



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:58 PM BST

PDB ID : 1M62
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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

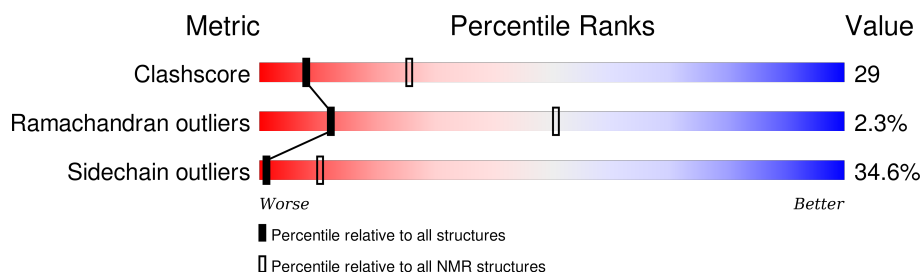
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	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)	0.51	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:

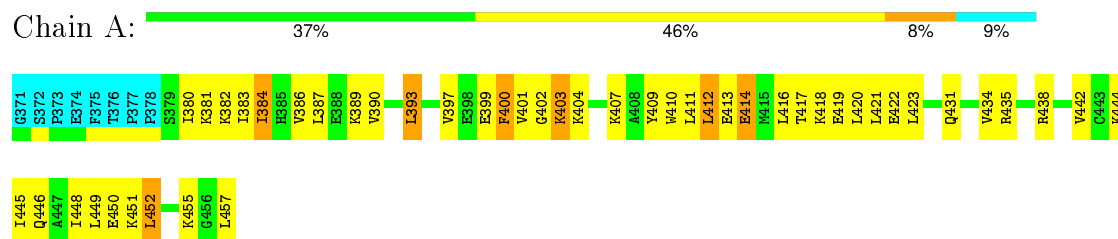
Chain	Residue	Modelled	Actual	Comment	Reference
A	371	GLY	-	CLONING ARTIFACT	UNP O95429
A	372	SER	-	CLONING ARTIFACT	UNP O95429
A	373	PRO	-	CLONING ARTIFACT	UNP O95429
A	374	GLU	-	CLONING ARTIFACT	UNP O95429
A	375	PHE	-	CLONING ARTIFACT	UNP O95429

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

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

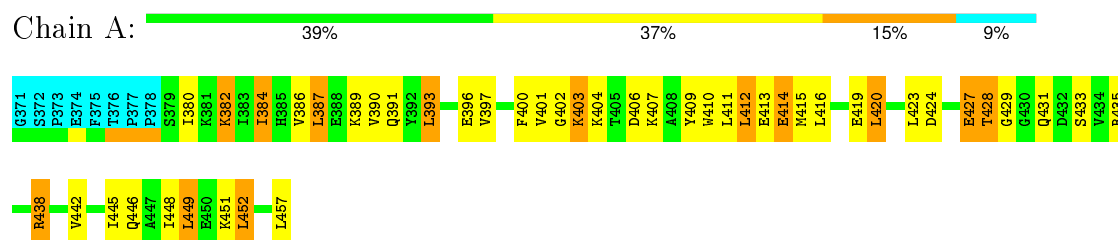


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

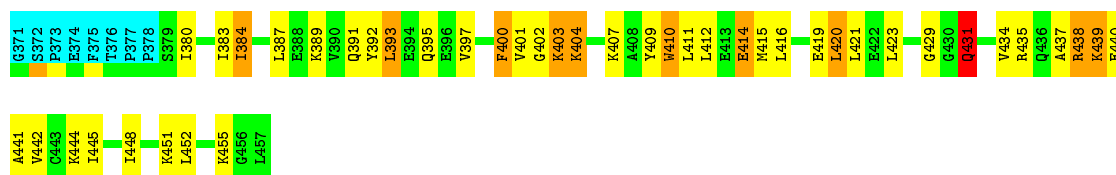
- Molecule 1: BAG-family molecular chaperone regulator-4



4.2.2 Score per residue for model 2

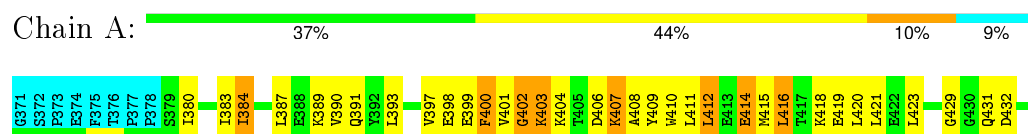
- Molecule 1: BAG-family molecular chaperone regulator-4





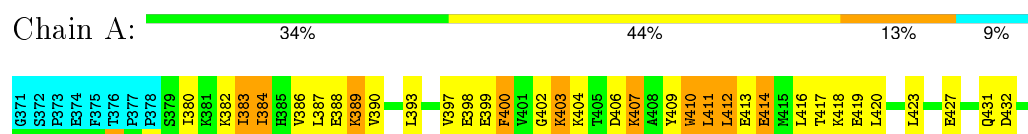
4.2.3 Score per residue for model 3 (medoid)

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



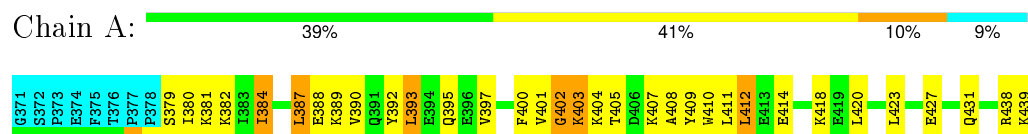
4.2.4 Score per residue for model 4

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



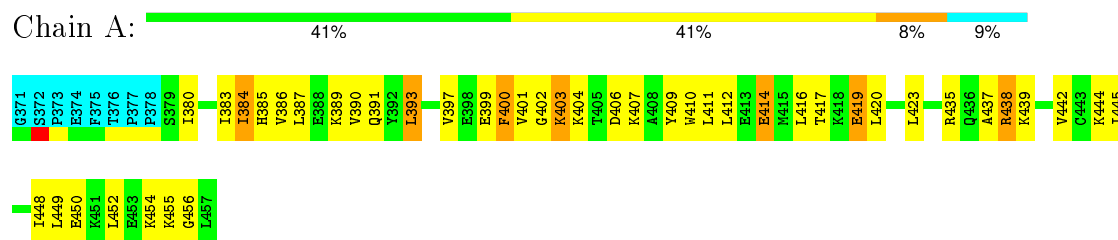
4.2.5 Score per residue for model 5

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



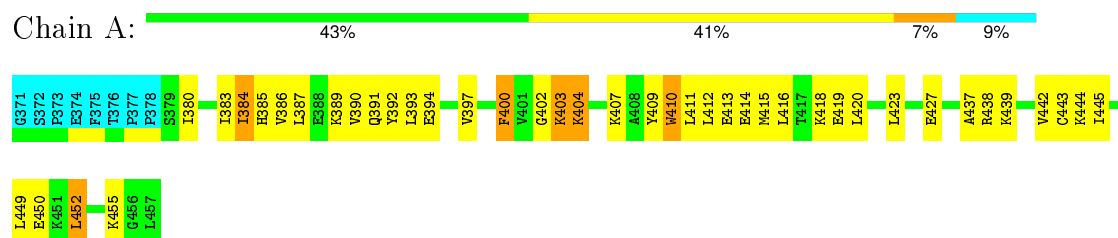
4.2.6 Score per residue for model 6

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



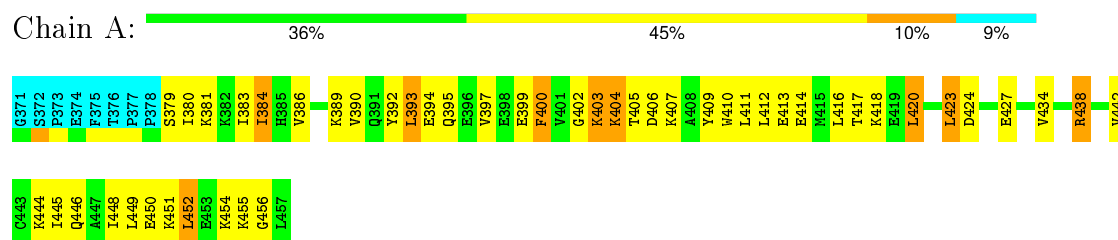
4.2.7 Score per residue for model 7

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



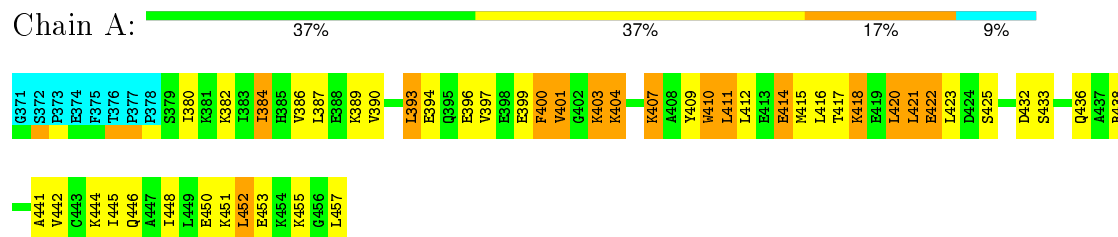
4.2.8 Score per residue for model 8

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



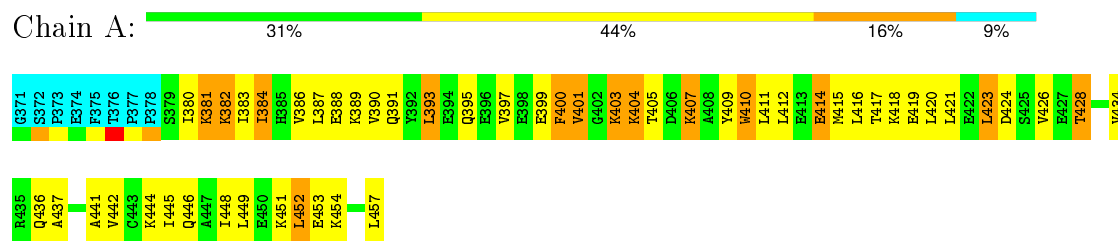
4.2.9 Score per residue for model 9

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



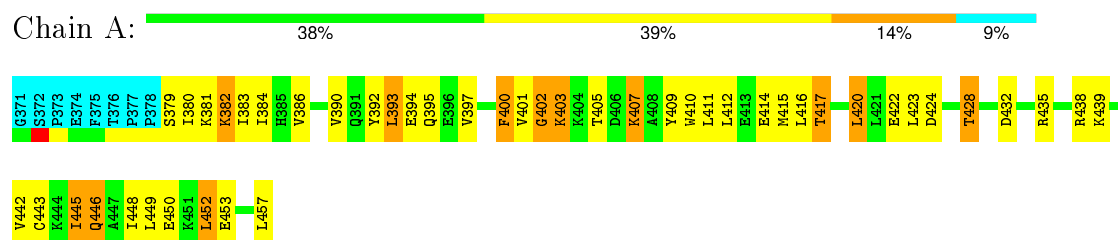
4.2.10 Score per residue for model 10

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



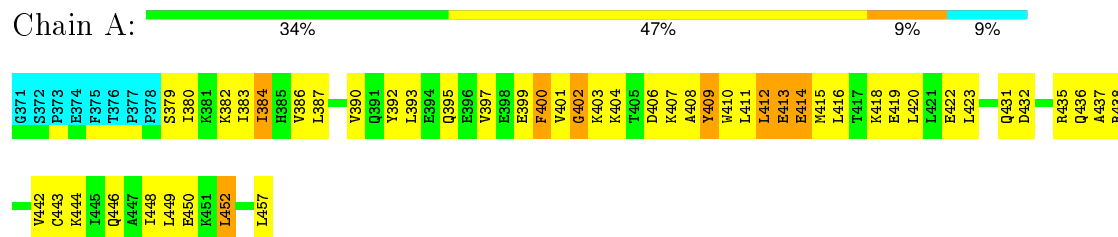
4.2.11 Score per residue for model 11

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



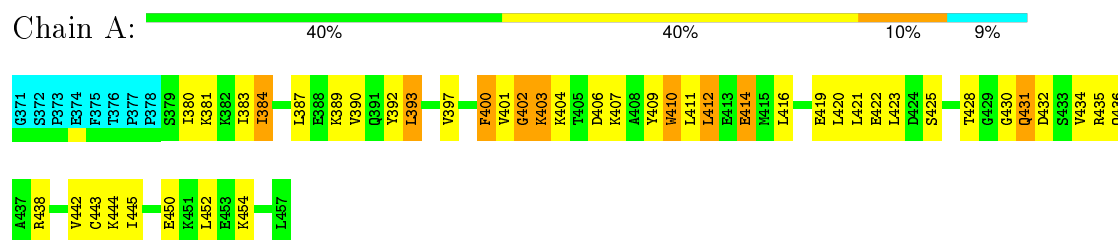
4.2.12 Score per residue for model 12

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



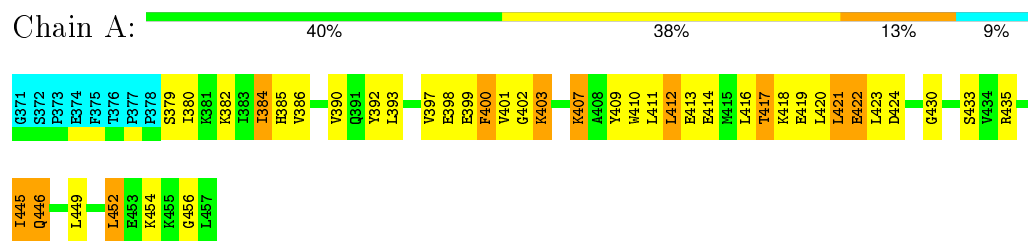
4.2.13 Score per residue for model 13

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



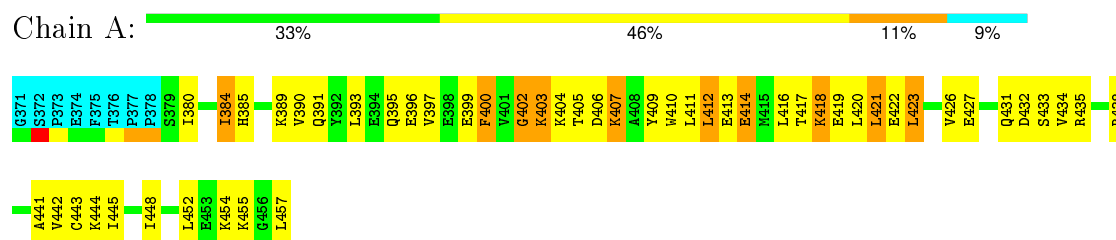
4.2.14 Score per residue for model 14

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



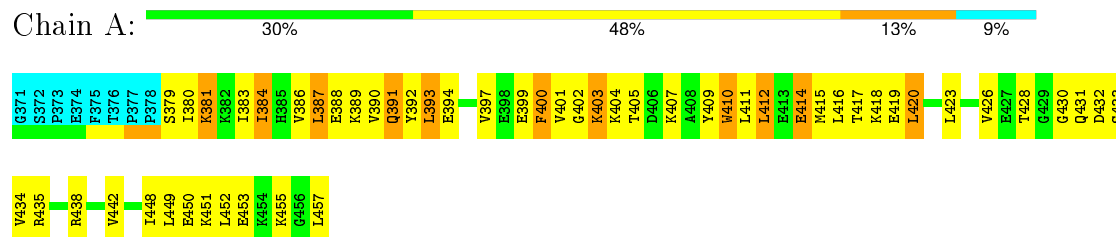
4.2.15 Score per residue for model 15

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



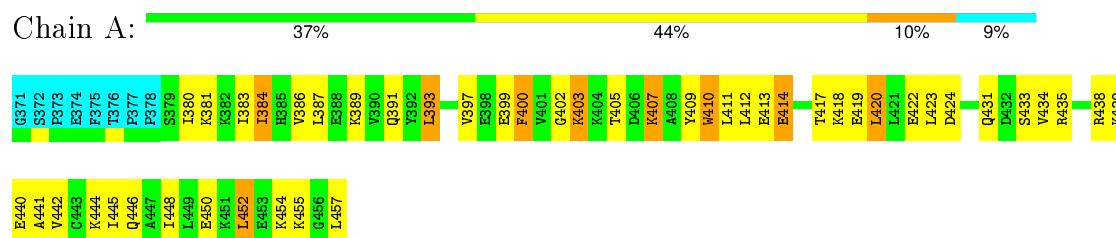
4.2.16 Score per residue for model 16

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



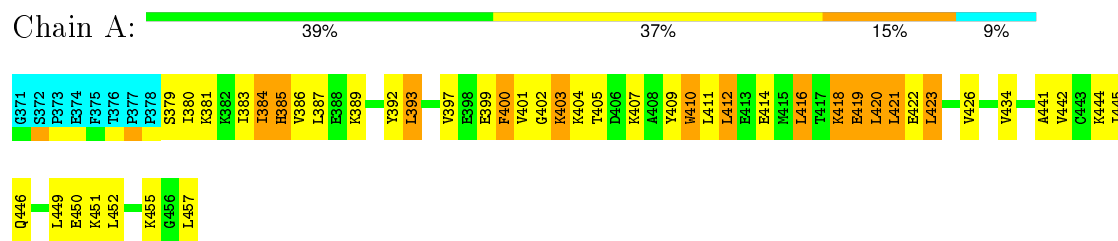
4.2.17 Score per residue for model 17

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



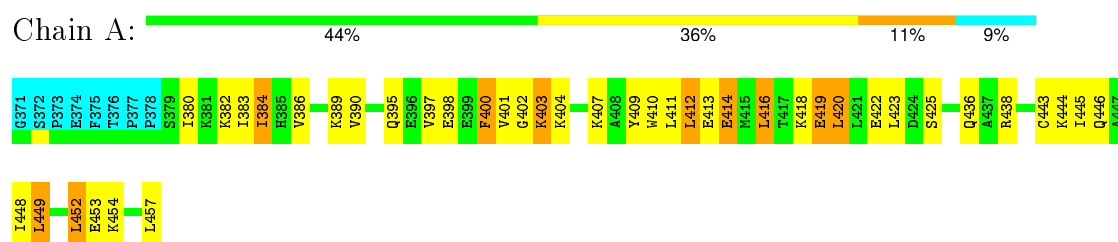
4.2.18 Score per residue for model 18

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



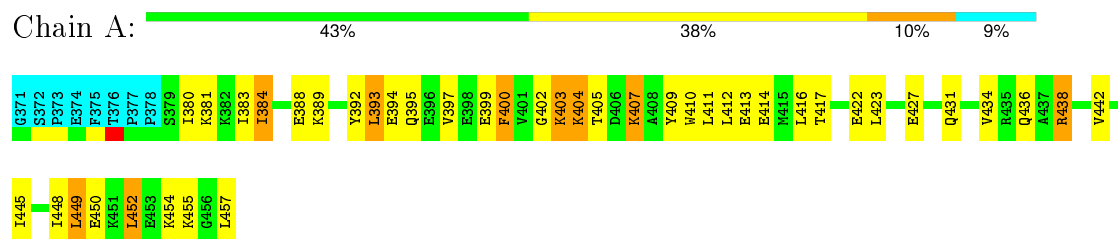
4.2.19 Score per residue for model 19

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



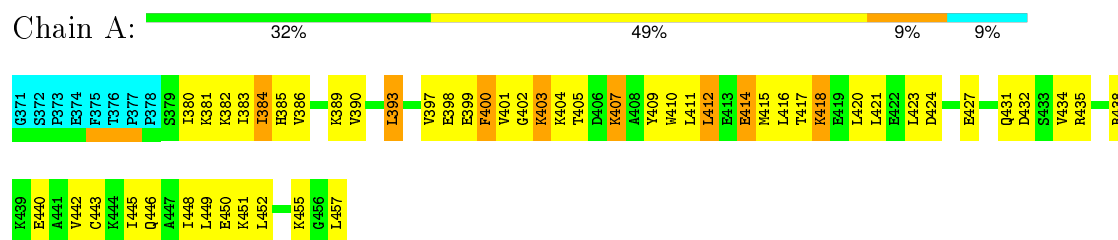
4.2.20 Score per residue for model 20

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



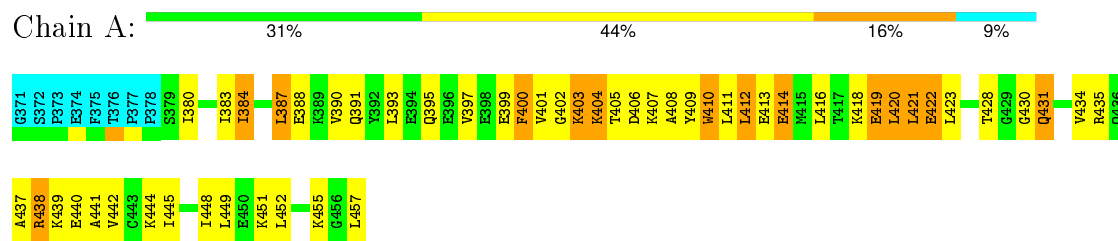
4.2.21 Score per residue for model 21

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



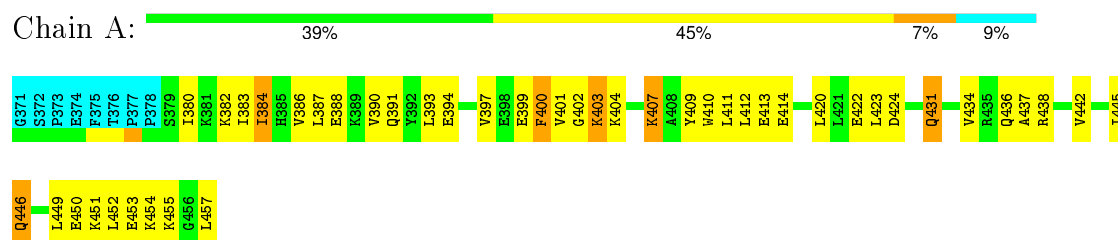
4.2.22 Score per residue for model 22

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



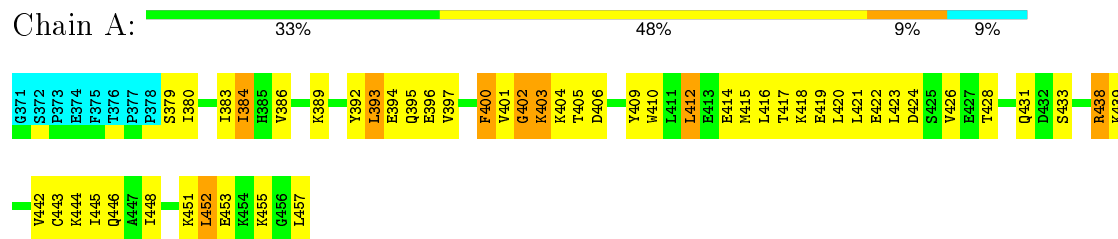
4.2.23 Score per residue for model 23

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



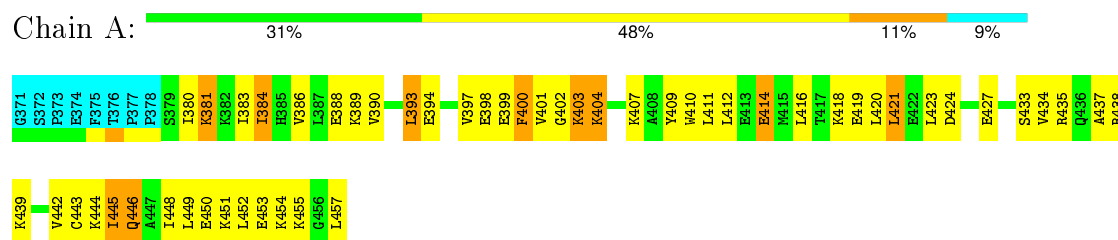
4.2.24 Score per residue for model 24

- 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	642	677	677	38±6
All	All	16050	16925	16925	952

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 29.

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: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:412:LEU:HD23	1:A:452:LEU:HD11	0.89	1.44	5	5
1:A:420:LEU:HD12	1:A:445:ILE:HD12	0.89	1.43	2	1
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:400:PHE:CD1	1:A:412:LEU:HD22	0.84	2.07	7	11
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:413:GLU:CG	1:A:452:LEU:HD13	0.74	2.12	20	1
1:A:423:LEU:HD22	1:A:441:ALA:HB3	0.74	1.59	18	2
1:A:448:ILE:O	1:A:452:LEU:HD12	0.74	1.82	19	3
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:420:LEU:HD22	1:A:423:LEU:HD11	0.72	1.61	17	2
1:A:407:LYS:HA	1:A:410:TRP:CE2	0.72	2.20	6	22
1:A:420:LEU:HD12	1:A:445:ILE:CG2	0.72	2.14	6	2
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
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:397:VAL:HG11	1:A:448:ILE:CG2	0.69	2.18	4	3
1:A:390:VAL:HG22	1:A:419:GLU:CD	0.68	2.08	19	1
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: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:O	1:A:416:LEU:HD13	0.66	1.91	7	2
1:A:420:LEU:CB	1:A:442:VAL:HG13	0.66	2.21	18	1
1:A:386:VAL:HG11	1:A:423:LEU:HB3	0.66	1.65	24	3
1:A:400:PHE:CG	1:A:412:LEU:HD13	0.66	2.25	11	1
1:A:421:LEU:HD22	1:A:421:LEU:C	0.65	2.11	22	2
1:A:400:PHE:CE2	1:A:402:GLY:CA	0.65	2.80	5	1
1:A:420:LEU:HD23	1:A:445:ILE:HG12	0.65	1.69	17	1
1:A:383:ILE:HD11	1:A:434:VAL:HG13	0.65	1.68	25	2
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:423:LEU:HD22	1:A:441:ALA:CB	0.64	2.22	10	4
1:A:421:LEU:C	1:A:421:LEU:HD22	0.64	2.11	9	3
1:A:420:LEU:HA	1:A:423:LEU:HD12	0.64	1.67	4	1
1:A:421:LEU:O	1:A:421:LEU:HD22	0.64	1.93	22	3
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:393:LEU:HD11	1:A:415:MET:CE	0.63	2.22	3	1
1:A:421:LEU:HD22	1:A:421:LEU:O	0.63	1.92	15	2
1:A:412:LEU:O	1:A:416:LEU:HD12	0.63	1.93	1	3
1:A:397:VAL:HG11	1:A:448:ILE:HG22	0.63	1.71	20	5
1:A:393:LEU:HD13	1:A:419:GLU:OE1	0.63	1.94	2	3
1:A:423:LEU:HD22	1:A:441:ALA:HB2	0.62	1.72	10	1
1:A:420:LEU:HD22	1:A:420:LEU:O	0.62	1.95	17	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:HD12	1:A:420:LEU:O	0.62	1.95	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:393:LEU:HD21	1:A:415:MET:HG2	0.61	1.72	21	1
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:445:ILE:HD12	1:A:446:GLN:N	0.61	2.11	23	4
1:A:386:VAL:HG11	1:A:423:LEU:HG	0.61	1.73	23	3
1:A:420:LEU:HD23	1:A:421:LEU:N	0.61	2.10	22	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:400:PHE:CG	1:A:412:LEU:HD23	0.60	2.32	13	1
1:A:393:LEU:HD11	1:A:415:MET:HG2	0.60	1.72	9	1
1:A:400:PHE:CD1	1:A:412:LEU:HD23	0.59	2.31	16	5
1:A:423:LEU:CD1	1:A:442:VAL:HG22	0.59	2.26	6	1
1:A:420:LEU:CG	1:A:445:ILE:HD12	0.59	2.27	2	1
1:A:416:LEU:HD13	1:A:416:LEU:O	0.59	1.98	10	3
1:A:390:VAL:HG22	1:A:419:GLU:CB	0.59	2.28	10	1
1:A:423:LEU:HD22	1:A:438:ARG:HA	0.59	1.74	9	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
1:A:401:VAL:O	1:A:401:VAL:HG22	0.57	1.99	18	4
1:A:420:LEU:HD22	1:A:445:ILE:HD13	0.57	1.76	3	2
1:A:420:LEU:HD21	1:A:442:VAL:CG2	0.57	2.29	1	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:401:VAL:HG22	1:A:401:VAL:O	0.56	2.01	16	4
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:393:LEU:HD13	1:A:419:GLU:CD	0.56	2.21	2	2
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: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:416:LEU:HD12	1:A:445:ILE:CG2	0.55	2.20	19	1
1:A:386:VAL:HG21	1:A:423:LEU:CG	0.55	2.30	18	1
1:A:420:LEU:HG	1:A:445:ILE:HD13	0.55	1.79	17	1
1:A:386:VAL:CG2	1:A:423:LEU:HD11	0.55	2.31	16	1
1:A:413:GLU:CD	1:A:452:LEU:HD22	0.55	2.22	12	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:445:ILE:N	1:A:445:ILE:HD13	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:415:MET:CE	0.54	2.32	2	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:O	1:A:401:VAL:HG12	0.53	2.03	6	4
1:A:420:LEU:O	1:A:420:LEU:HD13	0.53	2.03	12	1
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
1:A:416:LEU:O	1:A:416:LEU:HD12	0.53	2.02	2	2
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:403:LYS:O	1:A:409:TYR:CD1	0.52	2.62	9	2
1:A:416:LEU:CD2	1:A:452:LEU:HD11	0.52	2.34	21	1
1:A:401:VAL:HG12	1:A:401:VAL:O	0.52	2.05	23	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:383:ILE:HG13	1:A:434:VAL:HG13	0.52	1.81	18	1
1:A:397:VAL:HG13	1:A:452:LEU:CD1	0.52	2.34	3	2
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:N	1:A:384:ILE:HD13	0.52	2.19	14	6
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:412:LEU:HD23	1:A:452:LEU:HG	0.51	1.83	17	1
1:A:446:GLN:HA	1:A:449:LEU:HD12	0.51	1.82	14	1
1:A:431:GLN:HB3	1:A:434:VAL:HG23	0.51	1.82	17	3
1:A:420:LEU:C	1:A:420:LEU:HD13	0.51	2.26	23	5
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:416:LEU:C	1:A:416:LEU:HD12	0.51	2.26	9	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:393:LEU:HD21	1:A:415:MET:CE	0.51	2.36	12	1
1:A:384:ILE:HD13	1:A:384:ILE:N	0.50	2.21	1	8
1:A:411:LEU:HD11	1:A:415:MET:CE	0.50	2.36	7	1
1:A:400:PHE:CE2	1:A:402:GLY:HA3	0.50	2.41	5	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:399:GLU:O	1:A:401:VAL:N	0.50	2.44	9	2
1:A:417:THR:HA	1:A:420:LEU:HD23	0.50	1.81	16	1
1:A:399:GLU:O	1:A:400:PHE:C	0.50	2.50	4	8
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:420:LEU:C	1:A:420:LEU:HD12	0.50	2.27	21	4
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: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:O	1:A:420:LEU:HD23	0.49	2.06	6	1
1:A:445:ILE:HG22	1:A:449:LEU:HD12	0.49	1.84	1	1
1:A:406:ASP:OD2	1:A:408:ALA:HB3	0.49	2.07	22	2
1:A:445:ILE:CG2	1:A:449:LEU:HD12	0.49	2.38	1	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:420:LEU:HD23	1:A:420:LEU:C	0.49	2.28	6	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:420:LEU:HD12	1:A:420:LEU:C	0.49	2.29	15	2
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:416:LEU:HD13	1:A:416:LEU:C	0.48	2.29	24	2
1:A:420:LEU:HD11	1:A:445:ILE:CD1	0.48	2.21	7	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:400:PHE:CE2	1:A:402:GLY:HA2	0.48	2.43	5	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:423:LEU:C	1:A:423:LEU:HD12	0.48	2.29	19	1
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:420:LEU:HD23	1:A:445:ILE:HD13	0.47	1.85	18	1
1:A:416:LEU:HD12	1:A:449:LEU:HD12	0.47	1.87	18	1
1:A:441:ALA:O	1:A:445:ILE:HD13	0.47	2.09	22	1
1:A:401:VAL:O	1:A:402:GLY:O	0.47	2.32	5	3
1:A:383:ILE:CG2	1:A:384:ILE:HD13	0.47	2.39	20	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: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:CD2	1:A:421:LEU:C	0.46	2.84	18	1
1:A:400:PHE:CG	1:A:412:LEU:CD2	0.46	2.98	13	5
1:A:403:LYS:O	1:A:409:TYR:HB3	0.46	2.10	12	4
1:A:380:ILE:HD12	1:A:380:ILE:N	0.46	2.26	10	2
1:A:443:CYS:HA	1:A:446:GLN:HG3	0.46	1.86	25	2
1:A:407:LYS:CD	1:A:410:TRP:CH2	0.46	2.99	16	2
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:HB2	1:A:410:TRP:CZ2	0.46	2.45	9	4
1:A:407:LYS:CG	1:A:410:TRP:CH2	0.46	2.98	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:423:LEU:HD12	1:A:423:LEU:C	0.46	2.31	24	1
1:A:410:TRP:CZ3	1:A:411:LEU:HD12	0.45	2.45	22	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:407:LYS:CB	1:A:410:TRP:CZ2	0.45	2.99	17	4
1:A:442:VAL:HA	1:A:445:ILE:HD11	0.45	1.87	2	1
1:A:393:LEU:O	1:A:393:LEU:HD23	0.45	2.12	7	1
1:A:397:VAL:HG11	1:A:448:ILE:HG23	0.45	1.86	4	1
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:416:LEU:HD12	1:A:416:LEU:C	0.45	2.32	21	2
1:A:393:LEU:HD11	1:A:415:MET:HE1	0.45	1.88	3	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:421:LEU:C	1:A:421:LEU:CD2	0.45	2.84	14	2
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:420:LEU:HD13	1:A:420:LEU:O	0.44	2.12	5	1
1:A:403:LYS:HG2	1:A:406:ASP:HB2	0.44	1.90	24	2
1:A:393:LEU:HD13	1:A:416:LEU:HB3	0.44	1.89	8	1
1:A:400:PHE:CD1	1:A:412:LEU:CD1	0.44	3.00	11	1
1:A:404:LYS:O	1:A:409:TYR:CD2	0.44	2.70	10	2
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:400:PHE:CG	1:A:412:LEU:CD1	0.44	2.98	11	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:380:ILE:N	1:A:380:ILE:HD12	0.44	2.28	18	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:CD	1:A:403:LYS:N	0.43	2.81	2	1
1:A:423:LEU:HD11	1:A:442:VAL:HG22	0.43	1.88	6	1
1:A:427:GLU:O	1:A:428:THR:HG22	0.43	2.12	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:420:LEU:HD23	1:A:420:LEU:O	0.43	2.13	7	1
1:A:380:ILE:HD12	1:A:380:ILE:H	0.43	1.74	25	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:412:LEU:CD1	1:A:452:LEU:HD13	0.43	2.42	22	1
1:A:413:GLU:OE2	1:A:449:LEU:HD23	0.43	2.14	19	1
1:A:390:VAL:HG11	1:A:445:ILE:CD1	0.43	2.44	25	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:412:LEU:HD13	1:A:412:LEU:O	0.43	2.12	13	1
1:A:390:VAL:CG1	1:A:445:ILE:CD1	0.43	2.97	15	1
1:A:380:ILE:HD13	1:A:383:ILE:HD12	0.43	1.91	13	3
1:A:419:GLU:HG3	1:A:420:LEU:N	0.43	2.29	6	2
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:417:THR:O	1:A:421:LEU:HD13	0.42	2.15	24	1
1:A:416:LEU:CD1	1:A:445:ILE:HD13	0.42	2.44	18	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:423:LEU:HG	1:A:441:ALA:HB3	0.42	1.91	22	1
1:A:412:LEU:HD13	1:A:415:MET:CE	0.42	2.45	24	1
1:A:393:LEU:HD13	1:A:416:LEU:CB	0.42	2.45	8	1
1:A:412:LEU:CD2	1:A:452:LEU:HD21	0.42	2.35	7	1
1:A:445:ILE:HD12	1:A:445:ILE:C	0.42	2.35	23	1
1:A:445:ILE:HG22	1:A:449:LEU:CD1	0.42	2.44	20	1
1:A:402:GLY:O	1:A:455:LYS:O	0.42	2.37	5	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:404:LYS:HA	1:A:409:TYR:CD2	0.42	2.49	8	2
1:A:421:LEU:HD13	1:A:421:LEU:C	0.42	2.33	15	2
1:A:400:PHE:CD1	1:A:400:PHE:C	0.41	2.94	24	2
1:A:383:ILE:CD1	1:A:438:ARG:CZ	0.41	2.98	24	1
1:A:385:HIS:CG	1:A:386:VAL:N	0.41	2.88	18	1
1:A:411:LEU:O	1:A:415:MET:HG2	0.41	2.14	11	1
1:A:408:ALA:O	1:A:412:LEU:N	0.41	2.51	5	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:416:LEU:CD2	1:A:452:LEU:CD1	0.41	2.99	21	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: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:392:TYR:O	1:A:395:GLN:CG	0.41	2.69	11	1
1:A:383:ILE:CG2	1:A:437:ALA:CB	0.41	2.99	22	1
1:A:404:LYS:O	1:A:409:TYR:CE2	0.41	2.74	10	2
1:A:383:ILE:HD11	1:A:434:VAL:CG1	0.41	2.45	18	1
1:A:380:ILE:N	1:A:380:ILE:HD13	0.41	2.31	11	1
1:A:383:ILE:HD12	1:A:434:VAL:HG13	0.41	1.92	22	1
1:A:416:LEU:O	1:A:419:GLU:CG	0.41	2.69	1	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:409:TYR:CE2	1:A:457:LEU:O	0.41	2.74	5	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:431:GLN:O	1:A:434:VAL:HG12	0.40	2.16	21	1
1:A:405:THR:O	1:A:405:THR:HG22	0.40	2.15	11	1
1:A:413:GLU:CG	1:A:449:LEU:CD2	0.40	2.99	22	1
1:A:383:ILE:CD1	1:A:434:VAL:HG13	0.40	2.46	8	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:413:GLU:OE1	1:A:452:LEU:HD22	0.40	2.15	12	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: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%)	12	51
All	All	1950/2175 (90%)	1806 (93%)	99 (5%)	45 (2%)	12	51

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	430	GLY	4
1	A	428	THR	4
1	A	429	GLY	3
1	A	456	GLY	3
1	A	401	VAL	2
1	A	431	GLN	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%)	46±3 (65±5%)	25±3 (35±5%)	1	10
All	All	1775/1950 (91%)	1160 (65%)	615 (35%)	1	10

All 61 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	21
1	A	389	LYS	20
1	A	455	LYS	18
1	A	444	LYS	18
1	A	457	LEU	18
1	A	393	LEU	17
1	A	414	GLU	17
1	A	418	LYS	16
1	A	450	GLU	16
1	A	435	ARG	15
1	A	449	LEU	15
1	A	452	LEU	15
1	A	412	LEU	14

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Mol	Chain	Res	Type	Models (Total)
1	A	451	LYS	14
1	A	446	GLN	14
1	A	438	ARG	13
1	A	410	TRP	12
1	A	454	LYS	12
1	A	407	LYS	12
1	A	381	LYS	11
1	A	391	GLN	11
1	A	392	TYR	11
1	A	405	THR	11
1	A	422	GLU	11
1	A	439	LYS	11
1	A	395	GLN	10
1	A	420	LEU	10
1	A	453	GLU	10
1	A	431	GLN	10
1	A	432	ASP	9
1	A	387	LEU	9
1	A	427	GLU	8
1	A	394	GLU	8
1	A	423	LEU	8
1	A	436	GLN	8
1	A	379	SER	8
1	A	433	SER	8
1	A	388	GLU	8
1	A	421	LEU	7
1	A	424	ASP	7
1	A	443	CYS	7
1	A	413	GLU	7
1	A	398	GLU	6
1	A	440	GLU	6
1	A	385	HIS	6
1	A	382	LYS	5
1	A	419	GLU	5
1	A	406	ASP	5
1	A	417	THR	4
1	A	400	PHE	4
1	A	396	GLU	4
1	A	445	ILE	3
1	A	416	LEU	3
1	A	425	SER	3
1	A	428	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	411	LEU	2
1	A	409	TYR	1
1	A	415	MET	1
1	A	383	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided