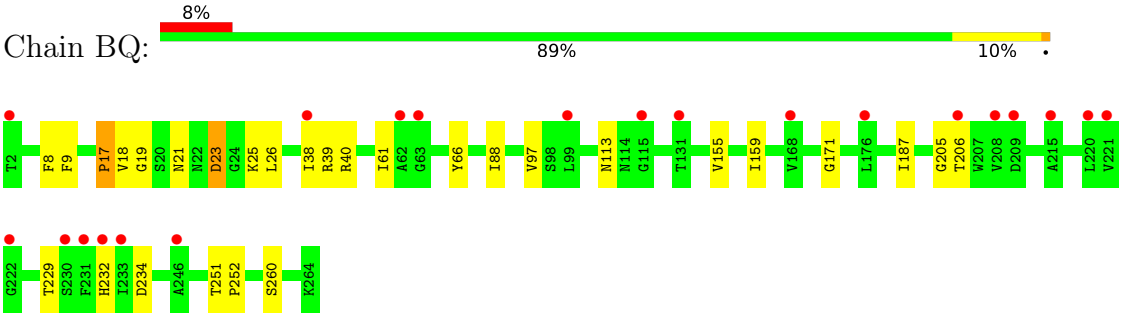
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BP:



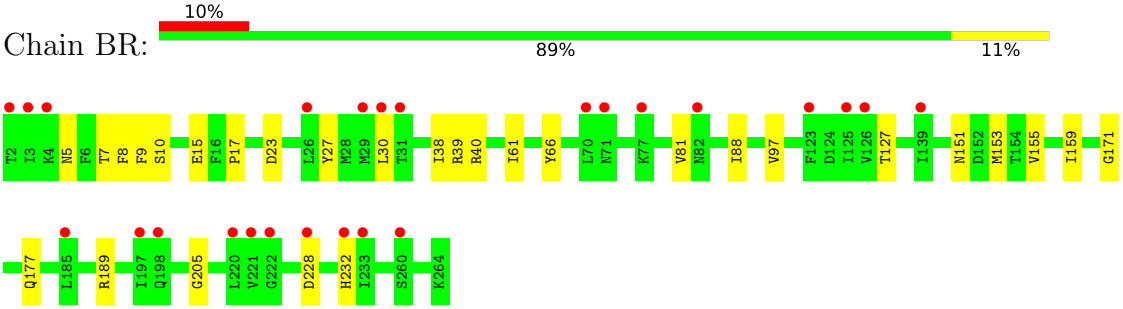
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BQ:



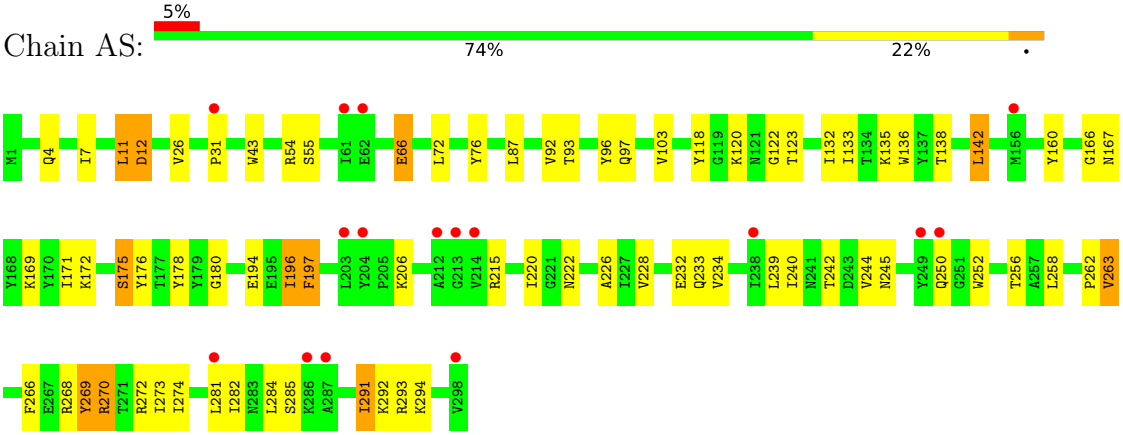
• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain BR:



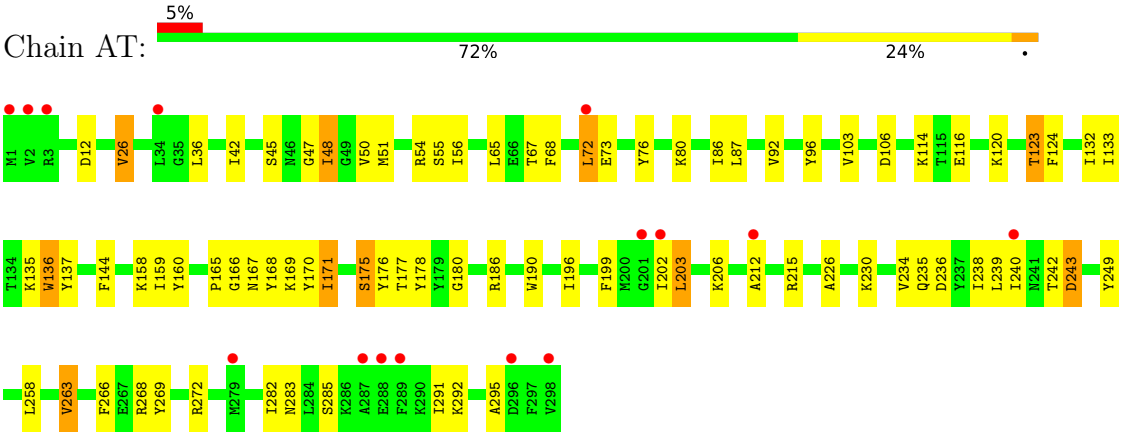
• Molecule 3: ORF15

Chain AS:



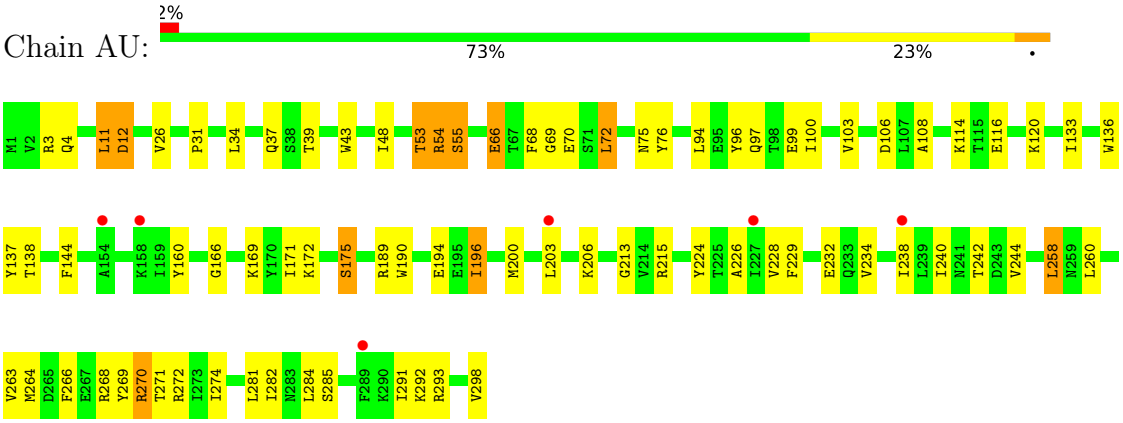
• Molecule 3: ORF15

Chain AT:



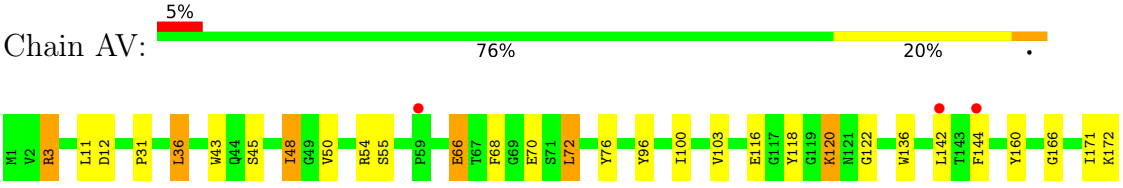
• Molecule 3: ORF15

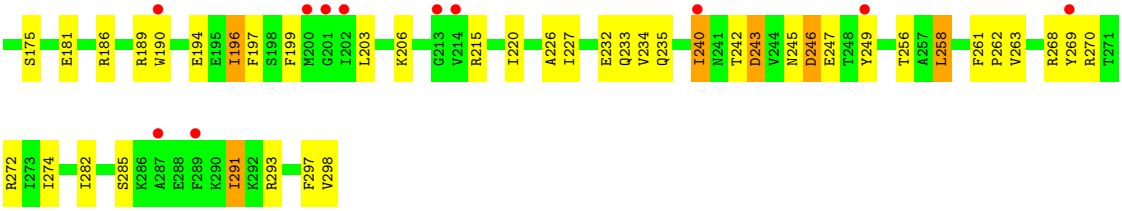
Chain AU:



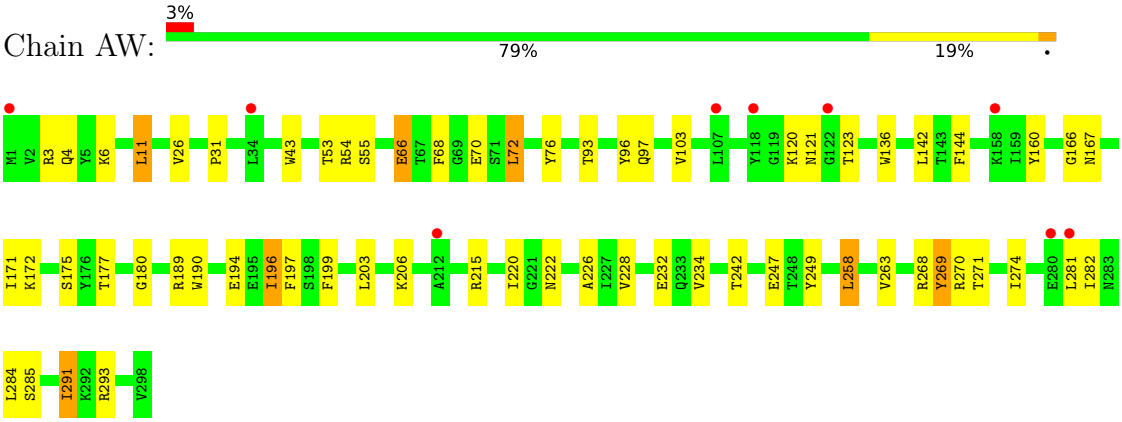
• Molecule 3: ORF15

Chain AV:

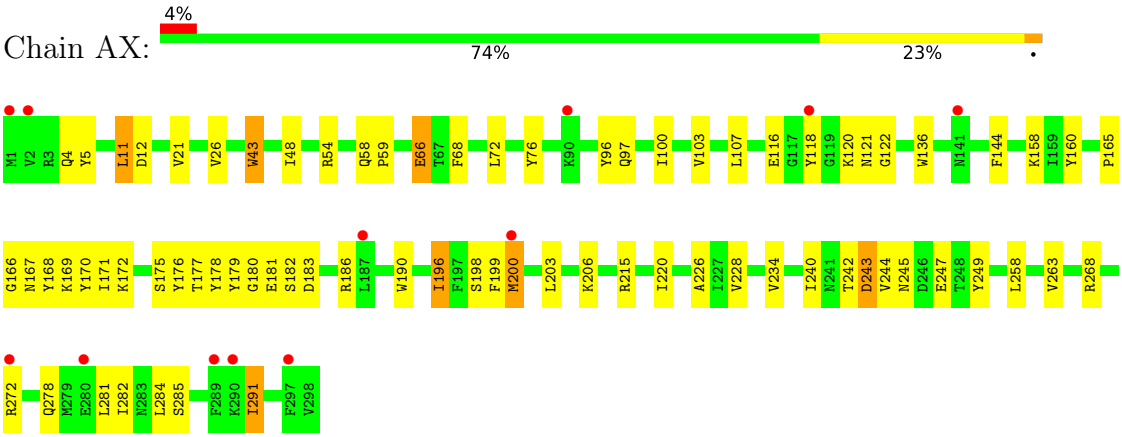




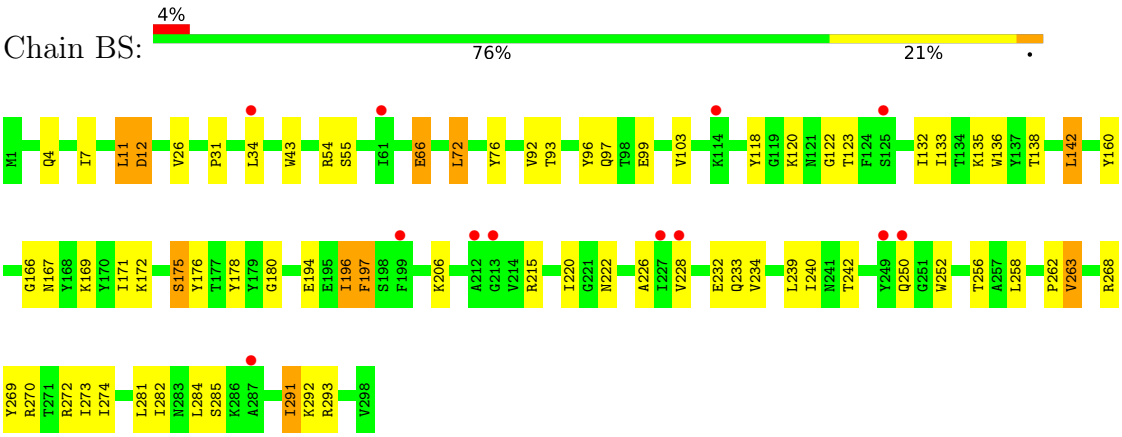
• Molecule 3: ORF15



• Molecule 3: ORF15

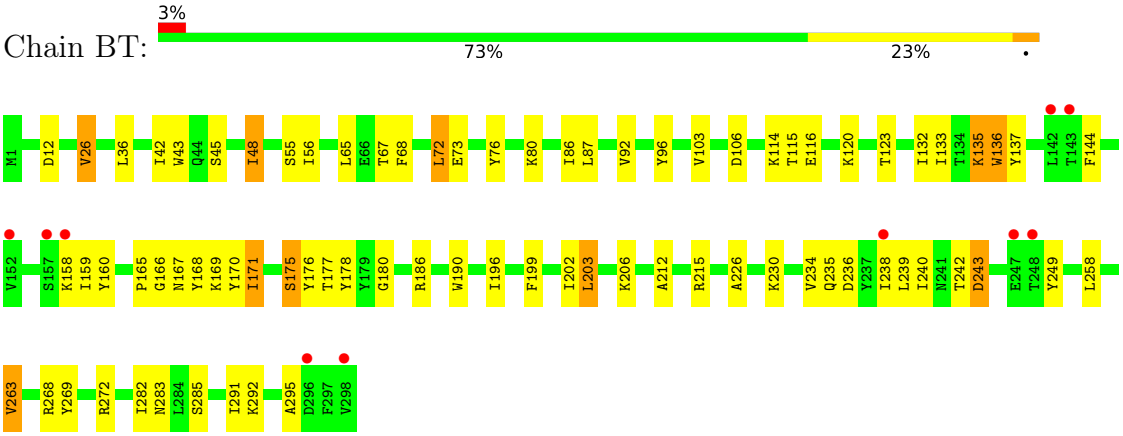


• Molecule 3: ORF15



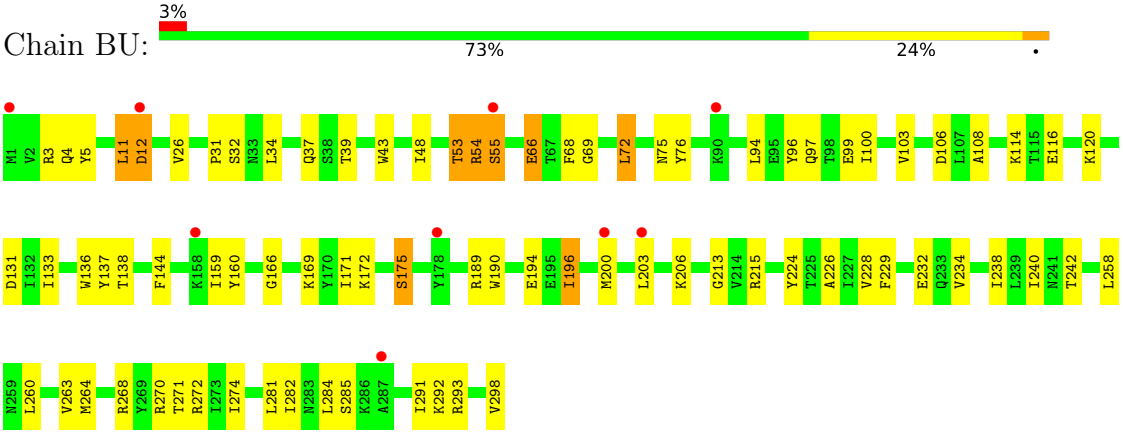
• Molecule 3: ORF15

Chain BT:



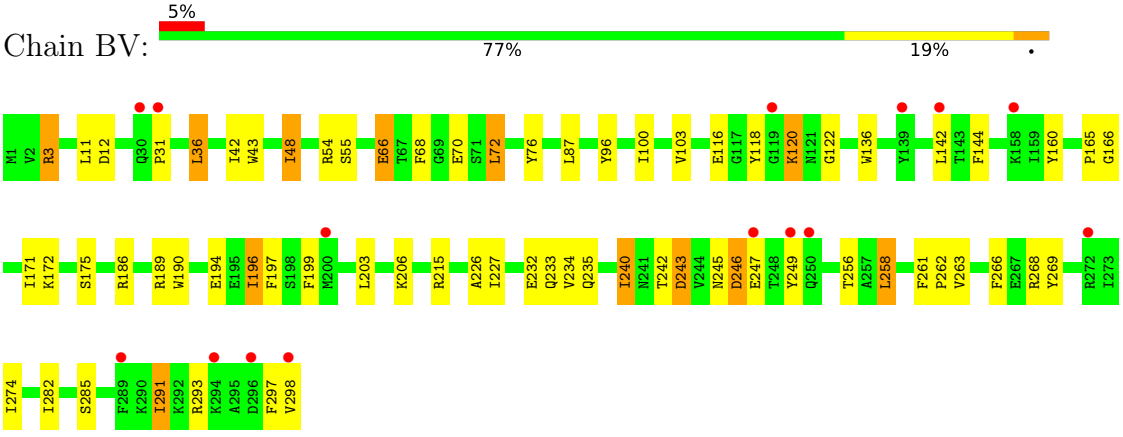
• Molecule 3: ORF15

Chain BU:



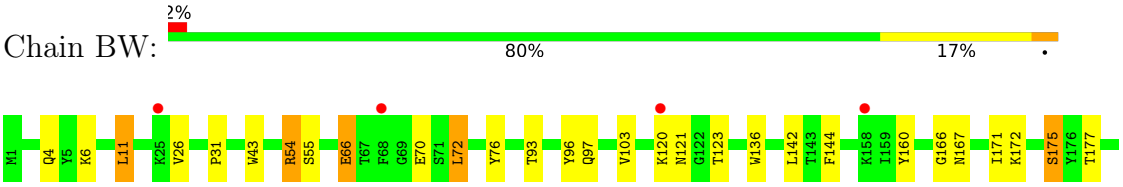
• Molecule 3: ORF15

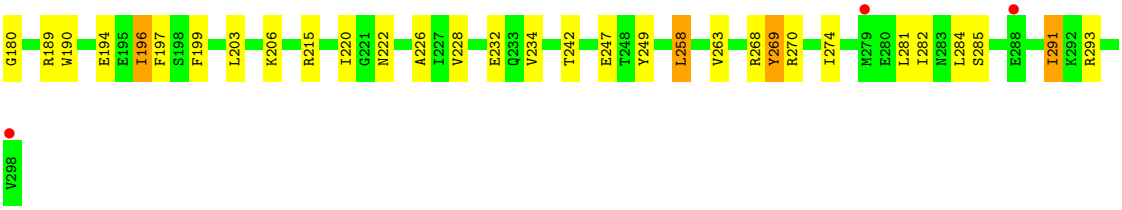
Chain BV:



• Molecule 3: ORF15

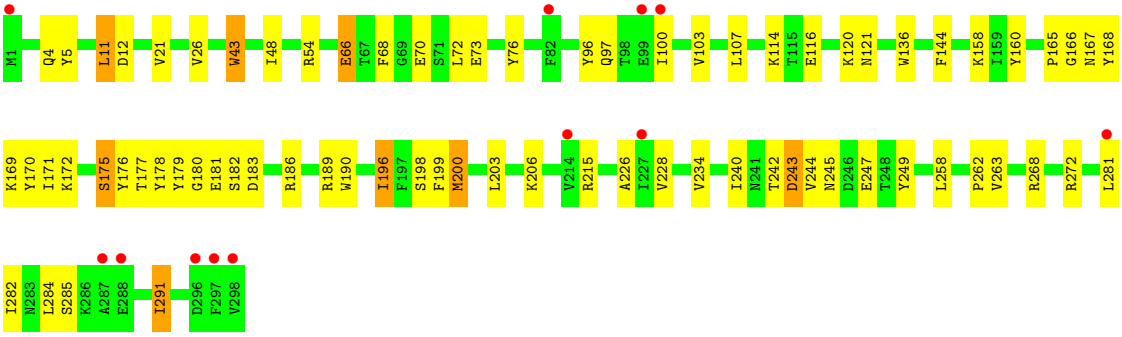
Chain BW:





• Molecule 3: ORF15

Chain BX:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	219.52Å 219.34Å 392.43Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	44.56 – 5.46 44.56 – 5.46	Depositor EDS
% Data completeness (in resolution range)	91.0 (44.56-5.46) 90.9 (44.56-5.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 5.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.291 , 0.297 0.298 , 0.301	Depositor DCC
R_{free} test set	5621 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	205.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 403.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.409 for k,h,-l 0.399 for -k,-h,-l 0.408 for h,-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	119484	wwPDB-VP
Average B, all atoms (Å^2)	343.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	A0	0.38	0/3069	0.64	0/4175
1	AY	0.38	0/3069	0.65	0/4175
1	AZ	0.37	0/3069	0.63	0/4175
1	B0	0.38	0/3069	0.64	0/4175
1	BY	0.38	0/3069	0.65	0/4175
1	BZ	0.37	0/3069	0.63	0/4175
2	AA	0.32	0/2048	0.63	0/2791
2	AB	0.36	0/2048	0.58	0/2791
2	AC	0.35	0/2048	0.59	0/2791
2	AD	0.32	0/2048	0.61	0/2791
2	AE	0.36	0/2048	0.58	0/2791
2	AF	0.36	0/2048	0.58	0/2791
2	AG	0.32	0/2048	0.62	0/2791
2	AH	0.37	0/2048	0.58	0/2791
2	AI	0.37	0/2048	0.58	0/2791
2	AJ	0.34	0/2048	0.63	0/2791
2	AK	0.36	0/2048	0.59	0/2791
2	AL	0.36	0/2048	0.58	0/2791
2	AM	0.34	0/2048	0.63	0/2791
2	AN	0.36	0/2048	0.58	0/2791
2	AO	0.36	0/2048	0.58	0/2791
2	AP	0.34	0/2048	0.63	0/2791
2	AQ	0.37	0/2048	0.58	0/2791
2	AR	0.37	0/2048	0.59	0/2791
2	BA	0.32	0/2048	0.63	0/2791
2	BB	0.36	0/2048	0.58	0/2791
2	BC	0.35	0/2048	0.59	0/2791
2	BD	0.32	0/2048	0.61	0/2791
2	BE	0.36	0/2048	0.58	0/2791
2	BF	0.36	0/2048	0.58	0/2791
2	BG	0.32	0/2048	0.62	0/2791
2	BH	0.37	0/2048	0.58	0/2791

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	BI	0.37	0/2048	0.58	0/2791
2	BJ	0.34	0/2048	0.63	0/2791
2	BK	0.35	0/2048	0.59	0/2791
2	BL	0.36	0/2048	0.58	0/2791
2	BM	0.34	0/2048	0.63	0/2791
2	BN	0.36	0/2048	0.58	0/2791
2	BO	0.36	0/2048	0.58	0/2791
2	BP	0.34	0/2048	0.63	0/2791
2	BQ	0.37	0/2048	0.58	0/2791
2	BR	0.37	0/2048	0.59	0/2791
3	AS	0.36	0/2485	0.69	0/3356
3	AT	0.36	0/2485	0.69	0/3356
3	AU	0.35	0/2485	0.67	0/3356
3	AV	0.36	0/2485	0.67	0/3356
3	AW	0.35	0/2485	0.66	0/3356
3	AX	0.36	0/2485	0.67	0/3356
3	BS	0.36	0/2485	0.69	0/3356
3	BT	0.36	0/2485	0.69	0/3356
3	BU	0.35	0/2485	0.67	0/3356
3	BV	0.36	0/2485	0.67	0/3356
3	BW	0.35	0/2485	0.66	0/3356
3	BX	0.36	0/2485	0.67	0/3356
All	All	0.36	0/121962	0.62	0/165798

There are no bond length outliers.

There are no bond angle outliers.

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	A0	3000	0	2956	55	0
1	AY	3000	0	2956	37	0
1	AZ	3000	0	2956	72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B0	3000	0	2956	45	0
1	BY	3000	0	2956	36	0
1	BZ	3000	0	2956	53	0
2	AA	2008	0	1971	22	0
2	AB	2008	0	1971	16	0
2	AC	2008	0	1971	15	0
2	AD	2008	0	1971	57	0
2	AE	2008	0	1971	34	0
2	AF	2008	0	1971	20	0
2	AG	2008	0	1971	34	0
2	AH	2008	0	1971	9	0
2	AI	2008	0	1971	10	0
2	AJ	2008	0	1971	11	0
2	AK	2008	0	1971	15	0
2	AL	2008	0	1971	10	0
2	AM	2008	0	1971	15	0
2	AN	2008	0	1971	38	0
2	AO	2008	0	1971	13	0
2	AP	2008	0	1971	35	0
2	AQ	2008	0	1971	42	0
2	AR	2008	0	1971	32	0
2	BA	2008	0	1971	18	0
2	BB	2008	0	1971	17	0
2	BC	2008	0	1971	15	0
2	BD	2008	0	1971	46	0
2	BE	2008	0	1971	35	0
2	BF	2008	0	1971	21	0
2	BG	2008	0	1971	25	0
2	BH	2008	0	1971	11	0
2	BI	2008	0	1971	10	0
2	BJ	2008	0	1971	10	0
2	BK	2008	0	1971	12	0
2	BL	2008	0	1971	11	0
2	BM	2008	0	1971	16	0
2	BN	2008	0	1971	37	0
2	BO	2008	0	1971	12	0
2	BP	2008	0	1971	23	0
2	BQ	2008	0	1971	31	0
2	BR	2008	0	1971	23	0
3	AS	2432	0	2392	117	0
3	AT	2432	0	2392	107	0
3	AU	2432	0	2392	100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AV	2432	0	2392	98	0
3	AW	2432	0	2392	74	0
3	AX	2432	0	2392	141	0
3	BS	2432	0	2392	96	0
3	BT	2432	0	2392	102	0
3	BU	2432	0	2392	92	0
3	BV	2432	0	2392	95	0
3	BW	2432	0	2392	74	0
3	BX	2432	0	2392	112	0
4	AS	1	0	0	0	0
4	AT	1	0	0	0	0
4	AU	1	0	0	0	0
4	AV	1	0	0	0	0
4	AW	1	0	0	0	0
4	AX	1	0	0	0	0
4	BS	1	0	0	0	0
4	BT	1	0	0	0	0
4	BU	1	0	0	0	0
4	BV	1	0	0	0	0
4	BW	1	0	0	0	0
4	BX	1	0	0	0	0
All	All	119484	0	117396	1507	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 6.

The worst 5 of 1507 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)
3:AW:120:LYS:HD3	3:BV:68:PHE:CE1	1.26	1.65
3:AV:68:PHE:CD1	3:BW:120:LYS:HD3	1.30	1.61
3:AV:68:PHE:CE1	3:BW:120:LYS:HD3	1.28	1.58
3:AU:68:PHE:CE1	3:BX:120:LYS:HD3	1.37	1.54
3:AW:120:LYS:HD3	3:BV:68:PHE:CD1	1.42	1.54

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	A0	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	AY	370/372 (100%)	355 (96%)	15 (4%)	0	100	100
1	AZ	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	B0	370/372 (100%)	358 (97%)	12 (3%)	0	100	100
1	BY	370/372 (100%)	355 (96%)	15 (4%)	0	100	100
1	BZ	370/372 (100%)	357 (96%)	13 (4%)	0	100	100
2	AA	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	AB	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	AC	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AE	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AF	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AG	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AH	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AI	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AJ	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AK	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AL	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AM	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	AN	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	AO	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	AP	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	AQ	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	AR	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BA	261/263 (99%)	254 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BB	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	BC	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BE	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BF	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BG	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	BH	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BI	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BJ	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BK	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BL	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BM	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BN	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	BO	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	BP	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	BQ	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	BR	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
3	AS	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	22	62
3	AT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	22	62
3	AU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	22	62
3	AV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	22	62
3	AW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	22	62
3	AX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	22	62
3	BS	296/298 (99%)	278 (94%)	16 (5%)	2 (1%)	22	62
3	BT	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	22	62
3	BU	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	22	62
3	BV	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	22	62
3	BW	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	22	62
3	BX	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	22	62
All	All	15168/15276 (99%)	14418 (95%)	726 (5%)	24 (0%)	47	81

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AS	175	SER
3	AT	175	SER
3	AU	175	SER
3	AV	175	SER
3	AW	175	SER

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	A0	337/337 (100%)	324 (96%)	13 (4%)	32	57
1	AY	337/337 (100%)	319 (95%)	18 (5%)	22	49
1	AZ	337/337 (100%)	321 (95%)	16 (5%)	26	52
1	B0	337/337 (100%)	324 (96%)	13 (4%)	32	57
1	BY	337/337 (100%)	319 (95%)	18 (5%)	22	49
1	BZ	337/337 (100%)	321 (95%)	16 (5%)	26	52
2	AA	227/227 (100%)	218 (96%)	9 (4%)	31	56
2	AB	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	AC	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	AD	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	AE	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	AF	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	AG	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	AH	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	AI	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	AJ	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	AK	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	AL	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	AM	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	AN	227/227 (100%)	221 (97%)	6 (3%)	46	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AO	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	AP	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	AQ	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	AR	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	BA	227/227 (100%)	218 (96%)	9 (4%)	31	56
2	BB	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	BC	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	BD	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	BE	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	BF	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	BG	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	BH	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	BI	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	BJ	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	BK	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	BL	227/227 (100%)	223 (98%)	4 (2%)	59	77
2	BM	227/227 (100%)	219 (96%)	8 (4%)	36	59
2	BN	227/227 (100%)	221 (97%)	6 (3%)	46	67
2	BO	227/227 (100%)	224 (99%)	3 (1%)	69	82
2	BP	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	BQ	227/227 (100%)	220 (97%)	7 (3%)	40	62
2	BR	227/227 (100%)	223 (98%)	4 (2%)	59	77
3	AS	264/265 (100%)	246 (93%)	18 (7%)	16	42
3	AT	264/265 (100%)	248 (94%)	16 (6%)	18	45
3	AU	264/265 (100%)	241 (91%)	23 (9%)	10	33
3	AV	264/265 (100%)	241 (91%)	23 (9%)	10	33
3	AW	264/265 (100%)	244 (92%)	20 (8%)	13	39
3	AX	264/265 (100%)	247 (94%)	17 (6%)	17	44
3	BS	264/265 (100%)	245 (93%)	19 (7%)	14	41
3	BT	264/265 (100%)	247 (94%)	17 (6%)	17	44
3	BU	264/265 (100%)	241 (91%)	23 (9%)	10	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	BV	264/265 (100%)	241 (91%)	23 (9%)	10 33
3	BW	264/265 (100%)	244 (92%)	20 (8%)	13 39
3	BX	264/265 (100%)	247 (94%)	17 (6%)	17 44
All	All	13362/13374 (100%)	12818 (96%)	544 (4%)	30 55

5 of 544 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	BV	227	ILE
3	BW	43	TRP
3	BV	203	LEU
1	BY	207	ASN
3	AV	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
2	BJ	82	ASN
3	BS	222	ASN
2	BK	71	ASN
2	BP	5	ASN
3	BU	75	ASN

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)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A0	372/372 (100%)	0.53	40 (10%) 5 8	351, 388, 435, 523	0
1	AY	372/372 (100%)	0.36	37 (9%) 7 9	359, 396, 449, 555	0
1	AZ	372/372 (100%)	0.42	38 (10%) 6 9	364, 394, 444, 557	0
1	B0	372/372 (100%)	0.41	29 (7%) 13 13	337, 377, 425, 485	0
1	BY	372/372 (100%)	0.14	15 (4%) 38 32	331, 361, 429, 557	0
1	BZ	372/372 (100%)	0.31	28 (7%) 14 14	332, 360, 422, 502	0
2	AA	263/263 (100%)	0.06	6 (2%) 60 52	248, 312, 407, 435	0
2	AB	263/263 (100%)	0.13	15 (5%) 23 22	284, 350, 440, 481	0
2	AC	263/263 (100%)	-0.11	13 (4%) 29 27	257, 345, 417, 473	0
2	AD	263/263 (100%)	0.21	16 (6%) 21 19	258, 320, 441, 485	0
2	AE	263/263 (100%)	-0.05	8 (3%) 50 41	277, 344, 466, 480	0
2	AF	263/263 (100%)	0.11	16 (6%) 21 19	265, 367, 471, 497	0
2	AG	263/263 (100%)	0.26	23 (8%) 10 11	265, 348, 500, 556	0
2	AH	263/263 (100%)	-0.08	9 (3%) 45 38	315, 402, 524, 572	0
2	AI	263/263 (100%)	0.14	20 (7%) 13 14	282, 416, 532, 576	0
2	AJ	263/263 (100%)	0.01	13 (4%) 29 27	264, 342, 429, 539	0
2	AK	263/263 (100%)	0.00	10 (3%) 40 34	255, 301, 456, 521	0
2	AL	263/263 (100%)	0.17	20 (7%) 13 14	277, 345, 485, 575	0
2	AM	263/263 (100%)	0.17	22 (8%) 11 12	266, 358, 425, 467	0
2	AN	263/263 (100%)	0.20	14 (5%) 26 25	252, 313, 386, 420	0
2	AO	263/263 (100%)	0.13	13 (4%) 29 27	276, 347, 419, 449	0
2	AP	263/263 (100%)	0.20	18 (6%) 17 16	267, 341, 556, 576	0
2	AQ	263/263 (100%)	0.30	25 (9%) 8 9	295, 397, 566, 605	0
2	AR	263/263 (100%)	0.20	17 (6%) 18 17	298, 417, 541, 571	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	BA	263/263 (100%)	0.08	11 (4%) 36 31	259, 312, 430, 466	0
2	BB	263/263 (100%)	0.05	13 (4%) 29 27	282, 346, 455, 506	0
2	BC	263/263 (100%)	-0.03	13 (4%) 29 27	273, 344, 419, 481	0
2	BD	263/263 (100%)	0.17	15 (5%) 23 22	252, 316, 445, 484	0
2	BE	263/263 (100%)	-0.01	11 (4%) 36 31	274, 342, 448, 477	0
2	BF	263/263 (100%)	0.34	21 (7%) 12 13	258, 361, 457, 487	0
2	BG	263/263 (100%)	0.27	21 (7%) 12 13	252, 346, 496, 557	0
2	BH	263/263 (100%)	0.15	20 (7%) 13 14	314, 408, 514, 559	0
2	BI	263/263 (100%)	0.00	11 (4%) 36 31	276, 420, 541, 584	0
2	BJ	263/263 (100%)	-0.17	7 (2%) 54 46	268, 345, 419, 521	0
2	BK	263/263 (100%)	0.10	20 (7%) 13 14	256, 305, 435, 496	0
2	BL	263/263 (100%)	0.19	22 (8%) 11 12	283, 341, 452, 534	0
2	BM	263/263 (100%)	0.37	24 (9%) 9 10	264, 357, 438, 484	0
2	BN	263/263 (100%)	0.18	17 (6%) 18 17	255, 316, 388, 433	0
2	BO	263/263 (100%)	0.07	15 (5%) 23 22	276, 348, 418, 453	0
2	BP	263/263 (100%)	0.31	31 (11%) 4 7	261, 365, 541, 549	0
2	BQ	263/263 (100%)	0.18	21 (7%) 12 13	312, 413, 547, 559	0
2	BR	263/263 (100%)	0.29	25 (9%) 8 9	308, 418, 537, 556	0
3	AS	298/298 (100%)	0.29	16 (5%) 25 24	219, 262, 346, 379	0
3	AT	298/298 (100%)	0.26	15 (5%) 28 26	230, 260, 318, 344	0
3	AU	298/298 (100%)	0.16	6 (2%) 65 57	228, 269, 334, 364	0
3	AV	298/298 (100%)	0.21	14 (4%) 31 28	229, 264, 317, 332	0
3	AW	298/298 (100%)	0.17	9 (3%) 50 41	213, 254, 317, 347	0
3	AX	298/298 (100%)	0.10	12 (4%) 38 32	216, 255, 347, 401	0
3	BS	298/298 (100%)	0.21	12 (4%) 38 32	222, 256, 339, 388	0
3	BT	298/298 (100%)	0.19	10 (3%) 45 38	218, 265, 316, 343	0
3	BU	298/298 (100%)	0.09	9 (3%) 50 41	228, 262, 338, 382	0
3	BV	298/298 (100%)	0.28	15 (5%) 28 26	218, 260, 305, 324	0
3	BW	298/298 (100%)	0.08	7 (2%) 60 52	215, 256, 341, 403	0
3	BX	298/298 (100%)	0.09	12 (4%) 38 32	228, 272, 370, 407	0
All	All	15276/15276 (100%)	0.17	920 (6%) 21 20	213, 344, 468, 605	0

The worst 5 of 920 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AQ	221	VAL	16.4
2	AQ	220	LEU	15.4
2	BN	260	SER	9.5
2	BO	260	SER	9.4
2	BF	260	SER	9.3

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	BX	301	1/1	0.79	0.26	287,287,287,287	0
4	CA	BS	301	1/1	0.80	0.34	267,267,267,267	0
4	CA	BV	301	1/1	0.80	0.26	272,272,272,272	0
4	CA	AW	301	1/1	0.80	0.29	266,266,266,266	0
4	CA	BW	301	1/1	0.81	0.26	268,268,268,268	0
4	CA	AS	301	1/1	0.82	0.33	281,281,281,281	0
4	CA	BU	301	1/1	0.83	0.32	269,269,269,269	0
4	CA	BT	301	1/1	0.85	0.35	279,279,279,279	0
4	CA	AU	301	1/1	0.88	0.35	275,275,275,275	0
4	CA	AV	301	1/1	0.89	0.36	276,276,276,276	0
4	CA	AX	301	1/1	0.92	0.29	275,275,275,275	0
4	CA	AT	301	1/1	0.94	0.25	275,275,275,275	0

6.5 Other polymers (i)

There are no such residues in this entry.