



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 AM UTC

PDB ID : 1BT7 / pdb_00001bt7
Title : THE SOLUTION NMR STRUCTURE OF THE N-TERMINAL PROTEASE
DOMAIN OF THE HEPATITIS C VIRUS (HCV) NS3-PROTEIN, FROM BK
STRAIN, 20 STRUCTURES
Authors : Barbato, G.; Cicero, D.O.; Nardi, M.C.; Steinkuhler, C.; Cortese, R.; De
Francesco, R.; Bazzo, R.
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

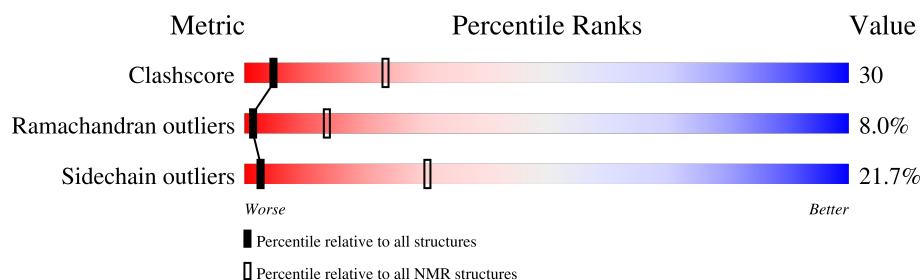
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

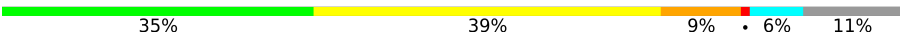
The overall completeness of chemical shifts assignment was not calculated.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	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)	1.04	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 (CCD ID: ZN) (formula: Zn).

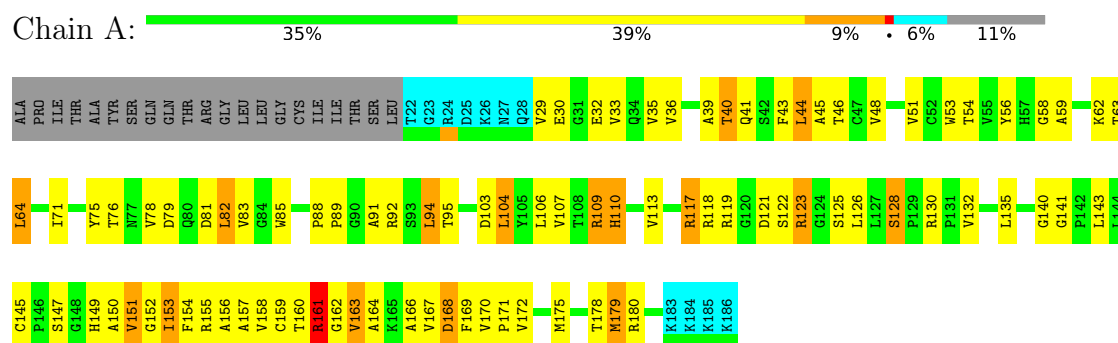
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: NS3 SERINE PROTEASE

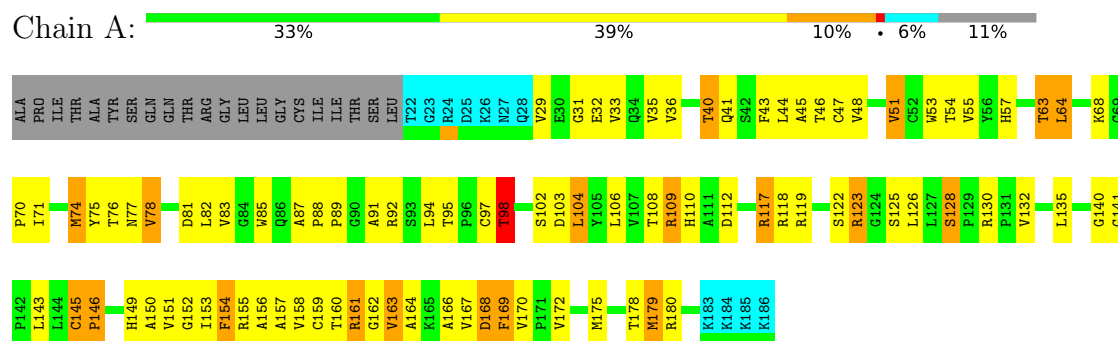


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: NS3 SERINE PROTEASE



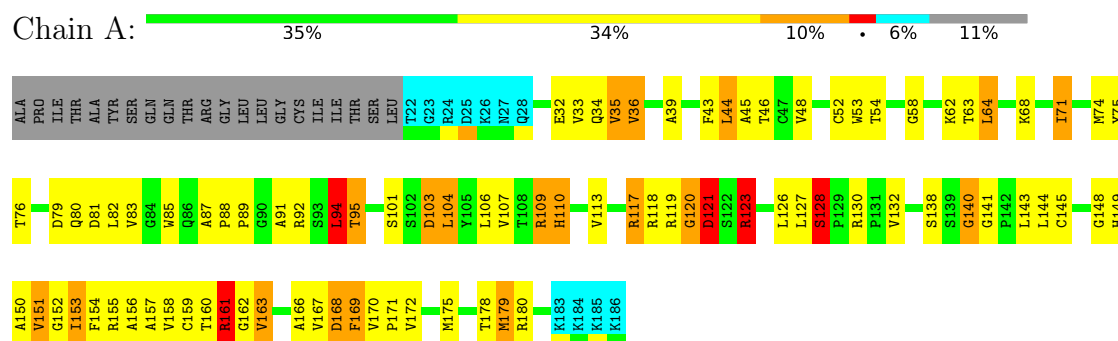
4.2.2 Score per residue for model 2

• Molecule 1: NS3 SERINE PROTEASE



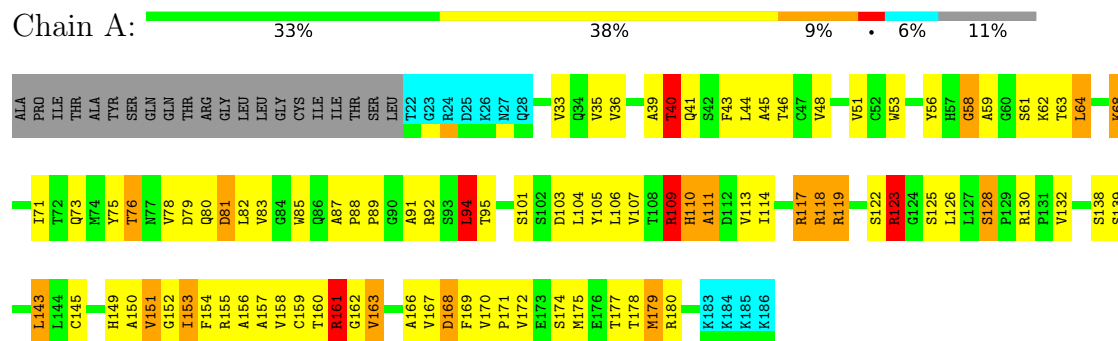
4.2.3 Score per residue for model 3

• Molecule 1: NS3 SERINE PROTEASE



4.2.4 Score per residue for model 4

• Molecule 1: NS3 SERINE PROTEASE



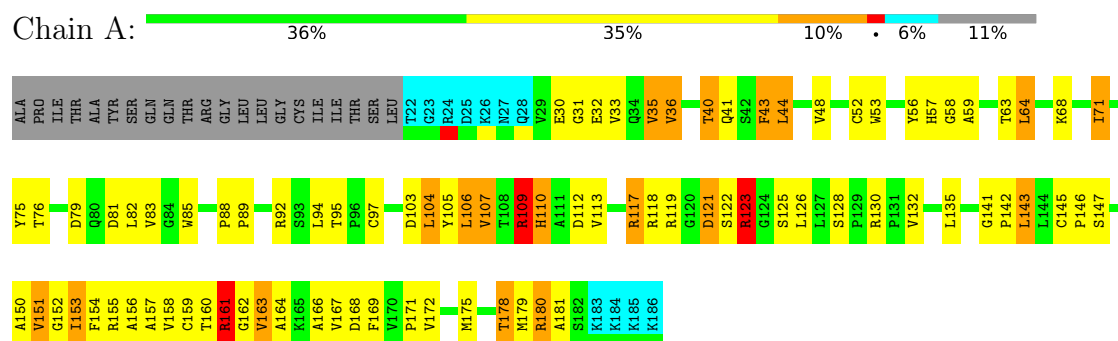
4.2.5 Score per residue for model 5

• Molecule 1: NS3 SERINE PROTEASE



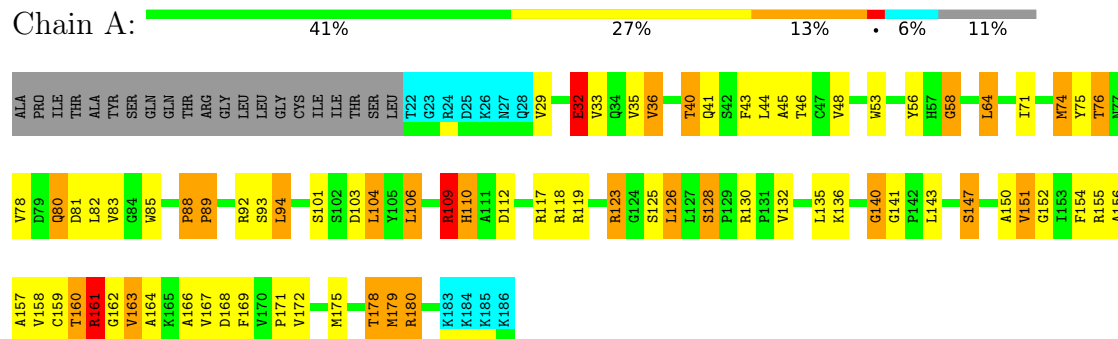
4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: NS3 SERINE PROTEASE



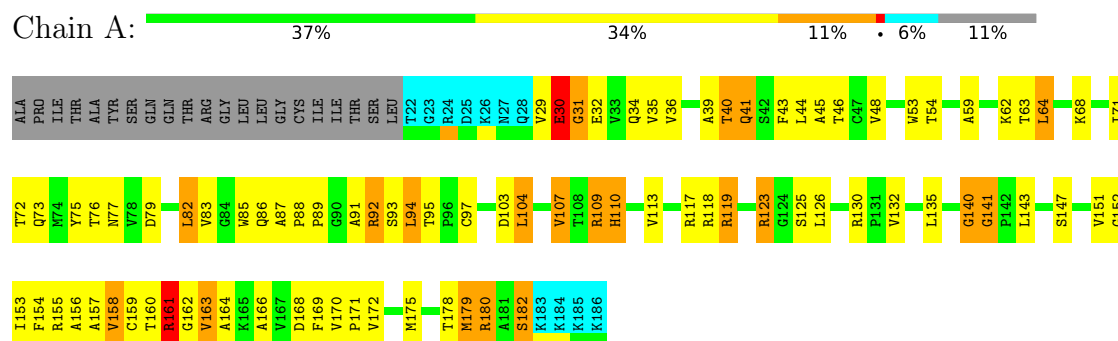
4.2.7 Score per residue for model 7

• Molecule 1: NS3 SERINE PROTEASE



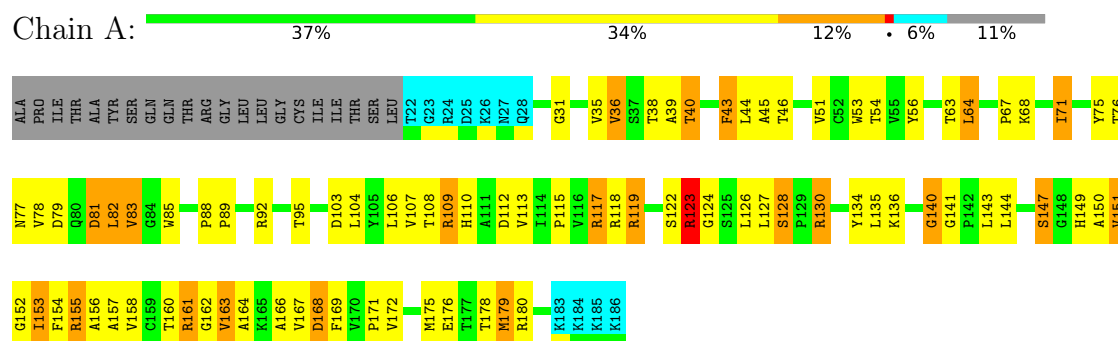
4.2.8 Score per residue for model 8

- Molecule 1: NS3 SERINE PROTEASE



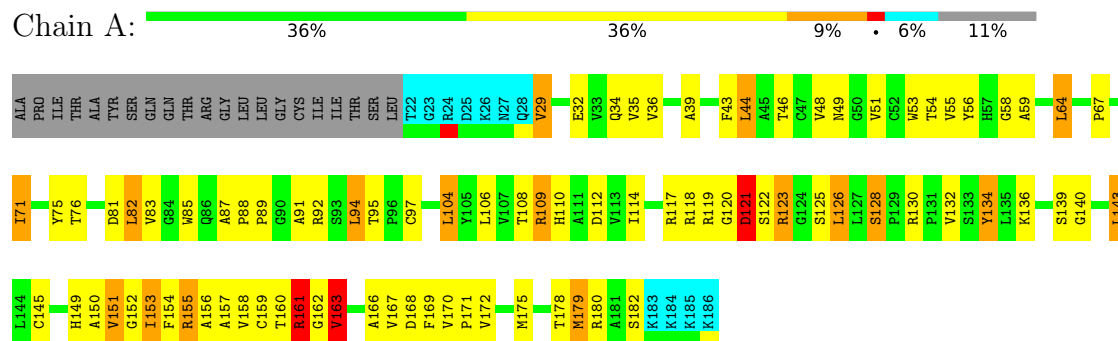
4.2.9 Score per residue for model 9

- Molecule 1: NS3 SERINE PROTEASE



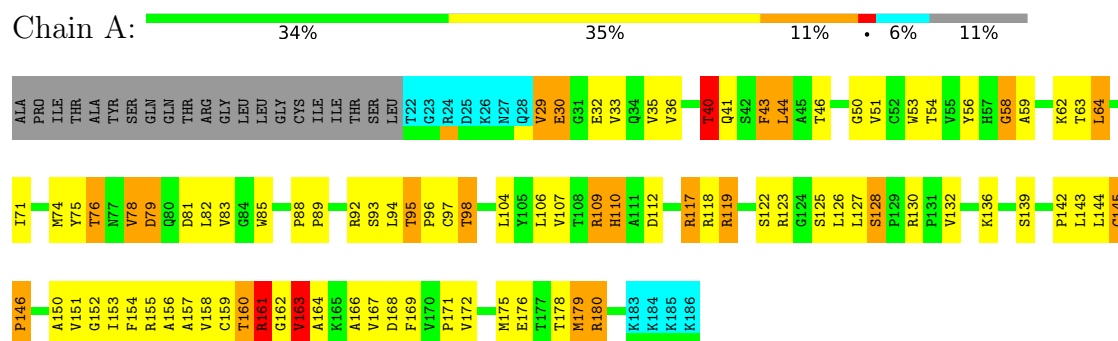
4.2.10 Score per residue for model 10

- Molecule 1: NS3 SERINE PROTEASE



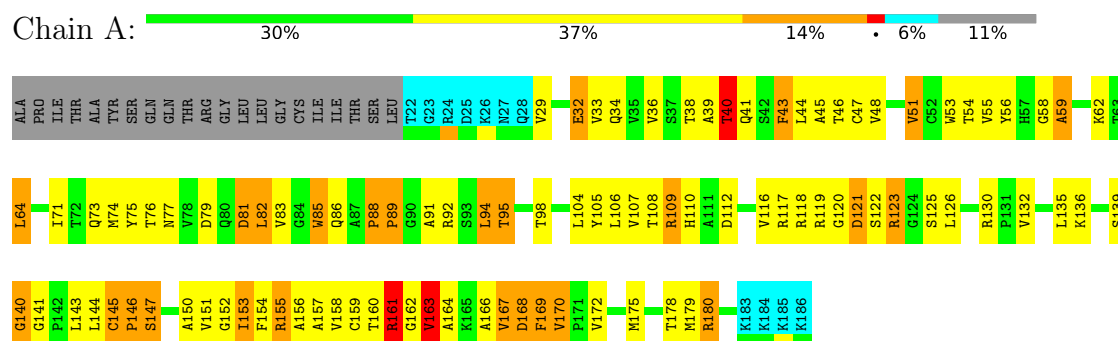
4.2.11 Score per residue for model 11

• Molecule 1: NS3 SERINE PROTEASE



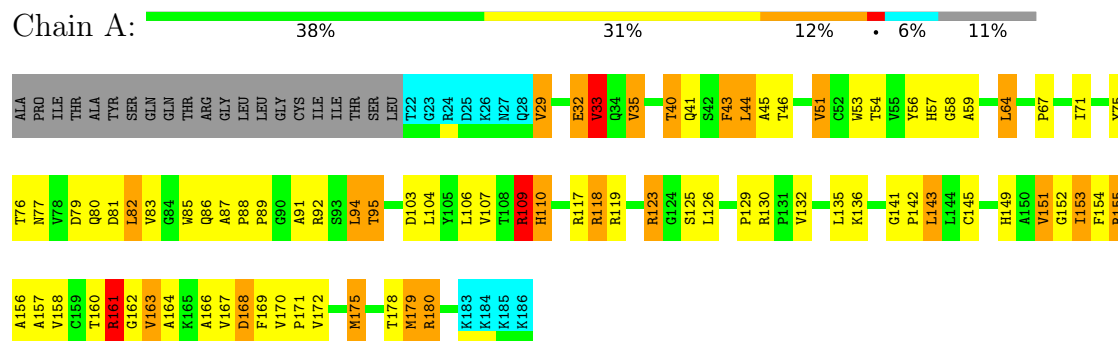
4.2.12 Score per residue for model 12

• Molecule 1: NS3 SERINE PROTEASE



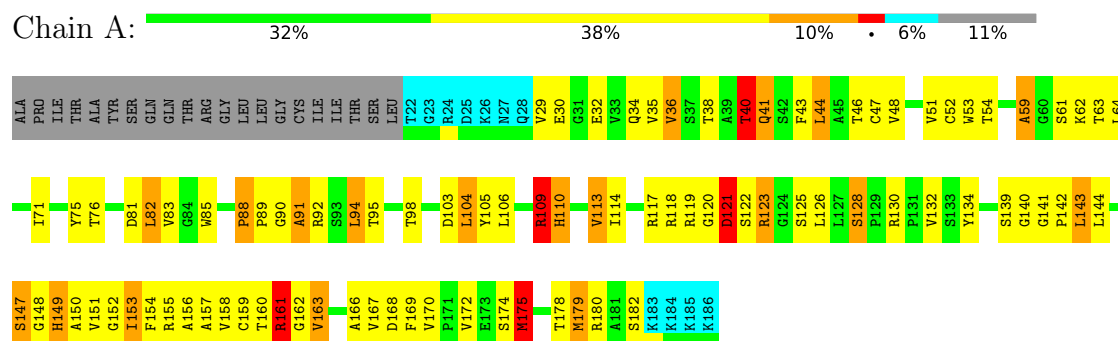
4.2.13 Score per residue for model 13

• Molecule 1: NS3 SERINE PROTEASE



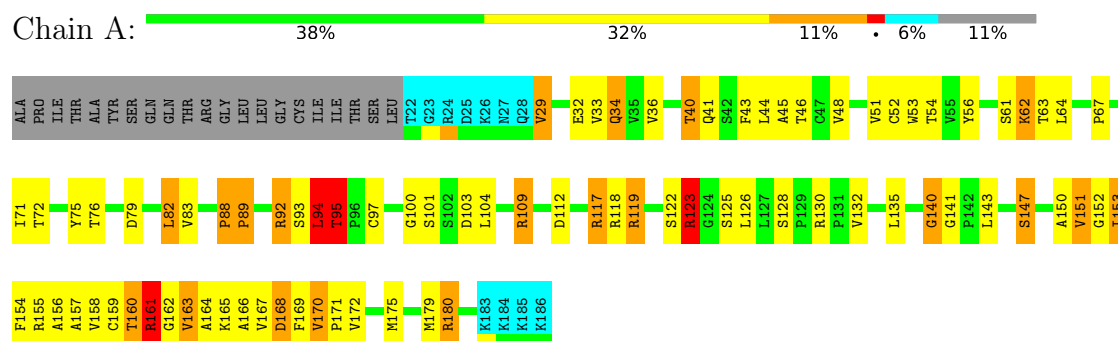
4.2.14 Score per residue for model 14

• Molecule 1: NS3 SERINE PROTEASE



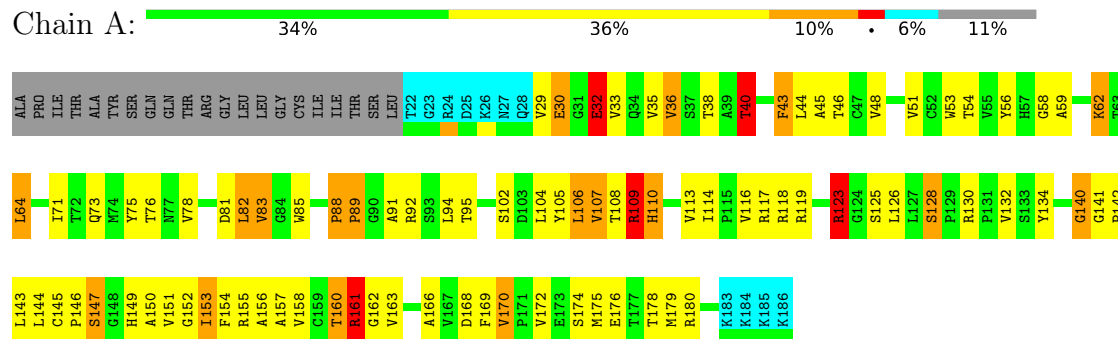
4.2.15 Score per residue for model 15

• Molecule 1: NS3 SERINE PROTEASE



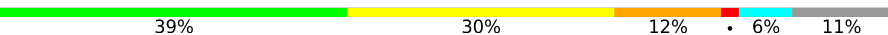
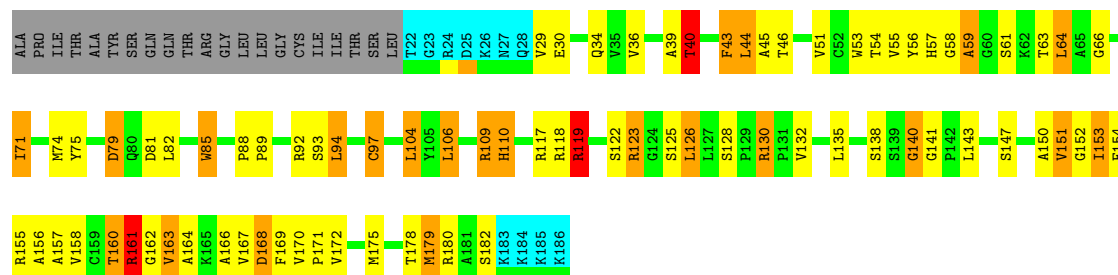
4.2.16 Score per residue for model 16

• Molecule 1: NS3 SERINE PROTEASE



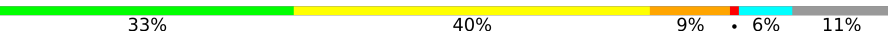
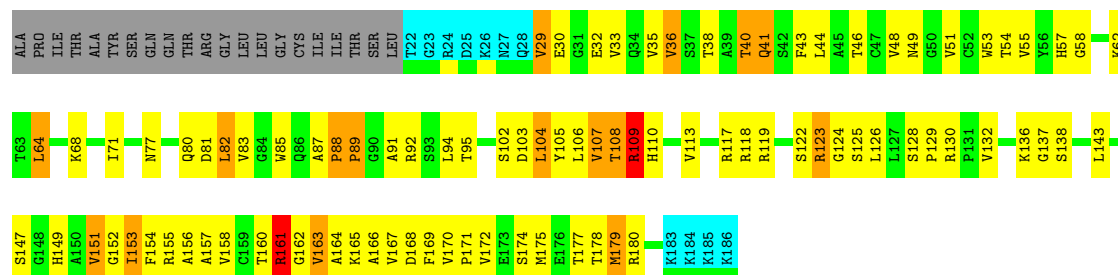
4.2.17 Score per residue for model 17

• Molecule 1: NS3 SERINE PROTEASE

Chain A:  39% 30% 12% • 6% 11%

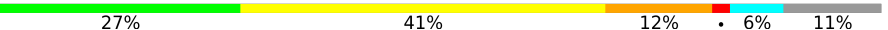
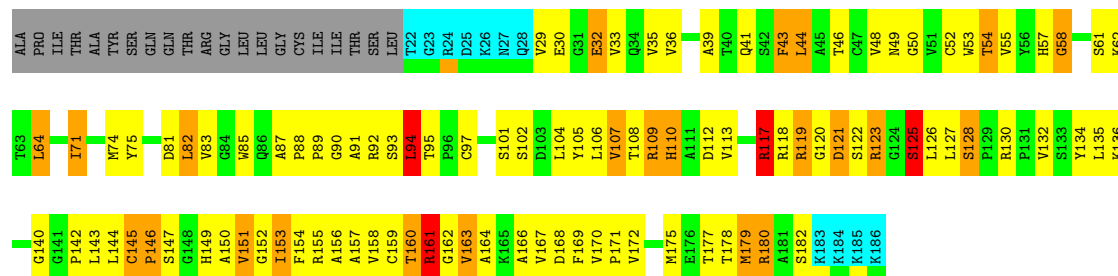
4.2.18 Score per residue for model 18

• Molecule 1: NS3 SERINE PROTEASE

Chain A:  33% 40% 9% • 6% 11%

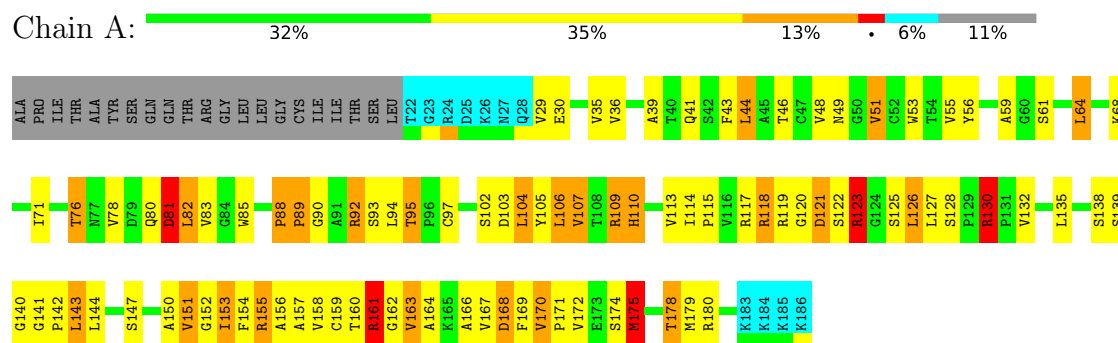
4.2.19 Score per residue for model 19

• Molecule 1: NS3 SERINE PROTEASE

Chain A:  27% 41% 12% • 6% 11%

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.

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	1.52±0.01	0±1/1151 (0.0± 0.0%)	1.52±0.02	5±1/1571 (0.3± 0.1%)
All	All	1.52	5/23020 (0.0%)	1.52	100/31420 (0.3%)

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

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	124	GLY	N-CA	5.49	1.50	1.45	18	2
1	A	175	MET	N-CA	5.32	1.52	1.46	14	2
1	A	82	LEU	N-CA	5.31	1.53	1.46	9	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	VAL	N-CA-CB	-6.93	104.17	112.07	13	2
1	A	140	GLY	N-CA-C	-6.51	106.73	114.48	2	14
1	A	163	VAL	N-CA-CB	-6.33	103.82	110.72	11	9
1	A	36	VAL	N-CA-CB	-6.27	105.43	112.45	7	8
1	A	35	VAL	N-CA-CB	-6.19	105.20	112.32	20	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	95	THR	N-CA-CB	-6.17	104.93	111.29	3	2
1	A	51	VAL	N-CA-CB	-6.06	104.47	112.34	17	12
1	A	107	VAL	N-CA-CB	-6.05	105.36	111.90	6	9
1	A	43	PHE	CA-CB-CG	-5.73	108.07	113.80	11	7
1	A	68	LYS	N-CA-CB	-5.69	104.96	111.79	3	5
1	A	122	SER	N-CA-CB	-5.68	103.70	111.65	4	1
1	A	71	ILE	N-CA-CB	-5.68	104.79	111.60	15	8
1	A	169	PHE	N-CA-CB	-5.67	102.42	111.43	2	1
1	A	44	LEU	N-CA-CB	-5.59	101.90	110.85	17	2
1	A	170	VAL	N-CA-CB	-5.56	106.48	112.37	3	1
1	A	90	GLY	N-CA-C	-5.41	108.65	115.08	14	1
1	A	137	GLY	N-CA-C	-5.32	108.36	114.69	18	1
1	A	98	THR	N-CA-CB	-5.20	105.55	111.79	12	1
1	A	125	SER	N-CA-CB	-5.19	102.62	110.77	20	2
1	A	91	ALA	N-CA-CB	-5.17	104.57	112.28	14	1
1	A	119	ARG	N-CA-CB	-5.09	103.83	110.59	11	3
1	A	179	MET	N-CA-CB	-5.08	102.64	110.01	5	1
1	A	123	ARG	N-CA-CB	-5.07	103.86	111.56	2	1
1	A	154	PHE	N-CA-CB	-5.00	103.35	110.46	1	1

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	92	ARG	Sidechain	20
1	A	109	ARG	Sidechain	20
1	A	117	ARG	Sidechain	20
1	A	118	ARG	Sidechain	20
1	A	119	ARG	Sidechain	20
1	A	123	ARG	Sidechain	20
1	A	130	ARG	Sidechain	20
1	A	155	ARG	Sidechain	20
1	A	161	ARG	Sidechain	20
1	A	180	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	68±7
All	All	22540	22480	22477	1350

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 30.

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:175:MET:O	1:A:179:MET:HE3	0.79	1.78	20	1
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:33:VAL:HG11	1:A:45:ALA:C	0.77	2.03	13	2
1:A:152:GLY:HA2	1:A:172:VAL:HG13	0.76	1.55	15	11
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:HD12	1:A:126:LEU:O	0.75	1.82	15	4
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:82:LEU:HD22	1:A:175:MET:HB3	0.73	1.57	2	5
1:A:44:LEU:HD21	1:A:109:ARG:CB	0.73	2.13	6	7
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:82:LEU:HD21	1:A:175:MET:HE2	0.71	1.62	1	6
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:44:LEU:HD22	1:A:140:GLY:C	0.69	2.13	17	9
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:107:VAL:HG22	1:A:113:VAL:CG1	0.68	2.18	4	4
1:A:82:LEU:HD22	1:A:175:MET:HG2	0.68	1.65	3	1
1:A:44:LEU:C	1:A:44:LEU:HD23	0.67	2.14	8	5
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:75:TYR:CD2	1:A:179:MET:HE1	0.66	2.25	5	2
1:A:44:LEU:HD22	1:A:141:GLY:N	0.66	2.05	9	10
1:A:126:LEU:HD21	1:A:164:ALA:C	0.66	2.15	18	4
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:53:TRP:CZ2	1:A:179:MET:HE1	0.66	2.26	14	15
1:A:76:THR:HG23	1:A:83:VAL:HG12	0.65	1.68	16	1
1:A:44:LEU:HD23	1:A:44:LEU:C	0.65	2.16	12	4
1:A:65:ALA:O	1:A:71:ILE:HD11	0.65	1.92	5	1
1:A:75:TYR:CD2	1:A:179:MET:HE2	0.65	2.26	3	12
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: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:53:TRP:CH2	1:A:179:MET:HE2	0.64	2.28	5	2
1:A:150:ALA:HB1	1:A:172:VAL:HG21	0.64	1.69	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:CD1	1:A:170:VAL:HG21	0.64	2.22	20	1
1:A:153:ILE:HG23	1:A:175:MET:HE1	0.64	1.68	6	8
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: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:52:CYS:SG	1:A:87:ALA:HB2	0.62	2.35	19	1
1:A:54:THR:HG23	1:A:83:VAL:CG2	0.61	2.25	8	4
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: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:36:VAL:HG21	1:A:64:LEU:CD2	0.60	2.26	16	1
1:A:94:LEU:O	1:A:95:THR:HG23	0.60	1.96	15	6
1:A:87:ALA:O	1:A:91:ALA:HB3	0.60	1.96	3	3
1:A:156:ALA:HB3	1:A:168:ASP:HB3	0.60	1.74	13	20
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:HD22	1:A:175:MET:CB	0.59	2.28	9	5
1:A:82:LEU:CD1	1:A:170:VAL:HG11	0.59	2.28	10	3
1:A:63:THR:HG23	1:A:63:THR:O	0.58	1.98	11	2
1:A:36:VAL:HG12	1:A:64:LEU:HD21	0.58	1.75	19	2
1:A:132:VAL:HG12	1:A:162:GLY:C	0.58	2.24	15	13
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
1:A:104:LEU:CD2	1:A:151:VAL:HG21	0.58	2.29	1	2
1:A:64:LEU:HD22	1:A:71:ILE:HB	0.58	1.76	11	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:53:TRP:HZ2	1:A:179:MET:HE1	0.57	1.60	18	7
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: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:34:GLN:O	1:A:45:ALA:HB3	0.55	2.01	8	3
1:A:81:ASP:O	1:A:82:LEU:HD12	0.55	2.02	14	7
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:150:ALA:HB1	1:A:172:VAL:HG11	0.55	1.78	1	1
1:A:71:ILE:HG22	1:A:71:ILE:O	0.55	2.02	2	1
1:A:76:THR:HG22	1:A:83:VAL:HG12	0.54	1.79	4	4
1:A:36:VAL:HG21	1:A:43:PHE:CD2	0.54	2.37	9	1
1:A:126:LEU:HD11	1:A:165:LYS:HA	0.54	1.78	18	2
1:A:82:LEU:HD11	1:A:170:VAL:HG11	0.54	1.79	20	3
1:A:151:VAL:O	1:A:171:PRO:HA	0.54	2.02	18	16
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:154:PHE:CE1	1:A:157:ALA:HB2	0.54	2.37	7	9
1:A:76:THR:CG2	1:A:83:VAL:HG12	0.54	2.33	7	4
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:105:TYR:HB3	1:A:113:VAL:HG13	0.54	1.79	6	2
1:A:107:VAL:HG22	1:A:113:VAL:CG2	0.54	2.13	5	1
1:A:105:TYR:HB2	1:A:113:VAL:HG13	0.54	1.79	14	1
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:56:TYR:CD1	1:A:76:THR:CG2	0.53	2.92	2	6
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:36:VAL:CG1	1:A:64:LEU:HD21	0.53	2.34	5	4
1:A:178:THR:O	1:A:181:ALA:HB3	0.53	2.04	6	1
1:A:152:GLY:N	1:A:172:VAL:HG23	0.53	2.18	18	3
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:33:VAL:HG23	1:A:45:ALA:O	0.52	2.05	4	2
1:A:56:TYR:HB2	1:A:83:VAL:HG11	0.52	1.80	20	6
1:A:172:VAL:HG12	1:A:175:MET:HE2	0.52	1.81	15	1
1:A:107:VAL:HA	1:A:113:VAL:HG12	0.52	1.82	19	1
1:A:106:LEU:HD13	1:A:143:LEU:HD12	0.52	1.81	4	1
1:A:83:VAL:HG23	1:A:83:VAL:O	0.52	2.05	8	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:126:LEU:HD12	1:A:126:LEU:C	0.51	2.29	2	3
1:A:32:GLU:C	1:A:33:VAL:CG2	0.51	2.83	5	2
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:N	1:A:43:PHE:CD1	0.51	2.77	9	11
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
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	0.50	2.06	11	9
1:A:150:ALA:CB	1:A:172:VAL:HG21	0.50	2.35	10	2
1:A:44:LEU:HD12	1:A:109:ARG:HB3	0.50	1.83	9	1
1:A:87:ALA:HB1	1:A:91:ALA:HB3	0.50	1.83	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:LEU:HD12	1:A:106:LEU:O	0.50	2.05	14	1
1:A:153:ILE:HG12	1:A:175:MET:HE1	0.50	1.84	20	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: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:CD2	1:A:110:HIS:N	0.49	2.80	8	14
1:A:88:PRO:N	1:A:89:PRO:HD2	0.49	2.23	19	8
1:A:160:THR:O	1:A:162:GLY:N	0.49	2.46	8	20
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: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:33:VAL:HG21	1:A:46:THR:HA	0.49	1.83	5	2
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:33:VAL:HG23	1:A:45:ALA:C	0.49	2.33	4	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:56:TYR:N	1:A:83:VAL:HG21	0.48	2.23	4	4
1:A:114:ILE:HD12	1:A:126:LEU:CD2	0.48	2.38	10	1
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: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
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:32:GLU:C	1:A:33:VAL:HG23	0.47	2.34	7	3
1:A:144:LEU:HD23	1:A:150:ALA:HA	0.47	1.86	9	1
1:A:94:LEU:HD23	1:A:150:ALA:HB2	0.47	1.85	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:THR:CB	1:A:83:VAL:HG13	0.47	2.40	1	1
1:A:36:VAL:CG1	1:A:43:PHE:CZ	0.47	2.98	3	1
1:A:114:ILE:HD11	1:A:134:TYR:CE2	0.47	2.43	14	1
1:A:97:CYS:C	1:A:98:THR:HG22	0.47	2.34	11	1
1:A:63:THR:HG22	1:A:70:PRO:HB2	0.47	1.87	1	1
1:A:172:VAL:O	1:A:172:VAL:HG12	0.47	2.10	10	5
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:81:ASP:O	1:A:82:LEU:CB	0.47	2.63	9	1
1:A:29:VAL:HG11	1:A:91:ALA:N	0.47	2.25	16	1
1:A:54:THR:HG23	1:A:83:VAL:HG22	0.47	1.87	16	1
1:A:53:TRP:CZ2	1:A:179:MET:CE	0.47	2.98	11	8
1:A:72:THR:HG23	1:A:72:THR:O	0.47	2.10	8	2
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:94:LEU:CD1	1:A:144:LEU:HD21	0.46	2.40	3	1
1:A:75:TYR:O	1:A:83:VAL:HG13	0.46	2.10	5	4
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:35:VAL:HG12	1:A:44:LEU:HD23	0.46	1.87	4	1
1:A:150:ALA:O	1:A:172:VAL:HG21	0.46	2.10	16	4
1:A:75:TYR:CD2	1:A:179:MET:CE	0.46	2.98	6	2
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:44:LEU:HD22	1:A:141:GLY:CA	0.46	2.41	20	1
1:A:56:TYR:N	1:A:83:VAL:CG2	0.46	2.79	4	2
1:A:64:LEU:HB3	1:A:71:ILE:HD12	0.46	1.88	5	1
1:A:39:ALA:O	1:A:40:THR:OG1	0.46	2.33	8	2
1:A:44:LEU:CD1	1:A:138:SER:HA	0.46	2.41	20	1
1:A:44:LEU:C	1:A:44:LEU:CD2	0.46	2.89	7	5
1:A:53:TRP:HE3	1:A:82:LEU:HD23	0.45	1.66	2	2
1:A:32:GLU:C	1:A:33:VAL:HG22	0.45	2.36	5	1
1:A:76:THR:HA	1:A:83:VAL:HG22	0.45	1.88	3	1
1:A:82:LEU:C	1:A:83:VAL:HG23	0.45	2.37	5	1
1:A:88:PRO:CD	1:A:89:PRO:CD	0.45	2.94	16	2
1:A:88:PRO:CB	1:A:89:PRO:HD3	0.45	2.42	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LEU:CD2	1:A:151:VAL:HG11	0.45	2.41	8	4
1:A:44:LEU:HD12	1:A:108:THR:C	0.45	2.36	12	1
1:A:45:ALA:HB1	1:A:52:CYS:SG	0.45	2.51	2	1
1:A:120:GLY:O	1:A:122:SER:N	0.45	2.50	14	5
1:A:116:VAL:CG1	1:A:167:VAL:HG21	0.45	2.41	12	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:53:TRP:CG	1:A:175:MET:SD	0.45	3.10	11	1
1:A:57:HIS:CD2	1:A:58:GLY:N	0.45	2.85	18	2
1:A:151:VAL:HG12	1:A:169:PHE:CE1	0.45	2.47	11	3
1:A:32:GLU:OE1	1:A:94:LEU:HD11	0.45	2.12	14	1
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:82:LEU:CD2	1:A:175:MET:HB3	0.45	2.41	16	1
1:A:43:PHE:CE1	1:A:58:GLY:O	0.45	2.70	7	3
1:A:82:LEU:C	1:A:83:VAL:HG13	0.45	2.37	15	1
1:A:64:LEU:CD1	1:A:85:TRP:CH2	0.45	2.99	16	1
1:A:75:TYR:CE1	1:A:179:MET:CB	0.45	2.99	16	1
1:A:88:PRO:CD	1:A:89:PRO:HD3	0.45	2.41	18	1
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:32:GLU:CD	1:A:94:LEU:HD11	0.44	2.38	10	1
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:87:ALA:HB1	1:A:91:ALA:HB2	0.44	1.89	2	1
1:A:151:VAL:CG1	1:A:169:PHE:CE2	0.44	3.01	4	2
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:143:LEU:CD2	1:A:169:PHE:CD1	0.44	2.99	8	1
1:A:56:TYR:CE1	1:A:59:ALA:O	0.44	2.70	17	2
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:34:GLN:C	1:A:35:VAL:HG13	0.44	2.37	10	1
1:A:171:PRO:O	1:A:175:MET:HG3	0.44	2.12	15	1
1:A:44:LEU:HD13	1:A:138:SER:O	0.44	2.12	17	1
1:A:126:LEU:HD21	1:A:130:ARG:NE	0.44	2.27	17	1
1:A:33:VAL:CG1	1:A:44:LEU:CD1	0.44	2.96	19	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TRP:CD2	1:A:82:LEU:HD23	0.44	2.46	3	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:74:MET:O	1:A:75:TYR:CD1	0.43	2.70	7	3
1:A:46:THR:HG21	1:A:153:ILE:HG22	0.43	1.85	5	1
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:43:PHE:CD1	1:A:58:GLY:C	0.43	2.97	6	1
1:A:105:TYR:O	1:A:105:TYR:CD2	0.43	2.71	14	1
1:A:143:LEU:HD12	1:A:143:LEU:N	0.43	2.27	8	2
1:A:30:GLU:O	1:A:31:GLY:C	0.43	2.62	8	1
1:A:44:LEU:HD12	1:A:109:ARG:CB	0.43	2.43	9	1
1:A:44:LEU:CD2	1:A:140:GLY:C	0.43	2.92	3	5
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:172:VAL:HA	1:A:175:MET:HE2	0.43	1.89	20	1
1:A:145:CYS:HB3	1:A:151:VAL:HG21	0.43	1.89	4	2
1:A:88:PRO:CG	1:A:89:PRO:HD3	0.43	2.44	2	1
1:A:78:VAL:O	1:A:80:GLN:N	0.43	2.52	4	1
1:A:66:GLY:HA3	1:A:71:ILE:HD11	0.43	1.90	17	1
1:A:44:LEU:HD13	1:A:109:ARG:HB2	0.43	1.89	18	1
1:A:44:LEU:HD13	1:A:45:ALA:N	0.43	2.29	5	1
1:A:59:ALA:HB1	1:A:85:TRP:CZ2	0.43	2.48	4	1
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:148:GLY:O	1:A:149:HIS:CG	0.43	2.72	3	2
1:A:50:GLY:C	1:A:51:VAL:HG23	0.43	2.39	11	1
1:A:43:PHE:CD1	1:A:43:PHE:N	0.43	2.87	13	2
1:A:77:ASN:C	1:A:78:VAL:HG22	0.42	2.38	2	1
1:A:172:VAL:HA	1:A:175:MET:HG2	0.42	1.91	2	1
1:A:75:TYR:C	1:A:76:THR:HG1	0.42	2.22	16	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
1:A:106:LEU:HD12	1:A:143:LEU:HG	0.42	1.91	2	1
1:A:172:VAL:HA	1:A:175:MET:HE3	0.42	1.89	12	2
1:A:44:LEU:HD13	1:A:138:SER:CA	0.42	2.44	20	1
1:A:78:VAL:HG22	1:A:79:ASP:N	0.42	2.29	11	1
1:A:46:THR:CG2	1:A:153:ILE:HG21	0.42	2.24	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LEU:C	1:A:105:TYR:CD2	0.42	2.97	19	1
1:A:152:GLY:N	1:A:172:VAL:HG13	0.42	2.29	1	1
1:A:127:LEU:O	1:A:128:SER:CB	0.42	2.67	3	1
1:A:82:LEU:CD2	1:A:175:MET:HE2	0.42	2.44	12	1
1:A:33:VAL:HG13	1:A:45:ALA:O	0.42	2.15	16	2
1:A:77:ASN:O	1:A:78:VAL:C	0.42	2.62	1	1
1:A:120:GLY:O	1:A:121:ASP:O	0.42	2.38	3	1
1:A:76:THR:HG22	1:A:83:VAL:CG1	0.42	2.44	4	1
1:A:161:ARG:O	1:A:161:ARG:CG	0.42	2.67	19	5
1:A:82:LEU:HD21	1:A:175:MET:SD	0.42	2.54	15	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:44:LEU:CD2	1:A:141:GLY:CA	0.42	2.98	20	1
1:A:141:GLY:O	1:A:153:ILE:HG22	0.42	2.15	13	1
1:A:108:THR:HG23	1:A:112:ASP:O	0.42	2.14	1	1
1:A:77:ASN:O	1:A:81:ASP:HB2	0.42	2.15	12	1
1:A:82:LEU:HD21	1:A:175:MET:HG2	0.42	1.91	14	1
1:A:55:VAL:HG21	1:A:57:HIS:NE2	0.42	2.30	19	1
1:A:66:GLY:N	1:A:69:GLY:O	0.42	2.53	2	1
1:A:53:TRP:HA	1:A:83:VAL:O	0.42	2.14	5	1
1:A:145:CYS:SG	1:A:146:PRO:CD	0.42	3.08	11	1
1:A:54:THR:CG2	1:A:85:TRP:CH2	0.42	2.97	12	1
1:A:105:TYR:CE1	1:A:144:LEU:O	0.42	2.73	14	1
1:A:55:VAL:HB	1:A:57:HIS:CE1	0.42	2.50	19	1
1:A:53:TRP:CE3	1:A:82:LEU:CD2	0.41	3.03	8	3
1:A:135:LEU:CD1	1:A:164:ALA:CB	0.41	2.98	12	2
1:A:43:PHE:CE2	1:A:58:GLY:C	0.41	2.98	17	1
1:A:126:LEU:HD21	1:A:164:ALA:O	0.41	2.14	2	1
1:A:57:HIS:CD2	1:A:57:HIS:C	0.41	2.97	18	2
1:A:122:SER:CA	1:A:169:PHE:O	0.41	2.68	15	3
1:A:132:VAL:HG23	1:A:159:CYS:SG	0.41	2.55	8	1
1:A:43:PHE:CD2	1:A:58:GLY:O	0.41	2.73	19	1
1:A:154:PHE:CE1	1:A:156:ALA:O	0.41	2.73	17	5
1:A:29:VAL:HG11	1:A:89:PRO:HB2	0.41	1.93	8	1
1:A:115:PRO:HB2	1:A:127:LEU:HD12	0.41	1.91	9	2
1:A:44:LEU:CD2	1:A:109:ARG:CB	0.41	2.98	14	2
1:A:47:CYS:CB	1:A:91:ALA:HB3	0.41	2.45	14	1
1:A:87:ALA:HB1	1:A:88:PRO:CD	0.41	2.45	2	1
1:A:44:LEU:CB	1:A:139:SER:O	0.41	2.68	20	2
1:A:170:VAL:CG2	1:A:175:MET:SD	0.41	3.09	15	1
1:A:104:LEU:C	1:A:105:TYR:CD1	0.41	2.98	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:THR:HG23	1:A:178:THR:N	0.41	2.30	4	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:88:PRO:CG	1:A:89:PRO:CD	0.41	2.99	2	2
1:A:54:THR:CG2	1:A:83:VAL:HG23	0.41	2.44	8	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:CZ2	0.41	2.99	13	1
1:A:29:VAL:HG21	1:A:89:PRO:HG3	0.41	1.91	14	1
1:A:54:THR:CG2	1:A:85:TRP:CZ3	0.41	3.03	14	1
1:A:71:ILE:HG21	1:A:85:TRP:CE3	0.41	2.50	16	1
1:A:103:ASP:O	1:A:145:CYS:HA	0.41	2.16	1	1
1:A:38:THR:O	1:A:40:THR:N	0.41	2.54	16	5
1:A:104:LEU:HD21	1:A:151:VAL:HG11	0.41	1.92	11	1
1:A:132:VAL:N	1:A:162:GLY:O	0.41	2.50	15	1
1:A:126:LEU:HD22	1:A:128:SER:O	0.41	2.16	7	1
1:A:46:THR:CG2	1:A:153:ILE:CG2	0.41	2.99	10	2
1:A:108:THR:HG21	1:A:134:TYR:CE1	0.41	2.51	10	1
1:A:114:ILE:O	1:A:116:VAL:HG23	0.41	2.15	16	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:145:CYS:HB2	1:A:146:PRO:HD2	0.41	1.93	16	1
1:A:50:GLY:N	1:A:93:SER:CB	0.41	2.84	19	1
1:A:75:TYR:CZ	1:A:179:MET:HG3	0.40	2.50	3	1
1:A:151:VAL:CG1	1:A:169:PHE:CZ	0.40	3.03	3	1
1:A:106:LEU:CD1	1:A:143:LEU:HD11	0.40	2.47	7	1
1:A:56:TYR:CB	1:A:78:VAL:CG1	0.40	2.99	9	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:105:TYR:CD1	1:A:105:TYR:N	0.40	2.89	14	1
1:A:88:PRO:O	1:A:90:GLY:N	0.40	2.55	19	1
1:A:117:ARG:O	1:A:125:SER:N	0.40	2.55	19	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
1:A:153:ILE:HG13	1:A:170:VAL:CG1	0.40	2.46	17	1
1:A:54:THR:CG2	1:A:83:VAL:CG2	0.40	2.99	18	1
1:A:107:VAL:CG2	1:A:113:VAL:HG12	0.40	2.40	4	1
1:A:43:PHE:CZ	1:A:58:GLY:C	0.40	2.99	12	1
1:A:175:MET:HG3	1:A:176:GLU:N	0.40	2.30	16	1
1:A:43:PHE:CG	1:A:58:GLY:O	0.40	2.74	19	1
1:A:54:THR:O	1:A:54:THR:HG23	0.40	2.16	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:CYS:HB2	1:A:146:PRO:CD	0.40	2.46	6	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:36:VAL:HG21	1:A:64:LEU:HD21	0.40	1.94	18	1
1:A:86:GLN:O	1:A:88:PRO:CD	0.40	2.70	8	1
1:A:35:VAL:HG13	1:A:109:ARG:CD	0.40	2.46	16	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	154/186 (83%)	114±4 (74±3%)	28±4 (18±2%)	12±3 (8±2%)	1	13
All	All	3080/3720 (83%)	2280 (74%)	554 (18%)	246 (8%)	1	13

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	94	LEU	9
1	A	106	LEU	9
1	A	149	HIS	9
1	A	147	SER	9
1	A	58	GLY	8
1	A	88	PRO	8
1	A	81	ASP	7
1	A	59	ALA	7
1	A	39	ALA	6
1	A	93	SER	6
1	A	63	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	A	89	PRO	6
1	A	62	LYS	6
1	A	31	GLY	5
1	A	121	ASP	5
1	A	79	ASP	5
1	A	29	VAL	4
1	A	41	GLN	4
1	A	145	CYS	4
1	A	146	PRO	4
1	A	182	SER	4
1	A	74	MET	4
1	A	30	GLU	4
1	A	67	PRO	4
1	A	78	VAL	3
1	A	110	HIS	3
1	A	80	GLN	3
1	A	98	THR	2
1	A	52	CYS	2
1	A	120	GLY	2
1	A	61	SER	2
1	A	73	GLN	2
1	A	33	VAL	2
1	A	142	PRO	2
1	A	129	PRO	2
1	A	72	THR	1
1	A	91	ALA	1
1	A	111	ALA	1
1	A	92	ARG	1
1	A	64	LEU	1
1	A	141	GLY	1
1	A	95	THR	1
1	A	96	PRO	1
1	A	100	GLY	1
1	A	101	SER	1
1	A	102	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%)	97±4 (78±3%)	27±4 (22±3%)	3	30
All	All	2480/3020 (82%)	1943 (78%)	537 (22%)	3	30

All 84 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	163	VAL	20
1	A	64	LEU	19
1	A	167	VAL	18
1	A	161	ARG	17
1	A	125	SER	16
1	A	126	LEU	16
1	A	128	SER	16
1	A	153	ILE	16
1	A	110	HIS	15
1	A	151	VAL	15
1	A	179	MET	14
1	A	94	LEU	13
1	A	95	THR	12
1	A	104	LEU	12
1	A	82	LEU	12
1	A	40	THR	11
1	A	168	ASP	10
1	A	178	THR	10
1	A	41	GLN	10
1	A	147	SER	10
1	A	44	LEU	9
1	A	136	LYS	9
1	A	109	ARG	9
1	A	180	ARG	9
1	A	117	ARG	8
1	A	170	VAL	8
1	A	121	ASP	8
1	A	123	ARG	8
1	A	30	GLU	8
1	A	62	LYS	7
1	A	79	ASP	7
1	A	143	LEU	7
1	A	112	ASP	7
1	A	122	SER	6
1	A	81	ASP	6
1	A	119	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	160	THR	6
1	A	36	VAL	5
1	A	68	LYS	5
1	A	76	THR	5
1	A	29	VAL	5
1	A	97	CYS	5
1	A	63	THR	4
1	A	102	SER	4
1	A	32	GLU	4
1	A	118	ARG	4
1	A	34	GLN	4
1	A	101	SER	4
1	A	139	SER	4
1	A	43	PHE	4
1	A	49	ASN	4
1	A	61	SER	4
1	A	74	MET	3
1	A	169	PHE	3
1	A	130	ARG	3
1	A	176	GLU	3
1	A	80	GLN	3
1	A	77	ASN	3
1	A	92	ARG	3
1	A	182	SER	3
1	A	155	ARG	3
1	A	175	MET	3
1	A	174	SER	3
1	A	133	SER	2
1	A	149	HIS	2
1	A	103	ASP	2
1	A	33	VAL	2
1	A	73	GLN	2
1	A	83	VAL	2
1	A	85	TRP	2
1	A	145	CYS	2
1	A	98	THR	1
1	A	138	SER	1
1	A	37	SER	1
1	A	158	VAL	1
1	A	134	TYR	1
1	A	86	GLN	1
1	A	113	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	52	CYS	1
1	A	106	LEU	1
1	A	108	THR	1
1	A	54	THR	1
1	A	177	THR	1
1	A	93	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 oligosaccharides 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