Full wwPDB NMR Structure Validation Report (i)

Feb 17, 2022 – 08:59 AM EST

PDB ID	:	1OWA
Title	:	Solution Structural Studies on Human Erythrocyte Alpha Spectrin N Terminal Tetramerization Domain
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Deposited on	:	2003-03-28

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:

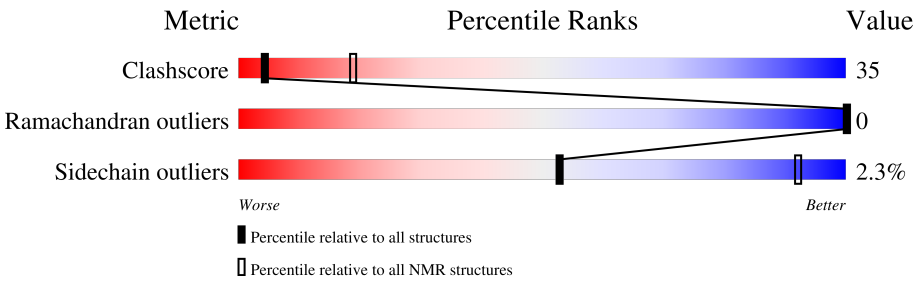
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	156	31% 32% 37%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:20-A:34 (15)	0.19	9
2	A:55-A:80, A:88-A:118, A:128-A:153 (83)	0.63	8

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, 5, 8, 10
2	2, 4, 7
3	3, 6, 9

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2597 atoms, of which 1294 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Spectrin alpha chain, erythrocyte.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	156	2597	810	1294	230	259	4	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: Spectrin alpha chain, erythrocyte

Chain A: 31% 32% 37%

M1 E2 Q3 F4 P5 K6 E7 T8 V9 V10 E11 S12 S13 G14 P15 K16 V17 L18 E19 T20 A21 E22 E23 I24 Q25 E26 R27 R28 V31 Y35 Q36 S37 F38 K39 E40 R41 V42 A43 E44 R45 G46 Q47 K48 L49 E50 D51 S52 Y53 H54 L55 Q56 V57 F58 K59 R60 D61 L65

G66 K67 W68 I69 M70 E71 K72 V73 N74 I75 L76 T77 D78 K79 S80 Y81 E82 D83 P84 T85 N86 I87 K90 K93 H94 Q95 S96 L97 E98 A99 E100 V101 K104 S105 R106 L107 M108 L111 R115 E116 E117 R118 F119 T120 M121 G122 H123 S124 A125 H126 E127 E128 T129 H132

L136 W140 D141 L142 L143 L146 T147 K150 L154 L155 R156

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: Spectrin alpha chain, erythrocyte

Chain A: 25% 37% • 37%

M1 E2 Q3 F4 P5 K6 E7 T8 V9 V10 E11 S12 S13 G14 P15 K16 V17 L18 E19 T20 A21 E22 E23 I24 Q25 E26 R27 V31 R34 Y35 Q36 S37 F38 K39 E40 R41 V42 A43 E44 R45 G46 Q47 K48 L49 E50 D51 S52 Y53 H54 L55 Q56 V57 F58 K59 R60 D61 L65

G66 K67 W68 I69 M70 E71 K72 V73 N74 I75 L76 T77 D78 K79 S80 Y81 E82 D83 P84 T85 N86 I87 K90 Y91 Q92 K93 H94 Q95 S96 L97 E98 A99 E100 V101 K104 S105 R106 L107 M108 S109 E110 L111 E112 K113 T114 R115 E116 E117 R118 F119 T120 M121 G122 H123 S124 A125 H126 E127

E128 T129 K130 L136 W140 D141 L142 L143 L146 T147 K150 G151 L154 L155 R156

4.2.2 Score per residue for model 2

• Molecule 1: Spectrin alpha chain, erythrocyte

Chain A: 31% 31% 37%

4.2.3 Score per residue for model 3

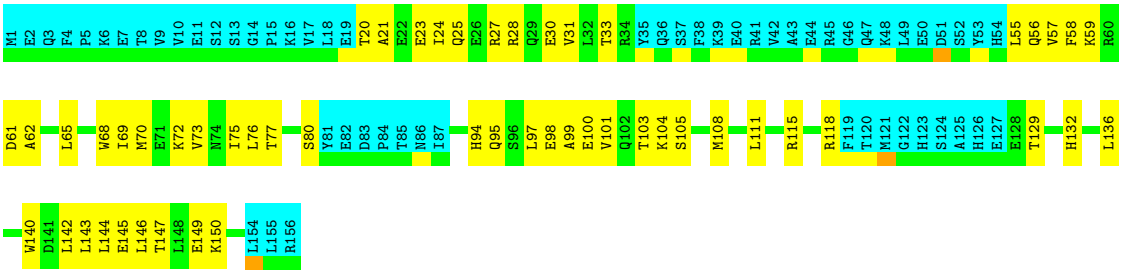
• Molecule 1: Spectrin alpha chain, erythrocyte

Chain A: 27% 36% 37%

4.2.4 Score per residue for model 4

• Molecule 1: Spectrin alpha chain, erythrocyte

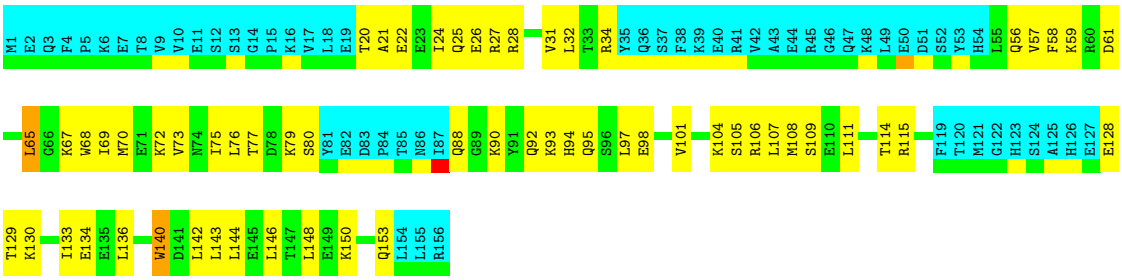
Chain A: 29% 34% 37%



4.2.5 Score per residue for model 5

• Molecule 1: Spectrin alpha chain, erythrocyte

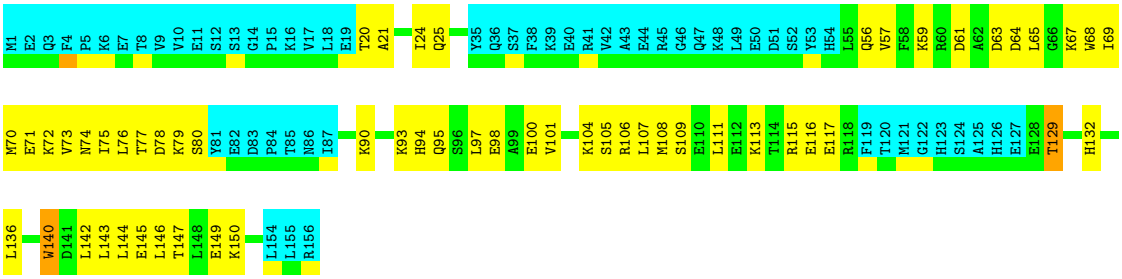
Chain A: 24% 37% • 37%



4.2.6 Score per residue for model 6

• Molecule 1: Spectrin alpha chain, erythrocyte

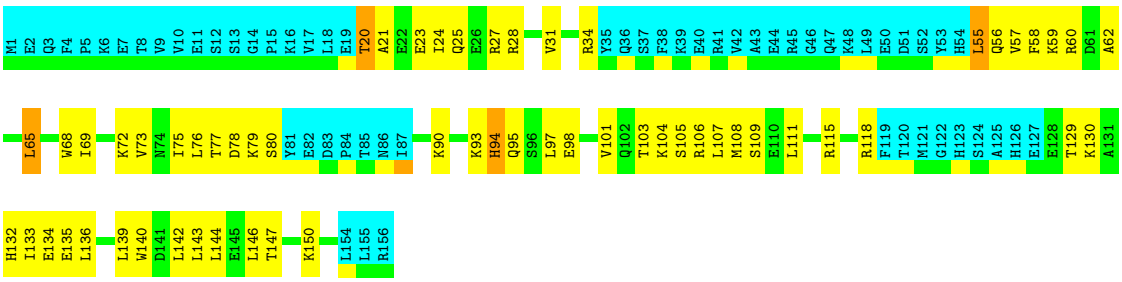
Chain A: 27% 35% • 37%



4.2.7 Score per residue for model 7

• Molecule 1: Spectrin alpha chain, erythrocyte

Chain A: 25% 35% • 37%



4.2.8 Score per residue for model 8 (medoid)

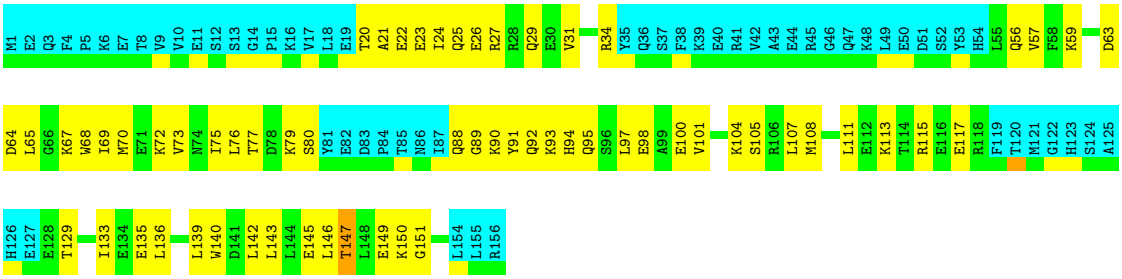
- Molecule 1: Spectrin alpha chain, erythrocyte

Chain A: 27% 35% • 37%

4.2.9 Score per residue for model 9

- Molecule 1: Spectrin alpha chain, erythrocyte

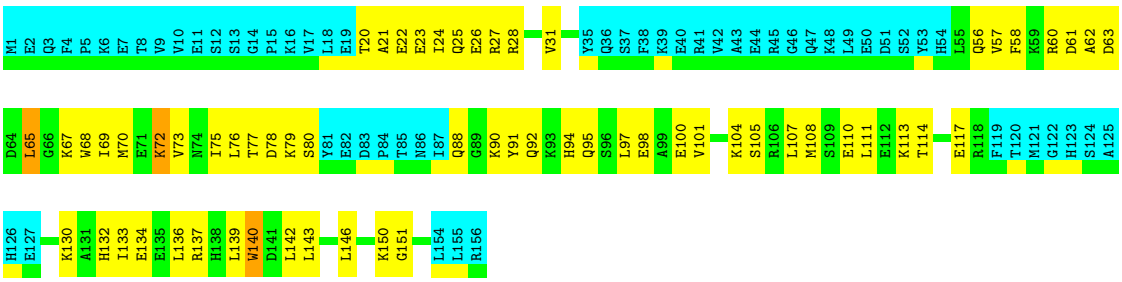
Chain A: 23% 39% • 37%



4.2.10 Score per residue for model 10

- Molecule 1: Spectrin alpha chain, erythrocyte

Chain A: 23% 38% • 37%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *Lowest Energy conformers*.

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)

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	824	836	833	59±5
All	All	8240	8360	8330	587

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ILE:HD11	1:A:93:LYS:HD2	0.96	1.36	7	2
1:A:65:LEU:HG	1:A:136:LEU:HD13	0.87	1.46	1	2
1:A:69:ILE:HG23	1:A:143:LEU:HD11	0.84	1.50	7	5
1:A:88:GLN:HA	1:A:91:TYR:CE2	0.83	2.08	9	1
1:A:62:ALA:HA	1:A:65:LEU:HD12	0.83	1.48	4	1
1:A:76:LEU:HD21	1:A:146:LEU:HD23	0.83	1.49	3	1
1:A:65:LEU:HD22	1:A:104:LYS:HE3	0.82	1.48	5	2
1:A:76:LEU:HD13	1:A:146:LEU:HD23	0.82	1.49	9	1
1:A:65:LEU:HD12	1:A:104:LYS:HE3	0.82	1.49	2	2
1:A:72:LYS:HD3	1:A:97:LEU:HD23	0.80	1.53	5	1
1:A:69:ILE:O	1:A:73:VAL:HG13	0.80	1.77	10	2
1:A:65:LEU:HB3	1:A:136:LEU:HD21	0.80	1.51	4	1
1:A:62:ALA:HB1	1:A:132:HIS:CD2	0.79	2.13	7	1
1:A:103:THR:O	1:A:106:ARG:HG2	0.78	1.79	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:THR:HA	1:A:150:LYS:HE2	0.77	1.55	6	1
1:A:72:LYS:HB2	1:A:143:LEU:HD21	0.76	1.57	1	1
1:A:65:LEU:HD23	1:A:136:LEU:HD13	0.76	1.57	2	2
1:A:68:TRP:CD1	1:A:104:LYS:HE3	0.75	2.17	7	2
1:A:68:TRP:HE1	1:A:100:GLU:HB3	0.75	1.42	1	7
1:A:72:LYS:HG2	1:A:97:LEU:HD22	0.74	1.59	1	1
1:A:69:ILE:O	1:A:73:VAL:HG23	0.74	1.83	7	2
1:A:76:LEU:O	1:A:79:LYS:HG2	0.74	1.83	7	7
1:A:65:LEU:HD23	1:A:136:LEU:HD23	0.73	1.58	10	1
1:A:97:LEU:O	1:A:101:VAL:HG23	0.73	1.84	5	9
1:A:72:LYS:HD2	1:A:97:LEU:HD11	0.72	1.61	7	1
1:A:65:LEU:HD22	1:A:136:LEU:HD23	0.71	1.62	6	1
1:A:90:LYS:HD2	1:A:151:GLY:HA2	0.71	1.62	9	1
1:A:27:ARG:O	1:A:31:VAL:HG23	0.71	1.85	9	6
1:A:111:LEU:O	1:A:114:THR:HG22	0.71	1.85	5	1
1:A:58:PHE:CZ	1:A:129:THR:HG23	0.70	2.20	1	1
1:A:93:LYS:O	1:A:97:LEU:HD13	0.70	1.86	3	4
1:A:90:LYS:O	1:A:93:LYS:HG2	0.70	1.87	6	2
1:A:72:LYS:HD3	1:A:143:LEU:HD13	0.70	1.62	10	1
1:A:142:LEU:O	1:A:146:LEU:HD23	0.70	1.87	4	1
1:A:69:ILE:O	1:A:72:LYS:HG2	0.69	1.88	10	1
1:A:28:ARG:O	1:A:32:LEU:HD23	0.69	1.87	5	1
1:A:105:SER:O	1:A:108:MET:HB2	0.69	1.86	5	6
1:A:90:LYS:CG	1:A:150:LYS:HE3	0.68	2.18	9	1
1:A:70:MET:O	1:A:73:VAL:HG22	0.68	1.88	9	2
1:A:76:LEU:CD1	1:A:146:LEU:HD23	0.68	2.18	9	1
1:A:90:LYS:HG3	1:A:150:LYS:HE3	0.68	1.64	9	1
1:A:147:THR:O	1:A:150:LYS:HG2	0.68	1.88	8	4
1:A:105:SER:O	1:A:108:MET:HB3	0.68	1.88	2	4
1:A:132:HIS:O	1:A:136:LEU:HD13	0.67	1.89	10	3
1:A:77:THR:O	1:A:80:SER:HB2	0.67	1.90	7	4
1:A:69:ILE:HG23	1:A:143:LEU:CD1	0.67	2.19	7	3
1:A:94:HIS:NE2	1:A:150:LYS:HE2	0.67	2.05	9	1
1:A:90:LYS:HA	1:A:93:LYS:HE2	0.66	1.66	7	1
1:A:109:SER:O	1:A:112:GLU:HG2	0.66	1.90	2	1
1:A:68:TRP:CD1	1:A:104:LYS:HE2	0.66	2.24	8	1
1:A:94:HIS:CE1	1:A:147:THR:HG22	0.66	2.25	7	2
1:A:108:MET:HG3	1:A:133:ILE:HD11	0.66	1.65	2	2
1:A:68:TRP:CZ2	1:A:72:LYS:HE2	0.66	2.26	5	1
1:A:70:MET:HA	1:A:73:VAL:HG12	0.65	1.67	8	6
1:A:94:HIS:CD2	1:A:147:THR:HG22	0.65	2.26	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:ARG:HD2	1:A:129:THR:HB	0.65	1.67	2	1
1:A:68:TRP:CH2	1:A:72:LYS:HE3	0.64	2.26	2	2
1:A:134:GLU:O	1:A:137:ARG:HG2	0.64	1.93	10	1
1:A:142:LEU:O	1:A:146:LEU:HG	0.64	1.93	7	6
1:A:20:THR:HB	1:A:23:GLU:CB	0.63	2.23	4	6
1:A:27:ARG:O	1:A:31:VAL:HG22	0.63	1.93	7	2
1:A:133:ILE:HA	1:A:136:LEU:HD12	0.63	1.70	9	1
1:A:97:LEU:HD23	1:A:100:GLU:OE1	0.63	1.93	1	2
1:A:65:LEU:HA	1:A:104:LYS:CE	0.63	2.24	10	2
1:A:104:LYS:HD3	1:A:107:LEU:HD12	0.63	1.71	6	1
1:A:62:ALA:HB1	1:A:132:HIS:NE2	0.63	2.08	3	3
1:A:63:ASP:O	1:A:67:LYS:HG3	0.63	1.94	9	4
1:A:76:LEU:CD2	1:A:146:LEU:HD13	0.63	2.24	7	2
1:A:108:MET:CG	1:A:133:ILE:HD11	0.63	2.24	10	2
1:A:115:ARG:HD3	1:A:129:THR:HG21	0.63	1.70	9	1
1:A:79:LYS:HA	1:A:90:LYS:NZ	0.62	2.08	7	2
1:A:65:LEU:HD12	1:A:136:LEU:HD13	0.62	1.71	3	2
1:A:73:VAL:O	1:A:77:THR:HG23	0.62	1.94	2	3
1:A:75:ILE:HD11	1:A:93:LYS:HD3	0.62	1.70	1	2
1:A:98:GLU:O	1:A:101:VAL:HG22	0.62	1.94	3	1
1:A:20:THR:O	1:A:24:ILE:HG22	0.61	1.95	8	2
1:A:68:TRP:CZ2	1:A:101:VAL:HA	0.61	2.30	5	1
1:A:72:LYS:HE2	1:A:97:LEU:HB3	0.61	1.71	2	3
1:A:72:LYS:HB3	1:A:143:LEU:HD11	0.61	1.72	1	1
1:A:68:TRP:CH2	1:A:101:VAL:HG22	0.61	2.31	10	3
1:A:95:GLN:O	1:A:98:GLU:HB2	0.61	1.95	7	2
1:A:94:HIS:HA	1:A:97:LEU:HD12	0.61	1.72	2	1
1:A:72:LYS:HG3	1:A:97:LEU:HD22	0.61	1.71	9	1
1:A:76:LEU:HD21	1:A:146:LEU:HB3	0.61	1.71	2	1
1:A:72:LYS:O	1:A:76:LEU:HG	0.60	1.95	5	3
1:A:135:GLU:O	1:A:139:LEU:HD23	0.60	1.96	9	3
1:A:90:LYS:HG2	1:A:93:LYS:NZ	0.60	2.11	7	1
1:A:69:ILE:HD11	1:A:140:TRP:CD1	0.60	2.31	3	2
1:A:145:GLU:O	1:A:149:GLU:HG3	0.60	1.96	9	3
1:A:68:TRP:CD2	1:A:104:LYS:HG3	0.60	2.31	3	1
1:A:95:GLN:O	1:A:98:GLU:HB3	0.60	1.97	1	8
1:A:73:VAL:HA	1:A:76:LEU:HD12	0.60	1.73	9	3
1:A:76:LEU:HD23	1:A:94:HIS:CE1	0.60	2.31	5	1
1:A:94:HIS:O	1:A:98:GLU:HG3	0.60	1.96	7	2
1:A:72:LYS:HE2	1:A:143:LEU:HB3	0.60	1.72	10	1
1:A:25:GLN:O	1:A:28:ARG:HG2	0.59	1.97	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LYS:HD2	1:A:143:LEU:HD13	0.59	1.74	9	1
1:A:26:GLU:O	1:A:29:GLN:HG2	0.59	1.98	9	1
1:A:68:TRP:CZ3	1:A:72:LYS:HD2	0.59	2.33	10	1
1:A:113:LYS:O	1:A:117:GLU:HG3	0.59	1.98	3	4
1:A:76:LEU:CD2	1:A:146:LEU:HD23	0.59	2.28	3	1
1:A:101:VAL:HG13	1:A:140:TRP:HE1	0.59	1.58	6	2
1:A:70:MET:HA	1:A:73:VAL:CG1	0.58	2.28	1	6
1:A:115:ARG:CD	1:A:129:THR:HB	0.58	2.27	2	1
1:A:93:LYS:HB2	1:A:150:LYS:NZ	0.58	2.13	9	1
1:A:72:LYS:CD	1:A:97:LEU:HD23	0.58	2.26	5	1
1:A:76:LEU:HG	1:A:146:LEU:HD13	0.58	1.75	2	1
1:A:97:LEU:O	1:A:97:LEU:HD23	0.58	1.97	7	1
1:A:68:TRP:CE2	1:A:104:LYS:HG3	0.58	2.33	7	1
1:A:142:LEU:O	1:A:146:LEU:HD13	0.58	1.99	9	3
1:A:72:LYS:CB	1:A:143:LEU:HD21	0.57	2.29	1	1
1:A:65:LEU:CD2	1:A:136:LEU:HD13	0.57	2.29	2	2
1:A:144:LEU:O	1:A:148:LEU:HD23	0.57	1.99	5	1
1:A:101:VAL:HG11	1:A:144:LEU:HD21	0.57	1.74	6	2
1:A:20:THR:HB	1:A:23:GLU:HB2	0.57	1.76	10	2
1:A:24:ILE:O	1:A:28:ARG:HG2	0.57	1.99	4	2
1:A:77:THR:O	1:A:80:SER:HB3	0.57	2.00	8	6
1:A:101:VAL:HG13	1:A:140:TRP:NE1	0.57	2.14	5	2
1:A:91:TYR:HA	1:A:94:HIS:CD2	0.56	2.35	3	2
1:A:75:ILE:O	1:A:79:LYS:HE2	0.56	2.00	8	1
1:A:75:ILE:HG21	1:A:97:LEU:CD2	0.56	2.29	5	1
1:A:68:TRP:CZ2	1:A:72:LYS:HE3	0.56	2.36	7	2
1:A:100:GLU:HA	1:A:103:THR:OG1	0.56	2.01	4	1
1:A:25:GLN:HA	1:A:28:ARG:CD	0.56	2.30	10	2
1:A:111:LEU:HD23	1:A:133:ILE:HD12	0.56	1.78	7	2
1:A:66:GLY:O	1:A:70:MET:HG3	0.56	2.01	1	1
1:A:143:LEU:HA	1:A:146:LEU:HD12	0.56	1.78	2	6
1:A:20:THR:HB	1:A:23:GLU:HB3	0.56	1.78	4	3
1:A:68:TRP:CH2	1:A:101:VAL:HG12	0.55	2.36	3	1
1:A:68:TRP:CH2	1:A:72:LYS:HG3	0.55	2.37	5	1
1:A:68:TRP:O	1:A:72:LYS:HD2	0.55	2.02	8	1
1:A:65:LEU:HD12	1:A:136:LEU:HD22	0.55	1.76	1	2
1:A:71:GLU:HA	1:A:74:ASN:ND2	0.55	2.17	6	1
1:A:65:LEU:HD13	1:A:136:LEU:HD22	0.55	1.78	6	1
1:A:132:HIS:NE2	1:A:136:LEU:HD11	0.55	2.15	8	1
1:A:76:LEU:HD21	1:A:146:LEU:HD13	0.55	1.79	7	1
1:A:90:LYS:CA	1:A:93:LYS:HE2	0.55	2.32	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:ARG:HH12	1:A:133:ILE:HD13	0.55	1.62	2	1
1:A:94:HIS:NE2	1:A:147:THR:HG22	0.55	2.17	4	2
1:A:145:GLU:O	1:A:149:GLU:HG2	0.55	2.01	6	1
1:A:68:TRP:CZ3	1:A:140:TRP:NE1	0.54	2.75	1	3
1:A:70:MET:CA	1:A:73:VAL:HG12	0.54	2.32	8	6
1:A:140:TRP:O	1:A:144:LEU:HG	0.54	2.01	4	2
1:A:72:LYS:HD3	1:A:97:LEU:CD2	0.54	2.30	5	1
1:A:76:LEU:CD1	1:A:150:LYS:HD3	0.54	2.33	6	1
1:A:55:LEU:HD12	1:A:118:ARG:NH1	0.54	2.17	3	1
1:A:118:ARG:NH1	1:A:118:ARG:HB3	0.54	2.17	3	1
1:A:74:ASN:OD1	1:A:75:ILE:N	0.54	2.40	6	1
1:A:72:LYS:HD2	1:A:97:LEU:CD1	0.54	2.31	7	1
1:A:104:LYS:O	1:A:107:LEU:HB3	0.54	2.03	5	1
1:A:115:ARG:HD2	1:A:129:THR:HG21	0.54	1.79	5	1
1:A:61:ASP:OD1	1:A:62:ALA:N	0.53	2.42	10	1
1:A:69:ILE:HD13	1:A:143:LEU:HD23	0.53	1.80	1	1
1:A:65:LEU:CD2	1:A:136:LEU:HD23	0.53	2.30	10	1
1:A:24:ILE:HG22	1:A:27:ARG:HH21	0.53	1.63	2	1
1:A:58:PHE:CE1	1:A:111:LEU:CD1	0.53	2.92	4	2
1:A:113:LYS:O	1:A:116:GLU:HG2	0.53	2.02	6	1
1:A:20:THR:O	1:A:24:ILE:HG12	0.53	2.04	2	2
1:A:72:LYS:HD2	1:A:143:LEU:HD21	0.53	1.80	3	2
1:A:69:ILE:CG2	1:A:143:LEU:HD11	0.53	2.31	7	3
1:A:143:LEU:HD23	1:A:146:LEU:HD12	0.53	1.79	7	3
1:A:55:LEU:O	1:A:59:LYS:HG3	0.53	2.04	7	2
1:A:72:LYS:CE	1:A:143:LEU:HB3	0.53	2.33	10	1
1:A:67:LYS:HA	1:A:70:MET:CE	0.52	2.35	5	2
1:A:22:GLU:O	1:A:26:GLU:HG3	0.52	2.03	9	4
1:A:21:ALA:O	1:A:25:GLN:HG3	0.52	2.04	8	1
1:A:68:TRP:NE1	1:A:72:LYS:HE2	0.52	2.19	8	1
1:A:72:LYS:HD2	1:A:143:LEU:CG	0.52	2.35	6	1
1:A:94:HIS:HD2	1:A:147:THR:HG22	0.52	1.64	9	1
1:A:68:TRP:CZ3	1:A:143:LEU:HD23	0.52	2.39	1	1
1:A:28:ARG:HA	1:A:31:VAL:CG2	0.51	2.34	7	2
1:A:104:LYS:HD2	1:A:140:TRP:CZ2	0.51	2.40	9	1
1:A:61:ASP:CB	1:A:111:LEU:HD21	0.51	2.36	1	1
1:A:20:THR:O	1:A:24:ILE:HG23	0.51	2.06	2	1
1:A:61:ASP:O	1:A:65:LEU:HB2	0.51	2.05	3	3
1:A:93:LYS:HB2	1:A:150:LYS:HZ1	0.51	1.65	9	1
1:A:72:LYS:HD2	1:A:143:LEU:CD2	0.51	2.36	3	2
1:A:68:TRP:HB3	1:A:104:LYS:HE2	0.51	1.82	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ILE:HD12	1:A:93:LYS:HE2	0.51	1.82	2	1
1:A:69:ILE:HG23	1:A:143:LEU:HD22	0.50	1.82	6	2
1:A:88:GLN:O	1:A:92:GLN:HG3	0.50	2.06	5	3
1:A:58:PHE:CE2	1:A:111:LEU:CD1	0.50	2.94	5	1
1:A:55:LEU:HD23	1:A:118:ARG:NH1	0.50	2.22	1	1
1:A:97:LEU:O	1:A:101:VAL:HG13	0.50	2.06	3	1
1:A:90:LYS:HG3	1:A:150:LYS:HG2	0.50	1.84	9	1
1:A:93:LYS:O	1:A:97:LEU:HG	0.50	2.07	9	1
1:A:65:LEU:HD13	1:A:136:LEU:CD2	0.50	2.36	6	1
1:A:72:LYS:CD	1:A:143:LEU:HD13	0.50	2.35	10	1
1:A:105:SER:N	1:A:140:TRP:HH2	0.50	2.04	10	1
1:A:90:LYS:HG3	1:A:93:LYS:HE2	0.50	1.83	6	1
1:A:107:LEU:O	1:A:111:LEU:HG	0.50	2.06	1	1
1:A:93:LYS:O	1:A:97:LEU:HD12	0.49	2.07	2	2
1:A:72:LYS:HE2	1:A:97:LEU:HD23	0.49	1.83	3	1
1:A:72:LYS:CE	1:A:97:LEU:HB3	0.49	2.36	2	1
1:A:147:THR:HG23	1:A:150:LYS:HE2	0.49	1.84	7	1
1:A:104:LYS:HD2	1:A:140:TRP:NE1	0.49	2.22	9	1
1:A:92:GLN:O	1:A:95:GLN:HG2	0.49	2.07	3	1
1:A:130:LYS:O	1:A:134:GLU:HG3	0.49	2.08	5	4
1:A:21:ALA:O	1:A:25:GLN:CG	0.49	2.60	8	1
1:A:21:ALA:O	1:A:25:GLN:CB	0.49	2.61	10	8
1:A:90:LYS:HE2	1:A:150:LYS:NZ	0.49	2.22	10	1
1:A:94:HIS:CD2	1:A:150:LYS:HE3	0.49	2.43	7	2
1:A:20:THR:O	1:A:24:ILE:HG13	0.49	2.08	6	5
1:A:72:LYS:HG3	1:A:97:LEU:CD2	0.49	2.38	8	1
1:A:76:LEU:HD23	1:A:94:HIS:HE1	0.49	1.64	5	1
1:A:65:LEU:HD22	1:A:104:LYS:CE	0.49	2.33	1	1
1:A:104:LYS:HB3	1:A:140:TRP:HZ2	0.49	1.68	9	2
1:A:64:ASP:HA	1:A:67:LYS:HD3	0.49	1.84	6	1
1:A:65:LEU:HA	1:A:104:LYS:NZ	0.48	2.23	10	1
1:A:90:LYS:HE2	1:A:150:LYS:HZ1	0.48	1.68	10	1
1:A:104:LYS:HD2	1:A:140:TRP:HE1	0.48	1.69	9	1
1:A:146:LEU:HD12	1:A:149:GLU:OE1	0.48	2.07	9	1
1:A:115:ARG:HD2	1:A:130:LYS:HE3	0.48	1.85	1	1
1:A:68:TRP:HB2	1:A:104:LYS:HE3	0.48	1.86	8	1
1:A:76:LEU:CG	1:A:146:LEU:HD13	0.48	2.38	2	1
1:A:108:MET:HE2	1:A:133:ILE:HD11	0.48	1.84	5	1
1:A:65:LEU:CD1	1:A:104:LYS:HE3	0.48	2.38	10	1
1:A:111:LEU:CD2	1:A:133:ILE:HD12	0.48	2.38	10	1
1:A:105:SER:HB2	1:A:140:TRP:HH2	0.48	1.69	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:TRP:HH2	1:A:101:VAL:HG22	0.48	1.67	10	3
1:A:56:GLN:O	1:A:60:ARG:HG3	0.48	2.08	10	1
1:A:65:LEU:O	1:A:104:LYS:HE3	0.47	2.08	4	1
1:A:91:TYR:HA	1:A:94:HIS:NE2	0.47	2.23	2	2
1:A:107:LEU:O	1:A:111:LEU:N	0.47	2.44	5	8
1:A:136:LEU:O	1:A:140:TRP:HB2	0.47	2.09	3	1
1:A:76:LEU:HD12	1:A:79:LYS:CE	0.47	2.40	7	1
1:A:91:TYR:CD1	1:A:92:GLN:N	0.47	2.82	9	1
1:A:58:PHE:CZ	1:A:115:ARG:HD2	0.47	2.44	5	1
1:A:106:ARG:O	1:A:109:SER:HB2	0.47	2.10	1	3
1:A:146:LEU:HA	1:A:149:GLU:OE1	0.47	2.10	9	1
1:A:61:ASP:O	1:A:65:LEU:N	0.47	2.46	10	5
1:A:65:LEU:HD22	1:A:108:MET:SD	0.47	2.50	4	1
1:A:58:PHE:HA	1:A:61:ASP:OD2	0.47	2.10	10	1
1:A:115:ARG:NH1	1:A:133:ILE:HG21	0.46	2.25	2	1
1:A:112:GLU:HB2	1:A:115:ARG:NH2	0.46	2.25	2	1
1:A:72:LYS:O	1:A:75:ILE:HG22	0.46	2.09	9	6
1:A:115:ARG:HD2	1:A:129:THR:CB	0.46	2.40	2	1
1:A:75:ILE:HD11	1:A:93:LYS:CD	0.46	2.40	6	1
1:A:94:HIS:CE1	1:A:147:THR:CG2	0.46	2.97	7	1
1:A:56:GLN:O	1:A:59:LYS:HB3	0.46	2.10	6	2
1:A:76:LEU:C	1:A:76:LEU:HD13	0.46	2.30	10	1
1:A:115:ARG:HG2	1:A:129:THR:HG21	0.46	1.86	6	1
1:A:90:LYS:HA	1:A:93:LYS:CE	0.46	2.41	7	1
1:A:115:ARG:HH12	1:A:133:ILE:HG21	0.46	1.69	2	1
1:A:64:ASP:HA	1:A:67:LYS:HD2	0.46	1.88	8	2
1:A:90:LYS:CD	1:A:151:GLY:HA2	0.45	2.39	9	1
1:A:68:TRP:CZ2	1:A:72:LYS:CE	0.45	2.99	7	1
1:A:68:TRP:NE1	1:A:100:GLU:HB3	0.45	2.27	4	3
1:A:58:PHE:HB2	1:A:118:ARG:NE	0.45	2.25	7	1
1:A:24:ILE:HG13	1:A:25:GLN:N	0.45	2.27	2	1
1:A:72:LYS:HB3	1:A:143:LEU:HD21	0.45	1.89	3	1
1:A:72:LYS:O	1:A:75:ILE:CG2	0.45	2.65	6	3
1:A:62:ALA:CA	1:A:65:LEU:HD12	0.45	2.32	4	1
1:A:69:ILE:O	1:A:73:VAL:HG12	0.45	2.10	4	1
1:A:24:ILE:O	1:A:28:ARG:N	0.45	2.49	5	1
1:A:91:TYR:CE2	1:A:95:GLN:NE2	0.45	2.84	10	1
1:A:21:ALA:O	1:A:25:GLN:N	0.45	2.47	4	2
1:A:75:ILE:O	1:A:78:ASP:HB3	0.45	2.11	6	3
1:A:72:LYS:NZ	1:A:97:LEU:HG	0.45	2.27	7	1
1:A:132:HIS:O	1:A:136:LEU:HG	0.45	2.12	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:O	1:A:76:LEU:HD13	0.45	2.12	2	1
1:A:90:LYS:HE2	1:A:150:LYS:HG3	0.45	1.89	8	1
1:A:25:GLN:HG2	1:A:28:ARG:HE	0.44	1.72	8	1
1:A:69:ILE:HG21	1:A:139:LEU:CD2	0.44	2.42	10	1
1:A:113:LYS:O	1:A:117:GLU:N	0.44	2.50	10	1
1:A:30:GLU:O	1:A:33:THR:HG22	0.44	2.13	4	1
1:A:68:TRP:CE2	1:A:72:LYS:CE	0.44	3.00	8	1
1:A:58:PHE:HB2	1:A:114:THR:HG21	0.44	1.89	1	1
1:A:101:VAL:HG23	1:A:102:GLN:N	0.44	2.28	3	1
1:A:56:GLN:O	1:A:59:LYS:HB2	0.44	2.13	5	5
1:A:76:LEU:HD21	1:A:146:LEU:HD12	0.44	1.88	4	1
1:A:65:LEU:CG	1:A:136:LEU:HD13	0.44	2.42	5	1
1:A:76:LEU:HD22	1:A:79:LYS:CE	0.44	2.42	10	1
1:A:68:TRP:CE3	1:A:140:TRP:NE1	0.44	2.86	1	1
1:A:61:ASP:O	1:A:65:LEU:HG	0.44	2.13	4	1
1:A:61:ASP:HB3	1:A:111:LEU:HD21	0.43	1.89	1	1
1:A:94:HIS:ND1	1:A:95:GLN:N	0.43	2.66	3	2
1:A:94:HIS:CD2	1:A:147:THR:CG2	0.43	3.01	8	1
1:A:65:LEU:CD1	1:A:136:LEU:HD13	0.43	2.40	3	1
1:A:97:LEU:HD23	1:A:101:VAL:HG23	0.43	1.90	7	1
1:A:55:LEU:CD1	1:A:118:ARG:NH1	0.43	2.80	3	1
1:A:72:LYS:HG2	1:A:143:LEU:HD11	0.43	1.90	3	1
1:A:68:TRP:CZ3	1:A:72:LYS:CD	0.43	3.02	10	1
1:A:68:TRP:CD1	1:A:72:LYS:HE2	0.43	2.48	8	1
1:A:24:ILE:HG23	1:A:25:GLN:N	0.43	2.28	5	1
1:A:104:LYS:HG2	1:A:140:TRP:HE1	0.43	1.73	1	1
1:A:104:LYS:HD2	1:A:107:LEU:HD12	0.43	1.90	1	1
1:A:68:TRP:CB	1:A:104:LYS:HE2	0.43	2.43	2	1
1:A:76:LEU:HD13	1:A:76:LEU:C	0.43	2.34	2	1
1:A:23:GLU:HG2	1:A:27:ARG:HH12	0.43	1.73	4	1
1:A:72:LYS:O	1:A:76:LEU:HB2	0.43	2.14	10	1
1:A:68:TRP:CZ2	1:A:72:LYS:HG3	0.43	2.49	5	1
1:A:130:LYS:O	1:A:133:ILE:HG22	0.43	2.14	5	1
1:A:58:PHE:HE1	1:A:111:LEU:O	0.43	1.95	8	1
1:A:104:LYS:HG2	1:A:140:TRP:NE1	0.42	2.30	1	1
1:A:25:GLN:HA	1:A:28:ARG:HD3	0.42	1.90	2	1
1:A:55:LEU:CD2	1:A:59:LYS:HE3	0.42	2.44	4	1
1:A:25:GLN:HA	1:A:28:ARG:HG2	0.42	1.91	10	2
1:A:72:LYS:CD	1:A:143:LEU:HD22	0.42	2.45	9	1
1:A:89:GLY:O	1:A:93:LYS:HD3	0.42	2.15	9	1
1:A:99:ALA:O	1:A:103:THR:HG23	0.42	2.15	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ALA:O	1:A:25:GLN:HB2	0.42	2.15	4	2
1:A:72:LYS:HA	1:A:75:ILE:HG22	0.42	1.91	1	1
1:A:115:ARG:NE	1:A:130:LYS:HE2	0.42	2.30	1	1
1:A:73:VAL:HG13	1:A:74:ASN:N	0.42	2.30	3	1
1:A:68:TRP:NE1	1:A:72:LYS:CE	0.42	2.82	8	1
1:A:65:LEU:CD1	1:A:104:LYS:HE2	0.42	2.44	9	1
1:A:104:LYS:HB3	1:A:140:TRP:CZ2	0.42	2.50	1	2
1:A:69:ILE:HG23	1:A:143:LEU:CD2	0.42	2.45	5	1
1:A:111:LEU:HD23	1:A:133:ILE:CD1	0.42	2.45	7	1
1:A:79:LYS:HA	1:A:90:LYS:CE	0.42	2.43	2	1
1:A:70:MET:C	1:A:73:VAL:HG12	0.42	2.35	3	2
1:A:65:LEU:HA	1:A:104:LYS:HE2	0.42	1.91	5	1
1:A:150:LYS:O	1:A:153:GLN:HG2	0.42	2.14	5	1
1:A:22:GLU:O	1:A:26:GLU:HG2	0.42	2.14	10	1
1:A:106:ARG:O	1:A:109:SER:HB3	0.41	2.13	2	2
1:A:56:GLN:O	1:A:60:ARG:N	0.41	2.53	7	2
1:A:68:TRP:CG	1:A:104:LYS:HG3	0.41	2.50	6	1
1:A:139:LEU:HD22	1:A:139:LEU:N	0.41	2.31	7	1
1:A:90:LYS:O	1:A:94:HIS:ND1	0.41	2.48	6	1
1:A:90:LYS:HE3	1:A:150:LYS:HE3	0.41	1.90	2	1
1:A:101:VAL:HB	1:A:140:TRP:CH2	0.41	2.51	3	1
1:A:70:MET:HA	1:A:73:VAL:CG2	0.41	2.46	2	1
1:A:101:VAL:HG11	1:A:144:LEU:CD2	0.41	2.45	6	1
1:A:112:GLU:CB	1:A:115:ARG:NH2	0.41	2.84	2	1
1:A:58:PHE:HZ	1:A:129:THR:HG23	0.41	1.75	4	1
1:A:115:ARG:CD	1:A:129:THR:HG21	0.41	2.46	5	1
1:A:94:HIS:CD2	1:A:150:LYS:HG3	0.41	2.51	6	1
1:A:64:ASP:O	1:A:67:LYS:HB2	0.41	2.15	8	2
1:A:88:GLN:HA	1:A:91:TYR:CZ	0.41	2.47	9	1
1:A:69:ILE:HA	1:A:143:LEU:CD2	0.41	2.46	1	1
1:A:114:THR:O	1:A:117:GLU:HB2	0.41	2.15	1	1
1:A:145:GLU:O	1:A:149:GLU:N	0.41	2.53	2	1
1:A:23:GLU:HG2	1:A:27:ARG:NH1	0.41	2.31	4	1
1:A:76:LEU:HD21	1:A:146:LEU:CD1	0.41	2.46	4	1
1:A:114:THR:O	1:A:117:GLU:HB3	0.41	2.16	8	1
1:A:68:TRP:HH2	1:A:101:VAL:HG12	0.41	1.73	3	1
1:A:75:ILE:O	1:A:78:ASP:HB2	0.41	2.15	8	1
1:A:110:GLU:O	1:A:114:THR:N	0.41	2.53	10	1
1:A:90:LYS:CE	1:A:150:LYS:HG3	0.40	2.46	8	1
1:A:68:TRP:CE2	1:A:72:LYS:HE2	0.40	2.51	5	1
1:A:56:GLN:O	1:A:60:ARG:HG2	0.40	2.16	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:THR:HB	1:A:23:GLU:H	0.40	1.76	7	1
1:A:104:LYS:HD2	1:A:140:TRP:CE2	0.40	2.50	9	1
1:A:65:LEU:CB	1:A:136:LEU:HD21	0.40	2.35	4	1
1:A:65:LEU:HD21	1:A:140:TRP:CZ3	0.40	2.51	6	1
1:A:71:GLU:O	1:A:74:ASN:ND2	0.40	2.55	6	1
1:A:74:ASN:CG	1:A:75:ILE:N	0.40	2.75	6	1
1:A:69:ILE:HG21	1:A:139:LEU:HD23	0.40	1.92	10	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	98/156 (63%)	98±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	980/1560 (63%)	979 (100%)	1 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	91/144 (63%)	89±2 (98±2%)	2±2 (2±2%)	53	92
All	All	910/1440 (63%)	889 (98%)	21 (2%)	53	92

All 10 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	140	TRP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	65	LEU	4
1	A	55	LEU	2
1	A	94	HIS	2
1	A	72	LYS	2
1	A	79	LYS	1
1	A	129	THR	1
1	A	20	THR	1
1	A	115	ARG	1
1	A	147	THR	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