Full wwPDB NMR Structure Validation Report (i)

Oct 11, 2021 – 08:57 PM EDT

PDB ID	:	2KJB
Title	:	Solution structure of CzrA in the DNA bound state
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Deposited on	:	2009-05-27

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

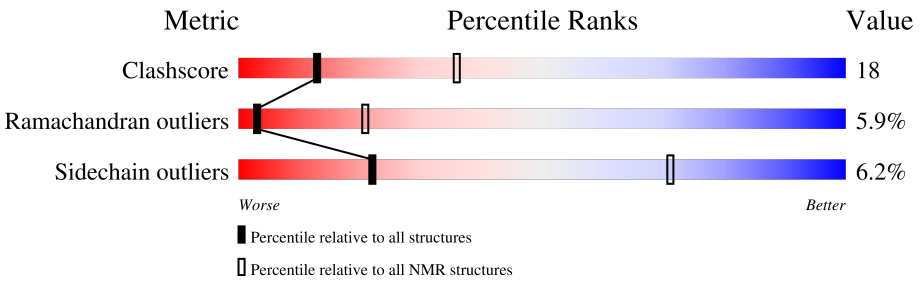
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	106	52% 30% 8% 10%
1	B	106	61% 21% 8% 10%

2 Ensemble composition and analysis (i)

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:11-A:97, B:11-B:97 (174)	0.62	1

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 7, 8, 9, 10, 11, 12, 13, 14, 15, 18, 19, 21
2	6, 16
3	5, 17
Single-model clusters	20

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3072 atoms, of which 1562 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CzrA protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1536	471	781	141	140	3	0
1	B	95	1536	471	781	141	140	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP O85142
B	2	ALA	SER	engineered mutation	UNP O85142

4 Residue-property plots (i)

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: CzrA protein

Chain A: 52% 30% 8% 10%

• Molecule 1: CzrA protein

Chain B: 61% 21% 8% 10%

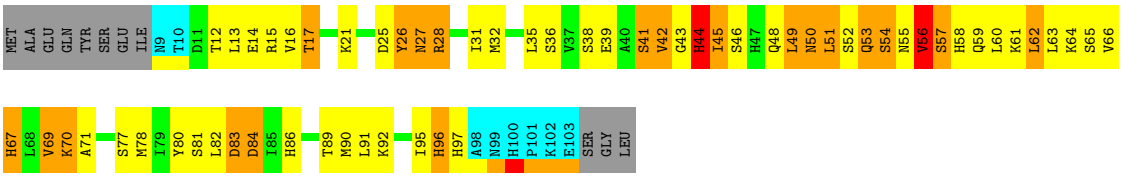
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: CzrA protein

Chain A: 25% 37% 19% • 8% 10%



• Molecule 1: CzrA protein

Chain B: 31% 25% 24% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 D11 T12 L13 E14 R15 V16 T17 E18 I19 F20 K21 A22 L23 G24 D25 Y26 N27 R28 I29 R30 I31 M32 L35 S36 V37 S38 E39 A40 S41 V42 G43 H44 I45 S46 H47 Q48 L49 N50 L51 S52 Q53 S54 N55 V56 S57 H58 Q59 L60 K61

L62 L63 K64 S65 V66 H67 L68 V69 S77 M78 I79 Y80 S81 L82 D83 H97 A98 N99 H100 P101 K102 E103 SER GLY LEU

4.2.2 Score per residue for model 2

- Molecule 1: CzrA protein

Chain A: 52% 28% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 D11 T12 L13 K21 N27 I31 M32 L35 S36 V37 S38 E39 N50 N55 V56 S57 H58 Q59 L63 K64 K70 A71 Q76 S77 M78 S81 L82 D83 D84 V87 A88 T89 M90 L91 I95 A98 N99

H100 P101 K102 E103 SER GLY LEU

- Molecule 1: CzrA protein

Chain B: 56% 23% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 D11 G24 I29 R30 I31 M32 L35 S36 V37 S38 G43 S46 N55 V56 S57 H58 Q59 L63 V66 G75 Q76 S77 M78 I79 L82 D83 D84 V87 A88 L91 A98 N99 H100 P101 K102 E103 SER

GLY LEU

4.2.3 Score per residue for model 3

- Molecule 1: CzrA protein

Chain A: 51% 25% 7% 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 D11 E14 R15 V16 F20 G24 R28 I29 R30 L34 S38 S41 V42 G43 H44 I45 S46 H47 Q48 L49 Q53 S54 N55 V56 Q59 L60 K61 L62 L63 L68 R73 Q76 S77 M78 D83 D84 I85

H86 V87 A88 A98 N99 H100 P101 K102 E103 SER GLY LEU

- Molecule 1: CzrA protein

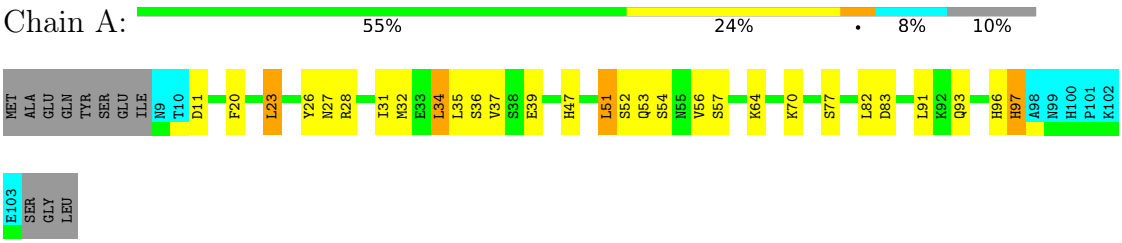
Chain B: 58% 17% 8% 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 M32 L35 S36 V37 S46 L49 S52 Q53 S54 N55 V56 S57 H58 Q59 L63 K64 S65 V66 Q76 S77 M78 I79 Y80 H86 M90 L91 K92 Q93 H96 H97 A98 N99 H100 P101 K102 E103 SER GLY LEU

4.2.4 Score per residue for model 4

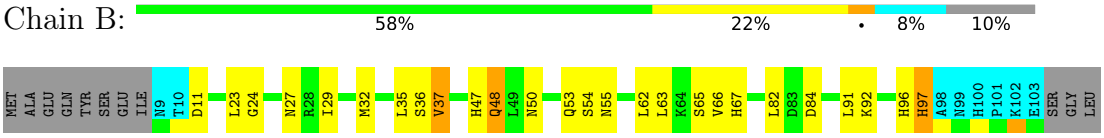
- Molecule 1: CzrA protein

Chain A:



- Molecule 1: CzrA protein

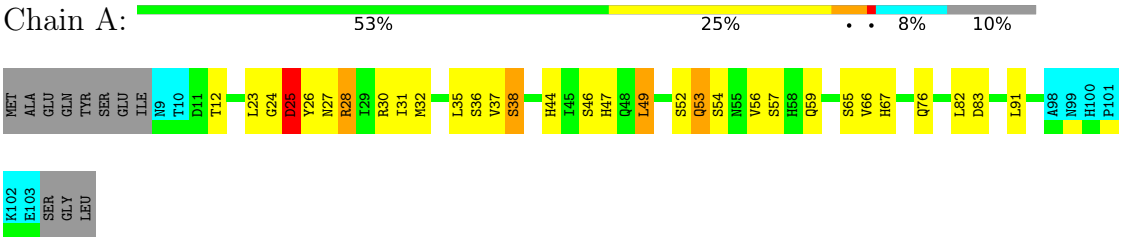
Chain B:



4.2.5 Score per residue for model 5

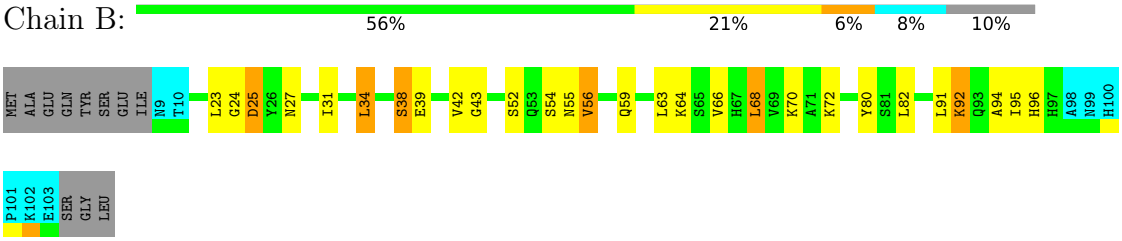
- Molecule 1: CzrA protein

Chain A:



- Molecule 1: CzrA protein

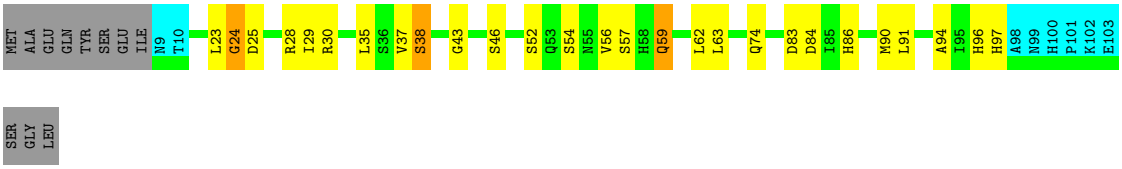
Chain B:



4.2.6 Score per residue for model 6

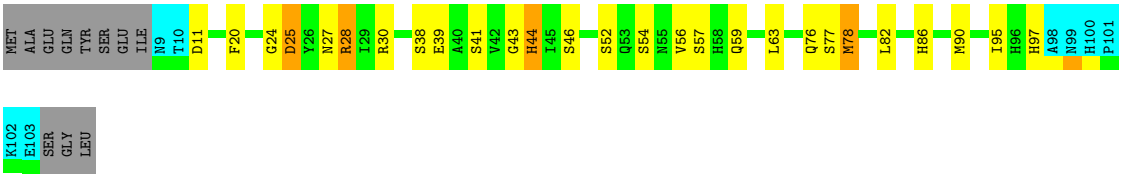
- Molecule 1: CzrA protein

Chain A:



• Molecule 1: CzrA protein

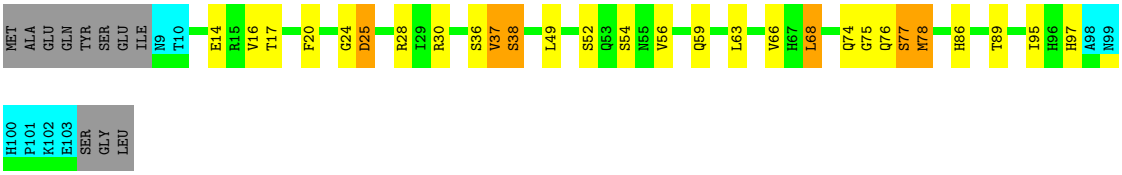
Chain B:



4.2.7 Score per residue for model 7

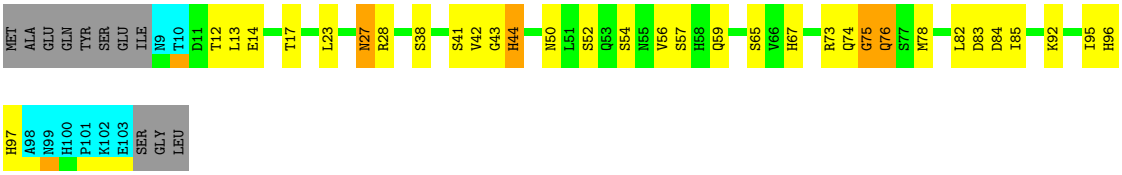
• Molecule 1: CzrA protein

Chain A:



• Molecule 1: CzrA protein

Chain B:



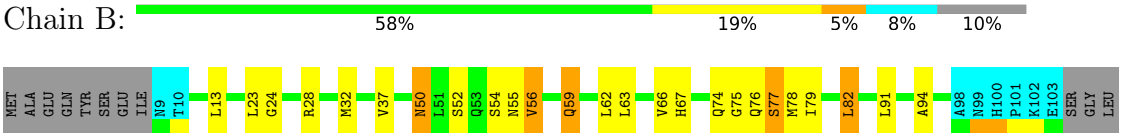
4.2.8 Score per residue for model 8

• Molecule 1: CzrA protein

Chain A:

• Molecule 1: CzrA protein

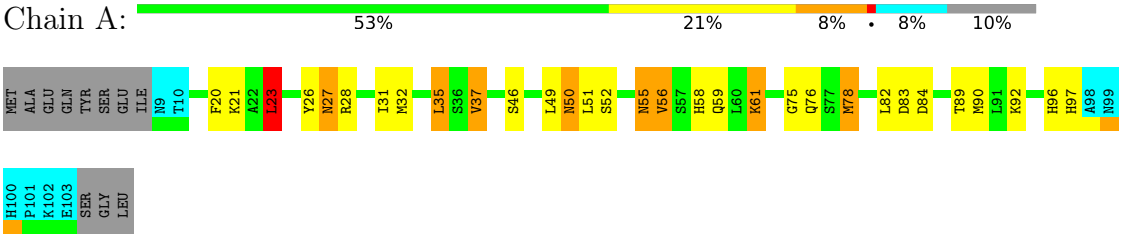
Chain B:



4.2.9 Score per residue for model 9

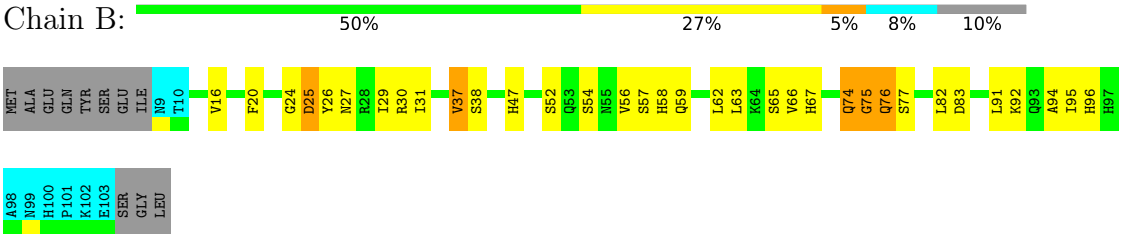
• Molecule 1: CzrA protein

Chain A:



• Molecule 1: CzrA protein

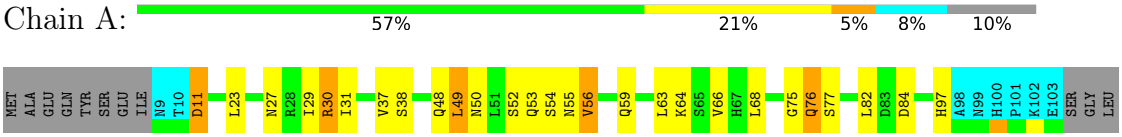
Chain B:



4.2.10 Score per residue for model 10

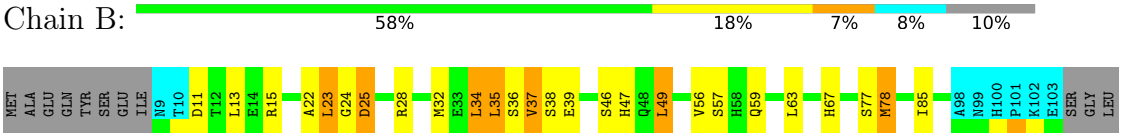
• Molecule 1: CzrA protein

Chain A:



• Molecule 1: CzrA protein

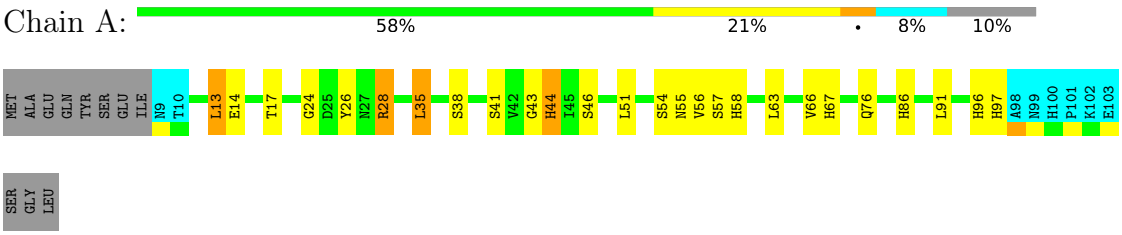
Chain B:



4.2.11 Score per residue for model 11

- Molecule 1: CzrA protein

Chain A:



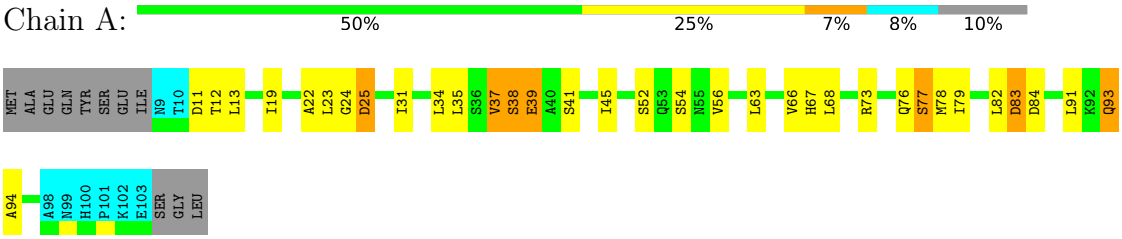
- Molecule 1: CzrA protein

Chain B:

4.2.12 Score per residue for model 12

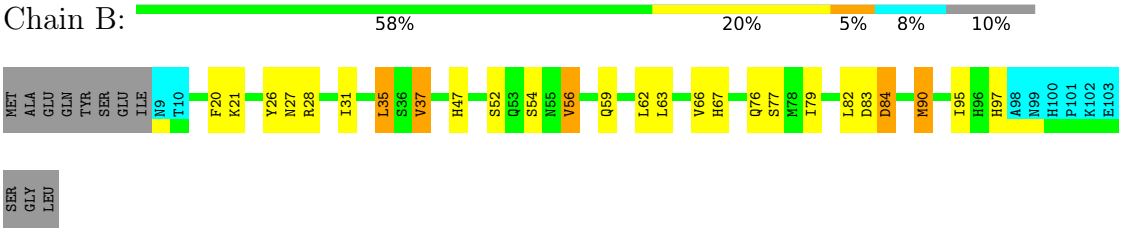
- Molecule 1: CzrA protein

Chain A:



- Molecule 1: CzrA protein

Chain B:



4.2.13 Score per residue for model 13

- Molecule 1: CzrA protein

Chain A: 51% 28% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 D11 G24 D25 Y26 N27 R28 I29 R30 I31 M32 L35 S36 V37 S38 E39 G43 S46 L49 N50 L51 S52 Q53 S54 N55 V56 S57 H58 Q59 L62 L63 K64 S65 R73 Q74 S77 M78 T79 Y80 D84 L91

A98 N99 H100 P101 K102 E103 SER GLY LEU

- Molecule 1: CzrA protein

Chain B: 58% 20% 5% 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 D11 G24 D25 Y26 N27 R28 I31 L34 L35 S36 V37 S46 H47 Q48 L49 N50 N55 V56 S57 H58 Q59 L62 V66 H67 G75 Q76 S77 D84 H97 A98 N99 H100 P101 K102 E103 SER GLY LEU

4.2.14 Score per residue for model 14

- Molecule 1: CzrA protein

Chain A: 55% 23% 5% 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 G24 R28 I29 R30 I31 L34 L35 S36 V37 S38 V42 G43 S46 H47 Q48 L49 N50 L51 S52 Q53 S54 N55 V56 L63 V66 H67 L68 G75 Q76 S77 M78 L82 D83 D84 L91 H97 A98 N99 H100

P101 K102 E103 SER GLY LEU

- Molecule 1: CzrA protein

Chain B: 54% 26% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 D11 T12 L13 E14 T17 D25 R28 I29 R30 L35 S36 V37 S38 G43 S46 H47 S52 Q53 S54 N55 V56 Q59 L62 S65 V66 H67 S77 M78 L82 I85 H86 L91 I95 A98

N99 H100 P101 K102 E103 SER GLY LEU

4.2.15 Score per residue for model 15

- Molecule 1: CzrA protein

Chain A: 58% 20% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 F20 Y26 N27 R28 M32 V37 S38 E39 Q53 S54 N55 V56 S57 K61 L62 L63 K64 S65 V66 H67 Q74 G75 Q76 S77 M78 H86 L91 A94 A98 N99 H100 P101 K102 E103 SER GLY LEU

- Molecule 1: CzrA protein

Chain B: 62% 18% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 L23 Y26 N27 R28 V37 V42 G43 S46 L51 V56 S57 H58 Q59 L60 L63 V66 H67 L82 D83 I95 H96 H97 A98 N99 H100 P101 K102 E103 SER GLY LEU

4.2.16 Score per residue for model 16

- Molecule 1: CzrA protein

Chain A: 52% 25% 6% 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 E14 T17 A22 L23 G24 D25 Y26 L35 S38 E39 A40 S41 V42 G43 H44 I45 S46 L49 V56 L63 K64 S65 V66 H67 K70 A71 K72 Y80 S81 L82 D83 D84 I85 H86 T89 A94 H97

A98 N99 H100 P101 K102 E103 SER GLY LEU

- Molecule 1: CzrA protein

Chain B: 53% 25% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 L13 V16 F20 G24 D25 Y26 N27 R28 I31 M32 E33 L34 L35 S36 V37 S38 E39 G43 H44 I45 S46 L49 N50 L51 S52 Q53 V56 S57 H58 Q59 V66 H67 L68 V69 K70 G75 Q76 I85

A98 N99 H100 P101 K102 E103 SER GLY LEU

4.2.17 Score per residue for model 17

- Molecule 1: CzrA protein

Chain A: 57% 23% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 I19 A22 L23 G24 D25 Y26 N27 R28 L35 S41 V42 G43 H44 H47 Q53 S54 N55 V56 Q59 L62 L63 V66 H67 S77 M78 I79 L82 L91 A94 A98 N99 H100 P101 K102 E103 SER

GLY LEU

- Molecule 1: CzrA protein

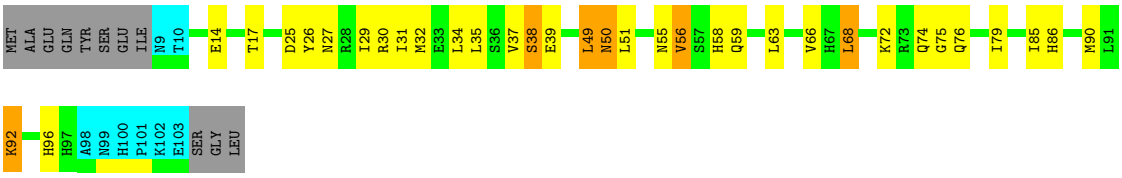
Chain B: 61% 18% • 8% 10%

MET ALA GLU GLN TYR SER GLU ILE N9 T10 E14 L23 G24 I29 R30 I31 L34 L35 S36 V37 S38 H44 S52 Q53 S54 N55 V56 S57 H58 L62 L63 L82 D83 D84 A94 I95 H96 H97 A98 N99 H100 P101 K102 E103 SER GLY LEU

4.2.18 Score per residue for model 18

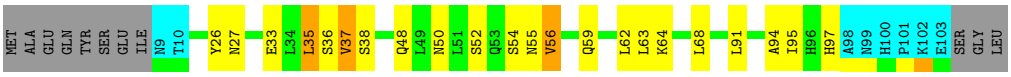
- Molecule 1: CzrA protein

Chain A: 50% 26% 6% 8% 10%



- Molecule 1: CzrA protein

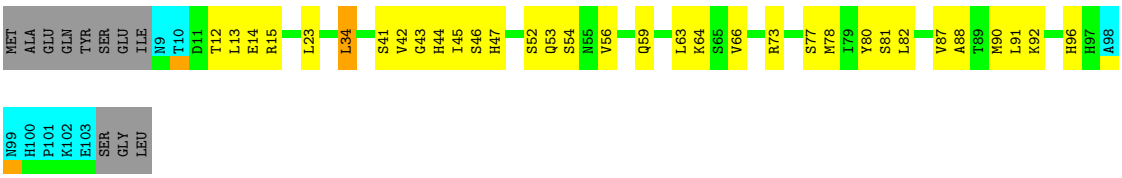
Chain B: 61% 18% • 8% 10%



4.2.19 Score per residue for model 19

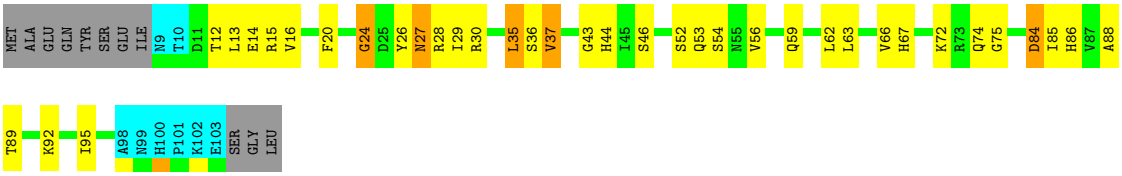
- Molecule 1: CzrA protein

Chain A: 51% 30% • 8% 10%



- Molecule 1: CzrA protein

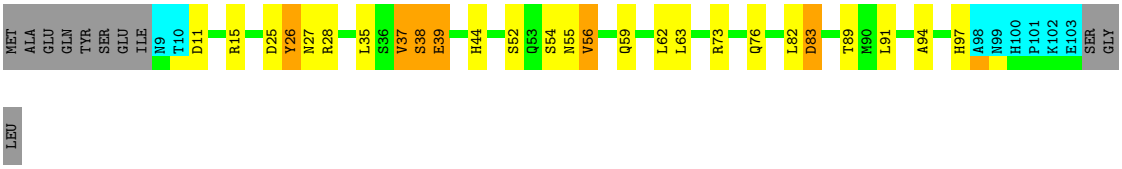
Chain B: 47% 30% 5% 8% 10%



4.2.20 Score per residue for model 20

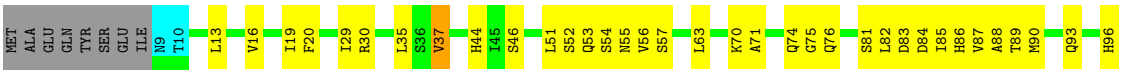
- Molecule 1: CzrA protein

Chain A: 58% 19% 6% 8% 10%



• Molecule 1: CzrA protein

Chain B: 48% 33% • 8% 10%



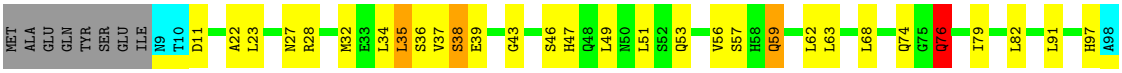
4.2.21 Score per residue for model 21

• Molecule 1: CzrA protein

Chain A: 58% 22% • 8% 10%

• Molecule 1: CzrA protein

Chain B: 54% 25% • • 8% 10%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 21 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
X-PLOR-NIH	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	692	723	716	26±10
1	B	692	723	716	26±10
All	All	29064	30366	30072	1093

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:TYR:CD1	1:B:26:TYR:N	1.12	2.12	1	2
1:A:53:GLN:HA	1:A:56:VAL:CG2	0.96	1.89	1	1
1:B:56:VAL:HG12	1:B:57:SER:N	0.94	1.75	1	1
1:A:28:ARG:NE	1:A:63:LEU:HD11	0.91	1.80	1	1
1:B:37:VAL:O	1:B:37:VAL:HG13	0.90	1.67	1	1
1:A:66:VAL:O	1:A:67:HIS:HB2	0.84	1.71	1	1
1:B:26:TYR:N	1:B:26:TYR:HD1	0.84	1.55	1	1
1:B:60:LEU:HD13	1:B:80:TYR:CE2	0.84	2.08	1	1
1:B:82:LEU:N	1:B:82:LEU:HD23	0.81	1.89	1	3
1:A:53:GLN:HA	1:A:56:VAL:HG23	0.79	1.53	1	1
1:B:37:VAL:O	1:B:37:VAL:CG1	0.79	2.30	1	1
1:A:43:GLY:O	1:A:46:SER:N	0.78	2.16	1	7
1:A:45:ILE:O	1:A:49:LEU:HB2	0.78	1.79	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:TYR:HD1	1:B:26:TYR:H	0.78	0.98	1	1
1:B:56:VAL:CG1	1:B:57:SER:N	0.76	2.48	1	7
1:B:60:LEU:HD13	1:B:80:TYR:CZ	0.76	2.14	1	1
1:B:11:ASP:N	1:B:11:ASP:OD1	0.76	2.18	1	2
1:A:28:ARG:NH1	1:A:28:ARG:HG2	0.74	1.96	1	1
1:A:53:GLN:HA	1:A:56:VAL:HG21	0.73	1.60	1	1
1:A:64:LYS:HE3	1:A:71:ALA:HB2	0.72	1.61	1	1
1:A:64:LYS:HE3	1:A:71:ALA:CB	0.72	2.14	1	1
1:A:84:ASP:N	1:A:84:ASP:OD1	0.72	2.18	1	3
1:B:25:ASP:N	1:B:25:ASP:OD1	0.71	2.23	1	3
1:A:28:ARG:CG	1:A:28:ARG:HH11	0.71	1.98	1	1
1:B:63:LEU:HB3	1:B:69:VAL:CG2	0.70	2.16	1	1
1:A:28:ARG:HE	1:A:63:LEU:HD11	0.70	1.43	1	1
1:A:45:ILE:O	1:A:49:LEU:CB	0.70	2.39	1	1
1:A:53:GLN:CA	1:A:56:VAL:HG23	0.70	2.17	1	1
1:B:37:VAL:O	1:B:38:SER:CB	0.69	2.40	1	2
1:B:62:LEU:O	1:B:65:SER:N	0.69	2.25	1	2
1:A:79:ILE:HD12	1:A:79:ILE:N	0.68	2.03	8	2
1:B:79:ILE:HD12	1:B:79:ILE:N	0.68	2.04	2	3
1:B:66:VAL:O	1:B:67:HIS:HB2	0.67	1.87	1	1
1:A:56:VAL:O	1:A:59:GLN:N	0.67	2.28	1	13
1:B:48:GLN:C	1:B:50:ASN:H	0.66	1.93	1	2
1:A:95:ILE:HD12	1:A:95:ILE:N	0.66	2.05	7	2
1:B:48:GLN:O	1:B:50:ASN:N	0.64	2.29	1	1
1:B:95:ILE:N	1:B:95:ILE:HD12	0.64	2.06	18	3
1:B:60:LEU:CD1	1:B:80:TYR:CZ	0.64	2.80	1	1
1:B:56:VAL:HG13	1:B:57:SER:H	0.63	1.53	9	4
1:A:26:TYR:O	1:A:28:ARG:N	0.63	2.31	1	4
1:A:26:TYR:HD2	1:B:17:THR:CG2	0.62	2.07	1	1
1:A:28:ARG:CZ	1:A:63:LEU:HD11	0.62	2.24	1	1
1:A:24:GLY:N	1:A:28:ARG:NH1	0.62	2.48	3	1
1:A:55:ASN:ND2	1:A:56:VAL:N	0.62	2.48	9	1
1:B:26:TYR:CD1	1:B:27:ASN:N	0.62	2.68	19	3
1:B:82:LEU:N	1:B:82:LEU:CD2	0.62	2.63	1	3
1:B:56:VAL:HG13	1:B:57:SER:N	0.62	2.08	9	7
1:A:56:VAL:HG23	1:A:57:SER:N	0.62	2.10	4	7
1:B:56:VAL:HG12	1:B:57:SER:H	0.62	1.51	1	1
1:B:85:ILE:N	1:B:85:ILE:HD12	0.62	2.10	10	1
1:B:63:LEU:H	1:B:63:LEU:HD12	0.61	1.54	1	2
1:B:59:GLN:O	1:B:60:LEU:C	0.61	2.38	1	1
1:B:80:TYR:O	1:B:81:SER:CB	0.61	2.49	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ARG:NH2	1:A:63:LEU:HG	0.61	2.11	1	1
1:B:34:LEU:C	1:B:34:LEU:HD13	0.61	2.16	21	1
1:A:64:LYS:NZ	1:A:71:ALA:N	0.60	2.48	2	1
1:A:43:GLY:O	1:A:44:HIS:C	0.60	2.39	1	1
1:A:80:TYR:CD1	1:A:80:TYR:N	0.60	2.69	1	2
1:A:56:VAL:HG23	1:A:57:SER:H	0.60	1.55	5	5
1:B:43:GLY:O	1:B:46:SER:OG	0.60	2.19	1	3
1:B:82:LEU:HD22	1:B:82:LEU:N	0.60	2.12	6	1
1:A:78:MET:N	1:A:78:MET:SD	0.59	2.76	9	4
1:A:41:SER:OG	1:A:42:VAL:N	0.59	2.36	1	1
1:B:78:MET:SD	1:B:78:MET:N	0.59	2.76	10	5
1:B:90:MET:N	1:B:90:MET:SD	0.58	2.76	3	1
1:A:28:ARG:HG2	1:A:28:ARG:HH11	0.58	1.52	1	1
1:A:44:HIS:N	1:A:44:HIS:ND1	0.58	2.52	20	2
1:B:27:ASN:HD22	1:B:28:ARG:N	0.58	1.97	13	2
1:B:80:TYR:N	1:B:80:TYR:CD1	0.57	2.72	1	1
1:B:56:VAL:HG23	1:B:57:SER:N	0.57	2.14	6	1
1:B:44:HIS:N	1:B:44:HIS:ND1	0.57	2.53	19	2
1:A:35:LEU:HD23	1:A:80:TYR:CE2	0.57	2.34	13	1
1:A:26:TYR:CZ	1:A:27:ASN:ND2	0.57	2.73	4	1
1:A:47:HIS:CD2	1:A:53:GLN:HE21	0.57	2.17	5	1
1:B:43:GLY:O	1:B:46:SER:N	0.56	2.37	1	6
1:A:70:LYS:HE2	1:A:83:ASP:CG	0.56	2.20	1	1
1:A:31:ILE:HD12	1:A:59:GLN:OE1	0.56	2.01	1	1
1:A:13:LEU:HD21	1:B:29:ILE:HG21	0.56	1.77	1	1
1:B:66:VAL:O	1:B:67:HIS:CB	0.56	2.54	1	4
1:B:79:ILE:N	1:B:79:ILE:CD1	0.56	2.69	21	3
1:A:23:LEU:CD1	1:B:20:PHE:CD1	0.56	2.89	12	2
1:A:60:LEU:HD13	1:A:80:TYR:CE2	0.56	2.36	1	1
1:A:25:ASP:H	1:A:28:ARG:HE	0.56	1.43	7	1
1:A:62:LEU:O	1:A:63:LEU:C	0.56	2.44	1	1
1:A:46:SER:OG	1:A:51:LEU:O	0.55	2.23	1	2
1:A:95:ILE:N	1:A:95:ILE:CD1	0.55	2.69	7	2
1:A:79:ILE:N	1:A:79:ILE:CD1	0.55	2.68	8	2
1:A:82:LEU:HD12	1:A:82:LEU:N	0.55	2.17	19	2
1:B:85:ILE:HD12	1:B:85:ILE:C	0.55	2.22	14	1
1:A:49:LEU:O	1:A:50:ASN:C	0.55	2.43	1	1
1:A:82:LEU:HD22	1:A:82:LEU:N	0.55	2.15	21	1
1:B:47:HIS:NE2	1:B:53:GLN:NE2	0.55	2.54	4	1
1:B:62:LEU:O	1:B:63:LEU:C	0.55	2.45	1	1
1:A:28:ARG:NH2	1:A:63:LEU:CG	0.55	2.70	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:GLN:C	1:B:50:ASN:N	0.55	2.60	1	1
1:B:63:LEU:HB3	1:B:69:VAL:HG23	0.55	1.77	1	1
1:A:27:ASN:ND2	1:A:59:GLN:HE21	0.54	2.01	13	1
1:A:13:LEU:CD2	1:B:29:ILE:HG21	0.54	2.32	1	1
1:B:66:VAL:O	1:B:67:HIS:CG	0.54	2.60	13	2
1:B:82:LEU:HD12	1:B:82:LEU:N	0.54	2.17	15	3
1:B:28:ARG:NH1	1:B:32:MET:SD	0.54	2.81	8	1
1:B:41:SER:OG	1:B:42:VAL:N	0.54	2.41	1	1
1:A:55:ASN:HD22	1:A:56:VAL:N	0.54	2.01	9	1
1:A:63:LEU:HD12	1:A:63:LEU:H	0.54	1.63	1	4
1:A:53:GLN:C	1:A:56:VAL:HG23	0.54	2.23	1	1
1:A:66:VAL:O	1:A:67:HIS:CB	0.54	2.49	1	2
1:B:42:VAL:O	1:B:45:ILE:HG22	0.54	2.03	1	1
1:B:49:LEU:H	1:B:49:LEU:CD2	0.54	2.16	16	1
1:B:75:GLY:O	1:B:77:SER:N	0.54	2.41	2	3
1:B:55:ASN:O	1:B:56:VAL:C	0.54	2.46	1	1
1:A:73:ARG:CZ	1:A:78:MET:SD	0.54	2.96	3	1
1:A:29:ILE:HG23	1:A:30:ARG:N	0.53	2.17	8	5
1:B:93:GLN:NE2	1:B:97:HIS:NE2	0.53	2.56	20	1
1:B:29:ILE:HG23	1:B:30:ARG:N	0.53	2.18	19	6
1:B:82:LEU:CD2	1:B:82:LEU:N	0.53	2.71	11	2
1:B:31:ILE:HG23	1:B:32:MET:N	0.53	2.18	16	1
1:B:23:LEU:HA	1:B:28:ARG:NH1	0.53	2.18	1	1
1:B:56:VAL:O	1:B:59:GLN:N	0.53	2.42	8	16
1:B:58:HIS:N	1:B:58:HIS:ND1	0.53	2.57	3	2
1:A:34:LEU:HD13	1:A:34:LEU:O	0.53	2.04	3	5
1:A:82:LEU:N	1:A:82:LEU:CD2	0.53	2.71	21	2
1:B:82:LEU:N	1:B:82:LEU:CD1	0.53	2.71	5	3
1:B:73:ARG:O	1:B:73:ARG:NE	0.53	2.42	7	1
1:A:92:LYS:O	1:A:96:HIS:CD2	0.53	2.62	9	1
1:B:52:SER:OG	1:B:55:ASN:ND2	0.53	2.42	3	1
1:A:63:LEU:HD12	1:A:63:LEU:N	0.53	2.19	11	11
1:A:16:VAL:O	1:A:20:PHE:CD2	0.53	2.62	3	2
1:B:92:LYS:O	1:B:96:HIS:CD2	0.53	2.62	7	3
1:B:46:SER:OG	1:B:47:HIS:N	0.53	2.42	13	3
1:A:89:THR:HG23	1:A:90:MET:N	0.53	2.19	9	2
1:B:35:LEU:O	1:B:37:VAL:N	0.53	2.42	10	8
1:A:11:ASP:N	1:A:14:GLU:OE1	0.53	2.42	3	1
1:B:95:ILE:N	1:B:95:ILE:CD1	0.53	2.72	18	3
1:B:22:ALA:O	1:B:28:ARG:NH1	0.53	2.42	21	2
1:B:82:LEU:O	1:B:84:ASP:N	0.53	2.42	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:SER:O	1:A:79:ILE:N	0.53	2.42	17	1
1:B:41:SER:OG	1:B:44:HIS:CG	0.52	2.62	7	2
1:A:73:ARG:N	1:A:73:ARG:CD	0.52	2.71	13	1
1:A:53:GLN:NE2	1:A:53:GLN:H	0.52	2.02	19	1
1:B:55:ASN:OD1	1:B:56:VAL:N	0.52	2.42	3	1
1:B:16:VAL:O	1:B:20:PHE:CD2	0.52	2.62	19	4
1:A:75:GLY:O	1:A:77:SER:N	0.52	2.42	14	3
1:A:41:SER:OG	1:A:44:HIS:CG	0.52	2.62	16	3
1:B:26:TYR:CE2	1:B:27:ASN:OD1	0.52	2.62	18	1
1:A:25:ASP:O	1:A:28:ARG:HB2	0.52	2.05	1	1
1:B:24:GLY:O	1:B:28:ARG:NH1	0.52	2.43	6	1
1:B:66:VAL:O	1:B:67:HIS:ND1	0.52	2.42	14	1
1:A:92:LYS:O	1:A:96:HIS:N	0.52	2.42	18	1
1:B:92:LYS:O	1:B:96:HIS:CG	0.52	2.62	5	2
1:A:65:SER:O	1:A:67:HIS:CD2	0.52	2.62	8	2
1:A:29:ILE:O	1:A:31:ILE:N	0.52	2.43	13	2
1:A:55:ASN:OD1	1:A:56:VAL:N	0.52	2.42	2	1
1:B:52:SER:O	1:B:55:ASN:ND2	0.52	2.42	3	1
1:A:25:ASP:N	1:A:25:ASP:OD1	0.52	2.42	5	1
1:A:25:ASP:OD2	1:A:28:ARG:N	0.52	2.43	8	1
1:A:94:ALA:O	1:A:97:HIS:CE1	0.52	2.62	16	1
1:A:55:ASN:O	1:A:59:GLN:N	0.52	2.42	18	6
1:B:55:ASN:O	1:B:59:GLN:N	0.52	2.42	13	6
1:B:23:LEU:HD12	1:B:23:LEU:N	0.52	2.20	17	4
1:B:48:GLN:O	1:B:48:GLN:NE2	0.52	2.42	4	1
1:B:74:GLN:O	1:B:76:GLN:N	0.52	2.43	8	2
1:A:27:ASN:ND2	1:A:59:GLN:OE1	0.52	2.43	9	1
1:A:50:ASN:O	1:A:50:ASN:ND2	0.52	2.42	14	1
1:B:91:LEU:CD2	1:B:91:LEU:N	0.52	2.72	21	1
1:B:46:SER:OG	1:B:53:GLN:NE2	0.52	2.43	3	1
1:A:64:LYS:NZ	1:A:70:LYS:O	0.52	2.43	4	1
1:B:59:GLN:O	1:B:59:GLN:NE2	0.52	2.43	15	1
1:B:54:SER:O	1:B:58:HIS:CD2	0.52	2.63	17	1
1:A:63:LEU:H	1:A:63:LEU:CD1	0.52	2.18	1	5
1:A:39:GLU:OE1	1:A:39:GLU:N	0.52	2.43	2	1
1:B:63:LEU:HD12	1:B:63:LEU:N	0.52	2.20	19	10
1:A:54:SER:O	1:A:58:HIS:CG	0.52	2.63	8	1
1:B:27:ASN:O	1:B:27:ASN:ND2	0.52	2.42	9	1
1:A:47:HIS:CD2	1:A:53:GLN:OE1	0.52	2.63	19	1
1:A:26:TYR:C	1:A:28:ARG:N	0.52	2.62	1	6
1:A:35:LEU:O	1:A:37:VAL:N	0.52	2.43	21	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:82:LEU:N	1:B:82:LEU:HD22	0.52	2.19	11	1
1:A:13:LEU:O	1:A:15:ARG:N	0.52	2.42	19	1
1:A:47:HIS:NE2	1:A:53:GLN:OE1	0.52	2.42	19	1
1:B:91:LEU:N	1:B:91:LEU:HD22	0.52	2.20	21	1
1:A:62:LEU:O	1:A:65:SER:N	0.51	2.43	13	2
1:A:21:LYS:CB	1:A:21:LYS:NZ	0.51	2.73	2	1
1:B:65:SER:O	1:B:67:HIS:CE1	0.51	2.63	9	1
1:A:65:SER:O	1:A:67:HIS:CE1	0.51	2.62	21	1
1:A:19:ILE:HG23	1:A:20:PHE:N	0.51	2.20	8	1
1:A:46:SER:O	1:A:50:ASN:N	0.51	2.43	9	1
1:B:93:GLN:NE2	1:B:97:HIS:CD2	0.51	2.78	20	1
1:B:65:SER:O	1:B:67:HIS:CD2	0.51	2.63	4	1
1:A:91:LEU:CD1	1:A:91:LEU:N	0.51	2.74	12	1
1:B:38:SER:OG	1:B:39:GLU:N	0.51	2.42	5	3
1:A:35:LEU:O	1:A:38:SER:N	0.51	2.44	21	4
1:A:23:LEU:HD12	1:A:23:LEU:N	0.51	2.20	17	2
1:B:29:ILE:O	1:B:31:ILE:N	0.51	2.44	11	1
1:A:92:LYS:O	1:A:96:HIS:CG	0.51	2.63	19	1
1:B:63:LEU:N	1:B:63:LEU:CD1	0.51	2.73	6	9
1:B:77:SER:OG	1:B:78:MET:N	0.51	2.42	6	2
1:A:82:LEU:N	1:A:82:LEU:CD1	0.51	2.73	19	2
1:A:63:LEU:O	1:A:66:VAL:N	0.51	2.44	1	3
1:A:97:HIS:O	1:A:97:HIS:CD2	0.51	2.63	10	1
1:B:21:LYS:CB	1:B:21:LYS:NZ	0.51	2.73	12	1
1:A:63:LEU:HB3	1:A:69:VAL:HG22	0.51	1.82	1	1
1:B:43:GLY:O	1:B:44:HIS:C	0.51	2.50	1	1
1:A:65:SER:O	1:A:67:HIS:NE2	0.51	2.44	8	1
1:B:50:ASN:N	1:B:50:ASN:OD1	0.50	2.44	8	1
1:B:35:LEU:N	1:B:35:LEU:CD2	0.50	2.74	13	2
1:A:85:ILE:C	1:A:85:ILE:HD12	0.50	2.26	18	1
1:A:17:THR:O	1:A:21:LYS:HB2	0.50	2.05	1	1
1:A:25:ASP:N	1:A:28:ARG:HE	0.50	2.03	7	2
1:B:85:ILE:HG23	1:B:86:HIS:N	0.50	2.20	19	1
1:A:78:MET:SD	1:A:78:MET:O	0.50	2.69	8	1
1:B:66:VAL:HG12	1:B:66:VAL:O	0.50	2.06	3	2
1:B:26:TYR:CE1	1:B:27:ASN:ND2	0.50	2.80	12	1
1:B:94:ALA:O	1:B:97:HIS:ND1	0.50	2.45	17	1
1:B:58:HIS:O	1:B:61:LYS:HB2	0.50	2.06	1	1
1:B:63:LEU:HD12	1:B:63:LEU:H	0.50	1.66	4	3
1:B:23:LEU:HD23	1:B:24:GLY:N	0.50	2.21	8	2
1:A:91:LEU:N	1:A:91:LEU:HD12	0.50	2.20	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:GLN:H	1:B:53:GLN:CD	0.50	2.10	19	2
1:B:75:GLY:O	1:B:76:GLN:CB	0.50	2.60	16	1
1:A:91:LEU:N	1:A:91:LEU:CD2	0.50	2.75	6	1
1:A:63:LEU:N	1:A:63:LEU:CD1	0.50	2.74	16	8
1:A:31:ILE:O	1:A:34:LEU:N	0.50	2.44	12	4
1:A:85:ILE:HD12	1:A:86:HIS:N	0.50	2.22	18	1
1:B:19:ILE:HG23	1:B:20:PHE:N	0.50	2.22	20	1
1:A:12:THR:HG23	1:A:13:LEU:N	0.49	2.22	12	2
1:A:64:LYS:HZ1	1:A:71:ALA:N	0.49	2.05	2	1
1:B:87:VAL:HG13	1:B:88:ALA:N	0.49	2.21	2	1
1:B:28:ARG:N	1:B:28:ARG:CD	0.49	2.74	11	1
1:B:24:GLY:N	1:B:28:ARG:NH1	0.49	2.60	16	2
1:B:69:VAL:HG22	1:B:70:LYS:N	0.49	2.22	16	1
1:B:32:MET:SD	1:B:36:SER:OG	0.49	2.70	21	1
1:A:27:ASN:ND2	1:A:27:ASN:N	0.49	2.58	2	1
1:B:86:HIS:O	1:B:90:MET:SD	0.49	2.70	3	1
1:B:92:LYS:O	1:B:96:HIS:N	0.49	2.45	4	1
1:B:91:LEU:O	1:B:94:ALA:N	0.49	2.45	8	4
1:A:26:TYR:CG	1:A:27:ASN:N	0.49	2.80	13	1
1:A:53:GLN:H	1:A:53:GLN:CD	0.49	2.10	19	3
1:A:23:LEU:O	1:A:25:ASP:N	0.49	2.44	16	2
1:A:35:LEU:CD2	1:A:35:LEU:N	0.49	2.75	18	1
1:A:90:MET:SD	1:A:90:MET:O	0.49	2.70	18	1
1:B:49:LEU:HD12	1:B:49:LEU:N	0.49	2.22	21	1
1:A:87:VAL:HG13	1:A:88:ALA:N	0.49	2.23	2	3
1:A:76:GLN:H	1:A:76:GLN:NE2	0.49	2.06	8	1
1:A:92:LYS:O	1:A:96:HIS:HB2	0.49	2.08	1	1
1:A:49:LEU:HD12	1:A:49:LEU:N	0.49	2.23	7	1
1:A:92:LYS:O	1:A:96:HIS:ND1	0.49	2.46	19	1
1:A:54:SER:O	1:A:58:HIS:ND1	0.49	2.46	11	1
1:B:35:LEU:N	1:B:35:LEU:HD22	0.49	2.23	13	2
1:A:77:SER:O	1:A:78:MET:SD	0.49	2.70	15	1
1:B:84:ASP:N	1:B:84:ASP:OD1	0.49	2.46	17	2
1:A:49:LEU:N	1:A:49:LEU:CD1	0.49	2.75	7	1
1:B:85:ILE:HD12	1:B:85:ILE:H	0.49	1.68	10	1
1:B:85:ILE:HD12	1:B:86:HIS:N	0.49	2.22	14	1
1:B:63:LEU:CD2	1:B:63:LEU:N	0.48	2.75	5	1
1:A:14:GLU:O	1:A:17:THR:N	0.48	2.46	11	1
1:B:51:LEU:HD23	1:B:52:SER:N	0.48	2.24	20	1
1:A:87:VAL:O	1:A:90:MET:N	0.48	2.45	8	1
1:A:27:ASN:N	1:A:27:ASN:HD22	0.48	2.06	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:93:GLN:O	1:B:97:HIS:ND1	0.48	2.46	3	1
1:A:25:ASP:H	1:A:28:ARG:HH21	0.48	1.51	6	1
1:A:31:ILE:HG23	1:A:32:MET:N	0.48	2.23	9	4
1:A:56:VAL:CG2	1:A:57:SER:N	0.48	2.77	15	6
1:A:92:LYS:N	1:A:92:LYS:CD	0.48	2.77	18	1
1:B:84:ASP:OD1	1:B:88:ALA:N	0.48	2.47	19	1
1:B:70:LYS:CG	1:B:71:ALA:N	0.48	2.77	20	1
1:A:97:HIS:O	1:A:97:HIS:ND1	0.48	2.47	6	1
1:B:63:LEU:HD22	1:B:63:LEU:N	0.48	2.24	11	1
1:B:28:ARG:NH2	1:B:31:ILE:CG2	0.48	2.76	12	1
1:A:26:TYR:CD1	1:A:26:TYR:N	0.48	2.82	16	1
1:A:83:ASP:O	1:A:85:ILE:N	0.48	2.46	16	1
1:B:35:LEU:C	1:B:37:VAL:N	0.48	2.67	2	11
1:A:55:ASN:N	1:A:55:ASN:OD1	0.48	2.44	3	2
1:A:51:LEU:HD13	1:A:52:SER:H	0.48	1.68	4	1
1:B:77:SER:O	1:B:78:MET:SD	0.48	2.72	8	1
1:B:56:VAL:O	1:B:57:SER:C	0.48	2.52	1	1
1:A:61:LYS:HZ3	1:A:61:LYS:CB	0.48	2.22	15	1
1:A:25:ASP:O	1:A:27:ASN:N	0.48	2.47	20	1
1:A:77:SER:OG	1:A:78:MET:N	0.48	2.47	13	5
1:B:57:SER:OG	1:B:58:HIS:N	0.48	2.46	2	1
1:B:76:GLN:N	1:B:76:GLN:CD	0.48	2.68	13	3
1:B:91:LEU:HD12	1:B:91:LEU:N	0.48	2.24	9	1
1:A:53:GLN:N	1:A:53:GLN:CD	0.48	2.67	10	1
1:A:64:LYS:CB	1:A:64:LYS:NZ	0.48	2.77	10	1
1:B:49:LEU:H	1:B:49:LEU:HD23	0.48	1.69	16	1
1:A:45:ILE:HG22	1:A:46:SER:N	0.48	2.23	1	1
1:B:26:TYR:O	1:B:28:ARG:N	0.48	2.47	15	3
1:A:49:LEU:O	1:A:49:LEU:HD23	0.48	2.09	10	5
1:B:35:LEU:O	1:B:35:LEU:HD13	0.48	2.09	18	3
1:A:20:PHE:O	1:A:23:LEU:CD2	0.48	2.62	9	1
1:A:26:TYR:H	1:A:28:ARG:HH21	0.48	1.51	11	1
1:A:14:GLU:N	1:A:14:GLU:CD	0.47	2.68	3	1
1:A:35:LEU:C	1:A:37:VAL:N	0.47	2.67	5	7
1:A:66:VAL:C	1:A:67:HIS:CG	0.47	2.88	11	6
1:B:28:ARG:NH2	1:B:31:ILE:HG21	0.47	2.23	12	1
1:A:91:LEU:HD12	1:A:91:LEU:N	0.47	2.24	21	1
1:A:59:GLN:HE22	1:A:63:LEU:CD1	0.47	2.22	6	1
1:B:59:GLN:NE2	1:B:59:GLN:C	0.47	2.67	15	1
1:B:84:ASP:OD1	1:B:85:ILE:N	0.47	2.47	7	1
1:B:79:ILE:HG23	1:B:79:ILE:O	0.47	2.10	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:HIS:NE2	1:B:53:GLN:CD	0.47	2.68	21	1
1:A:39:GLU:N	1:A:39:GLU:CD	0.47	2.68	2	3
1:A:64:LYS:HZ1	1:A:71:ALA:H	0.47	1.51	2	1
1:B:27:ASN:N	1:B:27:ASN:HD22	0.47	2.05	4	1
1:B:56:VAL:CG1	1:B:57:SER:H	0.47	2.23	9	2
1:A:42:VAL:HG13	1:A:43:GLY:N	0.47	2.24	17	3
1:B:25:ASP:O	1:B:27:ASN:N	0.47	2.47	16	1
1:B:55:ASN:O	1:B:58:HIS:N	0.47	2.48	1	1
1:B:39:GLU:N	1:B:39:GLU:CD	0.47	2.68	21	1
1:B:26:TYR:C	1:B:28:ARG:N	0.47	2.68	15	4
1:B:63:LEU:H	1:B:63:LEU:CD1	0.47	2.23	19	4
1:A:23:LEU:N	1:A:23:LEU:CD2	0.47	2.78	21	3
1:A:46:SER:OG	1:A:47:HIS:N	0.47	2.48	5	2
1:A:91:LEU:N	1:A:91:LEU:HD22	0.47	2.25	6	1
1:B:56:VAL:CG2	1:B:57:SER:N	0.47	2.78	6	1
1:A:66:VAL:HG12	1:A:66:VAL:O	0.47	2.09	19	6
1:B:16:VAL:O	1:B:20:PHE:CE2	0.47	2.66	11	1
1:B:28:ARG:HH21	1:B:31:ILE:CG2	0.47	2.23	12	1
1:A:42:VAL:HG23	1:A:43:GLY:N	0.47	2.24	14	3
1:B:45:ILE:O	1:B:49:LEU:CD2	0.47	2.62	16	1
1:A:49:LEU:O	1:A:50:ASN:ND2	0.47	2.48	18	1
1:B:51:LEU:O	1:B:53:GLN:NE2	0.47	2.48	21	1
1:B:37:VAL:O	1:B:38:SER:HB2	0.47	2.07	1	1
1:A:37:VAL:O	1:A:38:SER:CB	0.47	2.63	7	3
1:A:29:ILE:CG2	1:A:30:ARG:N	0.47	2.78	18	2
1:B:76:GLN:CD	1:B:77:SER:N	0.47	2.68	9	1
1:A:35:LEU:HD13	1:A:35:LEU:O	0.47	2.10	2	2
1:B:66:VAL:C	1:B:67:HIS:CG	0.47	2.88	19	5
1:B:67:HIS:O	1:B:67:HIS:ND1	0.47	2.48	10	3
1:A:53:GLN:C	1:A:55:ASN:N	0.47	2.68	15	1
1:B:85:ILE:C	1:B:87:VAL:N	0.47	2.68	20	1
1:A:26:TYR:CD2	1:B:17:THR:CG2	0.47	2.94	1	1
1:A:59:GLN:O	1:A:60:LEU:C	0.47	2.53	1	1
1:B:35:LEU:O	1:B:35:LEU:HD23	0.47	2.09	2	2
1:B:25:ASP:C	1:B:27:ASN:N	0.47	2.68	16	2
1:B:68:LEU:O	1:B:68:LEU:HD23	0.47	2.10	5	1
1:A:35:LEU:O	1:A:35:LEU:HD23	0.47	2.10	9	2
1:B:29:ILE:CG2	1:B:30:ARG:N	0.47	2.78	19	5
1:A:29:ILE:C	1:A:31:ILE:N	0.47	2.68	10	2
1:A:82:LEU:C	1:A:84:ASP:N	0.47	2.68	12	1
1:A:35:LEU:O	1:A:35:LEU:HD13	0.47	2.10	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:45:ILE:CG2	1:B:46:SER:N	0.46	2.78	1	1
1:B:34:LEU:HD23	1:B:34:LEU:O	0.46	2.10	10	2
1:A:58:HIS:O	1:A:58:HIS:ND1	0.46	2.48	13	1
1:A:47:HIS:CD2	1:A:53:GLN:NE2	0.46	2.83	5	1
1:B:82:LEU:HD23	1:B:82:LEU:H	0.46	1.70	17	1
1:A:36:SER:O	1:A:37:VAL:HG13	0.46	2.11	7	2
1:A:23:LEU:CD2	1:A:23:LEU:N	0.46	2.78	9	1
1:A:28:ARG:CZ	1:A:32:MET:SD	0.46	3.03	9	1
1:B:58:HIS:O	1:B:58:HIS:ND1	0.46	2.46	9	1
1:A:76:GLN:H	1:A:76:GLN:CD	0.46	2.13	11	1
1:A:43:GLY:O	1:A:45:ILE:N	0.46	2.48	1	1
1:A:80:TYR:HD1	1:A:80:TYR:H	0.46	1.52	1	1
1:B:59:GLN:O	1:B:61:LYS:N	0.46	2.48	1	1
1:A:60:LEU:O	1:A:63:LEU:N	0.46	2.48	3	1
1:A:68:LEU:O	1:A:68:LEU:HD23	0.46	2.10	7	3
1:B:67:HIS:CD2	1:B:67:HIS:N	0.46	2.84	4	1
1:A:46:SER:CB	1:A:51:LEU:O	0.46	2.63	9	1
1:B:17:THR:O	1:B:21:LYS:HB2	0.46	2.11	1	1
1:B:63:LEU:N	1:B:63:LEU:HD22	0.46	2.24	5	1
1:A:19:ILE:CG2	1:A:20:PHE:N	0.46	2.77	8	1
1:B:42:VAL:HG13	1:B:43:GLY:N	0.46	2.26	5	3
1:B:85:ILE:O	1:B:87:VAL:N	0.46	2.48	20	1
1:A:63:LEU:HD22	1:A:63:LEU:N	0.46	2.25	21	1
1:B:85:ILE:N	1:B:85:ILE:CD1	0.46	2.77	10	1
1:A:25:ASP:OD1	1:A:26:TYR:N	0.46	2.49	16	2
1:B:69:VAL:CG2	1:B:70:LYS:N	0.46	2.79	16	1
1:B:60:LEU:O	1:B:61:LYS:C	0.46	2.54	1	1
1:A:24:GLY:H	1:A:28:ARG:NE	0.46	2.09	6	1
1:A:91:LEU:O	1:A:94:ALA:N	0.46	2.48	6	3
1:A:86:HIS:O	1:A:89:THR:N	0.46	2.49	16	2
1:A:82:LEU:O	1:A:84:ASP:N	0.46	2.48	12	1
1:A:13:LEU:C	1:A:15:ARG:N	0.46	2.68	19	1
1:A:50:ASN:N	1:A:50:ASN:OD1	0.46	2.49	1	1
1:A:63:LEU:CD1	1:A:63:LEU:N	0.46	2.78	18	3
1:A:69:VAL:HG12	1:A:82:LEU:HD23	0.46	1.88	1	1
1:B:31:ILE:HD11	1:B:59:GLN:NE2	0.46	2.26	1	1
1:B:31:ILE:O	1:B:34:LEU:N	0.46	2.47	5	3
1:B:86:HIS:N	1:B:86:HIS:ND1	0.46	2.64	6	1
1:B:28:ARG:HE	1:B:28:ARG:C	0.46	2.14	14	1
1:A:83:ASP:N	1:A:83:ASP:OD1	0.45	2.47	20	2
1:B:47:HIS:CD2	1:B:53:GLN:NE2	0.45	2.84	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:46:SER:O	1:B:47:HIS:C	0.45	2.54	1	1
1:A:26:TYR:CD2	1:A:27:ASN:N	0.45	2.84	13	1
1:A:63:LEU:N	1:A:63:LEU:HD12	0.45	2.26	18	2
1:A:53:GLN:O	1:A:56:VAL:N	0.45	2.50	17	1
1:A:16:VAL:O	1:A:20:PHE:CE2	0.45	2.69	3	1
1:B:28:ARG:C	1:B:28:ARG:NE	0.45	2.69	14	1
1:A:38:SER:OG	1:A:39:GLU:N	0.45	2.50	16	1
1:B:85:ILE:O	1:B:88:ALA:N	0.45	2.50	20	1
1:B:29:ILE:O	1:B:32:MET:N	0.45	2.48	11	2
1:A:74:GLN:O	1:A:76:GLN:N	0.45	2.49	18	2
1:B:35:LEU:HD13	1:B:35:LEU:O	0.45	2.11	11	2
1:A:35:LEU:N	1:A:35:LEU:HD22	0.45	2.25	18	1
1:A:56:VAL:O	1:A:57:SER:C	0.45	2.55	1	1
1:B:61:LYS:O	1:B:62:LEU:C	0.45	2.54	1	1
1:A:76:GLN:CD	1:A:76:GLN:N	0.45	2.70	8	3
1:B:13:LEU:O	1:B:15:ARG:N	0.45	2.50	19	1
1:A:82:LEU:HD23	1:A:83:ASP:N	0.45	2.26	20	1
1:A:87:VAL:CG1	1:A:88:ALA:N	0.45	2.80	2	2
1:A:23:LEU:N	1:A:23:LEU:HD22	0.45	2.26	21	3
1:B:90:MET:O	1:B:90:MET:SD	0.45	2.74	6	1
1:B:90:MET:C	1:B:90:MET:SD	0.45	2.95	12	1
1:B:31:ILE:CG2	1:B:32:MET:N	0.45	2.79	16	1
1:A:93:GLN:HE21	1:A:97:HIS:CE1	0.45	2.29	4	1
1:B:34:LEU:HD13	1:B:34:LEU:O	0.45	2.11	5	1
1:A:32:MET:C	1:A:32:MET:SD	0.45	2.95	18	3
1:A:53:GLN:O	1:A:55:ASN:N	0.45	2.49	15	1
1:B:45:ILE:HG23	1:B:46:SER:N	0.45	2.27	1	1
1:B:62:LEU:O	1:B:66:VAL:HG23	0.45	2.12	1	1
1:A:23:LEU:N	1:A:23:LEU:HD23	0.45	2.25	9	1
1:B:27:ASN:ND2	1:B:27:ASN:C	0.45	2.69	13	1
1:A:77:SER:C	1:A:78:MET:SD	0.45	2.96	19	1
1:A:46:SER:HB2	1:A:56:VAL:HG21	0.45	1.88	1	1
1:B:32:MET:SD	1:B:32:MET:C	0.45	2.95	10	4
1:B:53:GLN:O	1:B:56:VAL:N	0.45	2.50	3	1
1:A:90:MET:C	1:A:90:MET:SD	0.45	2.96	6	2
1:B:77:SER:C	1:B:78:MET:SD	0.45	2.96	14	3
1:A:60:LEU:O	1:A:61:LYS:C	0.44	2.55	1	1
1:B:65:SER:C	1:B:67:HIS:N	0.44	2.70	7	1
1:B:49:LEU:HD23	1:B:49:LEU:N	0.44	2.27	16	1
1:B:29:ILE:C	1:B:31:ILE:N	0.44	2.70	11	1
1:B:14:GLU:O	1:B:17:THR:N	0.44	2.50	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:27:ASN:OD1	1:B:28:ARG:N	0.44	2.51	19	1
1:A:21:LYS:NZ	1:B:26:TYR:CE2	0.44	2.86	9	1
1:B:54:SER:O	1:B:58:HIS:ND1	0.44	2.50	11	1
1:A:31:ILE:CG2	1:A:32:MET:N	0.44	2.80	2	2
1:A:91:LEU:C	1:A:91:LEU:HD23	0.44	2.33	2	5
1:B:87:VAL:CG1	1:B:88:ALA:N	0.44	2.80	2	1
1:B:50:ASN:N	1:B:50:ASN:ND2	0.44	2.65	4	1
1:B:63:LEU:O	1:B:66:VAL:N	0.44	2.48	12	2
1:B:89:THR:HG23	1:B:90:MET:N	0.44	2.27	20	1
1:A:20:PHE:O	1:A:23:LEU:HD11	0.44	2.12	4	1
1:A:76:GLN:N	1:A:76:GLN:OE1	0.44	2.51	11	1
1:B:66:VAL:O	1:B:66:VAL:HG12	0.44	2.11	11	1
1:B:14:GLU:H	1:B:14:GLU:CD	0.44	2.15	17	1
1:A:63:LEU:N	1:A:63:LEU:CD2	0.44	2.81	21	1
1:B:27:ASN:OD1	1:B:30:ARG:NH2	0.44	2.51	6	1
1:A:90:MET:SD	1:A:90:MET:C	0.44	2.96	18	1
1:A:52:SER:O	1:A:54:SER:N	0.44	2.51	1	2
1:B:70:LYS:N	1:B:70:LYS:CD	0.44	2.81	5	1
1:A:87:VAL:HG23	1:A:88:ALA:N	0.44	2.27	8	1
1:B:48:GLN:O	1:B:50:ASN:ND2	0.44	2.51	18	2
1:A:63:LEU:HD11	1:A:68:LEU:CD2	0.44	2.43	14	1
1:B:63:LEU:N	1:B:63:LEU:HD12	0.44	2.28	20	2
1:B:19:ILE:CG2	1:B:20:PHE:N	0.44	2.80	20	1
1:A:52:SER:C	1:A:54:SER:N	0.44	2.71	1	8
1:A:23:LEU:C	1:A:23:LEU:HD12	0.44	2.33	8	2
1:B:91:LEU:C	1:B:91:LEU:HD23	0.44	2.34	4	2
1:B:90:MET:SD	1:B:90:MET:C	0.44	2.96	6	1
1:A:48:GLN:C	1:A:50:ASN:N	0.44	2.71	10	1
1:B:63:LEU:N	1:B:63:LEU:CD2	0.44	2.81	11	1
1:A:93:GLN:OE1	1:A:94:ALA:N	0.44	2.50	12	1
1:B:28:ARG:HE	1:B:29:ILE:N	0.44	2.11	14	1
1:A:25:ASP:C	1:A:27:ASN:N	0.44	2.71	20	1
1:A:82:LEU:HD23	1:A:82:LEU:C	0.44	2.33	20	1
1:A:26:TYR:HD2	1:B:17:THR:HG22	0.43	1.71	1	1
1:B:24:GLY:N	1:B:28:ARG:HH11	0.43	2.11	16	1
1:A:53:GLN:CG	1:A:54:SER:N	0.43	2.81	17	1
1:B:50:ASN:ND2	1:B:50:ASN:N	0.43	2.65	18	1
1:A:56:VAL:CG2	1:A:57:SER:H	0.43	2.26	4	2
1:A:27:ASN:N	1:A:27:ASN:OD1	0.43	2.51	10	1
1:B:22:ALA:O	1:B:28:ARG:CZ	0.43	2.66	10	1
1:B:85:ILE:H	1:B:85:ILE:CD1	0.43	2.25	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:HIS:ND1	1:B:67:HIS:C	0.43	2.71	13	1
1:B:49:LEU:CD2	1:B:49:LEU:N	0.43	2.81	16	1
1:A:63:LEU:HB3	1:A:69:VAL:CG2	0.43	2.44	1	1
1:A:41:SER:O	1:A:45:ILE:CG2	0.43	2.66	12	2
1:B:85:ILE:CD1	1:B:85:ILE:H	0.43	2.27	16	1
1:B:44:HIS:O	1:B:46:SER:N	0.43	2.51	20	1
1:A:86:HIS:ND1	1:A:86:HIS:N	0.43	2.67	11	2
1:B:22:ALA:C	1:B:24:GLY:H	0.43	2.17	10	1
1:A:29:ILE:O	1:A:32:MET:N	0.43	2.50	13	1
1:B:85:ILE:CD1	1:B:85:ILE:N	0.43	2.81	16	1
1:B:49:LEU:O	1:B:49:LEU:HD23	0.43	2.14	10	2
1:A:62:LEU:C	1:A:62:LEU:HD23	0.43	2.33	20	2
1:B:70:LYS:O	1:B:81:SER:O	0.43	2.37	20	1
1:A:24:GLY:O	1:A:25:ASP:O	0.43	2.37	12	2
1:A:52:SER:O	1:A:55:ASN:OD1	0.43	2.37	13	1
1:A:53:GLN:C	1:A:55:ASN:H	0.43	2.16	15	1
1:A:41:SER:OG	1:A:44:HIS:CD2	0.43	2.71	16	1
1:B:43:GLY:C	1:B:46:SER:HG	0.43	2.13	1	1
1:A:61:LYS:CB	1:A:61:LYS:NZ	0.43	2.81	9	1
1:B:35:LEU:O	1:B:38:SER:N	0.43	2.52	17	1
1:A:30:ARG:NH2	1:A:51:LEU:CD1	0.43	2.82	18	1
1:B:13:LEU:O	1:B:16:VAL:N	0.43	2.51	20	1
1:A:70:LYS:O	1:A:81:SER:O	0.43	2.37	2	2
1:B:52:SER:C	1:B:54:SER:H	0.43	2.17	20	9
1:B:72:LYS:CB	1:B:72:LYS:NZ	0.43	2.81	5	1
1:B:95:ILE:O	1:B:95:ILE:HG22	0.43	2.14	18	4
1:B:62:LEU:C	1:B:62:LEU:HD23	0.43	2.34	9	6
1:B:37:VAL:O	1:B:38:SER:O	0.43	2.37	21	1
1:B:82:LEU:HD23	1:B:83:ASP:N	0.43	2.29	2	1
1:B:54:SER:OG	1:B:55:ASN:N	0.43	2.52	4	1
1:A:74:GLN:O	1:A:77:SER:O	0.43	2.37	15	2
1:A:82:LEU:CD2	1:A:82:LEU:H	0.43	2.27	17	1
1:A:46:SER:OG	1:A:53:GLN:OE1	0.43	2.37	3	1
1:B:84:ASP:O	1:B:84:ASP:OD1	0.43	2.37	20	2
1:A:35:LEU:O	1:A:38:SER:O	0.43	2.37	6	1
1:A:22:ALA:C	1:A:24:GLY:H	0.43	2.17	16	1
1:B:85:ILE:N	1:B:85:ILE:HD13	0.43	2.28	16	1
1:A:26:TYR:O	1:A:27:ASN:C	0.42	2.57	1	1
1:B:52:SER:C	1:B:54:SER:N	0.42	2.72	1	9
1:B:24:GLY:O	1:B:25:ASP:O	0.42	2.37	6	3
1:A:14:GLU:O	1:A:17:THR:OG1	0.42	2.37	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:74:GLN:O	1:B:75:GLY:O	0.42	2.37	9	2
1:A:55:ASN:C	1:A:57:SER:N	0.42	2.72	13	1
1:A:82:LEU:N	1:A:82:LEU:HD23	0.42	2.28	17	1
1:A:80:TYR:O	1:A:81:SER:OG	0.42	2.37	19	1
1:A:65:SER:C	1:A:67:HIS:N	0.42	2.72	5	2
1:A:37:VAL:O	1:A:38:SER:OG	0.42	2.36	7	4
1:A:54:SER:O	1:A:58:HIS:CE1	0.42	2.72	11	1
1:A:39:GLU:OE2	1:A:80:TYR:O	0.42	2.37	16	1
1:A:67:HIS:CG	1:A:67:HIS:O	0.42	2.72	16	1
1:B:44:HIS:C	1:B:46:SER:N	0.42	2.72	20	1
1:B:52:SER:OG	1:B:54:SER:HB2	0.42	2.13	1	1
1:B:37:VAL:O	1:B:38:SER:OG	0.42	2.37	9	3
1:A:55:ASN:HD22	1:A:55:ASN:C	0.42	2.18	9	1
1:A:55:ASN:O	1:A:57:SER:N	0.42	2.52	13	1
1:B:28:ARG:NH2	1:B:63:LEU:HD11	0.42	2.29	1	1
1:B:80:TYR:H	1:B:80:TYR:HD1	0.42	1.56	1	1
1:A:72:LYS:O	1:A:79:ILE:O	0.42	2.37	18	1
1:B:64:LYS:CB	1:B:64:LYS:NZ	0.42	2.82	18	1
1:B:72:LYS:N	1:B:72:LYS:CD	0.42	2.83	19	1
1:B:34:LEU:C	1:B:34:LEU:CD1	0.42	2.87	21	1
1:A:62:LEU:O	1:A:66:VAL:HG23	0.42	2.14	1	1
1:A:43:GLY:O	1:A:46:SER:OG	0.42	2.37	3	1
1:A:52:SER:C	1:A:54:SER:H	0.42	2.18	13	6
1:B:55:ASN:OD1	1:B:55:ASN:N	0.42	2.53	5	1
1:B:82:LEU:CD2	1:B:82:LEU:H	0.42	2.27	8	1
1:B:60:LEU:O	1:B:63:LEU:N	0.42	2.53	15	1
1:B:68:LEU:C	1:B:68:LEU:HD23	0.42	2.34	21	2
1:B:35:LEU:HD23	1:B:35:LEU:O	0.42	2.14	21	1
1:B:49:LEU:N	1:B:49:LEU:CD1	0.42	2.83	21	1
1:A:67:HIS:CD2	1:A:67:HIS:N	0.42	2.84	15	2
1:B:23:LEU:HD12	1:B:23:LEU:H	0.42	1.73	17	1
1:A:26:TYR:C	1:A:28:ARG:H	0.42	2.18	17	5
1:B:12:THR:O	1:B:15:ARG:CG	0.42	2.68	19	1
1:A:27:ASN:OD1	1:A:59:GLN:NE2	0.42	2.51	21	1
1:A:82:LEU:O	1:A:83:ASP:OD1	0.42	2.37	2	1
1:B:84:ASP:OD1	1:B:84:ASP:N	0.42	2.50	2	1
1:B:35:LEU:HA	1:B:35:LEU:HD22	0.42	1.49	1	1
1:B:55:ASN:C	1:B:57:SER:N	0.42	2.73	2	2
1:A:84:ASP:OD1	1:A:85:ILE:N	0.42	2.52	3	1
1:B:95:ILE:HG22	1:B:95:ILE:O	0.42	2.15	6	4
1:B:75:GLY:O	1:B:76:GLN:C	0.42	2.57	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LEU:O	1:A:50:ASN:OD1	0.42	2.37	14	2
1:A:91:LEU:O	1:A:94:ALA:HB3	0.42	2.15	15	1
1:A:94:ALA:O	1:A:97:HIS:ND1	0.42	2.53	16	1
1:A:42:VAL:CG1	1:A:43:GLY:N	0.42	2.82	17	1
1:A:32:MET:SD	1:A:32:MET:O	0.42	2.77	21	1
1:B:76:GLN:NE2	1:B:76:GLN:C	0.42	2.73	21	1
1:B:15:ARG:C	1:B:17:THR:N	0.42	2.73	1	1
1:A:55:ASN:ND2	1:A:55:ASN:C	0.42	2.74	9	1
1:A:26:TYR:CE1	1:B:17:THR:CG2	0.42	3.03	11	1
1:B:85:ILE:C	1:B:85:ILE:CD1	0.42	2.88	14	1
1:B:46:SER:O	1:B:51:LEU:N	0.42	2.53	15	1
1:B:89:THR:O	1:B:92:LYS:N	0.42	2.53	19	1
1:B:64:LYS:C	1:B:66:VAL:H	0.41	2.19	5	1
1:B:50:ASN:O	1:B:50:ASN:OD1	0.41	2.38	7	1
1:A:23:LEU:N	1:A:23:LEU:CD1	0.41	2.83	17	2
1:B:25:ASP:OD2	1:B:59:GLN:OE1	0.41	2.37	10	1
1:A:55:ASN:C	1:A:57:SER:H	0.41	2.18	13	1
1:B:65:SER:O	1:B:67:HIS:NE2	0.41	2.53	4	1
1:A:58:HIS:O	1:A:61:LYS:CG	0.41	2.68	9	1
1:B:31:ILE:CD1	1:B:59:GLN:OE1	0.41	2.68	9	1
1:A:11:ASP:O	1:A:11:ASP:OD1	0.41	2.38	21	2
1:B:13:LEU:C	1:B:15:ARG:N	0.41	2.72	11	1
1:A:38:SER:O	1:A:39:GLU:O	0.41	2.37	15	3
1:B:27:ASN:O	1:B:30:ARG:HB2	0.41	2.14	1	1
1:B:80:TYR:CD1	1:B:80:TYR:N	0.41	2.88	5	1
1:B:27:ASN:HD22	1:B:27:ASN:C	0.41	2.18	7	1
1:A:20:PHE:CD1	1:B:23:LEU:CD1	0.41	3.04	15	1
1:A:55:ASN:O	1:A:56:VAL:C	0.41	2.59	1	1
1:A:41:SER:O	1:A:45:ILE:HG22	0.41	2.15	21	2
1:A:63:LEU:CD2	1:A:63:LEU:H	0.41	2.28	21	1
1:B:26:TYR:O	1:B:27:ASN:C	0.41	2.58	1	1
1:B:27:ASN:N	1:B:27:ASN:ND2	0.41	2.68	4	1
1:B:13:LEU:O	1:B:13:LEU:HD23	0.41	2.15	7	1
1:B:47:HIS:ND1	1:B:47:HIS:C	0.41	2.73	9	1
1:B:26:TYR:C	1:B:28:ARG:H	0.41	2.19	13	1
1:B:42:VAL:CG1	1:B:43:GLY:N	0.41	2.83	5	1
1:A:96:HIS:O	1:A:96:HIS:ND1	0.41	2.53	6	1
1:A:13:LEU:O	1:A:13:LEU:HD23	0.41	2.15	11	1
1:B:63:LEU:HD13	1:B:63:LEU:O	0.41	2.15	15	1
1:B:91:LEU:HD23	1:B:91:LEU:C	0.41	2.36	2	1
1:B:12:THR:OG1	1:B:13:LEU:N	0.41	2.53	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:HG13	1:A:37:VAL:O	0.41	2.16	20	1
1:A:12:THR:CG2	1:A:13:LEU:N	0.41	2.83	2	2
1:B:35:LEU:HD23	1:B:80:TYR:CE2	0.41	2.51	3	1
1:A:38:SER:OG	1:A:38:SER:O	0.41	2.36	5	1
1:B:25:ASP:C	1:B:27:ASN:H	0.41	2.19	5	1
1:A:59:GLN:O	1:A:59:GLN:NE2	0.41	2.54	6	1
1:A:42:VAL:CG2	1:A:43:GLY:N	0.41	2.84	14	1
1:A:65:SER:OG	1:A:66:VAL:N	0.41	2.54	16	1
1:B:14:GLU:CD	1:B:14:GLU:N	0.41	2.74	17	1
1:A:45:ILE:CG2	1:A:46:SER:N	0.41	2.83	1	1
1:A:95:ILE:O	1:A:95:ILE:HG22	0.41	2.15	2	1
1:A:95:ILE:HG22	1:A:95:ILE:O	0.41	2.16	7	1
1:A:19:ILE:O	1:A:22:ALA:HB3	0.41	2.15	12	2
1:A:11:ASP:CG	1:A:15:ARG:HH12	0.41	2.19	20	1
1:A:65:SER:C	1:A:67:HIS:H	0.41	2.19	5	1
1:A:96:HIS:C	1:A:96:HIS:HD1	0.41	2.18	6	1
1:B:28:ARG:HE	1:B:63:LEU:HD22	0.41	1.76	8	1
1:A:28:ARG:CG	1:A:29:ILE:N	0.41	2.84	14	1
1:B:74:GLN:CD	1:B:74:GLN:N	0.41	2.74	19	1
1:B:23:LEU:N	1:B:23:LEU:CD1	0.41	2.84	21	1
1:A:56:VAL:O	1:A:58:HIS:N	0.40	2.54	1	1
1:B:92:LYS:H	1:B:92:LYS:CD	0.40	2.29	5	1
1:A:68:LEU:HD23	1:A:68:LEU:C	0.40	2.36	12	1
1:A:48:GLN:C	1:A:50:ASN:H	0.40	2.20	14	1
1:B:83:ASP:OD1	1:B:83:ASP:N	0.40	2.52	15	1
1:A:50:ASN:O	1:A:50:ASN:OD1	0.40	2.38	18	1
1:A:78:MET:SD	1:A:78:MET:N	0.40	2.94	19	1
1:B:74:GLN:C	1:B:76:GLN:H	0.40	2.19	21	1
1:A:84:ASP:OD1	1:A:84:ASP:N	0.40	2.54	2	1
1:A:96:HIS:ND1	1:A:96:HIS:C	0.40	2.75	6	1
1:A:52:SER:OG	1:A:55:ASN:OD1	0.40	2.39	9	1
1:A:25:ASP:O	1:A:28:ARG:CB	0.40	2.70	17	1
1:B:80:TYR:O	1:B:81:SER:HB3	0.40	2.15	1	1
1:A:68:LEU:C	1:A:68:LEU:HD23	0.40	2.36	10	1
1:B:27:ASN:ND2	1:B:28:ARG:N	0.40	2.67	13	1
1:A:35:LEU:C	1:A:35:LEU:HD23	0.40	2.37	17	1
1:A:27:ASN:OD1	1:A:30:ARG:NH2	0.40	2.54	18	1
1:A:66:VAL:O	1:A:66:VAL:CG1	0.40	2.70	19	1
1:B:35:LEU:C	1:B:37:VAL:H	0.40	2.20	2	1
1:A:85:ILE:C	1:A:85:ILE:CD1	0.40	2.89	18	1
1:A:63:LEU:CD1	1:A:63:LEU:H	0.40	2.29	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:93:GLN:NE2	1:B:93:GLN:O	0.40	2.54	20	1
1:B:53:GLN:CD	1:B:53:GLN:N	0.40	2.75	21	1
1:B:92:LYS:CD	1:B:92:LYS:N	0.40	2.85	5	1
1:B:55:ASN:C	1:B:57:SER:H	0.40	2.20	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	87/106 (82%)	64±4 (74±4%)	17±3 (20±3%)	5±3 (6±3%)	3	21
1	B	87/106 (82%)	65±3 (74±3%)	17±2 (20±3%)	5±2 (6±2%)	3	21
All	All	3654/4452 (82%)	2710 (74%)	730 (20%)	214 (6%)	3	21

All 57 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	37	VAL	14
1	A	56	VAL	11
1	B	56	VAL	11
1	A	38	SER	11
1	A	37	VAL	9
1	B	76	GLN	9
1	A	76	GLN	9
1	B	38	SER	8
1	B	36	SER	7
1	A	24	GLY	7
1	B	24	GLY	6
1	B	75	GLY	6
1	A	39	GLU	6
1	B	62	LEU	5
1	B	77	SER	5
1	A	11	ASP	5
1	A	83	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	77	SER	4
1	A	36	SER	4
1	A	30	ARG	4
1	B	25	ASP	4
1	B	11	ASP	4
1	A	75	GLY	4
1	B	83	ASP	4
1	A	27	ASN	3
1	A	50	ASN	3
1	B	27	ASN	3
1	A	25	ASP	3
1	A	82	LEU	3
1	B	82	LEU	3
1	A	84	ASP	3
1	A	53	GLN	2
1	A	62	LEU	2
1	B	59	GLN	2
1	A	66	VAL	2
1	A	23	LEU	2
1	A	44	HIS	1
1	B	49	LEU	1
1	B	60	LEU	1
1	B	61	LYS	1
1	B	81	SER	1
1	B	66	VAL	1
1	B	54	SER	1
1	B	92	LYS	1
1	B	23	LEU	1
1	B	30	ARG	1
1	A	68	LEU	1
1	A	54	SER	1
1	B	26	TYR	1
1	B	39	GLU	1
1	A	78	MET	1
1	B	33	GLU	1
1	A	14	GLU	1
1	B	14	GLU	1
1	B	84	ASP	1
1	A	26	TYR	1
1	B	86	HIS	1

6.3.2 Protein sidechains (i)

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	79/95 (83%)	74±7 (93±8%)	5±7 (7±8%)	19	68
1	B	79/95 (83%)	75±6 (94±8%)	4±6 (6±8%)	24	73
All	All	3318/3990 (83%)	3111 (94%)	207 (6%)	22	71

All 107 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	B	35	LEU	9
1	A	49	LEU	8
1	A	35	LEU	7
1	A	44	HIS	6
1	A	78	MET	6
1	B	44	HIS	5
1	B	82	LEU	5
1	A	34	LEU	5
1	A	83	ASP	4
1	B	59	GLN	4
1	B	97	HIS	4
1	A	82	LEU	4
1	A	28	ARG	3
1	A	91	LEU	3
1	B	13	LEU	3
1	B	25	ASP	3
1	B	58	HIS	3
1	B	78	MET	3
1	A	55	ASN	3
1	A	68	LEU	3
1	B	49	LEU	3
1	A	97	HIS	3
1	B	34	LEU	3
1	B	27	ASN	3
1	A	73	ARG	3
1	A	12	THR	2
1	A	48	GLN	2
1	A	51	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	84	ASP	2
1	A	86	HIS	2
1	A	89	THR	2
1	B	11	ASP	2
1	B	12	THR	2
1	B	47	HIS	2
1	B	67	HIS	2
1	A	13	LEU	2
1	A	50	ASN	2
1	A	58	HIS	2
1	A	76	GLN	2
1	A	61	LYS	2
1	B	90	MET	2
1	A	23	LEU	2
1	A	47	HIS	2
1	B	53	GLN	2
1	A	16	VAL	1
1	A	17	THR	1
1	A	26	TYR	1
1	A	32	MET	1
1	A	36	SER	1
1	A	38	SER	1
1	A	39	GLU	1
1	A	41	SER	1
1	A	42	VAL	1
1	A	45	ILE	1
1	A	54	SER	1
1	A	56	VAL	1
1	A	57	SER	1
1	A	67	HIS	1
1	A	69	VAL	1
1	A	70	LYS	1
1	A	77	SER	1
1	A	81	SER	1
1	A	90	MET	1
1	A	95	ILE	1
1	A	96	HIS	1
1	B	16	VAL	1
1	B	17	THR	1
1	B	19	ILE	1
1	B	26	TYR	1
1	B	29	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	B	30	ARG	1
1	B	31	ILE	1
1	B	32	MET	1
1	B	36	SER	1
1	B	46	SER	1
1	B	54	SER	1
1	B	56	VAL	1
1	B	57	SER	1
1	B	65	SER	1
1	B	69	VAL	1
1	B	77	SER	1
1	B	81	SER	1
1	B	83	ASP	1
1	B	64	LYS	1
1	B	23	LEU	1
1	B	48	GLN	1
1	A	25	ASP	1
1	B	68	LEU	1
1	B	92	LYS	1
1	A	59	GLN	1
1	A	74	GLN	1
1	B	28	ARG	1
1	B	39	GLU	1
1	B	50	ASN	1
1	A	27	ASN	1
1	B	74	GLN	1
1	B	15	ARG	1
1	A	93	GLN	1
1	B	84	ASP	1
1	B	63	LEU	1
1	A	72	LYS	1
1	B	51	LEU	1
1	B	85	ILE	1
1	B	96	HIS	1
1	A	92	LYS	1
1	A	64	LYS	1
1	B	76	GLN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no 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 (i)

No chemical shift data were provided