



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:39 pm GMT

PDB ID : 1BT7  
Title : THE SOLUTION NMR STRUCTURE OF THE N-TERMINAL PROTEASE DOMAIN OF THE HEPATITIS C VIRUS (HCV) NS3-PROTEIN, FROM BK STRAIN, 20 STRUCTURES  
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Deposited on : 1998-09-01

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

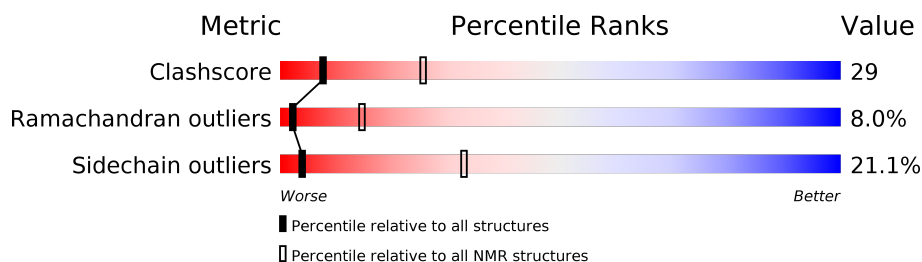
# 1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	186	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:29-A:182 (154)	0.60	6

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 4 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2450 atoms, of which 1230 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NS3 SERINE PROTEASE.

Mol	Chain	Residues	Atoms						Trace
1	A	165	Total	C	H	N	O	S	0
			2449	756	1230	224	230	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	TYR	PHE	CONFLICT	UNP P26663

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

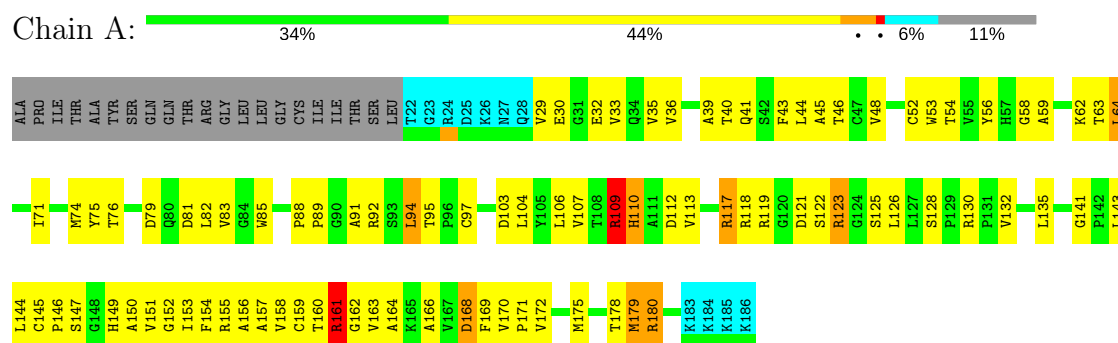
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

## 4 Residue-property plots

### 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: NS3 SERINE PROTEASE

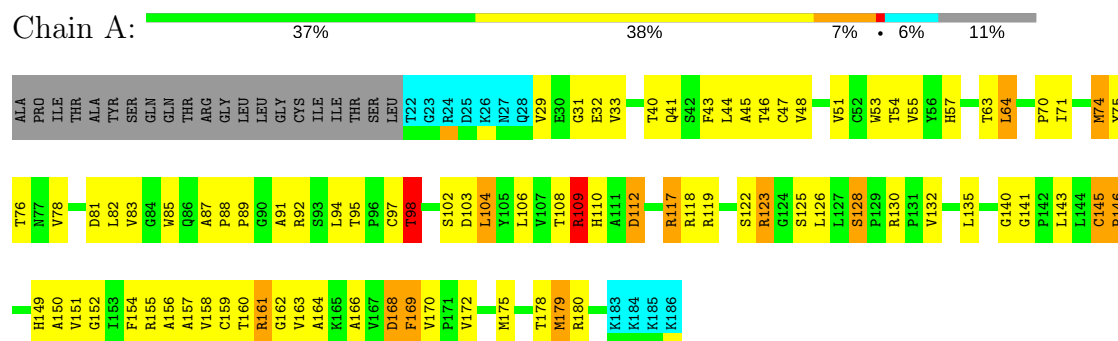


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

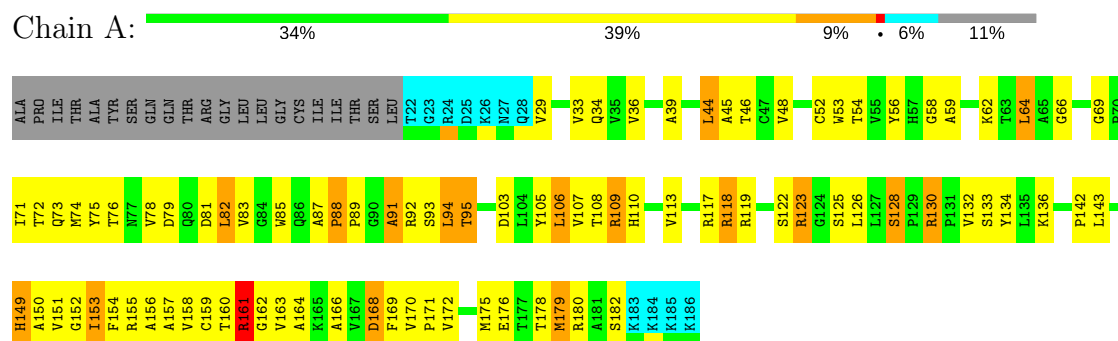
#### 4.2.1 Score per residue for model 1

#### • Molecule 1: NS3 SERINE PROTEASE



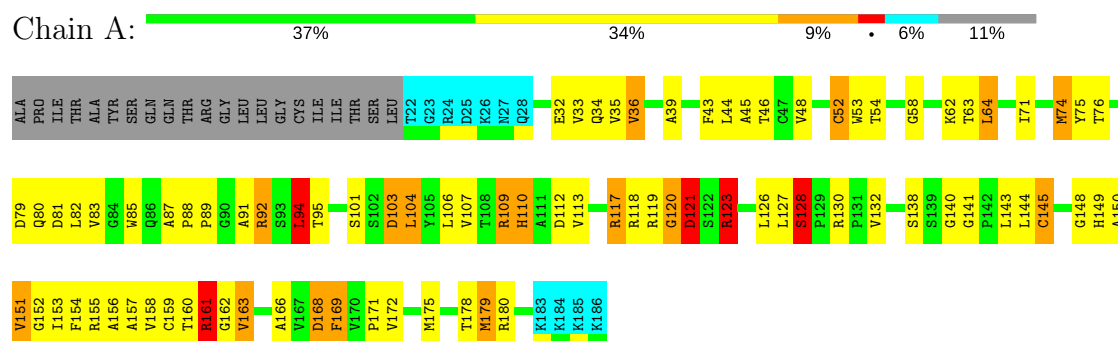
## 4.2.2 Score per residue for model 2

### • Molecule 1: NS3 SERINE PROTEASE



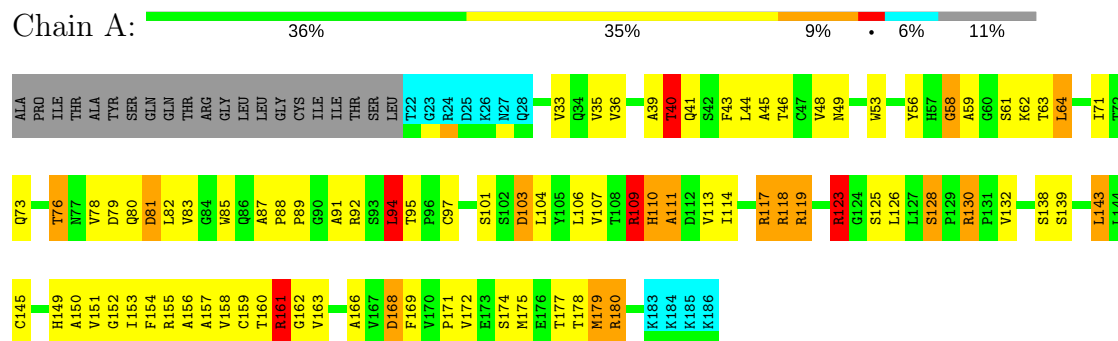
## 4.2.3 Score per residue for model 3

### • Molecule 1: NS3 SERINE PROTEASE



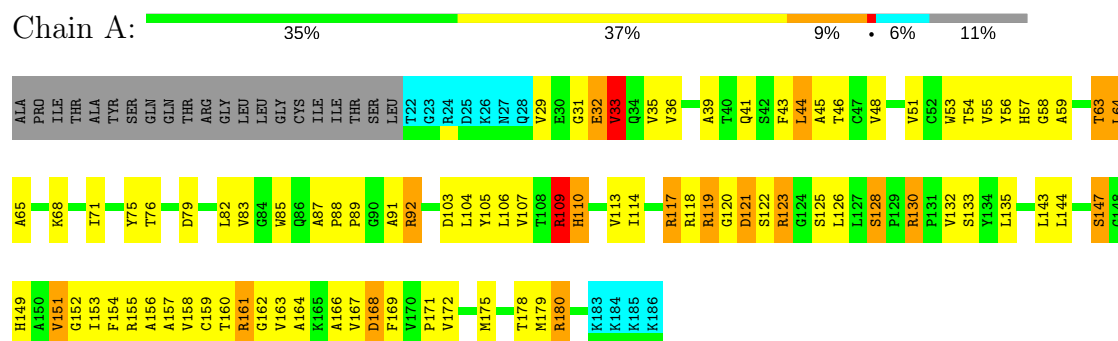
## 4.2.4 Score per residue for model 4

### • Molecule 1: NS3 SERINE PROTEASE



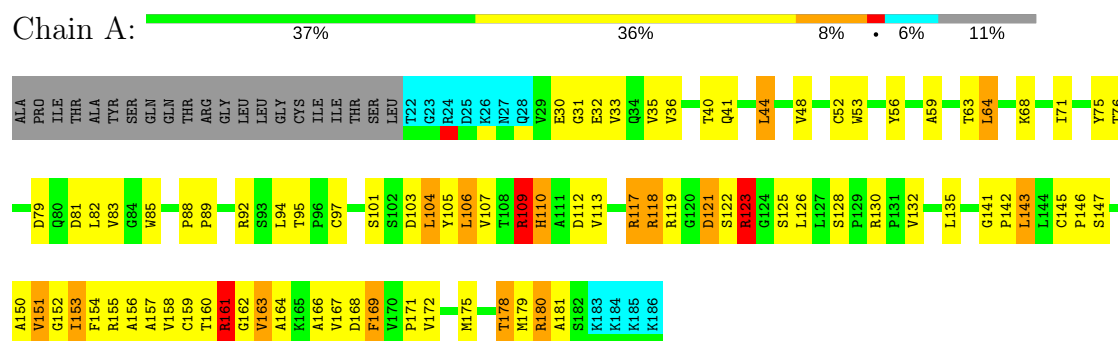
### 4.2.5 Score per residue for model 5

#### • Molecule 1: NS3 SERINE PROTEASE



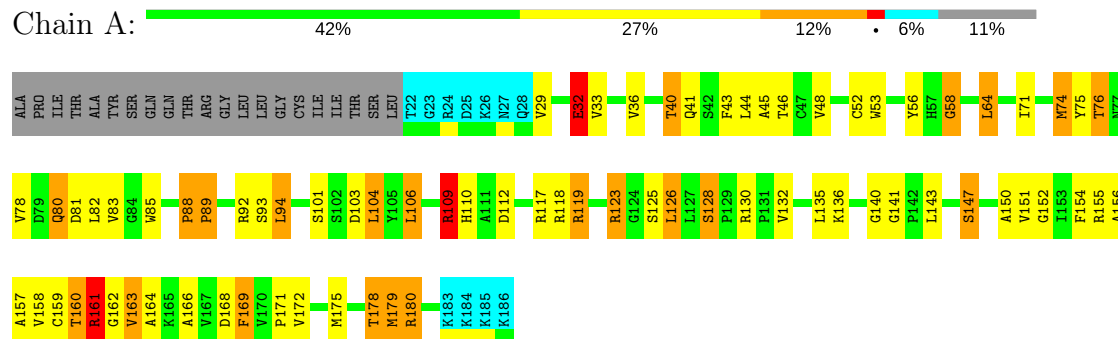
### 4.2.6 Score per residue for model 6 (medoid)

#### • Molecule 1: NS3 SERINE PROTEASE



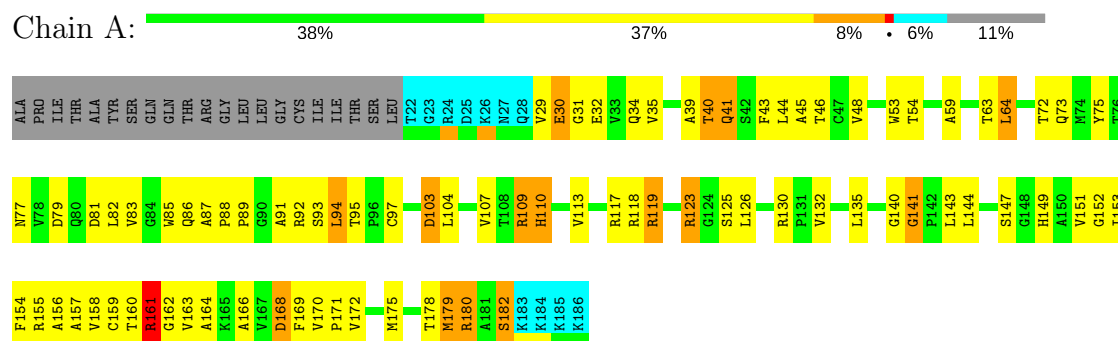
### 4.2.7 Score per residue for model 7

#### • Molecule 1: NS3 SERINE PROTEASE



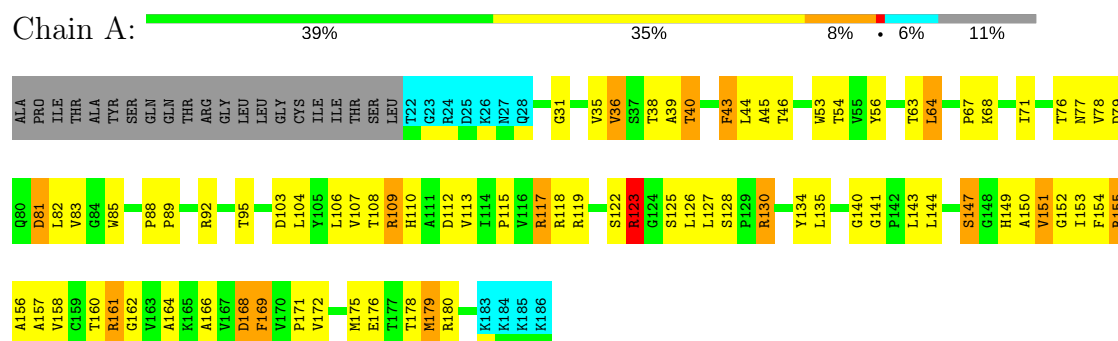
## 4.2.8 Score per residue for model 8

### • Molecule 1: NS3 SERINE PROTEASE



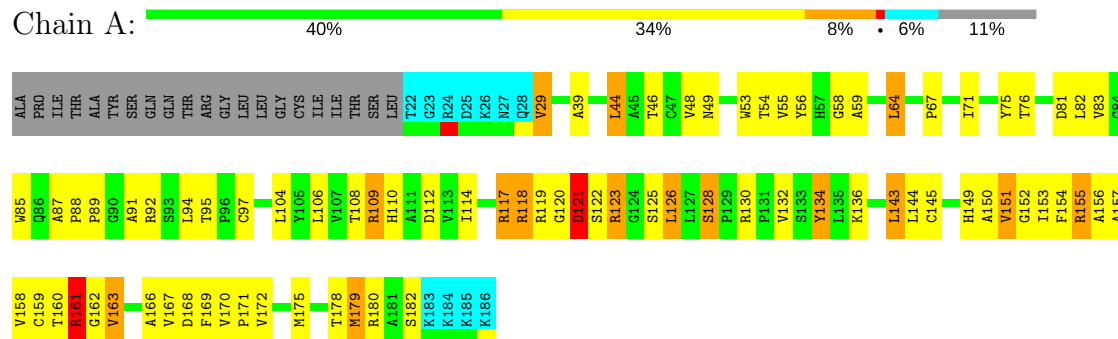
## 4.2.9 Score per residue for model 9

### • Molecule 1: NS3 SERINE PROTEASE



## 4.2.10 Score per residue for model 10

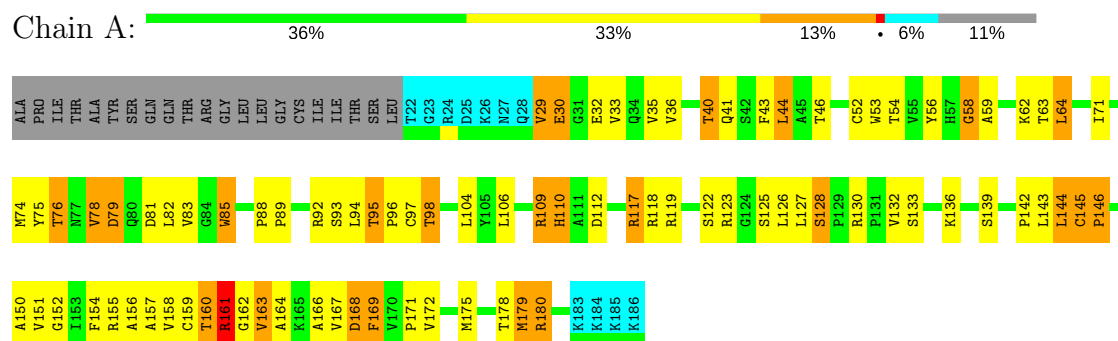
### • Molecule 1: NS3 SERINE PROTEASE





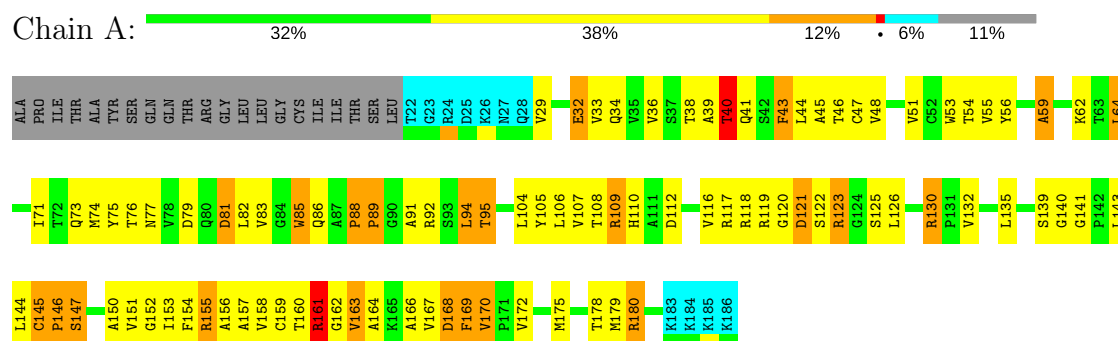
### 4.2.11 Score per residue for model 11

#### • Molecule 1: NS3 SERINE PROTEASE



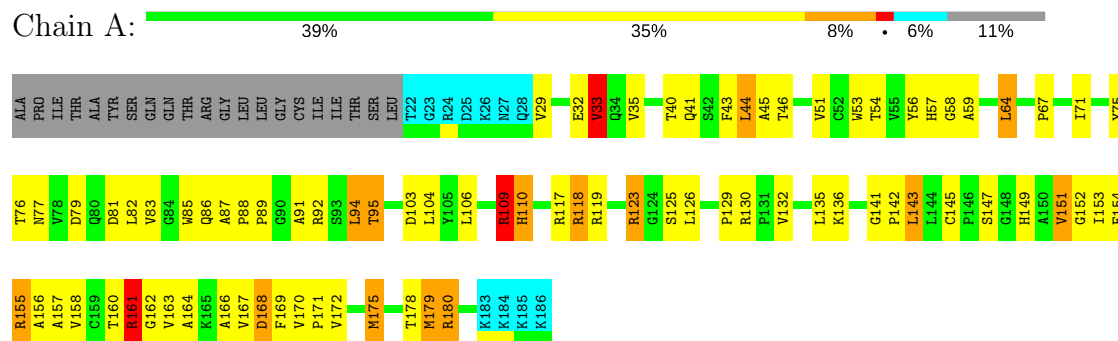
### 4.2.12 Score per residue for model 12

#### • Molecule 1: NS3 SERINE PROTEASE



### 4.2.13 Score per residue for model 13

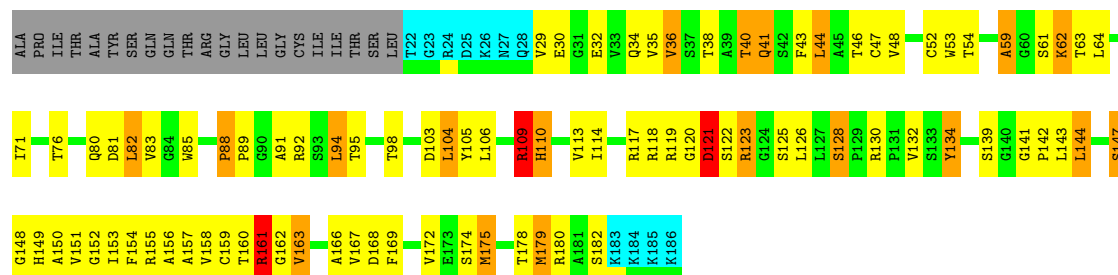
#### • Molecule 1: NS3 SERINE PROTEASE



### 4.2.14 Score per residue for model 14

#### • Molecule 1: NS3 SERINE PROTEASE

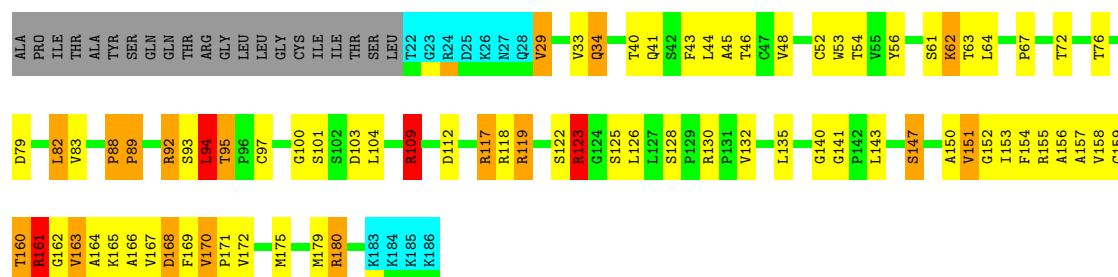
Chain A: 34% 37% 10% 6% 11%



### 4.2.15 Score per residue for model 15

#### • Molecule 1: NS3 SERINE PROTEASE

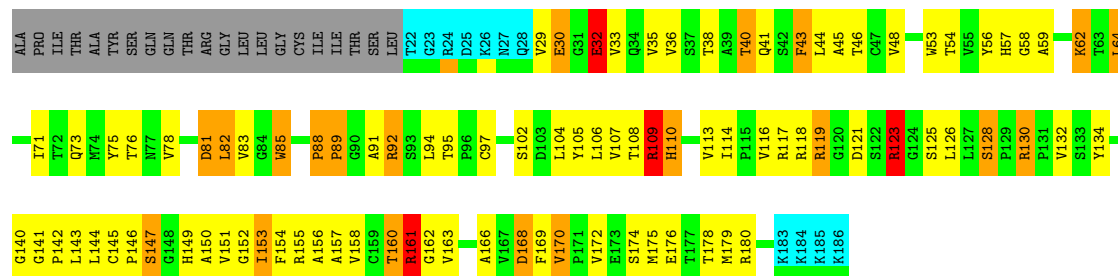
Chain A: 41% 31% 9% 6% 11%



### 4.2.16 Score per residue for model 16

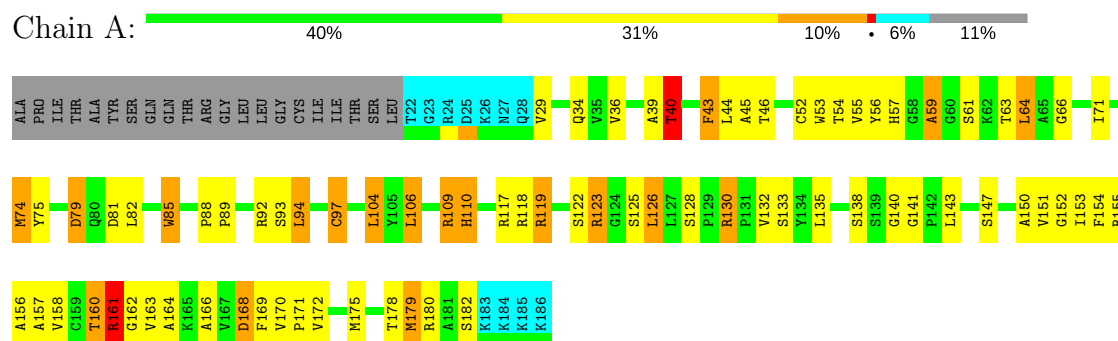
#### • Molecule 1: NS3 SERINE PROTEASE

Chain A: 33% 37% 11% 6% 11%



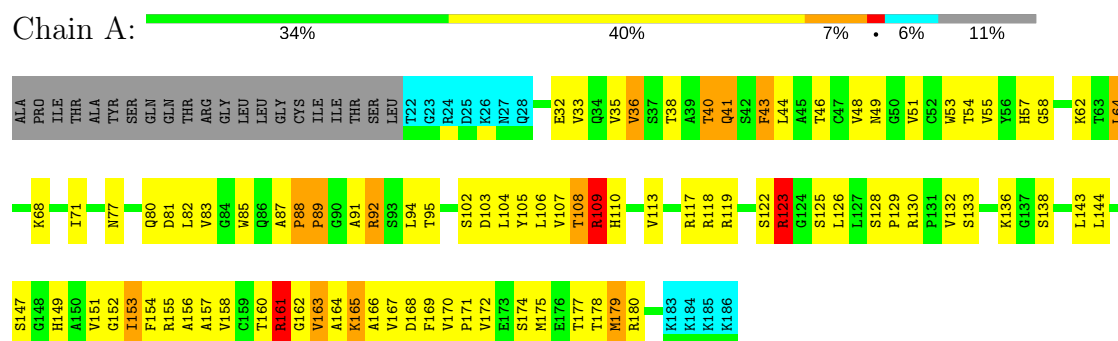
## 4.2.17 Score per residue for model 17

## • Molecule 1: NS3 SERINE PROTEASE



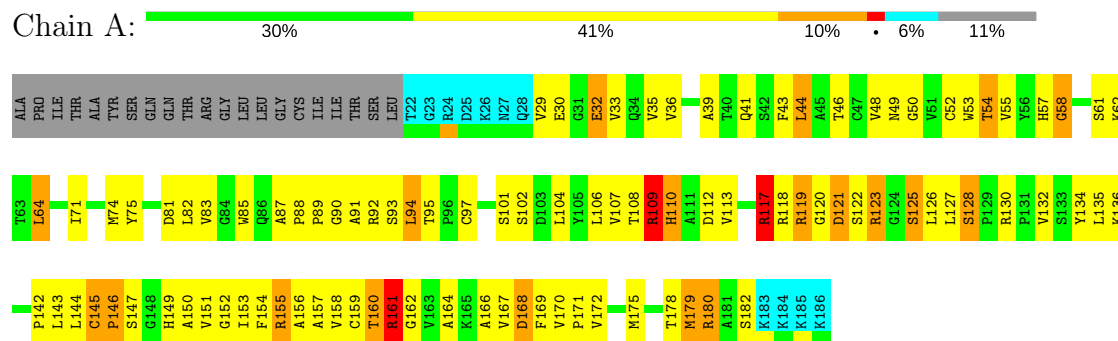
## 4.2.18 Score per residue for model 18

## • Molecule 1: NS3 SERINE PROTEASE



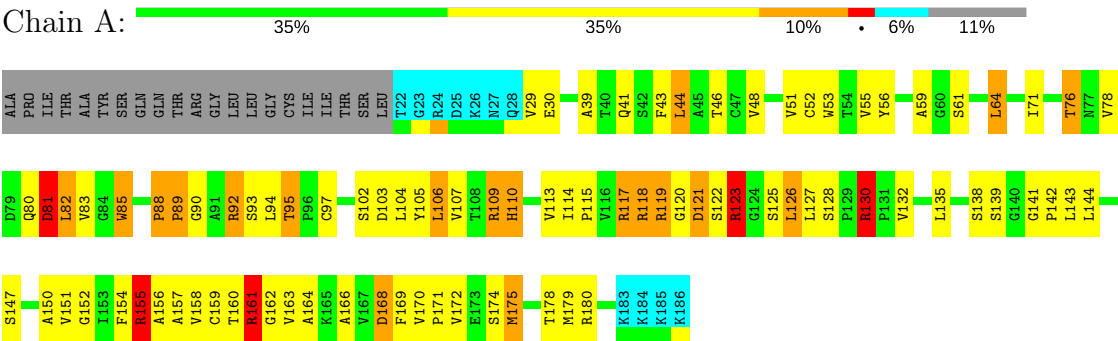
## 4.2.19 Score per residue for model 19

## • Molecule 1: NS3 SERINE PROTEASE



4.2.20 Score per residue for model 20

● Molecule 1: NS3 SERINE PROTEASE



## 5 Refinement protocol and experimental data overview

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

Of the 60 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATIONS/MINIMUM ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
NMRPIPE	structure solution	
NMRVIEW	structure solution	

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](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.04±0.00	0±0/1151 (0.0±0.0%)	1.21±0.01	0±0/1571 (0.0±0.0%)
All	All	1.04	0/23020 (0.0%)	1.21	2/31420 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	10.0±0.0
All	All	0	200

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	125	SER	N-CA-CB	-5.25	102.62	110.50	20	2

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	109	ARG	Sidechain	20
1	A	92	ARG	Sidechain	20
1	A	119	ARG	Sidechain	20
1	A	117	ARG	Sidechain	20
1	A	155	ARG	Sidechain	20
1	A	123	ARG	Sidechain	20

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	130	ARG	Sidechain	20
1	A	161	ARG	Sidechain	20
1	A	180	ARG	Sidechain	20
1	A	118	ARG	Sidechain	20

## 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	1126	1124	1124	64±8
All	All	22540	22480	22477	1286

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:VAL:HG22	1:A:113:VAL:HG22	1.02	1.20	5	2
1:A:46:THR:HG21	1:A:153:ILE:HG21	0.96	1.34	13	3
1:A:53:TRP:CE3	1:A:82:LEU:HD23	0.89	2.03	7	15
1:A:82:LEU:HD11	1:A:153:ILE:HD11	0.89	1.43	16	10
1:A:46:THR:HG21	1:A:153:ILE:CG2	0.84	2.03	13	5
1:A:175:MET:O	1:A:178:THR:HG22	0.83	1.72	9	8
1:A:54:THR:O	1:A:83:VAL:HG22	0.82	1.74	18	5
1:A:54:THR:HG21	1:A:85:TRP:CH2	0.82	2.09	8	9
1:A:44:LEU:HD23	1:A:45:ALA:N	0.80	1.91	17	9
1:A:82:LEU:CD1	1:A:153:ILE:HD11	0.80	2.06	16	7
1:A:64:LEU:CD2	1:A:71:ILE:HD12	0.80	2.07	14	16
1:A:132:VAL:HG12	1:A:162:GLY:O	0.79	1.76	17	17
1:A:107:VAL:HG22	1:A:113:VAL:HG12	0.79	1.52	16	4
1:A:108:THR:HG22	1:A:112:ASP:O	0.78	1.78	9	1
1:A:154:PHE:CZ	1:A:157:ALA:HB2	0.77	2.15	7	20
1:A:35:VAL:HG23	1:A:43:PHE:O	0.77	1.79	19	4
1:A:48:VAL:HG11	1:A:172:VAL:CG1	0.77	2.08	7	7
1:A:94:LEU:HD21	1:A:144:LEU:HD21	0.77	1.54	11	1
1:A:152:GLY:HA2	1:A:172:VAL:HG13	0.76	1.55	15	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:VAL:HG11	1:A:57:HIS:CE1	0.76	2.14	1	3
1:A:76:THR:HG23	1:A:83:VAL:CG1	0.76	2.11	1	10
1:A:54:THR:HG21	1:A:85:TRP:CZ2	0.75	2.16	2	5
1:A:126:LEU:O	1:A:126:LEU:HD12	0.75	1.82	15	2
1:A:82:LEU:HD13	1:A:170:VAL:HG11	0.74	1.59	10	5
1:A:44:LEU:HD12	1:A:109:ARG:N	0.74	1.97	9	7
1:A:64:LEU:HD22	1:A:71:ILE:HD12	0.74	1.57	13	12
1:A:44:LEU:HD21	1:A:109:ARG:CB	0.73	2.13	6	7
1:A:82:LEU:HD22	1:A:175:MET:HB3	0.73	1.57	2	5
1:A:33:VAL:HG11	1:A:46:THR:N	0.73	1.98	5	2
1:A:158:VAL:HB	1:A:166:ALA:HB3	0.73	1.60	8	20
1:A:143:LEU:HD22	1:A:169:PHE:CG	0.73	2.18	15	10
1:A:106:LEU:HD11	1:A:114:ILE:HD12	0.72	1.59	14	1
1:A:76:THR:HG23	1:A:83:VAL:HG13	0.72	1.61	1	3
1:A:33:VAL:HG11	1:A:45:ALA:C	0.72	2.03	13	2
1:A:152:GLY:CA	1:A:172:VAL:HG23	0.72	2.13	5	9
1:A:152:GLY:CA	1:A:172:VAL:HG13	0.71	2.15	12	11
1:A:43:PHE:CB	1:A:59:ALA:HB2	0.71	2.16	11	2
1:A:44:LEU:HD22	1:A:109:ARG:CB	0.71	2.16	18	2
1:A:36:VAL:HG21	1:A:43:PHE:CE2	0.70	2.21	12	2
1:A:35:VAL:HG12	1:A:44:LEU:HD22	0.70	1.63	13	3
1:A:152:GLY:HA2	1:A:172:VAL:HG23	0.70	1.62	5	8
1:A:54:THR:HG23	1:A:83:VAL:HG23	0.68	1.65	11	3
1:A:95:THR:O	1:A:150:ALA:HB3	0.68	1.89	3	5
1:A:82:LEU:HD22	1:A:175:MET:HG2	0.68	1.65	3	1
1:A:107:VAL:HG22	1:A:113:VAL:CG1	0.68	2.18	4	4
1:A:43:PHE:HB2	1:A:59:ALA:HB2	0.67	1.65	11	1
1:A:105:TYR:O	1:A:107:VAL:HG23	0.67	1.88	18	7
1:A:54:THR:OG1	1:A:59:ALA:HB3	0.67	1.88	11	2
1:A:143:LEU:HD22	1:A:169:PHE:CD1	0.67	2.23	8	7
1:A:48:VAL:HG11	1:A:172:VAL:HG11	0.66	1.64	6	6
1:A:44:LEU:HD22	1:A:141:GLY:N	0.66	2.05	9	10
1:A:108:THR:HG21	1:A:134:TYR:OH	0.66	1.91	19	3
1:A:174:SER:O	1:A:177:THR:HG22	0.66	1.91	18	2
1:A:104:LEU:HD13	1:A:143:LEU:HD23	0.66	1.66	18	19
1:A:33:VAL:HG22	1:A:46:THR:OG1	0.66	1.91	3	1
1:A:76:THR:HG23	1:A:83:VAL:HG12	0.65	1.68	16	1
1:A:65:ALA:O	1:A:71:ILE:HD11	0.65	1.92	5	1
1:A:36:VAL:HG11	1:A:85:TRP:CH2	0.65	2.27	12	6
1:A:44:LEU:HD22	1:A:109:ARG:HB2	0.65	1.67	18	2
1:A:44:LEU:HD22	1:A:140:GLY:C	0.64	2.13	17	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:CYS:O	1:A:98:THR:HG23	0.64	1.91	1	1
1:A:36:VAL:HG13	1:A:43:PHE:CZ	0.64	2.26	3	2
1:A:59:ALA:O	1:A:64:LEU:HD12	0.64	1.91	10	1
1:A:150:ALA:HB1	1:A:172:VAL:HG21	0.64	1.69	7	2
1:A:82:LEU:CD1	1:A:170:VAL:HG21	0.64	2.22	20	1
1:A:29:VAL:HG11	1:A:89:PRO:O	0.63	1.93	8	2
1:A:151:VAL:HG12	1:A:169:PHE:CE2	0.63	2.28	4	9
1:A:39:ALA:O	1:A:40:THR:HG23	0.63	1.94	17	3
1:A:44:LEU:C	1:A:44:LEU:HD23	0.63	2.14	8	6
1:A:132:VAL:HG21	1:A:159:CYS:SG	0.63	2.33	20	14
1:A:36:VAL:HG13	1:A:43:PHE:CE2	0.62	2.29	18	4
1:A:64:LEU:HD12	1:A:71:ILE:HD12	0.62	1.71	17	1
1:A:44:LEU:HD23	1:A:44:LEU:C	0.62	2.15	7	3
1:A:52:CYS:SG	1:A:87:ALA:HB2	0.62	2.35	19	1
1:A:126:LEU:HD21	1:A:164:ALA:C	0.62	2.15	18	4
1:A:54:THR:HG23	1:A:83:VAL:CG2	0.61	2.25	8	4
1:A:153:ILE:HG23	1:A:175:MET:HE1	0.61	1.73	3	7
1:A:55:VAL:HG21	1:A:57:HIS:CE1	0.61	2.30	18	1
1:A:53:TRP:CZ3	1:A:178:THR:HG21	0.60	2.31	18	9
1:A:29:VAL:HG12	1:A:89:PRO:O	0.60	1.96	11	3
1:A:154:PHE:HZ	1:A:157:ALA:HB2	0.60	1.54	19	20
1:A:36:VAL:HG21	1:A:64:LEU:CD2	0.60	2.26	16	1
1:A:107:VAL:HG13	1:A:113:VAL:HG12	0.60	1.72	19	5
1:A:29:VAL:HG21	1:A:89:PRO:O	0.60	1.96	8	1
1:A:94:LEU:O	1:A:95:THR:HG23	0.60	1.96	15	6
1:A:156:ALA:HB3	1:A:168:ASP:HB3	0.60	1.74	13	20
1:A:87:ALA:O	1:A:91:ALA:HB3	0.60	1.96	3	3
1:A:44:LEU:HD21	1:A:109:ARG:HB3	0.60	1.72	6	6
1:A:43:PHE:CG	1:A:59:ALA:HB2	0.60	2.32	20	2
1:A:47:CYS:SG	1:A:91:ALA:HB1	0.60	2.37	12	2
1:A:36:VAL:HG11	1:A:64:LEU:HD21	0.59	1.72	16	2
1:A:64:LEU:HD12	1:A:71:ILE:HB	0.59	1.74	17	1
1:A:88:PRO:N	1:A:89:PRO:CD	0.59	2.65	15	17
1:A:44:LEU:HD12	1:A:109:ARG:HG3	0.59	1.72	3	1
1:A:82:LEU:CD1	1:A:170:VAL:HG11	0.59	2.28	10	3
1:A:126:LEU:HD12	1:A:126:LEU:O	0.59	1.97	2	2
1:A:82:LEU:HD22	1:A:175:MET:CB	0.59	2.28	9	5
1:A:63:THR:O	1:A:63:THR:HG23	0.58	1.98	11	1
1:A:36:VAL:HG12	1:A:64:LEU:HD21	0.58	1.75	19	2
1:A:33:VAL:HG22	1:A:142:PRO:CD	0.58	2.29	11	3
1:A:44:LEU:HD12	1:A:141:GLY:HA2	0.58	1.76	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:LEU:HD22	1:A:71:ILE:HB	0.58	1.76	11	3
1:A:104:LEU:CD2	1:A:151:VAL:HG21	0.58	2.29	1	2
1:A:54:THR:HG21	1:A:85:TRP:CZ3	0.57	2.34	14	1
1:A:53:TRP:CZ3	1:A:82:LEU:HD23	0.57	2.34	16	3
1:A:76:THR:CG2	1:A:83:VAL:HG13	0.57	2.30	1	1
1:A:36:VAL:HG22	1:A:43:PHE:CZ	0.57	2.35	14	1
1:A:106:LEU:HD23	1:A:114:ILE:HD11	0.57	1.76	4	4
1:A:44:LEU:HD21	1:A:109:ARG:HB2	0.57	1.75	13	8
1:A:64:LEU:HD11	1:A:85:TRP:CZ2	0.57	2.34	2	3
1:A:55:VAL:HG12	1:A:81:ASP:O	0.57	2.00	18	2
1:A:94:LEU:CD2	1:A:144:LEU:HD21	0.57	2.30	11	1
1:A:35:VAL:HG13	1:A:109:ARG:HG2	0.57	1.74	13	2
1:A:44:LEU:HD13	1:A:138:SER:HA	0.56	1.76	20	1
1:A:29:VAL:HG21	1:A:91:ALA:HA	0.56	1.77	16	1
1:A:63:THR:HG23	1:A:63:THR:O	0.56	1.99	5	1
1:A:76:THR:HG23	1:A:83:VAL:CG2	0.56	2.30	5	6
1:A:82:LEU:HD11	1:A:153:ILE:CD1	0.56	2.26	16	1
1:A:64:LEU:HD23	1:A:71:ILE:HD12	0.56	1.76	19	4
1:A:35:VAL:HG13	1:A:109:ARG:HD2	0.56	1.77	5	1
1:A:81:ASP:O	1:A:82:LEU:HD12	0.55	2.02	14	7
1:A:34:GLN:O	1:A:45:ALA:HB3	0.55	2.01	8	3
1:A:32:GLU:HG3	1:A:33:VAL:HG23	0.55	1.77	12	1
1:A:97:CYS:CB	1:A:151:VAL:HG23	0.55	2.31	15	1
1:A:143:LEU:HD22	1:A:169:PHE:CD2	0.55	2.36	7	7
1:A:71:ILE:HG22	1:A:71:ILE:O	0.55	2.02	2	1
1:A:150:ALA:HB1	1:A:172:VAL:HG11	0.55	1.78	1	1
1:A:36:VAL:HG21	1:A:43:PHE:CD2	0.54	2.37	9	1
1:A:76:THR:HG22	1:A:83:VAL:HG12	0.54	1.79	4	4
1:A:126:LEU:HD11	1:A:165:LYS:HA	0.54	1.78	18	2
1:A:151:VAL:O	1:A:171:PRO:HA	0.54	2.02	18	16
1:A:82:LEU:HD11	1:A:170:VAL:HG11	0.54	1.79	20	3
1:A:135:LEU:HD11	1:A:164:ALA:CB	0.54	2.31	8	12
1:A:117:ARG:HG3	1:A:127:LEU:HD21	0.54	1.80	19	1
1:A:33:VAL:HG12	1:A:109:ARG:CG	0.54	2.32	18	2
1:A:76:THR:CG2	1:A:83:VAL:HG12	0.54	2.33	7	4
1:A:154:PHE:CE1	1:A:157:ALA:HB2	0.54	2.37	7	9
1:A:55:VAL:HG11	1:A:57:HIS:ND1	0.54	2.17	5	1
1:A:40:THR:HG22	1:A:41:GLN:HG2	0.54	1.79	18	3
1:A:56:TYR:HB3	1:A:78:VAL:HG11	0.54	1.80	20	4
1:A:53:TRP:HZ3	1:A:178:THR:HG21	0.54	1.63	18	6
1:A:107:VAL:HG22	1:A:113:VAL:CG2	0.54	2.13	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:TYR:HB3	1:A:113:VAL:HG13	0.54	1.79	6	2
1:A:105:TYR:HB2	1:A:113:VAL:HG13	0.54	1.79	14	1
1:A:132:VAL:HG12	1:A:162:GLY:C	0.53	2.24	15	9
1:A:56:TYR:CD1	1:A:76:THR:CG2	0.53	2.92	2	6
1:A:87:ALA:HB1	1:A:91:ALA:CB	0.53	2.33	19	6
1:A:145:CYS:CB	1:A:146:PRO:HD3	0.53	2.34	1	1
1:A:40:THR:HG22	1:A:41:GLN:CG	0.53	2.33	18	2
1:A:64:LEU:HD13	1:A:85:TRP:CZ2	0.53	2.39	10	1
1:A:51:VAL:HG13	1:A:85:TRP:O	0.53	2.03	1	4
1:A:38:THR:HG23	1:A:40:THR:OG1	0.53	2.04	12	1
1:A:46:THR:HG23	1:A:48:VAL:HG23	0.53	1.81	1	10
1:A:153:ILE:CG1	1:A:175:MET:HE2	0.53	2.34	19	2
1:A:36:VAL:CG1	1:A:64:LEU:HD21	0.53	2.34	5	4
1:A:152:GLY:N	1:A:172:VAL:HG23	0.53	2.18	18	3
1:A:178:THR:O	1:A:181:ALA:HB3	0.53	2.04	6	1
1:A:106:LEU:HD11	1:A:154:PHE:HB2	0.52	1.80	3	3
1:A:56:TYR:HB3	1:A:78:VAL:HG12	0.52	1.80	16	1
1:A:110:HIS:O	1:A:111:ALA:HB2	0.52	2.04	4	1
1:A:123:ARG:N	1:A:169:PHE:CE2	0.52	2.78	2	9
1:A:64:LEU:HD11	1:A:85:TRP:CH2	0.52	2.40	16	3
1:A:36:VAL:HG11	1:A:85:TRP:CZ3	0.52	2.40	4	2
1:A:64:LEU:CD1	1:A:71:ILE:HD12	0.52	2.34	17	1
1:A:142:PRO:O	1:A:144:LEU:HD12	0.52	2.05	14	5
1:A:35:VAL:HG12	1:A:44:LEU:HA	0.52	1.82	16	1
1:A:56:TYR:HB2	1:A:83:VAL:HG11	0.52	1.80	20	6
1:A:107:VAL:HA	1:A:113:VAL:HG12	0.52	1.82	19	1
1:A:33:VAL:HG23	1:A:45:ALA:O	0.52	2.05	4	2
1:A:83:VAL:O	1:A:83:VAL:HG23	0.52	2.05	8	1
1:A:106:LEU:HD13	1:A:143:LEU:HD12	0.52	1.81	4	1
1:A:106:LEU:HD13	1:A:143:LEU:CD1	0.52	2.35	19	4
1:A:160:THR:HG22	1:A:163:VAL:HG12	0.52	1.82	6	1
1:A:153:ILE:HG13	1:A:170:VAL:HG13	0.51	1.81	2	1
1:A:114:ILE:HD12	1:A:126:LEU:HD21	0.51	1.81	20	2
1:A:43:PHE:CD1	1:A:43:PHE:N	0.51	2.77	9	10
1:A:48:VAL:HG11	1:A:172:VAL:HG13	0.51	1.83	5	3
1:A:97:CYS:HB3	1:A:151:VAL:HG23	0.51	1.82	15	1
1:A:82:LEU:HD13	1:A:170:VAL:HG21	0.51	1.81	16	3
1:A:35:VAL:HG11	1:A:109:ARG:HB3	0.51	1.82	3	1
1:A:32:GLU:OE2	1:A:94:LEU:HD21	0.51	2.06	16	1
1:A:64:LEU:HD22	1:A:71:ILE:CD1	0.51	2.35	12	1
1:A:43:PHE:CE1	1:A:58:GLY:CA	0.51	2.94	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HD22	1:A:175:MET:SD	0.51	2.46	20	1
1:A:156:ALA:HB3	1:A:168:ASP:CB	0.51	2.35	1	7
1:A:46:THR:O	1:A:46:THR:HG23	0.51	2.06	11	5
1:A:150:ALA:CB	1:A:172:VAL:HG21	0.50	2.35	10	2
1:A:87:ALA:HB1	1:A:91:ALA:HB3	0.50	1.83	18	1
1:A:44:LEU:HD12	1:A:109:ARG:HB3	0.50	1.83	9	1
1:A:106:LEU:HD12	1:A:106:LEU:O	0.50	2.05	14	1
1:A:36:VAL:HG22	1:A:43:PHE:CE1	0.50	2.42	14	1
1:A:123:ARG:N	1:A:169:PHE:CE1	0.50	2.80	4	9
1:A:46:THR:HG22	1:A:53:TRP:O	0.50	2.07	13	2
1:A:150:ALA:HB3	1:A:172:VAL:HG21	0.50	1.84	10	1
1:A:106:LEU:HD23	1:A:114:ILE:HB	0.50	1.82	16	1
1:A:172:VAL:HG12	1:A:175:MET:HE3	0.50	1.83	12	1
1:A:53:TRP:CZ2	1:A:179:MET:HE1	0.50	2.41	12	2
1:A:82:LEU:CD2	1:A:175:MET:CB	0.50	2.90	16	1
1:A:55:VAL:HG11	1:A:155:ARG:HA	0.49	1.84	20	2
1:A:123:ARG:N	1:A:169:PHE:CD2	0.49	2.81	3	4
1:A:51:VAL:HG11	1:A:53:TRP:CZ2	0.49	2.42	20	1
1:A:110:HIS:N	1:A:110:HIS:CD2	0.49	2.80	8	10
1:A:160:THR:O	1:A:162:GLY:N	0.49	2.46	8	20
1:A:88:PRO:N	1:A:89:PRO:HD2	0.49	2.23	19	8
1:A:44:LEU:HD12	1:A:138:SER:O	0.49	2.07	4	1
1:A:33:VAL:CG2	1:A:46:THR:HA	0.49	2.38	13	2
1:A:43:PHE:N	1:A:43:PHE:CD1	0.49	2.80	12	3
1:A:33:VAL:HG21	1:A:46:THR:HA	0.49	1.83	5	2
1:A:160:THR:N	1:A:163:VAL:O	0.49	2.46	15	12
1:A:29:VAL:O	1:A:29:VAL:HG13	0.49	2.07	2	1
1:A:35:VAL:HG11	1:A:109:ARG:HD2	0.49	1.84	14	1
1:A:36:VAL:HG21	1:A:64:LEU:HG	0.49	1.85	14	1
1:A:36:VAL:CG2	1:A:43:PHE:CD2	0.49	2.96	17	3
1:A:33:VAL:CG1	1:A:44:LEU:HD11	0.49	2.38	19	1
1:A:82:LEU:HD11	1:A:170:VAL:CG1	0.49	2.38	20	1
1:A:53:TRP:CH2	1:A:179:MET:CE	0.49	2.96	9	18
1:A:43:PHE:CE2	1:A:59:ALA:N	0.49	2.80	17	2
1:A:114:ILE:HD12	1:A:126:LEU:CD2	0.48	2.38	10	1
1:A:56:TYR:N	1:A:83:VAL:HG21	0.48	2.23	4	4
1:A:36:VAL:CG1	1:A:85:TRP:CH2	0.48	2.96	14	3
1:A:98:THR:O	1:A:98:THR:HG22	0.48	2.07	14	1
1:A:110:HIS:CD2	1:A:110:HIS:N	0.48	2.81	9	4
1:A:64:LEU:CD1	1:A:85:TRP:CZ2	0.48	2.96	11	7
1:A:36:VAL:CG2	1:A:43:PHE:CE2	0.48	2.96	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:THR:HG23	1:A:83:VAL:HG11	0.48	1.83	9	1
1:A:33:VAL:HG11	1:A:46:THR:CA	0.47	2.39	5	1
1:A:107:VAL:HG13	1:A:113:VAL:CG1	0.47	2.39	19	1
1:A:82:LEU:HD22	1:A:175:MET:CG	0.47	2.39	3	1
1:A:29:VAL:HG23	1:A:91:ALA:HA	0.47	1.86	2	1
1:A:94:LEU:HD23	1:A:150:ALA:HB2	0.47	1.85	19	3
1:A:144:LEU:HD23	1:A:150:ALA:HA	0.47	1.86	9	1
1:A:36:VAL:CG1	1:A:43:PHE:CZ	0.47	2.98	3	1
1:A:76:THR:CB	1:A:83:VAL:HG13	0.47	2.40	1	1
1:A:114:ILE:HD11	1:A:134:TYR:CE2	0.47	2.43	14	1
1:A:53:TRP:CH2	1:A:179:MET:HE3	0.47	2.45	6	3
1:A:172:VAL:HG12	1:A:172:VAL:O	0.47	2.10	10	2
1:A:54:THR:HG23	1:A:83:VAL:HG22	0.47	1.87	16	1
1:A:29:VAL:HG11	1:A:91:ALA:N	0.47	2.25	16	1
1:A:75:TYR:CD2	1:A:179:MET:CE	0.47	2.98	6	2
1:A:81:ASP:O	1:A:82:LEU:CB	0.47	2.63	9	1
1:A:63:THR:HG22	1:A:70:PRO:HB2	0.47	1.87	1	1
1:A:44:LEU:HD12	1:A:109:ARG:HB2	0.47	1.87	8	2
1:A:97:CYS:SG	1:A:151:VAL:HG22	0.47	2.50	8	1
1:A:53:TRP:CZ2	1:A:179:MET:CE	0.47	2.98	11	8
1:A:126:LEU:HD12	1:A:126:LEU:C	0.47	2.29	2	1
1:A:32:GLU:C	1:A:33:VAL:CG2	0.47	2.83	5	1
1:A:72:THR:HG23	1:A:72:THR:O	0.47	2.10	8	1
1:A:106:LEU:HD23	1:A:114:ILE:CB	0.46	2.39	16	1
1:A:75:TYR:CE1	1:A:179:MET:CG	0.46	2.98	11	5
1:A:108:THR:HG22	1:A:138:SER:HB3	0.46	1.87	18	1
1:A:75:TYR:O	1:A:83:VAL:HG13	0.46	2.10	5	4
1:A:94:LEU:CD1	1:A:144:LEU:HD21	0.46	2.40	3	1
1:A:153:ILE:HG13	1:A:175:MET:HE2	0.46	1.86	19	1
1:A:55:VAL:CG2	1:A:57:HIS:CE1	0.46	2.99	18	1
1:A:33:VAL:HG12	1:A:109:ARG:HG3	0.46	1.87	2	1
1:A:52:CYS:HB2	1:A:85:TRP:CE2	0.46	2.45	14	1
1:A:29:VAL:HG11	1:A:90:GLY:N	0.46	2.26	20	1
1:A:75:TYR:CZ	1:A:179:MET:CG	0.46	2.98	3	5
1:A:32:GLU:O	1:A:33:VAL:HG22	0.46	2.10	5	1
1:A:121:ASP:O	1:A:169:PHE:CZ	0.46	2.69	14	5
1:A:51:VAL:HG22	1:A:86:GLN:HG2	0.46	1.87	12	1
1:A:150:ALA:O	1:A:172:VAL:HG21	0.46	2.10	16	4
1:A:44:LEU:HD22	1:A:141:GLY:CA	0.46	2.41	20	1
1:A:35:VAL:HG12	1:A:44:LEU:HD23	0.46	1.87	4	1
1:A:64:LEU:HB3	1:A:71:ILE:HD12	0.46	1.88	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ALA:O	1:A:40:THR:OG1	0.46	2.33	8	2
1:A:56:TYR:N	1:A:83:VAL:CG2	0.46	2.79	4	2
1:A:44:LEU:CD1	1:A:138:SER:HA	0.46	2.41	20	1
1:A:53:TRP:HE3	1:A:82:LEU:HD23	0.45	1.66	2	2
1:A:46:THR:HG23	1:A:46:THR:O	0.45	2.11	20	4
1:A:76:THR:HA	1:A:83:VAL:HG22	0.45	1.88	3	1
1:A:88:PRO:CD	1:A:89:PRO:CD	0.45	2.94	16	2
1:A:104:LEU:CD2	1:A:151:VAL:HG11	0.45	2.41	8	4
1:A:88:PRO:CB	1:A:89:PRO:HD3	0.45	2.42	2	2
1:A:120:GLY:O	1:A:122:SER:N	0.45	2.50	14	5
1:A:45:ALA:HB1	1:A:52:CYS:SG	0.45	2.51	2	1
1:A:116:VAL:CG1	1:A:167:VAL:HG21	0.45	2.41	12	1
1:A:57:HIS:CD2	1:A:58:GLY:N	0.45	2.85	18	2
1:A:53:TRP:CG	1:A:175:MET:SD	0.45	3.10	11	1
1:A:63:THR:HG22	1:A:70:PRO:CB	0.45	2.42	1	1
1:A:104:LEU:HD23	1:A:145:CYS:CA	0.45	2.41	4	1
1:A:151:VAL:HG12	1:A:169:PHE:CE1	0.45	2.47	11	3
1:A:82:LEU:CD2	1:A:175:MET:HB3	0.45	2.41	16	1
1:A:53:TRP:CH2	1:A:179:MET:HE1	0.45	2.47	5	2
1:A:82:LEU:HD21	1:A:175:MET:CG	0.45	2.42	18	2
1:A:114:ILE:HD11	1:A:134:TYR:CZ	0.45	2.46	14	1
1:A:32:GLU:OE1	1:A:94:LEU:HD11	0.45	2.12	14	1
1:A:75:TYR:CE1	1:A:179:MET:CB	0.45	2.99	16	1
1:A:64:LEU:CD1	1:A:85:TRP:CH2	0.45	2.99	16	1
1:A:43:PHE:CE1	1:A:58:GLY:O	0.45	2.70	7	3
1:A:88:PRO:CD	1:A:89:PRO:HD3	0.45	2.41	18	1
1:A:53:TRP:CZ2	1:A:179:MET:HE3	0.45	2.47	11	2
1:A:75:TYR:CZ	1:A:179:MET:CB	0.45	2.99	16	1
1:A:117:ARG:HG2	1:A:127:LEU:HD11	0.45	1.89	11	1
1:A:29:VAL:HG21	1:A:34:GLN:HG3	0.45	1.88	15	1
1:A:172:VAL:O	1:A:172:VAL:HG12	0.45	2.10	18	3
1:A:104:LEU:HD22	1:A:151:VAL:HG11	0.44	1.87	10	1
1:A:51:VAL:O	1:A:53:TRP:CD1	0.44	2.70	12	3
1:A:151:VAL:CG1	1:A:169:PHE:CE2	0.44	3.01	4	2
1:A:87:ALA:HB1	1:A:91:ALA:HB2	0.44	1.89	2	1
1:A:145:CYS:N	1:A:146:PRO:CD	0.44	2.80	12	2
1:A:43:PHE:CE1	1:A:59:ALA:HA	0.44	2.48	14	1
1:A:75:TYR:CE1	1:A:179:MET:HG3	0.44	2.48	11	6
1:A:33:VAL:HG23	1:A:45:ALA:C	0.44	2.33	4	1
1:A:56:TYR:CE1	1:A:59:ALA:O	0.44	2.70	17	2
1:A:143:LEU:CD2	1:A:169:PHE:CD1	0.44	2.99	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:PRO:HG2	1:A:89:PRO:HD3	0.44	1.90	2	2
1:A:35:VAL:HG12	1:A:109:ARG:HB2	0.44	1.89	9	1
1:A:53:TRP:HZ2	1:A:179:MET:HE1	0.44	1.71	12	1
1:A:171:PRO:O	1:A:175:MET:HG3	0.44	2.12	15	1
1:A:33:VAL:CG1	1:A:44:LEU:CD1	0.44	2.96	19	1
1:A:126:LEU:HD21	1:A:130:ARG:NE	0.44	2.27	17	1
1:A:44:LEU:HD13	1:A:138:SER:O	0.44	2.12	17	1
1:A:53:TRP:CD2	1:A:82:LEU:HD23	0.44	2.46	3	1
1:A:145:CYS:CB	1:A:146:PRO:CD	0.44	2.96	1	2
1:A:88:PRO:HB2	1:A:89:PRO:HD3	0.44	1.89	2	1
1:A:64:LEU:HD13	1:A:85:TRP:CE2	0.44	2.47	12	1
1:A:36:VAL:HG21	1:A:64:LEU:CG	0.44	2.43	18	2
1:A:153:ILE:CG1	1:A:175:MET:CE	0.44	2.96	19	1
1:A:46:THR:HG21	1:A:153:ILE:HG22	0.43	1.85	5	1
1:A:74:MET:O	1:A:75:TYR:CD1	0.43	2.70	7	3
1:A:106:LEU:CD1	1:A:143:LEU:CD1	0.43	2.96	7	3
1:A:35:VAL:CG1	1:A:109:ARG:CD	0.43	2.96	8	1
1:A:77:ASN:O	1:A:81:ASP:CB	0.43	2.66	9	1
1:A:105:TYR:CD2	1:A:105:TYR:O	0.43	2.71	14	1
1:A:44:LEU:HD12	1:A:109:ARG:CB	0.43	2.43	9	1
1:A:143:LEU:N	1:A:143:LEU:HD12	0.43	2.27	8	1
1:A:76:THR:HG23	1:A:83:VAL:HG22	0.43	1.91	13	2
1:A:56:TYR:CB	1:A:78:VAL:HB	0.43	2.43	11	1
1:A:53:TRP:CH2	1:A:175:MET:O	0.43	2.72	15	1
1:A:145:CYS:HB3	1:A:151:VAL:HG21	0.43	1.89	4	2
1:A:153:ILE:HG12	1:A:175:MET:HE2	0.43	1.89	6	1
1:A:88:PRO:CG	1:A:89:PRO:HD3	0.43	2.44	2	1
1:A:44:LEU:HD13	1:A:109:ARG:HB2	0.43	1.89	18	1
1:A:66:GLY:HA3	1:A:71:ILE:HD11	0.43	1.90	17	1
1:A:78:VAL:O	1:A:80:GLN:N	0.43	2.52	4	1
1:A:44:LEU:HD13	1:A:45:ALA:N	0.43	2.29	5	1
1:A:161:ARG:O	1:A:161:ARG:CG	0.43	2.67	19	3
1:A:76:THR:HG23	1:A:83:VAL:HB	0.43	1.90	15	1
1:A:71:ILE:HG21	1:A:85:TRP:CD1	0.43	2.49	19	1
1:A:32:GLU:C	1:A:33:VAL:HG23	0.43	2.34	7	2
1:A:59:ALA:HB1	1:A:85:TRP:CZ2	0.43	2.48	4	1
1:A:148:GLY:O	1:A:149:HIS:CG	0.43	2.72	3	2
1:A:97:CYS:C	1:A:98:THR:HG22	0.43	2.34	11	1
1:A:172:VAL:HA	1:A:175:MET:HG2	0.42	1.91	2	1
1:A:32:GLU:HB3	1:A:94:LEU:HD11	0.42	1.89	18	1
1:A:126:LEU:HD22	1:A:130:ARG:HB2	0.42	1.91	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:LEU:HD12	1:A:143:LEU:HG	0.42	1.91	2	1
1:A:44:LEU:HD13	1:A:138:SER:CA	0.42	2.44	20	1
1:A:46:THR:CG2	1:A:153:ILE:HG21	0.42	2.24	13	1
1:A:161:ARG:CG	1:A:161:ARG:O	0.42	2.67	16	3
1:A:78:VAL:HG22	1:A:79:ASP:N	0.42	2.29	11	1
1:A:127:LEU:O	1:A:128:SER:CB	0.42	2.67	3	1
1:A:33:VAL:HG13	1:A:45:ALA:O	0.42	2.15	16	2
1:A:152:GLY:N	1:A:172:VAL:HG13	0.42	2.29	1	1
1:A:120:GLY:O	1:A:121:ASP:O	0.42	2.38	3	1
1:A:29:VAL:HG12	1:A:89:PRO:HB2	0.42	1.90	16	1
1:A:108:THR:HG21	1:A:134:TYR:CZ	0.42	2.49	19	2
1:A:82:LEU:HD21	1:A:175:MET:SD	0.42	2.54	15	1
1:A:44:LEU:CD2	1:A:141:GLY:CA	0.42	2.98	20	1
1:A:76:THR:HG22	1:A:83:VAL:CG1	0.42	2.44	4	1
1:A:141:GLY:O	1:A:153:ILE:HG22	0.42	2.15	13	1
1:A:77:ASN:O	1:A:81:ASP:HB2	0.42	2.15	12	1
1:A:108:THR:HG23	1:A:112:ASP:O	0.42	2.14	1	1
1:A:55:VAL:HG21	1:A:57:HIS:NE2	0.42	2.30	19	1
1:A:82:LEU:HD21	1:A:175:MET:HG2	0.42	1.91	14	1
1:A:145:CYS:SG	1:A:146:PRO:CD	0.42	3.08	11	1
1:A:66:GLY:N	1:A:69:GLY:O	0.42	2.53	2	1
1:A:54:THR:CG2	1:A:85:TRP:CH2	0.42	2.97	12	1
1:A:53:TRP:HA	1:A:83:VAL:O	0.42	2.14	5	1
1:A:55:VAL:HB	1:A:57:HIS:CE1	0.42	2.50	19	1
1:A:105:TYR:CE1	1:A:144:LEU:O	0.42	2.73	14	1
1:A:177:THR:HG23	1:A:178:THR:N	0.42	2.30	4	1
1:A:126:LEU:HD21	1:A:164:ALA:O	0.41	2.14	2	1
1:A:135:LEU:CD1	1:A:164:ALA:CB	0.41	2.98	12	2
1:A:53:TRP:CE3	1:A:82:LEU:CD2	0.41	3.03	8	3
1:A:72:THR:O	1:A:72:THR:HG23	0.41	2.15	15	1
1:A:82:LEU:HD21	1:A:175:MET:CE	0.41	2.45	1	1
1:A:122:SER:CA	1:A:169:PHE:O	0.41	2.68	15	3
1:A:43:PHE:CD2	1:A:58:GLY:O	0.41	2.73	19	1
1:A:132:VAL:HG23	1:A:159:CYS:SG	0.41	2.55	8	1
1:A:44:LEU:CD2	1:A:109:ARG:CB	0.41	2.98	14	2
1:A:154:PHE:CE1	1:A:156:ALA:O	0.41	2.73	17	5
1:A:115:PRO:HB2	1:A:127:LEU:HD12	0.41	1.91	9	2
1:A:47:CYS:CB	1:A:91:ALA:HB3	0.41	2.45	14	1
1:A:29:VAL:HG11	1:A:89:PRO:HB2	0.41	1.93	8	1
1:A:44:LEU:CB	1:A:139:SER:O	0.41	2.68	20	2
1:A:87:ALA:HB1	1:A:88:PRO:CD	0.41	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:VAL:CG2	1:A:175:MET:SD	0.41	3.09	15	1
1:A:106:LEU:HD11	1:A:114:ILE:CD1	0.41	2.37	14	1
1:A:97:CYS:SG	1:A:151:VAL:HG23	0.41	2.55	17	1
1:A:54:THR:CG2	1:A:85:TRP:CZ2	0.41	2.99	13	1
1:A:88:PRO:CG	1:A:89:PRO:CD	0.41	2.99	2	2
1:A:71:ILE:HG21	1:A:85:TRP:CE3	0.41	2.50	16	1
1:A:143:LEU:O	1:A:151:VAL:HB	0.41	2.15	9	1
1:A:54:THR:CG2	1:A:85:TRP:CZ3	0.41	3.03	14	1
1:A:29:VAL:HG21	1:A:89:PRO:HG3	0.41	1.91	14	1
1:A:54:THR:CG2	1:A:83:VAL:HG23	0.41	2.44	8	1
1:A:104:LEU:HD21	1:A:151:VAL:HG11	0.41	1.92	11	1
1:A:38:THR:O	1:A:40:THR:N	0.41	2.54	16	5
1:A:132:VAL:N	1:A:162:GLY:O	0.41	2.50	15	1
1:A:103:ASP:O	1:A:145:CYS:HA	0.41	2.16	1	1
1:A:44:LEU:C	1:A:44:LEU:CD2	0.41	2.89	8	1
1:A:108:THR:HG21	1:A:134:TYR:CE1	0.41	2.51	10	1
1:A:46:THR:CG2	1:A:153:ILE:CG2	0.41	2.99	10	2
1:A:114:ILE:O	1:A:116:VAL:HG23	0.41	2.15	16	1
1:A:32:GLU:C	1:A:33:VAL:HG22	0.41	2.36	5	1
1:A:126:LEU:HD22	1:A:128:SER:O	0.41	2.16	7	1
1:A:44:LEU:CD2	1:A:44:LEU:C	0.41	2.89	7	1
1:A:36:VAL:HG11	1:A:85:TRP:CZ2	0.41	2.51	17	1
1:A:32:GLU:OE2	1:A:107:VAL:HG12	0.41	2.15	5	1
1:A:172:VAL:HA	1:A:175:MET:HG3	0.41	1.93	1	2
1:A:44:LEU:HD12	1:A:108:THR:C	0.41	2.36	12	1
1:A:145:CYS:HB2	1:A:146:PRO:HD2	0.41	1.93	16	1
1:A:82:LEU:C	1:A:83:VAL:HG23	0.41	2.37	5	1
1:A:50:GLY:N	1:A:93:SER:CB	0.41	2.84	19	1
1:A:151:VAL:CG1	1:A:169:PHE:CZ	0.40	3.03	3	1
1:A:75:TYR:CZ	1:A:179:MET:HG3	0.40	2.50	3	1
1:A:54:THR:O	1:A:54:THR:HG23	0.40	2.16	3	1
1:A:175:MET:O	1:A:178:THR:CB	0.40	2.69	18	2
1:A:97:CYS:O	1:A:98:THR:CG2	0.40	2.69	11	1
1:A:175:MET:HG3	1:A:176:GLU:N	0.40	2.30	16	1
1:A:117:ARG:O	1:A:125:SER:N	0.40	2.55	19	1
1:A:88:PRO:O	1:A:90:GLY:N	0.40	2.55	19	1
1:A:56:TYR:CB	1:A:78:VAL:CG1	0.40	2.99	9	1
1:A:106:LEU:CD1	1:A:143:LEU:HD11	0.40	2.47	7	1
1:A:105:TYR:N	1:A:105:TYR:CD1	0.40	2.89	14	1
1:A:144:LEU:HD22	1:A:147:SER:O	0.40	2.17	12	1
1:A:82:LEU:CD1	1:A:170:VAL:CG1	0.40	2.99	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:THR:CG2	1:A:83:VAL:CG2	0.40	2.99	18	1
1:A:143:LEU:HD12	1:A:143:LEU:N	0.40	2.30	7	1
1:A:153:ILE:HG13	1:A:170:VAL:CG1	0.40	2.46	17	1
1:A:82:LEU:HD21	1:A:175:MET:HE2	0.40	1.94	5	1
1:A:43:PHE:CG	1:A:58:GLY:O	0.40	2.74	19	1
1:A:107:VAL:CG2	1:A:113:VAL:HG12	0.40	2.40	4	1
1:A:104:LEU:HA	1:A:144:LEU:O	0.40	2.15	11	1
1:A:35:VAL:HG13	1:A:109:ARG:HD3	0.40	1.94	16	1
1:A:82:LEU:C	1:A:83:VAL:HG13	0.40	2.37	15	1
1:A:36:VAL:HG21	1:A:64:LEU:HD21	0.40	1.94	18	1
1:A:145:CYS:HB2	1:A:146:PRO:CD	0.40	2.46	6	1
1:A:35:VAL:HG13	1:A:109:ARG:CD	0.40	2.46	16	1
1:A:86:GLN:O	1:A:88:PRO:CD	0.40	2.70	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	154/186 (83%)	114±4 (74±3%)	28±4 (18±2%)	12±3 (8±2%)	2	14
All	All	3080/3720 (83%)	2280 (74%)	554 (18%)	246 (8%)	2	14

All 51 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	161	ARG	20
1	A	40	THR	14
1	A	128	SER	12
1	A	103	ASP	11
1	A	32	GLU	10
1	A	149	HIS	9
1	A	106	LEU	9
1	A	94	LEU	9
1	A	147	SER	9

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Mol	Chain	Res	Type	Models (Total)
1	A	88	PRO	8
1	A	58	GLY	8
1	A	81	ASP	7
1	A	59	ALA	7
1	A	93	SER	6
1	A	63	THR	6
1	A	39	ALA	6
1	A	89	PRO	6
1	A	62	LYS	6
1	A	121	ASP	5
1	A	79	ASP	5
1	A	31	GLY	5
1	A	67	PRO	4
1	A	182	SER	4
1	A	74	MET	4
1	A	41	GLN	4
1	A	146	PRO	4
1	A	145	CYS	4
1	A	30	GLU	4
1	A	29	VAL	4
1	A	78	VAL	3
1	A	110	HIS	3
1	A	80	GLN	3
1	A	61	SER	2
1	A	129	PRO	2
1	A	33	VAL	2
1	A	52	CYS	2
1	A	142	PRO	2
1	A	73	GLN	2
1	A	120	GLY	2
1	A	98	THR	2
1	A	96	PRO	1
1	A	64	LEU	1
1	A	91	ALA	1
1	A	102	SER	1
1	A	141	GLY	1
1	A	72	THR	1
1	A	95	THR	1
1	A	100	GLY	1
1	A	92	ARG	1
1	A	111	ALA	1
1	A	101	SER	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	124/151 (82%)	98±4 (79±3%)	26±4 (21±3%)	4	33
All	All	2480/3020 (82%)	1957 (79%)	523 (21%)	4	33

All 81 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	64	LEU	19
1	A	125	SER	17
1	A	161	ARG	17
1	A	126	LEU	16
1	A	163	VAL	15
1	A	168	ASP	15
1	A	128	SER	15
1	A	110	HIS	14
1	A	179	MET	14
1	A	109	ARG	12
1	A	94	LEU	12
1	A	95	THR	12
1	A	147	SER	11
1	A	41	GLN	11
1	A	117	ARG	10
1	A	180	ARG	10
1	A	119	ARG	9
1	A	167	VAL	9
1	A	44	LEU	9
1	A	178	THR	9
1	A	123	ARG	9
1	A	112	ASP	9
1	A	121	ASP	9
1	A	81	ASP	8
1	A	79	ASP	8
1	A	151	VAL	8
1	A	136	LYS	7
1	A	169	PHE	7
1	A	130	ARG	7

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Mol	Chain	Res	Type	Models (Total)
1	A	62	LYS	7
1	A	97	CYS	7
1	A	118	ARG	6
1	A	104	LEU	6
1	A	52	CYS	6
1	A	144	LEU	6
1	A	30	GLU	6
1	A	160	THR	6
1	A	122	SER	6
1	A	155	ARG	5
1	A	74	MET	5
1	A	85	TRP	5
1	A	92	ARG	5
1	A	82	LEU	5
1	A	133	SER	5
1	A	103	ASP	5
1	A	43	PHE	5
1	A	101	SER	5
1	A	153	ILE	4
1	A	143	LEU	4
1	A	61	SER	4
1	A	29	VAL	4
1	A	76	THR	4
1	A	102	SER	4
1	A	34	GLN	4
1	A	40	THR	4
1	A	68	LYS	4
1	A	49	ASN	4
1	A	36	VAL	4
1	A	149	HIS	3
1	A	182	SER	3
1	A	174	SER	3
1	A	170	VAL	3
1	A	32	GLU	3
1	A	73	GLN	3
1	A	77	ASN	3
1	A	139	SER	3
1	A	63	THR	3
1	A	145	CYS	3
1	A	80	GLN	3
1	A	175	MET	3
1	A	176	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	33	VAL	2
1	A	134	TYR	2
1	A	108	THR	1
1	A	165	LYS	1
1	A	57	HIS	1
1	A	54	THR	1
1	A	138	SER	1
1	A	86	GLN	1
1	A	93	SER	1
1	A	98	THR	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

No chemical shift data were provided