



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 03:00 AM UTC

PDB ID : 6KR8 / pdb_00006kr8
BMRB ID : 36284
Title : Structure of the beta2 adrenergic receptor in the full agonist bound state
Authors : Imai, S.; Shimada, I.
Deposited on : 2019-08-21

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

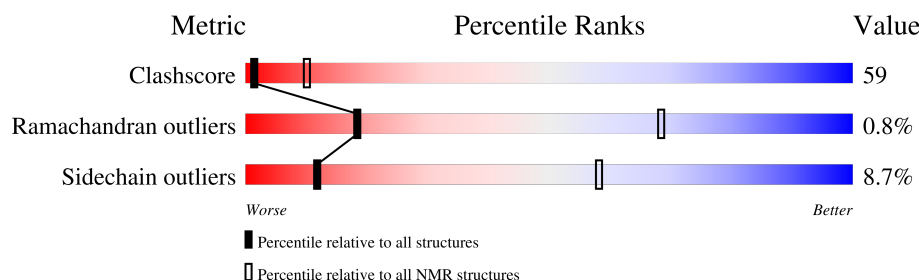
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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	336	

2 Ensemble composition and analysis

This entry contains 10 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:30-A:55, A:63-A:133, A:141-A:144, A:150-A:237, A:273-A:341 (258)	0.12	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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 7, 8, 9
2	3, 10
Single-model clusters	2

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5052 atoms, of which 2544 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called beta 2 adrenergic receptor.

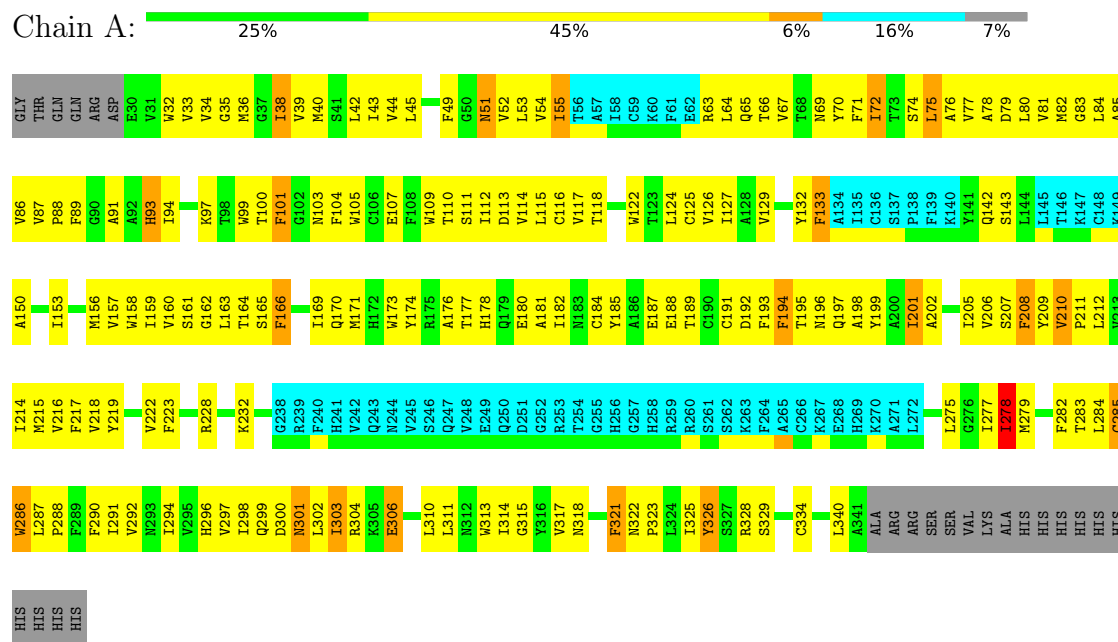
Mol	Chain	Residues	Atoms						Trace
1	A	312	Total	C	H	N	O	S	0
			5052	1651	2544	413	425	19	

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: beta 2 adrenergic receptor

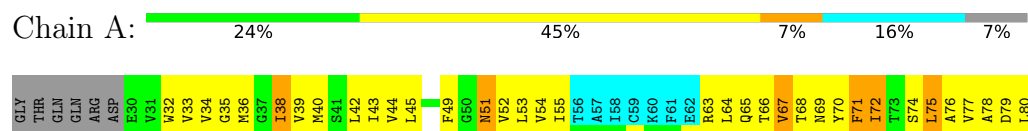


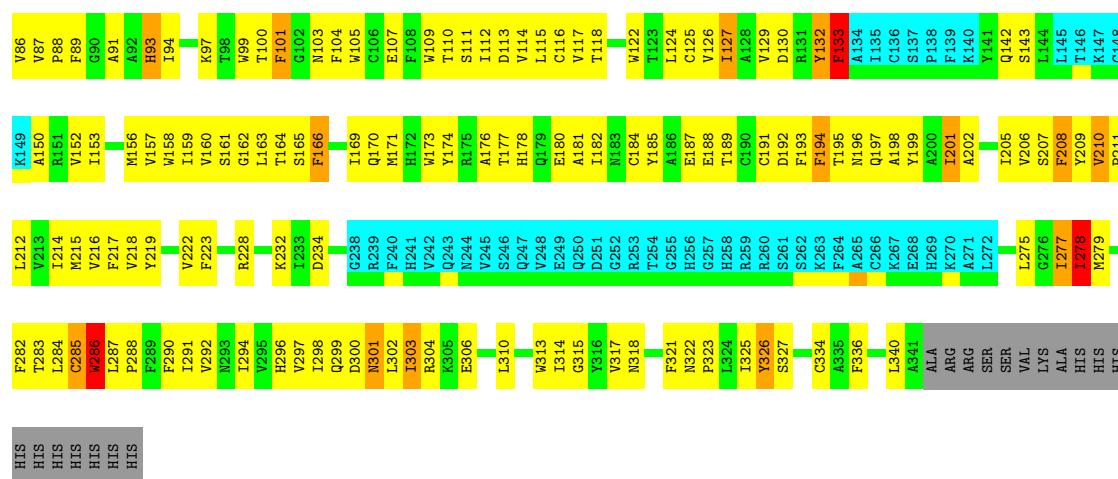
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: beta 2 adrenergic receptor

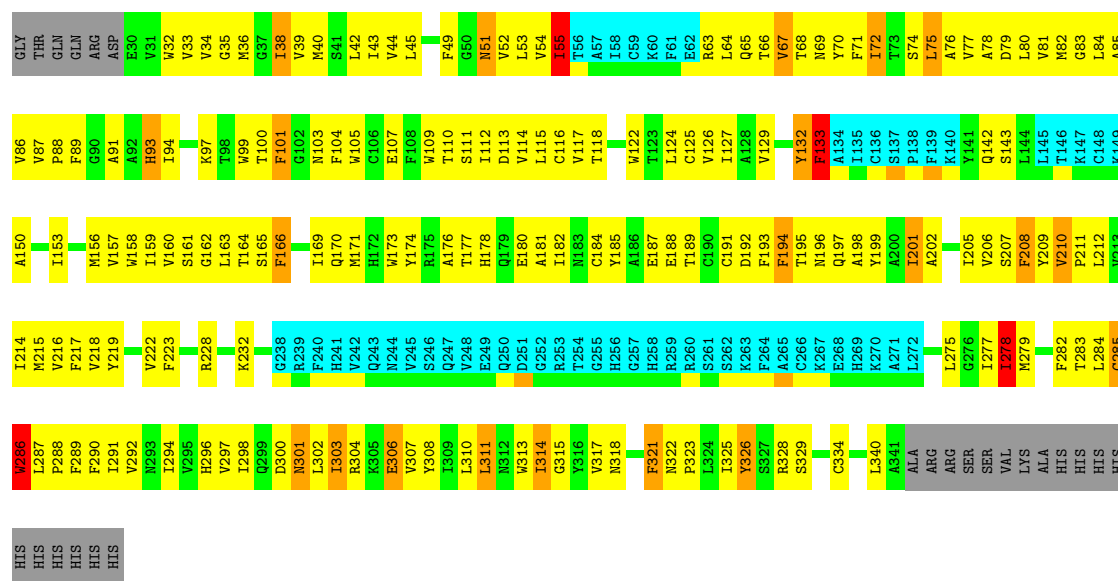




4.2.4 Score per residue for model 4

- Molecule 1: beta 2 adrenergic receptor

Chain A: 24% 45% 6% 16% 7%

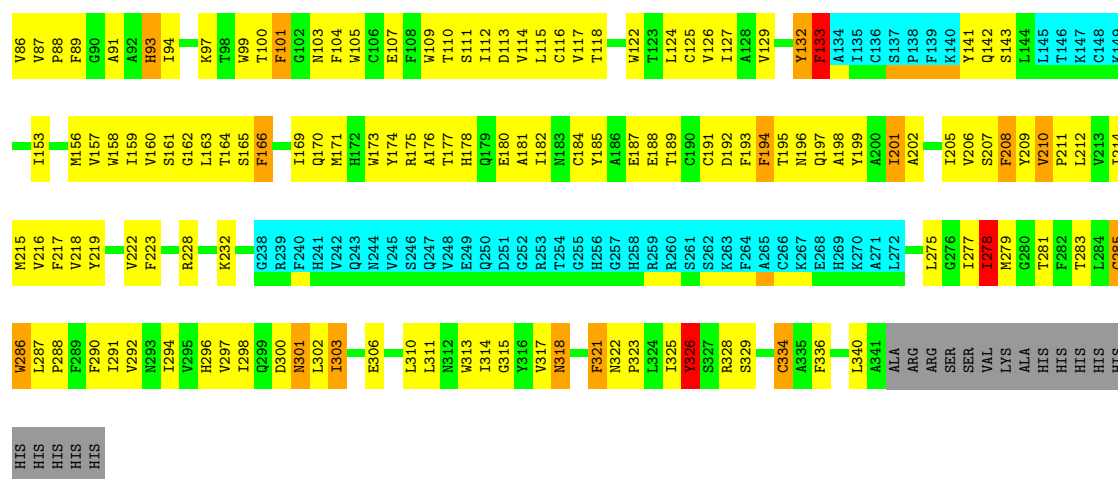


4.2.5 Score per residue for model 5

- Molecule 1: beta 2 adrenergic receptor

Chain A: 26% 44% 6% 16% 7%

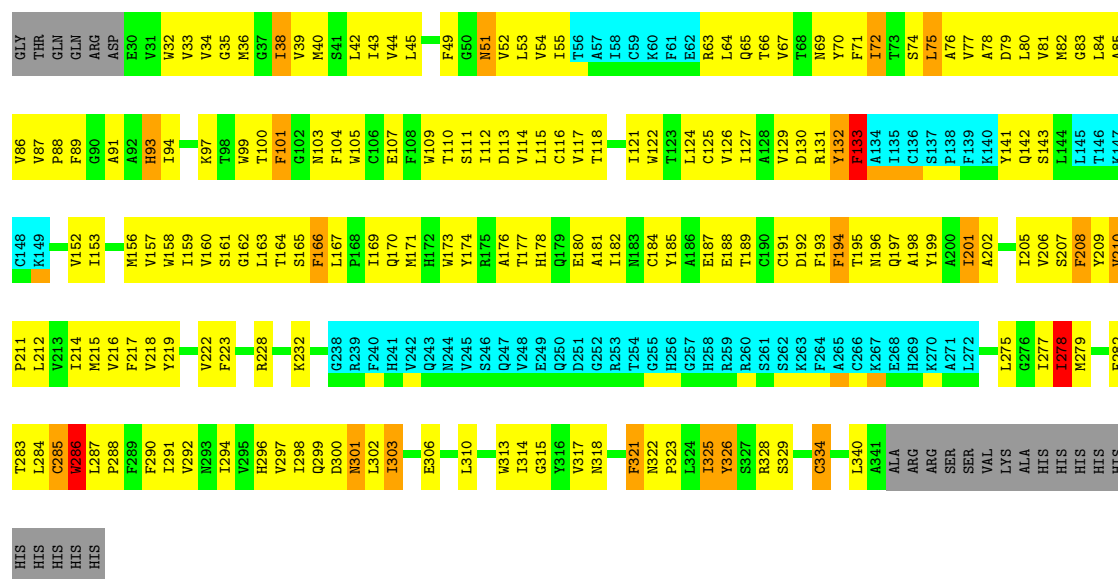




4.2.6 Score per residue for model 6

- Molecule 1: beta 2 adrenergic receptor

Chain A: 24% 46% 6% 16% 7%

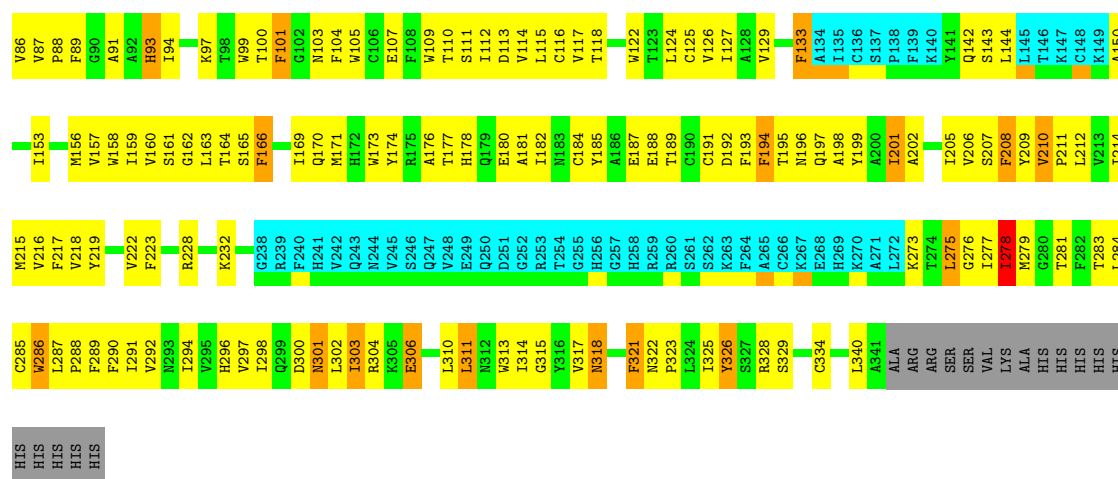


4.2.7 Score per residue for model 7

- Molecule 1: beta 2 adrenergic receptor

Chain A: 25% 46% 6% 16% 7%

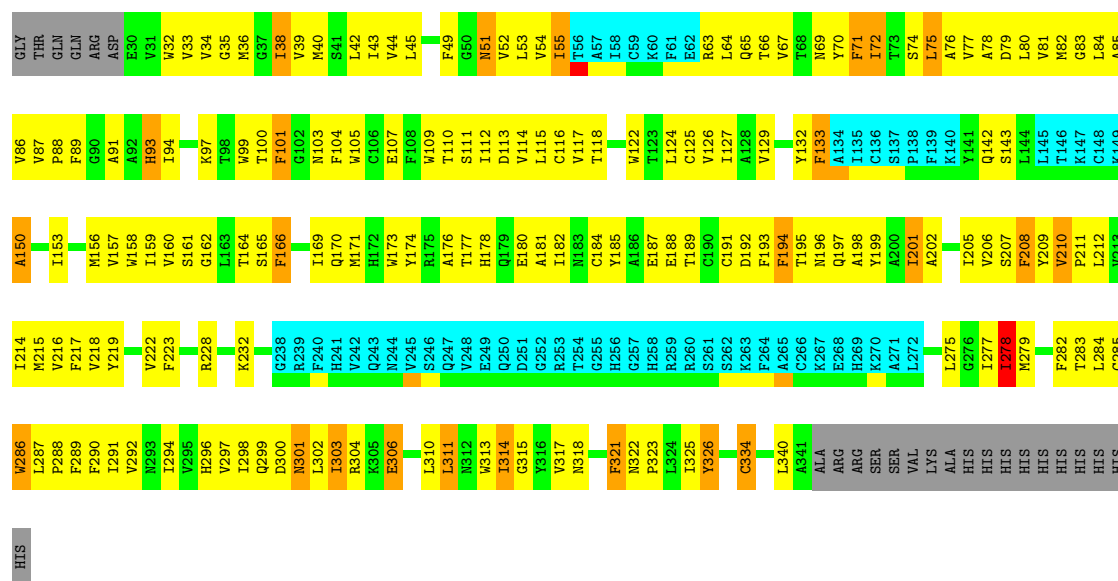




4.2.8 Score per residue for model 8

- Molecule 1: beta 2 adrenergic receptor

Chain A: 26% 43% 7% 16% 7%

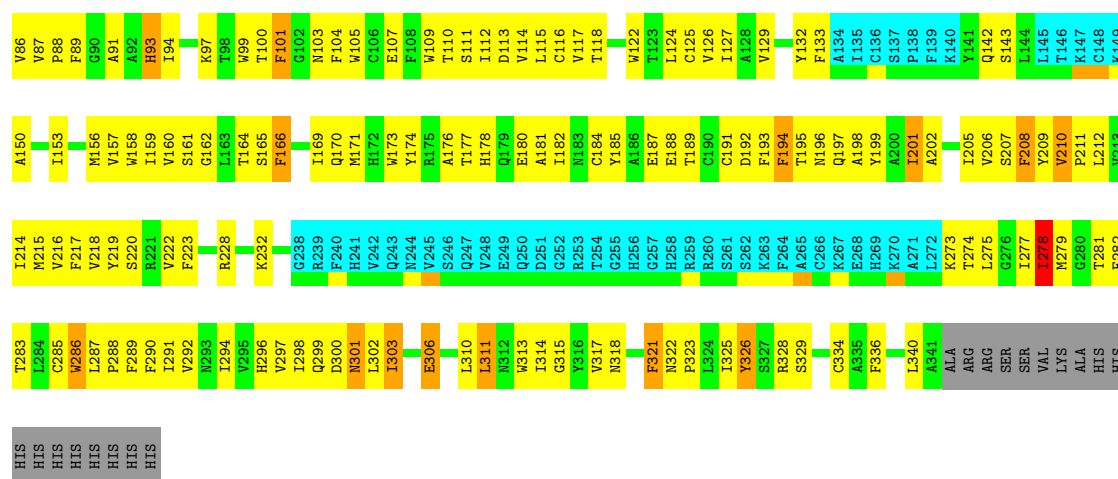


4.2.9 Score per residue for model 9

- Molecule 1: beta 2 adrenergic receptor

Chain A: 24% 47% 5% 16% 7%

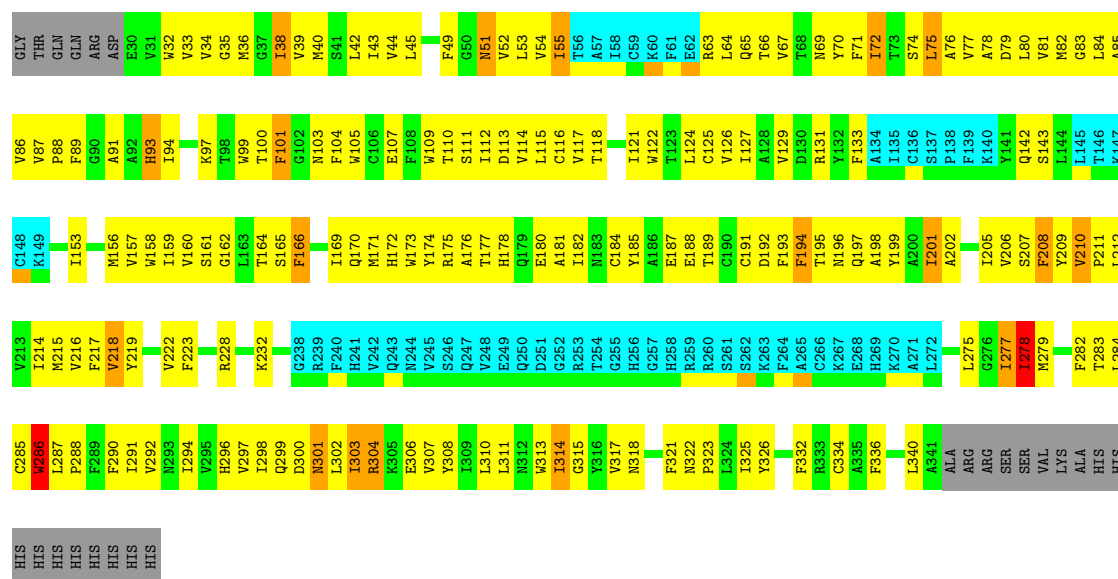




4.2.10 Score per residue for model 10

- Molecule 1: beta 2 adrenergic receptor

Chain A: 24% 46% 5% • 16% 7%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 500 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
X-PLOR NIH	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	38
Number of shifts mapped to atoms	38
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	1.32±0.00	1±0/2139 (0.0± 0.0%)	1.50±0.01	22±1/2922 (0.7± 0.0%)
All	All	1.32	10/21390 (0.0%)	1.50	218/29220 (0.7%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	210	VAL	CA-CB	-6.79	1.50	1.54	1	10

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	101	PHE	CA-CB-CG	-10.57	103.23	113.80	1	10
1	A	150	ALA	CA-C-N	8.71	131.95	120.28	7	1
1	A	150	ALA	C-N-CA	8.71	131.95	120.28	7	1
1	A	300	ASP	CA-CB-CG	-7.36	105.24	112.60	1	10
1	A	326	TYR	N-CA-C	7.36	120.00	111.02	2	2
1	A	300	ASP	N-CA-C	7.36	119.38	111.36	1	10
1	A	290	PHE	CA-CB-CG	-7.05	106.75	113.80	1	10
1	A	217	PHE	CA-CB-CG	-6.90	106.90	113.80	1	10
1	A	67	VAL	CB-CA-C	-6.74	103.05	112.14	3	4
1	A	321	PHE	CA-CB-CG	-6.30	107.50	113.80	2	10
1	A	334	CYS	O-C-N	6.28	128.80	122.08	7	10
1	A	104	PHE	CA-CB-CG	-6.27	107.53	113.80	1	10
1	A	166	PHE	CA-CB-CG	-6.25	107.55	113.80	1	10
1	A	150	ALA	O-C-N	6.24	129.64	123.46	7	1
1	A	194	PHE	CA-CB-CG	-6.10	107.70	113.80	1	10
1	A	336	PHE	CB-CA-C	-6.07	101.31	110.90	10	5
1	A	278	ILE	CB-CA-C	-6.05	104.09	112.02	5	10
1	A	71	PHE	CA-CB-CG	-5.76	108.04	113.80	1	10
1	A	283	THR	O-C-N	-5.74	115.89	122.09	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	55	ILE	CB-CA-C	-5.55	105.49	111.59	2	2
1	A	72	ILE	N-CA-CB	5.40	119.89	110.65	1	10
1	A	208	PHE	N-CA-C	5.24	119.58	112.04	1	10
1	A	300	ASP	CA-C-N	-5.23	114.27	122.79	1	10
1	A	300	ASP	C-N-CA	-5.23	114.27	122.79	1	10
1	A	127	ILE	CB-CA-C	-5.15	105.19	112.14	1	10
1	A	133	PHE	CA-CB-CG	-5.09	108.71	113.80	4	10
1	A	336	PHE	CA-CB-CG	-5.01	108.79	113.80	5	2
1	A	51	ASN	CA-CB-CG	-5.01	107.59	112.60	1	10

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2082	2114	2106	245±6
All	All	20820	21140	21060	2452

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 59.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:285:CYS:O	1:A:286:TRP:CG	1.07	2.08	7	10
1:A:285:CYS:O	1:A:286:TRP:CD1	0.98	2.17	7	8
1:A:176:ALA:HB3	1:A:194:PHE:HE2	0.90	1.25	1	10
1:A:285:CYS:HB3	1:A:314:ILE:O	0.90	1.66	5	10
1:A:285:CYS:CB	1:A:314:ILE:O	0.88	2.21	7	10
1:A:275:LEU:HD23	1:A:275:LEU:O	0.87	1.69	9	2
1:A:117:VAL:HG23	1:A:286:TRP:CZ2	0.84	2.07	10	2
1:A:287:LEU:HD13	1:A:291:ILE:HD13	0.84	1.50	1	10
1:A:117:VAL:HG23	1:A:286:TRP:CH2	0.83	2.07	10	10
1:A:176:ALA:HB3	1:A:194:PHE:CE2	0.82	2.09	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:285:CYS:O	1:A:286:TRP:CB	0.82	2.27	5	10
1:A:114:VAL:HG23	1:A:165:SER:HB3	0.81	1.51	1	10
1:A:275:LEU:HD23	1:A:276:GLY:N	0.81	1.90	7	1
1:A:314:ILE:O	1:A:317:VAL:HG12	0.81	1.75	1	10
1:A:54:VAL:O	1:A:55:ILE:C	0.80	2.22	5	1
1:A:219:TYR:HB2	1:A:275:LEU:HG	0.80	1.52	6	1
1:A:278:ILE:HG22	1:A:279:MET:N	0.79	1.90	4	10
1:A:275:LEU:HD23	1:A:275:LEU:C	0.79	2.03	9	3
1:A:169:ILE:HA	1:A:174:TYR:CE2	0.79	2.13	1	10
1:A:285:CYS:HB2	1:A:315:GLY:HA2	0.78	1.55	5	10
1:A:311:LEU:O	1:A:314:ILE:HG22	0.78	1.77	5	2
1:A:219:TYR:CD1	1:A:275:LEU:HD11	0.78	2.14	2	2
1:A:310:LEU:O	1:A:314:ILE:HG12	0.78	1.79	3	3
1:A:310:LEU:O	1:A:314:ILE:HG13	0.78	1.79	1	2
1:A:286:TRP:HA	1:A:286:TRP:CE3	0.77	2.14	6	10
1:A:49:PHE:CE2	1:A:53:LEU:HD11	0.76	2.15	1	10
1:A:36:MET:HG2	1:A:40:MET:HE2	0.75	1.56	1	10
1:A:210:VAL:HB	1:A:211:PRO:HD3	0.74	1.60	1	10
1:A:219:TYR:CD1	1:A:219:TYR:C	0.74	2.65	9	6
1:A:117:VAL:CG2	1:A:286:TRP:CH2	0.74	2.70	10	2
1:A:228:ARG:HB3	1:A:232:LYS:HE2	0.73	1.56	1	10
1:A:122:TRP:CD1	1:A:157:VAL:HG13	0.73	2.19	1	10
1:A:285:CYS:O	1:A:286:TRP:HB2	0.73	1.82	10	10
1:A:122:TRP:CD1	1:A:157:VAL:HG22	0.73	2.18	1	10
1:A:219:TYR:O	1:A:222:VAL:HG12	0.73	1.84	1	10
1:A:121:ILE:HD11	1:A:286:TRP:NE1	0.73	1.97	10	2
1:A:109:TRP:O	1:A:112:ILE:HG22	0.72	1.85	1	10
1:A:121:ILE:HD11	1:A:286:TRP:CD1	0.72	2.20	10	2
1:A:114:VAL:CG2	1:A:165:SER:HB3	0.71	2.15	1	10
1:A:82:MET:HB2	1:A:116:CYS:SG	0.71	2.26	1	10
1:A:83:GLY:HA2	1:A:87:VAL:HG12	0.71	1.63	1	10
1:A:285:CYS:HB3	1:A:314:ILE:C	0.70	2.11	1	4
1:A:67:VAL:HA	1:A:70:TYR:CD1	0.70	2.20	9	10
1:A:212:LEU:O	1:A:216:VAL:HG23	0.70	1.86	1	10
1:A:304:ARG:O	1:A:307:VAL:HG22	0.70	1.87	10	2
1:A:38:ILE:HD13	1:A:42:LEU:HD13	0.70	1.60	1	10
1:A:212:LEU:HD13	1:A:282:PHE:CD2	0.69	2.21	3	8
1:A:51:ASN:O	1:A:54:VAL:HG12	0.69	1.88	1	10
1:A:107:GLU:O	1:A:110:THR:HG22	0.69	1.87	1	10
1:A:156:MET:O	1:A:159:ILE:HG22	0.68	1.88	1	10
1:A:171:MET:HG2	1:A:173:TRP:NE1	0.68	2.02	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:MET:CE	1:A:94:ILE:HD12	0.68	2.18	1	10
1:A:287:LEU:O	1:A:291:ILE:HD13	0.68	1.87	1	10
1:A:75:LEU:HD21	1:A:124:LEU:CD2	0.68	2.19	1	10
1:A:99:TRP:O	1:A:189:THR:HG23	0.68	1.89	1	10
1:A:286:TRP:HA	1:A:286:TRP:HE3	0.67	1.48	6	7
1:A:284:LEU:O	1:A:314:ILE:CG2	0.67	2.42	10	8
1:A:82:MET:HE3	1:A:116:CYS:SG	0.66	2.31	1	10
1:A:197:GLN:HG2	1:A:297:VAL:CG2	0.66	2.20	1	10
1:A:178:HIS:CD2	1:A:180:GLU:H	0.65	2.08	1	10
1:A:74:SER:O	1:A:77:VAL:HG12	0.65	1.91	1	10
1:A:285:CYS:HB2	1:A:314:ILE:O	0.65	1.91	7	8
1:A:286:TRP:CZ2	1:A:315:GLY:O	0.65	2.49	7	2
1:A:40:MET:O	1:A:44:VAL:HG23	0.65	1.92	1	10
1:A:36:MET:HG2	1:A:40:MET:CE	0.64	2.22	1	10
1:A:285:CYS:HB3	1:A:314:ILE:HG22	0.64	1.67	7	7
1:A:40:MET:SD	1:A:91:ALA:HB1	0.64	2.32	1	10
1:A:153:ILE:O	1:A:157:VAL:HG23	0.64	1.93	1	10
1:A:71:PHE:CZ	1:A:150:ALA:HB1	0.64	2.27	2	4
1:A:219:TYR:HB2	1:A:275:LEU:CG	0.63	2.22	6	1
1:A:36:MET:HE2	1:A:94:ILE:HD12	0.63	1.69	1	10
1:A:169:ILE:HA	1:A:174:TYR:CD2	0.63	2.29	1	10
1:A:288:PRO:O	1:A:292:VAL:HG23	0.63	1.93	1	10
1:A:132:TYR:O	1:A:133:PHE:C	0.63	2.39	3	4
1:A:115:LEU:HB2	1:A:166:PHE:CE1	0.63	2.28	1	10
1:A:78:ALA:O	1:A:81:VAL:HG12	0.63	1.93	1	10
1:A:171:MET:HG2	1:A:173:TRP:CE2	0.62	2.30	1	10
1:A:197:GLN:HG2	1:A:297:VAL:HG21	0.62	1.70	1	10
1:A:275:LEU:C	1:A:275:LEU:CD2	0.61	2.72	9	3
1:A:36:MET:HE2	1:A:94:ILE:CD1	0.61	2.25	1	10
1:A:80:LEU:HD23	1:A:80:LEU:O	0.61	1.95	1	10
1:A:314:ILE:CG2	1:A:315:GLY:N	0.61	2.63	9	2
1:A:176:ALA:CB	1:A:194:PHE:HE2	0.61	2.07	1	10
1:A:219:TYR:CD1	1:A:275:LEU:HD12	0.61	2.30	7	1
1:A:187:GLU:OE1	1:A:189:THR:HB	0.61	1.96	1	10
1:A:205:ILE:HA	1:A:209:TYR:HD1	0.61	1.53	1	10
1:A:165:SER:O	1:A:169:ILE:HG12	0.60	1.95	1	10
1:A:161:SER:O	1:A:164:THR:HG22	0.60	1.96	1	10
1:A:36:MET:O	1:A:40:MET:HG3	0.60	1.96	1	10
1:A:228:ARG:O	1:A:232:LYS:HG3	0.60	1.96	1	10
1:A:86:VAL:HG22	1:A:112:ILE:HG23	0.60	1.74	1	10
1:A:275:LEU:CD2	1:A:279:MET:SD	0.60	2.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:277:ILE:HG21	1:A:326:TYR:CD1	0.59	2.32	3	8
1:A:306:GLU:O	1:A:310:LEU:HD13	0.59	1.98	1	10
1:A:285:CYS:HA	1:A:314:ILE:HG23	0.59	1.74	9	2
1:A:205:ILE:HA	1:A:209:TYR:CD1	0.59	2.33	1	10
1:A:55:ILE:HG23	1:A:55:ILE:O	0.59	1.95	3	2
1:A:115:LEU:HD11	1:A:158:TRP:CZ3	0.58	2.33	1	10
1:A:321:PHE:O	1:A:325:ILE:HG12	0.58	1.98	6	7
1:A:278:ILE:CG2	1:A:279:MET:N	0.58	2.60	4	6
1:A:55:ILE:HG21	1:A:73:THR:HG23	0.58	1.74	7	2
1:A:87:VAL:CG1	1:A:88:PRO:HD3	0.57	2.29	1	10
1:A:287:LEU:HD13	1:A:291:ILE:CD1	0.57	2.28	1	10
1:A:286:TRP:CZ3	1:A:315:GLY:HA3	0.57	2.33	6	2
1:A:215:MET:SD	1:A:278:ILE:CG2	0.57	2.93	7	4
1:A:103:ASN:HB2	1:A:188:GLU:HA	0.56	1.77	1	10
1:A:115:LEU:HD13	1:A:115:LEU:O	0.56	2.00	1	10
1:A:219:TYR:HB3	1:A:275:LEU:HD12	0.56	1.78	1	2
1:A:286:TRP:CE3	1:A:315:GLY:HA3	0.56	2.36	6	2
1:A:121:ILE:CD1	1:A:286:TRP:CD1	0.56	2.88	10	2
1:A:45:LEU:O	1:A:45:LEU:HD23	0.56	2.01	1	10
1:A:169:ILE:HA	1:A:174:TYR:HE2	0.56	1.59	1	10
1:A:285:CYS:HB2	1:A:315:GLY:CA	0.56	2.31	5	9
1:A:114:VAL:HG23	1:A:165:SER:CB	0.55	2.28	1	10
1:A:157:VAL:O	1:A:160:VAL:HG12	0.55	2.00	1	10
1:A:219:TYR:CB	1:A:275:LEU:HD13	0.55	2.31	5	2
1:A:33:VAL:HG13	1:A:34:VAL:N	0.55	2.17	1	10
1:A:211:PRO:O	1:A:215:MET:HG2	0.55	2.01	1	10
1:A:219:TYR:CG	1:A:275:LEU:HD23	0.55	2.37	3	1
1:A:67:VAL:HG13	1:A:68:THR:N	0.55	2.16	4	3
1:A:133:PHE:C	1:A:133:PHE:CD1	0.55	2.79	6	1
1:A:206:VAL:HG23	1:A:207:SER:N	0.55	2.16	1	10
1:A:133:PHE:CE1	1:A:141:TYR:CG	0.55	2.94	6	1
1:A:115:LEU:HD23	1:A:162:GLY:HA2	0.55	1.76	1	10
1:A:198:ALA:HA	1:A:201:ILE:CD1	0.55	2.31	1	10
1:A:89:PHE:CD2	1:A:101:PHE:CZ	0.55	2.95	1	10
1:A:277:ILE:HG22	1:A:278:ILE:N	0.55	2.17	2	1
1:A:208:PHE:CE1	1:A:282:PHE:CD2	0.55	2.94	3	1
1:A:38:ILE:O	1:A:42:LEU:HD13	0.54	2.01	1	10
1:A:89:PHE:CE2	1:A:101:PHE:CE2	0.54	2.95	1	10
1:A:36:MET:CG	1:A:40:MET:HE2	0.54	2.32	1	10
1:A:286:TRP:HE1	1:A:318:ASN:CG	0.54	2.10	7	2
1:A:307:VAL:CG2	1:A:308:TYR:N	0.54	2.70	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:285:CYS:C	1:A:286:TRP:CG	0.54	2.84	7	7
1:A:303:ILE:N	1:A:303:ILE:HD13	0.54	2.17	1	10
1:A:38:ILE:HD13	1:A:42:LEU:CD1	0.54	2.33	1	10
1:A:67:VAL:HG23	1:A:68:THR:N	0.54	2.16	3	1
1:A:288:PRO:HB2	1:A:311:LEU:HD22	0.54	1.78	10	1
1:A:294:ILE:O	1:A:297:VAL:HG12	0.54	2.02	1	10
1:A:178:HIS:HD2	1:A:180:GLU:H	0.53	1.46	1	10
1:A:287:LEU:HD13	1:A:287:LEU:O	0.53	2.03	1	10
1:A:117:VAL:CG2	1:A:286:TRP:CZ2	0.53	2.90	10	1
1:A:35:GLY:O	1:A:38:ILE:HG22	0.53	2.03	1	10
1:A:38:ILE:HD13	1:A:38:ILE:C	0.53	2.27	1	10
1:A:115:LEU:HB2	1:A:166:PHE:HE1	0.53	1.63	1	10
1:A:97:LYS:O	1:A:97:LYS:HG3	0.53	2.04	1	10
1:A:281:THR:O	1:A:285:CYS:O	0.53	2.27	5	3
1:A:285:CYS:CB	1:A:314:ILE:HG22	0.53	2.34	7	1
1:A:205:ILE:HG13	1:A:206:VAL:N	0.52	2.20	1	10
1:A:303:ILE:HD13	1:A:303:ILE:H	0.52	1.63	1	10
1:A:89:PHE:HD2	1:A:101:PHE:CZ	0.52	2.22	1	10
1:A:208:PHE:CE1	1:A:282:PHE:CE2	0.52	2.97	3	1
1:A:40:MET:HE2	1:A:94:ILE:CD1	0.52	2.34	1	10
1:A:114:VAL:O	1:A:117:VAL:HG12	0.52	2.05	1	10
1:A:288:PRO:HG2	1:A:311:LEU:HD11	0.52	1.79	7	4
1:A:277:ILE:HD11	1:A:325:ILE:HB	0.52	1.82	3	1
1:A:51:ASN:OD1	1:A:79:ASP:HB2	0.52	2.04	1	10
1:A:287:LEU:HB3	1:A:288:PRO:CD	0.52	2.34	1	10
1:A:322:ASN:O	1:A:326:TYR:N	0.52	2.42	5	8
1:A:125:CYS:HB3	1:A:211:PRO:HB3	0.52	1.81	1	10
1:A:289:PHE:HB2	1:A:311:LEU:HD12	0.52	1.82	7	4
1:A:178:HIS:O	1:A:182:ILE:HG13	0.52	2.04	1	10
1:A:103:ASN:HB2	1:A:188:GLU:CD	0.52	2.29	1	10
1:A:115:LEU:CD1	1:A:158:TRP:HZ3	0.52	2.18	1	10
1:A:169:ILE:HD13	1:A:174:TYR:CD2	0.52	2.39	1	10
1:A:196:ASN:HD21	1:A:199:TYR:HB2	0.51	1.65	1	10
1:A:177:THR:HG23	1:A:177:THR:O	0.51	2.05	1	10
1:A:277:ILE:HD13	1:A:277:ILE:N	0.51	2.19	10	1
1:A:36:MET:SD	1:A:94:ILE:HD12	0.51	2.45	1	10
1:A:67:VAL:HA	1:A:70:TYR:CE1	0.51	2.39	9	10
1:A:75:LEU:CD2	1:A:124:LEU:HD23	0.51	2.34	1	10
1:A:115:LEU:HD13	1:A:115:LEU:C	0.51	2.31	1	10
1:A:307:VAL:HG23	1:A:308:TYR:N	0.51	2.20	10	2
1:A:75:LEU:HD21	1:A:124:LEU:HD21	0.51	1.82	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:LEU:O	1:A:88:PRO:HG2	0.51	2.05	1	10
1:A:166:PHE:O	1:A:170:GLN:HG2	0.51	2.05	1	10
1:A:228:ARG:CB	1:A:232:LYS:HE2	0.51	2.34	1	10
1:A:212:LEU:HD13	1:A:282:PHE:HD2	0.51	1.66	10	1
1:A:284:LEU:O	1:A:314:ILE:HG22	0.50	2.04	10	5
1:A:202:ALA:O	1:A:206:VAL:HG22	0.50	2.06	1	10
1:A:328:ARG:O	1:A:329:SER:C	0.50	2.49	2	7
1:A:277:ILE:CG2	1:A:278:ILE:N	0.50	2.70	2	1
1:A:115:LEU:CB	1:A:166:PHE:HE1	0.50	2.19	1	10
1:A:193:PHE:CZ	1:A:195:THR:CG2	0.50	2.94	1	10
1:A:296:HIS:HA	1:A:303:ILE:HD11	0.50	1.83	1	10
1:A:228:ARG:HB3	1:A:232:LYS:CE	0.50	2.32	1	10
1:A:215:MET:CE	1:A:282:PHE:CZ	0.50	2.94	10	1
1:A:201:ILE:H	1:A:201:ILE:HD13	0.49	1.67	1	10
1:A:133:PHE:CE1	1:A:141:TYR:CD1	0.49	3.01	6	1
1:A:39:VAL:HG12	1:A:43:ILE:HD13	0.49	1.84	1	10
1:A:275:LEU:HD22	1:A:275:LEU:O	0.49	2.07	3	1
1:A:198:ALA:HA	1:A:201:ILE:HD11	0.49	1.84	1	10
1:A:133:PHE:O	1:A:133:PHE:CG	0.49	2.62	6	1
1:A:299:GLN:HG3	1:A:302:LEU:HD12	0.49	1.84	6	1
1:A:49:PHE:CE2	1:A:53:LEU:CD1	0.48	2.94	1	10
1:A:210:VAL:O	1:A:214:ILE:HD13	0.48	2.08	1	10
1:A:127:ILE:HG21	1:A:326:TYR:OH	0.48	2.08	3	1
1:A:169:ILE:CA	1:A:174:TYR:HE2	0.48	2.21	1	10
1:A:314:ILE:HG22	1:A:315:GLY:N	0.48	2.23	9	2
1:A:130:ASP:O	1:A:133:PHE:HB2	0.48	2.07	3	1
1:A:75:LEU:HD21	1:A:124:LEU:HD23	0.48	1.85	1	10
1:A:93:HIS:HB2	1:A:99:TRP:CZ3	0.48	2.44	1	10
1:A:219:TYR:HB2	1:A:275:LEU:HD13	0.48	1.84	5	1
1:A:54:VAL:CG1	1:A:76:ALA:HB1	0.48	2.39	1	10
1:A:122:TRP:CD1	1:A:157:VAL:CG1	0.48	2.95	1	10
1:A:130:ASP:O	1:A:133:PHE:HB3	0.48	2.08	6	1
1:A:193:PHE:CZ	1:A:195:THR:HG21	0.48	2.44	1	10
1:A:311:LEU:HD13	1:A:314:ILE:HG21	0.48	1.86	9	1
1:A:215:MET:SD	1:A:282:PHE:CE2	0.48	3.07	10	1
1:A:64:LEU:N	1:A:64:LEU:HD12	0.47	2.24	1	10
1:A:99:TRP:CD1	1:A:101:PHE:HB2	0.47	2.45	1	10
1:A:287:LEU:CD1	1:A:291:ILE:HD13	0.47	2.32	1	10
1:A:291:ILE:N	1:A:291:ILE:HD12	0.47	2.24	1	10
1:A:296:HIS:CG	1:A:303:ILE:HD11	0.47	2.44	1	10
1:A:55:ILE:O	1:A:55:ILE:HG13	0.47	2.09	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:VAL:HG13	1:A:55:ILE:N	0.47	2.24	1	10
1:A:122:TRP:HD1	1:A:157:VAL:HG22	0.47	1.66	1	10
1:A:122:TRP:HD1	1:A:157:VAL:CG2	0.47	2.22	1	10
1:A:307:VAL:HG12	1:A:311:LEU:HD22	0.47	1.86	1	1
1:A:99:TRP:CD2	1:A:191:CYS:HB3	0.47	2.45	2	10
1:A:210:VAL:CB	1:A:211:PRO:HD3	0.47	2.38	1	10
1:A:55:ILE:O	1:A:55:ILE:CG2	0.47	2.63	8	2
1:A:125:CYS:O	1:A:129:VAL:HG23	0.46	2.10	1	10
1:A:201:ILE:O	1:A:205:ILE:HG23	0.46	2.10	1	10
1:A:215:MET:SD	1:A:278:ILE:HG21	0.46	2.49	7	3
1:A:288:PRO:HB2	1:A:311:LEU:HD11	0.46	1.86	9	4
1:A:77:VAL:HG13	1:A:78:ALA:N	0.46	2.25	1	10
1:A:311:LEU:HA	1:A:314:ILE:HG13	0.46	1.87	10	3
1:A:67:VAL:HA	1:A:70:TYR:HD1	0.46	1.66	9	6
1:A:133:PHE:CZ	1:A:141:TYR:CD2	0.46	3.03	6	1
1:A:196:ASN:OD1	1:A:198:ALA:HB3	0.46	2.11	1	10
1:A:202:ALA:HA	1:A:205:ILE:HG12	0.46	1.87	1	10
1:A:38:ILE:CD1	1:A:42:LEU:CD1	0.46	2.94	1	10
1:A:66:THR:O	1:A:69:ASN:HB2	0.46	2.11	1	10
1:A:322:ASN:CB	1:A:323:PRO:HD3	0.46	2.41	4	10
1:A:38:ILE:HG23	1:A:39:VAL:N	0.45	2.26	1	10
1:A:287:LEU:HD13	1:A:287:LEU:C	0.45	2.35	1	10
1:A:121:ILE:CD1	1:A:286:TRP:NE1	0.45	2.74	10	1
1:A:87:VAL:HG12	1:A:88:PRO:HD3	0.45	1.86	1	10
1:A:169:ILE:HG23	1:A:174:TYR:CE2	0.45	2.46	1	10
1:A:285:CYS:CB	1:A:314:ILE:C	0.45	2.89	10	6
1:A:101:PHE:HB3	1:A:105:TRP:CD1	0.45	2.46	1	10
1:A:197:GLN:CG	1:A:297:VAL:CG2	0.45	2.94	1	10
1:A:40:MET:CE	1:A:94:ILE:CD1	0.45	2.95	1	10
1:A:294:ILE:HG22	1:A:298:ILE:CD1	0.45	2.42	1	10
1:A:54:VAL:CG1	1:A:76:ALA:CB	0.45	2.95	1	10
1:A:277:ILE:HD11	1:A:325:ILE:HG21	0.45	1.89	10	1
1:A:40:MET:SD	1:A:94:ILE:HD11	0.44	2.52	1	10
1:A:150:ALA:HA	1:A:153:ILE:HD12	0.44	1.87	9	1
1:A:55:ILE:C	1:A:55:ILE:HD12	0.44	2.38	1	1
1:A:87:VAL:HG22	1:A:313:TRP:CH2	0.44	2.47	1	10
1:A:159:ILE:HG23	1:A:160:VAL:N	0.44	2.27	1	10
1:A:130:ASP:O	1:A:133:PHE:HD2	0.44	1.95	6	1
1:A:52:VAL:O	1:A:55:ILE:O	0.44	2.36	7	1
1:A:171:MET:CG	1:A:173:TRP:NE1	0.44	2.78	1	10
1:A:215:MET:SD	1:A:278:ILE:HG23	0.44	2.53	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:TRP:NE1	1:A:36:MET:SD	0.44	2.91	1	10
1:A:201:ILE:HG12	1:A:202:ALA:N	0.44	2.27	1	10
1:A:38:ILE:HD13	1:A:38:ILE:O	0.44	2.13	1	10
1:A:91:ALA:O	1:A:94:ILE:HG12	0.44	2.12	1	10
1:A:287:LEU:CD1	1:A:291:ILE:CD1	0.44	2.95	1	10
1:A:89:PHE:CD2	1:A:101:PHE:CE2	0.43	3.06	1	10
1:A:83:GLY:HA2	1:A:87:VAL:CG1	0.43	2.39	1	10
1:A:100:THR:O	1:A:100:THR:HG22	0.43	2.13	1	10
1:A:275:LEU:HD13	1:A:275:LEU:C	0.43	2.38	3	1
1:A:219:TYR:CD1	1:A:220:SER:N	0.43	2.86	9	1
1:A:208:PHE:CE2	1:A:287:LEU:HD22	0.43	2.49	1	10
1:A:288:PRO:CG	1:A:311:LEU:HD11	0.43	2.43	9	4
1:A:322:ASN:HB2	1:A:323:PRO:HD3	0.43	1.89	10	2
1:A:114:VAL:CG2	1:A:165:SER:CB	0.43	2.95	1	10
1:A:115:LEU:HD11	1:A:158:TRP:HZ3	0.43	1.69	1	10
1:A:219:TYR:CD1	1:A:275:LEU:CD1	0.43	2.96	9	1
1:A:87:VAL:HG22	1:A:313:TRP:CZ3	0.43	2.49	1	10
1:A:87:VAL:CG2	1:A:313:TRP:CZ3	0.43	3.02	1	10
1:A:36:MET:CG	1:A:40:MET:CE	0.43	2.95	1	10
1:A:159:ILE:CG2	1:A:160:VAL:N	0.43	2.81	1	10
1:A:64:LEU:HD23	1:A:332:PHE:CE2	0.43	2.49	10	1
1:A:222:VAL:CG1	1:A:223:PHE:N	0.42	2.82	1	10
1:A:54:VAL:O	1:A:55:ILE:HD13	0.42	2.15	6	1
1:A:117:VAL:CG1	1:A:118:THR:N	0.42	2.82	1	10
1:A:52:VAL:CG1	1:A:53:LEU:N	0.42	2.82	1	10
1:A:122:TRP:CD1	1:A:157:VAL:CG2	0.42	2.95	1	10
1:A:184:CYS:SG	1:A:192:ASP:CG	0.42	3.03	1	10
1:A:285:CYS:CA	1:A:314:ILE:HG23	0.42	2.44	9	1
1:A:75:LEU:CD2	1:A:124:LEU:CD2	0.42	2.95	1	10
1:A:55:ILE:O	1:A:55:ILE:CG1	0.42	2.67	3	1
1:A:277:ILE:HD13	1:A:326:TYR:HA	0.42	1.92	9	1
1:A:45:LEU:C	1:A:45:LEU:CD2	0.42	2.93	1	10
1:A:110:THR:CG2	1:A:111:SER:N	0.42	2.82	1	10
1:A:33:VAL:CG1	1:A:34:VAL:N	0.42	2.82	1	10
1:A:54:VAL:CG1	1:A:55:ILE:N	0.42	2.82	1	10
1:A:297:VAL:CG1	1:A:298:ILE:N	0.42	2.83	1	10
1:A:288:PRO:CB	1:A:311:LEU:HD11	0.42	2.44	9	4
1:A:286:TRP:HE1	1:A:318:ASN:CB	0.41	2.28	7	1
1:A:291:ILE:CD1	1:A:291:ILE:N	0.41	2.83	1	10
1:A:93:HIS:CG	1:A:99:TRP:CZ3	0.41	3.08	3	10
1:A:115:LEU:CD1	1:A:158:TRP:CZ3	0.41	2.99	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:VAL:CG1	1:A:78:ALA:N	0.41	2.83	1	10
1:A:115:LEU:HD22	1:A:161:SER:OG	0.41	2.15	1	10
1:A:301:ASN:H	1:A:301:ASN:HD22	0.41	1.57	1	10
1:A:340:LEU:N	1:A:340:LEU:HD12	0.41	2.31	1	10
1:A:275:LEU:HD23	1:A:276:GLY:CA	0.41	2.44	7	1
1:A:45:LEU:HD23	1:A:45:LEU:C	0.41	2.40	1	10
1:A:115:LEU:CG	1:A:166:PHE:HE1	0.41	2.29	1	10
1:A:160:VAL:CG1	1:A:161:SER:N	0.41	2.83	1	10
1:A:206:VAL:CG2	1:A:207:SER:N	0.41	2.82	1	10
1:A:210:VAL:HG12	1:A:214:ILE:HD13	0.41	1.93	1	10
1:A:80:LEU:C	1:A:80:LEU:CD2	0.41	2.94	1	10
1:A:122:TRP:O	1:A:126:VAL:HG23	0.41	2.16	1	10
1:A:122:TRP:CE3	1:A:211:PRO:HG3	0.41	2.51	1	10
1:A:189:THR:O	1:A:189:THR:HG22	0.41	2.15	1	10
1:A:85:ALA:O	1:A:89:PHE:CD1	0.41	2.73	1	10
1:A:311:LEU:HD13	1:A:314:ILE:CG2	0.41	2.45	9	1
1:A:38:ILE:C	1:A:38:ILE:CD1	0.41	2.94	1	10
1:A:54:VAL:HG11	1:A:76:ALA:CB	0.41	2.46	1	10
1:A:110:THR:HG23	1:A:111:SER:N	0.41	2.30	1	10
1:A:112:ILE:CG2	1:A:113:ASP:N	0.41	2.84	1	10
1:A:117:VAL:HG13	1:A:118:THR:N	0.41	2.29	1	10
1:A:55:ILE:HD13	1:A:73:THR:HG23	0.41	1.92	3	1
1:A:310:LEU:O	1:A:314:ILE:CG1	0.41	2.69	10	3
1:A:54:VAL:HG13	1:A:55:ILE:HG12	0.41	1.92	10	1
1:A:115:LEU:CD1	1:A:115:LEU:C	0.41	2.94	1	10
1:A:202:ALA:CA	1:A:205:ILE:HG12	0.41	2.46	1	10
1:A:82:MET:CE	1:A:116:CYS:SG	0.40	3.07	1	10
1:A:181:ALA:O	1:A:185:TYR:CD1	0.40	2.74	1	10
1:A:302:LEU:HD23	1:A:302:LEU:HA	0.40	1.72	1	10
1:A:277:ILE:N	1:A:277:ILE:CD1	0.40	2.82	10	1
1:A:65:GLN:O	1:A:70:TYR:CE1	0.40	2.74	1	10
1:A:219:TYR:CG	1:A:275:LEU:HD13	0.40	2.51	8	2
1:A:115:LEU:CB	1:A:166:PHE:CE1	0.40	3.00	1	10
1:A:40:MET:HE2	1:A:94:ILE:HD11	0.40	1.93	1	10
1:A:275:LEU:HD12	1:A:275:LEU:O	0.40	2.17	5	1
1:A:218:VAL:HG12	1:A:219:TYR:N	0.40	2.31	10	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	256/336 (76%)	245±1 (96±0%)	9±1 (4±0%)	2±1 (1±0%)	18	68
All	All	2560/3360 (76%)	2447 (96%)	93 (4%)	20 (1%)	18	68

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	286	TRP	10
1	A	133	PHE	3
1	A	326	TYR	2
1	A	150	ALA	2
1	A	327	SER	1
1	A	55	ILE	1
1	A	141	TYR	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	229/296 (77%)	209±2 (91±1%)	20±2 (9±1%)	12	58
All	All	2290/2960 (77%)	2090 (91%)	200 (9%)	12	58

All 36 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	38	ILE	10
1	A	72	ILE	10
1	A	75	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	93	HIS	10
1	A	142	GLN	10
1	A	143	SER	10
1	A	201	ILE	10
1	A	218	VAL	10
1	A	278	ILE	10
1	A	301	ASN	10
1	A	303	ILE	10
1	A	318	ASN	10
1	A	132	TYR	7
1	A	163	LEU	7
1	A	326	TYR	7
1	A	285	CYS	6
1	A	306	GLU	6
1	A	299	GLN	5
1	A	286	TRP	4
1	A	304	ARG	4
1	A	311	LEU	4
1	A	277	ILE	3
1	A	55	ILE	3
1	A	314	ILE	3
1	A	334	CYS	3
1	A	167	LEU	2
1	A	172	HIS	2
1	A	275	LEU	2
1	A	325	ILE	2
1	A	133	PHE	2
1	A	175	ARG	2
1	A	273	LYS	2
1	A	234	ASP	1
1	A	327	SER	1
1	A	63	ARG	1
1	A	131	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *PeakList.star*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	38
Number of shifts mapped to atoms	38
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 34 atoms were assigned a chemical shift out of a possible 3695. 0 out of 56 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	34/1289 (3%)	17/521 (3%)	0/516 (0%)	17/252 (7%)
Sidechain	0/1977 (0%)	0/1317 (0%)	0/607 (0%)	0/53 (0%)
Aromatic	0/429 (0%)	0/209 (0%)	0/203 (0%)	0/17 (0%)
Overall	34/3695 (1%)	17/2047 (1%)	0/1326 (0%)	17/322 (5%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 38 atoms were assigned a chemical shift out of a possible 4437. 0 out of 61 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	38/1561 (2%)	19/632 (3%)	0/624 (0%)	19/305 (6%)
Sidechain	0/2375 (0%)	0/1572 (0%)	0/727 (0%)	0/76 (0%)
Aromatic	0/501 (0%)	0/245 (0%)	0/231 (0%)	0/25 (0%)
Overall	38/4437 (1%)	19/2449 (1%)	0/1582 (0%)	19/406 (5%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

