



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:27 pm BST

PDB ID : 2K6Q
Title : LC3 p62 complex structure
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Deposited on : 2008-07-17

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 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

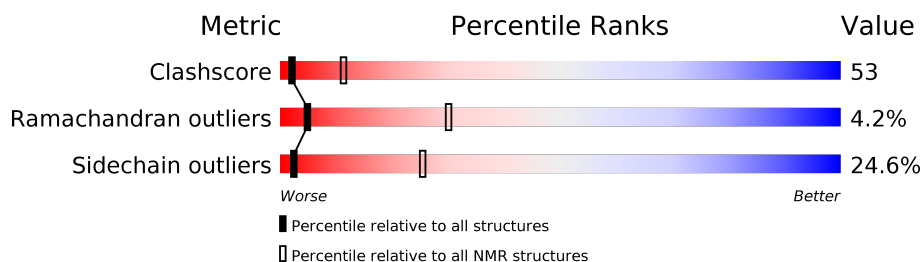
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	121	
2	B	17	

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:13-A:118, B:337-B:347 (117)	0.28	4

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2258 atoms, of which 1127 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Microtubule-associated proteins 1A/1B light chain 3B.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			2014	636	1013	176	185	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q62625

- Molecule 2 is a protein called p62_peptide from Sequestosome-1.

Mol	Chain	Residues	Atoms						Trace
2	B	17	Total	C	H	N	O	S	0
			244	77	114	21	31	1	

There is a discrepancy between the modelled and reference sequences:

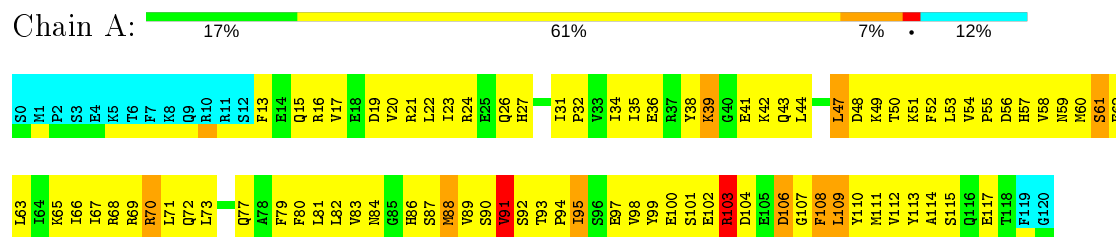
Chain	Residue	Modelled	Actual	Comment	Reference
B	331	MET	-	expression tag	UNP O08623

4 Residue-property plots

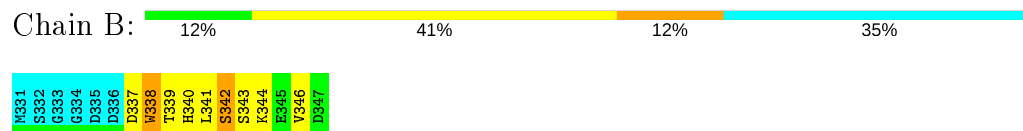
4.1 Average score per residue in the NMR ensemble

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: Microtubule-associated proteins 1A/1B light chain 3B



- Molecule 2: p62_peptide from Sequestosome-1

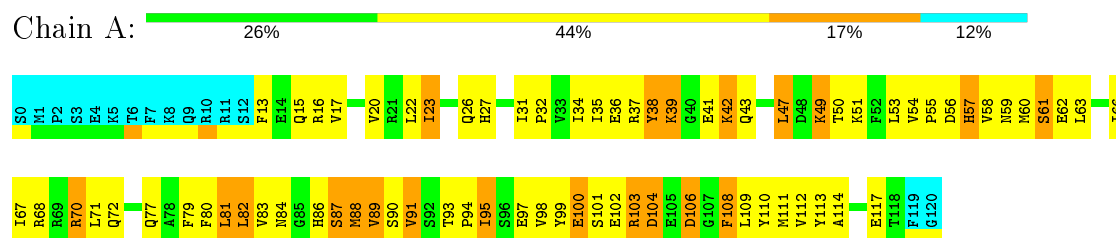


4.2 Scores per residue for each member of the ensemble

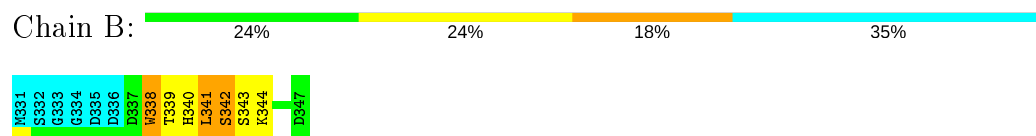
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

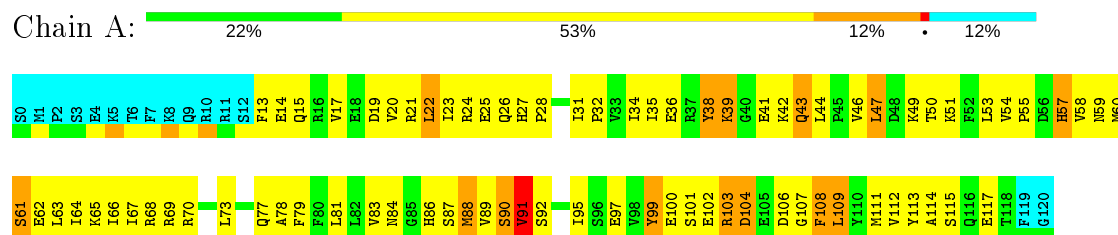


- Molecule 2: p62_peptide from Sequestosome-1

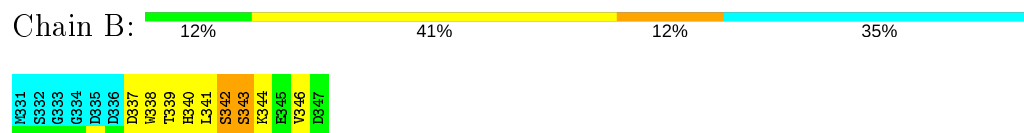


4.2.2 Score per residue for model 2

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

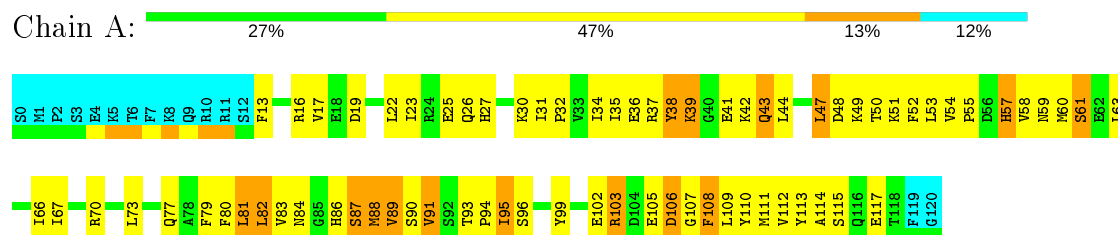


- Molecule 2: p62_peptide from Sequestosome-1

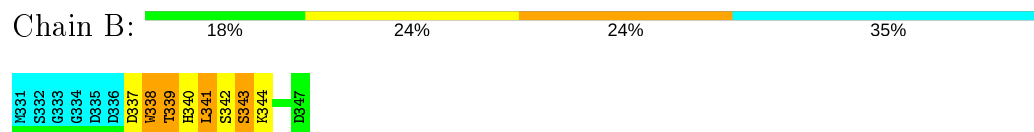


4.2.3 Score per residue for model 3

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

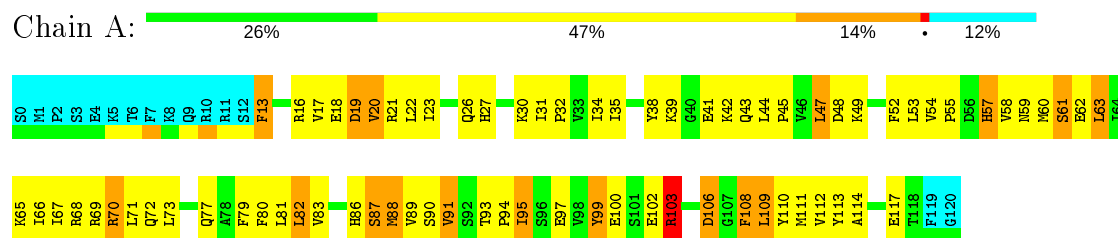


- Molecule 2: p62_peptide from Sequestosome-1

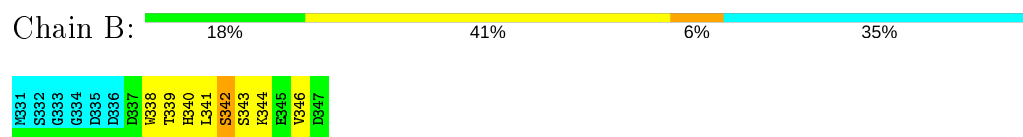


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

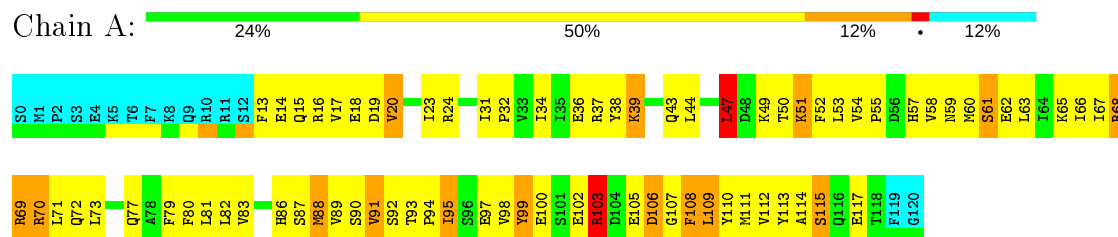


- Molecule 2: p62_peptide from Sequestosome-1

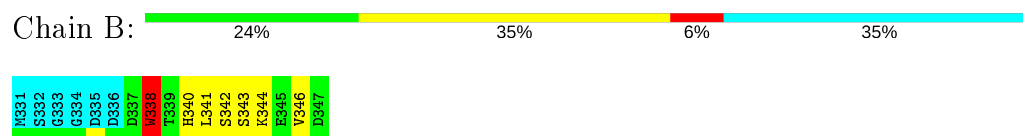


4.2.5 Score per residue for model 5

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

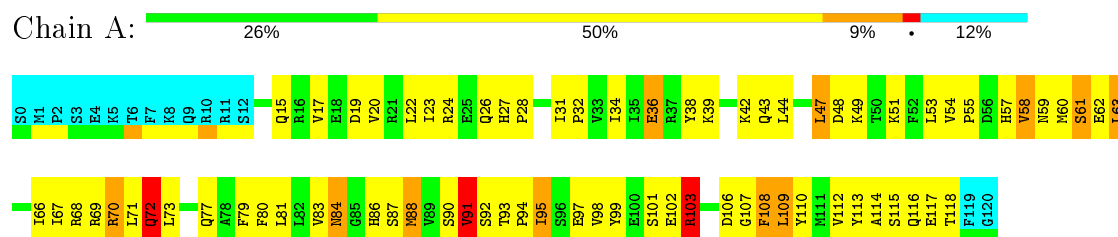


- Molecule 2: p62_peptide from Sequestosome-1

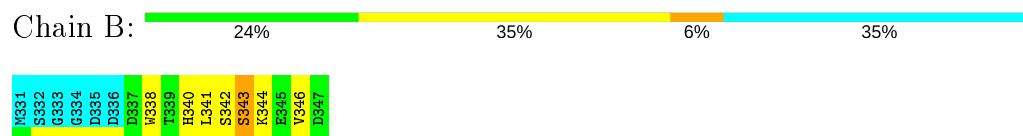


4.2.6 Score per residue for model 6

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

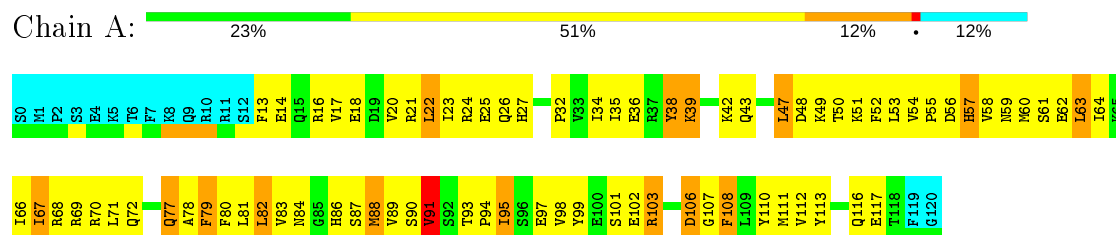


- Molecule 2: p62_peptide from Sequestosome-1

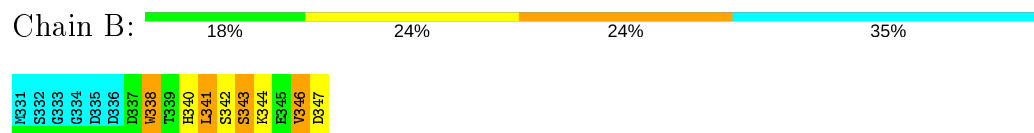


4.2.7 Score per residue for model 7

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

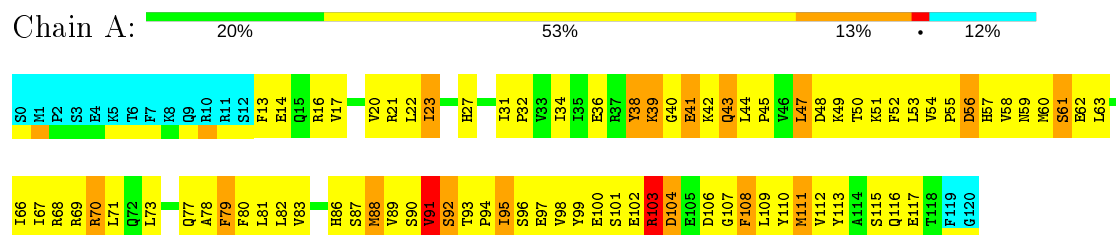


- Molecule 2: p62_peptide from Sequestosome-1

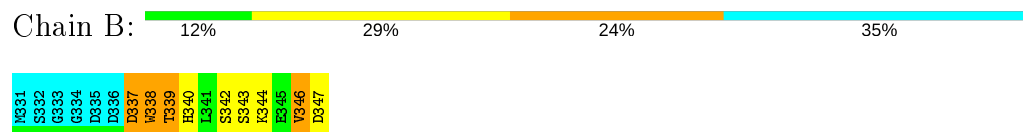


4.2.8 Score per residue for model 8

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

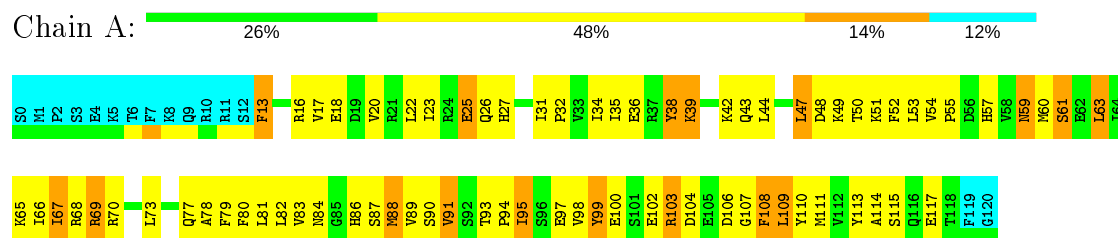


- Molecule 2: p62_peptide from Sequestosome-1



4.2.9 Score per residue for model 9

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

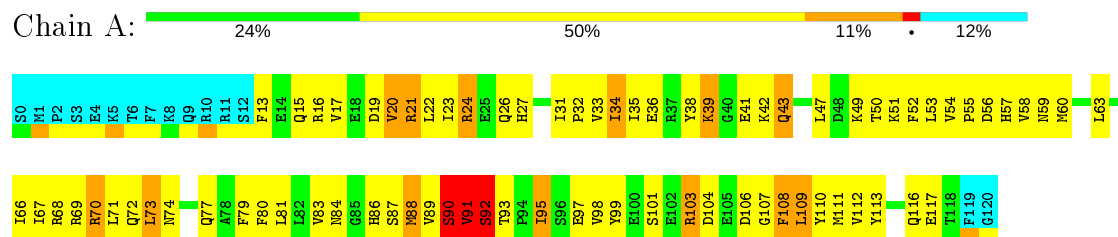


- Molecule 2: p62_peptide from Sequestosome-1

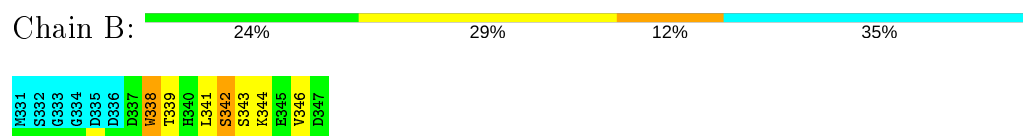


4.2.10 Score per residue for model 10

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

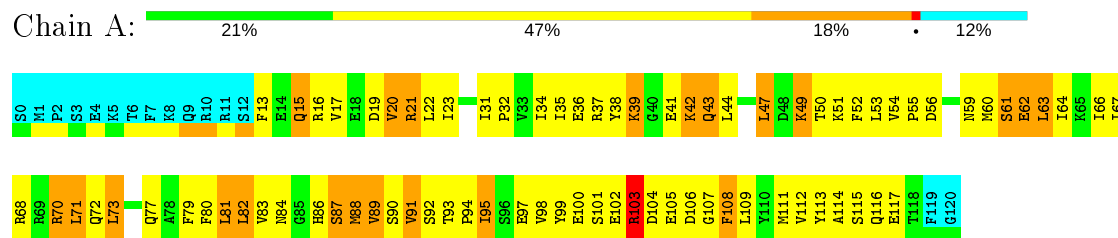


- Molecule 2: p62_peptide from Sequestosome-1

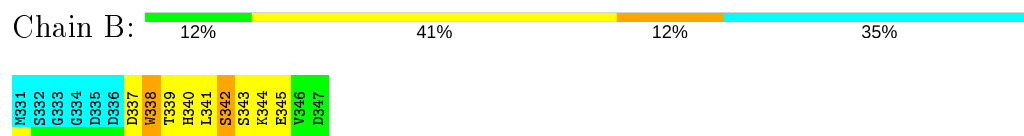


4.2.11 Score per residue for model 11

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

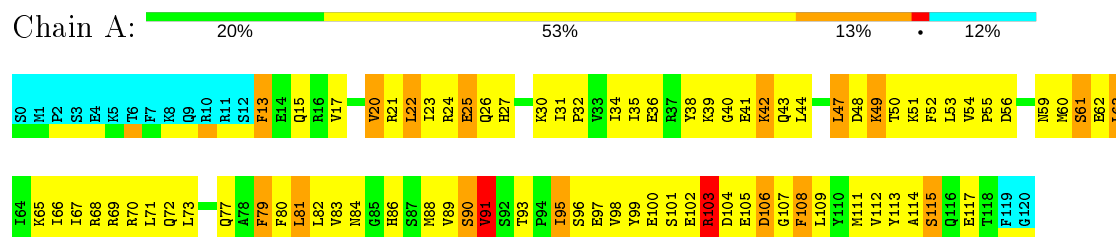


- Molecule 2: p62_peptide from Sequestosome-1



4.2.12 Score per residue for model 12

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

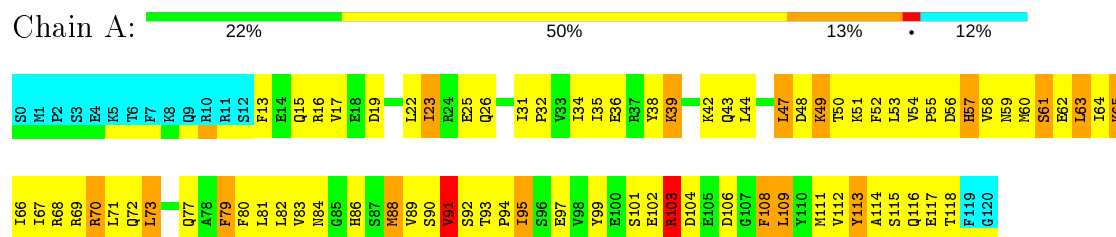


- Molecule 2: p62_peptide from Sequestosome-1



4.2.13 Score per residue for model 13

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

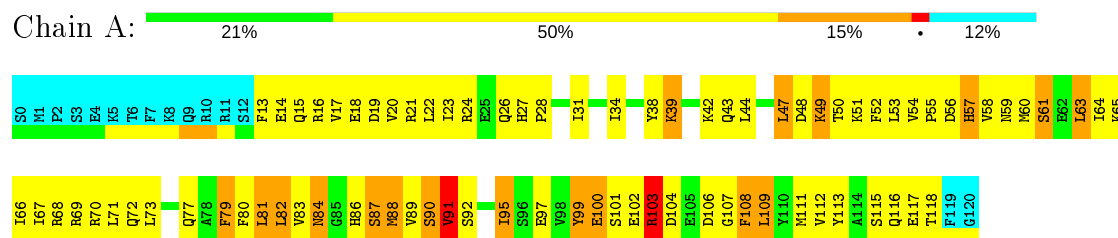


- Molecule 2: p62_peptide from Sequestosome-1

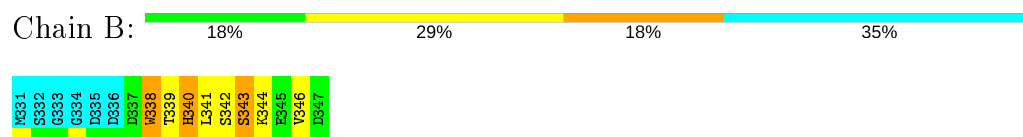


4.2.14 Score per residue for model 14

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

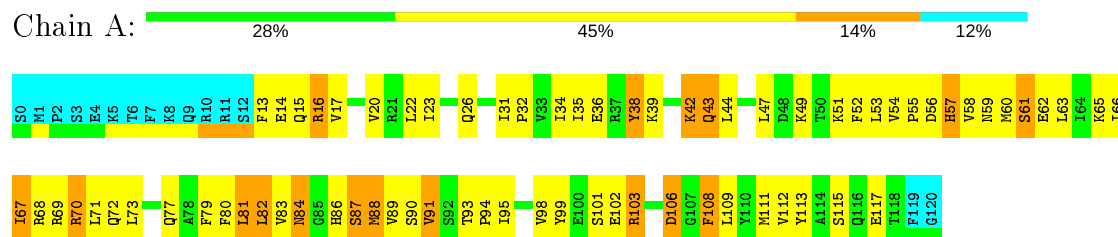


- Molecule 2: p62_peptide from Sequestosome-1



4.2.15 Score per residue for model 15

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

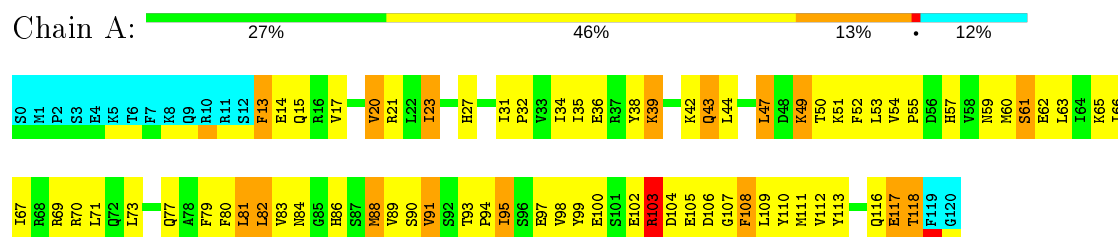


- Molecule 2: p62_peptide from Sequestosome-1

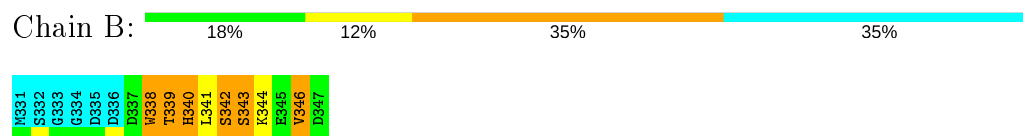


4.2.16 Score per residue for model 16

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

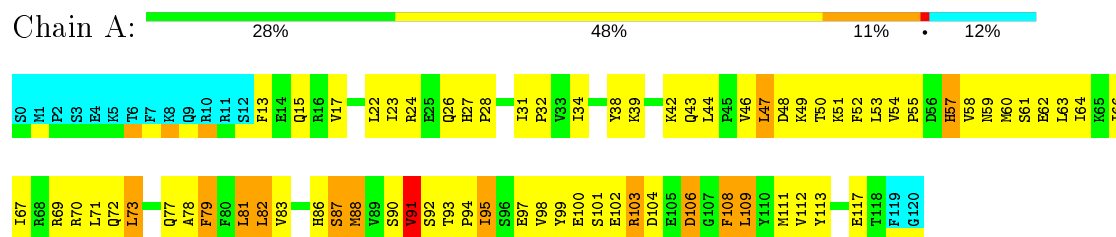


- Molecule 2: p62_peptide from Sequestosome-1

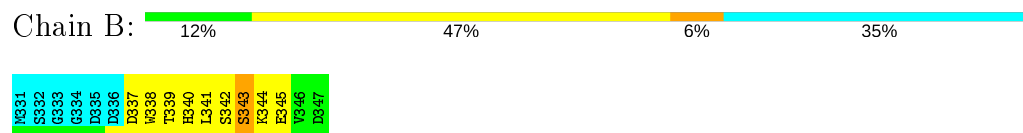


4.2.17 Score per residue for model 17

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

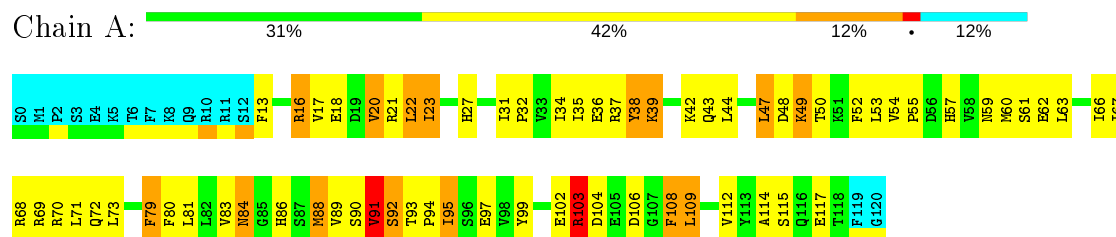


- Molecule 2: p62_peptide from Sequestosome-1

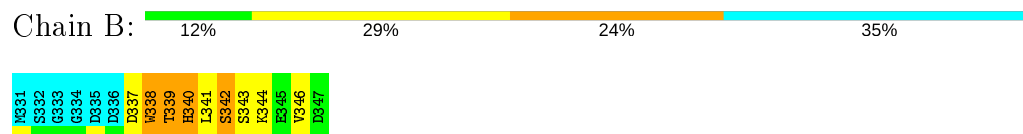


4.2.18 Score per residue for model 18

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

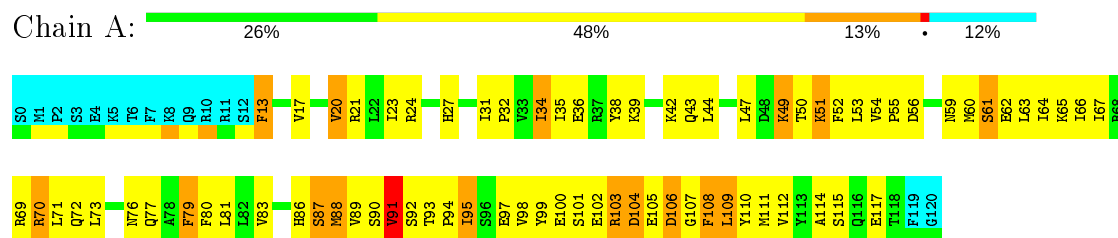


- Molecule 2: p62_peptide from Sequestosome-1



4.2.19 Score per residue for model 19

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B

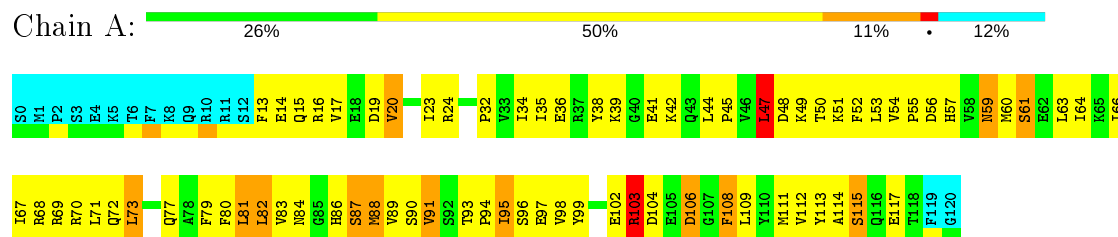


- Molecule 2: p62_peptide from Sequestosome-1

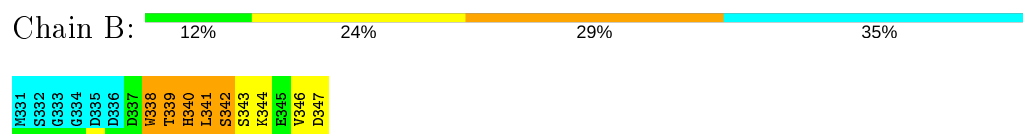


4.2.20 Score per residue for model 20

- Molecule 1: Microtubule-associated proteins 1A/1B light chain 3B



- Molecule 2: p62_peptide from Sequestosome-1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Sparky	refinement	3.110
CYANA	structure solution	2.1
CYANA	refinement	2.1

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1776
Number of shifts mapped to atoms	1776
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	877	890	888	99±9
2	B	92	83	81	21±4
All	All	19380	19460	19380	2047

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 53.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD22	1:A:71:LEU:HD21	1.03	1.28	16	8
1:A:35:ILE:HD13	1:A:67:ILE:HD11	0.99	1.34	18	10
1:A:63:LEU:HD22	1:A:63:LEU:O	0.95	1.60	13	1
1:A:13:PHE:O	1:A:17:VAL:HG13	0.94	1.63	16	5
1:A:66:ILE:HG21	2:B:341:LEU:HD13	0.90	1.39	20	8
1:A:17:VAL:HG12	1:A:106:ASP:CB	0.90	1.96	2	5
1:A:20:VAL:HG21	1:A:107:GLY:O	0.88	1.67	11	6
1:A:13:PHE:O	1:A:17:VAL:HG23	0.88	1.68	10	7
1:A:64:ILE:HG23	1:A:79:PHE:CE2	0.87	2.03	17	1
1:A:66:ILE:CG2	2:B:341:LEU:HD13	0.87	1.99	20	8
1:A:17:VAL:HG23	1:A:106:ASP:O	0.86	1.69	8	3
1:A:57:HIS:ND1	1:A:58:VAL:HG13	0.85	1.85	13	11
1:A:63:LEU:HD12	1:A:95:ILE:HD11	0.85	1.48	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HD11	1:A:63:LEU:HD11	0.84	1.47	19	3
1:A:34:ILE:HG22	1:A:36:GLU:OE1	0.83	1.70	12	1
1:A:23:ILE:HD13	2:B:338:TRP:CE2	0.82	2.09	11	17
1:A:17:VAL:HG12	1:A:106:ASP:HB3	0.81	1.52	19	4
1:A:82:LEU:HD21	1:A:116:GLN:O	0.80	1.76	13	2
1:A:23:ILE:HG12	1:A:53:LEU:HD21	0.80	1.52	11	8
1:A:108:PHE:CE1	2:B:338:TRP:CH2	0.79	2.70	4	20
1:A:20:VAL:HG11	1:A:107:GLY:O	0.79	1.76	8	1
1:A:108:PHE:CZ	2:B:338:TRP:CH2	0.79	2.70	8	19
1:A:83:VAL:HG22	1:A:111:MET:SD	0.79	2.17	13	12
1:A:36:GLU:OE1	1:A:112:VAL:HG22	0.79	1.77	6	1
1:A:17:VAL:HG22	1:A:106:ASP:HA	0.78	1.53	18	8
1:A:66:ILE:HG21	2:B:341:LEU:HB3	0.78	1.54	16	7
1:A:63:LEU:HD12	1:A:95:ILE:CD1	0.78	2.09	18	6
1:A:23:ILE:HD13	2:B:338:TRP:NE1	0.77	1.95	15	20
1:A:34:ILE:HG23	1:A:50:THR:HG22	0.76	1.56	12	4
1:A:61:SER:HA	1:A:64:ILE:HD12	0.76	1.56	14	4
1:A:23:ILE:CG1	1:A:53:LEU:HD21	0.76	2.10	12	9
1:A:35:ILE:CD1	1:A:67:ILE:HD11	0.75	2.10	16	10
2:B:343:SER:O	2:B:346:VAL:HG22	0.75	1.82	12	11
1:A:35:ILE:HD13	1:A:67:ILE:CD1	0.75	2.11	16	8
1:A:31:ILE:HG23	1:A:99:TYR:CD2	0.74	2.17	17	11
2:B:341:LEU:N	2:B:341:LEU:HD23	0.74	1.97	15	4
1:A:20:VAL:HG23	1:A:108:PHE:CE2	0.73	2.19	9	3
1:A:66:ILE:HD13	2:B:346:VAL:CG1	0.73	2.14	6	9
1:A:63:LEU:HD22	1:A:63:LEU:C	0.72	2.04	13	1
1:A:27:HIS:CG	1:A:53:LEU:HD13	0.71	2.20	17	7
1:A:57:HIS:CE1	1:A:58:VAL:HG13	0.71	2.21	13	9
1:A:67:ILE:CG2	1:A:79:PHE:CZ	0.71	2.74	11	15
1:A:67:ILE:HG21	1:A:79:PHE:CZ	0.71	2.21	19	12
1:A:73:LEU:HD22	1:A:77:GLN:HG2	0.70	1.63	19	15
1:A:63:LEU:HD23	2:B:341:LEU:HD12	0.70	1.62	11	2
1:A:99:TYR:CD2	1:A:109:LEU:HD23	0.70	2.21	18	9
1:A:13:PHE:O	1:A:17:VAL:HG12	0.69	1.87	14	4
1:A:54:VAL:HG11	1:A:95:ILE:HD13	0.69	1.63	19	13
1:A:35:ILE:O	1:A:50:THR:HG23	0.69	1.88	7	7
1:A:63:LEU:HD13	1:A:63:LEU:C	0.68	2.09	14	1
1:A:63:LEU:HD13	1:A:64:ILE:HD13	0.68	1.65	13	1
1:A:35:ILE:CD1	1:A:63:LEU:HD11	0.67	2.20	19	1
2:B:339:THR:HG23	2:B:340:HIS:N	0.67	2.04	16	3
1:A:34:ILE:HD11	1:A:108:PHE:CZ	0.67	2.24	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:HD23	1:A:63:LEU:O	0.66	1.89	18	2
1:A:16:ARG:NH2	1:A:34:ILE:HG21	0.66	2.04	9	1
1:A:16:ARG:CZ	1:A:108:PHE:CD2	0.66	2.79	18	1
1:A:16:ARG:NH2	1:A:110:TYR:CE1	0.66	2.64	9	2
1:A:93:THR:HG22	1:A:98:VAL:HG23	0.66	1.66	15	11
1:A:67:ILE:HG21	1:A:79:PHE:CE1	0.66	2.26	1	10
1:A:35:ILE:HD12	1:A:81:LEU:HD11	0.66	1.66	3	2
1:A:17:VAL:HG22	1:A:106:ASP:CB	0.65	2.21	13	1
1:A:16:ARG:NH1	1:A:108:PHE:CD2	0.65	2.64	18	1
1:A:82:LEU:HD22	1:A:82:LEU:N	0.65	2.06	20	7
1:A:47:LEU:HD22	1:A:71:LEU:CD2	0.65	2.15	16	4
1:A:89:VAL:HG12	1:A:117:GLU:OE2	0.64	1.93	5	2
1:A:57:HIS:CE1	1:A:58:VAL:CG1	0.64	2.81	13	6
1:A:106:ASP:C	1:A:106:ASP:OD1	0.64	2.37	15	1
1:A:93:THR:CG2	1:A:98:VAL:HG23	0.64	2.23	1	10
1:A:16:ARG:NH1	1:A:110:TYR:CE1	0.63	2.67	5	1
1:A:73:LEU:HD13	1:A:77:GLN:OE1	0.63	1.94	17	2
1:A:83:VAL:O	1:A:86:HIS:CE1	0.62	2.53	6	19
1:A:41:GLU:CD	1:A:114:ALA:HB1	0.62	2.14	1	1
1:A:108:PHE:CZ	2:B:338:TRP:CZ3	0.61	2.87	11	4
1:A:15:GLN:HB3	1:A:16:ARG:HH21	0.61	1.56	14	1
1:A:20:VAL:HG23	1:A:108:PHE:CD2	0.61	2.30	9	7
1:A:63:LEU:O	1:A:63:LEU:HD23	0.61	1.96	3	5
1:A:20:VAL:CG2	1:A:108:PHE:CD2	0.61	2.84	15	2
1:A:82:LEU:N	1:A:82:LEU:HD22	0.61	2.11	4	5
1:A:83:VAL:HG11	1:A:102:GLU:OE1	0.61	1.94	16	1
1:A:80:PHE:CD1	1:A:117:GLU:OE1	0.60	2.54	13	3
1:A:66:ILE:HG21	2:B:341:LEU:HD22	0.60	1.73	19	3
1:A:113:TYR:CD1	1:A:113:TYR:C	0.60	2.74	13	6
1:A:31:ILE:CG2	1:A:99:TYR:CG	0.60	2.85	11	7
1:A:38:TYR:CE1	1:A:39:LYS:O	0.60	2.55	15	18
1:A:83:VAL:O	1:A:86:HIS:CD2	0.60	2.54	6	16
1:A:52:PHE:HA	2:B:339:THR:HG22	0.60	1.71	20	7
1:A:60:MET:CE	1:A:83:VAL:HG21	0.60	2.27	8	5
1:A:27:HIS:CG	1:A:53:LEU:CD1	0.60	2.84	3	10
1:A:31:ILE:O	1:A:54:VAL:HG12	0.60	1.97	3	6
1:A:31:ILE:HG23	1:A:99:TYR:CG	0.59	2.32	13	12
1:A:108:PHE:CZ	2:B:338:TRP:CZ2	0.59	2.90	20	3
1:A:54:VAL:HG23	1:A:55:PRO:HD2	0.59	1.74	18	6
2:B:341:LEU:N	2:B:341:LEU:CD2	0.59	2.65	3	3
1:A:82:LEU:N	1:A:82:LEU:CD2	0.59	2.66	16	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:CG2	1:A:99:TYR:CD2	0.59	2.86	5	9
1:A:13:PHE:CE1	1:A:106:ASP:OD2	0.59	2.55	5	1
1:A:108:PHE:CE1	2:B:338:TRP:CZ3	0.59	2.90	11	14
1:A:63:LEU:CD2	2:B:341:LEU:CD1	0.59	2.80	14	2
1:A:38:TYR:HB3	1:A:114:ALA:HB2	0.59	1.72	20	3
1:A:108:PHE:O	1:A:110:TYR:CE2	0.59	2.56	6	5
1:A:64:ILE:HG22	1:A:68:ARG:HH21	0.59	1.58	13	1
1:A:16:ARG:NH1	1:A:108:PHE:CE2	0.59	2.71	18	1
1:A:79:PHE:C	1:A:79:PHE:CD1	0.58	2.77	7	3
1:A:91:VAL:HG22	1:A:92:SER:N	0.58	2.13	18	2
1:A:99:TYR:HA	1:A:109:LEU:HD21	0.58	1.75	17	11
1:A:61:SER:CB	1:A:91:VAL:HG21	0.58	2.28	11	13
1:A:60:MET:HG3	1:A:91:VAL:HG23	0.58	1.73	17	17
1:A:117:GLU:O	1:A:117:GLU:CG	0.58	2.51	20	10
1:A:52:PHE:HB3	2:B:341:LEU:HD11	0.58	1.74	10	6
1:A:109:LEU:HD13	1:A:111:MET:CE	0.58	2.29	15	2
1:A:23:ILE:HD13	2:B:338:TRP:CD1	0.58	2.34	15	12
1:A:117:GLU:CG	1:A:117:GLU:O	0.58	2.52	2	9
1:A:27:HIS:CD2	1:A:53:LEU:CD1	0.58	2.86	17	1
1:A:83:VAL:HG12	1:A:86:HIS:CE1	0.58	2.34	19	12
2:B:341:LEU:CD2	2:B:341:LEU:N	0.58	2.67	20	3
1:A:44:LEU:HD11	1:A:115:SER:N	0.58	2.13	14	6
1:A:41:GLU:OE1	1:A:113:TYR:CE1	0.57	2.57	12	1
1:A:16:ARG:HH21	1:A:106:ASP:HB2	0.57	1.58	18	1
1:A:91:VAL:HG22	1:A:91:VAL:O	0.57	1.97	4	7
1:A:113:TYR:C	1:A:113:TYR:CD1	0.57	2.77	8	10
1:A:57:HIS:CD2	1:A:57:HIS:O	0.57	2.57	10	3
1:A:91:VAL:O	1:A:91:VAL:HG22	0.57	1.97	15	5
1:A:67:ILE:HG22	1:A:79:PHE:CZ	0.57	2.34	8	8
1:A:26:GLN:O	1:A:27:HIS:CD2	0.57	2.57	17	2
1:A:102:GLU:HB2	1:A:109:LEU:HD21	0.57	1.77	11	5
2:B:338:TRP:N	2:B:338:TRP:CD1	0.57	2.73	12	12
1:A:93:THR:HG23	1:A:94:PRO:HD2	0.57	1.75	1	12
1:A:66:ILE:HG21	2:B:341:LEU:CD1	0.57	2.27	7	5
1:A:44:LEU:CD2	1:A:73:LEU:CD1	0.56	2.83	5	3
1:A:63:LEU:CD1	1:A:64:ILE:HD13	0.56	2.29	13	1
1:A:36:GLU:OE1	1:A:50:THR:HG23	0.56	2.00	19	2
1:A:83:VAL:O	1:A:86:HIS:CG	0.56	2.59	6	13
1:A:54:VAL:HG22	2:B:341:LEU:HD12	0.56	1.77	4	2
1:A:82:LEU:CD2	1:A:82:LEU:N	0.56	2.69	3	2
1:A:34:ILE:HG22	1:A:36:GLU:OE2	0.56	2.01	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:LEU:CD2	2:B:338:TRP:CE3	0.56	2.89	8	12
1:A:44:LEU:HD21	1:A:77:GLN:OE1	0.56	2.01	17	2
1:A:99:TYR:CD1	1:A:99:TYR:C	0.55	2.80	9	5
1:A:44:LEU:CD1	1:A:115:SER:N	0.55	2.69	2	10
1:A:47:LEU:HD22	1:A:71:LEU:CG	0.55	2.32	7	1
1:A:63:LEU:CD1	1:A:81:LEU:HD23	0.55	2.31	14	1
1:A:67:ILE:CG2	1:A:79:PHE:CE1	0.55	2.90	18	14
1:A:66:ILE:HG21	2:B:341:LEU:CB	0.55	2.31	4	7
1:A:16:ARG:NH2	1:A:34:ILE:CG2	0.54	2.70	9	1
1:A:26:GLN:O	1:A:27:HIS:CG	0.54	2.60	17	2
1:A:89:VAL:O	1:A:90:SER:CB	0.54	2.55	14	6
1:A:34:ILE:CG2	1:A:36:GLU:OE1	0.54	2.56	10	3
1:A:80:PHE:CG	1:A:117:GLU:CB	0.54	2.91	13	5
1:A:66:ILE:CG2	2:B:341:LEU:HD22	0.54	2.33	5	4
1:A:60:MET:HA	1:A:95:ILE:HD12	0.54	1.79	19	2
1:A:80:PHE:CD1	1:A:117:GLU:CB	0.54	2.90	13	2
1:A:63:LEU:HD23	2:B:341:LEU:CD1	0.54	2.32	11	2
1:A:32:PRO:HB3	2:B:338:TRP:CH2	0.54	2.38	8	16
1:A:38:TYR:CA	1:A:112:VAL:HG13	0.54	2.32	12	8
1:A:64:ILE:HG23	1:A:79:PHE:CE1	0.54	2.37	19	3
1:A:44:LEU:HD11	1:A:79:PHE:HA	0.54	1.78	17	1
1:A:38:TYR:C	1:A:38:TYR:CD1	0.54	2.81	18	9
1:A:23:ILE:CD1	2:B:338:TRP:CE2	0.54	2.90	5	8
1:A:44:LEU:HD12	1:A:114:ALA:C	0.54	2.22	4	2
1:A:71:LEU:O	1:A:72:GLN:C	0.54	2.46	6	5
1:A:66:ILE:HD13	2:B:346:VAL:HG13	0.54	1.78	6	1
1:A:64:ILE:HG23	1:A:79:PHE:HE1	0.54	1.61	14	3
1:A:61:SER:CB	1:A:91:VAL:HG11	0.54	2.33	12	1
1:A:44:LEU:HD21	1:A:77:GLN:NE2	0.54	2.18	16	1
1:A:20:VAL:HG13	1:A:108:PHE:CD2	0.53	2.38	8	1
1:A:36:GLU:CD	1:A:112:VAL:HG22	0.53	2.22	6	1
1:A:20:VAL:CG1	1:A:108:PHE:CD2	0.53	2.92	8	1
1:A:44:LEU:HD22	1:A:73:LEU:HD11	0.53	1.80	3	2
1:A:89:VAL:HG22	1:A:117:GLU:OE2	0.53	2.03	9	1
1:A:47:LEU:HD22	1:A:71:LEU:HG	0.53	1.80	7	2
1:A:66:ILE:HD13	2:B:346:VAL:HG11	0.53	1.80	15	1
1:A:69:ARG:HH21	2:B:347:ASP:CB	0.53	2.17	13	1
1:A:86:HIS:CE1	1:A:102:GLU:OE1	0.53	2.61	15	1
1:A:31:ILE:HB	1:A:54:VAL:HG13	0.53	1.80	2	5
1:A:80:PHE:CD1	1:A:117:GLU:HB2	0.53	2.39	10	3
1:A:38:TYR:CD1	1:A:38:TYR:C	0.52	2.82	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HG12	1:A:108:PHE:CE1	0.52	2.39	18	16
1:A:13:PHE:CZ	1:A:106:ASP:OD1	0.52	2.61	14	1
1:A:16:ARG:HH21	1:A:34:ILE:HG13	0.52	1.64	11	1
1:A:23:ILE:HD11	1:A:53:LEU:HD11	0.52	1.81	7	3
1:A:44:LEU:CD2	1:A:73:LEU:HD11	0.52	2.34	4	1
1:A:113:TYR:O	1:A:113:TYR:CD1	0.52	2.62	8	1
1:A:13:PHE:CE1	1:A:106:ASP:OD1	0.52	2.62	14	1
1:A:99:TYR:O	1:A:103:ARG:CG	0.52	2.58	15	19
1:A:34:ILE:HG12	1:A:108:PHE:CD1	0.52	2.40	9	8
1:A:99:TYR:C	1:A:99:TYR:CD1	0.52	2.83	4	2
2:B:338:TRP:CD1	2:B:338:TRP:N	0.52	2.78	11	5
1:A:81:LEU:C	1:A:82:LEU:HD22	0.52	2.25	20	2
1:A:80:PHE:CE1	1:A:117:GLU:OE1	0.52	2.63	13	3
1:A:44:LEU:CD2	1:A:77:GLN:NE2	0.52	2.73	16	1
1:A:47:LEU:CD2	1:A:71:LEU:HD21	0.52	2.35	20	2
1:A:17:VAL:HG12	1:A:106:ASP:HB2	0.52	1.80	2	3
1:A:44:LEU:HD12	1:A:115:SER:N	0.52	2.19	5	2
2:B:339:THR:CG2	2:B:341:LEU:CD2	0.52	2.88	9	2
1:A:87:SER:HB2	1:A:89:VAL:HG13	0.52	1.80	14	2
1:A:16:ARG:CZ	1:A:110:TYR:CE1	0.51	2.93	9	1
1:A:51:LYS:C	1:A:52:PHE:CD1	0.51	2.84	5	5
1:A:57:HIS:CD2	1:A:58:VAL:HG12	0.51	2.40	8	1
1:A:65:LYS:O	1:A:69:ARG:CG	0.51	2.58	16	4
1:A:47:LEU:HD11	1:A:70:ARG:CB	0.51	2.35	3	1
1:A:32:PRO:HB3	2:B:338:TRP:CZ3	0.51	2.41	3	17
1:A:83:VAL:CG1	1:A:102:GLU:OE2	0.51	2.59	16	1
1:A:38:TYR:HA	1:A:112:VAL:HG13	0.51	1.82	12	2
1:A:34:ILE:CG2	1:A:50:THR:HG22	0.51	2.31	12	1
1:A:66:ILE:CD1	2:B:342:SER:O	0.51	2.59	18	12
1:A:98:VAL:O	1:A:102:GLU:CG	0.51	2.59	17	6
1:A:54:VAL:HG11	1:A:95:ILE:CD1	0.51	2.36	11	3
1:A:34:ILE:CG1	1:A:108:PHE:CD1	0.51	2.94	7	4
1:A:63:LEU:HD12	1:A:67:ILE:HG12	0.51	1.82	20	5
1:A:63:LEU:HD11	1:A:81:LEU:CD2	0.51	2.35	14	1
2:B:339:THR:CG2	2:B:340:HIS:N	0.51	2.72	16	4
1:A:54:VAL:HG12	1:A:55:PRO:HD2	0.50	1.81	11	13
1:A:44:LEU:CD2	1:A:73:LEU:HD13	0.50	2.36	5	2
1:A:63:LEU:O	1:A:63:LEU:HD22	0.50	2.06	11	1
1:A:80:PHE:O	1:A:82:LEU:CD2	0.50	2.60	16	7
1:A:23:ILE:HB	2:B:338:TRP:CZ2	0.50	2.41	17	6
1:A:60:MET:C	1:A:60:MET:SD	0.50	2.90	14	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:CD1	1:A:114:ALA:C	0.50	2.80	4	8
1:A:52:PHE:N	1:A:52:PHE:CD1	0.50	2.78	5	3
1:A:38:TYR:CB	1:A:114:ALA:HB2	0.50	2.36	13	2
1:A:27:HIS:CD2	1:A:53:LEU:HD13	0.50	2.41	17	1
2:B:342:SER:O	2:B:343:SER:CB	0.50	2.57	19	1
1:A:35:ILE:HD12	1:A:52:PHE:CD2	0.50	2.42	7	1
1:A:64:ILE:CG2	1:A:68:ARG:HH21	0.50	2.18	13	1
1:A:17:VAL:HG22	1:A:106:ASP:CA	0.50	2.36	1	2
1:A:44:LEU:HD11	1:A:115:SER:CA	0.50	2.37	2	2
1:A:79:PHE:CE2	1:A:113:TYR:HB2	0.50	2.42	7	2
1:A:34:ILE:CG2	1:A:36:GLU:OE2	0.50	2.60	10	1
1:A:49:LYS:CE	2:B:339:THR:OG1	0.50	2.60	18	4
1:A:39:LYS:CB	1:A:39:LYS:NZ	0.50	2.75	1	1
1:A:71:LEU:O	1:A:72:GLN:CG	0.50	2.60	14	8
1:A:69:ARG:HH21	2:B:347:ASP:HB2	0.50	1.67	20	1
1:A:31:ILE:HG21	1:A:99:TYR:HB2	0.50	1.83	8	3
1:A:83:VAL:CG1	1:A:102:GLU:CD	0.50	2.80	16	1
1:A:63:LEU:C	1:A:63:LEU:CD2	0.49	2.80	7	5
1:A:36:GLU:O	1:A:113:TYR:CD2	0.49	2.65	8	1
1:A:47:LEU:HD23	1:A:71:LEU:HD21	0.49	1.83	20	1
1:A:16:ARG:CD	1:A:110:TYR:OH	0.49	2.60	3	1
2:B:341:LEU:HD23	2:B:341:LEU:N	0.49	2.22	9	3
1:A:69:ARG:HH21	2:B:347:ASP:CA	0.49	2.20	13	1
1:A:47:LEU:HD13	1:A:48:ASP:H	0.49	1.68	18	9
1:A:23:ILE:HG21	1:A:32:PRO:HB3	0.49	1.82	17	5
1:A:63:LEU:HD21	1:A:111:MET:SD	0.49	2.47	20	2
1:A:63:LEU:HD11	1:A:81:LEU:CD1	0.49	2.38	11	1
1:A:34:ILE:CG1	1:A:108:PHE:CE1	0.49	2.96	12	4
1:A:67:ILE:O	1:A:70:ARG:N	0.49	2.45	18	13
1:A:35:ILE:HB	1:A:52:PHE:CE1	0.49	2.43	10	2
1:A:82:LEU:HD13	1:A:87:SER:CA	0.49	2.38	1	8
1:A:56:ASP:O	1:A:56:ASP:CG	0.49	2.51	8	7
1:A:99:TYR:CD2	1:A:109:LEU:CD2	0.49	2.96	18	4
1:A:83:VAL:N	1:A:86:HIS:O	0.49	2.46	13	15
1:A:68:ARG:HB3	1:A:79:PHE:CD2	0.49	2.43	12	6
1:A:26:GLN:C	1:A:27:HIS:CD2	0.49	2.86	9	2
1:A:19:ASP:OD1	1:A:51:LYS:CE	0.49	2.61	10	1
1:A:80:PHE:CG	1:A:117:GLU:HB2	0.48	2.43	8	18
1:A:89:VAL:CG2	1:A:117:GLU:OE1	0.48	2.61	12	2
1:A:35:ILE:HB	1:A:52:PHE:CE2	0.48	2.43	12	1
1:A:65:LYS:CD	1:A:65:LYS:N	0.48	2.75	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ILE:HG21	1:A:79:PHE:CE2	0.48	2.42	19	1
1:A:32:PRO:HD2	1:A:99:TYR:CE2	0.48	2.43	2	4
1:A:20:VAL:CG1	1:A:21:ARG:N	0.48	2.75	12	7
1:A:40:GLY:O	1:A:42:LYS:CD	0.48	2.61	12	1
1:A:20:VAL:CG2	1:A:108:PHE:CE2	0.48	2.96	15	1
1:A:62:GLU:OE2	2:B:343:SER:CB	0.48	2.61	8	2
1:A:54:VAL:HB	2:B:341:LEU:HD12	0.48	1.83	18	1
1:A:13:PHE:CE1	1:A:106:ASP:HB3	0.48	2.44	17	5
1:A:16:ARG:NH2	1:A:34:ILE:CB	0.48	2.77	9	1
1:A:65:LYS:O	1:A:69:ARG:CD	0.48	2.61	16	1
1:A:49:LYS:HG2	1:A:52:PHE:CZ	0.48	2.44	19	2
1:A:68:ARG:CG	1:A:69:ARG:N	0.48	2.76	14	4
1:A:31:ILE:O	1:A:54:VAL:CG1	0.48	2.61	3	3
1:A:36:GLU:OE1	1:A:112:VAL:CG2	0.48	2.59	6	1
1:A:57:HIS:CD2	1:A:58:VAL:CG1	0.48	2.97	8	1
1:A:63:LEU:O	1:A:63:LEU:HD12	0.48	2.09	19	3
1:A:83:VAL:CG1	1:A:102:GLU:OE1	0.48	2.61	16	1
1:A:73:LEU:HD22	1:A:77:GLN:HG3	0.48	1.85	17	1
1:A:53:LEU:HD21	2:B:338:TRP:CE3	0.48	2.44	2	12
1:A:77:GLN:NE2	1:A:78:ALA:N	0.48	2.62	7	1
1:A:19:ASP:OD2	2:B:338:TRP:CZ2	0.48	2.67	10	1
1:A:99:TYR:O	1:A:109:LEU:HD21	0.48	2.09	10	1
1:A:32:PRO:CB	2:B:338:TRP:CZ3	0.48	2.97	4	13
1:A:63:LEU:CD2	2:B:341:LEU:HD12	0.48	2.37	14	1
1:A:61:SER:HB2	1:A:91:VAL:HG21	0.47	1.86	11	3
1:A:36:GLU:HG2	1:A:50:THR:HG23	0.47	1.85	11	1
2:B:340:HIS:C	2:B:341:LEU:HD23	0.47	2.30	15	1
1:A:51:LYS:HB2	2:B:338:TRP:CE3	0.47	2.44	5	2
1:A:68:ARG:HB3	1:A:79:PHE:CE2	0.47	2.45	12	6
1:A:90:SER:O	1:A:92:SER:N	0.47	2.47	8	6
1:A:77:GLN:NE2	1:A:78:ALA:H	0.47	2.07	2	3
1:A:32:PRO:HD2	1:A:99:TYR:CE1	0.47	2.44	6	2
1:A:79:PHE:CZ	1:A:113:TYR:HB2	0.47	2.44	7	1
2:B:343:SER:O	2:B:346:VAL:CG2	0.47	2.61	8	2
1:A:19:ASP:OD2	1:A:51:LYS:CE	0.47	2.63	11	2
1:A:60:MET:SD	1:A:60:MET:C	0.47	2.93	18	11
1:A:51:LYS:NZ	2:B:338:TRP:NE1	0.47	2.60	3	2
1:A:45:PRO:HD2	1:A:71:LEU:HD22	0.47	1.87	20	3
1:A:68:ARG:HH21	2:B:347:ASP:HB3	0.47	1.69	8	1
1:A:27:HIS:HE2	2:B:337:ASP:CG	0.47	2.13	17	1
1:A:63:LEU:CD2	1:A:63:LEU:C	0.47	2.82	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:SER:HB3	1:A:91:VAL:HG21	0.47	1.86	4	1
1:A:31:ILE:CG2	1:A:99:TYR:CD1	0.47	2.98	8	1
1:A:49:LYS:HE2	2:B:339:THR:HG21	0.47	1.87	12	1
1:A:62:GLU:OE1	2:B:343:SER:CB	0.47	2.63	17	2
1:A:99:TYR:O	1:A:103:ARG:N	0.47	2.48	8	7
1:A:80:PHE:CD2	1:A:117:GLU:HB3	0.47	2.45	16	1
1:A:34:ILE:CG1	1:A:108:PHE:CZ	0.47	2.98	19	1
1:A:67:ILE:HG13	1:A:81:LEU:HD12	0.46	1.87	11	4
1:A:50:THR:O	1:A:52:PHE:CD2	0.46	2.68	12	1
1:A:97:GLU:O	1:A:101:SER:N	0.46	2.49	8	12
1:A:22:LEU:O	1:A:26:GLN:N	0.46	2.47	2	12
1:A:62:GLU:O	1:A:65:LYS:N	0.46	2.49	12	7
1:A:89:VAL:HG12	1:A:117:GLU:OE1	0.46	2.10	4	1
1:A:64:ILE:HD11	1:A:88:MET:HG2	0.46	1.86	17	2
1:A:67:ILE:CG2	1:A:79:PHE:CE2	0.46	2.98	19	1
1:A:34:ILE:N	1:A:109:LEU:O	0.46	2.48	10	10
1:A:66:ILE:HD13	2:B:346:VAL:HG12	0.46	1.86	4	2
1:A:84:ASN:CB	1:A:86:HIS:NE2	0.46	2.78	3	1
1:A:56:ASP:OD1	1:A:96:SER:CB	0.46	2.64	8	1
1:A:34:ILE:HD11	1:A:108:PHE:CE1	0.46	2.45	12	1
1:A:38:TYR:CZ	1:A:116:GLN:OE1	0.46	2.69	7	1
1:A:87:SER:CB	1:A:117:GLU:CD	0.46	2.84	17	1
1:A:88:MET:O	1:A:91:VAL:HG12	0.46	2.11	17	1
1:A:88:MET:O	1:A:91:VAL:N	0.46	2.49	18	1
1:A:45:PRO:HG2	1:A:71:LEU:HD23	0.46	1.87	20	1
1:A:47:LEU:HG	1:A:52:PHE:CZ	0.46	2.46	11	2
1:A:36:GLU:CD	1:A:50:THR:HG21	0.46	2.31	16	1
1:A:88:MET:O	1:A:90:SER:N	0.46	2.49	3	9
1:A:88:MET:C	1:A:90:SER:N	0.46	2.69	5	10
1:A:23:ILE:O	1:A:27:HIS:N	0.46	2.49	12	6
1:A:83:VAL:O	1:A:86:HIS:NE2	0.46	2.49	17	7
1:A:91:VAL:O	1:A:93:THR:N	0.46	2.49	10	2
1:A:102:GLU:O	1:A:103:ARG:C	0.46	2.54	15	19
1:A:44:LEU:HD21	1:A:73:LEU:HD13	0.46	1.88	5	2
1:A:63:LEU:O	1:A:63:LEU:CD2	0.46	2.64	9	2
1:A:89:VAL:CG1	1:A:117:GLU:OE1	0.46	2.63	18	1
1:A:35:ILE:O	1:A:50:THR:CG2	0.46	2.64	20	1
1:A:42:LYS:CD	1:A:42:LYS:C	0.45	2.85	1	1
1:A:38:TYR:CE2	1:A:116:GLN:OE1	0.45	2.69	7	1
1:A:22:LEU:O	1:A:25:GLU:N	0.45	2.50	2	5
1:A:97:GLU:O	1:A:100:GLU:N	0.45	2.49	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HG12	2:B:338:TRP:CE2	0.45	2.46	9	3
1:A:20:VAL:O	1:A:23:ILE:N	0.45	2.50	20	3
1:A:106:ASP:OD1	1:A:110:TYR:CE2	0.45	2.69	10	1
1:A:52:PHE:CD2	2:B:339:THR:HG21	0.45	2.47	19	1
1:A:79:PHE:CE2	1:A:113:TYR:CD1	0.45	3.04	7	1
1:A:63:LEU:C	1:A:63:LEU:HD13	0.45	2.32	11	1
1:A:36:GLU:CD	1:A:50:THR:HG23	0.45	2.32	1	1
1:A:81:LEU:HD22	1:A:111:MET:HB3	0.45	1.89	12	2
1:A:84:ASN:ND2	1:A:102:GLU:OE1	0.45	2.50	18	3
1:A:48:ASP:CG	1:A:49:LYS:NZ	0.45	2.70	18	1
1:A:41:GLU:OE2	1:A:43:GLN:N	0.45	2.50	10	3
1:A:86:HIS:NE2	1:A:102:GLU:OE1	0.45	2.50	15	4
1:A:44:LEU:HD13	1:A:114:ALA:HA	0.45	1.88	11	1
1:A:89:VAL:HG21	1:A:117:GLU:OE1	0.45	2.11	12	1
1:A:63:LEU:HD22	1:A:95:ILE:HD11	0.45	1.89	17	1
1:A:103:ARG:CD	1:A:104:ASP:O	0.45	2.65	8	3
1:A:51:LYS:HB3	2:B:338:TRP:CD2	0.45	2.47	16	9
1:A:116:GLN:NE2	1:A:118:THR:O	0.45	2.50	6	2
1:A:84:ASN:ND2	1:A:102:GLU:OE2	0.45	2.50	15	3
1:A:68:ARG:O	1:A:72:GLN:N	0.45	2.50	1	1
1:A:32:PRO:CB	2:B:338:TRP:CH2	0.45	3.00	8	6
1:A:20:VAL:O	1:A:22:LEU:N	0.45	2.50	11	2
1:A:55:PRO:HB2	1:A:57:HIS:CE1	0.45	2.47	20	2
1:A:51:LYS:HB3	2:B:338:TRP:CG	0.45	2.47	12	7
1:A:63:LEU:CD2	1:A:111:MET:CE	0.45	2.95	10	1
1:A:66:ILE:O	1:A:69:ARG:N	0.45	2.49	14	2
1:A:48:ASP:CG	1:A:49:LYS:HZ3	0.45	2.14	18	1
1:A:13:PHE:O	1:A:16:ARG:N	0.45	2.50	1	3
1:A:77:GLN:CD	1:A:78:ALA:N	0.45	2.71	17	2
1:A:26:GLN:C	1:A:27:HIS:CG	0.45	2.91	9	1
1:A:69:ARG:NH1	1:A:69:ARG:O	0.45	2.50	10	1
1:A:24:ARG:NH2	1:A:30:LYS:O	0.45	2.50	12	1
1:A:19:ASP:OD1	2:B:338:TRP:NE1	0.45	2.50	13	1
1:A:99:TYR:HA	1:A:109:LEU:HD11	0.44	1.89	12	1
1:A:17:VAL:HG22	1:A:106:ASP:HB3	0.44	1.86	13	1
1:A:18:GLU:O	1:A:21:ARG:CB	0.44	2.64	14	1
1:A:109:LEU:HD13	1:A:111:MET:HE1	0.44	1.89	15	1
1:A:23:ILE:CG1	2:B:338:TRP:CE2	0.44	3.01	9	3
1:A:104:ASP:O	1:A:107:GLY:N	0.44	2.50	19	5
1:A:61:SER:HB2	1:A:91:VAL:HG11	0.44	1.87	12	1
1:A:66:ILE:O	1:A:70:ARG:NE	0.44	2.50	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HG13	1:A:108:PHE:CD1	0.44	2.47	4	1
1:A:36:GLU:OE2	1:A:36:GLU:N	0.44	2.51	8	2
1:A:44:LEU:HD12	1:A:71:LEU:HD13	0.44	1.88	8	1
1:A:62:GLU:CD	2:B:343:SER:CB	0.44	2.86	15	1
1:A:41:GLU:CD	1:A:114:ALA:CB	0.44	2.85	1	1
1:A:23:ILE:HG12	2:B:338:TRP:CD2	0.44	2.47	9	3
1:A:16:ARG:O	1:A:19:ASP:N	0.44	2.51	3	1
1:A:106:ASP:OD2	1:A:107:GLY:N	0.44	2.51	19	3
1:A:41:GLU:OE2	1:A:44:LEU:N	0.44	2.50	8	2
1:A:66:ILE:O	1:A:70:ARG:CD	0.44	2.65	10	1
1:A:76:ASN:ND2	1:A:76:ASN:C	0.44	2.71	19	1
1:A:20:VAL:O	1:A:21:ARG:C	0.44	2.55	8	3
1:A:31:ILE:HG23	1:A:99:TYR:CD1	0.44	2.48	19	2
1:A:14:GLU:HA	1:A:17:VAL:HG12	0.44	1.89	15	1
1:A:38:TYR:HB2	1:A:112:VAL:CG1	0.44	2.42	19	16
1:A:91:VAL:C	1:A:93:THR:N	0.44	2.70	10	2
1:A:36:GLU:CD	1:A:50:THR:CG2	0.44	2.86	16	1
1:A:19:ASP:CG	1:A:51:LYS:NZ	0.44	2.71	2	1
1:A:90:SER:O	1:A:91:VAL:C	0.44	2.57	7	7
1:A:94:PRO:O	1:A:97:GLU:N	0.44	2.51	19	4
1:A:20:VAL:CG2	1:A:32:PRO:CG	0.44	2.96	11	2
1:A:16:ARG:NE	1:A:110:TYR:OH	0.44	2.50	4	1
1:A:67:ILE:C	1:A:69:ARG:N	0.44	2.71	6	4
1:A:66:ILE:HG12	2:B:346:VAL:HG12	0.44	1.90	8	1
1:A:27:HIS:NE2	2:B:337:ASP:OD1	0.43	2.51	17	1
1:A:44:LEU:CD1	1:A:73:LEU:CD1	0.43	2.96	8	1
1:A:20:VAL:HG21	1:A:106:ASP:OD1	0.43	2.12	15	1
1:A:64:ILE:CD1	1:A:81:LEU:HB3	0.43	2.43	20	1
1:A:99:TYR:CD1	1:A:100:GLU:N	0.43	2.85	1	1
1:A:79:PHE:CZ	1:A:81:LEU:HB2	0.43	2.48	17	1
1:A:35:ILE:HG22	1:A:113:TYR:CD2	0.43	2.47	20	1
1:A:61:SER:O	1:A:64:ILE:N	0.43	2.51	2	2
1:A:14:GLU:HA	1:A:17:VAL:CG1	0.43	2.44	15	4
1:A:20:VAL:CG1	1:A:107:GLY:O	0.43	2.61	8	1
1:A:20:VAL:C	1:A:22:LEU:N	0.43	2.71	11	3
1:A:62:GLU:N	1:A:62:GLU:CD	0.43	2.71	11	1
1:A:18:GLU:CG	1:A:19:ASP:N	0.43	2.81	4	1
1:A:58:VAL:HG11	1:A:62:GLU:OE1	0.43	2.13	4	1
1:A:17:VAL:HG13	1:A:18:GLU:N	0.43	2.29	5	1
1:A:97:GLU:C	1:A:99:TYR:N	0.43	2.72	8	3
1:A:104:ASP:O	1:A:106:ASP:N	0.43	2.51	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:TYR:CD1	1:A:113:TYR:O	0.43	2.71	13	1
1:A:88:MET:O	1:A:89:VAL:C	0.43	2.57	20	9
1:A:62:GLU:O	1:A:63:LEU:C	0.43	2.57	18	5
1:A:70:ARG:O	1:A:72:GLN:NE2	0.43	2.51	6	1
1:A:31:ILE:HG21	1:A:99:TYR:CB	0.43	2.43	11	3
1:A:16:ARG:CG	1:A:106:ASP:OD2	0.43	2.67	15	1
1:A:99:TYR:O	1:A:103:ARG:CB	0.43	2.67	19	6
1:A:67:ILE:O	1:A:69:ARG:N	0.43	2.51	6	3
1:A:69:ARG:HG3	2:B:346:VAL:HG12	0.43	1.91	9	1
1:A:54:VAL:CG1	1:A:55:PRO:HD2	0.43	2.44	19	12
1:A:16:ARG:CZ	1:A:34:ILE:HG21	0.43	2.43	9	1
1:A:63:LEU:C	1:A:63:LEU:CD1	0.43	2.83	14	1
1:A:104:ASP:CB	1:A:106:ASP:OD1	0.43	2.66	20	1
1:A:22:LEU:N	1:A:22:LEU:HD23	0.43	2.29	10	1
1:A:63:LEU:HD12	1:A:63:LEU:O	0.43	2.14	17	1
1:A:68:ARG:HG2	1:A:79:PHE:CE2	0.42	2.49	1	2
1:A:77:GLN:HE21	1:A:78:ALA:N	0.42	2.12	9	2
1:A:77:GLN:NE2	1:A:115:SER:OG	0.42	2.52	12	1
1:A:91:VAL:O	1:A:91:VAL:CG2	0.42	2.67	15	1
1:A:44:LEU:HD22	1:A:73:LEU:CD1	0.42	2.44	3	1
1:A:18:GLU:O	1:A:21:ARG:N	0.42	2.52	7	2
1:A:35:ILE:C	1:A:36:GLU:OE2	0.42	2.58	10	1
1:A:49:LYS:HD3	1:A:52:PHE:CE2	0.42	2.49	11	1
1:A:35:ILE:HG12	1:A:52:PHE:CD2	0.42	2.49	12	1
1:A:36:GLU:OE1	1:A:50:THR:CG2	0.42	2.67	19	1
1:A:71:LEU:C	1:A:72:GLN:CG	0.42	2.88	20	1
1:A:77:GLN:NE2	1:A:78:ALA:O	0.42	2.52	2	1
1:A:88:MET:SD	1:A:88:MET:C	0.42	2.98	11	4
1:A:71:LEU:O	1:A:73:LEU:N	0.42	2.52	6	1
1:A:69:ARG:HH21	2:B:347:ASP:HB3	0.42	1.73	7	1
1:A:69:ARG:NH2	2:B:347:ASP:CB	0.42	2.82	7	1
2:B:337:ASP:N	2:B:337:ASP:OD2	0.42	2.52	8	1
1:A:13:PHE:N	1:A:16:ARG:HH21	0.42	2.13	13	1
1:A:63:LEU:HD13	1:A:64:ILE:CD1	0.42	2.40	13	1
1:A:63:LEU:HD23	1:A:63:LEU:C	0.42	2.34	18	1
1:A:35:ILE:CG1	1:A:52:PHE:CD1	0.42	3.03	20	1
1:A:51:LYS:HD2	2:B:338:TRP:CE2	0.42	2.50	15	10
1:A:116:GLN:O	1:A:116:GLN:CG	0.42	2.67	16	2
2:B:343:SER:OG	2:B:343:SER:O	0.42	2.37	15	2
1:A:24:ARG:CZ	1:A:24:ARG:HB3	0.42	2.45	10	1
1:A:86:HIS:O	1:A:86:HIS:ND1	0.42	2.53	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:GLU:OE1	1:A:43:GLN:N	0.42	2.53	3	1
1:A:63:LEU:CD2	1:A:67:ILE:HG12	0.42	2.45	6	6
1:A:19:ASP:C	1:A:21:ARG:N	0.42	2.73	14	1
1:A:60:MET:SD	1:A:88:MET:CB	0.42	3.08	17	1
1:A:51:LYS:HD2	2:B:338:TRP:CD2	0.42	2.50	19	1
1:A:59:ASN:ND2	1:A:59:ASN:H	0.42	2.12	20	1
1:A:47:LEU:HD23	1:A:113:TYR:CE2	0.42	2.50	1	1
1:A:15:GLN:N	1:A:15:GLN:OE1	0.42	2.53	1	1
1:A:17:VAL:C	1:A:19:ASP:N	0.42	2.73	5	1
1:A:34:ILE:O	1:A:36:GLU:OE2	0.42	2.38	10	1
1:A:63:LEU:HD13	1:A:63:LEU:O	0.42	2.14	14	1
1:A:24:ARG:NH1	1:A:28:PRO:HA	0.42	2.30	2	4
1:A:19:ASP:O	1:A:22:LEU:N	0.42	2.53	14	1
1:A:66:ILE:CG2	2:B:341:LEU:CD1	0.42	2.92	7	1
1:A:69:ARG:NH2	2:B:345:GLU:O	0.42	2.51	12	1
1:A:80:PHE:CD1	1:A:117:GLU:HB3	0.42	2.49	13	1
1:A:41:GLU:OE1	1:A:114:ALA:HB1	0.42	2.13	20	1
1:A:93:THR:CG2	1:A:94:PRO:HD2	0.42	2.45	11	12
1:A:103:ARG:CD	1:A:103:ARG:C	0.42	2.89	9	2
1:A:103:ARG:HB3	1:A:109:LEU:CD2	0.42	2.45	17	6
1:A:105:GLU:O	1:A:106:ASP:C	0.42	2.58	16	4
1:A:51:LYS:HB3	2:B:338:TRP:CE3	0.41	2.50	1	1
1:A:88:MET:C	1:A:88:MET:SD	0.41	2.98	18	14
1:A:34:ILE:HG23	1:A:50:THR:CG2	0.41	2.45	3	1
1:A:94:PRO:C	1:A:96:SER:N	0.41	2.74	20	2
1:A:54:VAL:CG2	1:A:95:ILE:HG21	0.41	2.45	5	1
1:A:36:GLU:OE2	1:A:112:VAL:CG2	0.41	2.68	6	1
1:A:36:GLU:N	1:A:36:GLU:OE1	0.41	2.53	7	1
1:A:91:VAL:O	1:A:92:SER:C	0.41	2.58	10	2
1:A:116:GLN:CG	1:A:116:GLN:O	0.41	2.67	11	1
1:A:34:ILE:HD13	1:A:51:LYS:HA	0.41	1.92	12	1
1:A:44:LEU:HD22	1:A:44:LEU:N	0.41	2.30	8	1
1:A:20:VAL:O	1:A:24:ARG:N	0.41	2.53	14	1
1:A:66:ILE:O	1:A:67:ILE:C	0.41	2.59	14	1
1:A:44:LEU:HD12	1:A:113:TYR:HD1	0.41	1.75	16	1
1:A:47:LEU:HD12	1:A:52:PHE:CZ	0.41	2.50	14	1
1:A:109:LEU:HD13	1:A:111:MET:HE2	0.41	1.91	15	1
1:A:91:VAL:CG2	1:A:92:SER:N	0.41	2.82	18	1
1:A:44:LEU:CD2	1:A:115:SER:HB3	0.41	2.45	20	1
1:A:106:ASP:OD1	1:A:107:GLY:N	0.41	2.53	6	1
1:A:20:VAL:HG23	1:A:21:ARG:N	0.41	2.30	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:ASP:O	1:A:105:GLU:C	0.41	2.57	19	2
1:A:69:ARG:CZ	2:B:345:GLU:O	0.41	2.68	15	1
1:A:23:ILE:HG21	2:B:338:TRP:CH2	0.41	2.50	17	1
1:A:38:TYR:HA	1:A:112:VAL:CG1	0.41	2.46	19	13
1:A:106:ASP:OD2	1:A:106:ASP:N	0.41	2.53	18	1
1:A:24:ARG:NE	1:A:24:ARG:HA	0.41	2.30	10	1
1:A:63:LEU:CD1	1:A:64:ILE:CD1	0.41	2.99	13	1
1:A:53:LEU:N	2:B:339:THR:O	0.41	2.54	13	1
1:A:63:LEU:CD2	1:A:67:ILE:CG1	0.41	2.98	16	1
1:A:60:MET:HG3	1:A:91:VAL:CG2	0.41	2.46	14	6
1:A:19:ASP:OD2	1:A:51:LYS:CD	0.41	2.68	6	1
1:A:38:TYR:O	1:A:40:GLY:N	0.41	2.53	8	1
1:A:44:LEU:CD2	1:A:44:LEU:N	0.41	2.84	8	1
1:A:13:PHE:C	1:A:17:VAL:HG13	0.41	2.34	9	1
1:A:23:ILE:O	1:A:27:HIS:C	0.41	2.58	18	2
1:A:71:LEU:HD13	1:A:73:LEU:HD11	0.41	1.93	15	1
1:A:67:ILE:HG22	1:A:79:PHE:CE1	0.41	2.51	3	1
1:A:102:GLU:O	1:A:103:ARG:O	0.41	2.39	6	4
1:A:36:GLU:C	1:A:36:GLU:OE1	0.41	2.59	6	1
1:A:71:LEU:N	1:A:71:LEU:CD2	0.41	2.82	11	1
1:A:91:VAL:CG2	1:A:91:VAL:O	0.41	2.69	11	1
1:A:23:ILE:CG2	1:A:53:LEU:HD21	0.41	2.46	12	1
1:A:66:ILE:HG12	2:B:346:VAL:CG1	0.41	2.45	14	1
2:B:339:THR:HG22	2:B:340:HIS:N	0.41	2.30	14	1
1:A:66:ILE:HD13	2:B:341:LEU:HB3	0.41	1.92	14	1
1:A:69:ARG:CG	2:B:346:VAL:HA	0.41	2.46	16	1
1:A:52:PHE:CE2	1:A:67:ILE:CD1	0.41	3.04	20	1
1:A:54:VAL:CG2	1:A:55:PRO:HD2	0.41	2.46	3	1
1:A:109:LEU:HD13	1:A:111:MET:HE3	0.41	1.91	8	1
1:A:39:LYS:O	1:A:39:LYS:CG	0.41	2.69	9	1
1:A:34:ILE:C	1:A:36:GLU:OE2	0.41	2.59	10	1
1:A:56:ASP:CG	1:A:56:ASP:O	0.41	2.58	13	3
1:A:51:LYS:HB2	1:A:51:LYS:HZ3	0.41	1.76	14	1
1:A:83:VAL:O	1:A:86:HIS:ND1	0.41	2.54	19	1
1:A:115:SER:O	1:A:115:SER:OG	0.41	2.38	20	1
1:A:46:VAL:O	1:A:47:LEU:C	0.41	2.60	2	2
1:A:44:LEU:HD21	1:A:73:LEU:CD1	0.41	2.46	4	1
1:A:59:ASN:C	1:A:61:SER:N	0.41	2.74	9	1
1:A:47:LEU:CD2	1:A:71:LEU:CD2	0.41	2.99	20	1
2:B:343:SER:O	2:B:343:SER:OG	0.40	2.39	3	1
1:A:47:LEU:HD21	1:A:67:ILE:HG23	0.40	1.93	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LYS:O	1:A:43:GLN:C	0.40	2.59	15	2
1:A:44:LEU:N	1:A:44:LEU:HD22	0.40	2.31	12	1
1:A:57:HIS:NE2	1:A:58:VAL:CG1	0.40	2.84	8	1
1:A:99:TYR:CD2	1:A:100:GLU:N	0.40	2.90	12	1
1:A:104:ASP:C	1:A:106:ASP:N	0.40	2.71	12	1
1:A:58:VAL:HG11	2:B:343:SER:OG	0.40	2.16	14	1
1:A:36:GLU:HG2	1:A:50:THR:CG2	0.40	2.46	16	1
1:A:19:ASP:CG	1:A:51:LYS:HZ1	0.40	2.20	2	1
1:A:47:LEU:CD1	1:A:70:ARG:CB	0.40	2.99	3	1
1:A:52:PHE:CD1	1:A:52:PHE:N	0.40	2.89	15	1
2:B:337:ASP:OD2	2:B:337:ASP:N	0.40	2.53	9	1
1:A:57:HIS:CG	1:A:57:HIS:O	0.40	2.74	10	1
1:A:74:ASN:O	1:A:77:GLN:O	0.40	2.40	10	1
1:A:69:ARG:NH1	1:A:69:ARG:HA	0.40	2.31	5	1
1:A:64:ILE:C	1:A:66:ILE:N	0.40	2.72	7	1
2:B:339:THR:CG2	2:B:341:LEU:HD21	0.40	2.47	9	1
1:A:25:GLU:OE2	1:A:25:GLU:C	0.40	2.60	12	1
1:A:23:ILE:CD1	2:B:338:TRP:NE1	0.40	2.82	12	1
1:A:26:GLN:OE1	2:B:337:ASP:OD2	0.40	2.40	15	1
1:A:14:GLU:HA	1:A:17:VAL:HG22	0.40	1.92	16	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	106/121 (88%)	86±2 (81±2%)	16±2 (15±2%)	4±1 (4±1%)	5	32
2	B	10/17 (59%)	8±1 (78±8%)	1±1 (14±10%)	1±1 (8±6%)	2	14
All	All	2320/2760 (84%)	1872 (81%)	350 (15%)	98 (4%)	5	30

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	103	ARG	20

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Mol	Chain	Res	Type	Models (Total)
1	A	43	GLN	19
1	A	39	LYS	14
2	B	338	TRP	12
1	A	91	VAL	11
1	A	90	SER	3
1	A	67	ILE	3
2	B	346	VAL	3
1	A	47	LEU	2
1	A	58	VAL	2
1	A	92	SER	2
1	A	89	VAL	2
1	A	21	ARG	1
2	B	337	ASP	1
1	A	68	ARG	1
1	A	105	GLU	1
1	A	72	GLN	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	100/114 (88%)	78±2 (78±2%)	22±2 (22±2%)	3	30
2	B	11/15 (73%)	6±1 (52±9%)	5±1 (48±9%)	0	1
All	All	2220/2580 (86%)	1673 (75%)	547 (25%)	2	25

All 76 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	88	MET	20
1	A	59	ASN	20
1	A	95	ILE	20
1	A	47	LEU	20
1	A	49	LYS	20
1	A	108	PHE	20
2	B	344	LYS	20
1	A	81	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	91	VAL	20
2	B	340	HIS	19
1	A	42	LYS	19
2	B	342	SER	18
1	A	61	SER	17
1	A	70	ARG	15
1	A	87	SER	15
2	B	343	SER	13
2	B	339	THR	13
1	A	84	ASN	12
1	A	103	ARG	11
1	A	82	LEU	11
1	A	109	LEU	11
1	A	106	ASP	10
1	A	104	ASP	9
1	A	20	VAL	9
1	A	79	PHE	9
1	A	57	HIS	9
1	A	63	LEU	8
1	A	38	TYR	8
2	B	341	LEU	7
1	A	100	GLU	6
1	A	73	LEU	6
2	B	337	ASP	6
1	A	23	ILE	5
1	A	24	ARG	5
1	A	13	PHE	5
1	A	99	TYR	5
2	B	338	TRP	5
1	A	92	SER	5
1	A	37	ARG	4
1	A	16	ARG	4
1	A	115	SER	4
1	A	69	ARG	4
1	A	68	ARG	4
1	A	22	LEU	4
1	A	14	GLU	3
1	A	48	ASP	3
2	B	345	GLU	3
1	A	90	SER	2
1	A	41	GLU	2
1	A	118	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	56	ASP	2
1	A	25	GLU	2
1	A	30	LYS	2
1	A	19	ASP	2
1	A	43	GLN	2
1	A	51	LYS	2
1	A	15	GLN	2
1	A	65	LYS	2
1	A	77	GLN	2
1	A	34	ILE	2
1	A	111	MET	2
1	A	62	GLU	1
1	A	117	GLU	1
1	A	21	ARG	1
1	A	50	THR	1
1	A	89	VAL	1
2	B	346	VAL	1
1	A	33	VAL	1
1	A	18	GLU	1
1	A	101	SER	1
1	A	71	LEU	1
1	A	96	SER	1
1	A	39	LYS	1
1	A	113	TYR	1
1	A	72	GLN	1
1	A	36	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1776
Number of shifts mapped to atoms	1776
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	76

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	138	-0.24 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	131	0.06 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	128	-0.09 ± 0.11	None needed (< 0.5 ppm)
^{15}N	130	0.60 ± 0.55	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 1406 atoms were assigned a chemical shift out of a possible 1534. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	569/575 (99%)	229/229 (100%)	228/234 (97%)	112/112 (100%)
Sidechain	741/842 (88%)	450/493 (91%)	277/308 (90%)	14/41 (34%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	96/117 (82%)	52/63 (83%)	43/49 (88%)	1/5 (20%)
Overall	1406/1534 (92%)	731/785 (93%)	548/591 (93%)	127/158 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1621 atoms were assigned a chemical shift out of a possible 1789. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	664/678 (98%)	268/270 (99%)	266/276 (96%)	130/132 (98%)
Sidechain	848/976 (87%)	520/575 (90%)	313/351 (89%)	15/50 (30%)
Aromatic	109/135 (81%)	59/73 (81%)	49/57 (86%)	1/5 (20%)
Overall	1621/1789 (91%)	847/918 (92%)	628/684 (92%)	146/187 (78%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	344	LYS	CE	72.06	46.00 – 37.80	36.8
2	B	339	THR	CG2	51.11	27.15 – 15.95	26.4
2	B	341	LEU	CG	56.68	32.55 – 21.05	26.0
2	B	344	LYS	CG	54.67	30.67 – 19.17	25.9
2	B	338	TRP	CZ3	161.54	129.20 – 113.60	25.7
2	B	344	LYS	CD	58.97	34.86 – 23.06	25.4
2	B	345	GLU	CG	66.84	42.24 – 29.94	25.0
2	B	331	MET	CG	61.86	38.33 – 25.73	23.7
2	B	334	GLY	CA	75.67	51.81 – 38.91	23.5
1	A	69	ARG	NE	121.89	92.63 – 76.73	23.4
2	B	333	GLY	CA	75.47	51.81 – 38.91	23.3
1	A	24	ARG	NE	119.16	92.63 – 76.73	21.7
1	A	37	ARG	NE	119.08	92.63 – 76.73	21.6
1	A	21	ARG	NE	118.97	92.63 – 76.73	21.6
2	B	342	SER	CB	95.11	71.24 – 56.34	21.0
2	B	346	VAL	CG1	49.98	28.40 – 14.60	20.6
2	B	332	SER	CB	93.93	71.24 – 56.34	20.2
2	B	338	TRP	CE3	155.09	129.06 – 111.96	20.2
2	B	338	TRP	CH2	160.82	133.06 – 114.56	20.0
2	B	343	SER	CB	93.47	71.24 – 56.34	19.9
2	B	338	TRP	CZ2	144.03	121.76 – 106.66	19.7
2	B	346	VAL	CG2	51.66	29.20 – 13.40	19.2

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	347	ASP	CB	72.28	49.06 – 32.66	19.2
2	B	337	ASP	CB	71.93	49.06 – 32.66	18.9
2	B	336	ASP	CB	71.55	49.06 – 32.66	18.7
2	B	341	LEU	CD1	54.91	32.77 – 16.57	18.7
2	B	335	ASP	CB	71.19	49.06 – 32.66	18.5
2	B	339	THR	CB	99.44	78.10 – 61.30	17.7
2	B	345	GLU	CB	60.18	38.65 – 21.35	17.4
2	B	344	LYS	CB	62.83	41.68 – 23.88	16.9
2	B	346	VAL	CB	63.11	41.76 – 23.66	16.8
2	B	341	LEU	CD2	52.53	32.60 – 15.60	16.7
2	B	341	LEU	CB	73.60	51.69 – 32.89	16.7
2	B	338	TRP	CD1	158.33	136.18 – 116.78	16.4
2	B	338	TRP	NE1	160.13	139.19 – 119.59	15.7
2	B	338	TRP	CB	61.22	40.02 – 19.92	15.5
2	B	347	ASP	CA	86.07	64.88 – 44.48	15.4
2	B	335	ASP	CA	85.07	64.88 – 44.48	14.9
2	B	340	HIS	CB	61.37	40.69 – 19.69	14.8
2	B	336	ASP	CA	84.71	64.88 – 44.48	14.7
2	B	343	SER	CA	89.55	69.25 – 48.25	14.7
2	B	337	ASP	CA	83.67	64.88 – 44.48	14.2
2	B	345	GLU	CA	87.15	67.86 – 46.86	14.2
2	B	332	SER	CA	88.44	69.25 – 48.25	14.1
2	B	344	LYS	CA	86.72	67.97 – 45.97	13.5
2	B	342	SER	CA	86.84	69.25 – 48.25	13.4
2	B	331	MET	CB	62.92	44.20 – 21.80	13.4
2	B	341	LEU	CA	83.68	66.36 – 44.96	13.1
2	B	340	HIS	CA	87.02	68.24 – 44.74	13.0
2	B	331	MET	CA	85.33	67.38 – 44.88	13.0
2	B	340	HIS	CE1	166.28	149.70 – 125.30	11.8
2	B	339	THR	CA	92.66	75.37 – 49.07	11.6
2	B	338	TRP	CA	87.02	70.54 – 44.84	11.4
2	B	346	VAL	CA	91.71	76.93 – 48.03	10.1
2	B	340	HIS	N	159.13	139.70 – 99.40	9.8
2	B	347	ASP	N	158.09	140.24 – 101.14	9.6
1	A	51	LYS	HE2	1.16	3.87 – 1.97	-9.3
2	B	343	SER	N	148.57	134.24 – 98.34	9.0
1	A	51	LYS	HE3	1.23	3.86 – 1.96	-8.8
2	B	332	SER	N	147.26	134.24 – 98.34	8.6
2	B	345	GLU	N	150.68	138.24 – 103.14	8.5
2	B	344	LYS	N	151.91	140.01 – 102.11	8.1
2	B	333	GLY	N	141.08	129.07 – 90.27	8.1
2	B	340	HIS	CD2	147.42	137.40 – 103.40	7.9

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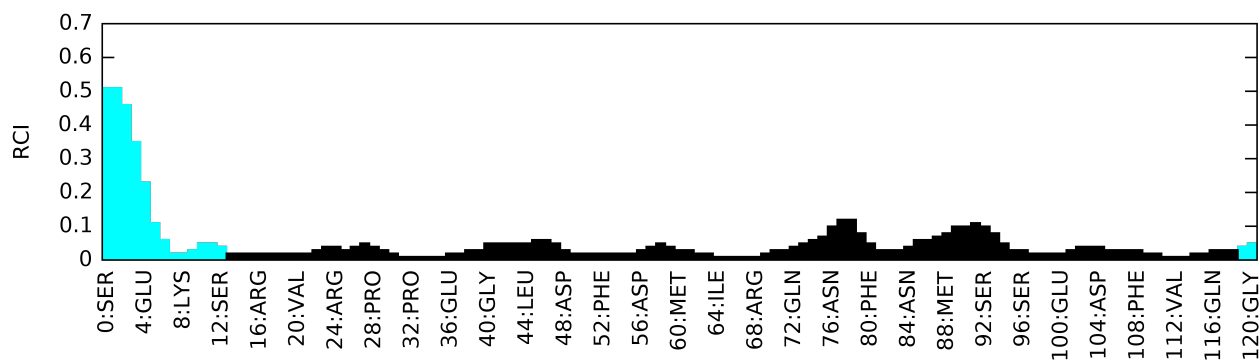
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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	341	LEU	N	153.30	141.70 – 102.00	7.9
2	B	342	SER	N	144.02	134.24 – 98.34	7.7
2	B	334	GLY	N	138.89	129.07 – 90.27	7.5
2	B	335	ASP	N	149.64	140.24 – 101.14	7.4
2	B	337	ASP	N	149.56	140.24 – 101.14	7.4
2	B	336	ASP	N	148.88	140.24 – 101.14	7.2
2	B	339	THR	N	149.50	139.35 – 91.55	7.1
2	B	338	TRP	N	150.17	142.48 – 100.78	6.8
1	A	34	ILE	HD12	-1.02	2.13 – -0.77	-5.9
1	A	34	ILE	HD13	-1.02	2.13 – -0.77	-5.9
1	A	34	ILE	HD11	-1.02	2.13 – -0.77	-5.9
2	B	346	VAL	N	146.72	144.09 – 98.19	5.6

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

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

