Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2G2B
Title	:	NMR structure of the human allograft inflammatory factor 1
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Deposited on	:	2006-02-15

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:

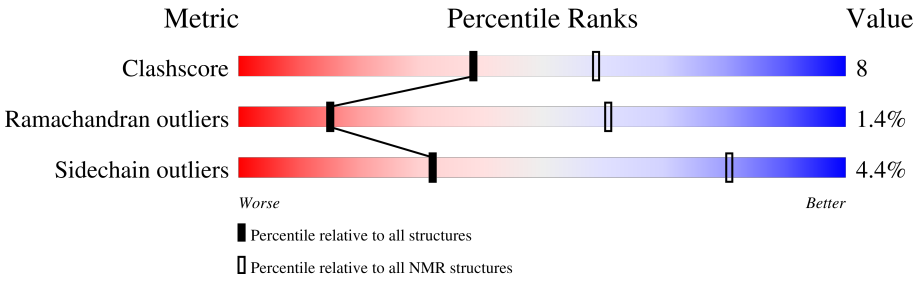
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	150	59% 15% 26%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:18-A:128 (111)	0.72	4

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 4 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2407 atoms, of which 1218 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Allograft inflammatory factor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	150	2407	753	1218	197	232	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P55008
A	2	PRO	-	cloning artifact	UNP P55008
A	3	LEU	-	cloning artifact	UNP P55008
A	4	GLU	-	cloning artifact	UNP P55008

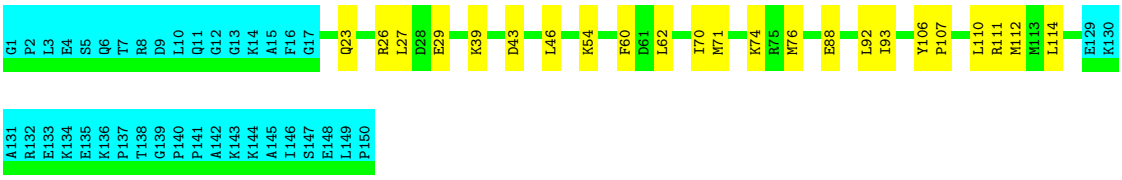
4 Residue-property plots (i)

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: Allograft inflammatory factor 1

Chain A: 59% 15% 26%



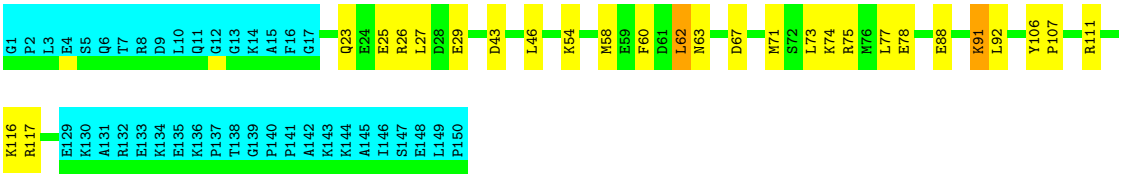
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Allograft inflammatory factor 1

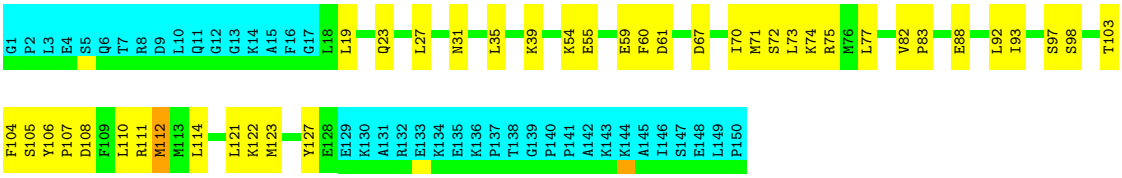
Chain A: 56% 17% • 26%



4.2.2 Score per residue for model 2

• Molecule 1: Allograft inflammatory factor 1

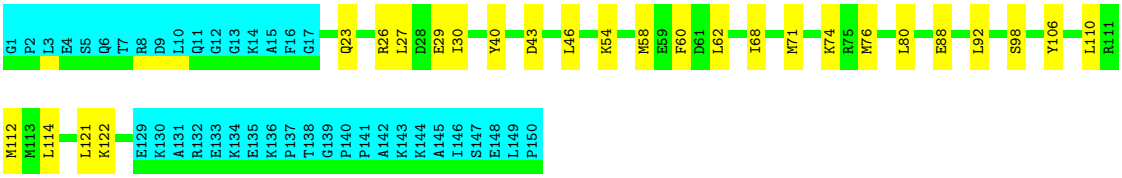
Chain A: 47% 26% • 26%



4.2.3 Score per residue for model 3

- Molecule 1: Allograft inflammatory factor 1

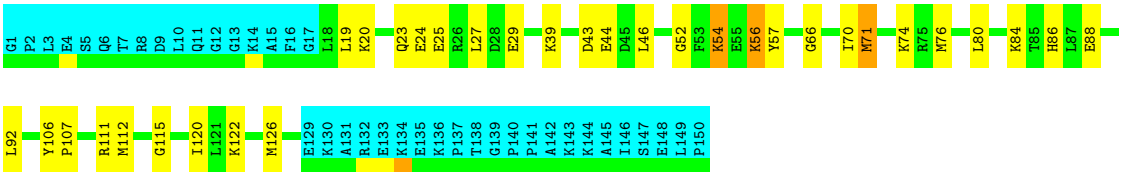
Chain A:



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Allograft inflammatory factor 1

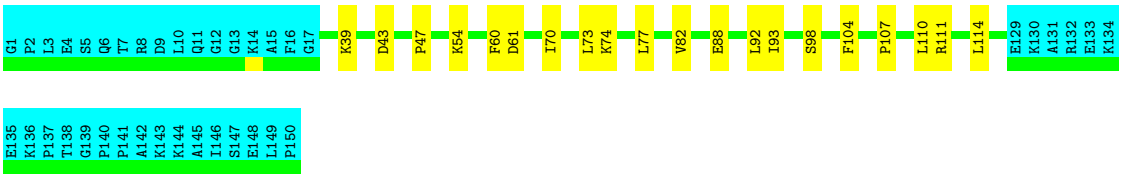
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Allograft inflammatory factor 1

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Allograft inflammatory factor 1

Chain A: 53% 20% • 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 L18 L19 Q22 Q23 L27 S41 S42 D43 L46 K54 E55 M58 E59 F60 D61 L62 L73 K74 L77 V82 P83 K84 L89 V96 S97 S98 S105 Y106 P107 D108 F109

L110 R111 L114 G115 K116 R117 L121 E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

4.2.7 Score per residue for model 7

- Molecule 1: Allograft inflammatory factor 1

Chain A: 58% 15% • 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 Q23 E24 E25 R26 L27 D28 E29 I30 K39 K54 E55 F60 D61 I70 M71 K74 E88 L89 L92 I93 Y106 M112 K116 R117 E128 E129 K130 A131 R132 E133 K134

E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

4.2.8 Score per residue for model 8

- Molecule 1: Allograft inflammatory factor 1

Chain A: 55% 19% 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 Q23 L27 K39 Y40 D43 L46 E51 E55 K56 F60 D61 L62 D69 I70 K74 R75 M76 L92 I93 G99 E102 T103 F104 S105 Y106 P107 R111 M112

S118 A119 I120 L121 K122 L125 E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

4.2.9 Score per residue for model 9

- Molecule 1: Allograft inflammatory factor 1

Chain A: 49% 24% • 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 K20 Q23 E24 E25 R26 L27 D28 E29 I30 Q33 D37 P38 K39 K49 Y57 D61 N65 G66 D67 I68 D69 I70 M71 K74 R75 M76 L77 E78 K79 L80 P83 K84

I93 E102 T103 F104 S105 Y106 L110 R111 M112 M113 L114 L121 K122 M126 Y127 E128 E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

4.2.10 Score per residue for model 10

- Molecule 1: Allograft inflammatory factor 1

Chain A: 56% 17% • 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 L18 A21 Q22 Q23 E24 E25 R26 E29 I30 Y40 L46 K54 F60 D61 L62 I68 D69 I70 M76 L80 E88 L92 I93 G99 F104 S105 Y106 P107 D108

M112 M113 L114 L121 K122 E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

4.2.11 Score per residue for model 11

- Molecule 1: Allograft inflammatory factor 1

Chain A: 54% 19% • 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 Q23 E24 E25 R26 L27 D28 E29 I30 Q33 S41 S42 D43 P47 S48 K49 K54 E55 E59 F60 D61 L62 S72 E88 L92 E102 P107 L110 R111 M112 M113 L114

R117 S118 E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

4.2.12 Score per residue for model 12

- Molecule 1: Allograft inflammatory factor 1

Chain A: 53% 21% 26%

G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 L18 L19 K20 Q23 E24 E25 R26 I30 L35 K39 Y40 L46 K54 Y57 F60 D61 L62 N71 K74 R75 M76 L77 E78 K79 L80 L89 K90 K91 G94 G101

Y106 P107 L110 R111 L114 G115 K116 E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

4.2.13 Score per residue for model 13

- Molecule 1: Allograft inflammatory factor 1

Chain A: 55% 19% • 26%

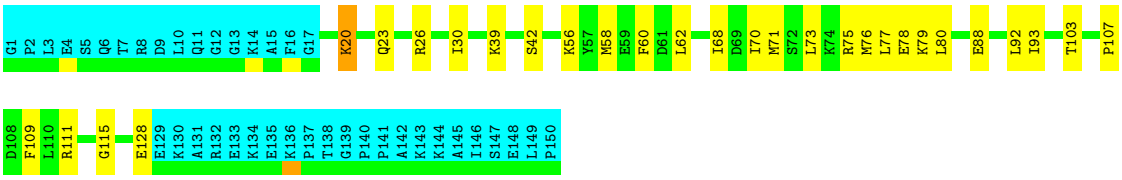
G1 P2 L3 E4 S5 Q6 T7 R8 D9 L10 Q11 G12 G13 K14 A15 F16 G17 L18 L19 K20 Q23 L27 N31 K39 Y40 D43 L46 L50 K56 D61 L62 N63 G64 D67 K74 L87 E88 K91 L92 V96 S97 S98 S105 Y106 P107

D108 R111 M112 I120 E129 K130 A131 R132 E133 K134 E135 K136 P137 T138 G139 P140 P141 A142 K143 K144 A145 I146 S147 E148 L149 P150

4.2.14 Score per residue for model 14

- Molecule 1: Allograft inflammatory factor 1

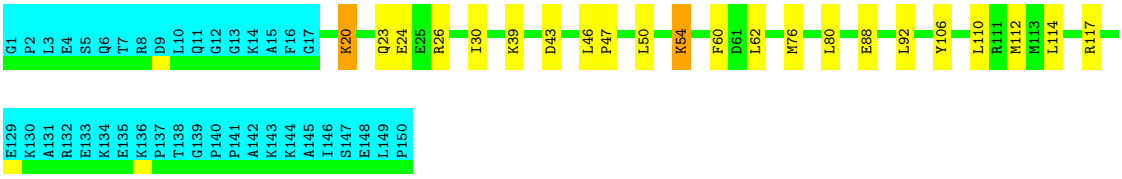
Chain A: 55% 19% • 26%



4.2.15 Score per residue for model 15

- Molecule 1: Allograft inflammatory factor 1

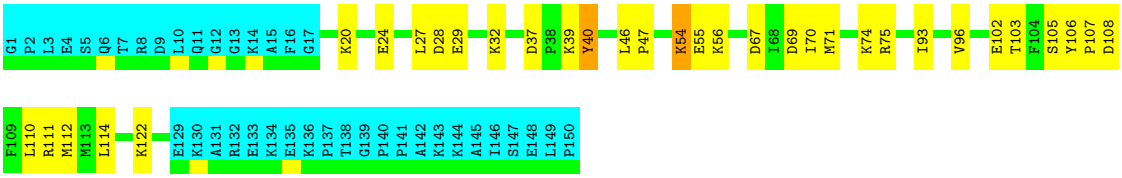
Chain A: 59% 13% • 26%



4.2.16 Score per residue for model 16

- Molecule 1: Allograft inflammatory factor 1

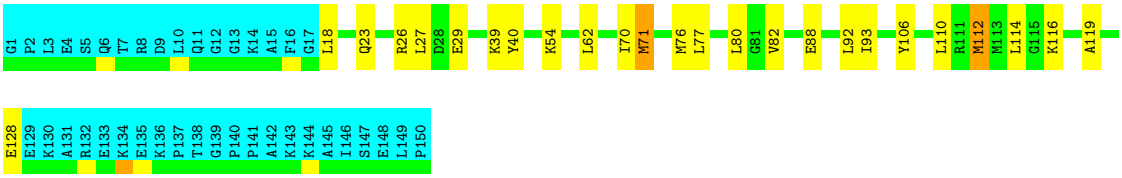
Chain A: 52% 21% • 26%



4.2.17 Score per residue for model 17

- Molecule 1: Allograft inflammatory factor 1

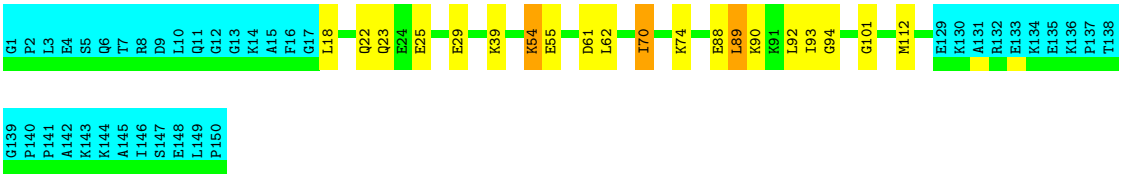
Chain A: 57% 15% • 26%



4.2.18 Score per residue for model 18

- Molecule 1: Allograft inflammatory factor 1

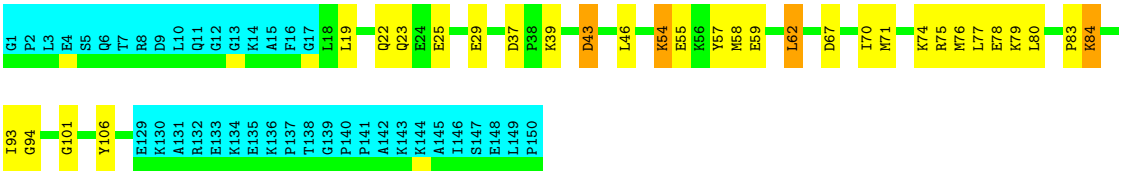
Chain A: 61% 11% • 26%



4.2.19 Score per residue for model 19

- Molecule 1: Allograft inflammatory factor 1

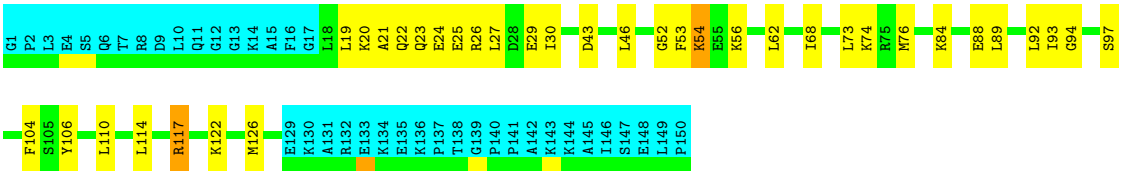
Chain A: 53% 18% • 26%



4.2.20 Score per residue for model 20

- Molecule 1: Allograft inflammatory factor 1

Chain A: 50% 23% • 26%



5 Refinement protocol and experimental data overview (i)

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

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
Xplor-NIH	refinement	2.9.3

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	117	ARG	Sidechain	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	897	915	914	14±3
All	All	17940	18300	18280	285

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:110:LEU:O	1:A:114:LEU:HG	0.68	1.88	9	9
1:A:93:ILE:HG12	1:A:104:PHE:CZ	0.65	2.26	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LYS:O	1:A:24:GLU:HG3	0.65	1.91	9	6
1:A:76:MET:O	1:A:80:LEU:HG	0.62	1.95	9	9
1:A:43:ASP:HB2	1:A:46:LEU:HB2	0.60	1.74	4	1
1:A:40:TYR:CE2	1:A:46:LEU:HD21	0.60	2.32	16	1
1:A:70:ILE:HG21	1:A:90:LYS:HG3	0.60	1.73	18	1
1:A:51:GLU:O	1:A:55:GLU:HG2	0.59	1.97	8	1
1:A:88:GLU:O	1:A:92:LEU:HG	0.59	1.97	7	14
1:A:122:LYS:O	1:A:126:MET:HG2	0.58	1.99	9	2
1:A:58:MET:HA	1:A:62:LEU:HD11	0.57	1.76	19	3
1:A:93:ILE:HG12	1:A:104:PHE:CE2	0.57	2.35	9	3
1:A:31:ASN:ND2	1:A:50:LEU:HB3	0.57	2.15	13	1
1:A:91:LYS:O	1:A:91:LYS:HE2	0.57	2.00	1	1
1:A:19:LEU:O	1:A:22:GLN:HG2	0.56	2.01	19	1
1:A:70:ILE:HG22	1:A:93:ILE:HG13	0.56	1.76	18	3
1:A:23:GLN:NE2	1:A:62:LEU:HD13	0.56	2.16	20	5
1:A:23:GLN:O	1:A:27:LEU:HG	0.55	2.00	13	8
1:A:23:GLN:HE22	1:A:62:LEU:HB3	0.55	1.61	8	4
1:A:68:ILE:O	1:A:103:THR:HA	0.54	2.02	14	1
1:A:27:LEU:HD22	1:A:106:TYR:CE2	0.54	2.37	1	8
1:A:60:PHE:CE1	1:A:73:LEU:HD12	0.54	2.38	1	3
1:A:19:LEU:O	1:A:23:GLN:HG3	0.54	2.02	13	5
1:A:40:TYR:O	1:A:46:LEU:HG	0.54	2.02	13	4
1:A:37:ASP:OD2	1:A:39:LYS:HB3	0.53	2.04	16	1
1:A:27:LEU:HD22	1:A:106:TYR:CD2	0.53	2.38	20	6
1:A:96:VAL:HG22	1:A:112:MET:HG2	0.53	1.79	13	1
1:A:105:SER:HB3	1:A:108:ASP:OD2	0.53	2.03	2	3
1:A:54:LYS:HB3	1:A:106:TYR:OH	0.53	2.03	7	5
1:A:54:LYS:HD3	1:A:55:GLU:N	0.53	2.18	19	1
1:A:25:GLU:O	1:A:29:GLU:HG2	0.52	2.04	20	6
1:A:27:LEU:HD22	1:A:106:TYR:CE1	0.52	2.40	13	2
1:A:60:PHE:HA	1:A:76:MET:SD	0.52	2.45	10	2
1:A:77:LEU:HB3	1:A:82:VAL:O	0.52	2.04	6	2
1:A:71:MET:O	1:A:75:ARG:HG3	0.52	2.04	9	4
1:A:107:PRO:O	1:A:111:ARG:HG2	0.51	2.05	12	7
1:A:37:ASP:OD1	1:A:39:LYS:HG2	0.51	2.05	9	1
1:A:43:ASP:N	1:A:46:LEU:HB2	0.51	2.21	19	1
1:A:112:MET:SD	1:A:122:LYS:HD2	0.51	2.46	10	1
1:A:54:LYS:HD2	1:A:55:GLU:N	0.51	2.21	16	2
1:A:74:LYS:HE3	1:A:84:LYS:O	0.51	2.06	4	1
1:A:18:LEU:O	1:A:22:GLN:HG3	0.51	2.06	18	2
1:A:43:ASP:HB3	1:A:46:LEU:HB2	0.50	1.83	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ASP:HA	1:A:102:GLU:O	0.50	2.06	8	2
1:A:26:ARG:O	1:A:29:GLU:HG2	0.50	2.06	3	3
1:A:28:ASP:OD2	1:A:32:LYS:HE3	0.50	2.07	16	1
1:A:96:VAL:CG1	1:A:108:ASP:HB3	0.49	2.37	6	1
1:A:107:PRO:O	1:A:111:ARG:HG3	0.49	2.07	8	4
1:A:74:LYS:HB3	1:A:89:LEU:CD2	0.49	2.37	12	1
1:A:60:PHE:CB	1:A:68:ILE:HG12	0.49	2.37	3	1
1:A:70:ILE:HG13	1:A:71:MET:N	0.49	2.21	7	4
1:A:89:LEU:O	1:A:93:ILE:HG12	0.49	2.07	7	3
1:A:27:LEU:HD22	1:A:106:TYR:CD1	0.49	2.43	13	1
1:A:67:ASP:OD1	1:A:103:THR:HB	0.49	2.08	2	1
1:A:55:GLU:O	1:A:59:GLU:HG3	0.48	2.07	2	2
1:A:65:ASN:HB3	1:A:67:ASP:OD1	0.48	2.08	9	1
1:A:105:SER:HB3	1:A:108:ASP:OD1	0.48	2.08	6	1
1:A:26:ARG:O	1:A:30:ILE:HG13	0.48	2.08	10	9
1:A:57:TYR:HA	1:A:60:PHE:CD2	0.48	2.44	12	1
1:A:23:GLN:NE2	1:A:62:LEU:HD22	0.48	2.24	19	1
1:A:75:ARG:O	1:A:79:LYS:HD3	0.48	2.08	19	1
1:A:74:LYS:HB2	1:A:89:LEU:HD21	0.47	1.85	6	1
1:A:94:GLY:HA2	1:A:101:GLY:HA2	0.47	1.87	19	3
1:A:112:MET:SD	1:A:119:ALA:HB3	0.47	2.49	8	2
1:A:40:TYR:CE1	1:A:114:LEU:HD22	0.47	2.44	17	1
1:A:77:LEU:HG	1:A:82:VAL:HG13	0.47	1.86	2	1
1:A:37:ASP:OD1	1:A:39:LYS:HB3	0.47	2.10	19	1
1:A:70:ILE:HG22	1:A:93:ILE:HD12	0.47	1.87	2	3
1:A:70:ILE:CG2	1:A:93:ILE:HD12	0.47	2.40	10	4
1:A:43:ASP:O	1:A:47:PRO:HD2	0.46	2.09	15	3
1:A:57:TYR:CD2	1:A:106:TYR:HD2	0.46	2.28	4	4
1:A:109:PHE:CE2	1:A:121:LEU:HD13	0.46	2.46	6	1
1:A:21:ALA:O	1:A:25:GLU:HG3	0.46	2.10	10	1
1:A:67:ASP:OD2	1:A:103:THR:HB	0.46	2.09	16	1
1:A:77:LEU:HD12	1:A:78:GLU:N	0.45	2.26	14	4
1:A:43:ASP:HA	1:A:46:LEU:CD1	0.45	2.41	20	1
1:A:49:LYS:HD3	1:A:113:MET:SD	0.45	2.50	11	1
1:A:70:ILE:HG23	1:A:102:GLU:HA	0.45	1.89	16	1
1:A:18:LEU:O	1:A:18:LEU:HD13	0.45	2.11	17	1
1:A:26:ARG:O	1:A:29:GLU:HB3	0.45	2.11	17	1
1:A:60:PHE:CE2	1:A:73:LEU:HD12	0.45	2.46	6	2
1:A:20:LYS:HE3	1:A:58:MET:SD	0.45	2.52	14	1
1:A:60:PHE:CD2	1:A:68:ILE:HD13	0.44	2.46	14	1
1:A:94:GLY:HA2	1:A:97:SER:O	0.44	2.11	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LEU:HD22	1:A:120:ILE:HB	0.44	1.89	4	1
1:A:84:LYS:HE3	1:A:84:LYS:HA	0.44	1.89	6	1
1:A:75:ARG:O	1:A:79:LYS:HB2	0.44	2.12	12	1
1:A:25:GLU:O	1:A:29:GLU:HG3	0.44	2.12	1	1
1:A:92:LEU:CD2	1:A:120:ILE:HB	0.44	2.43	13	2
1:A:54:LYS:HD2	1:A:54:LYS:C	0.44	2.33	11	1
1:A:87:LEU:O	1:A:91:LYS:HG3	0.44	2.12	13	1
1:A:31:ASN:HD21	1:A:54:LYS:HB2	0.43	1.72	2	1
1:A:112:MET:SD	1:A:122:LYS:HB2	0.43	2.53	2	2
1:A:60:PHE:CD2	1:A:76:MET:HG3	0.43	2.47	8	1
1:A:23:GLN:NE2	1:A:66:GLY:HA2	0.43	2.28	4	1
1:A:77:LEU:HB2	1:A:82:VAL:O	0.43	2.13	5	1
1:A:112:MET:HG2	1:A:117:ARG:O	0.43	2.13	11	1
1:A:71:MET:O	1:A:74:LYS:HB3	0.43	2.13	7	1
1:A:21:ALA:HA	1:A:24:GLU:OE2	0.43	2.14	20	1
1:A:96:VAL:HG12	1:A:108:ASP:HB3	0.43	1.91	16	2
1:A:60:PHE:O	1:A:72:SER:HB3	0.43	2.14	11	1
1:A:71:MET:O	1:A:75:ARG:HG2	0.43	2.13	1	1
1:A:112:MET:HA	1:A:117:ARG:HB2	0.43	1.89	15	1
1:A:63:ASN:HB2	1:A:67:ASP:OD1	0.43	2.13	13	2
1:A:68:ILE:HB	1:A:104:PHE:CD2	0.43	2.48	10	1
1:A:52:GLY:O	1:A:56:LYS:HD2	0.42	2.15	4	1
1:A:105:SER:O	1:A:108:ASP:HB2	0.42	2.14	6	1
1:A:121:LEU:H	1:A:121:LEU:HD22	0.42	1.74	8	2
1:A:54:LYS:O	1:A:58:MET:HG2	0.42	2.14	19	1
1:A:40:TYR:CE1	1:A:114:LEU:HD23	0.42	2.49	10	1
1:A:74:LYS:O	1:A:78:GLU:HG3	0.42	2.15	12	1
1:A:73:LEU:O	1:A:76:MET:HB2	0.42	2.15	20	1
1:A:92:LEU:O	1:A:121:LEU:HD21	0.42	2.14	8	1
1:A:19:LEU:HG	1:A:22:GLN:NE2	0.42	2.29	20	1
1:A:40:TYR:OH	1:A:114:LEU:HD13	0.42	2.14	3	1
1:A:30:ILE:O	1:A:33:GLN:HG2	0.42	2.15	9	1
1:A:52:GLY:O	1:A:56:LYS:HG3	0.42	2.15	20	1
1:A:46:LEU:O	1:A:50:LEU:HD13	0.42	2.15	15	1
1:A:71:MET:HA	1:A:71:MET:CE	0.42	2.45	17	1
1:A:68:ILE:HB	1:A:104:PHE:CE1	0.42	2.50	20	1
1:A:30:ILE:HA	1:A:33:GLN:NE2	0.41	2.30	11	1
1:A:26:ARG:HD3	1:A:29:GLU:OE1	0.41	2.16	1	1
1:A:112:MET:HG2	1:A:117:ARG:HB2	0.41	1.92	7	1
1:A:112:MET:SD	1:A:118:SER:HA	0.41	2.55	11	1
1:A:35:LEU:O	1:A:35:LEU:HD23	0.41	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ILE:HD12	1:A:71:MET:N	0.41	2.30	4	1
1:A:53:PHE:CD2	1:A:110:LEU:HD21	0.41	2.51	20	1
1:A:110:LEU:O	1:A:114:LEU:HB2	0.41	2.15	20	2
1:A:123:MET:O	1:A:127:TYR:HD1	0.41	1.99	2	1
1:A:71:MET:HE2	1:A:71:MET:HA	0.41	1.93	12	1
1:A:83:PRO:O	1:A:84:LYS:HE2	0.41	2.16	19	1
1:A:61:ASP:HB3	1:A:72:SER:HB3	0.40	1.93	2	1
1:A:122:LYS:HE2	1:A:126:MET:SD	0.40	2.56	20	1
1:A:83:PRO:O	1:A:84:LYS:HD2	0.40	2.17	9	1
1:A:46:LEU:N	1:A:47:PRO:HD2	0.40	2.32	16	1
1:A:121:LEU:HD12	1:A:122:LYS:N	0.40	2.32	10	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	111/150 (74%)	103±2 (93±2%)	7±2 (6±2%)	2±1 (1±1%)	15	61
All	All	2220/3000 (74%)	2056 (93%)	132 (6%)	32 (1%)	15	61

All 15 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	61	ASP	6
1	A	98	SER	5
1	A	62	LEU	3
1	A	116	LYS	3
1	A	117	ARG	2
1	A	115	GLY	2
1	A	41	SER	2
1	A	99	GLY	2
1	A	83	PRO	1
1	A	97	SER	1
1	A	60	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	118	SER	1
1	A	102	GLU	1
1	A	42	SER	1
1	A	43	ASP	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	101/131 (77%)	97±2 (96±2%)	4±2 (4±2%)	32 81
All	All	2020/2620 (77%)	1932 (96%)	88 (4%)	32 81

All 28 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	54	LYS	15
1	A	74	LYS	12
1	A	39	LYS	12
1	A	112	MET	7
1	A	56	LYS	5
1	A	128	GLU	4
1	A	71	MET	3
1	A	20	LYS	3
1	A	91	LYS	2
1	A	121	LEU	2
1	A	55	GLU	2
1	A	108	ASP	2
1	A	116	LYS	2
1	A	122	LYS	2
1	A	84	LYS	2
1	A	35	LEU	1
1	A	44	GLU	1
1	A	125	LEU	1
1	A	49	LYS	1
1	A	79	LYS	1
1	A	109	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	29	GLU	1
1	A	40	TYR	1
1	A	69	ASP	1
1	A	70	ILE	1
1	A	89	LEU	1
1	A	67	ASP	1
1	A	117	ARG	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