Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 09:11 AM EST

PDB ID	:	2KEN
Title	:	Solution NMR structure of the OB domain (residues 67-166) of MM0293 from Methanosarcina mazei. Northeast Structural Genomics Consortium target MaR214a.
Authors	:	Ramelot, T.A.; Ding, K.; Magliqui, M.; Jiang, M.; Ciccosanti, C.; Xiao, R.; Lui, J.; Everett, J.K.; Swapna, G.; Acton, T.B.; Rost, B.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-01-30

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:

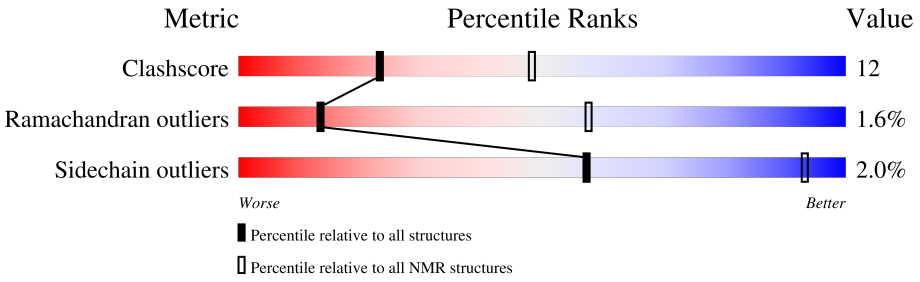
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	109	75% 9% 16%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 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:3-A:29, A:35-A:99 (92)	0.32	17

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 2 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1756 atoms, of which 872 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Conserved protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	109	1756	561	872	153	169	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8Q045
A	102	LEU	-	expression tag	UNP Q8Q045
A	103	GLU	-	expression tag	UNP Q8Q045
A	104	HIS	-	expression tag	UNP Q8Q045
A	105	HIS	-	expression tag	UNP Q8Q045
A	106	HIS	-	expression tag	UNP Q8Q045
A	107	HIS	-	expression tag	UNP Q8Q045
A	108	HIS	-	expression tag	UNP Q8Q045
A	109	HIS	-	expression tag	UNP Q8Q045

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: Conserved protein

Chain A: 75% 9% 16%

M1 E2 V12 N19 N30 T31 H32 E33 S34 I35 S36 D43 L61 Y77 N78 D79 R80 E99 V100 G101 L102 E103 H104 H105 H106 H107 H108 H109

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: Conserved protein

Chain A: 62% 19% • 16%

M1 E2 L5 I11 V12 E13 N14 I25 Q26 L27 N30 T31 H32 E33 S34 I35 G39 L40 L41 G42 D43 E44 L61 E62 Q63 Y67 Y77 R80 K87 N88 K93 L94 E99 V100 G101 L102 E103 H104 H105 H106 H107 H108 H109

4.2.2 Score per residue for model 2

• Molecule 1: Conserved protein

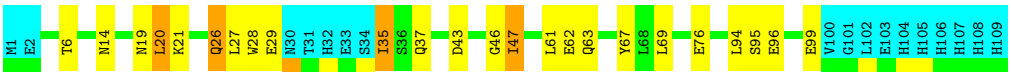
Chain A: 62% 21% • 16%

M1 E2 L5 I11 V12 E13 A18 N19 I25 N30 T31 H32 E33 S34 L41 G42 F50 T51 L61 L68 L69 R70 Y77 N78 D79 R80 F81 Q82 N86 K87 N88 L94 S95 E96 V100 G101 L102 E103 H104 H105 H106 H107 H108 H109

4.2.3 Score per residue for model 3

- Molecule 1: Conserved protein

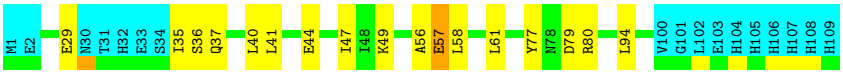
Chain A: 62% 18% • 16%



4.2.4 Score per residue for model 4

- Molecule 1: Conserved protein

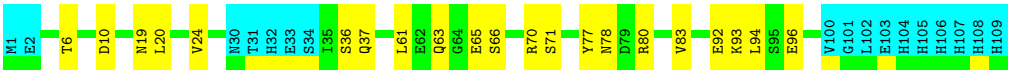
Chain A: 69% 15% • 16%



4.2.5 Score per residue for model 5

- Molecule 1: Conserved protein

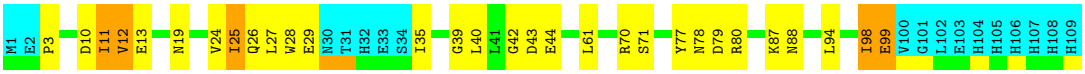
Chain A: 65% 19% 16%



4.2.6 Score per residue for model 6

- Molecule 1: Conserved protein

Chain A: 57% 23% 5% 16%



4.2.7 Score per residue for model 7

- Molecule 1: Conserved protein

Chain A: 58% 22% 5% 16%

4.2.8 Score per residue for model 8

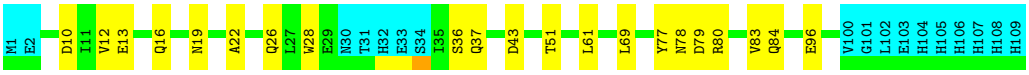
- Molecule 1: Conserved protein

Chain A: 62% 20% • 16%

4.2.9 Score per residue for model 9

- Molecule 1: Conserved protein

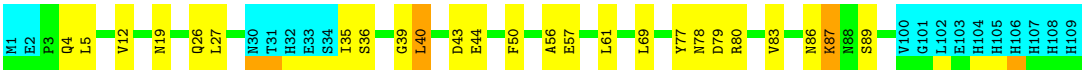
Chain A: 65% 19% 16%



4.2.10 Score per residue for model 10

- Molecule 1: Conserved protein

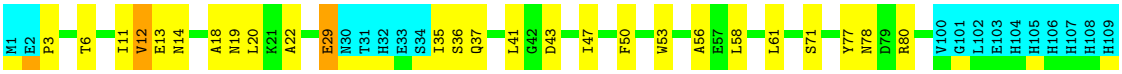
Chain A: 61% 21% • 16%



4.2.11 Score per residue for model 11

- Molecule 1: Conserved protein

Chain A: 61% 22% • 16%



4.2.12 Score per residue for model 12

- Molecule 1: Conserved protein

Chain A: 71% 11% • • 16%

4.2.13 Score per residue for model 13

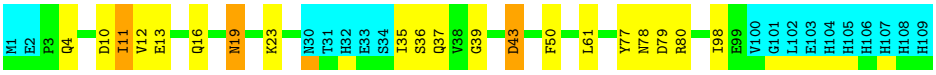
- Molecule 1: Conserved protein

Chain A: 61% 23% 16%

4.2.14 Score per residue for model 14

- Molecule 1: Conserved protein

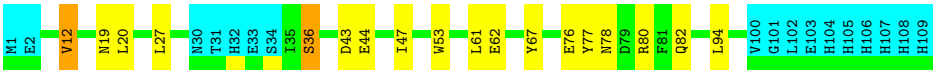
Chain A: 66% 16% • 16%



4.2.15 Score per residue for model 15

- Molecule 1: Conserved protein

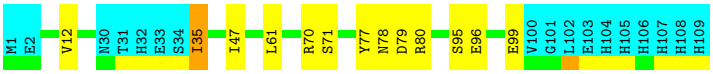
Chain A: 68% 15% • 16%



4.2.16 Score per residue for model 16

- Molecule 1: Conserved protein

Chain A: 72% 11% • 16%



4.2.17 Score per residue for model 17 (medoid)

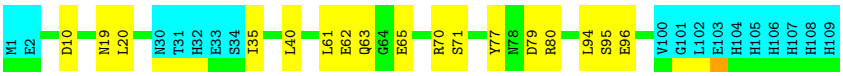
- Molecule 1: Conserved protein

Chain A: 73% 10% • 16%

4.2.18 Score per residue for model 18

- Molecule 1: Conserved protein

Chain A: 69% 16% 16%



4.2.19 Score per residue for model 19

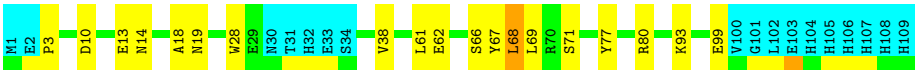
- Molecule 1: Conserved protein

Chain A: 70% 13% • 16%

4.2.20 Score per residue for model 20

- Molecule 1: Conserved protein

Chain A: 67% 17% • 16%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
AutoStructure	structure solution	2.2.1
X-PLOR NIH	refinement	2.20

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	738	753	753	18±5
All	All	14760	15060	15060	368

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HD23	1:A:27:LEU:H	0.80	1.37	13	5
1:A:40:LEU:N	1:A:40:LEU:HD23	0.77	1.94	10	1
1:A:27:LEU:H	1:A:27:LEU:HD23	0.73	1.43	17	1
1:A:56:ALA:O	1:A:58:LEU:N	0.67	2.27	4	1
1:A:77:TYR:CD2	1:A:78:ASN:ND2	0.63	2.67	6	1
1:A:27:LEU:HD23	1:A:27:LEU:N	0.62	2.08	10	6
1:A:86:ASN:N	1:A:86:ASN:HD22	0.62	1.93	7	1
1:A:19:ASN:HD22	1:A:19:ASN:N	0.61	1.93	14	1
1:A:61:LEU:N	1:A:61:LEU:HD12	0.60	2.10	13	16
1:A:86:ASN:N	1:A:86:ASN:ND2	0.60	2.48	7	1
1:A:11:ILE:O	1:A:13:GLU:N	0.60	2.34	11	5
1:A:20:LEU:C	1:A:20:LEU:HD22	0.60	2.17	7	1
1:A:47:ILE:HD12	1:A:47:ILE:C	0.60	2.16	19	4
1:A:11:ILE:O	1:A:12:VAL:C	0.60	2.39	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ILE:HD12	1:A:47:ILE:O	0.60	1.97	11	4
1:A:14:ASN:ND2	1:A:15:GLY:N	0.60	2.50	13	2
1:A:61:LEU:HD12	1:A:61:LEU:N	0.59	2.11	9	4
1:A:43:ASP:O	1:A:44:GLU:CB	0.59	2.50	12	1
1:A:47:ILE:H	1:A:47:ILE:HD13	0.58	1.57	3	1
1:A:39:GLY:C	1:A:40:LEU:HD12	0.58	2.19	1	1
1:A:41:LEU:HD21	1:A:50:PHE:CD1	0.58	2.34	2	1
1:A:20:LEU:HD13	1:A:21:LYS:N	0.57	2.14	3	1
1:A:20:LEU:HD13	1:A:20:LEU:N	0.57	2.13	7	1
1:A:99:GLU:H	1:A:99:GLU:CD	0.57	2.02	12	1
1:A:27:LEU:N	1:A:63:GLN:HE21	0.57	1.98	3	1
1:A:20:LEU:N	1:A:20:LEU:CD1	0.57	2.68	7	1
1:A:65:GLU:N	1:A:65:GLU:OE1	0.57	2.37	8	2
1:A:78:ASN:OD1	1:A:79:ASP:N	0.56	2.38	6	2
1:A:65:GLU:OE1	1:A:65:GLU:N	0.56	2.39	18	1
1:A:39:GLY:C	1:A:40:LEU:HD23	0.56	2.20	10	1
1:A:26:GLN:NE2	1:A:28:TRP:HE1	0.56	1.99	6	1
1:A:94:LEU:O	1:A:96:GLU:N	0.56	2.39	3	4
1:A:27:LEU:N	1:A:27:LEU:CD2	0.55	2.69	10	7
1:A:61:LEU:N	1:A:61:LEU:CD1	0.55	2.70	9	20
1:A:43:ASP:OD2	1:A:46:GLY:N	0.55	2.40	3	1
1:A:62:GLU:N	1:A:62:GLU:OE1	0.55	2.40	20	1
1:A:47:ILE:HD13	1:A:47:ILE:N	0.54	2.17	3	1
1:A:29:GLU:OE1	1:A:37:GLN:NE2	0.54	2.40	3	1
1:A:75:GLY:H	1:A:84:GLN:HE22	0.54	1.45	12	1
1:A:23:LYS:NZ	1:A:98:ILE:O	0.54	2.40	14	2
1:A:19:ASN:N	1:A:19:ASN:ND2	0.54	2.55	14	1
1:A:36:SER:OG	1:A:37:GLN:N	0.54	2.41	14	6
1:A:13:GLU:O	1:A:16:GLN:NE2	0.54	2.41	9	2
1:A:29:GLU:H	1:A:29:GLU:CD	0.54	2.05	6	2
1:A:50:PHE:CD1	1:A:50:PHE:O	0.54	2.61	12	1
1:A:14:ASN:ND2	1:A:74:VAL:O	0.53	2.42	13	2
1:A:29:GLU:OE1	1:A:29:GLU:N	0.53	2.41	13	1
1:A:43:ASP:N	1:A:43:ASP:OD1	0.53	2.42	19	3
1:A:99:GLU:N	1:A:99:GLU:OE1	0.53	2.42	13	2
1:A:70:ARG:NH2	1:A:92:GLU:OE2	0.53	2.42	5	1
1:A:44:GLU:N	1:A:44:GLU:OE2	0.53	2.41	4	2
1:A:19:ASN:OD1	1:A:71:SER:N	0.53	2.41	20	2
1:A:77:TYR:CD2	1:A:78:ASN:OD1	0.53	2.62	11	1
1:A:62:GLU:OE1	1:A:93:LYS:NZ	0.53	2.41	20	1
1:A:5:LEU:CD2	1:A:5:LEU:N	0.53	2.72	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:GLN:N	1:A:4:GLN:OE1	0.53	2.42	7	1
1:A:27:LEU:H	1:A:27:LEU:CD2	0.52	2.12	1	3
1:A:43:ASP:OD1	1:A:44:GLU:N	0.52	2.42	6	4
1:A:47:ILE:N	1:A:47:ILE:CD1	0.52	2.73	3	1
1:A:23:LYS:NZ	1:A:64:GLY:O	0.52	2.42	12	2
1:A:51:THR:OG1	1:A:82:GLN:NE2	0.52	2.43	2	1
1:A:19:ASN:ND2	1:A:71:SER:H	0.52	2.03	7	1
1:A:77:TYR:CB	1:A:82:GLN:HE21	0.52	2.18	13	1
1:A:77:TYR:CE2	1:A:78:ASN:OD1	0.51	2.62	14	3
1:A:70:ARG:NE	1:A:90:SER:OG	0.51	2.43	7	1
1:A:5:LEU:N	1:A:5:LEU:HD22	0.51	2.20	2	4
1:A:43:ASP:O	1:A:43:ASP:OD1	0.51	2.29	12	1
1:A:76:GLU:OE1	1:A:81:PHE:CE2	0.51	2.63	19	1
1:A:26:GLN:OE1	1:A:63:GLN:NE2	0.51	2.44	3	1
1:A:57:GLU:N	1:A:57:GLU:OE1	0.51	2.44	10	1
1:A:40:LEU:N	1:A:40:LEU:CD2	0.50	2.64	10	1
1:A:77:TYR:O	1:A:79:ASP:N	0.50	2.44	19	1
1:A:14:ASN:ND2	1:A:15:GLY:H	0.50	2.04	8	2
1:A:94:LEU:C	1:A:96:GLU:N	0.50	2.65	3	4
1:A:27:LEU:H	1:A:63:GLN:HE21	0.49	1.50	3	1
1:A:11:ILE:C	1:A:13:GLU:N	0.49	2.66	2	3
1:A:14:ASN:ND2	1:A:76:GLU:OE2	0.49	2.44	3	1
1:A:44:GLU:H	1:A:44:GLU:CD	0.49	2.11	10	1
1:A:66:SER:CB	1:A:96:GLU:O	0.49	2.60	5	1
1:A:6:THR:O	1:A:20:LEU:CD2	0.49	2.61	3	1
1:A:36:SER:OG	1:A:54:LYS:N	0.49	2.45	13	1
1:A:77:TYR:CG	1:A:82:GLN:NE2	0.49	2.81	13	1
1:A:70:ARG:NH2	1:A:90:SER:OG	0.49	2.46	7	1
1:A:19:ASN:C	1:A:20:LEU:HD22	0.49	2.28	18	2
1:A:87:LYS:C	1:A:89:SER:H	0.48	2.12	10	1
1:A:78:ASN:CG	1:A:79:ASP:N	0.48	2.67	16	3
1:A:40:LEU:HD21	1:A:49:LYS:NZ	0.48	2.23	4	1
1:A:94:LEU:C	1:A:96:GLU:H	0.48	2.12	2	2
1:A:87:LYS:O	1:A:88:ASN:CB	0.48	2.62	8	5
1:A:77:TYR:O	1:A:80:ARG:O	0.48	2.32	6	14
1:A:22:ALA:HB2	1:A:43:ASP:OD1	0.48	2.09	11	2
1:A:75:GLY:N	1:A:84:GLN:NE2	0.48	2.61	12	1
1:A:70:ARG:O	1:A:71:SER:OG	0.47	2.32	6	3
1:A:70:ARG:CZ	1:A:90:SER:OG	0.47	2.62	7	1
1:A:70:ARG:CZ	1:A:92:GLU:OE2	0.47	2.63	5	1
1:A:78:ASN:C	1:A:80:ARG:H	0.47	2.13	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:SER:C	1:A:67:TYR:CD1	0.47	2.88	20	1
1:A:40:LEU:HD12	1:A:40:LEU:N	0.47	2.25	1	1
1:A:86:ASN:O	1:A:87:LYS:O	0.47	2.33	10	3
1:A:50:PHE:CD1	1:A:50:PHE:C	0.47	2.88	12	2
1:A:21:LYS:O	1:A:43:ASP:OD1	0.47	2.33	12	1
1:A:41:LEU:HD21	1:A:50:PHE:CE1	0.47	2.44	17	2
1:A:39:GLY:C	1:A:50:PHE:CE2	0.46	2.88	14	2
1:A:29:GLU:CD	1:A:29:GLU:N	0.46	2.69	11	1
1:A:24:VAL:O	1:A:63:GLN:NE2	0.46	2.47	5	2
1:A:71:SER:O	1:A:71:SER:OG	0.46	2.33	11	2
1:A:36:SER:OG	1:A:54:LYS:CA	0.46	2.63	13	1
1:A:78:ASN:O	1:A:80:ARG:N	0.46	2.48	14	2
1:A:12:VAL:O	1:A:12:VAL:HG22	0.46	2.11	9	2
1:A:43:ASP:OD2	1:A:45:THR:OG1	0.46	2.34	13	1
1:A:76:GLU:OE2	1:A:79:ASP:N	0.46	2.49	7	1
1:A:12:VAL:O	1:A:12:VAL:CG2	0.46	2.64	9	1
1:A:11:ILE:C	1:A:13:GLU:H	0.46	2.13	14	1
1:A:76:GLU:OE2	1:A:78:ASN:O	0.45	2.34	15	1
1:A:19:ASN:OD1	1:A:69:LEU:O	0.45	2.34	10	4
1:A:84:GLN:NE2	1:A:84:GLN:N	0.45	2.65	12	1
1:A:6:THR:O	1:A:20:LEU:HD13	0.45	2.11	5	2
1:A:96:GLU:CD	1:A:96:GLU:N	0.45	2.69	9	1
1:A:10:ASP:O	1:A:10:ASP:OD1	0.45	2.35	9	6
1:A:63:GLN:O	1:A:65:GLU:OE1	0.45	2.35	18	3
1:A:26:GLN:CD	1:A:28:TRP:HE1	0.45	2.15	9	3
1:A:12:VAL:CG2	1:A:12:VAL:O	0.45	2.64	15	1
1:A:68:LEU:HD13	1:A:69:LEU:N	0.45	2.26	20	1
1:A:79:ASP:O	1:A:79:ASP:OD1	0.45	2.34	4	2
1:A:43:ASP:OD1	1:A:46:GLY:O	0.45	2.34	13	2
1:A:51:THR:CG2	1:A:84:GLN:OE1	0.45	2.65	9	1
1:A:87:LYS:O	1:A:89:SER:N	0.44	2.50	10	1
1:A:38:VAL:HG12	1:A:39:GLY:N	0.44	2.27	7	1
1:A:62:GLU:N	1:A:67:TYR:OH	0.44	2.50	1	4
1:A:83:VAL:O	1:A:83:VAL:HG23	0.44	2.12	10	1
1:A:25:ILE:HD11	1:A:42:GLY:CA	0.44	2.43	2	2
1:A:44:GLU:N	1:A:44:GLU:CD	0.44	2.71	4	1
1:A:63:GLN:CD	1:A:64:GLY:N	0.44	2.72	13	1
1:A:98:ILE:N	1:A:98:ILE:HD13	0.44	2.27	6	1
1:A:14:ASN:OD1	1:A:14:ASN:O	0.43	2.36	1	4
1:A:26:GLN:C	1:A:27:LEU:HD22	0.43	2.34	6	1
1:A:41:LEU:CD2	1:A:50:PHE:CD1	0.43	3.00	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ASN:C	1:A:80:ARG:N	0.43	2.72	14	2
1:A:50:PHE:C	1:A:50:PHE:CD1	0.43	2.92	14	1
1:A:86:ASN:N	1:A:89:SER:OG	0.43	2.50	19	1
1:A:18:ALA:O	1:A:19:ASN:ND2	0.43	2.50	7	1
1:A:5:LEU:CD2	1:A:19:ASN:HD22	0.43	2.27	10	1
1:A:79:ASP:OD1	1:A:79:ASP:O	0.43	2.36	9	1
1:A:41:LEU:HD11	1:A:50:PHE:CD1	0.43	2.49	12	1
1:A:96:GLU:N	1:A:96:GLU:OE1	0.43	2.51	16	1
1:A:62:GLU:OE1	1:A:63:GLN:O	0.43	2.37	3	1
1:A:77:TYR:CD2	1:A:82:GLN:NE2	0.43	2.87	13	1
1:A:79:ASP:N	1:A:79:ASP:OD1	0.43	2.51	19	2
1:A:18:ALA:O	1:A:19:ASN:OD1	0.43	2.36	2	3
1:A:76:GLU:O	1:A:76:GLU:OE1	0.43	2.36	7	1
1:A:28:TRP:N	1:A:38:VAL:O	0.43	2.51	20	1
1:A:77:TYR:O	1:A:78:ASN:C	0.43	2.57	11	4
1:A:26:GLN:CD	1:A:63:GLN:NE2	0.43	2.71	3	1
1:A:77:TYR:O	1:A:78:ASN:OD1	0.43	2.37	6	1
1:A:43:ASP:CG	1:A:44:GLU:N	0.43	2.71	13	1
1:A:11:ILE:HG22	1:A:13:GLU:H	0.43	1.74	2	1
1:A:25:ILE:CD1	1:A:42:GLY:N	0.43	2.82	6	1
1:A:77:TYR:CD1	1:A:82:GLN:NE2	0.43	2.86	15	1
1:A:47:ILE:C	1:A:47:ILE:CD1	0.43	2.87	16	2
1:A:13:GLU:OE1	1:A:14:ASN:O	0.43	2.36	20	1
1:A:73:VAL:HG22	1:A:74:VAL:N	0.42	2.29	8	1
1:A:26:GLN:HB3	1:A:40:LEU:HD21	0.42	1.92	10	1
1:A:68:LEU:HD21	1:A:70:ARG:NE	0.42	2.29	2	1
1:A:13:GLU:O	1:A:16:GLN:OE1	0.42	2.36	13	1
1:A:62:GLU:OE1	1:A:65:GLU:OE2	0.42	2.36	17	1
1:A:78:ASN:CG	1:A:79:ASP:H	0.42	2.16	9	2
1:A:77:TYR:CZ	1:A:78:ASN:OD1	0.42	2.73	5	1
1:A:14:ASN:OD1	1:A:76:GLU:OE1	0.42	2.37	19	1
1:A:93:LYS:C	1:A:94:LEU:HD22	0.42	2.35	1	3
1:A:3:PRO:CG	1:A:19:ASN:ND2	0.42	2.83	6	1
1:A:36:SER:OG	1:A:53:TRP:C	0.42	2.58	15	1
1:A:47:ILE:O	1:A:80:ARG:NH2	0.41	2.52	4	1
1:A:44:GLU:OE1	1:A:99:GLU:O	0.41	2.37	7	1
1:A:25:ILE:H	1:A:25:ILE:HD13	0.41	1.74	6	1
1:A:20:LEU:HD13	1:A:20:LEU:H	0.41	1.72	7	1
1:A:56:ALA:C	1:A:57:GLU:OE1	0.41	2.58	10	1
1:A:62:GLU:O	1:A:65:GLU:OE1	0.41	2.38	18	1
1:A:3:PRO:CB	1:A:19:ASN:ND2	0.41	2.83	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:GLU:OE1	1:A:99:GLU:N	0.41	2.47	1	1
1:A:41:LEU:O	1:A:47:ILE:HG23	0.41	2.16	4	1
1:A:56:ALA:O	1:A:57:GLU:C	0.41	2.58	4	1
1:A:20:LEU:HD22	1:A:21:LYS:N	0.41	2.30	7	1
1:A:51:THR:HG22	1:A:84:GLN:NE2	0.41	2.31	9	1
1:A:86:ASN:O	1:A:87:LYS:C	0.41	2.59	8	1
1:A:28:TRP:O	1:A:37:GLN:OE1	0.41	2.39	3	1
1:A:39:GLY:C	1:A:40:LEU:HD22	0.41	2.36	6	1
1:A:88:ASN:O	1:A:89:SER:O	0.41	2.39	7	1
1:A:27:LEU:HD22	1:A:63:GLN:OE1	0.40	2.16	1	1
1:A:29:GLU:OE2	1:A:37:GLN:NE2	0.40	2.55	4	1
1:A:38:VAL:CG1	1:A:39:GLY:N	0.40	2.83	7	1
1:A:44:GLU:O	1:A:44:GLU:CD	0.40	2.59	8	1
1:A:95:SER:OG	1:A:96:GLU:OE2	0.40	2.39	16	1
1:A:4:GLN:N	1:A:4:GLN:CD	0.40	2.74	8	1
1:A:56:ALA:HB1	1:A:58:LEU:HD13	0.40	1.92	11	1
1:A:77:TYR:C	1:A:78:ASN:OD1	0.40	2.60	11	1
1:A:13:GLU:OE2	1:A:14:ASN:O	0.40	2.39	20	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	92/109 (84%)	86±2 (94±2%)	4±1 (4±2%)	1±1 (2±1%)	13	57
All	All	1840/2180 (84%)	1729 (94%)	82 (4%)	29 (2%)	13	57

All 11 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	12	VAL	8
1	A	99	GLU	4
1	A	11	ILE	3
1	A	87	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	95	SER	3
1	A	35	ILE	2
1	A	79	ASP	2
1	A	57	GLU	1
1	A	89	SER	1
1	A	44	GLU	1
1	A	78	ASN	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	83/99 (84%)	81±1 (98±2%)	2±1 (2±2%)	57 93
All	All	1660/1980 (84%)	1626 (98%)	34 (2%)	57 93

All 23 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	94	LEU	3
1	A	4	GLN	3
1	A	20	LEU	2
1	A	47	ILE	2
1	A	83	VAL	2
1	A	68	LEU	2
1	A	88	ASN	2
1	A	40	LEU	2
1	A	43	ASP	2
1	A	26	GLN	1
1	A	24	VAL	1
1	A	25	ILE	1
1	A	98	ILE	1
1	A	86	ASN	1
1	A	29	GLU	1
1	A	50	PHE	1
1	A	99	GLU	1
1	A	28	TRP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	55	ASN	1
1	A	19	ASN	1
1	A	12	VAL	1
1	A	27	LEU	1
1	A	36	SER	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