

Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 08:23 PM EST

PDB ID	:	1TBO
Title	:	NMR STRUCTURE OF A PROTEIN KINASE C-G PHORBOL-BINDING
		DOMAIN, 30 STRUCTURES
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Deposited on	:	1997-04-15

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

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

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

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} \; { m archive} \ (\#{ m Entries})$
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		Qua	ality of chair	1	
1	А	82	7%	43%	11%	20%	20%



2 Ensemble composition and analysis (i)

This entry contains 30 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 30 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 mode						
1	A:102-A:151 (50)	0.36	30			

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1026 atoms, of which 497 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called PROTEIN KINASE C, GAMMA TYPE.

Mol	Chain	Residues	Atoms					Trace	
1	Δ	66	Total	С	Н	Ν	Ο	S	0
	A 66	1024	318	497	106	94	9	0	

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	А	2	Total Zn	
	11	2	2 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: PROTEIN KINASE C, GAMMA TYPE



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





4.2.2 Score per residue for model 2

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE

Chain A: 16% 39% 5% 20% 20%



RIC RIC PRD PRD

E157 R158 R158 GLY GLY LEU LEU LEU LEU ILEU ARG ALA ALA ALA ALA ALA ALA ALA CLU SER SER

4.2.3 Score per residue for model 3

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.4 Score per residue for model 4

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.5 Score per residue for model 5

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.6 Score per residue for model 6





4.2.7 Score per residue for model 7

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.8 Score per residue for model 8

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.9 Score per residue for model 9

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



H155 T156 E157 R158 R158 R159 GLY GLV GLV GLU THR ALA ALA ALA ALA ALA ALA ALA ALA CIU THR CIU



4.2.10 Score per residue for model 10

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



- 4.2.11 Score per residue for model 11
- Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.12 Score per residue for model 12

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.13 Score per residue for model 13



4.2.14 Score per residue for model 14

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



- 4.2.15 Score per residue for model 15
- Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.17 Score per residue for model 17



4.2.18 Score per residue for model 18

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



- 4.2.19 Score per residue for model 19
- Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.20 Score per residue for model 20

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.21 Score per residue for model 21



4.2.22 Score per residue for model 22

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



- 4.2.23 Score per residue for model 23
- Molecule 1: PROTEIN KINASE C, GAMMA TYPE



R158 R159 GLY ARG LEU GLU LEU GLU TLE ARG PRO PRO PRO PRO THR SER ASP

4.2.24 Score per residue for model 24

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.25 Score per residue for model 25



4.2.26 Score per residue for model 26

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



- 4.2.27 Score per residue for model 27
- Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.28 Score per residue for model 28

• Molecule 1: PROTEIN KINASE C, GAMMA TYPE



4.2.29 Score per residue for model 29



4.2.30 Score per residue for model 30 (medoid)





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: DG-SA.

Of the 1 calculated structures, 30 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	structure solution	
X-PLOR	refinement	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	А	$0.0{\pm}0.0$	$3.8{\pm}0.4$
All	All	0	115

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	А	145	ARG	Sidechain	30
1	А	105	ARG	Sidechain	29
1	А	142	ARG	Sidechain	29
1	А	141	ARG	Sidechain	27

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	А	393	374	376	47 ± 8
All	All	11850	11220	11281	1409

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 61.



A. 1				Mo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:122:LEU:HD23	1:A:140:HIS:CD2	1.07	1.85	5	30
1:A:117:HIS:ND1	1:A:147:VAL:HG22	0.90	1.81	29	4
1:A:122:LEU:HD13	1:A:129:GLY:HA3	0.86	1.47	18	21
1:A:143:CYS:O	1:A:147:VAL:HG23	0.81	1.75	16	13
1:A:122:LEU:HD13	1:A:129:GLY:CA	0.81	2.06	22	27
1:A:104:PHE:CE2	1:A:144:VAL:HG13	0.80	2.12	24	16
1:A:126:VAL:HG12	1:A:141:ARG:HB2	0.80	1.53	25	2
1:A:122:LEU:HD13	1:A:129:GLY:HA2	0.77	1.56	11	12
1:A:116:ASP:OD1	1:A:139:VAL:HG12	0.75	1.80	1	7
1:A:139:VAL:CG2	1:A:144:VAL:HG22	0.73	2.12	24	2
1:A:122:LEU:HD23	1:A:140:HIS:NE2	0.72	1.99	13	22
1:A:122:LEU:HD23	1:A:140:HIS:CG	0.71	2.20	26	19
1:A:107:HIS:CG	1:A:109:TYR:CZ	0.70	2.80	17	6
1:A:106:LEU:HD23	1:A:106:LEU:N	0.69	2.02	13	30
1:A:107:HIS:CD2	1:A:109:TYR:CE2	0.69	2.81	14	6
1:A:114:PHE:CZ	1:A:121:LEU:HD11	0.68	2.24	22	11
1:A:107:HIS:CE1	1:A:109:TYR:CD2	0.68	2.82	17	1
1:A:126:VAL:HG12	1:A:141:ARG:CB	0.67	2.20	25	1
1:A:122:LEU:HB3	1:A:126:VAL:HG21	0.67	1.67	27	3
1:A:104:PHE:CZ	1:A:139:VAL:HG21	0.65	2.27	5	6
1:A:126:VAL:HG21	1:A:130:MET:CE	0.65	2.21	5	1
1:A:107:HIS:CB	1:A:109:TYR:CZ	0.65	2.80	7	11
1:A:126:VAL:O	1:A:126:VAL:HG23	0.65	1.91	3	2
1:A:126:VAL:HG11	1:A:141:ARG:HB2	0.65	1.66	30	2
1:A:140:HIS:O	1:A:144:VAL:HG23	0.64	1.92	24	2
1:A:150:LEU:HD23	1:A:150:LEU:N	0.64	2.08	22	4
1:A:102:HIS:HE2	1:A:150:LEU:N	0.64	1.89	29	4
1:A:102:HIS:CB	1:A:104:PHE:CE2	0.64	2.81	7	4
1:A:114:PHE:CZ	1:A:121:LEU:CD1	0.64	2.81	14	10
1:A:104:PHE:CE1	1:A:139:VAL:CG2	0.64	2.81	6	13
1:A:139:VAL:HG23	1:A:144:VAL:CG2	0.63	2.22	24	1
1:A:125:LEU:CD1	1:A:140:HIS:CD2	0.63	2.81	1	1
1:A:114:PHE:CE1	1:A:121:LEU:HD11	0.63	2.27	14	6
1:A:102:HIS:CE1	1:A:151:CYS:N	0.63	2.66	13	5
1:A:126:VAL:HG11	1:A:141:ARG:CB	0.63	2.24	14	2
1:A:114:PHE:CD1	1:A:121:LEU:HD21	0.63	2.29	14	2
1:A:122:LEU:CD2	1:A:140:HIS:CD2	0.62	2.81	14	15
1:A:109:TYR:CE2	1:A:128:GLN:NE2	0.62	2.67	18	4
1:A:107:HIS:ND1	1:A:109:TYR:CE2	0.62	2.67	27	1
1:A:127:HIS:CE1	1:A:128:GLN:NE2	0.62	2.67	11	2
1:A:107:HIS:CD2	1:A:109:TYR:CZ	0.61	2.88	21	2

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



1	TBO
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	his as page			Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:102:HIS:CE1	1:A:151:CYS:CA	0.61	2.83	13	5	
1:A:107:HIS:CD2	1:A:109:TYR:CD2	0.61	2.88	28	2	
1:A:115:CYS:CB	1:A:140:HIS:CE1	0.61	2.84	21	10	
1:A:104:PHE:HE2	1:A:144:VAL:HG13	0.60	1.56	30	1	
1:A:107:HIS:CE1	1:A:109:TYR:CE2	0.60	2.89	17	4	
1:A:114:PHE:CD1	1:A:114:PHE:N	0.60	2.68	17	2	
1:A:147:VAL:HG13	1:A:150:LEU:HD12	0.60	1.74	13	1	
1:A:112:PRO:CG	1:A:123:TYR:CE1	0.59	2.84	8	3	
1:A:114:PHE:CE1	1:A:121:LEU:CG	0.59	2.85	14	5	
1:A:107:HIS:CG	1:A:109:TYR:CE2	0.59	2.90	14	3	
1:A:108:SER:O	1:A:109:TYR:CD1	0.59	2.56	10	2	
1:A:104:PHE:CD2	1:A:144:VAL:HG13	0.59	2.32	21	3	
1:A:122:LEU:O	1:A:123:TYR:CG	0.59	2.56	8	2	
1:A:106:LEU:N	1:A:106:LEU:CD2	0.59	2.66	5	30	
1:A:112:PRO:CG	1:A:123:TYR:CD1	0.58	2.86	3	2	
1:A:107:HIS:CE1	1:A:129:GLY:O	0.58	2.57	10	3	
1:A:139:VAL:HG21	1:A:144:VAL:HG22	0.58	1.73	24	2	
1:A:107:HIS:CG	1:A:109:TYR:OH	0.58	2.57	27	1	
1:A:127:HIS:ND1	1:A:128:GLN:NE2	0.58	2.51	17	2	
1:A:107:HIS:CD2	1:A:129:GLY:O	0.58	2.57	27	1	
1:A:148:PRO:HG2	1:A:150:LEU:HD11	0.58	1.75	12	2	
1:A:115:CYS:HB2	1:A:140:HIS:CE1	0.57	2.33	5	27	
1:A:109:TYR:CE2	1:A:128:GLN:OE1	0.57	2.57	5	3	
1:A:102:HIS:HE2	1:A:150:LEU:H	0.57	1.42	29	4	
1:A:118:CYS:SG	1:A:140:HIS:CE1	0.57	2.97	24	29	
1:A:122:LEU:CD1	1:A:129:GLY:CA	0.57	2.81	17	4	
1:A:109:TYR:CG	1:A:128:GLN:OE1	0.57	2.57	20	1	
1:A:109:TYR:CD2	1:A:128:GLN:OE1	0.57	2.57	20	1	
1:A:109:TYR:O	1:A:110:SER:CB	0.57	2.53	16	13	
1:A:104:PHE:CE1	1:A:139:VAL:HG22	0.57	2.35	14	8	
1:A:108:SER:OG	1:A:127:HIS:CE1	0.57	2.57	18	4	
1:A:126:VAL:CG1	1:A:141:ARG:CG	0.57	2.82	26	1	
1:A:114:PHE:CE1	1:A:121:LEU:HD21	0.57	2.34	14	8	
1:A:126:VAL:HG21	1:A:130:MET:HE3	0.56	1.77	5	1	
1:A:104:PHE:CE2	1:A:144:VAL:CG1	0.56	2.88	24	5	
1:A:112:PRO:CG	1:A:123:TYR:CZ	0.56	2.88	1	1	
1:A:114:PHE:CD1	1:A:121:LEU:CD2	0.56	2.88	14	2	
1:A:109:TYR:CD1	1:A:128:GLN:OE1	0.56	2.59	20	1	
1:A:109:TYR:CZ	1:A:128:GLN:NE2	0.56	2.74	13	2	
1:A:126:VAL:HG11	1:A:141:ARG:N	0.56	2.16	25	1	
1:A:109:TYR:CE2	1:A:128:GLN:CD	0.55	2.80	8	7	



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	the active page		D 1 (8)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:124:GLY:O	1:A:125:LEU:HD23	0.55	2.01	24	2	
1:A:125:LEU:HD13	1:A:140:HIS:CD2	0.55	2.36	29	2	
1:A:104:PHE:CD2	1:A:144:VAL:HG22	0.55	2.37	10	1	
1:A:126:VAL:HG11	1:A:141:ARG:CG	0.55	2.32	26	1	
1:A:107:HIS:HB3	1:A:109:TYR:CZ	0.55	2.36	23	14	
1:A:122:LEU:HD13	1:A:128:GLN:O	0.55	2.01	13	1	
1:A:117:HIS:CE1	1:A:147:VAL:HG22	0.55	2.37	29	2	
1:A:112:PRO:HG3	1:A:123:TYR:CD1	0.55	2.37	8	1	
1:A:116:ASP:OD1	1:A:139:VAL:HG13	0.55	2.01	11	2	
1:A:107:HIS:CG	1:A:109:TYR:CE1	0.54	2.95	8	2	
1:A:109:TYR:CZ	1:A:128:GLN:OE1	0.54	2.60	20	2	
1:A:126:VAL:O	1:A:127:HIS:CB	0.54	2.55	30	1	
1:A:107:HIS:HB3	1:A:109:TYR:CE1	0.54	2.37	8	10	
1:A:112:PRO:CD	1:A:123:TYR:CE1	0.54	2.90	3	1	
1:A:127:HIS:CE1	1:A:128:GLN:OE1	0.54	2.61	30	1	
1:A:109:TYR:CE1	1:A:128:GLN:OE1	0.54	2.60	20	1	
1:A:126:VAL:HG11	1:A:141:ARG:HG3	0.54	1.76	24	1	
1:A:112:PRO:CB	1:A:122:LEU:O	0.54	2.56	26	15	
1:A:127:HIS:O	1:A:128:GLN:CB	0.54	2.56	9	5	
1:A:122:LEU:O	1:A:123:TYR:CD2	0.54	2.61	8	1	
1:A:102:HIS:CE1	1:A:150:LEU:C	0.54	2.81	29	3	
1:A:107:HIS:O	1:A:128:GLN:NE2	0.54	2.41	21	2	
1:A:102:HIS:HB2	1:A:104:PHE:CE2	0.54	2.38	13	13	
1:A:108:SER:CB	1:A:128:GLN:OE1	0.54	2.56	30	1	
1:A:126:VAL:O	1:A:128:GLN:N	0.54	2.41	16	10	
1:A:107:HIS:O	1:A:128:GLN:CG	0.53	2.56	20	2	
1:A:147:VAL:CG1	1:A:150:LEU:HD21	0.53	2.32	27	1	
1:A:109:TYR:CD2	1:A:128:GLN:CD	0.53	2.81	5	2	
1:A:102:HIS:NE2	1:A:147:VAL:HG11	0.53	2.18	6	1	
1:A:106:LEU:HD13	1:A:141:ARG:HH22	0.53	1.64	7	1	
1:A:122:LEU:HD13	1:A:129:GLY:N	0.53	2.17	21	2	
1:A:112:PRO:HG3	1:A:123:TYR:CE1	0.53	2.38	1	1	
1:A:147:VAL:HG12	1:A:148:PRO:HD2	0.53	1.78	15	6	
1:A:135:CYS:O	1:A:136:GLU:CB	0.53	2.56	23	12	
1:A:126:VAL:O	1:A:126:VAL:CG2	0.53	2.57	3	1	
1:A:112:PRO:CG	1:A:122:LEU:O	0.53	2.56	8	1	
1:A:104:PHE:CE2	1:A:144:VAL:HG22	0.53	2.39	2	3	
1:A:105:ARG:NH2	1:A:107:HIS:NE2	0.53	2.57	1	1	
1:A:114:PHE:CZ	1:A:121:LEU:HG	0.53	2.38	14	9	
1:A:128:GLN:OE1	1:A:128:GLN:CA	0.53	2.56	14	2	
1:A:148:PRO:HD2	1:A:150:LEU:HD11	0.53	1.81	12	1	



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	A h a			Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:107:HIS:HB2	1:A:109:TYR:CZ	0.53	2.39	22	3	
1:A:139:VAL:HG23	1:A:144:VAL:HG22	0.53	1.77	24	1	
1:A:112:PRO:HD2	1:A:123:TYR:CE1	0.52	2.39	3	1	
1:A:123:TYR:O	1:A:125:LEU:N	0.52	2.42	13	6	
1:A:107:HIS:CE1	1:A:129:GLY:N	0.52	2.77	27	1	
1:A:148:PRO:O	1:A:149:SER:CB	0.52	2.58	3	11	
1:A:132:CYS:CB	1:A:135:CYS:SG	0.52	2.97	11	4	
1:A:116:ASP:OD1	1:A:117:HIS:N	0.52	2.43	7	8	
1:A:116:ASP:OD1	1:A:139:VAL:CG1	0.52	2.57	30	10	
1:A:128:GLN:OE1	1:A:128:GLN:N	0.52	2.43	14	2	
1:A:125:LEU:HD13	1:A:140:HIS:CG	0.52	2.39	1	1	
1:A:148:PRO:CG	1:A:150:LEU:HD11	0.52	2.34	12	1	
1:A:104:PHE:CD2	1:A:144:VAL:CG2	0.52	2.93	10	1	
1:A:134:CYS:CB	1:A:151:CYS:SG	0.52	2.98	17	1	
1:A:117:HIS:CE1	1:A:146:SER:HB2	0.52	2.40	22	2	
1:A:102:HIS:CE1	1:A:151:CYS:HA	0.52	2.40	17	6	
1:A:122:LEU:CD1	1:A:128:GLN:O	0.52	2.58	13	1	
1:A:127:HIS:CG	1:A:128:GLN:CD	0.52	2.83	11	2	
1:A:107:HIS:CD2	1:A:109:TYR:CE1	0.52	2.98	2	2	
1:A:116:ASP:OD2	1:A:137:MET:CE	0.52	2.57	4	1	
1:A:102:HIS:CE1	1:A:150:LEU:O	0.52	2.63	18	1	
1:A:148:PRO:O	1:A:150:LEU:N	0.52	2.43	25	2	
1:A:116:ASP:OD2	1:A:139:VAL:HG13	0.51	2.05	19	3	
1:A:126:VAL:HG23	1:A:128:GLN:O	0.51	2.06	14	2	
1:A:102:HIS:HB2	1:A:104:PHE:CZ	0.51	2.40	1	6	
1:A:104:PHE:CE1	1:A:139:VAL:HG21	0.51	2.41	6	8	
1:A:108:SER:OG	1:A:127:HIS:ND1	0.51	2.43	13	1	
1:A:109:TYR:CD2	1:A:128:GLN:HG3	0.51	2.40	16	3	
1:A:107:HIS:NE2	1:A:129:GLY:O	0.51	2.43	10	2	
1:A:112:PRO:HD2	1:A:123:TYR:CZ	0.51	2.41	3	1	
1:A:114:PHE:CE1	1:A:121:LEU:CD1	0.51	2.93	14	3	
1:A:107:HIS:HB3	1:A:109:TYR:CE2	0.51	2.40	2	2	
1:A:114:PHE:CD1	1:A:121:LEU:HG	0.51	2.41	13	3	
1:A:138:ASN:O	1:A:139:VAL:HG13	0.51	2.06	9	2	
1:A:107:HIS:HB2	1:A:109:TYR:CE1	0.51	2.41	24	6	
1:A:148:PRO:HG2	1:A:150:LEU:HD13	0.51	1.82	29	1	
1:A:121:LEU:O	1:A:123:TYR:N	0.51	2.44	6	4	
1:A:122:LEU:CB	1:A:128:GLN:O	0.51	2.58	20	2	
1:A:107:HIS:CD2	1:A:128:GLN:CD	0.51	2.85	24	1	
1:A:127:HIS:ND1	1:A:128:GLN:OE1	0.51	2.43	30	1	
1:A:122:LEU:HB3	1:A:126:VAL:HG22	0.50	1.81	29	2	



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Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:114:PHE:CE2	1:A:121:LEU:HG	0.50	2.42	2	17	
1:A:139:VAL:CG2	1:A:144:VAL:CG2	0.50	2.85	24	1	
1:A:123:TYR:O	1:A:126:VAL:HG22	0.50	2.05	28	1	
1:A:122:LEU:HA	1:A:140:HIS:HE2	0.50	1.65	10	6	
1:A:103:LYS:CE	1:A:134:CYS:SG	0.50	2.99	14	1	
1:A:107:HIS:CB	1:A:128:GLN:NE2	0.50	2.75	20	1	
1:A:112:PRO:HG2	1:A:123:TYR:CE2	0.50	2.41	1	1	
1:A:147:VAL:HG12	1:A:149:SER:H	0.50	1.67	2	2	
1:A:128:GLN:CD	1:A:129:GLY:N	0.50	2.64	8	5	
1:A:122:LEU:CD1	1:A:129:GLY:HA3	0.50	2.36	28	5	
1:A:104:PHE:CZ	1:A:139:VAL:CG2	0.50	2.94	5	1	
1:A:107:HIS:NE2	1:A:128:GLN:NE2	0.50	2.59	24	1	
1:A:121:LEU:HB3	1:A:123:TYR:CD1	0.50	2.42	14	1	
1:A:145:ARG:CD	1:A:145:ARG:O	0.50	2.60	24	1	
1:A:126:VAL:HG11	1:A:141:ARG:HB3	0.49	1.83	14	1	
1:A:126:VAL:HG11	1:A:141:ARG:HG2	0.49	1.83	26	1	
1:A:105:ARG:NH2	1:A:107:HIS:CD2	0.49	2.80	1	1	
1:A:126:VAL:HG21	1:A:129:GLY:HA2	0.49	1.83	1	1	
1:A:107:HIS:CE1	1:A:131:LYS:HB2	0.49	2.43	10	1	
1:A:149:SER:OG	1:A:149:SER:O	0.49	2.30	30	2	
1:A:122:LEU:CD1	1:A:129:GLY:HA2	0.49	2.35	11	2	
1:A:102:HIS:HE2	1:A:150:LEU:HG	0.49	1.67	27	1	
1:A:128:GLN:OE1	1:A:129:GLY:N	0.49	2.46	19	1	
1:A:114:PHE:CE1	1:A:121:LEU:CD2	0.49	2.96	7	2	
1:A:130:MET:SD	1:A:130:MET:N	0.49	2.85	16	4	
1:A:112:PRO:CB	1:A:128:GLN:O	0.49	2.60	9	2	
1:A:117:HIS:CE1	1:A:146:SER:CB	0.49	2.95	22	1	
1:A:102:HIS:HB3	1:A:104:PHE:CE2	0.49	2.43	25	1	
1:A:135:CYS:C	1:A:136:GLU:CG	0.48	2.82	23	2	
1:A:126:VAL:CG1	1:A:141:ARG:HB2	0.48	2.37	30	4	
1:A:103:LYS:NZ	1:A:134:CYS:SG	0.48	2.86	14	1	
1:A:128:GLN:HG2	1:A:129:GLY:N	0.48	2.23	21	1	
1:A:102:HIS:CB	1:A:104:PHE:CZ	0.48	2.96	27	2	
1:A:122:LEU:HA	1:A:140:HIS:CD2	0.48	2.42	24	3	
1:A:126:VAL:CG1	1:A:141:ARG:CB	0.48	2.90	14	2	
1:A:125:LEU:HD12	1:A:140:HIS:CD2	0.48	2.44	1	1	
1:A:107:HIS:NE2	1:A:129:GLY:C	0.48	2.67	27	2	
1:A:147:VAL:HG13	1:A:148:PRO:HD2	0.48	1.86	25	5	
1:A:126:VAL:CG1	1:A:141:ARG:HB3	0.48	2.38	14	1	
1:A:102:HIS:CE1	1:A:151:CYS:HB2	0.48	2.44	2	3	
1:A:107:HIS:CB	1:A:128:GLN:OE1	0.48	2.62	8	1	



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			\mathbf{D}	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:109:TYR:N	1:A:128:GLN:OE1	0.48	2.46	29	1	
1:A:102:HIS:CG	1:A:104:PHE:CZ	0.48	3.02	26	2	
1:A:128:GLN:N	1:A:128:GLN:CD	0.48	2.67	28	1	
1:A:112:PRO:HG2	1:A:123:TYR:CZ	0.48	2.44	1	2	
1:A:126:VAL:CG1	1:A:130:MET:SD	0.48	3.02	8	1	
1:A:127:HIS:CG	1:A:128:GLN:OE1	0.48	2.67	28	1	
1:A:130:MET:CE	1:A:141:ARG:HG3	0.48	2.39	8	1	
1:A:117:HIS:CD2	1:A:117:HIS:C	0.48	2.87	24	3	
1:A:114:PHE:CE1	1:A:121:LEU:HG	0.48	2.44	14	4	
1:A:147:VAL:CG1	1:A:148:PRO:HD2	0.47	2.39	14	18	
1:A:102:HIS:CD2	1:A:147:VAL:HG11	0.47	2.44	26	2	
1:A:111:SER:O	1:A:128:GLN:OE1	0.47	2.32	1	2	
1:A:114:PHE:CD2	1:A:121:LEU:HG	0.47	2.44	8	7	
1:A:126:VAL:O	1:A:127:HIS:O	0.47	2.32	20	3	
1:A:108:SER:HG	1:A:127:HIS:CE1	0.47	2.25	18	1	
1:A:106:LEU:O	1:A:106:LEU:HG	0.47	2.09	5	26	
1:A:122:LEU:O	1:A:123:TYR:O	0.47	2.32	27	12	
1:A:107:HIS:ND1	1:A:131:LYS:HB2	0.47	2.25	10	2	
1:A:105:ARG:CG	1:A:131:LYS:O	0.47	2.63	1	1	
1:A:127:HIS:O	1:A:128:GLN:HB2	0.47	2.10	9	5	
1:A:107:HIS:O	1:A:127:HIS:O	0.47	2.33	5	3	
1:A:128:GLN:NE2	1:A:129:GLY:N	0.47	2.63	16	2	
1:A:114:PHE:CZ	1:A:121:LEU:CG	0.47	2.97	14	4	
1:A:148:PRO:CD	1:A:150:LEU:HD11	0.47	2.39	12	1	
1:A:107:HIS:CE1	1:A:131:LYS:HD2	0.47	2.45	22	1	
1:A:150:LEU:H	1:A:150:LEU:HD23	0.47	1.69	24	1	
1:A:122:LEU:CD2	1:A:140:HIS:CG	0.47	2.97	26	1	
1:A:112:PRO:HA	1:A:128:GLN:NE2	0.47	2.25	1	1	
1:A:112:PRO:HG2	1:A:123:TYR:CD1	0.47	2.44	3	1	
1:A:116:ASP:OD2	1:A:138:ASN:O	0.47	2.33	18	16	
1:A:108:SER:O	1:A:109:TYR:CG	0.47	2.68	10	1	
1:A:107:HIS:NE2	1:A:109:TYR:CE2	0.47	2.82	28	2	
1:A:127:HIS:ND1	1:A:128:GLN:CD	0.47	2.68	30	2	
1:A:107:HIS:NE2	1:A:128:GLN:CD	0.47	2.69	24	1	
1:A:127:HIS:O	1:A:128:GLN:HB3	0.47	2.10	26	4	
1:A:130:MET:CE	1:A:141:ARG:HG2	0.47	2.40	21	2	
1:A:108:SER:HB3	1:A:127:HIS:CE1	0.46	2.45	8	2	
1:A:102:HIS:NE2	1:A:150:LEU:N	0.46	2.61	29	4	
1:A:123:TYR:O	1:A:124:GLY:O	0.46	2.33	5	1	
1:A:107:HIS:CE1	1:A:131:LYS:N	0.46	2.84	10	1	
1:A:142:ARG:CG	1:A:142:ARG:O	0.46	2.63	1	3	



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			D . (8)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:107:HIS:O	1:A:128:GLN:HG3	0.46	2.09	21	2	
1:A:112:PRO:HB3	1:A:122:LEU:O	0.46	2.10	14	1	
1:A:106:LEU:O	1:A:106:LEU:CG	0.46	2.64	1	21	
1:A:109:TYR:CD1	1:A:109:TYR:N	0.46	2.83	30	4	
1:A:121:LEU:HB3	1:A:123:TYR:CE1	0.46	2.46	14	1	
1:A:122:LEU:HD22	1:A:140:HIS:HA	0.46	1.86	8	2	
1:A:127:HIS:O	1:A:128:GLN:C	0.46	2.53	21	1	
1:A:124:GLY:O	1:A:126:VAL:N	0.46	2.48	8	3	
1:A:113:THR:O	1:A:122:LEU:HD12	0.46	2.11	1	1	
1:A:102:HIS:HE2	1:A:147:VAL:CG1	0.46	2.24	6	1	
1:A:102:HIS:CD2	1:A:104:PHE:CZ	0.46	3.04	26	1	
1:A:133:SER:O	1:A:133:SER:OG	0.45	2.34	17	1	
1:A:107:HIS:O	1:A:128:GLN:CD	0.45	2.54	17	4	
1:A:107:HIS:HB2	1:A:128:GLN:OE1	0.45	2.12	8	1	
1:A:130:MET:SD	1:A:141:ARG:CG	0.45	3.05	10	2	
1:A:122:LEU:HB3	1:A:126:VAL:CG2	0.45	2.41	8	8	
1:A:126:VAL:HG12	1:A:141:ARG:CD	0.45	2.42	11	1	
1:A:112:PRO:HB2	1:A:122:LEU:O	0.45	2.11	18	3	
1:A:107:HIS:CB	1:A:109:TYR:CE1	0.45	2.99	8	1	
1:A:122:LEU:HB2	1:A:128:GLN:O	0.45	2.11	20	1	
1:A:142:ARG:O	1:A:142:ARG:HG2	0.45	2.12	28	5	
1:A:111:SER:N	1:A:128:GLN:NE2	0.45	2.64	14	1	
1:A:126:VAL:O	1:A:127:HIS:C	0.45	2.55	28	19	
1:A:111:SER:C	1:A:128:GLN:NE2	0.45	2.70	4	1	
1:A:135:CYS:O	1:A:136:GLU:OE1	0.45	2.34	27	1	
1:A:125:LEU:HD13	1:A:140:HIS:NE2	0.45	2.27	29	1	
1:A:103:LYS:O	1:A:104:PHE:C	0.45	2.56	14	29	
1:A:122:LEU:HA	1:A:140:HIS:NE2	0.45	2.27	21	21	
1:A:150:LEU:N	1:A:150:LEU:CD2	0.45	2.78	2	3	
1:A:128:GLN:NE2	1:A:128:GLN:C	0.45	2.70	8	1	
1:A:114:PHE:HE1	1:A:121:LEU:HD21	0.45	1.71	13	1	
1:A:113:THR:OG1	1:A:128:GLN:NE2	0.45	2.50	19	1	
1:A:127:HIS:O	1:A:128:GLN:O	0.45	2.34	20	1	
1:A:112:PRO:HB3	1:A:128:GLN:O	0.44	2.12	3	1	
1:A:122:LEU:CD2	1:A:140:HIS:HA	0.44	2.42	6	2	
1:A:122:LEU:O	1:A:123:TYR:C	0.44	2.54	18	8	
1:A:128:GLN:NE2	1:A:128:GLN:HA	0.44	2.28	25	2	
1:A:126:VAL:HG12	1:A:130:MET:CE	0.44	2.42	8	1	
1:A:123:TYR:O	1:A:124:GLY:C	0.44	2.56	14	3	
1:A:116:ASP:OD1	1:A:138:ASN:O	0.44	2.35	21	1	
1:A:126:VAL:CG1	1:A:141:ARG:N	0.44	2.80	25	1	



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Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:130:MET:CE	1:A:141:ARG:HD3	0.44	2.42	21	1
1:A:142:ARG:O	1:A:142:ARG:CG	0.44	2.66	27	1
1:A:124:GLY:O	1:A:125:LEU:C	0.44	2.55	8	5
1:A:107:HIS:O	1:A:128:GLN:HB2	0.44	2.13	17	3
1:A:149:SER:O	1:A:149:SER:OG	0.44	2.34	8	2
1:A:121:LEU:HD13	1:A:123:TYR:CE1	0.44	2.47	14	1
1:A:126:VAL:O	1:A:127:HIS:HB3	0.44	2.12	30	1
1:A:102:HIS:ND1	1:A:151:CYS:HB2	0.44	2.27	9	5
1:A:135:CYS:O	1:A:136:GLU:HB2	0.44	2.13	28	21
1:A:112:PRO:HG2	1:A:123:TYR:CG	0.44	2.47	3	1
1:A:135:CYS:SG	1:A:137:MET:HB2	0.44	2.52	18	3
1:A:144:VAL:HA	1:A:147:VAL:CG2	0.44	2.43	7	1
1:A:134:CYS:HB2	1:A:151:CYS:SG	0.44	2.53	17	1
1:A:102:HIS:CE1	1:A:151:CYS:CB	0.44	3.01	29	1
1:A:148:PRO:C	1:A:149:SER:OG	0.43	2.57	17	2
1:A:134:CYS:HB3	1:A:151:CYS:SG	0.43	2.53	17	2
1:A:109:TYR:N	1:A:128:GLN:HG2	0.43	2.28	25	1
1:A:112:PRO:HG2	1:A:123:TYR:CE1	0.43	2.47	29	1
1:A:107:HIS:HB2	1:A:109:TYR:OH	0.43	2.14	22	3
1:A:107:HIS:O	1:A:128:GLN:CB	0.43	2.66	17	1
1:A:109:TYR:CD2	1:A:128:GLN:CG	0.43	3.00	19	1
1:A:107:HIS:ND1	1:A:109:TYR:CE1	0.43	2.87	23	1
1:A:107:HIS:CD2	1:A:128:GLN:HB3	0.43	2.48	28	1
1:A:116:ASP:CG	1:A:138:ASN:O	0.43	2.57	22	8
1:A:120:SER:O	1:A:121:LEU:C	0.43	2.57	1	2
1:A:148:PRO:HG2	1:A:150:LEU:CD1	0.43	2.42	12	4
1:A:126:VAL:CG1	1:A:141:ARG:HG3	0.43	2.43	10	1
1:A:126:VAL:CG1	1:A:141:ARG:HD3	0.43	2.44	17	1
1:A:148:PRO:O	1:A:149:SER:O	0.43	2.36	27	1
1:A:103:LYS:HB3	1:A:133:SER:OG	0.43	2.14	17	3
1:A:116:ASP:OD2	1:A:137:MET:CG	0.43	2.66	15	2
1:A:148:PRO:O	1:A:149:SER:C	0.43	2.56	4	5
1:A:127:HIS:O	1:A:128:GLN:CD	0.43	2.57	7	1
1:A:107:HIS:ND1	1:A:128:GLN:HB3	0.43	2.29	27	1
1:A:106:LEU:HB3	1:A:130:MET:CE	0.43	2.44	7	1
1:A:116:ASP:OD1	1:A:116:ASP:C	0.43	2.57	10	5
1:A:148:PRO:O	1:A:149:SER:HB2	0.43	2.13	19	1
1:A:111:SER:C	1:A:128:GLN:OE1	0.43	2.57	22	1
1:A:148:PRO:O	1:A:149:SER:OG	0.43	2.31	30	1
1:A:115:CYS:HB3	1:A:118:CYS:SG	0.43	2.54	14	25
1:A:107:HIS:HB3	1:A:128:GLN:OE1	0.43	2.13	5	1



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Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:107:HIS:CE1	1:A:129:GLY:C	0.43	2.92	10	1
1:A:110:SER:O	1:A:111:SER:OG	0.43	2.35	19	1
1:A:111:SER:O	1:A:128:GLN:CD	0.43	2.57	24	1
1:A:126:VAL:HG12	1:A:141:ARG:CG	0.43	2.44	10	1
1:A:122:LEU:HD23	1:A:140:HIS:CE1	0.43	2.48	28	1
1:A:107:HIS:O	1:A:128:GLN:HB3	0.42	2.14	1	3
1:A:109:TYR:O	1:A:128:GLN:NE2	0.42	2.51	4	1
1:A:102:HIS:CE1	1:A:137:MET:SD	0.42	3.13	7	1
1:A:124:GLY:O	1:A:125:LEU:HG	0.42	2.14	13	2
1:A:105:ARG:CZ	1:A:107:HIS:CD2	0.42	3.02	1	1
1:A:137:MET:O	1:A:138:ASN:OD1	0.42	2.37	29	2
1:A:105:ARG:O	1:A:105:ARG:CG	0.42	2.68	17	1
1:A:117:HIS:CD2	1:A:117:HIS:O	0.42	2.72	27	2
1:A:105:ARG:NH2	1:A:133:SER:OG	0.42	2.51	28	1
1:A:107:HIS:CD2	1:A:128:GLN:OE1	0.42	2.73	24	1
1:A:107:HIS:CE1	1:A:128:GLN:HB3	0.42	2.49	27	1
1:A:111:SER:HB3	1:A:112:PRO:HD2	0.42	1.91	30	1
1:A:105:ARG:HG3	1:A:131:LYS:O	0.42	2.15	1	1
1:A:112:PRO:HA	1:A:128:GLN:O	0.42	2.14	9	2
1:A:110:SER:C	1:A:111:SER:OG	0.42	2.57	19	1
1:A:109:TYR:N	1:A:128:GLN:HG3	0.42	2.29	10	1
1:A:127:HIS:O	1:A:128:GLN:HG2	0.42	2.14	21	1
1:A:108:SER:HA	1:A:128:GLN:CG	0.42	2.45	29	1
1:A:141:ARG:O	1:A:141:ARG:HG3	0.42	2.14	2	1
1:A:109:TYR:O	1:A:110:SER:C	0.42	2.57	4	1
1:A:122:LEU:C	1:A:123:TYR:CG	0.42	2.93	23	1
1:A:130:MET:N	1:A:130:MET:CE	0.42	2.82	18	1
1:A:113:THR:N	1:A:122:LEU:HD12	0.42	2.30	21	1
1:A:109:TYR:O	1:A:128:GLN:CD	0.42	2.58	23	1
1:A:109:TYR:O	1:A:110:SER:HB2	0.41	2.15	27	3
1:A:127:HIS:CD2	1:A:128:GLN:HG3	0.41	2.49	11	1
1:A:130:MET:SD	1:A:141:ARG:CD	0.41	3.08	19	1
1:A:147:VAL:HG13	1:A:150:LEU:HD21	0.41	1.91	23	1
1:A:107:HIS:C	1:A:128:GLN:HG2	0.41	2.36	8	1
1:A:117:HIS:O	1:A:117:HIS:CD2	0.41	2.73	26	2
1:A:140:HIS:N	1:A:143:CYS:SG	0.41	2.94	24	1
1:A:130:MET:N	1:A:130:MET:SD	0.41	2.91	3	1
1:A:131:LYS:HA	1:A:137:MET:O	0.41	2.15	5	2
1:A:127:HIS:CD2	1:A:128:GLN:OE1	0.41	2.74	6	1
1:A:130:MET:HE2	1:A:141:ARG:HG2	0.41	1.91	21	1
1:A:115:CYS:CB	1:A:118:CYS:SG	0.41	3.08	26	1



Clash(Å)

1:A:110:SER:OG	0.41	2.35	9
1:A:150:LEU:CD1	0.41	2.45	12
1:A:105:ARG:HG3	0.41	2.16	17
1:A:128:GLN:HG3	0.41	2.16	23
1:A:141:ARG:HG3	0.41	1.91	7
1:A:129:GLY:N	0.41	2.81	21
1:A:109:TYR:OH	0.41	2.69	22
1:A:141:ARG:HG3	0.41	1.93	8
1:A:109:TYR:OH	0.41	2.15	9
1:A:128:GLN:NE2	0.41	2.54	13
1:A:150:LEU:HA	0.41	1.75	20
1:A:128:GLN:OE1	0.41	2.68	30
1.A.127.MET.HC2	0.41	9.16	1

Continued from previous page...

Atom-2

Atom-1

1:A:109:TYR:O

1:A:148:PRO:HD2

1:A:105:ARG:O

1:A:111:SER:O

1:A:126:VAL:HG12

1:A:128:GLN:CG

1:A:107:HIS:CB	1:A:109:TYR:OH	0.41	2.69	22	1
1:A:130:MET:HE2	1:A:141:ARG:HG3	0.41	1.93	8	1
1:A:107:HIS:HB3	1:A:109:TYR:OH	0.41	2.15	9	1
1:A:109:TYR:OH	1:A:128:GLN:NE2	0.41	2.54	13	1
1:A:150:LEU:HD12	1:A:150:LEU:HA	0.41	1.75	20	1
1:A:108:SER:CA	1:A:128:GLN:OE1	0.41	2.68	30	1
1:A:116:ASP:OD2	1:A:137:MET:HG2	0.41	2.16	4	1
1:A:109:TYR:N	1:A:109:TYR:CD1	0.41	2.87	28	1
1:A:116:ASP:OD2	1:A:137:MET:HG3	0.40	2.15	28	1
1:A:102:HIS:ND1	1:A:151:CYS:CB	0.40	2.84	29	1
1:A:113:THR:O	1:A:122:LEU:HG	0.40	2.16	10	1
1:A:105:ARG:O	1:A:106:LEU:C	0.40	2.58	21	1
1:A:104:PHE:CD2	1:A:144:VAL:CG1	0.40	3.03	26	1
1:A:112:PRO:CA	1:A:128:GLN:O	0.40	2.69	9	1
1:A:116:ASP:OD2	1:A:138:ASN:N	0.40	2.54	13	1
1:A:122:LEU:O	1:A:123:TYR:CD1	0.40	2.74	23	1
1:A:106:LEU:HB3	1:A:130:MET:HE3	0.40	1.92	24	1
1:A:147:VAL:CG1	1:A:150:LEU:CD2	0.40	2.97	27	1

6.3 Torsion angles (i)

6.3.1Protein 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	Percentile	es
1	А	50/82~(61%)	$36\pm2~(72\pm3\%)$	$11\pm2(22\pm4\%)$	$3\pm2~(6\pm3\%)$	3 21	
All	All	1500/2460~(61%)	1082 (72%)	331 (22%)	87~(6%)	3 21	

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Models

Worst

Total

1

1

1

1

1

1

Distance(Å)



Mol	Chain	Res	Type	Models (Total)
1	А	123	TYR	19
1	А	127	HIS	13
1	А	110	SER	12
1	А	128	GLN	12
1	А	122	LEU	8
1	А	124	GLY	8
1	А	149	SER	6
1	А	102	HIS	4
1	А	109	TYR	2
1	А	148	PRO	2
1	А	125	LEU	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	Perce	entiles
1	А	47/75~(63%)	$36\pm2(78\pm4\%)$	$10\pm2~(22\pm4\%)$	3	29
All	All	1410/2250~(63%)	1095 (78%)	315 (22%)	3	29

All 28 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	113	THR	30
1	А	150	LEU	20
1	А	137	MET	19
1	А	141	ARG	19
1	А	130	MET	18
1	А	107	HIS	17
1	А	149	SER	17
1	А	133	SER	16
1	А	108	SER	16
1	А	105	ARG	15
1	А	145	ARG	14
1	А	131	LYS	14
1	А	103	LYS	13
1	А	142	ARG	13
1	А	134	CYS	13



Mol	Chain	Res	Type	Models (Total)
1	А	111	SER	11
1	А	128	GLN	10
1	А	127	HIS	8
1	А	110	SER	6
1	А	126	VAL	6
1	А	109	TYR	5
1	А	139	VAL	4
1	А	136	GLU	3
1	А	116	ASP	3
1	А	146	SER	2
1	А	106	LEU	1
1	А	104	PHE	1
1	А	120	SER	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

