



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:09 PM BST

PDB ID : 1VJ6
Title : PDZ2 from PTP-BL in complex with the C-terminal ligand from the APC protein
Authors : Walma, T.; Vuister, G.W.
Deposited on : 2004-02-03

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

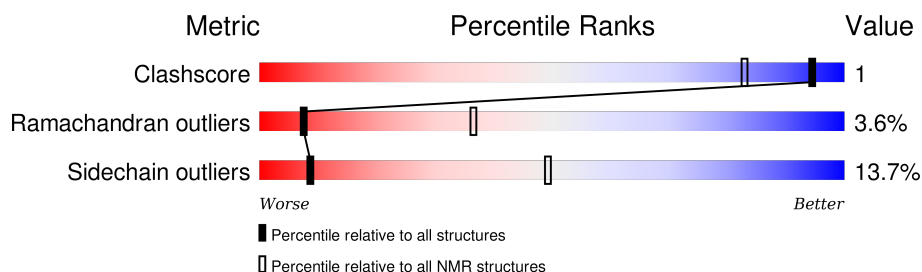
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	102	
2	B	12	

2 Ensemble composition and analysis ⓘ

This entry contains 35 models. Model 22 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:13-A:33, A:41-A:48, A:52-A:98, B:206-B:210 (81)	0.28	22

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 6 single-model clusters were found.

Cluster number	Models
1	4, 6, 7, 9, 10, 11, 12, 13, 15, 18, 22, 23, 26, 27, 30, 31, 33, 34
2	1, 14, 17, 20, 21, 24, 32
3	19, 28
4	2, 35
Single-model clusters	3; 5; 8; 16; 25; 29

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1509 atoms, of which 766 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called protein-tyrosine-phosphatase (nonreceptor type 13).

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1411	431	716	128	135	1	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q64512
A	2	HIS	-	EXPRESSION TAG	UNP Q64512
A	3	HIS	-	EXPRESSION TAG	UNP Q64512
A	4	HIS	-	EXPRESSION TAG	UNP Q64512
A	5	HIS	-	EXPRESSION TAG	UNP Q64512
A	6	HIS	-	EXPRESSION TAG	UNP Q64512
A	7	HIS	-	EXPRESSION TAG	UNP Q64512
A	8	MET	-	CLONING ARTIFACT	UNP Q64512

- Molecule 2 is a protein called Adenomatous polyposis coli protein.

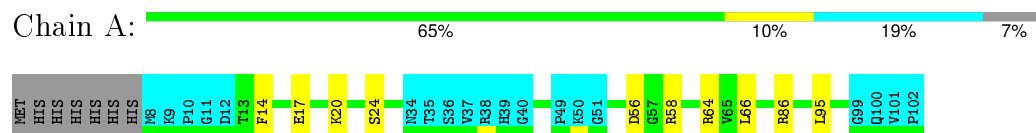
Mol	Chain	Residues	Atoms						Trace
2	B	6	Total	C	H	N	O		0
			98	32	50	6	10		

4 Residue-property plots [i](#)

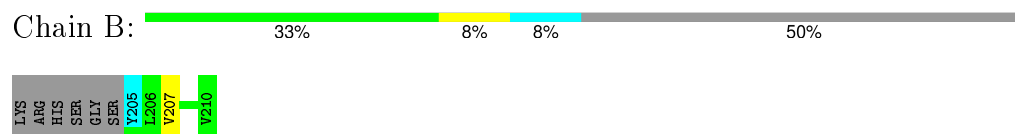
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)



- Molecule 2: Adenomatous polyposis coli protein

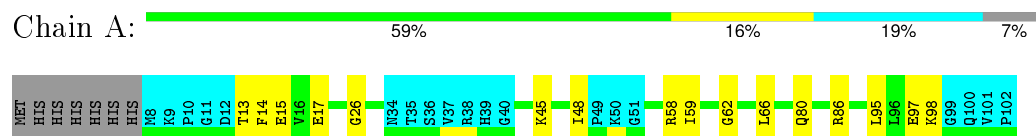


4.2 Scores per residue for each member of the ensemble

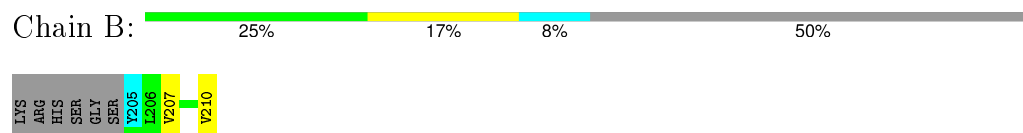
Colouring as in section 4.1 above.

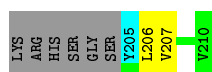
4.2.1 Score per residue for model 1

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)



- Molecule 2: Adenomatous polyposis coli protein

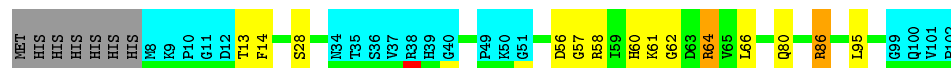




4.2.5 Score per residue for model 5

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

Chain A:



- Molecule 2: Adenomatous polyposis coli protein

Chain B:



4.2.6 Score per residue for model 6

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

Chain A:



- Molecule 2: Adenomatous polyposis coli protein

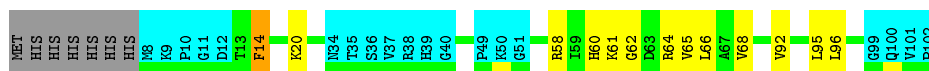
Chain B:



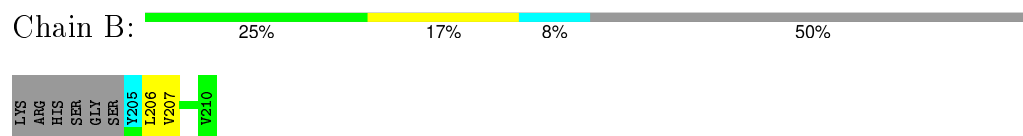
4.2.7 Score per residue for model 7

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

Chain A:

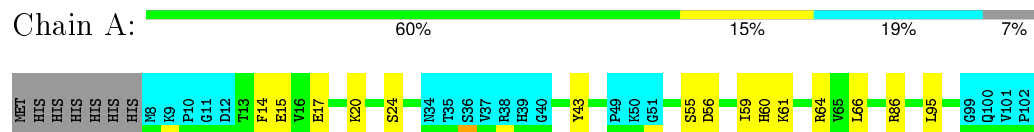


- Molecule 2: Adenomatous polyposis coli protein

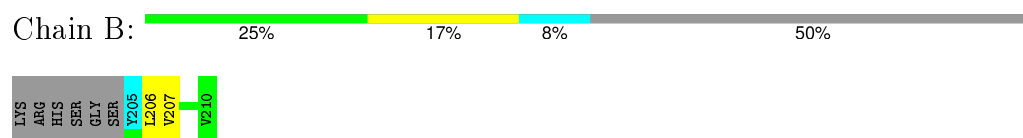


4.2.8 Score per residue for model 8

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

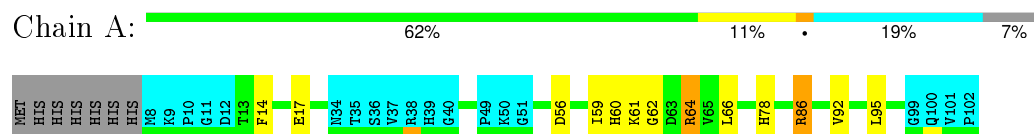


- Molecule 2: Adenomatous polyposis coli protein

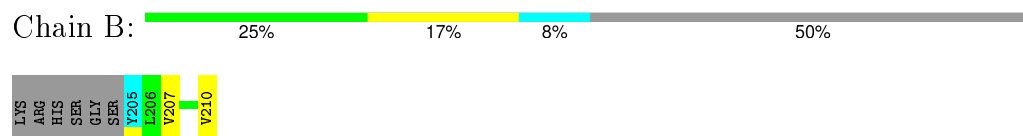


4.2.9 Score per residue for model 9

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

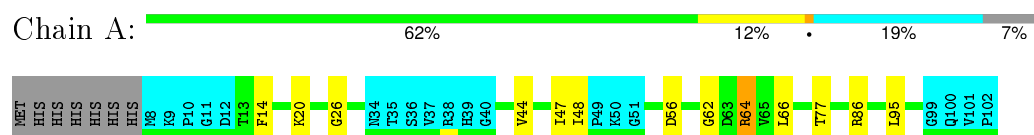


- Molecule 2: Adenomatous polyposis coli protein

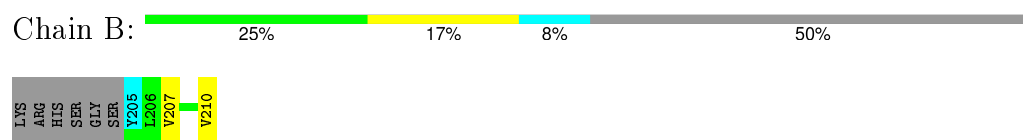


4.2.10 Score per residue for model 10

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

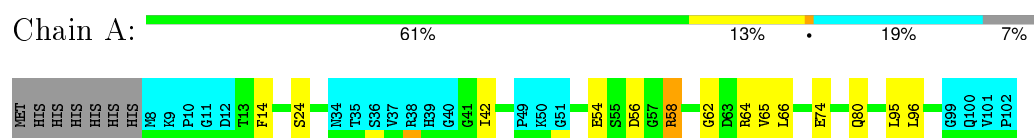


- Molecule 2: Adenomatous polyposis coli protein

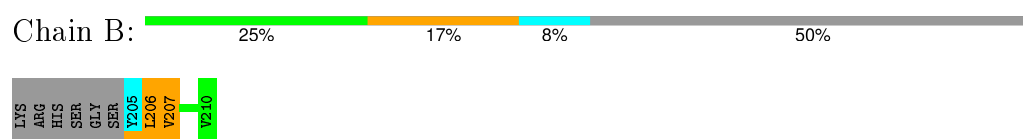


4.2.11 Score per residue for model 11

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

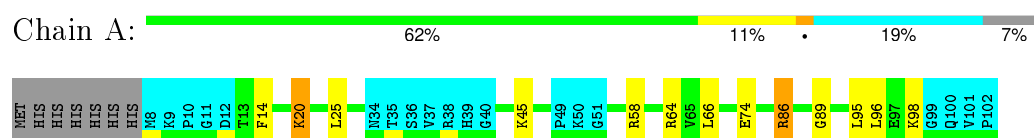


- Molecule 2: Adenomatous polyposis coli protein

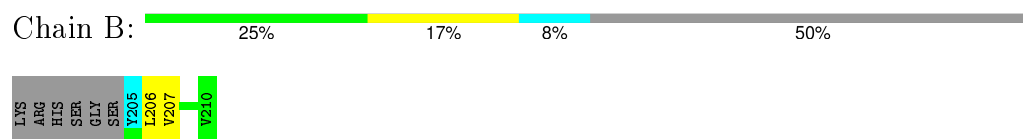


4.2.12 Score per residue for model 12

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)



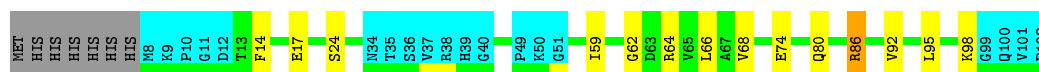
- Molecule 2: Adenomatous polyposis coli protein



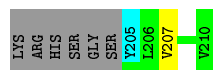
4.2.13 Score per residue for model 13

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)





- Molecule 2: Adenomatous polyposis coli protein



4.2.14 Score per residue for model 14

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)



- Molecule 2: Adenomatous polyposis coli protein



4.2.15 Score per residue for model 15

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

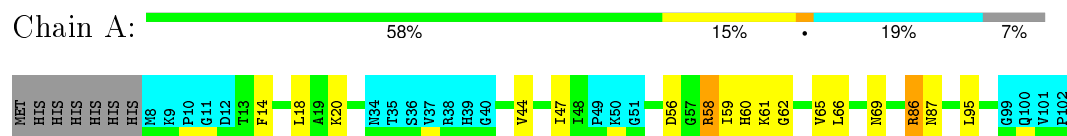


- Molecule 2: Adenomatous polyposis coli protein

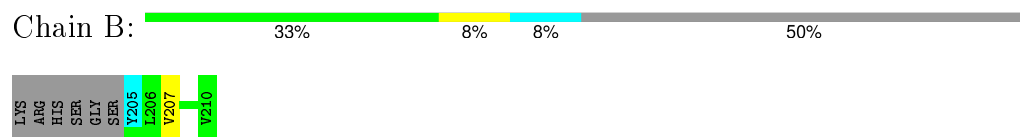


4.2.16 Score per residue for model 16

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

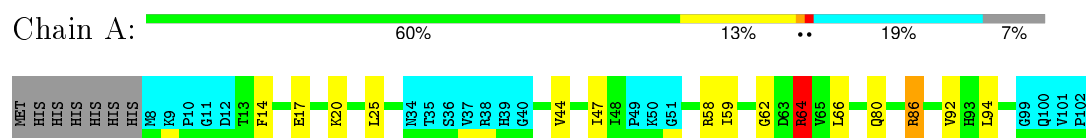


- Molecule 2: Adenomatous polyposis coli protein

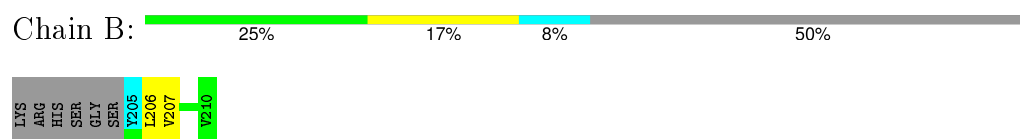


4.2.17 Score per residue for model 17

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

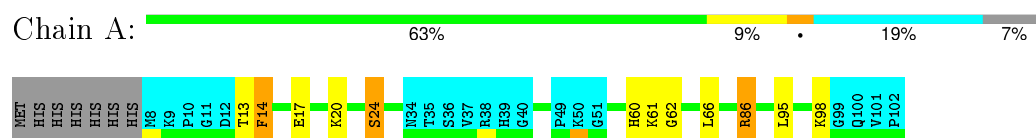


- Molecule 2: Adenomatous polyposis coli protein

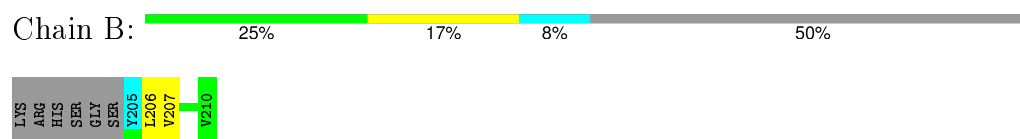


4.2.18 Score per residue for model 18

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

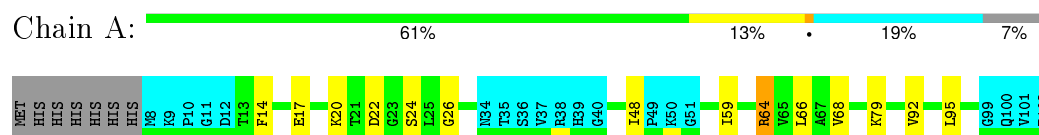


- Molecule 2: Adenomatous polyposis coli protein

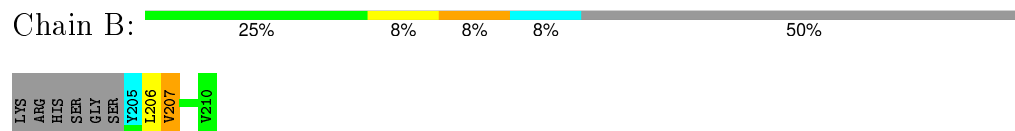


4.2.19 Score per residue for model 19

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

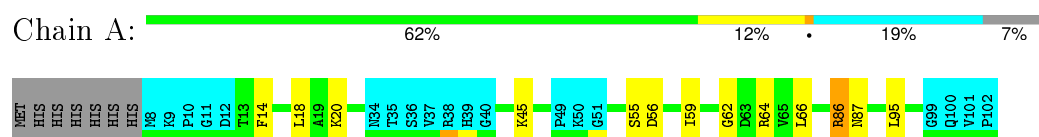


- Molecule 2: Adenomatous polyposis coli protein

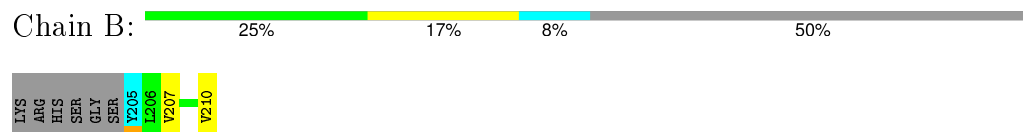


4.2.20 Score per residue for model 20

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

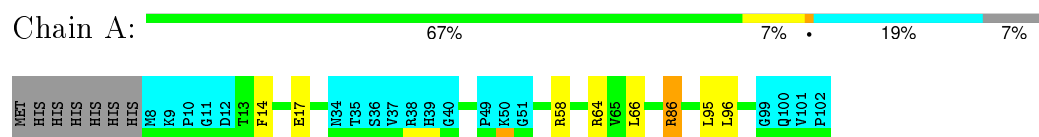


- Molecule 2: Adenomatous polyposis coli protein

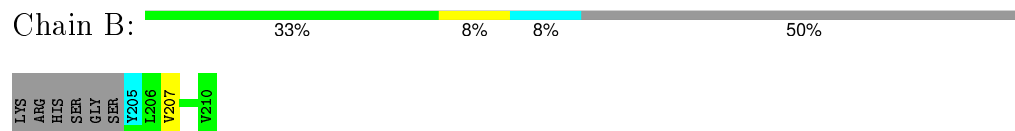


4.2.21 Score per residue for model 21

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

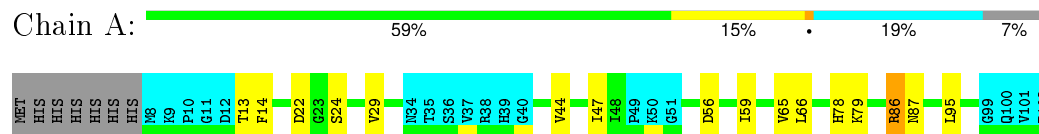


- Molecule 2: Adenomatous polyposis coli protein

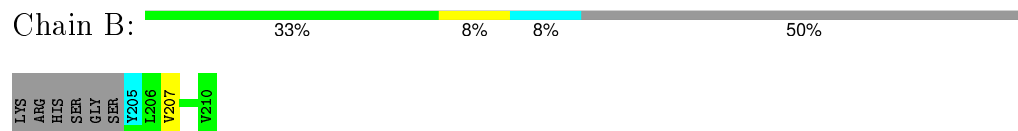


4.2.22 Score per residue for model 22 (medoid)

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

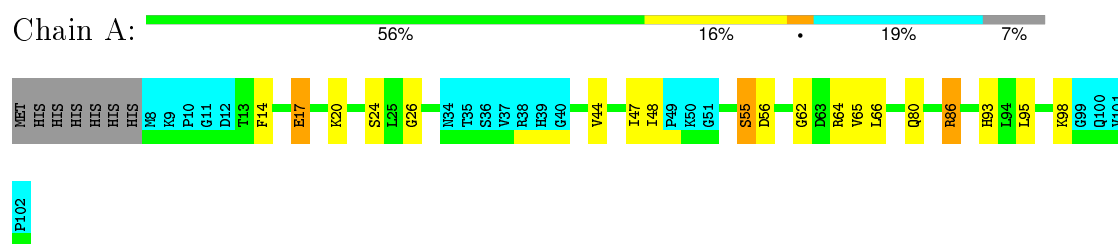


- Molecule 2: Adenomatous polyposis coli protein

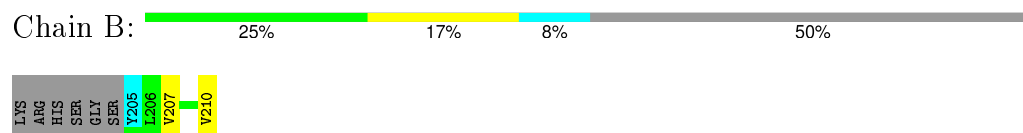


4.2.23 Score per residue for model 23

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

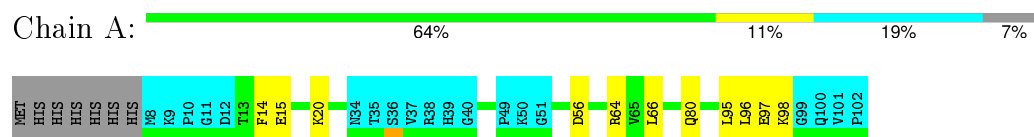


- Molecule 2: Adenomatous polyposis coli protein



4.2.24 Score per residue for model 24

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)



- Molecule 2: Adenomatous polyposis coli protein





4.2.25 Score per residue for model 25

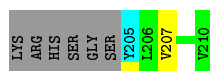
- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

Chain A: 61% 13% 19% 7%



- Molecule 2: Adenomatous polyposis coli protein

Chain B: 33% 8% 8% 50%



4.2.26 Score per residue for model 26

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

Chain A: 60% 13% 19% 7%



- Molecule 2: Adenomatous polyposis coli protein

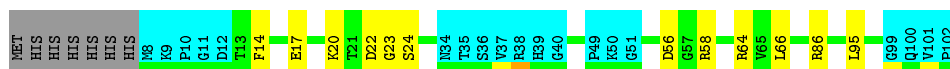
Chain B: 33% 8% 8% 50%



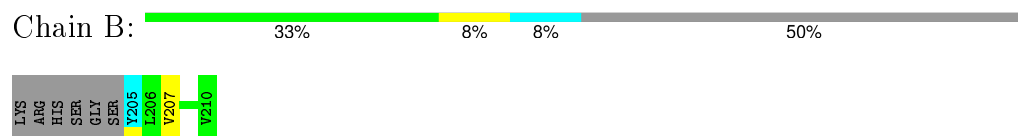
4.2.27 Score per residue for model 27

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

Chain A: 63% 12% 19% 7%

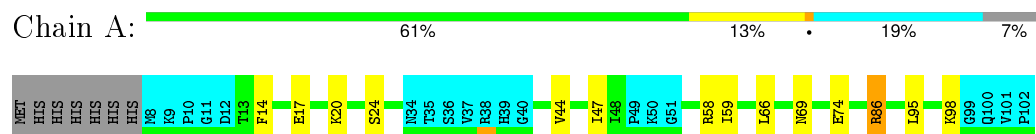


- Molecule 2: Adenomatous polyposis coli protein

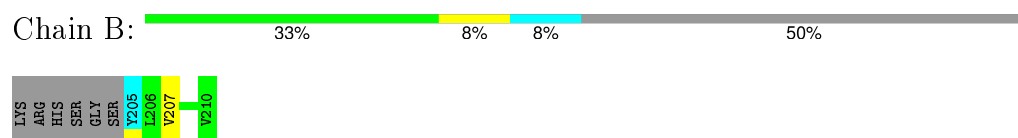


4.2.28 Score per residue for model 28

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

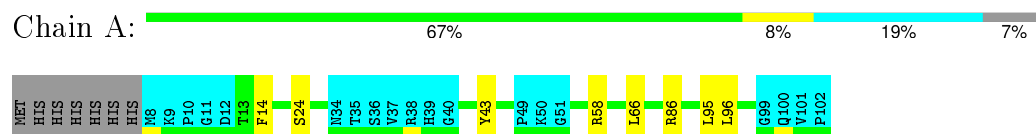


- Molecule 2: Adenomatous polyposis coli protein

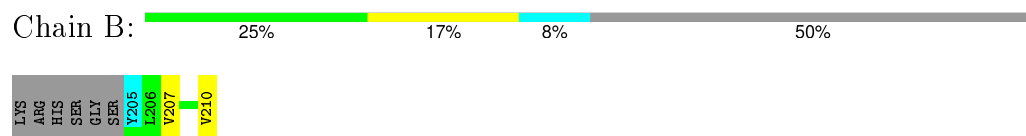


4.2.29 Score per residue for model 29

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

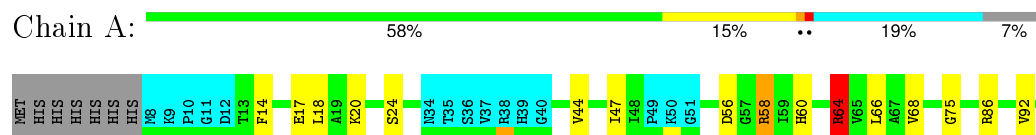


- Molecule 2: Adenomatous polyposis coli protein



4.2.30 Score per residue for model 30

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)



V101
P102

- Molecule 2: Adenomatous polyposis coli protein

Chain B:  25% 17% 8% 50%

LYS
ARG
HIS
HIS
SER
GLY
SER
Y205
L206
V207
V210

4.2.31 Score per residue for model 31

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

Chain A:  64% 9% 19% 7%

MET
HIS
HIS
HIS
HIS
HIS
HIS
H8
K9
P10
G11
D12
T13
F14
K20
L25
N34
T35
S36
V37
R38
R39
G40
P49
K50
G51
D56
G57
R58
G62
R63
R64
R65
L66
R86
L95
L96
G99
Q100
V101
P102

- Molecule 2: Adenomatous polyposis coli protein

Chain B:  33% 8% 8% 50%

LYS
ARG
HIS
HIS
SER
GLY
SER
Y205
L206
V207
V210

4.2.32 Score per residue for model 32

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

Chain A:  55% 18% 19% 7%

MET
HIS
HIS
HIS
HIS
HIS
HIS
H8
K9
P10
G11
D12
T13
F14
L18
G23
S24
L25
G26
N34
T35
S36
V37
R38
R39
G40
V44
K45
A46
I47
I48
P49
K50
G51
D56
G57
R58
I59
H60
R64
V65
L66
R69
R78
R86
L94
L95
L96
G99

Q100
V101
P102

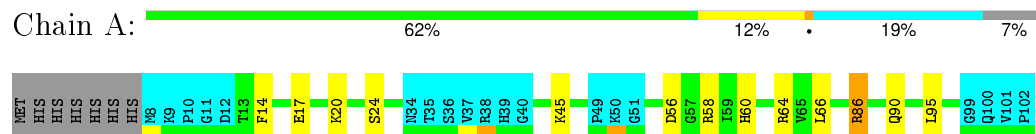
- Molecule 2: Adenomatous polyposis coli protein

Chain B:  33% 8% 8% 50%

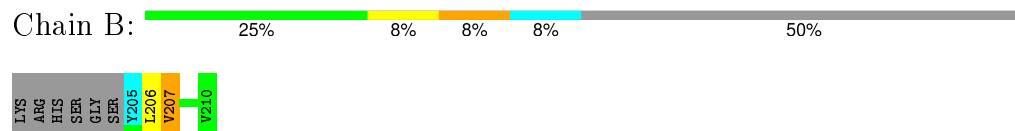
LYS
ARG
HIS
HIS
SER
GLY
SER
Y205
L206
V207
V210

4.2.33 Score per residue for model 33

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

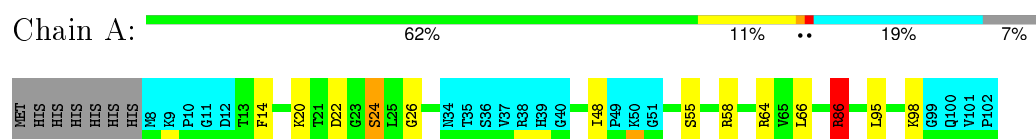


- Molecule 2: Adenomatous polyposis coli protein

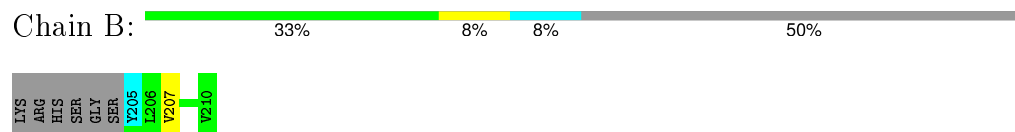


4.2.34 Score per residue for model 34

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)

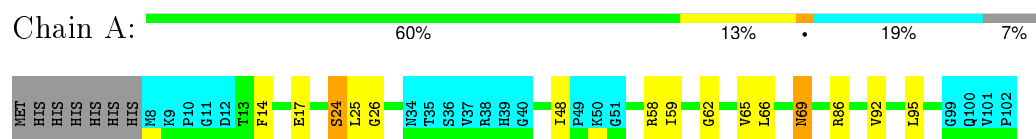


- Molecule 2: Adenomatous polyposis coli protein

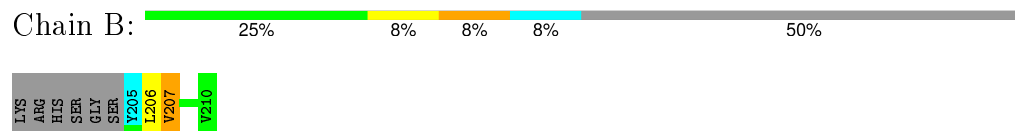


4.2.35 Score per residue for model 35

- Molecule 1: protein-tyrosine-phosphatase (nonreceptor type 13)



- Molecule 2: Adenomatous polyposis coli protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Initial calculations with XPLOR version 3.851, followed by restrained molecular dynamics protocol under a CHARMM22 forcefield..*

Of the 200 calculated structures, 35 were deposited, based on the following criterion: *structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.851
CHARMM	refinement	22

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 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 (average) 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	1.01±0.00	0±0/563 (0.0±0.0%)	1.18±0.03	2±1/762 (0.3±0.2%)
2	B	1.04±0.00	0±0/35 (0.0±0.0%)	1.43±0.09	0±0/46 (0.0±0.0%)
All	All	1.01	0/20930 (0.0%)	1.20	68/28280 (0.2%)

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	Planarity
1	A	0.0±0.0	0.8±0.7
All	All	0	29

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	ARG	NE-CZ-NH1	7.80	124.20	120.30	4	14
1	A	14	PHE	CB-CG-CD2	-7.48	115.56	120.80	25	1
1	A	64	ARG	NE-CZ-NH1	7.48	124.04	120.30	20	21
1	A	14	PHE	CB-CG-CD1	6.90	125.63	120.80	25	1
1	A	24	SER	N-CA-CB	6.60	120.40	110.50	34	5
1	A	86	ARG	NE-CZ-NH1	6.47	123.54	120.30	5	15
1	A	28	SER	N-CA-CB	5.97	119.45	110.50	5	1
1	A	86	ARG	CA-CB-CG	5.90	126.39	113.40	5	1
1	A	86	ARG	NE-CZ-NH2	-5.81	117.39	120.30	4	2
1	A	64	ARG	NE-CZ-NH2	-5.81	117.39	120.30	17	1
1	A	58	ARG	NE-CZ-NH2	-5.40	117.60	120.30	3	2
1	A	14	PHE	N-CA-CB	5.27	120.08	110.60	7	4

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	58	ARG	Sidechain	10
1	A	86	ARG	Sidechain	7
1	A	64	ARG	Sidechain	7
1	A	43	TYR	Sidechain	2
1	A	55	SER	Peptide	2
1	A	63	ASP	Peptide	1

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	558	580	579	2±1
2	B	36	41	41	0±0
All	All	20790	21735	21700	62

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:GLY:HA2	1:A:48:ILE:HD12	0.60	1.74	1	9
1:A:25:LEU:HD21	1:A:92:VAL:HG21	0.55	1.78	17	1
1:A:20:LYS:HB3	1:A:25:LEU:HD23	0.54	1.80	12	2
1:A:44:VAL:HG11	1:A:47:ILE:CD1	0.51	2.36	14	8
1:A:60:HIS:CG	1:A:61:LYS:H	0.50	2.25	18	7
1:A:17:GLU:HB2	1:A:93:HIS:CD2	0.49	2.43	14	1
1:A:44:VAL:HG11	1:A:47:ILE:HD13	0.47	1.87	28	7
1:A:25:LEU:CD2	1:A:92:VAL:HG21	0.47	2.40	17	3
2:B:206:LEU:HG	2:B:207:VAL:H	0.47	1.68	24	5
1:A:26:GLY:CA	1:A:48:ILE:HD12	0.46	2.40	35	7
1:A:60:HIS:CG	1:A:61:LYS:N	0.45	2.85	16	3
1:A:29:VAL:HG23	1:A:78:HIS:CE1	0.45	2.47	22	1
1:A:14:PHE:CE2	1:A:58:ARG:HB2	0.43	2.48	32	1
1:A:17:GLU:HB3	1:A:93:HIS:CD2	0.43	2.48	23	1
1:A:68:VAL:HG13	1:A:92:VAL:HG13	0.42	1.90	26	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:VAL:CG2	1:A:92:VAL:HG13	0.41	2.45	19	1
1:A:42:ILE:HG22	1:A:65:VAL:HG13	0.41	1.93	11	1

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	76/102 (75%)	65±2 (86±3%)	9±2 (12±3%)	2±1 (2±1%)	12	49
2	B	4/12 (33%)	2±0 (59±12%)	1±0 (15±12%)	1±0 (26±4%)	0	1
All	All	2800/3990 (70%)	2370 (85%)	330 (12%)	100 (4%)	7	36

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	207	VAL	35
1	A	56	ASP	18
1	A	62	GLY	17
1	A	24	SER	14
1	A	23	GLY	4
1	A	74	GLU	3
1	A	22	ASP	2
2	B	206	LEU	1
1	A	89	GLY	1
1	A	57	GLY	1
1	A	41	GLY	1
1	A	75	GLY	1
1	A	20	LYS	1
1	A	69	ASN	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	59/81 (73%)	51±2 (86±3%)	8±2 (14±3%)	8 48
2	B	5/11 (45%)	5±1 (90±11%)	0±1 (10±11%)	15 59
All	All	2240/3220 (70%)	1934 (86%)	306 (14%)	9 49

All 37 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	66	LEU	35
1	A	14	PHE	34
1	A	95	LEU	34
1	A	86	ARG	28
1	A	20	LYS	21
1	A	17	GLU	18
1	A	59	ILE	13
1	A	96	LEU	11
1	A	80	GLN	10
1	A	64	ARG	9
2	B	206	LEU	8
1	A	65	VAL	8
1	A	98	LYS	8
2	B	210	VAL	8
1	A	18	LEU	6
1	A	22	ASP	5
1	A	55	SER	5
1	A	45	LYS	5
1	A	15	GLU	4
1	A	13	THR	4
1	A	87	ASN	4
1	A	69	ASN	4
1	A	60	HIS	4
1	A	97	GLU	2
1	A	79	LYS	2
1	A	94	LEU	2
1	A	58	ARG	2
1	A	74	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	77	THR	2
1	A	90	GLN	1
1	A	78	HIS	1
1	A	25	LEU	1
1	A	56	ASP	1
1	A	54	GLU	1
1	A	16	VAL	1
2	B	207	VAL	1
1	A	92	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided