



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 11, 2024 – 07:57 PM EDT

PDB ID : 2JZB  
BMRB ID : 15614  
Title : Solution structure of the complex between E.coli NusA-AR2 and RNAP-aCTD  
Authors : Prasch, S.; Schweimer, K.; Roesch, P.  
Deposited on : 2008-01-02

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

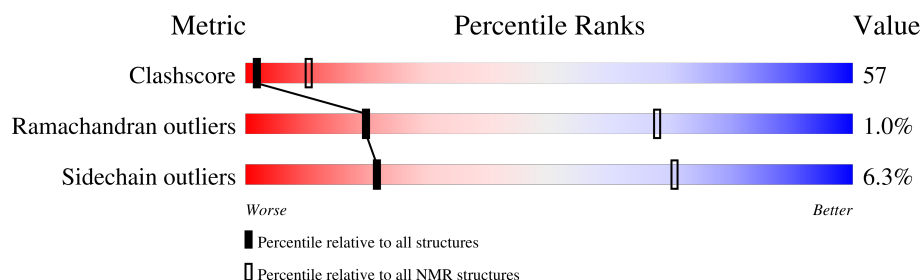
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 83%.

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  $\geq 3$ , 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	99	
2	B	74	

## 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:249-A:326, B:428-B:492 (143)	1.16	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	4, 5, 8, 12, 14, 15, 18, 19, 20
2	2, 3, 6, 9, 10, 11
3	7, 16
Single-model clusters	1; 13; 17

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2309 atoms, of which 1155 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1287	400	655	108	122	2	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	GLY	-	expression tag	UNP P0A7Z4
A	232	PRO	-	expression tag	UNP P0A7Z4

- Molecule 2 is a protein called Transcription elongation protein nusA.

Mol	Chain	Residues	Atoms						Trace
2	B	70	Total	C	H	N	O	S	0
			1022	321	500	87	111	3	

There are 2 discrepancies between the modelled and reference sequences:

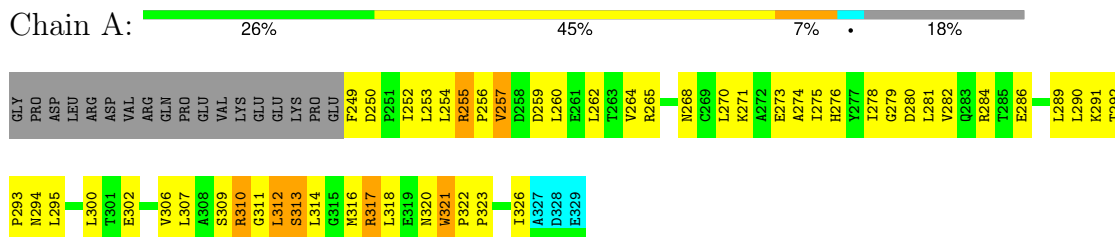
Chain	Residue	Modelled	Actual	Comment	Reference
B	422	GLY	-	expression tag	UNP P0AFF6
B	423	PRO	-	expression tag	UNP P0AFF6

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: Transcription elongation protein nusa

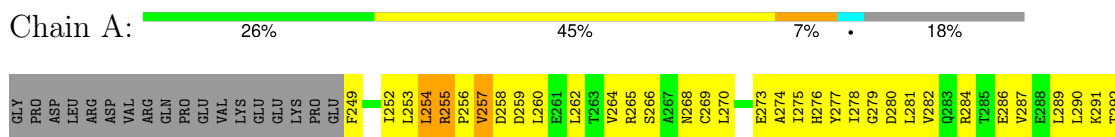


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: DNA-directed RNA polymerase subunit alpha





- Molecule 2: Transcription elongation protein nuaA

Chain B: 53% 28% 7% 7% 5%



#### 4.2.2 Score per residue for model 2

- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 27% 44% 7% 18%



- Molecule 2: Transcription elongation protein nuaA

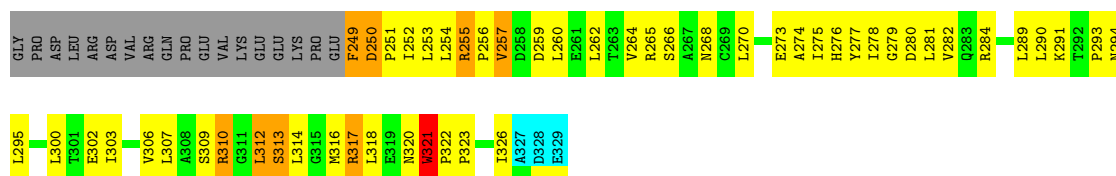
Chain B: 53% 32% 7% 5%



#### 4.2.3 Score per residue for model 3

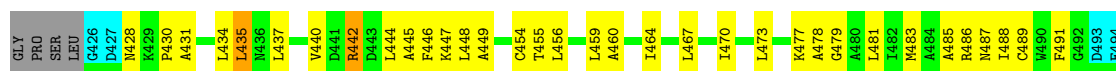
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 26% 43% 8% 18%



- Molecule 2: Transcription elongation protein nuaA

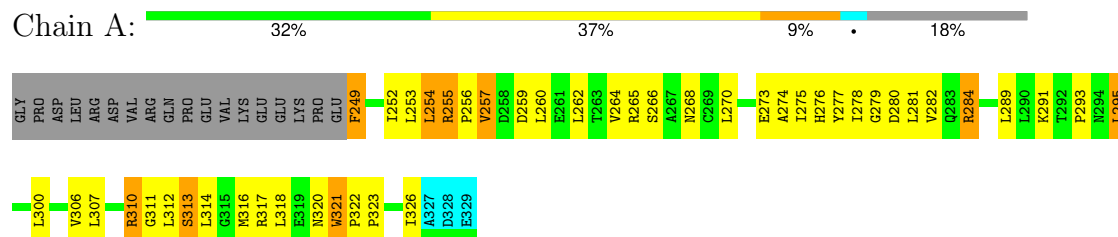
Chain B: 42% 43% 7% 5%



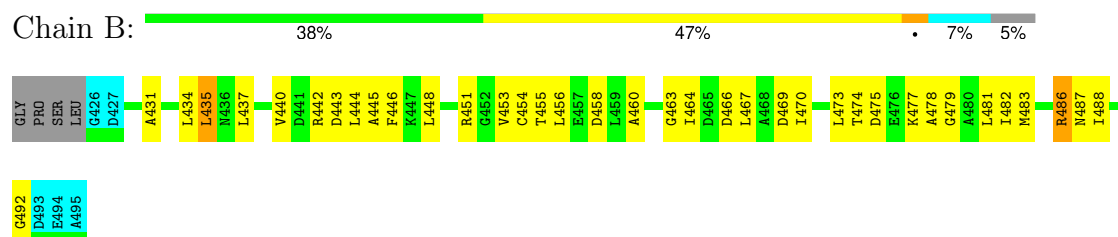
A495

#### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: DNA-directed RNA polymerase subunit alpha

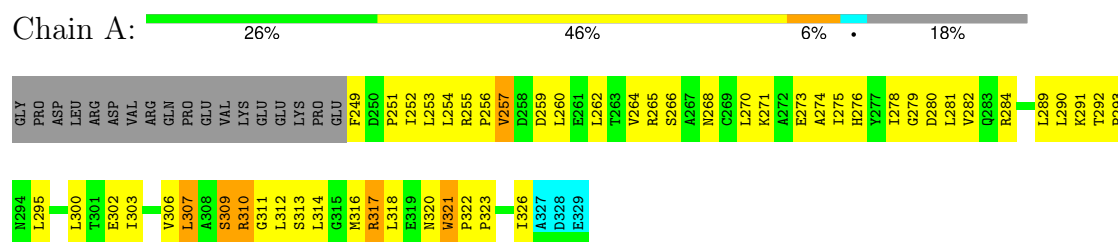


- Molecule 2: Transcription elongation protein nusa

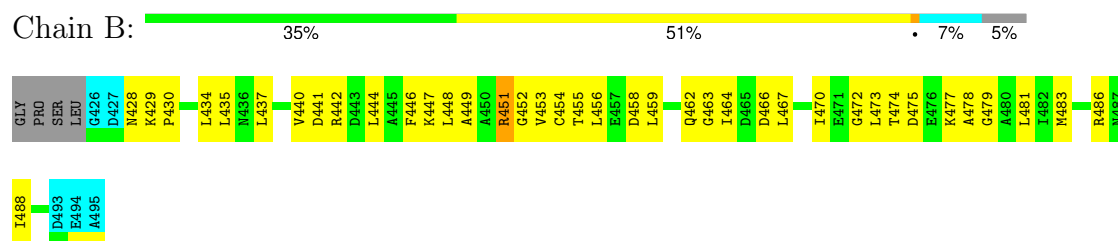


#### 4.2.5 Score per residue for model 5

- Molecule 1: DNA-directed RNA polymerase subunit alpha

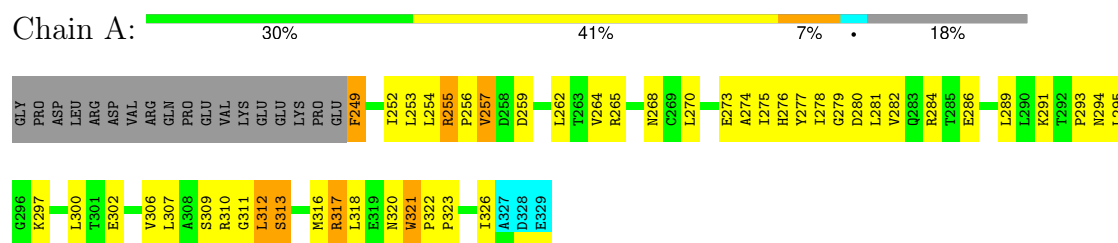


- Molecule 2: Transcription elongation protein nusa

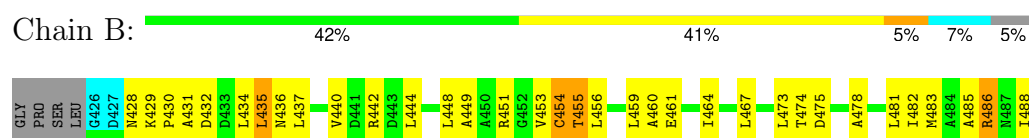


### 4.2.6 Score per residue for model 6

- Molecule 1: DNA-directed RNA polymerase subunit alpha

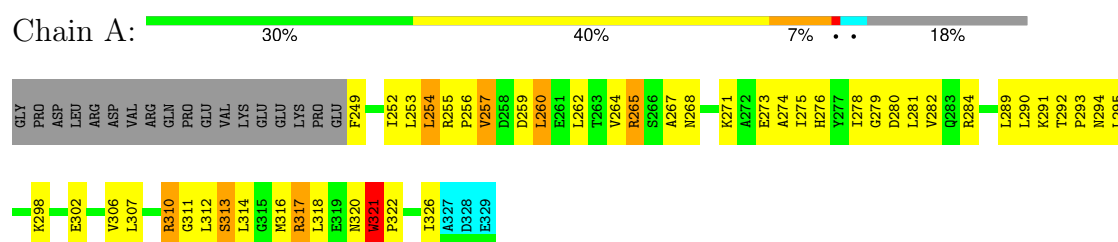


- Molecule 2: Transcription elongation protein nuaA

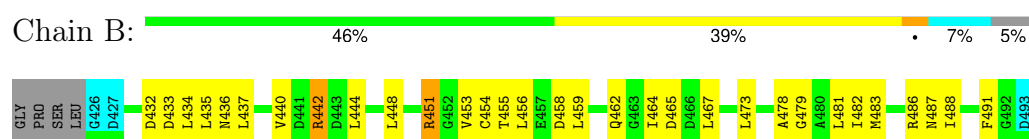


### 4.2.7 Score per residue for model 7

- Molecule 1: DNA-directed RNA polymerase subunit alpha

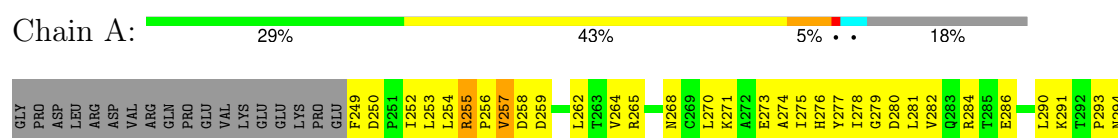


- Molecule 2: Transcription elongation protein nuaA

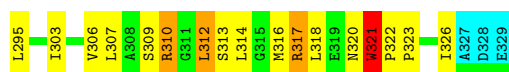


### 4.2.8 Score per residue for model 8

- Molecule 1: DNA-directed RNA polymerase subunit alpha

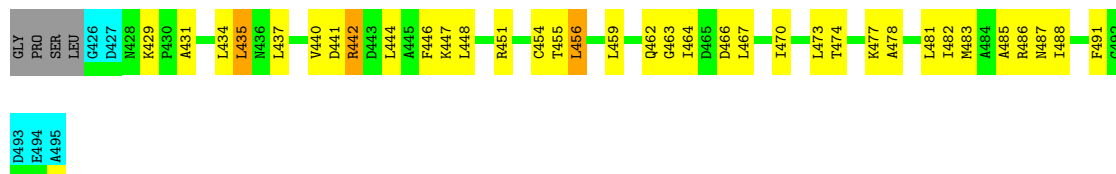






- Molecule 2: Transcription elongation protein nusA

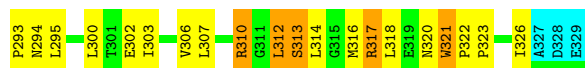
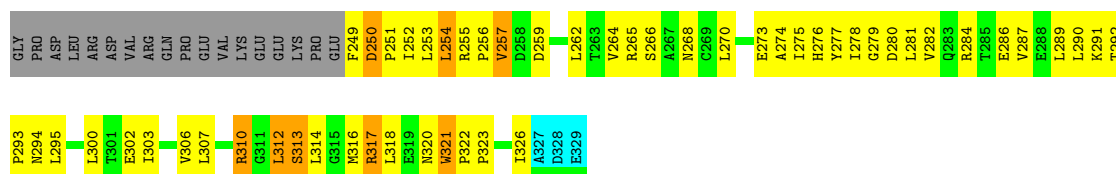
Chain B: 41% 43% 7% 5%



#### 4.2.9 Score per residue for model 9

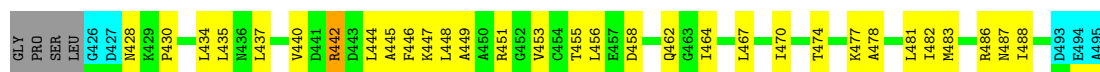
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 25% 45% 8% 18%



- Molecule 2: Transcription elongation protein nusA

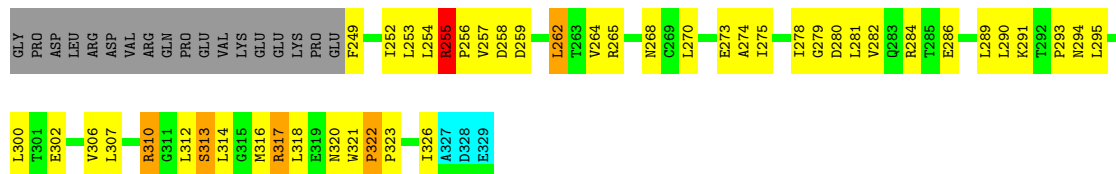
Chain B: 46% 41% 7% 5%



#### 4.2.10 Score per residue for model 10

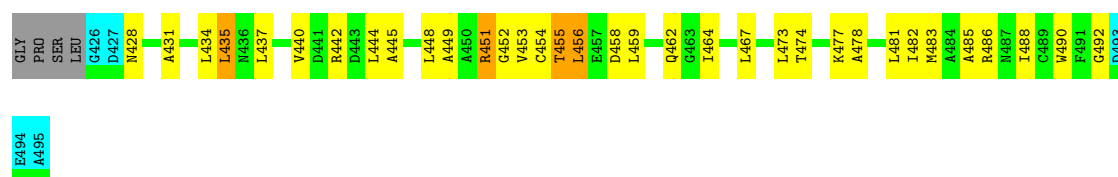
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 32% 40% 5% 18%



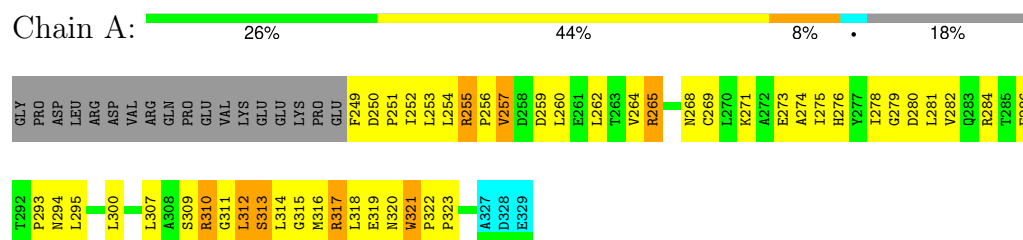
- Molecule 2: Transcription elongation protein nusA

Chain B: 42% 41% 5% 7%

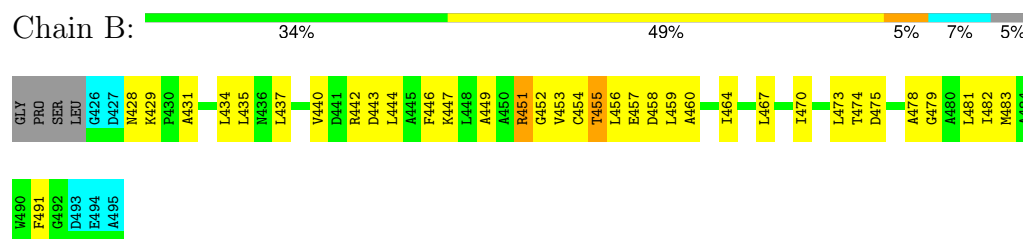


#### 4.2.11 Score per residue for model 11

- Molecule 1: DNA-directed RNA polymerase subunit alpha

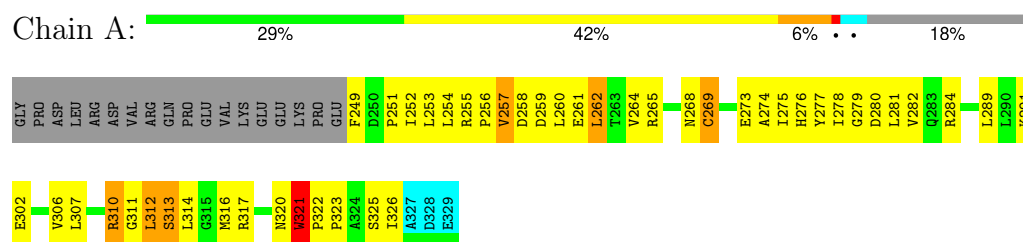


- Molecule 2: Transcription elongation protein nusa

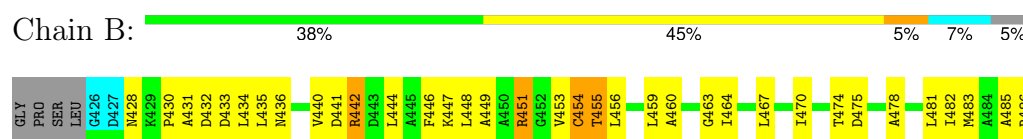


#### 4.2.12 Score per residue for model 12

- Molecule 1: DNA-directed RNA polymerase subunit alpha



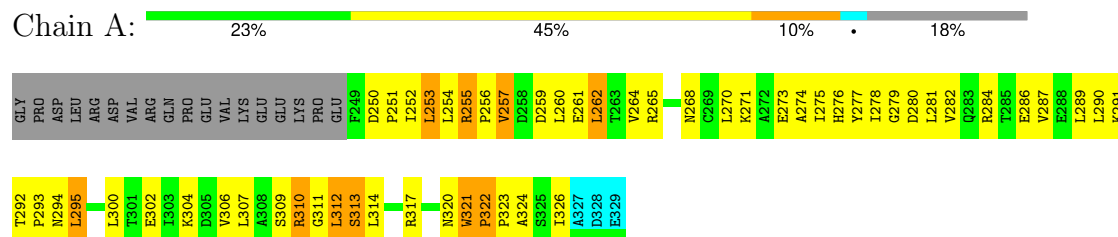
- Molecule 2: Transcription elongation protein nusa



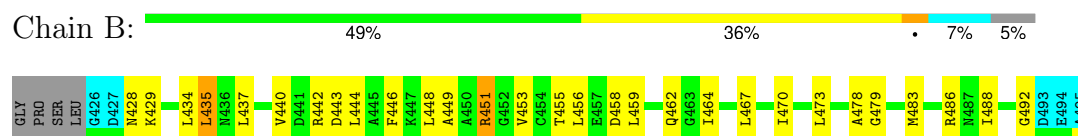
E494  
A495

## 4.2.13 Score per residue for model 13

- Molecule 1: DNA-directed RNA polymerase subunit alpha

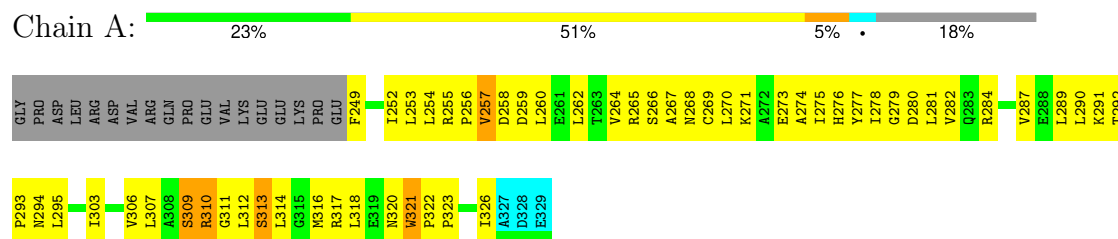


- Molecule 2: Transcription elongation protein nusa

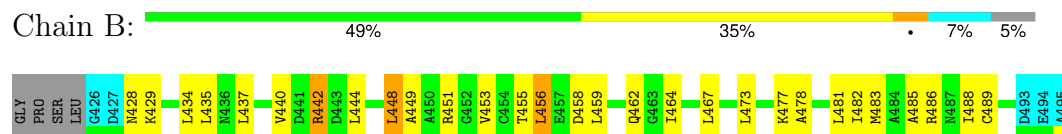


## 4.2.14 Score per residue for model 14

- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: Transcription elongation protein nusa



## 4.2.15 Score per residue for model 15

- Molecule 1: DNA-directed RNA polymerase subunit alpha

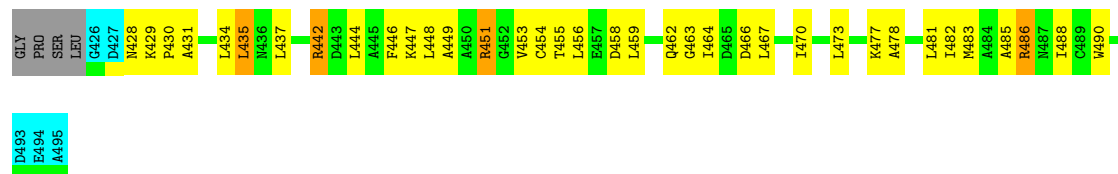






- Molecule 2: Transcription elongation protein nusA

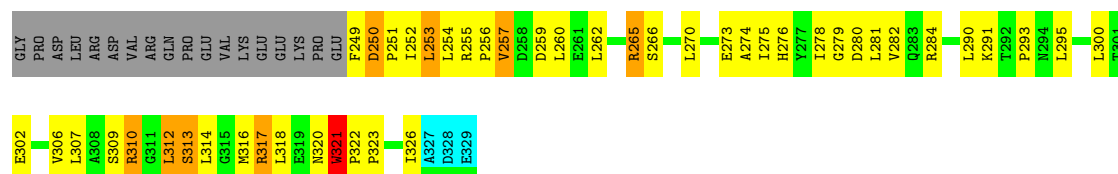
Chain B:



#### 4.2.18 Score per residue for model 18

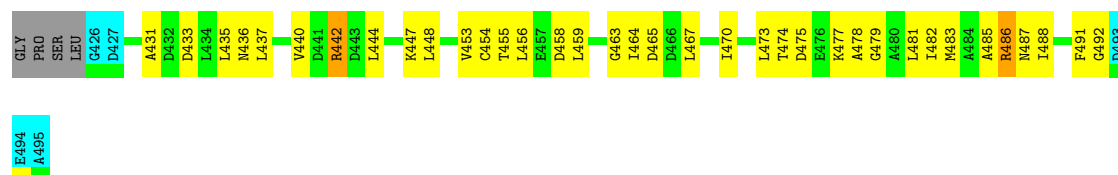
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



- Molecule 2: Transcription elongation protein nusA

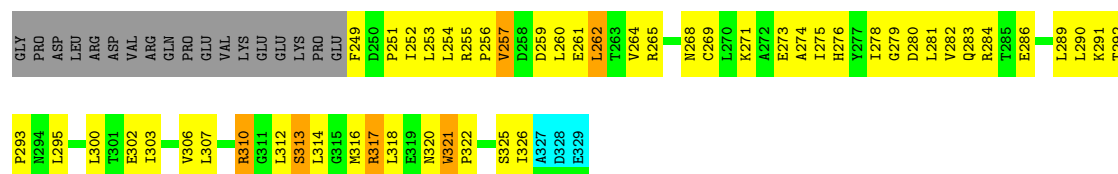
Chain B:



#### 4.2.19 Score per residue for model 19

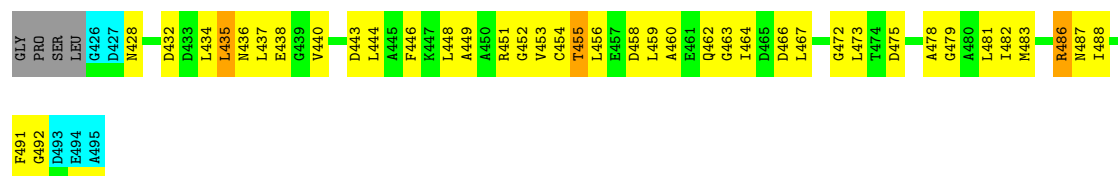
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



- Molecule 2: Transcription elongation protein nusA

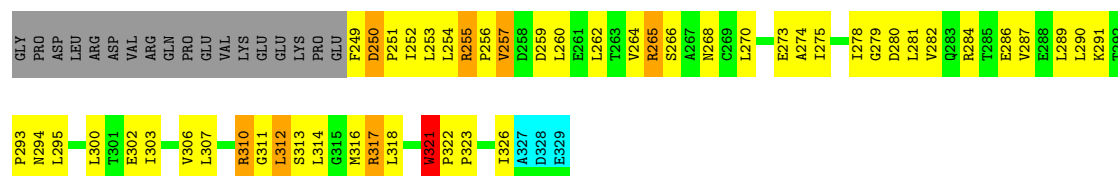
Chain B: 



#### 4.2.20 Score per residue for model 20

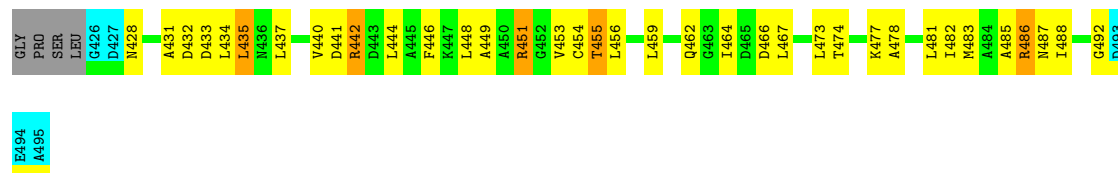
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 



- Molecule 2: Transcription elongation protein nusa

Chain B: 



## 5 Refinement protocol and experimental data overview

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

Of the 240 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1886
Number of shifts mapped to atoms	1678
Number of unparsed shifts	0
Number of shifts with mapping errors	208
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.0±0.0
2	B	0.0±0.0	2.7±0.5
All	All	0	154

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	255	ARG	Sidechain	20
1	A	265	ARG	Sidechain	20
1	A	284	ARG	Sidechain	20
1	A	310	ARG	Sidechain	20
1	A	317	ARG	Sidechain	20
2	B	442	ARG	Sidechain	19
2	B	451	ARG	Sidechain	18
2	B	486	ARG	Sidechain	17

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	609	640	639	80±8
2	B	487	478	478	56±7
All	All	21920	22360	22340	2503



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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:437:LEU:HD22	2:B:456:LEU:HD11	1.10	1.23	4	4
2:B:467:LEU:HD12	2:B:478:ALA:HB1	1.07	1.25	12	10
2:B:444:LEU:HD11	2:B:473:LEU:HD21	1.06	1.28	7	8
1:A:252:ILE:HD13	1:A:312:LEU:HD22	1.05	1.23	6	2
1:A:306:VAL:HG11	1:A:312:LEU:HD21	1.04	1.26	7	3
1:A:290:LEU:HD13	1:A:300:LEU:HD22	1.00	1.31	19	1
2:B:456:LEU:HD21	2:B:488:ILE:HD12	0.97	1.35	9	10
2:B:444:LEU:HD11	2:B:473:LEU:CD2	0.96	1.90	8	8
2:B:440:VAL:HG22	2:B:481:LEU:CD2	0.94	1.92	19	2
1:A:306:VAL:HG12	1:A:312:LEU:CD2	0.93	1.94	2	6
2:B:437:LEU:HD22	2:B:456:LEU:CD1	0.93	1.94	4	8
2:B:444:LEU:HD11	2:B:473:LEU:CD1	0.93	1.93	19	3
1:A:254:LEU:HD22	1:A:321:TRP:CZ2	0.92	1.98	7	5
1:A:279:GLY:O	1:A:282:VAL:HG22	0.92	1.64	19	20
1:A:323:PRO:O	1:A:326:ILE:HG22	0.92	1.65	5	6
1:A:281:LEU:HD22	1:A:312:LEU:HD11	0.92	1.36	5	1
2:B:456:LEU:CD2	2:B:488:ILE:HD12	0.92	1.95	3	10
1:A:270:LEU:HD21	1:A:281:LEU:HD12	0.92	1.42	5	1
2:B:440:VAL:HG13	2:B:444:LEU:HD12	0.91	1.37	10	1
1:A:290:LEU:O	1:A:290:LEU:HD13	0.90	1.65	3	4
2:B:434:LEU:HD13	2:B:434:LEU:O	0.89	1.68	2	11
1:A:306:VAL:HG12	1:A:312:LEU:HD21	0.89	1.44	9	5
1:A:270:LEU:CD2	1:A:281:LEU:HD12	0.89	1.98	5	1
1:A:278:ILE:HG21	1:A:312:LEU:HD23	0.89	1.41	11	3
1:A:252:ILE:CD1	1:A:312:LEU:HD22	0.88	1.99	6	2
1:A:254:LEU:HD21	1:A:326:ILE:HD11	0.88	1.45	20	6
2:B:444:LEU:HD11	2:B:473:LEU:HD11	0.88	1.43	3	3
1:A:253:LEU:CD2	1:A:282:VAL:HG11	0.88	1.97	17	2
1:A:281:LEU:HD23	1:A:312:LEU:HD13	0.88	1.45	20	1
2:B:435:LEU:O	2:B:435:LEU:HD13	0.88	1.69	5	15
1:A:289:LEU:O	1:A:295:LEU:HD11	0.88	1.67	2	3
2:B:437:LEU:HD13	2:B:456:LEU:HD11	0.87	1.45	8	5
2:B:467:LEU:HD22	2:B:478:ALA:HB1	0.87	1.47	5	9
2:B:453:VAL:HG21	2:B:462:GLN:HG3	0.86	1.46	5	8
1:A:293:PRO:HB2	2:B:482:ILE:HD12	0.86	1.47	18	11
1:A:281:LEU:HD11	1:A:289:LEU:HD11	0.86	1.45	9	4
1:A:310:ARG:O	1:A:314:LEU:HD21	0.86	1.69	3	9
1:A:281:LEU:HD22	1:A:312:LEU:CD1	0.85	2.01	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:307:LEU:HD21	1:A:313:SER:OG	0.85	1.71	11	2
1:A:275:ILE:HG23	1:A:280:ASP:HB2	0.85	1.49	8	16
1:A:310:ARG:O	1:A:314:LEU:HD11	0.85	1.72	7	6
1:A:300:LEU:HD13	1:A:300:LEU:O	0.85	1.70	4	3
1:A:278:ILE:CG2	1:A:312:LEU:HD13	0.84	2.02	19	2
1:A:287:VAL:HA	1:A:290:LEU:HD12	0.84	1.49	2	6
1:A:306:VAL:CG1	1:A:312:LEU:HD21	0.84	2.01	3	3
1:A:252:ILE:O	1:A:278:ILE:HD12	0.84	1.73	14	18
2:B:456:LEU:HD11	2:B:488:ILE:HD12	0.83	1.49	14	5
2:B:448:LEU:HD13	2:B:448:LEU:O	0.83	1.73	4	8
2:B:467:LEU:CD1	2:B:478:ALA:HB1	0.83	2.04	7	10
2:B:440:VAL:HG22	2:B:481:LEU:HD21	0.82	1.47	19	3
1:A:310:ARG:HA	1:A:314:LEU:HD21	0.82	1.49	7	2
1:A:278:ILE:HG21	1:A:312:LEU:CD2	0.81	2.04	11	2
1:A:293:PRO:HG2	2:B:464:ILE:HD11	0.81	1.52	17	20
1:A:249:PHE:CE2	1:A:318:LEU:HD21	0.81	2.10	5	4
1:A:253:LEU:HD21	1:A:311:GLY:O	0.80	1.76	11	3
2:B:467:LEU:HD12	2:B:478:ALA:CB	0.80	2.05	20	10
2:B:453:VAL:HG21	2:B:462:GLN:CG	0.80	2.05	7	9
2:B:453:VAL:HG13	2:B:458:ASP:CB	0.80	2.07	2	12
1:A:253:LEU:HD22	1:A:282:VAL:HG11	0.80	1.52	17	1
1:A:254:LEU:HD23	1:A:321:TRP:CZ2	0.79	2.13	14	1
1:A:322:PRO:HA	1:A:326:ILE:HD12	0.79	1.53	16	2
1:A:253:LEU:HD11	1:A:311:GLY:O	0.79	1.78	5	2
1:A:318:LEU:HD12	1:A:318:LEU:N	0.78	1.93	14	14
1:A:289:LEU:O	1:A:292:THR:HG22	0.78	1.78	1	2
1:A:290:LEU:CD1	1:A:300:LEU:HD22	0.78	2.08	19	2
1:A:295:LEU:HD12	1:A:295:LEU:N	0.77	1.93	17	9
1:A:323:PRO:CG	1:A:326:ILE:HD12	0.77	2.09	10	1
1:A:290:LEU:HD13	1:A:300:LEU:CD2	0.77	2.09	19	1
1:A:307:LEU:HD23	1:A:307:LEU:O	0.76	1.79	11	1
2:B:460:ALA:HB2	2:B:485:ALA:CB	0.76	2.09	12	3
2:B:460:ALA:HB1	2:B:486:ARG:HG2	0.76	1.56	6	3
2:B:448:LEU:HD11	2:B:459:LEU:CD2	0.76	2.11	8	2
2:B:440:VAL:HG13	2:B:444:LEU:HD23	0.75	1.57	7	7
2:B:444:LEU:CD1	2:B:473:LEU:HD21	0.75	2.09	7	8
2:B:428:ASN:O	2:B:449:ALA:HB1	0.75	1.82	20	9
1:A:314:LEU:HD22	1:A:314:LEU:N	0.75	1.97	17	10
2:B:467:LEU:HB3	2:B:473:LEU:HD23	0.75	1.59	6	1
1:A:254:LEU:HD22	1:A:321:TRP:CH2	0.75	2.16	17	2
2:B:467:LEU:HD22	2:B:478:ALA:CB	0.74	2.12	2	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:295:LEU:HD23	1:A:303:ILE:HD11	0.74	1.59	15	4
2:B:473:LEU:HD22	2:B:473:LEU:N	0.74	1.98	5	4
2:B:459:LEU:HD13	2:B:459:LEU:O	0.74	1.82	7	9
1:A:253:LEU:HD23	1:A:254:LEU:CD2	0.74	2.13	13	1
1:A:262:LEU:HD22	1:A:302:GLU:CG	0.74	2.11	13	2
1:A:257:VAL:HG11	1:A:270:LEU:HD12	0.74	1.59	13	2
2:B:430:PRO:HB3	2:B:434:LEU:HD23	0.74	1.58	6	3
1:A:310:ARG:HA	1:A:314:LEU:HD11	0.74	1.58	19	5
1:A:260:LEU:HD21	1:A:278:ILE:HD13	0.73	1.60	5	5
1:A:262:LEU:HD11	1:A:306:VAL:HG21	0.73	1.60	3	4
2:B:437:LEU:HD23	2:B:440:VAL:HG21	0.73	1.60	2	12
1:A:302:GLU:O	1:A:306:VAL:HG23	0.73	1.83	20	9
2:B:435:LEU:HD11	2:B:442:ARG:HG2	0.73	1.61	9	5
1:A:314:LEU:HD12	1:A:314:LEU:N	0.73	1.99	8	1
1:A:278:ILE:HG22	1:A:312:LEU:HD13	0.73	1.61	19	1
1:A:307:LEU:HD13	1:A:313:SER:OG	0.72	1.83	7	1
1:A:281:LEU:HD23	1:A:312:LEU:CD1	0.72	2.13	20	1
1:A:306:VAL:CG1	1:A:312:LEU:HD22	0.72	2.15	14	1
1:A:262:LEU:HD22	1:A:266:SER:OG	0.72	1.84	2	4
1:A:294:ASN:ND2	2:B:464:ILE:HD12	0.72	1.99	15	9
1:A:306:VAL:HG12	1:A:312:LEU:HD11	0.72	1.60	8	2
1:A:249:PHE:CZ	1:A:318:LEU:HD21	0.71	2.20	3	3
2:B:444:LEU:HD11	2:B:473:LEU:HD23	0.71	1.59	16	5
1:A:307:LEU:HD22	1:A:313:SER:CB	0.71	2.16	17	5
2:B:460:ALA:HB1	2:B:486:ARG:CG	0.71	2.15	6	3
1:A:295:LEU:HB2	1:A:300:LEU:HD21	0.71	1.62	6	4
1:A:250:ASP:HB2	1:A:253:LEU:HD13	0.71	1.62	15	1
2:B:456:LEU:C	2:B:456:LEU:HD13	0.71	2.06	12	3
1:A:306:VAL:HG11	1:A:312:LEU:CD2	0.71	2.10	7	1
1:A:270:LEU:HD21	1:A:295:LEU:HD21	0.71	1.63	18	1
2:B:459:LEU:C	2:B:459:LEU:HD13	0.70	2.07	1	8
1:A:278:ILE:CG2	1:A:312:LEU:HD23	0.70	2.16	11	2
1:A:250:ASP:O	1:A:254:LEU:HD12	0.70	1.86	20	1
2:B:456:LEU:HD23	2:B:488:ILE:HD12	0.70	1.63	11	2
1:A:264:VAL:HG12	1:A:268:ASN:OD1	0.70	1.86	1	3
2:B:453:VAL:HG13	2:B:458:ASP:HB2	0.70	1.62	2	2
2:B:467:LEU:CD2	2:B:478:ALA:HB1	0.70	2.17	3	5
2:B:447:LYS:HB3	2:B:470:ILE:HG21	0.70	1.63	11	3
2:B:448:LEU:HD11	2:B:453:VAL:HG21	0.70	1.62	12	4
2:B:434:LEU:C	2:B:434:LEU:HD13	0.69	2.07	9	4
1:A:312:LEU:HD23	1:A:312:LEU:N	0.69	2.02	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:434:LEU:HD13	2:B:434:LEU:C	0.69	2.07	14	7
2:B:444:LEU:C	2:B:444:LEU:HD13	0.69	2.08	10	1
1:A:281:LEU:HD13	1:A:281:LEU:C	0.69	2.08	1	2
2:B:456:LEU:HD21	2:B:488:ILE:CD1	0.69	2.18	15	5
2:B:448:LEU:HD11	2:B:459:LEU:HD21	0.69	1.64	8	1
1:A:317:ARG:C	1:A:318:LEU:HD12	0.69	2.07	19	13
1:A:253:LEU:HD21	1:A:326:ILE:HD11	0.69	1.65	13	1
1:A:313:SER:OG	1:A:314:LEU:HD22	0.69	1.88	11	1
1:A:312:LEU:HD12	1:A:312:LEU:O	0.69	1.88	13	1
1:A:254:LEU:HD11	1:A:326:ILE:HD12	0.68	1.64	17	2
2:B:437:LEU:HD13	2:B:456:LEU:CD1	0.68	2.19	10	9
2:B:448:LEU:HD13	2:B:448:LEU:C	0.68	2.09	3	8
1:A:257:VAL:HA	1:A:260:LEU:HD13	0.68	1.65	12	3
2:B:437:LEU:CD1	2:B:488:ILE:HD11	0.68	2.17	6	3
1:A:310:ARG:C	1:A:314:LEU:HD21	0.68	2.09	5	6
2:B:448:LEU:HD13	2:B:459:LEU:HD13	0.68	1.65	10	3
1:A:250:ASP:O	1:A:254:LEU:HD22	0.68	1.88	9	1
2:B:444:LEU:HD11	2:B:473:LEU:HD13	0.68	1.66	19	4
2:B:477:LYS:O	2:B:481:LEU:HD13	0.67	1.90	10	10
1:A:249:PHE:CE2	1:A:253:LEU:HD12	0.67	2.24	11	1
2:B:459:LEU:HD21	2:B:481:LEU:HB3	0.67	1.67	10	3
1:A:252:ILE:HD13	1:A:312:LEU:CD2	0.67	2.13	6	2
1:A:300:LEU:C	1:A:300:LEU:HD13	0.67	2.08	16	1
1:A:254:LEU:CD2	1:A:326:ILE:HD11	0.67	2.19	20	1
2:B:444:LEU:HD21	2:B:473:LEU:HD21	0.67	1.67	10	1
2:B:467:LEU:CB	2:B:478:ALA:HB1	0.67	2.20	16	10
2:B:456:LEU:HD11	2:B:488:ILE:CD1	0.67	2.19	14	4
2:B:430:PRO:CB	2:B:434:LEU:HD23	0.67	2.20	6	2
2:B:459:LEU:HD13	2:B:459:LEU:C	0.67	2.10	7	1
1:A:254:LEU:HD21	1:A:326:ILE:CD1	0.66	2.20	20	3
1:A:306:VAL:HG12	1:A:312:LEU:CD1	0.66	2.21	6	2
2:B:444:LEU:HD22	2:B:477:LYS:CE	0.66	2.21	14	3
2:B:437:LEU:CD2	2:B:456:LEU:HD11	0.66	2.13	4	2
2:B:460:ALA:HB2	2:B:485:ALA:HB1	0.66	1.67	12	2
1:A:260:LEU:HD21	1:A:278:ILE:CD1	0.66	2.20	5	7
1:A:257:VAL:HG22	1:A:276:HIS:O	0.66	1.91	8	2
1:A:323:PRO:HG2	1:A:326:ILE:HD12	0.66	1.68	10	1
2:B:440:VAL:CG2	2:B:481:LEU:HD22	0.66	2.20	12	4
1:A:281:LEU:HD23	1:A:312:LEU:HB3	0.66	1.67	8	1
1:A:289:LEU:HD22	1:A:289:LEU:N	0.66	2.06	3	9
1:A:318:LEU:HD22	1:A:318:LEU:N	0.66	2.06	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:PHE:N	1:A:325:SER:HG	0.65	1.89	2	2
1:A:307:LEU:HD22	1:A:313:SER:HB3	0.65	1.67	6	5
1:A:270:LEU:N	1:A:270:LEU:HD22	0.65	2.06	17	2
2:B:456:LEU:HD11	2:B:485:ALA:HA	0.65	1.66	6	2
2:B:448:LEU:CG	2:B:459:LEU:HD23	0.65	2.22	1	2
1:A:310:ARG:CA	1:A:314:LEU:HD21	0.65	2.21	7	3
1:A:293:PRO:CG	2:B:464:ILE:HD11	0.65	2.21	7	6
1:A:270:LEU:HD21	1:A:289:LEU:HD11	0.65	1.69	6	1
1:A:262:LEU:HD13	1:A:302:GLU:HB3	0.65	1.68	7	3
2:B:453:VAL:HG13	2:B:458:ASP:HB3	0.64	1.67	13	12
1:A:269:CYS:SG	1:A:295:LEU:HD23	0.64	2.33	14	1
1:A:253:LEU:CD1	1:A:282:VAL:HG21	0.64	2.21	13	1
1:A:303:ILE:HG22	1:A:307:LEU:HD22	0.64	1.67	8	1
2:B:448:LEU:HD13	2:B:459:LEU:HD12	0.64	1.68	15	1
1:A:311:GLY:C	1:A:312:LEU:HD12	0.64	2.13	14	1
1:A:275:ILE:HG23	1:A:280:ASP:HB3	0.64	1.70	1	1
1:A:312:LEU:H	1:A:312:LEU:HD23	0.64	1.53	4	5
1:A:303:ILE:HG22	1:A:307:LEU:HD13	0.64	1.70	3	1
1:A:306:VAL:HG12	1:A:312:LEU:HD22	0.63	1.68	2	5
1:A:293:PRO:CB	2:B:482:ILE:HD12	0.63	2.23	9	11
1:A:254:LEU:HD22	1:A:254:LEU:N	0.63	2.08	3	4
1:A:300:LEU:HD13	1:A:300:LEU:C	0.63	2.14	13	2
1:A:253:LEU:HD21	1:A:312:LEU:HA	0.63	1.70	6	4
1:A:249:PHE:CD1	1:A:323:PRO:CB	0.63	2.81	18	3
1:A:253:LEU:CD2	1:A:326:ILE:HD11	0.63	2.24	13	1
2:B:460:ALA:HB2	2:B:485:ALA:HB3	0.62	1.68	11	2
2:B:448:LEU:CD2	2:B:473:LEU:HD11	0.62	2.24	10	2
2:B:437:LEU:HD13	2:B:456:LEU:HD13	0.62	1.71	17	3
1:A:264:VAL:HG12	1:A:268:ASN:ND2	0.62	2.10	10	16
2:B:434:LEU:CD1	2:B:445:ALA:HB1	0.62	2.24	4	4
1:A:281:LEU:HD11	1:A:289:LEU:CD1	0.62	2.25	12	3
1:A:294:ASN:OD1	2:B:464:ILE:HD12	0.62	1.93	10	1
2:B:448:LEU:HD13	2:B:459:LEU:HD11	0.62	1.71	6	1
1:A:312:LEU:N	1:A:314:LEU:HD21	0.62	2.09	14	2
1:A:262:LEU:HD22	1:A:302:GLU:HG2	0.62	1.70	13	1
1:A:262:LEU:HD23	1:A:302:GLU:HB3	0.61	1.73	16	2
2:B:437:LEU:HD13	2:B:438:GLU:N	0.61	2.09	19	1
1:A:307:LEU:HD13	1:A:313:SER:HB3	0.61	1.73	10	3
1:A:254:LEU:CD2	1:A:321:TRP:CZ2	0.61	2.81	7	3
1:A:276:HIS:ND1	1:A:277:TYR:CD1	0.61	2.68	6	9
1:A:254:LEU:HD13	1:A:321:TRP:CZ2	0.61	2.30	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:254:LEU:HD22	1:A:321:TRP:HZ2	0.61	1.52	7	3
1:A:262:LEU:HD21	1:A:302:GLU:CB	0.61	2.25	20	1
1:A:264:VAL:HG12	1:A:268:ASN:HD21	0.61	1.56	20	10
2:B:434:LEU:HD11	2:B:448:LEU:CD1	0.61	2.26	7	1
1:A:282:VAL:HG11	1:A:316:MET:HE2	0.60	1.73	1	11
1:A:252:ILE:CG2	1:A:253:LEU:HD12	0.60	2.26	15	3
1:A:300:LEU:HD12	1:A:304:LYS:HE3	0.60	1.72	13	1
1:A:254:LEU:CD1	1:A:326:ILE:HD12	0.60	2.27	5	2
1:A:254:LEU:CD2	1:A:321:TRP:CH2	0.60	2.84	17	1
1:A:262:LEU:HD13	1:A:302:GLU:HG2	0.60	1.71	12	3
1:A:290:LEU:HD22	1:A:290:LEU:N	0.60	2.11	9	4
1:A:281:LEU:HD12	1:A:312:LEU:HD11	0.60	1.73	19	1
1:A:253:LEU:HD21	1:A:282:VAL:HG11	0.59	1.75	5	3
1:A:281:LEU:CD1	1:A:289:LEU:HD11	0.59	2.27	12	3
1:A:262:LEU:HD11	1:A:306:VAL:CG2	0.59	2.28	3	2
1:A:262:LEU:CD2	1:A:302:GLU:CG	0.59	2.81	13	1
1:A:321:TRP:CD1	1:A:321:TRP:O	0.59	2.56	17	1
1:A:281:LEU:HD12	1:A:312:LEU:CD1	0.59	2.27	19	1
2:B:437:LEU:HD13	2:B:437:LEU:C	0.59	2.18	19	1
2:B:444:LEU:HD22	2:B:473:LEU:HD21	0.59	1.74	17	2
1:A:270:LEU:HD11	1:A:281:LEU:HD13	0.59	1.75	13	3
1:A:306:VAL:CG1	1:A:312:LEU:CD1	0.59	2.81	6	1
1:A:251:PRO:HA	1:A:254:LEU:HD12	0.59	1.75	12	3
1:A:273:GLU:O	1:A:274:ALA:HB3	0.59	1.98	1	20
1:A:262:LEU:HD22	1:A:302:GLU:HB3	0.59	1.74	10	1
2:B:448:LEU:HG	2:B:459:LEU:HD23	0.58	1.75	1	1
1:A:282:VAL:HG12	1:A:313:SER:H	0.58	1.58	17	10
2:B:434:LEU:CD1	2:B:448:LEU:HD23	0.58	2.27	13	1
1:A:306:VAL:CG1	1:A:312:LEU:HD11	0.58	2.28	6	2
1:A:286:GLU:CD	1:A:307:LEU:HD13	0.58	2.19	9	1
1:A:260:LEU:HD11	1:A:278:ILE:HD11	0.58	1.74	12	2
1:A:262:LEU:HD21	1:A:302:GLU:HB2	0.58	1.74	20	1
2:B:431:ALA:HB3	2:B:455:THR:HA	0.58	1.76	15	6
2:B:433:ASP:CB	2:B:456:LEU:CB	0.58	2.81	20	2
2:B:453:VAL:HG11	2:B:459:LEU:HA	0.58	1.75	7	7
2:B:487:ASN:O	2:B:491:PHE:CG	0.58	2.56	12	4
1:A:307:LEU:HD12	1:A:312:LEU:HD13	0.58	1.75	8	1
2:B:451:ARG:CD	2:B:470:ILE:HD11	0.58	2.28	5	1
2:B:451:ARG:CG	2:B:470:ILE:HD11	0.58	2.29	5	3
2:B:437:LEU:HD23	2:B:440:VAL:CG2	0.58	2.29	11	9
1:A:269:CYS:SG	1:A:295:LEU:HD11	0.58	2.39	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:467:LEU:HB2	2:B:478:ALA:HB1	0.58	1.74	16	10
1:A:290:LEU:HD13	1:A:290:LEU:C	0.58	2.18	18	4
1:A:295:LEU:HD12	1:A:295:LEU:H	0.58	1.58	20	7
1:A:270:LEU:HD13	1:A:281:LEU:HD13	0.58	1.75	4	4
1:A:282:VAL:HG12	1:A:313:SER:N	0.58	2.13	18	6
1:A:314:LEU:HD13	1:A:316:MET:HE2	0.58	1.75	8	1
2:B:444:LEU:HD13	2:B:444:LEU:O	0.58	1.99	10	1
1:A:321:TRP:O	1:A:321:TRP:CG	0.58	2.57	17	1
1:A:314:LEU:N	1:A:314:LEU:CD2	0.57	2.67	4	9
2:B:437:LEU:CD1	2:B:488:ILE:CD1	0.57	2.81	7	4
1:A:249:PHE:O	1:A:249:PHE:CD2	0.57	2.57	7	9
1:A:286:GLU:CD	1:A:289:LEU:HD12	0.57	2.19	20	2
2:B:440:VAL:CG2	2:B:481:LEU:CD2	0.57	2.81	12	4
2:B:456:LEU:HD21	2:B:485:ALA:HA	0.57	1.76	18	1
1:A:286:GLU:OE1	1:A:289:LEU:HD12	0.57	1.99	20	2
2:B:456:LEU:HD21	2:B:485:ALA:HB2	0.57	1.75	20	3
2:B:453:VAL:HG21	2:B:462:GLN:CD	0.57	2.20	7	2
1:A:321:TRP:O	1:A:321:TRP:CE3	0.57	2.57	12	12
2:B:437:LEU:HD13	2:B:488:ILE:HD11	0.57	1.75	6	1
1:A:252:ILE:HD11	1:A:312:LEU:HD23	0.57	1.76	7	1
1:A:254:LEU:O	1:A:277:TYR:CD2	0.57	2.57	13	1
1:A:252:ILE:HD13	1:A:312:LEU:HD11	0.57	1.74	14	1
2:B:487:ASN:O	2:B:491:PHE:CD2	0.57	2.57	12	5
1:A:295:LEU:CB	1:A:300:LEU:HD21	0.57	2.29	20	4
2:B:456:LEU:HD22	2:B:456:LEU:O	0.57	1.99	12	4
2:B:447:LYS:HB3	2:B:470:ILE:HD13	0.57	1.74	15	2
1:A:253:LEU:CD1	1:A:316:MET:CE	0.57	2.82	19	3
1:A:253:LEU:HD11	1:A:282:VAL:HG21	0.57	1.75	20	3
1:A:260:LEU:CD1	1:A:278:ILE:HD11	0.57	2.30	12	2
1:A:257:VAL:HG23	1:A:271:LYS:HE3	0.57	1.75	15	1
1:A:318:LEU:N	1:A:318:LEU:CD1	0.56	2.67	14	13
1:A:253:LEU:CD1	1:A:316:MET:HE1	0.56	2.30	19	2
2:B:440:VAL:CG2	2:B:481:LEU:HD21	0.56	2.30	16	1
1:A:253:LEU:HD11	1:A:316:MET:CE	0.56	2.30	19	4
2:B:448:LEU:CD1	2:B:453:VAL:HG11	0.56	2.31	1	1
2:B:448:LEU:HD22	2:B:459:LEU:HD12	0.56	1.76	6	1
1:A:257:VAL:HA	1:A:260:LEU:HD23	0.56	1.77	7	1
1:A:270:LEU:HD21	1:A:281:LEU:HD13	0.56	1.76	9	1
1:A:317:ARG:O	1:A:318:LEU:HD13	0.56	1.99	17	1
1:A:312:LEU:O	1:A:313:SER:CB	0.56	2.53	11	9
2:B:444:LEU:HD22	2:B:477:LYS:HE2	0.56	1.77	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:262:LEU:H	1:A:262:LEU:HD12	0.56	1.61	11	9
1:A:295:LEU:N	1:A:295:LEU:CD1	0.56	2.67	6	8
2:B:448:LEU:CD1	2:B:459:LEU:CD2	0.56	2.84	17	2
1:A:294:ASN:ND2	2:B:464:ILE:CD1	0.56	2.69	12	9
1:A:321:TRP:CB	1:A:322:PRO:CD	0.56	2.84	15	12
1:A:270:LEU:CD2	1:A:289:LEU:HD12	0.56	2.30	2	1
2:B:444:LEU:CD2	2:B:477:LYS:CE	0.56	2.83	14	2
1:A:253:LEU:CD2	1:A:316:MET:CE	0.55	2.84	5	2
1:A:252:ILE:CD1	1:A:312:LEU:HD23	0.55	2.31	7	2
1:A:262:LEU:HD13	1:A:302:GLU:CG	0.55	2.31	13	2
1:A:249:PHE:CD1	1:A:323:PRO:HB3	0.55	2.36	8	2
1:A:254:LEU:O	1:A:277:TYR:CE2	0.55	2.59	13	1
1:A:321:TRP:N	1:A:322:PRO:CD	0.55	2.69	13	1
2:B:456:LEU:CD2	2:B:488:ILE:CD1	0.55	2.84	19	9
1:A:282:VAL:HG11	1:A:316:MET:CE	0.55	2.30	18	3
1:A:306:VAL:HG11	1:A:312:LEU:HD22	0.55	1.78	14	1
1:A:282:VAL:HB	1:A:316:MET:HE3	0.55	1.77	7	1
1:A:270:LEU:CD2	1:A:281:LEU:HD13	0.55	2.31	9	1
1:A:281:LEU:HD13	1:A:281:LEU:O	0.55	2.00	19	2
2:B:434:LEU:HD11	2:B:448:LEU:HD12	0.55	1.79	7	1
1:A:307:LEU:HD21	1:A:313:SER:HG	0.55	1.61	11	1
1:A:253:LEU:CD2	1:A:282:VAL:CG1	0.55	2.81	17	1
2:B:473:LEU:N	2:B:473:LEU:CD2	0.55	2.70	3	4
1:A:306:VAL:CG1	1:A:312:LEU:CD2	0.55	2.82	7	2
1:A:252:ILE:HD11	1:A:312:LEU:HD22	0.55	1.77	12	1
1:A:321:TRP:O	1:A:323:PRO:CD	0.55	2.55	17	3
1:A:279:GLY:O	1:A:282:VAL:CG2	0.54	2.56	8	15
2:B:435:LEU:HD13	2:B:435:LEU:C	0.54	2.22	5	9
1:A:267:ALA:HB1	1:A:271:LYS:HE3	0.54	1.79	14	1
2:B:437:LEU:HD23	2:B:456:LEU:HD13	0.54	1.78	19	1
1:A:289:LEU:N	1:A:289:LEU:CD2	0.54	2.70	19	9
2:B:467:LEU:HD22	2:B:478:ALA:CA	0.54	2.32	10	3
1:A:307:LEU:CD2	1:A:313:SER:CB	0.54	2.85	17	6
1:A:257:VAL:CG1	1:A:270:LEU:HD12	0.54	2.30	13	2
2:B:444:LEU:HD21	2:B:473:LEU:CD2	0.54	2.33	10	1
1:A:293:PRO:CB	2:B:479:GLY:CA	0.54	2.85	1	3
2:B:456:LEU:CD2	2:B:485:ALA:CB	0.54	2.86	10	5
2:B:434:LEU:CD1	2:B:459:LEU:HD13	0.54	2.32	12	1
1:A:252:ILE:HD13	1:A:311:GLY:HA3	0.54	1.79	7	1
1:A:249:PHE:CD1	1:A:323:PRO:CG	0.54	2.91	18	2
1:A:254:LEU:HD11	1:A:326:ILE:CD1	0.54	2.32	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:312:LEU:HD12	1:A:312:LEU:C	0.54	2.22	13	1
1:A:286:GLU:OE2	1:A:307:LEU:HD22	0.54	2.03	13	2
1:A:291:LYS:O	2:B:483:MET:HE2	0.53	2.03	11	12
1:A:260:LEU:CD2	1:A:278:ILE:CD1	0.53	2.86	5	1
1:A:313:SER:OG	1:A:314:LEU:N	0.53	2.39	11	1
1:A:252:ILE:HD13	1:A:312:LEU:HD23	0.53	1.79	15	1
2:B:444:LEU:CD1	2:B:473:LEU:HD11	0.53	2.28	3	3
2:B:434:LEU:HD11	2:B:445:ALA:HB1	0.53	1.80	4	1
1:A:252:ILE:O	1:A:278:ILE:CD1	0.53	2.57	18	9
1:A:249:PHE:CD1	1:A:325:SER:CB	0.53	2.91	16	2
1:A:291:LYS:O	2:B:483:MET:CE	0.53	2.57	6	16
1:A:275:ILE:HG23	1:A:280:ASP:CB	0.53	2.31	4	4
1:A:295:LEU:CD2	1:A:303:ILE:HD11	0.53	2.32	15	1
1:A:253:LEU:HD21	1:A:321:TRP:HE1	0.53	1.63	10	1
1:A:249:PHE:CE1	1:A:323:PRO:CB	0.53	2.92	14	2
1:A:262:LEU:CB	1:A:266:SER:OG	0.53	2.57	4	1
2:B:453:VAL:HG13	2:B:458:ASP:C	0.53	2.23	19	4
1:A:314:LEU:HD12	1:A:316:MET:HE1	0.53	1.80	20	1
1:A:294:ASN:HA	2:B:464:ILE:HD12	0.53	1.80	11	4
1:A:309:SER:O	1:A:310:ARG:CB	0.53	2.56	15	4
2:B:464:ILE:HG23	2:B:478:ALA:HB3	0.53	1.81	18	2
1:A:320:ASN:O	1:A:321:TRP:CB	0.53	2.57	2	16
2:B:456:LEU:HD21	2:B:485:ALA:CB	0.53	2.34	20	6
1:A:262:LEU:HD12	1:A:262:LEU:N	0.53	2.18	5	7
1:A:253:LEU:HD21	1:A:316:MET:CE	0.53	2.34	5	4
1:A:310:ARG:O	1:A:314:LEU:CD2	0.53	2.57	18	3
1:A:307:LEU:CD1	1:A:312:LEU:O	0.53	2.57	18	1
2:B:477:LYS:O	2:B:481:LEU:CD1	0.53	2.57	9	9
1:A:294:ASN:HD22	2:B:464:ILE:HD12	0.53	1.64	12	1
2:B:448:LEU:HG	2:B:459:LEU:HD13	0.53	1.81	14	1
2:B:428:ASN:O	2:B:449:ALA:CB	0.52	2.57	11	9
1:A:249:PHE:CD1	1:A:323:PRO:HG3	0.52	2.39	14	5
1:A:312:LEU:N	1:A:314:LEU:CD2	0.52	2.73	14	2
2:B:467:LEU:HD12	2:B:467:LEU:N	0.52	2.18	8	10
1:A:270:LEU:HD12	1:A:270:LEU:N	0.52	2.18	5	3
1:A:281:LEU:HD23	1:A:312:LEU:CB	0.52	2.35	8	1
1:A:323:PRO:CG	1:A:326:ILE:CD1	0.52	2.85	10	1
1:A:279:GLY:HA3	1:A:321:TRP:CH2	0.52	2.39	18	8
1:A:314:LEU:N	1:A:314:LEU:CD1	0.52	2.72	8	1
2:B:437:LEU:CD1	2:B:438:GLU:O	0.52	2.58	19	1
1:A:251:PRO:HA	1:A:254:LEU:HD23	0.52	1.81	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:291:LYS:CB	2:B:483:MET:CE	0.52	2.88	3	1
1:A:252:ILE:CG2	1:A:311:GLY:O	0.52	2.57	17	6
1:A:289:LEU:O	1:A:295:LEU:CD1	0.52	2.57	11	3
1:A:257:VAL:O	1:A:260:LEU:HD12	0.52	2.05	1	1
2:B:431:ALA:CB	2:B:454:CYS:O	0.52	2.57	3	5
2:B:470:ILE:HB	2:B:473:LEU:HD12	0.52	1.80	4	1
2:B:456:LEU:CD1	2:B:488:ILE:HD12	0.52	2.31	14	2
2:B:482:ILE:CG2	2:B:486:ARG:NE	0.52	2.73	19	2
1:A:322:PRO:CA	1:A:326:ILE:HD12	0.52	2.32	16	2
1:A:249:PHE:CD2	1:A:253:LEU:HD22	0.52	2.39	18	1
1:A:279:GLY:HA3	1:A:321:TRP:CZ3	0.52	2.39	12	8
1:A:250:ASP:O	1:A:254:LEU:CD2	0.52	2.58	18	2
1:A:321:TRP:N	1:A:322:PRO:HD3	0.52	2.20	10	1
2:B:456:LEU:HD22	2:B:488:ILE:HD12	0.52	1.78	19	1
1:A:249:PHE:O	1:A:249:PHE:CG	0.52	2.63	16	5
2:B:434:LEU:CB	2:B:454:CYS:O	0.52	2.58	19	6
2:B:448:LEU:CD2	2:B:467:LEU:HD22	0.52	2.35	14	1
1:A:275:ILE:HG23	1:A:280:ASP:OD2	0.52	2.04	20	1
1:A:312:LEU:N	1:A:312:LEU:CD2	0.52	2.73	6	5
1:A:275:ILE:HD12	1:A:280:ASP:HB3	0.52	1.80	4	1
1:A:291:LYS:O	2:B:483:MET:HE1	0.52	2.05	17	1
1:A:289:LEU:O	1:A:295:LEU:HD21	0.52	2.05	4	2
2:B:434:LEU:CD1	2:B:459:LEU:CD1	0.52	2.88	12	1
2:B:448:LEU:HD13	2:B:459:LEU:CD1	0.52	2.35	15	1
1:A:270:LEU:CD1	1:A:281:LEU:HD13	0.51	2.35	8	4
1:A:286:GLU:OE1	1:A:307:LEU:HD13	0.51	2.05	9	1
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	0.51	2.41	2	1
2:B:467:LEU:CD2	2:B:478:ALA:CB	0.51	2.87	2	5
2:B:433:ASP:CB	2:B:456:LEU:HB2	0.51	2.34	20	3
2:B:448:LEU:HD21	2:B:473:LEU:HD11	0.51	1.81	10	3
2:B:486:ARG:HG2	2:B:490:TRP:CD1	0.51	2.40	15	5
1:A:314:LEU:HD12	1:A:316:MET:CE	0.51	2.35	20	2
1:A:254:LEU:N	1:A:254:LEU:CD2	0.51	2.73	10	4
2:B:467:LEU:CB	2:B:478:ALA:CB	0.51	2.89	2	11
1:A:253:LEU:HD23	1:A:282:VAL:HG21	0.51	1.82	3	1
2:B:432:ASP:O	2:B:436:ASN:N	0.51	2.44	7	3
1:A:307:LEU:HD13	1:A:313:SER:O	0.51	2.05	13	1
1:A:252:ILE:CD1	1:A:312:LEU:CD2	0.51	2.88	15	1
2:B:459:LEU:HD12	2:B:485:ALA:HB2	0.51	1.81	16	2
1:A:269:CYS:SG	1:A:299:SER:CB	0.51	2.98	1	1
2:B:441:ASP:OD1	2:B:444:LEU:CG	0.51	2.58	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:LEU:HD13	1:A:311:GLY:O	0.51	2.05	2	1
1:A:307:LEU:CD2	1:A:313:SER:HB2	0.51	2.36	9	3
1:A:281:LEU:HD12	1:A:289:LEU:HD21	0.51	1.81	13	1
1:A:254:LEU:HD21	1:A:323:PRO:HG3	0.51	1.83	17	1
1:A:271:LYS:HE3	1:A:276:HIS:CE1	0.51	2.40	17	1
1:A:260:LEU:HB3	1:A:262:LEU:HD12	0.51	1.81	16	1
1:A:281:LEU:CD2	1:A:312:LEU:HD13	0.51	2.29	20	1
1:A:293:PRO:N	2:B:483:MET:SD	0.51	2.84	7	4
2:B:437:LEU:HD13	2:B:488:ILE:CD1	0.51	2.36	6	1
1:A:252:ILE:HG21	1:A:311:GLY:CA	0.51	2.36	7	2
1:A:249:PHE:CE1	1:A:323:PRO:HB3	0.51	2.41	14	4
1:A:321:TRP:HB3	1:A:322:PRO:CD	0.51	2.36	3	17
1:A:257:VAL:HG12	1:A:260:LEU:HD11	0.51	1.83	18	2
2:B:474:THR:HG22	2:B:475:ASP:N	0.51	2.21	6	8
1:A:254:LEU:HD21	1:A:326:ILE:HD12	0.51	1.83	6	1
1:A:258:ASP:OD1	1:A:259:ASP:N	0.51	2.43	10	1
2:B:440:VAL:HG13	2:B:444:LEU:CD1	0.51	2.26	10	1
2:B:437:LEU:HD13	2:B:456:LEU:CD2	0.51	2.35	11	1
1:A:254:LEU:CD2	1:A:254:LEU:N	0.51	2.73	13	1
1:A:318:LEU:HB3	1:A:321:TRP:CG	0.51	2.41	17	1
2:B:448:LEU:HD11	2:B:453:VAL:HG11	0.50	1.81	1	1
2:B:449:ALA:O	2:B:452:GLY:N	0.50	2.43	5	5
1:A:256:PRO:O	1:A:259:ASP:N	0.50	2.43	19	19
2:B:448:LEU:HD23	2:B:448:LEU:O	0.50	2.06	9	1
1:A:253:LEU:CD1	1:A:311:GLY:O	0.50	2.57	15	1
1:A:270:LEU:HD13	1:A:281:LEU:HD23	0.50	1.82	1	1
1:A:270:LEU:HD12	1:A:270:LEU:H	0.50	1.65	16	3
1:A:279:GLY:HA3	1:A:321:TRP:CE2	0.50	2.42	16	1
2:B:434:LEU:HD21	2:B:459:LEU:HD12	0.50	1.83	2	1
1:A:287:VAL:CA	1:A:290:LEU:HD12	0.50	2.35	13	1
2:B:444:LEU:CD2	2:B:477:LYS:HE2	0.50	2.36	14	3
1:A:260:LEU:HD11	1:A:278:ILE:CD1	0.50	2.36	12	1
1:A:290:LEU:CD2	1:A:300:LEU:CD1	0.50	2.90	1	1
2:B:467:LEU:HB2	2:B:478:ALA:CB	0.50	2.37	6	9
2:B:434:LEU:C	2:B:434:LEU:CD1	0.50	2.80	10	11
1:A:307:LEU:HD11	1:A:313:SER:CB	0.50	2.36	5	2
2:B:456:LEU:HG	2:B:488:ILE:HD12	0.50	1.82	6	1
1:A:320:ASN:O	1:A:321:TRP:HB2	0.50	2.07	16	12
1:A:252:ILE:HG21	1:A:311:GLY:O	0.50	2.07	16	3
1:A:253:LEU:CD1	1:A:282:VAL:HG11	0.50	2.37	9	2
1:A:250:ASP:N	1:A:250:ASP:OD1	0.50	2.45	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:433:ASP:HB2	2:B:456:LEU:CB	0.50	2.37	20	1
2:B:441:ASP:OD1	2:B:444:LEU:CB	0.50	2.59	16	3
2:B:444:LEU:HD22	2:B:473:LEU:CD2	0.50	2.36	1	2
2:B:442:ARG:NH1	2:B:442:ARG:CG	0.50	2.75	3	1
1:A:290:LEU:O	2:B:486:ARG:NH1	0.50	2.45	9	1
1:A:278:ILE:O	1:A:281:LEU:N	0.50	2.45	6	12
2:B:459:LEU:C	2:B:459:LEU:CD1	0.50	2.81	13	9
1:A:282:VAL:HG21	1:A:316:MET:HE3	0.50	1.83	20	3
1:A:249:PHE:CE2	1:A:318:LEU:HD22	0.50	2.42	4	1
1:A:254:LEU:HD11	1:A:326:ILE:HD11	0.50	1.82	10	1
1:A:323:PRO:HG2	1:A:326:ILE:CD1	0.50	2.35	10	1
2:B:434:LEU:HD11	2:B:459:LEU:CD1	0.50	2.36	12	1
1:A:321:TRP:O	1:A:323:PRO:HD3	0.49	2.07	13	10
2:B:447:LYS:HD2	2:B:473:LEU:HD21	0.49	1.84	5	1
2:B:456:LEU:HD11	2:B:485:ALA:CA	0.49	2.35	6	1
1:A:291:LYS:C	2:B:483:MET:CE	0.49	2.81	16	7
2:B:448:LEU:CD1	2:B:453:VAL:HG21	0.49	2.38	14	2
1:A:312:LEU:C	1:A:312:LEU:CD1	0.49	2.81	13	1
2:B:451:ARG:NH1	2:B:466:ASP:O	0.49	2.44	20	1
2:B:448:LEU:CD1	2:B:453:VAL:CB	0.49	2.91	12	2
1:A:253:LEU:HD11	1:A:282:VAL:CG1	0.49	2.36	2	1
1:A:262:LEU:CD2	1:A:302:GLU:HB3	0.49	2.38	3	3
1:A:303:ILE:O	1:A:307:LEU:CD1	0.49	2.60	14	2
2:B:456:LEU:C	2:B:456:LEU:CD1	0.49	2.80	12	2
2:B:487:ASN:O	2:B:491:PHE:CD1	0.49	2.65	11	1
1:A:254:LEU:CD2	1:A:326:ILE:HD13	0.49	2.38	14	1
2:B:437:LEU:HD23	2:B:456:LEU:CD1	0.49	2.38	19	1
1:A:300:LEU:C	1:A:300:LEU:CD1	0.49	2.80	16	3
2:B:448:LEU:C	2:B:448:LEU:CD1	0.49	2.81	18	8
1:A:310:ARG:O	1:A:314:LEU:CD1	0.49	2.59	9	3
1:A:253:LEU:O	1:A:279:GLY:N	0.49	2.45	17	5
2:B:453:VAL:HG22	2:B:462:GLN:OE1	0.49	2.08	14	1
1:A:293:PRO:CB	2:B:479:GLY:HA2	0.49	2.36	1	7
2:B:434:LEU:HD23	2:B:456:LEU:HD12	0.49	1.85	4	1
1:A:312:LEU:HD12	1:A:312:LEU:N	0.49	2.23	8	2
1:A:262:LEU:HD12	1:A:262:LEU:H	0.49	1.67	5	3
1:A:249:PHE:CD1	1:A:325:SER:HB3	0.49	2.43	16	1
1:A:249:PHE:CG	1:A:323:PRO:HG3	0.49	2.43	2	6
2:B:488:ILE:O	2:B:492:GLY:CA	0.49	2.61	10	2
2:B:437:LEU:HD12	2:B:488:ILE:HD11	0.49	1.82	7	1
1:A:307:LEU:CD2	1:A:313:SER:OG	0.49	2.61	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:292:THR:CG2	1:A:295:LEU:CD1	0.49	2.91	9	1
1:A:249:PHE:HD2	1:A:253:LEU:HD22	0.49	1.67	18	1
1:A:265:ARG:NH2	2:B:465:ASP:OD2	0.49	2.45	18	1
2:B:456:LEU:CD2	2:B:485:ALA:HB1	0.48	2.38	8	2
1:A:291:LYS:HB3	2:B:483:MET:CE	0.48	2.38	6	11
1:A:254:LEU:HG	1:A:326:ILE:HG21	0.48	1.84	8	1
1:A:290:LEU:HD21	1:A:300:LEU:HG	0.48	1.84	13	1
2:B:464:ILE:N	2:B:482:ILE:HD11	0.48	2.23	16	2
1:A:314:LEU:HD13	1:A:316:MET:CE	0.48	2.38	8	1
1:A:303:ILE:O	1:A:307:LEU:HD13	0.48	2.07	3	2
2:B:448:LEU:HD23	2:B:448:LEU:C	0.48	2.29	9	1
1:A:250:ASP:CB	1:A:253:LEU:HD13	0.48	2.35	15	1
1:A:293:PRO:HB2	2:B:464:ILE:HD11	0.48	1.85	16	2
1:A:306:VAL:O	1:A:312:LEU:CD1	0.48	2.61	18	1
2:B:430:PRO:HD3	2:B:446:PHE:CD1	0.48	2.43	5	2
2:B:442:ARG:NH1	2:B:442:ARG:HG3	0.48	2.23	3	1
1:A:254:LEU:CD1	1:A:321:TRP:CZ2	0.48	2.96	9	2
1:A:318:LEU:HB3	1:A:321:TRP:CD1	0.48	2.43	17	1
1:A:254:LEU:HG	1:A:321:TRP:CZ2	0.48	2.43	20	1
1:A:265:ARG:N	1:A:265:ARG:HD3	0.48	2.24	20	1
1:A:310:ARG:CA	1:A:314:LEU:HD11	0.48	2.38	13	3
2:B:435:LEU:O	2:B:435:LEU:CD1	0.48	2.59	10	9
2:B:456:LEU:CD1	2:B:488:ILE:CD1	0.48	2.91	14	2
2:B:444:LEU:C	2:B:444:LEU:CD1	0.48	2.81	10	1
1:A:289:LEU:N	1:A:289:LEU:CD1	0.48	2.75	13	2
1:A:293:PRO:HG3	2:B:479:GLY:CA	0.48	2.39	11	5
1:A:262:LEU:CD2	1:A:266:SER:OG	0.48	2.61	9	2
1:A:282:VAL:CG1	1:A:316:MET:HE2	0.48	2.39	18	4
2:B:434:LEU:HD12	2:B:445:ALA:HB1	0.48	1.85	10	3
2:B:431:ALA:N	2:B:454:CYS:O	0.48	2.45	6	8
1:A:271:LYS:HE2	1:A:276:HIS:CE1	0.48	2.44	5	1
2:B:451:ARG:HG3	2:B:470:ILE:HD11	0.48	1.84	11	3
1:A:318:LEU:HD22	1:A:321:TRP:HD1	0.48	1.68	10	1
1:A:293:PRO:CB	2:B:464:ILE:HD11	0.48	2.39	16	2
1:A:318:LEU:HG	1:A:321:TRP:CD2	0.48	2.43	17	1
1:A:281:LEU:C	1:A:281:LEU:CD1	0.48	2.81	19	2
1:A:269:CYS:SG	1:A:294:ASN:CB	0.48	3.02	12	1
2:B:459:LEU:HD12	2:B:485:ALA:CB	0.48	2.38	16	2
1:A:313:SER:O	1:A:314:LEU:HB2	0.48	2.09	11	2
1:A:253:LEU:HD13	1:A:282:VAL:HG21	0.48	1.86	12	1
2:B:488:ILE:O	2:B:492:GLY:N	0.48	2.45	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:317:ARG:C	1:A:318:LEU:HD22	0.48	2.28	17	1
2:B:451:ARG:CZ	2:B:451:ARG:HB3	0.47	2.39	10	3
2:B:451:ARG:CZ	2:B:469:ASP:CB	0.47	2.92	15	1
1:A:321:TRP:N	1:A:322:PRO:HD2	0.47	2.23	16	7
1:A:262:LEU:HB3	1:A:266:SER:CB	0.47	2.38	2	5
1:A:252:ILE:HG22	1:A:253:LEU:HD12	0.47	1.86	8	3
1:A:307:LEU:CD1	1:A:313:SER:HB3	0.47	2.38	5	1
1:A:276:HIS:CE1	1:A:277:TYR:CD1	0.47	3.02	6	1
1:A:291:LYS:HB2	2:B:483:MET:CE	0.47	2.39	3	1
1:A:254:LEU:CD2	1:A:326:ILE:CD1	0.47	2.89	20	1
1:A:290:LEU:HD21	1:A:300:LEU:CD1	0.47	2.39	1	1
2:B:437:LEU:HD22	2:B:456:LEU:HD13	0.47	1.85	5	2
2:B:433:ASP:O	2:B:436:ASN:OD1	0.47	2.32	18	1
1:A:312:LEU:C	1:A:314:LEU:HD22	0.47	2.30	14	3
1:A:249:PHE:CD1	1:A:253:LEU:HD12	0.47	2.44	4	1
1:A:286:GLU:OE2	1:A:313:SER:CB	0.47	2.63	8	1
1:A:306:VAL:HG11	1:A:312:LEU:HD23	0.47	1.86	19	1
2:B:443:ASP:HA	2:B:446:PHE:CD2	0.47	2.44	11	5
1:A:254:LEU:N	1:A:254:LEU:HD22	0.47	2.25	10	3
1:A:267:ALA:O	1:A:271:LYS:CB	0.47	2.62	17	1
1:A:286:GLU:OE2	1:A:303:ILE:HG21	0.47	2.09	20	1
2:B:448:LEU:CD1	2:B:453:VAL:CG1	0.47	2.93	1	1
2:B:430:PRO:CD	2:B:446:PHE:CE1	0.47	2.97	3	2
1:A:306:VAL:CB	1:A:312:LEU:HD11	0.47	2.40	6	2
2:B:433:ASP:CB	2:B:456:LEU:HB3	0.47	2.40	20	2
2:B:487:ASN:HB3	2:B:491:PHE:CE2	0.47	2.44	19	2
1:A:318:LEU:HD12	1:A:318:LEU:H	0.47	1.66	14	1
1:A:300:LEU:HA	1:A:303:ILE:HD12	0.47	1.85	20	1
1:A:307:LEU:HD21	1:A:313:SER:CB	0.47	2.38	3	1
2:B:482:ILE:HG22	2:B:486:ARG:CD	0.47	2.40	4	1
1:A:286:GLU:OE2	1:A:313:SER:O	0.47	2.33	9	1
2:B:486:ARG:CG	2:B:490:TRP:CD1	0.47	2.98	15	2
2:B:448:LEU:HD13	2:B:453:VAL:HB	0.47	1.87	1	1
1:A:273:GLU:O	1:A:274:ALA:CB	0.47	2.63	10	12
1:A:252:ILE:HG21	1:A:311:GLY:C	0.47	2.30	16	3
2:B:482:ILE:CG2	2:B:486:ARG:HD2	0.47	2.39	4	1
2:B:448:LEU:HD21	2:B:459:LEU:HD23	0.47	1.85	8	1
1:A:270:LEU:N	1:A:270:LEU:CD2	0.47	2.77	17	2
2:B:444:LEU:CD1	2:B:473:LEU:CD1	0.47	2.83	14	1
2:B:448:LEU:HD13	2:B:459:LEU:CD2	0.47	2.40	17	1
1:A:253:LEU:CD1	1:A:316:MET:HE3	0.47	2.40	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:ASP:HB2	1:A:253:LEU:CD1	0.46	2.38	15	3
1:A:286:GLU:CD	1:A:307:LEU:CD1	0.46	2.83	6	1
2:B:434:LEU:HD13	2:B:448:LEU:HD23	0.46	1.86	13	1
1:A:288:GLU:O	1:A:292:THR:OG1	0.46	2.33	15	1
1:A:264:VAL:CG1	1:A:268:ASN:ND2	0.46	2.77	16	1
1:A:286:GLU:OE2	1:A:300:LEU:HD11	0.46	2.09	19	1
1:A:250:ASP:CB	1:A:253:LEU:CD1	0.46	2.93	15	2
1:A:261:GLU:O	1:A:262:LEU:O	0.46	2.34	19	4
1:A:249:PHE:CE1	1:A:316:MET:CE	0.46	2.98	4	1
1:A:253:LEU:CD2	1:A:311:GLY:O	0.46	2.57	11	2
1:A:264:VAL:HG12	1:A:268:ASN:CG	0.46	2.29	8	1
2:B:486:ARG:NH2	2:B:490:TRP:CZ2	0.46	2.84	10	1
1:A:312:LEU:O	1:A:313:SER:OG	0.46	2.33	11	1
2:B:448:LEU:CD1	2:B:453:VAL:HB	0.46	2.40	1	4
1:A:275:ILE:CG2	1:A:280:ASP:HB2	0.46	2.41	5	10
1:A:307:LEU:HD11	1:A:313:SER:OG	0.46	2.11	5	1
2:B:433:ASP:HB3	2:B:456:LEU:CB	0.46	2.40	16	3
2:B:437:LEU:C	2:B:437:LEU:CD1	0.46	2.83	19	1
1:A:286:GLU:OE1	1:A:307:LEU:CD1	0.46	2.64	11	1
2:B:441:ASP:OD1	2:B:444:LEU:HD12	0.46	2.10	12	1
1:A:262:LEU:HD22	1:A:302:GLU:CD	0.46	2.30	13	1
1:A:254:LEU:CD1	1:A:326:ILE:HB	0.46	2.41	17	1
1:A:293:PRO:CG	2:B:479:GLY:HA3	0.46	2.40	16	3
2:B:463:GLY:O	2:B:467:LEU:CD1	0.46	2.64	2	1
1:A:290:LEU:C	1:A:290:LEU:CD1	0.46	2.84	18	4
2:B:434:LEU:HD11	2:B:445:ALA:CB	0.46	2.41	4	1
1:A:281:LEU:CD2	1:A:312:LEU:HD12	0.46	2.41	7	1
2:B:444:LEU:HD21	2:B:481:LEU:HD11	0.46	1.86	7	1
2:B:483:MET:O	2:B:487:ASN:ND2	0.46	2.49	20	2
1:A:291:LYS:CB	2:B:483:MET:HE2	0.46	2.41	3	1
2:B:470:ILE:CB	2:B:473:LEU:HD12	0.46	2.41	4	1
2:B:451:ARG:HD2	2:B:470:ILE:CD1	0.46	2.40	5	1
2:B:430:PRO:HG3	2:B:446:PHE:CD1	0.46	2.45	9	1
1:A:249:PHE:CE2	1:A:321:TRP:CZ3	0.46	3.03	11	1
2:B:453:VAL:HG22	2:B:462:GLN:CD	0.46	2.31	14	1
1:A:321:TRP:CD1	1:A:321:TRP:N	0.46	2.83	17	1
2:B:447:LYS:HD2	2:B:473:LEU:CD2	0.46	2.41	5	1
1:A:295:LEU:HD23	1:A:295:LEU:N	0.46	2.25	11	1
1:A:262:LEU:CD2	1:A:302:GLU:OE2	0.46	2.63	13	1
2:B:442:ARG:HB3	2:B:446:PHE:CZ	0.46	2.45	1	1
1:A:257:VAL:O	1:A:267:ALA:HB2	0.46	2.11	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:456:LEU:CD2	2:B:456:LEU:C	0.46	2.85	10	1
1:A:254:LEU:HG	1:A:321:TRP:CH2	0.46	2.46	20	1
1:A:249:PHE:HB2	1:A:323:PRO:CG	0.46	2.41	11	1
1:A:253:LEU:HD23	1:A:254:LEU:HD22	0.46	1.84	13	1
1:A:252:ILE:HG23	1:A:253:LEU:HD12	0.46	1.88	15	1
1:A:282:VAL:O	1:A:316:MET:O	0.45	2.34	4	8
1:A:307:LEU:HG	1:A:313:SER:CB	0.45	2.41	15	2
1:A:270:LEU:HD21	1:A:289:LEU:CD1	0.45	2.38	6	1
2:B:456:LEU:CD2	2:B:456:LEU:O	0.45	2.65	10	1
1:A:255:ARG:CD	1:A:259:ASP:OD2	0.45	2.65	1	1
2:B:447:LYS:HD3	2:B:470:ILE:CG2	0.45	2.40	8	5
2:B:448:LEU:CD2	2:B:453:VAL:HG11	0.45	2.41	6	1
1:A:281:LEU:CD1	1:A:312:LEU:HD11	0.45	2.41	19	1
1:A:312:LEU:HD12	1:A:313:SER:N	0.45	2.27	19	2
1:A:265:ARG:NH1	2:B:465:ASP:OD2	0.45	2.49	18	2
1:A:293:PRO:CG	2:B:479:GLY:CA	0.45	2.94	3	5
2:B:430:PRO:HD2	2:B:446:PHE:CE1	0.45	2.47	5	1
1:A:307:LEU:CD2	1:A:313:SER:HB3	0.45	2.40	6	1
1:A:290:LEU:N	1:A:290:LEU:CD2	0.45	2.80	10	4
1:A:269:CYS:SG	1:A:295:LEU:CD1	0.45	3.04	19	1
1:A:271:LYS:HG3	1:A:276:HIS:CE1	0.45	2.46	16	5
2:B:453:VAL:CG2	2:B:462:GLN:CD	0.45	2.84	7	2
1:A:303:ILE:HG22	1:A:307:LEU:CD2	0.45	2.41	8	1
1:A:290:LEU:HD11	1:A:300:LEU:HD11	0.45	1.88	10	1
1:A:253:LEU:CD1	1:A:279:GLY:HA2	0.45	2.42	13	1
1:A:292:THR:CG2	1:A:295:LEU:HD21	0.45	2.41	13	1
2:B:434:LEU:HB2	2:B:454:CYS:O	0.45	2.11	19	6
1:A:250:ASP:O	1:A:254:LEU:CD1	0.45	2.63	20	1
1:A:275:ILE:HG21	1:A:280:ASP:HB2	0.45	1.88	20	1
1:A:262:LEU:HB3	1:A:266:SER:OG	0.45	2.12	4	1
1:A:289:LEU:N	1:A:289:LEU:HD12	0.45	2.25	13	1
2:B:442:ARG:O	2:B:446:PHE:CD2	0.45	2.70	8	5
1:A:306:VAL:CG1	1:A:312:LEU:HD23	0.45	2.42	5	1
2:B:456:LEU:O	2:B:456:LEU:HD23	0.45	2.11	10	1
2:B:467:LEU:HD22	2:B:478:ALA:HA	0.45	1.88	10	1
2:B:429:LYS:O	2:B:454:CYS:SG	0.45	2.74	11	1
1:A:253:LEU:CD1	1:A:282:VAL:CG1	0.45	2.95	14	1
1:A:309:SER:O	1:A:310:ARG:HB2	0.45	2.10	15	5
1:A:321:TRP:CD2	1:A:321:TRP:C	0.45	2.90	7	5
1:A:254:LEU:HD22	1:A:254:LEU:H	0.45	1.71	8	1
1:A:286:GLU:OE2	1:A:313:SER:HB3	0.45	2.12	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:260:LEU:HD21	1:A:278:ILE:HD11	0.45	1.87	17	1
2:B:473:LEU:HD23	2:B:477:LYS:HD3	0.45	1.89	18	1
1:A:293:PRO:HB3	2:B:482:ILE:CG2	0.44	2.43	12	11
1:A:321:TRP:C	1:A:321:TRP:CD2	0.44	2.88	15	1
2:B:434:LEU:CD1	2:B:445:ALA:CB	0.44	2.95	15	1
1:A:310:ARG:HA	1:A:314:LEU:CD2	0.44	2.41	20	1
1:A:252:ILE:HG12	1:A:312:LEU:HD21	0.44	1.89	11	1
1:A:290:LEU:HD21	1:A:300:LEU:HD11	0.44	1.89	11	1
2:B:444:LEU:CD2	2:B:477:LYS:HE3	0.44	2.41	14	1
2:B:441:ASP:OD1	2:B:444:LEU:N	0.44	2.45	16	1
2:B:448:LEU:CD1	2:B:467:LEU:HD22	0.44	2.43	17	1
1:A:259:ASP:O	1:A:260:LEU:C	0.44	2.56	7	7
1:A:293:PRO:HD3	2:B:483:MET:CG	0.44	2.43	5	6
1:A:295:LEU:HB2	1:A:300:LEU:CD2	0.44	2.39	6	1
1:A:258:ASP:OD1	1:A:271:LYS:NZ	0.44	2.50	8	1
1:A:249:PHE:CD1	1:A:249:PHE:N	0.44	2.85	9	2
1:A:269:CYS:SG	1:A:294:ASN:O	0.44	2.76	11	1
1:A:257:VAL:CA	1:A:260:LEU:HD13	0.44	2.40	14	2
1:A:254:LEU:HD21	1:A:326:ILE:HD13	0.44	1.88	14	1
2:B:448:LEU:CD1	2:B:459:LEU:HD23	0.44	2.43	1	2
1:A:276:HIS:CG	1:A:277:TYR:N	0.44	2.86	8	4
2:B:466:ASP:O	2:B:469:ASP:OD1	0.44	2.35	4	1
1:A:312:LEU:O	1:A:313:SER:HB3	0.44	2.12	15	2
1:A:286:GLU:O	1:A:290:LEU:CD2	0.44	2.66	9	3
2:B:449:ALA:CB	2:B:454:CYS:SG	0.44	3.06	11	1
2:B:464:ILE:CG2	2:B:475:ASP:HA	0.44	2.42	18	3
1:A:260:LEU:CD2	1:A:278:ILE:HD11	0.44	2.43	17	1
1:A:296:GLY:N	1:A:299:SER:OG	0.44	2.48	2	1
2:B:440:VAL:HG22	2:B:481:LEU:HD22	0.44	1.89	3	2
2:B:463:GLY:O	2:B:466:ASP:N	0.44	2.50	5	4
1:A:321:TRP:O	1:A:326:ILE:HD12	0.44	2.12	13	1
1:A:281:LEU:HD12	1:A:289:LEU:CD1	0.44	2.42	16	1
2:B:435:LEU:C	2:B:435:LEU:CD1	0.44	2.86	5	3
2:B:432:ASP:O	2:B:436:ASN:CB	0.44	2.65	19	1
1:A:321:TRP:HB3	1:A:322:PRO:HD3	0.44	1.90	15	15
1:A:262:LEU:CD1	1:A:302:GLU:CG	0.44	2.96	13	1
2:B:430:PRO:HG3	2:B:446:PHE:CE1	0.44	2.48	15	2
2:B:436:ASN:OD1	2:B:436:ASN:C	0.44	2.55	18	1
1:A:266:SER:CB	1:A:302:GLU:OE1	0.44	2.65	1	1
1:A:313:SER:OG	1:A:313:SER:O	0.44	2.33	7	1
1:A:282:VAL:CG1	1:A:312:LEU:HA	0.44	2.43	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:295:LEU:HB3	1:A:300:LEU:HD21	0.43	1.90	3	2
1:A:271:LYS:HG3	1:A:276:HIS:ND1	0.43	2.28	11	4
1:A:311:GLY:HA2	1:A:314:LEU:HD11	0.43	1.88	5	1
1:A:271:LYS:CE	1:A:276:HIS:CE1	0.43	3.01	17	2
1:A:256:PRO:O	1:A:257:VAL:C	0.43	2.57	19	15
1:A:249:PHE:N	1:A:323:PRO:CG	0.43	2.81	4	1
2:B:444:LEU:CD1	2:B:473:LEU:CD2	0.43	2.84	7	1
2:B:448:LEU:CD1	2:B:459:LEU:HD21	0.43	2.42	17	2
1:A:253:LEU:CD1	1:A:282:VAL:CG2	0.43	2.96	13	1
1:A:290:LEU:O	2:B:483:MET:HE1	0.43	2.13	1	1
2:B:472:GLY:C	2:B:473:LEU:HD22	0.43	2.34	5	2
1:A:258:ASP:OD1	1:A:271:LYS:CE	0.43	2.66	8	1
1:A:323:PRO:HG3	1:A:326:ILE:HD12	0.43	1.87	10	1
1:A:307:LEU:HD12	1:A:312:LEU:HD12	0.43	1.91	15	1
1:A:291:LYS:C	2:B:483:MET:HE2	0.43	2.33	7	2
1:A:293:PRO:HB2	2:B:479:GLY:HA2	0.43	1.90	1	3
1:A:290:LEU:O	2:B:486:ARG:NH2	0.43	2.51	2	1
2:B:437:LEU:HD11	2:B:488:ILE:CD1	0.43	2.43	5	1
2:B:451:ARG:CD	2:B:470:ILE:CD1	0.43	2.97	5	1
1:A:292:THR:CG2	1:A:295:LEU:HG	0.43	2.44	1	1
2:B:451:ARG:HD2	2:B:470:ILE:HD11	0.43	1.89	5	1
1:A:318:LEU:HD22	1:A:321:TRP:HE3	0.43	1.74	11	1
1:A:253:LEU:HD11	1:A:316:MET:HE2	0.43	1.90	19	1
1:A:293:PRO:CA	2:B:483:MET:SD	0.43	3.07	7	2
2:B:448:LEU:HD12	2:B:453:VAL:HG11	0.43	1.91	2	1
2:B:448:LEU:CD2	2:B:459:LEU:HD23	0.43	2.43	8	2
1:A:293:PRO:HB2	2:B:464:ILE:CG1	0.43	2.44	5	7
1:A:298:LYS:O	1:A:302:GLU:OE1	0.43	2.36	7	1
1:A:322:PRO:CB	1:A:326:ILE:HD11	0.43	2.44	8	1
1:A:252:ILE:CD1	1:A:312:LEU:HD11	0.43	2.43	11	1
2:B:435:LEU:CD1	2:B:442:ARG:HA	0.43	2.43	7	2
1:A:290:LEU:HA	1:A:295:LEU:CD1	0.43	2.43	2	2
1:A:253:LEU:HD23	1:A:282:VAL:CG2	0.43	2.44	3	1
2:B:437:LEU:HB2	2:B:456:LEU:HD13	0.43	1.90	4	1
1:A:314:LEU:O	1:A:315:GLY:C	0.43	2.56	11	1
1:A:306:VAL:HB	1:A:312:LEU:HD11	0.43	1.90	13	1
1:A:318:LEU:N	1:A:318:LEU:CD2	0.43	2.78	17	1
2:B:462:GLN:OE1	2:B:462:GLN:CA	0.43	2.66	8	1
1:A:287:VAL:CG1	1:A:291:LYS:HE3	0.43	2.44	9	2
1:A:292:THR:HB	1:A:295:LEU:CD1	0.43	2.44	15	1
1:A:252:ILE:HG21	1:A:311:GLY:HA3	0.43	1.90	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:432:ASP:OD1	2:B:432:ASP:N	0.43	2.52	20	1
2:B:467:LEU:HD23	2:B:473:LEU:HD13	0.42	1.90	2	1
2:B:437:LEU:CD2	2:B:456:LEU:CD1	0.42	2.97	19	2
1:A:250:ASP:OD2	1:A:252:ILE:HG22	0.42	2.13	16	1
1:A:262:LEU:HD23	1:A:302:GLU:OE1	0.42	2.14	18	1
1:A:269:CYS:SG	1:A:299:SER:HB3	0.42	2.53	1	1
2:B:448:LEU:HD11	2:B:459:LEU:HD23	0.42	1.86	8	1
1:A:318:LEU:O	1:A:319:GLU:C	0.42	2.56	11	1
1:A:265:ARG:N	1:A:265:ARG:CD	0.42	2.81	20	1
1:A:294:ASN:OD1	2:B:464:ILE:CD1	0.42	2.67	2	1
1:A:262:LEU:CD2	1:A:302:GLU:CB	0.42	2.98	3	1
2:B:448:LEU:HG	2:B:459:LEU:CD1	0.42	2.43	14	2
1:A:262:LEU:CD1	1:A:302:GLU:HB3	0.42	2.44	15	1
1:A:293:PRO:HB2	2:B:482:ILE:CD1	0.42	2.39	17	1
1:A:266:SER:CA	1:A:302:GLU:OE1	0.42	2.67	1	1
1:A:278:ILE:O	1:A:279:GLY:C	0.42	2.58	13	7
1:A:253:LEU:HD12	1:A:253:LEU:H	0.42	1.74	3	1
1:A:257:VAL:O	1:A:260:LEU:CG	0.42	2.68	3	2
2:B:435:LEU:HD11	2:B:442:ARG:CG	0.42	2.40	9	1
2:B:437:LEU:CD1	2:B:456:LEU:HD11	0.42	2.36	10	1
1:A:255:ARG:CG	1:A:256:PRO:HD2	0.42	2.44	13	1
1:A:260:LEU:HD21	1:A:278:ILE:HG12	0.42	1.90	18	1
1:A:323:PRO:HD2	1:A:326:ILE:CD1	0.42	2.45	2	2
1:A:255:ARG:HG2	1:A:259:ASP:CB	0.42	2.44	10	2
1:A:323:PRO:HG2	1:A:326:ILE:CG1	0.42	2.44	10	1
1:A:271:LYS:HD2	1:A:276:HIS:ND1	0.42	2.29	13	1
1:A:252:ILE:HG21	1:A:312:LEU:HD11	0.42	1.91	14	1
1:A:275:ILE:CG2	1:A:280:ASP:HB3	0.42	2.44	1	1
1:A:257:VAL:HA	1:A:260:LEU:CD1	0.42	2.45	5	1
2:B:455:THR:O	2:B:456:LEU:C	0.42	2.58	6	3
2:B:467:LEU:CD1	2:B:478:ALA:CB	0.42	2.89	9	2
2:B:486:ARG:CZ	2:B:490:TRP:NE1	0.42	2.82	10	1
1:A:269:CYS:SG	1:A:294:ASN:HB3	0.42	2.54	12	1
1:A:262:LEU:HG	1:A:302:GLU:CG	0.42	2.44	16	1
1:A:292:THR:CG2	1:A:294:ASN:OD1	0.42	2.68	17	1
1:A:250:ASP:O	1:A:254:LEU:HD23	0.42	2.14	18	1
2:B:433:ASP:HB3	2:B:456:LEU:HB3	0.42	1.92	20	1
2:B:448:LEU:HD21	2:B:473:LEU:CD1	0.42	2.45	20	1
2:B:483:MET:O	2:B:487:ASN:CG	0.42	2.57	9	2
1:A:300:LEU:CD1	1:A:304:LYS:HE3	0.42	2.42	13	1
1:A:310:ARG:HB3	1:A:314:LEU:HD21	0.42	1.90	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:293:PRO:HB2	2:B:464:ILE:CD1	0.42	2.45	19	1
1:A:251:PRO:O	1:A:255:ARG:N	0.42	2.53	20	1
1:A:307:LEU:HD13	1:A:313:SER:CB	0.42	2.45	20	1
1:A:321:TRP:CB	1:A:322:PRO:HD3	0.42	2.45	3	2
1:A:318:LEU:HB3	1:A:322:PRO:CD	0.42	2.44	10	1
2:B:431:ALA:CB	2:B:455:THR:HA	0.42	2.45	20	2
1:A:252:ILE:CG2	1:A:312:LEU:HD11	0.42	2.45	14	1
2:B:451:ARG:NH1	2:B:470:ILE:CG1	0.42	2.83	17	1
1:A:291:LYS:O	2:B:486:ARG:NH1	0.42	2.53	18	1
1:A:322:PRO:HA	1:A:326:ILE:HD11	0.42	1.91	4	2
1:A:254:LEU:HD13	1:A:321:TRP:CH2	0.42	2.49	10	2
1:A:290:LEU:CD1	1:A:300:LEU:HD21	0.42	2.44	17	1
1:A:249:PHE:CD1	1:A:323:PRO:HB2	0.42	2.50	18	1
2:B:441:ASP:H	2:B:444:LEU:HD12	0.41	1.74	20	2
1:A:293:PRO:O	1:A:294:ASN:C	0.41	2.57	13	1
1:A:321:TRP:CE3	1:A:321:TRP:C	0.41	2.94	15	1
2:B:451:ARG:CZ	2:B:469:ASP:HB2	0.41	2.45	15	1
2:B:456:LEU:HD11	2:B:485:ALA:HB2	0.41	1.90	18	1
1:A:292:THR:C	2:B:483:MET:SD	0.41	2.99	7	3
1:A:278:ILE:O	1:A:281:LEU:HB3	0.41	2.15	8	2
2:B:453:VAL:CG2	2:B:462:GLN:CG	0.41	2.90	7	1
1:A:286:GLU:OE2	1:A:307:LEU:HD23	0.41	2.15	8	1
1:A:323:PRO:O	1:A:324:ALA:C	0.41	2.57	16	2
1:A:262:LEU:CG	1:A:302:GLU:OE1	0.41	2.68	18	1
1:A:290:LEU:CD2	1:A:300:LEU:CD2	0.41	2.98	18	1
1:A:264:VAL:O	1:A:268:ASN:CG	0.41	2.58	20	1
1:A:253:LEU:HD21	1:A:316:MET:HE2	0.41	1.91	5	1
1:A:314:LEU:HB2	1:A:316:MET:CG	0.41	2.46	7	1
2:B:486:ARG:NH2	2:B:490:TRP:CE2	0.41	2.88	10	1
1:A:307:LEU:HD13	1:A:313:SER:C	0.41	2.36	13	1
1:A:306:VAL:O	1:A:312:LEU:HD11	0.41	2.15	18	1
1:A:286:GLU:OE1	1:A:307:LEU:CD2	0.41	2.69	2	1
1:A:293:PRO:CG	2:B:479:GLY:HA2	0.41	2.45	4	2
2:B:453:VAL:CG1	2:B:458:ASP:C	0.41	2.88	19	2
1:A:293:PRO:HB3	2:B:482:ILE:HB	0.41	1.93	20	5
1:A:281:LEU:CD1	1:A:289:LEU:HG	0.41	2.46	11	1
1:A:291:LYS:C	2:B:483:MET:HE1	0.41	2.35	13	1
1:A:267:ALA:HB1	1:A:271:LYS:CE	0.41	2.44	14	1
1:A:295:LEU:HD23	1:A:303:ILE:CD1	0.41	2.44	5	1
1:A:292:THR:HG22	1:A:295:LEU:HD12	0.41	1.93	9	1
1:A:312:LEU:CD2	1:A:312:LEU:N	0.41	2.84	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:PHE:N	1:A:325:SER:CB	0.41	2.84	1	1
1:A:254:LEU:HD13	1:A:321:TRP:HZ2	0.41	1.68	3	1
2:B:463:GLY:O	2:B:464:ILE:C	0.41	2.58	19	7
1:A:282:VAL:HB	1:A:316:MET:CE	0.41	2.44	7	1
2:B:432:ASP:O	2:B:436:ASN:HB2	0.41	2.16	7	1
1:A:286:GLU:HA	1:A:289:LEU:HD23	0.41	1.93	17	1
1:A:253:LEU:CD2	1:A:316:MET:HE1	0.41	2.45	5	1
1:A:249:PHE:HB2	1:A:254:LEU:HD11	0.41	1.91	15	1
2:B:448:LEU:HD12	2:B:467:LEU:HD22	0.41	1.92	17	1
1:A:257:VAL:HG22	1:A:276:HIS:C	0.41	2.35	18	1
1:A:253:LEU:HD11	1:A:282:VAL:HG11	0.41	1.93	2	1
1:A:258:ASP:OD1	1:A:271:LYS:HE2	0.41	2.16	8	1
1:A:318:LEU:HD22	1:A:321:TRP:CE3	0.41	2.51	11	1
1:A:249:PHE:CE1	1:A:325:SER:HB3	0.41	2.51	19	1
1:A:256:PRO:O	1:A:258:ASP:N	0.41	2.53	14	5
1:A:289:LEU:HB3	1:A:295:LEU:HD11	0.41	1.93	1	1
1:A:292:THR:N	2:B:483:MET:HE1	0.41	2.31	1	1
2:B:430:PRO:CG	2:B:446:PHE:CE1	0.41	3.04	9	1
2:B:448:LEU:HD21	2:B:467:LEU:CD2	0.41	2.46	14	1
1:A:251:PRO:O	1:A:254:LEU:N	0.41	2.52	18	1
2:B:456:LEU:CD2	2:B:485:ALA:HB2	0.41	2.45	20	1
1:A:307:LEU:HG	1:A:313:SER:OG	0.41	2.15	3	1
1:A:249:PHE:N	1:A:323:PRO:HG3	0.41	2.31	4	1
2:B:441:ASP:OD1	2:B:442:ARG:N	0.41	2.54	8	1
2:B:441:ASP:OD1	2:B:444:LEU:HB2	0.40	2.16	1	1
2:B:430:PRO:CD	2:B:446:PHE:CD1	0.40	3.04	5	1
2:B:434:LEU:N	2:B:456:LEU:HB2	0.40	2.31	6	1
1:A:256:PRO:HB2	1:A:258:ASP:OD1	0.40	2.16	10	1
2:B:448:LEU:CD1	2:B:453:VAL:CG2	0.40	2.99	12	1
1:A:270:LEU:HD22	1:A:270:LEU:H	0.40	1.73	17	1
2:B:464:ILE:HG12	2:B:479:GLY:CA	0.40	2.45	19	1
1:A:271:LYS:HA	1:A:275:ILE:O	0.40	2.16	2	1
1:A:320:ASN:O	1:A:321:TRP:C	0.40	2.59	17	2
2:B:456:LEU:HG	2:B:485:ALA:CB	0.40	2.46	11	1
2:B:457:GLU:OE1	2:B:489:CYS:SG	0.40	2.74	11	1
1:A:251:PRO:HB2	1:A:255:ARG:NH2	0.40	2.31	13	1
1:A:255:ARG:HG2	1:A:259:ASP:OD2	0.40	2.17	1	1
2:B:451:ARG:NH1	2:B:469:ASP:CB	0.40	2.84	1	1
1:A:284:ARG:HG2	1:A:284:ARG:NH1	0.40	2.32	4	1
1:A:307:LEU:CD1	1:A:313:SER:CB	0.40	2.99	5	1
1:A:252:ILE:HD11	1:A:312:LEU:CD2	0.40	2.46	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:282:VAL:CG2	1:A:318:LEU:HD11	0.40	2.46	15	1
1:A:262:LEU:HB3	1:A:266:SER:HB2	0.40	1.93	16	1
1:A:287:VAL:HG12	1:A:291:LYS:HE3	0.40	1.92	2	1
1:A:297:LYS:CE	2:B:461:GLU:HA	0.40	2.46	6	1
1:A:312:LEU:CD1	1:A:312:LEU:N	0.40	2.84	8	1
1:A:307:LEU:CD2	1:A:313:SER:HG	0.40	2.28	11	1
2:B:448:LEU:HD21	2:B:459:LEU:HB2	0.40	1.94	13	1
1:A:280:ASP:O	1:A:283:GLN:HB3	0.40	2.17	19	1
2:B:437:LEU:HG	2:B:456:LEU:CD1	0.40	2.46	19	1
2:B:485:ALA:O	2:B:486:ARG:C	0.40	2.60	20	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	77/99 (78%)	70±1 (91±2%)	6±1 (7±2%)	1±1 (2±1%)	12	54
2	B	65/74 (88%)	63±1 (97±2%)	2±1 (3±2%)	0±0 (0±0%)	100	100
All	All	2840/3460 (82%)	2664 (94%)	148 (5%)	28 (1%)	20	68

All 4 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	321	TRP	18
1	A	262	LEU	5
1	A	322	PRO	3
1	A	313	SER	2

### 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	69/88 (78%)	64±2 (93±2%)	5±2 (7±2%)	19	67
2	B	49/55 (89%)	46±1 (95±2%)	3±1 (5±2%)	26	75
All	All	2360/2860 (83%)	2211 (94%)	149 (6%)	21	70

All 25 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	257	VAL	20
2	B	455	THR	20
1	A	313	SER	13
2	B	435	LEU	12
1	A	312	LEU	11
1	A	250	ASP	9
1	A	321	TRP	8
1	A	255	ARG	7
2	B	429	LYS	7
1	A	309	SER	5
1	A	254	LEU	4
1	A	249	PHE	4
2	B	456	LEU	4
1	A	295	LEU	4
1	A	292	THR	4
2	B	474	THR	4
2	B	454	CYS	3
2	B	489	CYS	2
1	A	253	LEU	2
1	A	300	LEU	1
1	A	307	LEU	1
1	A	260	LEU	1
1	A	265	ARG	1
1	A	269	CYS	1
2	B	448	LEU	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 [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_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	1886
Number of shifts mapped to atoms	1678
Number of unparsed shifts	0
Number of shifts with mapping errors	208
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 208 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	231	GLY	HA2	3.9	0.03	2
1	A	231	GLY	HA3	3.9	0.03	2
1	A	231	GLY	CA	45.37	0.2	1
1	A	232	PRO	HA	4.43	0.03	1
1	A	232	PRO	HB2	1.89	0.03	2
1	A	232	PRO	HB3	2.26	0.03	2
1	A	232	PRO	HD2	3.43	0.03	2
1	A	232	PRO	HD3	3.64	0.03	2
1	A	232	PRO	HG2	1.98	0.03	2
1	A	232	PRO	HG3	1.98	0.03	2
1	A	232	PRO	CA	63.04	0.2	1
1	A	232	PRO	CB	32.29	0.2	1
1	A	232	PRO	CD	49.63	0.2	1
1	A	232	PRO	CG	27.01	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	233	ASP	H	8.55	0.03	1
1	A	233	ASP	HA	4.57	0.03	1
1	A	233	ASP	HB2	2.56	0.03	2
1	A	233	ASP	HB3	2.72	0.03	2
1	A	233	ASP	CA	54.46	0.2	1
1	A	233	ASP	CB	41.12	0.2	1
1	A	233	ASP	N	120.98	0.2	1
1	A	234	LEU	H	8.33	0.03	1
1	A	234	LEU	HA	4.3	0.03	1
1	A	234	LEU	HB2	1.6	0.03	2
1	A	234	LEU	HB3	1.6	0.03	2
1	A	234	LEU	HD11	0.89	0.03	2
1	A	234	LEU	HD12	0.89	0.03	2
1	A	234	LEU	HD13	0.89	0.03	2
1	A	234	LEU	HD21	0.82	0.03	2
1	A	234	LEU	HD22	0.82	0.03	2
1	A	234	LEU	HD23	0.82	0.03	2
1	A	234	LEU	HG	1.79	0.03	1
1	A	234	LEU	CA	55.28	0.2	1
1	A	234	LEU	CB	41.89	0.2	1
1	A	234	LEU	CD1	25.0	0.2	2
1	A	234	LEU	CD2	23.24	0.2	2
1	A	234	LEU	CG	27.04	0.2	1
1	A	234	LEU	N	124.15	0.2	1
1	A	235	ARG	H	8.3	0.03	1
1	A	235	ARG	HA	4.21	0.03	1
1	A	235	ARG	HB2	1.6	0.03	2
1	A	235	ARG	HB3	1.78	0.03	2
1	A	235	ARG	HD2	3.17	0.03	2
1	A	235	ARG	HD3	3.17	0.03	2
1	A	235	ARG	HE	7.34	0.03	1
1	A	235	ARG	HG2	1.59	0.03	2
1	A	235	ARG	HG3	1.59	0.03	2
1	A	235	ARG	CA	56.53	0.2	1
1	A	235	ARG	CB	30.65	0.2	1
1	A	235	ARG	CD	43.4	0.2	1
1	A	235	ARG	CG	27.04	0.2	1
1	A	235	ARG	N	121.16	0.2	1
1	A	236	ASP	H	8.29	0.03	1
1	A	236	ASP	HA	4.58	0.03	1
1	A	236	ASP	HB2	2.72	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	236	ASP	HB3	2.56	0.03	2
1	A	236	ASP	CA	54.24	0.2	1
1	A	236	ASP	CB	41.12	0.2	1
1	A	236	ASP	N	120.88	0.2	1
1	A	237	VAL	H	7.96	0.03	1
1	A	237	VAL	HA	4.06	0.03	1
1	A	237	VAL	HB	2.09	0.03	1
1	A	237	VAL	HG11	0.88	0.03	2
1	A	237	VAL	HG12	0.88	0.03	2
1	A	237	VAL	HG13	0.88	0.03	2
1	A	237	VAL	HG21	0.88	0.03	2
1	A	237	VAL	HG22	0.88	0.03	2
1	A	237	VAL	HG23	0.88	0.03	2
1	A	237	VAL	CA	62.26	0.2	1
1	A	237	VAL	CB	32.52	0.2	1
1	A	237	VAL	CG1	21.15	0.2	2
1	A	237	VAL	CG2	21.15	0.2	2
1	A	237	VAL	N	120.43	0.2	1
1	A	238	ARG	H	8.36	0.03	1
1	A	238	ARG	HA	4.31	0.03	1
1	A	238	ARG	HB2	1.79	0.03	2
1	A	238	ARG	HB3	1.79	0.03	2
1	A	238	ARG	HD2	3.16	0.03	2
1	A	238	ARG	HD3	3.16	0.03	2
1	A	238	ARG	HE	7.41	0.03	1
1	A	238	ARG	HG2	1.59	0.03	2
1	A	238	ARG	HG3	1.59	0.03	2
1	A	238	ARG	CA	55.93	0.2	1
1	A	238	ARG	CB	30.73	0.2	1
1	A	238	ARG	CD	43.29	0.2	1
1	A	238	ARG	CG	27.04	0.2	1
1	A	238	ARG	N	124.66	0.2	1
1	A	239	GLN	H	8.41	0.03	1
1	A	239	GLN	HA	4.57	0.03	1
1	A	239	GLN	HB2	1.9	0.03	2
1	A	239	GLN	HB3	2.09	0.03	2
1	A	239	GLN	HE21	7.57	0.03	1
1	A	239	GLN	HE22	6.87	0.03	1
1	A	239	GLN	HG2	2.37	0.03	2
1	A	239	GLN	HG3	2.37	0.03	2
1	A	239	GLN	CA	53.64	0.2	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	239	GLN	CB	28.75	0.2	1
1	A	239	GLN	CG	33.47	0.2	1
1	A	239	GLN	N	122.96	0.2	1
1	A	239	GLN	NE2	112.77	0.2	1
1	A	240	PRO	HA	4.36	0.03	1
1	A	240	PRO	HB2	2.27	0.03	2
1	A	240	PRO	HB3	1.87	0.03	2
1	A	240	PRO	HD2	3.64	0.03	2
1	A	240	PRO	HD3	3.75	0.03	2
1	A	240	PRO	HG2	1.98	0.03	2
1	A	240	PRO	HG3	1.98	0.03	2
1	A	240	PRO	CA	63.19	0.2	1
1	A	240	PRO	CB	32.15	0.2	1
1	A	240	PRO	CD	50.62	0.2	1
1	A	240	PRO	CG	27.38	0.2	1
1	A	241	GLU	H	8.54	0.03	1
1	A	241	GLU	HA	4.22	0.03	1
1	A	241	GLU	HB2	1.88	0.03	2
1	A	241	GLU	HB3	1.97	0.03	2
1	A	241	GLU	HG2	2.18	0.03	2
1	A	241	GLU	HG3	2.27	0.03	2
1	A	241	GLU	CA	56.58	0.2	1
1	A	241	GLU	CB	30.28	0.2	1
1	A	241	GLU	CG	36.24	0.2	1
1	A	241	GLU	N	121.45	0.2	1
1	A	242	VAL	H	8.23	0.03	1
1	A	242	VAL	HA	4.06	0.03	1
1	A	242	VAL	HB	2.0	0.03	1
1	A	242	VAL	HG11	0.82	0.03	2
1	A	242	VAL	HG12	0.82	0.03	2
1	A	242	VAL	HG13	0.82	0.03	2
1	A	242	VAL	HG21	0.82	0.03	2
1	A	242	VAL	HG22	0.82	0.03	2
1	A	242	VAL	HG23	0.82	0.03	2
1	A	242	VAL	CA	62.26	0.2	1
1	A	242	VAL	CB	32.78	0.2	1
1	A	242	VAL	CG1	21.09	0.2	2
1	A	242	VAL	CG2	21.09	0.2	2
1	A	242	VAL	N	122.63	0.2	1
1	A	243	LYS	H	8.45	0.03	1
1	A	243	LYS	HA	4.31	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	243	LYS	HB2	1.7	0.03	2
1	A	243	LYS	HB3	1.77	0.03	2
1	A	243	LYS	HD2	1.64	0.03	2
1	A	243	LYS	HD3	1.64	0.03	2
1	A	243	LYS	HE2	2.95	0.03	2
1	A	243	LYS	HE3	2.95	0.03	2
1	A	243	LYS	HG2	1.36	0.03	2
1	A	243	LYS	HG3	1.36	0.03	2
1	A	243	LYS	CA	55.93	0.2	1
1	A	243	LYS	CB	33.24	0.2	1
1	A	243	LYS	CD	29.07	0.2	1
1	A	243	LYS	CE	42.13	0.2	1
1	A	243	LYS	CG	24.61	0.2	1
1	A	243	LYS	N	126.37	0.2	1
1	A	244	GLU	H	8.47	0.03	1
1	A	244	GLU	HA	4.26	0.03	1
1	A	244	GLU	HB2	1.92	0.03	2
1	A	244	GLU	HB3	1.92	0.03	2
1	A	244	GLU	HG2	2.2	0.03	2
1	A	244	GLU	HG3	2.2	0.03	2
1	A	244	GLU	CA	56.26	0.2	1
1	A	244	GLU	CB	30.31	0.2	1
1	A	244	GLU	CG	36.3	0.2	1
1	A	244	GLU	N	123.24	0.2	1
1	A	245	GLU	H	8.48	0.03	1
1	A	245	GLU	HA	4.31	0.03	1
1	A	245	GLU	HB2	1.87	0.03	2
1	A	245	GLU	HB3	1.97	0.03	2
1	A	245	GLU	HG2	2.2	0.03	2
1	A	245	GLU	HG3	2.2	0.03	2
1	A	245	GLU	CA	55.93	0.2	1
1	A	245	GLU	CB	30.44	0.2	1
1	A	245	GLU	CG	36.3	0.2	1
1	A	245	GLU	N	123.38	0.2	1
1	A	246	LYS	H	8.43	0.03	1
1	A	246	LYS	HA	4.61	0.03	1
1	A	246	LYS	HB2	1.67	0.03	2
1	A	246	LYS	HB3	1.78	0.03	2
1	A	246	LYS	HD2	1.65	0.03	2
1	A	246	LYS	HD3	1.65	0.03	2
1	A	246	LYS	HE2	2.96	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	246	LYS	HE3	2.96	0.03	2
1	A	246	LYS	HG2	1.4	0.03	2
1	A	246	LYS	HG3	1.4	0.03	2
1	A	246	LYS	CA	54.18	0.2	1
1	A	246	LYS	CB	32.52	0.2	1
1	A	246	LYS	CD	29.15	0.2	1
1	A	246	LYS	CE	42.26	0.2	1
1	A	246	LYS	CG	24.42	0.2	1
1	A	246	LYS	N	124.13	0.2	1
1	A	247	PRO	HA	4.66	0.03	1
1	A	247	PRO	HB2	2.09	0.03	2
1	A	247	PRO	HB3	2.36	0.03	2
1	A	247	PRO	HD2	3.53	0.03	2
1	A	247	PRO	HD3	3.59	0.03	2
1	A	247	PRO	HG2	1.81	0.03	2
1	A	247	PRO	HG3	1.93	0.03	2
1	A	247	PRO	CA	62.58	0.2	1
1	A	247	PRO	CB	34.34	0.2	1
1	A	247	PRO	CD	50.28	0.2	1
1	A	247	PRO	CG	24.78	0.2	1
1	A	248	GLU	H	8.56	0.03	1
1	A	248	GLU	HA	4.06	0.03	1
1	A	248	GLU	HB2	1.88	0.03	2
1	A	248	GLU	HB3	1.81	0.03	2
1	A	248	GLU	HG2	2.21	0.03	2
1	A	248	GLU	HG3	2.21	0.03	2
1	A	248	GLU	CA	57.02	0.2	1
1	A	248	GLU	CB	30.7	0.2	1
1	A	248	GLU	CG	36.3	0.2	1
1	A	248	GLU	N	121.84	0.2	1

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	167	$-0.19 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	156	$0.13 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	159	$0.74 \pm 0.26$	Should be applied

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1615 atoms were assigned a chemical shift out of a possible 1940. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	567/713 (80%)	289/290 (100%)	141/286 (49%)	137/137 (100%)
Sidechain	1006/1157 (87%)	696/755 (92%)	302/362 (83%)	8/40 (20%)
Aromatic	42/70 (60%)	24/35 (69%)	16/32 (50%)	2/3 (67%)
Overall	1615/1940 (83%)	1009/1080 (93%)	459/680 (68%)	147/180 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1677 atoms were assigned a chemical shift out of a possible 2015. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	600/754 (80%)	306/307 (100%)	149/302 (49%)	145/145 (100%)
Sidechain	1035/1191 (87%)	716/775 (92%)	311/376 (83%)	8/40 (20%)
Aromatic	42/70 (60%)	24/35 (69%)	16/32 (50%)	2/3 (67%)
Overall	1677/2015 (83%)	1046/1117 (94%)	476/710 (67%)	155/188 (82%)

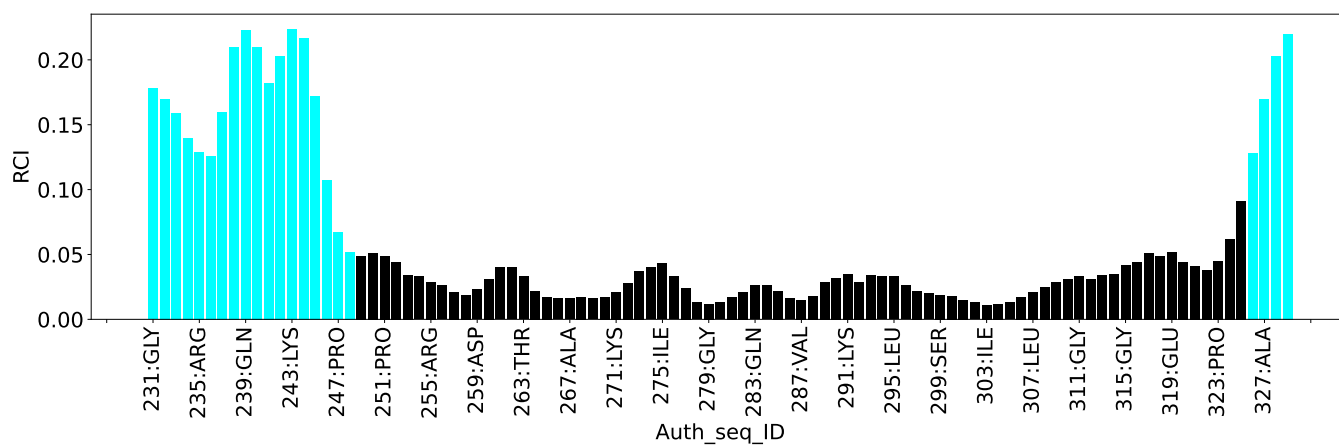
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

