Full wwPDB NMR Structure Validation Report (i)

Mar 7, 2022 – 03:47 AM EST

PDB ID	:	3PDZ
Title	:	SOLUTION STRUCTURE OF THE PDZ2 DOMAIN FROM HUMAN PHOSPHATASE HPTP1E
Authors	:	Kozlov, G.; Gehring, K.; Ekiel, I.
Deposited on	:	1999-05-10

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

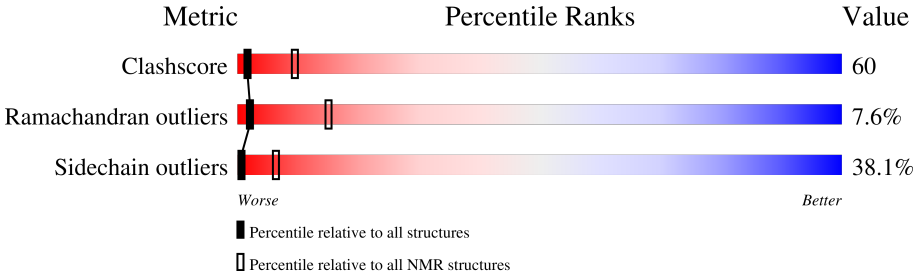
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	96	21% 48% 17% • 14%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 2 is the overall representative, medoid model (most similar to other models).

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:6-A:13, A:18-A:92 (83)	0.15	2

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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1426 atoms, of which 721 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1)).

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	96	1426	435	721	131	139	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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 (PTP-BAS, TYPE 1))

Chain A: 21% 48% 17% • 14%

P1 K2 P3 G4 D5 I6 F7 E8 V9 E10 L11 A12 K13 N14 D15 N16 S17 L18 G19 I20 S21 V22 T23 G24 G25 V26 V30 R31 H32 G33 G34 I35 Y36 V37 K38 A39 V40 I41 P42 Q43 G44 A45 A46 E47 S48 D49 G50 R51 I52 H53 K54 G55 D56 R57 V58 L59 A60 V61 N62

G63 V64 S65 L66 E67 G68 A69 T70 H71 K72 Q73 A74 V75 E76 T77 L78 R79 N80 T81 G82 Q83 V84 V85 H86 L87 L88 L89 E90 K91 G92 Q93 S94 P95 T96

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 (PTP-BAS, TYPE 1))

Chain A: 25% 41% 21% 14%

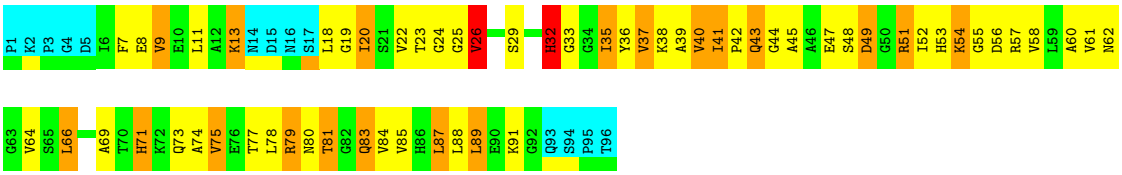
P1 K2 P3 G4 D5 I6 F7 E8 V9 E10 L11 A12 K13 N14 D15 N16 S17 L18 G19 I20 S21 V22 T23 G24 G25 V26 N27 T28 S29 V30 R31 I35 Y36 V37 K38 A39 V40 I41 P42 Q43 G44 A45 A46 E47 S48 D49 G50 R51 I52 H53 K54 G55 D56 R57 V58 L59 A60 V61 N62

G63 V64 S65 L66 E67 G68 A69 T70 H71 K72 Q73 A74 V75 E76 T77 L78 R79 N80 T81 G82 Q83 V84 V85 H86 L87 L88 L89 E90 K91 G92 Q93 S94 P95 T96

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

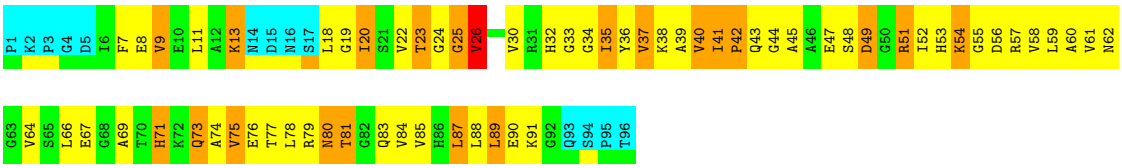
Chain A: 24% 41% 20% • 14%



4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

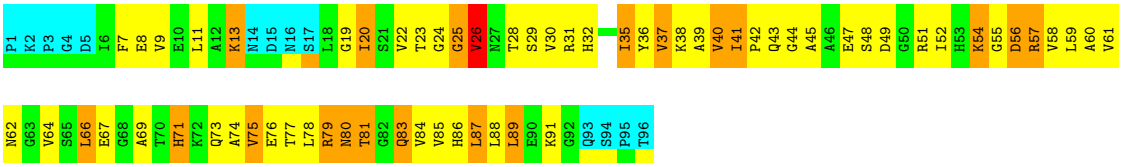
Chain A: 19% 46% 21% • 14%



4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

Chain A: 20% 46% 20% • 14%



4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

Chain A: 26% 41% 19% • 14%

4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

Chain A: 24% 41% 21% • 14%

P1 K2 P3 G4 D5 I6 F7 E8 V9 E10 L11 A12 K13 N14 D15 N16 S17 L18 G19 I20 S21 V22 T23 G24 G25 V26 R31 H32 I35 Y36 V37 K38 A39 V40 I41 P42 Q43 G44 A45 A46 E47 S48 D49 G50 R51 I52 H53 K54 G55 D56 R57 V58 L59 A60 V61 N62 G63 V64

S65 L66 E67 G68 A69 T70 H71 K72 Q73 A74 V75 E76 T77 L78 R79 N80 T81 G82 Q83 V84 V85 H86 L87 L88 L89 E90 K91 G92 Q93 S94 P95 T96

4.2.7 Score per residue for model 7

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

Chain A: 27% 40% 18% • 14%

P1 K2 P3 G4 D5 I6 F7 E8 V9 E10 L11 A12 K13 N14 D15 N16 S17 L18 G19 I20 S21 V22 T23 G24 G25 V26 N27 T28 S29 V30 R31 H32 G33 G34 I35 Y36 V37 K38 A39 V40 I41 P42 Q43 G44 A45 A46 E47 S48 D49 G50 R51 I52 H53 K54 G55 D56 R57 V58 L59 A60

V61 V64 S65 L66 E67 G68 A69 T70 H71 K72 Q73 A74 V75 E76 T77 L78 R79 N80 T81 G82 Q83 V84 V85 H86 L87 L88 L89 Q93 S94 P95 T96

4.2.8 Score per residue for model 8

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

Chain A: 25% 42% 20% 14%

P1 K2 P3 G4 D5 I6 F7 E8 V9 E10 L11 A12 K13 N14 D15 N16 S17 L18 G19 I20 S21 V22 T23 G24 G25 V26 N27 T28 S29 V30 G33 G34 I35 Y36 V37 K38 A39 V40 I41 P42 Q43 G44 A45 A46 E47 S48 D49 G50 R51 I52 H53 K54 G55 D56 R57 V58 L59 A60 V61

N62 G63 V64 S65 L66 E67 G68 A69 T70 H71 K72 Q73 A74 V75 E76 T77 L78 R79 N80 T81 G82 Q83 V84 V85 H86 L87 L88 L89 E90 K91 G92 Q93 S94 P95 T96

4.2.9 Score per residue for model 9

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

Chain A: 26% 39% 21% • 14%

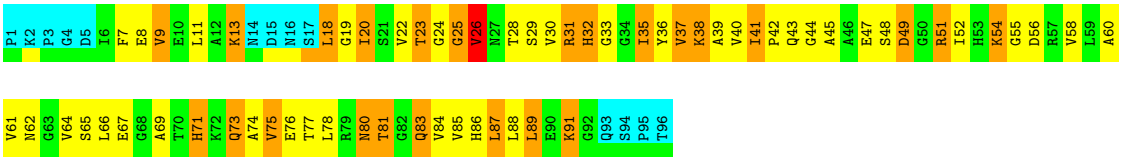
P1 K2 P3 G4 D5 I6 F7 E8 V9 E10 L11 A12 K13 N14 D15 N16 S17 L18 G19 I20 S21 V22 T23 G24 G25 V26 N27 T28 S29 V30 I35 Y36 V37 K38 A39 V40 I41 P42 Q43 G44 A45 A46 E47 S48 D49 G50 R51 I52 H53 K54 G55 D56 R57 V58 L59 A60 V61 N62 G63

V64 S65 L66 E67 G68 A69 T70 H71 K72 Q73 A74 V75 E76 T77 L78 R79 N80 T81 G82 Q83 V84 V85 H86 L87 L88 L89 E90 K91 G92 Q93 S94 P95 T96

4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

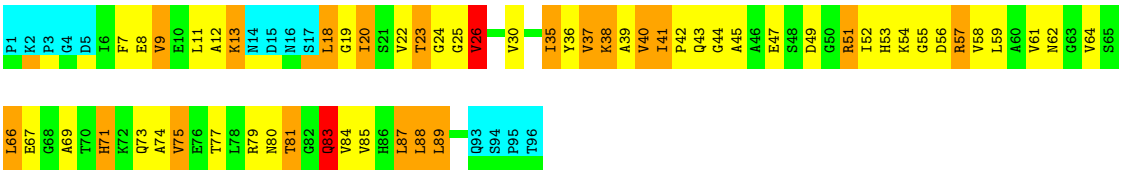
Chain A: 20% 41% 25% • 14%



4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

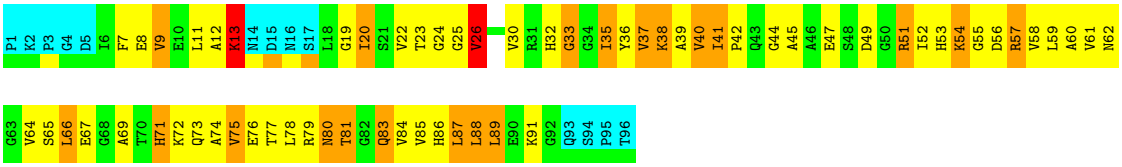
Chain A: 27% 38% 20% • 14%



4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

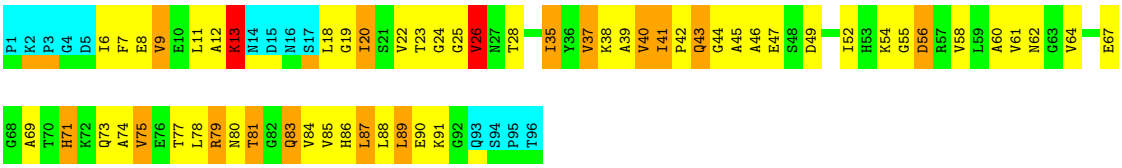
Chain A: 20% 44% 21% • 14%



4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

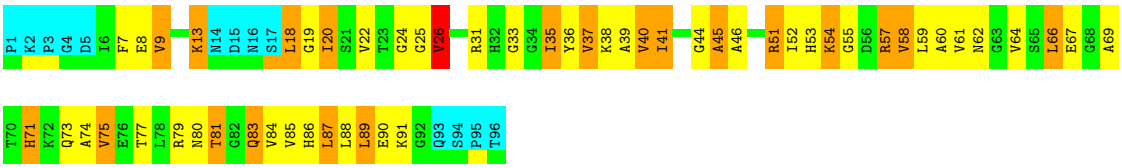
Chain A: 26% 43% 16% • 14%



4.2.14 Score per residue for model 14

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

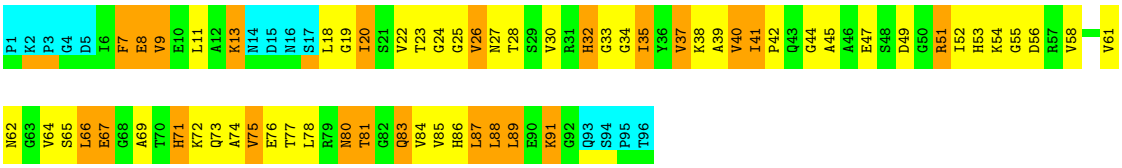
Chain A: 29% 35% 21% • 14%



4.2.15 Score per residue for model 15

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

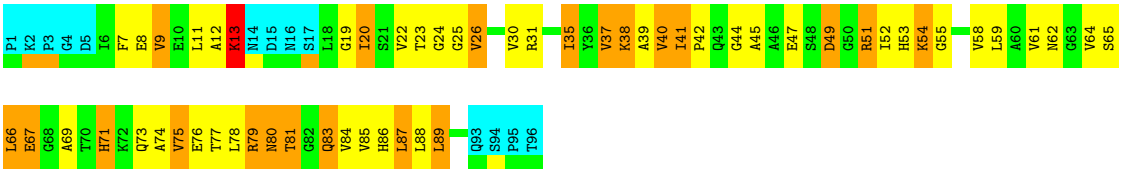
Chain A: 22% 41% 24% 14%



4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

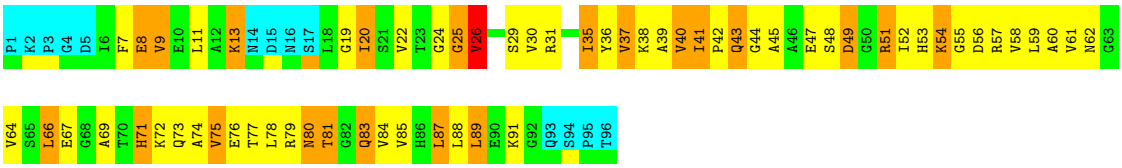
Chain A: 27% 36% 22% • 14%



4.2.17 Score per residue for model 17

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

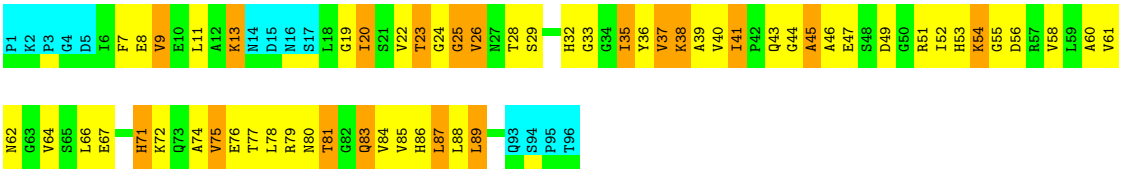
Chain A: 22% 42% 22% • 14%



4.2.18 Score per residue for model 18

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

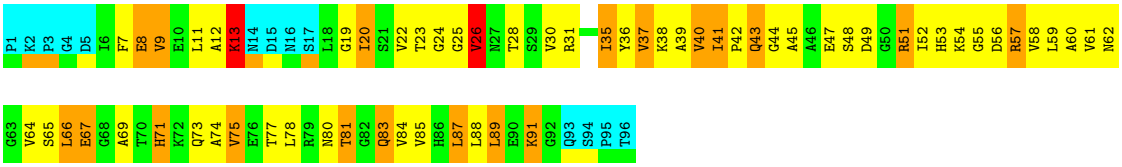
Chain A: 25% 43% 19% 14%



4.2.19 Score per residue for model 19

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

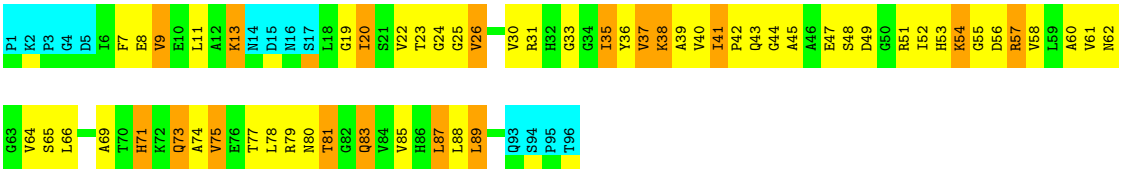
Chain A: 22% 43% 20% • 14%



4.2.20 Score per residue for model 20

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

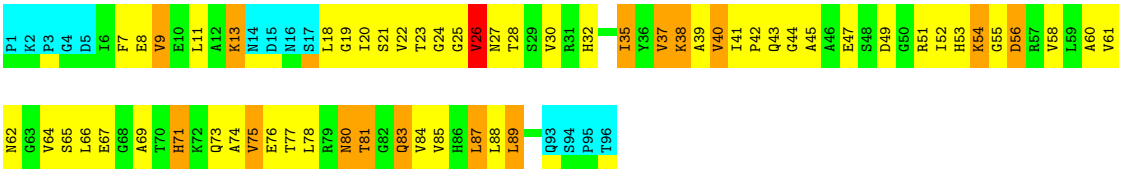
Chain A: 26% 43% 18% 14%



4.2.21 Score per residue for model 21

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

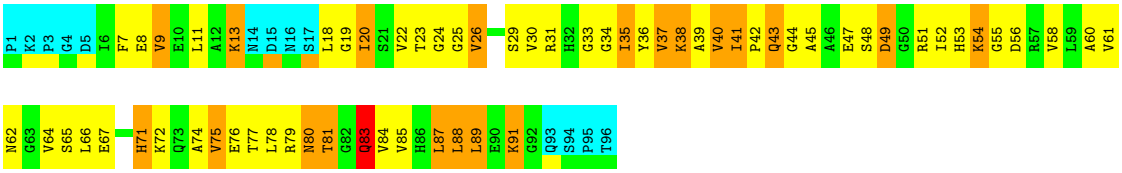
Chain A: 24% 46% 16% • 14%



4.2.22 Score per residue for model 22

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

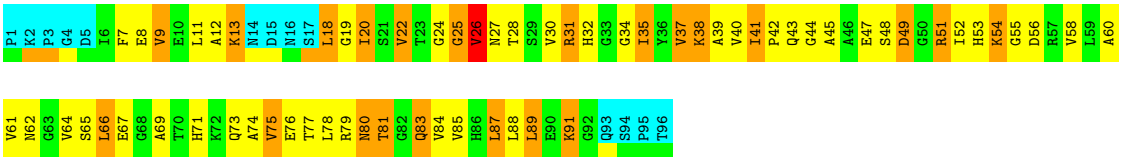
Chain A: 21% 44% 21% • 14%



4.2.23 Score per residue for model 23

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

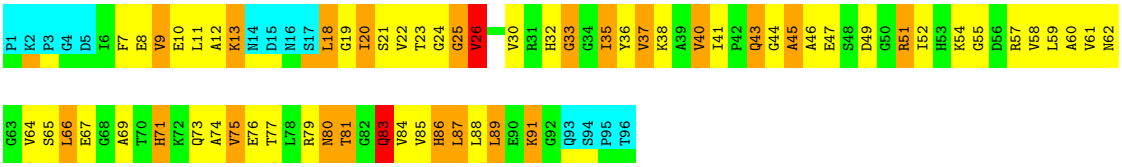
Chain A: 20% 43% 23% • 14%



4.2.24 Score per residue for model 24

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

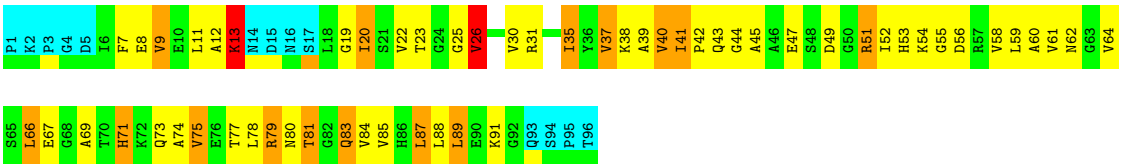
Chain A: 21% 42% 22% • 14%



4.2.25 Score per residue for model 25

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

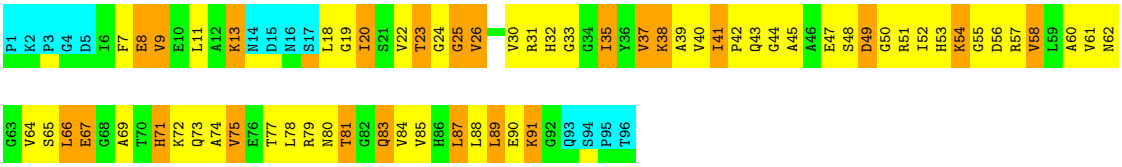
Chain A: 27% 42% 16% • 14%



4.2.26 Score per residue for model 26

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

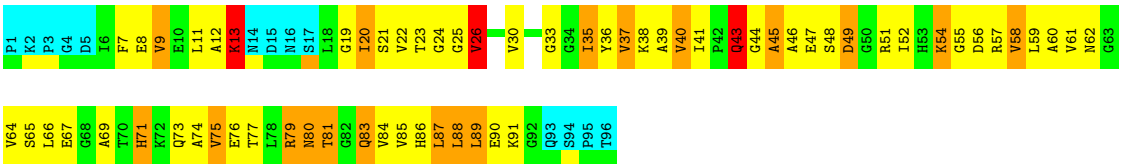
Chain A: 19% 44% 24% 14%



4.2.27 Score per residue for model 27

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

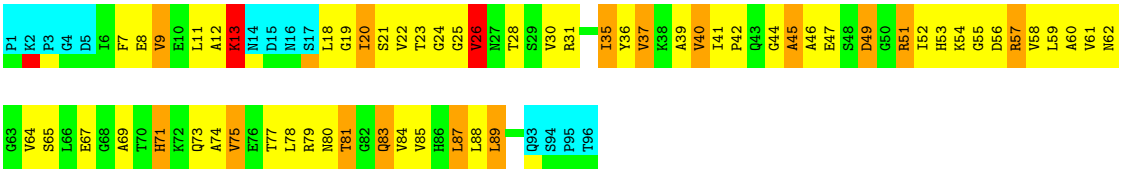
Chain A: 20% 45% 19% • 14%



4.2.28 Score per residue for model 28

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

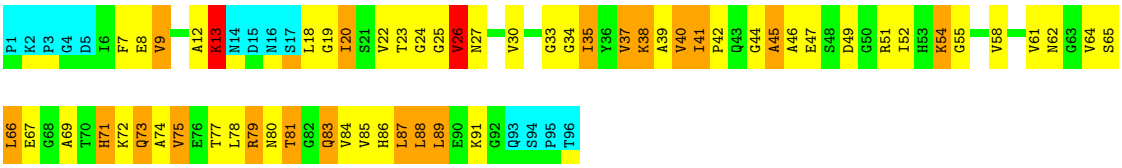
Chain A: 23% 46% 16% • 14%



4.2.29 Score per residue for model 29

• Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

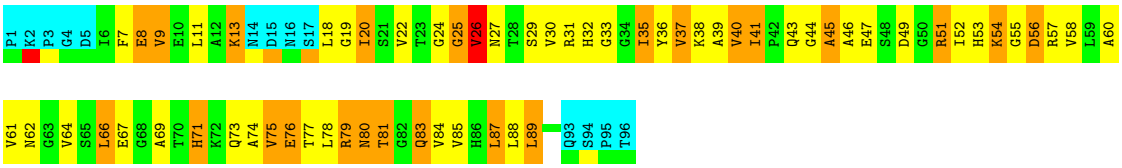
Chain A: 25% 40% 20% • 14%



4.2.30 Score per residue for model 30

- Molecule 1: PROTEIN (TYROSINE PHOSPHATASE (PTP-BAS, TYPE 1))

Chain A: 22% 40% 24% • 14%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 30 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
,RICE,SIMONSON,WARREN	refinement	
CNS	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 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	610	637	633	74±6
All	All	18300	19110	18990	2221

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 60.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HG22	1:A:58:VAL:HG22	0.94	1.38	27	30
1:A:22:VAL:HG21	1:A:75:VAL:HG23	0.89	1.42	14	25
1:A:7:PHE:CE1	1:A:89:LEU:HD12	0.86	2.06	26	22
1:A:35:ILE:HD12	1:A:74:ALA:HB3	0.85	1.45	17	7
1:A:22:VAL:CG2	1:A:75:VAL:HG23	0.82	2.05	26	30
1:A:35:ILE:CG2	1:A:58:VAL:HG22	0.82	2.04	22	30
1:A:61:VAL:HG11	1:A:77:THR:O	0.79	1.78	28	28
1:A:20:ILE:HG21	1:A:52:ILE:HG21	0.78	1.53	21	1
1:A:66:LEU:HD11	1:A:74:ALA:HB2	0.78	1.53	25	10
1:A:62:ASN:ND2	1:A:81:THR:HG22	0.78	1.93	30	25
1:A:58:VAL:HG12	1:A:89:LEU:HD22	0.78	1.55	22	6
1:A:61:VAL:HG23	1:A:66:LEU:HD11	0.78	1.56	4	2
1:A:37:VAL:HG22	1:A:55:GLY:N	0.76	1.95	20	30
1:A:11:LEU:HD13	1:A:51:ARG:CG	0.73	2.13	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:HD13	1:A:51:ARG:HG3	0.72	1.60	4	19
1:A:7:PHE:CZ	1:A:89:LEU:HD12	0.71	2.21	14	23
1:A:19:GLY:O	1:A:41:ILE:HB	0.71	1.84	17	30
1:A:61:VAL:HG21	1:A:77:THR:OG1	0.71	1.85	10	6
1:A:13:LYS:HB2	1:A:85:VAL:HG23	0.71	1.62	23	27
1:A:22:VAL:HG23	1:A:71:HIS:CD2	0.70	2.22	6	29
1:A:56:ASP:CG	1:A:89:LEU:HD13	0.69	2.08	20	2
1:A:8:GLU:CB	1:A:88:LEU:HD12	0.69	2.17	26	30
1:A:57:ARG:CD	1:A:59:LEU:HD21	0.69	2.17	9	4
1:A:60:ALA:HB3	1:A:88:LEU:HB2	0.69	1.63	21	17
1:A:57:ARG:HD2	1:A:59:LEU:HD21	0.68	1.65	12	6
1:A:35:ILE:HD13	1:A:36:TYR:N	0.68	2.04	27	4
1:A:61:VAL:HG21	1:A:78:LEU:HD23	0.67	1.66	9	17
1:A:58:VAL:CG1	1:A:89:LEU:HD22	0.67	2.19	22	2
1:A:58:VAL:HG23	1:A:66:LEU:HD13	0.67	1.67	24	4
1:A:13:LYS:CB	1:A:85:VAL:HG23	0.66	2.21	20	22
1:A:22:VAL:HG23	1:A:71:HIS:NE2	0.66	2.05	24	16
1:A:87:LEU:HB3	1:A:89:LEU:HD21	0.66	1.66	19	28
1:A:23:THR:O	1:A:36:TYR:O	0.66	2.13	3	3
1:A:85:VAL:O	1:A:85:VAL:HG12	0.66	1.91	19	30
1:A:8:GLU:HB2	1:A:88:LEU:HD12	0.66	1.67	26	22
1:A:19:GLY:HA3	1:A:44:GLY:HA3	0.65	1.67	16	28
1:A:20:ILE:HG12	1:A:39:ALA:O	0.65	1.92	17	28
1:A:69:ALA:HB1	1:A:73:GLN:HB3	0.65	1.69	9	12
1:A:58:VAL:HG21	1:A:78:LEU:HD21	0.64	1.70	23	11
1:A:22:VAL:HB	1:A:35:ILE:HD11	0.63	1.70	22	1
1:A:41:ILE:O	1:A:47:GLU:HB3	0.63	1.93	27	8
1:A:26:VAL:O	1:A:30:VAL:HG22	0.63	1.94	7	21
1:A:62:ASN:OD1	1:A:81:THR:HG22	0.63	1.94	17	4
1:A:8:GLU:HB3	1:A:88:LEU:HD12	0.63	1.70	11	19
1:A:69:ALA:HB1	1:A:73:GLN:CB	0.63	2.24	25	26
1:A:78:LEU:HD22	1:A:87:LEU:HD21	0.63	1.71	6	12
1:A:9:VAL:CG1	1:A:89:LEU:HD11	0.62	2.24	8	24
1:A:61:VAL:CG2	1:A:78:LEU:HD23	0.62	2.24	28	13
1:A:21:SER:CB	1:A:41:ILE:HD11	0.62	2.24	28	4
1:A:24:GLY:O	1:A:26:VAL:HG22	0.62	1.94	23	18
1:A:37:VAL:HG11	1:A:56:ASP:OD2	0.62	1.94	20	1
1:A:64:VAL:HG13	1:A:64:VAL:O	0.62	1.94	7	30
1:A:20:ILE:HD12	1:A:52:ILE:HB	0.62	1.72	23	3
1:A:18:LEU:N	1:A:18:LEU:HD22	0.61	2.11	14	16
1:A:69:ALA:HB1	1:A:73:GLN:CG	0.60	2.25	10	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ILE:HD13	1:A:41:ILE:N	0.60	2.09	5	4
1:A:20:ILE:HG21	1:A:52:ILE:CG2	0.60	2.25	21	1
1:A:56:ASP:OD1	1:A:58:VAL:HG12	0.59	1.97	20	1
1:A:61:VAL:HG23	1:A:66:LEU:CD1	0.59	2.28	30	2
1:A:9:VAL:HG23	1:A:51:ARG:CG	0.59	2.28	23	7
1:A:11:LEU:HD13	1:A:51:ARG:HB2	0.59	1.74	24	4
1:A:35:ILE:HG13	1:A:74:ALA:HB3	0.59	1.75	11	7
1:A:9:VAL:HG12	1:A:89:LEU:HD11	0.58	1.75	26	6
1:A:88:LEU:N	1:A:88:LEU:HD13	0.58	2.12	27	1
1:A:35:ILE:HG22	1:A:58:VAL:CG2	0.58	2.25	14	26
1:A:20:ILE:HD12	1:A:52:ILE:CG2	0.58	2.28	26	22
1:A:35:ILE:HG21	1:A:74:ALA:CB	0.58	2.28	22	3
1:A:20:ILE:CG2	1:A:22:VAL:HG12	0.58	2.28	23	5
1:A:41:ILE:CD1	1:A:41:ILE:N	0.58	2.66	14	25
1:A:61:VAL:HG11	1:A:77:THR:C	0.58	2.19	19	18
1:A:21:SER:HB3	1:A:41:ILE:HD11	0.57	1.73	5	4
1:A:20:ILE:HD13	1:A:37:VAL:HB	0.57	1.75	13	15
1:A:20:ILE:HD12	1:A:52:ILE:CG1	0.57	2.30	20	24
1:A:37:VAL:HG11	1:A:52:ILE:HG21	0.57	1.75	5	3
1:A:19:GLY:O	1:A:41:ILE:CB	0.57	2.53	24	4
1:A:87:LEU:HD22	1:A:89:LEU:CD2	0.57	2.30	20	25
1:A:30:VAL:HG21	1:A:34:GLY:O	0.56	2.00	3	2
1:A:20:ILE:HB	1:A:39:ALA:O	0.56	2.01	21	1
1:A:11:LEU:HD11	1:A:49:ASP:CB	0.56	2.30	3	27
1:A:11:LEU:HD13	1:A:51:ARG:HG2	0.55	1.76	5	1
1:A:35:ILE:HG22	1:A:58:VAL:HG13	0.55	1.79	20	1
1:A:37:VAL:O	1:A:55:GLY:N	0.55	2.39	28	26
1:A:38:LYS:HG3	1:A:39:ALA:N	0.55	2.15	14	2
1:A:37:VAL:CG2	1:A:54:LYS:HA	0.55	2.32	27	29
1:A:61:VAL:HG22	1:A:87:LEU:HD21	0.55	1.77	4	20
1:A:52:ILE:HG22	1:A:53:HIS:N	0.55	2.17	5	6
1:A:20:ILE:HG13	1:A:40:VAL:HG12	0.55	1.79	5	7
1:A:87:LEU:HD22	1:A:89:LEU:HD21	0.54	1.78	20	1
1:A:20:ILE:CG2	1:A:22:VAL:HG13	0.54	2.32	29	6
1:A:56:ASP:OD1	1:A:89:LEU:HD13	0.54	2.02	20	1
1:A:66:LEU:HD21	1:A:74:ALA:HA	0.54	1.80	6	5
1:A:61:VAL:HG22	1:A:87:LEU:CD2	0.54	2.33	30	10
1:A:61:VAL:CG2	1:A:66:LEU:HD11	0.54	2.32	30	2
1:A:42:PRO:HA	1:A:47:GLU:HG2	0.54	1.80	26	20
1:A:60:ALA:O	1:A:87:LEU:HD23	0.54	2.03	20	25
1:A:9:VAL:HG23	1:A:51:ARG:HG2	0.53	1.80	23	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LYS:NZ	1:A:18:LEU:HD22	0.53	2.18	23	1
1:A:42:PRO:HA	1:A:47:GLU:CG	0.53	2.34	4	20
1:A:37:VAL:HG11	1:A:52:ILE:CG2	0.53	2.34	23	5
1:A:64:VAL:O	1:A:64:VAL:CG1	0.53	2.57	19	30
1:A:78:LEU:HD22	1:A:87:LEU:HD11	0.52	1.81	18	4
1:A:20:ILE:HD12	1:A:52:ILE:HG12	0.52	1.82	24	12
1:A:74:ALA:HA	1:A:77:THR:OG1	0.52	2.05	6	2
1:A:20:ILE:HG22	1:A:40:VAL:HA	0.52	1.81	21	1
1:A:6:ILE:HD11	1:A:90:GLU:OE1	0.52	2.04	13	1
1:A:66:LEU:HD13	1:A:69:ALA:HB3	0.51	1.81	19	3
1:A:36:TYR:CE2	1:A:57:ARG:CG	0.51	2.92	30	3
1:A:58:VAL:CG2	1:A:58:VAL:O	0.51	2.58	20	24
1:A:61:VAL:HG21	1:A:77:THR:HB	0.51	1.83	6	2
1:A:61:VAL:HG22	1:A:87:LEU:CG	0.51	2.36	25	4
1:A:9:VAL:N	1:A:87:LEU:O	0.50	2.44	24	20
1:A:66:LEU:CD1	1:A:69:ALA:HB3	0.50	2.36	19	3
1:A:22:VAL:O	1:A:71:HIS:CE1	0.50	2.65	23	9
1:A:71:HIS:CD2	1:A:71:HIS:C	0.50	2.84	4	17
1:A:58:VAL:O	1:A:58:VAL:HG23	0.50	2.07	7	24
1:A:38:LYS:O	1:A:54:LYS:HG2	0.50	2.07	26	12
1:A:20:ILE:HG22	1:A:22:VAL:HG13	0.50	1.84	29	2
1:A:44:GLY:O	1:A:47:GLU:HG3	0.49	2.06	11	18
1:A:35:ILE:CG2	1:A:58:VAL:CG2	0.49	2.88	27	15
1:A:20:ILE:HD12	1:A:52:ILE:HG23	0.49	1.85	26	1
1:A:85:VAL:O	1:A:85:VAL:CG1	0.49	2.61	28	24
1:A:87:LEU:C	1:A:88:LEU:HD13	0.49	2.28	27	1
1:A:61:VAL:O	1:A:64:VAL:HG12	0.49	2.08	9	10
1:A:13:LYS:CA	1:A:85:VAL:HG23	0.49	2.38	21	8
1:A:69:ALA:HB1	1:A:73:GLN:CD	0.49	2.28	12	1
1:A:7:PHE:O	1:A:89:LEU:N	0.49	2.45	15	26
1:A:25:GLY:HA3	1:A:71:HIS:N	0.49	2.22	23	30
1:A:41:ILE:O	1:A:47:GLU:HG2	0.48	2.08	21	13
1:A:24:GLY:O	1:A:26:VAL:N	0.48	2.45	23	10
1:A:13:LYS:HZ1	1:A:18:LEU:HD22	0.48	1.68	23	1
1:A:19:GLY:O	1:A:41:ILE:N	0.48	2.46	24	5
1:A:66:LEU:HD11	1:A:74:ALA:CB	0.48	2.38	24	2
1:A:37:VAL:O	1:A:55:GLY:HA2	0.48	2.08	27	6
1:A:52:ILE:CG2	1:A:53:HIS:N	0.48	2.76	21	6
1:A:59:LEU:HD22	1:A:59:LEU:N	0.48	2.24	11	7
1:A:44:GLY:O	1:A:46:ALA:N	0.48	2.46	13	10
1:A:20:ILE:HG12	1:A:40:VAL:HA	0.48	1.84	13	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:HD12	1:A:52:ILE:CB	0.48	2.38	23	2
1:A:42:PRO:HA	1:A:47:GLU:OE1	0.48	2.09	29	2
1:A:61:VAL:HB	1:A:64:VAL:HG12	0.47	1.86	11	29
1:A:74:ALA:O	1:A:77:THR:N	0.47	2.47	29	30
1:A:87:LEU:CD2	1:A:89:LEU:CD2	0.47	2.92	28	28
1:A:53:HIS:N	1:A:56:ASP:OD2	0.47	2.47	2	9
1:A:57:ARG:NH1	1:A:59:LEU:HD11	0.47	2.24	3	3
1:A:58:VAL:CB	1:A:89:LEU:HD22	0.47	2.38	22	1
1:A:13:LYS:CG	1:A:13:LYS:O	0.47	2.63	23	4
1:A:8:GLU:CB	1:A:88:LEU:CD1	0.47	2.92	11	17
1:A:13:LYS:O	1:A:13:LYS:HD3	0.47	2.10	14	9
1:A:66:LEU:HD11	1:A:77:THR:OG1	0.47	2.09	20	1
1:A:58:VAL:O	1:A:58:VAL:CG2	0.47	2.62	7	4
1:A:57:ARG:HH11	1:A:59:LEU:HD11	0.47	1.69	19	1
1:A:21:SER:O	1:A:38:LYS:HB3	0.47	2.10	21	1
1:A:88:LEU:HD22	1:A:88:LEU:H	0.47	1.70	29	5
1:A:22:VAL:HG22	1:A:75:VAL:HG23	0.47	1.85	7	3
1:A:36:TYR:CZ	1:A:57:ARG:HG2	0.47	2.45	6	10
1:A:20:ILE:CG2	1:A:22:VAL:CG1	0.46	2.93	30	8
1:A:9:VAL:HG11	1:A:52:ILE:CD1	0.46	2.40	14	1
1:A:24:GLY:O	1:A:71:HIS:HB2	0.46	2.11	23	4
1:A:72:LYS:O	1:A:75:VAL:HG12	0.46	2.10	17	2
1:A:78:LEU:CD2	1:A:87:LEU:HD21	0.46	2.41	2	9
1:A:58:VAL:CG2	1:A:66:LEU:HD13	0.46	2.39	24	1
1:A:41:ILE:N	1:A:41:ILE:CD1	0.46	2.79	5	1
1:A:33:GLY:O	1:A:69:ALA:O	0.46	2.33	26	5
1:A:40:VAL:HG23	1:A:47:GLU:OE2	0.46	2.11	27	1
1:A:32:HIS:CD2	1:A:32:HIS:N	0.45	2.84	2	1
1:A:24:GLY:O	1:A:71:HIS:CB	0.45	2.64	21	16
1:A:20:ILE:CD1	1:A:52:ILE:CG2	0.45	2.94	3	2
1:A:11:LEU:HD21	1:A:45:ALA:O	0.45	2.10	21	1
1:A:76:GLU:O	1:A:80:ASN:HB2	0.45	2.11	17	8
1:A:37:VAL:CG2	1:A:53:HIS:O	0.45	2.65	20	6
1:A:76:GLU:O	1:A:80:ASN:N	0.45	2.47	10	1
1:A:41:ILE:O	1:A:43:GLN:N	0.45	2.50	9	14
1:A:11:LEU:HB3	1:A:85:VAL:HB	0.45	1.87	13	2
1:A:9:VAL:HG22	1:A:9:VAL:O	0.45	2.11	8	7
1:A:36:TYR:CZ	1:A:57:ARG:CG	0.45	3.00	28	2
1:A:19:GLY:CA	1:A:44:GLY:HA3	0.45	2.42	25	16
1:A:20:ILE:HD12	1:A:37:VAL:HB	0.45	1.89	21	1
1:A:61:VAL:HG21	1:A:77:THR:CB	0.44	2.43	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HA	1:A:87:LEU:HD11	0.44	1.87	2	1
1:A:25:GLY:O	1:A:26:VAL:C	0.44	2.55	27	18
1:A:66:LEU:HD21	1:A:77:THR:OG1	0.44	2.13	17	1
1:A:9:VAL:HG23	1:A:51:ARG:HB3	0.44	1.90	29	3
1:A:19:GLY:HA3	1:A:44:GLY:CA	0.44	2.42	18	10
1:A:20:ILE:CG1	1:A:40:VAL:HA	0.44	2.42	16	9
1:A:11:LEU:HD13	1:A:51:ARG:CD	0.44	2.42	23	3
1:A:30:VAL:HG11	1:A:34:GLY:O	0.44	2.12	22	3
1:A:32:HIS:CD2	1:A:33:GLY:N	0.44	2.85	24	1
1:A:84:VAL:HG12	1:A:85:VAL:N	0.44	2.26	23	21
1:A:18:LEU:HD22	1:A:18:LEU:H	0.44	1.72	30	2
1:A:23:THR:HA	1:A:71:HIS:ND1	0.44	2.27	26	3
1:A:21:SER:O	1:A:38:LYS:CB	0.44	2.66	21	1
1:A:7:PHE:CD1	1:A:7:PHE:C	0.44	2.91	4	12
1:A:71:HIS:CG	1:A:72:LYS:N	0.44	2.86	22	4
1:A:21:SER:O	1:A:38:LYS:HG2	0.44	2.13	21	1
1:A:59:LEU:O	1:A:66:LEU:N	0.44	2.51	25	1
1:A:36:TYR:CE2	1:A:57:ARG:HG2	0.44	2.48	5	4
1:A:56:ASP:OD1	1:A:58:VAL:CG1	0.44	2.66	20	1
1:A:11:LEU:HD11	1:A:49:ASP:HB2	0.43	1.89	22	4
1:A:9:VAL:CG2	1:A:51:ARG:HB3	0.43	2.43	22	4
1:A:11:LEU:HD11	1:A:49:ASP:HB3	0.43	1.88	5	1
1:A:23:THR:HA	1:A:71:HIS:CE1	0.43	2.48	24	3
1:A:84:VAL:CG1	1:A:85:VAL:N	0.43	2.81	7	28
1:A:9:VAL:HG11	1:A:89:LEU:HD11	0.43	1.88	8	3
1:A:53:HIS:O	1:A:56:ASP:HB2	0.43	2.13	22	2
1:A:88:LEU:HD22	1:A:88:LEU:N	0.43	2.28	22	2
1:A:20:ILE:CD1	1:A:52:ILE:HG23	0.43	2.43	26	1
1:A:69:ALA:HB1	1:A:73:GLN:HG2	0.43	1.89	10	1
1:A:43:GLN:N	1:A:47:GLU:HG2	0.43	2.29	2	14
1:A:7:PHE:C	1:A:7:PHE:CD1	0.43	2.92	1	8
1:A:20:ILE:HD13	1:A:37:VAL:CB	0.43	2.42	13	1
1:A:37:VAL:CG1	1:A:56:ASP:OD2	0.43	2.66	20	1
1:A:23:THR:HG22	1:A:38:LYS:HB2	0.43	1.91	5	1
1:A:37:VAL:HG22	1:A:55:GLY:H	0.43	1.74	21	3
1:A:23:THR:OG1	1:A:38:LYS:HB3	0.43	2.14	18	1
1:A:24:GLY:O	1:A:71:HIS:HB3	0.43	2.13	22	2
1:A:57:ARG:HD3	1:A:59:LEU:HD21	0.42	1.88	1	1
1:A:9:VAL:O	1:A:85:VAL:O	0.42	2.37	19	1
1:A:57:ARG:O	1:A:59:LEU:HD22	0.42	2.14	27	1
1:A:23:THR:OG1	1:A:38:LYS:CB	0.42	2.67	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:HG21	1:A:53:HIS:O	0.42	2.14	20	1
1:A:7:PHE:CZ	1:A:56:ASP:OD1	0.42	2.72	13	2
1:A:41:ILE:N	1:A:41:ILE:HD13	0.42	2.29	14	1
1:A:35:ILE:HG13	1:A:71:HIS:HA	0.42	1.91	8	3
1:A:59:LEU:N	1:A:59:LEU:CD2	0.42	2.83	16	2
1:A:59:LEU:HD12	1:A:67:GLU:HG3	0.42	1.91	16	1
1:A:88:LEU:N	1:A:88:LEU:CD1	0.42	2.82	27	1
1:A:30:VAL:CG1	1:A:36:TYR:CD1	0.42	3.03	5	1
1:A:36:TYR:CE2	1:A:57:ARG:HG3	0.42	2.50	30	1
1:A:35:ILE:HD13	1:A:36:TYR:H	0.42	1.72	3	1
1:A:51:ARG:O	1:A:53:HIS:CE1	0.42	2.73	12	2
1:A:61:VAL:HG22	1:A:87:LEU:HG	0.42	1.92	25	1
1:A:52:ILE:HD12	1:A:56:ASP:OD2	0.42	2.15	12	1
1:A:18:LEU:N	1:A:18:LEU:CD2	0.42	2.83	15	6
1:A:9:VAL:O	1:A:9:VAL:HG22	0.42	2.14	3	2
1:A:50:GLY:O	1:A:53:HIS:CE1	0.42	2.73	26	1
1:A:79:ARG:O	1:A:81:THR:N	0.41	2.53	20	16
1:A:13:LYS:HB3	1:A:83:GLN:O	0.41	2.15	22	1
1:A:13:LYS:HD3	1:A:13:LYS:O	0.41	2.15	24	2
1:A:66:LEU:CD2	1:A:74:ALA:CB	0.41	2.98	30	1
1:A:19:GLY:O	1:A:41:ILE:HG12	0.41	2.15	24	2
1:A:57:ARG:CD	1:A:59:LEU:CD2	0.41	2.96	9	1
1:A:76:GLU:O	1:A:80:ASN:CB	0.41	2.69	3	6
1:A:31:ARG:O	1:A:32:HIS:CD2	0.41	2.74	6	1
1:A:27:ASN:CB	1:A:32:HIS:O	0.41	2.68	15	4
1:A:20:ILE:HD12	1:A:52:ILE:HG21	0.41	1.93	17	2
1:A:57:ARG:NE	1:A:59:LEU:HD21	0.41	2.30	24	1
1:A:22:VAL:CG2	1:A:71:HIS:CD2	0.41	3.02	30	1
1:A:31:ARG:O	1:A:33:GLY:N	0.41	2.53	10	1
1:A:18:LEU:HD22	1:A:18:LEU:N	0.41	2.31	13	1
1:A:20:ILE:CB	1:A:39:ALA:O	0.41	2.69	21	1
1:A:47:GLU:OE1	1:A:47:GLU:C	0.41	2.59	29	1
1:A:58:VAL:HB	1:A:87:LEU:CD2	0.41	2.46	24	1
1:A:25:GLY:HA3	1:A:71:HIS:CA	0.40	2.47	10	1
1:A:30:VAL:HG11	1:A:36:TYR:CD1	0.40	2.51	12	1
1:A:10:GLU:OE1	1:A:86:HIS:CE1	0.40	2.74	24	1
1:A:11:LEU:O	1:A:85:VAL:N	0.40	2.48	25	1
1:A:41:ILE:C	1:A:47:GLU:CB	0.40	2.90	5	1
1:A:86:HIS:CE1	1:A:88:LEU:HD11	0.40	2.51	15	1
1:A:58:VAL:C	1:A:59:LEU:HD22	0.40	2.37	16	1
1:A:18:LEU:HD11	1:A:85:VAL:HG21	0.40	1.93	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:PRO:N	1:A:47:GLU:HG2	0.40	2.31	13	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	83/96 (86%)	57±2 (69±3%)	20±2 (24±3%)	6±2 (8±2%)	2 15
All	All	2490/2880 (86%)	1708 (69%)	592 (24%)	190 (8%)	2 15

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	26	VAL	30
1	A	80	ASN	30
1	A	83	GLN	28
1	A	67	GLU	26
1	A	91	LYS	13
1	A	25	GLY	12
1	A	33	GLY	11
1	A	45	ALA	10
1	A	13	LYS	10
1	A	32	HIS	9
1	A	24	GLY	3
1	A	31	ARG	2
1	A	43	GLN	2
1	A	42	PRO	1
1	A	92	GLY	1
1	A	18	LEU	1
1	A	30	VAL	1

6.3.2 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 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	64/76 (84%)	40±3 (62±4%)	24±3 (38±4%)	1 6
All	All	1920/2280 (84%)	1188 (62%)	732 (38%)	1 6

All 45 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	9	VAL	30
1	A	35	ILE	30
1	A	37	VAL	30
1	A	40	VAL	30
1	A	75	VAL	30
1	A	81	THR	30
1	A	83	GLN	30
1	A	87	LEU	30
1	A	89	LEU	30
1	A	13	LYS	29
1	A	20	ILE	29
1	A	71	HIS	29
1	A	38	LYS	28
1	A	66	LEU	26
1	A	41	ILE	25
1	A	26	VAL	23
1	A	54	LYS	22
1	A	23	THR	21
1	A	51	ARG	20
1	A	31	ARG	17
1	A	79	ARG	17
1	A	91	LYS	16
1	A	65	SER	16
1	A	49	ASP	15
1	A	56	ASP	15
1	A	28	THR	13
1	A	86	HIS	12
1	A	48	SER	12
1	A	57	ARG	11

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Mol	Chain	Res	Type	Models (Total)
1	A	29	SER	9
1	A	88	LEU	8
1	A	43	GLN	8
1	A	67	GLU	7
1	A	73	GLN	6
1	A	8	GLU	6
1	A	18	LEU	5
1	A	90	GLU	4
1	A	58	VAL	3
1	A	32	HIS	2
1	A	22	VAL	2
1	A	76	GLU	2
1	A	77	THR	1
1	A	7	PHE	1
1	A	72	LYS	1
1	A	27	ASN	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 monosaccharides 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 (i)

No chemical shift data were provided