



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 02:00 AM UTC

PDB ID : 1M62 / pdb_00001m62
Title : Solution structure of the BAG domain from BAG4/SODD
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Deposited on : 2002-07-11

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

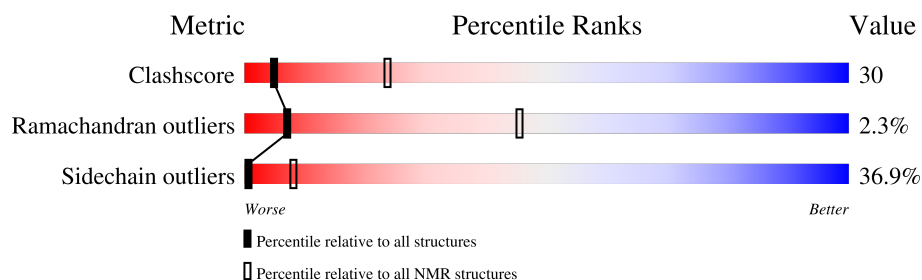
1 Overall quality at a glance

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	87	

2 Ensemble composition and analysis

This entry contains 25 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:379-A:457 (79)	0.88	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1430 atoms, of which 730 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BAG-family molecular chaperone regulator-4.

Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1430	448	730	113	137	2	

There are 5 discrepancies between the modelled and reference sequences:

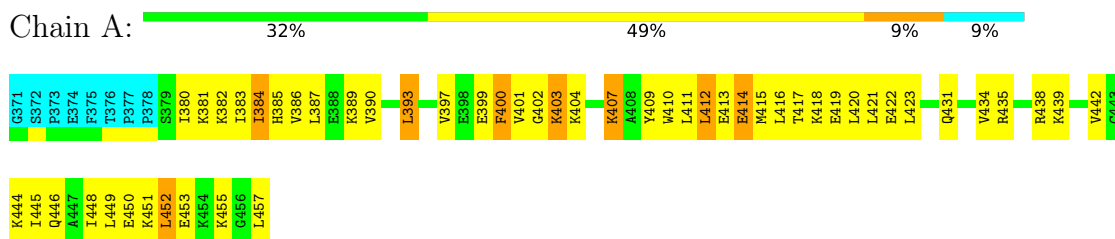
Chain	Residue	Modelled	Actual	Comment	Reference
A	371	GLY	-	cloning artifact	UNP O95429
A	372	SER	-	cloning artifact	UNP O95429
A	373	PRO	-	cloning artifact	UNP O95429
A	374	GLU	-	cloning artifact	UNP O95429
A	375	PHE	-	cloning artifact	UNP O95429

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: BAG-family molecular chaperone regulator-4

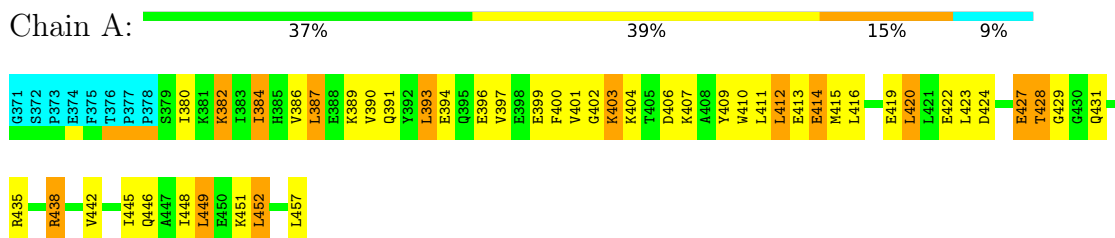


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

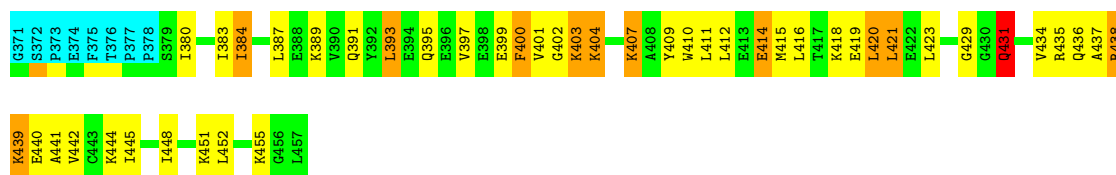
- Molecule 1: BAG-family molecular chaperone regulator-4



4.2.2 Score per residue for model 2

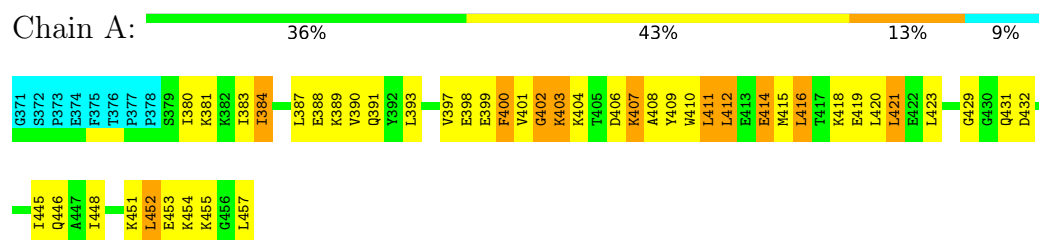
- Molecule 1: BAG-family molecular chaperone regulator-4





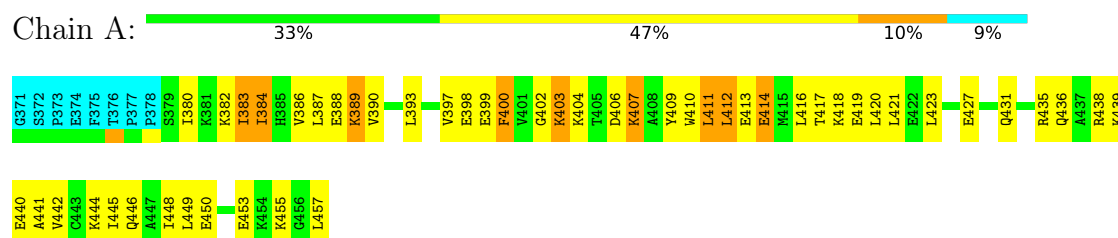
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: BAG-family molecular chaperone regulator-4



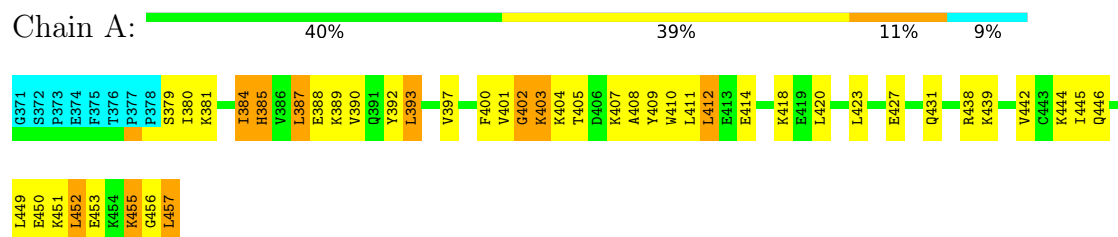
4.2.4 Score per residue for model 4

- Molecule 1: BAG-family molecular chaperone regulator-4



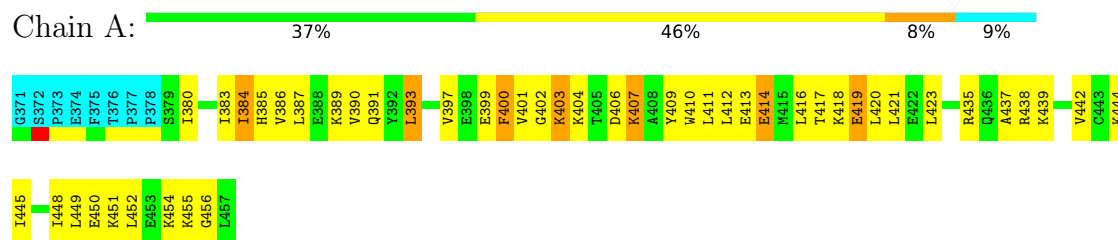
4.2.5 Score per residue for model 5

- Molecule 1: BAG-family molecular chaperone regulator-4



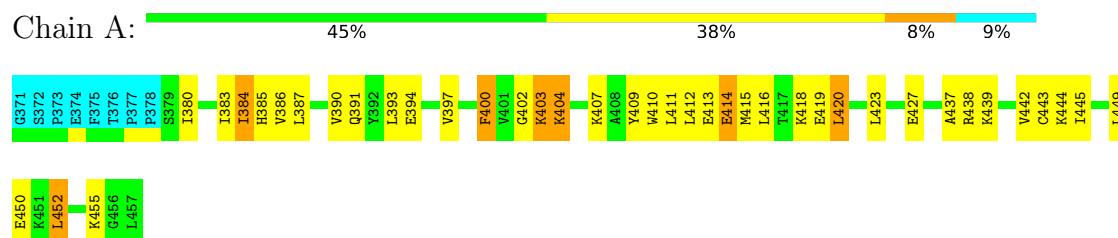
4.2.6 Score per residue for model 6

- Molecule 1: BAG-family molecular chaperone regulator-4



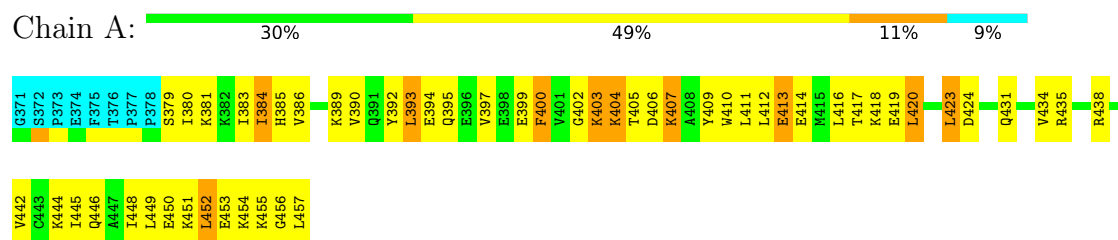
4.2.7 Score per residue for model 7

- Molecule 1: BAG-family molecular chaperone regulator-4



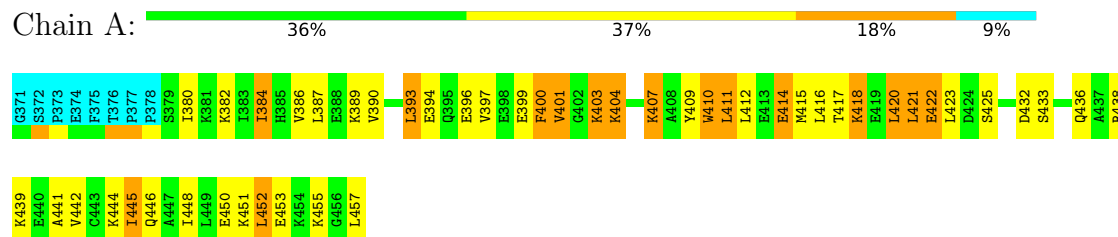
4.2.8 Score per residue for model 8

- Molecule 1: BAG-family molecular chaperone regulator-4



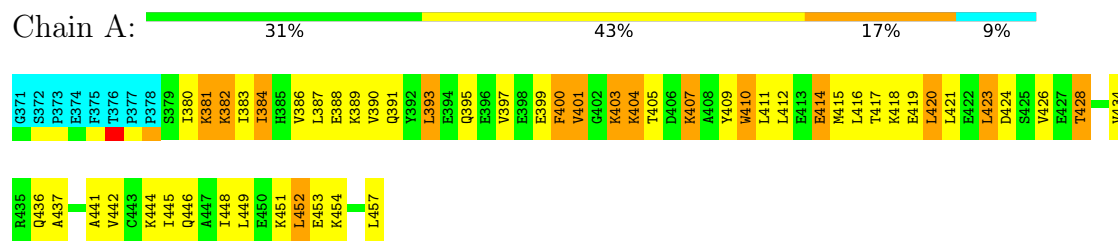
4.2.9 Score per residue for model 9

- Molecule 1: BAG-family molecular chaperone regulator-4



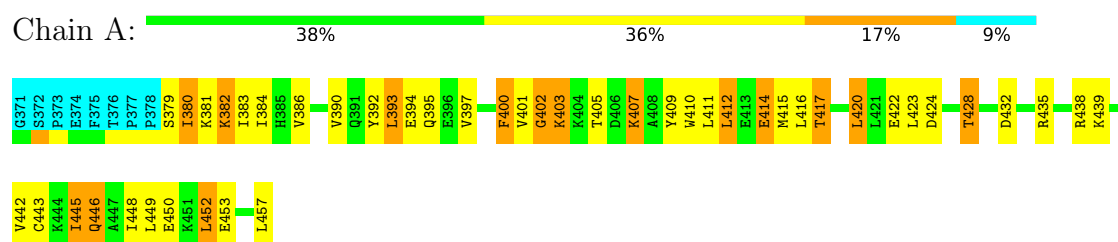
4.2.10 Score per residue for model 10

- Molecule 1: BAG-family molecular chaperone regulator-4



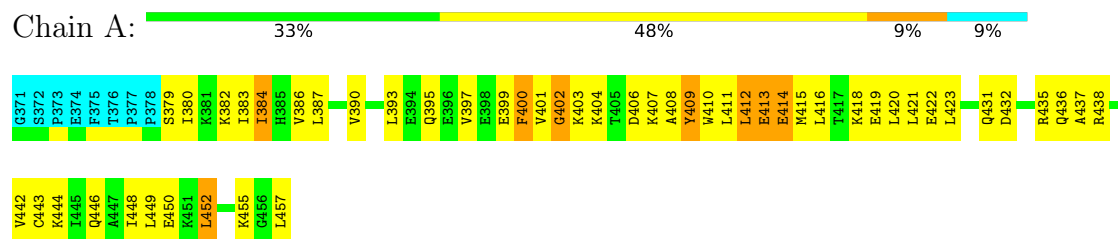
4.2.11 Score per residue for model 11

- Molecule 1: BAG-family molecular chaperone regulator-4



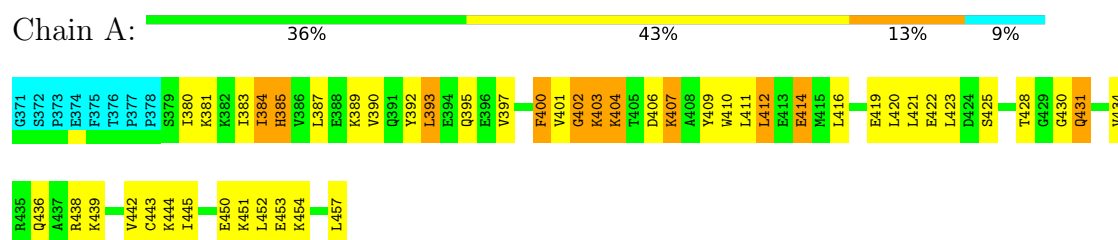
4.2.12 Score per residue for model 12

- Molecule 1: BAG-family molecular chaperone regulator-4



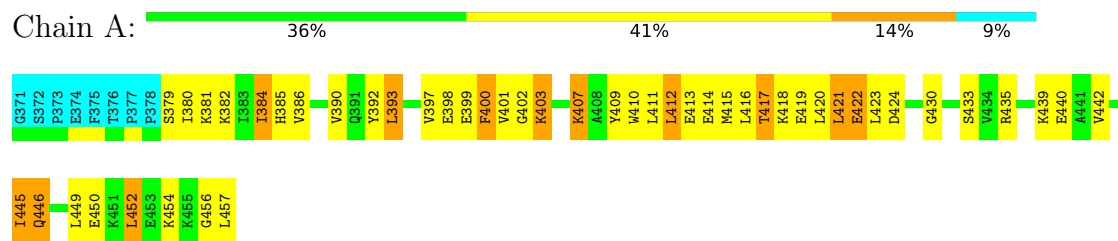
4.2.13 Score per residue for model 13

- Molecule 1: BAG-family molecular chaperone regulator-4



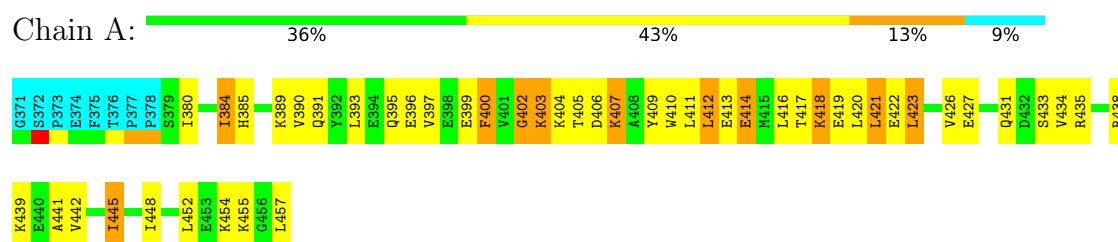
4.2.14 Score per residue for model 14

- Molecule 1: BAG-family molecular chaperone regulator-4



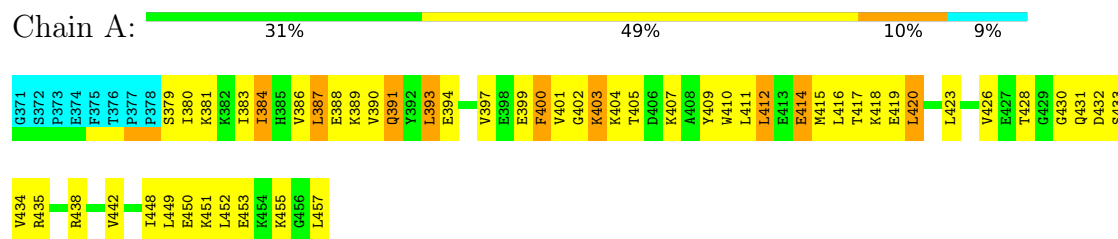
4.2.15 Score per residue for model 15

- Molecule 1: BAG-family molecular chaperone regulator-4



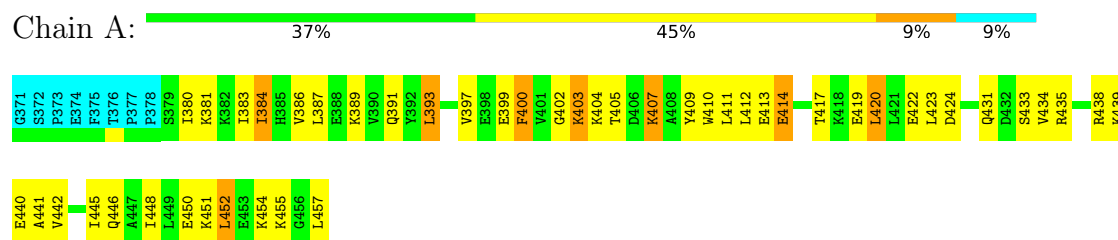
4.2.16 Score per residue for model 16

- Molecule 1: BAG-family molecular chaperone regulator-4



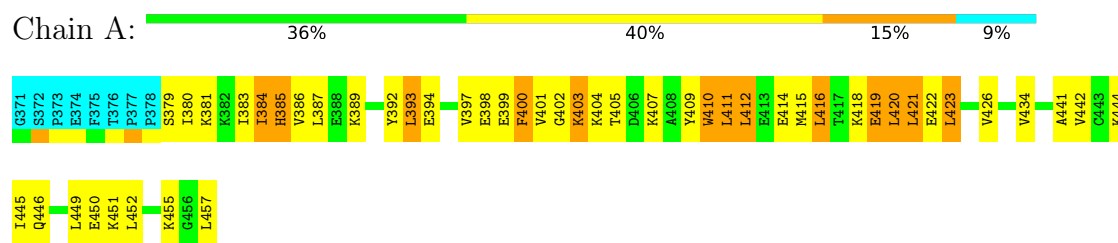
4.2.17 Score per residue for model 17

- Molecule 1: BAG-family molecular chaperone regulator-4



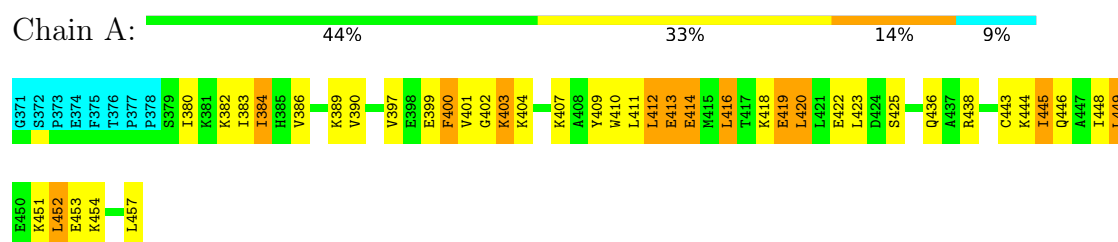
4.2.18 Score per residue for model 18

- Molecule 1: BAG-family molecular chaperone regulator-4



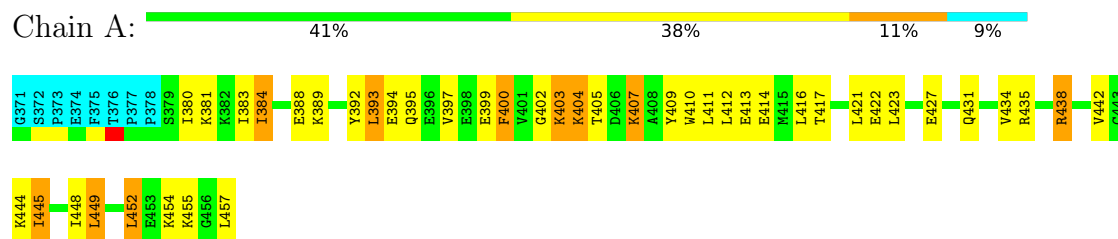
4.2.19 Score per residue for model 19

- Molecule 1: BAG-family molecular chaperone regulator-4



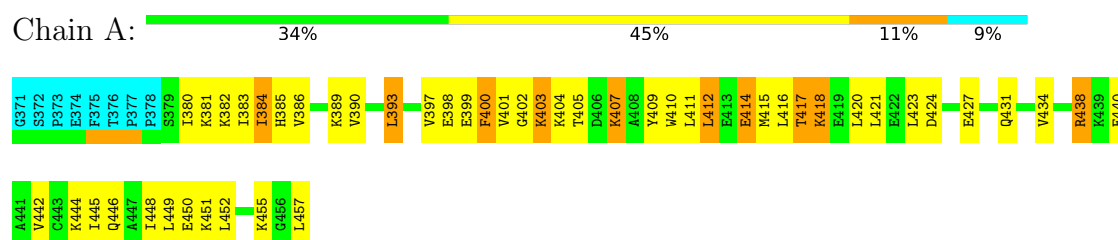
4.2.20 Score per residue for model 20

- Molecule 1: BAG-family molecular chaperone regulator-4



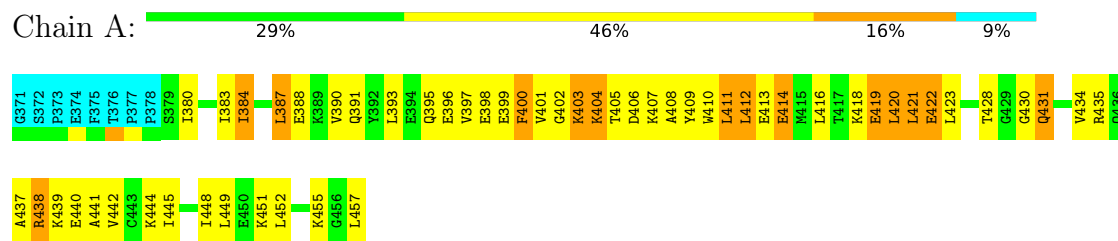
4.2.21 Score per residue for model 21

- Molecule 1: BAG-family molecular chaperone regulator-4



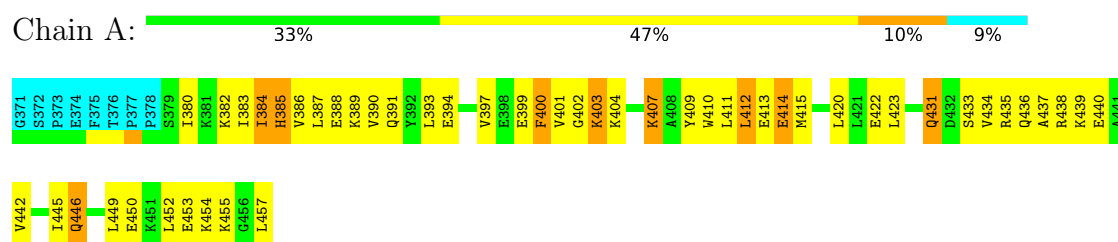
4.2.22 Score per residue for model 22

- Molecule 1: BAG-family molecular chaperone regulator-4



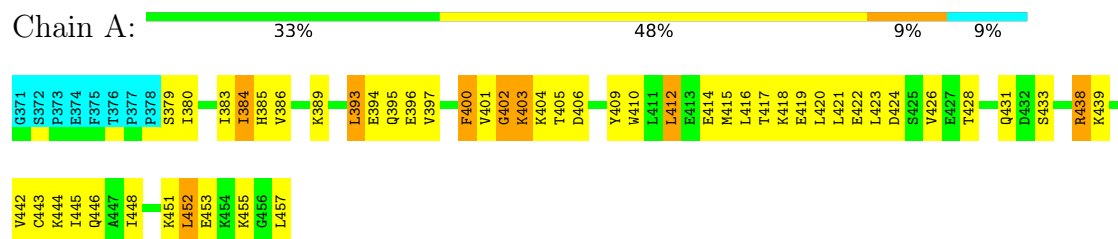
4.2.23 Score per residue for model 23

- Molecule 1: BAG-family molecular chaperone regulator-4



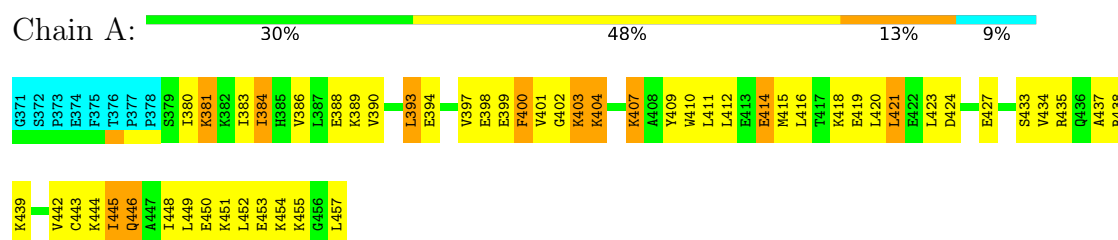
4.2.24 Score per residue for model 24

- Molecule 1: BAG-family molecular chaperone regulator-4



4.2.25 Score per residue for model 25

- Molecule 1: BAG-family molecular chaperone regulator-4



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 28 calculated structures, 25 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.0
CNS	refinement	1.0

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	642	677	677	39±6
All	All	16050	16925	16925	981

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:423:LEU:HD22	1:A:441:ALA:HB1	1.02	1.31	17	2
1:A:393:LEU:HD11	1:A:415:MET:HE2	1.02	1.29	3	2
1:A:420:LEU:HD11	1:A:445:ILE:HD13	1.00	1.28	7	1
1:A:416:LEU:HD12	1:A:445:ILE:HG23	0.99	1.31	19	1
1:A:383:ILE:HG21	1:A:437:ALA:HB1	0.99	1.30	2	7
1:A:400:PHE:CE1	1:A:412:LEU:HD22	0.91	2.01	14	12
1:A:420:LEU:HD12	1:A:445:ILE:HD12	0.89	1.43	2	1
1:A:412:LEU:HD23	1:A:452:LEU:HD11	0.89	1.44	5	5
1:A:421:LEU:HD13	1:A:422:GLU:N	0.88	1.84	14	5
1:A:412:LEU:HD12	1:A:452:LEU:HD11	0.86	1.46	3	2
1:A:400:PHE:CD2	1:A:412:LEU:HD22	0.86	2.06	12	10
1:A:412:LEU:HD13	1:A:415:MET:HE2	0.85	1.48	24	1
1:A:400:PHE:CD1	1:A:412:LEU:HD22	0.84	2.07	7	11
1:A:411:LEU:HD11	1:A:415:MET:HE2	0.84	1.47	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:400:PHE:CE2	1:A:412:LEU:HD13	0.83	2.08	14	1
1:A:387:LEU:O	1:A:390:VAL:HG12	0.83	1.74	22	7
1:A:400:PHE:CE1	1:A:412:LEU:HD13	0.82	2.09	23	9
1:A:397:VAL:HG21	1:A:448:ILE:CG2	0.82	2.03	1	14
1:A:412:LEU:HD23	1:A:452:LEU:HD21	0.82	1.48	7	4
1:A:393:LEU:O	1:A:397:VAL:HG23	0.80	1.76	12	22
1:A:420:LEU:CD1	1:A:445:ILE:HD12	0.80	2.05	2	1
1:A:442:VAL:HA	1:A:445:ILE:HD12	0.80	1.52	13	2
1:A:393:LEU:HD21	1:A:415:MET:HE2	0.80	1.52	12	1
1:A:380:ILE:O	1:A:383:ILE:HG22	0.80	1.75	4	3
1:A:423:LEU:O	1:A:426:VAL:HG13	0.80	1.77	16	1
1:A:420:LEU:HB2	1:A:445:ILE:HD13	0.79	1.55	13	2
1:A:438:ARG:O	1:A:442:VAL:HG23	0.78	1.76	11	14
1:A:420:LEU:HD21	1:A:442:VAL:HG22	0.77	1.55	1	4
1:A:416:LEU:HD12	1:A:417:THR:N	0.77	1.94	21	9
1:A:420:LEU:HD12	1:A:445:ILE:HG21	0.76	1.57	1	2
1:A:420:LEU:HD12	1:A:421:LEU:N	0.76	1.96	14	4
1:A:393:LEU:HD22	1:A:415:MET:HE3	0.76	1.55	23	1
1:A:390:VAL:HG13	1:A:419:GLU:OE2	0.76	1.81	7	3
1:A:397:VAL:HG11	1:A:452:LEU:HD11	0.76	1.55	2	1
1:A:390:VAL:HG22	1:A:419:GLU:OE2	0.75	1.79	6	4
1:A:423:LEU:HD13	1:A:441:ALA:HB3	0.75	1.59	2	2
1:A:420:LEU:CD1	1:A:445:ILE:HD13	0.75	2.09	7	1
1:A:420:LEU:HD23	1:A:423:LEU:HD11	0.74	1.58	1	1
1:A:423:LEU:HD22	1:A:441:ALA:HB3	0.74	1.59	18	2
1:A:413:GLU:CG	1:A:452:LEU:HD13	0.74	2.12	20	1
1:A:448:ILE:O	1:A:452:LEU:HD12	0.74	1.82	19	3
1:A:412:LEU:HD12	1:A:415:MET:HE2	0.74	1.60	2	1
1:A:456:GLY:O	1:A:457:LEU:HD12	0.74	1.83	5	1
1:A:397:VAL:HG21	1:A:448:ILE:HG21	0.73	1.59	4	7
1:A:399:GLU:O	1:A:401:VAL:HG23	0.73	1.84	14	1
1:A:390:VAL:HG22	1:A:419:GLU:CD	0.73	2.08	19	1
1:A:420:LEU:HD22	1:A:423:LEU:HD11	0.72	1.61	17	2
1:A:420:LEU:HD12	1:A:445:ILE:CG2	0.72	2.14	6	2
1:A:407:LYS:HA	1:A:410:TRP:CE2	0.72	2.20	6	22
1:A:400:PHE:CG	1:A:412:LEU:HD22	0.71	2.20	2	8
1:A:386:VAL:HG21	1:A:423:LEU:HG	0.71	1.61	18	2
1:A:423:LEU:HD12	1:A:424:ASP:N	0.71	1.99	24	3
1:A:412:LEU:HD23	1:A:452:LEU:CD2	0.71	2.16	7	4
1:A:420:LEU:CD2	1:A:442:VAL:HG22	0.71	2.16	1	2
1:A:420:LEU:CA	1:A:445:ILE:HD12	0.71	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:419:GLU:O	1:A:423:LEU:HD12	0.71	1.86	18	4
1:A:389:LYS:O	1:A:393:LEU:HD23	0.70	1.87	4	1
1:A:420:LEU:HG	1:A:442:VAL:HG13	0.70	1.61	22	2
1:A:420:LEU:HB2	1:A:442:VAL:HG13	0.70	1.63	18	2
1:A:412:LEU:CD1	1:A:452:LEU:HD21	0.70	2.17	13	2
1:A:421:LEU:C	1:A:421:LEU:HD22	0.70	2.11	22	5
1:A:400:PHE:CE2	1:A:412:LEU:HD22	0.69	2.21	5	4
1:A:412:LEU:HD12	1:A:452:LEU:HD21	0.69	1.62	13	4
1:A:397:VAL:HG11	1:A:448:ILE:CG2	0.69	2.18	4	3
1:A:445:ILE:HA	1:A:448:ILE:HD12	0.68	1.64	11	6
1:A:407:LYS:HA	1:A:410:TRP:NE1	0.68	2.04	8	22
1:A:423:LEU:HD13	1:A:441:ALA:CB	0.67	2.19	9	3
1:A:413:GLU:HG2	1:A:452:LEU:HD22	0.67	1.66	19	1
1:A:419:GLU:HG2	1:A:445:ILE:HG21	0.67	1.64	18	1
1:A:390:VAL:HG22	1:A:419:GLU:OE1	0.67	1.88	19	1
1:A:393:LEU:CD1	1:A:415:MET:HE2	0.67	2.17	3	1
1:A:416:LEU:HD21	1:A:448:ILE:HG21	0.67	1.66	20	1
1:A:412:LEU:HD12	1:A:452:LEU:HD13	0.66	1.67	22	2
1:A:416:LEU:HD13	1:A:416:LEU:O	0.66	1.91	7	5
1:A:420:LEU:CB	1:A:442:VAL:HG13	0.66	2.21	18	1
1:A:400:PHE:CG	1:A:412:LEU:HD13	0.66	2.25	11	1
1:A:386:VAL:HG11	1:A:423:LEU:HB3	0.66	1.65	24	3
1:A:412:LEU:CD1	1:A:415:MET:HE2	0.65	2.21	24	2
1:A:400:PHE:CE2	1:A:402:GLY:CA	0.65	2.80	5	1
1:A:383:ILE:HD11	1:A:434:VAL:HG13	0.65	1.68	25	2
1:A:420:LEU:HD23	1:A:445:ILE:HG12	0.65	1.69	17	1
1:A:413:GLU:HG2	1:A:452:LEU:HD13	0.65	1.68	14	2
1:A:423:LEU:HD21	1:A:445:ILE:HD11	0.64	1.70	6	1
1:A:397:VAL:HG22	1:A:412:LEU:HD11	0.64	1.69	22	4
1:A:420:LEU:HA	1:A:423:LEU:HD12	0.64	1.67	4	1
1:A:423:LEU:HD22	1:A:441:ALA:CB	0.64	2.22	10	4
1:A:421:LEU:HD22	1:A:421:LEU:O	0.64	1.93	22	5
1:A:420:LEU:HB3	1:A:445:ILE:HG21	0.64	1.69	21	1
1:A:393:LEU:HD22	1:A:419:GLU:OE1	0.64	1.92	25	1
1:A:400:PHE:CD1	1:A:412:LEU:HD13	0.64	2.28	17	6
1:A:420:LEU:CB	1:A:445:ILE:HG21	0.64	2.22	21	1
1:A:416:LEU:CD1	1:A:445:ILE:HG23	0.64	2.17	19	1
1:A:412:LEU:O	1:A:416:LEU:HD12	0.63	1.93	1	3
1:A:393:LEU:HD13	1:A:419:GLU:OE1	0.63	1.94	2	3
1:A:397:VAL:HG11	1:A:448:ILE:HG22	0.63	1.71	20	5
1:A:423:LEU:HD22	1:A:441:ALA:HB2	0.62	1.72	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:420:LEU:O	1:A:420:LEU:HD12	0.62	1.95	8	1
1:A:397:VAL:HG13	1:A:412:LEU:CD2	0.62	2.23	11	1
1:A:420:LEU:CB	1:A:445:ILE:HD13	0.62	2.24	13	1
1:A:390:VAL:HG22	1:A:445:ILE:HD11	0.62	1.72	14	1
1:A:420:LEU:HD22	1:A:420:LEU:O	0.62	1.95	17	1
1:A:420:LEU:CD2	1:A:423:LEU:HD11	0.62	2.25	17	2
1:A:413:GLU:HG3	1:A:452:LEU:HD13	0.62	1.71	20	2
1:A:413:GLU:HA	1:A:416:LEU:HD12	0.62	1.70	12	1
1:A:380:ILE:HA	1:A:383:ILE:HD12	0.62	1.70	2	6
1:A:393:LEU:HD21	1:A:415:MET:SD	0.61	2.35	1	1
1:A:393:LEU:HD22	1:A:416:LEU:HD23	0.61	1.71	7	2
1:A:383:ILE:HD13	1:A:437:ALA:CB	0.61	2.24	2	1
1:A:400:PHE:CZ	1:A:402:GLY:HA2	0.61	2.30	5	2
1:A:394:GLU:OE1	1:A:448:ILE:HD11	0.61	1.95	20	1
1:A:393:LEU:HD21	1:A:415:MET:HG2	0.61	1.72	21	1
1:A:420:LEU:HD23	1:A:421:LEU:N	0.61	2.10	22	2
1:A:386:VAL:HG11	1:A:423:LEU:HG	0.61	1.73	23	3
1:A:445:ILE:HD12	1:A:446:GLN:N	0.61	2.11	23	4
1:A:393:LEU:HD13	1:A:419:GLU:CD	0.61	2.21	2	2
1:A:386:VAL:HB	1:A:423:LEU:HD21	0.61	1.72	21	2
1:A:416:LEU:HD11	1:A:445:ILE:HG23	0.61	1.72	13	1
1:A:386:VAL:HG21	1:A:423:LEU:HD11	0.61	1.71	16	1
1:A:397:VAL:HG11	1:A:452:LEU:CD1	0.60	2.26	2	1
1:A:397:VAL:HG13	1:A:452:LEU:HG	0.60	1.71	24	2
1:A:397:VAL:HG21	1:A:448:ILE:HG23	0.60	1.71	21	3
1:A:400:PHE:CD2	1:A:412:LEU:HD13	0.60	2.31	14	2
1:A:382:LYS:O	1:A:386:VAL:HG23	0.60	1.97	21	8
1:A:393:LEU:HD11	1:A:415:MET:HG2	0.60	1.72	9	1
1:A:400:PHE:CG	1:A:412:LEU:HD23	0.60	2.32	13	1
1:A:413:GLU:CD	1:A:452:LEU:HD22	0.59	2.22	12	1
1:A:400:PHE:CD1	1:A:412:LEU:HD23	0.59	2.31	16	5
1:A:420:LEU:CG	1:A:445:ILE:HD12	0.59	2.27	2	1
1:A:423:LEU:CD1	1:A:442:VAL:HG22	0.59	2.26	6	1
1:A:423:LEU:HD22	1:A:438:ARG:HA	0.59	1.74	9	1
1:A:390:VAL:HG22	1:A:419:GLU:CB	0.59	2.28	10	1
1:A:400:PHE:CZ	1:A:402:GLY:HA3	0.58	2.33	3	22
1:A:387:LEU:CD2	1:A:441:ALA:HB2	0.58	2.28	22	1
1:A:410:TRP:CE3	1:A:411:LEU:HD12	0.58	2.33	22	1
1:A:400:PHE:CE1	1:A:412:LEU:HD23	0.58	2.34	19	7
1:A:431:GLN:HG2	1:A:434:VAL:HG23	0.58	1.76	2	4
1:A:420:LEU:HD13	1:A:445:ILE:HG12	0.58	1.75	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:401:VAL:O	1:A:401:VAL:HG22	0.57	1.99	18	8
1:A:420:LEU:HD21	1:A:442:VAL:CG2	0.57	2.29	1	1
1:A:420:LEU:HD22	1:A:445:ILE:HD13	0.57	1.76	3	2
1:A:390:VAL:HG22	1:A:419:GLU:HB3	0.57	1.75	10	1
1:A:418:LYS:HA	1:A:421:LEU:HD12	0.57	1.75	18	4
1:A:412:LEU:CD2	1:A:452:LEU:HD11	0.57	2.29	12	2
1:A:386:VAL:O	1:A:390:VAL:HG23	0.56	2.01	10	9
1:A:417:THR:HG22	1:A:421:LEU:HD13	0.56	1.77	10	1
1:A:403:LYS:O	1:A:409:TYR:HB2	0.56	1.99	10	13
1:A:383:ILE:HG23	1:A:384:ILE:HD13	0.56	1.76	4	3
1:A:431:GLN:CG	1:A:434:VAL:HG23	0.56	2.30	23	1
1:A:400:PHE:CZ	1:A:402:GLY:CA	0.56	2.88	14	2
1:A:403:LYS:O	1:A:409:TYR:CB	0.56	2.54	18	23
1:A:397:VAL:HG13	1:A:412:LEU:HD21	0.56	1.77	11	2
1:A:397:VAL:HG22	1:A:412:LEU:CD1	0.56	2.31	22	2
1:A:421:LEU:HD13	1:A:422:GLU:H	0.56	1.57	18	4
1:A:397:VAL:HG22	1:A:412:LEU:HD21	0.56	1.78	14	1
1:A:416:LEU:HD12	1:A:416:LEU:C	0.55	2.26	9	4
1:A:380:ILE:HG22	1:A:384:ILE:HD11	0.55	1.78	10	17
1:A:383:ILE:HG21	1:A:437:ALA:CB	0.55	2.20	2	1
1:A:386:VAL:HG21	1:A:423:LEU:CG	0.55	2.30	18	1
1:A:416:LEU:HD12	1:A:445:ILE:CG2	0.55	2.20	19	1
1:A:420:LEU:C	1:A:420:LEU:HD13	0.55	2.26	23	4
1:A:420:LEU:HG	1:A:445:ILE:HD13	0.55	1.79	17	1
1:A:399:GLU:O	1:A:400:PHE:C	0.55	2.50	4	11
1:A:386:VAL:CG2	1:A:423:LEU:HD11	0.55	2.31	16	1
1:A:416:LEU:HD11	1:A:445:ILE:HB	0.55	1.79	10	2
1:A:390:VAL:HG22	1:A:445:ILE:CD1	0.55	2.32	14	1
1:A:420:LEU:C	1:A:420:LEU:HD12	0.54	2.27	21	4
1:A:445:ILE:HD13	1:A:445:ILE:N	0.54	2.16	25	4
1:A:412:LEU:O	1:A:416:LEU:HD13	0.54	2.01	25	1
1:A:412:LEU:HD12	1:A:452:LEU:CD1	0.54	2.27	3	1
1:A:400:PHE:CZ	1:A:412:LEU:HD22	0.54	2.37	10	3
1:A:412:LEU:HD23	1:A:452:LEU:CD1	0.54	2.32	11	3
1:A:420:LEU:O	1:A:442:VAL:HG22	0.54	2.03	14	1
1:A:401:VAL:HG12	1:A:401:VAL:O	0.53	2.03	6	8
1:A:420:LEU:HD13	1:A:420:LEU:O	0.53	2.03	12	2
1:A:420:LEU:HD12	1:A:420:LEU:C	0.53	2.29	15	3
1:A:420:LEU:N	1:A:445:ILE:HD12	0.53	2.18	9	1
1:A:420:LEU:HA	1:A:442:VAL:HG22	0.53	1.80	18	1
1:A:412:LEU:CD1	1:A:452:LEU:HD11	0.53	2.28	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:416:LEU:O	1:A:416:LEU:HD12	0.53	2.02	2	2
1:A:420:LEU:C	1:A:420:LEU:HD23	0.53	2.28	6	1
1:A:420:LEU:HD13	1:A:420:LEU:C	0.53	2.29	12	1
1:A:420:LEU:CD1	1:A:421:LEU:HD12	0.53	2.34	13	1
1:A:386:VAL:HG21	1:A:423:LEU:HB3	0.53	1.80	6	1
1:A:428:THR:HG23	1:A:434:VAL:HB	0.53	1.79	10	1
1:A:412:LEU:HD12	1:A:415:MET:CE	0.53	2.32	2	1
1:A:403:LYS:O	1:A:409:TYR:CD1	0.52	2.62	9	2
1:A:423:LEU:C	1:A:423:LEU:HD12	0.52	2.29	19	1
1:A:383:ILE:HG13	1:A:434:VAL:HG13	0.52	1.81	18	1
1:A:416:LEU:CD2	1:A:452:LEU:HD11	0.52	2.34	21	1
1:A:397:VAL:HG13	1:A:452:LEU:CD1	0.52	2.34	3	2
1:A:416:LEU:HD13	1:A:416:LEU:C	0.52	2.29	24	3
1:A:383:ILE:CG2	1:A:437:ALA:HB1	0.52	2.20	2	2
1:A:441:ALA:O	1:A:445:ILE:HG23	0.52	2.04	18	1
1:A:384:ILE:HD13	1:A:384:ILE:N	0.52	2.19	14	14
1:A:400:PHE:CZ	1:A:412:LEU:HD13	0.52	2.39	12	3
1:A:400:PHE:CE1	1:A:402:GLY:CA	0.51	2.93	14	1
1:A:446:GLN:HA	1:A:449:LEU:HD12	0.51	1.82	14	1
1:A:412:LEU:HD23	1:A:452:LEU:HG	0.51	1.83	17	1
1:A:431:GLN:HB3	1:A:434:VAL:HG23	0.51	1.82	17	3
1:A:416:LEU:HD21	1:A:452:LEU:CD1	0.51	2.36	21	1
1:A:390:VAL:CG2	1:A:445:ILE:HD11	0.51	2.35	14	2
1:A:423:LEU:HD13	1:A:441:ALA:HB1	0.51	1.83	3	2
1:A:390:VAL:HG13	1:A:445:ILE:CD1	0.51	2.35	15	1
1:A:400:PHE:CE2	1:A:402:GLY:HA3	0.50	2.41	5	2
1:A:399:GLU:O	1:A:401:VAL:N	0.50	2.44	9	2
1:A:420:LEU:CD1	1:A:442:VAL:HG22	0.50	2.36	10	1
1:A:420:LEU:HD11	1:A:442:VAL:HG22	0.50	1.82	10	1
1:A:417:THR:HA	1:A:420:LEU:HD23	0.50	1.81	16	1
1:A:423:LEU:HD12	1:A:423:LEU:C	0.50	2.31	24	2
1:A:420:LEU:HG	1:A:445:ILE:HG21	0.50	1.82	7	1
1:A:387:LEU:O	1:A:387:LEU:HD23	0.50	2.07	12	1
1:A:412:LEU:HD23	1:A:452:LEU:CG	0.49	2.37	17	5
1:A:420:LEU:HB3	1:A:445:ILE:HD11	0.49	1.83	18	1
1:A:445:ILE:HG22	1:A:449:LEU:HD12	0.49	1.84	1	1
1:A:410:TRP:O	1:A:414:GLU:HB2	0.49	2.08	25	20
1:A:420:LEU:HD12	1:A:445:ILE:HG22	0.49	1.81	6	1
1:A:420:LEU:HD23	1:A:420:LEU:O	0.49	2.06	6	2
1:A:445:ILE:CG2	1:A:449:LEU:HD12	0.49	2.38	1	1
1:A:406:ASP:OD2	1:A:408:ALA:HB3	0.49	2.07	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:400:PHE:CE1	1:A:402:GLY:HA3	0.49	2.42	14	1
1:A:423:LEU:HD21	1:A:445:ILE:CD1	0.49	2.37	6	1
1:A:400:PHE:CD2	1:A:412:LEU:HD23	0.49	2.42	24	2
1:A:423:LEU:O	1:A:426:VAL:HG23	0.49	2.07	18	1
1:A:410:TRP:O	1:A:414:GLU:N	0.49	2.45	7	13
1:A:404:LYS:HA	1:A:409:TYR:CG	0.49	2.43	2	3
1:A:406:ASP:OD1	1:A:408:ALA:HB3	0.49	2.08	12	1
1:A:400:PHE:CE2	1:A:452:LEU:HD11	0.49	2.43	6	2
1:A:420:LEU:HA	1:A:445:ILE:HD12	0.49	1.85	9	1
1:A:397:VAL:HG21	1:A:448:ILE:HG22	0.48	1.85	15	2
1:A:452:LEU:O	1:A:452:LEU:HD13	0.48	2.08	15	1
1:A:420:LEU:HD11	1:A:421:LEU:CD1	0.48	2.38	13	1
1:A:420:LEU:HB3	1:A:445:ILE:HD12	0.48	1.85	14	1
1:A:442:VAL:HA	1:A:445:ILE:CG1	0.48	2.38	3	9
1:A:420:LEU:HD11	1:A:445:ILE:CD1	0.48	2.21	7	1
1:A:400:PHE:CE2	1:A:402:GLY:HA2	0.48	2.43	5	1
1:A:399:GLU:O	1:A:400:PHE:O	0.48	2.32	8	6
1:A:413:GLU:HA	1:A:416:LEU:HD21	0.48	1.86	14	1
1:A:404:LYS:HG2	1:A:457:LEU:HD23	0.48	1.86	22	1
1:A:418:LYS:O	1:A:421:LEU:CD1	0.48	2.61	18	4
1:A:410:TRP:CZ3	1:A:411:LEU:CD1	0.48	2.96	3	2
1:A:393:LEU:HD23	1:A:397:VAL:HG21	0.47	1.86	2	1
1:A:410:TRP:CZ3	1:A:411:LEU:CD2	0.47	2.97	4	2
1:A:421:LEU:C	1:A:421:LEU:CD2	0.47	2.83	9	3
1:A:416:LEU:HD12	1:A:449:LEU:HD12	0.47	1.87	18	1
1:A:420:LEU:HD23	1:A:445:ILE:HD13	0.47	1.85	18	1
1:A:441:ALA:O	1:A:445:ILE:HD13	0.47	2.09	22	1
1:A:383:ILE:CG2	1:A:384:ILE:HD13	0.47	2.39	20	3
1:A:401:VAL:O	1:A:402:GLY:O	0.47	2.32	5	3
1:A:420:LEU:HG	1:A:445:ILE:HD12	0.47	1.87	6	1
1:A:387:LEU:HD23	1:A:391:GLN:HE21	0.47	1.70	16	1
1:A:445:ILE:HD12	1:A:445:ILE:C	0.47	2.35	23	1
1:A:411:LEU:HA	1:A:414:GLU:HB2	0.47	1.87	11	23
1:A:400:PHE:CD1	1:A:412:LEU:CD2	0.46	2.98	22	12
1:A:421:LEU:HD13	1:A:421:LEU:C	0.46	2.33	15	5
1:A:400:PHE:CG	1:A:412:LEU:CD2	0.46	2.98	13	5
1:A:400:PHE:C	1:A:400:PHE:CD1	0.46	2.94	24	1
1:A:380:ILE:HD12	1:A:380:ILE:N	0.46	2.26	10	3
1:A:403:LYS:O	1:A:409:TYR:HB3	0.46	2.10	12	4
1:A:407:LYS:CD	1:A:410:TRP:CH2	0.46	2.99	16	2
1:A:443:CYS:HA	1:A:446:GLN:HG3	0.46	1.86	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:400:PHE:CE1	1:A:412:LEU:HG	0.46	2.45	24	2
1:A:416:LEU:HD21	1:A:448:ILE:CG2	0.46	2.38	20	1
1:A:407:LYS:CG	1:A:410:TRP:CH2	0.46	2.98	7	1
1:A:407:LYS:HB2	1:A:410:TRP:CZ2	0.46	2.45	9	4
1:A:400:PHE:CD1	1:A:400:PHE:C	0.46	2.94	13	2
1:A:393:LEU:HD13	1:A:416:LEU:HD23	0.46	1.88	12	1
1:A:419:GLU:O	1:A:423:LEU:HD23	0.46	2.11	22	1
1:A:420:LEU:HD22	1:A:445:ILE:HG21	0.46	1.88	13	1
1:A:397:VAL:CG1	1:A:452:LEU:HD12	0.45	2.41	1	1
1:A:403:LYS:O	1:A:409:TYR:CG	0.45	2.69	24	2
1:A:410:TRP:CZ3	1:A:411:LEU:HD12	0.45	2.45	22	1
1:A:442:VAL:HA	1:A:445:ILE:HD11	0.45	1.87	2	1
1:A:397:VAL:HG11	1:A:448:ILE:HG23	0.45	1.86	4	1
1:A:393:LEU:O	1:A:393:LEU:HD23	0.45	2.12	7	1
1:A:407:LYS:CB	1:A:410:TRP:CZ2	0.45	2.99	17	4
1:A:404:LYS:CD	1:A:409:TYR:CE2	0.45	3.00	13	1
1:A:393:LEU:HD11	1:A:415:MET:HB2	0.45	1.88	16	1
1:A:442:VAL:HA	1:A:445:ILE:HG12	0.45	1.89	24	1
1:A:442:VAL:O	1:A:446:GLN:CG	0.45	2.64	11	2
1:A:434:VAL:HG12	1:A:438:ARG:CD	0.45	2.42	16	1
1:A:416:LEU:O	1:A:419:GLU:HG3	0.45	2.11	16	1
1:A:383:ILE:CG1	1:A:434:VAL:HG13	0.45	2.41	18	1
1:A:380:ILE:HD13	1:A:383:ILE:CD1	0.45	2.42	7	2
1:A:397:VAL:HG13	1:A:452:LEU:HD23	0.45	1.88	15	1
1:A:397:VAL:HG22	1:A:412:LEU:CD2	0.44	2.41	14	1
1:A:393:LEU:HD12	1:A:416:LEU:HB3	0.44	1.89	16	1
1:A:393:LEU:CD2	1:A:415:MET:HE3	0.44	2.42	24	2
1:A:393:LEU:HD13	1:A:416:LEU:HB3	0.44	1.89	8	1
1:A:403:LYS:HG2	1:A:406:ASP:HB2	0.44	1.90	24	2
1:A:404:LYS:O	1:A:409:TYR:CD2	0.44	2.70	10	2
1:A:400:PHE:CD1	1:A:412:LEU:CD1	0.44	3.00	11	1
1:A:382:LYS:HG3	1:A:383:ILE:N	0.44	2.28	11	1
1:A:423:LEU:CD2	1:A:441:ALA:HB3	0.44	2.37	18	1
1:A:386:VAL:HG13	1:A:387:LEU:N	0.44	2.28	6	3
1:A:423:LEU:O	1:A:426:VAL:HG22	0.44	2.12	24	2
1:A:400:PHE:CG	1:A:412:LEU:CD1	0.44	2.98	11	1
1:A:393:LEU:HD21	1:A:415:MET:CE	0.44	2.36	12	1
1:A:400:PHE:C	1:A:401:VAL:HG23	0.43	2.38	9	1
1:A:407:LYS:O	1:A:411:LEU:HD23	0.43	2.13	1	1
1:A:383:ILE:HD13	1:A:437:ALA:HB3	0.43	1.89	2	1
1:A:403:LYS:N	1:A:403:LYS:CD	0.43	2.81	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:427:GLU:O	1:A:428:THR:HG22	0.43	2.12	1	1
1:A:423:LEU:HD11	1:A:442:VAL:HG22	0.43	1.88	6	1
1:A:423:LEU:C	1:A:426:VAL:HG23	0.43	2.38	18	1
1:A:407:LYS:HB3	1:A:410:TRP:CZ2	0.43	2.49	19	3
1:A:386:VAL:HG11	1:A:423:LEU:HD11	0.43	1.89	12	1
1:A:380:ILE:HD12	1:A:380:ILE:H	0.43	1.74	25	1
1:A:413:GLU:OE2	1:A:449:LEU:HD23	0.43	2.14	19	1
1:A:412:LEU:CD1	1:A:452:LEU:HD13	0.43	2.42	22	1
1:A:428:THR:HG23	1:A:438:ARG:NH1	0.43	2.28	16	1
1:A:420:LEU:HD23	1:A:445:ILE:CD1	0.43	2.44	18	1
1:A:390:VAL:HG11	1:A:445:ILE:CD1	0.43	2.44	25	1
1:A:412:LEU:O	1:A:412:LEU:HD13	0.43	2.12	13	1
1:A:390:VAL:CG1	1:A:445:ILE:CD1	0.43	2.97	15	1
1:A:419:GLU:HG3	1:A:420:LEU:N	0.43	2.29	6	2
1:A:380:ILE:HD13	1:A:383:ILE:HD12	0.43	1.91	13	3
1:A:393:LEU:HD13	1:A:416:LEU:CD2	0.43	2.44	24	1
1:A:420:LEU:HD11	1:A:421:LEU:HD12	0.42	1.91	25	2
1:A:400:PHE:CD2	1:A:412:LEU:CD2	0.42	2.98	5	2
1:A:416:LEU:CD1	1:A:445:ILE:HD13	0.42	2.44	18	1
1:A:417:THR:O	1:A:421:LEU:HD13	0.42	2.15	24	1
1:A:420:LEU:CB	1:A:445:ILE:HD12	0.42	2.44	9	1
1:A:423:LEU:CD2	1:A:441:ALA:CB	0.42	2.98	18	1
1:A:415:MET:O	1:A:418:LYS:HG3	0.42	2.13	21	1
1:A:393:LEU:HG	1:A:415:MET:HE3	0.42	1.91	21	1
1:A:423:LEU:HG	1:A:441:ALA:HB3	0.42	1.91	22	1
1:A:409:TYR:CD1	1:A:409:TYR:C	0.42	2.97	14	2
1:A:412:LEU:CD2	1:A:452:LEU:HD21	0.42	2.35	7	1
1:A:393:LEU:HD13	1:A:416:LEU:CB	0.42	2.45	8	1
1:A:402:GLY:O	1:A:455:LYS:O	0.42	2.37	5	1
1:A:445:ILE:HG22	1:A:449:LEU:CD1	0.42	2.44	20	1
1:A:426:VAL:HG11	1:A:438:ARG:HG3	0.42	1.91	15	1
1:A:442:VAL:O	1:A:445:ILE:HG13	0.42	2.14	18	1
1:A:393:LEU:HD12	1:A:419:GLU:CD	0.42	2.40	8	1
1:A:404:LYS:HA	1:A:409:TYR:CD2	0.42	2.49	8	2
1:A:385:HIS:CG	1:A:386:VAL:N	0.41	2.88	18	1
1:A:383:ILE:CD1	1:A:438:ARG:CZ	0.41	2.98	24	1
1:A:408:ALA:O	1:A:412:LEU:N	0.41	2.51	5	1
1:A:411:LEU:O	1:A:415:MET:HG2	0.41	2.14	11	1
1:A:393:LEU:HD22	1:A:416:LEU:CD2	0.41	2.45	12	1
1:A:420:LEU:HB2	1:A:445:ILE:HG21	0.41	1.92	11	1
1:A:442:VAL:HA	1:A:445:ILE:CD1	0.41	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:420:LEU:CD1	1:A:442:VAL:HG13	0.41	2.45	8	1
1:A:416:LEU:CD2	1:A:452:LEU:CD1	0.41	2.99	21	1
1:A:428:THR:OG1	1:A:434:VAL:HG11	0.41	2.16	13	1
1:A:400:PHE:CE2	1:A:412:LEU:HD23	0.41	2.50	24	1
1:A:416:LEU:O	1:A:419:GLU:HG2	0.41	2.16	14	1
1:A:385:HIS:CD2	1:A:385:HIS:C	0.41	2.99	5	3
1:A:404:LYS:O	1:A:409:TYR:CE2	0.41	2.74	10	2
1:A:392:TYR:O	1:A:395:GLN:CG	0.41	2.69	11	1
1:A:383:ILE:HD11	1:A:434:VAL:CG1	0.41	2.45	18	1
1:A:383:ILE:CG2	1:A:437:ALA:CB	0.41	2.99	22	1
1:A:416:LEU:O	1:A:419:GLU:CG	0.41	2.69	1	1
1:A:409:TYR:CE2	1:A:457:LEU:O	0.41	2.74	5	1
1:A:407:LYS:CG	1:A:410:TRP:CZ2	0.41	3.04	10	1
1:A:407:LYS:HG3	1:A:410:TRP:CH2	0.41	2.51	10	1
1:A:380:ILE:HD13	1:A:380:ILE:N	0.41	2.31	11	1
1:A:383:ILE:HD12	1:A:434:VAL:HG13	0.41	1.92	22	1
1:A:402:GLY:C	1:A:403:LYS:CD	0.41	2.94	24	1
1:A:438:ARG:CD	1:A:439:LYS:N	0.41	2.84	2	1
1:A:413:GLU:HG3	1:A:452:LEU:HD22	0.41	1.93	20	1
1:A:405:THR:HG22	1:A:405:THR:O	0.40	2.15	11	1
1:A:431:GLN:O	1:A:434:VAL:HG12	0.40	2.16	21	1
1:A:383:ILE:CD1	1:A:434:VAL:HG13	0.40	2.46	8	1
1:A:413:GLU:CG	1:A:449:LEU:CD2	0.40	2.99	22	1
1:A:413:GLU:OE1	1:A:452:LEU:HD22	0.40	2.15	12	1
1:A:420:LEU:CD1	1:A:421:LEU:CD1	0.40	2.98	13	1
1:A:384:ILE:N	1:A:384:ILE:CD1	0.40	2.84	14	1
1:A:420:LEU:HD21	1:A:442:VAL:CB	0.40	2.46	1	1
1:A:420:LEU:O	1:A:423:LEU:HG	0.40	2.16	19	1
1:A:393:LEU:CG	1:A:415:MET:HE3	0.40	2.46	21	1
1:A:413:GLU:CG	1:A:452:LEU:HD22	0.40	2.43	19	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	78/87 (90%)	72±1 (93±2%)	4±1 (5±2%)	2±1 (2±1%)	7	45
All	All	1950/2175 (90%)	1806 (93%)	99 (5%)	45 (2%)	7	45

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	400	PHE	19
1	A	402	GLY	7
1	A	428	THR	4
1	A	430	GLY	4
1	A	429	GLY	3
1	A	456	GLY	3
1	A	431	GLN	2
1	A	401	VAL	2
1	A	427	GLU	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	71/78 (91%)	45±3 (63±4%)	26±3 (37±4%)	1	8
All	All	1775/1950 (91%)	1120 (63%)	655 (37%)	1	8

All 63 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	384	ILE	25
1	A	403	LYS	24
1	A	404	LYS	23
1	A	457	LEU	21
1	A	389	LYS	20
1	A	414	GLU	20
1	A	455	LYS	19
1	A	393	LEU	18
1	A	451	LYS	17

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Mol	Chain	Res	Type	Models (Total)
1	A	407	LYS	17
1	A	444	LYS	17
1	A	412	LEU	16
1	A	435	ARG	16
1	A	418	LYS	16
1	A	450	GLU	16
1	A	449	LEU	15
1	A	452	LEU	15
1	A	439	LYS	15
1	A	446	GLN	14
1	A	421	LEU	13
1	A	453	GLU	13
1	A	420	LEU	12
1	A	422	GLU	12
1	A	381	LYS	12
1	A	454	LYS	12
1	A	391	GLN	11
1	A	431	GLN	11
1	A	438	ARG	11
1	A	385	HIS	11
1	A	405	THR	11
1	A	394	GLU	10
1	A	413	GLU	10
1	A	387	LEU	9
1	A	395	GLN	9
1	A	388	GLU	9
1	A	436	GLN	8
1	A	379	SER	8
1	A	423	LEU	8
1	A	433	SER	8
1	A	427	GLU	7
1	A	440	GLU	7
1	A	398	GLU	7
1	A	445	ILE	7
1	A	392	TYR	6
1	A	424	ASP	6
1	A	396	GLU	5
1	A	406	ASP	5
1	A	410	TRP	5
1	A	411	LEU	5
1	A	432	ASP	5
1	A	419	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	443	CYS	5
1	A	417	THR	5
1	A	382	LYS	4
1	A	400	PHE	4
1	A	416	LEU	3
1	A	425	SER	3
1	A	415	MET	3
1	A	428	THR	2
1	A	399	GLU	1
1	A	383	ILE	1
1	A	380	ILE	1
1	A	409	TYR	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