



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:28 PM BST

PDB ID : 1A0N
Title : NMR STUDY OF THE SH3 DOMAIN FROM FYN PROTO-ONCOGENE
TYROSINE KINASE COMPLEXED WITH THE SYNTHETIC PEPTIDE
P2L CORRESPONDING TO RESIDUES 91-104 OF THE P85 SUBUNIT
OF PI3-KINASE, FAMILY OF 25 STRUCTURES
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Waterfield, M.D.; Campbell, I.D.; Ladbury, J.E.
Deposited on : 1997-12-05

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

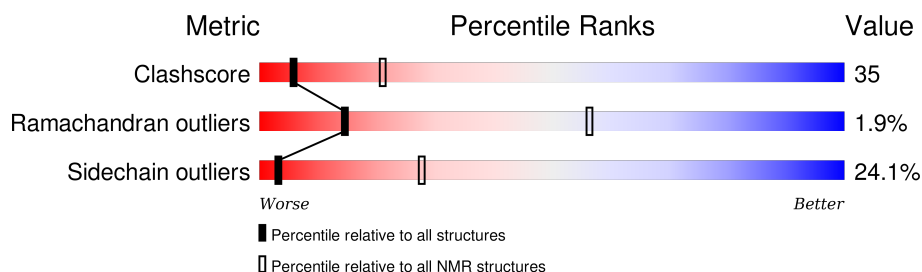
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	14	 7% 7% 86%
2	B	69	 17% 58% • 7% 16%

2 Ensemble composition and analysis

This entry contains 25 models. Model 5 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:95-A:96, B:86-B:89, B:100-B:124, B:128-B:151 (55)	0.30	5

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	1, 4, 8, 11, 13, 14, 20, 21, 25
2	5, 6, 7, 17, 18, 23
3	2, 3
4	15, 16
5	12, 24
6	10, 22
Single-model clusters	9; 19

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1108 atoms, of which 540 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR.

Mol	Chain	Residues	Atoms					Trace
1	A	14	Total	C	H	N	O	0
			207	63	108	18	18	

- Molecule 2 is a protein called FYN.

Mol	Chain	Residues	Atoms					Trace
2	B	58	Total	C	H	N	O	0
			901	301	432	73	95	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	81	SER	GLY	CONFLICT	UNP P06241

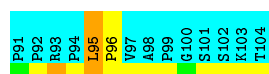
4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

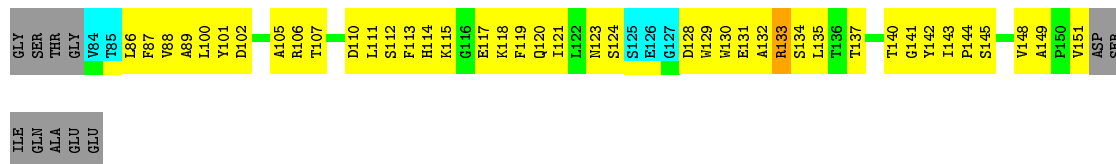
- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A: 



- Molecule 2: FYN

Chain B: 



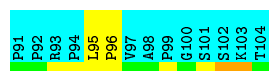
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

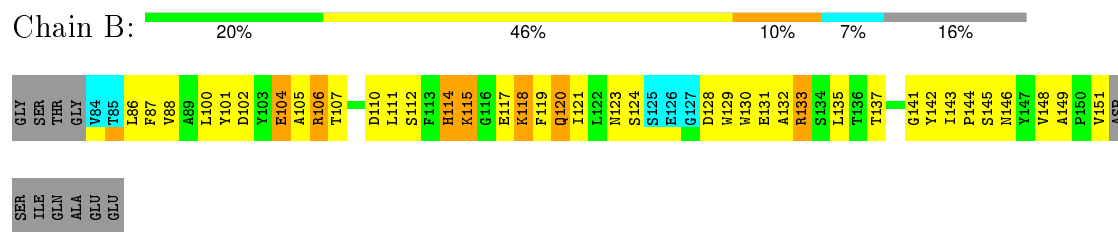
4.2.1 Score per residue for model 1

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A: 



- Molecule 2: FYN

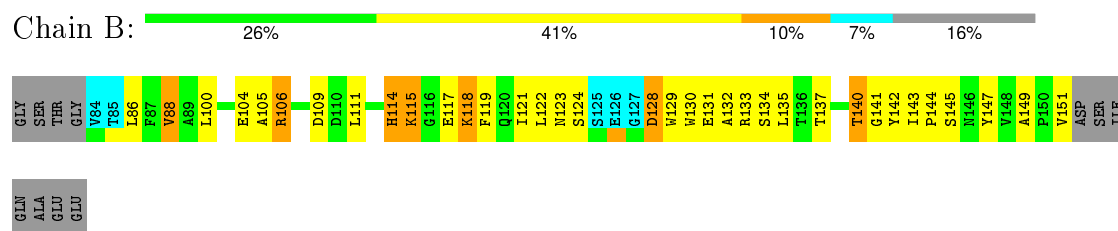


4.2.2 Score per residue for model 2

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



- Molecule 2: FYN

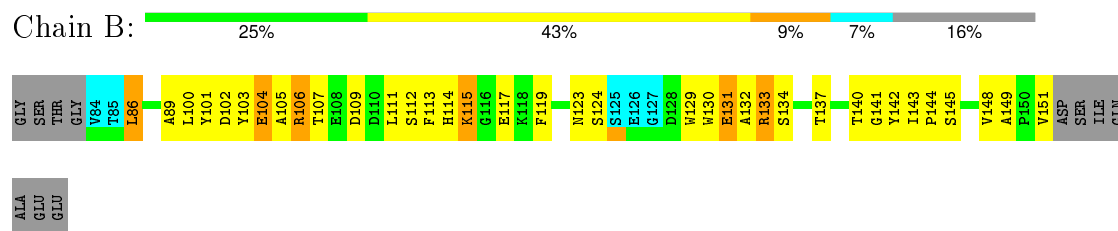


4.2.3 Score per residue for model 3

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



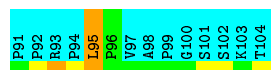
- Molecule 2: FYN



4.2.4 Score per residue for model 4

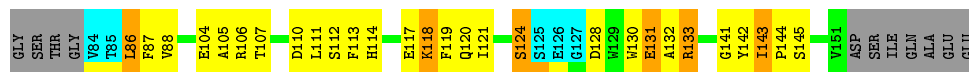
- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A: 



- Molecule 2: FYN

Chain B: 



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A: 



- Molecule 2: FYN

Chain B: 



4.2.6 Score per residue for model 6

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A: 



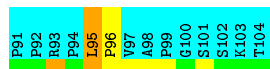
- Molecule 2: FYN

Chain B: 

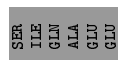


4.2.7 Score per residue for model 7

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

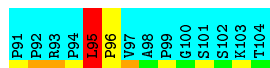


- Molecule 2: FYN

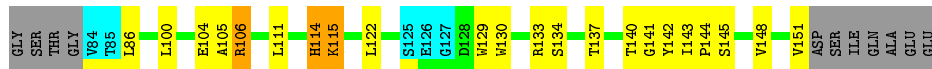


4.2.8 Score per residue for model 8

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



- Molecule 2: FYN



4.2.9 Score per residue for model 9

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



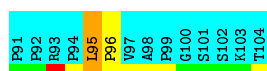


- Molecule 2: FYN

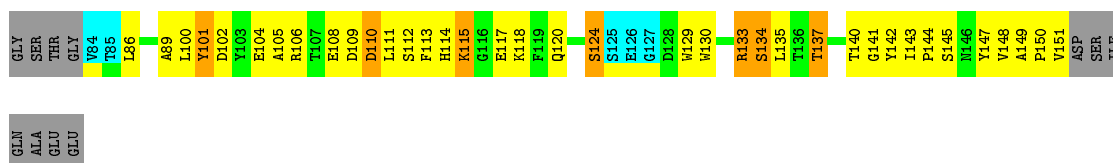
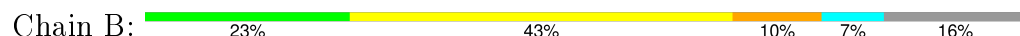


4.2.10 Score per residue for model 10

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

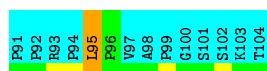


- Molecule 2: FYN

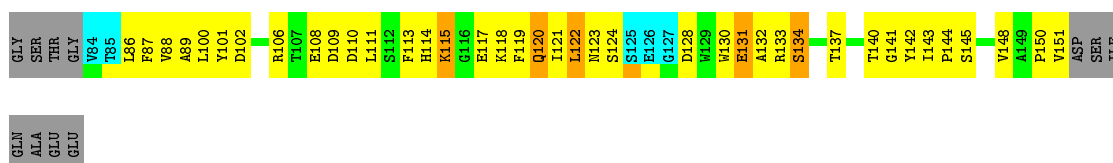


4.2.11 Score per residue for model 11

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



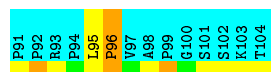
- Molecule 2: FYN



4.2.12 Score per residue for model 12

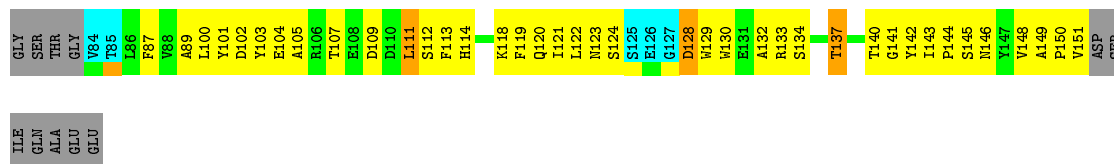
- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A: 



- Molecule 2: FYN

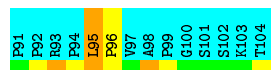
Chain B: 



4.2.13 Score per residue for model 13

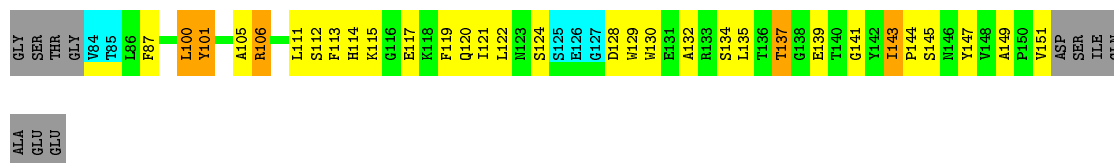
- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A: 



- Molecule 2: FYN

Chain B: 



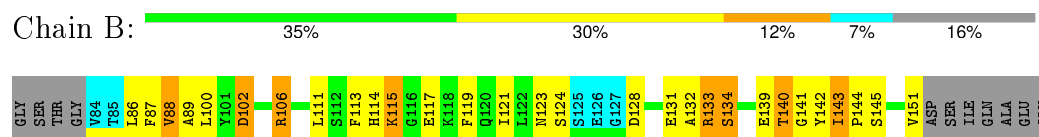
4.2.14 Score per residue for model 14

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A: 



- Molecule 2: FYN

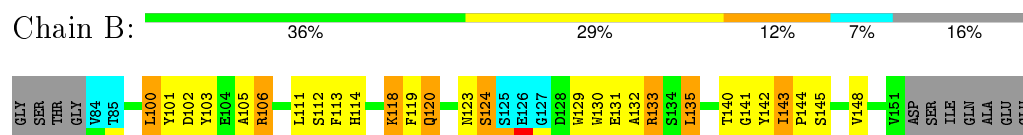


4.2.15 Score per residue for model 15

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



- Molecule 2: FYN

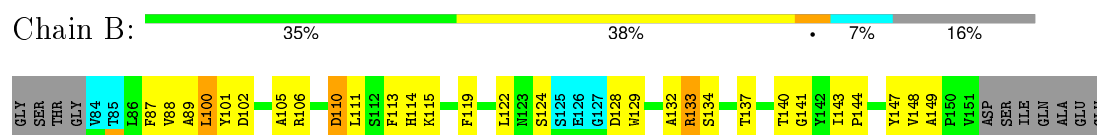


4.2.16 Score per residue for model 16

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



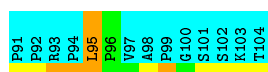
- Molecule 2: FYN



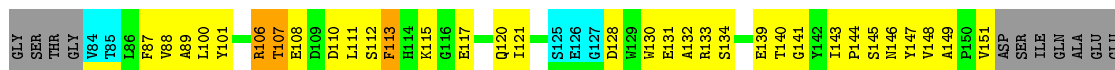
4.2.17 Score per residue for model 17

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



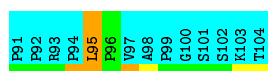


• Molecule 2: FYN

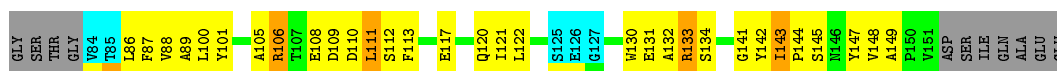


4.2.18 Score per residue for model 18

• Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-TH R

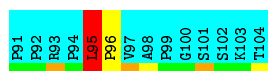


• Molecule 2: FYN

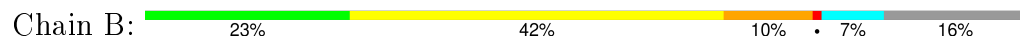


4.2.19 Score per residue for model 19

• Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-TH R



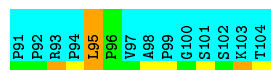
• Molecule 2: FYN



4.2.20 Score per residue for model 20

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-TH R

Chain A: 



- Molecule 2: FYN

Chain B: 



4.2.21 Score per residue for model 21

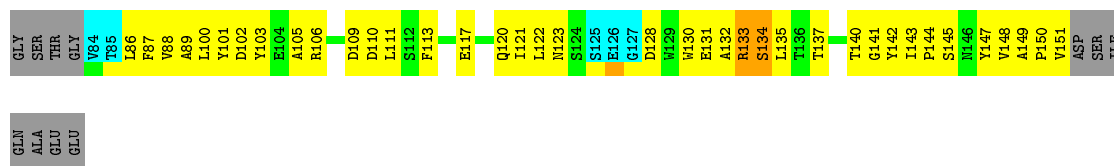
- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-TH R

Chain A: 



- Molecule 2: FYN

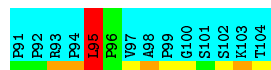
Chain B: 



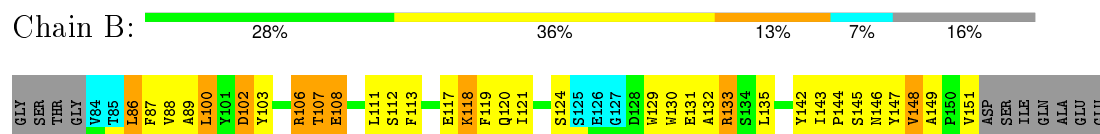
4.2.22 Score per residue for model 22

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-TH R

Chain A: 



- Molecule 2: FYN

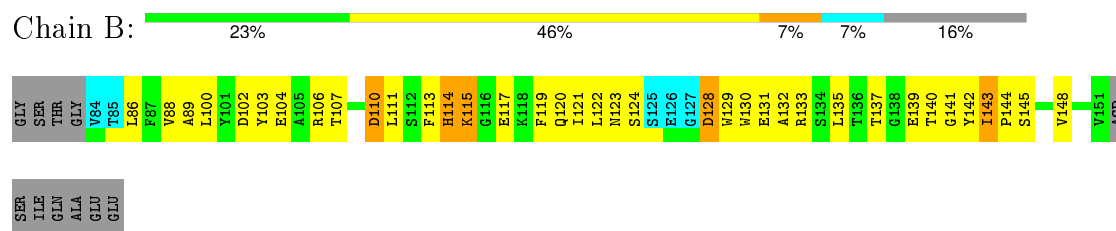


4.2.23 Score per residue for model 23

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



- Molecule 2: FYN

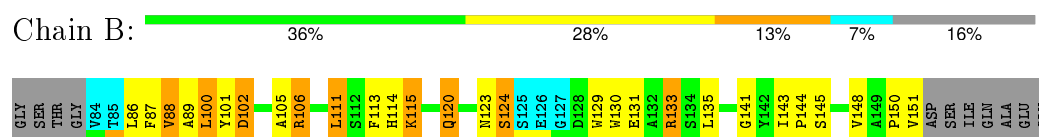


4.2.24 Score per residue for model 24

- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR



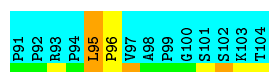
- Molecule 2: FYN



4.2.25 Score per residue for model 25

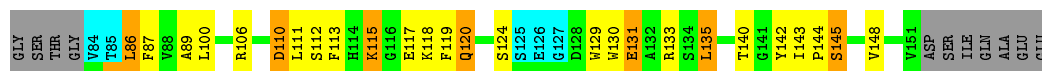
- Molecule 1: PRO-PRO-ARG-PRO-LEU-PRO-VAL-ALA-PRO-GLY-SER-SER-LYS-THR

Chain A:  7% 7% 86%



- Molecule 2: FYN

Chain B: 



5 Refinement protocol and experimental data overview

Of the 50 calculated structures, 25 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

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
2	B	0.0±0.0	1.9±0.3
All	All	0	48

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)
2	B	133	ARG	Sidechain	24
2	B	106	ARG	Sidechain	24

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	15	18	18	1±1
2	B	436	403	403	30±5
All	All	11275	10525	10525	755

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:121:ILE:HD13	2:B:132:ALA:HB2	0.94	1.35	9	11
2:B:111:LEU:HD21	2:B:140:THR:C	0.89	1.87	16	10
2:B:111:LEU:HD12	2:B:143:ILE:HG23	0.87	1.47	2	24
2:B:143:ILE:CD1	2:B:148:VAL:HG11	0.85	2.02	21	9
2:B:105:ALA:HB2	2:B:111:LEU:O	0.83	1.72	13	8
2:B:111:LEU:HD11	2:B:141:GLY:N	0.81	1.91	16	5
2:B:105:ALA:HB1	2:B:110:ASP:OD1	0.79	1.77	18	1
2:B:86:LEU:O	2:B:151:VAL:HG23	0.78	1.79	8	4
1:A:95:LEU:HD12	1:A:95:LEU:O	0.78	1.77	2	2
2:B:143:ILE:HD11	2:B:148:VAL:HG11	0.76	1.58	16	15
2:B:111:LEU:HD21	2:B:141:GLY:N	0.74	1.98	10	12
2:B:143:ILE:HD11	2:B:148:VAL:CG1	0.74	2.12	7	5
2:B:143:ILE:HD12	2:B:143:ILE:O	0.73	1.83	5	1
2:B:111:LEU:HD12	2:B:143:ILE:CG2	0.71	2.16	14	6
2:B:100:LEU:HD11	2:B:149:ALA:HB2	0.70	1.62	3	10
2:B:133:ARG:HB3	2:B:140:THR:HG23	0.70	1.64	14	1
1:A:95:LEU:N	1:A:95:LEU:HD12	0.70	2.02	10	2
2:B:120:GLN:HG3	2:B:135:LEU:HD21	0.69	1.62	7	4
2:B:120:GLN:O	2:B:122:LEU:HD23	0.69	1.86	11	1
2:B:121:ILE:CD1	2:B:132:ALA:HB2	0.69	2.18	1	9
2:B:143:ILE:H	2:B:143:ILE:HD13	0.68	1.48	13	3
2:B:89:ALA:HB1	2:B:113:PHE:CE2	0.68	2.24	23	10
2:B:143:ILE:HD12	2:B:143:ILE:C	0.66	2.10	5	1
2:B:111:LEU:HD11	2:B:141:GLY:C	0.65	2.12	13	12
2:B:119:PHE:HB3	2:B:132:ALA:HB1	0.64	1.68	13	6
2:B:133:ARG:CB	2:B:140:THR:HG23	0.64	2.22	14	1
2:B:120:GLN:OE1	2:B:135:LEU:HD21	0.64	1.91	15	1
2:B:149:ALA:HB1	2:B:150:PRO:HD2	0.63	1.70	10	3
2:B:111:LEU:HD11	2:B:141:GLY:CA	0.63	2.23	12	13
2:B:143:ILE:N	2:B:143:ILE:HD13	0.62	2.10	13	1
1:A:95:LEU:HD22	2:B:146:ASN:OD1	0.61	1.96	17	1
2:B:142:TYR:N	2:B:142:TYR:CD1	0.61	2.69	23	8
1:A:95:LEU:HD23	2:B:128:ASP:OD2	0.61	1.95	2	1
2:B:142:TYR:CD1	2:B:142:TYR:N	0.61	2.69	22	9
1:A:95:LEU:HD11	2:B:128:ASP:HB3	0.60	1.73	11	1
2:B:120:GLN:HG3	2:B:135:LEU:HD11	0.60	1.73	13	3
2:B:143:ILE:CD1	2:B:148:VAL:CG1	0.60	2.80	15	14
2:B:120:GLN:CD	2:B:135:LEU:HD21	0.59	2.18	15	2
2:B:120:GLN:CG	2:B:135:LEU:HD21	0.59	2.27	10	2
2:B:111:LEU:HD21	2:B:141:GLY:HA3	0.59	1.72	20	5
2:B:133:ARG:HB2	2:B:140:THR:HG23	0.59	1.74	3	1
2:B:124:SER:CB	2:B:130:TRP:CD2	0.59	2.85	23	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:151:VAL:O	2:B:151:VAL:HG12	0.58	1.98	13	2
1:A:95:LEU:HD12	1:A:96:PRO:O	0.58	1.98	12	1
2:B:105:ALA:HB2	2:B:111:LEU:C	0.58	2.18	16	7
2:B:87:PHE:CD1	2:B:87:PHE:N	0.58	2.72	11	3
2:B:89:ALA:HB1	2:B:113:PHE:HE2	0.58	1.56	23	9
2:B:118:LYS:CD	2:B:118:LYS:N	0.57	2.66	15	1
2:B:89:ALA:CB	2:B:113:PHE:CE2	0.57	2.87	23	9
2:B:100:LEU:O	2:B:101:TYR:CD1	0.57	2.57	21	8
2:B:128:ASP:O	2:B:129:TRP:CD1	0.57	2.58	2	3
2:B:88:VAL:CG2	2:B:151:VAL:HG22	0.57	2.29	2	6
2:B:130:TRP:CE2	2:B:145:SER:CB	0.57	2.88	11	13
2:B:124:SER:HB2	2:B:130:TRP:CD2	0.57	2.35	6	8
2:B:151:VAL:HG12	2:B:151:VAL:O	0.56	2.01	3	1
2:B:130:TRP:CE2	2:B:145:SER:HB2	0.56	2.35	10	16
2:B:124:SER:CB	2:B:130:TRP:CG	0.56	2.89	1	6
2:B:100:LEU:HD12	2:B:147:TYR:C	0.56	2.20	16	1
1:A:95:LEU:CD1	2:B:146:ASN:ND2	0.56	2.69	19	1
2:B:110:ASP:OD2	2:B:129:TRP:CZ3	0.56	2.59	1	1
1:A:95:LEU:CD1	1:A:95:LEU:O	0.56	2.54	2	2
1:A:95:LEU:HD21	2:B:128:ASP:O	0.56	2.01	20	2
2:B:113:PHE:CD2	2:B:119:PHE:CZ	0.55	2.93	4	6
1:A:95:LEU:HD23	2:B:144:PRO:HB3	0.55	1.76	17	1
2:B:143:ILE:HB	2:B:144:PRO:HD2	0.55	1.79	25	25
2:B:111:LEU:HD11	2:B:141:GLY:H	0.55	1.59	16	1
2:B:124:SER:HB3	2:B:130:TRP:CG	0.54	2.37	1	2
2:B:100:LEU:HD21	2:B:149:ALA:CB	0.54	2.32	16	2
2:B:118:LYS:O	2:B:119:PHE:CD1	0.54	2.61	1	1
1:A:95:LEU:HD21	2:B:128:ASP:OD1	0.54	2.02	7	1
2:B:130:TRP:CD2	2:B:145:SER:HB2	0.54	2.38	21	2
2:B:100:LEU:O	2:B:101:TYR:CG	0.54	2.61	5	1
2:B:102:ASP:OD1	2:B:102:ASP:N	0.54	2.40	22	1
2:B:128:ASP:C	2:B:129:TRP:CD1	0.54	2.81	16	3
2:B:124:SER:HB3	2:B:130:TRP:CD2	0.54	2.38	4	8
2:B:109:ASP:OD2	2:B:142:TYR:CD1	0.54	2.60	2	1
2:B:131:GLU:CD	2:B:142:TYR:CE2	0.54	2.81	7	2
2:B:131:GLU:OE1	2:B:142:TYR:CE2	0.53	2.60	4	1
2:B:89:ALA:HB1	2:B:113:PHE:CE1	0.53	2.38	7	6
1:A:95:LEU:O	1:A:95:LEU:HD12	0.53	2.03	12	2
2:B:134:SER:CB	2:B:137:THR:OG1	0.53	2.57	11	1
2:B:130:TRP:CZ2	2:B:145:SER:HB2	0.53	2.39	10	12
2:B:143:ILE:CD1	2:B:148:VAL:HG13	0.53	2.33	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:131:GLU:HB3	2:B:142:TYR:CE2	0.53	2.38	15	3
2:B:131:GLU:CG	2:B:131:GLU:O	0.53	2.57	17	3
2:B:115:LYS:CG	2:B:115:LYS:O	0.52	2.57	11	4
2:B:86:LEU:C	2:B:87:PHE:CD1	0.52	2.83	11	8
1:A:95:LEU:CD2	2:B:146:ASN:OD1	0.52	2.57	1	1
2:B:124:SER:HA	2:B:130:TRP:CD1	0.52	2.39	25	3
2:B:86:LEU:HD13	2:B:87:PHE:N	0.52	2.19	4	1
2:B:86:LEU:HD23	2:B:119:PHE:O	0.52	2.04	22	3
2:B:131:GLU:O	2:B:131:GLU:CG	0.52	2.58	20	5
2:B:110:ASP:OD1	2:B:129:TRP:CZ3	0.52	2.63	25	1
2:B:120:GLN:O	2:B:122:LEU:CD2	0.52	2.57	6	2
1:A:95:LEU:HD13	1:A:96:PRO:HD2	0.52	1.79	8	1
2:B:124:SER:HA	2:B:130:TRP:CG	0.52	2.39	7	4
2:B:128:ASP:N	2:B:128:ASP:OD1	0.52	2.43	12	1
2:B:106:ARG:O	2:B:107:THR:HG23	0.52	2.05	7	1
2:B:120:GLN:HE21	2:B:135:LEU:HD11	0.52	1.65	21	1
2:B:114:HIS:N	2:B:114:HIS:CD2	0.52	2.77	19	1
2:B:102:ASP:OD2	2:B:114:HIS:CD2	0.52	2.63	11	2
2:B:122:LEU:N	2:B:122:LEU:HD23	0.51	2.19	12	4
2:B:121:ILE:CG2	2:B:124:SER:OG	0.51	2.57	13	1
2:B:141:GLY:C	2:B:142:TYR:CD1	0.51	2.84	9	1
2:B:111:LEU:HD21	2:B:141:GLY:CA	0.51	2.35	20	5
2:B:102:ASP:N	2:B:102:ASP:OD1	0.51	2.43	24	2
1:A:95:LEU:CD1	1:A:95:LEU:N	0.51	2.70	10	1
2:B:111:LEU:HD21	2:B:140:THR:CA	0.51	2.34	16	1
2:B:143:ILE:N	2:B:143:ILE:CD1	0.51	2.73	13	1
2:B:113:PHE:CD1	2:B:119:PHE:CZ	0.51	2.98	19	4
2:B:131:GLU:HG2	2:B:142:TYR:CE2	0.51	2.40	7	3
2:B:88:VAL:HG23	2:B:151:VAL:HG22	0.51	1.82	17	3
2:B:100:LEU:HD11	2:B:149:ALA:CB	0.51	2.35	13	3
2:B:100:LEU:C	2:B:101:TYR:CD1	0.51	2.84	18	1
2:B:104:GLU:OE2	2:B:106:ARG:NH1	0.51	2.44	8	1
2:B:102:ASP:HB2	2:B:114:HIS:CD2	0.50	2.41	23	1
2:B:113:PHE:N	2:B:113:PHE:CD1	0.50	2.79	9	4
2:B:124:SER:HB2	2:B:130:TRP:CE2	0.50	2.42	2	7
2:B:120:GLN:NE2	2:B:135:LEU:HD21	0.50	2.20	13	2
2:B:121:ILE:CG2	2:B:124:SER:HG	0.50	2.19	13	1
2:B:131:GLU:HB3	2:B:142:TYR:CE1	0.50	2.41	18	1
2:B:129:TRP:CZ3	2:B:144:PRO:HD3	0.50	2.42	24	15
2:B:124:SER:HB3	2:B:130:TRP:CE3	0.50	2.41	7	1
2:B:117:GLU:HB3	2:B:119:PHE:CE2	0.50	2.41	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:113:PHE:CG	2:B:119:PHE:CZ	0.49	3.00	23	5
2:B:87:PHE:N	2:B:87:PHE:CD1	0.49	2.80	21	6
2:B:88:VAL:HG13	2:B:118:LYS:HD3	0.49	1.84	19	1
2:B:89:ALA:CB	2:B:113:PHE:CE1	0.49	2.95	7	3
2:B:131:GLU:HB3	2:B:142:TYR:CD2	0.49	2.42	15	1
2:B:120:GLN:OE1	2:B:135:LEU:CD2	0.49	2.59	15	1
1:A:95:LEU:CD1	2:B:146:ASN:CG	0.49	2.80	19	1
2:B:131:GLU:HB2	2:B:142:TYR:CE2	0.49	2.43	11	1
2:B:103:TYR:HB3	2:B:113:PHE:CE1	0.49	2.43	23	2
2:B:86:LEU:HD11	2:B:135:LEU:HD11	0.49	1.83	21	1
1:A:95:LEU:HD12	1:A:95:LEU:C	0.49	2.27	12	1
2:B:117:GLU:OE1	2:B:118:LYS:N	0.49	2.46	4	1
2:B:113:PHE:CD1	2:B:113:PHE:N	0.49	2.81	23	3
2:B:130:TRP:CD2	2:B:145:SER:CB	0.49	2.95	20	2
2:B:89:ALA:CB	2:B:113:PHE:CD2	0.49	2.96	23	1
2:B:101:TYR:HB3	2:B:147:TYR:CE2	0.48	2.42	7	3
2:B:145:SER:O	2:B:148:VAL:HG23	0.48	2.07	24	2
2:B:117:GLU:OE1	2:B:119:PHE:CE1	0.48	2.66	4	1
2:B:124:SER:CB	2:B:130:TRP:CD1	0.48	2.96	9	1
2:B:115:LYS:O	2:B:115:LYS:CG	0.48	2.62	25	2
2:B:100:LEU:HB2	2:B:101:TYR:CE2	0.48	2.43	15	2
1:A:96:PRO:HD3	2:B:129:TRP:CZ2	0.48	2.43	7	3
2:B:110:ASP:N	2:B:110:ASP:OD1	0.47	2.47	17	2
2:B:128:ASP:O	2:B:145:SER:CB	0.47	2.62	19	2
2:B:130:TRP:CE2	2:B:145:SER:HB3	0.47	2.45	22	2
2:B:100:LEU:HD21	2:B:149:ALA:HB3	0.47	1.86	20	2
2:B:88:VAL:CG2	2:B:151:VAL:CG2	0.47	2.93	24	1
2:B:114:HIS:N	2:B:114:HIS:ND1	0.47	2.62	14	1
2:B:87:PHE:CD2	2:B:149:ALA:C	0.47	2.87	16	1
2:B:131:GLU:HG2	2:B:142:TYR:CD2	0.47	2.44	7	2
2:B:117:GLU:CD	2:B:119:PHE:CE1	0.47	2.88	4	1
2:B:103:TYR:HB3	2:B:113:PHE:CZ	0.47	2.45	15	2
2:B:101:TYR:HB2	2:B:147:TYR:CE2	0.47	2.45	21	2
1:A:95:LEU:HD11	2:B:146:ASN:CG	0.47	2.29	19	1
2:B:110:ASP:OD1	2:B:110:ASP:N	0.47	2.48	16	2
1:A:96:PRO:HG2	2:B:147:TYR:CZ	0.47	2.45	10	1
2:B:104:GLU:CG	2:B:104:GLU:O	0.47	2.63	1	1
2:B:88:VAL:HG13	2:B:118:LYS:CD	0.47	2.40	19	1
2:B:100:LEU:HD21	2:B:149:ALA:HB2	0.47	1.87	16	1
2:B:117:GLU:CD	2:B:118:LYS:N	0.46	2.68	4	1
2:B:143:ILE:CD1	2:B:143:ILE:C	0.46	2.80	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:109:ASP:O	2:B:110:ASP:O	0.46	2.33	10	1
2:B:87:PHE:CD1	2:B:121:ILE:HG12	0.46	2.46	12	2
2:B:100:LEU:HB2	2:B:101:TYR:CE1	0.46	2.46	18	1
2:B:102:ASP:OD1	2:B:103:TYR:N	0.46	2.48	15	1
2:B:103:TYR:HH	2:B:129:TRP:HH2	0.46	1.52	22	1
2:B:130:TRP:CD2	2:B:145:SER:HB3	0.46	2.46	25	1
2:B:131:GLU:HG3	2:B:131:GLU:O	0.46	2.11	19	2
2:B:129:TRP:N	2:B:129:TRP:CD1	0.46	2.84	22	1
2:B:130:TRP:CD1	2:B:130:TRP:N	0.45	2.84	17	4
2:B:107:THR:O	2:B:110:ASP:OD1	0.45	2.33	17	1
2:B:100:LEU:O	2:B:115:LYS:HD2	0.45	2.11	24	1
2:B:104:GLU:OE2	2:B:105:ALA:O	0.45	2.34	3	1
2:B:101:TYR:HB2	2:B:147:TYR:CD2	0.45	2.46	16	2
2:B:86:LEU:HD22	2:B:120:GLN:HG2	0.45	1.87	19	1
2:B:87:PHE:CD1	2:B:121:ILE:CG1	0.45	3.00	12	1
2:B:145:SER:O	2:B:148:VAL:CG2	0.45	2.64	24	1
2:B:101:TYR:HB2	2:B:147:TYR:CG	0.45	2.46	17	1
2:B:130:TRP:N	2:B:130:TRP:CD1	0.45	2.84	11	6
2:B:121:ILE:HD13	2:B:132:ALA:CB	0.45	2.35	21	2
2:B:117:GLU:OE1	2:B:118:LYS:O	0.45	2.34	4	1
2:B:103:TYR:CD2	2:B:111:LEU:O	0.45	2.69	21	1
2:B:120:GLN:HG3	2:B:135:LEU:CD1	0.45	2.42	6	1
2:B:131:GLU:CG	2:B:142:TYR:CE2	0.45	2.99	7	1
2:B:114:HIS:CD2	2:B:114:HIS:O	0.45	2.70	15	1
2:B:115:LYS:HG2	2:B:115:LYS:O	0.45	2.12	3	2
2:B:105:ALA:HB1	2:B:110:ASP:HB2	0.45	1.87	1	1
2:B:131:GLU:O	2:B:131:GLU:HG3	0.45	2.12	14	2
2:B:87:PHE:CD2	2:B:150:PRO:N	0.45	2.85	11	2
2:B:134:SER:HB2	2:B:137:THR:OG1	0.44	2.12	11	4
2:B:105:ALA:CB	2:B:110:ASP:OD1	0.44	2.59	18	1
2:B:124:SER:OG	2:B:124:SER:O	0.44	2.33	5	1
2:B:100:LEU:C	2:B:101:TYR:CG	0.44	2.91	15	2
2:B:117:GLU:OE1	2:B:119:PHE:CE2	0.44	2.70	14	1
1:A:95:LEU:O	1:A:95:LEU:CD1	0.44	2.65	9	1
2:B:118:LYS:HB2	2:B:135:LEU:HD12	0.44	1.88	2	1
2:B:123:ASN:CB	2:B:131:GLU:OE2	0.44	2.65	2	1
2:B:139:GLU:O	2:B:139:GLU:CG	0.44	2.64	13	1
2:B:103:TYR:CD1	2:B:104:GLU:N	0.44	2.86	12	1
2:B:145:SER:O	2:B:148:VAL:HG22	0.44	2.12	25	1
2:B:122:LEU:HD23	2:B:122:LEU:N	0.44	2.28	8	1
2:B:103:TYR:OH	2:B:110:ASP:OD2	0.44	2.34	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:129:TRP:CH2	2:B:144:PRO:HD3	0.44	2.48	1	1
2:B:104:GLU:O	2:B:105:ALA:C	0.44	2.57	2	3
2:B:111:LEU:CG	2:B:141:GLY:HA3	0.43	2.43	4	2
2:B:111:LEU:CD2	2:B:141:GLY:HA3	0.43	2.42	20	1
2:B:123:ASN:HB2	2:B:131:GLU:OE2	0.43	2.13	24	1
2:B:113:PHE:CD2	2:B:119:PHE:CE2	0.43	3.05	4	1
2:B:128:ASP:O	2:B:145:SER:OG	0.43	2.32	4	2
2:B:111:LEU:HD23	2:B:139:GLU:OE1	0.43	2.13	19	1
2:B:111:LEU:CD1	2:B:143:ILE:HG23	0.43	2.33	22	3
2:B:114:HIS:O	2:B:115:LYS:C	0.43	2.57	24	9
2:B:102:ASP:CB	2:B:114:HIS:HA	0.43	2.44	12	2
2:B:143:ILE:HD12	2:B:144:PRO:O	0.43	2.14	6	1
2:B:107:THR:OG1	2:B:110:ASP:OD2	0.43	2.34	17	2
2:B:100:LEU:HB2	2:B:101:TYR:CD1	0.43	2.48	18	1
2:B:120:GLN:NE2	2:B:135:LEU:HD11	0.43	2.29	21	1
2:B:110:ASP:OD1	2:B:142:TYR:O	0.43	2.36	19	1
2:B:123:ASN:HB3	2:B:131:GLU:CG	0.43	2.44	3	1
2:B:150:PRO:O	2:B:151:VAL:C	0.43	2.57	12	1
2:B:105:ALA:CB	2:B:110:ASP:HB3	0.43	2.44	21	1
2:B:117:GLU:OE1	2:B:119:PHE:CZ	0.43	2.72	14	2
2:B:113:PHE:HB3	2:B:117:GLU:OE1	0.43	2.14	5	1
2:B:143:ILE:HD13	2:B:143:ILE:N	0.42	2.28	14	2
2:B:128:ASP:C	2:B:145:SER:OG	0.42	2.58	2	1
2:B:120:GLN:CG	2:B:135:LEU:HD11	0.42	2.43	23	1
2:B:102:ASP:HB3	2:B:114:HIS:ND1	0.42	2.29	1	1
2:B:123:ASN:CB	2:B:131:GLU:CD	0.42	2.87	2	2
2:B:104:GLU:OE2	2:B:105:ALA:C	0.42	2.57	3	1
2:B:151:VAL:HG13	2:B:151:VAL:O	0.42	2.13	22	1
2:B:134:SER:HB3	2:B:137:THR:OG1	0.42	2.15	13	1
2:B:134:SER:OG	2:B:139:GLU:O	0.42	2.38	14	1
2:B:151:VAL:HG22	2:B:151:VAL:O	0.42	2.13	7	1
1:A:95:LEU:HD23	2:B:129:TRP:NE1	0.42	2.30	15	1
2:B:120:GLN:HG3	2:B:135:LEU:CG	0.42	2.44	23	1
2:B:107:THR:OG1	2:B:108:GLU:N	0.42	2.53	22	1
1:A:96:PRO:HB2	2:B:147:TYR:OH	0.42	2.15	13	1
2:B:109:ASP:OD1	2:B:109:ASP:O	0.41	2.37	20	1
2:B:123:ASN:HB3	2:B:131:GLU:OE2	0.41	2.15	2	2
2:B:100:LEU:O	2:B:115:LYS:CD	0.41	2.68	24	1
2:B:128:ASP:O	2:B:145:SER:HB3	0.41	2.15	23	1
1:A:95:LEU:HD22	2:B:129:TRP:NE1	0.41	2.30	8	1
2:B:120:GLN:HG3	2:B:135:LEU:CD2	0.41	2.43	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:105:ALA:CB	2:B:111:LEU:O	0.41	2.58	13	1
2:B:113:PHE:O	2:B:114:HIS:CD2	0.41	2.73	6	1
2:B:120:GLN:O	2:B:120:GLN:CG	0.41	2.68	11	1
2:B:102:ASP:OD1	2:B:102:ASP:C	0.41	2.58	16	1
2:B:112:SER:O	2:B:113:PHE:HB3	0.41	2.16	17	1
2:B:123:ASN:HB2	2:B:131:GLU:CD	0.41	2.36	3	1
2:B:143:ILE:HD12	2:B:148:VAL:CG1	0.41	2.44	21	1
2:B:124:SER:CA	2:B:130:TRP:CD1	0.41	3.03	25	1
1:A:95:LEU:CD2	2:B:146:ASN:CG	0.41	2.88	1	1
2:B:88:VAL:HG13	2:B:117:GLU:O	0.41	2.15	4	1
2:B:102:ASP:OD1	2:B:102:ASP:O	0.41	2.39	3	1
2:B:146:ASN:O	2:B:146:ASN:ND2	0.41	2.53	12	1
2:B:89:ALA:HA	2:B:147:TYR:O	0.41	2.15	17	1
2:B:118:LYS:CB	2:B:135:LEU:HD13	0.41	2.46	22	1
2:B:87:PHE:HA	2:B:149:ALA:O	0.41	2.15	1	1
2:B:88:VAL:CG2	2:B:151:VAL:HB	0.41	2.46	1	1
2:B:115:LYS:O	2:B:115:LYS:HG2	0.40	2.16	7	1
2:B:86:LEU:CD2	2:B:86:LEU:N	0.40	2.84	24	1
1:A:96:PRO:HG2	2:B:144:PRO:HG3	0.40	1.93	16	1
2:B:104:GLU:O	2:B:104:GLU:HG2	0.40	2.15	1	1
1:A:96:PRO:CG	2:B:144:PRO:HG3	0.40	2.47	7	1
2:B:123:ASN:HB2	2:B:131:GLU:CG	0.40	2.47	6	1
2:B:130:TRP:O	2:B:142:TYR:HA	0.40	2.16	8	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	2/14 (14%)	1±1 (36±27%)	1±1 (26±32%)	1±1 (38±32%)	0	0
2	B	52/69 (75%)	49±1 (94±3%)	3±1 (6±2%)	0±1 (0±1%)	38	79
All	All	1350/2075 (65%)	1234 (91%)	91 (7%)	25 (2%)	14	56

All 7 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	95	LEU	15
1	A	96	PRO	4
2	B	110	ASP	2
2	B	113	PHE	1
2	B	124	SER	1
2	B	128	ASP	1
2	B	105	ALA	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	2/12 (17%)	1±0 (64±22%)	1±0 (36±22%)	1	9
2	B	46/58 (79%)	35±3 (76±6%)	11±3 (24±6%)	3	29
All	All	1200/1750 (69%)	911 (76%)	289 (24%)	3	28

All 34 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	95	LEU	18
2	B	100	LEU	16
2	B	117	GLU	16
2	B	115	LYS	15
2	B	133	ARG	14
2	B	137	THR	13
2	B	112	SER	12
2	B	134	SER	12
2	B	118	LYS	11
2	B	106	ARG	11
2	B	120	GLN	11
2	B	107	THR	10
2	B	128	ASP	9
2	B	86	LEU	8
2	B	108	GLU	8
2	B	123	ASN	8
2	B	102	ASP	8
2	B	88	VAL	8

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Mol	Chain	Res	Type	Models (Total)
2	B	143	ILE	7
2	B	131	GLU	7
2	B	122	LEU	7
2	B	124	SER	7
2	B	109	ASP	7
2	B	140	THR	6
2	B	104	GLU	6
2	B	114	HIS	5
2	B	111	LEU	5
2	B	101	TYR	4
2	B	110	ASP	4
2	B	139	GLU	4
2	B	148	VAL	4
2	B	147	TYR	4
2	B	135	LEU	2
2	B	145	SER	2

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 carbohydrates 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