Full wwPDB NMR Structure Validation Report ⓘ

Feb 19, 2022 – 11:27 PM EST

PDB ID : 1SRZ
Title : Solution structure of the second complement control protein (CCP) module of the GABA(B)R1a receptor, Pro-119 trans conformer
Authors : Blein, S.; Uhrin, D.; Smith, B.O.; White, J.H.; Barlow, P.N.
Deposited on : 2004-03-23

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

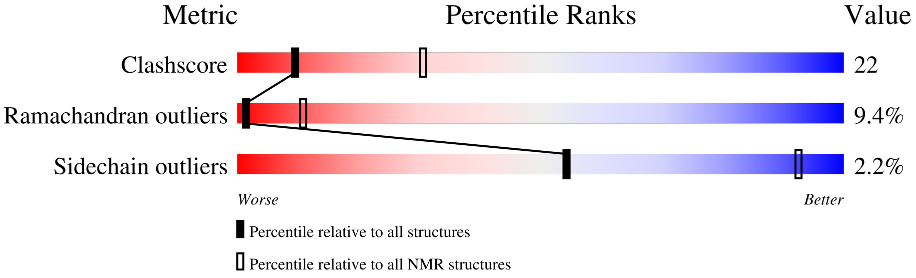
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance ⓘ

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	68	

2 Ensemble composition and analysis (i)

This entry contains 24 models. Model 14 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:98-A:159 (62)	0.43	14

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 5 clusters and 4 single-model clusters were found.

Cluster number	**Models**
1	1, 3, 8, 10, 14, 15, 16, 17, 20, 21, 23
2	6, 18, 19
3	13, 22
4	2, 5
5	4, 11
Single-model clusters	7; 9; 12; 24

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1029 atoms, of which 504 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gamma-aminobutyric acid type B receptor, subunit 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	68	1029	327	504	93	101	4	0

There are 4 discrepancies between the modelled and reference sequences:

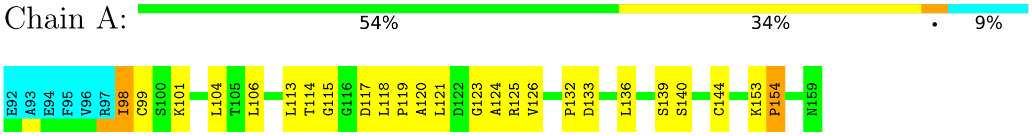
Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLU	-	cloning artifact	UNP Q9Z0U4
A	93	ALA	-	cloning artifact	UNP Q9Z0U4
A	94	GLU	-	cloning artifact	UNP Q9Z0U4
A	95	PHE	-	cloning artifact	UNP Q9Z0U4

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: Gamma-aminobutyric acid type B receptor, subunit 1

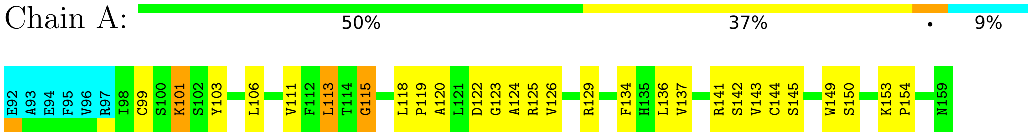


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

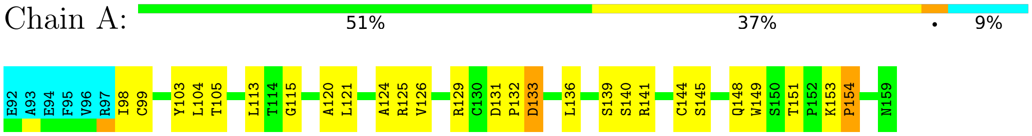
4.2.1 Score per residue for model 1

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



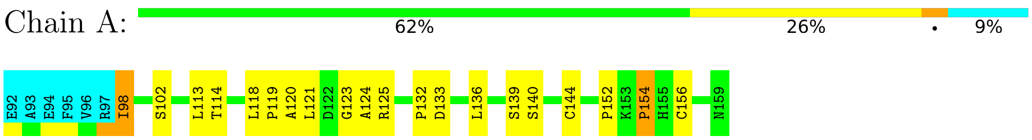
4.2.2 Score per residue for model 2

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



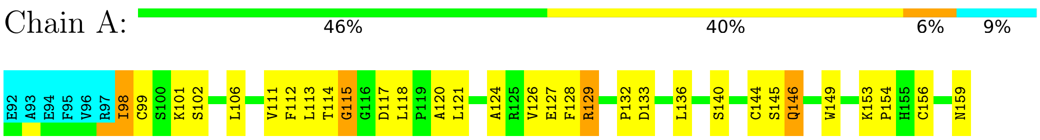
4.2.3 Score per residue for model 3

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



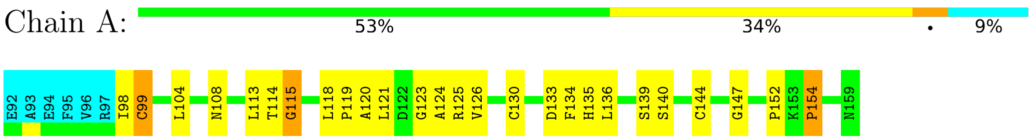
4.2.4 Score per residue for model 4

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



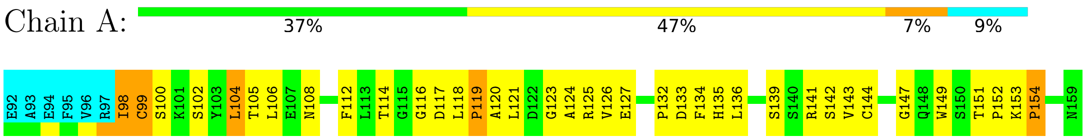
4.2.5 Score per residue for model 5

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



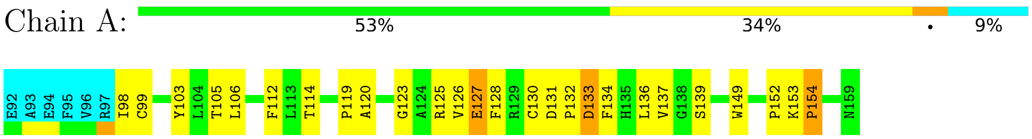
4.2.6 Score per residue for model 6

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



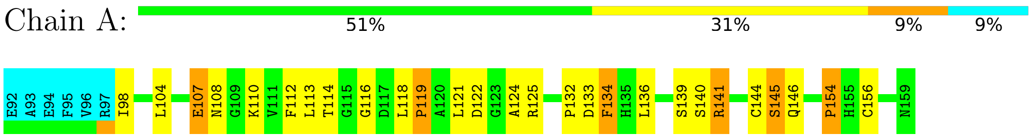
4.2.7 Score per residue for model 7

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



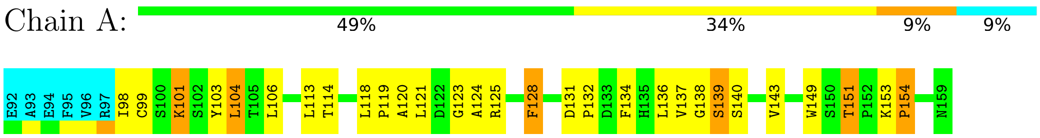
4.2.8 Score per residue for model 8

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



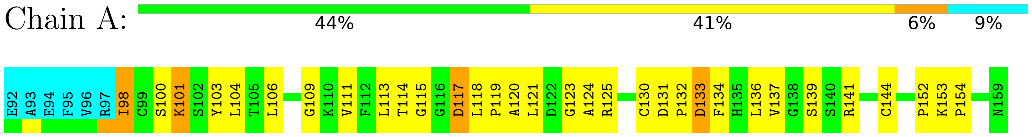
4.2.9 Score per residue for model 9

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



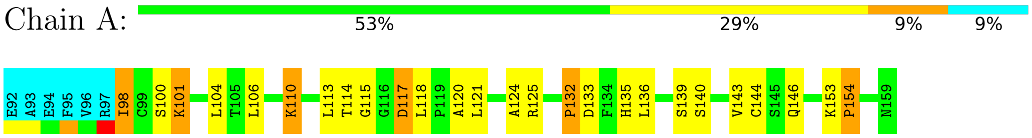
4.2.10 Score per residue for model 10

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



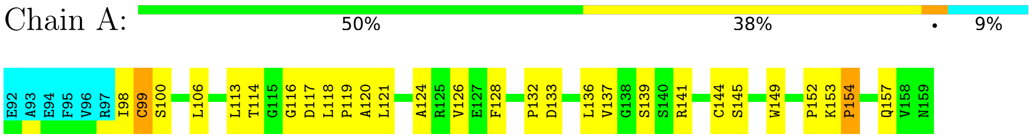
4.2.11 Score per residue for model 11

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



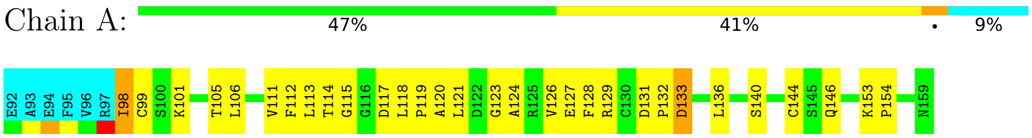
4.2.12 Score per residue for model 12

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



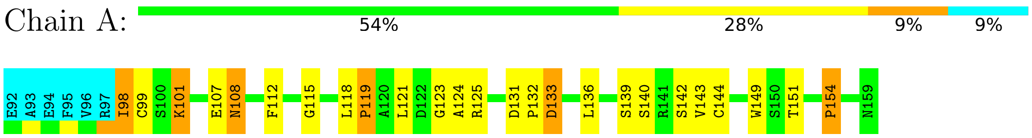
4.2.13 Score per residue for model 13

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



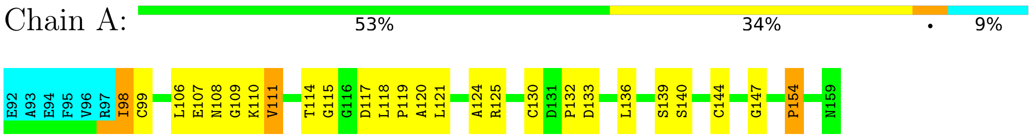
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



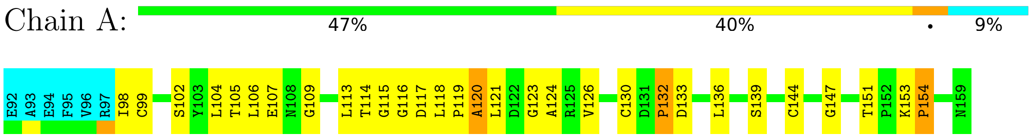
4.2.15 Score per residue for model 15

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



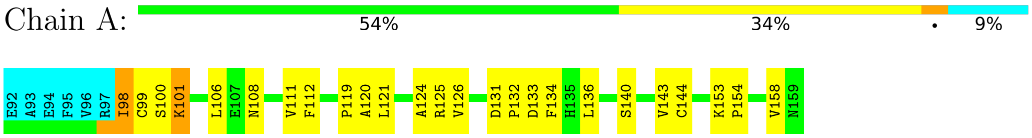
4.2.16 Score per residue for model 16

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



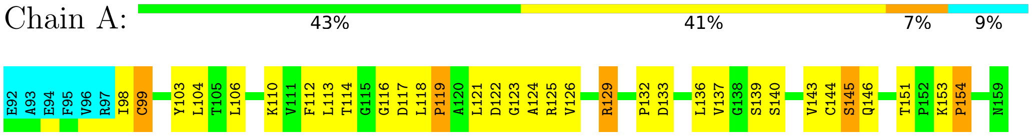
4.2.17 Score per residue for model 17

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



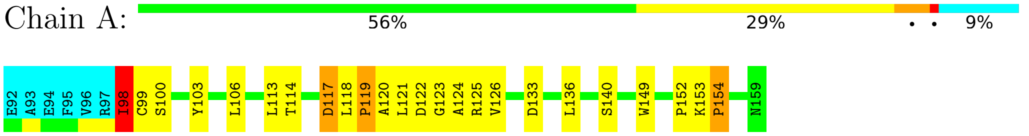
4.2.18 Score per residue for model 18

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



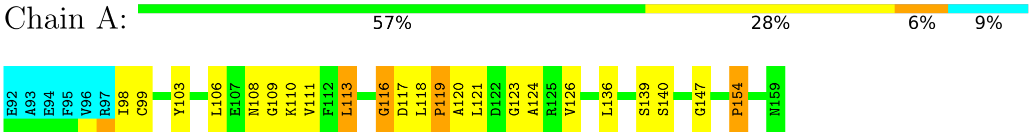
4.2.19 Score per residue for model 19

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



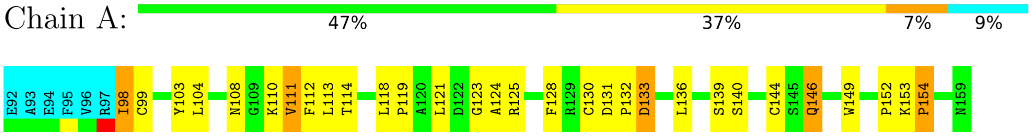
4.2.20 Score per residue for model 20

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



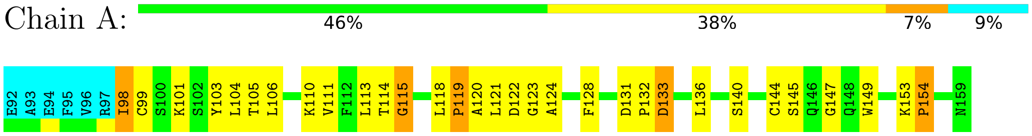
4.2.21 Score per residue for model 21

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



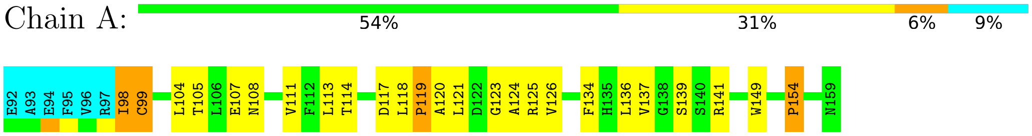
4.2.22 Score per residue for model 22

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



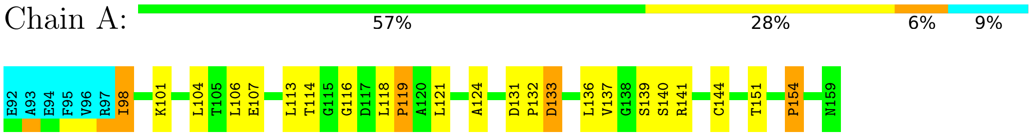
4.2.23 Score per residue for model 23

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



4.2.24 Score per residue for model 24

- Molecule 1: Gamma-aminobutyric acid type B receptor, subunit 1



5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 24 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure solution	1.0
CNS	refinement	1.0

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	473	454	452	21±4
All	All	11352	10896	10848	498

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:ALA:HB3	1:A:144:CYS:HB3	0.86	1.48	8	8
1:A:113:LEU:HA	1:A:126:VAL:HG12	0.84	1.45	1	8
1:A:98:ILE:HA	1:A:121:LEU:HB2	0.83	1.50	11	3
1:A:98:ILE:HG22	1:A:121:LEU:HB2	0.76	1.55	16	2
1:A:121:LEU:HG	1:A:124:ALA:HB2	0.75	1.57	11	7
1:A:124:ALA:HB3	1:A:144:CYS:HB2	0.73	1.59	18	7
1:A:139:SER:HB3	1:A:154:PRO:HD3	0.73	1.58	9	5
1:A:103:TYR:HA	1:A:153:LYS:HD2	0.72	1.61	2	3
1:A:136:LEU:HD21	1:A:140:SER:HA	0.71	1.61	5	13
1:A:122:ASP:HA	1:A:145:SER:HA	0.68	1.65	1	4
1:A:106:LEU:HD13	1:A:153:LYS:HE3	0.68	1.64	6	4
1:A:138:GLY:HA3	1:A:154:PRO:HB3	0.67	1.65	9	1
1:A:113:LEU:HD23	1:A:114:THR:N	0.66	2.05	4	2
1:A:136:LEU:HD11	1:A:154:PRO:HG2	0.66	1.67	9	3

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:120:ALA:HB1	1:A:147:GLY:N	0.66	2.06	22	4
1:A:117:ASP:C	1:A:118:LEU:HD22	0.66	2.11	19	6
1:A:153:LYS:HD3	1:A:154:PRO:HD2	0.65	1.69	9	1
1:A:106:LEU:HD13	1:A:153:LYS:HE2	0.65	1.68	7	4
1:A:139:SER:OG	1:A:151:THR:HG23	0.64	1.93	9	3
1:A:104:LEU:HD12	1:A:105:THR:N	0.62	2.07	6	1
1:A:117:ASP:C	1:A:118:LEU:HD12	0.62	2.14	15	3
1:A:98:ILE:O	1:A:98:ILE:HD12	0.62	1.94	5	2
1:A:113:LEU:HD13	1:A:114:THR:N	0.61	2.10	5	10
1:A:139:SER:N	1:A:154:PRO:HB3	0.61	2.11	2	15
1:A:118:LEU:O	1:A:121:LEU:HD12	0.61	1.95	14	2
1:A:98:ILE:N	1:A:98:ILE:HD13	0.60	2.10	14	4
1:A:118:LEU:O	1:A:120:ALA:N	0.60	2.35	22	6
1:A:110:LYS:HD3	1:A:111:VAL:N	0.60	2.11	22	1
1:A:98:ILE:HD12	1:A:98:ILE:O	0.60	1.96	2	2
1:A:98:ILE:HG21	1:A:117:ASP:HA	0.60	1.74	23	1
1:A:98:ILE:HG23	1:A:118:LEU:O	0.59	1.97	16	1
1:A:125:ARG:HD2	1:A:141:ARG:HH21	0.58	1.58	2	1
1:A:121:LEU:HB2	1:A:144:CYS:SG	0.58	2.38	5	1
1:A:98:ILE:HA	1:A:121:LEU:HD13	0.58	1.75	13	3
1:A:104:LEU:HD12	1:A:105:THR:HG23	0.58	1.74	23	1
1:A:153:LYS:HD2	1:A:154:PRO:HD2	0.58	1.74	12	1
1:A:113:LEU:HD22	1:A:113:LEU:O	0.58	1.98	20	1
1:A:104:LEU:HD12	1:A:105:THR:H	0.58	1.56	6	1
1:A:106:LEU:HD22	1:A:109:GLY:H	0.57	1.58	15	1
1:A:103:TYR:HA	1:A:153:LYS:HD3	0.57	1.76	19	1
1:A:104:LEU:HD22	1:A:113:LEU:HD22	0.57	1.76	18	1
1:A:136:LEU:HD13	1:A:137:VAL:N	0.57	2.15	18	5
1:A:125:ARG:CD	1:A:143:VAL:HG22	0.57	2.30	14	2
1:A:121:LEU:HG	1:A:124:ALA:CB	0.57	2.28	11	4
1:A:139:SER:H	1:A:154:PRO:HB3	0.57	1.60	15	12
1:A:99:CYS:SG	1:A:121:LEU:HB2	0.56	2.41	22	2
1:A:101:LYS:HB3	1:A:101:LYS:NZ	0.56	2.15	10	1
1:A:124:ALA:H	1:A:144:CYS:HB2	0.56	1.59	24	1
1:A:114:THR:HB	1:A:125:ARG:O	0.56	2.01	18	12
1:A:104:LEU:HD21	1:A:113:LEU:HD13	0.56	1.78	11	1
1:A:111:VAL:HG22	1:A:128:PHE:HA	0.55	1.78	13	2
1:A:116:GLY:H	1:A:121:LEU:HD21	0.55	1.61	24	4
1:A:115:GLY:C	1:A:121:LEU:HD11	0.55	2.21	15	1
1:A:98:ILE:HG22	1:A:118:LEU:H	0.55	1.60	18	1
1:A:117:ASP:O	1:A:118:LEU:HD22	0.54	2.02	4	3

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:101:LYS:NZ	1:A:101:LYS:HB2	0.54	2.17	4	2
1:A:141:ARG:O	1:A:141:ARG:HD2	0.54	2.01	12	1
1:A:99:CYS:HA	1:A:147:GLY:HA2	0.54	1.80	16	1
1:A:121:LEU:HB3	1:A:124:ALA:HB3	0.54	1.79	5	3
1:A:101:LYS:HD2	1:A:104:LEU:HD12	0.54	1.79	22	1
1:A:113:LEU:C	1:A:113:LEU:HD22	0.53	2.23	1	1
1:A:129:ARG:O	1:A:129:ARG:HD3	0.53	2.03	4	2
1:A:118:LEU:HB3	1:A:119:PRO:HD2	0.53	1.81	8	1
1:A:118:LEU:HB2	1:A:121:LEU:HD23	0.53	1.79	18	2
1:A:104:LEU:HD12	1:A:104:LEU:N	0.53	2.18	8	2
1:A:121:LEU:HD23	1:A:144:CYS:SG	0.53	2.43	4	4
1:A:101:LYS:HA	1:A:104:LEU:HD23	0.53	1.81	24	1
1:A:136:LEU:HD23	1:A:137:VAL:N	0.53	2.19	1	2
1:A:153:LYS:NZ	1:A:153:LYS:HB3	0.53	2.18	19	1
1:A:103:TYR:O	1:A:111:VAL:HG21	0.52	2.05	10	3
1:A:117:ASP:O	1:A:118:LEU:HD13	0.52	2.03	11	2
1:A:130:CYS:SG	1:A:134:PHE:HB2	0.52	2.44	5	2
1:A:106:LEU:HD13	1:A:153:LYS:NZ	0.52	2.19	19	4
1:A:110:LYS:NZ	1:A:110:LYS:HB2	0.52	2.19	20	2
1:A:115:GLY:O	1:A:121:LEU:HD11	0.52	2.05	11	1
1:A:110:LYS:HB2	1:A:129:ARG:HD2	0.52	1.80	18	1
1:A:115:GLY:HA3	1:A:124:ALA:HB2	0.52	1.82	1	1
1:A:136:LEU:HD12	1:A:140:SER:HB3	0.52	1.82	24	2
1:A:101:LYS:H	1:A:101:LYS:HD2	0.52	1.63	14	3
1:A:121:LEU:HB3	1:A:124:ALA:HB2	0.52	1.81	22	4
1:A:99:CYS:HB3	1:A:149:TRP:CD1	0.52	2.39	7	4
1:A:136:LEU:CD2	1:A:140:SER:HA	0.52	2.35	9	2
1:A:121:LEU:HD22	1:A:124:ALA:HB2	0.52	1.80	21	3
1:A:111:VAL:HG12	1:A:126:VAL:HB	0.52	1.82	23	1
1:A:111:VAL:HA	1:A:128:PHE:HA	0.51	1.81	21	1
1:A:114:THR:HG21	1:A:125:ARG:NH2	0.51	2.20	8	1
1:A:141:ARG:N	1:A:141:ARG:HD2	0.51	2.20	8	1
1:A:99:CYS:HB2	1:A:121:LEU:HD22	0.51	1.82	5	1
1:A:113:LEU:HD22	1:A:114:THR:H	0.51	1.64	10	2
1:A:136:LEU:HD12	1:A:140:SER:HB2	0.51	1.83	18	1
1:A:131:ASP:O	1:A:133:ASP:N	0.51	2.44	10	8
1:A:118:LEU:HB2	1:A:121:LEU:HG	0.50	1.83	20	1
1:A:101:LYS:NZ	1:A:101:LYS:HB3	0.50	2.21	17	1
1:A:112:PHE:C	1:A:126:VAL:HG23	0.50	2.27	18	2
1:A:117:ASP:O	1:A:118:LEU:HD12	0.50	2.07	15	2
1:A:121:LEU:HD23	1:A:124:ALA:HB2	0.50	1.83	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:ARG:HD2	1:A:142:SER:N	0.50	2.22	6	1
1:A:99:CYS:SG	1:A:121:LEU:HD22	0.50	2.46	13	1
1:A:98:ILE:HD13	1:A:98:ILE:H	0.49	1.66	14	1
1:A:136:LEU:HD11	1:A:154:PRO:HB2	0.49	1.83	21	1
1:A:143:VAL:HG13	1:A:150:SER:OG	0.49	2.07	1	1
1:A:132:PRO:O	1:A:133:ASP:HB3	0.49	2.07	15	2
1:A:98:ILE:HD12	1:A:101:LYS:NZ	0.49	2.23	13	1
1:A:113:LEU:HD22	1:A:113:LEU:C	0.49	2.27	20	1
1:A:140:SER:OG	1:A:141:ARG:HD2	0.49	2.08	24	1
1:A:106:LEU:HD13	1:A:153:LYS:CE	0.49	2.37	7	7
1:A:115:GLY:O	1:A:118:LEU:HD23	0.49	2.08	4	1
1:A:128:PHE:O	1:A:136:LEU:HD22	0.49	2.07	4	2
1:A:112:PHE:O	1:A:126:VAL:HA	0.49	2.08	7	4
1:A:126:VAL:HG23	1:A:128:PHE:CE1	0.48	2.43	7	2
1:A:99:CYS:HB3	1:A:149:TRP:CE2	0.48	2.42	14	1
1:A:113:LEU:CA	1:A:126:VAL:HG12	0.48	2.34	20	1
1:A:106:LEU:HB2	1:A:153:LYS:HZ3	0.48	1.67	9	1
1:A:100:SER:HB2	1:A:149:TRP:HD1	0.48	1.69	6	1
1:A:139:SER:OG	1:A:154:PRO:HD3	0.48	2.08	12	1
1:A:126:VAL:HG22	1:A:127:GLU:N	0.48	2.24	6	1
1:A:134:PHE:HB3	1:A:156:CYS:HB3	0.48	1.85	8	1
1:A:102:SER:O	1:A:105:THR:HG22	0.48	2.09	16	1
1:A:136:LEU:HD23	1:A:156:CYS:SG	0.48	2.49	3	1
1:A:124:ALA:HB3	1:A:144:CYS:SG	0.48	2.49	12	3
1:A:113:LEU:C	1:A:113:LEU:HD13	0.48	2.29	10	1
1:A:144:CYS:HA	1:A:149:TRP:HA	0.48	1.84	22	1
1:A:146:GLN:N	1:A:146:GLN:OE1	0.47	2.47	13	2
1:A:129:ARG:HA	1:A:129:ARG:HE	0.47	1.69	2	1
1:A:98:ILE:N	1:A:98:ILE:CD1	0.47	2.77	14	2
1:A:113:LEU:HD13	1:A:113:LEU:C	0.47	2.30	13	9
1:A:106:LEU:HB3	1:A:109:GLY:O	0.47	2.09	20	1
1:A:118:LEU:HD12	1:A:118:LEU:N	0.47	2.25	24	4
1:A:132:PRO:O	1:A:133:ASP:HB2	0.47	2.09	17	7
1:A:107:GLU:HG2	1:A:107:GLU:O	0.47	2.09	15	1
1:A:110:LYS:HB3	1:A:110:LYS:NZ	0.47	2.25	8	1
1:A:136:LEU:C	1:A:136:LEU:HD13	0.47	2.31	3	3
1:A:99:CYS:HB2	1:A:149:TRP:CE2	0.46	2.46	1	1
1:A:113:LEU:HD23	1:A:113:LEU:C	0.46	2.30	19	1
1:A:104:LEU:HD22	1:A:104:LEU:N	0.46	2.25	24	1
1:A:133:ASP:HB3	1:A:159:ASN:ND2	0.46	2.26	4	1
1:A:118:LEU:HD22	1:A:118:LEU:N	0.46	2.26	23	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ILE:HG12	1:A:118:LEU:O	0.46	2.10	12	1
1:A:153:LYS:HB3	1:A:153:LYS:HZ2	0.46	1.70	19	1
1:A:99:CYS:HB2	1:A:149:TRP:NE1	0.46	2.25	1	2
1:A:113:LEU:HD22	1:A:114:THR:N	0.46	2.26	10	1
1:A:128:PHE:CD1	1:A:128:PHE:N	0.45	2.85	9	2
1:A:136:LEU:HD11	1:A:154:PRO:CG	0.45	2.41	2	3
1:A:111:VAL:HA	1:A:127:GLU:O	0.45	2.12	4	2
1:A:109:GLY:HA2	1:A:130:CYS:HA	0.45	1.88	15	1
1:A:118:LEU:HB2	1:A:121:LEU:CD2	0.45	2.42	21	1
1:A:139:SER:HB3	1:A:151:THR:OG1	0.45	2.11	18	2
1:A:137:VAL:HG13	1:A:137:VAL:O	0.45	2.10	9	1
1:A:118:LEU:HD23	1:A:121:LEU:HD13	0.45	1.89	16	1
1:A:115:GLY:C	1:A:118:LEU:HD13	0.45	2.31	5	1
1:A:109:GLY:HA2	1:A:131:ASP:OD1	0.45	2.12	10	1
1:A:98:ILE:HB	1:A:117:ASP:HA	0.45	1.87	19	1
1:A:117:ASP:O	1:A:118:LEU:HD23	0.45	2.11	20	2
1:A:125:ARG:NH2	1:A:141:ARG:HD3	0.44	2.27	1	1
1:A:129:ARG:NH1	1:A:129:ARG:HB3	0.44	2.27	13	1
1:A:129:ARG:HA	1:A:129:ARG:NE	0.44	2.27	2	1
1:A:136:LEU:HD23	1:A:136:LEU:C	0.44	2.32	12	1
1:A:124:ALA:O	1:A:143:VAL:HG13	0.44	2.12	18	3
1:A:104:LEU:O	1:A:104:LEU:HD12	0.44	2.13	9	1
1:A:107:GLU:O	1:A:107:GLU:HG3	0.44	2.13	16	1
1:A:142:SER:OG	1:A:149:TRP:HB3	0.44	2.13	14	1
1:A:100:SER:HB3	1:A:149:TRP:CD1	0.44	2.47	19	1
1:A:109:GLY:HA3	1:A:130:CYS:HA	0.44	1.89	16	1
1:A:111:VAL:CG1	1:A:126:VAL:HB	0.44	2.42	17	2
1:A:98:ILE:HD12	1:A:121:LEU:HD22	0.44	1.88	3	1
1:A:134:PHE:CD1	1:A:134:PHE:N	0.44	2.85	8	4
1:A:153:LYS:HZ2	1:A:154:PRO:HD2	0.44	1.73	19	1
1:A:113:LEU:HD13	1:A:113:LEU:N	0.44	2.28	20	1
1:A:115:GLY:HA3	1:A:124:ALA:CB	0.44	2.43	10	1
1:A:121:LEU:O	1:A:123:GLY:N	0.44	2.51	19	1
1:A:104:LEU:N	1:A:104:LEU:CD2	0.44	2.81	24	1
1:A:98:ILE:HG22	1:A:121:LEU:HD11	0.43	1.90	9	2
1:A:101:LYS:HD2	1:A:101:LYS:N	0.43	2.28	11	1
1:A:128:PHE:CE2	1:A:153:LYS:HG3	0.43	2.48	13	1
1:A:104:LEU:HD12	1:A:104:LEU:H	0.43	1.72	2	2
1:A:115:GLY:O	1:A:118:LEU:HG	0.43	2.13	22	1
1:A:99:CYS:SG	1:A:121:LEU:HB3	0.43	2.54	15	1
1:A:113:LEU:H	1:A:113:LEU:CD1	0.43	2.27	20	1

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:101:LYS:H	1:A:101:LYS:CD	0.43	2.27	11	3
1:A:130:CYS:SG	1:A:136:LEU:HB2	0.43	2.52	21	1
1:A:136:LEU:HD21	1:A:154:PRO:CG	0.43	2.44	23	1
1:A:98:ILE:HD13	1:A:117:ASP:HA	0.43	1.90	12	2
1:A:106:LEU:HD22	1:A:153:LYS:HZ1	0.43	1.72	12	1
1:A:106:LEU:HD13	1:A:109:GLY:HA3	0.43	1.90	15	1
1:A:139:SER:HB3	1:A:151:THR:HB	0.43	1.91	16	1
1:A:134:PHE:HA	1:A:158:VAL:HA	0.43	1.90	17	1
1:A:99:CYS:HB3	1:A:149:TRP:NE1	0.43	2.29	4	2
1:A:136:LEU:C	1:A:136:LEU:HD23	0.43	2.34	6	1
1:A:110:LYS:O	1:A:111:VAL:O	0.43	2.37	21	2
1:A:107:GLU:HG2	1:A:108:ASN:ND2	0.43	2.29	23	1
1:A:104:LEU:CD2	1:A:104:LEU:H	0.43	2.27	24	1
1:A:98:ILE:O	1:A:99:CYS:O	0.42	2.36	18	1
1:A:146:GLN:O	1:A:146:GLN:HG3	0.42	2.14	4	1
1:A:106:LEU:HD23	1:A:107:GLU:N	0.42	2.28	24	1
1:A:125:ARG:HD2	1:A:141:ARG:NH2	0.42	2.27	2	2
1:A:121:LEU:HD12	1:A:121:LEU:N	0.42	2.28	22	2
1:A:100:SER:HB2	1:A:149:TRP:CD1	0.42	2.49	6	1
1:A:106:LEU:HD13	1:A:153:LYS:HZ3	0.42	1.74	19	1
1:A:107:GLU:OE1	1:A:108:ASN:ND2	0.42	2.52	8	1
1:A:125:ARG:HG2	1:A:143:VAL:HG22	0.42	1.91	9	1
1:A:126:VAL:HG22	1:A:142:SER:O	0.42	2.15	1	1
1:A:108:ASN:N	1:A:108:ASN:HD22	0.42	2.12	6	1
1:A:142:SER:HB3	1:A:149:TRP:HB3	0.42	1.91	6	1
1:A:104:LEU:O	1:A:111:VAL:HB	0.42	2.14	10	1
1:A:137:VAL:HG21	1:A:157:GLN:NE2	0.42	2.30	12	1
1:A:116:GLY:N	1:A:121:LEU:HD21	0.42	2.29	8	3
1:A:103:TYR:O	1:A:153:LYS:NZ	0.42	2.53	9	1
1:A:131:ASP:O	1:A:134:PHE:HB2	0.42	2.15	9	1
1:A:121:LEU:HD23	1:A:124:ALA:CB	0.42	2.44	13	1
1:A:107:GLU:O	1:A:108:ASN:CG	0.42	2.58	14	1
1:A:125:ARG:HD2	1:A:126:VAL:N	0.42	2.29	18	1
1:A:136:LEU:HD21	1:A:154:PRO:HB2	0.42	1.92	24	1
1:A:118:LEU:N	1:A:118:LEU:HD12	0.42	2.29	3	1
1:A:119:PRO:O	1:A:120:ALA:HB3	0.42	2.15	19	3
1:A:115:GLY:HA3	1:A:121:LEU:HD11	0.42	1.91	16	1
1:A:98:ILE:HG22	1:A:118:LEU:O	0.42	2.15	18	1
1:A:104:LEU:HA	1:A:111:VAL:HB	0.41	1.91	23	1
1:A:139:SER:OG	1:A:151:THR:HB	0.41	2.14	24	1
1:A:127:GLU:OE1	1:A:127:GLU:N	0.41	2.53	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:HD11	1:A:154:PRO:CB	0.41	2.45	21	1
1:A:104:LEU:HD23	1:A:113:LEU:HD13	0.41	1.91	9	1
1:A:138:GLY:O	1:A:140:SER:N	0.41	2.53	9	1
1:A:130:CYS:HB2	1:A:134:PHE:O	0.41	2.15	10	1
1:A:98:ILE:HG22	1:A:98:ILE:O	0.41	2.15	12	1
1:A:104:LEU:HD11	1:A:113:LEU:HD13	0.41	1.92	21	1
1:A:99:CYS:HA	1:A:147:GLY:O	0.41	2.15	6	1
1:A:126:VAL:CG2	1:A:127:GLU:N	0.41	2.84	6	1
1:A:112:PHE:N	1:A:112:PHE:CD1	0.41	2.89	8	2
1:A:103:TYR:OH	1:A:152:PRO:HA	0.41	2.16	7	1
1:A:125:ARG:HD2	1:A:141:ARG:HH22	0.41	1.76	10	1
1:A:139:SER:HB2	1:A:152:PRO:O	0.41	2.16	10	1
1:A:112:PHE:CD1	1:A:112:PHE:N	0.41	2.89	14	2
1:A:108:ASN:HB3	1:A:131:ASP:OD1	0.41	2.16	17	1
1:A:125:ARG:NE	1:A:143:VAL:HG22	0.41	2.31	17	1
1:A:121:LEU:CD2	1:A:124:ALA:HB2	0.41	2.46	23	1
1:A:104:LEU:HD21	1:A:113:LEU:HD23	0.41	1.93	5	1
1:A:104:LEU:H	1:A:104:LEU:CD1	0.40	2.28	2	1
1:A:113:LEU:HD23	1:A:114:THR:H	0.40	1.74	4	1
1:A:136:LEU:HD13	1:A:156:CYS:SG	0.40	2.55	4	1
1:A:116:GLY:O	1:A:117:ASP:HB3	0.40	2.15	6	1
1:A:129:ARG:NE	1:A:129:ARG:HA	0.40	2.32	1	1
1:A:131:ASP:CG	1:A:132:PRO:HD2	0.40	2.37	9	1
1:A:119:PRO:O	1:A:120:ALA:HB2	0.40	2.17	16	1
1:A:103:TYR:CD1	1:A:103:TYR:N	0.40	2.89	18	1
1:A:145:SER:O	1:A:148:GLN:HG2	0.40	2.16	2	1
1:A:115:GLY:O	1:A:121:LEU:HG	0.40	2.16	13	1
1:A:99:CYS:O	1:A:100:SER:C	0.40	2.60	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	61/68 (90%)	44±3 (72±5%)	12±2 (19±4%)	6±2 (9±3%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1464/1632 (90%)	1047 (72%)	280 (19%)	137 (9%)	1 11

All 22 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	154	PRO	24
1	A	123	GLY	15
1	A	119	PRO	13
1	A	98	ILE	12
1	A	132	PRO	11
1	A	133	ASP	11
1	A	115	GLY	6
1	A	152	PRO	6
1	A	108	ASN	5
1	A	99	CYS	5
1	A	105	THR	4
1	A	145	SER	4
1	A	146	GLN	4
1	A	102	SER	3
1	A	100	SER	3
1	A	117	ASP	3
1	A	111	VAL	2
1	A	116	GLY	2
1	A	139	SER	1
1	A	104	LEU	1
1	A	120	ALA	1
1	A	122	ASP	1

6.3.2 Protein sidechains ⓘ

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	54/59 (92%)	53±1 (98±2%)	1±1 (2±2%)	54 92
All	All	1296/1416 (92%)	1268 (98%)	28 (2%)	54 92

All 15 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	101	LYS	6
1	A	98	ILE	4
1	A	135	HIS	3
1	A	113	LEU	2
1	A	129	ARG	2
1	A	104	LEU	2
1	A	99	CYS	1
1	A	127	GLU	1
1	A	107	GLU	1
1	A	134	PHE	1
1	A	141	ARG	1
1	A	128	PHE	1
1	A	151	THR	1
1	A	110	LYS	1
1	A	146	GLN	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided