



Full wwPDB NMR Structure Validation Report ⓘ

Jun 13, 2024 – 12:28 PM EDT

PDB ID : 1OH1
Title : Solution structure of staphostatin A from *Staphylococcus aureus* confirms the discovery of a novel class of cysteine proteinase inhibitors.
Authors : Dubin, G.; Popowicz, G.; Krajewski, M.; Stec, J.; Bochtler, M.; Potempa, J.; Dubin, A.; Holak, T.A.
Deposited on : 2003-05-21

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	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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)	:	2.36.2

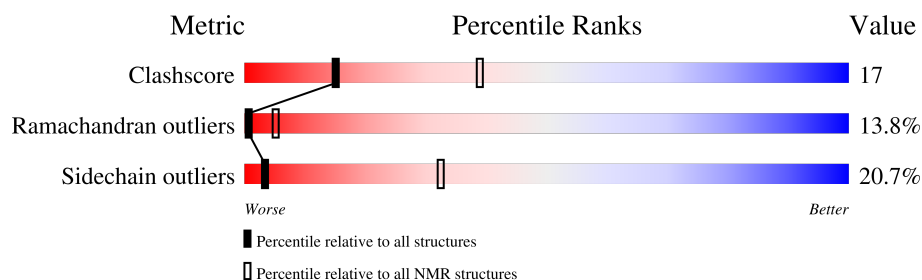
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	109	<div> <div></div> <div>36%</div> <div>56%</div> <div>6%</div> <div>.</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 5 as representative.

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:4-A:109 (106)	1.27	14

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 and 5 single-model clusters were found.

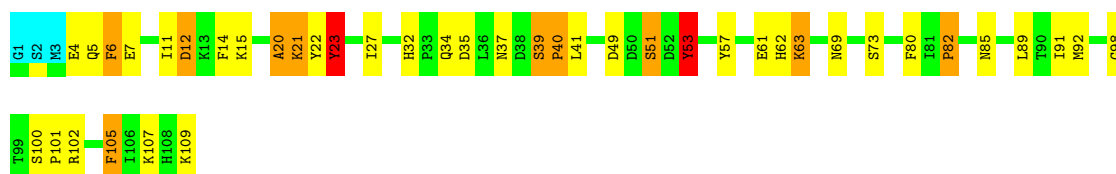
Cluster number	Models
1	2, 3, 4, 5, 9, 11, 12, 14, 16, 17, 20
2	7, 13
3	8, 19
Single-model clusters	1; 6; 10; 15; 18

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1141 atoms, of which 249 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called STAPHOSTATIN A.

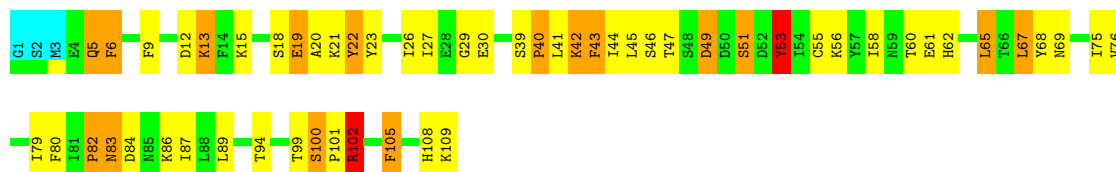
Mol	Chain	Residues	Atoms						Trace
1	A	109	Total	C	H	N	O	S	0
			1141	570	249	142	175	5	



4.2.3 Score per residue for model 3

- Molecule 1: STAPHOSTATIN A

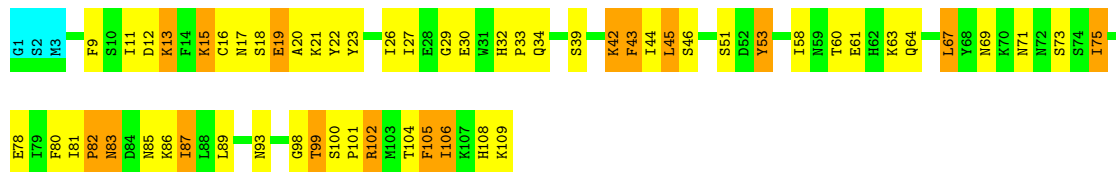
Chain A: 46% 35% 15% . .



4.2.4 Score per residue for model 4

- Molecule 1: STAPHOSTATIN A

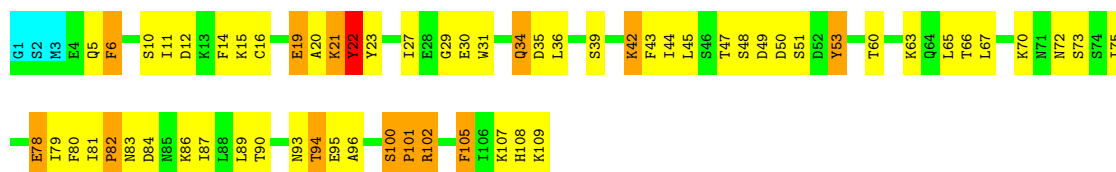
Chain A: 44% 39% 15% .



4.2.5 Score per residue for model 5

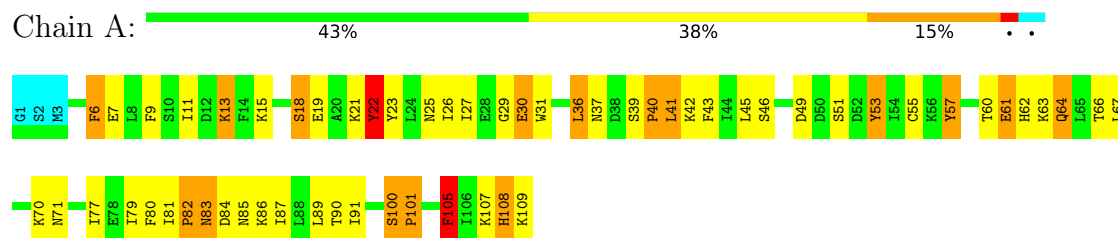
- Molecule 1: STAPHOSTATIN A

Chain A: 40% 44% 12% . .



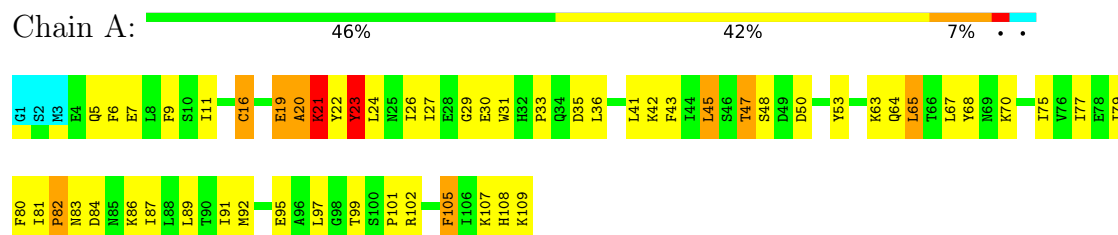
4.2.6 Score per residue for model 6

- Molecule 1: STAPHOSTATIN A



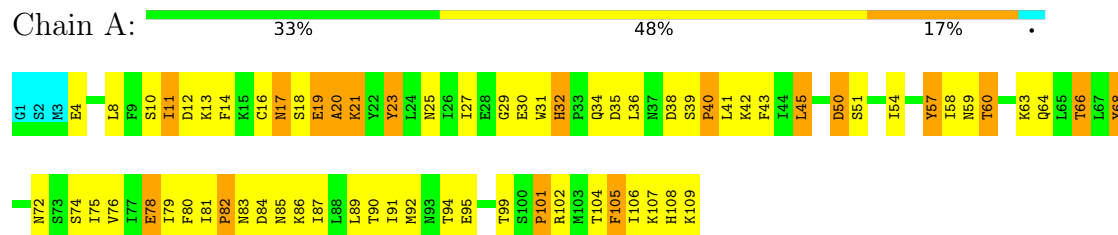
4.2.7 Score per residue for model 7

- Molecule 1: STAPHOSTATIN A



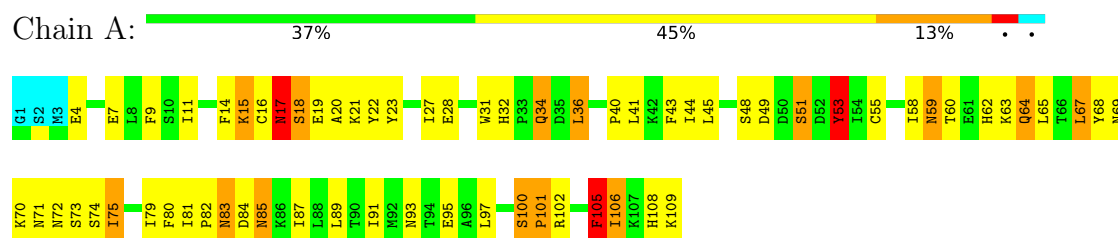
4.2.8 Score per residue for model 8

- Molecule 1: STAPHOSTATIN A



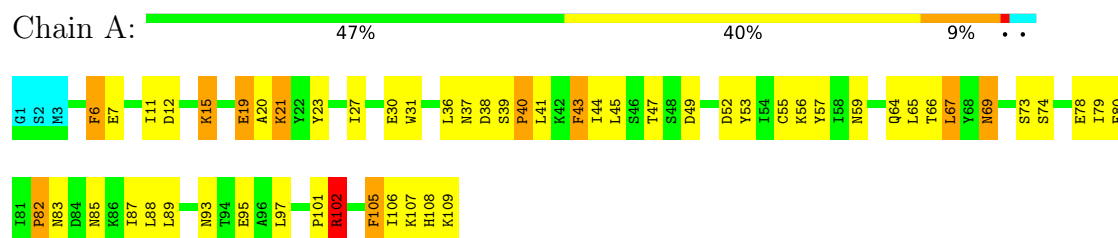
4.2.9 Score per residue for model 9

- Molecule 1: STAPHOSTATIN A



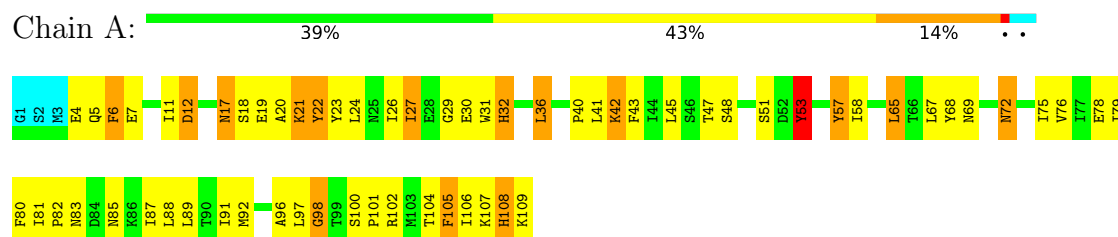
4.2.10 Score per residue for model 10

- Molecule 1: STAPHOSTATIN A



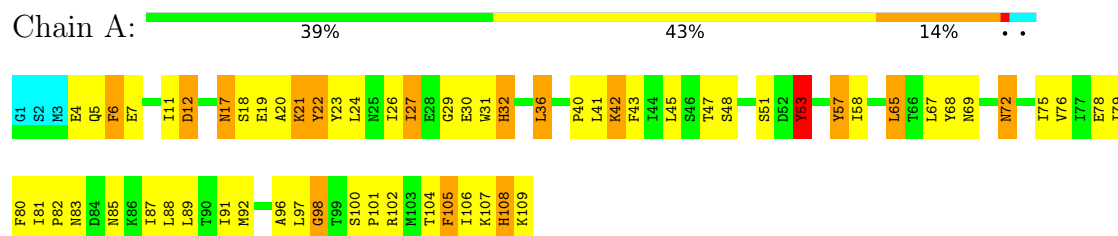
4.2.11 Score per residue for model 11

- Molecule 1: STAPHOSTATIN A



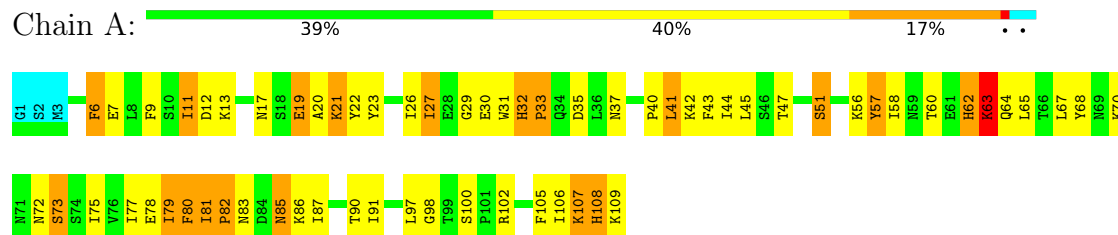
4.2.12 Score per residue for model 12

- Molecule 1: STAPHOSTATIN A



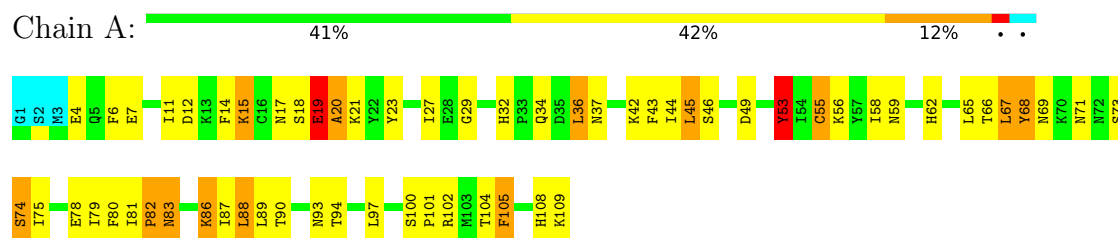
4.2.13 Score per residue for model 13

- Molecule 1: STAPHOSTATIN A



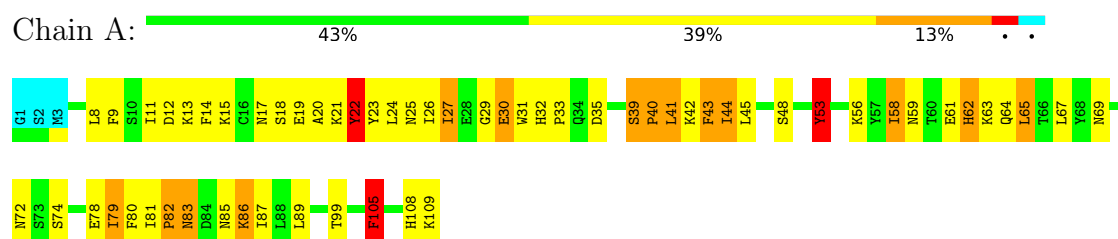
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: STAPHOSTATIN A



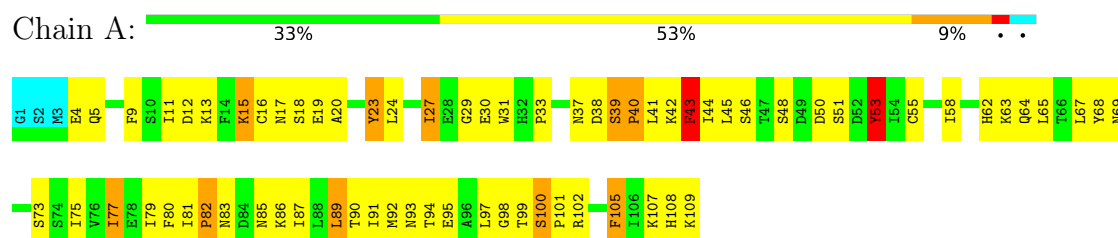
4.2.15 Score per residue for model 15

- Molecule 1: STAPHOSTATIN A



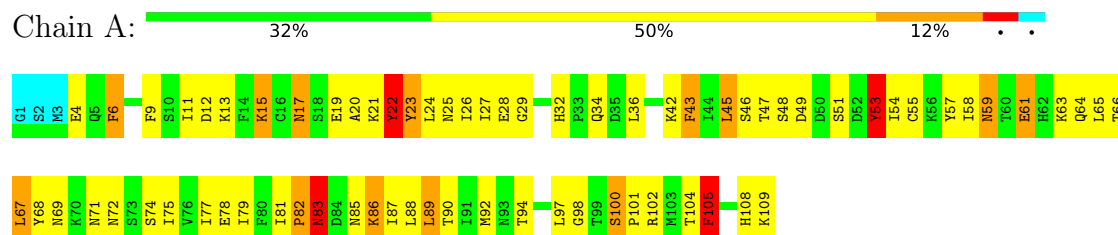
4.2.16 Score per residue for model 16

- Molecule 1: STAPHOSTATIN A



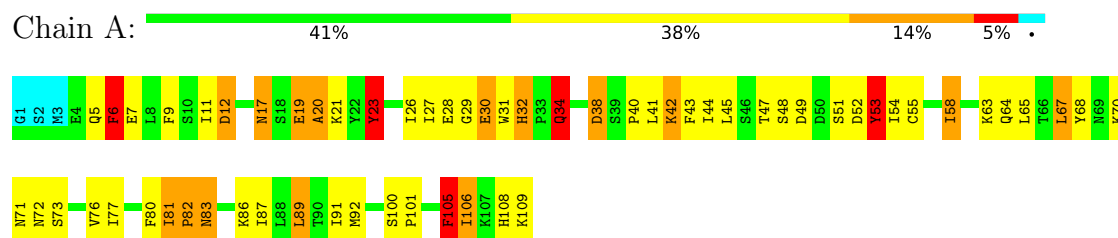
4.2.17 Score per residue for model 17

- Molecule 1: STAPHOSTATIN A



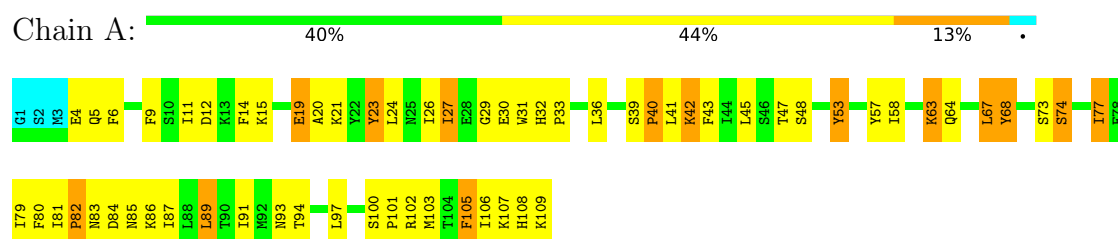
4.2.18 Score per residue for model 18

• Molecule 1: STAPHOSTATIN A



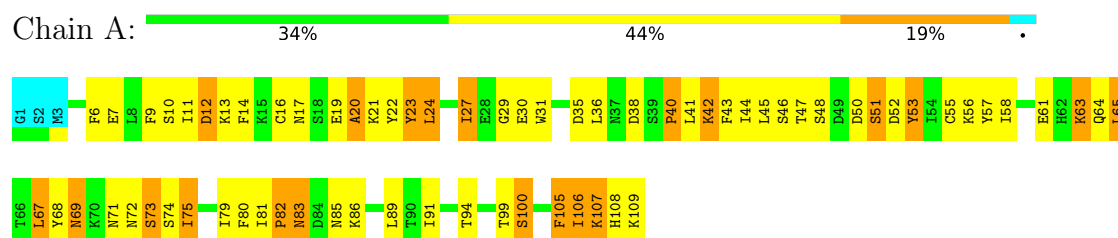
4.2.19 Score per residue for model 19

• Molecule 1: STAPHOSTATIN A



4.2.20 Score per residue for model 20

• Molecule 1: STAPHOSTATIN A



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *SIMMULATED ANNEALING*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *FINAL ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	

No chemical shift data was provided.

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	0.69±0.02	0±0/892 (0.0± 0.0%)	1.10±0.02	2±1/1203 (0.1± 0.1%)
All	All	0.69	0/17840 (0.0%)	1.10	30/24060 (0.1%)

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	3.5±1.6
All	All	0	70

There are no bond-length outliers.

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	22	TYR	CB-CG-CD2	-7.77	116.34	121.00	1	8
1	A	57	TYR	CB-CG-CD2	-6.47	117.12	121.00	13	2
1	A	23	TYR	CB-CG-CD2	-6.46	117.12	121.00	7	1
1	A	6	PHE	CB-CG-CD2	-6.22	116.45	120.80	3	2
1	A	102	ARG	NE-CZ-NH1	6.21	123.41	120.30	3	2
1	A	89	LEU	CA-CB-CG	5.89	128.84	115.30	19	1
1	A	43	PHE	CB-CG-CD1	-5.57	116.90	120.80	16	5
1	A	18	SER	N-CA-CB	5.52	118.78	110.50	9	1
1	A	20	ALA	N-CA-CB	5.50	117.81	110.10	18	1
1	A	22	TYR	CB-CG-CD1	5.45	124.27	121.00	1	1
1	A	57	TYR	CB-CG-CD1	5.43	124.26	121.00	13	1
1	A	105	PHE	CB-CG-CD1	-5.38	117.03	120.80	8	3
1	A	14	PHE	CB-CG-CD2	-5.11	117.22	120.80	2	1
1	A	53	TYR	CB-CG-CD2	-5.02	117.99	121.00	9	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	53	TYR	Sidechain	16
1	A	22	TYR	Sidechain	9
1	A	24	LEU	Mainchain	7
1	A	57	TYR	Sidechain	7
1	A	105	PHE	Sidechain	7
1	A	34	GLN	Mainchain	6
1	A	20	ALA	Mainchain	4
1	A	5	GLN	Mainchain	3
1	A	23	TYR	Sidechain	2
1	A	73	SER	Mainchain	2
1	A	36	LEU	Mainchain	1
1	A	62	HIS	Mainchain	1
1	A	16	CYS	Mainchain	1
1	A	51	SER	Mainchain	1
1	A	6	PHE	Sidechain	1
1	A	17	ASN	Mainchain	1
1	A	35	ASP	Mainchain	1

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	874	243	854	29±6
All	All	17480	4860	17080	576

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:LYS:CA	1:A:109:LYS:CG	0.87	2.52	10	19
1:A:109:LYS:CG	1:A:109:LYS:CA	0.85	2.55	2	1
1:A:79:ILE:HG22	1:A:89:LEU:HA	0.85	1.47	10	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:SER:HB2	1:A:58:ILE:HG12	0.79	1.54	14	2
1:A:13:LYS:HB2	1:A:46:SER:HB3	0.79	1.54	16	2
1:A:68:TYR:HB3	1:A:76:VAL:HB	0.77	1.56	8	2
1:A:64:GLN:HE21	1:A:80:PHE:HB2	0.77	1.37	8	4
1:A:91:ILE:HB	1:A:101:PRO:HG3	0.76	1.57	9	1
1:A:11:ILE:HG22	1:A:45:LEU:HA	0.76	1.56	16	18
1:A:72:ASN:HB2	1:A:75:ILE:HD11	0.76	1.58	9	2
1:A:55:CYS:HA	1:A:67:LEU:HB3	0.74	1.58	10	6
1:A:66:THR:HG22	1:A:78:GLU:HG2	0.71	1.60	14	2
1:A:18:SER:H	1:A:58:ILE:HG21	0.71	1.46	1	1
1:A:47:THR:HB	1:A:51:SER:HA	0.71	1.63	13	1
1:A:27:ILE:HB	1:A:81:ILE:HG12	0.70	1.63	16	5
1:A:11:ILE:HG23	1:A:13:LYS:H	0.70	1.46	20	3
1:A:26:ILE:HB	1:A:81:ILE:HD11	0.70	1.61	18	3
1:A:55:CYS:HB2	1:A:65:LEU:HD11	0.69	1.64	18	2
1:A:17:ASN:HB3	1:A:58:ILE:HG12	0.69	1.62	8	1
1:A:86:LYS:HA	1:A:106:ILE:HG22	0.68	1.66	19	3
1:A:19:GLU:HG2	1:A:65:LEU:HD23	0.67	1.64	17	1
1:A:63:LYS:HB2	1:A:80:PHE:CE1	0.66	2.25	19	8
1:A:83:ASN:ND2	1:A:84:ASP:H	0.66	1.88	3	1
1:A:59:ASN:HB2	1:A:64:GLN:HB3	0.66	1.68	8	1
1:A:76:VAL:HB	1:A:92:MET:HB3	0.66	1.67	11	2
1:A:7:GLU:HB2	1:A:41:LEU:HA	0.65	1.67	11	8
1:A:39:SER:H	1:A:40:PRO:HD3	0.65	1.52	2	2
1:A:76:VAL:HG13	1:A:92:MET:HB2	0.65	1.68	8	2
1:A:19:GLU:HB2	1:A:23:TYR:CD2	0.65	2.26	14	1
1:A:30:GLU:HB3	1:A:42:LYS:HB3	0.64	1.69	15	9
1:A:83:ASN:HD22	1:A:84:ASP:H	0.64	1.32	3	1
1:A:78:GLU:HG3	1:A:90:THR:HB	0.64	1.69	8	1
1:A:87:ILE:HG23	1:A:105:PHE:CD1	0.64	2.27	15	9
1:A:26:ILE:HB	1:A:81:ILE:HG23	0.64	1.69	17	1
1:A:31:TRP:CD1	1:A:41:LEU:HD23	0.63	2.28	19	3
1:A:11:ILE:HB	1:A:43:PHE:CE2	0.63	2.28	16	9
1:A:100:SER:H	1:A:101:PRO:HD2	0.63	1.52	6	4
1:A:72:ASN:HB3	1:A:75:ILE:HG12	0.62	1.71	11	2
1:A:66:THR:HG22	1:A:78:GLU:HB3	0.62	1.71	5	1
1:A:65:LEU:HD13	1:A:67:LEU:HG	0.62	1.71	10	1
1:A:85:ASN:O	1:A:106:ILE:HB	0.62	1.94	19	3
1:A:11:ILE:HB	1:A:43:PHE:CZ	0.61	2.30	17	11
1:A:26:ILE:HG12	1:A:83:ASN:HA	0.61	1.72	3	5
1:A:44:ILE:HG22	1:A:45:LEU:H	0.61	1.56	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HA	1:A:28:GLU:HB3	0.61	1.70	1	1
1:A:34:GLN:HB2	1:A:38:ASP:HA	0.60	1.73	18	1
1:A:85:ASN:HA	1:A:107:LYS:HB3	0.60	1.73	6	1
1:A:31:TRP:HZ2	1:A:81:ILE:HG12	0.60	1.55	13	1
1:A:30:GLU:HA	1:A:41:LEU:O	0.60	1.96	19	14
1:A:31:TRP:CH2	1:A:87:ILE:HB	0.60	2.32	10	4
1:A:80:PHE:CZ	1:A:82:PRO:HB3	0.60	2.32	1	3
1:A:64:GLN:HG3	1:A:79:ILE:O	0.60	1.96	13	2
1:A:55:CYS:HA	1:A:67:LEU:HA	0.59	1.74	9	1
1:A:26:ILE:HB	1:A:81:ILE:HG22	0.59	1.74	19	1
1:A:23:TYR:OH	1:A:64:GLN:HA	0.58	1.99	7	2
1:A:53:TYR:HB3	1:A:67:LEU:HD23	0.58	1.75	17	3
1:A:19:GLU:HG2	1:A:65:LEU:HB2	0.57	1.76	16	1
1:A:57:TYR:CE1	1:A:66:THR:HG21	0.57	2.34	8	1
1:A:12:ASP:HA	1:A:51:SER:HB2	0.57	1.77	8	1
1:A:39:SER:N	1:A:40:PRO:HD3	0.57	2.14	2	8
1:A:29:GLY:O	1:A:42:LYS:HA	0.57	1.99	20	17
1:A:89:LEU:O	1:A:102:ARG:HA	0.57	2.00	14	9
1:A:52:ASP:HB3	1:A:69:ASN:HD21	0.56	1.60	10	1
1:A:33:PRO:HA	1:A:108:HIS:ND1	0.56	2.15	13	1
1:A:59:ASN:HB3	1:A:64:GLN:HG3	0.56	1.75	9	2
1:A:53:TYR:CE1	1:A:69:ASN:HB2	0.56	2.35	15	11
1:A:82:PRO:HD2	1:A:86:LYS:O	0.56	2.01	15	12
1:A:77:ILE:HG22	1:A:91:ILE:HA	0.55	1.77	6	5
1:A:5:GLN:HA	1:A:39:SER:HB2	0.55	1.77	16	2
1:A:59:ASN:HB3	1:A:61:GLU:HG2	0.55	1.78	15	1
1:A:19:GLU:HB2	1:A:23:TYR:CD1	0.55	2.37	19	3
1:A:82:PRO:HG2	1:A:86:LYS:HE2	0.55	1.77	3	1
1:A:23:TYR:HA	1:A:81:ILE:HD12	0.54	1.78	18	1
1:A:85:ASN:HB2	1:A:106:ILE:HB	0.54	1.78	10	3
1:A:12:ASP:HB2	1:A:53:TYR:O	0.54	2.03	10	1
1:A:44:ILE:HG13	1:A:45:LEU:H	0.54	1.62	3	2
1:A:6:PHE:N	1:A:39:SER:HB2	0.54	2.17	1	1
1:A:91:ILE:H	1:A:101:PRO:HD2	0.54	1.62	7	1
1:A:77:ILE:HB	1:A:90:THR:O	0.54	2.02	16	1
1:A:89:LEU:HB3	1:A:103:MET:HB3	0.53	1.80	19	1
1:A:90:THR:HA	1:A:101:PRO:O	0.53	2.04	17	1
1:A:31:TRP:CZ3	1:A:107:LYS:HB2	0.53	2.39	10	7
1:A:88:LEU:HG	1:A:104:THR:HB	0.52	1.81	14	1
1:A:105:PHE:CD1	1:A:105:PHE:N	0.52	2.77	19	2
1:A:91:ILE:H	1:A:101:PRO:HB3	0.52	1.64	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:SER:HB3	1:A:46:SER:O	0.52	2.04	20	1
1:A:19:GLU:HG2	1:A:65:LEU:HD13	0.52	1.81	14	1
1:A:92:MET:HA	1:A:98:GLY:HA3	0.52	1.82	2	1
1:A:56:LYS:HG2	1:A:68:TYR:CE1	0.52	2.39	1	1
1:A:19:GLU:HB3	1:A:58:ILE:HD13	0.52	1.81	14	4
1:A:68:TYR:HA	1:A:75:ILE:O	0.52	2.04	16	10
1:A:23:TYR:O	1:A:27:ILE:HG22	0.52	2.05	17	13
1:A:27:ILE:HG23	1:A:43:PHE:CE1	0.52	2.40	3	2
1:A:27:ILE:HB	1:A:81:ILE:HD13	0.52	1.82	9	2
1:A:27:ILE:HG13	1:A:31:TRP:HE1	0.52	1.64	10	1
1:A:23:TYR:HA	1:A:81:ILE:HG21	0.51	1.82	17	1
1:A:85:ASN:HD22	1:A:107:LYS:HB3	0.51	1.64	19	3
1:A:58:ILE:HB	1:A:64:GLN:O	0.51	2.04	13	1
1:A:78:GLU:HG2	1:A:90:THR:HB	0.51	1.82	5	1
1:A:23:TYR:CD1	1:A:81:ILE:HG13	0.51	2.40	6	1
1:A:61:GLU:HB3	1:A:64:GLN:HB3	0.51	1.82	6	1
1:A:23:TYR:HA	1:A:81:ILE:HG12	0.51	1.82	11	3
1:A:74:SER:O	1:A:93:ASN:HA	0.51	2.05	10	3
1:A:13:LYS:NZ	1:A:45:LEU:HB3	0.51	2.20	16	1
1:A:80:PHE:CD1	1:A:81:ILE:N	0.51	2.79	9	8
1:A:90:THR:HA	1:A:101:PRO:HB2	0.51	1.83	8	2
1:A:106:ILE:H	1:A:106:ILE:HD13	0.51	1.66	20	1
1:A:11:ILE:HB	1:A:43:PHE:CE1	0.51	2.40	20	3
1:A:27:ILE:HB	1:A:81:ILE:HG21	0.51	1.82	13	3
1:A:79:ILE:CG2	1:A:89:LEU:HG	0.51	2.35	15	1
1:A:23:TYR:CD1	1:A:81:ILE:HG21	0.51	2.40	9	2
1:A:9:PHE:O	1:A:43:PHE:HA	0.51	2.06	16	13
1:A:4:GLU:HA	1:A:7:GLU:OE2	0.51	2.05	14	2
1:A:16:CYS:HB3	1:A:19:GLU:OE1	0.51	2.06	7	1
1:A:82:PRO:HG2	1:A:86:LYS:HG3	0.50	1.82	16	2
1:A:31:TRP:HA	1:A:107:LYS:NZ	0.50	2.20	6	1
1:A:69:ASN:HB3	1:A:75:ILE:HG23	0.50	1.84	4	2
1:A:65:LEU:O	1:A:78:GLU:HA	0.50	2.06	11	3
1:A:19:GLU:HG3	1:A:23:TYR:CD1	0.50	2.42	5	1
1:A:80:PHE:O	1:A:87:ILE:HG13	0.49	2.07	16	7
1:A:80:PHE:CE2	1:A:82:PRO:HG3	0.49	2.42	6	3
1:A:92:MET:HA	1:A:98:GLY:O	0.49	2.06	11	2
1:A:53:TYR:HB3	1:A:67:LEU:HD12	0.49	1.83	16	1
1:A:21:LYS:H	1:A:21:LYS:HD3	0.49	1.66	13	1
1:A:23:TYR:CZ	1:A:81:ILE:HD13	0.49	2.42	17	1
1:A:26:ILE:HG22	1:A:31:TRP:CZ2	0.49	2.42	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TYR:CZ	1:A:77:ILE:HG12	0.49	2.43	17	2
1:A:32:HIS:HD2	1:A:35:ASP:HA	0.48	1.67	13	1
1:A:12:ASP:OD2	1:A:14:PHE:HB2	0.48	2.08	15	1
1:A:17:ASN:O	1:A:58:ILE:HG21	0.48	2.08	16	1
1:A:26:ILE:HB	1:A:81:ILE:CG2	0.48	2.38	19	1
1:A:12:ASP:HB3	1:A:53:TYR:O	0.48	2.09	14	1
1:A:26:ILE:HB	1:A:81:ILE:CD1	0.48	2.36	18	1
1:A:19:GLU:HB3	1:A:58:ILE:HD12	0.48	1.86	4	1
1:A:21:LYS:HE3	1:A:21:LYS:HA	0.48	1.86	7	1
1:A:34:GLN:CB	1:A:38:ASP:HA	0.48	2.37	18	1
1:A:100:SER:N	1:A:101:PRO:HD2	0.47	2.24	6	1
1:A:19:GLU:HG3	1:A:65:LEU:HB3	0.47	1.86	7	1
1:A:64:GLN:HB2	1:A:80:PHE:CD2	0.47	2.44	7	2
1:A:31:TRP:CZ2	1:A:87:ILE:HD11	0.47	2.44	8	1
1:A:32:HIS:CD2	1:A:35:ASP:HA	0.47	2.43	13	1
1:A:13:LYS:HB2	1:A:46:SER:HB2	0.47	1.86	4	1
1:A:75:ILE:HD13	1:A:93:ASN:OD1	0.47	2.09	16	1
1:A:16:CYS:HB2	1:A:19:GLU:HB2	0.47	1.87	20	1
1:A:19:GLU:HB2	1:A:23:TYR:HB2	0.47	1.85	6	1
1:A:47:THR:HG22	1:A:48:SER:H	0.47	1.68	17	3
1:A:31:TRP:CD1	1:A:41:LEU:HG	0.47	2.44	13	1
1:A:12:ASP:HA	1:A:51:SER:HB3	0.47	1.87	18	1
1:A:27:ILE:HB	1:A:81:ILE:HG13	0.47	1.85	18	1
1:A:22:TYR:CE2	1:A:63:LYS:HB3	0.47	2.45	5	3
1:A:68:TYR:CD1	1:A:74:SER:HA	0.47	2.45	19	1
1:A:53:TYR:CE1	1:A:67:LEU:HD13	0.47	2.45	4	1
1:A:31:TRP:CZ3	1:A:87:ILE:HG22	0.47	2.44	16	1
1:A:23:TYR:CE1	1:A:81:ILE:HG12	0.47	2.45	19	1
1:A:87:ILE:HG22	1:A:105:PHE:CD1	0.47	2.45	4	1
1:A:90:THR:HG22	1:A:102:ARG:HG3	0.47	1.87	14	1
1:A:23:TYR:CD1	1:A:81:ILE:HG22	0.46	2.45	13	1
1:A:68:TYR:CE1	1:A:74:SER:HA	0.46	2.46	14	1
1:A:12:ASP:HA	1:A:51:SER:CB	0.46	2.41	13	10
1:A:94:THR:HG23	1:A:95:GLU:H	0.46	1.70	5	1
1:A:38:ASP:C	1:A:40:PRO:HD3	0.46	2.30	20	2
1:A:62:HIS:O	1:A:63:LYS:HB2	0.46	2.10	13	1
1:A:64:GLN:HG2	1:A:80:PHE:HB2	0.46	1.88	20	1
1:A:23:TYR:CE1	1:A:65:LEU:HD11	0.46	2.45	15	1
1:A:92:MET:HA	1:A:98:GLY:CA	0.46	2.41	16	1
1:A:87:ILE:HG23	1:A:105:PHE:HD1	0.46	1.71	3	3
1:A:23:TYR:HA	1:A:81:ILE:CG2	0.46	2.41	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:ILE:HG22	1:A:101:PRO:HB3	0.45	1.88	8	1
1:A:91:ILE:H	1:A:101:PRO:CG	0.45	2.23	18	1
1:A:12:ASP:HA	1:A:51:SER:OG	0.45	2.11	3	3
1:A:83:ASN:O	1:A:86:LYS:HG2	0.45	2.11	14	1
1:A:54:ILE:O	1:A:67:LEU:HG	0.45	2.10	17	1
1:A:20:ALA:O	1:A:24:LEU:HG	0.45	2.10	20	1
1:A:18:SER:O	1:A:19:GLU:HG2	0.45	2.12	3	1
1:A:28:GLU:OE2	1:A:44:ILE:HA	0.45	2.12	18	1
1:A:80:PHE:O	1:A:87:ILE:HG12	0.45	2.11	4	1
1:A:90:THR:HB	1:A:100:SER:OG	0.45	2.12	13	1
1:A:23:TYR:CE1	1:A:81:ILE:HG13	0.45	2.47	6	1
1:A:58:ILE:HG22	1:A:65:LEU:HB3	0.45	1.88	17	1
1:A:31:TRP:CZ2	1:A:87:ILE:HD12	0.45	2.46	19	1
1:A:58:ILE:HG22	1:A:65:LEU:HD13	0.44	1.88	9	1
1:A:59:ASN:ND2	1:A:61:GLU:HB2	0.44	2.26	17	1
1:A:26:ILE:HG13	1:A:82:PRO:O	0.44	2.12	7	1
1:A:27:ILE:HG12	1:A:31:TRP:HE1	0.44	1.72	20	1
1:A:19:GLU:OE1	1:A:65:LEU:HG	0.44	2.12	3	1
1:A:77:ILE:H	1:A:77:ILE:HD13	0.44	1.73	19	1
1:A:19:GLU:HB2	1:A:58:ILE:HD13	0.44	1.88	15	1
1:A:61:GLU:HG3	1:A:62:HIS:H	0.44	1.73	15	1
1:A:79:ILE:HG21	1:A:89:LEU:HG	0.44	1.89	15	1
1:A:27:ILE:HD11	1:A:41:LEU:HD21	0.44	1.89	19	1
1:A:13:LYS:HB3	1:A:46:SER:HB2	0.44	1.89	3	1
1:A:66:THR:OG1	1:A:78:GLU:HB3	0.44	2.13	8	1
1:A:89:LEU:HB3	1:A:105:PHE:HE1	0.43	1.73	20	1
1:A:13:LYS:HB3	1:A:46:SER:HB3	0.43	1.89	6	1
1:A:23:TYR:CZ	1:A:65:LEU:HG	0.43	2.48	10	2
1:A:31:TRP:O	1:A:40:PRO:HB3	0.43	2.13	15	1
1:A:67:LEU:O	1:A:77:ILE:HD13	0.43	2.13	19	1
1:A:19:GLU:HB2	1:A:23:TYR:CG	0.43	2.49	4	1
1:A:69:ASN:OD1	1:A:71:ASN:HB2	0.43	2.13	4	1
1:A:5:GLN:C	1:A:39:SER:HB2	0.43	2.34	5	1
1:A:41:LEU:HD22	1:A:105:PHE:CE2	0.43	2.49	15	1
1:A:27:ILE:CB	1:A:81:ILE:HG12	0.43	2.40	16	1
1:A:23:TYR:CZ	1:A:81:ILE:HG12	0.43	2.47	20	1
1:A:27:ILE:HB	1:A:81:ILE:CD1	0.43	2.44	5	1
1:A:6:PHE:H	1:A:39:SER:HB2	0.43	1.74	1	1
1:A:89:LEU:HB2	1:A:105:PHE:HE1	0.43	1.74	18	1
1:A:27:ILE:HG13	1:A:81:ILE:HD12	0.43	1.89	19	1
1:A:52:ASP:HB3	1:A:69:ASN:OD1	0.43	2.14	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:SER:O	1:A:53:TYR:HB2	0.43	2.14	5	1
1:A:74:SER:HB2	1:A:94:THR:HB	0.42	1.90	8	1
1:A:91:ILE:HB	1:A:101:PRO:HG2	0.42	1.91	2	3
1:A:68:TYR:HB3	1:A:76:VAL:HG22	0.42	1.91	3	1
1:A:54:ILE:HG23	1:A:68:TYR:CE1	0.42	2.49	8	1
1:A:74:SER:HB3	1:A:94:THR:OG1	0.42	2.13	17	1
1:A:55:CYS:CA	1:A:67:LEU:HB3	0.42	2.39	18	1
1:A:23:TYR:CE2	1:A:81:ILE:HD13	0.42	2.49	4	1
1:A:100:SER:H	1:A:101:PRO:CD	0.42	2.27	9	1
1:A:93:ASN:HB2	1:A:96:ALA:HB3	0.42	1.90	5	1
1:A:7:GLU:HB3	1:A:9:PHE:CE2	0.42	2.49	13	1
1:A:17:ASN:O	1:A:58:ILE:HG23	0.42	2.15	18	1
1:A:80:PHE:O	1:A:87:ILE:HD12	0.42	2.14	9	1
1:A:89:LEU:HB2	1:A:105:PHE:CZ	0.42	2.49	19	1
1:A:31:TRP:CE3	1:A:107:LYS:HG2	0.42	2.49	7	1
1:A:17:ASN:O	1:A:58:ILE:HG12	0.42	2.15	9	1
1:A:23:TYR:CE1	1:A:81:ILE:HG22	0.42	2.50	13	1
1:A:5:GLN:O	1:A:39:SER:HB2	0.41	2.15	5	1
1:A:31:TRP:CE2	1:A:87:ILE:HD11	0.41	2.50	8	1
1:A:85:ASN:HB3	1:A:107:LYS:O	0.41	2.15	13	1
1:A:74:SER:HB3	1:A:94:THR:HB	0.41	1.92	20	1
1:A:14:PHE:O	1:A:15:LYS:HB2	0.41	2.15	1	1
1:A:81:ILE:HA	1:A:87:ILE:HG12	0.41	1.91	18	1
1:A:23:TYR:CE2	1:A:81:ILE:HG12	0.41	2.51	20	1
1:A:12:ASP:HB2	1:A:54:ILE:HA	0.41	1.90	18	1
1:A:90:THR:HA	1:A:101:PRO:CB	0.41	2.46	8	1
1:A:21:LYS:H	1:A:21:LYS:HE2	0.41	1.76	10	1
1:A:41:LEU:O	1:A:41:LEU:HG	0.41	2.14	15	1
1:A:98:GLY:O	1:A:101:PRO:HD2	0.41	2.16	4	1
1:A:87:ILE:O	1:A:104:THR:HA	0.41	2.16	8	1
1:A:106:ILE:HD13	1:A:106:ILE:H	0.41	1.76	18	1
1:A:9:PHE:CD1	1:A:53:TYR:CE2	0.41	3.09	19	1
1:A:7:GLU:HG2	1:A:9:PHE:CE2	0.41	2.51	20	1
1:A:18:SER:HB3	1:A:58:ILE:HG21	0.41	1.93	4	1
1:A:31:TRP:O	1:A:40:PRO:HB2	0.41	2.16	8	1
1:A:27:ILE:HG23	1:A:43:PHE:CD1	0.40	2.51	11	2
1:A:19:GLU:OE2	1:A:65:LEU:HD22	0.40	2.16	14	1
1:A:64:GLN:HB2	1:A:79:ILE:O	0.40	2.15	10	1
1:A:56:LYS:HD2	1:A:68:TYR:HB3	0.40	1.94	14	1
1:A:55:CYS:HA	1:A:67:LEU:CD1	0.40	2.46	17	1
1:A:31:TRP:O	1:A:32:HIS:HB2	0.40	2.16	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ILE:N	1:A:81:ILE:HD12	0.40	2.31	15	1
1:A:12:ASP:OD1	1:A:14:PHE:HB2	0.40	2.15	14	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	105/109 (96%)	67±4 (64±4%)	23±4 (22±4%)	14±3 (14±2%)	1	5
All	All	2100/2180 (96%)	1342 (64%)	468 (22%)	290 (14%)	1	5

All 45 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	82	PRO	20
1	A	20	ALA	19
1	A	83	ASN	19
1	A	108	HIS	19
1	A	21	LYS	18
1	A	40	PRO	15
1	A	100	SER	15
1	A	73	SER	12
1	A	32	HIS	11
1	A	6	PHE	10
1	A	15	LYS	9
1	A	101	PRO	9
1	A	17	ASN	9
1	A	36	LEU	8
1	A	48	SER	8
1	A	19	GLU	7
1	A	102	ARG	6
1	A	49	ASP	6
1	A	33	PRO	6
1	A	4	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	51	SER	5
1	A	63	LYS	5
1	A	99	THR	5
1	A	47	THR	4
1	A	60	THR	4
1	A	18	SER	4
1	A	98	GLY	4
1	A	12	ASP	3
1	A	39	SER	3
1	A	38	ASP	3
1	A	34	GLN	2
1	A	85	ASN	2
1	A	96	ALA	2
1	A	61	GLU	1
1	A	94	THR	1
1	A	37	ASN	1
1	A	50	ASP	1
1	A	14	PHE	1
1	A	16	CYS	1
1	A	84	ASP	1
1	A	97	LEU	1
1	A	62	HIS	1
1	A	46	SER	1
1	A	27	ILE	1
1	A	72	ASN	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	101/104 (97%)	80±3 (79±3%)	21±3 (21±3%)	3	32
All	All	2020/2080 (97%)	1602 (79%)	418 (21%)	3	32

All 86 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	105	PHE	18
1	A	6	PHE	14
1	A	67	LEU	14
1	A	53	TYR	13
1	A	36	LEU	10
1	A	97	LEU	10
1	A	15	LYS	10
1	A	62	HIS	8
1	A	23	TYR	8
1	A	42	LYS	8
1	A	65	LEU	8
1	A	19	GLU	8
1	A	27	ILE	8
1	A	22	TYR	7
1	A	21	LYS	7
1	A	44	ILE	7
1	A	72	ASN	7
1	A	13	LYS	6
1	A	35	ASP	6
1	A	37	ASN	6
1	A	60	THR	6
1	A	88	LEU	6
1	A	64	GLN	6
1	A	102	ARG	6
1	A	106	ILE	6
1	A	70	LYS	6
1	A	71	ASN	6
1	A	83	ASN	5
1	A	104	THR	5
1	A	47	THR	5
1	A	56	LYS	5
1	A	61	GLU	5
1	A	45	LEU	5
1	A	78	GLU	5
1	A	50	ASP	5
1	A	84	ASP	5
1	A	57	TYR	5
1	A	95	GLU	5
1	A	17	ASN	5
1	A	32	HIS	5
1	A	85	ASN	5
1	A	12	ASP	4
1	A	68	TYR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	69	ASN	4
1	A	74	SER	4
1	A	63	LYS	4
1	A	49	ASP	4
1	A	58	ILE	4
1	A	94	THR	4
1	A	30	GLU	4
1	A	75	ILE	4
1	A	14	PHE	4
1	A	16	CYS	4
1	A	34	GLN	4
1	A	25	ASN	4
1	A	41	LEU	4
1	A	107	LYS	3
1	A	5	GLN	3
1	A	11	ILE	3
1	A	100	SER	3
1	A	99	THR	3
1	A	18	SER	3
1	A	66	THR	3
1	A	108	HIS	3
1	A	59	ASN	3
1	A	86	LYS	3
1	A	89	LEU	3
1	A	4	GLU	2
1	A	43	PHE	2
1	A	80	PHE	2
1	A	93	ASN	2
1	A	92	MET	2
1	A	8	LEU	2
1	A	28	GLU	2
1	A	79	ILE	2
1	A	81	ILE	2
1	A	77	ILE	2
1	A	24	LEU	2
1	A	51	SER	1
1	A	39	SER	1
1	A	87	ILE	1
1	A	10	SER	1
1	A	26	ILE	1
1	A	55	CYS	1
1	A	52	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	91	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

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