WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2017 – 09:57 pm GMT

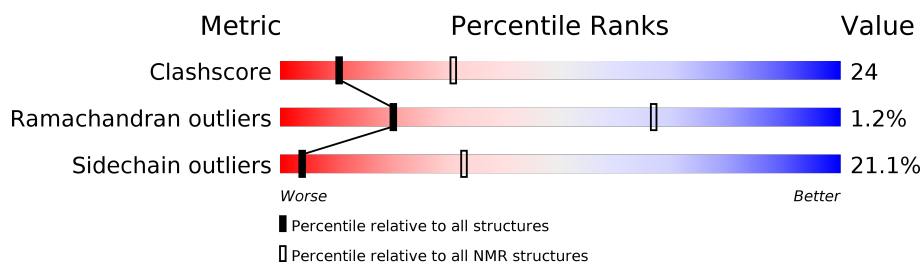|		
PDB ID	:	2GD7
Title	:	The Structure of the Cyclin T-binding domain of Hexim1 reveals the molecular basis for regulation of transcription elongation
Authors	:	Dames, S.A.
Deposited on	:	2006-03-15

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment was not calculated.

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

Metric	Percentile Ranks	Value
Clashscore		24
Ramachandran outliers		1.2%
Sidechain outliers		21.1%

Worse   *Better*

▌ Percentile relative to all structures
⫿ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	107	11% 23% • 62%
1	B	107	22% 33% 6% 39%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 16 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:23-A:63, B:23-B:87 (106)	0.95	16

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. No single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 3500 atoms, of which 1726 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HEXIM1 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1750	538	863	163	182	4	
1	B	107	Total	C	H	N	O	S	0
			1750	538	863	163	182	4	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	GB 5453682
A	2	ALA	-	EXPRESSION TAG	GB 5453682
A	4	ALA	GLY	ENGINEERED	GB 5453682
B	1	GLY	-	EXPRESSION TAG	GB 5453682
B	2	ALA	-	EXPRESSION TAG	GB 5453682
B	4	ALA	GLY	ENGINEERED	GB 5453682

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

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

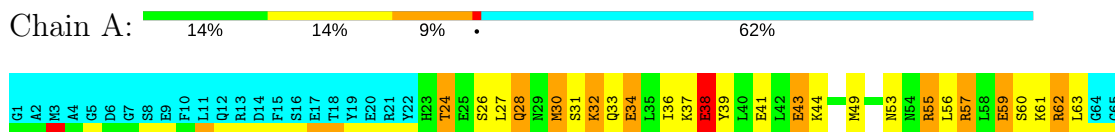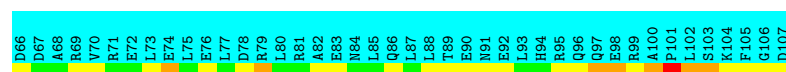- Molecule 1: HEXIM1 protein
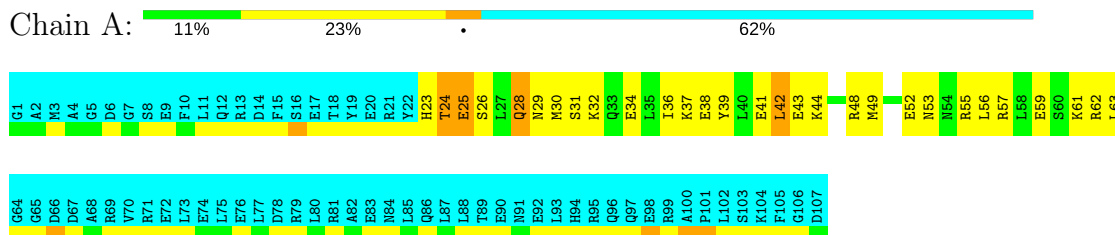
- Molecule 1: HEXIM1 protein
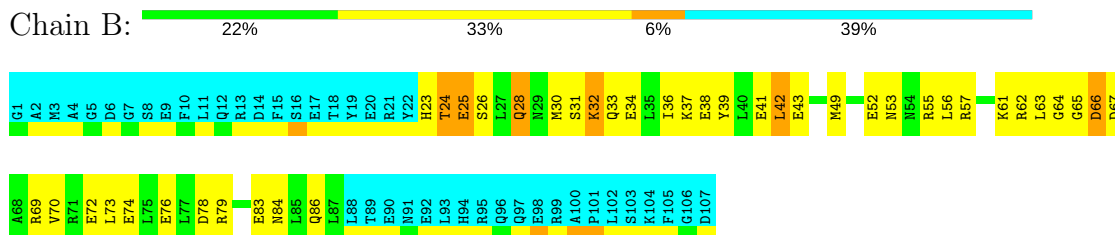
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

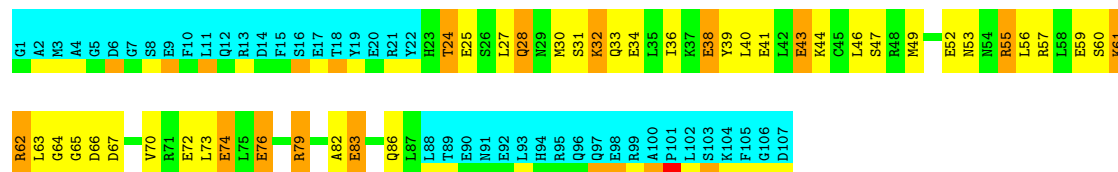### 4.2.1 Score per residue for model 1

- Molecule 1: HEXIM1 protein

D66 D67 A68 R69 V70 R71 E72 L73 E74 L75 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

• Molecule 1: HEXIM1 protein

Chain B: 21% 28% 11% 39%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 E34 L35 I36 K37 E38 Y39 L40 E41 L42 E43 K44 C45 L46 S47 R48 M49 E52 N53 N54 R55 L56 L58 E59 S60 K61

R62 L63 G64 G65 D66 D67 V70 R71 E72 L73 E74 L75 E76 R79 A82 E83 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

4.2.2 Score per residue for model 2

• Molecule 1: HEXIM1 protein

Chain A: 14% 19% 6% 62%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 I36 K37 E38 Y39 L40 E41 L42 E43 K44 C45 L46 M49 N53 N54 R55 L56 E59 S60 K61 R62 L63 G64 G65

D66 D67 A68 R69 V70 R71 E72 L73 E74 L75 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

• Molecule 1: HEXIM1 protein

Chain B: 23% 30% 7% 39%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 E34 L35 I36 K37 E38 Y39 L40 E41 L42 E43 K44 C45 L46 M49 E52 N53 N54 R55 L56 S60 K61 R62 L63 G64

G65 D66 D67 A68 R69 V70 R71 E72 L73 E74 L75 E76 R79 L80 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

4.2.3 Score per residue for model 3

• Molecule 1: HEXIM1 protein

Chain A: 12% 21% 5% 62%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 E34 L35 I36 K37 E38 Y39 L40 E41 L42 M49 E50 D51 E52 N53 N54 R55 L56 R57 L58 E59 S60 K61 R62 L63 G64 G65

D66 D67 A68 R69 V70 R71 E72 L73 E74 L75 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

• Molecule 1: HEXIM1 protein

Chain B: 23% 31% 6% • 39%

4.2.4 Score per residue for model 4

• Molecule 1: HEXIM1 protein

Chain A: 15% 18% 5% • 62%

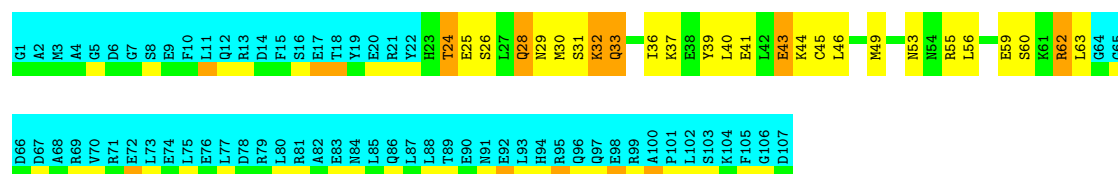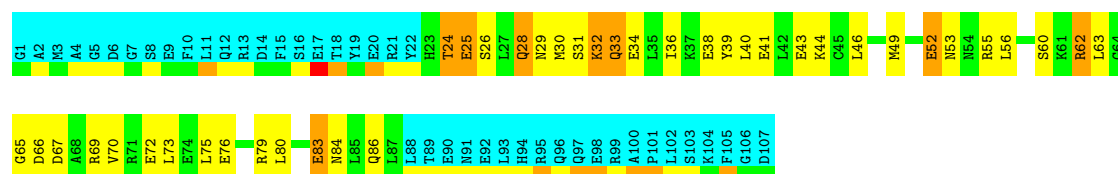• Molecule 1: HEXIM1 protein

Chain B: 27% 28% 6% 39%

4.2.5 Score per residue for model 5

• Molecule 1: HEXIM1 protein

Chain A: 10% 21% 7% • 62%
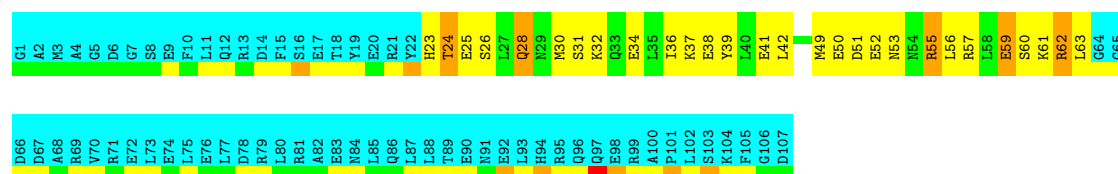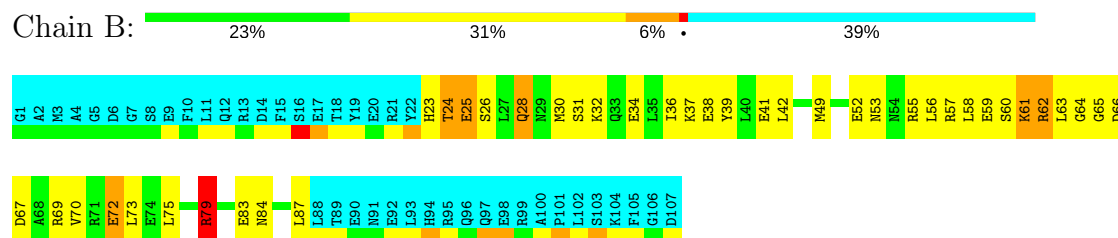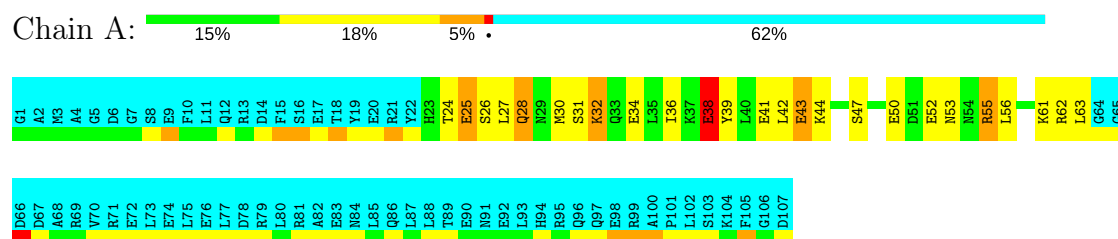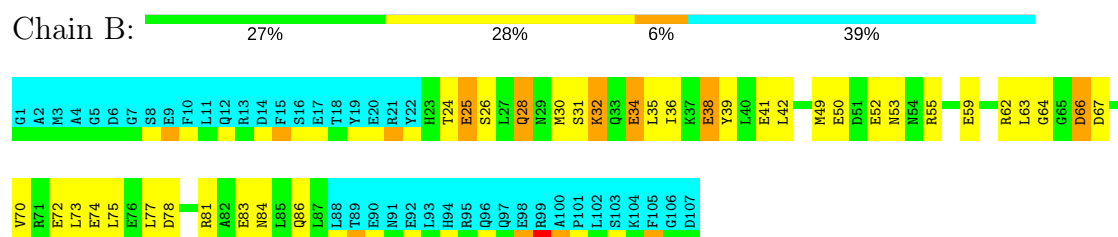

• Molecule 1: HEXIM1 protein

Chain B: 26% 26% 8% 39%

R69 E72 E76 R79 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

4.2.6 Score per residue for model 6

• Molecule 1: HEXIM1 protein

Chain A: 17% 13% 8% 62%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 S31 K32 Q33 E34 L35 I36 K37 E38 Y39 L42 E43 K44 M49 N53 N54 R55 L56 R57 I58 E59 S60 K61 R62 L63 G64 G65 D66 D67

A68 R69 V70 R71 E72 L73 E74 L75 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

• Molecule 1: HEXIM1 protein

Chain B: 24% 28% 8% 39%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 E34 L35 I36 K37 E38 Y39 L42 E43 K44 M49 E52 N53 N54 R55 L56 R57 L58 E59 S60 K61 R62 L63 G64 G65

D66 R69 V70 L73 E76 L77 D78 R79 L80 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

4.2.7 Score per residue for model 7

• Molecule 1: HEXIM1 protein

Chain A: 14% 20% 5% 62%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 L35 I36 K37 E38 Y39 L40 E41 L42 E43 K44 R48 M49 E50 D51 E52 N53 L56 R57 K61 R62 L63 G64 G65 D66

D67 A68 R69 V70 R71 E72 L73 E74 L75 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

• Molecule 1: HEXIM1 protein

Chain B: 23% 31% 7% 39%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 E34 L35 I36 K37 E38 Y39 L40 E41 L42 R48 M49 E50 N53 L56 R57 K61 R62 L63 G64 G65 D66 D67 A68

R69 V70 R71 E72 L73 E74 D78 R79 L80 R81 A82 E83 N84 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

4.2.8　Score per residue for model 8

• Molecule 1: HEXIM1 protein

Chain A:

• Molecule 1: HEXIM1 protein

Chain B:

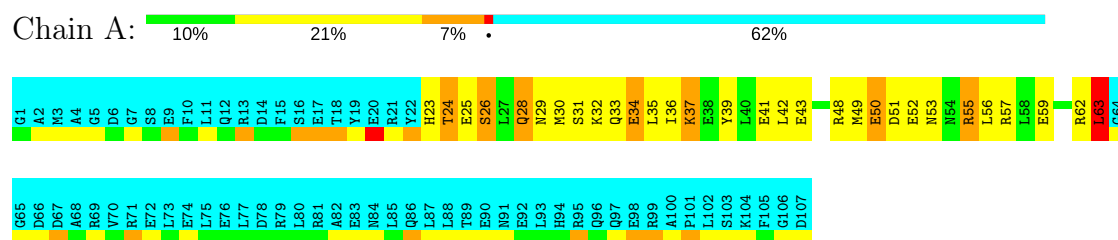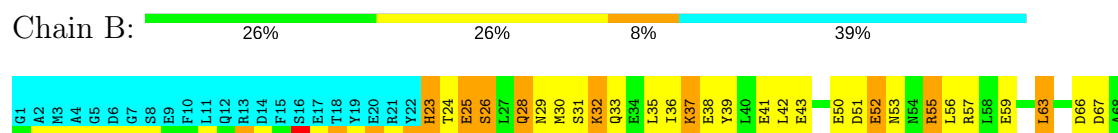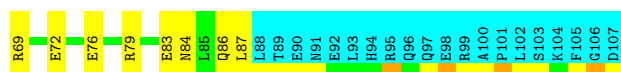### 4.2.9　Score per residue for model 9

• Molecule 1: HEXIM1 protein

Chain A:

• Molecule 1: HEXIM1 protein

Chain B:
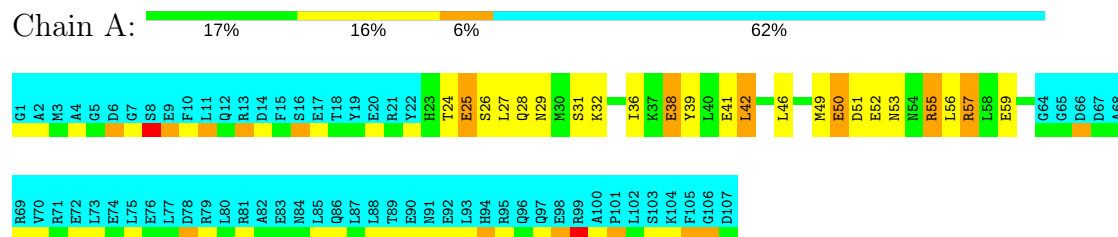
4.2.10　Score per residue for model 10

• Molecule 1: HEXIM1 protein

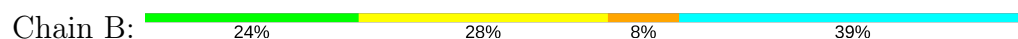Chain A:

• Molecule 1: HEXIM1 protein

Chain B:

4.2.11   Score per residue for model 11

• Molecule 1: HEXIM1 protein

Chain A:

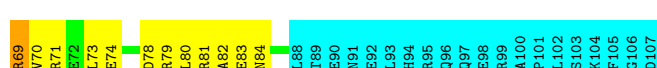• Molecule 1: HEXIM1 protein

Chain B:

4.2.12   Score per residue for model 12

• Molecule 1: HEXIM1 protein

Chain A:

• Molecule 1: HEXIM1 protein

Chain B: 24% 30% 7% 39%
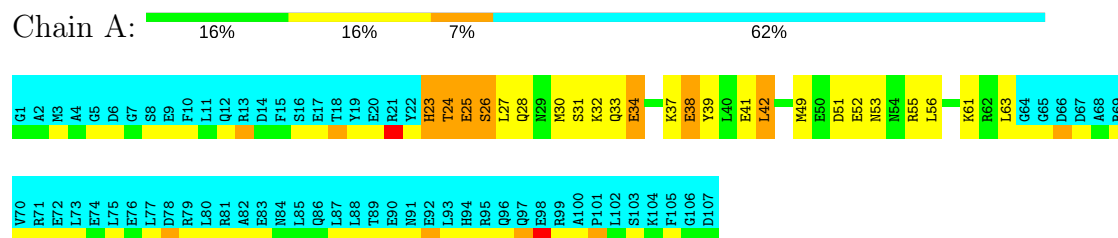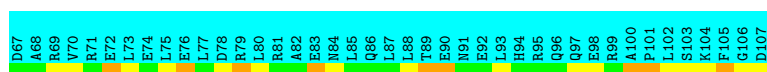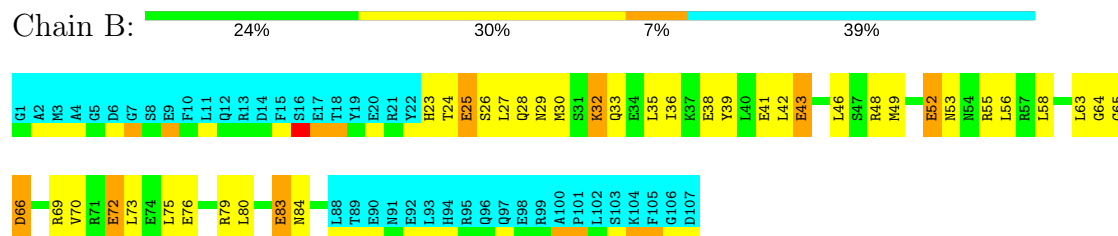
4.2.13 Score per residue for model 13

• Molecule 1: HEXIM1 protein

Chain A: 16% 16% 6% 62%

• Molecule 1: HEXIM1 protein

Chain B: 28% 25% 7% 39%
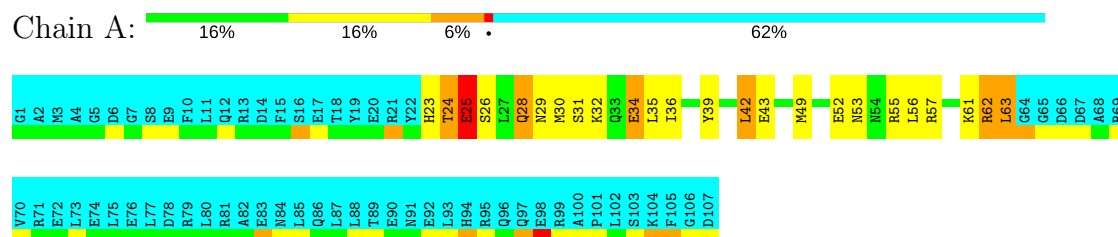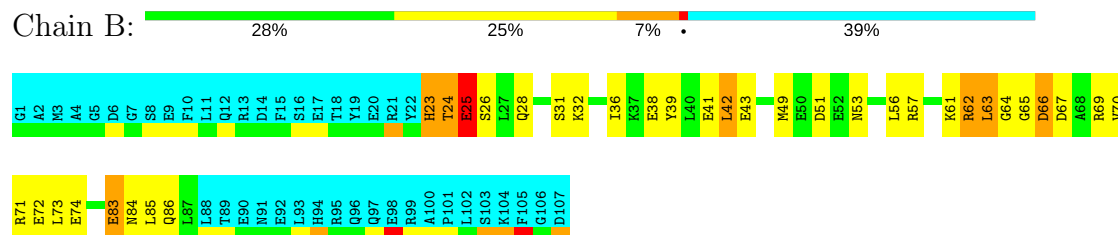
4.2.14 Score per residue for model 14

• Molecule 1: HEXIM1 protein

Chain A: 17% 17% 62%

• Molecule 1: HEXIM1 protein

Chain B: 25%   26%   9%   39%
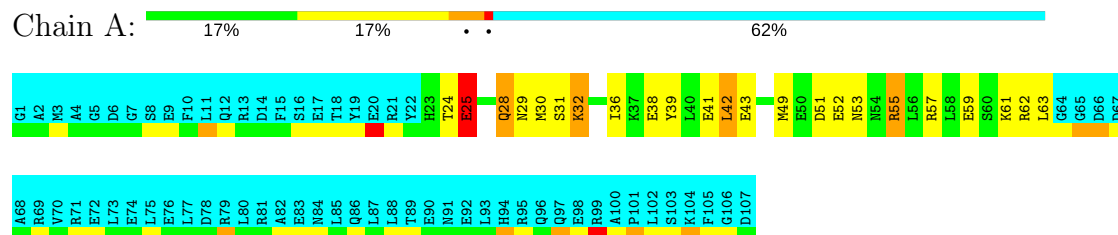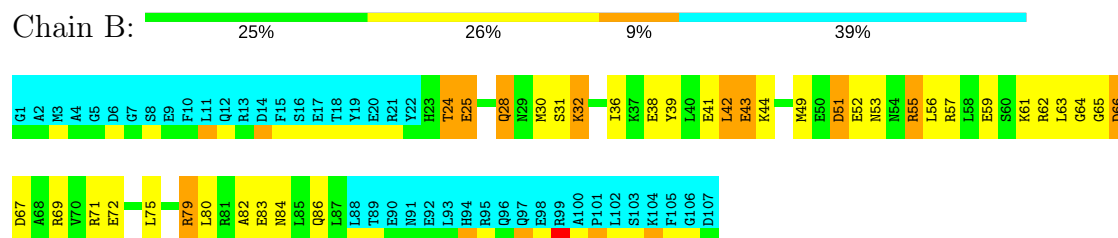
4.2.15 Score per residue for model 15

• Molecule 1: HEXIM1 protein

Chain A: 14%   21%   •   62%

• Molecule 1: HEXIM1 protein

Chain B: 30%   24%   7%   39%
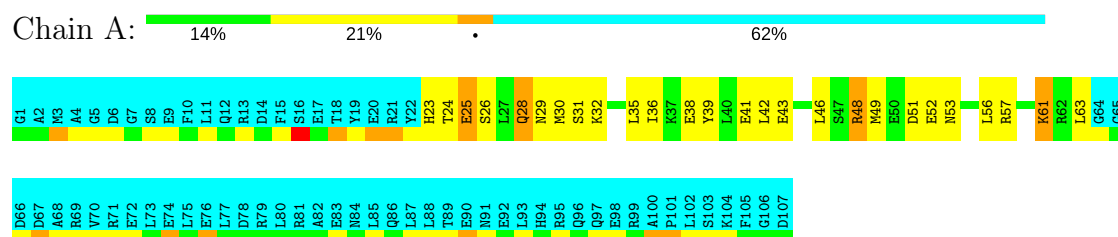
4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: HEXIM1 protein

Chain A: 12%   20%   7%   62%

• Molecule 1: HEXIM1 protein

Chain B: 23%   30%   7%   •   39%

D67 V70 L73 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107
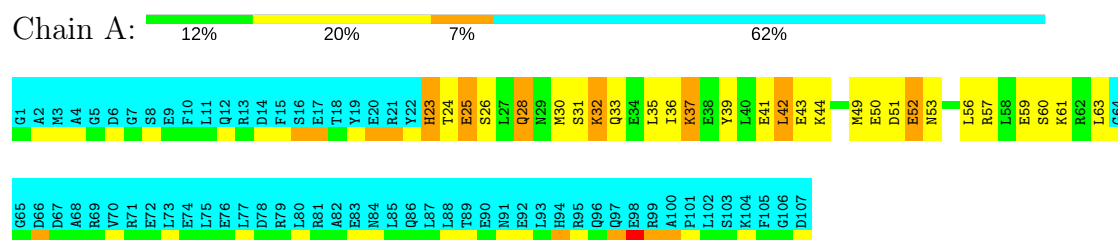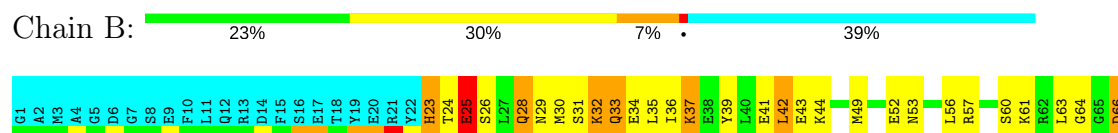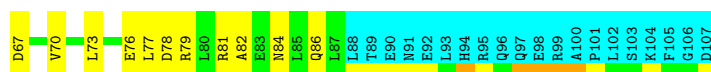
4.2.17 Score per residue for model 17

• Molecule 1: HEXIM1 protein

Chain A: 15% 17% 5% • 62%

G1 A2 M3 A4 G5 D6 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 I36 K37 E38 Y39 L40 E41 L42 E43 K44 C45 R48 N53 N54 R55 L56 E59 S60 K61 R62 L63 G64 G65 D66

D67 A68 R69 V70 R71 E72 L73 E74 L75 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

• Molecule 1: HEXIM1 protein

Chain B: 22% 28% 8% • 39%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 E34 L35 I36 K37 E38 Y39 L40 E41 L42 E43 K44 C45 R48 E52 N53 E59 S60 K61 R62 L63 D66 R69

V70 R71 E72 L73 E74 L75 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

4.2.18 Score per residue for model 18

• Molecule 1: HEXIM1 protein

Chain A: 14% 19% 5% • 62%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 E34 L35 I36 K37 E38 E41 L42 E43 K44 C45 R48 M49 E50 R55 L56 R57 L58 K61 R62 L63 G64 G65 D66

D67 A68 R69 V70 R71 E72 L73 E74 L75 E76 L77 D78 R79 L80 R81 A82 E83 N84 L85 Q86 L87 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107

• Molecule 1: HEXIM1 protein

Chain B: 32% 21% 7% • 39%

G1 A2 M3 A4 G5 D6 G7 S8 E9 F10 L11 Q12 R13 D14 F15 S16 E17 T18 Y19 E20 R21 Y22 H23 T24 E25 S26 L27 Q28 N29 M30 S31 K32 Q33 E34 L35 I36 K37 L42 E43 R48 M49 E52 R55 L56 R57 L58 K61 R62 L63 D66 D67 A68 R69 V70

R71 L75 E76 R79 E83 N84 L88 T89 E90 N91 E92 L93 H94 R95 Q96 Q97 E98 R99 A100 P101 L102 S103 K104 F105 G106 D107
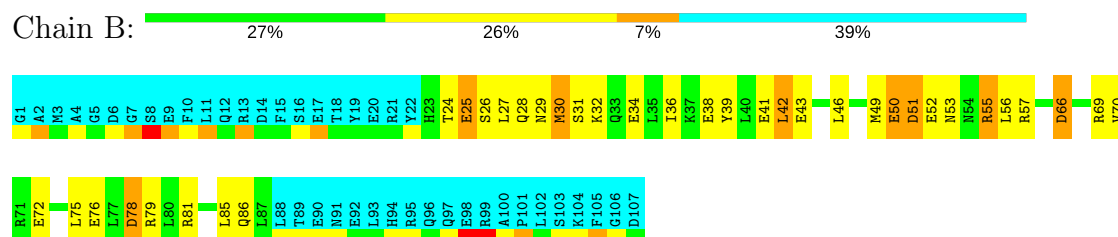
4.2.19 Score per residue for model 19

• Molecule 1: HEXIM1 protein

Chain A:

• Molecule 1: HEXIM1 protein

Chain B:

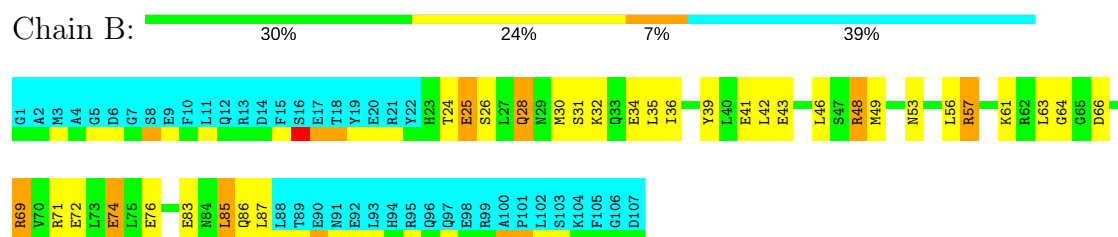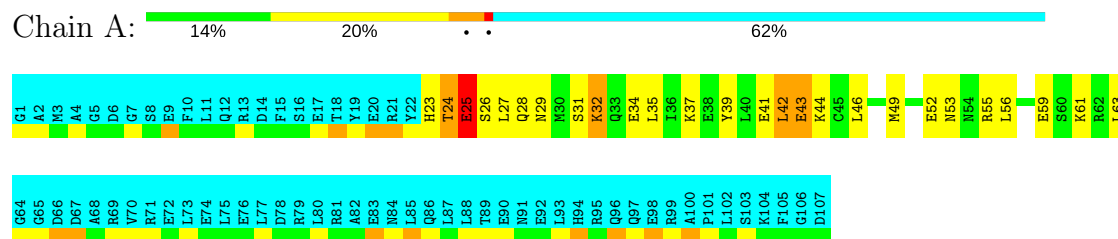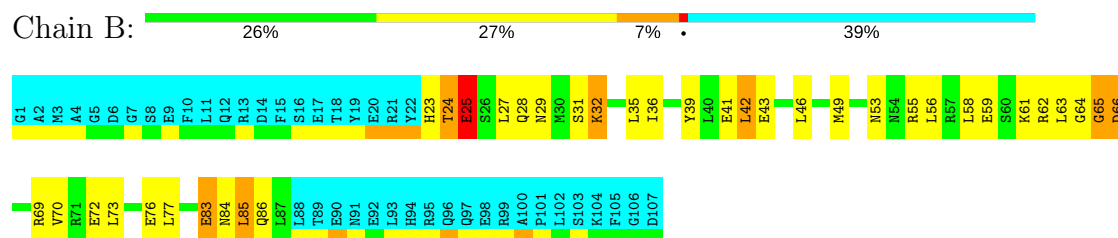#### 4.2.20 Score per residue for model 20

• Molecule 1: HEXIM1 protein

Chain A:

• Molecule 1: HEXIM1 protein

Chain B:
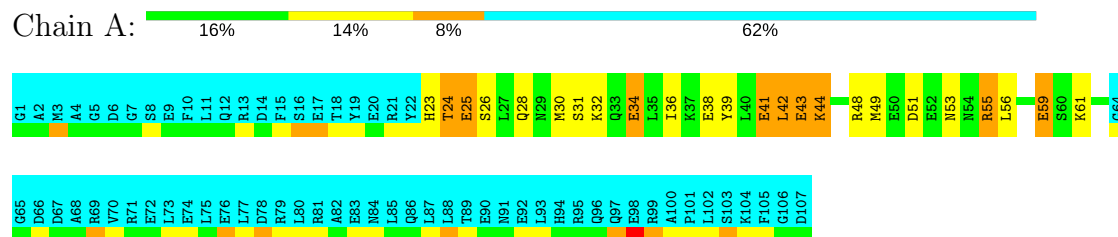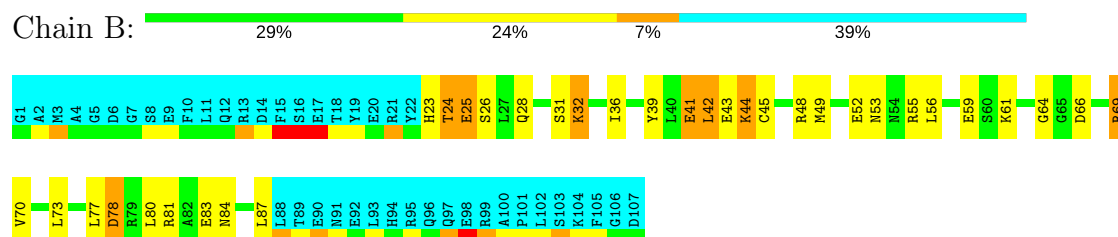
5　Refinement protocol and experimental data overview ⓘ

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

Of the 200 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	2.9.9
X-PLOR-NIH	refinement	2.9.9

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.46±0.03	4±2/351 (1.3±0.6%)	0.89±0.02	0±0/466 (0.0±0.0%)
1	B	1.47±0.02	6±2/545 (1.1±0.4%)	0.89±0.01	0±0/726 (0.0±0.0%)
All	All	1.47	213/17920 (1.2%)	0.89	0/23840 (0.0%)

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	0.1±0.2
1	B	0.0±0.0	0.1±0.5
All	All	0	4

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models Worst	Total
1	B	38	GLU	CD-OE2	-6.59	1.18	1.25	12	9
1	A	38	GLU	CD-OE2	-6.51	1.18	1.25	12	11
1	A	41	GLU	CD-OE2	-6.14	1.18	1.25	12	11
1	A	25	GLU	CD-OE2	-6.12	1.19	1.25	20	9
1	A	41	GLU	CD-OE1	-6.00	1.19	1.25	12	6
1	B	25	GLU	CD-OE2	-5.99	1.19	1.25	12	12
1	B	43	GLU	CD-OE2	-5.95	1.19	1.25	6	9
1	B	83	GLU	CD-OE1	-5.91	1.19	1.25	17	6
1	A	43	GLU	CD-OE2	-5.90	1.19	1.25	6	7
1	B	34	GLU	CD-OE1	-5.89	1.19	1.25	16	5
1	B	74	GLU	CD-OE2	-5.83	1.19	1.25	10	6
1	B	72	GLU	CD-OE2	-5.82	1.19	1.25	12	7
1	B	25	GLU	CD-OE1	-5.80	1.19	1.25	1	7
1	B	41	GLU	CD-OE1	-5.75	1.19	1.25	16	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models Worst	Total
1	B	41	GLU	CD-OE2	-5.74	1.19	1.25	4	14
1	A	34	GLU	CD-OE1	-5.69	1.19	1.25	18	8
1	B	52	GLU	CD-OE1	-5.69	1.19	1.25	8	4
1	A	59	GLU	CD-OE1	-5.67	1.19	1.25	20	4
1	A	43	GLU	CD-OE1	-5.66	1.19	1.25	15	1
1	B	72	GLU	CD-OE1	-5.61	1.19	1.25	12	4
1	B	34	GLU	CD-OE2	-5.60	1.19	1.25	4	5
1	B	76	GLU	CD-OE2	-5.59	1.19	1.25	18	8
1	A	59	GLU	CD-OE2	-5.53	1.19	1.25	19	8
1	A	50	GLU	CD-OE2	-5.52	1.19	1.25	5	4
1	B	52	GLU	CD-OE2	-5.48	1.19	1.25	20	7
1	B	59	GLU	CD-OE2	-5.46	1.19	1.25	4	2
1	A	52	GLU	CD-OE2	-5.45	1.19	1.25	13	5
1	B	74	GLU	CD-OE1	-5.41	1.19	1.25	1	2
1	A	52	GLU	CD-OE1	-5.40	1.19	1.25	16	1
1	A	50	GLU	CD-OE1	-5.39	1.19	1.25	12	5
1	A	34	GLU	CD-OE2	-5.34	1.19	1.25	10	5
1	B	76	GLU	CD-OE1	-5.27	1.19	1.25	12	2
1	B	50	GLU	CD-OE1	-5.27	1.19	1.25	9	1
1	A	25	GLU	CD-OE1	-5.22	1.20	1.25	20	3
1	B	50	GLU	CD-OE2	-5.11	1.20	1.25	7	2
1	B	83	GLU	CD-OE2	-5.11	1.20	1.25	5	7
1	B	59	GLU	CD-OE1	-5.08	1.20	1.25	14	2
1	B	43	GLU	CD-OE1	-5.07	1.20	1.25	15	1

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	B	81	ARG	Sidechain	1
1	B	79	ARG	Sidechain	1
1	A	62	ARG	Sidechain	1
1	B	62	ARG	Sidechain	1

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	349	356	355	29±5
1	B	543	549	548	32±5
All	All	17840	18100	18060	847

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:24:THR:HG22	1:B:28:GLN:HE22	0.89	1.25	12	10
1:A:42:LEU:HD23	1:B:42:LEU:HD23	0.87	1.47	5	3
1:A:36:ILE:HD13	1:B:28:GLN:NE2	0.83	1.88	2	8
1:A:24:THR:HG22	1:A:28:GLN:HE22	0.81	1.36	19	11
1:A:56:LEU:HD21	1:B:57:ARG:HE	0.80	1.34	16	1
1:B:24:THR:HG22	1:B:28:GLN:NE2	0.80	1.92	12	19
1:A:28:GLN:NE2	1:B:36:ILE:HD13	0.79	1.92	13	9
1:A:63:LEU:HD23	1:B:63:LEU:HD23	0.79	1.53	6	1
1:A:24:THR:HG22	1:A:28:GLN:NE2	0.79	1.92	19	19
1:A:57:ARG:HE	1:B:56:LEU:HD21	0.72	1.41	16	1
1:A:63:LEU:HD23	1:B:63:LEU:HA	0.70	1.62	5	3
1:A:63:LEU:HA	1:B:63:LEU:HD23	0.70	1.63	5	3
1:A:42:LEU:HD12	1:B:42:LEU:HD12	0.70	1.62	19	12
1:A:46:LEU:HD11	1:B:49:MET:SD	0.70	2.27	12	5
1:A:36:ILE:HG21	1:B:28:GLN:HE22	0.67	1.49	13	8
1:A:28:GLN:HE22	1:B:36:ILE:HG21	0.66	1.51	13	8
1:A:63:LEU:CB	1:B:63:LEU:HD13	0.65	2.22	15	1
1:A:49:MET:SD	1:B:46:LEU:HD11	0.65	2.31	12	5
1:A:39:TYR:CE2	1:B:39:TYR:CE2	0.65	2.85	9	19
1:B:49:MET:O	1:B:53:ASN:ND2	0.64	2.30	10	16
1:A:30:MET:O	1:B:32:LYS:NZ	0.63	2.32	3	11
1:A:53:ASN:HD21	1:B:53:ASN:HD21	0.62	1.35	10	9
1:A:49:MET:O	1:A:53:ASN:ND2	0.62	2.31	10	16
1:A:28:GLN:OE1	1:B:36:ILE:HD13	0.61	1.96	5	1
1:A:53:ASN:ND2	1:B:53:ASN:HD21	0.60	1.95	10	18
1:A:36:ILE:HD13	1:B:28:GLN:HG3	0.60	1.73	7	6
1:A:53:ASN:HD21	1:B:53:ASN:ND2	0.60	1.95	20	16
1:A:63:LEU:HB3	1:B:63:LEU:HB3	0.59	1.73	8	11
1:A:36:ILE:HD13	1:B:28:GLN:HE22	0.59	1.53	13	1
1:A:28:GLN:HG3	1:B:36:ILE:HD13	0.58	1.75	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:71:ARG:O	1:B:75:LEU:HD12	0.58	1.97	8	2
1:A:32:LYS:NZ	1:B:28:GLN:O	0.58	2.35	3	17
1:A:32:LYS:NZ	1:B:30:MET:O	0.58	2.33	3	11
1:A:53:ASN:OD1	1:A:57:ARG:NH1	0.57	2.35	6	2
1:A:63:LEU:HD13	1:B:63:LEU:CB	0.57	2.29	15	1
1:B:32:LYS:HA	1:B:35:LEU:HD12	0.57	1.76	12	8
1:B:53:ASN:OD1	1:B:57:ARG:NH1	0.57	2.37	3	2
1:A:32:LYS:HG2	1:A:36:ILE:HD11	0.57	1.76	14	1
1:A:57:ARG:NE	1:A:57:ARG:HA	0.56	2.14	16	1
1:A:28:GLN:O	1:B:32:LYS:NZ	0.56	2.38	15	18
1:B:51:ASP:CB	1:B:55:ARG:HH12	0.56	2.13	9	2
1:B:32:LYS:HG2	1:B:36:ILE:HD11	0.56	1.76	14	1
1:A:24:THR:O	1:A:28:GLN:NE2	0.56	2.38	10	12
1:A:32:LYS:HA	1:A:35:LEU:HD12	0.56	1.77	5	7
1:A:63:LEU:CB	1:B:63:LEU:HB3	0.56	2.31	17	2
1:B:57:ARG:NE	1:B:57:ARG:HA	0.56	2.15	16	1
1:A:28:GLN:HE22	1:B:36:ILE:HD13	0.56	1.60	13	2
1:B:24:THR:O	1:B:28:GLN:NE2	0.55	2.39	10	14
1:A:63:LEU:HB3	1:B:63:LEU:CB	0.55	2.31	17	2
1:B:60:SER:HA	1:B:63:LEU:HD12	0.55	1.78	2	1
1:B:43:GLU:OE1	1:B:44:LYS:NZ	0.55	2.39	1	1
1:A:53:ASN:ND2	1:B:53:ASN:ND2	0.55	2.54	17	13
1:B:62:ARG:O	1:B:64:GLY:N	0.54	2.37	11	4
1:B:72:GLU:HA	1:B:75:LEU:HD12	0.54	1.78	14	8
1:B:62:ARG:O	1:B:62:ARG:NH1	0.54	2.37	17	1
1:B:48:ARG:CG	1:B:49:MET:N	0.54	2.71	18	1
1:A:63:LEU:HD23	1:B:64:GLY:O	0.54	2.03	10	6
1:B:66:ASP:O	1:B:70:VAL:HG23	0.54	2.02	6	3
1:B:62:ARG:NH2	1:B:64:GLY:O	0.54	2.35	6	1
1:B:66:ASP:O	1:B:69:ARG:N	0.54	2.41	13	13
1:A:63:LEU:HB3	1:B:63:LEU:HD13	0.54	1.79	15	1
1:A:28:GLN:NE2	1:B:36:ILE:HG21	0.53	2.17	3	7
1:A:36:ILE:HD11	1:B:28:GLN:HA	0.53	1.78	6	1
1:A:43:GLU:OE1	1:A:44:LYS:NZ	0.53	2.41	19	4
1:A:52:GLU:CG	1:B:57:ARG:HH21	0.53	2.16	14	1
1:A:28:GLN:HA	1:B:36:ILE:HD11	0.53	1.78	6	1
1:B:25:GLU:O	1:B:28:GLN:N	0.53	2.41	13	2
1:A:27:LEU:HD22	1:B:39:TYR:CD2	0.53	2.39	19	3
1:B:25:GLU:O	1:B:29:ASN:N	0.53	2.38	7	10
1:B:59:GLU:O	1:B:62:ARG:N	0.53	2.40	11	3
1:B:69:ARG:CZ	1:B:69:ARG:HB2	0.53	2.33	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ARG:CG	1:A:49:MET:N	0.53	2.72	18	1
1:B:66:ASP:CG	1:B:67:ASP:N	0.52	2.62	14	1
1:A:60:SER:HA	1:A:63:LEU:HD12	0.52	1.79	2	1
1:A:32:LYS:HD3	1:A:36:ILE:HD11	0.52	1.82	12	1
1:B:25:GLU:H	1:B:25:GLU:CD	0.52	2.07	3	1
1:B:28:GLN:N	1:B:28:GLN:NE2	0.52	2.58	10	3
1:A:62:ARG:NH1	1:A:62:ARG:O	0.52	2.36	17	1
1:A:57:ARG:O	1:A:61:LYS:CG	0.52	2.58	15	1
1:B:79:ARG:NH1	1:B:83:GLU:OE1	0.52	2.40	17	3
1:A:39:TYR:CE1	1:B:39:TYR:CE1	0.52	2.97	9	4
1:A:25:GLU:CD	1:A:25:GLU:H	0.52	2.08	3	1
1:A:28:GLN:HE21	1:B:36:ILE:HD13	0.52	1.64	14	2
1:A:25:GLU:O	1:A:28:GLN:N	0.52	2.43	13	2
1:A:36:ILE:HG21	1:B:28:GLN:NE2	0.51	2.20	15	6
1:B:51:ASP:OD1	1:B:55:ARG:NH2	0.51	2.43	5	1
1:B:24:THR:O	1:B:25:GLU:C	0.51	2.49	19	15
1:B:57:ARG:NH2	1:B:60:SER:OG	0.51	2.39	16	1
1:B:64:GLY:O	1:B:66:ASP:N	0.51	2.44	13	2
1:B:65:GLY:O	1:B:66:ASP:CB	0.51	2.58	14	1
1:B:79:ARG:O	1:B:82:ALA:HB3	0.51	2.05	1	4
1:A:57:ARG:HH21	1:B:52:GLU:CG	0.50	2.20	14	1
1:A:25:GLU:O	1:A:29:ASN:N	0.50	2.40	7	10
1:A:52:GLU:OE2	1:B:57:ARG:NH1	0.50	2.44	5	1
1:A:59:GLU:O	1:B:63:LEU:HD21	0.50	2.05	11	1
1:A:24:THR:O	1:A:25:GLU:C	0.50	2.49	7	14
1:A:33:GLN:O	1:A:37:LYS:NZ	0.50	2.41	18	1
1:A:53:ASN:HD21	1:B:53:ASN:CG	0.50	2.10	20	5
1:A:59:GLU:O	1:A:62:ARG:N	0.50	2.45	17	3
1:B:69:ARG:CZ	1:B:69:ARG:HA	0.50	2.37	17	1
1:A:39:TYR:CD2	1:B:27:LEU:HD22	0.49	2.42	19	3
1:B:62:ARG:NE	1:B:62:ARG:O	0.49	2.41	1	2
1:B:67:ASP:O	1:B:70:VAL:N	0.49	2.45	11	1
1:B:28:GLN:H	1:B:28:GLN:NE2	0.49	2.05	10	4
1:A:32:LYS:CE	1:B:30:MET:O	0.49	2.60	12	3
1:A:55:ARG:HH12	1:A:59:GLU:CD	0.49	2.10	17	1
1:A:51:ASP:CB	1:A:55:ARG:HH12	0.49	2.20	14	3
1:B:76:GLU:OE2	1:B:79:ARG:NH1	0.49	2.44	6	1
1:B:44:LYS:NZ	1:B:47:SER:OG	0.49	2.41	1	1
1:A:36:ILE:HG23	1:B:27:LEU:HD13	0.49	1.85	1	1
1:A:36:ILE:HD13	1:B:28:GLN:HE21	0.48	1.68	14	1
1:A:56:LEU:HD11	1:B:57:ARG:HD2	0.48	1.84	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ASN:CG	1:B:49:MET:SD	0.48	2.91	4	1
1:A:57:ARG:HD2	1:B:56:LEU:HD11	0.48	1.85	13	1
1:B:78:ASP:HA	1:B:81:ARG:CZ	0.48	2.38	20	1
1:A:25:GLU:CD	1:A:26:SER:N	0.48	2.67	4	1
1:B:58:LEU:O	1:B:62:ARG:NH1	0.48	2.38	19	1
1:A:56:LEU:HB3	1:B:56:LEU:HD13	0.48	1.85	7	3
1:A:44:LYS:HD3	1:A:44:LYS:N	0.48	2.23	20	1
1:A:56:LEU:HD22	1:B:56:LEU:HB3	0.48	1.85	16	1
1:B:44:LYS:HD3	1:B:44:LYS:N	0.48	2.23	20	1
1:A:39:TYR:N	1:B:39:TYR:OH	0.48	2.45	17	5
1:B:78:ASP:CG	1:B:81:ARG:HH21	0.48	2.12	4	1
1:A:42:LEU:HD12	1:B:42:LEU:CD1	0.48	2.38	8	8
1:A:57:ARG:NH2	1:A:60:SER:OG	0.47	2.39	16	1
1:A:28:GLN:CD	1:B:36:ILE:HD13	0.47	2.29	16	1
1:A:57:ARG:NH1	1:B:52:GLU:OE1	0.47	2.43	1	4
1:A:56:LEU:HD13	1:B:56:LEU:HB3	0.47	1.85	7	3
1:A:26:SER:C	1:A:30:MET:SD	0.47	2.92	5	1
1:B:26:SER:C	1:B:30:MET:SD	0.47	2.92	5	1
1:B:66:ASP:O	1:B:67:ASP:C	0.47	2.52	11	1
1:A:63:LEU:HD23	1:B:66:ASP:HB2	0.47	1.86	14	1
1:A:28:GLN:NE2	1:A:28:GLN:N	0.47	2.62	17	2
1:A:42:LEU:CD1	1:B:42:LEU:HD12	0.47	2.39	16	10
1:A:28:GLN:N	1:A:28:GLN:NE2	0.47	2.63	10	1
1:B:75:LEU:O	1:B:79:ARG:NH2	0.47	2.41	3	1
1:B:69:ARG:HH21	1:B:72:GLU:CD	0.47	2.12	14	2
1:A:28:GLN:NE2	1:A:28:GLN:H	0.47	2.07	10	4
1:A:28:GLN:N	1:A:28:GLN:HE21	0.47	2.08	13	1
1:A:63:LEU:HD13	1:B:63:LEU:HB3	0.47	1.85	15	1
1:B:37:LYS:HD3	1:B:37:LYS:N	0.47	2.25	16	1
1:B:24:THR:O	1:B:27:LEU:N	0.46	2.48	9	5
1:A:53:ASN:OD1	1:B:53:ASN:ND2	0.46	2.48	1	2
1:A:53:ASN:N	1:A:53:ASN:HD22	0.46	2.08	11	1
1:B:33:GLN:O	1:B:37:LYS:NZ	0.46	2.43	18	1
1:B:76:GLU:CD	1:B:79:ARG:HH21	0.46	2.12	5	2
1:A:63:LEU:HB2	1:B:63:LEU:HD13	0.46	1.86	15	2
1:A:55:ARG:NH1	1:A:59:GLU:OE2	0.46	2.46	1	2
1:B:69:ARG:NH1	1:B:72:GLU:OE1	0.46	2.46	2	2
1:A:39:TYR:OH	1:B:39:TYR:N	0.46	2.48	17	5
1:A:37:LYS:N	1:A:37:LYS:HD3	0.46	2.26	16	1
1:B:48:ARG:CZ	1:B:48:ARG:HB3	0.46	2.40	15	2
1:A:55:ARG:N	1:A:55:ARG:HD3	0.46	2.26	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:LEU:O	1:B:44:LYS:NZ	0.46	2.37	2	1
1:B:78:ASP:OD1	1:B:81:ARG:NH1	0.46	2.48	7	1
1:A:48:ARG:CZ	1:A:48:ARG:HB3	0.45	2.41	15	1
1:B:23:HIS:NE2	1:B:25:GLU:OE1	0.45	2.49	10	1
1:B:33:GLN:H	1:B:33:GLN:CD	0.45	2.15	12	2
1:A:33:GLN:H	1:A:33:GLN:CD	0.45	2.15	2	1
1:B:28:GLN:NE2	1:B:28:GLN:N	0.45	2.63	9	2
1:A:48:ARG:HB3	1:A:48:ARG:CZ	0.45	2.41	17	1
1:A:30:MET:O	1:B:32:LYS:CE	0.45	2.65	12	2
1:B:37:LYS:NZ	1:B:41:GLU:OE2	0.45	2.42	17	1
1:A:61:LYS:C	1:A:63:LEU:H	0.45	2.15	14	1
1:A:55:ARG:O	1:A:58:LEU:N	0.45	2.50	18	1
1:B:25:GLU:CD	1:B:26:SER:N	0.45	2.70	4	1
1:A:53:ASN:CG	1:B:53:ASN:HD21	0.45	2.13	8	3
1:A:27:LEU:HD13	1:B:36:ILE:HG23	0.45	1.87	4	2
1:B:85:LEU:HG	1:B:86:GLN:N	0.45	2.27	15	1
1:B:62:ARG:C	1:B:64:GLY:H	0.45	2.15	11	1
1:A:55:ARG:CD	1:A:55:ARG:N	0.45	2.79	20	1
1:A:43:GLU:O	1:A:47:SER:OG	0.44	2.35	4	1
1:B:39:TYR:O	1:B:43:GLU:CB	0.44	2.65	1	1
1:A:61:LYS:O	1:A:63:LEU:N	0.44	2.49	14	1
1:A:62:ARG:O	1:A:62:ARG:NE	0.44	2.42	1	2
1:A:35:LEU:O	1:B:39:TYR:OH	0.44	2.31	19	2
1:B:55:ARG:O	1:B:56:LEU:C	0.44	2.54	8	12
1:A:57:ARG:HH22	1:B:52:GLU:CD	0.44	2.16	18	1
1:A:40:LEU:O	1:A:44:LYS:NZ	0.44	2.38	2	1
1:A:62:ARG:NE	1:A:62:ARG:HA	0.44	2.27	2	1
1:B:41:GLU:O	1:B:45:CYS:SG	0.44	2.66	17	2
1:A:63:LEU:HD22	1:B:63:LEU:HB3	0.44	1.88	15	1
1:B:71:ARG:HH21	1:B:74:GLU:CD	0.44	2.12	15	1
1:A:34:GLU:N	1:A:34:GLU:CD	0.44	2.69	20	1
1:A:34:GLU:O	1:A:38:GLU:HG2	0.44	2.13	10	1
1:B:51:ASP:O	1:B:55:ARG:HD3	0.44	2.12	8	1
1:A:63:LEU:HD23	1:B:65:GLY:N	0.44	2.27	8	1
1:A:39:TYR:O	1:A:43:GLU:CB	0.44	2.66	1	2
1:A:37:LYS:NZ	1:A:41:GLU:OE2	0.44	2.47	17	1
1:A:48:ARG:HB3	1:A:48:ARG:NH1	0.44	2.28	7	1
1:A:55:ARG:O	1:A:56:LEU:C	0.44	2.55	8	16
1:B:69:ARG:NH2	1:B:73:LEU:HD21	0.44	2.27	6	1
1:A:39:TYR:OH	1:B:35:LEU:O	0.44	2.31	19	2
1:A:63:LEU:HD13	1:B:63:LEU:HB2	0.44	1.89	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:48:ARG:HH21	1:B:52:GLU:CD	0.44	2.16	17	1
1:A:30:MET:O	1:B:32:LYS:HE3	0.44	2.12	20	1
1:A:63:LEU:HD21	1:B:59:GLU:O	0.44	2.13	11	1
1:A:63:LEU:HB3	1:B:63:LEU:HD22	0.44	1.89	15	1
1:A:24:THR:O	1:A:27:LEU:N	0.43	2.51	9	5
1:A:51:ASP:OD1	1:A:55:ARG:NH2	0.43	2.51	5	2
1:B:51:ASP:HB3	1:B:55:ARG:NH2	0.43	2.28	10	1
1:B:78:ASP:OD1	1:B:81:ARG:NH2	0.43	2.45	16	1
1:A:38:GLU:HG3	1:B:39:TYR:OH	0.43	2.13	4	4
1:A:34:GLU:OE2	1:A:37:LYS:NZ	0.43	2.44	1	1
1:A:57:ARG:O	1:A:61:LYS:HG2	0.43	2.12	15	1
1:B:67:ASP:OD2	1:B:71:ARG:NH2	0.43	2.43	10	1
1:B:78:ASP:CG	1:B:81:ARG:HH22	0.43	2.17	9	2
1:A:39:TYR:CZ	1:B:39:TYR:CE2	0.43	3.07	16	1
1:A:52:GLU:CD	1:B:57:ARG:NH1	0.43	2.72	5	1
1:B:61:LYS:C	1:B:63:LEU:H	0.43	2.16	14	1
1:B:37:LYS:HE2	1:B:40:LEU:HD12	0.43	1.89	17	1
1:A:56:LEU:CB	1:B:56:LEU:HD13	0.43	2.43	6	2
1:B:33:GLN:CD	1:B:33:GLN:H	0.43	2.17	2	1
1:B:69:ARG:HH12	1:B:72:GLU:CD	0.43	2.15	17	1
1:B:33:GLN:O	1:B:37:LYS:HG3	0.43	2.14	18	2
1:A:41:GLU:O	1:A:45:CYS:SG	0.43	2.74	17	3
1:B:82:ALA:O	1:B:86:GLN:NE2	0.43	2.48	16	1
1:B:23:HIS:ND1	1:B:23:HIS:O	0.43	2.51	8	1
1:A:37:LYS:HD3	1:A:37:LYS:N	0.42	2.28	2	1
1:A:48:ARG:NH2	1:A:52:GLU:OE2	0.42	2.50	15	2
1:B:79:ARG:NE	1:B:83:GLU:OE1	0.42	2.43	1	1
1:A:63:LEU:CA	1:B:63:LEU:HD23	0.42	2.42	11	1
1:B:28:GLN:NE2	1:B:28:GLN:H	0.42	2.13	19	2
1:A:39:TYR:OH	1:B:38:GLU:HG3	0.42	2.14	13	5
1:A:51:ASP:O	1:A:55:ARG:HD3	0.42	2.13	8	1
1:A:32:LYS:HE2	1:B:30:MET:O	0.42	2.15	6	1
1:B:79:ARG:HH11	1:B:83:GLU:CD	0.42	2.16	7	1
1:B:67:ASP:CG	1:B:68:ALA:N	0.42	2.73	11	1
1:B:85:LEU:O	1:B:85:LEU:HD12	0.42	2.15	19	1
1:B:26:SER:O	1:B:30:MET:SD	0.42	2.76	5	1
1:B:53:ASN:O	1:B:57:ARG:HD2	0.42	2.15	9	1
1:A:58:LEU:O	1:A:61:LYS:NZ	0.42	2.38	8	2
1:A:59:GLU:O	1:A:60:SER:C	0.42	2.58	3	4
1:A:53:ASN:ND2	1:B:53:ASN:OD1	0.42	2.47	20	3
1:B:55:ARG:O	1:B:58:LEU:N	0.42	2.53	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:62:ARG:NE	1:B:62:ARG:HA	0.42	2.29	2	1
1:A:53:ASN:O	1:A:57:ARG:CG	0.42	2.68	7	1
1:B:59:GLU:O	1:B:60:SER:C	0.42	2.57	11	3
1:B:55:ARG:NH1	1:B:59:GLU:OE2	0.42	2.46	11	2
1:B:79:ARG:NH1	1:B:83:GLU:CD	0.42	2.72	7	1
1:A:36:ILE:HD13	1:B:28:GLN:CD	0.41	2.35	16	1
1:B:79:ARG:NH1	1:B:83:GLU:OE2	0.41	2.46	2	1
1:B:39:TYR:O	1:B:43:GLU:HB2	0.41	2.15	12	1
1:A:53:ASN:HD22	1:A:53:ASN:N	0.41	2.13	1	1
1:A:40:LEU:O	1:A:44:LYS:CD	0.41	2.68	7	1
1:A:52:GLU:OE1	1:B:57:ARG:NH1	0.41	2.46	15	2
1:A:48:ARG:NH2	1:A:51:ASP:OD2	0.41	2.46	12	1
1:A:55:ARG:NH1	1:A:59:GLU:CD	0.41	2.73	17	1
1:A:53:ASN:O	1:A:57:ARG:HD2	0.41	2.15	9	1
1:B:23:HIS:O	1:B:24:THR:C	0.41	2.56	16	1
1:A:33:GLN:CD	1:A:33:GLN:H	0.41	2.14	12	1
1:A:23:HIS:ND1	1:A:23:HIS:O	0.41	2.54	16	1
1:A:52:GLU:HG3	1:B:57:ARG:HH21	0.41	1.73	14	1
1:A:36:ILE:HD13	1:B:28:GLN:OE1	0.41	2.16	5	1
1:B:58:LEU:O	1:B:61:LYS:NZ	0.41	2.40	3	1
1:A:56:LEU:HB3	1:B:56:LEU:HD22	0.41	1.92	16	1
1:B:51:ASP:HB3	1:B:55:ARG:HH12	0.41	1.73	9	1
1:A:63:LEU:CB	1:B:63:LEU:CB	0.41	2.97	17	1
1:A:51:ASP:O	1:A:55:ARG:NH1	0.41	2.50	9	1
1:A:49:MET:HE2	1:B:46:LEU:HD11	0.41	1.91	1	1
1:B:53:ASN:O	1:B:57:ARG:CG	0.41	2.69	7	1
1:B:61:LYS:O	1:B:63:LEU:N	0.41	2.53	14	1
1:B:26:SER:O	1:B:30:MET:N	0.41	2.54	5	1
1:A:56:LEU:HD21	1:B:57:ARG:CZ	0.41	2.45	15	1
1:A:33:GLN:OE1	1:A:37:LYS:NZ	0.41	2.38	5	1
1:A:51:ASP:CB	1:A:55:ARG:NH2	0.41	2.83	3	1
1:A:63:LEU:CD2	1:B:63:LEU:HD23	0.41	2.38	6	1
1:B:61:LYS:HG3	1:B:62:ARG:N	0.41	2.30	1	1
1:A:55:ARG:HD3	1:A:55:ARG:N	0.41	2.31	20	1
1:A:37:LYS:CB	1:A:37:LYS:NZ	0.41	2.84	8	1
1:A:52:GLU:OE1	1:B:57:ARG:NE	0.41	2.53	9	1
1:A:25:GLU:O	1:A:26:SER:C	0.40	2.59	10	1
1:B:82:ALA:C	1:B:86:GLN:HE21	0.40	2.18	1	1
1:A:23:HIS:NE2	1:A:25:GLU:OE1	0.40	2.48	10	1
1:A:55:ARG:HH11	1:A:55:ARG:CG	0.40	2.30	4	1
1:A:63:LEU:HD21	1:B:64:GLY:O	0.40	2.15	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:ARG:CB	1:B:69:ARG:CZ	0.40	2.99	7	1
1:B:33:GLN:OE1	1:B:37:LYS:NZ	0.40	2.36	5	1
1:B:80:LEU:HA	1:B:80:LEU:HD23	0.40	1.81	14	1
1:A:48:ARG:NH1	1:A:52:GLU:OE2	0.40	2.54	15	1
1:B:48:ARG:HB3	1:B:48:ARG:HH11	0.40	1.76	7	1
1:A:63:LEU:CD2	1:B:64:GLY:O	0.40	2.69	10	1
1:A:33:GLN:O	1:A:37:LYS:HG3	0.40	2.16	18	1
1:A:56:LEU:HD13	1:B:56:LEU:CB	0.40	2.47	6	1
1:A:57:ARG:CZ	1:B:56:LEU:HD21	0.40	2.46	15	1
1:A:59:GLU:C	1:B:63:LEU:HD21	0.40	2.37	11	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	41/107 (38%)	34±2 (84±4%)	6±2 (15±4%)	0±0 (1±1%)	21	68
1	B	65/107 (61%)	56±3 (86±4%)	8±2 (13±4%)	1±1 (1±1%)	20	66
All	All	2120/4280 (50%)	1804 (85%)	291 (14%)	25 (1%)	20	66

All 10 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	65	GLY	7
1	B	23	HIS	5
1	A	23	HIS	5
1	A	63	LEU	2
1	A	25	GLU	1
1	B	62	ARG	1
1	A	62	ARG	1
1	B	25	GLU	1
1	B	63	LEU	1
1	B	66	ASP	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	41/96 (43%)	32±2 (78±6%)	9±2 (22±6%)	3	31
1	B	61/96 (64%)	49±3 (80±4%)	13±3 (20±4%)	4	34
All	All	2040/3840 (53%)	1609 (79%)	431 (21%)	4	33

All 65 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	26	SER	18
1	B	31	SER	17
1	A	31	SER	16
1	B	26	SER	16
1	B	42	LEU	16
1	A	42	LEU	15
1	A	24	THR	14
1	A	61	LYS	14
1	B	61	LYS	13
1	B	66	ASP	13
1	B	24	THR	13
1	A	28	GLN	12
1	B	67	ASP	12
1	B	32	LYS	11
1	B	28	GLN	10
1	A	32	LYS	10
1	B	86	GLN	9
1	A	55	ARG	9
1	B	55	ARG	8
1	B	83	GLU	8
1	B	43	GLU	8
1	B	25	GLU	7
1	A	37	LYS	7
1	A	25	GLU	7
1	B	62	ARG	7
1	A	62	ARG	7
1	B	79	ARG	7
1	A	43	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	B	78	ASP	6
1	B	37	LYS	6
1	B	30	MET	5
1	A	44	LYS	5
1	B	85	LEU	5
1	A	48	ARG	5
1	B	69	ARG	5
1	A	30	MET	5
1	B	48	ARG	5
1	B	71	ARG	5
1	B	23	HIS	4
1	A	50	GLU	4
1	A	38	GLU	4
1	B	57	ARG	4
1	B	33	GLN	4
1	B	44	LYS	4
1	A	23	HIS	3
1	A	41	GLU	3
1	B	74	GLU	3
1	A	57	ARG	3
1	A	33	GLN	3
1	B	51	ASP	3
1	B	52	GLU	2
1	A	63	LEU	2
1	A	59	GLU	2
1	B	50	GLU	2
1	A	51	ASP	2
1	A	34	GLU	2
1	B	76	GLU	2
1	B	81	ARG	2
1	B	63	LEU	2
1	B	38	GLU	2
1	B	34	GLU	2
1	B	59	GLU	2
1	A	60	SER	1
1	A	52	GLU	1
1	A	53	ASN	1

6.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7   Chemical shift validation ⓘ

No chemical shift data were provided