Full wwPDB NMR Structure Validation Report (i)

Oct 2, 2021 – 01:37 PM EDT

PDB ID	:	2KM7
Title	:	Solution Structure of BamE, a component of the outer membrane protein assembly machinery in Escherichia coli
Authors	:	Knowles, T.J.; Sridhar, P.; Rajesh, S.; Manoli, E.; Henderson, I.R.; Overduin, M.
Deposited on	:	2009-07-24

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:

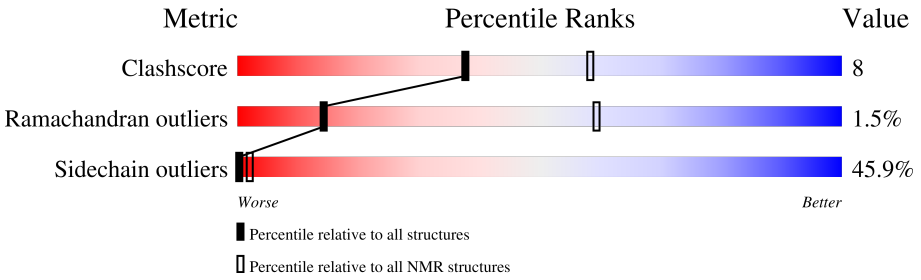
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	102	31% 41% • 26%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:36-A:110 (75)	0.84	11

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1585 atoms, of which 777 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Small protein A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	102	1585	504	777	147	155	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	CYS	engineered mutation	UNP P0A937
A	114	LEU	-	expression tag	UNP P0A937
A	115	GLU	-	expression tag	UNP P0A937
A	116	HIS	-	expression tag	UNP P0A937
A	117	HIS	-	expression tag	UNP P0A937
A	118	HIS	-	expression tag	UNP P0A937
A	119	HIS	-	expression tag	UNP P0A937
A	120	HIS	-	expression tag	UNP P0A937
A	121	HIS	-	expression tag	UNP P0A937

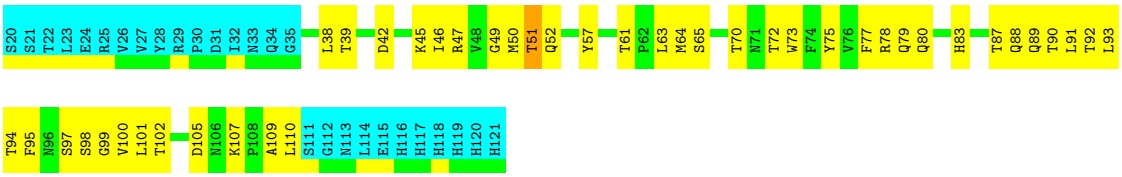
4 Residue-property plots (i)

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: Small protein A

Chain A: 31% 41% • 26%



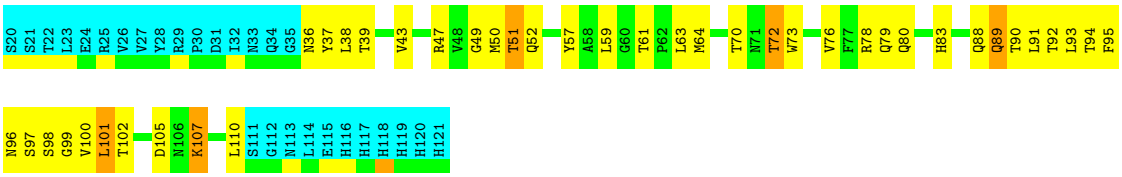
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Small protein A

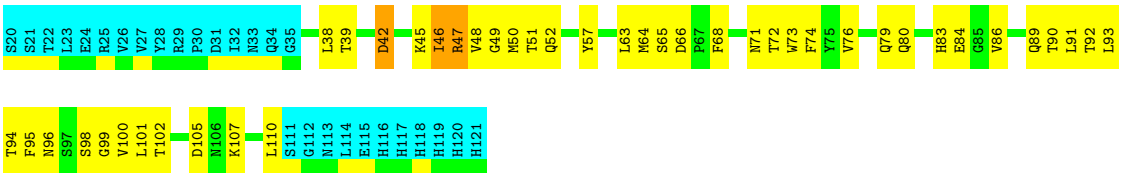
Chain A: 33% 35% 5% 26%



4.2.2 Score per residue for model 2

• Molecule 1: Small protein A

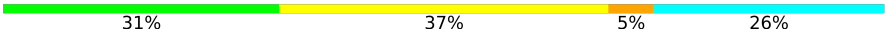
Chain A: 31% 39% • 26%

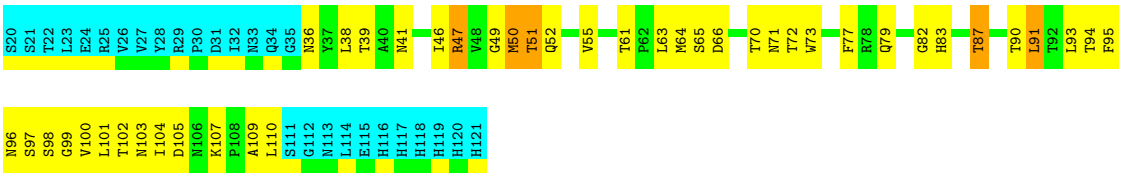


4.2.3 Score per residue for model 3

- Molecule 1: Small protein A

Chain A:

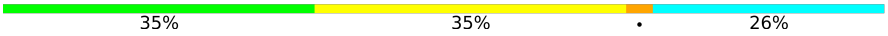


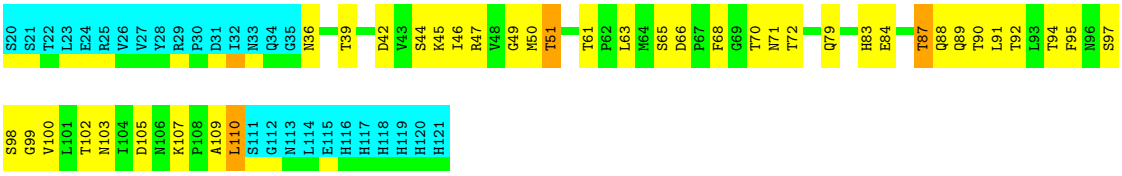


4.2.4 Score per residue for model 4

- Molecule 1: Small protein A

Chain A:

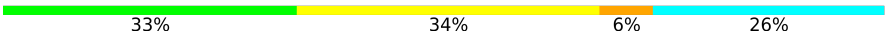


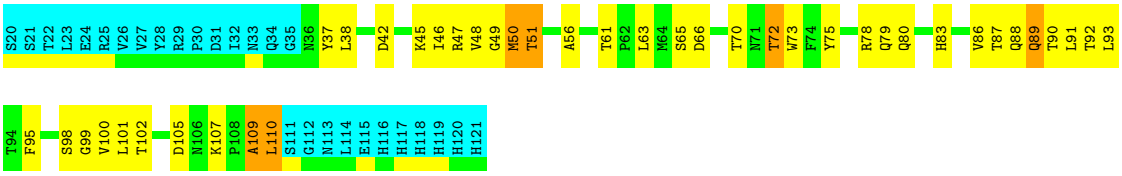


4.2.5 Score per residue for model 5

- Molecule 1: Small protein A

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: Small protein A

Chain A: 32% 36% 5% 26%

S20 S21 T22 L23 E24 R25 V26 V27 Y28 R29 P30 D31 I32 N33 Q34 G35 L38 T39 D42 K45 I46 R47 V48 G49 M50 T51 V55 A56 Y57 T61 P62 L63 M64 S65 D66 T72 W73 F74 Y75 Q79 H83 V86 T87 Q88 Q89 T90 L91 T92 L93 T94 F95

N96 S97 S98 G99 V100 L101 T102 N106 K107 P108 A109 L110 S111 G112 N113 L114 E115 H116 H117 H118 H119 H120 H121

4.2.7 Score per residue for model 7

- Molecule 1: Small protein A

Chain A: 33% 32% 8% 26%

S20 S21 T22 L23 E24 R25 V26 V27 Y28 R29 P30 D31 I32 N33 Q34 G35 T39 D42 K45 I46 R47 V48 G49 M50 T51 Q54 Y57 A58 M64 S65 T70 N71 T72 W73 F74 Y75 V76 F77 R78 Q79 Q80 H83 V86 T87 Q88 Q89 T90 L91 T92 L93 T94

F95 N96 S97 S98 G99 V100 L101 T102 D105 N106 K107 P108 A109 L110 S111 G112 N113 L114 E115 H116 H117 H118 H119 H120 H121

4.2.8 Score per residue for model 8

- Molecule 1: Small protein A

Chain A: 32% 35% 6% 26%

S20 S21 T22 L23 E24 R25 V26 V27 Y28 R29 P30 D31 I32 N33 Q34 G35 N36 Y37 L38 T39 D42 V43 S44 K45 I46 R47 V48 G49 M50 T51 Q52 Y57 A58 L59 G60 T61 P62 L63 M64 S65 T70 N71 T72 W73 F74 Y75 V76 Q79 H83 V86 T87 Q88 Q89 T90

L91 T92 L93 T94 F95 N96 S97 S98 G99 V100 L101 T102 N103 I104 P108 A109 L110 S111 G112 N113 L114 E115 H116 H117 H118 H119 H120 H121

4.2.9 Score per residue for model 9

- Molecule 1: Small protein A

Chain A: 29% 34% 10% 26%

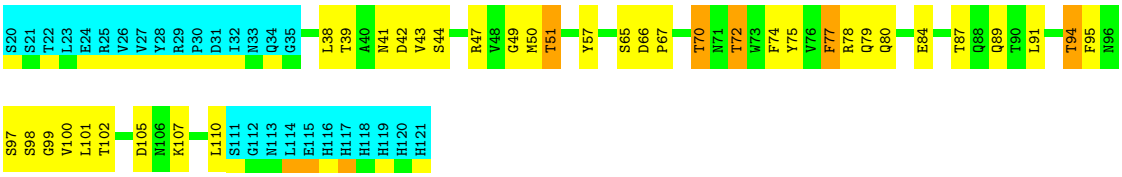
S20 S21 T22 L23 E24 R25 V26 V27 Y28 R29 P30 D31 I32 N33 Q34 G35 D42 V43 S44 K45 I46 R47 V48 G49 M50 T51 Q52 Q53 Q54 V55 A56 Y57 A58 L59 G60 T61 P62 L63 M64 S65 T72 W73 F77 R78 Q79 Q80 P81 G82 H83 E84 G85 V86 T87 Q88 Q89 T90 L91

T92 L93 T94 F95 N96 S97 S98 G99 V100 L101 T102 N103 K107 P108 A109 L110 S111 G112 N113 L114 E115 H116 H117 H118 H119 H120 H121

4.2.10 Score per residue for model 10

- Molecule 1: Small protein A

Chain A: 37% 31% 5% 26%



4.2.11 Score per residue for model 11 (medoid)

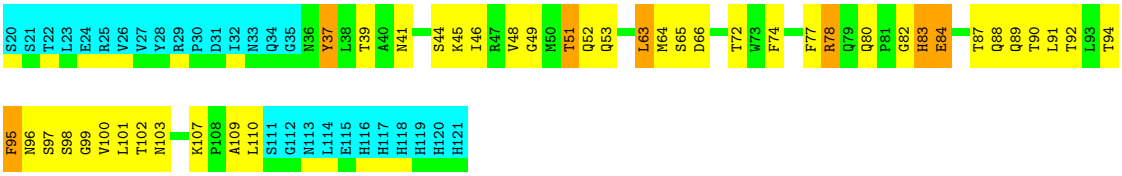
- Molecule 1: Small protein A

Chain A: 34% 35% • 26%

4.2.12 Score per residue for model 12

- Molecule 1: Small protein A

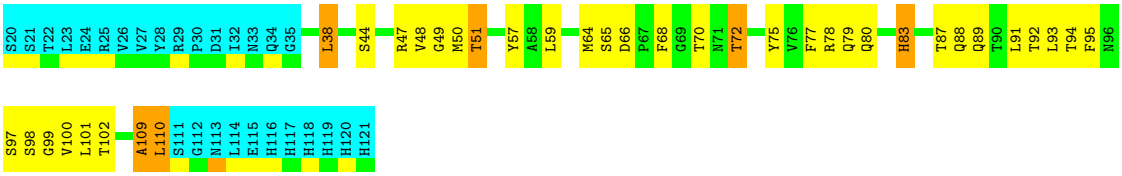
Chain A: 32% 34% 7% 26%



4.2.13 Score per residue for model 13

- Molecule 1: Small protein A

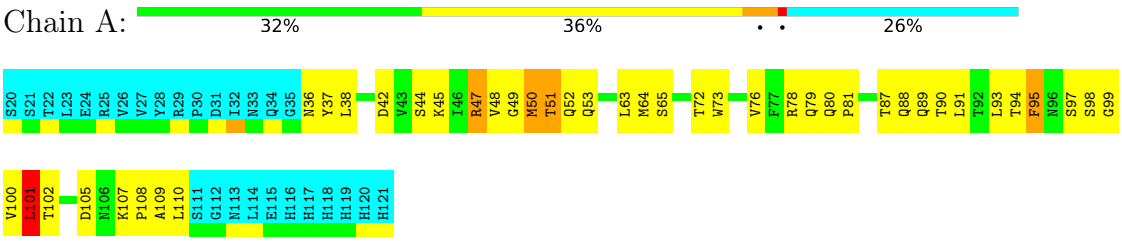
Chain A: 37% 30% 6% 26%



4.2.14 Score per residue for model 14

- Molecule 1: Small protein A

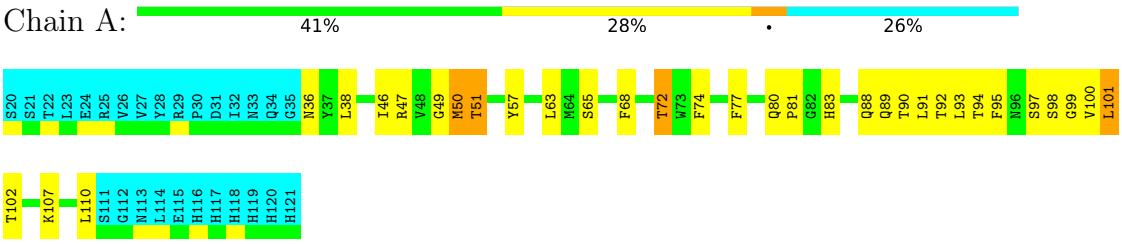
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Small protein A

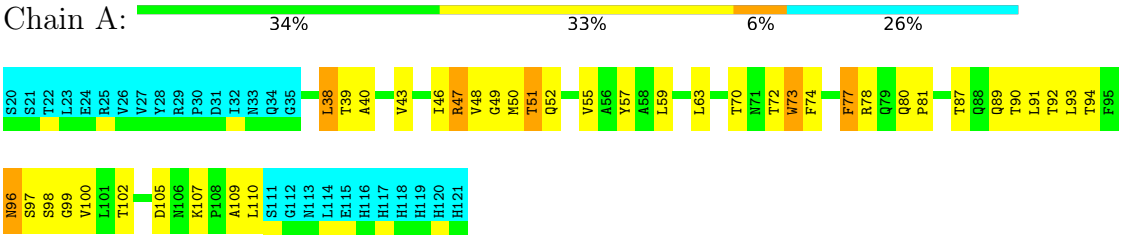
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Small protein A

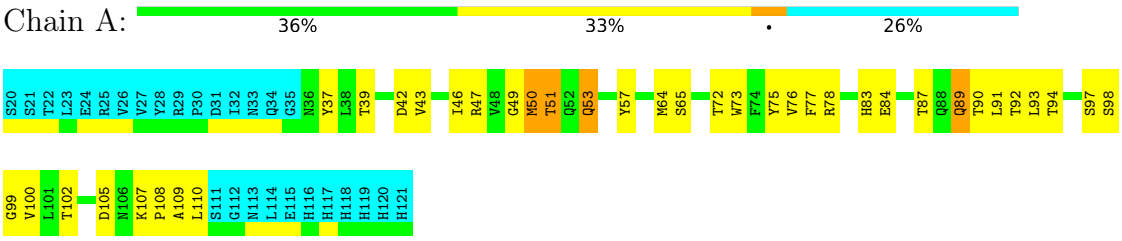
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Small protein A

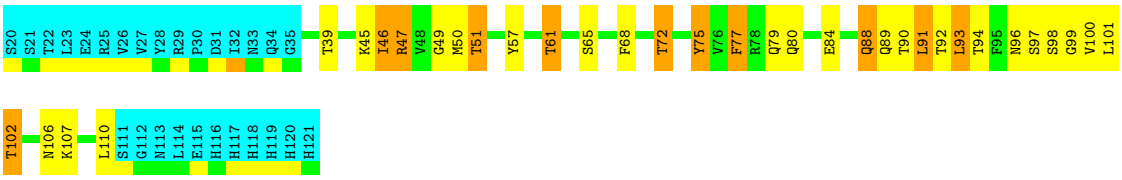
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Small protein A

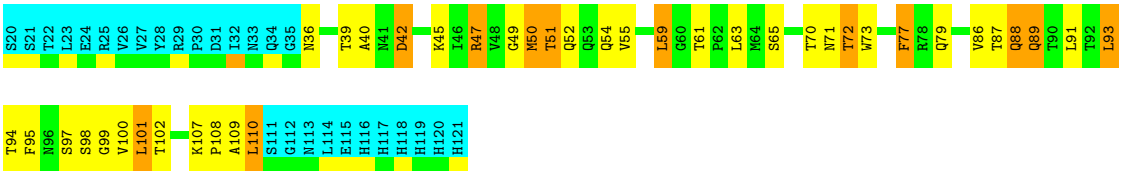
Chain A: 40% 23% 11% 26%



4.2.19 Score per residue for model 19

- Molecule 1: Small protein A

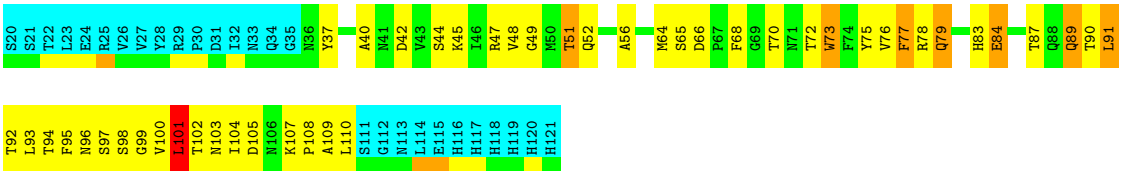
Chain A: 34% 27% 12% 26%



4.2.20 Score per residue for model 20

- Molecule 1: Small protein A

Chain A: 27% 38% 7% • 26%



5 Refinement protocol and experimental data overview (i)

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

Of the 150 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
CYANA	structure solution	1.0.5
CYANA	refinement	1.0.5

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	584	570	569	9±3
All	All	11680	11400	11380	187

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLY:HA2	1:A:100:VAL:HG13	0.82	1.49	8	20
1:A:87:THR:HG23	1:A:109:ALA:HB1	0.75	1.56	5	3
1:A:42:ASP:HA	1:A:45:LYS:HE3	0.73	1.59	14	1
1:A:47:ARG:HB3	1:A:50:MET:HG3	0.71	1.61	18	1
1:A:87:THR:HG22	1:A:109:ALA:HB1	0.69	1.62	12	3
1:A:39:THR:HG22	1:A:41:ASN:H	0.68	1.49	10	1
1:A:38:LEU:HD21	1:A:59:LEU:HD11	0.68	1.66	16	1
1:A:51:THR:HA	1:A:99:GLY:O	0.66	1.89	9	19
1:A:49:GLY:H	1:A:101:LEU:HB2	0.64	1.51	18	4
1:A:75:TYR:HB2	1:A:91:LEU:HD12	0.63	1.69	6	1
1:A:79:GLN:CG	1:A:89:GLN:HG3	0.62	2.24	20	2
1:A:78:ARG:O	1:A:78:ARG:HG3	0.60	1.96	12	1
1:A:46:ILE:HG21	1:A:55:VAL:HA	0.60	1.71	6	2
1:A:51:THR:HB	1:A:53:GLN:OE1	0.58	1.97	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:PHE:HE2	1:A:91:LEU:HG	0.57	1.58	7	2
1:A:42:ASP:O	1:A:45:LYS:HG2	0.57	1.99	7	1
1:A:79:GLN:HG3	1:A:89:GLN:HG3	0.57	1.76	20	1
1:A:91:LEU:HD23	1:A:106:ASN:HB2	0.57	1.76	6	1
1:A:73:TRP:HB2	1:A:93:LEU:HB2	0.56	1.76	17	6
1:A:96:ASN:HB2	1:A:102:THR:HG23	0.56	1.78	18	1
1:A:37:TYR:HE2	1:A:77:PHE:HA	0.56	1.60	12	1
1:A:95:PHE:HB3	1:A:101:LEU:HD22	0.56	1.77	1	2
1:A:93:LEU:HG	1:A:101:LEU:HD11	0.55	1.76	20	2
1:A:92:THR:HB	1:A:105:ASP:HB3	0.55	1.79	7	1
1:A:89:GLN:HG3	1:A:108:PRO:HA	0.54	1.77	14	1
1:A:95:PHE:HB3	1:A:101:LEU:HD23	0.53	1.79	12	3
1:A:87:THR:HG23	1:A:109:ALA:HB3	0.53	1.81	20	5
1:A:43:VAL:HA	1:A:59:LEU:HD21	0.52	1.81	1	1
1:A:61:THR:HG23	1:A:75:TYR:HE2	0.52	1.64	18	1
1:A:52:GLN:HG2	1:A:99:GLY:HA3	0.52	1.80	12	2
1:A:95:PHE:HB3	1:A:101:LEU:HA	0.52	1.82	9	1
1:A:38:LEU:HB3	1:A:77:PHE:HB3	0.52	1.82	13	1
1:A:47:ARG:O	1:A:50:MET:HB2	0.52	2.05	14	12
1:A:89:GLN:HB3	1:A:108:PRO:HA	0.52	1.81	8	2
1:A:95:PHE:HE1	1:A:101:LEU:HD22	0.51	1.64	14	1
1:A:72:THR:HA	1:A:93:LEU:O	0.51	2.06	5	6
1:A:55:VAL:HG21	1:A:101:LEU:HD23	0.51	1.83	19	1
1:A:63:LEU:O	1:A:63:LEU:HG	0.50	2.06	12	1
1:A:45:LYS:HE3	1:A:58:ALA:HB1	0.50	1.83	7	1
1:A:66:ASP:N	1:A:67:PRO:HD3	0.50	2.22	10	1
1:A:87:THR:HG23	1:A:109:ALA:CB	0.49	2.37	8	1
1:A:40:ALA:HA	1:A:77:PHE:CZ	0.49	2.43	20	3
1:A:89:GLN:NE2	1:A:108:PRO:HA	0.49	2.23	19	1
1:A:56:ALA:HB2	1:A:73:TRP:CH2	0.49	2.43	5	2
1:A:38:LEU:HD13	1:A:75:TYR:HE1	0.49	1.68	8	1
1:A:49:GLY:H	1:A:101:LEU:HB3	0.49	1.68	15	1
1:A:71:ASN:HB3	1:A:95:PHE:O	0.48	2.08	2	2
1:A:72:THR:HG23	1:A:94:THR:HG23	0.48	1.86	10	1
1:A:47:ARG:HB2	1:A:50:MET:HG3	0.48	1.85	13	1
1:A:74:PHE:HA	1:A:91:LEU:O	0.48	2.07	7	1
1:A:40:ALA:HA	1:A:77:PHE:CE2	0.48	2.44	16	1
1:A:42:ASP:HA	1:A:45:LYS:HG3	0.48	1.85	2	1
1:A:88:GLN:C	1:A:109:ALA:HB2	0.47	2.29	8	1
1:A:55:VAL:O	1:A:59:LEU:HB3	0.46	2.10	16	1
1:A:88:GLN:O	1:A:109:ALA:HB2	0.46	2.10	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:GLN:HB3	1:A:107:LYS:O	0.46	2.10	1	1
1:A:56:ALA:HB2	1:A:73:TRP:HH2	0.46	1.71	5	1
1:A:66:ASP:HA	1:A:70:THR:OG1	0.45	2.11	10	1
1:A:49:GLY:HA2	1:A:100:VAL:CG1	0.45	2.38	9	2
1:A:88:GLN:NE2	1:A:88:GLN:HA	0.45	2.24	19	2
1:A:55:VAL:O	1:A:59:LEU:HB2	0.45	2.12	19	1
1:A:55:VAL:O	1:A:59:LEU:HG	0.45	2.11	9	1
1:A:89:GLN:NE2	1:A:109:ALA:H	0.45	2.09	5	1
1:A:89:GLN:HB2	1:A:107:LYS:O	0.45	2.12	9	1
1:A:77:PHE:HB3	1:A:89:GLN:HG2	0.45	1.89	19	1
1:A:42:ASP:HA	1:A:45:LYS:HD3	0.44	1.89	19	2
1:A:89:GLN:OE1	1:A:108:PRO:HA	0.44	2.13	17	1
1:A:56:ALA:HA	1:A:61:THR:OG1	0.44	2.13	6	1
1:A:79:GLN:HG3	1:A:79:GLN:O	0.44	2.12	20	1
1:A:88:GLN:H	1:A:109:ALA:HB3	0.43	1.73	4	2
1:A:56:ALA:HA	1:A:61:THR:HB	0.43	1.89	5	1
1:A:87:THR:HA	1:A:109:ALA:HB3	0.43	1.90	4	1
1:A:46:ILE:HD12	1:A:93:LEU:HD21	0.43	1.90	2	1
1:A:43:VAL:O	1:A:46:ILE:HG13	0.43	2.12	9	3
1:A:56:ALA:HB1	1:A:61:THR:O	0.43	2.13	11	1
1:A:95:PHE:CB	1:A:101:LEU:HA	0.42	2.44	9	1
1:A:77:PHE:CE2	1:A:91:LEU:HG	0.42	2.45	7	1
1:A:79:GLN:HE21	1:A:80:GLN:NE2	0.42	2.11	11	1
1:A:42:ASP:O	1:A:45:LYS:HB2	0.42	2.13	6	1
1:A:83:HIS:HB3	1:A:87:THR:OG1	0.42	2.15	13	1
1:A:77:PHE:CE1	1:A:91:LEU:HG	0.42	2.50	18	2
1:A:88:GLN:OE1	1:A:88:GLN:HA	0.42	2.15	18	1
1:A:71:ASN:HA	1:A:95:PHE:CE2	0.41	2.49	19	1
1:A:83:HIS:O	1:A:84:GLU:HB2	0.41	2.15	12	1
1:A:56:ALA:HB1	1:A:61:THR:OG1	0.41	2.16	9	1
1:A:39:THR:O	1:A:42:ASP:HB2	0.41	2.16	10	1
1:A:43:VAL:CG2	1:A:77:PHE:HZ	0.41	2.28	10	1
1:A:43:VAL:HG21	1:A:77:PHE:HZ	0.41	1.76	10	1
1:A:37:TYR:CE2	1:A:77:PHE:HA	0.41	2.46	12	1
1:A:46:ILE:HG21	1:A:55:VAL:HG13	0.41	1.91	16	1
1:A:96:ASN:ND2	1:A:100:VAL:HB	0.41	2.31	16	1
1:A:56:ALA:HA	1:A:61:THR:CG2	0.41	2.45	11	1
1:A:48:VAL:HG22	1:A:104:ILE:HD12	0.41	1.91	20	1
1:A:49:GLY:CA	1:A:100:VAL:HG13	0.41	2.43	18	1
1:A:93:LEU:HD12	1:A:104:ILE:HG12	0.40	1.92	3	1
1:A:79:GLN:O	1:A:81:PRO:HD3	0.40	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:THR:HB	1:A:42:ASP:HB2	0.40	1.92	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	75/102 (74%)	67±2 (89±3%)	7±2 (10±3%)	1±1 (1±1%)	14	59
All	All	1500/2040 (74%)	1332 (89%)	146 (10%)	22 (1%)	14	59

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	36	ASN	5
1	A	110	LEU	3
1	A	109	ALA	3
1	A	81	PRO	3
1	A	83	HIS	2
1	A	82	GLY	2
1	A	101	LEU	2
1	A	84	GLU	1
1	A	46	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	65/90 (72%)	35±3 (54±4%)	30±3 (46±4%)	0	2
All	All	1300/1800 (72%)	703 (54%)	597 (46%)	0	2

All 59 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	72	THR	20
1	A	91	LEU	20
1	A	102	THR	20
1	A	110	LEU	20
1	A	51	THR	19
1	A	94	THR	19
1	A	98	SER	19
1	A	97	SER	18
1	A	107	LYS	18
1	A	90	THR	17
1	A	65	SER	17
1	A	89	GLN	16
1	A	92	THR	15
1	A	47	ARG	14
1	A	83	HIS	14
1	A	57	TYR	13
1	A	63	LEU	13
1	A	79	GLN	13
1	A	39	THR	12
1	A	50	MET	12
1	A	70	THR	12
1	A	78	ARG	12
1	A	80	GLN	12
1	A	38	LEU	11
1	A	64	MET	11
1	A	95	PHE	11
1	A	88	GLN	10
1	A	101	LEU	10
1	A	105	ASP	10
1	A	52	GLN	9
1	A	42	ASP	9
1	A	46	ILE	9
1	A	44	SER	9
1	A	61	THR	8
1	A	48	VAL	8
1	A	66	ASP	8
1	A	75	TYR	8
1	A	77	PHE	8
1	A	73	TRP	7
1	A	68	PHE	7
1	A	84	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	86	VAL	7
1	A	45	LYS	7
1	A	37	TYR	6
1	A	76	VAL	6
1	A	96	ASN	6
1	A	103	ASN	6
1	A	74	PHE	5
1	A	71	ASN	4
1	A	87	THR	4
1	A	59	LEU	4
1	A	41	ASN	3
1	A	36	ASN	3
1	A	54	GLN	3
1	A	53	GLN	3
1	A	93	LEU	2
1	A	100	VAL	1
1	A	104	ILE	1
1	A	106	ASN	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