Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2HFD
Title	:	NMR structure of protein Hydrogenase-1 operon protein hyaE from Escherichia coli: Northeast Structural Genomics Consortium Target ER415
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Deposited on	:	2006-06-23

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

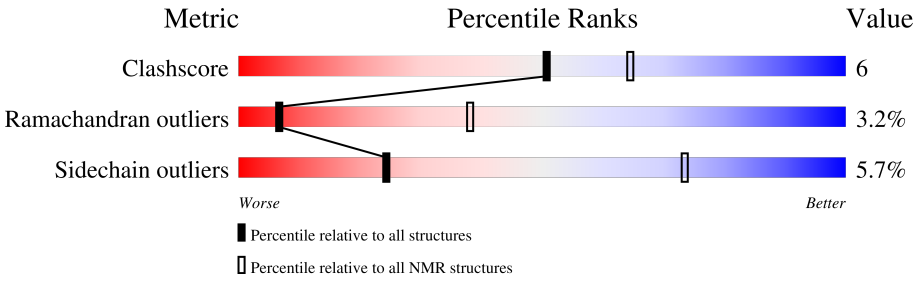
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	140	67% 12% • 14% 6%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 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:5-A:42, A:52-A:125 (112)	1.33	1

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2064 atoms, of which 1014 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hydrogenase-1 operon protein hyaE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	132	2064	667	1014	181	198	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	LEU	-	cloning artifact	UNP P19931
A	134	GLU	-	cloning artifact	UNP P19931
A	135	HIS	-	expression tag	UNP P19931
A	136	HIS	-	expression tag	UNP P19931
A	137	HIS	-	expression tag	UNP P19931
A	138	HIS	-	expression tag	UNP P19931
A	139	HIS	-	expression tag	UNP P19931
A	140	HIS	-	expression tag	UNP P19931

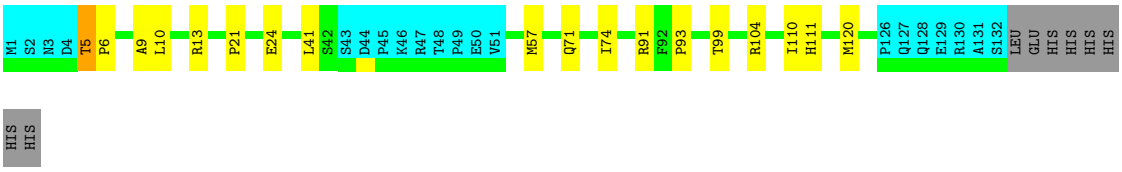
4 Residue-property plots (i)

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: Hydrogenase-1 operon protein hyaE

Chain A: 67% 12% • 14% 6%



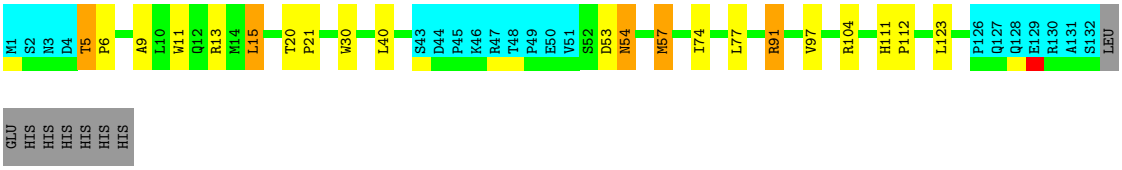
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Hydrogenase-1 operon protein hyaE

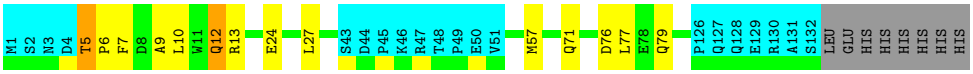
Chain A: 65% 11% • 14% 6%



4.2.2 Score per residue for model 2

• Molecule 1: Hydrogenase-1 operon protein hyaE

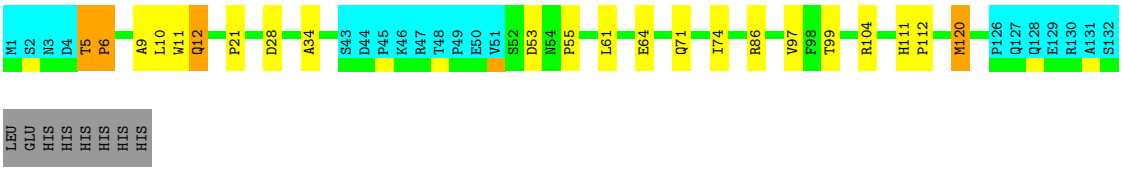
Chain A: 70% 9% • 14% 6%



4.2.3 Score per residue for model 3

- Molecule 1: Hydrogenase-1 operon protein hyaE

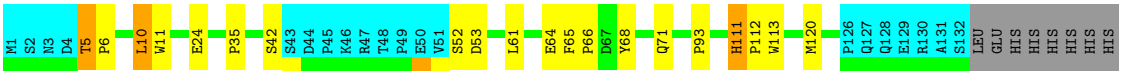
Chain A: 64% 13% • 14% 6%



4.2.4 Score per residue for model 4

- Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A: 66% 12% • 14% 6%



4.2.5 Score per residue for model 5

- Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A: 59% 20% • 14% 6%

4.2.6 Score per residue for model 6

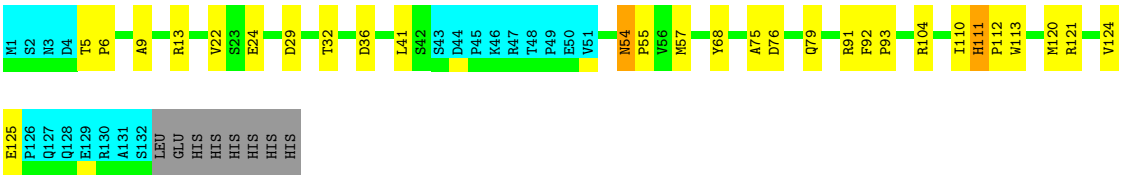
- Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A: 64% 13% • • 14% 6%

4.2.7 Score per residue for model 7

• Molecule 1: Hydrogenase-1 operon protein hyaE

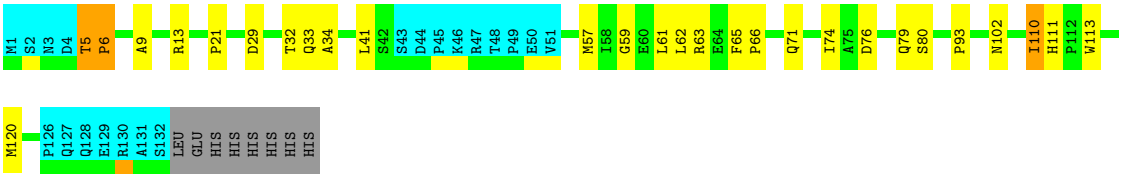
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Hydrogenase-1 operon protein hyaE

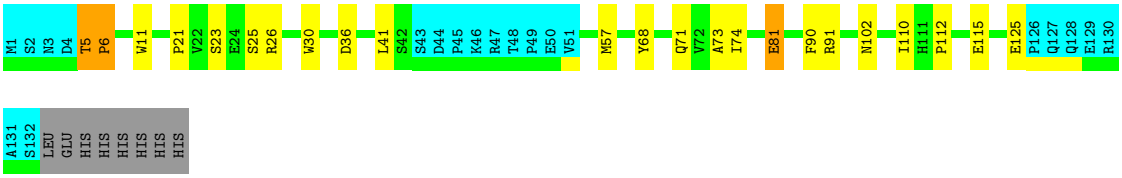
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Hydrogenase-1 operon protein hyaE

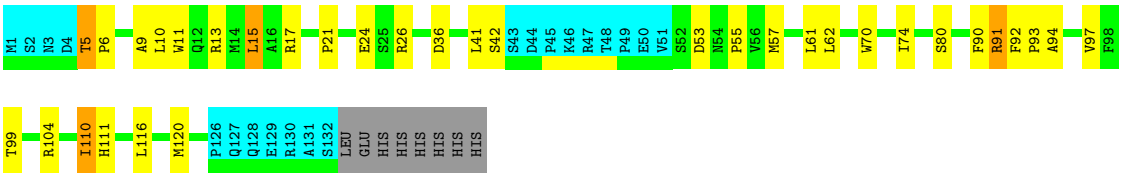
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Hydrogenase-1 operon protein hyaE

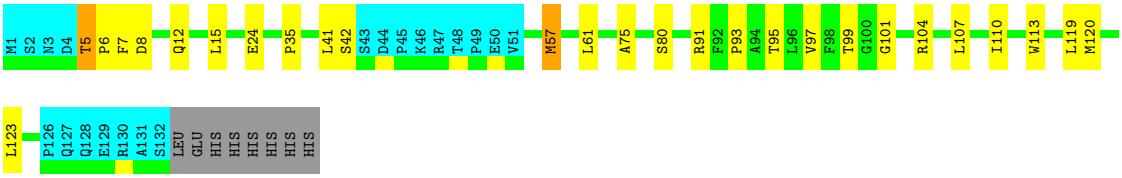
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Hydrogenase-1 operon protein hyaE

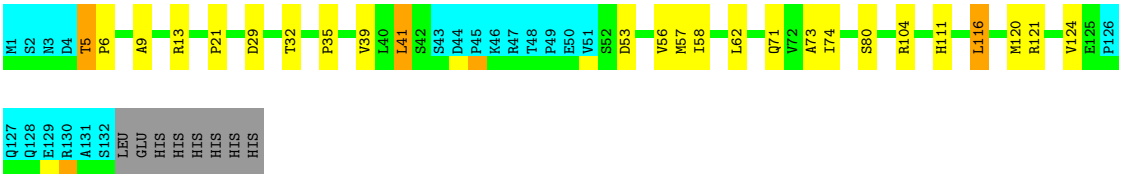
Chain A: 61% 18% • 14% 6%



4.2.12 Score per residue for model 12

- Molecule 1: Hydrogenase-1 operon protein hyaE

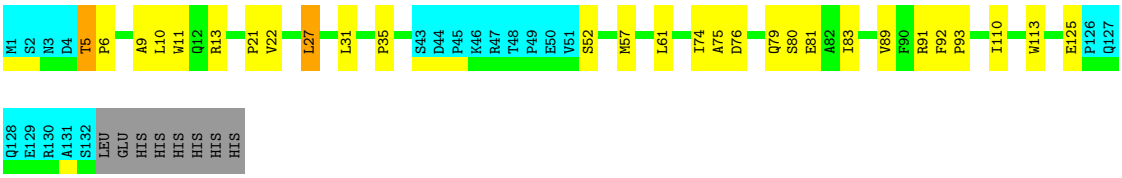
Chain A: 62% 16% • 14% 6%



4.2.13 Score per residue for model 13

- Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A: 60% 19% • 14% 6%



4.2.14 Score per residue for model 14

- Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A: 66% 13% • 14% 6%

M1 S2 N3 D4 T5 P6 A9 Q12 R13 E24 D36 S43 D44 P45 K46 R47 T48 P49 E50 V51 M57 F65 Q71 Q79 T99 R104 I110 H111 P112 W113 A114 E115 L116 I117 M120 P126 Q127 Q128 E129 R130 A131 S132 LEU GLU HIS HIS

HIS HIS HIS HIS

4.2.15 Score per residue for model 15

• Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A: 69% 9% • 14% 6%

M1 S2 N3 D4 T5 P6 A9 R13 P35 S43 D44 P45 K46 R47 T48 P49 E50 V51 P55 G59 E60 L61 L62 R63 R91 F92 R104 I110 H111 P112 M120 P126 Q127 Q128 E129 R130 A131 S132 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.16 Score per residue for model 16

• Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A: 66% 11% • • 14% 6%

M1 S2 N3 D4 T5 P6 L10 W11 S23 E24 S25 D29 W30 L31 T32 Q33 S43 D44 P45 K46 R47 T48 P49 E50 V51 S52 D53 M57 Y68 P93 T99 P112 W113 L116 P126 Q127 Q128 E129 R130 A131 S132 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.17 Score per residue for model 17

• Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A: 61% 16% • 14% 6%

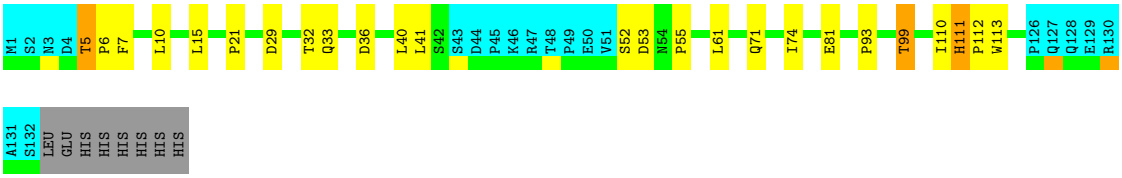
M1 S2 N3 D4 T5 P6 L10 P21 E24 D36 L41 S42 S43 D44 P45 K46 R47 T48 P49 E50 V51 M57 I58 G59 E60 L61 L62 R63 E64 F65 W70 Q71 I74 A75 S80 P93 A94 T99 G100 G101 N102 Y103 R104 W113 L116 M120

P126 Q127 Q128 E129 R130 A131 S132 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.18 Score per residue for model 18

• Molecule 1: Hydrogenase-1 operon protein hyaE

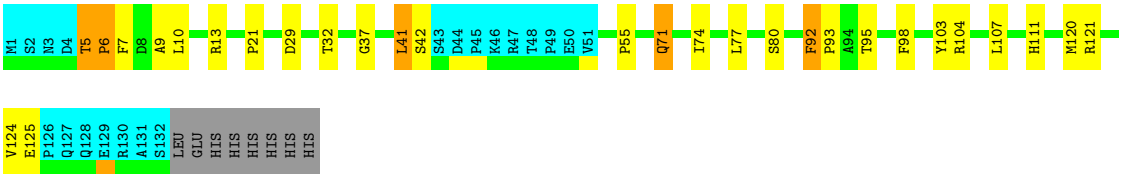
Chain A: 62% 16% • 14% 6%



4.2.19 Score per residue for model 19

- Molecule 1: Hydrogenase-1 operon protein hyaE

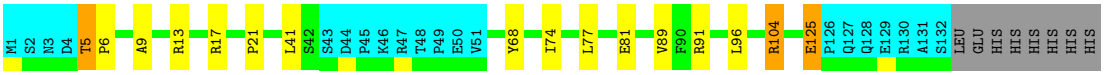
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Hydrogenase-1 operon protein hyaE

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry simulated annealing molecular 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
CYANA	refinement	2.1
CNS	refinement	1.1

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.

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	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	24	GLU	Peptide	1

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	893	867	866	10±3
All	All	17860	17340	17320	207

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:VAL:HG13	1:A:104:ARG:HB2	0.76	1.57	1	4
1:A:110:ILE:HG22	1:A:111:HIS:H	0.68	1.48	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLN:HE21	1:A:33:GLN:HA	0.66	1.49	16	1
1:A:12:GLN:HE21	1:A:12:GLN:HA	0.64	1.52	6	2
1:A:61:LEU:HB2	1:A:113:TRP:HH2	0.63	1.50	8	5
1:A:76:ASP:HB2	1:A:79:GLN:HG2	0.63	1.68	5	2
1:A:35:PRO:HG2	1:A:71:GLN:HB2	0.61	1.71	12	1
1:A:5:THR:OG1	1:A:6:PRO:HD3	0.61	1.95	6	1
1:A:15:LEU:HD21	1:A:21:PRO:HG3	0.60	1.73	1	1
1:A:42:SER:HB2	1:A:93:PRO:HB3	0.60	1.73	10	1
1:A:61:LEU:HD21	1:A:120:MET:HB2	0.60	1.72	10	1
1:A:61:LEU:HD21	1:A:120:MET:HG3	0.60	1.73	3	2
1:A:111:HIS:HB3	1:A:112:PRO:HD3	0.60	1.74	1	3
1:A:111:HIS:H	1:A:112:PRO:HD2	0.59	1.56	4	1
1:A:21:PRO:HA	1:A:74:ILE:O	0.58	1.97	17	11
1:A:111:HIS:HB2	1:A:112:PRO:HD3	0.58	1.74	18	2
1:A:7:PHE:HE1	1:A:42:SER:HB2	0.58	1.59	11	1
1:A:89:VAL:HG11	1:A:96:LEU:HD21	0.56	1.77	5	2
1:A:36:ASP:HB2	1:A:68:TYR:HE2	0.56	1.60	7	1
1:A:41:LEU:HA	1:A:80:SER:HB3	0.56	1.75	8	1
1:A:5:THR:HB	1:A:6:PRO:HD3	0.56	1.78	12	13
1:A:9:ALA:O	1:A:13:ARG:HG2	0.56	2.01	12	10
1:A:61:LEU:HD21	1:A:120:MET:HG2	0.56	1.77	8	2
1:A:35:PRO:HB2	1:A:101:GLY:HA2	0.55	1.77	11	1
1:A:29:ASP:O	1:A:33:GLN:HG2	0.55	2.01	18	1
1:A:8:ASP:O	1:A:12:GLN:HG2	0.55	2.01	11	1
1:A:112:PRO:HG2	1:A:115:GLU:HB2	0.54	1.78	9	1
1:A:7:PHE:CE2	1:A:77:LEU:HB2	0.54	2.37	2	1
1:A:104:ARG:HA	1:A:104:ARG:HE	0.53	1.61	15	4
1:A:111:HIS:HB3	1:A:116:LEU:HD23	0.53	1.80	12	1
1:A:104:ARG:NE	1:A:104:ARG:HA	0.52	2.19	12	3
1:A:92:PHE:HB3	1:A:93:PRO:HD2	0.52	1.81	5	1
1:A:41:LEU:O	1:A:93:PRO:HA	0.52	2.04	18	3
1:A:36:ASP:OD2	1:A:99:THR:HA	0.50	2.05	14	2
1:A:5:THR:HB	1:A:6:PRO:CD	0.50	2.37	16	7
1:A:41:LEU:O	1:A:93:PRO:HB3	0.50	2.06	17	1
1:A:61:LEU:HA	1:A:113:TRP:HH2	0.50	1.66	5	1
1:A:104:ARG:CZ	1:A:104:ARG:HA	0.50	2.36	17	1
1:A:41:LEU:HB2	1:A:94:ALA:H	0.50	1.66	17	1
1:A:42:SER:HA	1:A:93:PRO:HB3	0.50	1.83	4	2
1:A:36:ASP:HB2	1:A:68:TYR:CE2	0.50	2.41	7	1
1:A:7:PHE:CE1	1:A:42:SER:HB2	0.49	2.40	11	1
1:A:76:ASP:HB3	1:A:79:GLN:HB2	0.49	1.84	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:GLU:HG3	1:A:90:PHE:CE1	0.49	2.42	9	1
1:A:13:ARG:O	1:A:17:ARG:HG2	0.49	2.07	20	1
1:A:90:PHE:HB3	1:A:92:PHE:HD1	0.48	1.68	10	1
1:A:53:ASP:O	1:A:54:ASN:HB3	0.48	2.08	1	1
1:A:110:ILE:O	1:A:111:HIS:HB2	0.48	2.09	7	2
1:A:36:ASP:OD2	1:A:99:THR:HB	0.48	2.09	10	1
1:A:29:ASP:O	1:A:32:THR:HG22	0.47	2.08	16	6
1:A:75:ALA:HB3	1:A:80:SER:HB3	0.47	1.86	11	3
1:A:89:VAL:HG12	1:A:92:PHE:HB2	0.47	1.85	13	1
1:A:119:LEU:O	1:A:123:LEU:HG	0.47	2.09	5	2
1:A:120:MET:O	1:A:124:VAL:HG22	0.47	2.09	19	3
1:A:53:ASP:HA	1:A:110:ILE:HG13	0.47	1.87	18	1
1:A:9:ALA:O	1:A:13:ARG:HG3	0.46	2.10	10	2
1:A:11:TRP:CH2	1:A:76:ASP:HA	0.46	2.45	13	1
1:A:112:PRO:O	1:A:116:LEU:HB2	0.46	2.11	16	1
1:A:65:PHE:HB2	1:A:70:TRP:HE1	0.46	1.69	17	1
1:A:59:GLY:O	1:A:63:ARG:HG2	0.46	2.10	17	3
1:A:62:LEU:O	1:A:65:PHE:HD2	0.46	1.93	8	1
1:A:65:PHE:HB2	1:A:68:TYR:O	0.46	2.10	4	1
1:A:11:TRP:O	1:A:15:LEU:HB2	0.46	2.11	10	2
1:A:9:ALA:O	1:A:12:GLN:HG3	0.46	2.09	3	1
1:A:36:ASP:OD1	1:A:99:THR:HA	0.46	2.10	17	1
1:A:58:ILE:O	1:A:62:LEU:HD13	0.45	2.12	12	1
1:A:110:ILE:HG22	1:A:111:HIS:N	0.45	2.23	10	1
1:A:34:ALA:HB1	1:A:71:GLN:NE2	0.45	2.26	3	1
1:A:41:LEU:HG	1:A:80:SER:HB3	0.45	1.88	10	1
1:A:76:ASP:HB3	1:A:79:GLN:HG2	0.45	1.89	2	1
1:A:41:LEU:HD22	1:A:80:SER:HB2	0.45	1.88	19	1
1:A:77:LEU:O	1:A:81:GLU:HG3	0.45	2.12	20	1
1:A:104:ARG:CG	1:A:124:VAL:HA	0.44	2.42	6	1
1:A:62:LEU:HD23	1:A:70:TRP:HB3	0.44	1.89	10	1
1:A:37:GLY:O	1:A:98:PHE:HB2	0.44	2.12	19	1
1:A:104:ARG:NH1	1:A:125:GLU:HB3	0.44	2.27	20	1
1:A:29:ASP:O	1:A:32:THR:HB	0.44	2.12	18	1
1:A:89:VAL:CG1	1:A:92:PHE:HB2	0.44	2.43	13	1
1:A:90:PHE:HB2	1:A:92:PHE:CE2	0.44	2.48	6	1
1:A:57:MET:HB2	1:A:113:TRP:CE3	0.44	2.48	7	1
1:A:34:ALA:HB2	1:A:71:GLN:NE2	0.44	2.27	8	1
1:A:121:ARG:O	1:A:125:GLU:HB3	0.43	2.13	19	1
1:A:57:MET:SD	1:A:57:MET:N	0.43	2.90	11	2
1:A:24:GLU:H	1:A:24:GLU:CD	0.43	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD22	1:A:80:SER:HB3	0.43	1.89	12	1
1:A:12:GLN:HE21	1:A:12:GLN:CA	0.43	2.25	2	2
1:A:39:VAL:HA	1:A:73:ALA:O	0.43	2.13	12	2
1:A:121:ARG:HA	1:A:124:VAL:HG12	0.43	1.90	6	1
1:A:90:PHE:O	1:A:91:ARG:HG2	0.43	2.14	10	1
1:A:98:PHE:CD1	1:A:103:TYR:HA	0.43	2.48	19	1
1:A:112:PRO:HG2	1:A:115:GLU:HB3	0.43	1.91	14	1
1:A:22:VAL:O	1:A:75:ALA:HA	0.43	2.14	7	1
1:A:104:ARG:HA	1:A:104:ARG:NE	0.42	2.29	17	2
1:A:113:TRP:HA	1:A:113:TRP:CE3	0.42	2.49	16	1
1:A:61:LEU:O	1:A:64:GLU:HG2	0.42	2.15	4	2
1:A:94:ALA:HB1	1:A:106:VAL:CG2	0.42	2.44	5	1
1:A:104:ARG:HD2	1:A:123:LEU:O	0.42	2.15	1	1
1:A:27:LEU:O	1:A:31:LEU:HG	0.42	2.15	13	1
1:A:40:LEU:HB2	1:A:74:ILE:HG22	0.42	1.91	18	2
1:A:29:ASP:O	1:A:33:GLN:HG3	0.42	2.15	8	1
1:A:5:THR:CB	1:A:6:PRO:HD3	0.42	2.45	6	1
1:A:22:VAL:HG11	1:A:27:LEU:HG	0.42	1.90	13	1
1:A:61:LEU:CD2	1:A:120:MET:HG3	0.41	2.42	3	1
1:A:7:PHE:CD2	1:A:77:LEU:HD13	0.41	2.50	19	1
1:A:63:ARG:HG3	1:A:63:ARG:HH11	0.41	1.74	6	1
1:A:95:THR:HB	1:A:107:LEU:HB2	0.41	1.91	11	2
1:A:61:LEU:HA	1:A:113:TRP:CH2	0.41	2.50	13	1
1:A:28:ASP:HB2	1:A:86:ARG:HH12	0.41	1.74	3	1
1:A:11:TRP:CZ2	1:A:76:ASP:HA	0.41	2.51	13	1
1:A:115:GLU:O	1:A:119:LEU:HG	0.41	2.16	6	1
1:A:81:GLU:HG3	1:A:90:PHE:CZ	0.41	2.51	9	1
1:A:113:TRP:O	1:A:117:ILE:HG13	0.41	2.15	14	1
1:A:54:ASN:HD22	1:A:54:ASN:N	0.41	2.13	7	1
1:A:76:ASP:HB2	1:A:79:GLN:HB2	0.41	1.92	7	1
1:A:41:LEU:HD22	1:A:93:PRO:HA	0.41	1.92	10	1
1:A:92:PHE:HA	1:A:93:PRO:HD3	0.41	1.80	19	1
1:A:98:PHE:HD1	1:A:103:TYR:HA	0.41	1.76	19	1
1:A:121:ARG:O	1:A:125:GLU:HA	0.40	2.16	7	1
1:A:30:TRP:HZ3	1:A:73:ALA:HB2	0.40	1.75	9	1
1:A:23:SER:O	1:A:24:GLU:C	0.40	2.59	16	1
1:A:79:GLN:O	1:A:83:ILE:HG13	0.40	2.16	13	1
1:A:91:ARG:O	1:A:92:PHE:HB3	0.40	2.16	15	1
1:A:91:ARG:O	1:A:92:PHE:HB2	0.40	2.17	5	1
1:A:37:GLY:HA2	1:A:71:GLN:O	0.40	2.17	19	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	112/140 (80%)	100±3 (89±3%)	9±3 (8±2%)	4±1 (3±1%)	7 38
All	All	2240/2800 (80%)	1997 (89%)	172 (8%)	71 (3%)	7 38

All 19 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	5	THR	20
1	A	6	PRO	7
1	A	55	PRO	6
1	A	53	ASP	5
1	A	111	HIS	5
1	A	110	ILE	4
1	A	91	ARG	3
1	A	35	PRO	3
1	A	125	GLU	3
1	A	92	PHE	3
1	A	66	PRO	2
1	A	56	VAL	2
1	A	25	SER	2
1	A	54	ASN	1
1	A	100	GLY	1
1	A	36	ASP	1
1	A	94	ALA	1
1	A	24	GLU	1
1	A	101	GLY	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	94/121 (78%)	89±3 (94±3%)	5±3 (6±3%)	24 73
All	All	1880/2420 (78%)	1772 (94%)	108 (6%)	24 73

All 32 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	57	MET	11
1	A	10	LEU	9
1	A	24	GLU	8
1	A	71	GLN	7
1	A	99	THR	7
1	A	11	TRP	6
1	A	120	MET	5
1	A	116	LEU	5
1	A	15	LEU	4
1	A	12	GLN	4
1	A	52	SER	4
1	A	102	ASN	4
1	A	104	ARG	4
1	A	41	LEU	4
1	A	31	LEU	3
1	A	68	TYR	3
1	A	27	LEU	2
1	A	81	GLU	2
1	A	91	ARG	2
1	A	26	ARG	2
1	A	20	THR	1
1	A	30	TRP	1
1	A	32	THR	1
1	A	5	THR	1
1	A	125	GLU	1
1	A	54	ASN	1
1	A	23	SER	1
1	A	17	ARG	1
1	A	121	ARG	1
1	A	65	PHE	1
1	A	79	GLN	1
1	A	33	GLN	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