



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 09:00 pm BST

PDB ID : 1XN5
Title : Solution Structure of Bacillus halodurans Protein BH1534: The Northeast Structural Genomics Consortium Target BhR29
Authors : Liu, G.; Ma, L.; Shen, Y.; Acton, T.; Atreya, H.S.; Xiao, R.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-10-04

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 ⓘ 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
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

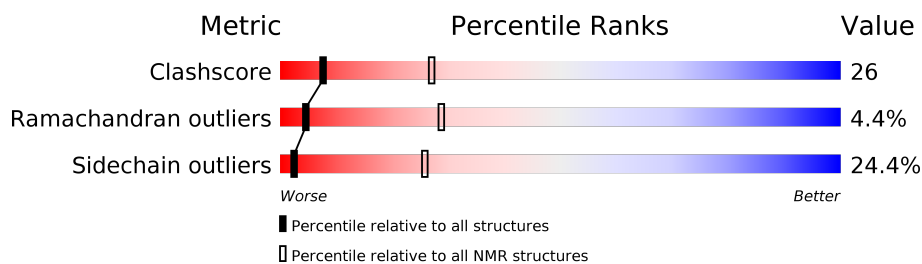
1 Overall quality at a glance i

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	146	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:73, A:78-A:98, A:121-A:138 (106)	0.19	4

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 3 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2199 atoms, of which 1075 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BH1534 unknown conserved protein.

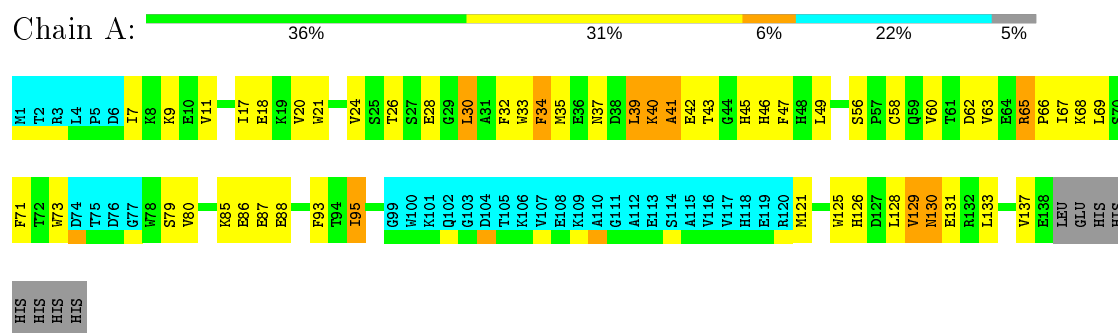
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	138	2199	714	1075	196	210	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	LEU	-	EXPRESSION TAG	UNP Q9KCN5
A	140	GLU	-	EXPRESSION TAG	UNP Q9KCN5
A	141	HIS	-	EXPRESSION TAG	UNP Q9KCN5
A	142	HIS	-	EXPRESSION TAG	UNP Q9KCN5
A	143	HIS	-	EXPRESSION TAG	UNP Q9KCN5
A	144	HIS	-	EXPRESSION TAG	UNP Q9KCN5
A	145	HIS	-	EXPRESSION TAG	UNP Q9KCN5
A	146	HIS	-	EXPRESSION TAG	UNP Q9KCN5

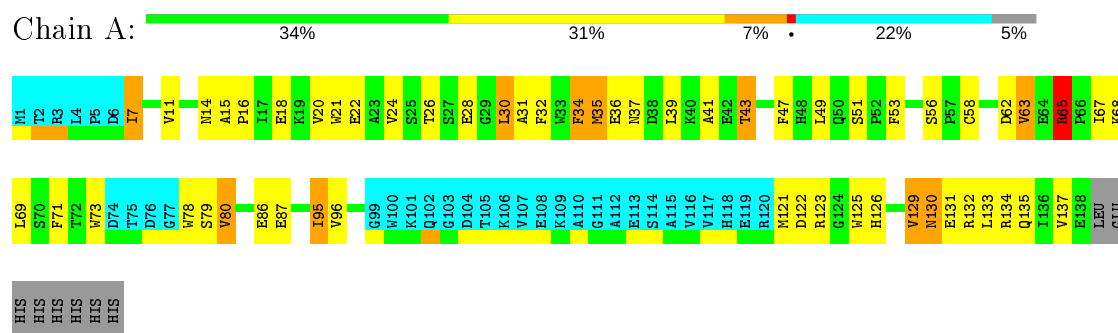
4.2.5 Score per residue for model 5

- Molecule 1: BH1534 unknown conserved protein



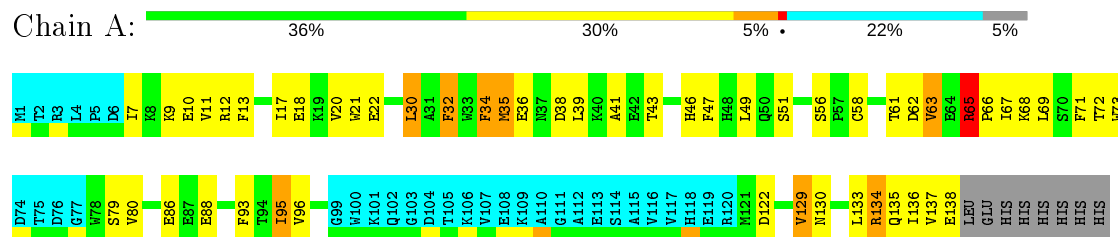
4.2.6 Score per residue for model 6

- Molecule 1: BH1534 unknown conserved protein



4.2.7 Score per residue for model 7

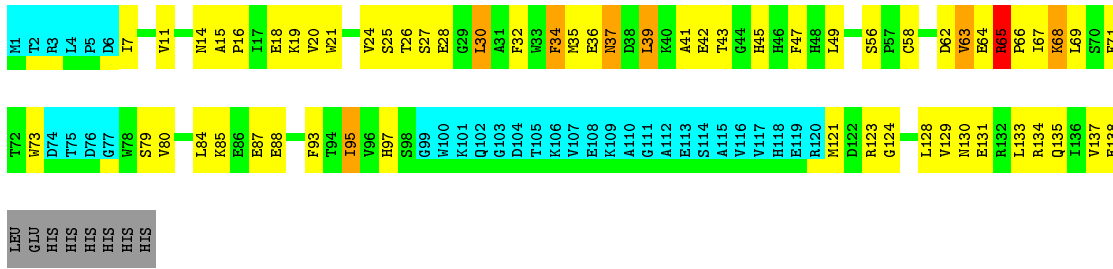
- Molecule 1: BH1534 unknown conserved protein



4.2.8 Score per residue for model 8

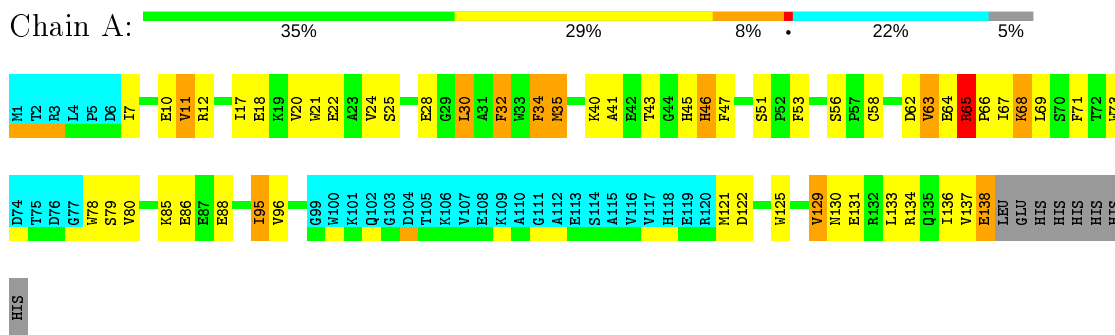
- Molecule 1: BH1534 unknown conserved protein





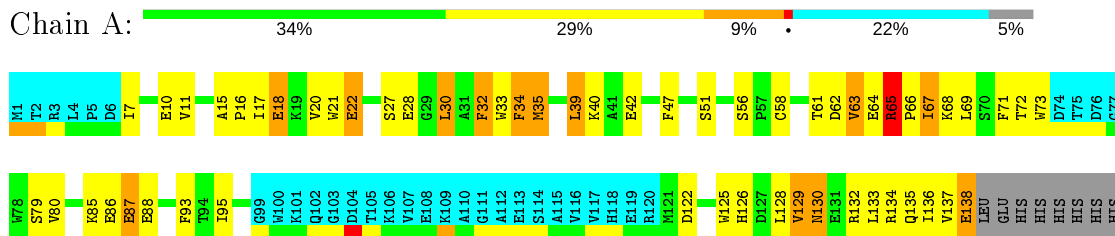
4.2.9 Score per residue for model 9

- Molecule 1: BH1534 unknown conserved protein



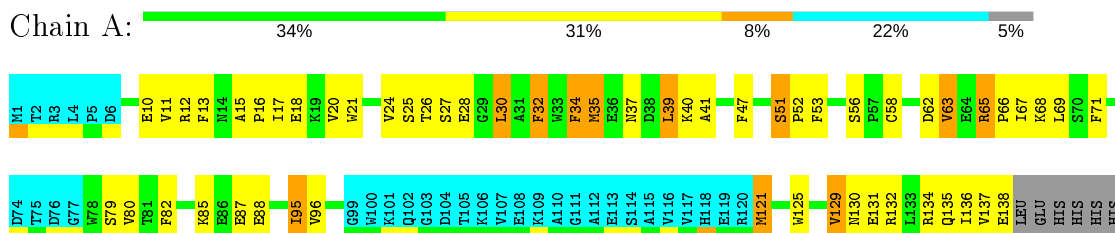
4.2.10 Score per residue for model 10

- Molecule 1: BH1534 unknown conserved protein



4.2.11 Score per residue for model 11

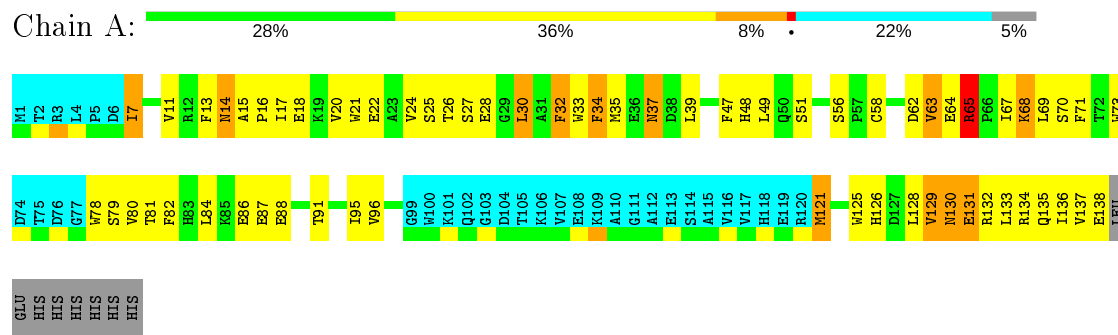
- Molecule 1: BH1534 unknown conserved protein



HIS
HIS

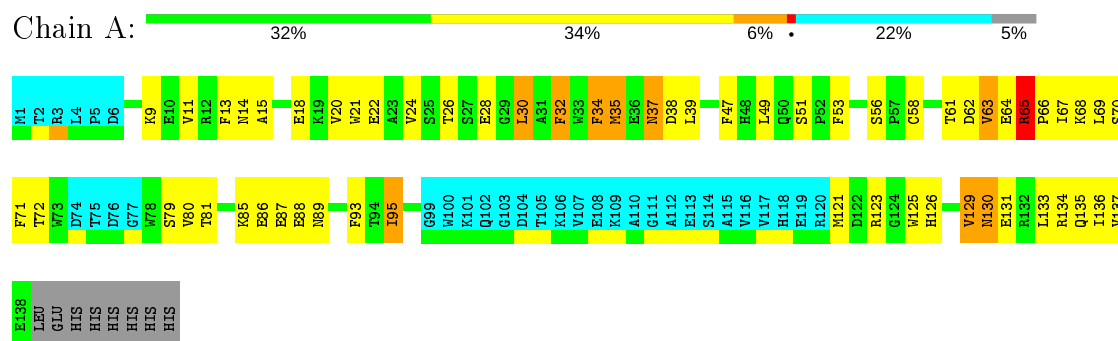
4.2.12 Score per residue for model 12

- Molecule 1: BH1534 unknown conserved protein



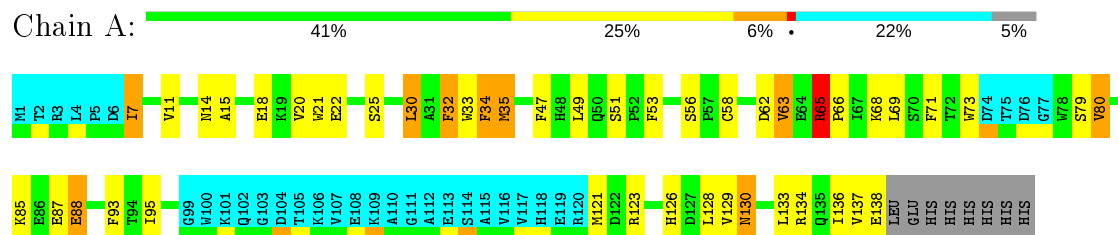
4.2.13 Score per residue for model 13

- Molecule 1: BH1534 unknown conserved protein



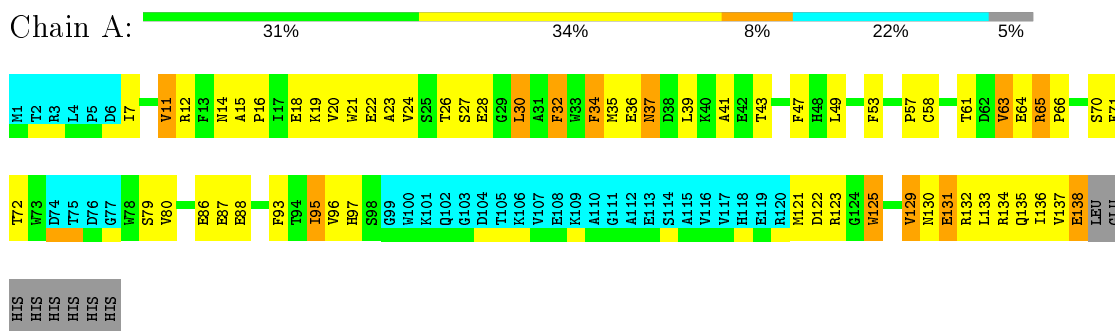
4.2.14 Score per residue for model 14

- Molecule 1: BH1534 unknown conserved protein



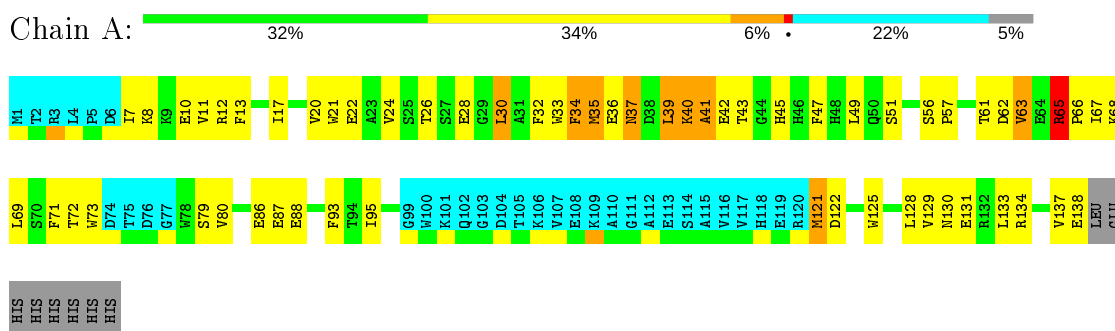
4.2.15 Score per residue for model 15

- Molecule 1: BH1534 unknown conserved protein



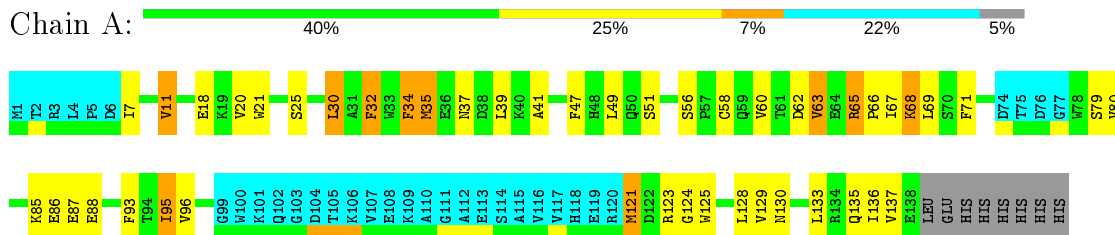
4.2.16 Score per residue for model 16

- Molecule 1: BH1534 unknown conserved protein



4.2.17 Score per residue for model 17

- Molecule 1: BH1534 unknown conserved protein



4.2.18 Score per residue for model 18

- Molecule 1: BH1534 unknown conserved protein



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	1.5

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 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	881	844	844	44±6
All	All	17620	16880	16880	882

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:VAL:HG22	1:A:137:VAL:HG11	0.95	1.38	16	19
1:A:63:VAL:HG23	1:A:69:LEU:CD1	0.90	1.97	2	19
1:A:11:VAL:HG11	1:A:129:VAL:O	0.86	1.71	8	11
1:A:63:VAL:HG23	1:A:69:LEU:HD13	0.86	1.45	4	19
1:A:11:VAL:HG21	1:A:129:VAL:O	0.86	1.71	9	15
1:A:67:ILE:HD12	1:A:68:LYS:N	0.85	1.87	17	14
1:A:32:PHE:CG	1:A:136:ILE:HD12	0.81	2.11	9	12
1:A:71:PHE:CE2	1:A:80:VAL:HG13	0.80	2.12	16	7
1:A:30:LEU:CD1	1:A:39:LEU:HD22	0.80	2.06	16	3
1:A:129:VAL:HG23	1:A:133:LEU:HD23	0.80	1.50	8	15
1:A:71:PHE:CE1	1:A:82:PHE:CE2	0.79	2.70	12	3
1:A:30:LEU:HD13	1:A:39:LEU:HD22	0.78	1.55	5	4
1:A:36:GLU:O	1:A:49:LEU:HD12	0.78	1.78	7	6
1:A:125:TRP:O	1:A:129:VAL:HG12	0.78	1.79	6	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:PHE:CE2	1:A:133:LEU:HD21	0.76	2.15	17	5
1:A:20:VAL:O	1:A:24:VAL:HG13	0.76	1.78	6	10
1:A:11:VAL:HG21	1:A:129:VAL:HG22	0.73	1.57	3	13
1:A:71:PHE:CE1	1:A:80:VAL:HG13	0.73	2.19	4	12
1:A:71:PHE:CZ	1:A:80:VAL:CG1	0.70	2.75	5	13
1:A:71:PHE:CE2	1:A:80:VAL:CG1	0.70	2.75	20	8
1:A:95:ILE:HD13	1:A:95:ILE:C	0.69	2.08	5	4
1:A:26:THR:O	1:A:30:LEU:HD12	0.69	1.88	16	12
1:A:22:GLU:O	1:A:26:THR:HG23	0.68	1.88	6	2
1:A:61:THR:CG2	1:A:72:THR:HG23	0.68	2.18	20	7
1:A:32:PHE:CD1	1:A:136:ILE:CD1	0.67	2.77	17	10
1:A:7:ILE:HG22	1:A:7:ILE:O	0.67	1.89	9	8
1:A:95:ILE:C	1:A:95:ILE:HD13	0.67	2.10	4	4
1:A:7:ILE:HG23	1:A:122:ASP:OD1	0.67	1.88	16	1
1:A:41:ALA:HA	1:A:63:VAL:HG21	0.66	1.66	20	14
1:A:49:LEU:CD2	1:A:73:TRP:CZ2	0.66	2.78	16	2
1:A:7:ILE:O	1:A:7:ILE:HG22	0.66	1.90	18	6
1:A:47:PHE:CZ	1:A:58:CYS:CB	0.66	2.79	3	15
1:A:95:ILE:HD12	1:A:96:VAL:H	0.65	1.50	7	2
1:A:15:ALA:HB1	1:A:16:PRO:HD2	0.64	1.70	2	9
1:A:11:VAL:CG2	1:A:129:VAL:HG22	0.64	2.23	7	11
1:A:37:ASN:HB3	1:A:49:LEU:HD12	0.64	1.69	16	4
1:A:32:PHE:CD1	1:A:136:ILE:HD12	0.63	2.28	9	11
1:A:71:PHE:CE1	1:A:80:VAL:CG1	0.63	2.81	1	5
1:A:80:VAL:HG23	1:A:96:VAL:O	0.62	1.94	15	4
1:A:25:SER:O	1:A:39:LEU:HD23	0.62	1.94	8	2
1:A:21:TRP:HA	1:A:24:VAL:HG22	0.61	1.71	12	6
1:A:21:TRP:CZ2	1:A:65:ARG:C	0.61	2.74	15	20
1:A:95:ILE:HG21	1:A:129:VAL:HG11	0.61	1.71	18	7
1:A:14:ASN:O	1:A:15:ALA:HB2	0.61	1.96	18	10
1:A:63:VAL:CG2	1:A:69:LEU:CD1	0.60	2.80	1	19
1:A:21:TRP:CH2	1:A:65:ARG:O	0.60	2.54	5	19
1:A:49:LEU:CD2	1:A:73:TRP:CE2	0.59	2.85	16	7
1:A:34:PHE:CZ	1:A:49:LEU:HD11	0.59	2.33	5	3
1:A:95:ILE:HD12	1:A:96:VAL:N	0.58	2.12	7	2
1:A:21:TRP:O	1:A:24:VAL:HG22	0.58	1.98	11	2
1:A:21:TRP:CZ2	1:A:65:ARG:CA	0.57	2.86	15	7
1:A:20:VAL:CG2	1:A:137:VAL:HG11	0.57	2.30	15	4
1:A:34:PHE:CE2	1:A:49:LEU:HD11	0.57	2.34	14	5
1:A:34:PHE:CG	1:A:35:MET:N	0.56	2.72	1	20
1:A:129:VAL:HG23	1:A:133:LEU:HD22	0.56	1.78	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:TRP:CH2	1:A:65:ARG:C	0.56	2.79	15	7
1:A:21:TRP:CZ2	1:A:65:ARG:O	0.56	2.59	18	8
1:A:33:TRP:O	1:A:128:LEU:HD11	0.56	2.01	16	5
1:A:71:PHE:CD1	1:A:71:PHE:C	0.55	2.79	15	4
1:A:49:LEU:HD22	1:A:73:TRP:CD1	0.55	2.36	6	1
1:A:21:TRP:CE3	1:A:66:PRO:HA	0.54	2.38	9	17
1:A:70:SER:HB2	1:A:81:THR:HG23	0.54	1.79	20	4
1:A:49:LEU:HD21	1:A:73:TRP:CZ2	0.54	2.38	7	2
1:A:49:LEU:CD2	1:A:73:TRP:NE1	0.53	2.71	6	3
1:A:129:VAL:HG23	1:A:133:LEU:CD2	0.53	2.33	9	8
1:A:47:PHE:CZ	1:A:58:CYS:HB3	0.53	2.39	2	16
1:A:32:PHE:HB3	1:A:136:ILE:HD12	0.53	1.79	19	4
1:A:15:ALA:HB1	1:A:16:PRO:CD	0.53	2.33	2	4
1:A:21:TRP:CZ3	1:A:66:PRO:HA	0.53	2.39	17	16
1:A:129:VAL:O	1:A:129:VAL:HG13	0.52	2.04	17	2
1:A:47:PHE:CZ	1:A:58:CYS:HB2	0.52	2.39	3	3
1:A:126:HIS:CG	1:A:130:ASN:OD1	0.52	2.63	10	1
1:A:49:LEU:HD22	1:A:73:TRP:NE1	0.51	2.20	19	1
1:A:134:ARG:O	1:A:137:VAL:HG22	0.51	2.04	20	7
1:A:126:HIS:CD2	1:A:130:ASN:OD1	0.51	2.63	10	1
1:A:93:PHE:CE2	1:A:133:LEU:CD2	0.51	2.90	17	1
1:A:17:ILE:HD12	1:A:91:THR:HG23	0.51	1.83	12	2
1:A:21:TRP:CE3	1:A:66:PRO:HB3	0.51	2.41	15	6
1:A:126:HIS:CD2	1:A:130:ASN:ND2	0.51	2.79	13	2
1:A:71:PHE:CD1	1:A:71:PHE:O	0.51	2.64	15	2
1:A:20:VAL:HG12	1:A:84:LEU:HD21	0.50	1.83	12	2
1:A:47:PHE:CE2	1:A:58:CYS:HB2	0.50	2.42	10	10
1:A:47:PHE:CG	1:A:47:PHE:O	0.50	2.65	8	2
1:A:17:ILE:O	1:A:21:TRP:CB	0.50	2.60	19	7
1:A:36:GLU:O	1:A:49:LEU:CD1	0.50	2.60	18	1
1:A:21:TRP:CE3	1:A:66:PRO:CA	0.50	2.95	19	9
1:A:20:VAL:HG22	1:A:137:VAL:CG1	0.50	2.30	14	3
1:A:7:ILE:CG2	1:A:7:ILE:O	0.50	2.60	5	4
1:A:22:GLU:O	1:A:26:THR:CG2	0.49	2.60	6	1
1:A:47:PHE:CE2	1:A:58:CYS:HB3	0.49	2.42	2	1
1:A:47:PHE:CE1	1:A:58:CYS:HB2	0.49	2.42	3	3
1:A:71:PHE:C	1:A:71:PHE:CD1	0.49	2.85	9	2
1:A:93:PHE:CD2	1:A:133:LEU:HD21	0.49	2.42	20	3
1:A:47:PHE:CD1	1:A:47:PHE:O	0.49	2.65	3	1
1:A:7:ILE:O	1:A:7:ILE:CG2	0.49	2.61	18	4
1:A:34:PHE:CZ	1:A:49:LEU:CD1	0.49	2.95	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LEU:CD2	1:A:73:TRP:CD1	0.49	2.95	6	1
1:A:131:GLU:OE2	1:A:132:ARG:CZ	0.49	2.61	12	1
1:A:129:VAL:O	1:A:129:VAL:HG22	0.48	2.09	6	2
1:A:93:PHE:CE1	1:A:129:VAL:HG21	0.48	2.43	14	3
1:A:49:LEU:HD22	1:A:73:TRP:CE2	0.48	2.43	12	2
1:A:47:PHE:N	1:A:47:PHE:CD1	0.48	2.82	9	2
1:A:71:PHE:O	1:A:71:PHE:CD1	0.48	2.66	9	1
1:A:124:GLY:O	1:A:128:LEU:CB	0.48	2.61	17	3
1:A:129:VAL:HG13	1:A:129:VAL:O	0.48	2.07	14	1
1:A:42:GLU:O	1:A:45:HIS:CB	0.48	2.61	2	4
1:A:80:VAL:CG2	1:A:95:ILE:HD11	0.48	2.38	9	1
1:A:13:PHE:CD1	1:A:134:ARG:HG3	0.48	2.44	3	6
1:A:40:LYS:HB3	1:A:45:HIS:CD2	0.47	2.44	5	1
1:A:47:PHE:CD1	1:A:47:PHE:N	0.47	2.82	19	3
1:A:41:ALA:CA	1:A:63:VAL:HG21	0.47	2.39	20	5
1:A:121:MET:SD	1:A:125:TRP:CD1	0.47	3.07	12	1
1:A:40:LYS:O	1:A:42:GLU:N	0.47	2.48	16	2
1:A:95:ILE:O	1:A:95:ILE:HD13	0.47	2.08	15	1
1:A:49:LEU:HD23	1:A:73:TRP:NE1	0.47	2.25	4	4
1:A:45:HIS:CG	1:A:46:HIS:N	0.47	2.82	5	4
1:A:49:LEU:HD23	1:A:73:TRP:CE2	0.47	2.44	3	1
1:A:63:VAL:CB	1:A:69:LEU:HD12	0.46	2.41	1	3
1:A:42:GLU:N	1:A:63:VAL:HG11	0.46	2.25	2	2
1:A:48:HIS:CE1	1:A:57:PRO:HB3	0.46	2.45	4	1
1:A:60:VAL:HG11	1:A:63:VAL:CG1	0.46	2.40	5	2
1:A:35:MET:CE	1:A:49:LEU:HD21	0.46	2.41	1	3
1:A:30:LEU:O	1:A:34:PHE:N	0.46	2.47	17	20
1:A:43:THR:N	1:A:63:VAL:CG1	0.46	2.79	8	4
1:A:95:ILE:C	1:A:95:ILE:CD1	0.46	2.81	15	3
1:A:21:TRP:O	1:A:25:SER:N	0.46	2.49	1	3
1:A:126:HIS:HA	1:A:129:VAL:HG12	0.46	1.88	2	2
1:A:93:PHE:CD1	1:A:129:VAL:HG21	0.46	2.46	5	1
1:A:71:PHE:CZ	1:A:80:VAL:HG13	0.46	2.46	12	3
1:A:93:PHE:CZ	1:A:133:LEU:HD21	0.46	2.45	16	1
1:A:131:GLU:O	1:A:134:ARG:N	0.46	2.49	6	2
1:A:80:VAL:HB	1:A:97:HIS:CD2	0.46	2.46	20	3
1:A:37:ASN:N	1:A:37:ASN:HD22	0.45	2.09	1	2
1:A:34:PHE:CE2	1:A:49:LEU:CD1	0.45	3.00	14	3
1:A:134:ARG:O	1:A:138:GLU:N	0.45	2.50	2	7
1:A:95:ILE:HD13	1:A:96:VAL:N	0.45	2.26	6	1
1:A:47:PHE:CE2	1:A:58:CYS:CB	0.45	2.99	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:HIS:O	1:A:130:ASN:ND2	0.45	2.50	6	4
1:A:71:PHE:CZ	1:A:82:PHE:CE2	0.45	3.04	12	1
1:A:87:GLU:N	1:A:87:GLU:OE1	0.45	2.50	10	1
1:A:63:VAL:HG23	1:A:69:LEU:HD12	0.45	1.84	18	1
1:A:17:ILE:HD11	1:A:66:PRO:HB2	0.44	1.88	9	1
1:A:11:VAL:HG21	1:A:13:PHE:CZ	0.44	2.47	16	1
1:A:13:PHE:CE1	1:A:134:ARG:HB2	0.44	2.47	11	1
1:A:33:TRP:CE2	1:A:133:LEU:HD13	0.44	2.46	14	2
1:A:61:THR:CG2	1:A:72:THR:CG2	0.44	2.95	20	2
1:A:124:GLY:O	1:A:128:LEU:N	0.44	2.50	8	2
1:A:63:VAL:HB	1:A:69:LEU:HD12	0.44	1.89	1	4
1:A:9:LYS:HG2	1:A:126:HIS:CD2	0.44	2.47	5	1
1:A:134:ARG:O	1:A:137:VAL:CG2	0.44	2.65	12	8
1:A:131:GLU:O	1:A:135:GLN:N	0.43	2.50	3	1
1:A:126:HIS:NE2	1:A:130:ASN:ND2	0.43	2.64	14	1
1:A:11:VAL:CG2	1:A:129:VAL:O	0.43	2.60	20	1
1:A:87:GLU:CA	1:A:87:GLU:OE1	0.43	2.66	10	1
1:A:121:MET:O	1:A:125:TRP:N	0.43	2.51	4	5
1:A:21:TRP:O	1:A:24:VAL:CG2	0.43	2.66	11	1
1:A:27:SER:OG	1:A:39:LEU:N	0.43	2.52	12	5
1:A:95:ILE:HG13	1:A:125:TRP:CZ3	0.43	2.48	15	1
1:A:71:PHE:CZ	1:A:80:VAL:HG11	0.43	2.49	9	4
1:A:24:VAL:HG11	1:A:93:PHE:HE2	0.43	1.73	13	2
1:A:63:VAL:O	1:A:63:VAL:HG13	0.43	2.14	2	1
1:A:35:MET:HE3	1:A:49:LEU:HD21	0.42	1.92	8	1
1:A:31:ALA:HB2	1:A:36:GLU:HA	0.42	1.91	6	1
1:A:70:SER:CB	1:A:81:THR:HG23	0.42	2.45	13	2
1:A:47:PHE:CD1	1:A:47:PHE:C	0.42	2.92	3	1
1:A:10:GLU:OE2	1:A:11:VAL:N	0.42	2.53	11	1
1:A:61:THR:HG23	1:A:72:THR:HG23	0.42	1.91	15	1
1:A:21:TRP:CG	1:A:66:PRO:HG3	0.42	2.50	15	1
1:A:131:GLU:O	1:A:132:ARG:C	0.42	2.57	18	3
1:A:67:ILE:HD12	1:A:68:LYS:CB	0.42	2.45	20	2
1:A:51:SER:CB	1:A:52:PRO:CD	0.42	2.98	11	2
1:A:131:GLU:OE1	1:A:132:ARG:N	0.42	2.53	15	1
1:A:34:PHE:O	1:A:35:MET:CG	0.42	2.68	20	2
1:A:69:LEU:O	1:A:82:PHE:N	0.41	2.49	20	1
1:A:71:PHE:CZ	1:A:80:VAL:HG12	0.41	2.48	5	1
1:A:7:ILE:HG23	1:A:122:ASP:OD2	0.41	2.16	15	1
1:A:134:ARG:CZ	1:A:138:GLU:OE2	0.41	2.68	15	1
1:A:14:ASN:O	1:A:15:ALA:CB	0.41	2.62	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:HIS:N	1:A:46:HIS:CD2	0.41	2.89	19	1
1:A:69:LEU:HD23	1:A:82:PHE:HD2	0.41	1.76	11	2
1:A:9:LYS:HG2	1:A:126:HIS:CG	0.41	2.51	5	1
1:A:24:VAL:HG21	1:A:84:LEU:HD11	0.41	1.92	8	1
1:A:30:LEU:C	1:A:32:PHE:N	0.41	2.74	15	1
1:A:131:GLU:C	1:A:131:GLU:OE1	0.41	2.59	15	1
1:A:40:LYS:CB	1:A:45:HIS:CE1	0.41	3.03	16	1
1:A:11:VAL:CG2	1:A:13:PHE:CZ	0.41	3.04	16	1
1:A:64:GLU:O	1:A:65:ARG:O	0.41	2.39	15	1
1:A:19:LYS:O	1:A:23:ALA:N	0.40	2.52	15	1
1:A:21:TRP:CZ2	1:A:65:ARG:HA	0.40	2.50	15	1
1:A:7:ILE:N	1:A:97:HIS:O	0.40	2.53	3	1
1:A:24:VAL:O	1:A:30:LEU:HD11	0.40	2.15	5	1
1:A:35:MET:HE1	1:A:73:TRP:CZ2	0.40	2.52	5	1
1:A:37:ASN:OD1	1:A:39:LEU:CB	0.40	2.69	8	1
1:A:18:GLU:O	1:A:22:GLU:CD	0.40	2.60	10	1
1:A:20:VAL:O	1:A:24:VAL:N	0.40	2.53	12	1
1:A:34:PHE:CE1	1:A:35:MET:HE2	0.40	2.51	20	1
1:A:63:VAL:CG2	1:A:69:LEU:HD12	0.40	2.46	1	1
1:A:21:TRP:CD2	1:A:66:PRO:HB3	0.40	2.51	8	1
1:A:80:VAL:CG2	1:A:95:ILE:CD1	0.40	2.99	9	1
1:A:17:ILE:O	1:A:21:TRP:N	0.40	2.51	16	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	105/146 (72%)	87±2 (83±2%)	13±2 (13±2%)	5±1 (4±1%)	4	29
All	All	2100/2920 (72%)	1742 (83%)	266 (13%)	92 (4%)	4	29

All 9 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	65	ARG	20
1	A	34	PHE	20
1	A	63	VAL	17
1	A	129	VAL	14
1	A	88	GLU	13
1	A	7	ILE	4
1	A	41	ALA	2
1	A	15	ALA	1
1	A	67	ILE	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	97/130 (75%)	73±3 (76±3%)	24±3 (24±3%)	2 26
All	All	1940/2600 (75%)	1467 (76%)	473 (24%)	2 26

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	130	ASN	20
1	A	95	ILE	20
1	A	79	SER	20
1	A	32	PHE	20
1	A	30	LEU	20
1	A	18	GLU	19
1	A	56	SER	19
1	A	62	ASP	19
1	A	121	MET	17
1	A	28	GLU	17
1	A	87	GLU	17
1	A	39	LEU	14
1	A	131	GLU	14
1	A	65	ARG	14
1	A	135	GLN	14
1	A	35	MET	13
1	A	51	SER	12

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Mol	Chain	Res	Type	Models (Total)
1	A	22	GLU	12
1	A	138	GLU	11
1	A	86	GLU	11
1	A	85	LYS	11
1	A	12	ARG	10
1	A	123	ARG	10
1	A	37	ASN	10
1	A	64	GLU	10
1	A	43	THR	10
1	A	53	PHE	8
1	A	40	LYS	7
1	A	11	VAL	7
1	A	68	LYS	7
1	A	88	GLU	6
1	A	9	LYS	5
1	A	132	ARG	5
1	A	14	ASN	5
1	A	10	GLU	5
1	A	38	ASP	4
1	A	27	SER	4
1	A	134	ARG	4
1	A	46	HIS	3
1	A	19	LYS	3
1	A	36	GLU	2
1	A	25	SER	2
1	A	80	VAL	2
1	A	48	HIS	2
1	A	78	TRP	2
1	A	59	GLN	1
1	A	89	ASN	1
1	A	70	SER	1
1	A	42	GLU	1
1	A	125	TRP	1
1	A	8	LYS	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