Full wwPDB NMR Structure Validation Report (i)

Jun 13, 2024 – 12:07 AM EDT

PDB ID	:	1GCF
Title	:	NMR STRUCTURE OF THE C-TERMINAL DOMAIN OF THE LIGAND-BINDING REGION OF MURINE GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR, 12 STRUCTURES
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Deposited on	:	1997-04-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

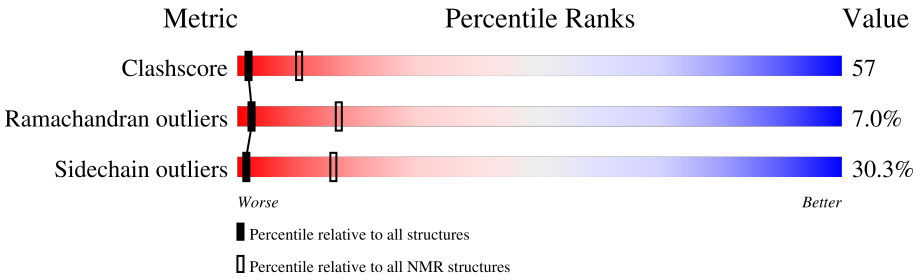
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	109	8% 35% 15% • 41%

2 Ensemble composition and analysis (i)

This entry contains 12 models. Model 12 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:10-A:13, A:25-A:30, A:43-A:86, A:98-A:107 (64)	0.43	12

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 2 single-model clusters were found.

Cluster number	Models
1	1, 4, 6, 8, 9, 10, 12
2	3, 5, 11
Single-model clusters	2; 7

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1739 atoms, of which 858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	109	1739	570	858	148	155	8	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	DELETION	UNP P40223
A	?	-	SER	DELETION	UNP P40223
A	?	-	PRO	DELETION	UNP P40223
A	?	-	LYS	DELETION	UNP P40223
A	?	-	LEU	DELETION	UNP P40223
A	?	-	CYS	DELETION	UNP P40223
A	?	-	LEU	DELETION	UNP P40223
A	?	-	ASP	DELETION	UNP P40223
A	?	-	PRO	DELETION	UNP P40223
A	?	-	MET	DELETION	UNP P40223
A	?	-	ASP	DELETION	UNP P40223
A	?	-	VAL	DELETION	UNP P40223
A	?	-	VAL	DELETION	UNP P40223
A	?	-	LYS	DELETION	UNP P40223

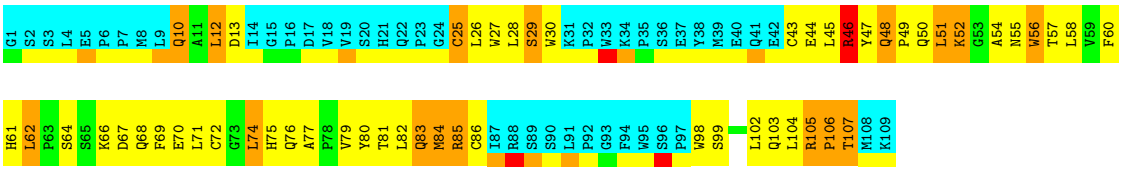
4 Residue-property plots (i)

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: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

Chain A: 8% 35% 15% • 41%



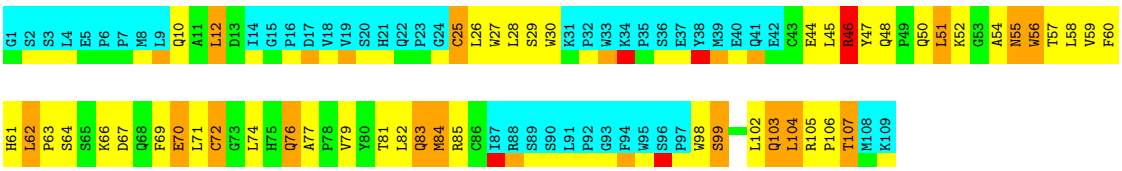
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

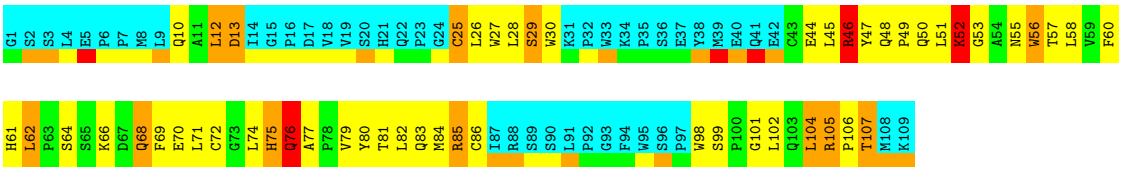
Chain A: 13% 31% 14% • 41%



4.2.2 Score per residue for model 2

• Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

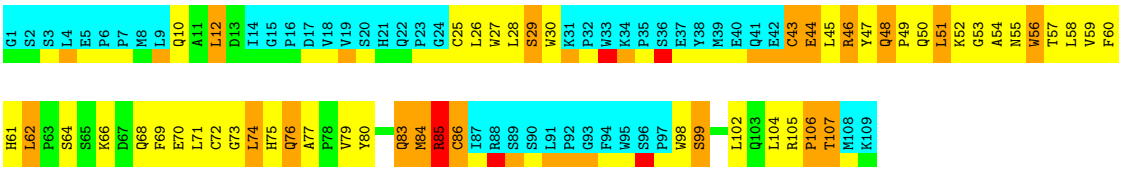
Chain A: 10% 35% 11% • 41%



4.2.3 Score per residue for model 3

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

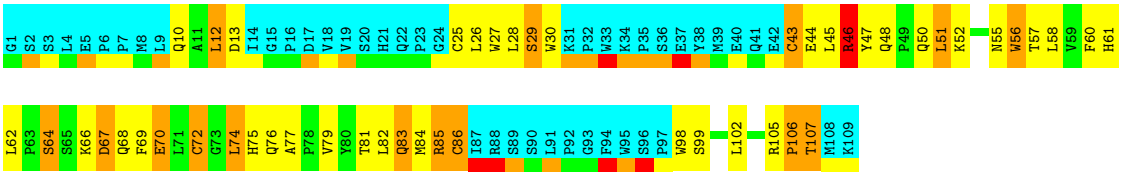
Chain A: 10% 32% 16% • 41%



4.2.4 Score per residue for model 4

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

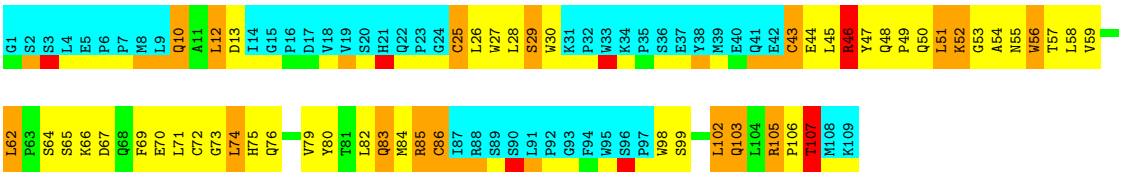
Chain A: 14% 30% 14% • 41%



4.2.5 Score per residue for model 5

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

Chain A: 10% 32% 15% • 41%



4.2.6 Score per residue for model 6

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

Chain A: 14% 28% 17% 41%

G1 S2 S3 L4 E5 P6 P7 M8 L9 Q10 A11 L12 D13 I14 G15 P16 D17 V18 V19 S20 H21 Q22 P23 G24 C25 L26 W27 L28 S29 W30 K31 P32 W33 K34 P35 S36 E37 Y38 M39 E40 Q41 E42 C43 E44 L45 R46 Y47 Q48 P49 Q50 L51 K52 N55 W56 T57 L58 L62

S65 K66 D67 Q68 F69 E70 L71 C72 G73 L74 H75 Q76 A77 P78 V79 Y80 T81 L82 Q83 M84 R85 C86 I87 R88 S89 S90 L91 P92 G93 F94 W95 S96 P97 W98 S99 L102 Q103 L104 R105 P106 T107 M108 K109

4.2.7 Score per residue for model 7

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

Chain A: 13% 28% 17% • 41%

G1 S2 S3 L4 E5 P6 P7 M8 L9 Q10 A11 L12 D13 I14 G15 P16 D17 V18 V19 S20 H21 Q22 P23 G24 C25 L26 W27 L28 S29 W30 K31 P32 W33 K34 P35 S36 E37 Y38 M39 E40 Q41 E42 C43 E44 L45 R46 Y47 Q48 P49 Q50 L51 K52 G53 A54 N55 W56 T57 L58 V59 F60

H61 L62 P63 S64 S65 K66 D67 Q68 F69 E70 L71 C72 G73 L74 H75 Q76 V79 Y80 T81 L82 Q83 M84 R85 C86 I87 R88 S89 S90 L91 P92 G93 F94 W95 S96 P97 W98 S99 L102 Q103 L104 R105 P106 T107 M108 K109

4.2.8 Score per residue for model 8

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

Chain A: 11% 36% 11% • 41%

G1 S2 S3 L4 E5 P6 P7 M8 L9 Q10 A11 L12 D13 I14 G15 P16 D17 V18 V19 S20 H21 Q22 P23 G24 C25 L26 W27 L28 S29 W30 K31 P32 W33 K34 P35 S36 E37 Y38 M39 E40 Q41 E42 C43 E44 L45 R46 Y47 Q48 P49 Q50 L51 K52 G53 A54 N55 W56 T57 L58 V59 F60

H61 L62 P63 S64 S65 K66 D67 Q68 F69 E70 L71 C72 G73 L74 H75 Q76 A77 P78 V79 Y80 T81 L82 Q83 M84 R85 C86 I87 R88 S89 S90 L91 P92 G93 F94 W95 S96 P97 W98 S99 L102 Q103 L104 R105 P106 T107 M108 K109

4.2.9 Score per residue for model 9

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

Chain A: 13% 32% 12% • 41%

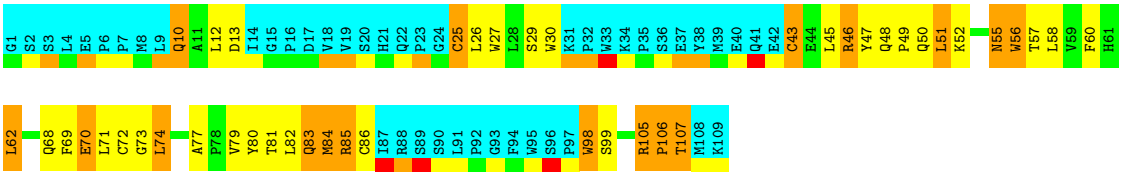
G1 S2 S3 L4 E5 P6 P7 M8 L9 Q10 A11 L12 D13 I14 G15 P16 D17 V18 V19 S20 H21 Q22 P23 G24 C25 L26 W27 L28 S29 W30 K31 P32 W33 K34 P35 S36 E37 Y38 M39 E40 Q41 E42 C43 E44 L45 R46 Y47 Q48 P49 Q50 L51 K52 N55 W56 T57 L58 V59 F60 H61

L62 P63 S64 S65 K66 D67 Q68 F69 E70 L71 C72 G73 L74 H75 Q76 A77 P78 V79 Y80 T81 L82 Q83 M84 R85 C86 I87 R88 S89 S90 L91 P92 G93 F94 W95 S96 P97 W98 S99 L102 Q103 L104 R105 P106 T107 M108 K109

4.2.10 Score per residue for model 10

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

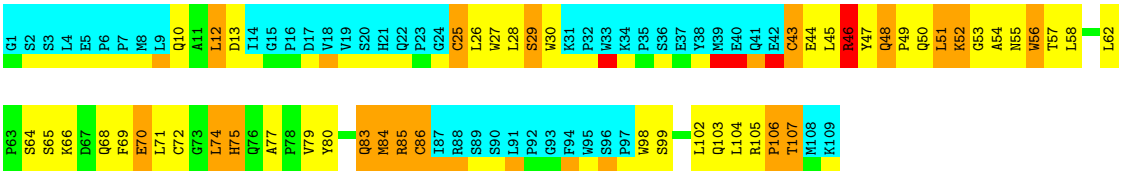
Chain A: 18% 25% 16% 41%



4.2.11 Score per residue for model 11

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

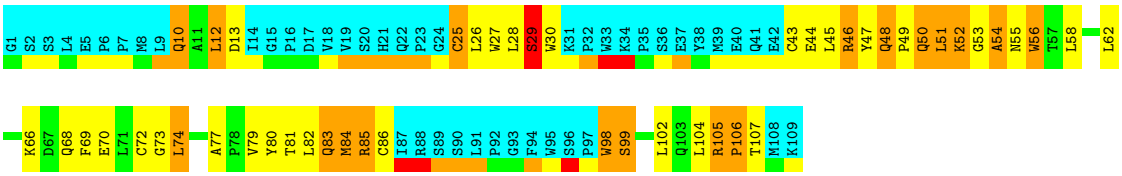
Chain A: 12% 30% 16% • 41%



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR RECEPTOR

Chain A: 15% 27% 17% • 41%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *RANDOM.INP/DGSA.INP/ REFINE.INP*.

Of the 100 calculated structures, 12 were deposited, based on the following criterion: *TOTAL OF NOE, DIHEDRAL, AND VAN DER WAALS ENERGIES*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	3.1

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	2.8±0.4
All	All	0	34

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	46	ARG	Sidechain	12
1	A	105	ARG	Sidechain	12
1	A	85	ARG	Sidechain	10

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	527	512	512	59±7
All	All	6324	6144	6144	712

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD12	1:A:74:LEU:CD1	0.97	1.88	7	11
1:A:57:THR:O	1:A:58:LEU:HD23	0.94	1.63	11	11
1:A:28:LEU:HD12	1:A:69:PHE:CG	0.90	2.01	8	4
1:A:50:GLN:HB3	1:A:79:VAL:HG13	0.83	1.49	2	11
1:A:57:THR:C	1:A:58:LEU:HD23	0.83	1.94	10	10
1:A:25:CYS:N	1:A:107:THR:HG21	0.81	1.90	12	7
1:A:81:THR:C	1:A:82:LEU:HD12	0.78	1.98	4	8
1:A:73:GLY:C	1:A:74:LEU:HD23	0.77	2.00	3	4
1:A:51:LEU:HD22	1:A:76:GLN:O	0.77	1.80	2	1
1:A:26:LEU:HD12	1:A:74:LEU:HD13	0.75	1.58	7	7
1:A:51:LEU:CD2	1:A:77:ALA:HB2	0.73	2.13	4	4
1:A:77:ALA:HB3	1:A:80:TYR:CE1	0.72	2.20	2	1
1:A:30:TRP:CZ3	1:A:84:MET:HE1	0.71	2.20	1	4
1:A:46:ARG:HG3	1:A:58:LEU:HD22	0.71	1.63	7	12
1:A:46:ARG:CG	1:A:58:LEU:HD22	0.71	2.16	7	10
1:A:49:PRO:HB2	1:A:77:ALA:HB2	0.70	1.63	2	2
1:A:26:LEU:HD11	1:A:106:PRO:HB3	0.67	1.65	6	6
1:A:30:TRP:CE2	1:A:84:MET:HE1	0.67	2.23	7	1
1:A:103:GLN:O	1:A:104:LEU:HD12	0.67	1.89	1	2
1:A:51:LEU:HD12	1:A:52:LYS:N	0.65	2.07	2	4
1:A:49:PRO:O	1:A:51:LEU:HD23	0.65	1.91	5	3
1:A:69:PHE:CD1	1:A:70:GLU:N	0.64	2.66	6	12
1:A:102:LEU:HD23	1:A:102:LEU:N	0.64	2.08	4	8
1:A:30:TRP:CZ2	1:A:84:MET:CE	0.64	2.80	7	1
1:A:51:LEU:HD23	1:A:77:ALA:HB2	0.63	1.69	2	7
1:A:62:LEU:HD11	1:A:69:PHE:CE2	0.62	2.28	4	1
1:A:30:TRP:CD1	1:A:30:TRP:O	0.62	2.53	3	1
1:A:51:LEU:HD11	1:A:53:GLY:O	0.62	1.95	2	1
1:A:28:LEU:CD1	1:A:45:LEU:HD21	0.62	2.23	11	4
1:A:26:LEU:HD12	1:A:74:LEU:HD12	0.62	1.71	7	4
1:A:46:ARG:NE	1:A:56:TRP:CE3	0.61	2.68	6	2
1:A:71:LEU:HG	1:A:74:LEU:HD21	0.61	1.72	10	3
1:A:66:LYS:CE	1:A:69:PHE:CD2	0.61	2.84	11	1
1:A:73:GLY:O	1:A:74:LEU:HD23	0.60	1.96	3	2
1:A:28:LEU:CD1	1:A:45:LEU:CD2	0.60	2.80	6	6
1:A:47:TYR:CD2	1:A:47:TYR:O	0.59	2.56	2	4
1:A:47:TYR:CD1	1:A:47:TYR:O	0.59	2.56	7	8
1:A:25:CYS:H	1:A:107:THR:HG21	0.59	1.55	7	2
1:A:66:LYS:HE3	1:A:69:PHE:CD2	0.59	2.33	11	2
1:A:49:PRO:CB	1:A:77:ALA:HB2	0.59	2.27	2	1
1:A:46:ARG:CG	1:A:58:LEU:CD2	0.59	2.81	7	7
1:A:53:GLY:O	1:A:54:ALA:HB2	0.59	1.98	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:CB	1:A:62:LEU:CD2	0.58	2.80	10	8
1:A:47:TYR:O	1:A:47:TYR:CG	0.58	2.56	4	12
1:A:60:PHE:O	1:A:61:HIS:CG	0.58	2.56	1	4
1:A:75:HIS:O	1:A:75:HIS:CG	0.58	2.57	5	5
1:A:75:HIS:O	1:A:76:GLN:CG	0.58	2.52	2	1
1:A:85:ARG:NH2	1:A:98:TRP:N	0.58	2.52	7	1
1:A:28:LEU:HD13	1:A:45:LEU:HD21	0.56	1.77	5	3
1:A:60:PHE:C	1:A:61:HIS:CG	0.56	2.78	3	4
1:A:30:TRP:CD2	1:A:84:MET:SD	0.56	2.98	6	2
1:A:30:TRP:CH2	1:A:84:MET:HE1	0.56	2.36	10	3
1:A:46:ARG:HD2	1:A:98:TRP:CZ2	0.55	2.37	7	2
1:A:25:CYS:N	1:A:107:THR:CG2	0.55	2.70	3	5
1:A:47:TYR:OH	1:A:57:THR:HG21	0.55	2.02	6	4
1:A:60:PHE:CD1	1:A:60:PHE:N	0.55	2.75	10	3
1:A:106:PRO:O	1:A:107:THR:O	0.55	2.25	9	5
1:A:51:LEU:HD12	1:A:52:LYS:H	0.54	1.62	11	3
1:A:30:TRP:CZ2	1:A:84:MET:HE1	0.54	2.36	7	1
1:A:50:GLN:CB	1:A:79:VAL:O	0.54	2.56	2	6
1:A:44:GLU:OE1	1:A:98:TRP:CH2	0.54	2.61	6	1
1:A:50:GLN:O	1:A:77:ALA:HB1	0.54	2.03	11	5
1:A:30:TRP:CE2	1:A:84:MET:CE	0.54	2.91	7	1
1:A:74:LEU:HB3	1:A:80:TYR:CZ	0.54	2.38	2	2
1:A:46:ARG:HB2	1:A:98:TRP:CH2	0.54	2.38	2	6
1:A:85:ARG:HB2	1:A:98:TRP:CE3	0.53	2.39	11	9
1:A:83:GLN:CG	1:A:99:SER:O	0.53	2.57	10	9
1:A:25:CYS:O	1:A:107:THR:CG2	0.53	2.56	12	3
1:A:25:CYS:O	1:A:27:TRP:CZ3	0.53	2.62	7	1
1:A:80:TYR:CD1	1:A:106:PRO:HG3	0.53	2.38	11	3
1:A:102:LEU:N	1:A:102:LEU:CD2	0.52	2.72	6	6
1:A:43:CYS:O	1:A:62:LEU:CB	0.52	2.57	10	3
1:A:12:LEU:HD22	1:A:27:TRP:HB3	0.52	1.82	10	4
1:A:68:GLN:CG	1:A:68:GLN:O	0.52	2.58	8	1
1:A:46:ARG:CD	1:A:98:TRP:CZ2	0.52	2.93	7	3
1:A:48:GLN:HB3	1:A:56:TRP:CD2	0.52	2.40	1	9
1:A:46:ARG:CZ	1:A:56:TRP:CE3	0.52	2.93	11	1
1:A:46:ARG:HB2	1:A:98:TRP:CZ3	0.52	2.40	9	10
1:A:46:ARG:HD3	1:A:98:TRP:CD2	0.52	2.40	11	1
1:A:25:CYS:HB3	1:A:27:TRP:CH2	0.51	2.39	2	8
1:A:85:ARG:NE	1:A:98:TRP:CD1	0.51	2.78	1	1
1:A:49:PRO:HB3	1:A:80:TYR:CZ	0.51	2.39	2	8
1:A:85:ARG:NH2	1:A:86:CYS:O	0.51	2.43	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:HD12	1:A:69:PHE:CB	0.51	2.35	8	1
1:A:48:GLN:OE1	1:A:54:ALA:CB	0.51	2.59	1	2
1:A:85:ARG:CZ	1:A:98:TRP:CD1	0.51	2.94	1	1
1:A:12:LEU:HD23	1:A:13:ASP:O	0.51	2.06	10	1
1:A:48:GLN:OE1	1:A:56:TRP:CE2	0.51	2.64	12	3
1:A:85:ARG:HB2	1:A:98:TRP:CH2	0.51	2.41	9	1
1:A:51:LEU:HD22	1:A:77:ALA:HB2	0.50	1.80	4	2
1:A:45:LEU:HB2	1:A:62:LEU:CD2	0.50	2.36	12	9
1:A:62:LEU:HD21	1:A:69:PHE:HE2	0.50	1.67	10	2
1:A:85:ARG:HB2	1:A:98:TRP:CZ3	0.50	2.42	5	4
1:A:75:HIS:O	1:A:75:HIS:ND1	0.50	2.45	3	3
1:A:25:CYS:O	1:A:107:THR:HG23	0.49	2.07	12	1
1:A:48:GLN:HB3	1:A:56:TRP:CE3	0.49	2.42	3	8
1:A:84:MET:C	1:A:98:TRP:CZ3	0.49	2.86	11	2
1:A:46:ARG:HD3	1:A:98:TRP:CH2	0.49	2.42	1	1
1:A:45:LEU:HB2	1:A:62:LEU:HD23	0.49	1.85	6	2
1:A:46:ARG:CD	1:A:98:TRP:CE2	0.48	2.96	11	1
1:A:50:GLN:OE1	1:A:81:THR:OG1	0.48	2.32	8	3
1:A:68:GLN:O	1:A:68:GLN:HG3	0.48	2.07	9	2
1:A:48:GLN:HG2	1:A:56:TRP:CZ2	0.48	2.43	1	7
1:A:45:LEU:HG	1:A:46:ARG:N	0.48	2.23	1	3
1:A:26:LEU:CG	1:A:106:PRO:HB3	0.48	2.37	8	2
1:A:30:TRP:CZ3	1:A:84:MET:CE	0.48	2.94	1	1
1:A:47:TYR:CZ	1:A:71:LEU:HD21	0.48	2.44	5	1
1:A:85:ARG:HG2	1:A:86:CYS:N	0.48	2.23	2	1
1:A:47:TYR:HB3	1:A:82:LEU:CD2	0.48	2.37	5	1
1:A:12:LEU:HD22	1:A:27:TRP:CB	0.48	2.38	10	1
1:A:85:ARG:HD2	1:A:98:TRP:CE2	0.48	2.43	1	1
1:A:85:ARG:CG	1:A:86:CYS:N	0.47	2.77	11	2
1:A:47:TYR:CE2	1:A:71:LEU:HD21	0.47	2.45	5	1
1:A:47:TYR:CD1	1:A:47:TYR:C	0.47	2.87	11	3
1:A:69:PHE:CD1	1:A:69:PHE:C	0.47	2.87	6	5
1:A:44:GLU:CB	1:A:59:VAL:O	0.47	2.62	8	2
1:A:25:CYS:SG	1:A:71:LEU:O	0.47	2.72	1	8
1:A:26:LEU:CD1	1:A:106:PRO:HB3	0.47	2.40	8	6
1:A:60:PHE:C	1:A:61:HIS:CD2	0.47	2.87	8	3
1:A:85:ARG:N	1:A:98:TRP:CZ3	0.47	2.82	9	3
1:A:48:GLN:HG2	1:A:56:TRP:CH2	0.47	2.44	3	4
1:A:46:ARG:CD	1:A:98:TRP:CH2	0.47	2.98	1	1
1:A:103:GLN:O	1:A:104:LEU:CD1	0.47	2.63	1	1
1:A:47:TYR:CB	1:A:82:LEU:HG	0.47	2.39	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ARG:NH1	1:A:85:ARG:HG3	0.47	2.24	3	1
1:A:71:LEU:O	1:A:72:CYS:SG	0.47	2.73	9	1
1:A:26:LEU:C	1:A:27:TRP:CE3	0.47	2.88	4	3
1:A:85:ARG:HB2	1:A:98:TRP:CD2	0.47	2.44	3	2
1:A:103:GLN:O	1:A:103:GLN:OE1	0.47	2.33	5	1
1:A:30:TRP:CE3	1:A:84:MET:SD	0.47	3.08	1	1
1:A:28:LEU:CB	1:A:69:PHE:HB3	0.47	2.40	2	3
1:A:49:PRO:HB3	1:A:80:TYR:CE2	0.47	2.44	2	3
1:A:43:CYS:SG	1:A:85:ARG:O	0.47	2.73	4	3
1:A:28:LEU:HD12	1:A:69:PHE:CD1	0.47	2.42	8	1
1:A:12:LEU:HB3	1:A:27:TRP:CB	0.46	2.40	8	6
1:A:83:GLN:HG2	1:A:99:SER:O	0.46	2.10	10	3
1:A:48:GLN:OE1	1:A:56:TRP:CZ2	0.46	2.68	8	1
1:A:106:PRO:O	1:A:107:THR:C	0.46	2.54	5	8
1:A:45:LEU:HB3	1:A:62:LEU:CD2	0.46	2.40	10	1
1:A:12:LEU:CB	1:A:27:TRP:HB3	0.46	2.41	1	2
1:A:46:ARG:HG3	1:A:58:LEU:CD2	0.46	2.40	3	3
1:A:12:LEU:CB	1:A:27:TRP:O	0.46	2.63	8	4
1:A:66:LYS:HE3	1:A:69:PHE:CG	0.46	2.45	11	1
1:A:30:TRP:CH2	1:A:84:MET:CE	0.46	2.98	12	3
1:A:28:LEU:O	1:A:29:SER:CB	0.46	2.64	11	3
1:A:81:THR:O	1:A:82:LEU:HG	0.46	2.11	2	7
1:A:12:LEU:HB2	1:A:27:TRP:O	0.46	2.11	9	8
1:A:79:VAL:HG23	1:A:104:LEU:O	0.46	2.11	2	1
1:A:83:GLN:HG3	1:A:99:SER:O	0.46	2.11	8	6
1:A:81:THR:O	1:A:82:LEU:HD12	0.46	2.10	12	2
1:A:60:PHE:O	1:A:61:HIS:C	0.46	2.55	1	5
1:A:48:GLN:CB	1:A:56:TRP:HA	0.45	2.41	4	4
1:A:44:GLU:HB2	1:A:59:VAL:O	0.45	2.11	5	2
1:A:46:ARG:HG2	1:A:58:LEU:CD2	0.45	2.41	5	6
1:A:68:GLN:O	1:A:68:GLN:CG	0.45	2.63	9	2
1:A:68:GLN:O	1:A:69:PHE:C	0.45	2.55	4	8
1:A:85:ARG:HG3	1:A:86:CYS:N	0.45	2.27	3	2
1:A:50:GLN:HB3	1:A:79:VAL:O	0.45	2.11	7	4
1:A:49:PRO:HA	1:A:80:TYR:CE2	0.45	2.46	8	2
1:A:43:CYS:O	1:A:62:LEU:HB2	0.45	2.12	3	2
1:A:59:VAL:O	1:A:60:PHE:CD1	0.45	2.70	1	1
1:A:85:ARG:CB	1:A:98:TRP:CZ3	0.45	3.00	11	1
1:A:84:MET:C	1:A:98:TRP:CE3	0.45	2.90	11	2
1:A:26:LEU:CD1	1:A:74:LEU:CD1	0.45	2.80	7	2
1:A:66:LYS:HG3	1:A:67:ASP:N	0.45	2.26	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:TRP:CZ2	1:A:84:MET:HE3	0.44	2.47	2	1
1:A:25:CYS:SG	1:A:70:GLU:OE2	0.44	2.75	8	1
1:A:28:LEU:HB2	1:A:69:PHE:CB	0.44	2.42	8	1
1:A:74:LEU:HD23	1:A:74:LEU:N	0.44	2.28	12	2
1:A:45:LEU:HD13	1:A:84:MET:SD	0.44	2.52	8	1
1:A:26:LEU:HG	1:A:106:PRO:HB3	0.44	1.88	9	1
1:A:71:LEU:HG	1:A:72:CYS:N	0.44	2.28	1	1
1:A:81:THR:C	1:A:82:LEU:CD1	0.44	2.81	4	1
1:A:28:LEU:HB2	1:A:69:PHE:HB3	0.44	1.90	8	4
1:A:49:PRO:HA	1:A:80:TYR:CD2	0.44	2.48	2	3
1:A:51:LEU:O	1:A:52:LYS:C	0.44	2.56	10	2
1:A:51:LEU:CD2	1:A:76:GLN:O	0.44	2.61	2	1
1:A:46:ARG:HD3	1:A:98:TRP:CE3	0.44	2.47	11	1
1:A:48:GLN:HG2	1:A:56:TRP:CE2	0.43	2.47	1	1
1:A:74:LEU:N	1:A:74:LEU:HD23	0.43	2.28	2	3
1:A:85:ARG:NH1	1:A:86:CYS:O	0.43	2.51	3	1
1:A:25:CYS:N	1:A:107:THR:HG22	0.43	2.28	10	1
1:A:55:ASN:O	1:A:56:TRP:HB2	0.43	2.12	3	11
1:A:81:THR:O	1:A:82:LEU:CG	0.43	2.66	2	1
1:A:60:PHE:HB2	1:A:61:HIS:CD2	0.43	2.48	7	2
1:A:12:LEU:HB3	1:A:27:TRP:HB2	0.43	1.89	2	4
1:A:48:GLN:OE1	1:A:56:TRP:NE1	0.43	2.51	12	1
1:A:59:VAL:C	1:A:60:PHE:CD1	0.43	2.92	1	2
1:A:63:PRO:O	1:A:64:SER:C	0.43	2.57	8	2
1:A:25:CYS:HB2	1:A:27:TRP:CH2	0.43	2.49	4	1
1:A:83:GLN:HB3	1:A:98:TRP:CE3	0.43	2.48	5	1
1:A:30:TRP:CZ2	1:A:84:MET:HE2	0.43	2.48	12	1
1:A:26:LEU:HD21	1:A:106:PRO:HB3	0.43	1.90	8	1
1:A:75:HIS:O	1:A:76:GLN:CB	0.43	2.65	2	1
1:A:51:LEU:HB3	1:A:77:ALA:CB	0.43	2.43	1	3
1:A:98:TRP:O	1:A:99:SER:C	0.43	2.57	2	1
1:A:48:GLN:NE2	1:A:54:ALA:CB	0.43	2.82	8	1
1:A:68:GLN:HG2	1:A:68:GLN:O	0.43	2.14	12	1
1:A:46:ARG:HD3	1:A:56:TRP:CZ3	0.43	2.49	6	1
1:A:12:LEU:CB	1:A:27:TRP:CB	0.42	2.97	1	2
1:A:28:LEU:O	1:A:29:SER:HB2	0.42	2.14	4	1
1:A:61:HIS:CD2	1:A:61:HIS:N	0.42	2.88	2	1
1:A:81:THR:O	1:A:82:LEU:CD1	0.42	2.67	2	1
1:A:27:TRP:NE1	1:A:70:GLU:HG3	0.42	2.29	3	1
1:A:75:HIS:N	1:A:75:HIS:CD2	0.42	2.86	11	1
1:A:46:ARG:HD2	1:A:98:TRP:CE2	0.42	2.49	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ARG:HH11	1:A:58:LEU:HD21	0.42	1.75	11	1
1:A:60:PHE:O	1:A:61:HIS:CD2	0.42	2.72	1	1
1:A:45:LEU:HD12	1:A:83:GLN:O	0.42	2.14	2	2
1:A:50:GLN:HB2	1:A:79:VAL:O	0.42	2.13	6	1
1:A:49:PRO:HB2	1:A:51:LEU:CD2	0.42	2.44	8	1
1:A:60:PHE:O	1:A:62:LEU:N	0.42	2.52	8	1
1:A:58:LEU:HD23	1:A:58:LEU:N	0.42	2.27	10	2
1:A:12:LEU:CD1	1:A:68:GLN:HG2	0.42	2.45	11	1
1:A:57:THR:HG22	1:A:58:LEU:N	0.41	2.30	10	2
1:A:43:CYS:O	1:A:62:LEU:O	0.41	2.38	10	1
1:A:81:THR:CG2	1:A:82:LEU:N	0.41	2.83	4	1
1:A:83:GLN:OE1	1:A:99:SER:O	0.41	2.38	2	1
1:A:43:CYS:C	1:A:44:GLU:OE1	0.41	2.58	9	1
1:A:28:LEU:O	1:A:29:SER:HB3	0.41	2.16	5	4
1:A:47:TYR:CZ	1:A:57:THR:HG21	0.41	2.51	6	1
1:A:43:CYS:O	1:A:62:LEU:HB3	0.41	2.16	10	1
1:A:49:PRO:HB2	1:A:51:LEU:HD23	0.41	1.92	2	1
1:A:48:GLN:HB3	1:A:56:TRP:HA	0.41	1.93	1	1
1:A:51:LEU:CD2	1:A:77:ALA:CB	0.41	2.95	4	1
1:A:30:TRP:CZ3	1:A:84:MET:HE3	0.41	2.51	7	1
1:A:44:GLU:HB3	1:A:59:VAL:O	0.41	2.16	9	1
1:A:85:ARG:HB2	1:A:98:TRP:CZ2	0.41	2.51	9	1
1:A:45:LEU:CB	1:A:62:LEU:HD21	0.40	2.47	7	1
1:A:45:LEU:HD13	1:A:84:MET:HE1	0.40	1.93	1	1
1:A:51:LEU:HD23	1:A:77:ALA:CB	0.40	2.44	2	1
1:A:51:LEU:CG	1:A:52:LYS:N	0.40	2.83	7	1
1:A:66:LYS:HG2	1:A:69:PHE:N	0.40	2.32	11	1
1:A:81:THR:HG22	1:A:82:LEU:N	0.40	2.31	4	1
1:A:45:LEU:HA	1:A:84:MET:HE3	0.40	1.92	1	1
1:A:47:TYR:CB	1:A:82:LEU:CD2	0.40	3.00	5	1
1:A:62:LEU:HD12	1:A:62:LEU:HA	0.40	1.74	7	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	64/109 (59%)	49±2 (77±4%)	10±2 (16±3%)	4±1 (7±1%)	2 17
All	All	768/1308 (59%)	590 (77%)	124 (16%)	54 (7%)	2 17

All 11 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	29	SER	12
1	A	56	TRP	12
1	A	107	THR	8
1	A	106	PRO	6
1	A	76	GLN	5
1	A	98	TRP	5
1	A	65	SER	2
1	A	52	LYS	1
1	A	75	HIS	1
1	A	101	GLY	1
1	A	54	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	58/99 (59%)	40±3 (70±5%)	18±3 (30±5%)	1 16
All	All	696/1188 (59%)	485 (70%)	211 (30%)	1 16

All 36 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	51	LEU	11
1	A	52	LYS	11
1	A	72	CYS	11
1	A	83	GLN	11
1	A	12	LEU	10
1	A	25	CYS	9
1	A	62	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	84	MET	9
1	A	74	LEU	8
1	A	104	LEU	8
1	A	86	CYS	8
1	A	46	ARG	7
1	A	76	GLN	7
1	A	66	LYS	7
1	A	43	CYS	7
1	A	44	GLU	6
1	A	13	ASP	6
1	A	64	SER	6
1	A	105	ARG	6
1	A	48	GLN	6
1	A	10	GLN	6
1	A	70	GLU	5
1	A	50	GLN	4
1	A	99	SER	4
1	A	103	GLN	4
1	A	85	ARG	4
1	A	55	ASN	3
1	A	102	LEU	3
1	A	67	ASP	3
1	A	29	SER	3
1	A	79	VAL	2
1	A	68	GLN	2
1	A	107	THR	2
1	A	28	LEU	1
1	A	65	SER	1
1	A	75	HIS	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