Full wwPDB NMR Structure Validation Report (i)

Feb 14, 2022 – 09:04 AM EST

PDB ID	:	1K0S
Title	:	Solution structure of the chemotaxis protein CheW from the thermophilic organism Thermotoga maritima
Authors	:	Griswold, I.J.; Zhou, H.; Swanson, R.V.; Simon, M.I.; Dahlquist, F.W.
Deposited on	:	2001-09-20

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:

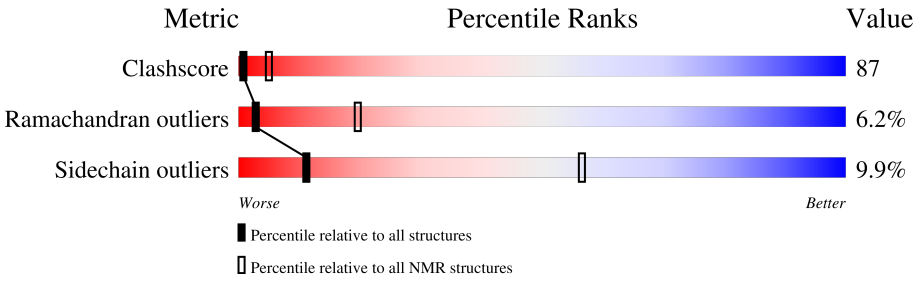
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	151	15% 52% 7% 27%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 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:9-A:36, A:49-A:53, A:60-A:108, A:118-A:122, A:126-A:148 (110)	0.38	13

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 4 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2455 atoms, of which 1264 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CHEMOTAXIS PROTEIN CHEW.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	151	2455	765	1264	197	226	3	0

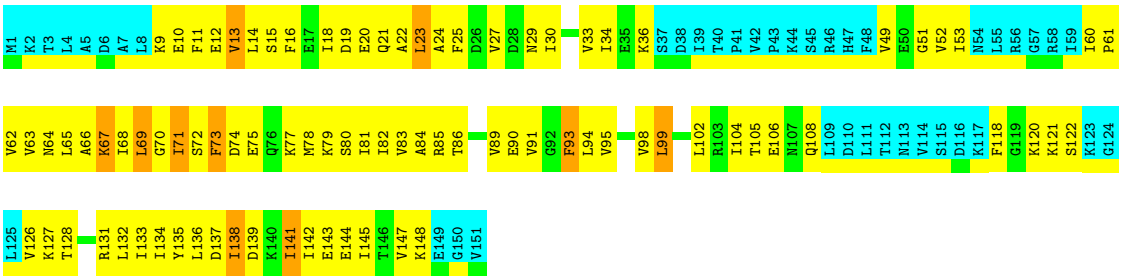
4 Residue-property plots (i)

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: CHEMOTAXIS PROTEIN CHEW

Chain A: 15% 52% 7% 27%



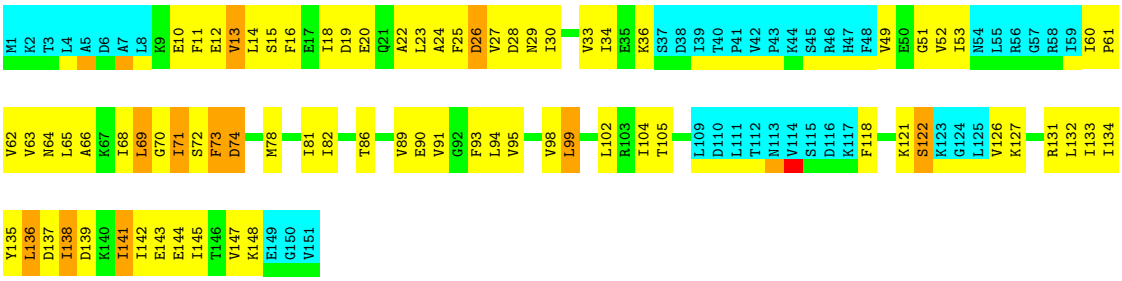
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CHEMOTAXIS PROTEIN CHEW

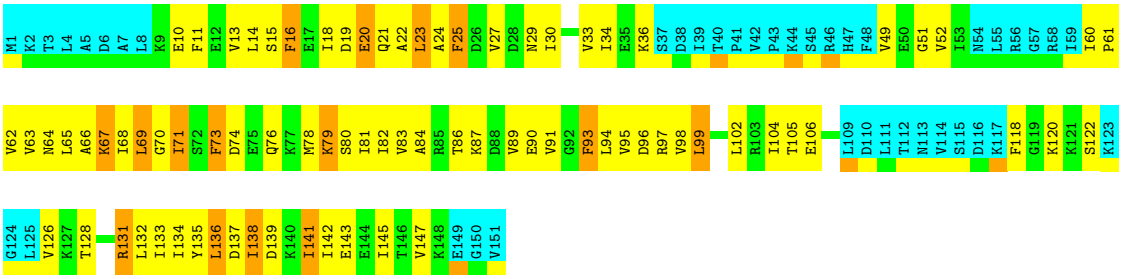
Chain A: 23% 43% 7% 27%



4.2.2 Score per residue for model 2

• Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 20% 43% 10% 27%



4.2.3 Score per residue for model 3

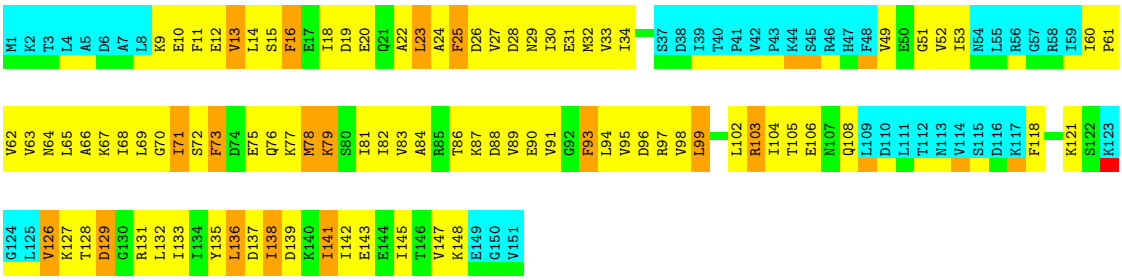
• Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 23% 40% 9% • 27%

4.2.4 Score per residue for model 4

• Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 13% 49% 11% 27%



4.2.5 Score per residue for model 5

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 17% 45% 11% 27%

M1 K2 T3 L4 A5 D6 A7 L8 K9 E10 F11 E12 V13 L14 S15 F16 E17 I18 D19 E20 Q21 A22 L23 A24 F25 D26 V27 D28 N29 I30 E31 M32 V33 I34 E35 K36 S37 D38 I39 T40 P41 V42 P43 K44 S45 R46 H47 F48 V49 E50 G51 V52 I53 N54 L55 R56 G57 R58 I59 I60

P61 V62 V63 N64 L65 A66 K67 I68 L69 G70 I71 S72 F73 D74 K77 M78 K79 S80 I81 I82 V83 A84 R85 T86 K87 D88 V89 E90 V91 G92 F93 L94 V95 V98 L99 L102 R103 I104 T105 E106 L109 D110 L111 T112 N113 V114 S115 D116 K117 F118 K121 S122 K123 G124 L125

V126 K127 T128 R131 L132 I133 I134 Y135 L136 D137 I138 I141 I142 E143 E144 I145 T146 V147 K148 E149 G150 V151

4.2.6 Score per residue for model 6

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 18% 45% 10% 27%

M1 K2 T3 L4 A5 D6 A7 L8 K9 E10 F11 E12 V13 L14 S15 F16 E17 I18 D19 E20 Q21 A22 L23 A24 F25 D26 V27 D28 N29 I30 E31 M32 V33 S37 D38 I39 T40 P41 V42 P43 K44 S45 R46 H47 F48 V49 E50 G51 V52 I53 N54 L55 R56 G57 R58 I59 I60 P61 V62

V63 N64 L65 A66 K67 I68 L69 G70 I71 S72 F73 M78 K79 S80 I81 I82 V83 A84 R85 T86 K87 D88 V89 E90 V91 G92 F93 L94 V95 V98 L99 L102 R103 I104 T105 E106 N107 Q108 L109 D110 L111 T112 N113 V114 S115 D116 K117 F118 G119 S122 K123 G124 L125 V126 K127 T128

R131 L132 I133 I134 Y135 L136 D137 I138 D139 K140 I141 I142 E143 E144 I145 T146 V147 K148 E149 G150 V151

4.2.7 Score per residue for model 7

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 19% 44% 9% • 27%

M1 K2 T3 L4 A5 D6 A7 L8 K9 E10 F11 E12 V13 L14 S15 F16 E17 I18 D19 E20 Q21 A22 L23 A24 F25 D26 V27 D28 N29 I30 V33 S37 D38 I39 T40 P41 V42 P43 K44 S45 R46 H47 F48 V49 E50 G51 V52 I53 N54 L55 R56 G57 R58 I59 I60 P61 V62 V63

N64 L65 A66 K67 I68 L69 G70 I71 S72 F73 D74 K77 M78 K79 S80 I81 I82 V83 A84 R85 T86 V89 E90 V91 G92 F93 L94 V95 V98 L99 G100 V101 L102 R103 I104 T105 E106 L109 D110 L111 T112 N113 V114 S115 D116 K117 F118 G119 K120 K121 S122 K123 G124 L125 V126 K127

T128 D129 G130 R131 L132 I133 I134 Y135 L136 D137 I138 D139 K140 I141 I142 E143 E144 I145 T146 V147 K148 E149 G150 V151

4.2.8 Score per residue for model 8

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 19% 45% 9% 27%

M1 K2 T3 L4 A5 D6 A7 L8 K9 E10 F11 E12 V13 L14 S15 F16 E17 I18 D19 E20 Q21 A22 L23 A24 F25 D26 V27 D28 N29 I30 E31 M32 V33 K36 S37 D38 I39 T40 P41 V42 P43 K44 S45 R46 H47 F48 V49 E50 G51 V52 I53 N54 L55 R56 G57 R58 I59 I60 P61

V62 V63 N64 L65 A66 K67 I68 L69 G70 I71 S72 F73 D74 E75 Q76 K77 M78 K79 S80 I81 I82 V83 A84 R85 T86 V89 E90 V91 G92 F93 L94 V95 D96 R97 V98 L99 L102 R103 I104 T105 E106 N107 Q108 L109 D110 L111 T112 N113 V114 S115 D116 K117 F118 G119 K123 G124 L125

V126 K127 T128 D129 G130 R131 L132 I133 I134 Y135 L136 D137 I138 I141 I142 E143 E144 I145 T146 V147 K148 E149 G150 V151

4.2.9 Score per residue for model 9

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 15% 47% 11% 27%

M1 K2 T3 L4 A5 D6 A7 L8 K9 E10 F11 E12 V13 L14 S15 F16 E17 I18 D19 E20 Q21 A22 L23 A24 F25 D26 V27 D28 N29 I30 V33 I34 S37 D38 I39 T40 P41 V42 P43 K44 S45 R46 H47 F48 V49 E50 G51 V52 I53 N54 L55 R56 G57 R58 I59 I60 P61 V62

V63 N64 L65 A66 K67 I68 L69 G70 I71 S72 F73 D74 E75 Q76 K77 M78 K79 S80 I81 I82 V83 A84 R85 T86 V89 E90 V91 G92 F93 L94 V95 V98 L99 L102 R103 I104 T105 E106 L109 D110 L111 T112 N113 V114 S115 D116 K117 F118 G119 K120 K121 S122 K123 G124 L125 V126

K127 T128 R131 L132 I133 I134 Y135 L136 D137 I138 D139 K140 I141 I142 E143 E144 I145 T146 V147 K148 E149 G150 V151

4.2.10 Score per residue for model 10

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 19% 44% 10% • 27%

M1 K2 T3 L4 A5 D6 A7 L8 F11 E12 V13 L14 S15 F16 E17 I18 D19 E20 Q21 A22 L23 A24 F25 D26 V27 D28 N29 I30 V33 I34 E35 K36 S37 D38 I39 T40 P41 V42 P43 K44 S45 R46 H47 F48 V49 E50 G51 V52 I53 N54 L55 R56 G57 R58 I59 I60 P61 V62

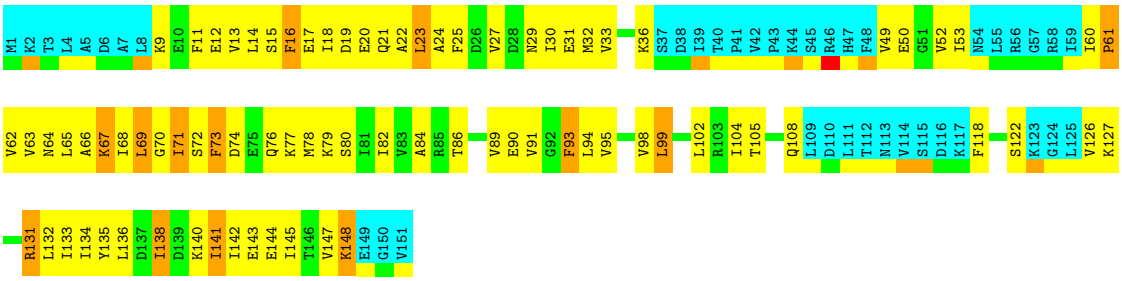
V63 N64 L65 A66 K67 I68 L69 G70 I71 S72 F73 D74 E75 Q76 K77 M78 K79 S80 I81 I82 V83 A84 R85 T86 V89 E90 V91 G92 F93 L94 V95 D96 R97 V98 L99 L102 R103 I104 T105 E106 N107 Q108 L109 D110 L111 T112 N113 V114 S115 D116 K117 F118 G119 K120 K121 S122 K123 G124

L125 V126 K127 T128 R131 L132 I133 I134 Y135 L136 D137 I138 I141 I142 E143 E144 I145 T146 V147 K148 E149 G150 V151

4.2.11 Score per residue for model 11

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

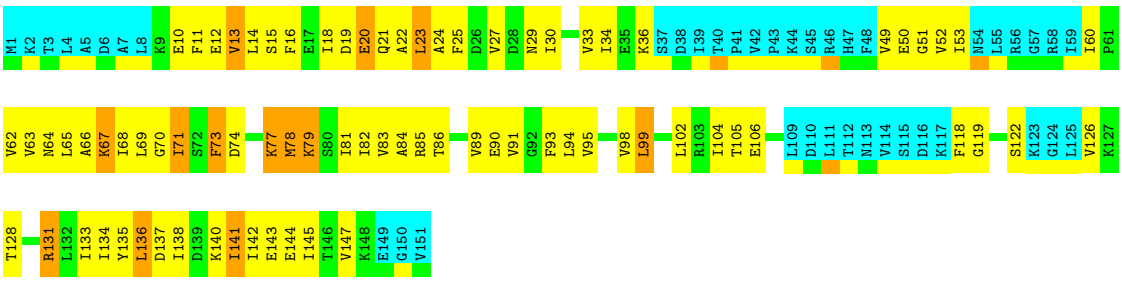
Chain A: 19% 45% 9% 27%



4.2.12 Score per residue for model 12

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

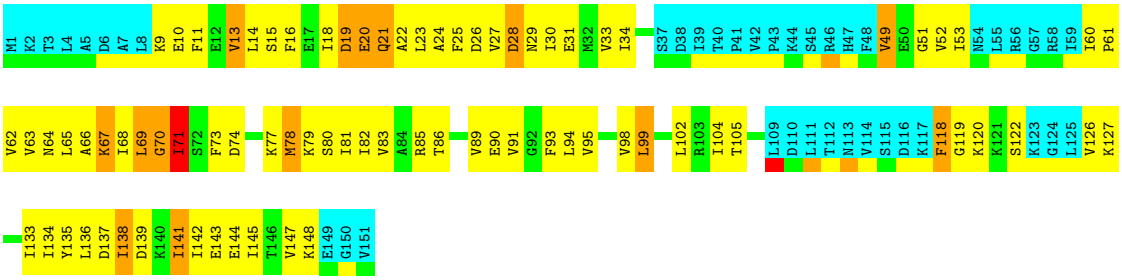
Chain A: 21% 44% 9% 27%



4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

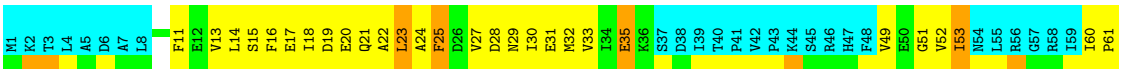
Chain A: 19% 44% 9% • 27%

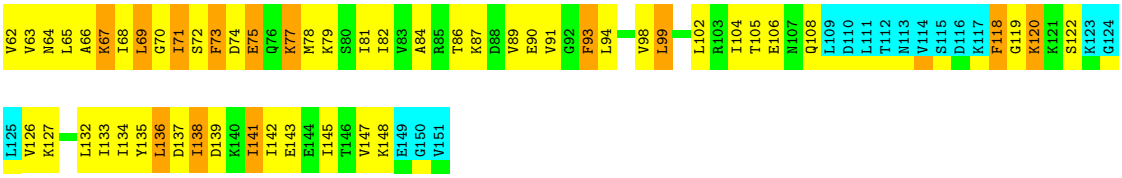


4.2.14 Score per residue for model 14

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A: 19% 43% 11% 27%

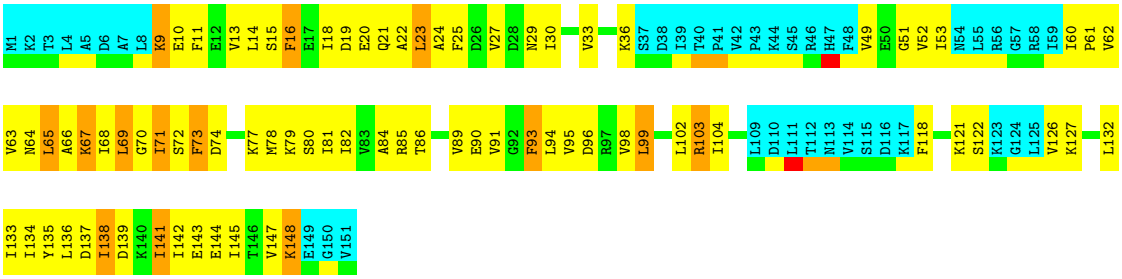




4.2.15 Score per residue for model 15

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

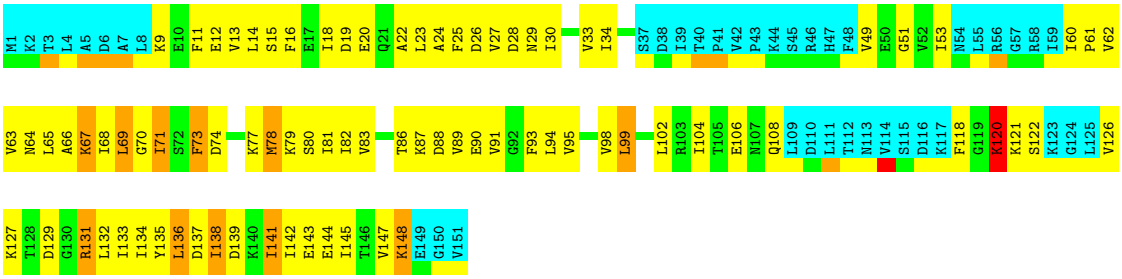
Chain A: 20% 44% 9% 27%



4.2.16 Score per residue for model 16

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

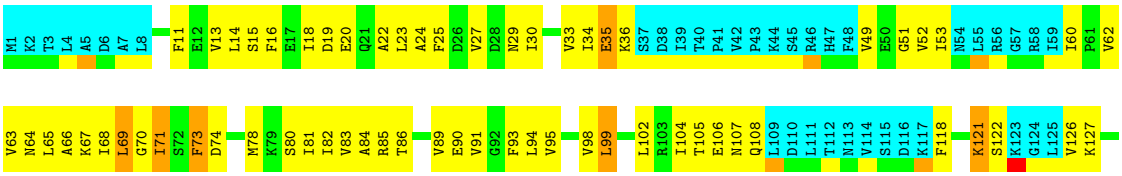
Chain A: 18% 47% 7% • 27%



4.2.17 Score per residue for model 17

- Molecule 1: CHEMOTAXIS PROTEIN CHEW

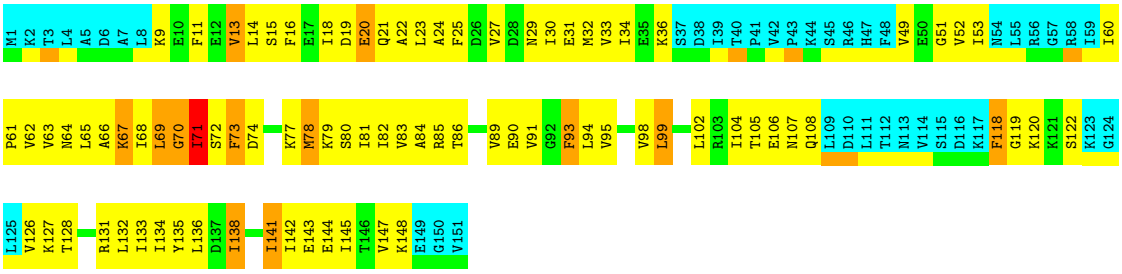
Chain A: 23% 44% 6% 27%



4.2.18 Score per residue for model 18

• Molecule 1: CHEMOTAXIS PROTEIN CHEW

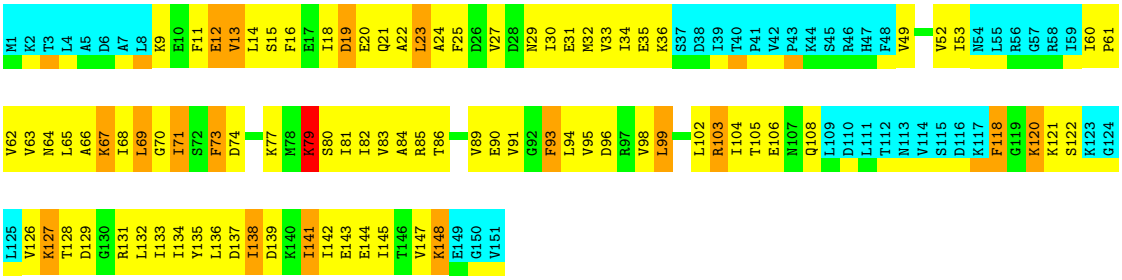
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: CHEMOTAXIS PROTEIN CHEW

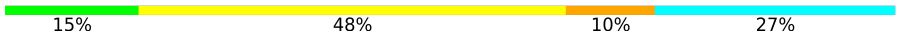
Chain A:

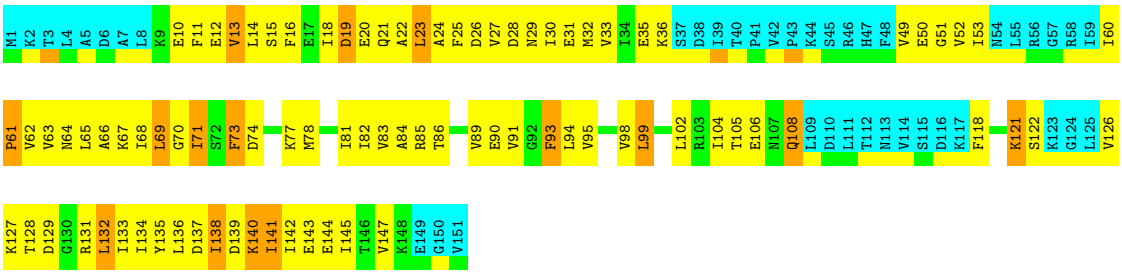


4.2.20 Score per residue for model 20

• Molecule 1: CHEMOTAXIS PROTEIN CHEW

Chain A:





5 Refinement protocol and experimental data overview (i)

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

Of the 50 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
CNS	structure solution	1.0
ARIA	structure solution	1.0
ARIA	refinement	1.0

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	876	929	929	156±10
All	All	17520	18580	18580	3129

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 87.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HG21	1:A:71:ILE:HD12	1.00	1.22	16	20
1:A:25:PHE:CE2	1:A:65:LEU:HD13	0.98	1.94	9	4
1:A:33:VAL:HG11	1:A:98:VAL:HG11	0.97	1.37	20	16
1:A:16:PHE:CE2	1:A:95:VAL:HG11	0.93	1.99	4	7
1:A:69:LEU:HD21	1:A:118:PHE:CE2	0.92	1.98	1	11
1:A:49:VAL:HG22	1:A:63:VAL:HG22	0.92	1.41	12	1
1:A:66:ALA:HB1	1:A:71:ILE:HD11	0.92	1.42	9	20
1:A:91:VAL:HG21	1:A:142:ILE:HD13	0.92	1.41	19	20
1:A:66:ALA:CB	1:A:71:ILE:HD11	0.92	1.95	17	17
1:A:104:ILE:HD12	1:A:126:VAL:HG11	0.91	1.39	18	9
1:A:22:ALA:HB3	1:A:133:ILE:HG12	0.90	1.42	2	20
1:A:104:ILE:HD12	1:A:126:VAL:HG21	0.90	1.41	1	6
1:A:25:PHE:CE2	1:A:136:LEU:HD22	0.89	2.02	19	8
1:A:14:LEU:HD11	1:A:82:ILE:HD13	0.88	1.44	19	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:HD11	1:A:60:ILE:HD11	0.87	1.45	5	5
1:A:29:ASN:ND2	1:A:138:ILE:HG21	0.87	1.84	19	12
1:A:13:VAL:HG11	1:A:104:ILE:CG1	0.86	1.99	17	20
1:A:80:SER:O	1:A:94:LEU:HD12	0.86	1.71	10	13
1:A:25:PHE:CZ	1:A:136:LEU:HD12	0.85	2.06	15	1
1:A:25:PHE:CZ	1:A:65:LEU:HD13	0.85	2.07	16	5
1:A:36:LYS:HB2	1:A:81:ILE:HD12	0.84	1.49	10	5
1:A:25:PHE:CD2	1:A:136:LEU:HD21	0.83	2.08	5	7
1:A:65:LEU:HD23	1:A:65:LEU:O	0.83	1.74	6	16
1:A:69:LEU:HD11	1:A:71:ILE:HG23	0.83	1.50	15	19
1:A:89:VAL:HG12	1:A:91:VAL:HG22	0.83	1.50	1	20
1:A:69:LEU:C	1:A:69:LEU:HD13	0.83	1.94	20	17
1:A:65:LEU:O	1:A:68:ILE:HG22	0.82	1.74	17	20
1:A:65:LEU:HD22	1:A:93:PHE:CD2	0.82	2.09	15	2
1:A:138:ILE:HA	1:A:141:ILE:CG2	0.82	2.04	9	20
1:A:135:TYR:O	1:A:136:LEU:HD23	0.82	1.74	15	1
1:A:23:LEU:HD13	1:A:134:ILE:HB	0.82	1.50	18	18
1:A:60:ILE:HG22	1:A:90:GLU:HB2	0.81	1.51	4	14
1:A:15:SER:HB3	1:A:102:LEU:HD22	0.81	1.51	19	16
1:A:25:PHE:CE2	1:A:136:LEU:HD21	0.81	2.11	2	6
1:A:69:LEU:HD13	1:A:69:LEU:C	0.81	1.95	14	3
1:A:126:VAL:HG13	1:A:133:ILE:HB	0.81	1.53	8	11
1:A:143:GLU:O	1:A:147:VAL:HG12	0.81	1.73	7	12
1:A:138:ILE:HA	1:A:141:ILE:HG23	0.81	1.53	12	20
1:A:23:LEU:HD12	1:A:24:ALA:N	0.80	1.91	11	20
1:A:65:LEU:HD22	1:A:93:PHE:CE2	0.80	2.11	15	3
1:A:49:VAL:HA	1:A:63:VAL:HG22	0.79	1.51	17	18
1:A:22:ALA:O	1:A:133:ILE:HG23	0.79	1.78	4	1
1:A:13:VAL:HA	1:A:27:VAL:HG13	0.79	1.53	15	16
1:A:16:PHE:CD2	1:A:95:VAL:HG11	0.78	2.13	4	8
1:A:132:LEU:HD23	1:A:133:ILE:N	0.78	1.94	2	1
1:A:29:ASN:CG	1:A:138:ILE:HG21	0.77	1.99	20	17
1:A:138:ILE:O	1:A:142:ILE:HG22	0.77	1.79	12	20
1:A:69:LEU:HD23	1:A:122:SER:OG	0.77	1.79	16	1
1:A:25:PHE:CZ	1:A:136:LEU:HD22	0.77	2.14	10	8
1:A:69:LEU:HD12	1:A:71:ILE:HD13	0.77	1.55	3	2
1:A:64:ASN:O	1:A:67:LYS:HG3	0.77	1.80	15	8
1:A:65:LEU:HD11	1:A:136:LEU:CD1	0.76	2.10	9	1
1:A:69:LEU:HD21	1:A:118:PHE:CE1	0.76	2.15	17	7
1:A:66:ALA:HB3	1:A:73:PHE:CD2	0.76	2.15	13	17
1:A:33:VAL:HG12	1:A:82:ILE:HG23	0.76	1.57	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:HD22	1:A:136:LEU:O	0.75	1.80	1	2
1:A:49:VAL:HG22	1:A:63:VAL:CG2	0.75	2.11	17	7
1:A:25:PHE:CE2	1:A:65:LEU:HD11	0.75	2.16	10	4
1:A:15:SER:CB	1:A:102:LEU:HD22	0.75	2.12	3	20
1:A:104:ILE:CD1	1:A:126:VAL:HG11	0.74	2.12	18	6
1:A:66:ALA:CB	1:A:73:PHE:CD2	0.74	2.71	13	20
1:A:85:ARG:O	1:A:86:THR:HG23	0.73	1.82	6	1
1:A:60:ILE:O	1:A:60:ILE:HD12	0.73	1.83	19	14
1:A:18:ILE:CG2	1:A:71:ILE:HD12	0.73	2.11	16	15
1:A:25:PHE:CE1	1:A:136:LEU:HD11	0.73	2.19	1	3
1:A:136:LEU:HD23	1:A:141:ILE:HG21	0.72	1.59	14	12
1:A:91:VAL:HG21	1:A:142:ILE:CD1	0.72	2.14	9	18
1:A:18:ILE:HG21	1:A:71:ILE:CD1	0.72	2.14	13	6
1:A:22:ALA:HB3	1:A:133:ILE:CG1	0.72	2.14	2	19
1:A:21:GLN:NE2	1:A:134:ILE:HD11	0.72	1.99	20	2
1:A:13:VAL:HG11	1:A:104:ILE:HG13	0.71	1.61	10	17
1:A:15:SER:HB2	1:A:102:LEU:HD22	0.71	1.62	16	4
1:A:63:VAL:HG12	1:A:64:ASN:H	0.71	1.45	1	3
1:A:71:ILE:HG13	1:A:73:PHE:HB3	0.71	1.61	15	19
1:A:29:ASN:ND2	1:A:138:ILE:HD13	0.71	2.01	20	3
1:A:122:SER:CB	1:A:136:LEU:HD22	0.71	2.16	15	1
1:A:138:ILE:O	1:A:142:ILE:CG2	0.71	2.39	11	20
1:A:53:ILE:HD12	1:A:53:ILE:O	0.70	1.86	13	2
1:A:16:PHE:CE1	1:A:95:VAL:HG11	0.70	2.21	9	7
1:A:132:LEU:HD13	1:A:133:ILE:N	0.70	2.02	18	1
1:A:65:LEU:HD11	1:A:136:LEU:HG	0.70	1.63	16	1
1:A:29:ASN:OD1	1:A:86:THR:HG22	0.70	1.86	20	2
1:A:25:PHE:CD1	1:A:136:LEU:HD21	0.69	2.22	12	1
1:A:65:LEU:HD12	1:A:141:ILE:HD11	0.69	1.62	10	5
1:A:69:LEU:CD1	1:A:71:ILE:HG23	0.69	2.17	9	20
1:A:16:PHE:CD1	1:A:82:ILE:HD11	0.69	2.23	3	4
1:A:61:PRO:HD2	1:A:90:GLU:O	0.69	1.88	4	16
1:A:64:ASN:OD1	1:A:94:LEU:HD23	0.69	1.86	3	2
1:A:29:ASN:HD21	1:A:138:ILE:HD13	0.68	1.48	20	1
1:A:51:GLY:C	1:A:62:VAL:HG22	0.68	2.08	5	18
1:A:22:ALA:O	1:A:133:ILE:HA	0.68	1.89	15	3
1:A:29:ASN:HD21	1:A:86:THR:HG22	0.68	1.48	16	9
1:A:21:GLN:OE1	1:A:132:LEU:HD22	0.68	1.89	2	1
1:A:69:LEU:HD23	1:A:122:SER:HG	0.68	1.49	16	1
1:A:13:VAL:CG2	1:A:24:ALA:HB1	0.67	2.19	1	13
1:A:18:ILE:HG22	1:A:19:ASP:OD2	0.67	1.87	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:C	1:A:65:LEU:HD23	0.67	2.10	15	6
1:A:69:LEU:HD12	1:A:71:ILE:HG12	0.67	1.66	20	13
1:A:65:LEU:HD12	1:A:141:ILE:CD1	0.67	2.19	9	3
1:A:89:VAL:HG12	1:A:91:VAL:CG2	0.67	2.20	14	20
1:A:14:LEU:HG	1:A:30:ILE:HG21	0.66	1.66	9	20
1:A:29:ASN:OD1	1:A:85:ARG:O	0.66	2.12	20	8
1:A:72:SER:O	1:A:73:PHE:O	0.65	2.15	6	1
1:A:18:ILE:HG22	1:A:19:ASP:OD1	0.65	1.91	10	2
1:A:67:LYS:HD2	1:A:68:ILE:N	0.65	2.06	18	4
1:A:16:PHE:CD2	1:A:82:ILE:HD11	0.65	2.26	19	9
1:A:89:VAL:CG1	1:A:91:VAL:HG22	0.65	2.21	1	20
1:A:18:ILE:HD11	1:A:95:VAL:HG12	0.65	1.68	12	4
1:A:126:VAL:HG13	1:A:133:ILE:O	0.65	1.90	16	9
1:A:69:LEU:HD11	1:A:118:PHE:CZ	0.65	2.27	20	2
1:A:65:LEU:HA	1:A:68:ILE:HG22	0.65	1.67	7	20
1:A:21:GLN:NE2	1:A:134:ILE:HD13	0.65	2.07	13	2
1:A:16:PHE:CE2	1:A:23:LEU:HG	0.65	2.27	11	9
1:A:80:SER:OG	1:A:95:VAL:HG23	0.64	1.91	19	4
1:A:128:THR:O	1:A:131:ARG:HB2	0.64	1.92	5	2
1:A:65:LEU:HD11	1:A:136:LEU:HD11	0.64	1.70	9	1
1:A:69:LEU:C	1:A:69:LEU:CD1	0.64	2.66	1	20
1:A:126:VAL:HG13	1:A:133:ILE:CB	0.64	2.23	20	7
1:A:16:PHE:CE1	1:A:18:ILE:HD11	0.64	2.27	5	3
1:A:65:LEU:HD23	1:A:65:LEU:C	0.63	2.13	7	14
1:A:141:ILE:O	1:A:145:ILE:HG13	0.63	1.93	1	19
1:A:63:VAL:O	1:A:93:PHE:HA	0.63	1.92	9	10
1:A:23:LEU:HD13	1:A:134:ILE:CB	0.63	2.24	10	11
1:A:91:VAL:HG11	1:A:145:ILE:CD1	0.63	2.24	8	20
1:A:84:ALA:O	1:A:90:GLU:HA	0.63	1.93	20	17
1:A:91:VAL:HG11	1:A:145:ILE:HD13	0.62	1.70	16	8
1:A:23:LEU:HD13	1:A:134:ILE:CG2	0.62	2.24	16	6
1:A:36:LYS:HB3	1:A:81:ILE:HD12	0.62	1.69	8	3
1:A:60:ILE:HG22	1:A:90:GLU:HB3	0.62	1.70	20	4
1:A:16:PHE:CE1	1:A:23:LEU:HB3	0.62	2.29	14	7
1:A:23:LEU:HD11	1:A:136:LEU:HD13	0.62	1.69	18	2
1:A:50:GLU:HG3	1:A:62:VAL:HG23	0.62	1.72	11	2
1:A:134:ILE:HD12	1:A:134:ILE:N	0.62	2.10	6	8
1:A:25:PHE:CE2	1:A:136:LEU:HD12	0.62	2.30	15	1
1:A:136:LEU:CD1	1:A:136:LEU:N	0.61	2.62	17	3
1:A:33:VAL:HG11	1:A:98:VAL:CG1	0.61	2.22	9	6
1:A:65:LEU:HD12	1:A:141:ILE:CG1	0.61	2.25	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:HD12	1:A:141:ILE:HG13	0.61	1.72	12	4
1:A:135:TYR:C	1:A:136:LEU:HD12	0.61	2.15	8	6
1:A:22:ALA:HB3	1:A:133:ILE:CD1	0.61	2.26	15	4
1:A:19:ASP:OD2	1:A:73:PHE:HA	0.61	1.96	8	2
1:A:25:PHE:CG	1:A:136:LEU:HD21	0.61	2.29	12	2
1:A:9:LYS:HE3	1:A:9:LYS:HA	0.61	1.71	6	1
1:A:16:PHE:CZ	1:A:23:LEU:HG	0.61	2.31	14	13
1:A:13:VAL:HG13	1:A:102:LEU:HB3	0.60	1.73	6	15
1:A:66:ALA:HB1	1:A:73:PHE:CD2	0.60	2.30	16	13
1:A:86:THR:OG1	1:A:89:VAL:HB	0.60	1.95	6	5
1:A:136:LEU:HD21	1:A:141:ILE:HG22	0.60	1.73	16	1
1:A:23:LEU:HD12	1:A:24:ALA:H	0.60	1.56	1	18
1:A:122:SER:HB2	1:A:136:LEU:HG	0.60	1.73	10	5
1:A:16:PHE:CD1	1:A:18:ILE:HD11	0.60	2.31	5	5
1:A:53:ILE:HD13	1:A:53:ILE:N	0.60	2.11	14	1
1:A:49:VAL:HG22	1:A:63:VAL:HG21	0.60	1.73	17	2
1:A:66:ALA:HB3	1:A:73:PHE:CE2	0.60	2.32	15	15
1:A:16:PHE:CD1	1:A:95:VAL:HG11	0.60	2.32	19	7
1:A:69:LEU:HD13	1:A:69:LEU:O	0.60	1.97	12	18
1:A:23:LEU:HD11	1:A:136:LEU:CD1	0.60	2.27	18	5
1:A:136:LEU:HD22	1:A:137:ASP:N	0.60	2.11	16	1
1:A:126:VAL:O	1:A:133:ILE:O	0.60	2.20	6	9
1:A:33:VAL:CG1	1:A:98:VAL:HG11	0.59	2.27	7	10
1:A:31:GLU:OE2	1:A:83:VAL:HG12	0.59	1.97	13	1
1:A:122:SER:OG	1:A:136:LEU:HD22	0.59	1.96	15	1
1:A:16:PHE:CE1	1:A:82:ILE:CD1	0.59	2.86	15	9
1:A:69:LEU:HD21	1:A:118:PHE:CZ	0.59	2.32	20	1
1:A:132:LEU:HD22	1:A:132:LEU:N	0.59	2.13	8	2
1:A:14:LEU:CD1	1:A:82:ILE:HD13	0.59	2.26	8	5
1:A:136:LEU:N	1:A:136:LEU:HD13	0.59	2.12	1	7
1:A:16:PHE:CE2	1:A:82:ILE:CD1	0.59	2.86	13	9
1:A:16:PHE:CZ	1:A:93:PHE:CE2	0.59	2.91	14	12
1:A:51:GLY:O	1:A:62:VAL:HG22	0.58	1.98	13	11
1:A:36:LYS:HE3	1:A:36:LYS:HA	0.58	1.73	8	1
1:A:132:LEU:N	1:A:132:LEU:HD12	0.58	2.13	16	2
1:A:66:ALA:HB1	1:A:71:ILE:CD1	0.58	2.24	17	6
1:A:13:VAL:HG22	1:A:24:ALA:HB1	0.58	1.76	9	11
1:A:16:PHE:HZ	1:A:25:PHE:CE1	0.58	2.17	9	8
1:A:25:PHE:CZ	1:A:93:PHE:CD2	0.58	2.91	12	3
1:A:132:LEU:HD12	1:A:132:LEU:N	0.58	2.13	17	7
1:A:23:LEU:HD13	1:A:134:ILE:HG22	0.58	1.76	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:ARG:HG2	1:A:103:ARG:O	0.58	1.99	9	4
1:A:67:LYS:HD3	1:A:68:ILE:N	0.58	2.14	5	1
1:A:15:SER:HB3	1:A:102:LEU:CD2	0.57	2.29	3	15
1:A:65:LEU:HB3	1:A:93:PHE:CG	0.57	2.34	14	15
1:A:26:ASP:OD2	1:A:28:ASP:HB2	0.57	1.99	16	3
1:A:90:GLU:N	1:A:90:GLU:OE1	0.57	2.37	14	3
1:A:121:LYS:O	1:A:122:SER:HB3	0.57	1.99	19	1
1:A:91:VAL:CG1	1:A:145:ILE:HD13	0.57	2.28	16	20
1:A:99:LEU:CD2	1:A:99:LEU:N	0.57	2.68	1	20
1:A:86:THR:HG21	1:A:138:ILE:HG12	0.57	1.75	11	3
1:A:14:LEU:O	1:A:24:ALA:HA	0.57	2.00	4	10
1:A:23:LEU:CD2	1:A:71:ILE:HD13	0.57	2.29	16	7
1:A:122:SER:HA	1:A:136:LEU:HD23	0.57	1.77	16	1
1:A:15:SER:HA	1:A:23:LEU:O	0.57	2.00	4	1
1:A:138:ILE:HG13	1:A:141:ILE:HD12	0.57	1.75	17	4
1:A:144:GLU:O	1:A:148:LYS:HB2	0.57	1.99	7	3
1:A:63:VAL:HG12	1:A:64:ASN:N	0.57	2.13	1	19
1:A:14:LEU:HD21	1:A:33:VAL:CG1	0.57	2.30	14	1
1:A:16:PHE:CE1	1:A:23:LEU:HG	0.57	2.35	18	6
1:A:136:LEU:N	1:A:136:LEU:CD1	0.57	2.68	5	3
1:A:25:PHE:CD2	1:A:136:LEU:CD2	0.57	2.87	5	4
1:A:65:LEU:HD12	1:A:141:ILE:HD12	0.57	1.75	9	1
1:A:94:LEU:HD23	1:A:95:VAL:N	0.56	2.15	1	1
1:A:11:PHE:HB3	1:A:104:ILE:O	0.56	1.99	4	12
1:A:49:VAL:HG13	1:A:62:VAL:O	0.56	2.00	6	8
1:A:33:VAL:HG21	1:A:98:VAL:CG1	0.56	2.30	15	1
1:A:11:PHE:CE2	1:A:13:VAL:HB	0.56	2.36	14	14
1:A:66:ALA:HB2	1:A:93:PHE:CE1	0.56	2.36	15	4
1:A:18:ILE:HG22	1:A:18:ILE:O	0.56	2.00	4	1
1:A:67:LYS:N	1:A:73:PHE:HE2	0.56	1.98	6	5
1:A:23:LEU:HD11	1:A:136:LEU:HD11	0.56	1.75	12	1
1:A:49:VAL:CG2	1:A:63:VAL:HG22	0.56	2.25	12	1
1:A:122:SER:HB2	1:A:136:LEU:CB	0.55	2.31	2	3
1:A:69:LEU:CD2	1:A:118:PHE:CE2	0.55	2.90	9	5
1:A:78:MET:SD	1:A:95:VAL:HA	0.55	2.41	10	6
1:A:16:PHE:HD1	1:A:98:VAL:HG23	0.55	1.60	4	4
1:A:60:ILE:HD12	1:A:60:ILE:C	0.55	2.21	13	14
1:A:68:ILE:HD11	1:A:144:GLU:HB2	0.55	1.77	10	13
1:A:147:VAL:HG22	1:A:147:VAL:O	0.55	2.00	3	15
1:A:64:ASN:O	1:A:67:LYS:HD3	0.55	2.01	5	1
1:A:17:GLU:HG2	1:A:99:LEU:HD21	0.55	1.79	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:HB3	1:A:93:PHE:CD1	0.55	2.37	11	15
1:A:69:LEU:HD12	1:A:71:ILE:HG23	0.55	1.79	9	2
1:A:25:PHE:CZ	1:A:65:LEU:HD11	0.55	2.36	10	1
1:A:13:VAL:HG11	1:A:104:ILE:HB	0.55	1.78	3	18
1:A:21:GLN:OE1	1:A:21:GLN:C	0.55	2.45	6	2
1:A:25:PHE:HZ	1:A:65:LEU:HD21	0.55	1.62	10	2
1:A:19:ASP:O	1:A:20:GLU:CB	0.54	2.56	10	12
1:A:33:VAL:HG21	1:A:98:VAL:HG11	0.54	1.78	15	1
1:A:136:LEU:HD22	1:A:138:ILE:H	0.54	1.62	5	5
1:A:85:ARG:O	1:A:86:THR:CG2	0.54	2.53	6	7
1:A:53:ILE:HD12	1:A:53:ILE:C	0.54	2.22	13	2
1:A:16:PHE:CE2	1:A:23:LEU:HB3	0.54	2.38	4	4
1:A:13:VAL:HG23	1:A:25:PHE:O	0.54	2.02	5	19
1:A:19:ASP:O	1:A:20:GLU:HB2	0.54	2.03	10	20
1:A:122:SER:HB2	1:A:136:LEU:HB3	0.54	1.78	14	4
1:A:13:VAL:HG11	1:A:104:ILE:HG12	0.54	1.79	17	2
1:A:65:LEU:O	1:A:68:ILE:CG2	0.54	2.53	17	7
1:A:67:LYS:HE3	1:A:68:ILE:N	0.54	2.17	19	4
1:A:142:ILE:HA	1:A:145:ILE:HD12	0.54	1.78	16	6
1:A:70:GLY:O	1:A:71:ILE:O	0.54	2.26	12	17
1:A:69:LEU:HD13	1:A:70:GLY:O	0.54	2.03	3	3
1:A:53:ILE:CD1	1:A:60:ILE:HD11	0.54	2.28	5	2
1:A:137:ASP:O	1:A:141:ILE:HG22	0.54	2.03	12	1
1:A:35:GLU:OE1	1:A:35:GLU:N	0.54	2.41	14	2
1:A:15:SER:HB2	1:A:24:ALA:HB2	0.54	1.79	18	1
1:A:102:LEU:CD2	1:A:104:ILE:HG12	0.53	2.33	11	17
1:A:25:PHE:CD1	1:A:25:PHE:N	0.53	2.76	5	4
1:A:77:LYS:N	1:A:77:LYS:HD2	0.53	2.18	13	1
1:A:50:GLU:OE1	1:A:94:LEU:HD22	0.53	2.04	20	1
1:A:25:PHE:CE1	1:A:136:LEU:HD21	0.53	2.38	12	1
1:A:21:GLN:NE2	1:A:71:ILE:HG22	0.53	2.18	14	1
1:A:121:LYS:O	1:A:140:LYS:HB2	0.53	2.04	9	1
1:A:13:VAL:CG2	1:A:14:LEU:N	0.53	2.71	9	20
1:A:25:PHE:CZ	1:A:136:LEU:HD13	0.53	2.38	20	2
1:A:65:LEU:O	1:A:65:LEU:HD23	0.53	2.03	17	2
1:A:132:LEU:C	1:A:132:LEU:HD22	0.53	2.24	20	1
1:A:138:ILE:O	1:A:138:ILE:HG12	0.53	2.04	14	8
1:A:16:PHE:CE2	1:A:93:PHE:CE2	0.53	2.97	4	6
1:A:86:THR:O	1:A:89:VAL:HB	0.53	2.04	16	12
1:A:16:PHE:CD1	1:A:16:PHE:N	0.53	2.77	11	6
1:A:93:PHE:CD1	1:A:94:LEU:N	0.53	2.77	17	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:PHE:CZ	1:A:95:VAL:CG1	0.53	2.92	10	5
1:A:67:LYS:N	1:A:73:PHE:CE2	0.53	2.77	6	13
1:A:134:ILE:N	1:A:134:ILE:HD12	0.53	2.19	14	3
1:A:16:PHE:CD2	1:A:82:ILE:CD1	0.52	2.91	17	6
1:A:25:PHE:CB	1:A:30:ILE:HD11	0.52	2.34	6	3
1:A:34:ILE:HD13	1:A:83:VAL:CG2	0.52	2.34	18	5
1:A:65:LEU:HD11	1:A:136:LEU:HD13	0.52	1.81	9	1
1:A:70:GLY:O	1:A:71:ILE:HG23	0.52	2.03	3	2
1:A:65:LEU:CD1	1:A:141:ILE:HD11	0.52	2.35	15	4
1:A:78:MET:HE3	1:A:95:VAL:HA	0.52	1.82	11	5
1:A:70:GLY:C	1:A:71:ILE:HG12	0.52	2.25	6	5
1:A:65:LEU:CA	1:A:68:ILE:HG22	0.52	2.35	16	12
1:A:29:ASN:ND2	1:A:86:THR:HG22	0.52	2.17	16	4
1:A:49:VAL:CA	1:A:63:VAL:HG22	0.52	2.30	17	4
1:A:65:LEU:HD11	1:A:141:ILE:CD1	0.52	2.35	11	8
1:A:104:ILE:CG2	1:A:105:THR:N	0.52	2.73	17	6
1:A:132:LEU:HD13	1:A:132:LEU:C	0.52	2.25	18	1
1:A:16:PHE:HB3	1:A:98:VAL:HA	0.52	1.82	7	20
1:A:126:VAL:CG2	1:A:127:LYS:N	0.52	2.73	8	16
1:A:136:LEU:HD23	1:A:141:ILE:CG2	0.52	2.34	4	4
1:A:13:VAL:HG21	1:A:135:TYR:CE1	0.52	2.40	16	4
1:A:9:LYS:O	1:A:105:THR:HG22	0.51	2.05	5	6
1:A:22:ALA:O	1:A:133:ILE:CG2	0.51	2.57	4	1
1:A:25:PHE:CD2	1:A:136:LEU:HD11	0.51	2.40	5	1
1:A:69:LEU:HD13	1:A:70:GLY:N	0.51	2.20	19	3
1:A:73:PHE:CD1	1:A:78:MET:HE2	0.51	2.40	9	4
1:A:20:GLU:N	1:A:20:GLU:OE1	0.51	2.42	12	1
1:A:73:PHE:CD1	1:A:78:MET:CE	0.51	2.93	9	10
1:A:126:VAL:CG1	1:A:133:ILE:O	0.51	2.58	16	5
1:A:126:VAL:HG13	1:A:133:ILE:C	0.51	2.26	12	3
1:A:10:GLU:HG2	1:A:105:THR:HG22	0.51	1.82	4	9
1:A:13:VAL:CA	1:A:27:VAL:HG13	0.51	2.32	15	10
1:A:16:PHE:CD2	1:A:18:ILE:HD11	0.51	2.41	3	2
1:A:66:ALA:HB1	1:A:73:PHE:CG	0.51	2.41	7	4
1:A:14:LEU:C	1:A:14:LEU:HD13	0.51	2.25	18	10
1:A:23:LEU:HD12	1:A:134:ILE:O	0.51	2.05	8	5
1:A:49:VAL:CG1	1:A:52:VAL:CG1	0.51	2.88	10	2
1:A:13:VAL:HG11	1:A:104:ILE:CB	0.51	2.36	13	18
1:A:70:GLY:O	1:A:71:ILE:HG13	0.51	2.05	12	12
1:A:93:PHE:CE2	1:A:95:VAL:CG1	0.51	2.94	17	4
1:A:70:GLY:O	1:A:71:ILE:CG1	0.50	2.59	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HG13	1:A:23:LEU:HB2	0.50	1.82	4	1
1:A:31:GLU:O	1:A:32:MET:HG3	0.50	2.06	6	3
1:A:128:THR:O	1:A:131:ARG:HG2	0.50	2.06	18	9
1:A:142:ILE:HG23	1:A:143:GLU:N	0.50	2.21	8	20
1:A:25:PHE:CZ	1:A:93:PHE:CE2	0.50	2.99	12	1
1:A:64:ASN:O	1:A:67:LYS:CD	0.50	2.60	5	1
1:A:121:LYS:O	1:A:121:LYS:HG3	0.50	2.07	1	2
1:A:142:ILE:HD12	1:A:145:ILE:HD12	0.50	1.84	17	10
1:A:34:ILE:HG13	1:A:81:ILE:HB	0.50	1.82	4	3
1:A:16:PHE:CD1	1:A:82:ILE:CD1	0.50	2.95	6	2
1:A:26:ASP:OD2	1:A:28:ASP:HB3	0.50	2.07	10	1
1:A:23:LEU:CD1	1:A:134:ILE:HG22	0.50	2.36	16	1
1:A:136:LEU:HD13	1:A:138:ILE:H	0.50	1.67	16	1
1:A:143:GLU:O	1:A:147:VAL:HG23	0.50	2.07	14	2
1:A:13:VAL:CG1	1:A:104:ILE:HB	0.50	2.36	4	7
1:A:16:PHE:CZ	1:A:25:PHE:HE1	0.50	2.25	5	1
1:A:144:GLU:O	1:A:148:LYS:HG2	0.50	2.07	19	2
1:A:73:PHE:CE1	1:A:78:MET:CE	0.49	2.94	15	3
1:A:13:VAL:HA	1:A:27:VAL:CG1	0.49	2.37	9	3
1:A:24:ALA:HB2	1:A:102:LEU:CD2	0.49	2.37	19	6
1:A:36:LYS:CB	1:A:81:ILE:HD12	0.49	2.32	3	2
1:A:16:PHE:CE1	1:A:23:LEU:CB	0.49	2.95	14	1
1:A:16:PHE:CZ	1:A:25:PHE:CE1	0.49	3.01	5	5
1:A:87:LYS:O	1:A:88:ASP:CG	0.49	2.50	4	2
1:A:66:ALA:O	1:A:70:GLY:N	0.49	2.45	13	12
1:A:87:LYS:O	1:A:87:LYS:CE	0.49	2.61	2	1
1:A:25:PHE:CD2	1:A:136:LEU:HD22	0.49	2.43	9	1
1:A:14:LEU:N	1:A:27:VAL:HG13	0.49	2.22	12	2
1:A:67:LYS:HD3	1:A:68:ILE:H	0.49	1.66	5	1
1:A:134:ILE:N	1:A:134:ILE:CD1	0.49	2.76	13	9
1:A:11:PHE:CE2	1:A:135:TYR:OH	0.49	2.60	10	11
1:A:122:SER:HB2	1:A:136:LEU:HB2	0.49	1.83	12	3
1:A:126:VAL:CG1	1:A:135:TYR:HB2	0.49	2.38	2	2
1:A:29:ASN:CG	1:A:85:ARG:O	0.49	2.51	5	1
1:A:23:LEU:HA	1:A:134:ILE:O	0.49	2.08	9	1
1:A:65:LEU:HA	1:A:68:ILE:CG2	0.49	2.37	12	9
1:A:103:ARG:HD2	1:A:103:ARG:H	0.49	1.67	15	2
1:A:69:LEU:HD11	1:A:118:PHE:CE2	0.49	2.43	5	2
1:A:21:GLN:NE2	1:A:134:ILE:CD1	0.49	2.74	13	4
1:A:22:ALA:HB3	1:A:133:ILE:HA	0.49	1.83	9	1
1:A:104:ILE:HG22	1:A:105:THR:N	0.49	2.23	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:VAL:O	1:A:53:ILE:HG23	0.48	2.08	6	9
1:A:131:ARG:HD2	1:A:133:ILE:CG1	0.48	2.38	11	1
1:A:87:LYS:CE	1:A:87:LYS:O	0.48	2.61	14	1
1:A:36:LYS:HD2	1:A:94:LEU:HD11	0.48	1.84	11	1
1:A:102:LEU:HG	1:A:104:ILE:HG12	0.48	1.85	2	14
1:A:93:PHE:CE1	1:A:94:LEU:O	0.48	2.66	9	16
1:A:104:ILE:HG22	1:A:105:THR:O	0.48	2.09	8	4
1:A:64:ASN:CB	1:A:67:LYS:HG3	0.48	2.38	5	3
1:A:25:PHE:CE1	1:A:136:LEU:HD13	0.48	2.43	10	2
1:A:18:ILE:HG23	1:A:73:PHE:HB2	0.48	1.85	14	3
1:A:15:SER:HB2	1:A:102:LEU:CD2	0.48	2.36	16	3
1:A:69:LEU:CD2	1:A:118:PHE:CE1	0.48	2.97	13	4
1:A:74:ASP:O	1:A:75:GLU:CB	0.48	2.62	3	4
1:A:67:LYS:HE2	1:A:68:ILE:N	0.48	2.24	7	3
1:A:93:PHE:HD1	1:A:94:LEU:N	0.48	2.06	19	6
1:A:73:PHE:CD1	1:A:74:ASP:N	0.48	2.82	8	4
1:A:30:ILE:HD13	1:A:84:ALA:HB2	0.48	1.85	5	2
1:A:25:PHE:HB2	1:A:30:ILE:HD11	0.48	1.86	6	1
1:A:15:SER:OG	1:A:102:LEU:HB2	0.48	2.09	10	3
1:A:34:ILE:O	1:A:81:ILE:HB	0.48	2.09	16	3
1:A:136:LEU:CD2	1:A:138:ILE:H	0.48	2.22	14	4
1:A:74:ASP:O	1:A:74:ASP:OD1	0.48	2.32	7	5
1:A:94:LEU:HD23	1:A:94:LEU:C	0.48	2.29	1	1
1:A:66:ALA:HB2	1:A:93:PHE:CZ	0.48	2.44	10	6
1:A:65:LEU:C	1:A:65:LEU:CD2	0.48	2.82	7	15
1:A:75:GLU:OE1	1:A:76:GLN:N	0.48	2.47	3	1
1:A:16:PHE:CZ	1:A:95:VAL:HG11	0.47	2.44	1	3
1:A:16:PHE:HA	1:A:99:LEU:HD23	0.47	1.84	4	3
1:A:144:GLU:HA	1:A:147:VAL:HG12	0.47	1.85	13	5
1:A:136:LEU:CD2	1:A:141:ILE:HG21	0.47	2.37	14	3
1:A:136:LEU:HD13	1:A:141:ILE:HG21	0.47	1.86	7	1
1:A:136:LEU:HD21	1:A:141:ILE:CG2	0.47	2.39	16	1
1:A:65:LEU:C	1:A:68:ILE:HG22	0.47	2.29	10	3
1:A:33:VAL:CB	1:A:98:VAL:HG11	0.47	2.39	7	2
1:A:13:VAL:CG1	1:A:104:ILE:CG1	0.47	2.87	10	5
1:A:25:PHE:CE2	1:A:136:LEU:HD11	0.47	2.44	5	2
1:A:16:PHE:CD2	1:A:23:LEU:HB3	0.47	2.44	4	1
1:A:122:SER:OG	1:A:136:LEU:HG	0.47	2.09	19	1
1:A:25:PHE:CZ	1:A:136:LEU:HD11	0.47	2.44	2	1
1:A:14:LEU:HD11	1:A:82:ILE:CD1	0.47	2.35	5	3
1:A:18:ILE:O	1:A:21:GLN:HG3	0.47	2.09	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:PHE:CZ	1:A:65:LEU:HD21	0.47	2.44	15	2
1:A:52:VAL:O	1:A:53:ILE:CG2	0.47	2.62	13	12
1:A:69:LEU:HD21	1:A:118:PHE:CD2	0.47	2.45	3	4
1:A:82:ILE:HG22	1:A:83:VAL:N	0.47	2.25	5	4
1:A:22:ALA:CB	1:A:133:ILE:HG12	0.47	2.36	9	2
1:A:148:LYS:HA	1:A:148:LYS:HE2	0.47	1.84	11	1
1:A:66:ALA:CA	1:A:71:ILE:HD11	0.47	2.40	5	4
1:A:12:GLU:OE2	1:A:101:VAL:HG12	0.47	2.10	7	1
1:A:16:PHE:HD2	1:A:98:VAL:HG23	0.47	1.69	18	3
1:A:23:LEU:CD1	1:A:25:PHE:CE1	0.47	2.98	4	1
1:A:16:PHE:CD1	1:A:98:VAL:HG23	0.47	2.43	4	3
1:A:21:GLN:OE1	1:A:134:ILE:HD11	0.46	2.10	2	1
1:A:136:LEU:CD1	1:A:138:ILE:H	0.46	2.23	16	1
1:A:13:VAL:HA	1:A:27:VAL:HG12	0.46	1.87	6	2
1:A:33:VAL:HG11	1:A:98:VAL:HG21	0.46	1.87	7	3
1:A:132:LEU:N	1:A:132:LEU:CD1	0.46	2.78	17	9
1:A:136:LEU:HD22	1:A:136:LEU:C	0.46	2.31	1	1
1:A:145:ILE:O	1:A:148:LYS:HD2	0.46	2.10	3	1
1:A:13:VAL:HG21	1:A:24:ALA:HB1	0.46	1.86	1	1
1:A:69:LEU:CD2	1:A:118:PHE:CZ	0.46	2.99	12	7
1:A:81:ILE:HG22	1:A:82:ILE:N	0.46	2.26	7	4
1:A:65:LEU:HD12	1:A:141:ILE:HG21	0.46	1.87	16	1
1:A:137:ASP:O	1:A:137:ASP:OD1	0.46	2.34	1	4
1:A:140:LYS:N	1:A:140:LYS:HD2	0.46	2.26	11	5
1:A:13:VAL:HG22	1:A:14:LEU:N	0.46	2.25	17	10
1:A:77:LYS:HB3	1:A:77:LYS:NZ	0.46	2.25	7	1
1:A:21:GLN:OE1	1:A:22:ALA:O	0.46	2.34	11	3
1:A:33:VAL:O	1:A:34:ILE:HG23	0.46	2.10	19	2
1:A:63:VAL:CG1	1:A:64:ASN:N	0.46	2.79	13	17
1:A:29:ASN:ND2	1:A:85:ARG:O	0.46	2.49	6	3
1:A:9:LYS:NZ	1:A:105:THR:HG21	0.46	2.26	11	1
1:A:53:ILE:CD1	1:A:62:VAL:HG13	0.45	2.40	14	1
1:A:77:LYS:O	1:A:78:MET:C	0.45	2.54	16	5
1:A:23:LEU:CD1	1:A:134:ILE:O	0.45	2.64	19	6
1:A:9:LYS:HE3	1:A:10:GLU:CB	0.45	2.42	15	1
1:A:68:ILE:HD13	1:A:141:ILE:HA	0.45	1.88	16	1
1:A:99:LEU:N	1:A:99:LEU:HD22	0.45	2.26	4	5
1:A:13:VAL:O	1:A:102:LEU:N	0.45	2.50	19	11
1:A:19:ASP:HB2	1:A:72:SER:CB	0.45	2.40	14	2
1:A:25:PHE:CE2	1:A:65:LEU:CD1	0.45	3.00	8	6
1:A:29:ASN:ND2	1:A:84:ALA:HB1	0.45	2.26	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ILE:CG2	1:A:90:GLU:HB2	0.45	2.42	12	5
1:A:34:ILE:CD1	1:A:83:VAL:CG2	0.45	2.94	18	5
1:A:128:THR:CG2	1:A:129:ASP:N	0.45	2.79	20	3
1:A:18:ILE:HG13	1:A:23:LEU:CB	0.45	2.42	18	2
1:A:18:ILE:HB	1:A:21:GLN:NE2	0.45	2.26	12	1
1:A:68:ILE:HD11	1:A:144:GLU:CB	0.45	2.41	3	2
1:A:127:LYS:N	1:A:127:LYS:HD3	0.45	2.27	3	2
1:A:71:ILE:O	1:A:72:SER:O	0.45	2.35	6	1
1:A:49:VAL:HG21	1:A:61:PRO:HB2	0.45	1.87	7	1
1:A:140:LYS:HA	1:A:140:LYS:HE2	0.45	1.88	17	1
1:A:108:GLN:OE1	1:A:108:GLN:N	0.45	2.50	18	1
1:A:14:LEU:HD13	1:A:15:SER:N	0.45	2.27	6	2
1:A:67:LYS:C	1:A:67:LYS:HD2	0.45	2.32	9	5
1:A:16:PHE:CE1	1:A:82:ILE:HD11	0.45	2.47	10	3
1:A:126:VAL:HG22	1:A:127:LYS:N	0.45	2.27	20	7
1:A:77:LYS:O	1:A:96:ASP:OD1	0.45	2.35	8	3
1:A:25:PHE:CD1	1:A:136:LEU:HD11	0.45	2.47	1	2
1:A:141:ILE:HD11	1:A:145:ILE:HD11	0.45	1.88	5	1
1:A:19:ASP:CG	1:A:72:SER:HB3	0.45	2.31	11	1
1:A:120:LYS:O	1:A:120:LYS:CD	0.45	2.65	14	1
1:A:9:LYS:HG2	1:A:10:GLU:HG3	0.45	1.86	4	1
1:A:10:GLU:HG3	1:A:105:THR:HG22	0.45	1.89	1	1
1:A:11:PHE:CE1	1:A:12:GLU:O	0.45	2.70	7	11
1:A:65:LEU:CD1	1:A:141:ILE:HG13	0.45	2.41	12	2
1:A:24:ALA:O	1:A:135:TYR:HA	0.44	2.12	13	2
1:A:21:GLN:CD	1:A:134:ILE:HD13	0.44	2.31	6	1
1:A:119:GLY:O	1:A:120:LYS:CG	0.44	2.65	18	2
1:A:29:ASN:ND2	1:A:138:ILE:CG2	0.44	2.80	5	2
1:A:35:GLU:O	1:A:36:LYS:CG	0.44	2.65	20	3
1:A:64:ASN:HB3	1:A:67:LYS:HG3	0.44	1.88	5	1
1:A:12:GLU:O	1:A:27:VAL:HG12	0.44	2.11	9	1
1:A:135:TYR:C	1:A:136:LEU:HD23	0.44	2.32	15	1
1:A:19:ASP:HB2	1:A:72:SER:HB2	0.44	1.87	7	5
1:A:78:MET:CE	1:A:95:VAL:HA	0.44	2.43	4	3
1:A:85:ARG:O	1:A:85:ARG:HD3	0.44	2.11	7	1
1:A:15:SER:O	1:A:99:LEU:N	0.44	2.51	9	2
1:A:138:ILE:HG13	1:A:141:ILE:CD1	0.44	2.42	17	2
1:A:148:LYS:HE2	1:A:148:LYS:HA	0.44	1.89	16	1
1:A:11:PHE:CZ	1:A:135:TYR:OH	0.44	2.70	3	2
1:A:65:LEU:CD1	1:A:141:ILE:CD1	0.44	2.95	5	7
1:A:102:LEU:HD21	1:A:104:ILE:HD11	0.44	1.90	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:PHE:CD2	1:A:95:VAL:CG1	0.44	2.98	7	2
1:A:137:ASP:O	1:A:139:ASP:N	0.44	2.50	15	9
1:A:15:SER:CA	1:A:23:LEU:O	0.44	2.66	4	1
1:A:69:LEU:CD1	1:A:118:PHE:CZ	0.44	3.00	20	2
1:A:23:LEU:HD22	1:A:71:ILE:HD13	0.44	1.88	16	1
1:A:70:GLY:C	1:A:71:ILE:CG1	0.44	2.86	15	15
1:A:18:ILE:O	1:A:21:GLN:O	0.44	2.36	15	2
1:A:60:ILE:HG21	1:A:90:GLU:OE2	0.44	2.13	15	1
1:A:93:PHE:CD1	1:A:93:PHE:C	0.44	2.89	8	8
1:A:49:VAL:HG12	1:A:51:GLY:O	0.44	2.12	7	1
1:A:25:PHE:CZ	1:A:65:LEU:HD22	0.44	2.47	12	1
1:A:132:LEU:HD23	1:A:132:LEU:C	0.43	2.33	2	1
1:A:49:VAL:CG1	1:A:51:GLY:O	0.43	2.66	5	4
1:A:74:ASP:O	1:A:75:GLU:OE2	0.43	2.36	9	1
1:A:122:SER:HB2	1:A:136:LEU:CD2	0.43	2.43	7	1
1:A:93:PHE:CZ	1:A:95:VAL:HG12	0.43	2.47	17	1
1:A:19:ASP:OD2	1:A:76:GLN:NE2	0.43	2.51	2	2
1:A:10:GLU:HA	1:A:105:THR:HA	0.43	1.90	6	2
1:A:132:LEU:N	1:A:132:LEU:CD2	0.43	2.81	8	2
1:A:77:LYS:O	1:A:78:MET:O	0.43	2.36	16	1
1:A:68:ILE:HG23	1:A:69:LEU:N	0.43	2.28	3	13
1:A:119:GLY:O	1:A:120:LYS:HB2	0.43	2.14	10	2
1:A:35:GLU:HG2	1:A:35:GLU:O	0.43	2.13	14	1
1:A:19:ASP:CG	1:A:72:SER:HB2	0.43	2.33	15	1
1:A:87:LYS:O	1:A:88:ASP:OD1	0.43	2.37	16	1
1:A:77:LYS:O	1:A:79:LYS:HG3	0.43	2.14	4	1
1:A:78:MET:HA	1:A:96:ASP:HB2	0.43	1.90	4	1
1:A:76:GLN:C	1:A:77:LYS:HD2	0.43	2.33	11	1
1:A:22:ALA:O	1:A:134:ILE:HG12	0.43	2.14	20	2
1:A:16:PHE:CB	1:A:98:VAL:HA	0.43	2.42	14	5
1:A:18:ILE:O	1:A:21:GLN:HG2	0.43	2.13	2	1
1:A:78:MET:N	1:A:78:MET:SD	0.43	2.92	6	1
1:A:25:PHE:CG	1:A:136:LEU:CD2	0.43	3.01	12	1
1:A:15:SER:O	1:A:98:VAL:HG23	0.43	2.13	14	1
1:A:16:PHE:HZ	1:A:93:PHE:CE2	0.43	2.29	14	2
1:A:81:ILE:HG12	1:A:94:LEU:HD13	0.43	1.91	4	1
1:A:127:LYS:HA	1:A:131:ARG:O	0.43	2.12	5	1
1:A:82:ILE:O	1:A:92:GLY:HA2	0.43	2.14	9	1
1:A:129:ASP:OD1	1:A:129:ASP:O	0.43	2.37	16	1
1:A:34:ILE:CD1	1:A:83:VAL:HG23	0.43	2.43	18	1
1:A:148:LYS:HA	1:A:148:LYS:HE3	0.43	1.89	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:PHE:CE1	1:A:18:ILE:CD1	0.43	3.02	5	1
1:A:67:LYS:CD	1:A:68:ILE:N	0.43	2.82	5	1
1:A:25:PHE:HZ	1:A:65:LEU:HD22	0.43	1.74	6	2
1:A:93:PHE:C	1:A:93:PHE:CD1	0.43	2.92	19	1
1:A:107:ASN:N	1:A:108:GLN:OE1	0.42	2.49	18	1
1:A:127:LYS:NZ	1:A:127:LYS:HB3	0.42	2.30	1	1
1:A:106:GLU:OE1	1:A:135:TYR:CE2	0.42	2.72	5	1
1:A:19:ASP:OD2	1:A:73:PHE:N	0.42	2.51	15	1
1:A:103:ARG:O	1:A:103:ARG:CG	0.42	2.67	19	1
1:A:68:ILE:CG2	1:A:69:LEU:N	0.42	2.82	1	8
1:A:142:ILE:O	1:A:145:ILE:HB	0.42	2.13	3	2
1:A:104:ILE:HD11	1:A:133:ILE:HG21	0.42	1.91	4	1
1:A:61:PRO:CD	1:A:90:GLU:O	0.42	2.68	5	2
1:A:9:LYS:HD2	1:A:9:LYS:C	0.42	2.35	19	2
1:A:28:ASP:OD1	1:A:29:ASN:N	0.42	2.52	14	2
1:A:104:ILE:CD1	1:A:126:VAL:HG21	0.42	2.44	14	2
1:A:25:PHE:HE2	1:A:65:LEU:HD11	0.42	1.74	20	1
1:A:98:VAL:HG13	1:A:98:VAL:O	0.42	2.14	11	6
1:A:91:VAL:CG1	1:A:145:ILE:CD1	0.42	2.98	6	4
1:A:69:LEU:HA	1:A:121:LYS:HE2	0.42	1.90	7	1
1:A:67:LYS:C	1:A:67:LYS:CD	0.42	2.88	9	1
1:A:16:PHE:CE1	1:A:82:ILE:HD12	0.42	2.49	2	1
1:A:19:ASP:OD1	1:A:77:LYS:CG	0.42	2.67	8	1
1:A:36:LYS:HB2	1:A:36:LYS:NZ	0.42	2.29	19	1
1:A:102:LEU:CD2	1:A:104:ILE:CG1	0.42	2.97	1	4
1:A:66:ALA:C	1:A:73:PHE:CD2	0.42	2.93	20	6
1:A:97:ARG:NH1	1:A:99:LEU:HD22	0.42	2.29	2	1
1:A:66:ALA:N	1:A:93:PHE:CE1	0.42	2.88	14	3
1:A:145:ILE:O	1:A:148:LYS:CD	0.42	2.68	13	1
1:A:136:LEU:HD11	1:A:141:ILE:HG21	0.42	1.92	16	1
1:A:34:ILE:HD11	1:A:81:ILE:HG22	0.42	1.92	18	1
1:A:122:SER:HB3	1:A:136:LEU:HD12	0.42	1.90	9	1
1:A:19:ASP:OD2	1:A:72:SER:CB	0.42	2.67	18	2
1:A:83:VAL:HG12	1:A:84:ALA:N	0.42	2.30	2	1
1:A:138:ILE:CA	1:A:141:ILE:HG23	0.42	2.36	10	3
1:A:31:GLU:O	1:A:32:MET:CE	0.42	2.68	19	5
1:A:126:VAL:HG12	1:A:135:TYR:N	0.42	2.30	11	1
1:A:73:PHE:CE1	1:A:78:MET:SD	0.42	3.13	14	1
1:A:16:PHE:CZ	1:A:93:PHE:HE2	0.42	2.33	16	1
1:A:15:SER:O	1:A:98:VAL:CG2	0.42	2.68	8	3
1:A:14:LEU:HD13	1:A:14:LEU:C	0.42	2.35	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:N	1:A:53:ILE:CD1	0.42	2.81	14	1
1:A:18:ILE:CG1	1:A:23:LEU:HB3	0.42	2.45	18	1
1:A:106:GLU:HG2	1:A:106:GLU:O	0.42	2.15	18	1
1:A:21:GLN:HE21	1:A:134:ILE:HD11	0.42	1.74	20	1
1:A:49:VAL:CG1	1:A:52:VAL:HG12	0.41	2.45	3	1
1:A:122:SER:CB	1:A:136:LEU:HG	0.41	2.45	13	1
1:A:71:ILE:CG2	1:A:134:ILE:HG12	0.41	2.45	2	1
1:A:25:PHE:CE2	1:A:136:LEU:HB2	0.41	2.50	10	1
1:A:104:ILE:HD12	1:A:126:VAL:CG2	0.41	2.38	11	2
1:A:69:LEU:HD22	1:A:118:PHE:CZ	0.41	2.49	2	1
1:A:79:LYS:HG3	1:A:96:ASP:O	0.41	2.16	2	1
1:A:74:ASP:O	1:A:75:GLU:HB3	0.41	2.15	3	2
1:A:16:PHE:CB	1:A:97:ARG:O	0.41	2.68	4	1
1:A:49:VAL:HG11	1:A:52:VAL:HG12	0.41	1.91	5	1
1:A:67:LYS:C	1:A:67:LYS:HE3	0.41	2.36	5	1
1:A:21:GLN:OE1	1:A:21:GLN:O	0.41	2.38	6	2
1:A:73:PHE:CE1	1:A:78:MET:HG3	0.41	2.50	17	2
1:A:79:LYS:HB2	1:A:79:LYS:NZ	0.41	2.30	10	2
1:A:128:THR:HG22	1:A:129:ASP:OD1	0.41	2.15	8	2
1:A:53:ILE:HG12	1:A:60:ILE:HD11	0.41	1.92	8	2
1:A:11:PHE:N	1:A:104:ILE:O	0.41	2.53	16	3
1:A:16:PHE:CE1	1:A:93:PHE:CE2	0.41	3.09	20	1
1:A:121:LYS:NZ	1:A:121:LYS:HB2	0.41	2.30	20	1
1:A:87:LYS:O	1:A:88:ASP:HB2	0.41	2.15	6	2
1:A:19:ASP:OD2	1:A:73:PHE:CA	0.41	2.69	6	1
1:A:140:LYS:N	1:A:140:LYS:CD	0.41	2.84	20	2
1:A:50:GLU:OE1	1:A:51:GLY:N	0.41	2.54	5	1
1:A:25:PHE:CE2	1:A:136:LEU:CB	0.41	3.03	10	1
1:A:16:PHE:CE1	1:A:95:VAL:CG1	0.41	3.02	19	1
1:A:11:PHE:CZ	1:A:26:ASP:OD1	0.41	2.73	20	1
1:A:64:ASN:O	1:A:67:LYS:HB3	0.41	2.16	4	1
1:A:16:PHE:CD1	1:A:18:ILE:CD1	0.41	3.04	5	1
1:A:78:MET:O	1:A:79:LYS:CG	0.41	2.68	6	2
1:A:87:LYS:HA	1:A:87:LYS:CE	0.41	2.45	6	1
1:A:34:ILE:HD12	1:A:53:ILE:CD1	0.41	2.46	9	1
1:A:77:LYS:HE3	1:A:77:LYS:N	0.41	2.31	14	1
1:A:137:ASP:OD1	1:A:139:ASP:CB	0.41	2.69	14	1
1:A:13:VAL:CG1	1:A:104:ILE:HG12	0.41	2.46	17	1
1:A:51:GLY:CA	1:A:62:VAL:CG2	0.41	2.98	5	1
1:A:86:THR:CG2	1:A:138:ILE:HD13	0.41	2.46	5	1
1:A:26:ASP:HB3	1:A:135:TYR:OH	0.41	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:GLU:O	1:A:147:VAL:CG2	0.41	2.68	14	1
1:A:75:GLU:HA	1:A:78:MET:CG	0.41	2.46	4	1
1:A:25:PHE:CD2	1:A:136:LEU:HB2	0.41	2.51	6	3
1:A:67:LYS:HD2	1:A:67:LYS:C	0.41	2.36	10	1
1:A:23:LEU:HD12	1:A:23:LEU:C	0.41	2.33	11	1
1:A:50:GLU:OE2	1:A:62:VAL:HG23	0.41	2.16	12	1
1:A:120:LYS:HB2	1:A:120:LYS:NZ	0.41	2.31	16	2
1:A:133:ILE:HG22	1:A:134:ILE:N	0.41	2.30	12	1
1:A:106:GLU:O	1:A:106:GLU:CG	0.41	2.68	14	1
1:A:22:ALA:HB2	1:A:131:ARG:HH12	0.41	1.76	16	1
1:A:69:LEU:O	1:A:118:PHE:CZ	0.41	2.74	18	1
1:A:16:PHE:HB3	1:A:98:VAL:HG23	0.41	1.93	20	1
1:A:139:ASP:O	1:A:142:ILE:HG22	0.41	2.16	20	1
1:A:90:GLU:OE1	1:A:90:GLU:N	0.40	2.52	2	1
1:A:66:ALA:CB	1:A:73:PHE:CG	0.40	3.04	7	2
1:A:36:LYS:O	1:A:81:ILE:HD11	0.40	2.16	19	1
1:A:63:VAL:CG1	1:A:64:ASN:H	0.40	2.22	1	1
1:A:99:LEU:CD2	1:A:99:LEU:H	0.40	2.29	4	1
1:A:72:SER:O	1:A:73:PHE:C	0.40	2.58	9	1
1:A:121:LYS:NZ	1:A:141:ILE:HB	0.40	2.30	15	1
1:A:35:GLU:O	1:A:36:LYS:HG3	0.40	2.17	17	1
1:A:118:PHE:CD2	1:A:121:LYS:HB3	0.40	2.51	17	1
1:A:67:LYS:O	1:A:67:LYS:HD2	0.40	2.16	7	1
1:A:25:PHE:CG	1:A:136:LEU:HD11	0.40	2.52	5	1
1:A:53:ILE:CD1	1:A:62:VAL:CG1	0.40	2.99	14	1
1:A:86:THR:OG1	1:A:142:ILE:HG12	0.40	2.17	14	1
1:A:77:LYS:HB3	1:A:96:ASP:OD2	0.40	2.16	19	1
1:A:26:ASP:OD1	1:A:28:ASP:CB	0.40	2.70	4	1
1:A:24:ALA:C	1:A:25:PHE:CD1	0.40	2.95	5	1
1:A:121:LYS:O	1:A:122:SER:HB2	0.40	2.17	9	1
1:A:50:GLU:OE2	1:A:62:VAL:CG2	0.40	2.70	12	1
1:A:138:ILE:O	1:A:138:ILE:CG1	0.40	2.68	14	1
1:A:49:VAL:HG11	1:A:61:PRO:CB	0.40	2.47	16	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	110/151 (73%)	86±3 (78±3%)	18±2 (16±2%)	7±2 (6±1%)	3 19
All	All	2200/3020 (73%)	1712 (78%)	352 (16%)	136 (6%)	3 19

All 20 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	71	ILE	20
1	A	138	ILE	19
1	A	73	PHE	18
1	A	79	LYS	15
1	A	74	ASP	10
1	A	120	LYS	8
1	A	20	GLU	7
1	A	118	PHE	6
1	A	78	MET	6
1	A	75	GLU	4
1	A	26	ASP	3
1	A	122	SER	3
1	A	49	VAL	3
1	A	70	GLY	3
1	A	121	LYS	3
1	A	61	PRO	3
1	A	119	GLY	2
1	A	72	SER	1
1	A	27	VAL	1
1	A	108	GLN	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	100/136 (74%)	90±2 (90±2%)	10±2 (10±2%)	11 56
All	All	2000/2720 (74%)	1801 (90%)	199 (10%)	11 56

All 39 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	99	LEU	20
1	A	141	ILE	20
1	A	69	LEU	17
1	A	67	LYS	16
1	A	93	PHE	12
1	A	13	VAL	11
1	A	23	LEU	11
1	A	136	LEU	9
1	A	16	PHE	7
1	A	131	ARG	6
1	A	148	LYS	6
1	A	25	PHE	5
1	A	127	LYS	5
1	A	77	LYS	5
1	A	79	LYS	4
1	A	103	ARG	4
1	A	126	VAL	4
1	A	71	ILE	3
1	A	9	LYS	3
1	A	21	GLN	3
1	A	120	LYS	3
1	A	35	GLU	3
1	A	19	ASP	3
1	A	129	ASP	2
1	A	121	LYS	2
1	A	65	LEU	2
1	A	73	PHE	1
1	A	75	GLU	1
1	A	50	GLU	1
1	A	78	MET	1
1	A	85	ARG	1
1	A	32	MET	1
1	A	36	LYS	1
1	A	20	GLU	1
1	A	28	ASP	1
1	A	53	ILE	1
1	A	12	GLU	1
1	A	132	LEU	1
1	A	140	LYS	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