Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 01:02 PM EST

PDB ID	:	1POQ
Title	:	Solution Structure of a Superantigen from Yersinia pseudotuberculosis
Authors	:	Donadini, R.; Liew, C.W.; Kwan, A.H.; Mackay, J.P.; Fields, B.A.
Deposited on	:	2003-06-16

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:

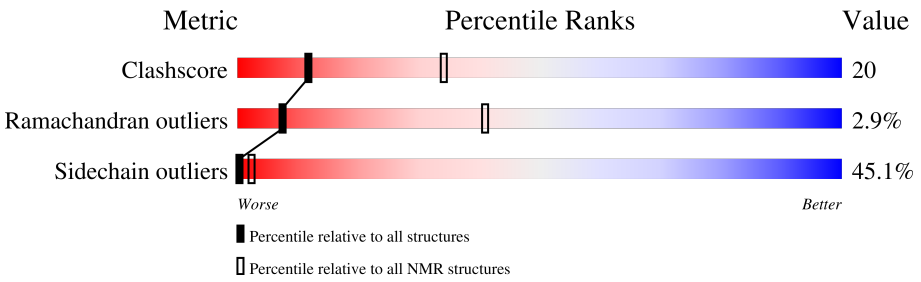
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	118	20% 47% 5% 28%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:19-A:33, A:46-A:115 (85)	1.11	1

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

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

The models can be grouped into 2 clusters and 8 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1825 atoms, of which 904 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called YPM.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	118	1825	574	904	158	186	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: YPM

Chain A: 20% 47% 5% 28%

R14 I15 P16 N17 I18 A19 T20 Y21 T22 G23 T24 I25 Q26 G27 K28 G29 E30 V31 C32 I33 I34 G35 N36 K37 E38 G39 K40 T41 R42 G43 G44 E45 L46 Y47 A48 V49 L50 H51 S52 T53 N54 V55 D58 M59 T60 L61 I62 L63 L64 R65 N66 W72 G73 E74 I75 K76 R77 N78

D79 I80 D81 K82 P83 L84 K85 Y86 E87 D88 Y89 Y90 T91 S92 G93 L94 S95 W96 I97 W98 K99 I100 K101 S104 S105 E106 T107 S108 S111 L112 D113 A114 T115 Y116 H117 D118 D119 K120 E121 D122 S123 D124 V125 L126 T127 K128 C129 P130 V131

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: YPM

Chain A: 36% 27% 9% 28%

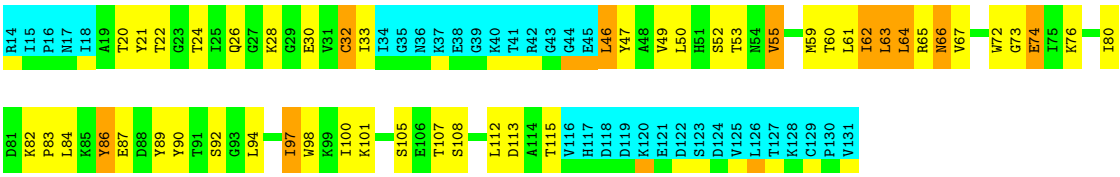
R14 I15 P16 N17 I18 A19 T20 Y21 T22 G23 T24 K28 C32 I33 I34 G35 N36 K37 E38 G39 K40 T41 R42 G43 G44 E45 L46 V49 S52 V55 D58 M59 T60 L61 I62 L63 L64 R65 N66 V67 W72 G73 E74 I75 K76 R77 N78 D79 I80 D81 K82 P83 L84

K85 Y86 S92 I97 W98 K99 N103 S104 S105 E106 T107 S108 N109 L112 T115 Y116 H117 D118 D119 K120 E121 D122 S123 D124 V125 L126 T127 K128 C129 P130 V131

4.2.2 Score per residue for model 2

• Molecule 1: YPM

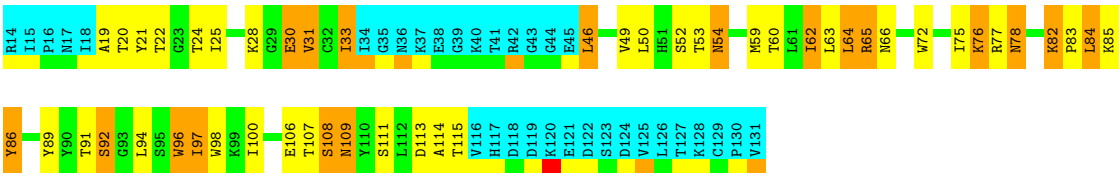
Chain A: 31% 33% 8% 28%



4.2.3 Score per residue for model 3

- Molecule 1: YPM

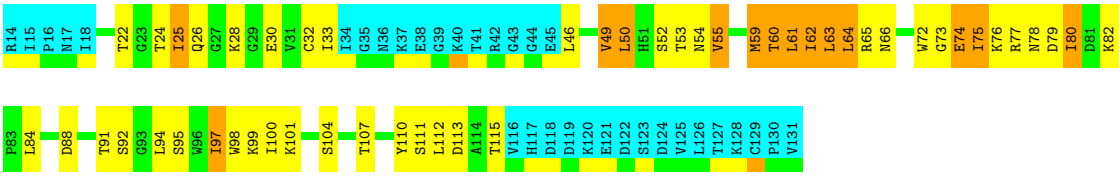
Chain A: 31% 26% 15% 28%



4.2.4 Score per residue for model 4

- Molecule 1: YPM

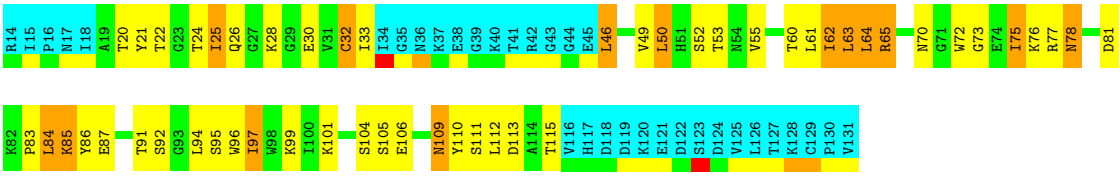
Chain A: 29% 31% 12% 28%



4.2.5 Score per residue for model 5

- Molecule 1: YPM

Chain A: 28% 32% 12% 28%



4.2.6 Score per residue for model 6

- Molecule 1: YPM

Chain A: 25% 36% 10% 28%

R14 I15 P16 N17 I18 A19 T20 Y21 T22 G23 T24 I25 Q26 E30 V31 C32 I33 I34 G35 N36 K37 E38 G39 K40 T41 R42 G43 G44 E45 L46 V49 S52 T53 N54 D58 M59 T60 L61 I62 L63 L64 R65 N66 W72 G73 E74 I75 K76 R77 N78 D79 I80 D81 K82 P83

L84 K85 Y86 Y89 Y90 T91 L94 S95 W96 I97 W98 K99 I100 K101 N102 N103 S104 S105 E106 T107 S108 N109 Y110 S111 L112 D113 A114 T115 V116 H117 D118 D119 K120 E121 D122 S123 D124 V125 L126 T127 K128 C129 P130 V131

4.2.7 Score per residue for model 7

- Molecule 1: YPM

Chain A: 29% 35% 8% 28%

R14 I15 P16 N17 I18 A19 T20 Y21 T22 G23 T24 I25 Q26 E30 V31 C32 I33 I34 G35 N36 K37 E38 G39 K40 T41 R42 G43 G44 E45 L46 Y47 A48 V49 L50 N54 V55 N56 A57 D58 M59 T60 L61 I62 L63 L64 R65 N66 N70 G71 W72 G73 E74 I75 K76 R77 N78 D79

I80 D81 K82 P83 L84 K85 Y86 Y89 Y90 T91 S92 G93 L94 I97 I100 N103 S104 S105 E106 T107 S108 N109 Y110 D113 A114 T115 V116 H117 D118 D119 K120 E121 D122 S123 D124 V125 L126 T127 K128 C129 P130 V131

4.2.8 Score per residue for model 8

- Molecule 1: YPM

Chain A: 28% 36% 8% 28%

R14 I15 P16 N17 I18 A19 T20 Y21 T22 G23 T24 K28 G29 E30 V31 C32 I33 I34 G35 N36 K37 E38 G39 K40 T41 R42 G43 G44 E45 L46 Y47 A48 V49 L50 H51 S52 T53 N54 V55 N56 A57 D58 M59 T60 L61 I62 L63 L64 R65 N66 V67 W72 G73 E74 I75 K76 R77 N78

D79 I80 D81 K82 P83 L84 K85 Y86 E87 T91 S92 G93 L94 W98 K99 I100 K101 N102 N103 S104 S105 E106 T107 S108 N109 Y110 S111 L112 T115 V116 H117 D118 D119 K120 E121 D122 S123 D124 V125 L126 T127 K128 C129 P130 V131

4.2.9 Score per residue for model 9

- Molecule 1: YPM

Chain A: 34% 31% 8% 28%

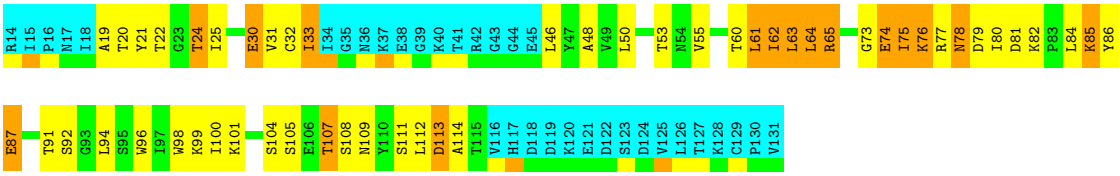
R14 I15 P16 N17 I18 T22 G23 T24 K28 G29 E30 V31 C32 I33 I34 G35 N36 K37 E38 G39 K40 T41 R42 G43 G44 E45 L46 V49 L50 H51 S52 V55 M59 T60 L61 I62 L63 L64 R65 N66 V67 W72 G73 E74 I75 K76 D81 K82 P83 L84 K85 Y86

T91 S92 S95 W96 I97 W98 K99 I100 S105 E106 T107 S108 N109 Y110 S111 L112 D113 A114 T115 V116 H117 D118 D119 K120 E121 D122 S123 D124 V125 L126 T127 K128 C129 P130 V131

4.2.10 Score per residue for model 10

- Molecule 1: YPM

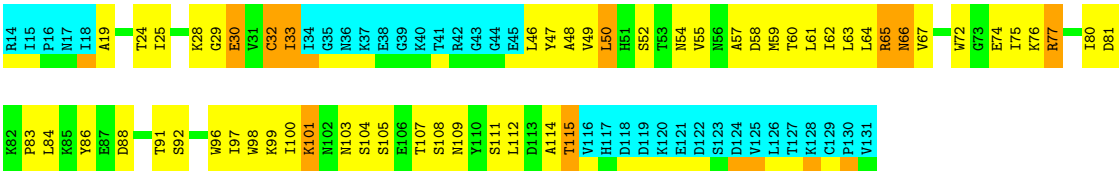
Chain A: 28% 31% 14% 28%



4.2.11 Score per residue for model 11

- Molecule 1: YPM

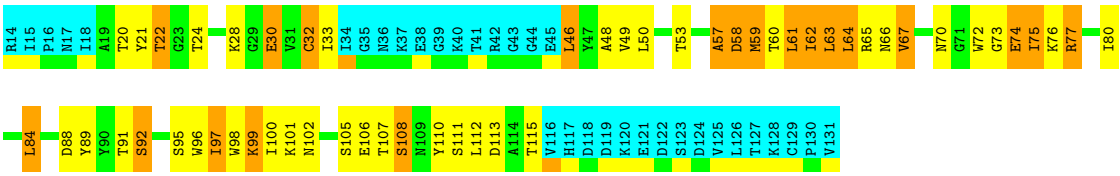
Chain A: 25% 40% 8% 28%



4.2.12 Score per residue for model 12

- Molecule 1: YPM

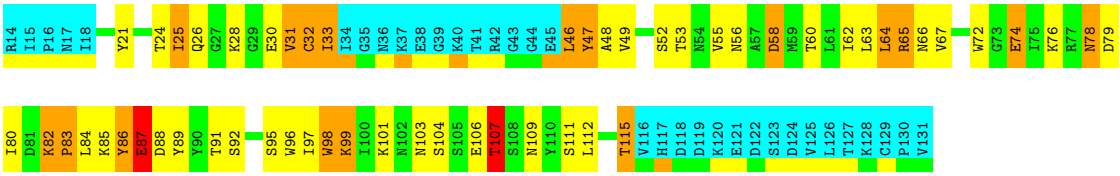
Chain A: 26% 29% 17% 28%



4.2.13 Score per residue for model 13

- Molecule 1: YPM

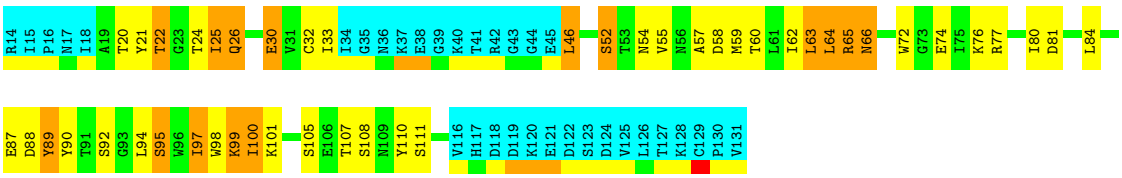
Chain A: 25% 31% 14% • 28%



4.2.14 Score per residue for model 14

- Molecule 1: YPM

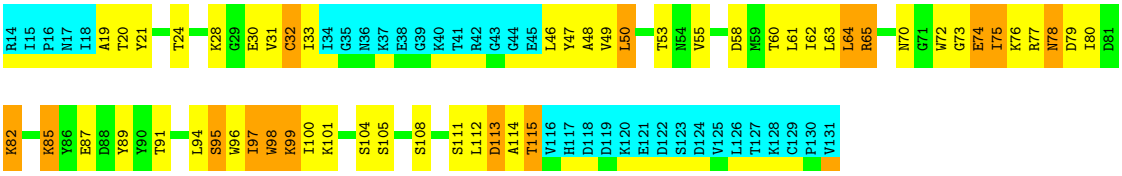
Chain A: 33% 26% 13% 28%



4.2.15 Score per residue for model 15

- Molecule 1: YPM

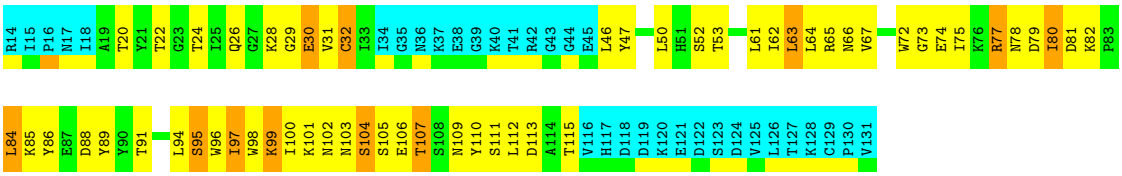
Chain A: 26% 33% 13% 28%



4.2.16 Score per residue for model 16

- Molecule 1: YPM

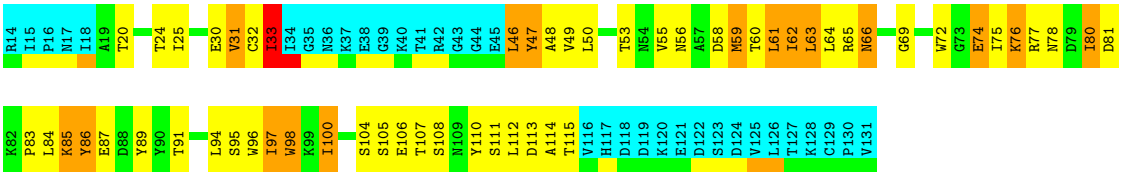
Chain A: 24% 39% 9% 28%



4.2.17 Score per residue for model 17

- Molecule 1: YPM

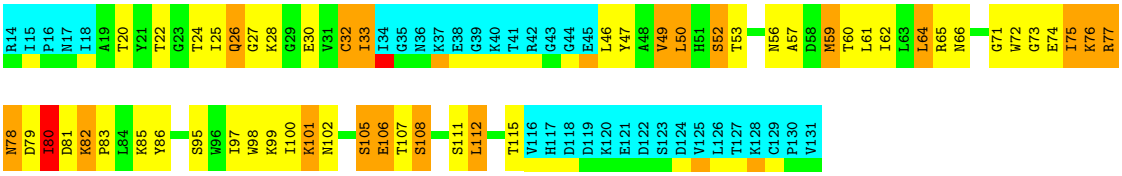
Chain A: 24% 34% 14% • 28%



4.2.18 Score per residue for model 18

- Molecule 1: YPM

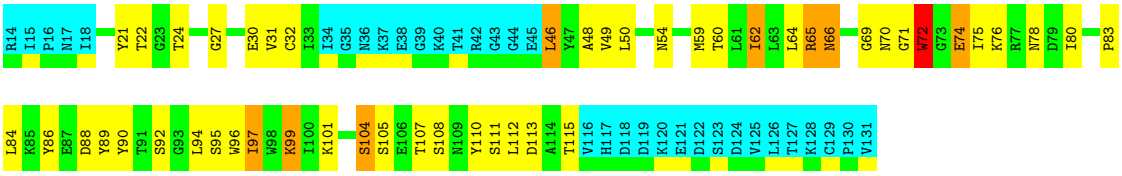
Chain A: 26% 30% 15% • 28%



4.2.19 Score per residue for model 19

- Molecule 1: YPM

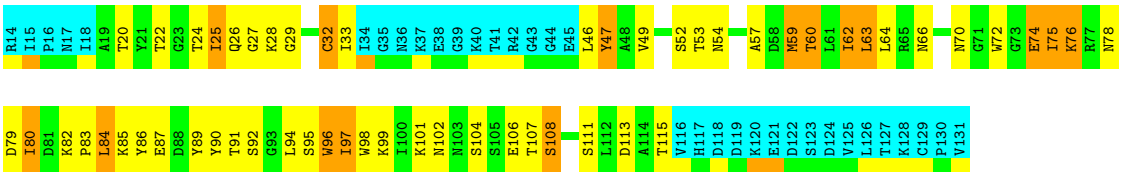
Chain A: 31% 34% 7% • 28%



4.2.20 Score per residue for model 20

- Molecule 1: YPM

Chain A: 25% 35% 13% 28%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, molecular dynamics, torsion angle dynamics.*

Of the 100 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
DYANA	refinement	1.5
ARIA	structure solution	1.1.2

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.

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	30	GLU	Peptide	1
1	A	106	GLU	Peptide	1

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	668	652	651	26±7
All	All	13360	13040	13020	520

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HA	1:A:85:LYS:HB3	0.97	1.32	13	1
1:A:64:LEU:HA	1:A:74:GLU:HB2	0.93	1.39	1	1
1:A:79:ASP:HB3	1:A:82:LYS:HD3	0.93	1.38	16	1
1:A:62:ILE:HD11	1:A:75:ILE:HA	0.91	1.41	6	2
1:A:64:LEU:HD22	1:A:99:LYS:HB2	0.91	1.43	20	2
1:A:31:VAL:HG23	1:A:100:ILE:HB	0.87	1.46	3	1
1:A:79:ASP:HB3	1:A:82:LYS:HD2	0.87	1.47	6	2
1:A:65:ARG:HG2	1:A:74:GLU:HG3	0.87	1.46	1	1
1:A:29:GLY:HA3	1:A:102:ASN:HB3	0.86	1.45	16	1
1:A:60:THR:HA	1:A:79:ASP:HB3	0.84	1.47	20	2
1:A:64:LEU:HD23	1:A:97:ILE:HD11	0.83	1.50	18	1
1:A:25:ILE:HG23	1:A:108:SER:HB2	0.83	1.50	18	2
1:A:46:LEU:HB2	1:A:86:TYR:HB3	0.82	1.51	9	1
1:A:21:TYR:HB2	1:A:112:LEU:HB3	0.82	1.47	15	7
1:A:64:LEU:HG	1:A:99:LYS:HD3	0.81	1.51	14	1
1:A:62:ILE:HB	1:A:77:ARG:HG3	0.81	1.51	11	1
1:A:46:LEU:HD21	1:A:87:GLU:HB3	0.81	1.51	15	1
1:A:48:ALA:HB2	1:A:85:LYS:HB2	0.80	1.53	17	1
1:A:62:ILE:HG21	1:A:74:GLU:HA	0.79	1.54	12	4
1:A:62:ILE:HD12	1:A:74:GLU:HA	0.78	1.56	18	3
1:A:62:ILE:HA	1:A:77:ARG:HB2	0.77	1.53	12	1
1:A:47:TYR:N	1:A:85:LYS:HB2	0.76	1.96	20	2
1:A:53:THR:HB	1:A:109:ASN:HB3	0.76	1.57	13	1
1:A:60:THR:HB	1:A:77:ARG:HD2	0.76	1.58	4	1
1:A:63:LEU:HG	1:A:98:TRP:CZ3	0.74	2.17	12	9
1:A:27:GLY:O	1:A:102:ASN:HB3	0.74	1.82	20	2
1:A:28:LYS:HG3	1:A:104:SER:HA	0.73	1.60	13	1
1:A:65:ARG:HG2	1:A:74:GLU:HB2	0.73	1.60	6	1
1:A:63:LEU:HG	1:A:98:TRP:HZ3	0.73	1.44	12	2
1:A:46:LEU:HD23	1:A:86:TYR:HB2	0.72	1.62	17	1
1:A:63:LEU:HB3	1:A:76:LYS:HB3	0.72	1.62	11	3
1:A:85:LYS:HA	1:A:98:TRP:CH2	0.71	2.19	17	1
1:A:64:LEU:HB2	1:A:97:ILE:HG22	0.71	1.60	11	4
1:A:49:VAL:H	1:A:113:ASP:HB3	0.71	1.43	15	1
1:A:62:ILE:HG23	1:A:64:LEU:HD11	0.71	1.61	17	1
1:A:64:LEU:HD23	1:A:72:TRP:HA	0.70	1.62	19	1
1:A:66:ASN:HD22	1:A:72:TRP:HE3	0.70	1.28	19	1
1:A:49:VAL:N	1:A:113:ASP:HB3	0.70	2.01	15	1
1:A:46:LEU:HB3	1:A:98:TRP:CZ2	0.70	2.21	8	2
1:A:48:ALA:HB1	1:A:112:LEU:HD11	0.70	1.63	8	3
1:A:62:ILE:HB	1:A:77:ARG:HG2	0.70	1.64	4	1
1:A:33:ILE:HG13	1:A:100:ILE:HB	0.70	1.64	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:HD12	1:A:112:LEU:HB2	0.69	1.65	8	1
1:A:21:TYR:HE2	1:A:33:ILE:HB	0.69	1.47	8	1
1:A:47:TYR:HA	1:A:84:LEU:O	0.69	1.86	2	4
1:A:47:TYR:N	1:A:85:LYS:H	0.69	1.86	17	1
1:A:25:ILE:HD13	1:A:31:VAL:HG22	0.68	1.64	3	1
1:A:62:ILE:HD11	1:A:75:ILE:H	0.68	1.48	15	1
1:A:49:VAL:HG13	1:A:113:ASP:HB2	0.68	1.62	4	6
1:A:50:LEU:HD11	1:A:110:TYR:HB2	0.68	1.65	17	2
1:A:30:GLU:HB2	1:A:99:LYS:HE3	0.68	1.63	14	1
1:A:48:ALA:HB3	1:A:84:LEU:O	0.68	1.89	13	3
1:A:86:TYR:HB3	1:A:98:TRP:CZ2	0.68	2.23	10	1
1:A:46:LEU:HD23	1:A:86:TYR:HB3	0.68	1.65	1	1
1:A:33:ILE:HG12	1:A:100:ILE:HD11	0.67	1.67	18	1
1:A:64:LEU:HB3	1:A:71:GLY:C	0.67	2.09	19	1
1:A:30:GLU:HA	1:A:100:ILE:O	0.67	1.89	6	9
1:A:32:CYS:HB3	1:A:98:TRP:HB2	0.67	1.67	11	1
1:A:65:ARG:HA	1:A:71:GLY:N	0.67	2.04	19	1
1:A:30:GLU:HB3	1:A:101:LYS:HD3	0.67	1.66	14	1
1:A:32:CYS:SG	1:A:97:ILE:HG12	0.67	2.29	5	2
1:A:86:TYR:HB2	1:A:96:TRP:CE3	0.66	2.25	5	1
1:A:46:LEU:HD22	1:A:86:TYR:HA	0.66	1.68	10	1
1:A:64:LEU:HG	1:A:74:GLU:H	0.66	1.50	1	1
1:A:75:ILE:HG23	1:A:76:LYS:H	0.66	1.50	12	1
1:A:32:CYS:HA	1:A:97:ILE:HD11	0.65	1.68	4	5
1:A:26:GLN:HA	1:A:107:THR:HG23	0.65	1.67	16	1
1:A:78:ASN:HB2	1:A:84:LEU:HD22	0.65	1.67	10	2
1:A:50:LEU:HB2	1:A:61:LEU:HD22	0.65	1.68	11	1
1:A:64:LEU:HD23	1:A:72:TRP:CB	0.65	2.22	1	1
1:A:63:LEU:HD21	1:A:86:TYR:HB2	0.65	1.68	10	1
1:A:48:ALA:H	1:A:84:LEU:N	0.64	1.91	17	2
1:A:62:ILE:HA	1:A:76:LYS:O	0.64	1.93	4	6
1:A:64:LEU:HG	1:A:65:ARG:N	0.64	2.07	18	2
1:A:59:MET:HB3	1:A:79:ASP:OD2	0.64	1.93	4	2
1:A:86:TYR:HB3	1:A:89:TYR:CE1	0.64	2.27	17	1
1:A:62:ILE:HG12	1:A:74:GLU:HB3	0.64	1.69	17	1
1:A:64:LEU:HD23	1:A:72:TRP:HB3	0.63	1.69	1	2
1:A:57:ALA:HB1	1:A:80:ILE:HG21	0.63	1.68	14	1
1:A:33:ILE:HB	1:A:98:TRP:HB2	0.63	1.70	15	4
1:A:92:SER:HB2	1:A:96:TRP:HH2	0.63	1.54	12	1
1:A:64:LEU:HG	1:A:73:GLY:O	0.63	1.93	2	2
1:A:65:ARG:O	1:A:65:ARG:HG2	0.62	1.93	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ASN:HB3	1:A:72:TRP:HA	0.62	1.71	7	2
1:A:64:LEU:HB3	1:A:97:ILE:HG22	0.62	1.71	20	1
1:A:66:ASN:HA	1:A:95:SER:HB2	0.62	1.71	6	2
1:A:48:ALA:HB2	1:A:85:LYS:CB	0.62	2.24	17	1
1:A:46:LEU:HD23	1:A:89:TYR:HA	0.62	1.71	19	1
1:A:86:TYR:HB3	1:A:98:TRP:CE2	0.62	2.29	13	1
1:A:66:ASN:ND2	1:A:72:TRP:CE3	0.62	2.68	19	1
1:A:98:TRP:HA	1:A:98:TRP:CE3	0.62	2.30	13	1
1:A:62:ILE:HG23	1:A:99:LYS:HB3	0.62	1.72	4	5
1:A:49:VAL:HA	1:A:83:PRO:HA	0.61	1.71	18	11
1:A:63:LEU:HD12	1:A:84:LEU:HB2	0.61	1.71	5	1
1:A:46:LEU:HD11	1:A:96:TRP:HZ3	0.61	1.55	3	1
1:A:46:LEU:HD13	1:A:63:LEU:HD21	0.61	1.71	3	1
1:A:72:TRP:CD2	1:A:72:TRP:N	0.61	2.68	19	1
1:A:49:VAL:HB	1:A:83:PRO:HB3	0.61	1.72	9	3
1:A:30:GLU:HB3	1:A:101:LYS:HG2	0.61	1.71	8	1
1:A:97:ILE:HG23	1:A:98:TRP:O	0.61	1.96	6	1
1:A:85:LYS:HA	1:A:98:TRP:CZ2	0.61	2.31	17	1
1:A:64:LEU:HD12	1:A:75:ILE:HG22	0.60	1.73	12	1
1:A:64:LEU:HA	1:A:74:GLU:HB3	0.60	1.72	13	2
1:A:61:LEU:HD13	1:A:78:ASN:HB3	0.60	1.72	17	1
1:A:63:LEU:CB	1:A:76:LYS:HB3	0.60	2.26	1	3
1:A:50:LEU:HD21	1:A:59:MET:HB3	0.60	1.72	9	1
1:A:62:ILE:CA	1:A:77:ARG:HB2	0.60	2.26	12	1
1:A:31:VAL:HG13	1:A:100:ILE:C	0.60	2.17	16	1
1:A:20:THR:HG23	1:A:113:ASP:HB3	0.60	1.74	17	1
1:A:46:LEU:HD23	1:A:87:GLU:H	0.59	1.55	10	1
1:A:64:LEU:HD22	1:A:73:GLY:O	0.59	1.96	4	4
1:A:70:ASN:HB3	1:A:96:TRP:HA	0.59	1.74	19	1
1:A:66:ASN:OD1	1:A:72:TRP:HA	0.59	1.97	13	3
1:A:64:LEU:CD2	1:A:72:TRP:HB3	0.59	2.27	16	2
1:A:78:ASN:ND2	1:A:82:LYS:HD3	0.59	2.13	7	2
1:A:46:LEU:HB3	1:A:85:LYS:C	0.59	2.18	10	1
1:A:48:ALA:CB	1:A:85:LYS:HA	0.59	2.27	13	1
1:A:72:TRP:CE3	1:A:72:TRP:N	0.59	2.71	19	1
1:A:61:LEU:HG	1:A:84:LEU:HD21	0.58	1.74	5	1
1:A:64:LEU:HA	1:A:74:GLU:CB	0.58	2.25	1	2
1:A:61:LEU:HD21	1:A:98:TRP:CE3	0.58	2.33	2	1
1:A:19:ALA:HB3	1:A:114:ALA:HB3	0.58	1.75	10	2
1:A:46:LEU:HD22	1:A:86:TYR:CE1	0.58	2.33	5	1
1:A:58:ASP:HB3	1:A:103:ASN:HB2	0.58	1.74	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:HG22	1:A:99:LYS:HB3	0.57	1.76	5	1
1:A:86:TYR:HB3	1:A:89:TYR:CD1	0.57	2.34	17	1
1:A:33:ILE:HG13	1:A:98:TRP:HB2	0.57	1.75	20	1
1:A:28:LYS:HE2	1:A:105:SER:HA	0.57	1.76	1	1
1:A:66:ASN:HB3	1:A:72:TRP:CE3	0.57	2.35	3	5
1:A:50:LEU:HB3	1:A:79:ASP:OD1	0.57	1.99	4	1
1:A:62:ILE:HG12	1:A:99:LYS:HB3	0.57	1.75	18	2
1:A:33:ILE:HG13	1:A:112:LEU:HD13	0.57	1.76	18	1
1:A:65:ARG:HB2	1:A:96:TRP:HA	0.57	1.76	13	1
1:A:49:VAL:HB	1:A:113:ASP:HB2	0.57	1.76	12	1
1:A:64:LEU:HG	1:A:99:LYS:HB2	0.56	1.77	14	1
1:A:46:LEU:HB3	1:A:98:TRP:CH2	0.56	2.34	2	1
1:A:48:ALA:HB2	1:A:85:LYS:HA	0.56	1.77	13	1
1:A:50:LEU:HD21	1:A:110:TYR:HB2	0.56	1.77	4	1
1:A:63:LEU:HG	1:A:76:LYS:HE2	0.56	1.77	13	1
1:A:66:ASN:H	1:A:71:GLY:H	0.56	1.42	19	1
1:A:21:TYR:HD2	1:A:112:LEU:HD23	0.56	1.61	6	1
1:A:54:ASN:ND2	1:A:108:SER:HA	0.56	2.15	7	1
1:A:30:GLU:HG2	1:A:101:LYS:HA	0.56	1.76	4	1
1:A:86:TYR:HA	1:A:89:TYR:CE2	0.56	2.35	3	1
1:A:62:ILE:CD1	1:A:74:GLU:HA	0.56	2.30	10	4
1:A:78:ASN:HB2	1:A:84:LEU:HG	0.56	1.77	1	1
1:A:29:GLY:O	1:A:101:LYS:HA	0.56	2.01	11	2
1:A:63:LEU:HD13	1:A:98:TRP:CH2	0.55	2.35	3	1
1:A:78:ASN:HD21	1:A:84:LEU:HB2	0.55	1.60	4	1
1:A:66:ASN:O	1:A:67:VAL:HB	0.55	2.01	9	2
1:A:21:TYR:HE2	1:A:86:TYR:HE1	0.55	1.44	13	1
1:A:32:CYS:HB3	1:A:97:ILE:HG21	0.55	1.78	20	1
1:A:78:ASN:HB3	1:A:82:LYS:HD3	0.55	1.79	7	1
1:A:78:ASN:HB2	1:A:84:LEU:HD23	0.55	1.78	5	1
1:A:19:ALA:HB2	1:A:115:THR:HG23	0.55	1.78	8	1
1:A:94:LEU:HG	1:A:95:SER:H	0.54	1.62	16	1
1:A:65:ARG:HG3	1:A:74:GLU:HG3	0.54	1.78	11	1
1:A:26:GLN:C	1:A:106:GLU:HB3	0.54	2.23	18	1
1:A:46:LEU:O	1:A:86:TYR:HB2	0.54	2.02	8	1
1:A:31:VAL:HG13	1:A:101:LYS:N	0.54	2.18	16	1
1:A:63:LEU:HD22	1:A:98:TRP:HZ3	0.54	1.61	11	1
1:A:64:LEU:HD21	1:A:72:TRP:HB3	0.54	1.79	13	1
1:A:59:MET:HB3	1:A:100:ILE:HG23	0.53	1.80	6	1
1:A:64:LEU:HG	1:A:74:GLU:HA	0.53	1.80	17	2
1:A:32:CYS:CB	1:A:98:TRP:HB2	0.53	2.33	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ASN:HD22	1:A:82:LYS:HD3	0.53	1.62	7	1
1:A:21:TYR:CE2	1:A:33:ILE:HB	0.53	2.36	8	1
1:A:19:ALA:HB1	1:A:33:ILE:HG13	0.53	1.81	10	1
1:A:46:LEU:CD2	1:A:86:TYR:HA	0.53	2.33	10	1
1:A:59:MET:HA	1:A:101:LYS:O	0.53	2.04	11	1
1:A:62:ILE:HD12	1:A:77:ARG:HG3	0.53	1.80	15	1
1:A:31:VAL:HG22	1:A:101:LYS:HA	0.53	1.79	16	1
1:A:32:CYS:O	1:A:97:ILE:HG13	0.53	2.03	11	1
1:A:49:VAL:HG22	1:A:83:PRO:HB3	0.53	1.81	11	1
1:A:46:LEU:HA	1:A:85:LYS:CB	0.53	2.23	13	1
1:A:65:ARG:HA	1:A:71:GLY:H	0.53	1.62	19	1
1:A:52:SER:HA	1:A:109:ASN:O	0.53	2.04	3	1
1:A:64:LEU:HD23	1:A:72:TRP:CA	0.53	2.33	19	1
1:A:22:THR:HA	1:A:110:TYR:O	0.53	2.03	7	5
1:A:25:ILE:HD12	1:A:31:VAL:HG22	0.53	1.81	10	1
1:A:64:LEU:HB2	1:A:74:GLU:CB	0.52	2.34	13	1
1:A:33:ILE:O	1:A:98:TRP:HB2	0.52	2.05	17	1
1:A:62:ILE:HG12	1:A:64:LEU:CD1	0.52	2.34	1	1
1:A:32:CYS:SG	1:A:100:ILE:HD12	0.52	2.43	11	1
1:A:62:ILE:HD12	1:A:77:ARG:HE	0.52	1.65	11	1
1:A:72:TRP:CH2	1:A:97:ILE:HB	0.52	2.39	20	2
1:A:25:ILE:HD13	1:A:100:ILE:HB	0.52	1.80	14	1
1:A:64:LEU:HD11	1:A:74:GLU:HA	0.52	1.79	16	1
1:A:30:GLU:HG2	1:A:101:LYS:HB2	0.52	1.81	18	1
1:A:64:LEU:HD22	1:A:72:TRP:HB3	0.52	1.80	17	2
1:A:62:ILE:HD11	1:A:74:GLU:HA	0.52	1.82	15	1
1:A:30:GLU:HG2	1:A:101:LYS:HG3	0.51	1.82	11	1
1:A:54:ASN:HB2	1:A:57:ALA:HB2	0.51	1.82	7	1
1:A:64:LEU:CD2	1:A:99:LYS:HD2	0.51	2.35	16	1
1:A:47:TYR:HB3	1:A:115:THR:O	0.51	2.05	18	1
1:A:49:VAL:HG22	1:A:83:PRO:HA	0.51	1.80	2	1
1:A:25:ILE:HD13	1:A:102:ASN:HB2	0.51	1.80	6	1
1:A:65:ARG:HB2	1:A:96:TRP:N	0.51	2.21	15	1
1:A:20:THR:HG22	1:A:113:ASP:HA	0.51	1.82	10	1
1:A:61:LEU:HD13	1:A:84:LEU:HD23	0.51	1.83	10	1
1:A:21:TYR:HE2	1:A:86:TYR:CE1	0.51	2.24	13	1
1:A:46:LEU:HA	1:A:87:GLU:N	0.51	2.21	10	1
1:A:57:ALA:HB1	1:A:108:SER:HB3	0.51	1.81	12	1
1:A:29:GLY:CA	1:A:102:ASN:HB3	0.51	2.27	16	1
1:A:19:ALA:N	1:A:114:ALA:HB3	0.50	2.21	7	1
1:A:64:LEU:CB	1:A:97:ILE:HG22	0.50	2.37	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:LEU:HD22	1:A:99:LYS:HD2	0.50	1.82	16	1
1:A:59:MET:SD	1:A:110:TYR:HB3	0.50	2.47	19	2
1:A:19:ALA:O	1:A:114:ALA:HA	0.50	2.06	15	1
1:A:32:CYS:SG	1:A:112:LEU:HD22	0.50	2.47	6	1
1:A:65:ARG:CZ	1:A:95:SER:HA	0.50	2.37	15	1
1:A:96:TRP:CD1	1:A:96:TRP:N	0.50	2.80	3	2
1:A:61:LEU:O	1:A:77:ARG:HB3	0.50	2.06	12	1
1:A:20:THR:HA	1:A:112:LEU:O	0.50	2.07	12	2
1:A:46:LEU:HG	1:A:63:LEU:HD11	0.49	1.83	1	1
1:A:53:THR:HA	1:A:109:ASN:O	0.49	2.06	5	1
1:A:46:LEU:HB3	1:A:86:TYR:HB3	0.49	1.83	7	1
1:A:64:LEU:CD2	1:A:72:TRP:HA	0.49	2.35	19	1
1:A:64:LEU:HA	1:A:75:ILE:HD12	0.49	1.84	4	2
1:A:25:ILE:HG13	1:A:26:GLN:N	0.49	2.23	5	2
1:A:46:LEU:HD23	1:A:63:LEU:HD21	0.49	1.83	13	1
1:A:63:LEU:HD12	1:A:76:LYS:HD2	0.49	1.82	17	1
1:A:50:LEU:HD12	1:A:61:LEU:HB2	0.49	1.85	18	1
1:A:64:LEU:HD12	1:A:74:GLU:HA	0.49	1.83	19	1
1:A:47:TYR:O	1:A:85:LYS:HB2	0.49	2.07	17	2
1:A:47:TYR:CD2	1:A:47:TYR:O	0.49	2.66	17	1
1:A:84:LEU:O	1:A:98:TRP:HZ2	0.48	1.91	13	1
1:A:59:MET:SD	1:A:100:ILE:HG23	0.48	2.49	3	1
1:A:65:ARG:H	1:A:75:ILE:HG13	0.48	1.67	5	1
1:A:78:ASN:OD1	1:A:82:LYS:HB3	0.48	2.09	13	1
1:A:72:TRP:HB3	1:A:99:LYS:HD2	0.48	1.84	9	1
1:A:46:LEU:HB3	1:A:86:TYR:HA	0.48	1.85	10	1
1:A:48:ALA:HA	1:A:113:ASP:O	0.48	2.08	10	1
1:A:22:THR:HG23	1:A:111:SER:HB2	0.48	1.86	16	1
1:A:46:LEU:O	1:A:85:LYS:HA	0.48	2.08	1	2
1:A:63:LEU:O	1:A:75:ILE:HG23	0.48	2.09	9	2
1:A:49:VAL:CG1	1:A:113:ASP:HB2	0.48	2.37	3	1
1:A:114:ALA:O	1:A:115:THR:HG23	0.47	2.09	15	1
1:A:63:LEU:HD22	1:A:98:TRP:CZ3	0.47	2.44	11	1
1:A:46:LEU:CD2	1:A:87:GLU:HB3	0.47	2.35	15	1
1:A:64:LEU:HD13	1:A:72:TRP:HB3	0.47	1.86	5	1
1:A:57:ALA:O	1:A:80:ILE:HG21	0.47	2.09	8	1
1:A:46:LEU:HD11	1:A:63:LEU:HD21	0.47	1.85	12	1
1:A:52:SER:OG	1:A:80:ILE:HB	0.47	2.09	14	1
1:A:48:ALA:CB	1:A:85:LYS:HB2	0.47	2.35	17	1
1:A:63:LEU:HD21	1:A:85:LYS:HE2	0.47	1.87	15	1
1:A:60:THR:HB	1:A:77:ARG:CD	0.47	2.37	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:HD11	1:A:75:ILE:N	0.47	2.20	15	1
1:A:60:THR:CB	1:A:77:ARG:HD2	0.47	2.34	4	1
1:A:64:LEU:HD23	1:A:97:ILE:HG22	0.46	1.85	3	1
1:A:82:LYS:HZ3	1:A:84:LEU:HB2	0.46	1.70	3	1
1:A:85:LYS:HE3	1:A:115:THR:N	0.46	2.25	13	1
1:A:54:ASN:HB3	1:A:109:ASN:HB3	0.46	1.87	8	1
1:A:33:ILE:HG13	1:A:98:TRP:HD1	0.46	1.70	10	1
1:A:46:LEU:HD13	1:A:84:LEU:HD22	0.46	1.86	17	1
1:A:62:ILE:HD13	1:A:74:GLU:HG3	0.46	1.88	20	1
1:A:27:GLY:HA2	1:A:104:SER:O	0.46	2.10	19	1
1:A:47:TYR:HA	1:A:85:LYS:HG3	0.46	1.87	15	1
1:A:61:LEU:HD22	1:A:84:LEU:HD12	0.46	1.86	17	1
1:A:89:TYR:CE1	1:A:96:TRP:HB2	0.46	2.46	17	1
1:A:32:CYS:HB3	1:A:97:ILE:HD13	0.46	1.88	18	1
1:A:57:ALA:O	1:A:58:ASP:HB3	0.46	2.10	12	1
1:A:32:CYS:HA	1:A:98:TRP:O	0.46	2.10	13	2
1:A:27:GLY:CA	1:A:106:GLU:HA	0.46	2.41	18	1
1:A:87:GLU:HB2	1:A:96:TRP:CH2	0.45	2.45	5	1
1:A:72:TRP:CZ3	1:A:97:ILE:HB	0.45	2.46	6	1
1:A:48:ALA:HB1	1:A:112:LEU:HD22	0.45	1.88	11	1
1:A:33:ILE:HG13	1:A:98:TRP:HB3	0.45	1.86	13	1
1:A:54:ASN:HB3	1:A:108:SER:HA	0.45	1.88	3	1
1:A:63:LEU:HD22	1:A:96:TRP:CE3	0.45	2.45	10	1
1:A:84:LEU:O	1:A:98:TRP:CZ2	0.45	2.69	13	1
1:A:31:VAL:CG1	1:A:100:ILE:N	0.45	2.80	16	1
1:A:71:GLY:CA	1:A:72:TRP:CE3	0.45	2.99	19	1
1:A:72:TRP:HB3	1:A:99:LYS:HE3	0.45	1.87	6	1
1:A:64:LEU:HD13	1:A:73:GLY:C	0.45	2.32	12	1
1:A:72:TRP:HB2	1:A:99:LYS:HE3	0.45	1.88	12	2
1:A:52:SER:HB3	1:A:57:ALA:HB1	0.45	1.88	18	1
1:A:46:LEU:C	1:A:85:LYS:HB3	0.45	2.32	10	1
1:A:58:ASP:O	1:A:103:ASN:HB2	0.45	2.12	7	1
1:A:98:TRP:HA	1:A:98:TRP:HE3	0.45	1.66	13	1
1:A:46:LEU:C	1:A:85:LYS:H	0.45	2.15	20	1
1:A:63:LEU:O	1:A:75:ILE:HB	0.45	2.12	4	3
1:A:92:SER:HB3	1:A:96:TRP:CH2	0.44	2.47	3	1
1:A:50:LEU:HD12	1:A:61:LEU:HB3	0.44	1.88	4	1
1:A:64:LEU:HD11	1:A:73:GLY:O	0.44	2.11	5	1
1:A:64:LEU:O	1:A:96:TRP:HA	0.44	2.11	6	1
1:A:63:LEU:HD13	1:A:98:TRP:CZ3	0.44	2.46	11	1
1:A:31:VAL:O	1:A:99:LYS:HA	0.44	2.11	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:HD22	1:A:61:LEU:HB2	0.44	1.89	16	1
1:A:80:ILE:O	1:A:82:LYS:HD2	0.44	2.12	16	1
1:A:32:CYS:CA	1:A:97:ILE:HD11	0.44	2.41	4	2
1:A:28:LYS:HA	1:A:102:ASN:O	0.44	2.13	18	2
1:A:24:THR:HB	1:A:107:THR:HG22	0.44	1.88	10	1
1:A:65:ARG:O	1:A:72:TRP:CZ3	0.44	2.70	14	1
1:A:84:LEU:O	1:A:98:TRP:CH2	0.44	2.70	20	2
1:A:71:GLY:CA	1:A:97:ILE:HB	0.44	2.42	19	1
1:A:85:LYS:HE3	1:A:115:THR:H	0.44	1.73	13	1
1:A:49:VAL:HA	1:A:82:LYS:O	0.44	2.11	20	3
1:A:31:VAL:O	1:A:99:LYS:HG2	0.44	2.12	16	1
1:A:46:LEU:O	1:A:85:LYS:HB3	0.44	2.12	10	1
1:A:46:LEU:HD12	1:A:88:ASP:O	0.44	2.13	11	1
1:A:63:LEU:HG	1:A:76:LYS:CE	0.44	2.43	13	1
1:A:62:ILE:HD12	1:A:77:ARG:HB2	0.44	1.89	1	2
1:A:63:LEU:HB2	1:A:76:LYS:HB3	0.44	1.90	17	3
1:A:85:LYS:HG3	1:A:86:TYR:N	0.44	2.27	13	1
1:A:86:TYR:HB2	1:A:96:TRP:CZ3	0.43	2.47	5	1
1:A:19:ALA:H	1:A:114:ALA:HA	0.43	1.74	15	1
1:A:64:LEU:HB3	1:A:71:GLY:CA	0.43	2.43	19	1
1:A:50:LEU:HB3	1:A:61:LEU:HD22	0.43	1.90	5	1
1:A:46:LEU:HB2	1:A:89:TYR:HB3	0.43	1.90	14	1
1:A:31:VAL:HA	1:A:100:ILE:O	0.43	2.14	16	1
1:A:84:LEU:HD13	1:A:98:TRP:CH2	0.43	2.48	3	1
1:A:86:TYR:HD2	1:A:96:TRP:HB2	0.43	1.73	20	1
1:A:63:LEU:HD21	1:A:86:TYR:HD2	0.43	1.73	5	1
1:A:59:MET:O	1:A:80:ILE:HG22	0.43	2.14	7	1
1:A:98:TRP:CE3	1:A:98:TRP:HA	0.43	2.49	9	1
1:A:65:ARG:HB2	1:A:96:TRP:CA	0.43	2.44	15	1
1:A:25:ILE:HB	1:A:110:TYR:CD1	0.43	2.48	4	1
1:A:86:TYR:CZ	1:A:96:TRP:HB2	0.43	2.49	10	1
1:A:72:TRP:CZ2	1:A:97:ILE:HD13	0.43	2.48	7	1
1:A:63:LEU:HB2	1:A:98:TRP:CZ3	0.43	2.49	8	1
1:A:86:TYR:CE1	1:A:96:TRP:HB2	0.43	2.48	10	1
1:A:19:ALA:HB3	1:A:114:ALA:O	0.43	2.14	11	1
1:A:71:GLY:HA3	1:A:72:TRP:CE3	0.43	2.49	19	1
1:A:63:LEU:HD21	1:A:98:TRP:CZ3	0.43	2.49	17	1
1:A:46:LEU:H	1:A:86:TYR:HB2	0.42	1.74	2	1
1:A:65:ARG:HG2	1:A:65:ARG:O	0.42	2.14	9	1
1:A:31:VAL:HG22	1:A:33:ILE:HG12	0.42	1.92	17	1
1:A:63:LEU:N	1:A:63:LEU:HD23	0.42	2.30	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:TYR:HB2	1:A:112:LEU:CB	0.42	2.33	15	1
1:A:33:ILE:HD13	1:A:33:ILE:HA	0.42	1.72	18	1
1:A:66:ASN:N	1:A:71:GLY:H	0.42	2.11	19	1
1:A:76:LYS:HE3	1:A:84:LEU:HD11	0.42	1.91	14	1
1:A:50:LEU:HG	1:A:61:LEU:HB2	0.42	1.91	15	1
1:A:76:LYS:HD2	1:A:76:LYS:HA	0.42	1.61	1	1
1:A:46:LEU:HD22	1:A:63:LEU:HD11	0.42	1.91	3	1
1:A:25:ILE:O	1:A:107:THR:HA	0.42	2.15	13	1
1:A:48:ALA:H	1:A:85:LYS:HG3	0.42	1.75	15	1
1:A:61:LEU:HD23	1:A:78:ASN:HD21	0.42	1.75	15	1
1:A:75:ILE:HG23	1:A:76:LYS:N	0.42	2.23	12	1
1:A:46:LEU:HD12	1:A:46:LEU:HA	0.42	1.77	14	1
1:A:31:VAL:HG12	1:A:99:LYS:HG2	0.42	1.90	16	1
1:A:77:ARG:CZ	1:A:84:LEU:HB3	0.41	2.45	12	1
1:A:46:LEU:HD13	1:A:46:LEU:HA	0.41	1.76	19	1
1:A:57:ALA:HB1	1:A:59:MET:SD	0.41	2.55	11	1
1:A:63:LEU:HD22	1:A:96:TRP:HE3	0.41	1.74	17	1
1:A:80:ILE:HG13	1:A:82:LYS:CE	0.41	2.45	18	1
1:A:49:VAL:CA	1:A:83:PRO:HA	0.41	2.45	20	1
1:A:66:ASN:CB	1:A:72:TRP:HA	0.41	2.46	11	2
1:A:64:LEU:HD12	1:A:75:ILE:CG2	0.41	2.41	12	1
1:A:19:ALA:H	1:A:114:ALA:CA	0.41	2.29	15	1
1:A:48:ALA:HB3	1:A:85:LYS:CE	0.41	2.45	15	1
1:A:47:TYR:O	1:A:85:LYS:CB	0.41	2.68	17	1
1:A:29:GLY:HA3	1:A:102:ASN:CB	0.41	2.33	16	1
1:A:64:LEU:CD1	1:A:74:GLU:HA	0.41	2.46	16	1
1:A:47:TYR:N	1:A:85:LYS:CB	0.41	2.84	13	1
1:A:21:TYR:HE2	1:A:33:ILE:CB	0.41	2.24	8	1
1:A:57:ALA:HB3	1:A:59:MET:SD	0.41	2.56	12	1
1:A:61:LEU:C	1:A:77:ARG:HB3	0.41	2.36	12	1
1:A:64:LEU:CG	1:A:74:GLU:H	0.41	2.27	1	1
1:A:64:LEU:HB2	1:A:74:GLU:HB3	0.41	1.92	13	1
1:A:31:VAL:HG12	1:A:99:LYS:CG	0.41	2.46	16	1
1:A:20:THR:HA	1:A:113:ASP:HA	0.41	1.92	17	1
1:A:62:ILE:HG22	1:A:77:ARG:HA	0.41	1.91	18	1
1:A:59:MET:O	1:A:79:ASP:HB2	0.41	2.16	20	1
1:A:60:THR:HA	1:A:79:ASP:CB	0.41	2.33	20	1
1:A:58:ASP:O	1:A:103:ASN:HB3	0.41	2.16	8	1
1:A:61:LEU:H	1:A:79:ASP:HB2	0.41	1.75	18	1
1:A:85:LYS:HG2	1:A:98:TRP:CZ2	0.40	2.51	17	1
1:A:61:LEU:HB3	1:A:78:ASN:O	0.40	2.16	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ILE:HG22	1:A:76:LYS:N	0.40	2.31	3	1
1:A:74:GLU:CD	1:A:77:ARG:HH12	0.40	2.19	4	1
1:A:63:LEU:HD22	1:A:98:TRP:CE3	0.40	2.52	15	1
1:A:63:LEU:HD21	1:A:86:TYR:CD2	0.40	2.52	5	1
1:A:62:ILE:CD1	1:A:74:GLU:HG3	0.40	2.46	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	85/118 (72%)	71±2 (84±3%)	11±3 (13±3%)	2±1 (3±2%)	7	41
All	All	1700/2360 (72%)	1424 (84%)	226 (13%)	50 (3%)	7	41

All 21 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	75	ILE	9
1	A	67	VAL	8
1	A	55	VAL	6
1	A	46	LEU	3
1	A	80	ILE	3
1	A	33	ILE	2
1	A	70	ASN	2
1	A	57	ALA	2
1	A	87	GLU	2
1	A	69	GLY	2
1	A	90	TYR	1
1	A	54	ASN	1
1	A	94	LEU	1
1	A	58	ASP	1
1	A	83	PRO	1
1	A	88	ASP	1
1	A	107	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	104	SER	1
1	A	71	GLY	1
1	A	105	SER	1
1	A	72	TRP	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	73/102 (72%)	40±3 (55±4%)	33±3 (45±4%)	0 2
All	All	1460/2040 (72%)	802 (55%)	658 (45%)	0 2

All 71 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	24	THR	20
1	A	60	THR	18
1	A	32	CYS	16
1	A	97	ILE	16
1	A	105	SER	16
1	A	107	THR	16
1	A	111	SER	16
1	A	92	SER	15
1	A	65	ARG	15
1	A	91	THR	15
1	A	108	SER	14
1	A	115	THR	14
1	A	62	ILE	14
1	A	52	SER	13
1	A	63	LEU	13
1	A	80	ILE	13
1	A	94	LEU	13
1	A	95	SER	13
1	A	22	THR	12
1	A	28	LYS	12
1	A	74	GLU	12

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Mol	Chain	Res	Type	Models (Total)
1	A	77	ARG	12
1	A	84	LEU	12
1	A	104	SER	12
1	A	53	THR	12
1	A	64	LEU	12
1	A	78	ASN	12
1	A	46	LEU	11
1	A	66	ASN	11
1	A	76	LYS	11
1	A	82	LYS	11
1	A	50	LEU	11
1	A	101	LYS	11
1	A	30	GLU	11
1	A	55	VAL	10
1	A	81	ASP	10
1	A	106	GLU	10
1	A	20	THR	10
1	A	33	ILE	10
1	A	85	LYS	10
1	A	86	TYR	9
1	A	89	TYR	9
1	A	99	LYS	8
1	A	26	GLN	8
1	A	59	MET	8
1	A	25	ILE	7
1	A	54	ASN	7
1	A	58	ASP	6
1	A	109	ASN	6
1	A	113	ASP	6
1	A	31	VAL	6
1	A	112	LEU	6
1	A	75	ILE	5
1	A	87	GLU	5
1	A	61	LEU	5
1	A	88	ASP	5
1	A	56	ASN	5
1	A	98	TRP	4
1	A	100	ILE	4
1	A	47	TYR	4
1	A	79	ASP	3
1	A	70	ASN	3
1	A	90	TYR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	96	TRP	2
1	A	49	VAL	2
1	A	103	ASN	2
1	A	83	PRO	1
1	A	21	TYR	1
1	A	102	ASN	1
1	A	110	TYR	1
1	A	72	TRP	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