



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 08:53 PM BST

PDB ID : 2J8P
Title : NMR STRUCTURE OF C-TERMINAL DOMAIN OF HUMAN CSTF-64
Authors : Qu, X.; Perez-Canadillas, J.M.; Agrawal, S.; De Baecke, J.; Cheng, H.; Varani, G.; Moore, C.
Deposited on : 2006-10-27

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

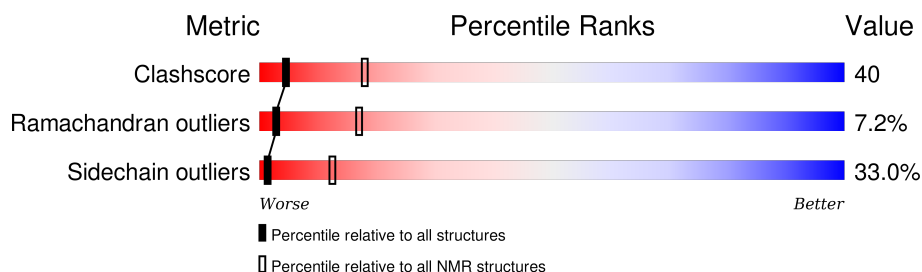
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	49	<div> <div></div> <div>31%</div> <div>41%</div> <div>16%</div> <div>12%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 1 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:530-A:572 (43)	0.50	1

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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 15, 16, 17, 18, 20, 23, 27, 29, 30
2	4, 13, 22, 24, 26, 28
3	14, 19, 21, 25

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 782 atoms, of which 400 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT.

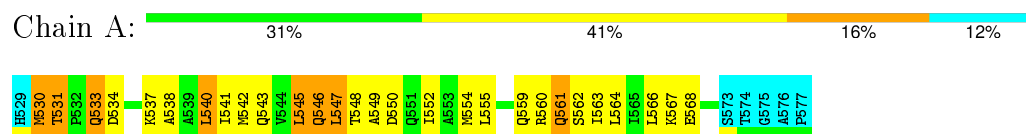
Mol	Chain	Residues	Atoms						Trace
1	A	49	Total	C	H	N	O	S	0
			782	240	400	67	72	3	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT

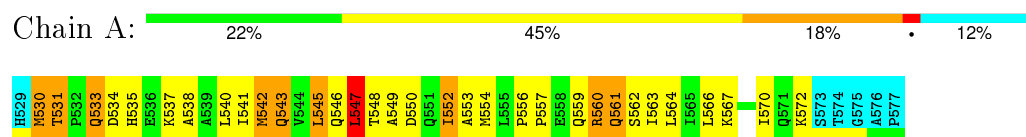


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

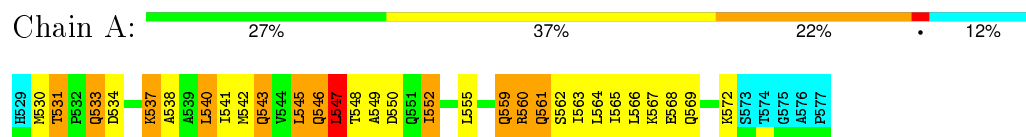
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



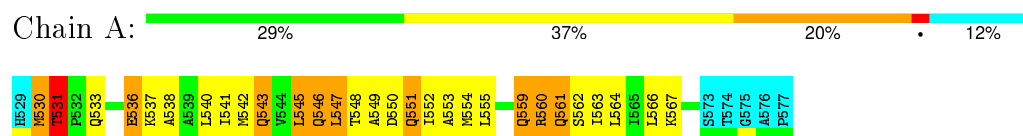
4.2.2 Score per residue for model 2

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



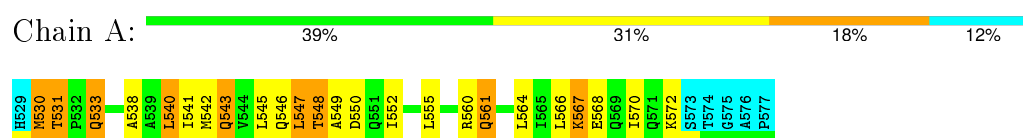
4.2.3 Score per residue for model 3

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



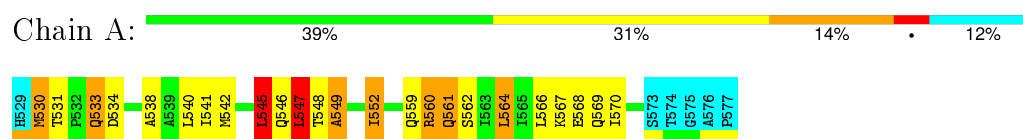
4.2.4 Score per residue for model 4

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



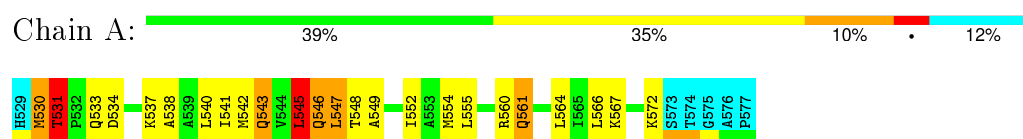
4.2.5 Score per residue for model 5

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



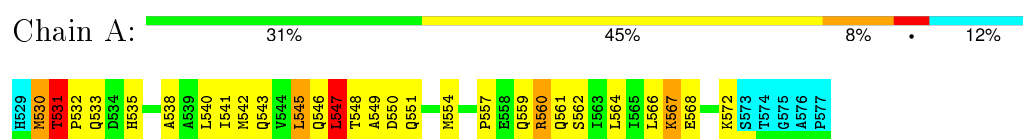
4.2.6 Score per residue for model 6

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



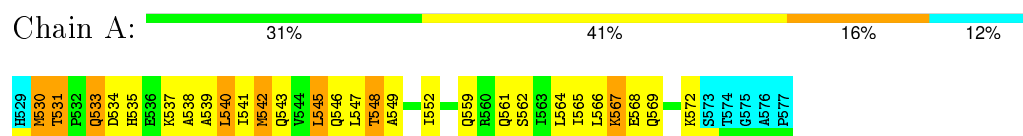
4.2.7 Score per residue for model 7

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



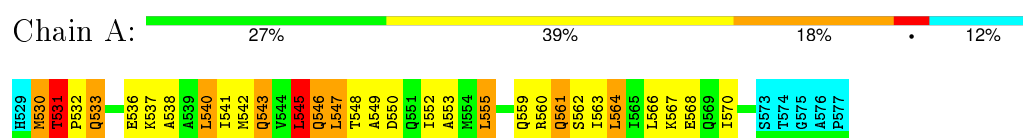
4.2.8 Score per residue for model 8

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



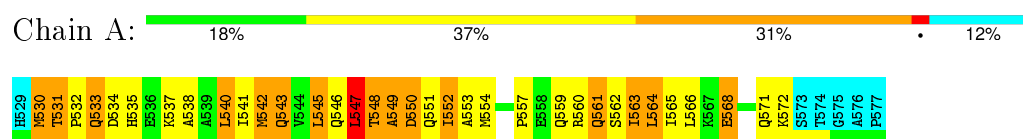
4.2.9 Score per residue for model 9

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



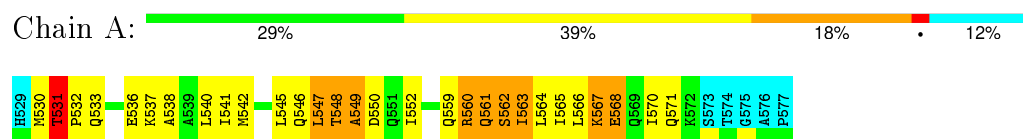
4.2.10 Score per residue for model 10

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



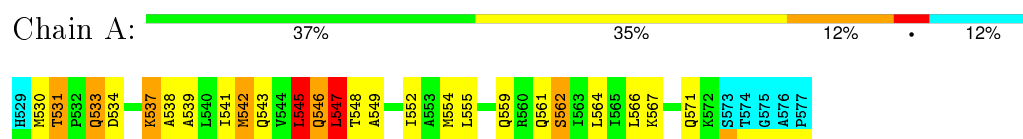
4.2.11 Score per residue for model 11

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



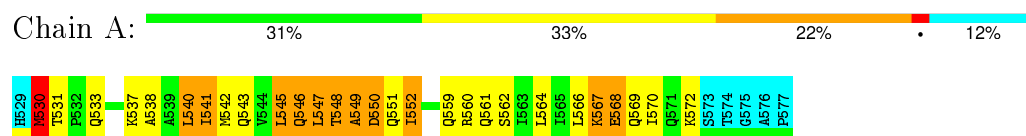
4.2.12 Score per residue for model 12

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



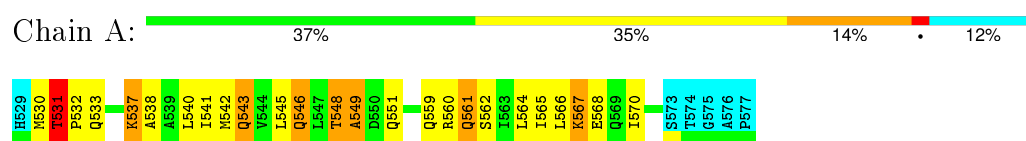
4.2.13 Score per residue for model 13

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



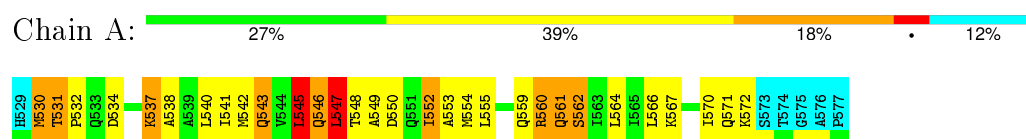
4.2.14 Score per residue for model 14

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



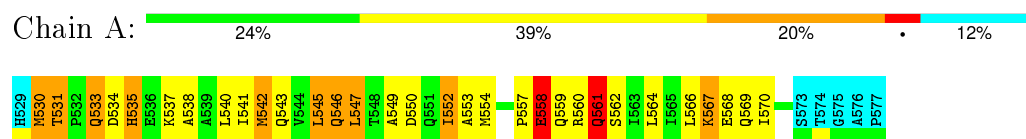
4.2.15 Score per residue for model 15

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



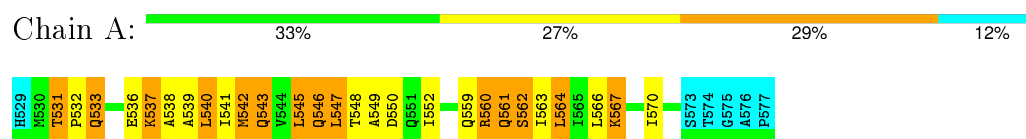
4.2.16 Score per residue for model 16

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



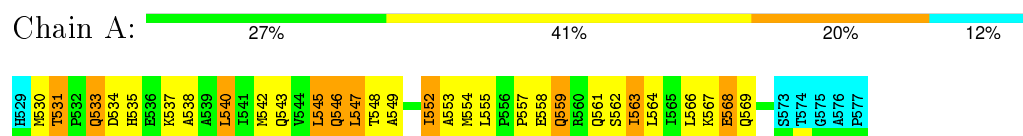
4.2.17 Score per residue for model 17

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



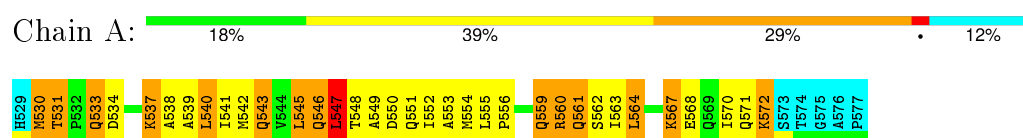
4.2.18 Score per residue for model 18

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



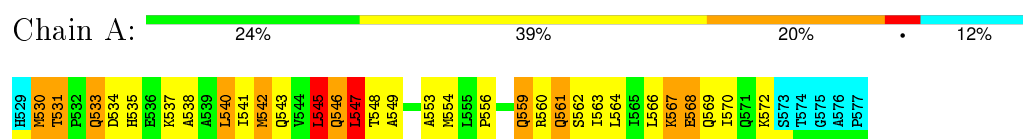
4.2.19 Score per residue for model 19

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



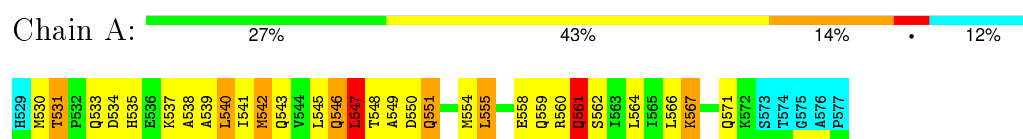
4.2.20 Score per residue for model 20

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



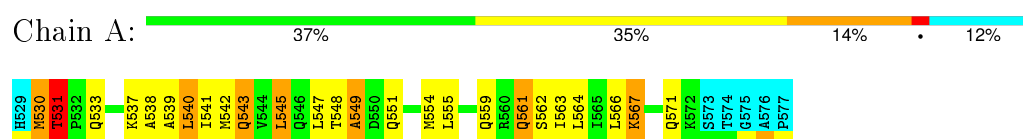
4.2.21 Score per residue for model 21

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



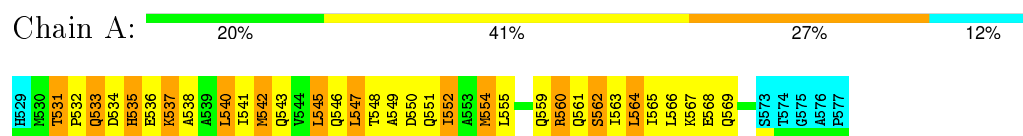
4.2.22 Score per residue for model 22

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



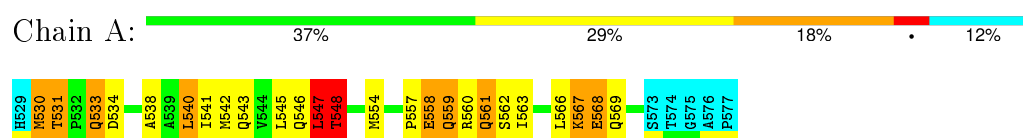
4.2.23 Score per residue for model 23

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



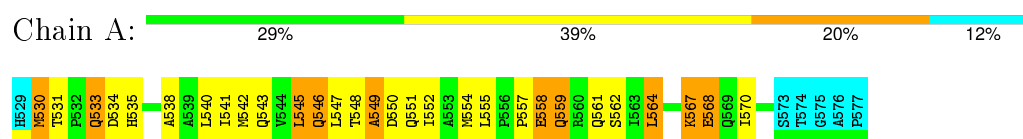
4.2.24 Score per residue for model 24

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



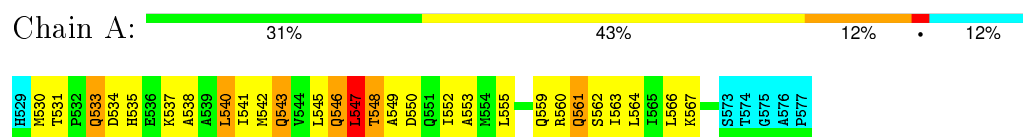
4.2.25 Score per residue for model 25

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



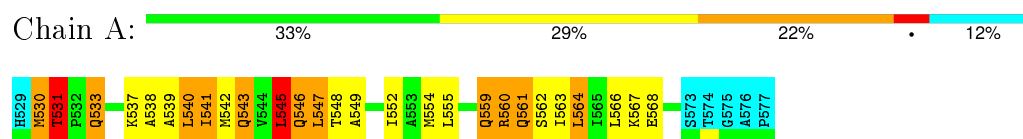
4.2.26 Score per residue for model 26

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



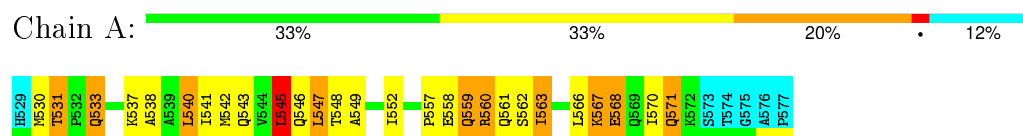
4.2.27 Score per residue for model 27

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



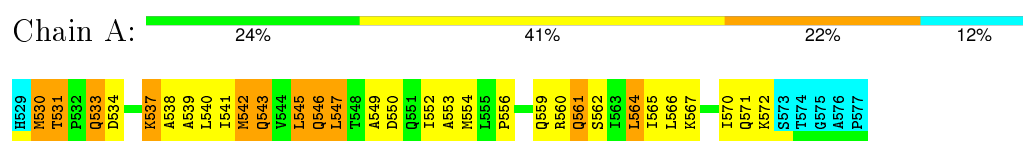
4.2.28 Score per residue for model 28

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



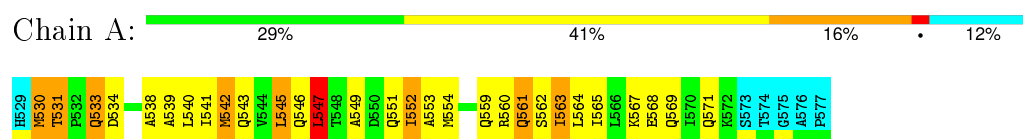
4.2.29 Score per residue for model 29

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



4.2.30 Score per residue for model 30

- Molecule 1: CLEAVAGE STIMULATION FACTOR 64 KDA SUBUNIT



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 35 calculated structures, 30 were deposited, based on the following criterion: *STRUCTURES HAVING NO DISTANCE RESTRAINT VIOLATION LARGER THAN 0.2 Å OR NO VIOLATION OF DIHEDRAL ANGLE CONSTRAINTS LARGER THAN 5 DEGREES*.

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

Software name	Classification	Version
CYANA	refinement	
ANSIG	structure solution	
TALOS	structure solution	
CYANA	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 ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	343	366	366	28±6
All	All	10290	10980	10980	844

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:545:LEU:HD22	1:A:552:ILE:HD11	1.04	1.21	19	5
1:A:552:ILE:HD13	1:A:555:LEU:HD12	0.97	1.36	12	5
1:A:545:LEU:HD23	1:A:546:GLN:OE1	0.93	1.63	23	4
1:A:541:ILE:HG22	1:A:545:LEU:CD1	0.92	1.94	1	1
1:A:545:LEU:CD2	1:A:552:ILE:HD11	0.92	1.94	19	3
1:A:540:LEU:HD12	1:A:540:LEU:O	0.91	1.66	9	11
1:A:540:LEU:O	1:A:540:LEU:HD12	0.90	1.66	24	12
1:A:545:LEU:HD23	1:A:546:GLN:CD	0.87	1.90	16	2
1:A:538:ALA:HB2	1:A:560:ARG:O	0.86	1.70	6	11
1:A:545:LEU:CD2	1:A:563:ILE:HD11	0.85	2.01	27	1
1:A:547:LEU:O	1:A:548:THR:HG23	0.84	1.73	24	6
1:A:541:ILE:HG22	1:A:545:LEU:HD13	0.84	1.48	1	1
1:A:542:MET:SD	1:A:549:ALA:HB2	0.79	2.18	20	6
1:A:552:ILE:HA	1:A:555:LEU:HD12	0.78	1.53	23	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:561:GLN:OE1	1:A:564:LEU:HD22	0.78	1.78	26	3
1:A:537:LYS:O	1:A:541:ILE:HD12	0.78	1.77	8	4
1:A:537:LYS:CB	1:A:564:LEU:HD12	0.77	2.10	17	10
1:A:541:ILE:HG22	1:A:545:LEU:HD12	0.77	1.57	12	2
1:A:537:LYS:HB3	1:A:564:LEU:HD12	0.75	1.57	29	9
1:A:567:LYS:HA	1:A:570:ILE:HD12	0.74	1.57	25	10
1:A:563:ILE:HG22	1:A:567:LYS:CD	0.73	2.13	22	1
1:A:542:MET:CE	1:A:552:ILE:HD13	0.73	2.13	13	1
1:A:563:ILE:HG22	1:A:567:LYS:HD2	0.72	1.60	22	1
1:A:545:LEU:HD22	1:A:546:GLN:OE1	0.72	1.85	30	1
1:A:530:MET:C	1:A:531:THR:HG23	0.71	2.06	14	5
1:A:541:ILE:HG22	1:A:545:LEU:HD23	0.70	1.63	5	3
1:A:547:LEU:C	1:A:547:LEU:HD12	0.70	2.07	11	2
1:A:545:LEU:HD13	1:A:546:GLN:OE1	0.70	1.85	30	1
1:A:538:ALA:HB1	1:A:563:ILE:HB	0.70	1.64	30	2
1:A:541:ILE:HG21	1:A:567:LYS:CG	0.69	2.16	26	14
1:A:541:ILE:HD13	1:A:564:LEU:HA	0.69	1.65	25	3
1:A:541:ILE:HD13	1:A:567:LYS:CE	0.69	2.18	22	1
1:A:546:GLN:O	1:A:547:LEU:CB	0.67	2.41	17	18
1:A:548:THR:O	1:A:549:ALA:HB3	0.67	1.89	13	17
1:A:564:LEU:HD23	1:A:564:LEU:C	0.67	2.09	10	11
1:A:545:LEU:HD23	1:A:551:GLN:OE1	0.67	1.89	25	1
1:A:541:ILE:HD13	1:A:567:LYS:HE2	0.67	1.65	22	1
1:A:545:LEU:HD13	1:A:546:GLN:N	0.66	2.05	29	1
1:A:545:LEU:HD22	1:A:552:ILE:CD1	0.66	2.12	19	1
1:A:541:ILE:HG21	1:A:567:LYS:HG3	0.66	1.67	26	13
1:A:537:LYS:CD	1:A:564:LEU:HD12	0.66	2.20	10	1
1:A:551:GLN:H	1:A:551:GLN:NE2	0.66	1.88	7	1
1:A:547:LEU:HD13	1:A:547:LEU:O	0.66	1.91	25	1
1:A:547:LEU:O	1:A:547:LEU:HD12	0.66	1.91	5	1
1:A:545:LEU:HD12	1:A:546:GLN:HG3	0.65	1.67	9	2
1:A:564:LEU:C	1:A:564:LEU:HD23	0.65	2.11	25	11
1:A:548:THR:HG22	1:A:550:ASP:H	0.64	1.51	3	4
1:A:546:GLN:NE2	1:A:551:GLN:HE22	0.64	1.90	3	1
1:A:547:LEU:HD12	1:A:547:LEU:O	0.64	1.91	28	4
1:A:541:ILE:O	1:A:545:LEU:HD13	0.64	1.93	1	1
1:A:567:LYS:HE2	1:A:570:ILE:HD12	0.64	1.70	29	4
1:A:542:MET:CE	1:A:549:ALA:HB1	0.63	2.24	17	1
1:A:546:GLN:O	1:A:547:LEU:HD23	0.63	1.94	1	2
1:A:552:ILE:HD13	1:A:555:LEU:CD1	0.62	2.20	12	2
1:A:538:ALA:O	1:A:542:MET:N	0.62	2.32	23	30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:543:GLN:CB	1:A:547:LEU:HD12	0.62	2.25	3	1
1:A:555:LEU:N	1:A:555:LEU:HD23	0.61	2.09	9	1
1:A:546:GLN:NE2	1:A:547:LEU:N	0.61	2.48	13	2
1:A:545:LEU:HD13	1:A:563:ILE:HD11	0.61	1.73	18	1
1:A:538:ALA:HB3	1:A:560:ARG:HG2	0.61	1.70	15	4
1:A:531:THR:CB	1:A:532:PRO:CD	0.61	2.79	17	7
1:A:545:LEU:CG	1:A:563:ILE:HD11	0.60	2.25	27	1
1:A:545:LEU:HG	1:A:563:ILE:HD11	0.60	1.73	27	2
1:A:535:HIS:CE1	1:A:558:GLU:CG	0.60	2.84	25	1
1:A:535:HIS:CE1	1:A:557:PRO:O	0.60	2.55	10	2
1:A:549:ALA:O	1:A:553:ALA:HB2	0.60	1.96	20	5
1:A:557:PRO:O	1:A:558:GLU:CB	0.60	2.50	18	5
1:A:537:LYS:HD3	1:A:564:LEU:HD12	0.59	1.74	10	1
1:A:540:LEU:HD12	1:A:540:LEU:C	0.58	2.19	24	7
1:A:541:ILE:O	1:A:545:LEU:HD23	0.58	1.98	2	3
1:A:537:LYS:O	1:A:540:LEU:HD23	0.58	1.98	18	1
1:A:559:GLN:O	1:A:562:SER:CB	0.58	2.52	29	26
1:A:541:ILE:O	1:A:541:ILE:CG2	0.57	2.51	19	6
1:A:546:GLN:C	1:A:546:GLN:CD	0.57	2.62	29	1
1:A:541:ILE:HD13	1:A:567:LYS:HB3	0.57	1.75	19	1
1:A:548:THR:O	1:A:549:ALA:CB	0.57	2.53	5	17
1:A:541:ILE:HG21	1:A:567:LYS:HG2	0.57	1.76	20	2
1:A:547:LEU:CG	1:A:547:LEU:O	0.57	2.52	26	5
1:A:547:LEU:O	1:A:547:LEU:HD23	0.57	2.00	16	2
1:A:538:ALA:HB3	1:A:560:ARG:CG	0.56	2.30	27	3
1:A:542:MET:SD	1:A:552:ILE:HD13	0.56	2.41	13	1
1:A:532:PRO:HA	1:A:535:HIS:CD2	0.56	2.35	23	1
1:A:546:GLN:O	1:A:547:LEU:CG	0.56	2.54	5	2
1:A:530:MET:CG	1:A:530:MET:O	0.56	2.51	14	1
1:A:542:MET:CE	1:A:549:ALA:HB2	0.56	2.31	27	4
1:A:547:LEU:CD1	1:A:547:LEU:O	0.55	2.54	26	4
1:A:530:MET:C	1:A:531:THR:CG2	0.55	2.74	14	5
1:A:539:ALA:O	1:A:542:MET:HE2	0.55	2.02	30	1
1:A:542:MET:CE	1:A:560:ARG:NH1	0.55	2.69	19	1
1:A:538:ALA:HB3	1:A:560:ARG:HG3	0.55	1.78	23	1
1:A:552:ILE:HG22	1:A:560:ARG:HD2	0.55	1.77	28	2
1:A:540:LEU:O	1:A:543:GLN:NE2	0.55	2.38	19	20
1:A:545:LEU:CD1	1:A:546:GLN:N	0.55	2.70	29	1
1:A:530:MET:O	1:A:530:MET:CG	0.55	2.53	15	1
1:A:564:LEU:HD23	1:A:565:ILE:HD13	0.55	1.78	14	1
1:A:564:LEU:CD2	1:A:565:ILE:HD13	0.55	2.32	10	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:546:GLN:CB	1:A:551:GLN:NE2	0.55	2.70	10	2
1:A:560:ARG:CZ	1:A:560:ARG:HA	0.55	2.32	23	1
1:A:561:GLN:NE2	1:A:565:ILE:HD11	0.55	2.17	11	2
1:A:530:MET:CE	1:A:535:HIS:NE2	0.55	2.70	10	1
1:A:563:ILE:O	1:A:567:LYS:N	0.54	2.41	22	2
1:A:551:GLN:CD	1:A:551:GLN:N	0.54	2.61	7	1
1:A:540:LEU:C	1:A:540:LEU:HD12	0.54	2.21	20	7
1:A:537:LYS:CG	1:A:564:LEU:HD12	0.54	2.33	10	4
1:A:542:MET:O	1:A:546:GLN:N	0.53	2.41	14	4
1:A:551:GLN:O	1:A:555:LEU:CD2	0.53	2.56	21	1
1:A:535:HIS:CE1	1:A:558:GLU:HG2	0.53	2.39	25	1
1:A:547:LEU:O	1:A:547:LEU:CD1	0.53	2.57	5	2
1:A:541:ILE:HG22	1:A:541:ILE:O	0.53	2.03	2	2
1:A:538:ALA:CB	1:A:560:ARG:O	0.52	2.57	30	4
1:A:546:GLN:NE2	1:A:546:GLN:C	0.52	2.62	17	1
1:A:547:LEU:O	1:A:548:THR:CG2	0.52	2.57	28	5
1:A:547:LEU:HG	1:A:547:LEU:O	0.52	2.04	26	3
1:A:545:LEU:HD21	1:A:567:LYS:HD3	0.52	1.80	13	1
1:A:541:ILE:O	1:A:541:ILE:HG22	0.52	2.05	10	4
1:A:542:MET:O	1:A:546:GLN:CB	0.52	2.57	19	4
1:A:547:LEU:HD12	1:A:547:LEU:C	0.52	2.25	26	2
1:A:531:THR:CB	1:A:532:PRO:HD2	0.52	2.35	17	5
1:A:541:ILE:HG23	1:A:567:LYS:HE3	0.52	1.82	3	1
1:A:549:ALA:O	1:A:553:ALA:CB	0.52	2.57	20	5
1:A:541:ILE:HG22	1:A:545:LEU:CD2	0.51	2.32	5	2
1:A:556:PRO:O	1:A:560:ARG:CG	0.51	2.58	1	4
1:A:542:MET:SD	1:A:549:ALA:CB	0.51	2.99	16	5
1:A:559:GLN:O	1:A:562:SER:N	0.51	2.43	29	5
1:A:532:PRO:O	1:A:536:GLU:CB	0.51	2.58	23	3
1:A:545:LEU:CD1	1:A:546:GLN:OE1	0.51	2.58	30	1
1:A:545:LEU:CD2	1:A:546:GLN:OE1	0.51	2.57	30	2
1:A:564:LEU:O	1:A:568:GLU:CB	0.51	2.59	14	6
1:A:538:ALA:HB1	1:A:563:ILE:CB	0.51	2.34	30	1
1:A:541:ILE:HD12	1:A:567:LYS:HD2	0.51	1.83	14	3
1:A:555:LEU:HD23	1:A:555:LEU:N	0.50	2.21	21	1
1:A:547:LEU:O	1:A:547:LEU:HG	0.50	2.06	4	1
1:A:546:GLN:CD	1:A:547:LEU:N	0.50	2.64	11	3
1:A:534:ASP:O	1:A:537:LYS:CG	0.50	2.60	19	1
1:A:533:GLN:HE21	1:A:534:ASP:N	0.50	2.05	10	13
1:A:564:LEU:O	1:A:568:GLU:CG	0.50	2.59	9	3
1:A:537:LYS:O	1:A:540:LEU:CD2	0.50	2.59	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:542:MET:SD	1:A:552:ILE:HG21	0.50	2.46	29	1
1:A:546:GLN:OE1	1:A:548:THR:CB	0.50	2.60	6	1
1:A:555:LEU:HB3	1:A:560:ARG:NH2	0.50	2.22	23	1
1:A:551:GLN:O	1:A:554:MET:CG	0.50	2.59	23	4
1:A:547:LEU:O	1:A:547:LEU:CG	0.49	2.60	1	1
1:A:565:ILE:O	1:A:568:GLU:CG	0.49	2.60	30	4
1:A:546:GLN:CD	1:A:546:GLN:O	0.49	2.51	17	1
1:A:561:GLN:O	1:A:564:LEU:N	0.49	2.45	29	19
1:A:542:MET:O	1:A:546:GLN:CG	0.49	2.61	19	3
1:A:551:GLN:NE2	1:A:551:GLN:N	0.49	2.60	7	1
1:A:541:ILE:HD13	1:A:567:LYS:CB	0.49	2.36	19	1
1:A:533:GLN:O	1:A:537:LYS:CG	0.49	2.61	9	1
1:A:546:GLN:O	1:A:548:THR:N	0.49	2.46	21	4
1:A:545:LEU:C	1:A:545:LEU:HD13	0.49	2.28	29	1
1:A:530:MET:HB3	1:A:535:HIS:CE1	0.49	2.43	8	2
1:A:539:ALA:O	1:A:542:MET:CG	0.49	2.61	8	1
1:A:539:ALA:O	1:A:543:GLN:OE1	0.49	2.31	27	1
1:A:545:LEU:HD21	1:A:563:ILE:HD12	0.48	1.83	1	1
1:A:535:HIS:C	1:A:535:HIS:ND1	0.48	2.67	16	2
1:A:546:GLN:HE22	1:A:548:THR:N	0.48	2.07	13	1
1:A:539:ALA:O	1:A:542:MET:CE	0.48	2.62	12	1
1:A:547:LEU:C	1:A:548:THR:HG23	0.48	2.29	28	1
1:A:530:MET:O	1:A:531:THR:HG23	0.48	2.09	14	3
1:A:546:GLN:NE2	1:A:548:THR:OG1	0.48	2.46	17	1
1:A:540:LEU:C	1:A:543:GLN:OE1	0.48	2.52	27	1
1:A:542:MET:SD	1:A:549:ALA:CA	0.48	3.02	6	3
1:A:552:ILE:HD11	1:A:563:ILE:CD1	0.48	2.38	3	1
1:A:552:ILE:HG23	1:A:560:ARG:CG	0.48	2.39	26	2
1:A:541:ILE:HG23	1:A:567:LYS:HG2	0.48	1.85	11	2
1:A:546:GLN:O	1:A:547:LEU:CD2	0.48	2.62	1	2
1:A:542:MET:HG3	1:A:552:ILE:HG21	0.48	1.85	17	1
1:A:546:GLN:CG	1:A:551:GLN:NE2	0.48	2.76	10	1
1:A:560:ARG:O	1:A:562:SER:N	0.48	2.47	21	2
1:A:542:MET:O	1:A:546:GLN:NE2	0.48	2.46	5	1
1:A:531:THR:CB	1:A:533:GLN:NE2	0.47	2.77	26	1
1:A:542:MET:CE	1:A:552:ILE:CD1	0.47	2.90	13	1
1:A:548:THR:HG22	1:A:550:ASP:N	0.47	2.22	21	1
1:A:546:GLN:NE2	1:A:551:GLN:NE2	0.47	2.59	3	1
1:A:538:ALA:HB1	1:A:563:ILE:CG2	0.47	2.40	30	1
1:A:542:MET:SD	1:A:552:ILE:CG2	0.47	3.03	5	2
1:A:549:ALA:O	1:A:553:ALA:N	0.47	2.48	29	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:560:ARG:C	1:A:562:SER:N	0.47	2.68	21	2
1:A:547:LEU:O	1:A:548:THR:OG1	0.47	2.33	4	1
1:A:546:GLN:CD	1:A:546:GLN:C	0.47	2.73	17	1
1:A:533:GLN:CD	1:A:533:GLN:C	0.47	2.73	24	3
1:A:542:MET:HE1	1:A:552:ILE:HD13	0.47	1.84	13	1
1:A:550:ASP:O	1:A:554:MET:CG	0.47	2.63	25	2
1:A:546:GLN:NE2	1:A:548:THR:CB	0.47	2.78	17	1
1:A:533:GLN:C	1:A:533:GLN:CD	0.46	2.74	4	4
1:A:543:GLN:O	1:A:547:LEU:HA	0.46	2.09	29	2
1:A:546:GLN:O	1:A:547:LEU:C	0.46	2.54	21	3
1:A:545:LEU:HD11	1:A:563:ILE:HD12	0.46	1.85	20	1
1:A:567:LYS:CE	1:A:570:ILE:HD12	0.46	2.40	20	1
1:A:552:ILE:HG23	1:A:560:ARG:CD	0.46	2.40	26	1
1:A:550:ASP:O	1:A:553:ALA:HB3	0.46	2.10	26	2
1:A:546:GLN:C	1:A:548:THR:N	0.46	2.68	14	4
1:A:535:HIS:CD2	1:A:535:HIS:N	0.46	2.84	26	1
1:A:545:LEU:HD12	1:A:567:LYS:HD3	0.46	1.88	19	1
1:A:545:LEU:HD13	1:A:563:ILE:CG1	0.46	2.41	19	1
1:A:546:GLN:O	1:A:547:LEU:HB3	0.46	2.11	18	5
1:A:561:GLN:OE1	1:A:564:LEU:CD2	0.45	2.58	26	1
1:A:542:MET:SD	1:A:549:ALA:N	0.45	2.89	6	3
1:A:542:MET:HG2	1:A:543:GLN:N	0.45	2.26	28	5
1:A:533:GLN:O	1:A:537:LYS:N	0.45	2.49	23	2
1:A:555:LEU:CD2	1:A:555:LEU:N	0.45	2.77	9	1
1:A:561:GLN:HE22	1:A:565:ILE:HD11	0.45	1.70	11	1
1:A:541:ILE:HD13	1:A:567:LYS:HG3	0.45	1.87	30	3
1:A:568:GLU:HG3	1:A:569:GLN:N	0.45	2.27	13	3
1:A:551:GLN:O	1:A:555:LEU:HD21	0.45	2.12	21	1
1:A:538:ALA:HB2	1:A:560:ARG:C	0.45	2.31	27	1
1:A:542:MET:SD	1:A:552:ILE:CG1	0.45	3.05	26	1
1:A:535:HIS:CE1	1:A:558:GLU:HG3	0.45	2.45	25	1
1:A:543:GLN:O	1:A:547:LEU:CA	0.45	2.64	30	1
1:A:546:GLN:NE2	1:A:548:THR:O	0.45	2.50	23	1
1:A:552:ILE:HD11	1:A:563:ILE:HD12	0.45	1.88	10	2
1:A:537:LYS:HB3	1:A:564:LEU:HD13	0.44	1.89	14	1
1:A:539:ALA:O	1:A:543:GLN:NE2	0.44	2.49	17	2
1:A:542:MET:HE1	1:A:549:ALA:HB2	0.44	1.88	27	2
1:A:540:LEU:HG	1:A:541:ILE:HD12	0.44	1.88	22	1
1:A:567:LYS:O	1:A:571:GLN:NE2	0.44	2.51	12	3
1:A:546:GLN:HG3	1:A:551:GLN:NE2	0.44	2.28	10	1
1:A:535:HIS:CD2	1:A:558:GLU:HA	0.44	2.46	21	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:548:THR:HG22	1:A:550:ASP:HB2	0.44	1.90	13	4
1:A:545:LEU:HD21	1:A:563:ILE:HG12	0.44	1.90	2	1
1:A:546:GLN:CD	1:A:551:GLN:NE2	0.44	2.71	3	1
1:A:541:ILE:CG2	1:A:567:LYS:HG3	0.43	2.43	14	7
1:A:542:MET:CG	1:A:548:THR:O	0.43	2.66	27	1
1:A:534:ASP:OD1	1:A:561:GLN:CG	0.43	2.66	15	1
1:A:530:MET:O	1:A:531:THR:O	0.43	2.36	10	16
1:A:535:HIS:ND1	1:A:557:PRO:O	0.43	2.51	1	2
1:A:540:LEU:O	1:A:543:GLN:OE1	0.43	2.36	27	1
1:A:560:ARG:CZ	1:A:560:ARG:CA	0.43	2.96	23	1
1:A:545:LEU:HD23	1:A:563:ILE:HD11	0.43	1.85	27	1
1:A:542:MET:CE	1:A:552:ILE:HG21	0.43	2.43	29	1
1:A:564:LEU:C	1:A:564:LEU:CD2	0.43	2.85	25	2
1:A:552:ILE:CG2	1:A:560:ARG:HD2	0.43	2.43	26	2
1:A:541:ILE:HG21	1:A:567:LYS:CD	0.43	2.43	20	1
1:A:542:MET:CE	1:A:542:MET:HA	0.43	2.44	21	1
1:A:530:MET:SD	1:A:535:HIS:CD2	0.43	3.12	10	1
1:A:538:ALA:HA	1:A:563:ILE:CG2	0.43	2.43	27	1
1:A:547:LEU:C	1:A:548:THR:CG2	0.43	2.88	28	1
1:A:546:GLN:O	1:A:547:LEU:HB2	0.43	2.13	17	3
1:A:537:LYS:O	1:A:541:ILE:CD1	0.43	2.60	8	1
1:A:557:PRO:O	1:A:558:GLU:HB2	0.42	2.14	28	1
1:A:539:ALA:HA	1:A:542:MET:CG	0.42	2.45	19	1
1:A:545:LEU:CG	1:A:546:GLN:OE1	0.42	2.67	30	1
1:A:545:LEU:CD2	1:A:567:LYS:NZ	0.42	2.82	28	1
1:A:542:MET:SD	1:A:546:GLN:OE1	0.42	2.77	26	2
1:A:552:ILE:CG2	1:A:560:ARG:CD	0.42	2.97	26	1
1:A:545:LEU:HD13	1:A:563:ILE:HG13	0.42	1.91	19	1
1:A:568:GLU:C	1:A:568:GLU:OE2	0.42	2.58	18	2
1:A:539:ALA:O	1:A:542:MET:HB2	0.42	2.15	21	1
1:A:547:LEU:C	1:A:548:THR:OG1	0.42	2.58	2	3
1:A:541:ILE:HD12	1:A:567:LYS:HG3	0.42	1.91	7	1
1:A:530:MET:O	1:A:534:ASP:HB2	0.42	2.14	15	1
1:A:541:ILE:HG23	1:A:545:LEU:HD23	0.42	1.90	22	1
1:A:540:LEU:O	1:A:543:GLN:CD	0.42	2.58	14	1
1:A:541:ILE:CG2	1:A:567:LYS:HG2	0.42	2.45	13	6
1:A:541:ILE:O	1:A:545:LEU:CD1	0.42	2.67	1	1
1:A:540:LEU:HD23	1:A:541:ILE:CD1	0.42	2.45	2	1
1:A:545:LEU:CD2	1:A:551:GLN:OE1	0.42	2.66	25	1
1:A:541:ILE:HD13	1:A:563:ILE:HG22	0.42	1.92	26	1
1:A:532:PRO:O	1:A:536:GLU:N	0.42	2.50	23	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:541:ILE:HG21	1:A:567:LYS:HD3	0.42	1.91	20	1
1:A:530:MET:O	1:A:531:THR:OG1	0.42	2.22	15	1
1:A:568:GLU:C	1:A:568:GLU:CD	0.42	2.78	11	3
1:A:541:ILE:O	1:A:545:LEU:N	0.41	2.46	29	1
1:A:538:ALA:O	1:A:542:MET:SD	0.41	2.78	29	1
1:A:554:MET:SD	1:A:554:MET:C	0.41	2.98	6	1
1:A:542:MET:HB2	1:A:552:ILE:CD1	0.41	2.45	30	1
1:A:542:MET:SD	1:A:548:THR:C	0.41	2.99	27	1
1:A:559:GLN:O	1:A:560:ARG:C	0.41	2.58	21	2
1:A:546:GLN:H	1:A:546:GLN:NE2	0.41	2.12	1	1
1:A:546:GLN:N	1:A:546:GLN:CD	0.41	2.73	30	1
1:A:530:MET:SD	1:A:534:ASP:CG	0.41	2.99	26	1
1:A:550:ASP:O	1:A:554:MET:CB	0.41	2.68	21	1
1:A:568:GLU:OE1	1:A:568:GLU:C	0.41	2.58	13	1
1:A:547:LEU:CD1	1:A:547:LEU:C	0.41	2.84	28	1
1:A:546:GLN:OE1	1:A:547:LEU:C	0.41	2.59	11	1
1:A:539:ALA:HB2	1:A:560:ARG:HH22	0.41	1.76	29	1
1:A:546:GLN:HG2	1:A:547:LEU:N	0.41	2.30	24	2
1:A:557:PRO:O	1:A:558:GLU:OE2	0.41	2.39	28	1
1:A:543:GLN:HA	1:A:547:LEU:CB	0.41	2.45	13	1
1:A:546:GLN:HB3	1:A:551:GLN:NE2	0.41	2.30	10	1
1:A:537:LYS:HB3	1:A:564:LEU:CD1	0.41	2.46	11	3
1:A:571:GLN:OE1	1:A:571:GLN:CA	0.41	2.69	28	1
1:A:571:GLN:O	1:A:572:LYS:CG	0.41	2.68	19	1
1:A:559:GLN:O	1:A:562:SER:OG	0.41	2.36	29	1
1:A:536:GLU:O	1:A:536:GLU:CD	0.41	2.59	3	1
1:A:542:MET:CE	1:A:552:ILE:HG12	0.41	2.46	26	1
1:A:541:ILE:CG1	1:A:567:LYS:HG3	0.41	2.46	30	1
1:A:541:ILE:CG2	1:A:567:LYS:HE3	0.41	2.46	3	1
1:A:539:ALA:O	1:A:542:MET:SD	0.41	2.80	8	1
1:A:537:LYS:HD3	1:A:564:LEU:HD13	0.40	1.93	21	1
1:A:530:MET:CG	1:A:534:ASP:HB3	0.40	2.46	26	1
1:A:534:ASP:OD2	1:A:561:GLN:CD	0.40	2.60	6	1
1:A:540:LEU:HA	1:A:543:GLN:NE2	0.40	2.32	24	1
1:A:564:LEU:CD2	1:A:564:LEU:C	0.40	2.88	5	1
1:A:567:LYS:N	1:A:567:LYS:HD2	0.40	2.31	20	1
1:A:534:ASP:OD1	1:A:561:GLN:OE1	0.40	2.39	24	1
1:A:565:ILE:O	1:A:568:GLU:HG2	0.40	2.17	30	1
1:A:543:GLN:HG2	1:A:547:LEU:CD2	0.40	2.46	13	1
1:A:541:ILE:CD1	1:A:567:LYS:HG3	0.40	2.47	2	1
1:A:547:LEU:CD2	1:A:547:LEU:O	0.40	2.68	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:531:THR:HB	1:A:532:PRO:HD2	0.40	1.93	10	1
1:A:537:LYS:HG3	1:A:564:LEU:CD1	0.40	2.46	8	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	43/49 (88%)	36±1 (84±3%)	4±2 (9±4%)	3±1 (7±2%)	3	17
All	All	1290/1470 (88%)	1082 (84%)	115 (9%)	93 (7%)	3	17

All 9 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	545	LEU	25
1	A	531	THR	24
1	A	547	LEU	20
1	A	549	ALA	7
1	A	548	THR	7
1	A	572	LYS	6
1	A	561	GLN	2
1	A	558	GLU	1
1	A	530	MET	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	Percentiles	
1	A	39/43 (91%)	26±2 (67±6%)	13±2 (33±6%)	1	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1170/1290 (91%)	784 (67%)	386 (33%)	1 12

All 33 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	561	GLN	29
1	A	533	GLN	28
1	A	566	LEU	27
1	A	530	MET	25
1	A	547	LEU	20
1	A	546	GLN	20
1	A	540	LEU	18
1	A	543	GLN	17
1	A	567	LYS	16
1	A	545	LEU	16
1	A	531	THR	16
1	A	560	ARG	15
1	A	554	MET	12
1	A	537	LYS	11
1	A	568	GLU	11
1	A	552	ILE	11
1	A	542	MET	11
1	A	559	GLN	10
1	A	550	ASP	9
1	A	564	LEU	9
1	A	563	ILE	8
1	A	569	GLN	7
1	A	571	GLN	6
1	A	572	LYS	5
1	A	562	SER	5
1	A	551	GLN	5
1	A	535	HIS	4
1	A	548	THR	4
1	A	555	LEU	3
1	A	558	GLU	3
1	A	536	GLU	2
1	A	541	ILE	2
1	A	534	ASP	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](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided