



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 11:46 PM UTC

PDB ID : 1E8L / pdb_00001e8l
Title : NMR solution structure of hen lysozyme
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Deposited on : 2000-09-27

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

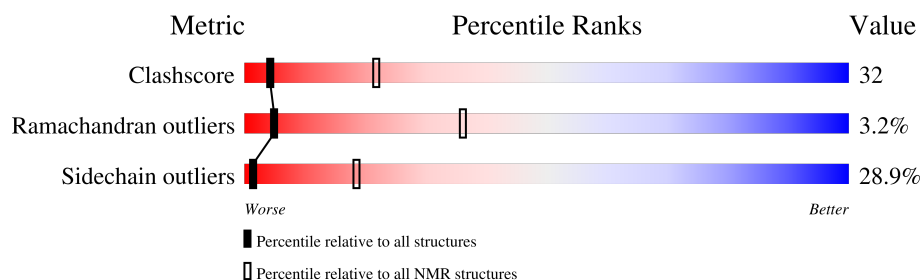
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	129	32% 57% 11%

2 Ensemble composition and analysis

This entry contains 50 models. Model 24 is the overall representative, medoid model (most similar to other models). The authors have identified model 49 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:1-A:129 (129)	0.59	24

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 14, 15, 16, 17, 18, 19, 21, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37
2	40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50
3	11, 12, 13
4	20, 22
5	38, 39

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1961 atoms, of which 960 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LYSOZYME.

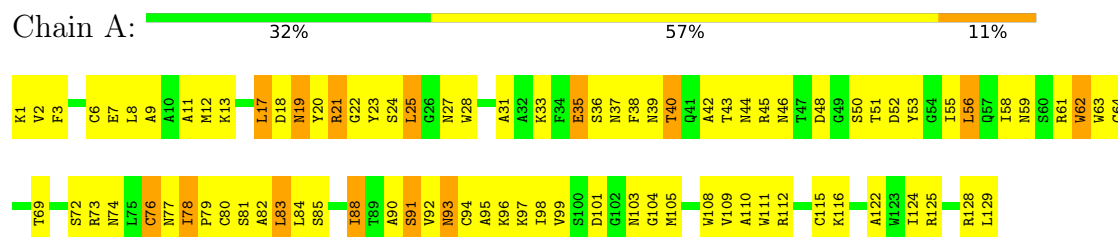
Mol	Chain	Residues	Atoms						Trace
1	A	129	Total	C	H	N	O	S	0
			1961	613	960	193	185	10	

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: LYSOZYME

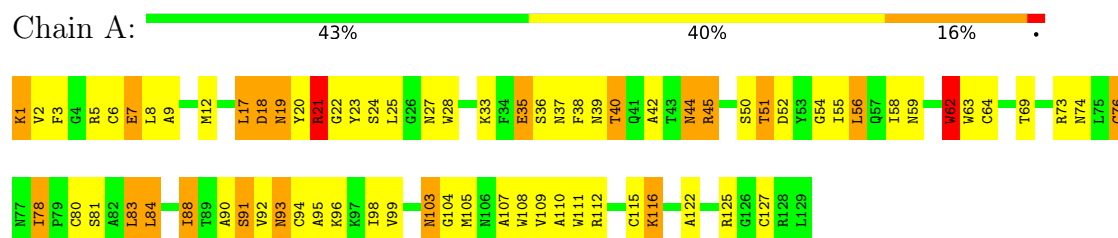


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

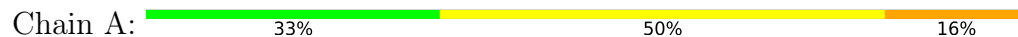
4.2.1 Score per residue for model 1

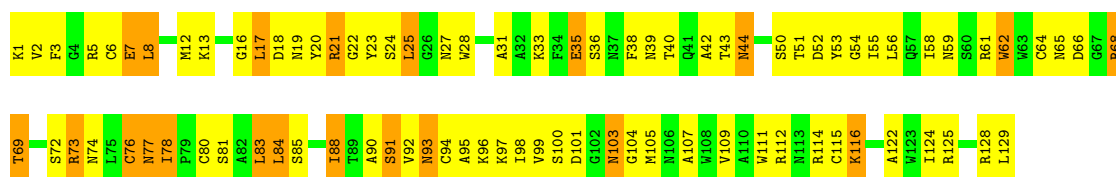
• Molecule 1: LYSOZYME



4.2.2 Score per residue for model 2

• Molecule 1: LYSOZYME

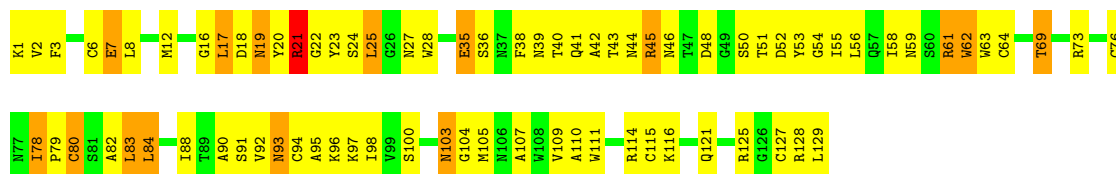




4.2.3 Score per residue for model 3

- Molecule 1: LYSOZYME

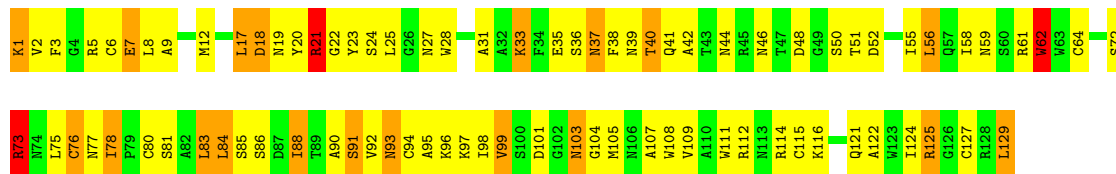
Chain A: 39% 49% 12% .



4.2.4 Score per residue for model 4

- Molecule 1: LYSOZYME

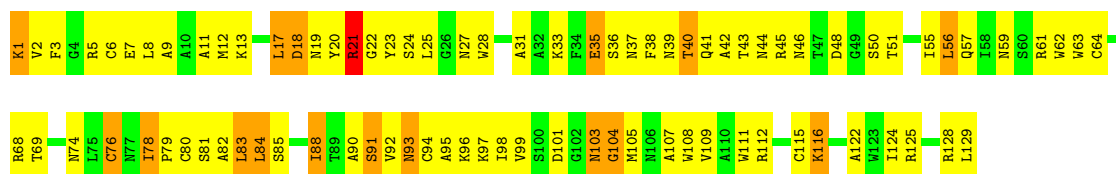
Chain A: 35% 48% 15% .



4.2.5 Score per residue for model 5

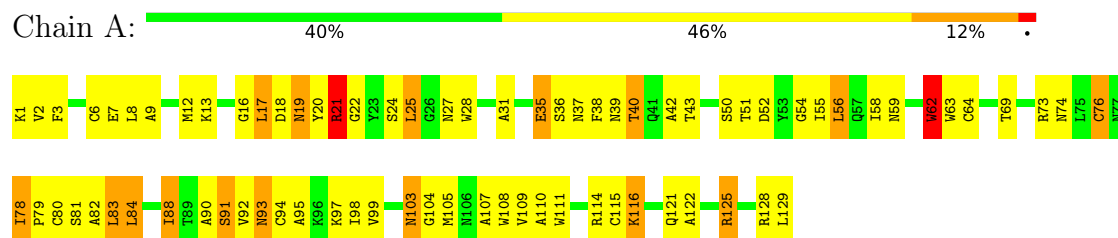
- Molecule 1: LYSOZYME

Chain A: 33% 53% 12% .



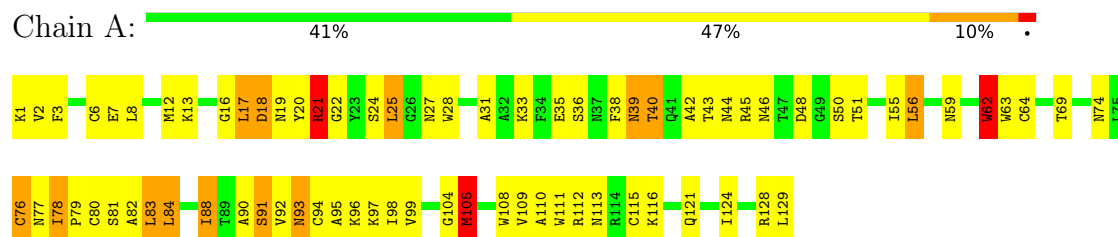
4.2.6 Score per residue for model 6

- Molecule 1: LYSOZYME



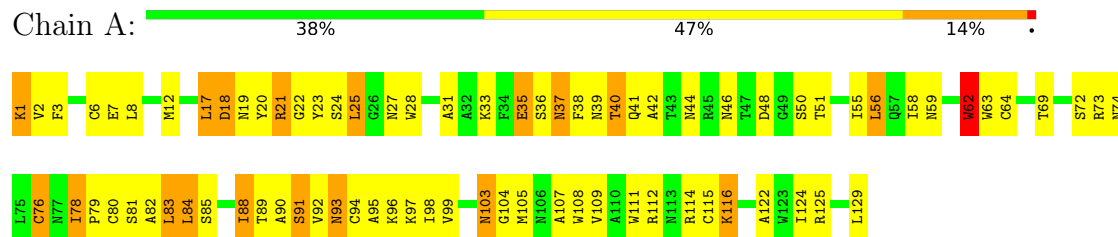
4.2.7 Score per residue for model 7

- Molecule 1: LYSOZYME



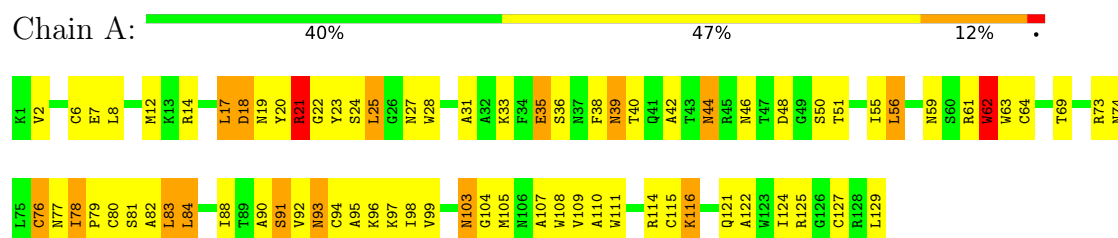
4.2.8 Score per residue for model 8

- Molecule 1: LYSOZYME



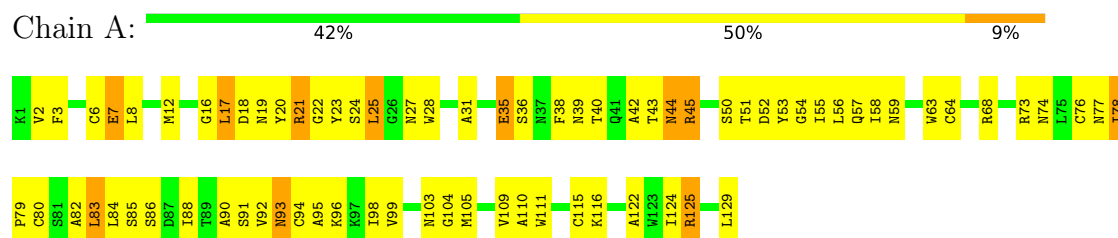
4.2.9 Score per residue for model 9

- Molecule 1: LYSOZYME



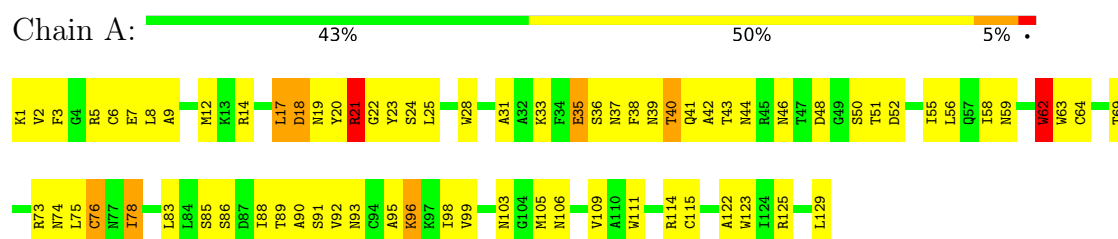
4.2.10 Score per residue for model 10

• Molecule 1: LYSOZYME



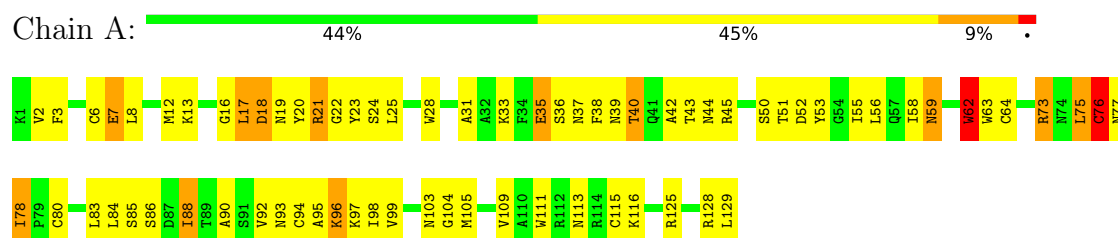
4.2.11 Score per residue for model 11

• Molecule 1: LYSOZYME



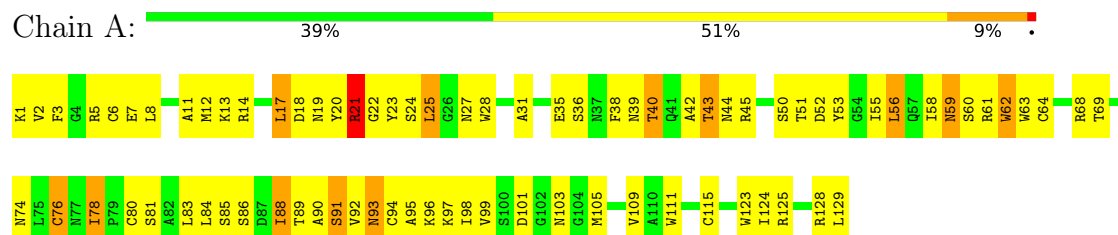
4.2.12 Score per residue for model 12

• Molecule 1: LYSOZYME



4.2.13 Score per residue for model 13

• Molecule 1: LYSOZYME



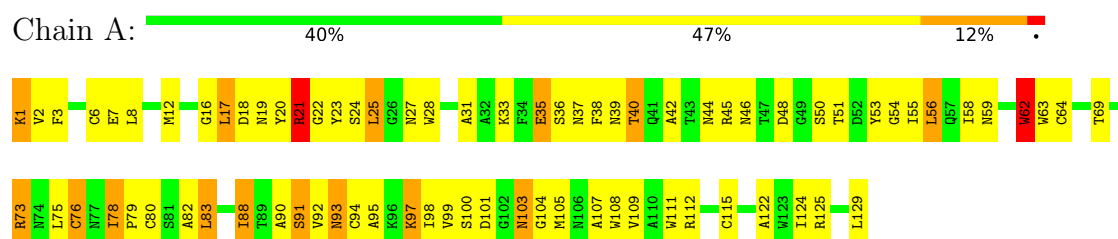
4.2.14 Score per residue for model 14

- Molecule 1: LYSOZYME



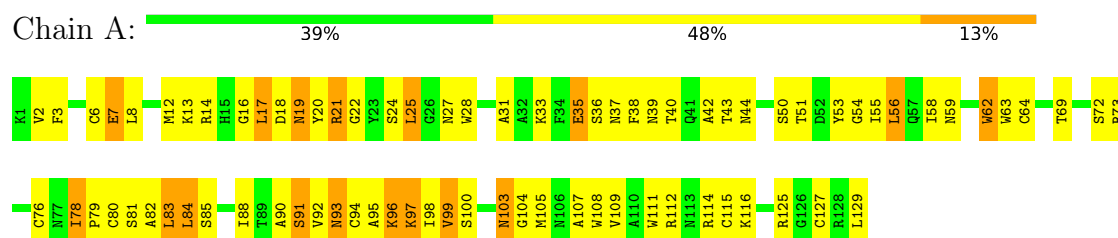
4.2.15 Score per residue for model 15

- Molecule 1: LYSOZYME



4.2.16 Score per residue for model 16

- Molecule 1: LYSOZYME



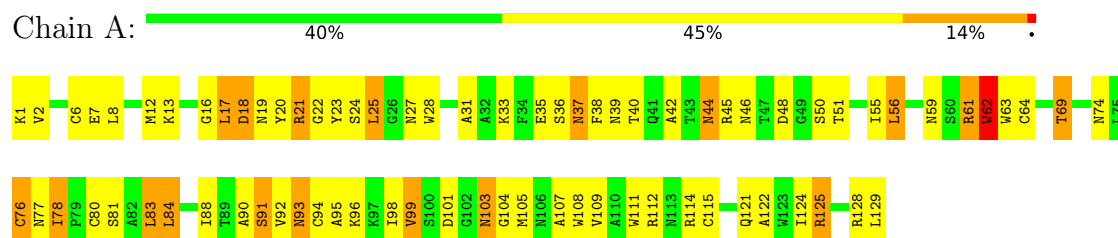
4.2.17 Score per residue for model 17

- Molecule 1: LYSOZYME



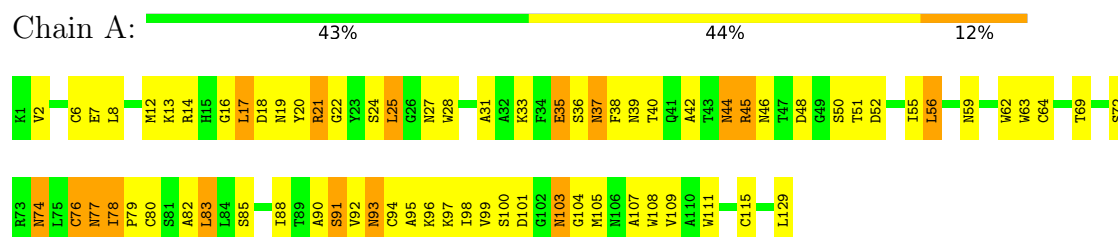
4.2.18 Score per residue for model 18

- Molecule 1: LYSOZYME



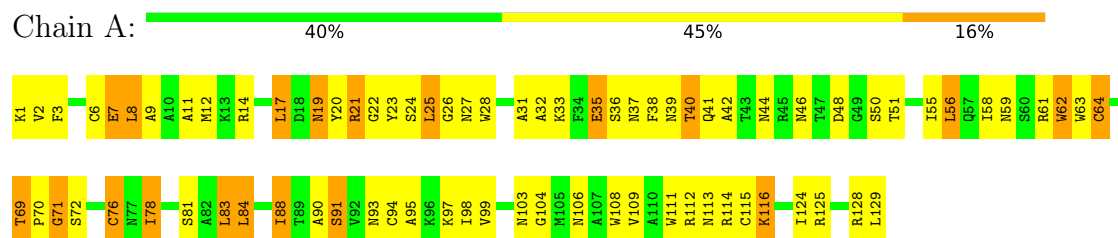
4.2.19 Score per residue for model 19

- Molecule 1: LYSOZYME



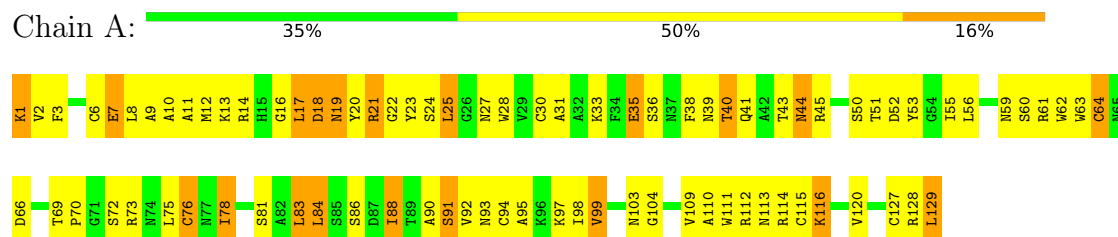
4.2.20 Score per residue for model 20

- Molecule 1: LYSOZYME



4.2.21 Score per residue for model 21

- Molecule 1: LYSOZYME



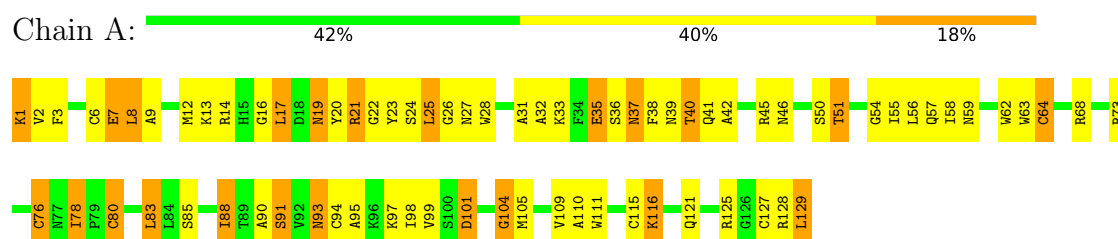
4.2.22 Score per residue for model 22

- Molecule 1: LYSOZYME



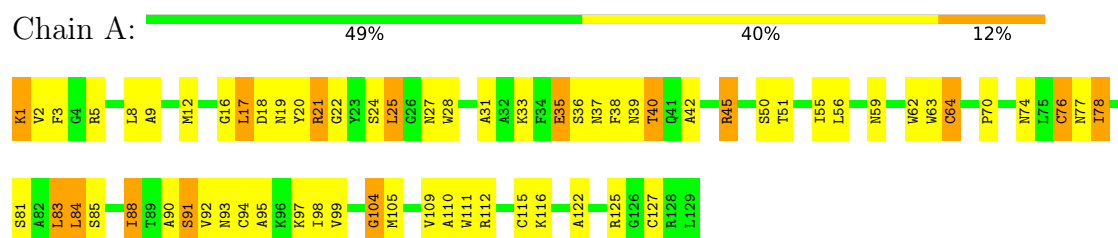
4.2.23 Score per residue for model 23

- Molecule 1: LYSOZYME



4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: LYSOZYME



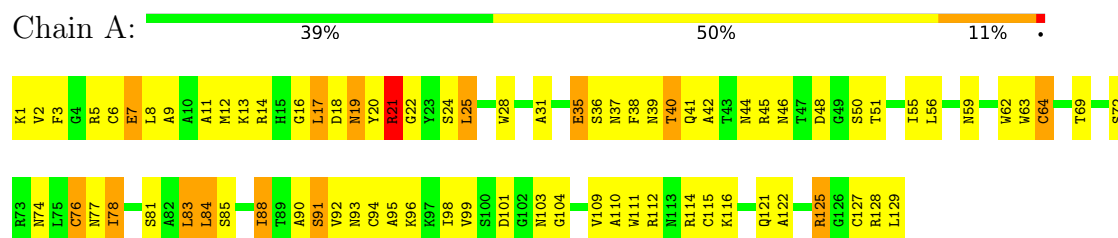
4.2.25 Score per residue for model 25

- Molecule 1: LYSOZYME



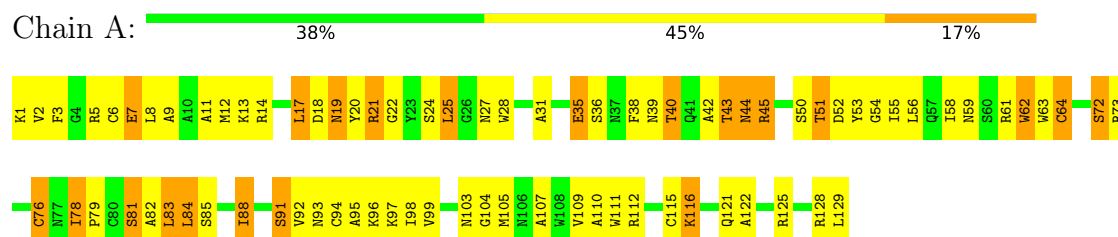
4.2.26 Score per residue for model 26

- Molecule 1: LYSOZYME



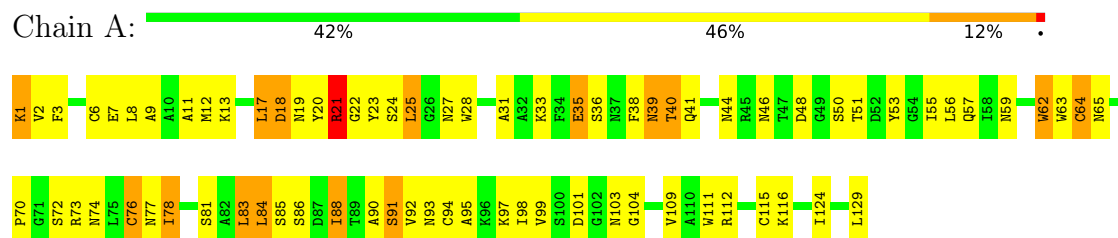
4.2.27 Score per residue for model 27

- Molecule 1: LYSOZYME



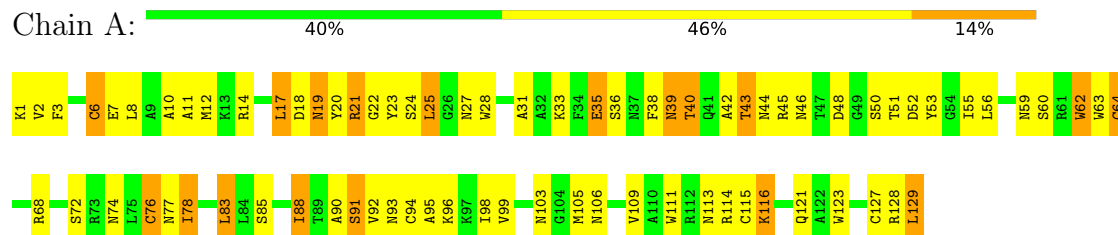
4.2.28 Score per residue for model 28

- Molecule 1: LYSOZYME



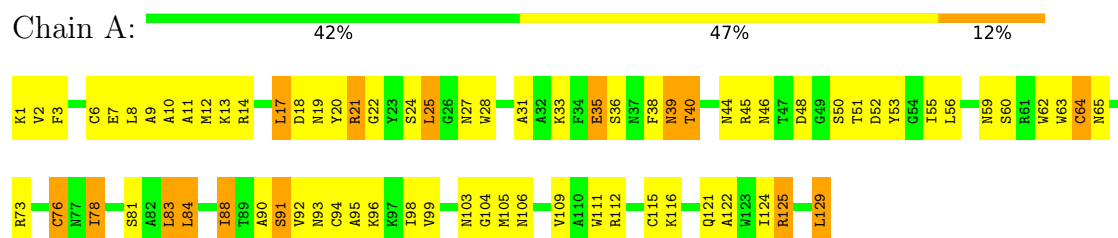
4.2.29 Score per residue for model 29

- Molecule 1: LYSOZYME



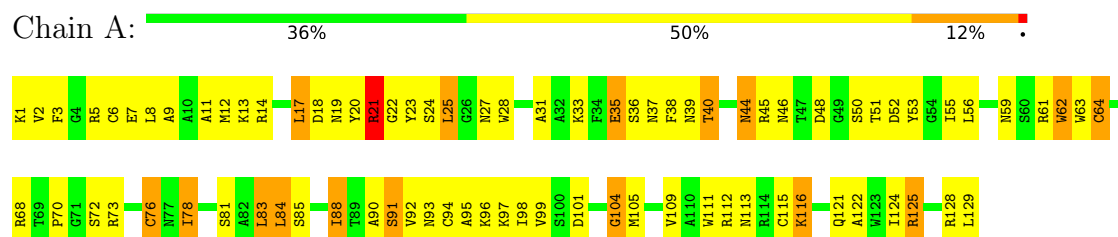
4.2.30 Score per residue for model 30

- Molecule 1: LYSOZYME



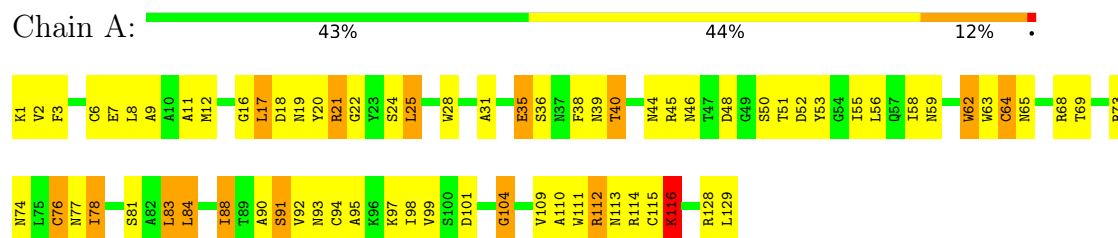
4.2.31 Score per residue for model 31

- Molecule 1: LYSOZYME



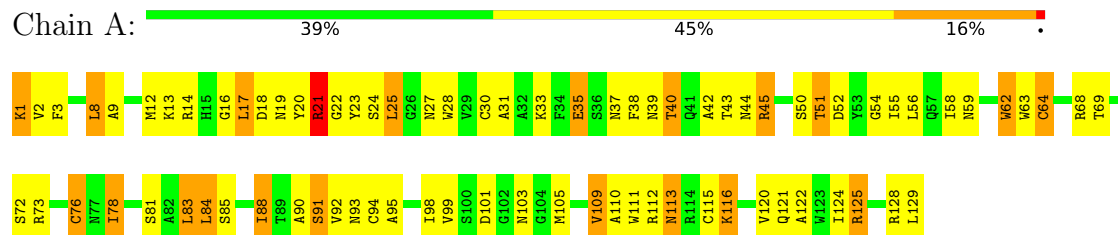
4.2.32 Score per residue for model 32

- Molecule 1: LYSOZYME



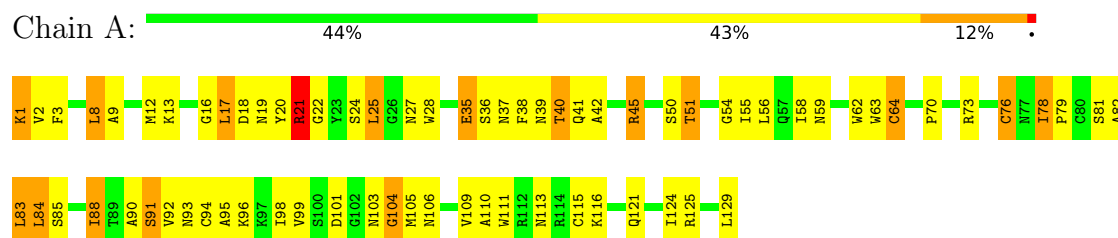
4.2.33 Score per residue for model 33

- Molecule 1: LYSOZYME



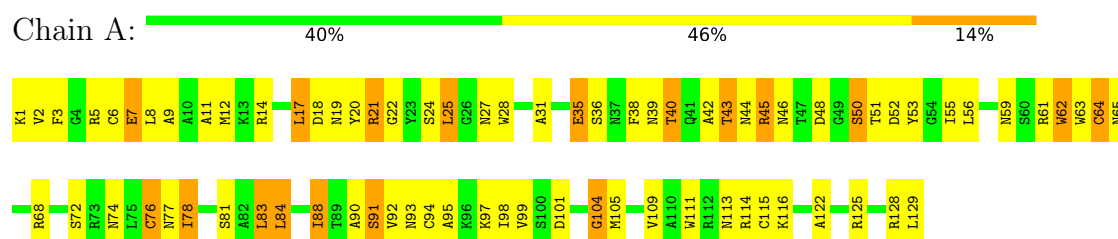
4.2.34 Score per residue for model 34

- Molecule 1: LYSOZYME



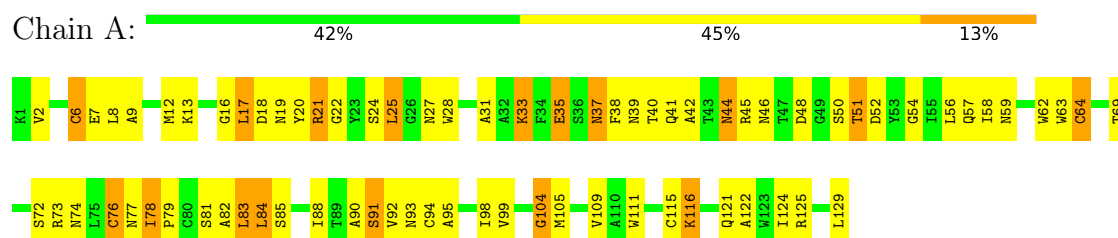
4.2.35 Score per residue for model 35

- Molecule 1: LYSOZYME



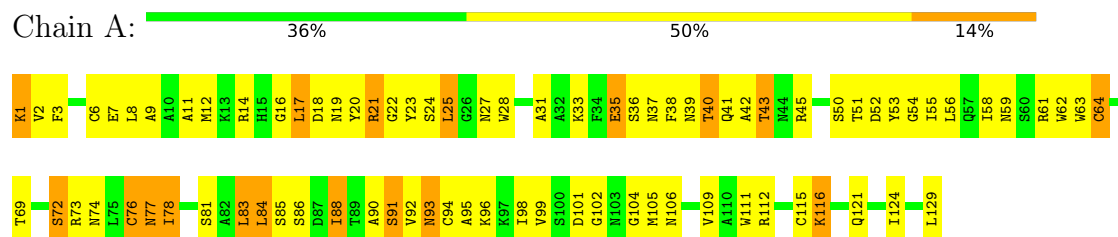
4.2.36 Score per residue for model 36

- Molecule 1: LYSOZYME



4.2.37 Score per residue for model 37

- Molecule 1: LYSOZYME



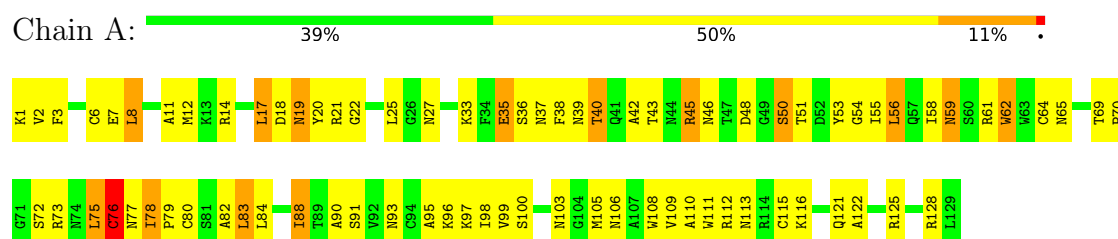
4.2.38 Score per residue for model 38

• Molecule 1: LYSOZYME



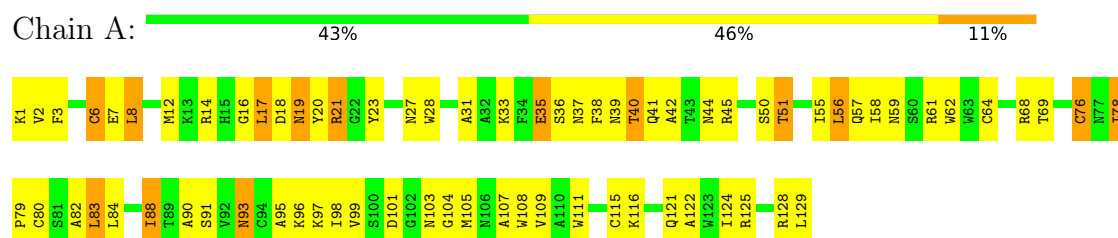
4.2.39 Score per residue for model 39

• Molecule 1: LYSOZYME



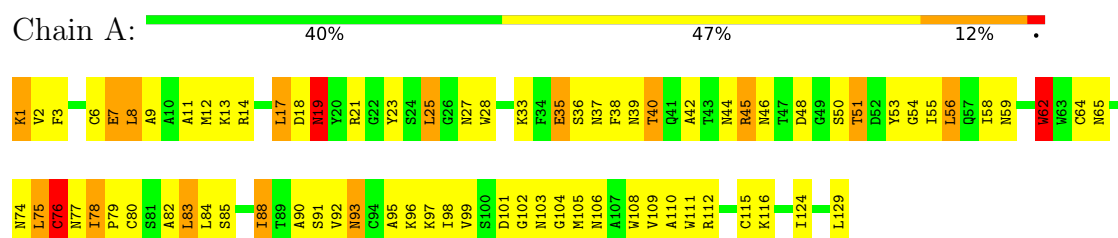
4.2.40 Score per residue for model 40

• Molecule 1: LYSOZYME



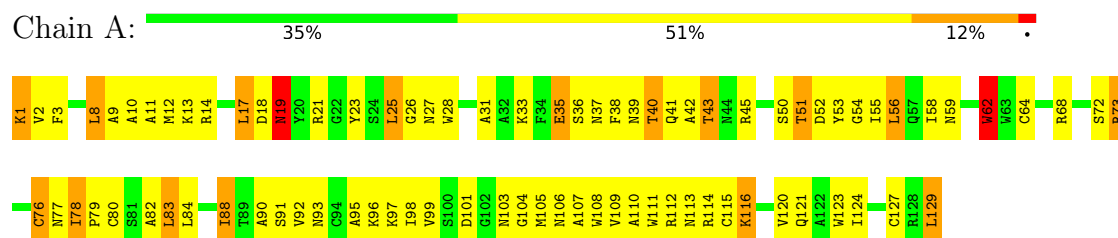
4.2.41 Score per residue for model 41

• Molecule 1: LYSOZYME



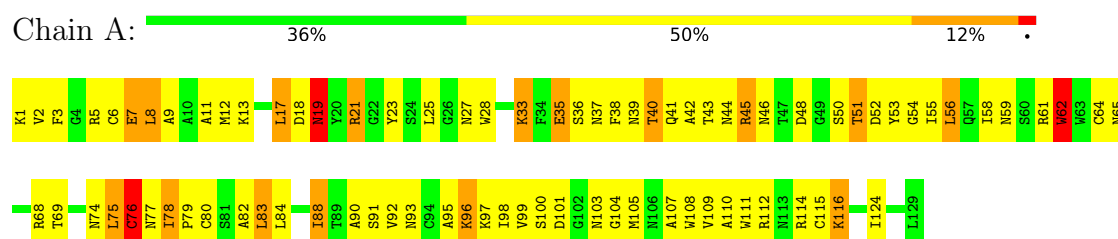
4.2.42 Score per residue for model 42

- Molecule 1: LYSOZYME



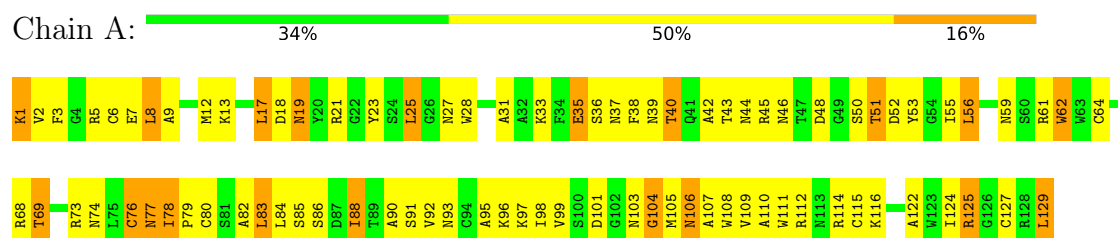
4.2.43 Score per residue for model 43

- Molecule 1: LYSOZYME



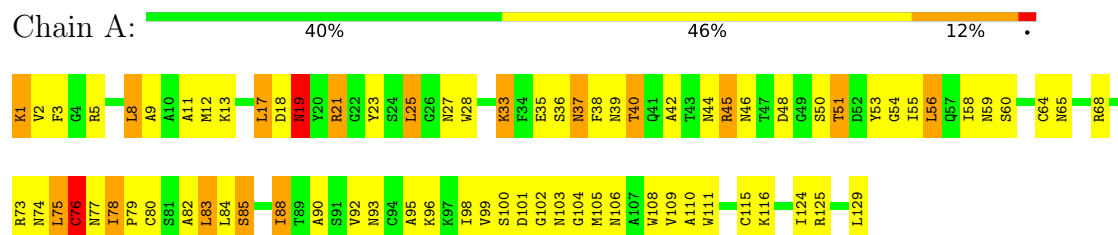
4.2.44 Score per residue for model 44

- Molecule 1: LYSOZYME



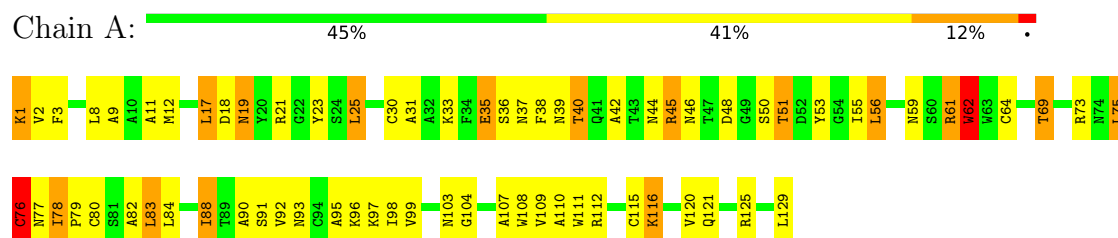
4.2.45 Score per residue for model 45

- Molecule 1: LYSOZYME



4.2.46 Score per residue for model 46

- Molecule 1: LYSOZYME



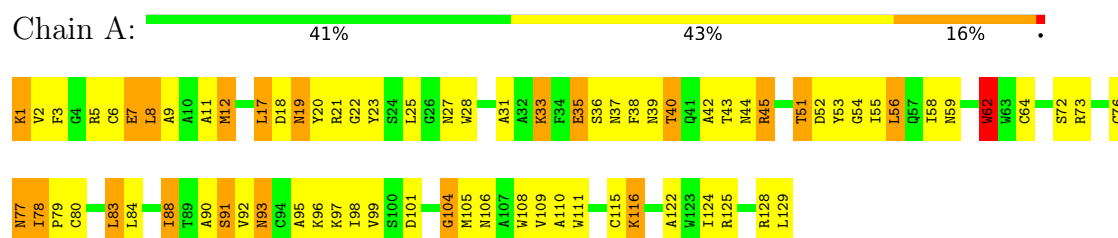
4.2.47 Score per residue for model 47

- Molecule 1: LYSOZYME



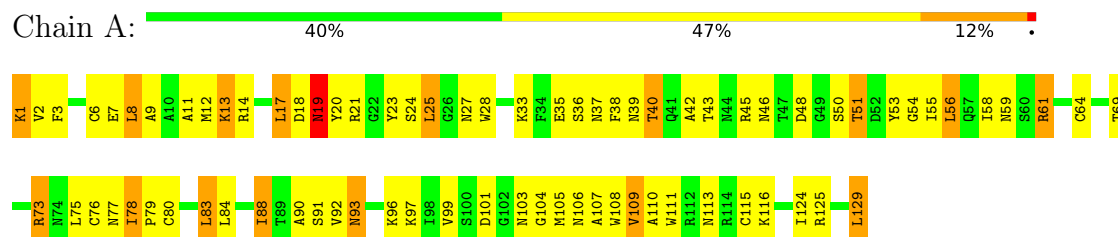
4.2.48 Score per residue for model 48

- Molecule 1: LYSOZYME



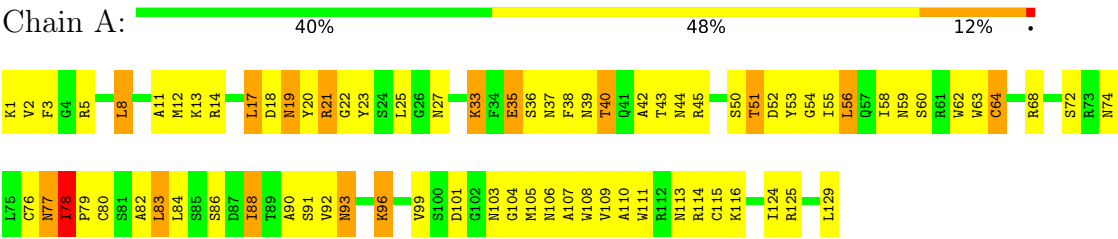
4.2.49 Score per residue for model 49

- Molecule 1: LYSOZYME



4.2.50 Score per residue for model 50

● Molecule 1: LYSOZYME



5 Refinement protocol and experimental data overview ⓘ

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

Of the 300 calculated structures, 50 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	
X-PLOR	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	0.37±0.01	0±0/1021 (0.0± 0.0%)	0.72±0.02	0±0/1379 (0.0± 0.0%)
All	All	0.37	0/51050 (0.0%)	0.72	2/68950 (0.0%)

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	78	ILE	N-CA-CB	-6.01	107.68	111.83	50	1
1	A	78	ILE	N-CA-C	5.32	113.75	107.84	50	1

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	1001	960	959	63±5
All	All	50050	48000	47950	3142

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:MET:HE3	1:A:17:LEU:HD12	0.94	1.39	40	34
1:A:39:ASN:HB3	1:A:42:ALA:HB2	0.94	1.39	46	38
1:A:99:VAL:HG23	1:A:104:GLY:HA2	0.87	1.46	34	42
1:A:58:ILE:HD11	1:A:91:SER:HA	0.87	1.44	13	2
1:A:19:ASN:H	1:A:24:SER:HA	0.85	1.31	8	38
1:A:80:CYS:HA	1:A:83:LEU:HD23	0.85	1.49	46	25
1:A:83:LEU:HD23	1:A:90:ALA:HB1	0.81	1.50	50	3
1:A:12:MET:HE1	1:A:28:TRP:HB3	0.80	1.52	6	8
1:A:79:PRO:HB2	1:A:82:ALA:HB3	0.78	1.54	47	12
1:A:2:VAL:HG13	1:A:38:PHE:C	0.77	2.04	15	50
1:A:17:LEU:HD23	1:A:17:LEU:N	0.77	1.94	40	50
1:A:54:GLY:HA3	1:A:58:ILE:HD12	0.76	1.55	48	1
1:A:12:MET:HE2	1:A:28:TRP:HB3	0.75	1.58	37	36
1:A:12:MET:HE1	1:A:28:TRP:CB	0.75	2.12	45	7
1:A:58:ILE:HG21	1:A:83:LEU:HD13	0.75	1.57	50	3
1:A:8:LEU:O	1:A:12:MET:HG2	0.74	1.83	50	43
1:A:19:ASN:N	1:A:24:SER:HA	0.73	1.99	25	37
1:A:2:VAL:HG22	1:A:39:ASN:HA	0.73	1.60	5	50
1:A:8:LEU:HD12	1:A:88:ILE:HD13	0.73	1.61	40	24
1:A:69:THR:N	1:A:70:PRO:HD2	0.72	1.98	38	2
1:A:83:LEU:HD22	1:A:90:ALA:HB2	0.72	1.61	11	1
1:A:27:ASN:HB3	1:A:105:MET:HG3	0.72	1.62	48	39
1:A:64:CYS:HB3	1:A:78:ILE:HD13	0.71	1.61	3	7
1:A:18:ASP:HB2	1:A:25:LEU:HG	0.71	1.62	46	7
1:A:10:ALA:HB2	1:A:129:LEU:HD22	0.70	1.64	42	3
1:A:9:ALA:HA	1:A:12:MET:HG3	0.70	1.64	6	7
1:A:103:ASN:HB3	1:A:107:ALA:HB2	0.69	1.62	42	15
1:A:12:MET:CE	1:A:17:LEU:HD12	0.69	2.18	48	50
1:A:38:PHE:HD1	1:A:55:ILE:HD11	0.69	1.47	4	37
1:A:83:LEU:HB3	1:A:90:ALA:HB3	0.68	1.66	18	23
1:A:25:LEU:H	1:A:25:LEU:HD23	0.68	1.48	21	1
1:A:64:CYS:HB3	1:A:78:ILE:HG22	0.68	1.65	49	3
1:A:83:LEU:HD13	1:A:91:SER:HB3	0.67	1.66	23	31
1:A:20:TYR:O	1:A:22:GLY:N	0.67	2.28	31	37
1:A:12:MET:HB2	1:A:25:LEU:HD21	0.67	1.66	7	39
1:A:55:ILE:HG21	1:A:88:ILE:HG22	0.66	1.67	49	16
1:A:64:CYS:HB2	1:A:78:ILE:O	0.65	1.91	15	49
1:A:27:ASN:HB3	1:A:105:MET:SD	0.65	2.31	7	1
1:A:35:GLU:HG3	1:A:110:ALA:HB3	0.65	1.68	44	25
1:A:3:PHE:CE2	1:A:88:ILE:HG23	0.65	2.27	38	27
1:A:12:MET:HE2	1:A:28:TRP:CB	0.64	2.22	21	36
1:A:76:CYS:HB3	1:A:78:ILE:HG23	0.63	1.69	43	41

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:PHE:CE1	1:A:88:ILE:HG23	0.62	2.29	45	1
1:A:103:ASN:ND2	1:A:107:ALA:HB2	0.62	2.09	2	1
1:A:111:TRP:O	1:A:115:CYS:HB2	0.62	1.95	13	23
1:A:8:LEU:O	1:A:12:MET:HG3	0.61	1.94	44	6
1:A:12:MET:HE1	1:A:17:LEU:HD12	0.61	1.71	46	32
1:A:44:ASN:HB2	1:A:52:ASP:HB2	0.61	1.72	44	14
1:A:56:LEU:HD12	1:A:108:TRP:NE1	0.61	2.10	5	13
1:A:17:LEU:HD11	1:A:92:VAL:HG13	0.61	1.72	3	31
1:A:9:ALA:HA	1:A:12:MET:HG2	0.61	1.72	22	17
1:A:56:LEU:HB2	1:A:91:SER:HB3	0.61	1.72	13	1
1:A:20:TYR:O	1:A:21:ARG:C	0.60	2.44	5	37
1:A:83:LEU:HD22	1:A:90:ALA:HB1	0.60	1.74	45	1
1:A:2:VAL:HG22	1:A:39:ASN:CA	0.60	2.27	6	50
1:A:83:LEU:HA	1:A:90:ALA:HB3	0.60	1.72	49	12
1:A:17:LEU:N	1:A:17:LEU:CD2	0.60	2.65	40	50
1:A:61:ARG:HG3	1:A:69:THR:HG21	0.60	1.73	44	9
1:A:58:ILE:HG13	1:A:83:LEU:HD13	0.59	1.73	10	2
1:A:79:PRO:HG2	1:A:82:ALA:HB3	0.59	1.73	50	9
1:A:1:LYS:H3	1:A:41:GLN:HB2	0.59	1.57	28	1
1:A:81:SER:HA	1:A:84:LEU:HD12	0.59	1.75	27	28
1:A:78:ILE:HD12	1:A:94:CYS:HB2	0.59	1.72	23	5
1:A:45:ARG:HA	1:A:51:THR:HG23	0.59	1.72	48	27
1:A:44:ASN:HB3	1:A:52:ASP:HB2	0.59	1.73	32	4
1:A:83:LEU:HD13	1:A:90:ALA:HB2	0.59	1.74	12	1
1:A:20:TYR:C	1:A:22:GLY:N	0.58	2.61	11	41
1:A:83:LEU:HD13	1:A:90:ALA:HB1	0.58	1.74	45	2
1:A:51:THR:O	1:A:59:ASN:HA	0.58	1.99	30	46
1:A:44:ASN:C	1:A:51:THR:HG23	0.58	2.24	22	15
1:A:63:TRP:O	1:A:76:CYS:HB3	0.57	1.98	10	5
1:A:63:TRP:CZ3	1:A:75:LEU:HB3	0.57	2.33	21	1
1:A:2:VAL:HG13	1:A:38:PHE:O	0.57	1.99	40	49
1:A:3:PHE:CE1	1:A:40:THR:HG21	0.57	2.35	13	5
1:A:76:CYS:SG	1:A:78:ILE:HD13	0.57	2.40	48	4
1:A:64:CYS:CB	1:A:78:ILE:HG22	0.57	2.30	49	4
1:A:58:ILE:HD11	1:A:91:SER:HB2	0.57	1.77	11	1
1:A:83:LEU:CB	1:A:90:ALA:HB2	0.57	2.30	13	1
1:A:3:PHE:HE2	1:A:88:ILE:HG23	0.56	1.60	26	11
1:A:93:ASN:HA	1:A:96:LYS:HD3	0.56	1.75	49	4
1:A:54:GLY:HA3	1:A:58:ILE:HG12	0.56	1.75	50	15
1:A:39:ASN:HB3	1:A:42:ALA:CB	0.56	2.28	41	9
1:A:83:LEU:HD12	1:A:83:LEU:O	0.56	2.00	39	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ASN:ND2	1:A:62:TRP:HB2	0.56	2.16	25	33
1:A:112:ARG:HG2	1:A:116:LYS:HD2	0.56	1.76	21	2
1:A:69:THR:N	1:A:70:PRO:CD	0.56	2.68	39	2
1:A:60:SER:HA	1:A:64:CYS:SG	0.55	2.41	50	3
1:A:78:ILE:HD11	1:A:93:ASN:OD1	0.55	2.02	10	2
1:A:99:VAL:HA	1:A:103:ASN:O	0.55	2.01	8	23
1:A:92:VAL:O	1:A:96:LYS:N	0.55	2.38	13	10
1:A:21:ARG:HD2	1:A:100:SER:HA	0.55	1.79	39	2
1:A:36:SER:OG	1:A:55:ILE:HA	0.55	2.01	12	41
1:A:76:CYS:HB3	1:A:78:ILE:CG2	0.55	2.32	12	7
1:A:17:LEU:HD21	1:A:92:VAL:HG11	0.55	1.78	11	15
1:A:2:VAL:HG11	1:A:37:ASN:O	0.54	2.03	46	30
1:A:11:ALA:HB1	1:A:88:ILE:HD11	0.54	1.79	21	12
1:A:78:ILE:HD11	1:A:83:LEU:HD22	0.54	1.78	46	9
1:A:62:TRP:HA	1:A:73:ARG:HB2	0.54	1.77	39	2
1:A:78:ILE:HB	1:A:93:ASN:HD21	0.54	1.62	23	1
1:A:3:PHE:CD2	1:A:40:THR:HG22	0.54	2.37	44	14
1:A:103:ASN:HB2	1:A:107:ALA:HB2	0.54	1.79	40	3
1:A:80:CYS:O	1:A:84:LEU:HG	0.53	2.03	39	14
1:A:3:PHE:CZ	1:A:40:THR:HG21	0.53	2.39	7	12
1:A:80:CYS:O	1:A:83:LEU:HG	0.53	2.04	10	1
1:A:31:ALA:O	1:A:35:GLU:HB2	0.53	2.04	17	40
1:A:3:PHE:CD1	1:A:40:THR:HG22	0.53	2.39	45	1
1:A:36:SER:HB2	1:A:42:ALA:HB3	0.53	1.81	45	13
1:A:94:CYS:O	1:A:98:ILE:HG13	0.53	2.04	3	34
1:A:58:ILE:HD12	1:A:58:ILE:N	0.53	2.17	32	7
1:A:63:TRP:O	1:A:64:CYS:O	0.53	2.26	20	19
1:A:111:TRP:O	1:A:115:CYS:HB3	0.52	2.04	2	27
1:A:103:ASN:CG	1:A:107:ALA:HB2	0.52	2.28	3	3
1:A:78:ILE:HG13	1:A:83:LEU:HG	0.52	1.80	45	1
1:A:78:ILE:HB	1:A:93:ASN:ND2	0.52	2.19	23	1
1:A:83:LEU:CB	1:A:90:ALA:HB3	0.52	2.34	19	32
1:A:8:LEU:CD2	1:A:88:ILE:HD13	0.52	2.35	48	14
1:A:83:LEU:HD13	1:A:91:SER:CB	0.52	2.35	18	16
1:A:122:ALA:HA	1:A:125:ARG:HB2	0.52	1.82	30	24
1:A:99:VAL:HG23	1:A:104:GLY:CA	0.52	2.32	17	4
1:A:74:ASN:ND2	1:A:77:ASN:HA	0.52	2.20	17	11
1:A:17:LEU:HB3	1:A:28:TRP:CE2	0.52	2.40	21	28
1:A:64:CYS:CB	1:A:78:ILE:HD13	0.52	2.35	16	5
1:A:58:ILE:HG21	1:A:78:ILE:HD11	0.51	1.81	40	7
1:A:3:PHE:HD2	1:A:55:ILE:HD12	0.51	1.65	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ASN:CB	1:A:42:ALA:HB2	0.51	2.35	16	17
1:A:38:PHE:CD1	1:A:55:ILE:HD11	0.51	2.39	5	9
1:A:103:ASN:OD1	1:A:107:ALA:HB2	0.51	2.06	3	2
1:A:111:TRP:HA	1:A:115:CYS:SG	0.51	2.45	18	7
1:A:60:SER:HB2	1:A:64:CYS:SG	0.51	2.46	45	2
1:A:83:LEU:HG	1:A:84:LEU:HG	0.51	1.81	3	8
1:A:1:LYS:O	1:A:40:THR:HG23	0.50	2.06	47	28
1:A:3:PHE:CD2	1:A:8:LEU:HD23	0.50	2.41	11	8
1:A:39:ASN:CG	1:A:42:ALA:HB2	0.50	2.31	13	8
1:A:40:THR:HG22	1:A:55:ILE:HB	0.50	1.82	13	6
1:A:54:GLY:HA3	1:A:58:ILE:HD13	0.50	1.82	36	6
1:A:12:MET:CB	1:A:25:LEU:HD22	0.50	2.36	4	5
1:A:56:LEU:O	1:A:108:TRP:NE1	0.50	2.45	49	13
1:A:92:VAL:HG12	1:A:96:LYS:HG3	0.50	1.83	38	4
1:A:1:LYS:HD2	1:A:86:SER:HB2	0.50	1.81	28	1
1:A:69:THR:HG22	1:A:71:GLY:H	0.50	1.66	22	1
1:A:45:ARG:N	1:A:51:THR:HG23	0.50	2.22	37	3
1:A:83:LEU:HD22	1:A:89:THR:HB	0.50	1.82	13	1
1:A:36:SER:HB3	1:A:57:GLN:HE22	0.50	1.67	40	1
1:A:95:ALA:HA	1:A:98:ILE:HB	0.50	1.84	13	48
1:A:2:VAL:HG22	1:A:39:ASN:CB	0.50	2.37	2	13
1:A:2:VAL:HA	1:A:38:PHE:O	0.50	2.07	13	14
1:A:127:CYS:HB3	1:A:129:LEU:HD23	0.50	1.84	14	9
1:A:31:ALA:HB2	1:A:111:TRP:HB2	0.50	1.82	14	6
1:A:69:THR:HA	1:A:72:SER:HB2	0.49	1.84	39	2
1:A:17:LEU:HD11	1:A:92:VAL:CG1	0.49	2.37	3	20
1:A:45:ARG:HG2	1:A:51:THR:HG23	0.49	1.84	42	1
1:A:51:THR:HB	1:A:53:TYR:CE1	0.49	2.43	21	3
1:A:2:VAL:CG1	1:A:38:PHE:HB2	0.49	2.38	34	10
1:A:21:ARG:HG3	1:A:99:VAL:HG13	0.49	1.84	39	1
1:A:43:THR:HA	1:A:52:ASP:O	0.49	2.07	37	11
1:A:83:LEU:HD12	1:A:84:LEU:HG	0.49	1.83	10	1
1:A:76:CYS:O	1:A:77:ASN:C	0.49	2.55	50	4
1:A:11:ALA:CB	1:A:88:ILE:HD11	0.49	2.37	48	23
1:A:21:ARG:HG2	1:A:99:VAL:O	0.49	2.08	50	2
1:A:51:THR:HB	1:A:53:TYR:CE2	0.49	2.43	13	18
1:A:1:LYS:H2	1:A:41:GLN:HB2	0.49	1.68	21	1
1:A:3:PHE:HD2	1:A:8:LEU:HD23	0.48	1.68	7	3
1:A:8:LEU:CD1	1:A:88:ILE:HD13	0.48	2.38	43	12
1:A:12:MET:HB2	1:A:25:LEU:CD2	0.48	2.39	13	26
1:A:83:LEU:HD13	1:A:90:ALA:CB	0.48	2.38	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:GLY:O	1:A:105:MET:CB	0.48	2.61	7	11
1:A:23:TYR:CE2	1:A:104:GLY:HA3	0.48	2.43	48	12
1:A:33:LYS:O	1:A:37:ASN:HA	0.48	2.08	47	28
1:A:35:GLU:OE2	1:A:108:TRP:HB3	0.48	2.09	14	1
1:A:58:ILE:HD11	1:A:91:SER:HB3	0.48	1.86	48	2
1:A:110:ALA:O	1:A:114:ARG:HB2	0.48	2.09	32	1
1:A:44:ASN:O	1:A:51:THR:HG23	0.47	2.08	22	6
1:A:64:CYS:HB2	1:A:78:ILE:HG12	0.47	1.86	11	1
1:A:23:TYR:HB3	1:A:27:ASN:ND2	0.47	2.24	25	15
1:A:63:TRP:O	1:A:74:ASN:HA	0.47	2.09	18	11
1:A:23:TYR:HB2	1:A:105:MET:SD	0.47	2.49	37	6
1:A:78:ILE:O	1:A:78:ILE:HG12	0.47	2.09	11	1
1:A:83:LEU:HD22	1:A:90:ALA:CB	0.47	2.38	45	1
1:A:65:ASN:HB2	1:A:74:ASN:ND2	0.47	2.23	32	6
1:A:18:ASP:HB2	1:A:25:LEU:HD12	0.47	1.85	8	6
1:A:1:LYS:HZ2	1:A:41:GLN:HG3	0.47	1.69	37	1
1:A:20:TYR:C	1:A:22:GLY:H	0.47	2.18	31	3
1:A:1:LYS:HE2	1:A:86:SER:HB2	0.47	1.86	37	1
1:A:64:CYS:CB	1:A:78:ILE:HG12	0.47	2.40	45	2
1:A:12:MET:HB2	1:A:25:LEU:HD22	0.47	1.87	12	1
1:A:53:TYR:O	1:A:58:ILE:HB	0.47	2.09	13	7
1:A:13:LYS:HD3	1:A:129:LEU:HD12	0.47	1.86	49	1
1:A:16:GLY:O	1:A:20:TYR:HB2	0.47	2.10	17	20
1:A:95:ALA:O	1:A:98:ILE:N	0.47	2.48	3	29
1:A:12:MET:CE	1:A:28:TRP:HB3	0.47	2.33	6	2
1:A:46:ASN:HB2	1:A:48:ASP:OD1	0.46	2.10	39	32
1:A:73:ARG:HG2	1:A:75:LEU:HG	0.46	1.88	12	3
1:A:23:TYR:HE2	1:A:104:GLY:HA3	0.46	1.70	49	8
1:A:78:ILE:HD11	1:A:93:ASN:HD21	0.46	1.70	49	1
1:A:61:ARG:HD3	1:A:69:THR:HG21	0.46	1.88	2	1
1:A:8:LEU:O	1:A:8:LEU:HD22	0.46	2.11	45	11
1:A:83:LEU:N	1:A:83:LEU:HD23	0.46	2.26	45	1
1:A:104:GLY:O	1:A:105:MET:HB2	0.46	2.10	7	5
1:A:38:PHE:HA	1:A:55:ILE:HG13	0.46	1.87	42	4
1:A:3:PHE:CZ	1:A:88:ILE:HG23	0.46	2.45	45	4
1:A:45:ARG:CA	1:A:51:THR:HG23	0.46	2.41	24	9
1:A:30:CYS:HB2	1:A:120:VAL:HG12	0.46	1.88	33	4
1:A:71:GLY:O	1:A:72:SER:HB3	0.46	2.10	20	2
1:A:112:ARG:HA	1:A:116:LYS:HB2	0.46	1.88	32	1
1:A:79:PRO:O	1:A:83:LEU:HG	0.46	2.11	48	3
1:A:23:TYR:HB3	1:A:27:ASN:OD1	0.45	2.11	23	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLU:HG2	1:A:57:GLN:HG3	0.45	1.87	23	3
1:A:25:LEU:HG	1:A:26:GLY:N	0.45	2.26	20	3
1:A:18:ASP:O	1:A:19:ASN:HB2	0.45	2.11	39	2
1:A:98:ILE:O	1:A:102:GLY:N	0.45	2.50	37	4
1:A:99:VAL:HA	1:A:103:ASN:HB2	0.45	1.89	5	2
1:A:89:THR:O	1:A:93:ASN:HB3	0.45	2.11	13	2
1:A:17:LEU:O	1:A:28:TRP:NE1	0.45	2.50	49	25
1:A:73:ARG:HD3	1:A:75:LEU:HG	0.45	1.89	4	1
1:A:69:THR:HG22	1:A:70:PRO:HD2	0.45	1.89	20	1
1:A:75:LEU:O	1:A:77:ASN:N	0.45	2.50	38	5
1:A:1:LYS:N	1:A:41:GLN:HB2	0.45	2.27	21	1
1:A:106:ASN:HA	1:A:112:ARG:HG3	0.45	1.89	39	2
1:A:63:TRP:HB3	1:A:94:CYS:SG	0.44	2.52	12	5
1:A:22:GLY:HA3	1:A:99:VAL:HG21	0.44	1.88	36	8
1:A:83:LEU:C	1:A:84:LEU:HD23	0.44	2.37	48	3
1:A:22:GLY:HA3	1:A:99:VAL:CG2	0.44	2.42	32	10
1:A:50:SER:HB2	1:A:59:ASN:OD1	0.44	2.11	39	1
1:A:53:TYR:O	1:A:83:LEU:HD11	0.44	2.12	30	3
1:A:50:SER:HA	1:A:61:ARG:HD3	0.44	1.88	35	1
1:A:33:LYS:HB2	1:A:38:PHE:CZ	0.44	2.48	36	13
1:A:2:VAL:CG1	1:A:37:ASN:O	0.44	2.66	40	16
1:A:95:ALA:HA	1:A:98:ILE:HD12	0.44	1.88	13	28
1:A:78:ILE:HD12	1:A:83:LEU:HD12	0.44	1.90	45	1
1:A:103:ASN:CB	1:A:107:ALA:HB2	0.44	2.43	4	9
1:A:60:SER:HB2	1:A:66:ASP:HB3	0.44	1.88	21	1
1:A:78:ILE:HG12	1:A:83:LEU:HD21	0.44	1.90	48	1
1:A:6:CYS:O	1:A:7:GLU:C	0.43	2.61	13	42
1:A:92:VAL:O	1:A:93:ASN:C	0.43	2.60	16	18
1:A:18:ASP:HB2	1:A:25:LEU:HD22	0.43	1.90	21	1
1:A:83:LEU:HB2	1:A:91:SER:OG	0.43	2.13	10	1
1:A:74:ASN:CG	1:A:77:ASN:HA	0.43	2.39	10	1
1:A:32:ALA:HB1	1:A:55:ILE:HG12	0.43	1.91	22	3
1:A:9:ALA:CA	1:A:12:MET:HG2	0.43	2.41	22	3
1:A:97:LYS:O	1:A:101:ASP:HB2	0.43	2.12	23	1
1:A:93:ASN:O	1:A:96:LYS:HB2	0.43	2.14	50	4
1:A:103:ASN:O	1:A:106:ASN:HB2	0.43	2.13	41	1
1:A:65:ASN:HB2	1:A:74:ASN:CG	0.43	2.38	45	2
1:A:79:PRO:HB2	1:A:82:ALA:CB	0.43	2.44	9	8
1:A:59:ASN:OD1	1:A:62:TRP:HB2	0.43	2.14	27	5
1:A:10:ALA:N	1:A:129:LEU:HD22	0.43	2.29	30	1
1:A:109:VAL:O	1:A:113:ASN:HB2	0.43	2.14	33	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ARG:HA	1:A:72:SER:OG	0.43	2.13	38	2
1:A:123:TRP:HA	1:A:123:TRP:CE3	0.43	2.49	29	3
1:A:21:ARG:HD3	1:A:100:SER:HA	0.43	1.90	45	1
1:A:12:MET:HB3	1:A:25:LEU:HD22	0.43	1.91	4	2
1:A:75:LEU:C	1:A:77:ASN:N	0.43	2.75	12	8
1:A:83:LEU:HB3	1:A:90:ALA:HB2	0.43	1.91	13	1
1:A:35:GLU:OE2	1:A:110:ALA:HB3	0.43	2.14	14	2
1:A:3:PHE:CE2	1:A:40:THR:HG21	0.43	2.49	30	4
1:A:95:ALA:HA	1:A:98:ILE:CG1	0.42	2.44	10	4
1:A:84:LEU:HD23	1:A:84:LEU:N	0.42	2.29	50	1
1:A:60:SER:O	1:A:64:CYS:O	0.42	2.37	13	1
1:A:11:ALA:HB3	1:A:88:ILE:HD11	0.42	1.91	48	4
1:A:16:GLY:C	1:A:17:LEU:HD23	0.42	2.39	16	12
1:A:61:ARG:O	1:A:73:ARG:HB2	0.42	2.14	21	1
1:A:78:ILE:HG13	1:A:79:PRO:CD	0.42	2.44	48	2
1:A:43:THR:HB	1:A:53:TYR:CD1	0.42	2.49	44	6
1:A:80:CYS:HA	1:A:83:LEU:HD12	0.42	1.92	48	1
1:A:80:CYS:HA	1:A:83:LEU:CD1	0.42	2.45	50	1
1:A:9:ALA:HA	1:A:12:MET:CG	0.42	2.44	49	7
1:A:10:ALA:HB2	1:A:129:LEU:HD13	0.42	1.90	21	1
1:A:61:ARG:O	1:A:61:ARG:HD2	0.42	2.14	4	1
1:A:83:LEU:HD13	1:A:91:SER:OG	0.42	2.15	8	1
1:A:18:ASP:O	1:A:19:ASN:CB	0.42	2.67	38	12
1:A:17:LEU:HA	1:A:20:TYR:HB2	0.42	1.92	49	1
1:A:63:TRP:CZ3	1:A:75:LEU:HD13	0.42	2.50	11	1
1:A:56:LEU:HD12	1:A:108:TRP:CE2	0.42	2.50	20	1
1:A:55:ILE:HG21	1:A:88:ILE:CG2	0.42	2.45	33	3
1:A:12:MET:HE1	1:A:28:TRP:HB2	0.42	1.91	42	3
1:A:74:ASN:OD1	1:A:77:ASN:HA	0.42	2.15	14	4
1:A:26:GLY:C	1:A:120:VAL:HB	0.42	2.40	42	1
1:A:95:ALA:C	1:A:97:LYS:N	0.41	2.76	16	3
1:A:66:ASP:CG	1:A:68:ARG:HG2	0.41	2.40	2	1
1:A:51:THR:H	1:A:59:ASN:ND2	0.41	2.12	24	1
1:A:52:ASP:HB3	1:A:57:GLN:HB3	0.41	1.92	36	2
1:A:64:CYS:HB3	1:A:78:ILE:CG2	0.41	2.44	48	1
1:A:25:LEU:HA	1:A:28:TRP:CD1	0.41	2.50	22	3
1:A:3:PHE:HE2	1:A:88:ILE:HG12	0.41	1.75	27	2
1:A:95:ALA:O	1:A:96:LYS:C	0.41	2.63	37	4
1:A:17:LEU:HD21	1:A:92:VAL:CG1	0.41	2.45	12	1
1:A:2:VAL:HG12	1:A:3:PHE:O	0.41	2.16	15	3
1:A:23:TYR:CD1	1:A:105:MET:HG2	0.41	2.51	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ASN:O	1:A:105:MET:HE2	0.41	2.15	49	2
1:A:31:ALA:HB2	1:A:111:TRP:CD1	0.41	2.51	48	2
1:A:54:GLY:HA3	1:A:58:ILE:CD1	0.41	2.46	45	1
1:A:25:LEU:HD12	1:A:25:LEU:C	0.41	2.41	23	1
1:A:58:ILE:HG13	1:A:83:LEU:HD22	0.40	1.93	20	3
1:A:25:LEU:O	1:A:28:TRP:N	0.40	2.54	21	1
1:A:122:ALA:O	1:A:125:ARG:HG2	0.40	2.16	33	1
1:A:83:LEU:CD1	1:A:90:ALA:HB1	0.40	2.46	45	1
1:A:112:ARG:O	1:A:116:LYS:HB3	0.40	2.15	32	1
1:A:79:PRO:O	1:A:83:LEU:HB3	0.40	2.15	46	1
1:A:3:PHE:CE2	1:A:40:THR:HG22	0.40	2.52	46	2
1:A:120:VAL:HA	1:A:123:TRP:CD1	0.40	2.51	42	1
1:A:41:GLN:O	1:A:43:THR:HG23	0.40	2.17	5	1
1:A:56:LEU:O	1:A:57:GLN:HB2	0.40	2.16	5	1
1:A:56:LEU:HD13	1:A:56:LEU:HA	0.40	1.82	18	1
1:A:53:TYR:HB2	1:A:58:ILE:O	0.40	2.17	12	1
1:A:25:LEU:C	1:A:25:LEU:HD12	0.40	2.41	20	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	127/129 (98%)	108±2 (85±2%)	15±3 (12±2%)	4±1 (3±1%)	5	36
All	All	6350/6450 (98%)	5395 (85%)	754 (12%)	201 (3%)	5	36

All 17 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	116	LYS	41
1	A	21	ARG	37
1	A	62	TRP	27
1	A	64	CYS	19
1	A	104	GLY	13

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Mol	Chain	Res	Type	Models (Total)
1	A	19	ASN	13
1	A	103	ASN	12
1	A	75	LEU	8
1	A	76	CYS	8
1	A	72	SER	7
1	A	70	PRO	5
1	A	73	ARG	3
1	A	127	CYS	2
1	A	59	ASN	2
1	A	71	GLY	2
1	A	105	MET	1
1	A	85	SER	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	105/105 (100%)	75±4 (71±4%)	30±4 (29±4%)	1	18
All	All	5250/5250 (100%)	3733 (71%)	1517 (29%)	1	18

All 68 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	17	LEU	50
1	A	40	THR	50
1	A	56	LEU	50
1	A	78	ILE	50
1	A	88	ILE	50
1	A	93	ASN	50
1	A	109	VAL	50
1	A	50	SER	49
1	A	83	LEU	47
1	A	91	SER	46
1	A	76	CYS	44
1	A	35	GLU	42
1	A	129	LEU	41

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Mol	Chain	Res	Type	Models (Total)
1	A	25	LEU	39
1	A	1	LYS	35
1	A	18	ASP	34
1	A	97	LYS	32
1	A	73	ARG	31
1	A	124	ILE	30
1	A	13	LYS	29
1	A	84	LEU	28
1	A	21	ARG	27
1	A	62	TRP	27
1	A	69	THR	27
1	A	85	SER	26
1	A	101	ASP	26
1	A	128	ARG	26
1	A	112	ARG	24
1	A	125	ARG	24
1	A	14	ARG	24
1	A	44	ASN	23
1	A	45	ARG	23
1	A	96	LYS	23
1	A	114	ARG	23
1	A	116	LYS	23
1	A	121	GLN	21
1	A	7	GLU	20
1	A	5	ARG	19
1	A	51	THR	19
1	A	8	LEU	18
1	A	68	ARG	17
1	A	19	ASN	16
1	A	113	ASN	15
1	A	72	SER	15
1	A	43	THR	14
1	A	41	GLN	14
1	A	61	ARG	14
1	A	37	ASN	13
1	A	106	ASN	13
1	A	77	ASN	11
1	A	33	LYS	9
1	A	86	SER	9
1	A	100	SER	5
1	A	39	ASN	5
1	A	99	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	6	CYS	4
1	A	80	CYS	3
1	A	127	CYS	3
1	A	65	ASN	3
1	A	103	ASN	2
1	A	52	ASP	1
1	A	105	MET	1
1	A	89	THR	1
1	A	74	ASN	1
1	A	46	ASN	1
1	A	81	SER	1
1	A	59	ASN	1
1	A	12	MET	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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