Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 01:07 PM EDT

PDB ID	:	2EXN
Title	:	Solution structure for the protein coded by gene locus BB0938 of Bordetella bronchiseptica. Northeast Structural Genomics target BoR11.
Authors	:	Rossi, P.; Ramelot, T.; Xiao, R.; Ho, C.K.; Ma, L.-C.; Acton, T.B.; Kennedy, M.A.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2005-11-08

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:

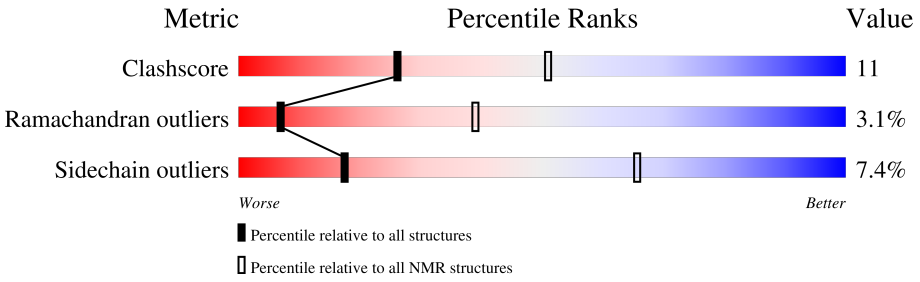
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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	136	65% 18% • 11% •

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 5 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 target function*.

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:71, A:80-A:127 (115)	0.84	5

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	2, 5, 7
2	1, 6, 8
Single-model clusters	3; 4; 9; 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2010 atoms, of which 999 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein BoR11.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	130	2010	635	999	174	194	8	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MET	-	expression tag	UNP Q7WNU7
A	122	ALA	-	expression tag	UNP Q7WNU7
A	123	GLU	-	expression tag	UNP Q7WNU7
A	124	VAL	-	expression tag	UNP Q7WNU7
A	125	ARG	-	expression tag	UNP Q7WNU7
A	126	TRP	-	expression tag	UNP Q7WNU7
A	127	PRO	-	expression tag	UNP Q7WNU7
A	128	SER	-	expression tag	UNP Q7WNU7
A	129	LEU	-	expression tag	UNP Q7WNU7
A	130	GLU	-	expression tag	UNP Q7WNU7
A	131	HIS	-	expression tag	UNP Q7WNU7
A	132	HIS	-	expression tag	UNP Q7WNU7
A	133	HIS	-	expression tag	UNP Q7WNU7
A	134	HIS	-	expression tag	UNP Q7WNU7
A	135	HIS	-	expression tag	UNP Q7WNU7
A	136	HIS	-	expression tag	UNP Q7WNU7

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: Hypothetical protein BoR11

Chain A: 65% 18% • 11% •

M1 S2 T3 T4 A5 Y6 Q7 P8 I9 A10 E11 C12 A20 Q24 W27 L28 V29 A30 N31 W36 L45 V48 S49 V50 A61 M64 L65 D72 V73 I74 E75 D76 D77 D78 S79 M84 D95 V110 P111 C112 L115 H118 V124 R125 W126

P127 S128 L129 E130 HIS HIS HIS HIS HIS HIS

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: Hypothetical protein BoR11

Chain A: 57% 25% • 11% •

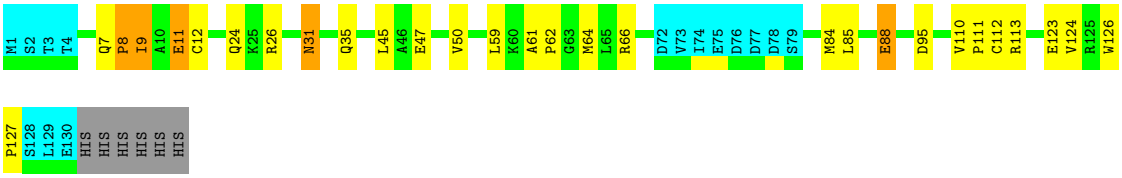
M1 S2 T3 T4 A5 P8 I9 A10 E11 C12 G13 A14 T15 T16 A20 Q24 W27 L28 V29 A30 N31 W36 R39 L45 V48 S49 V50 E51 L52 L57 A61 M64 L65 L71 D72 V73 I74 E75 D76 D77 D78 S79 V86 G87 E88 D92

D95 L99 V110 P111 C112 R113 I114 H118 A122 E123 V124 R125 W126 P127 S128 L129 E130 HIS HIS HIS HIS HIS HIS

4.2.2 Score per residue for model 2

• Molecule 1: Hypothetical protein BoR11

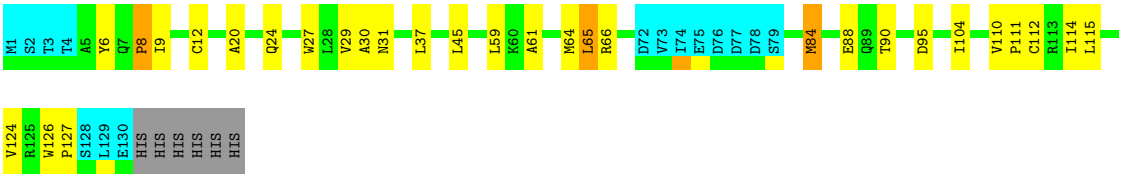
Chain A: 63% 18% • 11% •



4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical protein BoR11

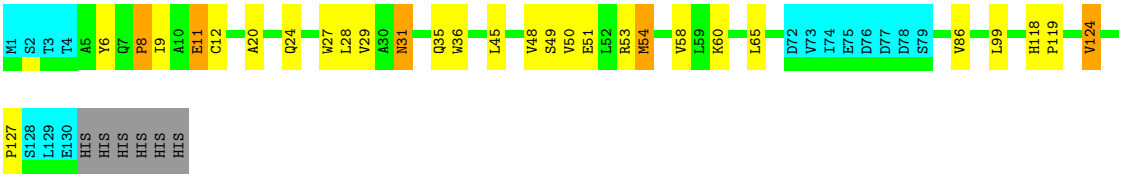
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein BoR11

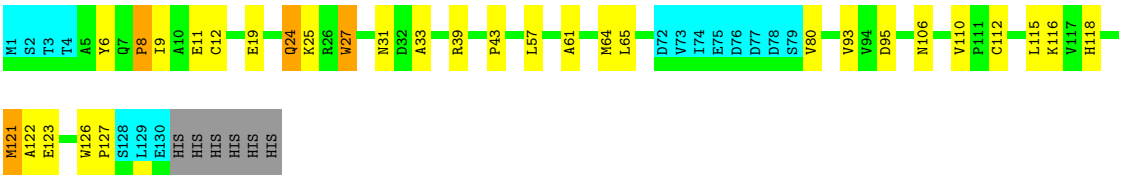
Chain A:



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Hypothetical protein BoR11

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein BoR11

Chain A: 60% 21% • 11% •

M1 S2 T3 T4 A5 Y6 Q7 P8 I9 A10 E11 C12 A20 W27 L28 V29 W36 V48 S49 V50 E51 L52 R53 M54 L59 K60 A61 M64 L65 R66 L67 D72 V73 I74 E75 D76 D77 D78 S79 V80 R81 Y82 Q83 M84 Q89 T90 V91 D92 V93 A102

S105 L115 K116 V117 H118 V124 R125 W126 P127 S128 L129 E130 HIS HIS HIS HIS HIS HIS

4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein BoR11

Chain A: 61% 23% • 11% •

M1 S2 T3 T4 A5 Y6 Q7 P8 I9 A10 E11 C12 G13 A14 A20 Q24 W27 L37 L45 A46 E47 V48 S49 V50 E51 L52 R53 M54 L65 D72 V73 I74 E75 D76 D77 D78 S79 Y82 Q83 M84 T90 V91 D92 V93 V94 D95 V110 P111 C112 R113

I114 L115 H118 P119 R125 W126 P127 S128 L129 E130 HIS HIS HIS HIS HIS HIS

4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein BoR11

Chain A: 60% 20% • 11% •

M1 S2 T3 T4 P8 I9 A10 E11 C12 Q24 K25 R26 W27 L28 V29 W36 L37 C42 L45 A46 E47 V48 S49 V50 R53 Y56 L65 P70 L71 D72 V73 I74 E75 D76 D77 D78 S79 M84 D92 V93 V94 D95 L99 V110 P111 C112

L115 H118 A122 E123 V124 R125 W126 P127 S128 L129 E130 HIS HIS HIS HIS HIS HIS

4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical protein BoR11

Chain A: 55% 27% • 11% •

M1 S2 T3 T4 A5 Y6 Q7 P8 I9 A10 E11 C12 Q17 A20 Q24 K25 R26 W27 L28 V29 A30 N31 W36 L37 N38 L41 C42 P43 R44 L45 A46 E47 V48 M54 A61 M64 L65 D72 V73 I74 E75 D76 D77 D78 S79 V80 R81 V86 G87 E88

D92 D95 E96 I104 H107 V110 P111 C112 L115 V124 S128 L129 E130 HIS HIS HIS HIS HIS HIS

4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein BoR11

Chain A: 53% 26% 6% 11% •

M1 S2 T3 T4 A5 P8 I9 A10 E11 C12 G13 A14 Q24 K25 R26 W27 L28 V29 Q35 W36 L45 A46 E47 V48 S49 V50 L57 V58 L59 K60 A61 M64 L65 R66 L67 D68 I69 P70 L71 D72 V73 I74 E75 D76 D77 D78 S79 H84 L85 V86 Q89

A101 I104 A108 G109 V110 P111 C112 R113 H118 P119 D120 M121 A122 E123 V124 R125 W126 P127 S128 L129 E130 HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *CS assignment: Backbone AutoAssign, manual sidechain HcCH-COSY and TOCSYs. AutoStructure for noesy assign. Hyper Dihedral, Dyana, Xplor(nih), and CNS force-field for simulated annealing (Dyana,xplor run within AutoStructure GUI).*

Of the 56 calculated structures, 10 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
AutoStructure	structure solution	2.1.1
CNS	refinement	1.1
xplor(nih)	structure solution	2.0.6
DYANA	structure solution	1.5

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	898	900	898	20±3
All	All	8980	9000	8980	201

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 11.

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:ILE:HB	1:A:12:CYS:SG	0.71	2.24	3	4
1:A:9:ILE:HD11	1:A:57:LEU:HD21	0.71	1.62	5	2
1:A:11:GLU:HG2	1:A:29:VAL:HG23	0.69	1.63	1	3
1:A:8:PRO:HG3	1:A:20:ALA:HB1	0.68	1.63	9	4
1:A:12:CYS:HA	1:A:48:VAL:HB	0.68	1.62	4	7
1:A:29:VAL:HG22	1:A:114:ILE:HD13	0.67	1.67	3	1
1:A:85:LEU:HG	1:A:88:GLU:HA	0.67	1.64	2	1
1:A:11:GLU:HB2	1:A:45:LEU:HB3	0.65	1.68	9	1
1:A:8:PRO:HA	1:A:24:GLN:CB	0.65	2.22	7	5
1:A:11:GLU:HB2	1:A:45:LEU:HG	0.65	1.69	8	2
1:A:44:ARG:O	1:A:47:GLU:HG2	0.63	1.94	9	1
1:A:31:ASN:HD21	1:A:35:GLN:HB3	0.62	1.52	2	2
1:A:29:VAL:HG23	1:A:37:LEU:HB3	0.62	1.71	8	1
1:A:65:LEU:H	1:A:65:LEU:HD12	0.61	1.54	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:GLU:OE2	1:A:28:LEU:HA	0.61	1.96	10	2
1:A:36:TRP:CZ2	1:A:124:VAL:HG21	0.61	2.30	9	1
1:A:6:TYR:O	1:A:8:PRO:HD3	0.60	1.96	7	6
1:A:37:LEU:HG	1:A:42:CYS:SG	0.59	2.37	8	2
1:A:126:TRP:CG	1:A:127:PRO:HD2	0.59	2.32	2	7
1:A:47:GLU:O	1:A:62:PRO:HD2	0.58	1.98	2	1
1:A:11:GLU:O	1:A:46:ALA:HA	0.58	1.97	10	4
1:A:36:TRP:CH2	1:A:124:VAL:HB	0.57	2.34	1	2
1:A:61:ALA:HB3	1:A:64:MET:HB2	0.57	1.74	10	7
1:A:11:GLU:HB3	1:A:45:LEU:HG	0.57	1.76	7	3
1:A:86:VAL:HG21	1:A:124:VAL:HB	0.57	1.75	9	1
1:A:118:HIS:CD2	1:A:119:PRO:HD2	0.57	2.34	10	3
1:A:99:LEU:H	1:A:99:LEU:HD23	0.57	1.59	1	2
1:A:110:VAL:HG23	1:A:112:CYS:SG	0.57	2.40	10	8
1:A:95:ASP:HA	1:A:115:LEU:HD23	0.57	1.76	9	2
1:A:5:ALA:HB1	1:A:14:ALA:HB1	0.56	1.77	1	3
1:A:9:ILE:HG23	1:A:27:TRP:HB3	0.56	1.76	5	1
1:A:30:ALA:HB3	1:A:115:LEU:HD12	0.56	1.76	3	2
1:A:95:ASP:OD2	1:A:113:ARG:HD3	0.56	2.01	2	1
1:A:42:CYS:SG	1:A:45:LEU:HD22	0.55	2.40	9	2
1:A:9:ILE:HD11	1:A:57:LEU:HD11	0.55	1.78	1	1
1:A:45:LEU:O	1:A:48:VAL:HG23	0.55	2.02	9	3
1:A:84:MET:HA	1:A:84:MET:CE	0.55	2.32	7	1
1:A:9:ILE:HB	1:A:12:CYS:HB2	0.54	1.79	1	3
1:A:26:ARG:NH1	1:A:123:GLU:HA	0.54	2.18	2	1
1:A:86:VAL:HG12	1:A:127:PRO:HD3	0.54	1.78	10	3
1:A:36:TRP:CD1	1:A:86:VAL:HG22	0.54	2.38	4	1
1:A:95:ASP:OD1	1:A:113:ARG:HD3	0.53	2.04	7	2
1:A:9:ILE:HD11	1:A:57:LEU:CD2	0.53	2.33	5	1
1:A:92:ASP:O	1:A:118:HIS:HB2	0.53	2.04	8	1
1:A:84:MET:O	1:A:90:THR:HA	0.52	2.04	6	2
1:A:125:ARG:O	1:A:126:TRP:HB2	0.52	2.02	10	1
1:A:39:ARG:O	1:A:43:PRO:HA	0.52	2.04	5	1
1:A:12:CYS:HB3	1:A:50:VAL:HG22	0.52	1.81	10	4
1:A:9:ILE:HB	1:A:12:CYS:HG	0.52	1.63	5	1
1:A:99:LEU:HD23	1:A:99:LEU:H	0.52	1.65	4	1
1:A:37:LEU:HD22	1:A:112:CYS:SG	0.51	2.46	7	1
1:A:8:PRO:HA	1:A:24:GLN:HB3	0.51	1.81	7	2
1:A:11:GLU:CD	1:A:11:GLU:H	0.50	2.09	6	5
1:A:12:CYS:HB3	1:A:50:VAL:HB	0.50	1.81	6	1
1:A:12:CYS:HB2	1:A:50:VAL:HG22	0.50	1.82	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:GLN:HE21	1:A:124:VAL:HG13	0.50	1.66	10	1
1:A:8:PRO:HA	1:A:24:GLN:HA	0.50	1.84	9	4
1:A:91:VAL:HG21	1:A:124:VAL:HG21	0.49	1.83	6	1
1:A:86:VAL:HG21	1:A:124:VAL:CG1	0.49	2.37	4	2
1:A:81:ARG:HB2	1:A:92:ASP:HB2	0.49	1.83	9	1
1:A:84:MET:HE2	1:A:115:LEU:HD12	0.49	1.83	8	1
1:A:12:CYS:SG	1:A:50:VAL:HG22	0.49	2.48	2	1
1:A:85:LEU:CG	1:A:88:GLU:HA	0.49	2.37	2	1
1:A:59:LEU:O	1:A:66:ARG:HA	0.48	2.08	10	3
1:A:9:ILE:HA	1:A:27:TRP:HB3	0.48	1.85	7	3
1:A:49:SER:HB2	1:A:60:LYS:HG3	0.48	1.85	4	1
1:A:38:ASN:OD1	1:A:41:LEU:HG	0.47	2.09	9	1
1:A:42:CYS:HB2	1:A:45:LEU:HD13	0.46	1.86	9	1
1:A:11:GLU:HG2	1:A:29:VAL:CG2	0.46	2.38	1	2
1:A:36:TRP:HB2	1:A:126:TRP:CD1	0.46	2.46	1	1
1:A:20:ALA:HA	1:A:52:LEU:HD22	0.45	1.86	1	3
1:A:9:ILE:HG22	1:A:11:GLU:OE2	0.44	2.13	1	2
1:A:93:VAL:HG21	1:A:115:LEU:HD13	0.44	1.89	5	2
1:A:59:LEU:HB2	1:A:67:LEU:HB3	0.44	1.89	6	1
1:A:95:ASP:HA	1:A:115:LEU:CD2	0.44	2.42	8	1
1:A:30:ALA:HB3	1:A:115:LEU:CD1	0.43	2.43	3	1
1:A:31:ASN:ND2	1:A:33:ALA:H	0.43	2.10	5	1
1:A:89:GLN:HE21	1:A:124:VAL:HG22	0.43	1.73	6	1
1:A:121:MET:SD	1:A:122:ALA:N	0.43	2.91	5	1
1:A:11:GLU:OE1	1:A:29:VAL:HG23	0.43	2.14	10	1
1:A:51:GLU:HB3	1:A:58:VAL:HB	0.43	1.91	4	1
1:A:110:VAL:HG23	1:A:112:CYS:HG	0.43	1.71	8	1
1:A:86:VAL:HG12	1:A:127:PRO:CD	0.42	2.43	10	1
1:A:9:ILE:HD13	1:A:50:VAL:HG11	0.42	1.90	4	1
1:A:104:ILE:HD12	1:A:107:HIS:HB3	0.42	1.92	9	1
1:A:84:MET:SD	1:A:93:VAL:HG11	0.42	2.54	8	1
1:A:82:TYR:O	1:A:93:VAL:HG22	0.42	2.15	6	2
1:A:104:ILE:HG22	1:A:112:CYS:HB2	0.42	1.91	3	1
1:A:80:VAL:HB	1:A:95:ASP:HB3	0.42	1.91	5	1
1:A:36:TRP:NE1	1:A:84:MET:SD	0.42	2.93	10	2
1:A:84:MET:HA	1:A:84:MET:HE2	0.42	1.89	7	1
1:A:37:LEU:HD23	1:A:45:LEU:HD22	0.42	1.90	3	1
1:A:31:ASN:HA	1:A:112:CYS:SG	0.42	2.55	9	1
1:A:12:CYS:CB	1:A:50:VAL:HG22	0.41	2.45	2	1
1:A:29:VAL:HG22	1:A:114:ILE:HG12	0.41	1.92	1	1
1:A:116:LYS:HZ3	1:A:116:LYS:HB3	0.41	1.76	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:VAL:HB	1:A:111:PRO:HD2	0.41	1.92	2	1
1:A:5:ALA:HB1	1:A:14:ALA:CB	0.41	2.46	7	1
1:A:53:ARG:HB3	1:A:56:TYR:HB2	0.41	1.93	8	1
1:A:47:GLU:HB3	1:A:62:PRO:HG2	0.41	1.92	2	1
1:A:102:ALA:HA	1:A:105:SER:OG	0.41	2.15	6	1
1:A:101:ALA:HA	1:A:113:ARG:HA	0.41	1.92	10	1
1:A:24:GLN:O	1:A:25:LYS:HG3	0.40	2.15	5	1
1:A:104:ILE:O	1:A:108:ALA:N	0.40	2.54	10	1
1:A:121:MET:SD	1:A:121:MET:N	0.40	2.94	10	1
1:A:11:GLU:CG	1:A:29:VAL:HG23	0.40	2.42	1	1
1:A:39:ARG:H	1:A:39:ARG:CD	0.40	2.29	1	1
1:A:9:ILE:HA	1:A:27:TRP:CB	0.40	2.46	10	1
1:A:26:ARG:HD2	1:A:122:ALA:O	0.40	2.17	8	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	115/136 (85%)	101±1 (88±1%)	10±1 (9±1%)	4±1 (3±1%)	7	39
All	All	1150/1360 (85%)	1011 (88%)	103 (9%)	36 (3%)	7	39

All 12 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	LEU	9
1	A	8	PRO	7
1	A	124	VAL	4
1	A	111	PRO	3
1	A	54	MET	3
1	A	122	ALA	2
1	A	126	TRP	2
1	A	125	ARG	2
1	A	71	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	123	GLU	1
1	A	127	PRO	1
1	A	119	PRO	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	93/114 (82%)	86±2 (93±2%)	7±2 (7±2%)	17 65
All	All	930/1140 (82%)	861 (93%)	69 (7%)	17 65

All 30 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	27	TRP	8
1	A	11	GLU	7
1	A	31	ASN	4
1	A	88	GLU	4
1	A	118	HIS	4
1	A	24	GLN	4
1	A	7	GLN	3
1	A	9	ILE	3
1	A	84	MET	3
1	A	50	VAL	3
1	A	92	ASP	2
1	A	28	LEU	2
1	A	54	MET	2
1	A	121	MET	2
1	A	81	ARG	2
1	A	90	THR	2
1	A	16	THR	1
1	A	39	ARG	1
1	A	53	ARG	1
1	A	19	GLU	1
1	A	106	ASN	1
1	A	116	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	29	VAL	1
1	A	17	GLN	1
1	A	25	LYS	1
1	A	96	GLU	1
1	A	26	ARG	1
1	A	35	GLN	1
1	A	68	ASP	1
1	A	86	VAL	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