wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:24 AM GMT

PDB ID	:	3LK4
Title	:	Crystal structure of CapZ bound to the uncapping motif from CD2AP
Authors	:	Hernandez-Valladares, M.; Kim, T.; Kannan, B.; Tung, A.; Cooper, J.A.; Robinson, R.C.
Deposited on	:	2010-01-27
Resolution	:	1.99 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

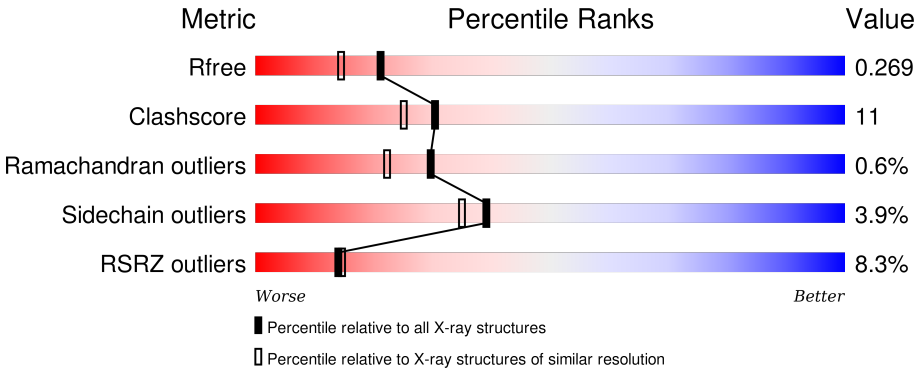
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.99 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	1	286	9% 73% 18% • 6%
1	4	286	9% 73% 19% • 6%
1	7	286	5% 73% 18% • 6%
1	A	286	9% 73% 19% • 6%
1	D	286	6% 74% 18% • 6%

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Mol	Chain	Length	Quality of chain
1	G	286	6% 75% 16% • 6%
1	J	286	7% 74% 17% • 6%
1	M	286	7% 73% 19% • 6%
1	P	286	11% 73% 19% • 6%
1	S	286	6% 74% 18% • 6%
1	V	286	6% 73% 20% • 6%
1	Y	286	11% 74% 17% • 6%
2	2	277	9% 71% 12% • 14%
2	5	277	4% 72% 13% • 14%
2	8	277	4% 71% 12% • 14%
2	B	277	9% 71% 13% • 14%
2	E	277	5% 74% 11% • 14%
2	H	277	4% 73% 12% • 14%
2	K	277	3% 72% 12% • 14%
2	N	277	4% 71% 13% • 14%
2	Q	277	8% 71% 13% • 14%
2	T	277	4% 73% 12% • 14%
2	W	277	3% 74% 10% • 14%
2	Z	277	7% 73% 12% • 14%
3	0	29	28% 55% 41% •
3	3	29	34% 52% 45% •
3	6	29	38% 55% 41% •
3	9	29	24% 59% 38% •
3	C	29	34% 55% 41% •
3	F	29	31% 55% 41% •

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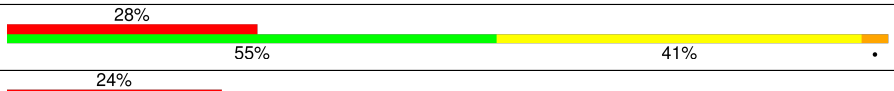
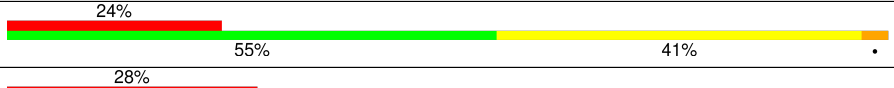
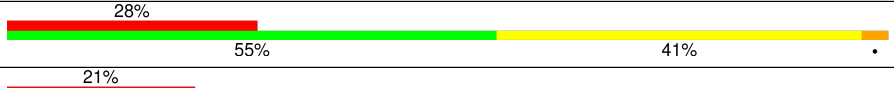
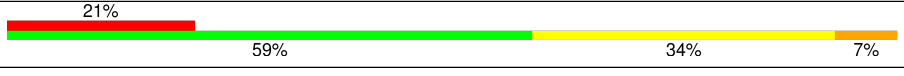
Mol	Chain	Length	Quality of chain
3	I	29	
3	L	29	
3	O	29	
3	R	29	
3	U	29	
3	X	29	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 54370 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 F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	D	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	G	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	J	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	M	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	P	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	S	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	V	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	Y	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	1	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	4	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			
1	7	269	Total	C	N	O	S	0	0	0
			2185	1378	381	421	5			

- Molecule 2 is a protein called F-actin-capping protein subunit beta isoforms 1 and 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			
2	E	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			
2	K	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			
2	N	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			
2	Q	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			
2	T	237	Total	C	N	O	S	0	0	0
			1870	1171	322	367	10			
2	W	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			
2	Z	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			
2	2	238	Total	C	N	O	S	0	0	0
			1878	1175	323	370	10			
2	5	237	Total	C	N	O	S	0	0	0
			1870	1171	322	367	10			
2	8	239	Total	C	N	O	S	0	0	0
			1884	1178	324	372	10			

- Molecule 3 is a protein called CD2-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	F	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	I	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	L	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	O	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	R	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	U	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	X	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	0	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	6	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			
3	9	29	Total	C	N	O	S	0	0	0
			225	139	44	41	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	90	Total	O	0	0
			90	90		
4	C	14	Total	O	0	0
			14	14		
4	D	131	Total	O	0	0
			131	131		
4	E	103	Total	O	0	0
			103	103		
4	F	13	Total	O	0	0
			13	13		
4	G	126	Total	O	0	0
			126	126		
4	H	155	Total	O	0	0
			155	155		
4	I	10	Total	O	0	0
			10	10		
4	J	135	Total	O	0	0
			135	135		
4	K	103	Total	O	0	0
			103	103		
4	L	14	Total	O	0	0
			14	14		
4	M	123	Total	O	0	0
			123	123		
4	N	138	Total	O	0	0
			138	138		
4	O	10	Total	O	0	0
			10	10		
4	P	93	Total	O	0	0
			93	93		

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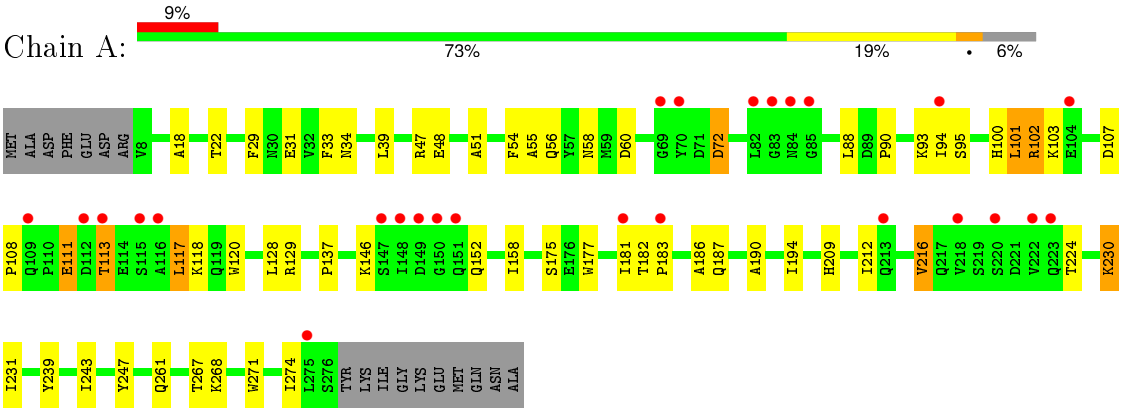
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	76	Total O 76 76	0	0
4	R	17	Total O 17 17	0	0
4	S	115	Total O 115 115	0	0
4	T	110	Total O 110 110	0	0
4	U	12	Total O 12 12	0	0
4	V	137	Total O 137 137	0	0
4	W	134	Total O 134 134	0	0
4	X	14	Total O 14 14	0	0
4	Y	91	Total O 91 91	0	0
4	Z	80	Total O 80 80	0	0
4	0	13	Total O 13 13	0	0
4	1	90	Total O 90 90	0	0
4	2	91	Total O 91 91	0	0
4	3	14	Total O 14 14	0	0
4	4	114	Total O 114 114	0	0
4	5	119	Total O 119 119	0	0
4	6	10	Total O 10 10	0	0
4	7	138	Total O 138 138	0	0
4	8	148	Total O 148 148	0	0
4	9	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

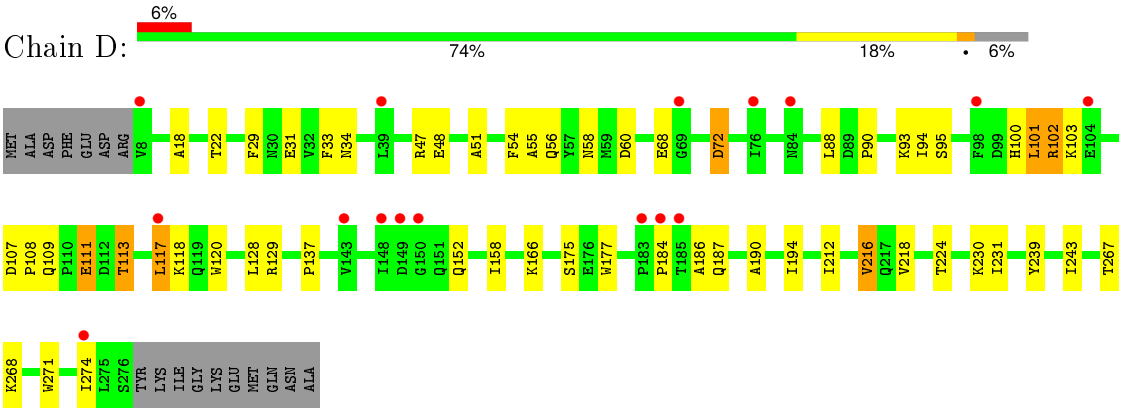
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain A:



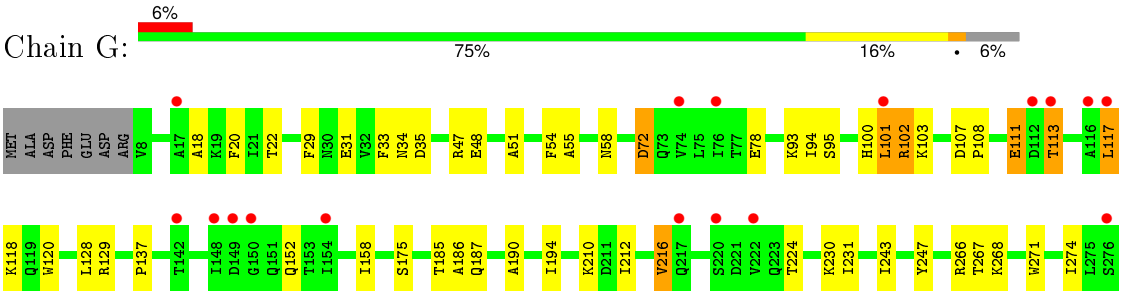
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain D:



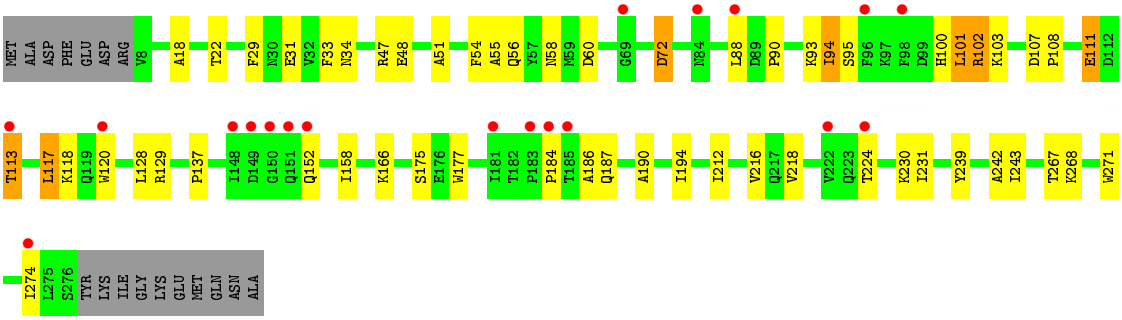
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain G:



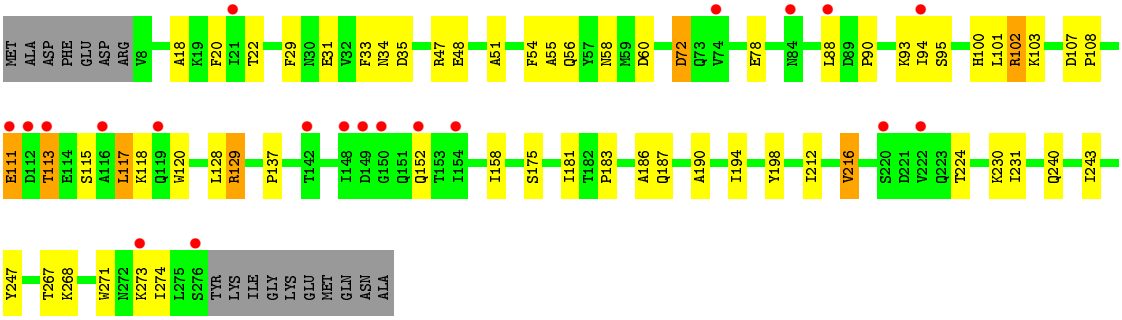
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain J:



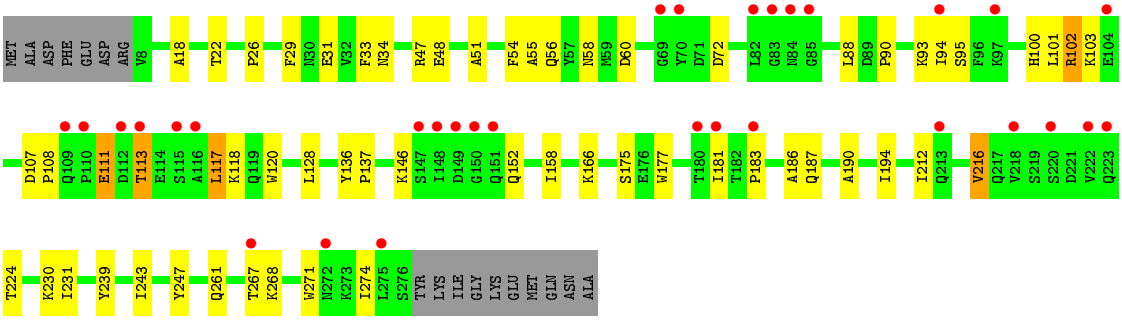
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain M:



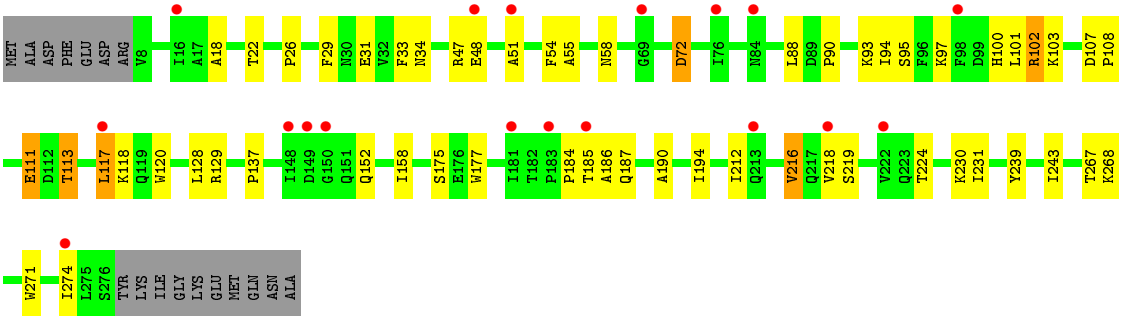
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain P:



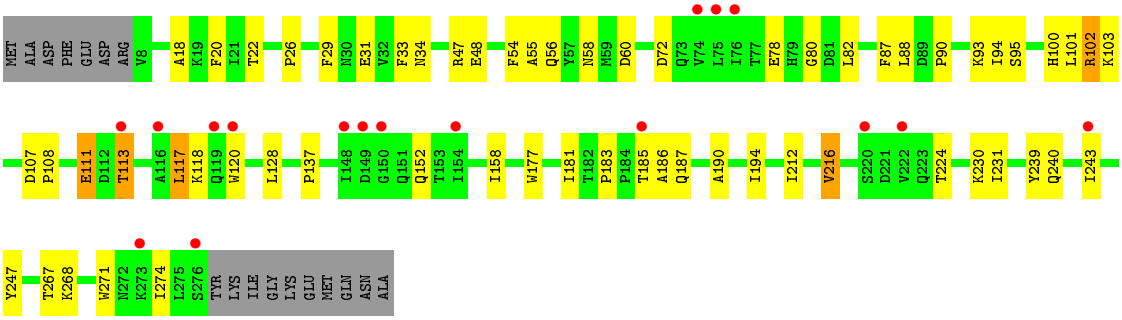
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain S:



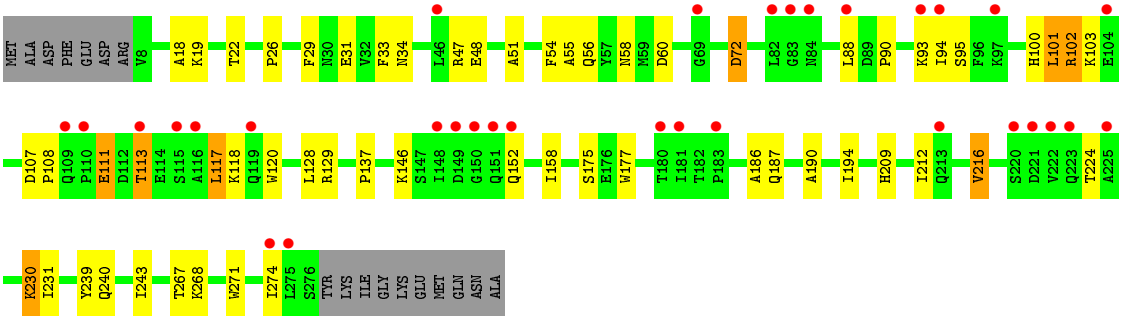
• Molecule 1: F-actin-capping protein subunit alpha-1

Chain V:



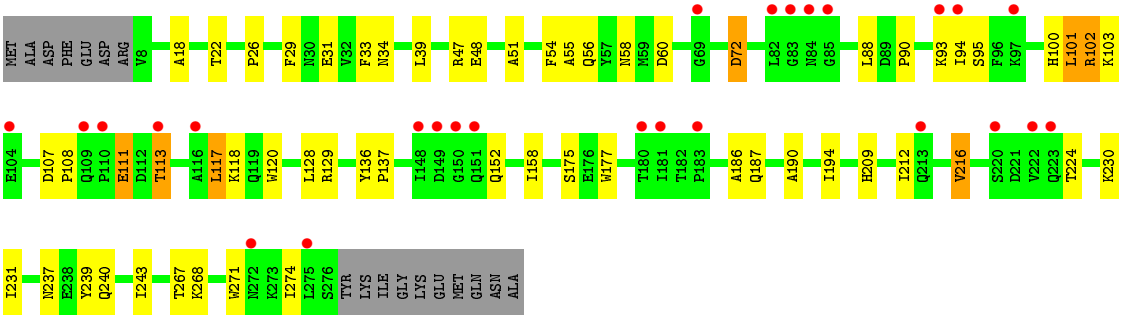
• Molecule 1: F-actin-capping protein subunit alpha-1

Chain Y:



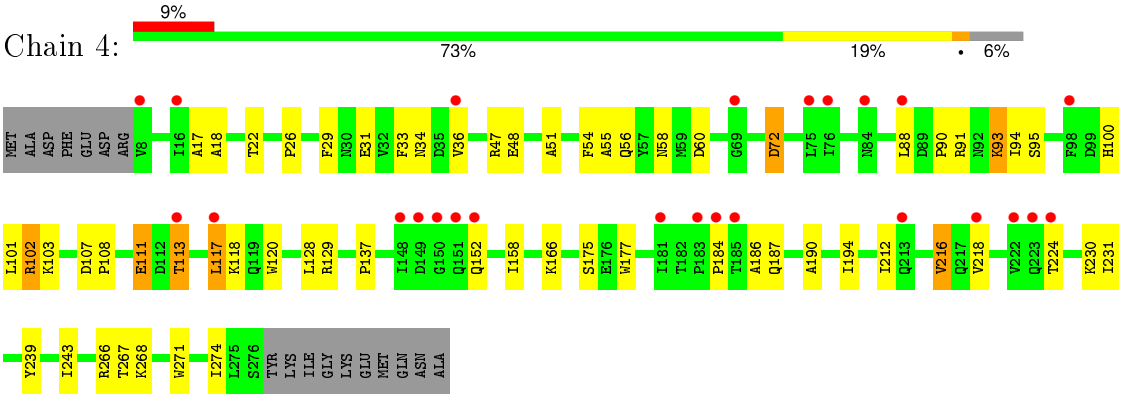
• Molecule 1: F-actin-capping protein subunit alpha-1

Chain 1:



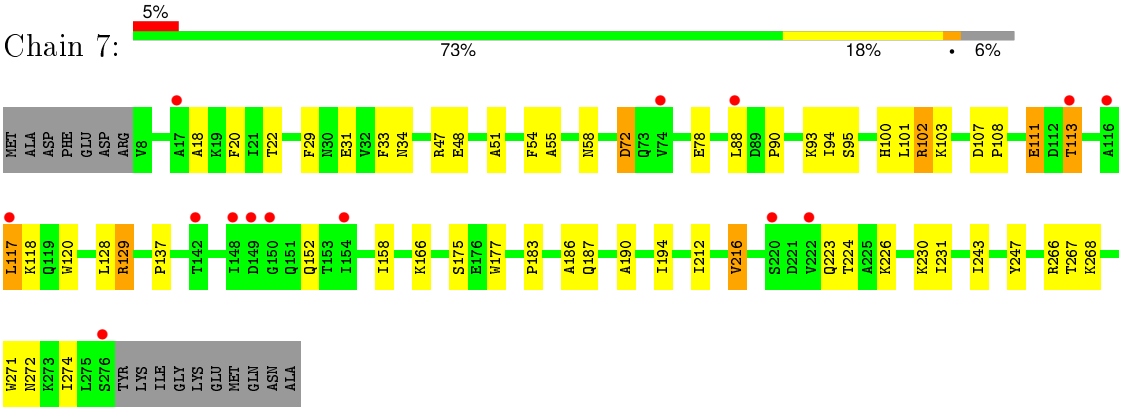
• Molecule 1: F-actin-capping protein subunit alpha-1

Chain 4:



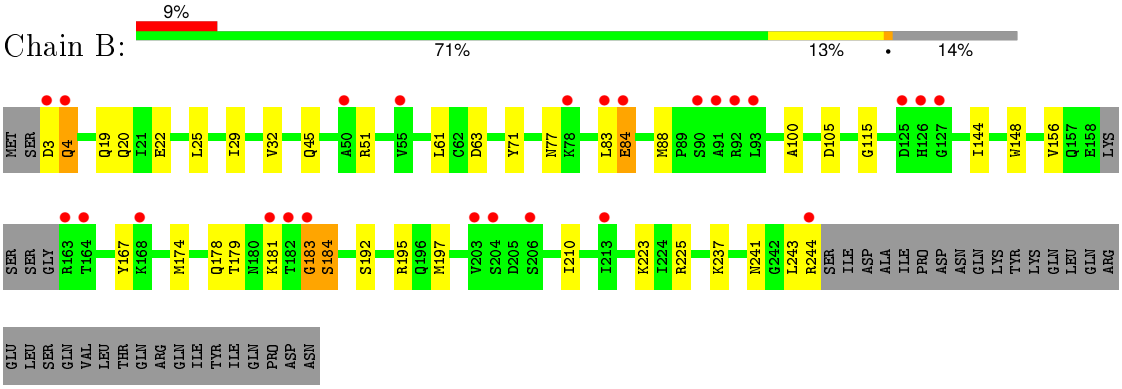
• Molecule 1: F-actin-capping protein subunit alpha-1

Chain 7:



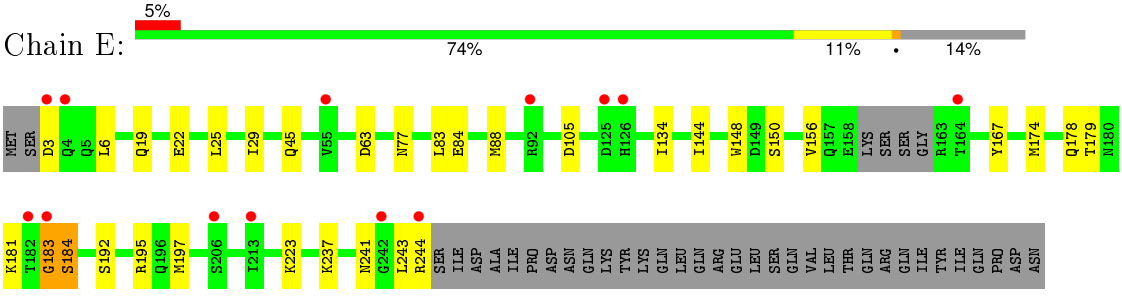
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B:



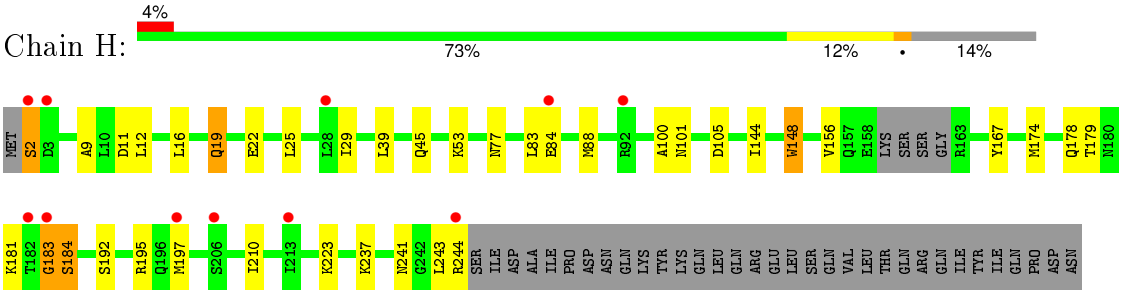
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain E:



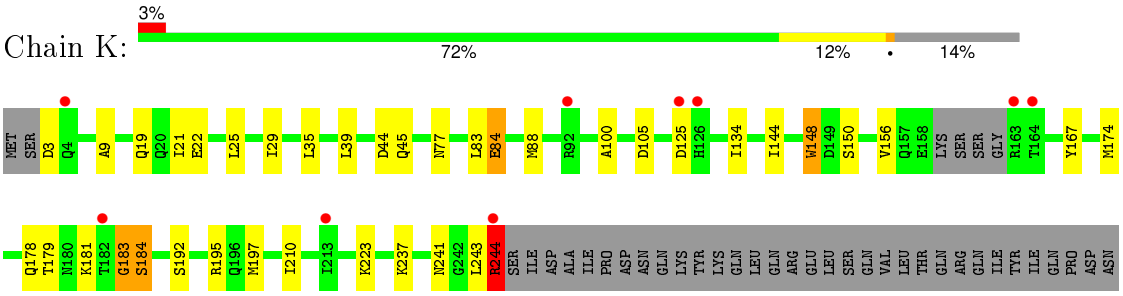
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain H:



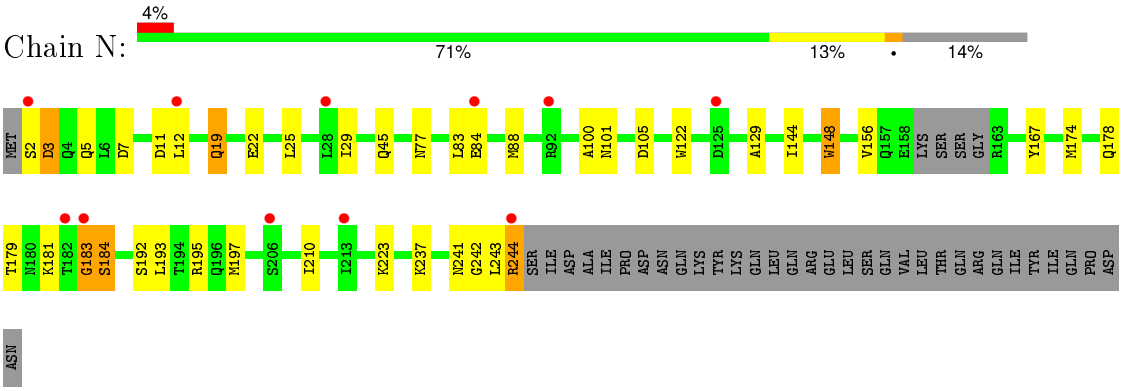
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain K:



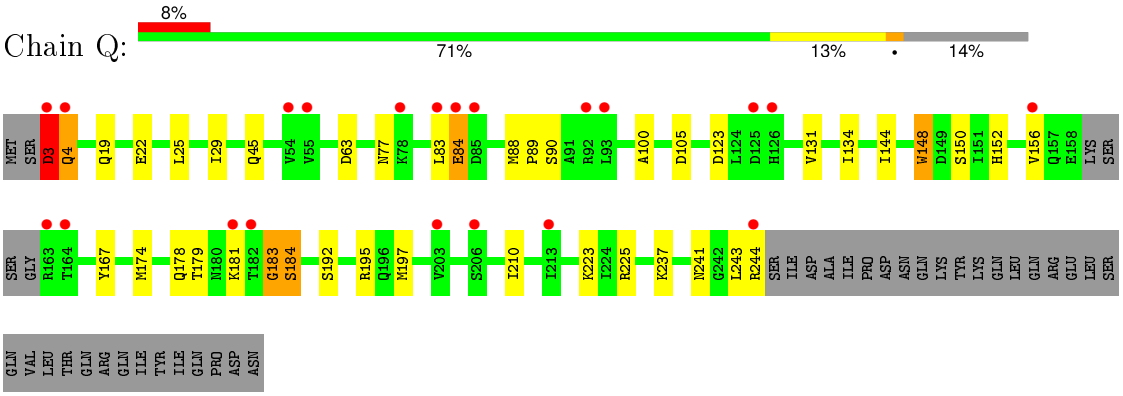
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain N:



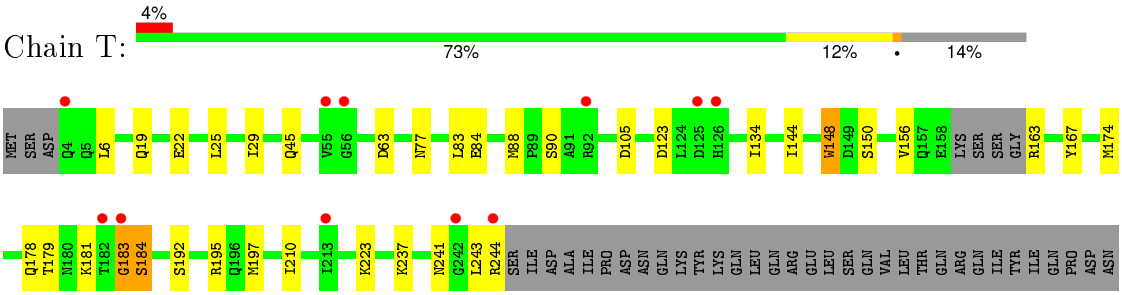
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain Q:



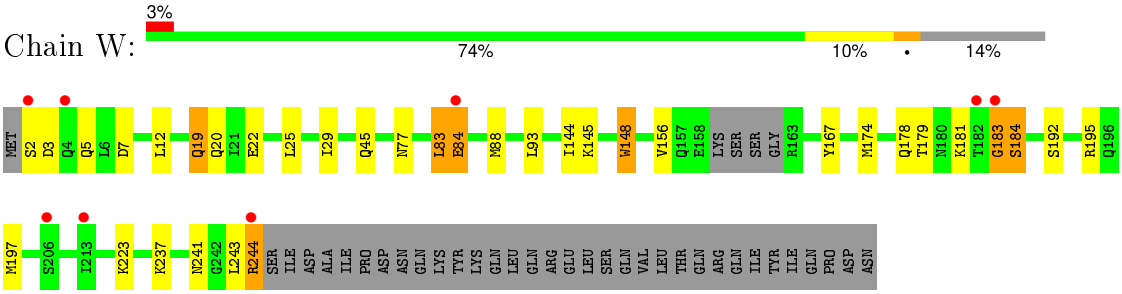
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain T:



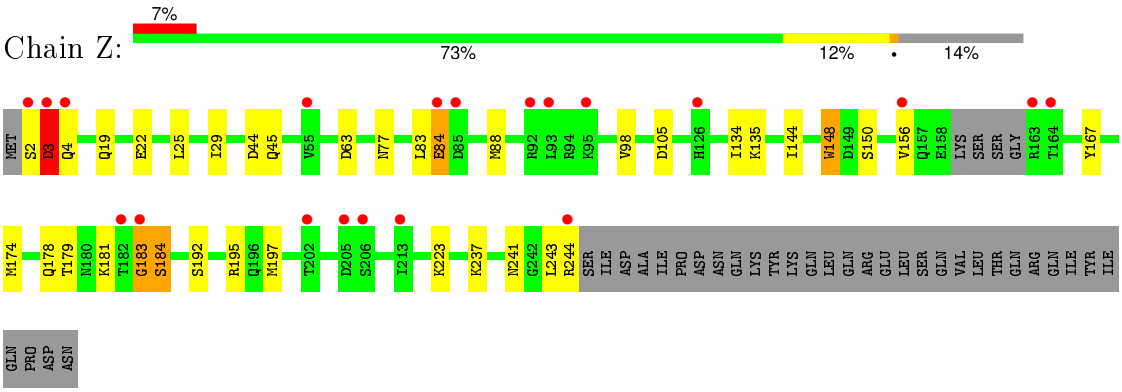
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain W:



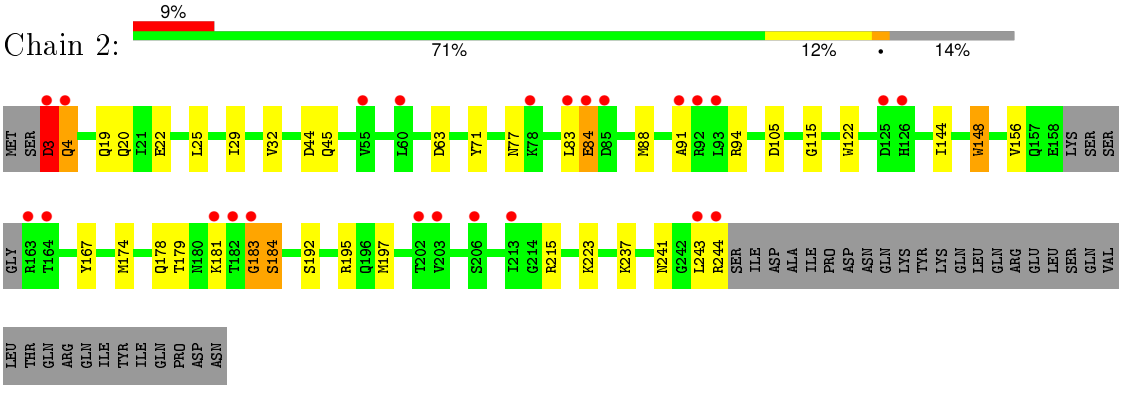
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain Z:



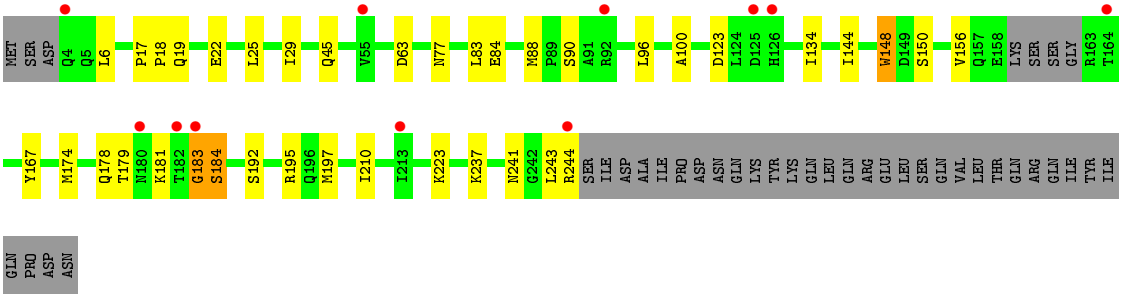
• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain 2:

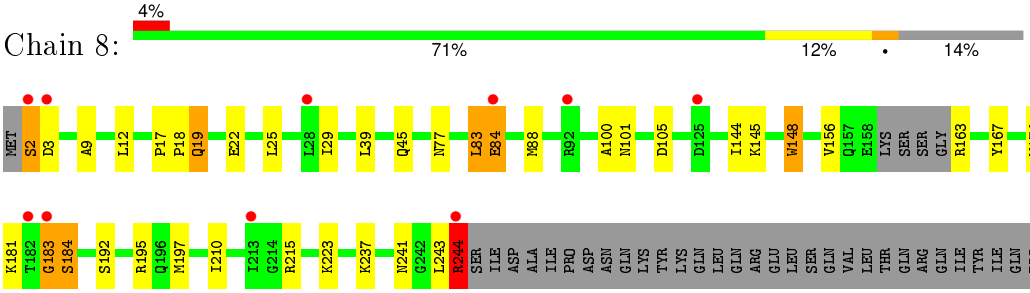


• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

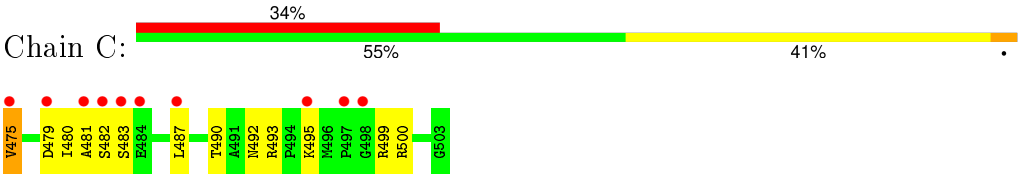
Chain 5:



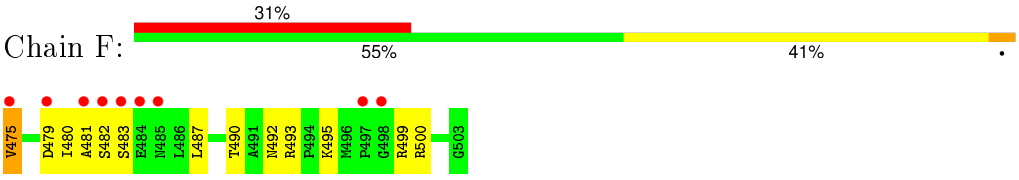
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



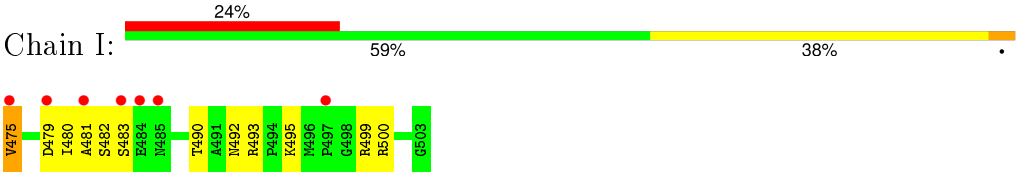
- Molecule 3: CD2-associated protein



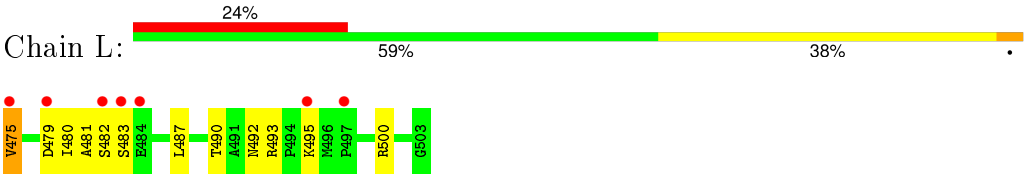
- Molecule 3: CD2-associated protein



- Molecule 3: CD2-associated protein

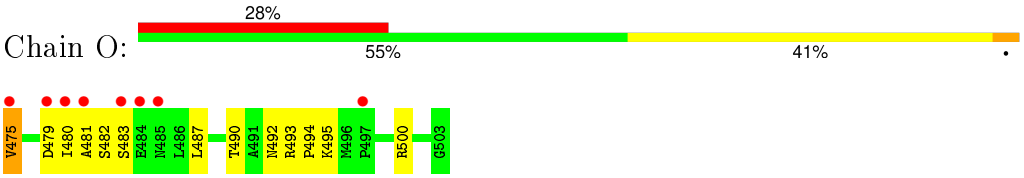


- Molecule 3: CD2-associated protein



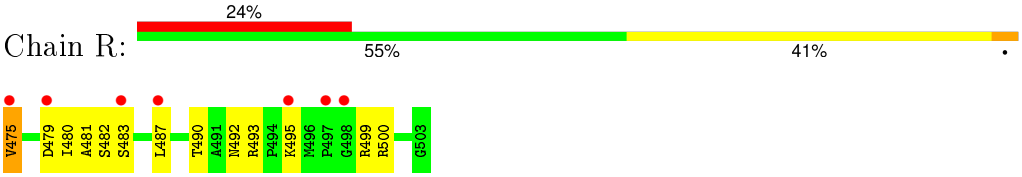
- Molecule 3: CD2-associated protein

Chain O:



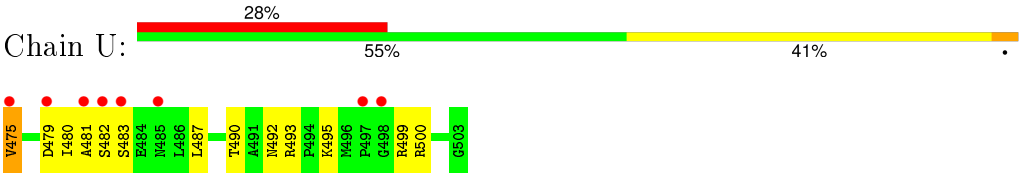
• Molecule 3: CD2-associated protein

Chain R:



• Molecule 3: CD2-associated protein

Chain U:

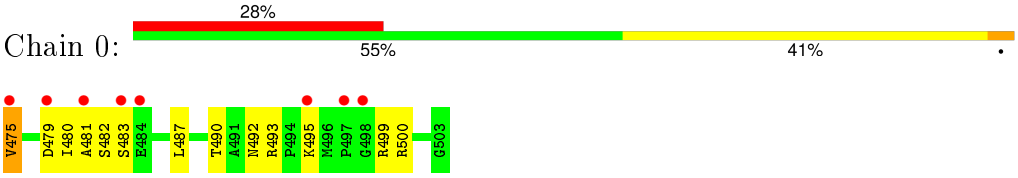


• Molecule 3: CD2-associated protein

Chain X:

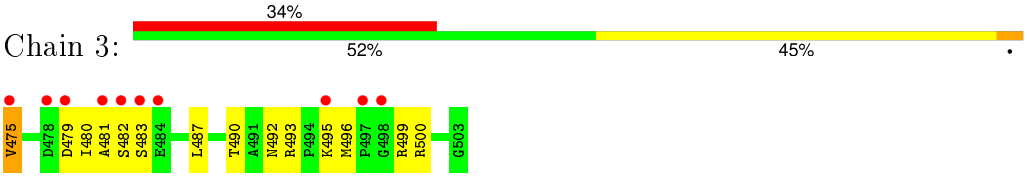
• Molecule 3: CD2-associated protein

Chain 0:



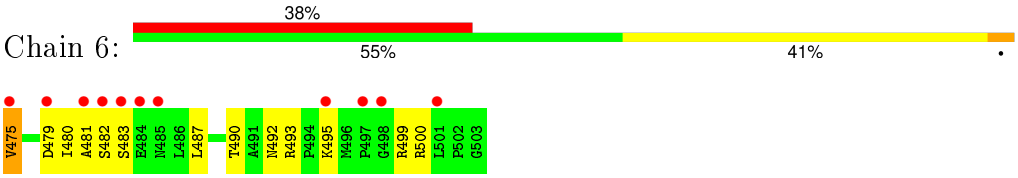
• Molecule 3: CD2-associated protein

Chain 3:



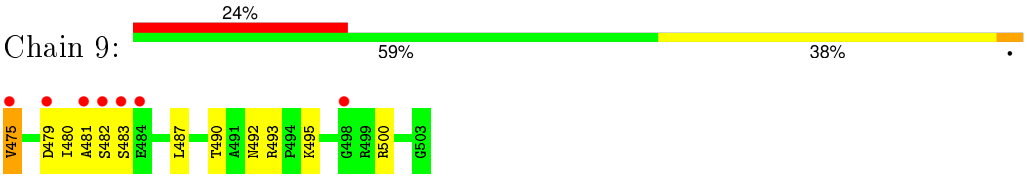
• Molecule 3: CD2-associated protein

Chain 6:



• Molecule 3: CD2-associated protein

Chain 9:


24%
59%
38%
V475
D479
I480
A481
S482
S483
E484
L487
T490
A491
N492
R493
P494
K495
G498
R499
R500
G503

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.73Å 142.34Å 193.00Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	19.98 – 1.99 19.98 – 1.99	Depositor EDS
% Data completeness (in resolution range)	82.2 (19.98-1.99) 82.5 (19.98-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.225 , 0.272 0.222 , 0.269	Depositor DCC
R_{free} test set	17972 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.6	EDS
Estimated twinning fraction	0.470 for h,-k,-l 0.478 for -h,k,-l 0.487 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 359377 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	54370	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.06 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.4815e-07.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1	0.36	0/2236	0.50	0/3032
1	4	0.36	0/2236	0.51	0/3032
1	7	0.39	0/2236	0.52	0/3032
1	A	0.37	0/2236	0.51	0/3032
1	D	0.37	0/2236	0.51	0/3032
1	G	0.38	0/2236	0.51	0/3032
1	J	0.37	0/2236	0.52	0/3032
1	M	0.37	0/2236	0.51	0/3032
1	P	0.37	0/2236	0.51	0/3032
1	S	0.36	0/2236	0.51	0/3032
1	V	0.40	0/2236	0.52	0/3032
1	Y	0.36	0/2236	0.50	0/3032
2	2	0.39	0/1910	0.54	0/2580
2	5	0.39	0/1902	0.53	0/2569
2	8	0.44	0/1916	0.57	1/2588 (0.0%)
2	B	0.40	0/1910	0.53	0/2580
2	E	0.40	0/1910	0.53	0/2580
2	H	0.42	0/1916	0.56	0/2588
2	K	0.41	0/1910	0.54	1/2580 (0.0%)
2	N	0.43	0/1916	0.57	1/2588 (0.0%)
2	Q	0.40	0/1910	0.55	0/2580
2	T	0.39	0/1902	0.53	0/2569
2	W	0.45	0/1916	0.57	1/2588 (0.0%)
2	Z	0.39	0/1916	0.53	0/2588
3	0	0.37	0/229	0.63	0/309
3	3	0.36	0/229	0.64	0/309
3	6	0.36	0/229	0.67	0/309
3	9	0.38	0/229	0.67	0/309
3	C	0.37	0/229	0.63	0/309
3	F	0.36	0/229	0.64	0/309
3	I	0.38	0/229	0.67	0/309
3	L	0.35	0/229	0.66	0/309
3	O	0.36	0/229	0.64	0/309
3	R	0.35	0/229	0.64	0/309

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
3	U	0.36	0/229	0.65	0/309
3	X	0.40	0/229	0.69	1/309 (0.3%)
All	All	0.39	0/52514	0.54	5/71070 (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
2	2	0	1
2	Q	0	1
2	Z	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	244	ARG	NE-CZ-NH1	-5.57	117.52	120.30
2	N	244	ARG	NE-CZ-NH1	-5.33	117.64	120.30
2	K	244	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	8	244	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	X	493	ARG	NE-CZ-NH2	-5.17	117.71	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	3	ASP	Peptide
2	Q	3	ASP	Peptide
2	Z	3	ASP	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	1	2185	0	2104	57	0
1	4	2185	0	2104	56	0
1	7	2185	0	2104	55	0
1	A	2185	0	2104	61	0
1	D	2185	0	2104	52	0
1	G	2185	0	2104	58	0
1	J	2185	0	2104	54	0
1	M	2185	0	2104	57	0
1	P	2185	0	2104	53	0
1	S	2185	0	2104	58	0
1	V	2185	0	2104	60	0
1	Y	2185	0	2104	50	0
2	2	1878	0	1852	52	0
2	5	1870	0	1848	39	0
2	8	1884	0	1857	43	0
2	B	1878	0	1852	49	0
2	E	1878	0	1852	39	0
2	H	1884	0	1857	48	0
2	K	1878	0	1852	42	0
2	N	1884	0	1857	49	0
2	Q	1878	0	1852	42	0
2	T	1870	0	1848	39	0
2	W	1884	0	1857	50	0
2	Z	1884	0	1857	33	0
3	0	225	0	226	16	0
3	3	225	0	226	16	0
3	6	225	0	226	16	0
3	9	225	0	226	14	0
3	C	225	0	226	16	0
3	F	225	0	226	14	0
3	I	225	0	226	14	0
3	L	225	0	226	14	0
3	O	225	0	226	16	0
3	R	225	0	226	15	0
3	U	225	0	226	15	0
3	X	225	0	226	14	0
4	0	13	0	0	0	0
4	1	90	0	0	5	0
4	2	91	0	0	8	0
4	3	14	0	0	0	0
4	4	114	0	0	4	0
4	5	119	0	0	5	0
4	6	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	7	138	0	0	7	0
4	8	148	0	0	4	0
4	9	11	0	0	0	0
4	A	108	0	0	5	0
4	B	90	0	0	3	0
4	C	14	0	0	1	0
4	D	131	0	0	4	0
4	E	103	0	0	0	0
4	F	13	0	0	0	0
4	G	126	0	0	6	0
4	H	155	0	0	3	0
4	I	10	0	0	1	0
4	J	135	0	0	2	0
4	K	103	0	0	4	0
4	L	14	0	0	0	0
4	M	123	0	0	9	0
4	N	138	0	0	3	0
4	O	10	0	0	0	0
4	P	93	0	0	3	0
4	Q	76	0	0	5	0
4	R	17	0	0	0	0
4	S	115	0	0	5	0
4	T	110	0	0	5	0
4	U	12	0	0	0	0
4	V	137	0	0	11	0
4	W	134	0	0	7	0
4	X	14	0	0	0	0
4	Y	91	0	0	9	0
4	Z	80	0	0	2	0
All	All	54370	0	50201	1122	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 11.

The worst 5 of 1122 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)
1:1:137:PRO:HD3	2:2:244:ARG:NH1	1.50	1.26
2:B:3:ASP:HA	2:B:4:GLN:CB	1.77	1.14
1:1:137:PRO:CD	2:2:244:ARG:NH1	2.10	1.14
1:G:137:PRO:HD3	2:H:244:ARG:HG3	1.12	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PRO:HD3	2:B:244:ARG:HG3	1.22	1.10

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	1	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
1	4	267/286 (93%)	259 (97%)	7 (3%)	1 (0%)	39	33
1	7	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	A	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
1	D	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	G	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
1	J	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	M	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	P	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
1	S	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	V	267/286 (93%)	258 (97%)	8 (3%)	1 (0%)	39	33
1	Y	267/286 (93%)	257 (96%)	9 (3%)	1 (0%)	39	33
2	2	234/277 (84%)	227 (97%)	4 (2%)	3 (1%)	15	7
2	5	233/277 (84%)	227 (97%)	4 (2%)	2 (1%)	21	13
2	8	235/277 (85%)	228 (97%)	5 (2%)	2 (1%)	21	13
2	B	234/277 (84%)	225 (96%)	6 (3%)	3 (1%)	15	7
2	E	234/277 (84%)	228 (97%)	4 (2%)	2 (1%)	21	13
2	H	235/277 (85%)	230 (98%)	3 (1%)	2 (1%)	21	13
2	K	234/277 (84%)	228 (97%)	4 (2%)	2 (1%)	21	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	N	235/277 (85%)	230 (98%)	3 (1%)	2 (1%)	21 13
2	Q	234/277 (84%)	227 (97%)	4 (2%)	3 (1%)	15 7
2	T	233/277 (84%)	228 (98%)	3 (1%)	2 (1%)	21 13
2	W	235/277 (85%)	229 (97%)	4 (2%)	2 (1%)	21 13
2	Z	235/277 (85%)	228 (97%)	4 (2%)	3 (1%)	15 7
3	0	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	3	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	6	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	9	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	C	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	F	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	I	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	L	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	O	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	R	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	U	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
3	X	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
All	All	6339/7104 (89%)	6139 (97%)	160 (2%)	40 (1%)	30 22

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	184	SER
2	E	184	SER
2	H	184	SER
2	K	184	SER
2	N	184	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	1	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	4	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	7	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	A	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	D	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	G	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	J	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	M	238/252 (94%)	228 (96%)	10 (4%)	36	31
1	P	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	S	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	V	238/252 (94%)	229 (96%)	9 (4%)	40	36
1	Y	238/252 (94%)	228 (96%)	10 (4%)	36	31
2	2	210/248 (85%)	203 (97%)	7 (3%)	45	43
2	5	209/248 (84%)	205 (98%)	4 (2%)	65	67
2	8	211/248 (85%)	202 (96%)	9 (4%)	35	30
2	B	210/248 (85%)	205 (98%)	5 (2%)	57	58
2	E	210/248 (85%)	206 (98%)	4 (2%)	65	67
2	H	211/248 (85%)	205 (97%)	6 (3%)	51	50
2	K	210/248 (85%)	203 (97%)	7 (3%)	45	43
2	N	211/248 (85%)	205 (97%)	6 (3%)	51	50
2	Q	210/248 (85%)	203 (97%)	7 (3%)	45	43
2	T	209/248 (84%)	204 (98%)	5 (2%)	57	58
2	W	211/248 (85%)	205 (97%)	6 (3%)	51	50
2	Z	211/248 (85%)	204 (97%)	7 (3%)	45	43
3	0	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	3	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	6	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	9	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	C	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	F	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	I	25/25 (100%)	22 (88%)	3 (12%)	6	3
3	L	25/25 (100%)	22 (88%)	3 (12%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	O	25/25 (100%)	22 (88%)	3 (12%)	6 3
3	R	25/25 (100%)	22 (88%)	3 (12%)	6 3
3	U	25/25 (100%)	22 (88%)	3 (12%)	6 3
3	X	25/25 (100%)	22 (88%)	3 (12%)	6 3
All	All	5679/6300 (90%)	5455 (96%)	224 (4%)	39 35

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	3	ASP
3	U	475	VAL
1	7	113	THR
2	Q	105	ASP
1	S	94	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	164	GLN
1	S	248	GLN
1	7	44	ASN
1	P	240	GLN
1	S	34	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	1	269/286 (94%)	0.71	26 (9%) 10 10	23, 48, 94, 120	0
1	4	269/286 (94%)	0.62	25 (9%) 11 11	28, 47, 89, 116	0
1	7	269/286 (94%)	0.54	14 (5%) 31 33	20, 40, 88, 116	0
1	A	269/286 (94%)	0.67	26 (9%) 10 10	20, 48, 94, 119	0
1	D	269/286 (94%)	0.56	16 (5%) 26 27	23, 44, 89, 116	0
1	G	269/286 (94%)	0.56	17 (6%) 23 24	22, 42, 88, 116	0
1	J	269/286 (94%)	0.53	19 (7%) 19 20	24, 44, 87, 115	0
1	M	269/286 (94%)	0.61	20 (7%) 17 18	22, 42, 88, 116	0
1	P	269/286 (94%)	0.69	31 (11%) 6 7	22, 47, 92, 118	0
1	S	269/286 (94%)	0.60	18 (6%) 21 22	27, 46, 89, 116	0
1	V	269/286 (94%)	0.57	17 (6%) 23 24	19, 40, 87, 116	0
1	Y	269/286 (94%)	0.70	32 (11%) 6 6	26, 49, 91, 118	0
2	2	238/277 (85%)	0.59	24 (10%) 9 10	25, 46, 77, 117	0
2	5	237/277 (85%)	0.35	11 (4%) 36 38	28, 42, 69, 114	0
2	8	239/277 (86%)	0.37	10 (4%) 40 41	21, 34, 68, 116	0
2	B	238/277 (85%)	0.52	25 (10%) 8 9	24, 42, 74, 116	0
2	E	238/277 (85%)	0.38	13 (5%) 29 30	26, 40, 70, 113	0
2	H	239/277 (86%)	0.41	11 (4%) 36 38	23, 36, 69, 116	0
2	K	238/277 (85%)	0.29	9 (3%) 44 45	24, 39, 71, 113	0
2	N	239/277 (86%)	0.41	11 (4%) 36 38	23, 36, 68, 116	0
2	Q	238/277 (85%)	0.49	21 (8%) 12 13	23, 44, 74, 117	0
2	T	237/277 (85%)	0.35	11 (4%) 36 38	29, 42, 68, 113	0
2	W	239/277 (86%)	0.33	8 (3%) 50 51	20, 34, 67, 116	0
2	Z	239/277 (86%)	0.61	20 (8%) 14 14	26, 47, 75, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
3	0	29/29 (100%)	1.78	8 (27%)	1 1	44, 72, 107, 129	0
3	3	29/29 (100%)	1.76	10 (34%)	0 1	42, 71, 107, 129	0
3	6	29/29 (100%)	1.65	11 (37%)	0 1	40, 67, 107, 129	0
3	9	29/29 (100%)	1.29	7 (24%)	1 1	35, 66, 104, 127	0
3	C	29/29 (100%)	1.54	10 (34%)	0 1	39, 68, 106, 128	0
3	F	29/29 (100%)	1.37	9 (31%)	1 1	40, 69, 106, 129	0
3	I	29/29 (100%)	1.57	7 (24%)	1 1	38, 68, 107, 127	0
3	L	29/29 (100%)	1.41	7 (24%)	1 1	38, 66, 106, 128	0
3	O	29/29 (100%)	1.59	8 (27%)	1 1	39, 66, 106, 128	0
3	R	29/29 (100%)	1.59	7 (24%)	1 1	38, 70, 106, 129	0
3	U	29/29 (100%)	1.40	8 (27%)	1 1	39, 68, 107, 128	0
3	X	29/29 (100%)	1.56	6 (20%)	1 1	35, 66, 104, 128	0
All	All	6435/7104 (90%)	0.58	533 (8%)	14 15	19, 44, 89, 148	0

The worst 5 of 533 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	3	ASP	9.5
1	1	150	GLY	9.3
1	1	148	ILE	9.2
1	D	150	GLY	9.2
1	P	148	ILE	8.3

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 carbohydrates 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.