Full wwPDB NMR Structure Validation Report (i)

Oct 21, 2021 – 08:09 AM EDT

PDB ID	:	2RGF
Title	:	RBD OF RAL GUANOSINE-NUCLEOTIDE EXCHANGE FACTOR (PROTEIN), NMR, 10 STRUCTURES
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Deposited on	:	1997-02-13

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:

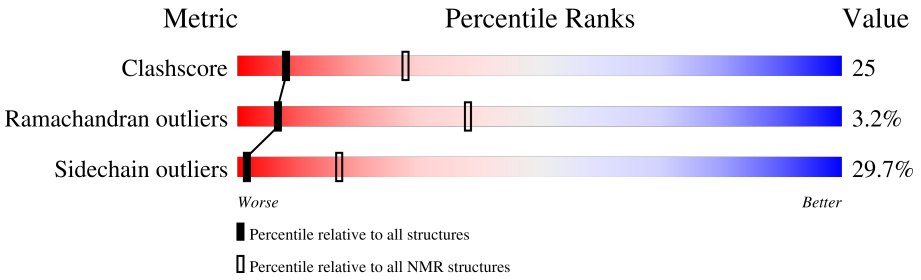
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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	97	45% 44% 9% •

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 6 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:1-A:97 (97)	0.36	6

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 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1557 atoms, of which 778 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RALGEF-RBD.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	97	1557	488	778	131	155	5	0

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: RALGEF-RBD

Chain A: 45% 44% 9%

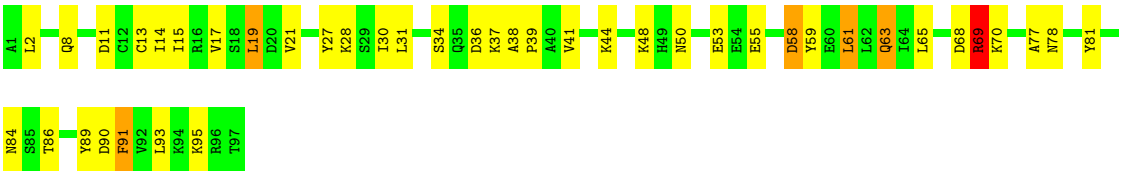
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: RALGEF-RBD

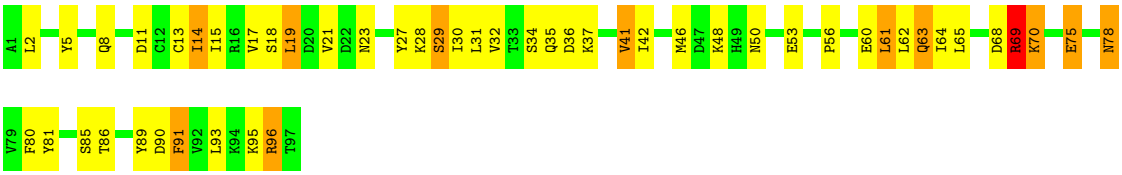
Chain A: 57% 37% 5%



4.2.2 Score per residue for model 2

• Molecule 1: RALGEF-RBD

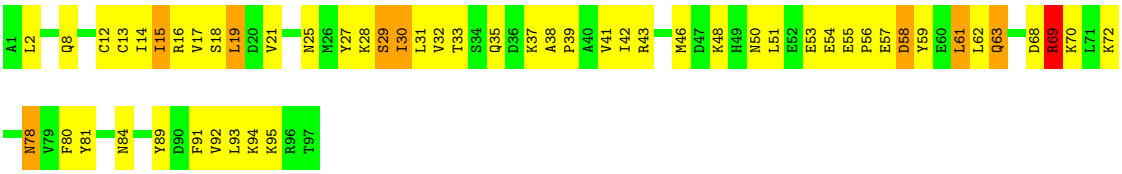
Chain A: 48% 39% 11%



4.2.3 Score per residue for model 3

- Molecule 1: RALGEF-RBD

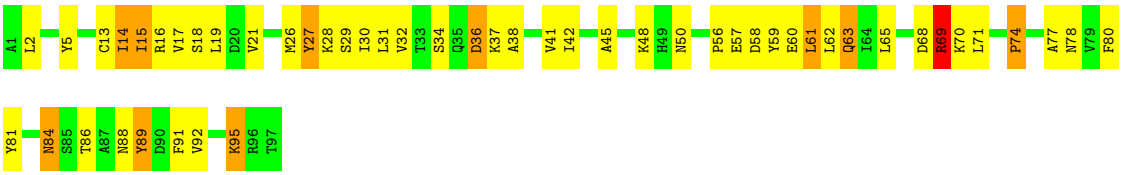
Chain A: 44% 46% 8%



4.2.4 Score per residue for model 4

- Molecule 1: RALGEF-RBD

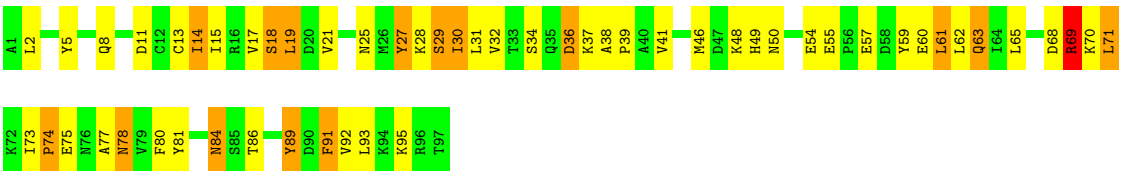
Chain A: 47% 41% 10%



4.2.5 Score per residue for model 5

- Molecule 1: RALGEF-RBD

Chain A: 43% 40% 15%



4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: RALGEF-RBD

Chain A: 38% 45% 16%

A1 L2 Y5 Q8 D11 C12 C13 I14 I15 R16 V17 S18 L19 D20 V21 N25 M26 Y27 K28 S29 I30 L31 V32 T33 S34 Q35 D36 K37 A38 P39 A40 V41 K44 A45 M46 D47 K48 H49 N50 L51 E52 E53 E54 E55 P56 E57 D58 Y59 E60 L61 L62 Q63 I64 L65

D68 R69 K70 L71 K72 I73 P74 E75 N76 A77 N78 V79 F80 Y81 N84 S85 T86 A87 N88 Y89 D90 F91 V92 L93 K94 K95 R96 T97

4.2.7 Score per residue for model 7

- Molecule 1: RALGEF-RBD

Chain A: 47% 37% 14%

A1 L2 Q8 D11 C12 C13 I14 I15 R16 V17 S18 L19 D20 V21 N25 M26 Y27 K28 S29 I30 L31 V32 T33 S34 Q35 D36 K37 V41 I42 R43 K44 A45 M46 D47 K48 H49 N50 E55 P56 E57 D58 Y59 E60 L61 L62 Q63 I64 L65 D68 R69 K70 L71 K72 I73

P74 E75 N76 A77 N78 V79 F80 Y81 N84 S85 T86 Y89 D90 F91 V92 K95 R96 T97

4.2.8 Score per residue for model 8

- Molecule 1: RALGEF-RBD

Chain A: 45% 46% 7%

A1 L2 Q8 D11 C12 C13 I14 I15 R16 V17 S18 L19 D20 V21 Y27 K28 S29 I30 L31 V32 T33 S34 Q35 A38 P39 A40 V41 I42 M46 D47 K48 H49 E52 E55 P56 E57 D58 Y59 E60 L61 L62 Q63 D68 R69 K70 L71 K72 I73 P74 E75 N76 A77

N78 V79 F80 Y81 N84 S85 Y89 D90 F91 V92 L93 K94 K95 R96 T97

4.2.9 Score per residue for model 9

- Molecule 1: RALGEF-RBD

Chain A: 47% 44% 7%

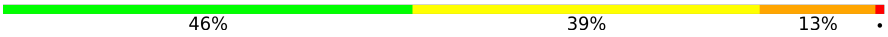
A1 L2 Q8 C12 C13 I14 I15 R16 V17 S18 L19 D20 V21 N25 M26 Y27 K28 S29 I30 L31 V32 T33 S34 Q35 D36 K37 A38 P39 A40 V41 I42 R43 K44 A45 K48 H49 N50 P56 E57 D58 Y59 E60 L61 L62 Q63 D68 R69 K70 I73 P74 E75 N76 A77

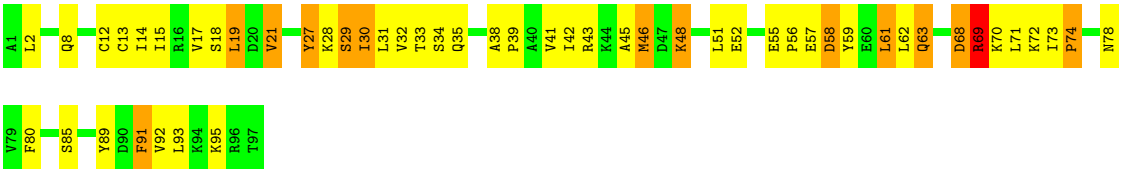
N78 V79 F80 Y81 N84 Y89 D90 F91 V92 L93 T97

4.2.10 Score per residue for model 10

- Molecule 1: RALGEF-RBD

Chain A:





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING*.

Of the 40 calculated structures, 10 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
X-PLOR	refinement	3.851
AURELIA	structure calculation	2.0
X-PLOR	structure calculation	3.851

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	779	778	777	39±10
All	All	7790	7780	7770	387

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:VAL:HG11	1:A:61:LEU:HD11	0.96	1.31	10	7
1:A:41:VAL:HG11	1:A:61:LEU:HD21	0.87	1.44	1	3
1:A:41:VAL:HG21	1:A:81:TYR:CE2	0.82	2.09	8	1
1:A:61:LEU:HD13	1:A:77:ALA:HB2	0.79	1.52	8	1
1:A:15:ILE:HG13	1:A:32:VAL:HG21	0.77	1.56	6	3
1:A:41:VAL:CG1	1:A:61:LEU:HD11	0.76	2.11	10	7
1:A:17:VAL:HG23	1:A:91:PHE:CZ	0.70	2.22	6	10
1:A:61:LEU:HD13	1:A:77:ALA:CB	0.69	2.18	7	7
1:A:41:VAL:HG22	1:A:81:TYR:CE1	0.69	2.22	7	3
1:A:17:VAL:HB	1:A:91:PHE:CE1	0.65	2.27	3	7
1:A:71:LEU:HD11	1:A:80:PHE:CE1	0.64	2.27	8	1
1:A:17:VAL:HB	1:A:91:PHE:CE2	0.64	2.27	5	3
1:A:18:SER:HB3	1:A:27:TYR:CE1	0.62	2.29	6	7
1:A:17:VAL:HG12	1:A:28:LYS:O	0.62	1.93	3	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:VAL:HG11	1:A:61:LEU:CD1	0.62	2.24	7	6
1:A:36:ASP:HB3	1:A:81:TYR:CD2	0.61	2.30	7	3
1:A:62:LEU:HD23	1:A:72:LYS:HB2	0.61	1.70	10	4
1:A:15:ILE:CG2	1:A:91:PHE:CD1	0.61	2.84	2	4
1:A:65:LEU:HD22	1:A:86:THR:HG23	0.60	1.72	4	1
1:A:15:ILE:HD12	1:A:32:VAL:HG21	0.60	1.72	2	2
1:A:71:LEU:HD11	1:A:80:PHE:HE1	0.60	1.57	8	1
1:A:17:VAL:CG2	1:A:91:PHE:CZ	0.60	2.85	6	9
1:A:15:ILE:CG1	1:A:32:VAL:HG21	0.60	2.27	5	2
1:A:61:LEU:HD13	1:A:77:ALA:HB1	0.59	1.73	7	3
1:A:61:LEU:HB3	1:A:80:PHE:CD2	0.59	2.32	10	7
1:A:41:VAL:HG21	1:A:81:TYR:CE1	0.59	2.33	2	1
1:A:32:VAL:HG13	1:A:81:TYR:CE2	0.57	2.35	7	1
1:A:36:ASP:HB3	1:A:81:TYR:CE2	0.57	2.34	1	2
1:A:19:LEU:HD11	1:A:93:LEU:HD23	0.57	1.76	10	2
1:A:61:LEU:HB3	1:A:80:PHE:CE2	0.56	2.36	8	2
1:A:19:LEU:CD1	1:A:93:LEU:HD23	0.56	2.30	10	2
1:A:71:LEU:HD21	1:A:84:ASN:HB3	0.55	1.78	7	3
1:A:5:TYR:CZ	1:A:14:ILE:HD11	0.55	2.36	4	4
1:A:15:ILE:O	1:A:29:SER:HA	0.54	2.02	10	8
1:A:65:LEU:HD22	1:A:86:THR:HG22	0.54	1.80	5	4
1:A:17:VAL:HG13	1:A:49:HIS:HE1	0.54	1.62	9	4
1:A:59:TYR:CZ	1:A:95:LYS:CD	0.54	2.91	8	1
1:A:41:VAL:HG22	1:A:81:TYR:CZ	0.53	2.39	6	2
1:A:15:ILE:HG21	1:A:91:PHE:CE1	0.53	2.38	6	1
1:A:71:LEU:HD21	1:A:84:ASN:CB	0.53	2.34	5	4
1:A:59:TYR:CD2	1:A:93:LEU:HG	0.53	2.39	1	4
1:A:37:LYS:O	1:A:41:VAL:HG23	0.53	2.03	1	6
1:A:15:ILE:HG12	1:A:89:TYR:CD1	0.53	2.38	7	3
1:A:37:LYS:HD3	1:A:78:ASN:HB2	0.52	1.81	2	6
1:A:59:TYR:CE1	1:A:95:LYS:HD2	0.52	2.39	8	1
1:A:17:VAL:HG23	1:A:91:PHE:CE2	0.52	2.39	4	2
1:A:38:ALA:HB3	1:A:39:PRO:CD	0.52	2.35	10	6
1:A:18:SER:HB3	1:A:27:TYR:CD1	0.51	2.40	3	5
1:A:73:ILE:HG23	1:A:74:PRO:HD2	0.51	1.82	10	6
1:A:41:VAL:HG22	1:A:81:TYR:CE2	0.50	2.40	1	2
1:A:29:SER:O	1:A:30:ILE:HD13	0.50	2.05	6	4
1:A:32:VAL:HG11	1:A:81:TYR:OH	0.50	2.06	3	2
1:A:41:VAL:CG2	1:A:81:TYR:CE1	0.50	2.95	5	3
1:A:29:SER:C	1:A:30:ILE:HD13	0.50	2.27	5	3
1:A:30:ILE:HG21	1:A:44:LYS:HB3	0.50	1.83	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TYR:CZ	1:A:95:LYS:HD3	0.50	2.42	6	2
1:A:21:VAL:HG11	1:A:95:LYS:O	0.50	2.07	10	1
1:A:42:ILE:HD13	1:A:56:PRO:O	0.49	2.07	4	3
1:A:17:VAL:HG22	1:A:18:SER:N	0.49	2.22	6	3
1:A:15:ILE:HG21	1:A:91:PHE:CE2	0.49	2.43	5	1
1:A:63:GLN:HG2	1:A:91:PHE:CB	0.49	2.37	3	7
1:A:59:TYR:CE1	1:A:95:LYS:CD	0.49	2.96	6	1
1:A:42:ILE:HG22	1:A:56:PRO:HA	0.49	1.84	2	1
1:A:63:GLN:HB2	1:A:80:PHE:CZ	0.49	2.43	2	6
1:A:42:ILE:HD11	1:A:59:TYR:HB2	0.49	1.84	9	2
1:A:16:ARG:HG2	1:A:27:TYR:CD1	0.48	2.43	3	2
1:A:62:LEU:CD2	1:A:72:LYS:HB2	0.48	2.38	10	1
1:A:43:ARG:HA	1:A:46:MET:SD	0.48	2.48	10	1
1:A:63:GLN:HB3	1:A:71:LEU:HD23	0.48	1.84	6	3
1:A:38:ALA:CA	1:A:77:ALA:HB3	0.48	2.38	8	2
1:A:62:LEU:O	1:A:91:PHE:HB2	0.47	2.08	10	7
1:A:63:GLN:HG3	1:A:84:ASN:HB2	0.47	1.86	4	1
1:A:19:LEU:HD22	1:A:53:GLU:HG2	0.47	1.86	1	2
1:A:42:ILE:HG21	1:A:55:GLU:O	0.47	2.10	3	4
1:A:59:TYR:CZ	1:A:95:LYS:HD2	0.47	2.44	8	2
1:A:30:ILE:CG2	1:A:44:LYS:HB3	0.47	2.39	1	1
1:A:41:VAL:HG11	1:A:61:LEU:CD2	0.47	2.31	1	1
1:A:17:VAL:CB	1:A:91:PHE:CE1	0.47	2.98	6	5
1:A:80:PHE:C	1:A:80:PHE:CD1	0.46	2.88	4	6
1:A:59:TYR:CZ	1:A:95:LYS:HB2	0.46	2.45	10	3
1:A:55:GLU:HB3	1:A:58:ASP:HB2	0.46	1.87	10	3
1:A:54:GLU:O	1:A:54:GLU:CG	0.46	2.63	5	3
1:A:15:ILE:CD1	1:A:32:VAL:HG21	0.46	2.39	2	2
1:A:17:VAL:HA	1:A:91:PHE:O	0.46	2.11	4	1
1:A:65:LEU:HD23	1:A:88:ASN:N	0.46	2.25	4	1
1:A:55:GLU:HB2	1:A:59:TYR:CE1	0.46	2.46	5	2
1:A:65:LEU:HD22	1:A:86:THR:CG2	0.46	2.41	4	3
1:A:18:SER:HB3	1:A:27:TYR:CZ	0.46	2.44	6	2
1:A:19:LEU:HD21	1:A:93:LEU:HD23	0.46	1.88	5	2
1:A:63:GLN:CG	1:A:91:PHE:HB3	0.46	2.41	6	3
1:A:62:LEU:HB2	1:A:92:VAL:HB	0.45	1.87	10	4
1:A:62:LEU:O	1:A:92:VAL:N	0.45	2.47	6	2
1:A:42:ILE:CG2	1:A:56:PRO:HA	0.45	2.41	2	1
1:A:64:ILE:HA	1:A:69:ARG:O	0.45	2.10	6	1
1:A:28:LYS:HB2	1:A:49:HIS:CE1	0.45	2.46	6	2
1:A:19:LEU:HD21	1:A:59:TYR:HE2	0.45	1.71	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TYR:CE1	1:A:95:LYS:HD3	0.45	2.47	1	5
1:A:37:LYS:CD	1:A:78:ASN:HB2	0.45	2.42	2	1
1:A:15:ILE:CG2	1:A:91:PHE:CE1	0.45	3.00	10	3
1:A:41:VAL:HB	1:A:61:LEU:HD11	0.45	1.88	1	1
1:A:75:GLU:HG3	1:A:96:ARG:CZ	0.45	2.42	2	1
1:A:12:CYS:HA	1:A:33:THR:HA	0.45	1.89	3	3
1:A:68:ASP:O	1:A:69:ARG:C	0.44	2.56	4	9
1:A:59:TYR:HA	1:A:95:LYS:HA	0.44	1.88	3	3
1:A:17:VAL:CB	1:A:91:PHE:CE2	0.44	3.00	5	1
1:A:28:LYS:HB3	1:A:48:LYS:HB3	0.44	1.90	10	1
1:A:38:ALA:O	1:A:42:ILE:HD12	0.44	2.12	4	2
1:A:92:VAL:HG12	1:A:94:LYS:HG3	0.44	1.89	3	1
1:A:30:ILE:HD12	1:A:45:ALA:HA	0.44	1.89	4	1
1:A:32:VAL:HG13	1:A:81:TYR:HE2	0.43	1.71	7	1
1:A:42:ILE:HB	1:A:56:PRO:HA	0.43	1.90	8	2
1:A:15:ILE:HG23	1:A:89:TYR:CD1	0.43	2.48	9	2
1:A:60:GLU:HG2	1:A:74:PRO:HA	0.43	1.90	4	3
1:A:17:VAL:HB	1:A:91:PHE:CZ	0.43	2.47	3	1
1:A:17:VAL:CG2	1:A:93:LEU:CB	0.43	2.97	2	1
1:A:63:GLN:CG	1:A:91:PHE:CB	0.43	2.96	6	2
1:A:71:LEU:HD21	1:A:84:ASN:HB2	0.43	1.90	8	1
1:A:16:ARG:HA	1:A:29:SER:HA	0.43	1.91	4	2
1:A:54:GLU:O	1:A:54:GLU:HG2	0.43	2.14	3	1
1:A:58:ASP:O	1:A:95:LYS:HG3	0.42	2.14	6	2
1:A:38:ALA:N	1:A:39:PRO:HD2	0.42	2.29	1	1
1:A:71:LEU:HD11	1:A:80:PHE:CE2	0.42	2.48	4	1
1:A:18:SER:OG	1:A:92:VAL:HG13	0.42	2.14	7	1
1:A:77:ALA:HA	1:A:80:PHE:HB3	0.42	1.91	8	1
1:A:59:TYR:CE2	1:A:95:LYS:HB2	0.42	2.50	10	1
1:A:61:LEU:HG	1:A:91:PHE:CE2	0.42	2.49	2	1
1:A:38:ALA:HA	1:A:77:ALA:HB3	0.42	1.91	9	1
1:A:15:ILE:HD12	1:A:81:TYR:CZ	0.42	2.49	7	1
1:A:41:VAL:HB	1:A:81:TYR:OH	0.42	2.15	2	1
1:A:64:ILE:HG23	1:A:70:LYS:HD2	0.42	1.91	2	1
1:A:38:ALA:HB2	1:A:77:ALA:N	0.42	2.30	4	1
1:A:41:VAL:CB	1:A:61:LEU:HD11	0.41	2.45	1	1
1:A:19:LEU:HD13	1:A:53:GLU:OE2	0.41	2.15	3	1
1:A:41:VAL:HG21	1:A:81:TYR:HE2	0.41	1.64	8	1
1:A:45:ALA:CB	1:A:93:LEU:HD22	0.41	2.45	10	2
1:A:63:GLN:HA	1:A:91:PHE:HA	0.41	1.92	1	1
1:A:61:LEU:HD13	1:A:77:ALA:HB3	0.41	1.93	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:TYR:HA	1:A:84:ASN:ND2	0.41	2.30	6	2
1:A:68:ASP:O	1:A:70:LYS:N	0.41	2.54	6	1
1:A:19:LEU:HG	1:A:93:LEU:O	0.41	2.15	1	1
1:A:15:ILE:CG2	1:A:91:PHE:CD2	0.40	3.04	5	1
1:A:15:ILE:CG2	1:A:91:PHE:CE2	0.40	3.04	5	1
1:A:80:PHE:CD1	1:A:80:PHE:C	0.40	2.94	9	1
1:A:41:VAL:CG2	1:A:81:TYR:CE2	0.40	3.04	1	1
1:A:63:GLN:HG2	1:A:91:PHE:HB3	0.40	1.94	6	1
1:A:37:LYS:HA	1:A:78:ASN:HA	0.40	1.93	7	1
1:A:15:ILE:CD1	1:A:32:VAL:HB	0.40	2.46	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	95/97 (98%)	71±1 (75±1%)	21±2 (22±2%)	3±1 (3±1%)	7	38
All	All	950/970 (98%)	712 (75%)	208 (22%)	30 (3%)	7	38

All 5 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	21	VAL	10
1	A	69	ARG	10
1	A	74	PRO	6
1	A	85	SER	3
1	A	87	ALA	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	88/88 (100%)	62±3 (70±3%)	26±3 (30±3%)	1 17
All	All	880/880 (100%)	619 (70%)	261 (30%)	1 17

All 44 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	2	LEU	10
1	A	13	CYS	10
1	A	14	ILE	10
1	A	19	LEU	10
1	A	31	LEU	10
1	A	48	LYS	10
1	A	63	GLN	10
1	A	70	LYS	10
1	A	78	ASN	10
1	A	89	TYR	10
1	A	8	GLN	9
1	A	61	LEU	9
1	A	69	ARG	9
1	A	34	SER	8
1	A	50	ASN	8
1	A	58	ASP	8
1	A	91	PHE	8
1	A	29	SER	8
1	A	30	ILE	8
1	A	57	GLU	8
1	A	84	ASN	7
1	A	46	MET	7
1	A	11	ASP	6
1	A	27	TYR	6
1	A	75	GLU	6
1	A	35	GLN	5
1	A	25	ASN	5
1	A	36	ASP	4
1	A	71	LEU	4
1	A	15	ILE	3
1	A	95	LYS	3
1	A	18	SER	3
1	A	52	GLU	3
1	A	90	ASP	2
1	A	60	GLU	2
1	A	43	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	51	LEU	2
1	A	68	ASP	2
1	A	23	ASN	1
1	A	41	VAL	1
1	A	96	ARG	1
1	A	26	MET	1
1	A	81	TYR	1
1	A	55	GLU	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