Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 05:29 PM EST

PDB ID	:	1S6I
Title	:	Ca2+-regulatory region (CLD) from soybean calcium-dependent protein kinase-alpha (CDPK) in the presence of Ca2+ and the junction domain (JD)
Authors	:	Weljie, A.M.; Vogel, H.J.
Deposited on	:	2004-01-23

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:

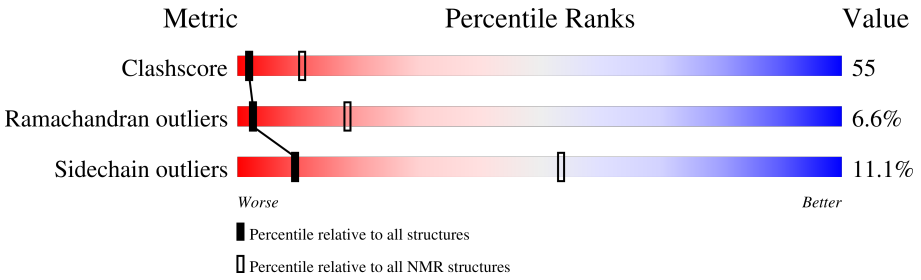
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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

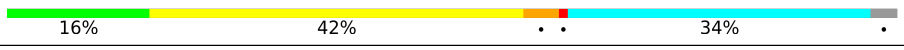
The overall completeness of chemical shifts assignment was not calculated.

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	188	

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 2 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:12-A:71 (60)	0.36	2
2	A:85-A:142 (58)	0.43	4

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 11, 15
2	2, 7, 8, 12, 13, 14
3	9, 10

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2821 atoms, of which 1389 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-dependent protein kinase SK5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	182	2817	883	1389	240	297	8	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	ARG	-	insertion	UNP P28583
A	144	LYS	-	insertion	UNP P28583
A	183	HIS	-	expression tag	UNP P28583
A	184	HIS	-	expression tag	UNP P28583
A	185	HIS	-	expression tag	UNP P28583
A	186	HIS	-	expression tag	UNP P28583
A	187	HIS	-	expression tag	UNP P28583
A	188	HIS	-	expression tag	UNP P28583

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	4	4	4

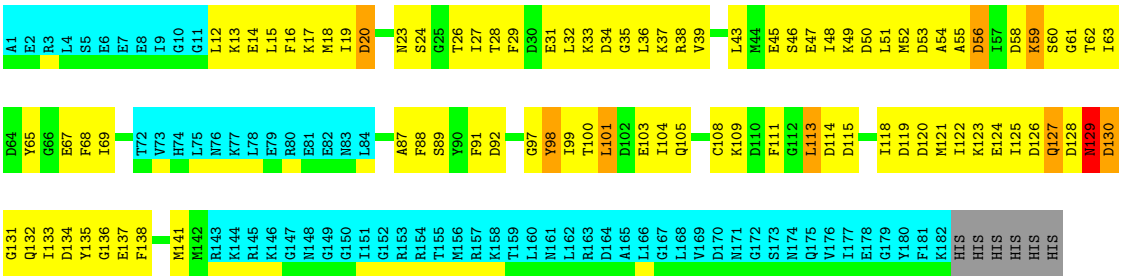
4 Residue-property plots (i)

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: Calcium-dependent protein kinase SK5

Chain A: 16% 42% • • 34% •



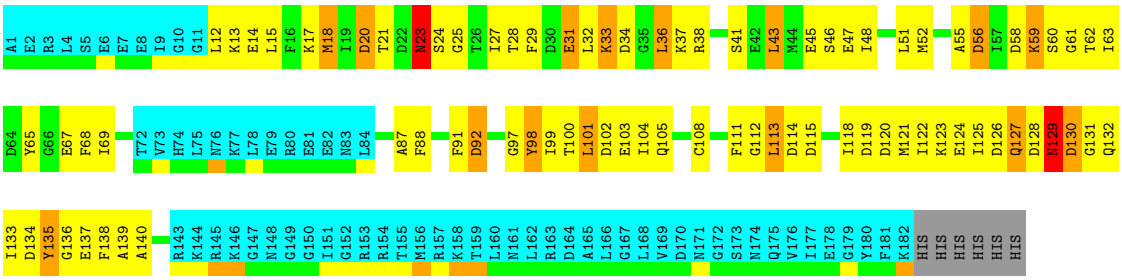
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Calcium-dependent protein kinase SK5

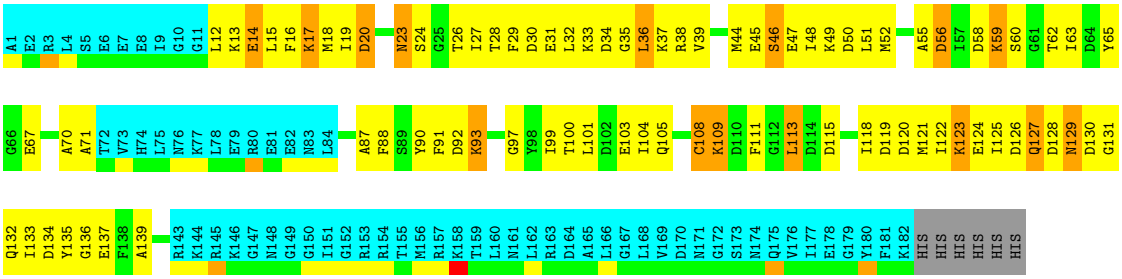
Chain A: 19% 35% 8% • 34% •



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Calcium-dependent protein kinase SK5

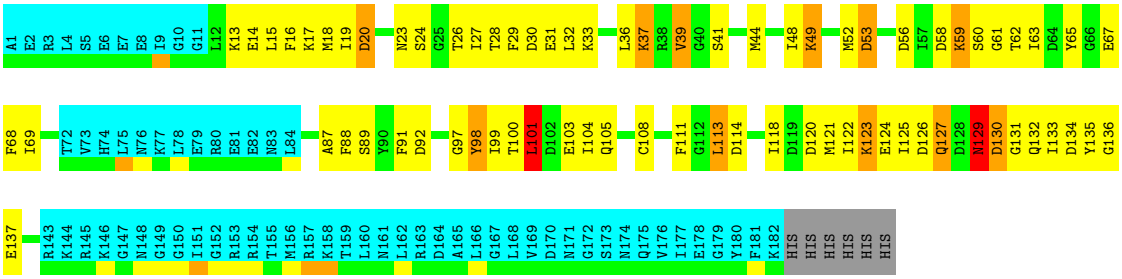
Chain A: 18% 37% 8% 34%



4.2.3 Score per residue for model 3

• Molecule 1: Calcium-dependent protein kinase SK5

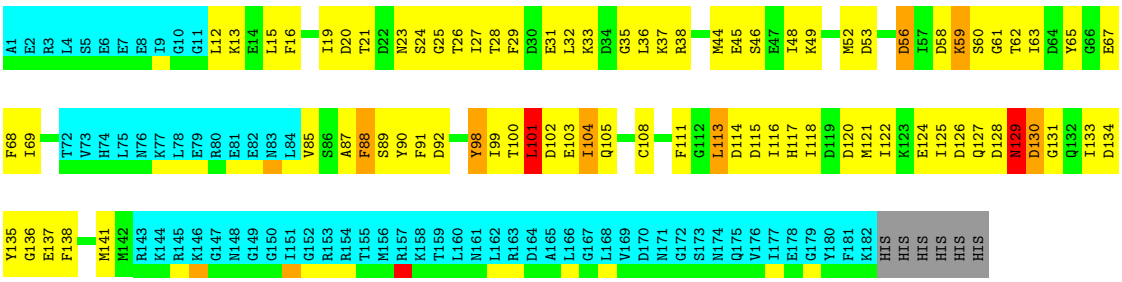
Chain A: 24% 32% 6% • 34% •



4.2.4 Score per residue for model 4

• Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 20% 38% • • 34% •



4.2.5 Score per residue for model 5

• Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 20% 36% 6% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 K13 E14 L15 F16 K17 M18 I19 D20 N23 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 M44 E45 S46 E47 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61 T62 I63 D64

Y65 G66 E67 F68 I69 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 V85 S86 A87 F88 F91 D92 G97 Y98 I99 T100 L101 D102 E103 I104 Q105 F111 G112 L113 D114 D115 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129 D130 G131 Q132 I133 D134

Y135 G136 E137 F138 A139 A140 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS HIS

4.2.6 Score per residue for model 6

• Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 19% 35% 8% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 K13 E14 L15 F16 K17 M18 I19 D20 T21 D22 N23 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 S41 E42 L43 M44 E45 S46 E47 I48 L51 M52 A55 D56 I57 D58 K59 S60 G61 T62 I63

D64 Y65 G66 E67 F68 I69 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 A87 F88 S89 Y90 F91 D92 G97 Y98 I99 T100 L101 D102 E103 I104 Q105 C108 F111 G112 L113 D114 D115 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129 D130 G131

Q132 I133 D134 Y135 G136 E137 F138 A139 A140 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS

4.2.7 Score per residue for model 7

• Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 19% 38% 5% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 K13 E14 L15 M18 I19 D20 N23 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61 T62 I63 D64 Y65 G66 E67 F68 I69

A70 A71 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 A87 F88 S89 Y90 F91 D92 K93 G97 Y98 I99 T100 L101 D102 E103 I104 Q105 C108 F111 G112 L113 D114 D115 I116 H117 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129 D130 G131 Q132 I133 D134

Y135 G136 E137 F138 M141 M142 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS HIS

4.2.8 Score per residue for model 8

- Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 21% 36% 5% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 K13 E14 L15 F16 K17 M18 I19 S24 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 G40 S41 E42 L43 E47 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61 T62 I63 D64 Y65 G66

E67 F68 I69 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 A87 F88 S89 Y90 F91 D92 G97 Y98 I99 T100 L101 D102 E103 I104 Q105 C108 K109 D110 F111 G112 L113 D114 D115 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129 D130 G131 Q132 I133

D134 Y135 G136 E137 F138 A139 A140 M141 M142 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS HIS

4.2.9 Score per residue for model 9

- Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 19% 37% 6% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 L15 F16 K17 M18 I19 D20 N23 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 G40 S41 S46 E47 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61 T62 I63 D64 Y65

G66 E67 F68 I69 A70 A71 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 V85 S86 A87 F88 S89 Y90 F91 D92 K93 G97 Y98 I99 T100 L101 I104 Q105 C108 K109 D110 F111 G112 L113 D114 D115 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129 D130

G131 Q132 I133 D134 Y135 G136 E137 F138 M141 M142 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS HIS

4.2.10 Score per residue for model 10

- Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 19% 34% 9% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L15 F16 K17 M18 I19 D20 N23 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 G40 S41 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61 T62 I63 D64 Y65 G66 E67 F68

I69 A70 A71 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 A87 F88 S89 Y90 F91 D92 K93 D94 Y98 I99 T100 L101 D102 E103 I104 Q105 Q106 A107 C108 F111 G112 L113 D114 D115 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129 D130 G131 Q132 I133

D134 Y135 G136 E137 F138 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS HIS

4.2.11 Score per residue for model 11

- Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 19% 35% 9% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 K13 E14 L15 M18 I19 D20 T21 D22 N23 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 M44 E47 I48 K49 D50 L51 M52 D53 D56 I57 D58 K59 S60 G61 T62 I63 D64 Y65 G66

E67 F68 I69 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 A87 F88 S89 D92 G97 Y98 I99 T100 L101 D102 E103 I104 Q105 Q106 A107 C108 K109 D110 F111 G112 L113 D114 H117 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129 D130 G131 Q132 I133

D134 Y135 G136 E137 F138 A139 A140 M141 M142 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS HIS

4.2.12 Score per residue for model 12

- Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 18% 38% 5% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 E14 L15 F16 K17 M18 I19 D20 T21 D22 N23 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 E45 S46 E47 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61 T62 I63 D64 Y65

G66 E67 F68 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 V85 S86 A87 F88 S89 Y90 F91 D92 K93 D94 G95 S96 G97 Y98 I99 T100 L101 D102 E103 I104 Q105 Q106 A107 C108 F111 G112 L113 D114 D115 I116 H117 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128

N129 D130 G131 Q132 I133 D134 Y135 G136 E137 F138 M141 M142 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS

4.2.13 Score per residue for model 13

- Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 18% 37% 8% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 K13 E14 L15 F16 K17 M18 I19 D20 N23 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 L43 M44 E45 S46 E47 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61 T62 I63

D64 Y65 G66 E67 F68 I69 A70 A71 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 V85 S86 A87 F88 S89 Y90 F91 D92 K93 Y98 I99 T100 L101 I104 Q105 C108 L113 D114 D115 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129 D130 G131 Q132

I133 D134 Y135 G136 E137 F138 M141 M142 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS

4.2.14 Score per residue for model 14

- Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 17% 40% 5% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 K13 E14 L15 F16 K17 M18 I19 D20 T21 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 G40 S41 E42 L43 M44 E45 S46 E47 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61

T62 I63 D64 Y65 G66 E67 F68 I69 A70 A71 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 A87 F88 F91 D92 K93 G97 Y98 I99 T100 L101 D102 E103 I104 Q105 C108 K109 D110 F111 G112 L113 D114 D115 I116 H117 I118 D119 D120 M121 I122 K123 E124 I125 D126

Q127 D128 N129 D130 G131 Q132 I133 D134 Y135 G136 E137 F138 A139 A140 M141 M142 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS

HIS HIS

4.2.15 Score per residue for model 15

- Molecule 1: Calcium-dependent protein kinase SK5

Chain A: 19% 36% 7% • 34% •

A1 E2 R3 L4 S5 E6 E7 E8 I9 G10 G11 L12 K13 E14 L15 F16 K17 M18 I19 D20 S24 G25 T26 I27 T28 F29 D30 E31 L32 K33 D34 G35 L36 K37 R38 V39 E42 L43 M44 E45 S46 E47 I48 K49 D50 L51 M52 D53 A54 A55 D56 I57 D58 K59 S60 G61 T62 I63

D64 Y65 G66 E67 F68 I69 T72 V73 H74 L75 N76 K77 L78 E79 R80 E81 E82 N83 L84 A87 F88 S89 Y90 F91 D92 G95 Y98 I99 T100 L101 D102 E103 I104 Q105 C108 K109 D110 F111 G112 L113 D114 D115 I118 D119 D120 M121 I122 K123 E124 I125 D126 Q127 D128 N129

D130 G131 Q132 I133 D134 Y135 G136 E137 F138 A139 R143 K144 R145 K146 G147 N148 G149 G150 I151 G152 R153 R154 T155 M156 R157 K158 T159 L160 N161 L162 R163 D164 A165 L166 G167 L168 V169 D170 N171 G172 S173 N174 Q175 V176 I177 E178 G179 Y180 F181 K182 HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing; molecular dynamics; matrix relaxation.*

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *structures with acceptable covalent geometry,structures with favorable non-bond energy,structures with the least restraint violations.*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	921	867	866	99±9
All	All	13875	13005	12971	1488

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 55.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:ILE:HG22	1:A:133:ILE:HD11	0.90	1.41	15	7
1:A:121:MET:HA	1:A:124:GLU:HB3	0.89	1.42	6	15
1:A:32:LEU:HD13	1:A:48:ILE:HG23	0.89	1.40	4	2
1:A:32:LEU:HD12	1:A:48:ILE:HD12	0.87	1.46	14	1
1:A:126:ASP:HB2	1:A:131:GLY:HA2	0.84	1.49	7	11
1:A:134:ASP:H	1:A:137:GLU:HB2	0.84	1.33	15	12
1:A:133:ILE:HD13	1:A:137:GLU:HB3	0.83	1.48	6	3
1:A:113:LEU:HA	1:A:118:ILE:HG13	0.83	1.50	4	8
1:A:49:LYS:HD3	1:A:93:LYS:HD2	0.82	1.50	2	1
1:A:27:ILE:HB	1:A:63:ILE:HB	0.78	1.52	4	15
1:A:113:LEU:HA	1:A:118:ILE:HD12	0.78	1.56	10	2
1:A:27:ILE:O	1:A:62:THR:HA	0.78	1.78	14	15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:GLN:HE21	1:A:137:GLU:HG2	0.78	1.38	1	3
1:A:105:GLN:NE2	1:A:118:ILE:HG22	0.76	1.93	5	7
1:A:125:ILE:HG21	1:A:133:ILE:HD11	0.75	1.57	5	3
1:A:52:MET:HB3	1:A:59:LYS:HD3	0.74	1.56	5	2
1:A:32:LEU:HD13	1:A:48:ILE:CG2	0.74	2.12	4	2
1:A:92:ASP:HA	1:A:99:ILE:HG12	0.74	1.59	9	15
1:A:125:ILE:O	1:A:133:ILE:HD11	0.73	1.83	4	6
1:A:125:ILE:HG22	1:A:133:ILE:CD1	0.73	2.13	8	9
1:A:105:GLN:NE2	1:A:118:ILE:HG23	0.72	1.99	3	2
1:A:113:LEU:HD22	1:A:113:LEU:O	0.72	1.83	11	1
1:A:43:LEU:HD13	1:A:48:ILE:HD11	0.72	1.62	13	5
1:A:127:GLN:NE2	1:A:137:GLU:HA	0.71	2.00	4	3
1:A:105:GLN:NE2	1:A:122:ILE:HD11	0.71	2.00	3	9
1:A:99:ILE:O	1:A:132:GLN:HB2	0.71	1.85	10	3
1:A:63:ILE:HG23	1:A:67:GLU:HB2	0.70	1.62	8	15
1:A:108:CYS:HB2	1:A:111:PHE:CD1	0.70	2.21	11	1
1:A:32:LEU:HD12	1:A:48:ILE:HG13	0.70	1.63	15	11
1:A:33:LYS:HB2	1:A:37:LYS:HE3	0.70	1.61	2	6
1:A:88:PHE:O	1:A:92:ASP:HB3	0.70	1.86	7	8
1:A:88:PHE:CE1	1:A:135:TYR:HB2	0.70	2.22	1	14
1:A:125:ILE:HG21	1:A:133:ILE:CD1	0.70	2.17	5	6
1:A:50:ASP:O	1:A:54:ALA:HB3	0.69	1.87	13	7
1:A:51:LEU:HD13	1:A:52:MET:N	0.69	2.01	9	1
1:A:132:GLN:O	1:A:133:ILE:HD13	0.69	1.87	11	2
1:A:53:ASP:HA	1:A:59:LYS:HG3	0.69	1.64	13	1
1:A:105:GLN:HB3	1:A:113:LEU:HD12	0.69	1.65	6	2
1:A:98:TYR:HA	1:A:134:ASP:HA	0.68	1.63	5	9
1:A:121:MET:O	1:A:125:ILE:HG12	0.68	1.89	1	4
1:A:105:GLN:HE21	1:A:118:ILE:HG22	0.68	1.48	7	3
1:A:36:LEU:O	1:A:39:VAL:HG12	0.68	1.88	13	6
1:A:108:CYS:HB3	1:A:111:PHE:HB2	0.68	1.66	10	4
1:A:55:ALA:HB1	1:A:71:ALA:HA	0.68	1.66	2	4
1:A:19:ILE:HA	1:A:35:GLY:HA3	0.67	1.66	10	2
1:A:98:TYR:HB3	1:A:132:GLN:NE2	0.67	2.04	3	7
1:A:113:LEU:HD23	1:A:118:ILE:HG12	0.67	1.65	12	1
1:A:32:LEU:HD21	1:A:51:LEU:HD23	0.67	1.66	15	1
1:A:125:ILE:HG22	1:A:133:ILE:CG1	0.67	2.20	4	6
1:A:125:ILE:HG21	1:A:133:ILE:HD13	0.67	1.67	13	3
1:A:20:ASP:HB3	1:A:26:THR:O	0.66	1.90	14	6
1:A:32:LEU:HD22	1:A:48:ILE:HG13	0.66	1.66	4	2
1:A:51:LEU:O	1:A:55:ALA:HB3	0.66	1.90	13	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLU:HA	1:A:17:LYS:HE2	0.66	1.67	12	2
1:A:127:GLN:NE2	1:A:137:GLU:HG2	0.66	2.05	6	2
1:A:121:MET:O	1:A:125:ILE:HG13	0.66	1.91	7	3
1:A:113:LEU:HD23	1:A:118:ILE:HG21	0.66	1.68	4	2
1:A:99:ILE:HG23	1:A:103:GLU:HB2	0.66	1.66	4	12
1:A:19:ILE:HG23	1:A:35:GLY:HA3	0.66	1.67	12	5
1:A:32:LEU:HD11	1:A:51:LEU:HD12	0.66	1.66	14	1
1:A:99:ILE:HG22	1:A:104:ILE:HG13	0.66	1.68	5	11
1:A:15:LEU:O	1:A:19:ILE:HG12	0.66	1.91	4	3
1:A:111:PHE:O	1:A:118:ILE:HD11	0.66	1.90	8	1
1:A:52:MET:O	1:A:56:ASP:HB3	0.65	1.90	12	12
1:A:134:ASP:HB3	1:A:137:GLU:HG3	0.65	1.67	2	2
1:A:101:LEU:HB3	1:A:122:ILE:HG23	0.65	1.68	12	5
1:A:32:LEU:CD1	1:A:48:ILE:HG23	0.65	2.18	4	4
1:A:33:LYS:HB3	1:A:48:ILE:HD11	0.65	1.69	13	3
1:A:33:LYS:HB3	1:A:43:LEU:HD11	0.65	1.68	15	3
1:A:15:LEU:HA	1:A:18:MET:HB2	0.65	1.69	8	8
1:A:134:ASP:OD1	1:A:137:GLU:HG3	0.65	1.91	10	5
1:A:32:LEU:HD11	1:A:51:LEU:HD11	0.65	1.66	8	1
1:A:88:PHE:HA	1:A:92:ASP:HB2	0.64	1.70	6	6
1:A:115:ASP:HA	1:A:119:ASP:HB2	0.64	1.69	10	9
1:A:120:ASP:O	1:A:124:GLU:HB2	0.64	1.91	11	1
1:A:123:LYS:HA	1:A:123:LYS:HE2	0.64	1.69	5	2
1:A:36:LEU:HG	1:A:43:LEU:HD23	0.64	1.69	15	1
1:A:33:LYS:HG2	1:A:48:ILE:HG12	0.64	1.68	8	4
1:A:104:ILE:HG21	1:A:125:ILE:HD12	0.64	1.69	7	2
1:A:118:ILE:HD12	1:A:118:ILE:H	0.64	1.52	7	1
1:A:122:ILE:HG22	1:A:131:GLY:HA3	0.64	1.69	6	13
1:A:21:THR:HG21	1:A:38:ARG:HD2	0.64	1.70	4	2
1:A:127:GLN:NE2	1:A:127:GLN:H	0.63	1.90	5	3
1:A:28:THR:HG22	1:A:62:THR:OG1	0.63	1.93	3	11
1:A:36:LEU:HD22	1:A:43:LEU:HD11	0.63	1.71	14	1
1:A:129:ASN:ND2	1:A:130:ASP:H	0.63	1.92	13	12
1:A:114:ASP:O	1:A:118:ILE:HG22	0.63	1.94	3	1
1:A:113:LEU:HA	1:A:118:ILE:HG12	0.63	1.71	12	1
1:A:113:LEU:HD12	1:A:113:LEU:O	0.62	1.93	2	3
1:A:113:LEU:CD2	1:A:118:ILE:HG21	0.62	2.24	3	2
1:A:88:PHE:HE1	1:A:135:TYR:HB2	0.62	1.54	8	3
1:A:133:ILE:CD1	1:A:137:GLU:HB3	0.62	2.24	4	1
1:A:105:GLN:NE2	1:A:118:ILE:HA	0.62	2.09	11	1
1:A:51:LEU:HD13	1:A:51:LEU:C	0.62	2.15	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LYS:O	1:A:36:LEU:HD13	0.62	1.95	6	2
1:A:127:GLN:HE22	1:A:137:GLU:HA	0.62	1.55	4	2
1:A:28:THR:O	1:A:30:ASP:N	0.62	2.33	7	5
1:A:92:ASP:CA	1:A:99:ILE:HG12	0.61	2.24	8	7
1:A:101:LEU:O	1:A:105:GLN:HG2	0.61	1.95	9	6
1:A:105:GLN:CD	1:A:122:ILE:HD11	0.61	2.14	3	2
1:A:52:MET:HA	1:A:56:ASP:HB2	0.61	1.70	9	2
1:A:53:ASP:O	1:A:93:LYS:HG3	0.61	1.95	9	1
1:A:104:ILE:HD11	1:A:133:ILE:HG12	0.61	1.70	11	2
1:A:88:PHE:CE1	1:A:135:TYR:HA	0.61	2.31	12	1
1:A:52:MET:HB3	1:A:59:LYS:HG2	0.61	1.73	8	7
1:A:12:LEU:HD12	1:A:15:LEU:HD23	0.61	1.71	4	4
1:A:105:GLN:HB3	1:A:113:LEU:HD22	0.61	1.70	12	1
1:A:32:LEU:HD11	1:A:52:MET:HB2	0.60	1.73	4	1
1:A:123:LYS:HD2	1:A:123:LYS:N	0.60	2.11	14	4
1:A:92:ASP:HB2	1:A:99:ILE:HD11	0.60	1.73	2	5
1:A:111:PHE:CD2	1:A:113:LEU:HD21	0.60	2.31	12	1
1:A:15:LEU:HA	1:A:18:MET:HB3	0.60	1.73	10	4
1:A:130:ASP:HB3	1:A:132:GLN:HG2	0.60	1.72	2	3
1:A:14:GLU:O	1:A:18:MET:HG2	0.60	1.96	14	3
1:A:111:PHE:CE2	1:A:113:LEU:HB2	0.60	2.31	7	2
1:A:121:MET:HA	1:A:124:GLU:CB	0.60	2.25	6	9
1:A:105:GLN:O	1:A:113:LEU:HD23	0.60	1.97	14	2
1:A:51:LEU:O	1:A:51:LEU:HD22	0.59	1.95	9	1
1:A:105:GLN:HB3	1:A:113:LEU:CD2	0.59	2.26	12	1
1:A:113:LEU:HD13	1:A:113:LEU:O	0.59	1.97	3	5
1:A:32:LEU:HD12	1:A:48:ILE:HG23	0.59	1.72	10	3
1:A:127:GLN:NE2	1:A:137:GLU:HB3	0.59	2.12	11	2
1:A:14:GLU:HG3	1:A:17:LYS:HE2	0.59	1.75	6	3
1:A:87:ALA:HB3	1:A:138:PHE:CE2	0.59	2.32	11	4
1:A:121:MET:SD	1:A:125:ILE:HD12	0.59	2.37	8	1
1:A:15:LEU:HD12	1:A:68:PHE:HZ	0.59	1.57	10	1
1:A:105:GLN:NE2	1:A:118:ILE:HG12	0.59	2.12	11	1
1:A:105:GLN:HE22	1:A:118:ILE:HG23	0.59	1.55	3	1
1:A:104:ILE:HG22	1:A:105:GLN:N	0.59	2.11	13	2
1:A:134:ASP:N	1:A:137:GLU:HB2	0.59	2.08	15	7
1:A:32:LEU:CG	1:A:48:ILE:HG23	0.58	2.28	13	10
1:A:36:LEU:HD12	1:A:37:LYS:N	0.58	2.13	9	1
1:A:29:PHE:HE2	1:A:49:LYS:HB2	0.58	1.58	7	2
1:A:33:LYS:HD3	1:A:37:LYS:NZ	0.58	2.12	7	2
1:A:99:ILE:N	1:A:133:ILE:O	0.58	2.37	6	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD12	1:A:43:LEU:HD23	0.58	1.76	8	1
1:A:91:PHE:HB3	1:A:99:ILE:HD13	0.58	1.74	8	8
1:A:54:ALA:HB1	1:A:89:SER:OG	0.58	1.97	10	1
1:A:113:LEU:HD23	1:A:113:LEU:O	0.58	1.98	6	2
1:A:118:ILE:O	1:A:121:MET:HB3	0.58	1.99	8	11
1:A:19:ILE:HG21	1:A:27:ILE:HG23	0.58	1.74	14	2
1:A:118:ILE:O	1:A:122:ILE:HG13	0.58	1.99	11	1
1:A:113:LEU:HD22	1:A:114:ASP:N	0.58	2.14	4	3
1:A:32:LEU:HG	1:A:51:LEU:HD23	0.58	1.75	5	1
1:A:52:MET:HG2	1:A:59:LYS:HG2	0.57	1.75	13	1
1:A:19:ILE:HG21	1:A:27:ILE:HD13	0.57	1.76	4	7
1:A:129:ASN:HD22	1:A:129:ASN:N	0.57	1.98	12	10
1:A:104:ILE:HG22	1:A:105:GLN:OE1	0.57	1.98	4	2
1:A:105:GLN:HE21	1:A:118:ILE:HG23	0.57	1.60	12	2
1:A:33:LYS:O	1:A:37:LYS:HB3	0.57	1.98	10	2
1:A:88:PHE:HZ	1:A:97:GLY:HA2	0.57	1.59	11	2
1:A:36:LEU:O	1:A:39:VAL:HG22	0.57	1.99	2	6
1:A:44:MET:SD	1:A:46:SER:HB2	0.57	2.40	5	1
1:A:34:ASP:O	1:A:38:ARG:HB3	0.57	1.98	12	2
1:A:126:ASP:CG	1:A:131:GLY:H	0.57	2.02	14	2
1:A:21:THR:HG21	1:A:38:ARG:NH2	0.57	2.15	6	2
1:A:104:ILE:HD11	1:A:133:ILE:HG13	0.56	1.78	10	2
1:A:36:LEU:C	1:A:36:LEU:HD22	0.56	2.21	1	2
1:A:98:TYR:HB3	1:A:132:GLN:HE22	0.56	1.58	8	5
1:A:30:ASP:OD1	1:A:31:GLU:HG3	0.56	2.00	5	1
1:A:32:LEU:HD11	1:A:51:LEU:HD23	0.56	1.76	10	1
1:A:63:ILE:HA	1:A:67:GLU:OE1	0.56	2.00	8	6
1:A:20:ASP:HB2	1:A:26:THR:O	0.56	2.01	7	2
1:A:133:ILE:CG2	1:A:138:PHE:HB2	0.55	2.31	15	5
1:A:109:LYS:HD3	1:A:109:LYS:H	0.55	1.60	15	2
1:A:111:PHE:N	1:A:111:PHE:CD1	0.55	2.73	12	2
1:A:116:ILE:HG23	1:A:117:HIS:H	0.55	1.60	7	1
1:A:58:ASP:O	1:A:60:SER:N	0.55	2.39	10	13
1:A:125:ILE:HG23	1:A:141:MET:SD	0.55	2.42	4	1
1:A:58:ASP:HB3	1:A:67:GLU:OE2	0.55	2.01	11	5
1:A:32:LEU:CD1	1:A:52:MET:HB2	0.55	2.31	4	1
1:A:105:GLN:HE22	1:A:118:ILE:HG22	0.55	1.61	4	1
1:A:128:ASP:HB3	1:A:137:GLU:OE1	0.55	2.02	14	1
1:A:28:THR:O	1:A:31:GLU:N	0.55	2.40	7	10
1:A:51:LEU:HD23	1:A:51:LEU:O	0.55	2.02	2	2
1:A:116:ILE:HG13	1:A:117:HIS:H	0.55	1.62	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:HG	1:A:68:PHE:HZ	0.55	1.62	7	8
1:A:113:LEU:HB3	1:A:118:ILE:HG21	0.54	1.79	12	1
1:A:52:MET:SD	1:A:61:GLY:HA2	0.54	2.43	3	5
1:A:114:ASP:OD2	1:A:116:ILE:HG22	0.54	2.02	14	2
1:A:56:ASP:OD1	1:A:63:ILE:HG12	0.54	2.03	5	4
1:A:65:TYR:O	1:A:69:ILE:HG13	0.54	2.03	14	4
1:A:14:GLU:HA	1:A:17:LYS:NZ	0.54	2.17	13	1
1:A:33:LYS:HB3	1:A:48:ILE:HG12	0.54	1.78	7	3
1:A:130:ASP:HB2	1:A:132:GLN:HG2	0.54	1.79	3	5
1:A:29:PHE:CE2	1:A:49:LYS:HB2	0.54	2.37	11	4
1:A:93:LYS:HB2	1:A:93:LYS:NZ	0.54	2.17	14	1
1:A:33:LYS:HG3	1:A:34:ASP:H	0.54	1.62	5	1
1:A:34:ASP:O	1:A:38:ARG:HB2	0.54	2.03	11	4
1:A:108:CYS:SG	1:A:111:PHE:HB3	0.54	2.43	7	1
1:A:20:ASP:OD2	1:A:25:GLY:HA2	0.54	2.03	12	3
1:A:32:LEU:HG	1:A:48:ILE:HG23	0.53	1.78	15	8
1:A:65:TYR:O	1:A:69:ILE:HG12	0.53	2.03	5	7
1:A:19:ILE:HD12	1:A:27:ILE:HD13	0.53	1.80	3	3
1:A:13:LYS:HG3	1:A:14:GLU:OE1	0.53	2.03	2	1
1:A:43:LEU:C	1:A:43:LEU:HD12	0.53	2.23	15	1
1:A:52:MET:HB3	1:A:59:LYS:CD	0.53	2.31	5	4
1:A:55:ALA:O	1:A:57:ILE:N	0.53	2.41	9	1
1:A:32:LEU:HD21	1:A:51:LEU:HD22	0.53	1.79	12	1
1:A:20:ASP:HA	1:A:31:GLU:CD	0.53	2.23	11	2
1:A:54:ALA:HB1	1:A:89:SER:HB3	0.53	1.79	9	1
1:A:32:LEU:HD21	1:A:51:LEU:HD11	0.53	1.78	8	2
1:A:123:LYS:HE3	1:A:123:LYS:HA	0.53	1.79	3	4
1:A:53:ASP:HA	1:A:59:LYS:HD3	0.53	1.79	3	2
1:A:125:ILE:CG2	1:A:133:ILE:HG13	0.53	2.34	7	6
1:A:132:GLN:NE2	1:A:134:ASP:OD1	0.53	2.41	9	1
1:A:23:ASN:HB2	1:A:31:GLU:OE2	0.53	2.04	7	4
1:A:43:LEU:HD12	1:A:43:LEU:O	0.53	2.04	8	4
1:A:99:ILE:HG23	1:A:103:GLU:CB	0.52	2.35	11	9
1:A:127:GLN:HE22	1:A:137:GLU:CG	0.52	2.17	5	3
1:A:32:LEU:HD22	1:A:48:ILE:HG23	0.52	1.81	5	1
1:A:122:ILE:CG2	1:A:131:GLY:HA3	0.52	2.34	11	2
1:A:125:ILE:HG22	1:A:133:ILE:HG13	0.52	1.80	4	5
1:A:44:MET:O	1:A:48:ILE:HD13	0.52	2.05	4	5
1:A:108:CYS:O	1:A:112:GLY:HA2	0.52	2.04	11	1
1:A:134:ASP:H	1:A:137:GLU:CG	0.52	2.18	3	3
1:A:116:ILE:HG23	1:A:117:HIS:N	0.52	2.19	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:GLY:O	1:A:134:ASP:HB2	0.52	2.05	6	2
1:A:113:LEU:HD22	1:A:118:ILE:HG21	0.52	1.80	3	1
1:A:113:LEU:HB2	1:A:118:ILE:HD11	0.52	1.82	11	1
1:A:101:LEU:H	1:A:101:LEU:HD23	0.52	1.64	4	9
1:A:32:LEU:CD1	1:A:48:ILE:HD12	0.52	2.30	14	1
1:A:122:ILE:HG22	1:A:131:GLY:CA	0.52	2.35	1	11
1:A:92:ASP:OD1	1:A:99:ILE:HG13	0.52	2.04	4	4
1:A:43:LEU:CD1	1:A:48:ILE:HD11	0.52	2.35	15	4
1:A:120:ASP:O	1:A:124:GLU:N	0.52	2.43	2	15
1:A:20:ASP:HB2	1:A:23:ASN:HB3	0.52	1.80	4	1
1:A:125:ILE:C	1:A:133:ILE:HD11	0.52	2.24	11	4
1:A:57:ILE:HA	1:A:94:ASP:O	0.52	2.05	10	1
1:A:113:LEU:CD2	1:A:118:ILE:HG12	0.51	2.35	12	1
1:A:32:LEU:HB3	1:A:48:ILE:HG23	0.51	1.83	14	2
1:A:59:LYS:HD3	1:A:59:LYS:C	0.51	2.26	10	7
1:A:114:ASP:H	1:A:118:ILE:HB	0.51	1.66	3	5
1:A:108:CYS:SG	1:A:111:PHE:HB2	0.51	2.45	4	3
1:A:28:THR:HA	1:A:61:GLY:O	0.51	2.05	12	13
1:A:87:ALA:O	1:A:91:PHE:N	0.51	2.44	2	10
1:A:19:ILE:HG23	1:A:31:GLU:O	0.51	2.06	14	1
1:A:29:PHE:HE1	1:A:49:LYS:HB2	0.51	1.65	4	1
1:A:113:LEU:CA	1:A:118:ILE:HD12	0.51	2.33	10	1
1:A:118:ILE:HG23	1:A:121:MET:CE	0.51	2.36	10	1
1:A:129:ASN:N	1:A:129:ASN:ND2	0.51	2.59	12	2
1:A:108:CYS:O	1:A:113:LEU:HB2	0.51	2.06	4	1
1:A:52:MET:C	1:A:59:LYS:HD3	0.51	2.26	2	1
1:A:88:PHE:CZ	1:A:97:GLY:HA2	0.51	2.41	3	4
1:A:123:LYS:HA	1:A:126:ASP:OD1	0.50	2.06	9	1
1:A:22:ASP:HB2	1:A:31:GLU:OE2	0.50	2.06	12	1
1:A:19:ILE:HA	1:A:35:GLY:HA2	0.50	1.81	13	1
1:A:88:PHE:O	1:A:92:ASP:HB2	0.50	2.06	15	1
1:A:33:LYS:NZ	1:A:48:ILE:HG12	0.50	2.21	12	2
1:A:36:LEU:HD23	1:A:41:SER:CB	0.50	2.37	6	2
1:A:129:ASN:ND2	1:A:129:ASN:N	0.50	2.59	4	10
1:A:27:ILE:O	1:A:62:THR:CA	0.50	2.58	5	2
1:A:105:GLN:CD	1:A:118:ILE:HG22	0.50	2.27	5	2
1:A:127:GLN:HE22	1:A:137:GLU:HB3	0.50	1.66	12	1
1:A:28:THR:HG22	1:A:62:THR:HB	0.50	1.83	14	1
1:A:105:GLN:HA	1:A:108:CYS:SG	0.50	2.47	3	2
1:A:20:ASP:CG	1:A:20:ASP:O	0.50	2.50	7	1
1:A:88:PHE:HE1	1:A:97:GLY:HA2	0.50	1.67	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASN:ND2	1:A:26:THR:OG1	0.50	2.45	4	2
1:A:16:PHE:CZ	1:A:65:TYR:N	0.50	2.80	2	7
1:A:52:MET:HG2	1:A:59:LYS:CD	0.49	2.37	4	2
1:A:33:LYS:O	1:A:37:LYS:HG2	0.49	2.06	9	2
1:A:33:LYS:O	1:A:36:LEU:HG	0.49	2.07	9	1
1:A:17:LYS:HB2	1:A:17:LYS:NZ	0.49	2.22	10	1
1:A:125:ILE:O	1:A:127:GLN:NE2	0.49	2.45	11	1
1:A:101:LEU:HA	1:A:104:ILE:HD12	0.49	1.83	10	1
1:A:36:LEU:HD13	1:A:43:LEU:HD12	0.49	1.83	14	1
1:A:33:LYS:HE2	1:A:37:LYS:NZ	0.49	2.21	15	1
1:A:51:LEU:HD12	1:A:55:ALA:HB3	0.49	1.84	5	1
1:A:43:LEU:HD12	1:A:43:LEU:C	0.49	2.28	8	1
1:A:56:ASP:OD2	1:A:59:LYS:HA	0.49	2.06	5	3
1:A:121:MET:SD	1:A:121:MET:C	0.49	2.91	8	1
1:A:63:ILE:HG23	1:A:67:GLU:CB	0.49	2.37	12	3
1:A:113:LEU:HA	1:A:118:ILE:CG1	0.49	2.31	14	5
1:A:105:GLN:NE2	1:A:118:ILE:CG2	0.49	2.74	3	1
1:A:108:CYS:HB3	1:A:111:PHE:HB3	0.49	1.82	8	2
1:A:37:LYS:HG2	1:A:37:LYS:O	0.49	2.07	10	1
1:A:108:CYS:SG	1:A:113:LEU:N	0.49	2.86	11	1
1:A:136:GLY:O	1:A:139:ALA:HB3	0.49	2.08	15	5
1:A:32:LEU:HD12	1:A:52:MET:CE	0.49	2.36	4	1
1:A:127:GLN:OE1	1:A:141:MET:HB3	0.49	2.07	11	1
1:A:113:LEU:HA	1:A:118:ILE:HD13	0.49	1.85	2	1
1:A:129:ASN:N	1:A:129:ASN:HD22	0.49	2.06	4	1
1:A:15:LEU:HD13	1:A:15:LEU:O	0.49	2.07	8	1
1:A:33:LYS:HB2	1:A:37:LYS:HE2	0.49	1.83	3	2
1:A:49:LYS:HE2	1:A:91:PHE:CE1	0.49	2.43	3	1
1:A:108:CYS:SG	1:A:113:LEU:HB3	0.49	2.48	14	1
1:A:36:LEU:HD21	1:A:43:LEU:HG	0.48	1.85	1	2
1:A:15:LEU:HD12	1:A:68:PHE:CZ	0.48	2.42	10	1
1:A:98:TYR:HB2	1:A:132:GLN:NE2	0.48	2.23	1	3
1:A:58:ASP:HB2	1:A:67:GLU:OE2	0.48	2.08	14	5
1:A:108:CYS:HB2	1:A:111:PHE:CG	0.48	2.43	14	2
1:A:27:ILE:O	1:A:63:ILE:N	0.48	2.46	4	10
1:A:33:LYS:HZ3	1:A:45:GLU:HG3	0.48	1.68	13	1
1:A:37:LYS:HA	1:A:41:SER:O	0.48	2.08	3	6
1:A:33:LYS:HB3	1:A:48:ILE:CG1	0.48	2.38	3	4
1:A:105:GLN:NE2	1:A:119:ASP:HA	0.48	2.24	2	4
1:A:21:THR:HG21	1:A:38:ARG:HH22	0.48	1.68	1	2
1:A:32:LEU:HD11	1:A:51:LEU:HD21	0.48	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASN:HB3	1:A:31:GLU:OE1	0.48	2.08	9	1
1:A:55:ALA:HB1	1:A:71:ALA:HB1	0.48	1.85	14	1
1:A:133:ILE:HG21	1:A:138:PHE:HD1	0.48	1.67	13	4
1:A:23:ASN:HB2	1:A:31:GLU:HG2	0.48	1.84	13	1
1:A:134:ASP:O	1:A:137:GLU:N	0.48	2.47	10	8
1:A:115:ASP:HA	1:A:119:ASP:CG	0.48	2.28	5	1
1:A:92:ASP:N	1:A:99:ILE:HD11	0.48	2.24	15	1
1:A:129:ASN:HD22	1:A:130:ASP:H	0.48	1.52	8	1
1:A:43:LEU:HD13	1:A:48:ILE:CD1	0.47	2.39	6	5
1:A:17:LYS:HA	1:A:20:ASP:OD1	0.47	2.09	15	3
1:A:97:GLY:O	1:A:134:ASP:HA	0.47	2.08	2	3
1:A:133:ILE:HD13	1:A:137:GLU:OE1	0.47	2.09	4	2
1:A:126:ASP:HB2	1:A:131:GLY:CA	0.47	2.39	13	3
1:A:49:LYS:NZ	1:A:109:LYS:HE2	0.47	2.24	11	1
1:A:14:GLU:O	1:A:18:MET:HB2	0.47	2.10	11	1
1:A:46:SER:OG	1:A:87:ALA:HB2	0.47	2.09	15	1
1:A:100:THR:O	1:A:102:ASP:N	0.47	2.46	15	5
1:A:118:ILE:HG23	1:A:121:MET:SD	0.47	2.49	14	3
1:A:97:GLY:O	1:A:135:TYR:N	0.47	2.48	5	1
1:A:53:ASP:HB2	1:A:59:LYS:NZ	0.47	2.24	11	1
1:A:15:LEU:HG	1:A:68:PHE:CZ	0.47	2.45	7	4
1:A:97:GLY:O	1:A:134:ASP:HB3	0.47	2.10	14	2
1:A:53:ASP:N	1:A:59:LYS:HD3	0.47	2.25	11	1
1:A:45:GLU:O	1:A:47:GLU:N	0.47	2.48	2	2
1:A:88:PHE:CZ	1:A:135:TYR:HB2	0.47	2.44	11	3
1:A:36:LEU:HD23	1:A:41:SER:HB3	0.47	1.86	6	2
1:A:32:LEU:CG	1:A:51:LEU:HD23	0.47	2.39	5	1
1:A:118:ILE:HG22	1:A:119:ASP:N	0.47	2.24	11	1
1:A:105:GLN:N	1:A:105:GLN:OE1	0.47	2.47	11	1
1:A:33:LYS:NZ	1:A:45:GLU:HA	0.47	2.25	13	1
1:A:18:MET:CE	1:A:18:MET:HA	0.47	2.40	6	3
1:A:127:GLN:OE1	1:A:137:GLU:HB3	0.47	2.10	2	1
1:A:13:LYS:HB3	1:A:13:LYS:NZ	0.47	2.25	1	2
1:A:36:LEU:HD22	1:A:36:LEU:N	0.47	2.24	7	3
1:A:108:CYS:HB2	1:A:111:PHE:HD1	0.47	1.61	11	1
1:A:47:GLU:O	1:A:50:ASP:HB3	0.47	2.10	12	7
1:A:111:PHE:CD1	1:A:112:GLY:N	0.47	2.83	8	3
1:A:133:ILE:HG21	1:A:138:PHE:CD1	0.47	2.45	14	2
1:A:113:LEU:C	1:A:113:LEU:HD13	0.46	2.31	4	3
1:A:45:GLU:O	1:A:48:ILE:N	0.46	2.48	1	5
1:A:133:ILE:HD13	1:A:137:GLU:CB	0.46	2.34	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ALA:HB3	1:A:138:PHE:CZ	0.46	2.46	5	1
1:A:28:THR:C	1:A:30:ASP:N	0.46	2.69	7	1
1:A:105:GLN:NE2	1:A:118:ILE:CA	0.46	2.78	11	1
1:A:127:GLN:HG3	1:A:140:ALA:HB3	0.46	1.87	6	2
1:A:108:CYS:HB2	1:A:111:PHE:HB2	0.46	1.86	14	2
1:A:101:LEU:HD22	1:A:122:ILE:HD13	0.46	1.87	12	1
1:A:109:LYS:HA	1:A:109:LYS:HE3	0.46	1.86	8	1
1:A:15:LEU:O	1:A:18:MET:HB3	0.46	2.10	10	2
1:A:52:MET:O	1:A:56:ASP:CB	0.46	2.63	13	1
1:A:104:ILE:CG2	1:A:105:GLN:N	0.46	2.78	13	1
1:A:56:ASP:OD1	1:A:67:GLU:HB3	0.46	2.10	13	1
1:A:104:ILE:HD11	1:A:133:ILE:CD1	0.46	2.41	13	1
1:A:37:LYS:HB3	1:A:37:LYS:NZ	0.46	2.26	3	2
1:A:28:THR:O	1:A:32:LEU:N	0.46	2.48	9	2
1:A:113:LEU:HD23	1:A:118:ILE:CG2	0.46	2.41	10	2
1:A:117:HIS:CD2	1:A:121:MET:HG3	0.46	2.46	11	1
1:A:31:GLU:HA	1:A:34:ASP:HB2	0.46	1.88	6	2
1:A:117:HIS:O	1:A:121:MET:HB2	0.46	2.11	11	2
1:A:13:LYS:HA	1:A:65:TYR:HE1	0.46	1.71	7	5
1:A:117:HIS:O	1:A:121:MET:N	0.46	2.49	12	1
1:A:108:CYS:CB	1:A:111:PHE:HB3	0.46	2.40	8	1
1:A:122:ILE:O	1:A:126:ASP:HB3	0.46	2.10	9	1
1:A:33:LYS:HG3	1:A:34:ASP:N	0.45	2.25	5	1
1:A:111:PHE:CD1	1:A:111:PHE:N	0.45	2.84	8	1
1:A:113:LEU:C	1:A:113:LEU:HD23	0.45	2.32	8	1
1:A:35:GLY:O	1:A:38:ARG:HB3	0.45	2.11	10	2
1:A:121:MET:O	1:A:124:GLU:N	0.45	2.50	11	3
1:A:109:LYS:C	1:A:109:LYS:HD3	0.45	2.32	2	1
1:A:138:PHE:O	1:A:142:MET:HG2	0.45	2.12	9	1
1:A:122:ILE:O	1:A:126:ASP:HB2	0.45	2.11	1	3
1:A:88:PHE:CA	1:A:92:ASP:HB2	0.45	2.41	13	2
1:A:118:ILE:HD12	1:A:121:MET:HE1	0.45	1.88	9	1
1:A:33:LYS:HB3	1:A:48:ILE:CD1	0.45	2.40	13	2
1:A:13:LYS:N	1:A:13:LYS:HD2	0.45	2.26	14	1
1:A:12:LEU:CD1	1:A:15:LEU:HD23	0.45	2.41	4	4
1:A:111:PHE:CD2	1:A:113:LEU:CD2	0.45	2.99	12	1
1:A:68:PHE:O	1:A:71:ALA:HB3	0.45	2.12	13	1
1:A:101:LEU:HD12	1:A:102:ASP:N	0.45	2.27	6	4
1:A:132:GLN:HG3	1:A:137:GLU:OE1	0.45	2.11	1	3
1:A:134:ASP:OD1	1:A:135:TYR:N	0.45	2.50	7	1
1:A:12:LEU:HA	1:A:15:LEU:HB3	0.45	1.87	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ASN:CG	1:A:130:ASP:H	0.45	2.16	2	2
1:A:112:GLY:O	1:A:113:LEU:HB3	0.45	2.11	11	1
1:A:34:ASP:HA	1:A:37:LYS:HE3	0.45	1.89	13	1
1:A:118:ILE:HG23	1:A:121:MET:HE2	0.45	1.88	2	1
1:A:49:LYS:HZ1	1:A:109:LYS:HE2	0.45	1.72	11	1
1:A:134:ASP:H	1:A:137:GLU:CB	0.44	2.25	5	2
1:A:104:ILE:HG22	1:A:121:MET:CE	0.44	2.42	7	1
1:A:13:LYS:NZ	1:A:13:LYS:HB2	0.44	2.26	15	1
1:A:43:LEU:C	1:A:43:LEU:CD1	0.44	2.85	15	1
1:A:98:TYR:CB	1:A:132:GLN:NE2	0.44	2.80	15	1
1:A:16:PHE:HB2	1:A:68:PHE:CD2	0.44	2.48	4	4
1:A:126:ASP:CB	1:A:131:GLY:HA2	0.44	2.41	12	2
1:A:115:ASP:HA	1:A:119:ASP:OD2	0.44	2.13	5	1
1:A:51:LEU:HD12	1:A:51:LEU:C	0.44	2.33	8	1
1:A:58:ASP:HB2	1:A:67:GLU:OE1	0.44	2.12	9	1
1:A:37:LYS:HE3	1:A:43:LEU:CD1	0.44	2.42	15	1
1:A:121:MET:CA	1:A:124:GLU:HB3	0.44	2.31	4	3
1:A:44:MET:HE3	1:A:86:SER:HB3	0.44	1.89	5	1
1:A:113:LEU:O	1:A:113:LEU:CD2	0.44	2.63	11	1
1:A:122:ILE:HG23	1:A:131:GLY:O	0.44	2.12	2	2
1:A:133:ILE:HG23	1:A:138:PHE:N	0.44	2.27	8	4
1:A:127:GLN:HE22	1:A:137:GLU:CB	0.44	2.26	5	1
1:A:92:ASP:CB	1:A:99:ILE:HG12	0.44	2.43	7	1
1:A:49:LYS:O	1:A:53:ASP:OD1	0.44	2.35	10	1
1:A:32:LEU:HB3	1:A:48:ILE:CG2	0.44	2.42	14	1
1:A:128:ASP:OD1	1:A:129:ASN:ND2	0.44	2.51	6	2
1:A:116:ILE:HG13	1:A:117:HIS:N	0.44	2.28	4	1
1:A:19:ILE:HA	1:A:35:GLY:CA	0.44	2.43	12	2
1:A:23:ASN:HB2	1:A:31:GLU:OE1	0.44	2.13	5	1
1:A:26:THR:O	1:A:31:GLU:OE1	0.44	2.36	9	2
1:A:91:PHE:O	1:A:103:GLU:HB3	0.44	2.13	8	1
1:A:129:ASN:ND2	1:A:130:ASP:N	0.44	2.65	10	2
1:A:107:ALA:O	1:A:108:CYS:C	0.44	2.56	11	1
1:A:133:ILE:HA	1:A:137:GLU:OE1	0.44	2.12	8	1
1:A:108:CYS:HB3	1:A:111:PHE:CG	0.43	2.47	9	2
1:A:121:MET:SD	1:A:125:ILE:CD1	0.43	3.05	8	1
1:A:33:LYS:CG	1:A:48:ILE:HG13	0.43	2.42	14	1
1:A:12:LEU:O	1:A:16:PHE:N	0.43	2.52	13	1
1:A:105:GLN:NE2	1:A:118:ILE:O	0.43	2.51	12	1
1:A:13:LYS:HD3	1:A:13:LYS:C	0.43	2.34	13	1
1:A:113:LEU:HB2	1:A:118:ILE:HG21	0.43	1.90	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ALA:C	1:A:89:SER:N	0.43	2.72	7	8
1:A:118:ILE:HD12	1:A:118:ILE:N	0.43	2.28	2	1
1:A:26:THR:HB	1:A:62:THR:CG2	0.43	2.43	10	3
1:A:88:PHE:CE1	1:A:97:GLY:HA2	0.43	2.48	9	2
1:A:15:LEU:CA	1:A:18:MET:HB3	0.43	2.43	9	2
1:A:114:ASP:O	1:A:118:ILE:HG13	0.43	2.12	11	1
1:A:29:PHE:HZ	1:A:45:GLU:HB3	0.43	1.74	13	1
1:A:12:LEU:C	1:A:12:LEU:HD13	0.43	2.34	14	1
1:A:32:LEU:HD11	1:A:51:LEU:CD1	0.43	2.41	14	1
1:A:134:ASP:C	1:A:136:GLY:N	0.43	2.72	10	2
1:A:31:GLU:HA	1:A:34:ASP:HB3	0.43	1.89	11	3
1:A:36:LEU:HD22	1:A:37:LYS:N	0.43	2.29	1	2
1:A:99:ILE:CG2	1:A:104:ILE:HG13	0.43	2.44	6	2
1:A:134:ASP:O	1:A:136:GLY:N	0.43	2.52	6	2
1:A:127:GLN:NE2	1:A:137:GLU:CA	0.43	2.79	4	1
1:A:126:ASP:O	1:A:126:ASP:CG	0.43	2.57	9	2
1:A:100:THR:O	1:A:103:GLU:N	0.43	2.52	14	3
1:A:19:ILE:CG2	1:A:31:GLU:O	0.43	2.67	10	1
1:A:44:MET:HE3	1:A:47:GLU:HG3	0.43	1.91	5	1
1:A:65:TYR:CZ	1:A:69:ILE:HD11	0.43	2.49	11	1
1:A:105:GLN:HE21	1:A:118:ILE:CG2	0.43	2.27	11	1
1:A:14:GLU:O	1:A:18:MET:N	0.42	2.52	1	3
1:A:108:CYS:SG	1:A:118:ILE:HD11	0.42	2.53	3	1
1:A:125:ILE:CG2	1:A:133:ILE:CD1	0.42	2.94	3	1
1:A:138:PHE:HA	1:A:141:MET:SD	0.42	2.54	13	1
1:A:100:THR:O	1:A:101:LEU:C	0.42	2.57	12	5
1:A:121:MET:O	1:A:125:ILE:N	0.42	2.52	4	1
1:A:38:ARG:C	1:A:38:ARG:HD3	0.42	2.33	9	2
1:A:113:LEU:O	1:A:113:LEU:HD13	0.42	2.14	11	1
1:A:49:LYS:CE	1:A:93:LYS:HD3	0.42	2.44	13	1
1:A:125:ILE:HD12	1:A:133:ILE:HD11	0.42	1.91	13	1
1:A:12:LEU:HD12	1:A:15:LEU:HB3	0.42	1.90	2	1
1:A:48:ILE:HD12	1:A:48:ILE:N	0.42	2.28	5	2
1:A:108:CYS:O	1:A:112:GLY:CA	0.42	2.66	11	1
1:A:105:GLN:OE1	1:A:121:MET:HE1	0.42	2.14	12	1
1:A:19:ILE:CG2	1:A:27:ILE:HD13	0.42	2.43	14	1
1:A:33:LYS:HB2	1:A:37:LYS:CE	0.42	2.44	15	1
1:A:14:GLU:C	1:A:18:MET:HG2	0.42	2.35	3	2
1:A:32:LEU:HD22	1:A:48:ILE:HA	0.42	1.89	5	1
1:A:51:LEU:O	1:A:51:LEU:HD23	0.42	2.15	6	2
1:A:87:ALA:O	1:A:89:SER:N	0.42	2.53	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ASP:HB3	1:A:131:GLY:HA2	0.42	1.90	5	2
1:A:49:LYS:NZ	1:A:93:LYS:NZ	0.42	2.67	7	1
1:A:92:ASP:HB2	1:A:99:ILE:CG1	0.42	2.45	7	1
1:A:104:ILE:HD11	1:A:133:ILE:HD12	0.42	1.91	13	1
1:A:52:MET:O	1:A:56:ASP:N	0.42	2.53	11	1
1:A:114:ASP:OD1	1:A:115:ASP:N	0.42	2.53	4	1
1:A:13:LYS:C	1:A:13:LYS:HD2	0.42	2.35	8	1
1:A:53:ASP:OD2	1:A:90:TYR:HB2	0.42	2.14	8	1
1:A:120:ASP:O	1:A:124:GLU:CB	0.42	2.64	11	1
1:A:128:ASP:OD1	1:A:137:GLU:OE2	0.42	2.38	1	2
1:A:108:CYS:SG	1:A:118:ILE:HD12	0.42	2.53	4	1
1:A:18:MET:SD	1:A:18:MET:O	0.42	2.78	15	1
1:A:49:LYS:HB2	1:A:49:LYS:NZ	0.42	2.30	13	2
1:A:56:ASP:OD1	1:A:67:GLU:OE1	0.42	2.37	9	1
1:A:20:ASP:CG	1:A:25:GLY:H	0.41	2.19	9	1
1:A:65:TYR:CE1	1:A:69:ILE:HD11	0.41	2.50	9	1
1:A:100:THR:HA	1:A:132:GLN:CB	0.41	2.45	13	1
1:A:137:GLU:C	1:A:139:ALA:N	0.41	2.72	15	1
1:A:113:LEU:HD22	1:A:113:LEU:C	0.41	2.36	3	1
1:A:44:MET:O	1:A:47:GLU:HB2	0.41	2.15	5	1
1:A:51:LEU:HD12	1:A:55:ALA:CB	0.41	2.45	5	1
1:A:54:ALA:CB	1:A:89:SER:HB3	0.41	2.45	9	1
1:A:105:GLN:HB3	1:A:113:LEU:HG	0.41	1.92	10	1
1:A:114:ASP:OD2	1:A:116:ILE:HB	0.41	2.15	12	1
1:A:13:LYS:HD2	1:A:13:LYS:H	0.41	1.75	14	1
1:A:138:PHE:O	1:A:141:MET:HG3	0.41	2.15	14	1
1:A:138:PHE:CD1	1:A:141:MET:SD	0.41	3.14	4	1
1:A:111:PHE:N	1:A:111:PHE:HD1	0.41	2.13	7	1
1:A:133:ILE:CG2	1:A:138:PHE:N	0.41	2.83	8	2
1:A:33:LYS:O	1:A:37:LYS:HG3	0.41	2.15	13	1
1:A:134:ASP:OD1	1:A:134:ASP:N	0.41	2.54	13	1
1:A:98:TYR:HB3	1:A:134:ASP:HB2	0.41	1.93	10	1
1:A:108:CYS:HB3	1:A:111:PHE:CB	0.41	2.41	10	1
1:A:46:SER:O	1:A:50:ASP:HB2	0.41	2.16	2	1
1:A:128:ASP:O	1:A:129:ASN:HB3	0.41	2.15	2	2
1:A:140:ALA:C	1:A:142:MET:N	0.41	2.73	14	1
1:A:127:GLN:HB2	1:A:137:GLU:CD	0.41	2.36	8	1
1:A:138:PHE:CD1	1:A:141:MET:HG2	0.41	2.49	14	1
1:A:47:GLU:OE1	1:A:47:GLU:N	0.41	2.53	1	2
1:A:32:LEU:CB	1:A:48:ILE:HG23	0.41	2.45	5	1
1:A:127:GLN:H	1:A:127:GLN:CD	0.41	2.18	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:PHE:HD2	1:A:69:ILE:HD13	0.41	1.76	6	1
1:A:103:GLU:O	1:A:107:ALA:HB2	0.41	2.16	10	2
1:A:21:THR:HG22	1:A:38:ARG:HH22	0.41	1.75	11	1
1:A:64:ASP:O	1:A:65:TYR:C	0.41	2.58	11	1
1:A:113:LEU:O	1:A:114:ASP:C	0.41	2.59	11	1
1:A:27:ILE:CG2	1:A:32:LEU:HA	0.41	2.45	13	1
1:A:34:ASP:HA	1:A:37:LYS:HD2	0.41	1.92	1	2
1:A:46:SER:HB2	1:A:87:ALA:HB2	0.41	1.92	1	2
1:A:125:ILE:CG2	1:A:133:ILE:HD11	0.41	2.40	3	1
1:A:19:ILE:HG13	1:A:68:PHE:CE1	0.41	2.50	5	1
1:A:104:ILE:HD11	1:A:132:GLN:HA	0.41	1.91	9	1
1:A:98:TYR:HA	1:A:133:ILE:O	0.41	2.15	11	1
1:A:45:GLU:N	1:A:45:GLU:OE1	0.41	2.53	14	2
1:A:33:LYS:CE	1:A:48:ILE:HG12	0.41	2.46	4	1
1:A:32:LEU:CD2	1:A:48:ILE:HG23	0.41	2.46	5	1
1:A:49:LYS:HE2	1:A:91:PHE:HE1	0.41	1.76	5	1
1:A:121:MET:C	1:A:124:GLU:H	0.41	2.20	8	1
1:A:33:LYS:O	1:A:37:LYS:N	0.41	2.53	11	1
1:A:105:GLN:HE21	1:A:118:ILE:CB	0.41	2.29	11	1
1:A:33:LYS:NZ	1:A:37:LYS:NZ	0.41	2.69	14	1
1:A:87:ALA:HB1	1:A:91:PHE:HB2	0.41	1.91	4	2
1:A:36:LEU:O	1:A:41:SER:HB2	0.41	2.16	10	1
1:A:105:GLN:HE21	1:A:118:ILE:HG12	0.41	1.76	11	1
1:A:112:GLY:O	1:A:113:LEU:C	0.40	2.59	1	1
1:A:113:LEU:HD23	1:A:114:ASP:N	0.40	2.31	7	1
1:A:126:ASP:OD1	1:A:129:ASN:N	0.40	2.54	8	1
1:A:105:GLN:OE1	1:A:118:ILE:HG22	0.40	2.16	10	1
1:A:105:GLN:O	1:A:108:CYS:SG	0.40	2.70	11	1
1:A:134:ASP:O	1:A:135:TYR:C	0.40	2.59	1	1
1:A:115:ASP:HA	1:A:119:ASP:CB	0.40	2.47	2	1
1:A:19:ILE:HG21	1:A:27:ILE:CG2	0.40	2.46	5	1
1:A:98:TYR:CD1	1:A:98:TYR:N	0.40	2.89	14	1
1:A:17:LYS:HD3	1:A:17:LYS:C	0.40	2.37	2	1
1:A:20:ASP:OD2	1:A:25:GLY:N	0.40	2.55	4	1
1:A:36:LEU:C	1:A:38:ARG:N	0.40	2.75	5	1
1:A:94:ASP:C	1:A:96:SER:H	0.40	2.20	12	1
1:A:134:ASP:HB2	1:A:137:GLU:OE2	0.40	2.17	15	1
1:A:118:ILE:HD12	1:A:121:MET:SD	0.40	2.56	14	1
1:A:126:ASP:OD2	1:A:129:ASN:HB3	0.40	2.16	14	1
1:A:127:GLN:HG3	1:A:140:ALA:CB	0.40	2.46	1	1
1:A:15:LEU:CA	1:A:18:MET:HB2	0.40	2.47	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:LYS:H	1:A:109:LYS:CD	0.40	2.28	9	1
1:A:121:MET:HB3	1:A:121:MET:HE2	0.40	1.85	12	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	118/188 (63%)	88±3 (75±2%)	22±3 (19±2%)	8±1 (7±1%)	2 18
All	All	1770/2820 (63%)	1320 (75%)	334 (19%)	116 (7%)	2 18

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	24	SER	15
1	A	59	LYS	15
1	A	129	ASN	14
1	A	29	PHE	13
1	A	56	ASP	12
1	A	130	ASP	11
1	A	101	LEU	7
1	A	23	ASN	5
1	A	46	SER	4
1	A	113	LEU	4
1	A	88	PHE	3
1	A	39	VAL	3
1	A	126	ASP	3
1	A	135	TYR	2
1	A	108	CYS	1
1	A	114	ASP	1
1	A	118	ILE	1
1	A	111	PHE	1
1	A	95	GLY	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	100/159 (63%)	89±2 (89±2%)	11±2 (11±2%)	9 53
All	All	1500/2385 (63%)	1333 (89%)	167 (11%)	9 53

All 38 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	98	TYR	12
1	A	129	ASN	12
1	A	20	ASP	10
1	A	127	GLN	10
1	A	113	LEU	9
1	A	101	LEU	9
1	A	18	MET	8
1	A	31	GLU	8
1	A	36	LEU	7
1	A	123	LYS	7
1	A	37	LYS	7
1	A	23	ASN	5
1	A	111	PHE	5
1	A	33	LYS	4
1	A	43	LEU	4
1	A	92	ASP	4
1	A	38	ARG	4
1	A	109	LYS	4
1	A	141	MET	4
1	A	134	ASP	4
1	A	17	LYS	3
1	A	90	TYR	3
1	A	45	GLU	3
1	A	104	ILE	3
1	A	14	GLU	2
1	A	39	VAL	2
1	A	53	ASP	2
1	A	13	LYS	2
1	A	93	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	49	LYS	1
1	A	44	MET	1
1	A	51	LEU	1
1	A	15	LEU	1
1	A	105	GLN	1
1	A	19	ILE	1
1	A	52	MET	1
1	A	32	LEU	1
1	A	42	GLU	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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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