Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 01:23 PM EST

PDB ID	:	1VFI
Title	:	Solution Structure of Vanabin2 (RUH-017), a Vanadium-binding Protein from Ascidia sydneiensis samea
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Deposited on	:	2004-04-13

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:

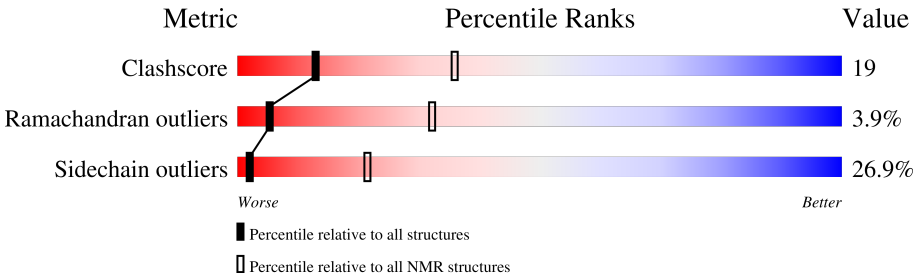
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	95	46% 43% • 6%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:7-A:95 (89)	0.83	9

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 12, 15, 16, 18, 19, 20
2	3, 4, 5, 6, 8, 9, 11
3	13, 14, 17
4	7, 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1391 atoms, of which 680 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called vanadium-binding protein 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1391	416	680	135	140	20	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ILE	-	cloning artifact	UNP Q86BW2
A	2	SER	-	cloning artifact	UNP Q86BW2
A	3	GLU	-	cloning artifact	UNP Q86BW2
A	4	PHE	-	cloning artifact	UNP Q86BW2

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: vanadium-binding protein 2

Chain A: 46% 43% • 6%

I1 S2 E3 F4 A5 P6 V7 D8 C9 K10 C13 T14 T15 P16 C17 E18 P19 L20 E25 K26 S30 S34 K37 K38 R41 R42 N43 C44 K45 E50 P51 C56 D57 A58 M61 K62 C63 H64 K65 A66 C67 R68 A69 A70 N71 C72 A73 S74 K78 H79

E80 H81 K82 T85 N93 C94 K95

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: vanadium-binding protein 2

Chain A: 57% 32% 5% 6%

I1 S2 E3 F4 A5 P6 K10 T14 T15 P16 C17 E18 P19 L20 E25 K26 C27 A28 E29 S30 C31 S34 K37 R42 K45 E50 P51 C56 D57 A58 C59 R60 M61 K62 C63 H64 A70 N71 C72 A73 S74 H81 T85 C86 R87 K91

C94 K95

4.2.2 Score per residue for model 2

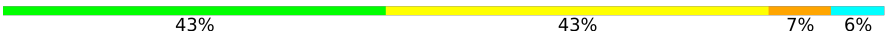
• Molecule 1: vanadium-binding protein 2

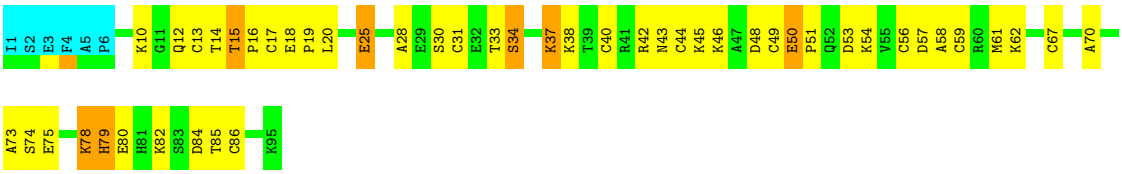
Chain A: 42% 41% 9% • 6%

4.2.3 Score per residue for model 3

- Molecule 1: vanadium-binding protein 2

Chain A:

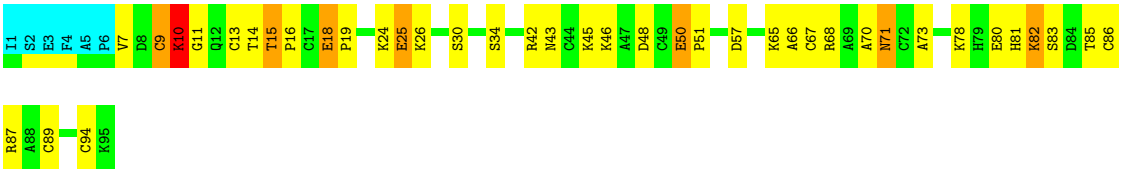




4.2.4 Score per residue for model 4

- Molecule 1: vanadium-binding protein 2

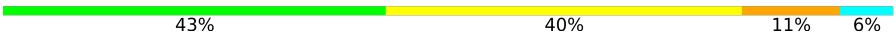
Chain A:

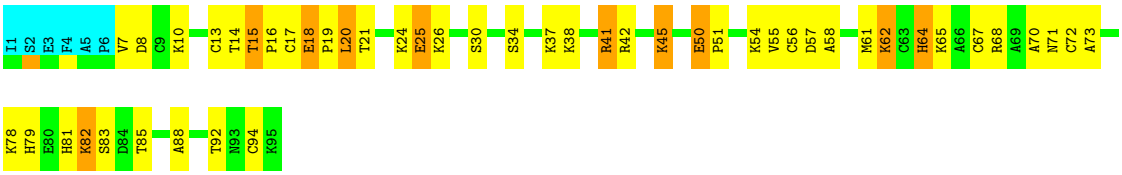


4.2.5 Score per residue for model 5

- Molecule 1: vanadium-binding protein 2

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: vanadium-binding protein 2

Chain A: 48% 35% 7% • 6%

I1 S2 E3 F4 A5 P6 V7 D8 C9 K10 C13 T14 T15 P16 C17 E18 P19 L20 T21 E25 K26 C27 A28 E29 S30 T33 S34 R42 N43 C44 K45 K46 A47 D48 C49 E50 P51 V55 C56 D57 A58 K62 K65 R68 A69 A70 A73 S74 H79 E80

H81 K82 S83 R87 K91 K95

4.2.7 Score per residue for model 7

- Molecule 1: vanadium-binding protein 2

Chain A: 38% 43% 13% 6%

I1 S2 E3 F4 A5 P6 V7 D8 C9 K10 G11 Q12 C13 T14 T15 P16 C17 E18 P19 L20 C23 K24 E25 K26 C27 A28 E29 S30 C31 E32 K38 R41 R42 K45 E50 P51 V55 C56 D57 A58 C59 R60 C63 H64 K65 A66 C67 R68 A69 A70 N71 C72 A73

S74 K78 H79 E80 H81 K82 T85 C86 R87 A88 C89 M90 K91 T92 N93 C94 K95

4.2.8 Score per residue for model 8

- Molecule 1: vanadium-binding protein 2

Chain A: 46% 36% 12% 6%

I1 S2 E3 F4 A5 P6 V7 K10 T14 T15 P16 C17 E18 P19 L20 T21 E25 K26 S30 C31 E32 T33 S34 K37 K38 R41 R42 K45 K46 E50 P51 K54 V55 C56 D57 A58 K62 A66 C67 R68 A69 A70 N71 C72 A73 S74 P77 K78

H79 E80 H81 K82 C86 R87 A88 C89 M90 K91 T92 N93 C94 K95

4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: vanadium-binding protein 2

Chain A: 46% 35% 12% • 6%

I1 S2 E3 F4 A5 P6 V7 D8 C13 T14 T15 P16 C17 E18 P19 L20 C23 K24 E25 K26 C27 S30 C31 E32 T33 S34 K37 K38 T39 C40 N43 C44 K45 D48 C49 E50 P51 Q52 D53 C56 M61 K62 C63 H64 C67 R68 A69 A70 N71 C72 A73

S74 E80 H81 K82 A88 T92 N93 C94 K95

4.2.10 Score per residue for model 10

- Molecule 1: vanadium-binding protein 2

Chain A: 46% 37% 9% • 6%

I1 S2 E3 F4 A5 P6 V7 D8 C9 K10 C13 T14 T15 P16 C17 E18 P19 L20 C23 K24 E25 K26 C27 S30 C31 C40 R41 R42 N43 C44 K45 K46 A47 D48 C49 E50 P51 C56 D57 R60 M61 K62 A66 A70 N71 C72 A73 S74 E75 C76 P77 K78

H79 E80 H81 K82 S83 D84 T85 C86 C89 K95

4.2.11 Score per residue for model 11

- Molecule 1: vanadium-binding protein 2

Chain A: 44% 40% 8% • 6%

I1 S2 E3 F4 A5 P6 V7 D8 C9 K10 G11 Q12 C13 T14 T15 P16 C17 E18 P19 L20 T21 K24 E25 K26 C27 S30 C31 S34 R42 N43 C44 K45 K46 A47 D48 C49 E50 P51 D57 A58 M61 K62 C63 H64 K65 A66 C67 A70 K78 H79 E80 H81

K82 S83 D84 T85 A88 K91 K95

4.2.12 Score per residue for model 12

- Molecule 1: vanadium-binding protein 2

Chain A: 47% 37% 9% 6%

I1 S2 E3 F4 A5 P6 V7 D8 C9 K10 T15 P16 C17 E18 P19 L20 C23 K24 E25 K26 C27 S30 C31 E32 K38 R41 R42 N43 C44 K45 K46 A47 D48 C49 E50 P51 Q52 D53 K54 V55 C56 D57 A58 K62 C63 A66 C67 R68 A69 A70 N71 E75

C76 P77 K78 H79 E80 H81 K82 N93 C94 K95

4.2.13 Score per residue for model 13

- Molecule 1: vanadium-binding protein 2

Chain A: 49% 36% 8% 6%

I1 S2 E3 F4 A5 P6 V7 K10 G11 Q12 C13 T14 T15 P16 C17 E18 P19 L20 T21 E25 K26 C27 A28 E29 S30 S34 K38 R42 N43 C44 K45 K46 A47 D48 C49 E50 P51 V55 C56 D57 A58 C59 K62 C63 H64 K65 A66 C67 R68 A69 A70 N71 C72

H79 K82 C89 M90 K95

4.2.14 Score per residue for model 14

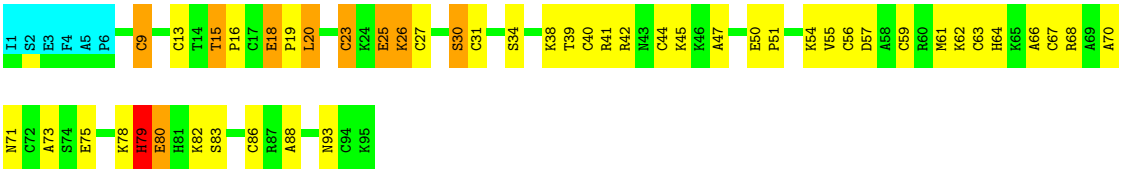
- Molecule 1: vanadium-binding protein 2

Chain A: 43% 42% 8% 6%

4.2.15 Score per residue for model 15

- Molecule 1: vanadium-binding protein 2

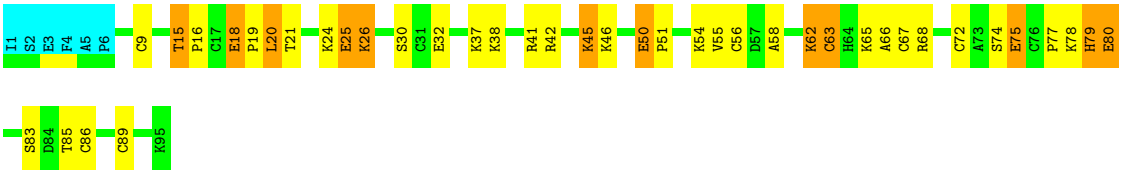
Chain A: 43% 40% 9% • 6%



4.2.16 Score per residue for model 16

- Molecule 1: vanadium-binding protein 2

Chain A: 51% 31% 13% 6%



4.2.17 Score per residue for model 17

- Molecule 1: vanadium-binding protein 2

Chain A: 46% 36% 12% 6%

4.2.18 Score per residue for model 18

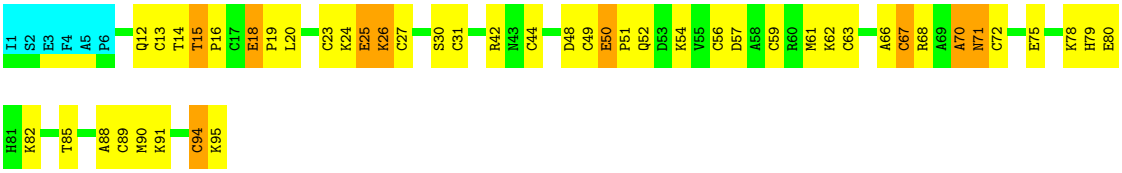
- Molecule 1: vanadium-binding protein 2

Chain A: 43% 38% 13% 6%

4.2.19 Score per residue for model 19

- Molecule 1: vanadium-binding protein 2

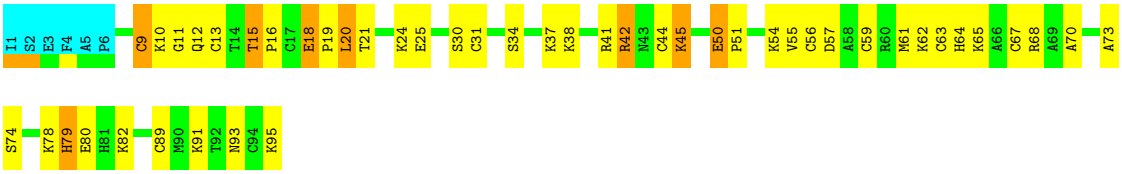
Chain A: 44% 40% 9% 6%



4.2.20 Score per residue for model 20

- Molecule 1: vanadium-binding protein 2

Chain A: 44% 41% 8% 6%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function*.

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

Software name	Classification	Version
KUJIRA	structure solution	0.8995
CYANA	structure solution	1.0.7
CYANA	refinement	1.0.7

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	665	637	637	24±4
All	All	13300	12740	12741	482

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:CYS:SG	1:A:13:CYS:SG	1.05	2.54	15	3
1:A:9:CYS:SG	1:A:59:CYS:SG	0.88	2.70	20	2
1:A:20:LEU:HD22	1:A:20:LEU:O	0.84	1.72	15	9
1:A:20:LEU:HD13	1:A:21:THR:N	0.82	1.90	6	8
1:A:43:ASN:O	1:A:47:ALA:HB2	0.78	1.78	10	2
1:A:51:PRO:O	1:A:55:VAL:HG23	0.74	1.83	14	6
1:A:67:CYS:O	1:A:70:ALA:HB3	0.70	1.87	13	6
1:A:20:LEU:HD22	1:A:20:LEU:C	0.68	2.09	17	6
1:A:55:VAL:O	1:A:58:ALA:HB3	0.68	1.89	13	4
1:A:20:LEU:C	1:A:20:LEU:HD22	0.67	2.09	20	3
1:A:13:CYS:CB	1:A:59:CYS:SG	0.65	2.84	19	1
1:A:13:CYS:CB	1:A:59:CYS:HG	0.65	2.05	19	1
1:A:44:CYS:SG	1:A:49:CYS:SG	0.64	2.95	19	3
1:A:20:LEU:HD12	1:A:56:CYS:SG	0.64	2.32	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:CYS:O	1:A:47:ALA:HB3	0.64	1.93	12	4
1:A:7:VAL:HG12	1:A:9:CYS:H	0.61	1.53	12	1
1:A:15:THR:N	1:A:16:PRO:CD	0.60	2.64	19	20
1:A:81:HIS:CD2	1:A:81:HIS:O	0.60	2.55	10	1
1:A:33:THR:HG23	1:A:33:THR:O	0.60	1.97	8	2
1:A:13:CYS:SG	1:A:59:CYS:CB	0.59	2.89	19	1
1:A:32:GLU:O	1:A:33:THR:HG22	0.58	1.99	14	1
1:A:20:LEU:O	1:A:20:LEU:HD22	0.57	2.00	16	1
1:A:67:CYS:HA	1:A:70:ALA:HB3	0.57	1.75	3	2
1:A:50:GLU:N	1:A:51:PRO:CD	0.57	2.68	15	20
1:A:7:VAL:HG11	1:A:67:CYS:HB2	0.56	1.77	2	1
1:A:32:GLU:O	1:A:33:THR:CB	0.56	2.54	14	1
1:A:20:LEU:HD22	1:A:56:CYS:HB2	0.56	1.75	19	2
1:A:7:VAL:HG21	1:A:67:CYS:HA	0.55	1.78	11	1
1:A:18:GLU:N	1:A:19:PRO:CD	0.54	2.70	19	19
1:A:63:CYS:O	1:A:66:ALA:HB3	0.54	2.03	16	4
1:A:72:CYS:O	1:A:73:ALA:HB3	0.53	2.02	10	1
1:A:20:LEU:HD13	1:A:53:ASP:HA	0.53	1.80	3	4
1:A:72:CYS:O	1:A:73:ALA:HB2	0.53	2.04	17	2
1:A:81:HIS:O	1:A:82:LYS:C	0.52	2.47	11	1
1:A:92:THR:HG22	1:A:93:ASN:OD1	0.51	2.05	9	1
1:A:20:LEU:HD13	1:A:20:LEU:C	0.51	2.25	6	1
1:A:63:CYS:O	1:A:67:CYS:CB	0.50	2.59	20	2
1:A:20:LEU:HD22	1:A:56:CYS:CB	0.50	2.37	18	5
1:A:45:LYS:CE	1:A:53:ASP:OD2	0.50	2.59	17	1
1:A:82:LYS:CG	1:A:82:LYS:O	0.50	2.59	11	2
1:A:66:ALA:O	1:A:70:ALA:CB	0.50	2.60	10	2
1:A:80:GLU:C	1:A:81:HIS:CD2	0.49	2.86	4	1
1:A:31:CYS:O	1:A:37:LYS:CD	0.49	2.60	20	1
1:A:31:CYS:O	1:A:37:LYS:CB	0.49	2.61	9	1
1:A:88:ALA:O	1:A:91:LYS:CB	0.49	2.61	2	3
1:A:17:CYS:HB3	1:A:20:LEU:HD12	0.49	1.84	11	1
1:A:32:GLU:O	1:A:33:THR:CG2	0.49	2.60	14	1
1:A:15:THR:N	1:A:16:PRO:HD2	0.49	2.23	19	20
1:A:78:LYS:O	1:A:79:HIS:CB	0.48	2.61	3	2
1:A:64:HIS:CD2	1:A:64:HIS:C	0.48	2.86	5	1
1:A:71:ASN:O	1:A:73:ALA:N	0.48	2.46	5	3
1:A:72:CYS:CB	1:A:76:CYS:SG	0.47	3.02	10	2
1:A:75:GLU:O	1:A:85:THR:CG2	0.47	2.62	19	1
1:A:20:LEU:HD13	1:A:53:ASP:CA	0.47	2.39	3	2
1:A:7:VAL:HG11	1:A:67:CYS:SG	0.47	2.49	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LYS:CG	1:A:11:GLY:N	0.47	2.77	20	1
1:A:8:ASP:O	1:A:10:LYS:N	0.47	2.47	10	4
1:A:85:THR:CG2	1:A:86:CYS:N	0.47	2.78	3	3
1:A:78:LYS:O	1:A:80:GLU:N	0.46	2.48	10	1
1:A:58:ALA:O	1:A:61:MET:N	0.46	2.48	18	3
1:A:40:CYS:O	1:A:44:CYS:N	0.46	2.49	10	2
1:A:90:MET:O	1:A:94:CYS:N	0.46	2.49	7	1
1:A:65:LYS:O	1:A:68:ARG:N	0.45	2.50	7	2
1:A:18:GLU:CB	1:A:19:PRO:HD3	0.45	2.41	11	9
1:A:81:HIS:O	1:A:82:LYS:CB	0.45	2.62	5	1
1:A:14:THR:O	1:A:18:GLU:N	0.45	2.50	3	12
1:A:72:CYS:SG	1:A:90:MET:N	0.45	2.90	19	1
1:A:43:ASN:O	1:A:46:LYS:N	0.45	2.50	13	3
1:A:66:ALA:O	1:A:70:ALA:N	0.45	2.50	11	6
1:A:41:ARG:O	1:A:45:LYS:N	0.45	2.50	8	5
1:A:9:CYS:O	1:A:13:CYS:N	0.45	2.50	6	2
1:A:56:CYS:O	1:A:59:CYS:N	0.45	2.50	13	5
1:A:68:ARG:O	1:A:72:CYS:C	0.45	2.55	5	3
1:A:87:ARG:O	1:A:91:LYS:N	0.45	2.50	8	2
1:A:56:CYS:SG	1:A:60:ARG:CZ	0.45	3.05	7	2
1:A:89:CYS:O	1:A:93:ASN:ND2	0.45	2.49	7	1
1:A:54:LYS:O	1:A:57:ASP:N	0.45	2.50	19	3
1:A:93:ASN:O	1:A:95:LYS:N	0.45	2.50	18	3
1:A:64:HIS:NE2	1:A:95:LYS:C	0.45	2.70	18	1
1:A:25:GLU:O	1:A:28:ALA:N	0.45	2.49	2	3
1:A:58:ALA:O	1:A:62:LYS:N	0.45	2.49	11	5
1:A:88:ALA:O	1:A:92:THR:N	0.45	2.49	5	2
1:A:50:GLU:N	1:A:51:PRO:HD2	0.45	2.27	12	18
1:A:40:CYS:O	1:A:43:ASN:N	0.45	2.49	9	1
1:A:90:MET:O	1:A:95:LYS:N	0.45	2.50	14	1
1:A:58:ALA:HB1	1:A:62:LYS:HE2	0.45	1.89	16	1
1:A:27:CYS:O	1:A:31:CYS:N	0.45	2.50	2	6
1:A:41:ARG:O	1:A:44:CYS:N	0.45	2.50	2	5
1:A:86:CYS:O	1:A:89:CYS:N	0.45	2.50	14	5
1:A:79:HIS:O	1:A:81:HIS:N	0.45	2.49	10	2
1:A:20:LEU:HD22	1:A:56:CYS:HB3	0.45	1.87	18	2
1:A:9:CYS:CB	1:A:13:CYS:SG	0.45	3.05	15	1
1:A:63:CYS:O	1:A:67:CYS:N	0.44	2.49	20	2
1:A:20:LEU:O	1:A:23:CYS:N	0.44	2.50	7	2
1:A:67:CYS:O	1:A:70:ALA:N	0.44	2.51	15	2
1:A:9:CYS:O	1:A:11:GLY:N	0.44	2.50	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:CYS:C	1:A:58:ALA:N	0.44	2.70	3	2
1:A:7:VAL:HG23	1:A:71:ASN:ND2	0.44	2.28	4	1
1:A:57:ASP:O	1:A:61:MET:N	0.44	2.49	1	5
1:A:59:CYS:O	1:A:62:LYS:N	0.44	2.50	2	1
1:A:90:MET:O	1:A:94:CYS:CA	0.44	2.65	7	1
1:A:27:CYS:O	1:A:30:SER:N	0.44	2.51	14	3
1:A:34:SER:O	1:A:36:ASP:N	0.44	2.51	2	1
1:A:20:LEU:CD1	1:A:21:THR:N	0.44	2.76	6	1
1:A:18:GLU:N	1:A:19:PRO:HD2	0.44	2.28	19	6
1:A:79:HIS:O	1:A:80:GLU:CB	0.44	2.65	15	2
1:A:89:CYS:O	1:A:93:ASN:N	0.43	2.50	20	1
1:A:31:CYS:O	1:A:37:LYS:CG	0.43	2.67	3	2
1:A:64:HIS:CE1	1:A:90:MET:CE	0.43	3.01	13	1
1:A:87:ARG:O	1:A:91:LYS:CB	0.43	2.67	6	2
1:A:54:LYS:C	1:A:56:CYS:N	0.43	2.70	15	4
1:A:45:LYS:O	1:A:49:CYS:N	0.43	2.52	10	1
1:A:63:CYS:O	1:A:66:ALA:N	0.43	2.51	16	2
1:A:90:MET:O	1:A:94:CYS:C	0.43	2.57	17	2
1:A:80:GLU:OE1	1:A:83:SER:N	0.43	2.50	11	1
1:A:20:LEU:CD2	1:A:56:CYS:SG	0.43	3.07	19	1
1:A:85:THR:HG23	1:A:86:CYS:N	0.43	2.29	3	1
1:A:88:ALA:O	1:A:91:LYS:N	0.43	2.51	7	1
1:A:54:LYS:O	1:A:56:CYS:N	0.43	2.51	15	1
1:A:67:CYS:O	1:A:71:ASN:N	0.42	2.51	2	2
1:A:62:LYS:O	1:A:66:ALA:N	0.42	2.49	10	2
1:A:14:THR:O	1:A:18:GLU:CB	0.42	2.67	19	1
1:A:56:CYS:O	1:A:58:ALA:N	0.42	2.53	3	1
1:A:54:LYS:O	1:A:55:VAL:C	0.42	2.58	15	3
1:A:16:PRO:CG	1:A:59:CYS:SG	0.42	3.08	18	2
1:A:75:GLU:N	1:A:75:GLU:CD	0.42	2.73	12	1
1:A:9:CYS:O	1:A:10:LYS:C	0.42	2.58	6	5
1:A:56:CYS:O	1:A:57:ASP:C	0.42	2.58	15	3
1:A:7:VAL:CG1	1:A:67:CYS:SG	0.42	3.08	13	1
1:A:86:CYS:C	1:A:88:ALA:N	0.42	2.72	15	1
1:A:20:LEU:C	1:A:20:LEU:CD2	0.42	2.83	17	2
1:A:33:THR:OG1	1:A:34:SER:N	0.42	2.52	3	1
1:A:25:GLU:O	1:A:26:LYS:C	0.42	2.59	6	16
1:A:43:ASN:O	1:A:47:ALA:N	0.41	2.53	6	1
1:A:78:LYS:HE3	1:A:79:HIS:CE1	0.41	2.50	10	1
1:A:68:ARG:O	1:A:72:CYS:O	0.41	2.38	5	3
1:A:45:LYS:O	1:A:49:CYS:CA	0.41	2.68	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ARG:O	1:A:45:LYS:N	0.41	2.53	20	1
1:A:11:GLY:C	1:A:13:CYS:N	0.41	2.73	4	2
1:A:91:LYS:C	1:A:93:ASN:N	0.41	2.74	7	1
1:A:33:THR:O	1:A:33:THR:CG2	0.41	2.67	8	1
1:A:56:CYS:SG	1:A:60:ARG:NH1	0.41	2.93	7	1
1:A:86:CYS:O	1:A:87:ARG:C	0.41	2.59	7	1
1:A:25:GLU:O	1:A:28:ALA:HB3	0.41	2.14	13	1
1:A:59:CYS:O	1:A:63:CYS:N	0.41	2.49	2	1
1:A:62:LYS:O	1:A:63:CYS:C	0.41	2.59	14	2
1:A:41:ARG:O	1:A:44:CYS:CB	0.41	2.69	12	1
1:A:55:VAL:O	1:A:58:ALA:CB	0.41	2.65	17	1
1:A:13:CYS:HB2	1:A:59:CYS:SG	0.41	2.56	19	1
1:A:27:CYS:O	1:A:28:ALA:C	0.41	2.60	1	2
1:A:13:CYS:O	1:A:17:CYS:SG	0.41	2.79	11	5
1:A:55:VAL:O	1:A:56:CYS:C	0.41	2.59	17	2
1:A:39:THR:O	1:A:43:ASN:N	0.41	2.52	9	1
1:A:63:CYS:O	1:A:64:HIS:C	0.41	2.59	9	1
1:A:45:LYS:O	1:A:49:CYS:C	0.41	2.59	17	2
1:A:23:CYS:O	1:A:27:CYS:SG	0.41	2.79	12	2
1:A:12:GLN:O	1:A:13:CYS:SG	0.41	2.79	17	2
1:A:86:CYS:O	1:A:88:ALA:N	0.41	2.53	15	1
1:A:36:ASP:O	1:A:37:LYS:C	0.40	2.60	2	1
1:A:10:LYS:O	1:A:13:CYS:N	0.40	2.54	6	1
1:A:39:THR:O	1:A:40:CYS:C	0.40	2.59	15	1
1:A:70:ALA:O	1:A:71:ASN:C	0.40	2.60	1	1
1:A:87:ARG:HB3	1:A:87:ARG:CZ	0.40	2.46	14	2
1:A:71:ASN:OD1	1:A:94:CYS:SG	0.40	2.80	9	1
1:A:57:ASP:O	1:A:58:ALA:C	0.40	2.60	12	1
1:A:19:PRO:O	1:A:52:GLN:CD	0.40	2.60	19	1
1:A:20:LEU:O	1:A:23:CYS:CB	0.40	2.69	10	1
1:A:94:CYS:O	1:A:95:LYS:C	0.40	2.60	18	1
1:A:16:PRO:CG	1:A:59:CYS:HB2	0.40	2.47	1	2
1:A:7:VAL:O	1:A:8:ASP:C	0.40	2.59	2	1
1:A:44:CYS:O	1:A:49:CYS:SG	0.40	2.79	3	1
1:A:89:CYS:SG	1:A:93:ASN:ND2	0.40	2.94	8	1
1:A:50:GLU:CB	1:A:51:PRO:HD3	0.40	2.46	10	1
1:A:23:CYS:SG	1:A:52:GLN:OE1	0.40	2.80	19	1
1:A:66:ALA:O	1:A:69:ALA:N	0.40	2.50	8	1
1:A:67:CYS:O	1:A:70:ALA:CB	0.40	2.67	13	1
1:A:7:VAL:HG12	1:A:8:ASP:N	0.40	2.31	14	1
1:A:74:SER:O	1:A:75:GLU:C	0.40	2.59	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:VAL:O	1:A:8:ASP:CB	0.40	2.69	18	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	88/95 (93%)	61±3 (70±4%)	23±4 (26±4%)	3±1 (4±2%)	5	32
All	All	1760/1900 (93%)	1228 (70%)	464 (26%)	68 (4%)	5	32

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	73	ALA	10
1	A	79	HIS	9
1	A	48	ASP	8
1	A	70	ALA	7
1	A	80	GLU	6
1	A	8	ASP	5
1	A	82	LYS	4
1	A	10	LYS	3
1	A	7	VAL	3
1	A	77	PRO	3
1	A	9	CYS	2
1	A	81	HIS	2
1	A	94	CYS	2
1	A	35	ALA	1
1	A	34	SER	1
1	A	72	CYS	1
1	A	75	GLU	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	78/83 (94%)	57±3 (73±3%)	21±3 (27±3%)	2 21
All	All	1560/1660 (94%)	1141 (73%)	419 (27%)	2 21

All 51 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	15	THR	20
1	A	30	SER	20
1	A	25	GLU	19
1	A	62	LYS	17
1	A	18	GLU	16
1	A	42	ARG	16
1	A	45	LYS	16
1	A	50	GLU	16
1	A	34	SER	14
1	A	38	LYS	14
1	A	82	LYS	14
1	A	78	LYS	13
1	A	95	LYS	12
1	A	10	LYS	11
1	A	26	LYS	11
1	A	74	SER	11
1	A	68	ARG	11
1	A	79	HIS	11
1	A	80	GLU	11
1	A	24	LYS	10
1	A	20	LEU	10
1	A	65	LYS	9
1	A	83	SER	9
1	A	61	MET	8
1	A	64	HIS	8
1	A	37	LYS	7
1	A	85	THR	7
1	A	12	GLN	7
1	A	94	CYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	57	ASP	6
1	A	46	LYS	6
1	A	71	ASN	6
1	A	32	GLU	5
1	A	9	CYS	5
1	A	93	ASN	4
1	A	63	CYS	4
1	A	8	ASP	3
1	A	67	CYS	3
1	A	75	GLU	3
1	A	91	LYS	3
1	A	89	CYS	3
1	A	81	HIS	2
1	A	43	ASN	2
1	A	41	ARG	2
1	A	7	VAL	2
1	A	40	CYS	1
1	A	84	ASP	1
1	A	54	LYS	1
1	A	33	THR	1
1	A	36	ASP	1
1	A	23	CYS	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