Full wwPDB NMR Structure Validation Report (i)

Feb 13, 2022 – 09:35 PM EST

PDB ID	:	1HUN
Title	:	SOLUTION STRUCTURE OF THE CHEMOKINE HMIP-1BETA(SLASH) ACT-2 BY MULTI-DIMENSIONAL NMR: A NOVEL CHEMOKINE DIMER
Authors	:	Clore, G.M.; Lodi, P.J.; Garrett, D.S.; Gronenborn, A.M.
Deposited on	:	1994-01-31

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:

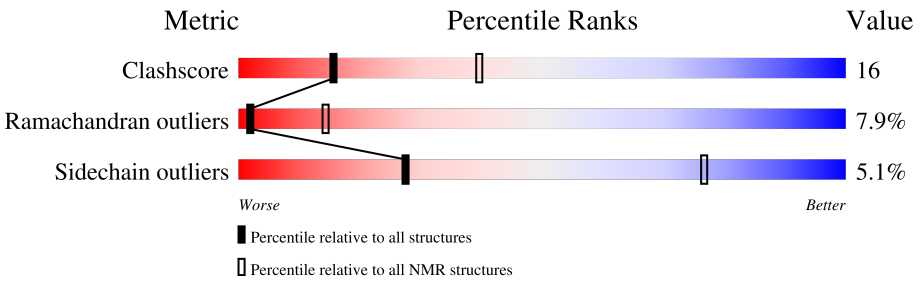
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	69	62% 25% • 9%
1	B	69	61% 26% • 9%

2 Ensemble composition and analysis (i)

This entry contains 35 models. Model 10 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:5-A:67, B:5-B:67 (126)	0.17	10

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 6 clusters and 2 single-model clusters were found.

Cluster number	Models
1	8, 10, 11, 12, 14, 16, 17, 20, 21, 23, 29, 30
2	5, 6, 7, 13, 22, 24, 26, 31, 34
3	3, 4, 9, 18, 35
4	2, 19, 32
5	1, 15
6	28, 33
Single-model clusters	25; 27

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2140 atoms, of which 1040 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	69	1064	346	516	88	109	5	0
1	B	69	1064	346	516	88	109	5	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		
			Total	H	O
2	A	2	6	4	2
2	B	2	6	4	2

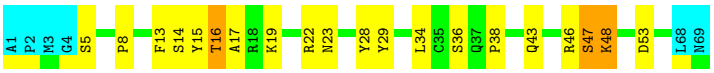
4 Residue-property plots (i)

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.

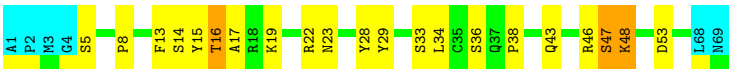
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 62% 25% • 9%



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 61% 26% • 9%



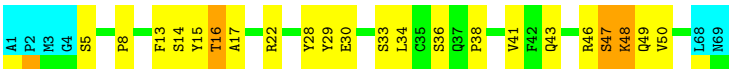
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

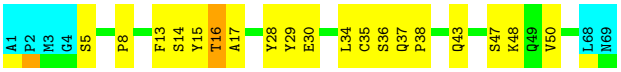
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 59% 28% • 9%



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

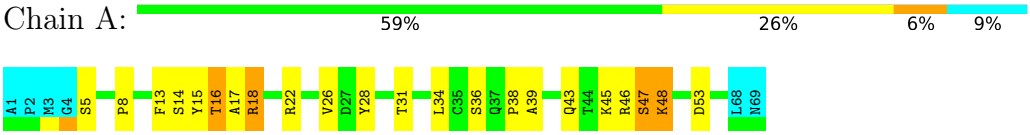
Chain B: 64% 26% • 9%



4.2.2 Score per residue for model 2

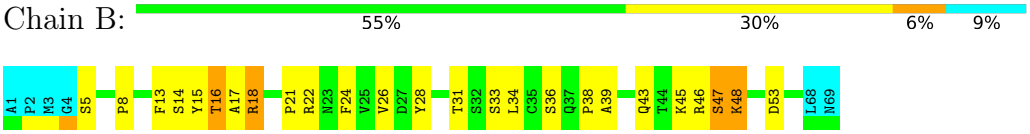
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A:



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

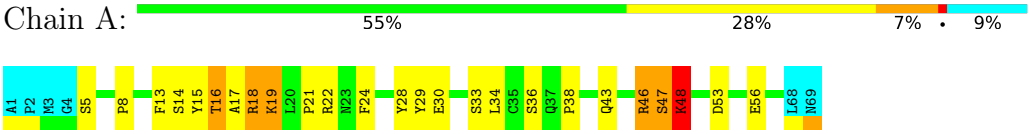
Chain B:



4.2.3 Score per residue for model 3

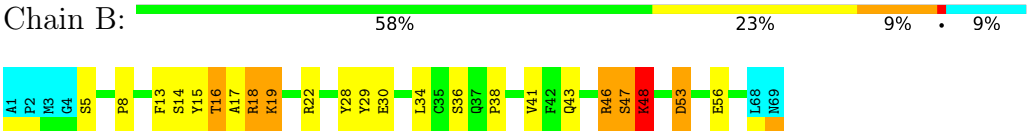
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A:



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

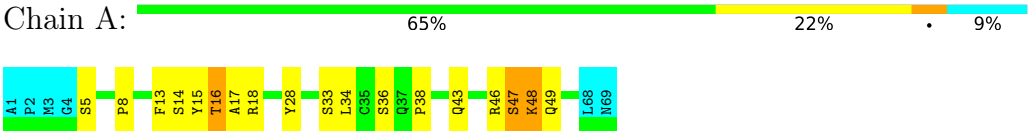
Chain B:



4.2.4 Score per residue for model 4

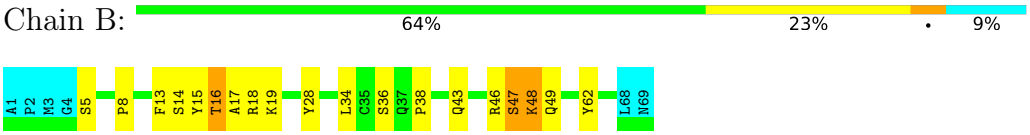
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A:



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

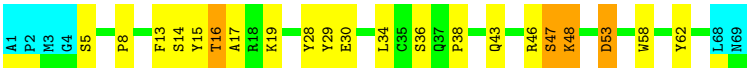
Chain B:



4.2.5 Score per residue for model 5

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 61% 25% 6% 9%



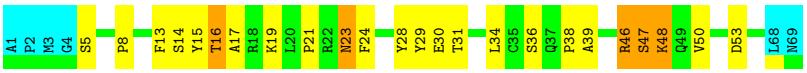
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 55% 30% 6% 9%

4.2.6 Score per residue for model 6

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 57% 28% 7% 9%



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 52% 32% 7% 9%

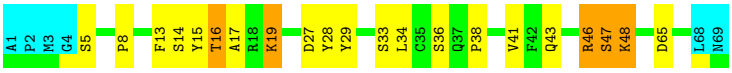
4.2.7 Score per residue for model 7

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 64% 20% 7% 9%

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 61% 23% 7% 9%



4.2.8 Score per residue for model 8

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 65% 20% 6% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 K19 R22 D27 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 D53 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 62% 23% 6% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 K19 R22 D27 Y28 Y29 L34 C35 S36 Q37 P38 V41 F42 Q43 R46 S47 K48 D53 L68 N69

4.2.9 Score per residue for model 9

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 58% 26% 7% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 K19 V26 D27 Y28 Y29 E30 S33 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 Q49 V50 D53 E61 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 59% 25% 7% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 K19 V26 D27 Y28 Y29 E30 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 Q49 V50 D53 E61 L68 N69

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 59% 28% • 9%

A1 P2 M3 G4 S5 D6 P7 P8 F13 S14 Y15 T16 A17 R18 K19 R22 Y28 Y29 L34 C35 S36 Q37 P38 V41 F42 Q43 R46 S47 K48 Q49 V50 D53 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

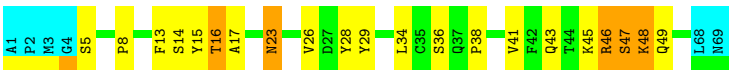
Chain B: 58% 29% • 9%

A1 P2 M3 G4 S5 D6 P7 P8 F13 S14 Y15 T16 A17 R18 K19 R22 Y28 S33 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 Q49 V50 D53 L68 N69

4.2.11 Score per residue for model 11

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 61% 23% 7% 9%



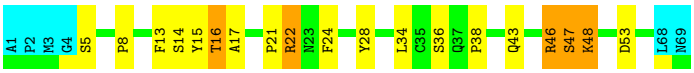
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 61% 23% 7% 9%

4.2.12 Score per residue for model 12

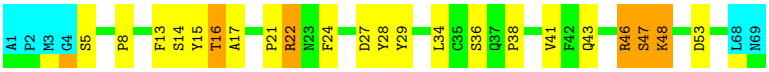
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 64% 20% 7% 9%



- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

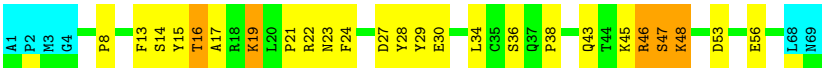
Chain B: 59% 25% 7% 9%



4.2.13 Score per residue for model 13

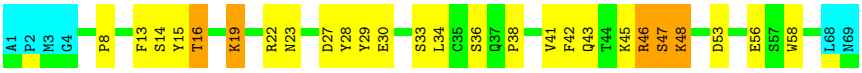
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 55% 29% 7% 9%



- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 54% 30% 7% 9%



4.2.14 Score per residue for model 14

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 68% 14% 9% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 K19 N23 L34 C35 S36 Q37 P38 R46 S47 K48 D53 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 62% 20% 9% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 K19 L20 P21 R22 N23 F24 Y29 L34 C35 S36 Q37 P38 V41 R46 S47 K48 D53 L68 N69

4.2.15 Score per residue for model 15

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 62% 23% 6% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 P21 F24 Y28 Y29 S33 L34 C35 S36 Q37 P38 V41 F42 Q43 R46 S47 K48 D53 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 65% 20% 6% 9%

A1 P2 M3 G4 S5 D6 P7 P8 F13 S14 Y15 T16 Y28 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 D53 L68 N69

4.2.16 Score per residue for model 16

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 57% 26% 9% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 R22 N23 V26 D27 Y28 Y29 E30 L34 C35 S36 Q37 P38 Q43 T44 K45 R46 S47 K48 Q49 V50 D53 P54 S55 E56 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

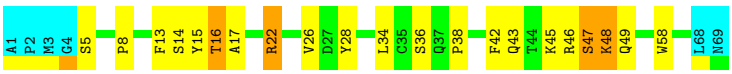
Chain B: 54% 29% 9% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 R22 N23 V26 D27 Y28 Y29 E30 S33 L34 C35 S36 Q37 P38 V41 F42 Q43 T44 K45 R46 S47 K48 Q49 V50 D53 P54 S55 E56 L68 N69

4.2.17 Score per residue for model 17

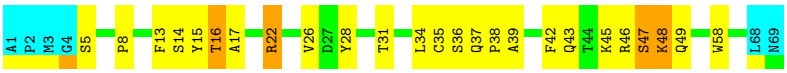
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 61% 25% 6% 9%



- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

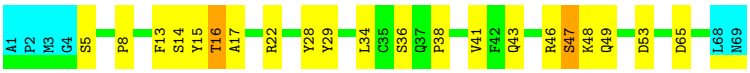
Chain B: 55% 30% 6% 9%



4.2.18 Score per residue for model 18

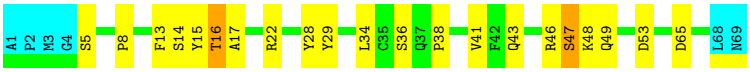
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 61% 28% • 9%



- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

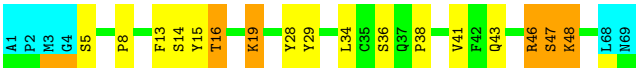
Chain B: 61% 28% • 9%



4.2.19 Score per residue for model 19

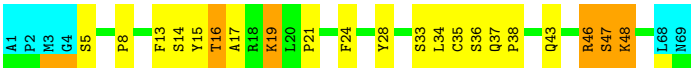
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 67% 17% 7% 9%



- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

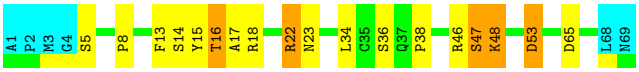
Chain B: 61% 23% 7% 9%



4.2.20 Score per residue for model 20

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 65% 19% 7% 9%



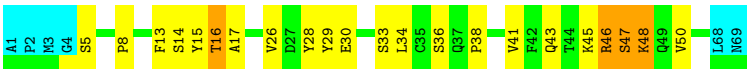
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 61% 23% 7% 9%

4.2.21 Score per residue for model 21

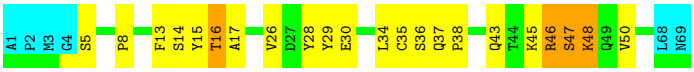
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 59% 26% 6% 9%



- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

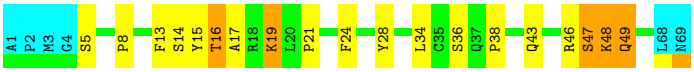
Chain B: 59% 26% 6% 9%



4.2.22 Score per residue for model 22

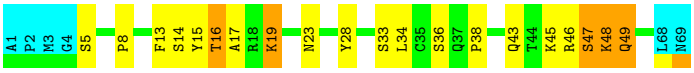
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 64% 20% 7% 9%



- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 62% 22% 7% 9%



4.2.23 Score per residue for model 23

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 57% 29% 6% 9%

A1 P2 M3 G4 S5 D6 P7 P8 F13 S14 Y15 T16 A17 R22 N23 D27 Y28 Y29 E30 S33 L34 C35 S36 Q37 P38 Q43 T44 K45 R46 S47 K48 Q49 V50 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 55% 30% 6% 9%

A1 P2 M3 G4 S5 D6 P7 P8 F13 S14 Y15 T16 A17 R22 N23 D27 Y28 Y29 E30 S33 L34 C35 S36 Q37 P38 V41 F42 Q43 T44 K45 R46 S47 K48 Q49 V50 L68 N69

4.2.24 Score per residue for model 24

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 65% 20% • • 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 Y28 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 Q49 V50 D53 E56 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 62% 23% • • 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 Y28 T31 L34 C35 S36 Q37 P38 A39 Q43 R46 S47 K48 Q49 V50 D53 E56 L68 N69

4.2.25 Score per residue for model 25

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 55% 29% 7% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 P21 R22 N23 F24 Y28 Y29 E30 S33 L34 C35 S36 Q37 P38 V41 F42 Q43 R46 S47 K48 D53 W58 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 61% 23% 7% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 N23 Y28 Y29 E30 L34 C35 S36 Q37 P38 F42 Q43 R46 S47 K48 D53 W58 L68 N69

4.2.26 Score per residue for model 26

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 51% 30% 10% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 K19 R22 N23 V26 D27 Y28 Y29 E30 T31 L34 C35 S36 Q37 P38 A39 F42 K45 R46 S47 K48 Q49 D53 W58 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 51% 30% 10% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 K19 R22 N23 V26 D27 Y28 Y29 E30 T31 L34 C35 S36 Q37 P38 A39 F42 K45 R46 S47 K48 Q49 D53 W58 L68 N69

4.2.27 Score per residue for model 27

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 65% 20% 6% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 Y28 L34 C35 S36 Q37 P38 F42 Q43 R46 S47 K48 W58 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 64% 22% 6% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 Y28 S33 L34 C35 S36 Q37 P38 F42 Q43 R46 S47 K48 W58 L68 N69

4.2.28 Score per residue for model 28

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 64% 23% • 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 Y28 Y29 E30 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 Q49 V50 D53 L68 N69

- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 62% 25% • 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 Y28 Y29 E30 S33 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 Q49 V50 D53 L68 N69

4.2.29 Score per residue for model 29

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 64% 22% 6% 9%

A1 P2 M3 G4 S5 D6 P7 P8 F13 S14 Y15 T16 A17 Y28 L34 C35 S36 Q37 P38 F42 Q43 R46 S47 K48 Q49 V50 W58 L68 N69

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 59% 26% 6% 9%

A1 P2 M3 G4 S5 D6 P7 P8 F13 S14 Y15 T16 A17 Y28 Y29 S33 L34 C35 S36 Q37 P38 V41 F42 Q43 R46 S47 K48 Q49 V50 W58 L68 N69

4.2.30 Score per residue for model 30

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 65% 22% • 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 K19 V26 D27 Y28 S33 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 D65 L68 N69

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B: 62% 25% • 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R18 K19 V26 D27 Y28 L34 C35 S36 Q37 P38 Q43 R46 S47 K48 D65 L68 N69

4.2.31 Score per residue for model 31

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 61% 25% 6% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R22 Y28 Y29 E30 S33 L34 C35 S36 Q37 P38 F42 Q43 S47 K48 D53 W58 L68 N69

• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

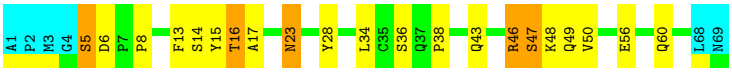
Chain B: 57% 29% 6% 9%

A1 P2 M3 G4 S5 P8 F13 S14 Y15 T16 A17 R22 Y28 Y29 E30 T31 S32 S33 L34 C35 S36 Q37 P38 A39 V40 V41 F42 Q43 S47 K48 D53 W58 L68 N69

4.2.32 Score per residue for model 32

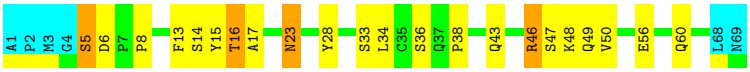
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 61% 23% 7% 9%



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

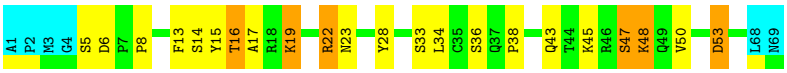
Chain B: 59% 26% 6% 9%



4.2.33 Score per residue for model 33

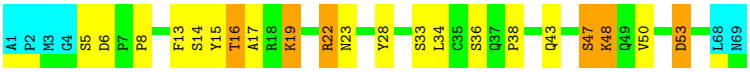
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 59% 23% 9% 9%



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

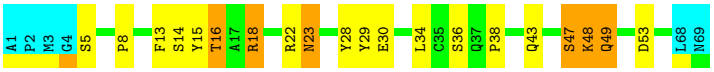
Chain B: 61% 22% 9% 9%



4.2.34 Score per residue for model 34

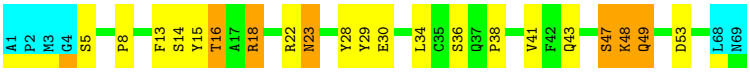
• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A: 62% 20% 9% 9%



• Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

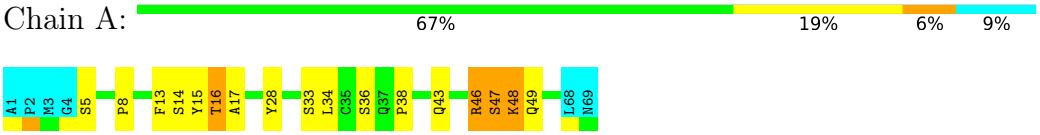
Chain B: 61% 22% 9% 9%



4.2.35 Score per residue for model 35

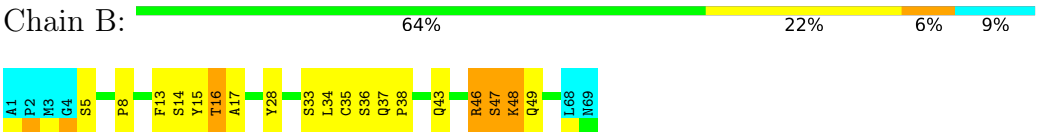
- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain A:



- Molecule 1: HUMAN MACROPHAGE INFLAMMATORY PROTEIN 1 BETA

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *?*.

Of the ? calculated structures, 35 were deposited, based on the following criterion: *?*.

The authors did not provide any information on software used for structure solution, optimization or refinement.

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	507	473	473	17±4
1	B	507	473	473	18±4
2	A	2	4	0	1±0
2	B	2	4	0	1±0
All	All	35630	33390	33110	1123

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:23:ASN:HD22	1:B:23:ASN:N	0.61	1.93	14	4
1:A:23:ASN:N	1:A:23:ASN:HD22	0.61	1.93	32	4
1:B:23:ASN:N	1:B:23:ASN:ND2	0.58	2.51	32	5
1:A:23:ASN:N	1:A:23:ASN:ND2	0.58	2.51	6	5
1:A:28:TYR:N	1:A:43:GLN:HE21	0.58	1.97	19	4
1:B:46:ARG:O	1:B:46:ARG:NE	0.57	2.37	26	2
1:A:46:ARG:O	1:A:46:ARG:NE	0.57	2.37	26	2
1:B:28:TYR:N	1:B:43:GLN:HE21	0.57	1.97	19	4
1:B:26:VAL:CG1	1:B:45:LYS:NZ	0.56	2.68	11	5
1:A:13:PHE:CE1	1:B:34:LEU:HD13	0.56	2.35	35	35
1:A:34:LEU:HD13	1:B:13:PHE:CE1	0.56	2.35	33	35

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:VAL:CG1	1:A:45:LYS:NZ	0.56	2.68	11	5
1:B:19:LYS:NZ	1:B:62:TYR:CZ	0.55	2.75	5	1
1:A:19:LYS:NZ	1:A:62:TYR:CE1	0.55	2.75	5	1
1:A:47:SER:OG	1:A:48:LYS:N	0.55	2.40	33	28
1:A:5:SER:HB2	1:B:50:VAL:HG22	0.55	1.79	28	1
1:B:56:GLU:N	1:B:56:GLU:OE1	0.54	2.41	3	2
1:A:19:LYS:NZ	1:A:62:TYR:CZ	0.54	2.75	5	1
1:B:47:SER:OG	1:B:48:LYS:N	0.54	2.40	33	28
1:B:19:LYS:NZ	1:B:62:TYR:CE1	0.54	2.75	5	1
1:A:50:VAL:HG22	1:B:5:SER:HB2	0.54	1.79	28	1
1:A:56:GLU:N	1:A:56:GLU:OE1	0.54	2.41	16	2
1:A:48:LYS:O	1:A:49:GLN:NE2	0.53	2.42	34	1
1:B:14:SER:O	1:B:15:TYR:CD1	0.53	2.61	13	32
1:A:14:SER:O	1:A:15:TYR:CD1	0.53	2.61	13	32
1:A:15:TYR:CD2	1:A:53:ASP:OD2	0.53	2.62	33	9
1:B:15:TYR:CD2	1:B:53:ASP:OD2	0.53	2.62	33	9
1:B:15:TYR:CG	1:B:53:ASP:OD1	0.53	2.62	34	11
1:A:15:TYR:CG	1:A:53:ASP:OD1	0.53	2.62	34	11
1:B:15:TYR:CD1	1:B:53:ASP:OD2	0.53	2.62	31	2
1:B:15:TYR:CG	1:B:53:ASP:OD2	0.53	2.62	2	2
1:A:29:TYR:CE1	1:A:30:GLU:O	0.53	2.62	5	8
1:A:28:TYR:O	1:A:43:GLN:NE2	0.53	2.42	32	12
1:A:15:TYR:CG	1:A:53:ASP:OD2	0.53	2.62	2	2
1:B:15:TYR:CE2	1:B:53:ASP:OD2	0.53	2.62	12	3
1:B:46:ARG:NE	1:B:46:ARG:C	0.53	2.62	28	2
1:B:18:ARG:CG	1:B:18:ARG:HH11	0.53	2.17	3	6
1:A:15:TYR:CD1	1:A:53:ASP:OD2	0.53	2.62	5	2
1:B:28:TYR:O	1:B:43:GLN:NE2	0.53	2.42	32	12
1:A:15:TYR:CE2	1:A:53:ASP:OD2	0.53	2.62	34	3
1:B:15:TYR:CE1	1:B:53:ASP:OD2	0.53	2.62	18	2
1:A:56:GLU:O	1:A:60:GLN:NE2	0.53	2.42	32	1
1:B:22:ARG:NH1	1:B:22:ARG:CG	0.52	2.72	12	10
1:A:23:ASN:C	1:A:45:LYS:HZ3	0.52	2.07	26	1
1:B:48:LYS:O	1:B:49:GLN:NE2	0.52	2.42	34	1
1:B:15:TYR:CE2	1:B:53:ASP:OD1	0.52	2.62	2	2
1:B:29:TYR:CE1	1:B:30:GLU:O	0.52	2.62	5	8
1:A:46:ARG:NE	1:A:46:ARG:C	0.52	2.62	28	2
1:B:60:GLN:N	1:B:60:GLN:OE1	0.52	2.43	32	1
1:B:22:ARG:CG	1:B:22:ARG:HH11	0.52	2.18	12	9
1:B:17:ALA:HB3	1:B:18:ARG:HE	0.52	1.64	2	1
1:A:15:TYR:CD2	1:A:53:ASP:OD1	0.52	2.63	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:TYR:CD2	1:B:53:ASP:OD1	0.52	2.63	12	3
1:A:18:ARG:NH1	1:A:18:ARG:CG	0.52	2.72	26	3
1:A:60:GLN:N	1:A:60:GLN:OE1	0.52	2.43	32	1
1:A:17:ALA:HB3	1:A:18:ARG:HE	0.52	1.64	2	1
1:B:18:ARG:CG	1:B:18:ARG:NH1	0.52	2.71	27	2
1:A:18:ARG:CG	1:A:18:ARG:HH11	0.52	2.17	3	6
1:A:28:TYR:CE2	1:A:30:GLU:OE2	0.52	2.62	23	4
1:A:53:ASP:OD1	1:A:53:ASP:N	0.52	2.43	33	10
1:B:28:TYR:CE2	1:B:30:GLU:OE2	0.52	2.62	23	4
1:B:56:GLU:O	1:B:60:GLN:NE2	0.52	2.42	32	1
1:A:15:TYR:CE2	1:A:53:ASP:OD1	0.52	2.62	2	2
1:B:30:GLU:N	1:B:30:GLU:OE2	0.52	2.43	26	2
1:A:15:TYR:CE1	1:A:53:ASP:OD2	0.52	2.62	18	2
1:A:30:GLU:N	1:A:30:GLU:OE2	0.52	2.43	5	1
1:B:18:ARG:NH1	1:B:18:ARG:CG	0.51	2.72	26	4
1:A:50:VAL:HG22	1:B:5:SER:OG	0.51	2.05	29	4
1:A:16:THR:OG1	1:A:17:ALA:N	0.51	2.42	24	27
1:A:22:ARG:NH1	1:A:22:ARG:CG	0.51	2.73	26	9
1:B:30:GLU:OE2	1:B:30:GLU:N	0.51	2.43	23	2
1:B:16:THR:OG1	1:B:17:ALA:N	0.51	2.42	24	29
1:A:22:ARG:CG	1:A:22:ARG:HH11	0.51	2.18	12	9
1:A:30:GLU:OE2	1:A:30:GLU:N	0.51	2.43	26	3
1:B:53:ASP:N	1:B:53:ASP:OD1	0.51	2.43	33	6
1:A:18:ARG:CG	1:A:18:ARG:NH1	0.51	2.71	3	3
1:B:23:ASN:HD22	1:B:23:ASN:H	0.51	1.48	11	2
1:A:5:SER:OG	1:B:50:VAL:HG22	0.51	2.05	29	4
1:B:15:TYR:CD1	1:B:53:ASP:OD1	0.51	2.64	18	1
1:B:23:ASN:C	1:B:45:LYS:HZ3	0.51	2.09	26	1
1:B:23:ASN:O	1:B:45:LYS:NZ	0.50	2.43	23	4
1:A:22:ARG:CG	1:A:22:ARG:NH1	0.50	2.72	12	2
1:A:15:TYR:CD1	1:A:53:ASP:OD1	0.50	2.64	18	1
1:A:28:TYR:N	1:A:43:GLN:OE1	0.50	2.45	34	1
1:B:14:SER:C	1:B:15:TYR:CG	0.50	2.85	31	35
1:B:53:ASP:OD1	1:B:53:ASP:N	0.50	2.44	5	5
1:A:23:ASN:H	1:A:23:ASN:HD22	0.50	1.48	11	1
1:A:19:LYS:CB	1:A:19:LYS:NZ	0.50	2.75	3	9
1:B:19:LYS:CB	1:B:19:LYS:NZ	0.50	2.75	3	9
1:B:28:TYR:N	1:B:43:GLN:OE1	0.50	2.45	34	1
1:A:14:SER:C	1:A:15:TYR:CG	0.50	2.85	18	35
1:B:23:ASN:O	1:B:23:ASN:ND2	0.49	2.45	25	2
1:A:5:SER:CB	1:B:50:VAL:HG22	0.49	2.37	10	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:HG22	1:B:5:SER:CB	0.49	2.37	10	8
1:B:29:TYR:CZ	1:B:30:GLU:O	0.49	2.65	6	8
1:A:23:ASN:O	1:A:45:LYS:NZ	0.49	2.43	23	3
1:A:29:TYR:CZ	1:A:30:GLU:O	0.49	2.65	6	8
1:A:23:ASN:O	1:A:23:ASN:ND2	0.49	2.45	25	2
1:B:46:ARG:C	1:B:46:ARG:HE	0.49	2.11	28	2
1:A:46:ARG:CG	1:A:46:ARG:NH1	0.48	2.75	3	2
1:A:15:TYR:CB	1:A:53:ASP:OD1	0.48	2.62	20	6
1:A:48:LYS:C	1:A:49:GLN:NE2	0.48	2.67	9	2
1:A:60:GLN:N	1:A:60:GLN:CD	0.48	2.67	32	1
1:B:46:ARG:NH1	1:B:46:ARG:CG	0.48	2.75	3	5
1:B:15:TYR:CB	1:B:53:ASP:OD1	0.47	2.62	20	6
1:A:23:ASN:C	1:A:45:LYS:NZ	0.47	2.68	26	1
1:B:23:ASN:C	1:B:45:LYS:NZ	0.47	2.68	26	1
1:B:48:LYS:C	1:B:49:GLN:NE2	0.47	2.67	9	2
1:A:46:ARG:C	1:A:46:ARG:HE	0.47	2.11	28	2
1:B:42:PHE:CE2	1:B:58:TRP:CZ3	0.47	3.03	17	7
1:A:42:PHE:CE2	1:A:58:TRP:CZ3	0.47	3.03	17	6
1:A:23:ASN:HD22	1:A:23:ASN:H	0.47	1.52	34	1
1:A:46:ARG:CD	1:A:46:ARG:O	0.47	2.63	3	24
1:B:46:ARG:CD	1:B:46:ARG:O	0.46	2.63	8	26
1:B:60:GLN:N	1:B:60:GLN:CD	0.46	2.67	32	1
1:A:30:GLU:N	1:A:30:GLU:CD	0.46	2.69	23	4
1:B:22:ARG:HH12	1:B:65:ASP:CB	0.46	2.24	20	1
1:A:31:THR:OG1	1:A:39:ALA:N	0.46	2.49	26	3
1:B:30:GLU:N	1:B:30:GLU:CD	0.46	2.69	23	4
1:A:48:LYS:N	1:A:48:LYS:CD	0.46	2.79	33	1
1:A:46:ARG:O	1:A:46:ARG:CD	0.45	2.65	4	4
1:B:48:LYS:N	1:B:48:LYS:CD	0.45	2.79	33	1
1:A:46:ARG:NE	1:A:46:ARG:CA	0.45	2.80	17	2
1:B:31:THR:OG1	1:B:39:ALA:N	0.45	2.49	2	7
1:B:19:LYS:NZ	1:B:19:LYS:CB	0.45	2.79	30	2
1:B:46:ARG:NE	1:B:46:ARG:CA	0.45	2.80	28	2
1:A:19:LYS:NZ	1:A:19:LYS:CB	0.45	2.79	30	2
1:A:26:VAL:CG1	1:A:45:LYS:HZ1	0.45	2.25	11	1
1:A:22:ARG:HH12	1:A:65:ASP:CB	0.45	2.24	20	1
1:A:46:ARG:O	1:A:47:SER:OG	0.45	2.35	18	7
1:B:15:TYR:O	1:B:16:THR:O	0.45	2.35	4	20
1:A:15:TYR:O	1:A:16:THR:O	0.44	2.35	4	19
1:A:38:PRO:N	2:A:202:HOH:O	0.44	2.50	15	35
1:B:38:PRO:N	2:B:302:HOH:O	0.44	2.51	19	35

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ARG:CG	1:A:46:ARG:HH11	0.44	2.25	3	1
1:B:27:ASP:OD2	1:B:43:GLN:NE2	0.44	2.51	23	3
1:B:46:ARG:CG	1:B:46:ARG:HH11	0.44	2.25	3	1
1:A:27:ASP:OD2	1:A:43:GLN:NE2	0.43	2.51	23	2
1:B:14:SER:O	1:B:15:TYR:CG	0.43	2.72	28	9
1:A:28:TYR:O	1:A:43:GLN:OE1	0.43	2.37	28	17
1:B:28:TYR:O	1:B:43:GLN:OE1	0.43	2.37	2	17
1:B:53:ASP:O	1:B:53:ASP:OD1	0.43	2.37	6	1
1:B:26:VAL:CG1	1:B:45:LYS:HZ1	0.43	2.26	11	1
1:A:5:SER:O	1:A:6:ASP:OD1	0.43	2.37	32	3
1:A:17:ALA:HB3	1:A:18:ARG:HH11	0.43	1.73	4	1
1:A:53:ASP:OD2	1:A:55:SER:OG	0.43	2.37	16	1
1:B:46:ARG:O	1:B:47:SER:OG	0.43	2.37	10	5
1:B:17:ALA:HB3	1:B:18:ARG:HH11	0.43	1.73	4	1
1:A:23:ASN:H	1:A:23:ASN:ND2	0.43	2.12	11	1
1:A:14:SER:O	1:A:15:TYR:CG	0.42	2.72	28	10
1:A:49:GLN:CD	1:A:49:GLN:N	0.42	2.72	22	1
1:B:49:GLN:CD	1:B:49:GLN:N	0.42	2.72	22	1
1:B:23:ASN:H	1:B:23:ASN:ND2	0.42	2.12	11	1
1:B:53:ASP:OD2	1:B:55:SER:OG	0.42	2.37	16	1
1:B:21:PRO:O	1:B:24:PHE:N	0.42	2.52	12	5
1:B:29:TYR:N	1:B:41:VAL:O	0.42	2.52	18	14
1:B:13:PHE:CE2	1:B:14:SER:OG	0.42	2.70	10	1
1:B:53:ASP:OD1	1:B:53:ASP:O	0.42	2.37	13	2
1:A:21:PRO:O	1:A:24:PHE:N	0.42	2.52	6	8
1:B:5:SER:OG	1:B:6:ASP:N	0.42	2.52	29	1
1:A:47:SER:O	1:A:48:LYS:CG	0.42	2.68	34	11
1:B:47:SER:O	1:B:48:LYS:CG	0.42	2.68	23	7
1:B:5:SER:O	1:B:6:ASP:OD1	0.42	2.37	10	3
1:A:61:GLU:O	1:A:61:GLU:OE2	0.42	2.38	9	1
1:B:19:LYS:NZ	1:B:58:TRP:CE3	0.42	2.88	5	1
1:A:53:ASP:OD1	1:A:53:ASP:O	0.42	2.37	6	3
1:A:27:ASP:OD2	1:A:43:GLN:OE1	0.42	2.38	8	1
1:A:29:TYR:N	1:A:41:VAL:O	0.42	2.53	15	8
1:A:23:ASN:OD1	1:A:23:ASN:O	0.42	2.38	20	1
1:B:23:ASN:O	1:B:23:ASN:OD1	0.42	2.38	20	1
1:B:27:ASP:OD2	1:B:43:GLN:OE1	0.41	2.38	8	1
1:B:53:ASP:OD1	1:B:56:GLU:OE2	0.41	2.38	13	1
1:B:19:LYS:NZ	1:B:62:TYR:OH	0.41	2.42	4	1
1:B:46:ARG:O	1:B:46:ARG:CD	0.41	2.68	26	2
1:A:33:SER:O	1:A:34:LEU:C	0.41	2.59	3	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:35:CYS:O	1:B:37:GLN:N	0.41	2.54	1	10
1:B:61:GLU:O	1:B:61:GLU:OE2	0.41	2.38	9	1
1:A:46:ARG:NH1	1:A:46:ARG:CG	0.41	2.82	15	1
1:B:23:ASN:C	1:B:23:ASN:ND2	0.41	2.74	16	1
1:B:33:SER:O	1:B:34:LEU:C	0.41	2.59	7	18
1:A:48:LYS:CB	1:A:48:LYS:NZ	0.41	2.84	13	1
1:B:14:SER:O	1:B:15:TYR:CD2	0.41	2.74	5	2
1:A:53:ASP:OD1	1:A:56:GLU:OE2	0.41	2.38	13	1
1:A:23:ASN:ND2	1:A:23:ASN:C	0.41	2.74	16	1
1:A:14:SER:O	1:A:15:TYR:CD2	0.41	2.74	18	2
1:A:19:LYS:NZ	1:A:58:TRP:CE3	0.41	2.88	5	1
1:A:53:ASP:OD1	1:A:56:GLU:OE1	0.41	2.39	24	1
1:A:48:LYS:NZ	1:A:49:GLN:HE21	0.40	2.14	1	1
1:A:34:LEU:HD13	1:B:13:PHE:CZ	0.40	2.51	9	1
1:A:5:SER:HB3	1:B:50:VAL:HG22	0.40	1.93	10	1
1:B:48:LYS:NZ	1:B:48:LYS:CB	0.40	2.84	13	1
1:B:53:ASP:OD1	1:B:56:GLU:OE1	0.40	2.39	24	1
1:A:5:SER:OG	1:A:6:ASP:N	0.40	2.52	29	1
1:A:13:PHE:CZ	1:B:34:LEU:HD13	0.40	2.50	9	2
1:B:27:ASP:CG	1:B:28:TYR:H	0.40	2.20	12	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	63/69 (91%)	45±1 (72±1%)	13±1 (20±1%)	5±0 (8±0%)	2	14
1	B	63/69 (91%)	45±1 (72±1%)	13±1 (20±1%)	5±0 (8±0%)	2	14
All	All	4410/4830 (91%)	3183 (72%)	879 (20%)	348 (8%)	2	14

All 10 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	8	PRO	35

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Mol	Chain	Res	Type	Models (Total)
1	A	16	THR	35
1	A	36	SER	35
1	A	47	SER	35
1	B	8	PRO	35
1	B	16	THR	35
1	B	36	SER	35
1	B	47	SER	35
1	A	48	LYS	34
1	B	48	LYS	34

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	59/63 (94%)	56±2 (95±3%)	3±2 (5±3%)	28	77
1	B	59/63 (94%)	56±2 (95±3%)	3±2 (5±3%)	27	77
All	All	4130/4410 (94%)	3921 (95%)	209 (5%)	27	77

All 26 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	5	SER	26
1	B	5	SER	26
1	A	46	ARG	15
1	B	46	ARG	15
1	A	19	LYS	12
1	A	22	ARG	12
1	B	19	LYS	12
1	B	22	ARG	12
1	A	49	GLN	10
1	B	49	GLN	10
1	A	53	ASP	7
1	B	53	ASP	7
1	A	23	ASN	7
1	B	23	ASN	7
1	A	18	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	B	18	ARG	5
1	A	65	ASP	3
1	B	65	ASP	3
1	A	26	VAL	3
1	B	26	VAL	3
1	A	48	LYS	2
1	B	48	LYS	2
1	B	7	PRO	2
1	A	7	PRO	1
1	A	16	THR	1
1	B	16	THR	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