Full wwPDB NMR Structure Validation Report (i)

Feb 28, 2022 – 12:15 AM EST

PDB ID	:	2DAW
Title	:	Solution structure of the RWD domain of human RWD omain containing protein 2
Authors	:	Yoneyama, M.; Kigawa, T.; Sato, M.; Tochio, N.; Koshiba, S.; Inoue, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-12-14

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:

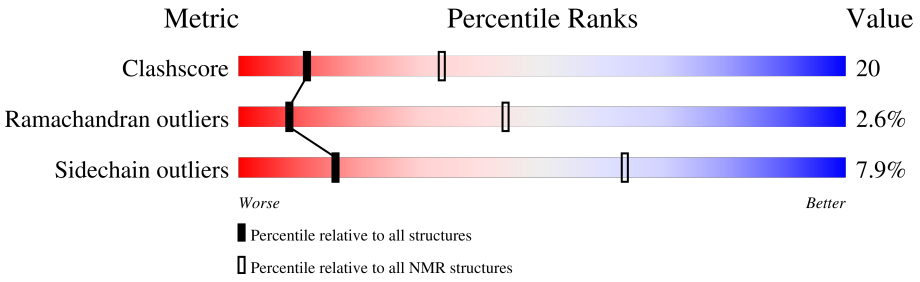
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	154	60% 21% •• 17%

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:11-A:53, A:58-A:142 (128)	0.32	1

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2410 atoms, of which 1210 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RWD domain containing protein 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	154	2410	763	1210	198	232	7	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9UIY3
A	2	SER	-	cloning artifact	UNP Q9UIY3
A	3	SER	-	cloning artifact	UNP Q9UIY3
A	4	GLY	-	cloning artifact	UNP Q9UIY3
A	5	SER	-	cloning artifact	UNP Q9UIY3
A	6	SER	-	cloning artifact	UNP Q9UIY3
A	7	GLY	-	cloning artifact	UNP Q9UIY3
A	90	LEU	VAL	SEE REMARK 999	UNP Q9UIY3
A	149	SER	-	cloning artifact	UNP Q9UIY3
A	150	GLY	-	cloning artifact	UNP Q9UIY3
A	151	PRO	-	cloning artifact	UNP Q9UIY3
A	152	SER	-	cloning artifact	UNP Q9UIY3
A	153	SER	-	cloning artifact	UNP Q9UIY3
A	154	GLY	-	cloning artifact	UNP Q9UIY3

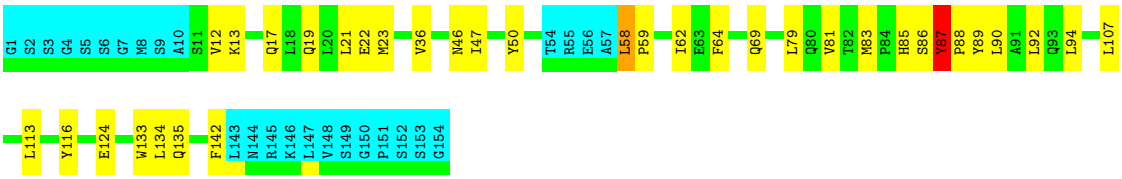
4 Residue-property plots (i)

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: RWD domain containing protein 2

Chain A: 60% 21% •• 17%



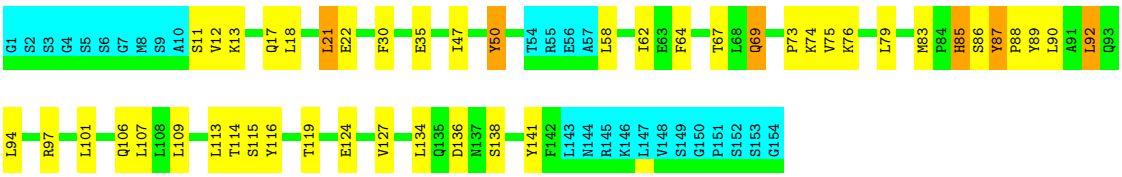
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: RWD domain containing protein 2

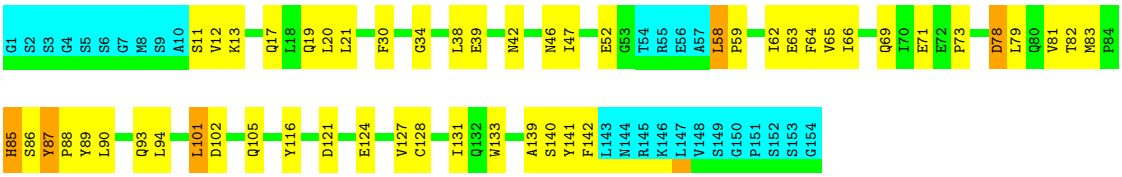
Chain A: 53% 26% • 17%



4.2.2 Score per residue for model 2

• Molecule 1: RWD domain containing protein 2

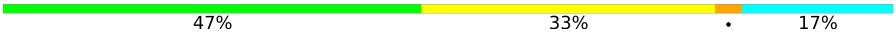
Chain A: 49% 31% • 17%

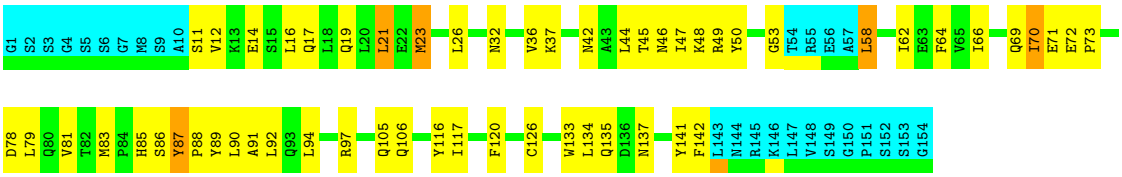


4.2.3 Score per residue for model 3

- Molecule 1: RWD domain containing protein 2

Chain A:

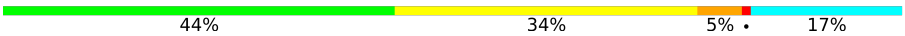


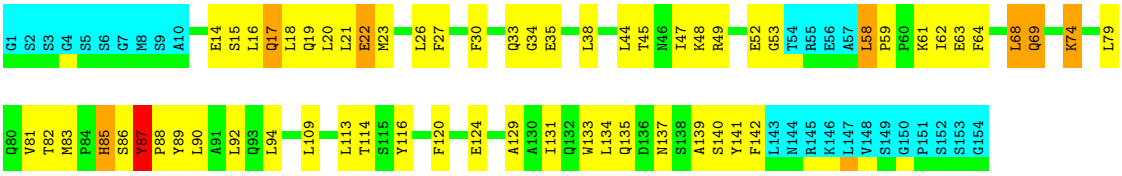


4.2.4 Score per residue for model 4

- Molecule 1: RWD domain containing protein 2

Chain A:

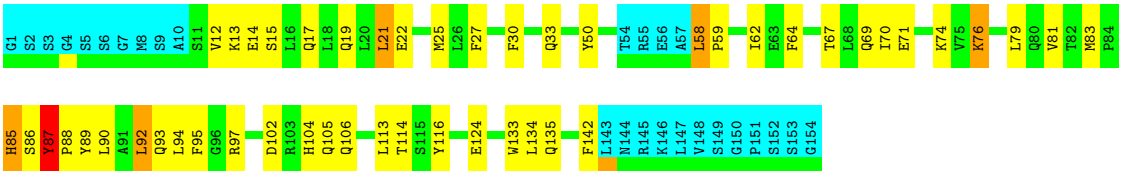




4.2.5 Score per residue for model 5

- Molecule 1: RWD domain containing protein 2

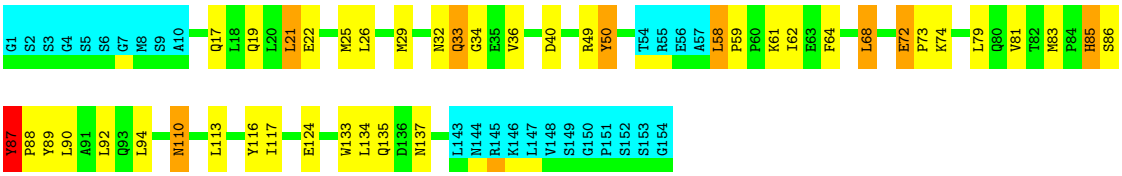
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: RWD domain containing protein 2

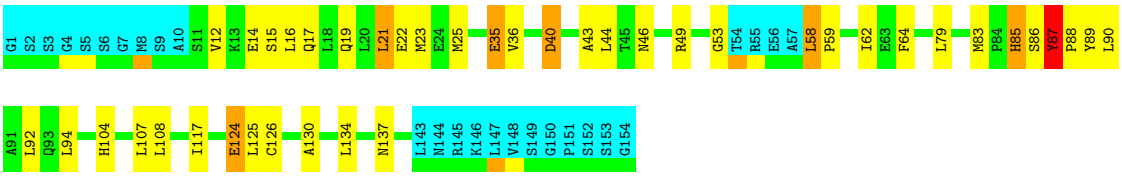
Chain A: 55% 22% 5% • 17%



4.2.7 Score per residue for model 7

- Molecule 1: RWD domain containing protein 2

Chain A: 56% 23% • • 17%



4.2.8 Score per residue for model 8

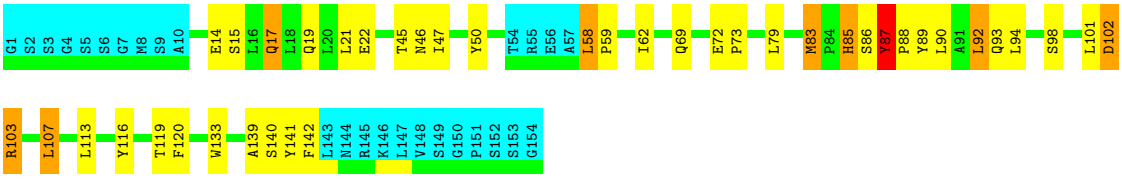
- Molecule 1: RWD domain containing protein 2

Chain A: 51% 27% • • 17%

4.2.9 Score per residue for model 9

- Molecule 1: RWD domain containing protein 2

Chain A: 56% 21% 5% • 17%



4.2.10 Score per residue for model 10

- Molecule 1: RWD domain containing protein 2

Chain A: 48% 30% 5% 17%

G1 S2 S3 G4 S5 S6 G7 M8 S9 A10 S11 V12 K13 L16 Q17 L18 Q19 L20 L21 E22 M23 E24 M25 L26 F30 P31 N32 Q33 G34 E35 V36 N42 T45 N46 I47 E52 G53 T54 R55 E56 A57 L58 P59 I62 E63 F64 L68 Q69 I70 P73 L79

M83 P84 H85 S86 Y87 P88 Y89 L90 A91 L92 Q93 L94 L101 L113 Y116 I117 D121 E124 L125 C126 A130 I131 Q132 W133 L134 Q135 F142 L143 N144 R145 K146 L147 V148 S149 G150 P151 S152 S153 G154

4.2.11 Score per residue for model 11

- Molecule 1: RWD domain containing protein 2

Chain A: 50% 30% • 17%

G1 S2 S3 G4 S5 S6 G7 M8 S9 A10 S11 V12 K13 Q17 L18 Q19 L20 L21 E22 Q33 V36 K37 N42 N46 I47 K48 R49 Y50 T54 R55 E56 A57 L58 P59 I62 E63 F64 V65 V75 L79 M83 P84 H85 S86 Y87 P88 Y89 L90 A91 L92

Q93 L94 R97 Q105 Q106 L107 L113 T114 S115 Y116 T119 L125 C126 V127 C128 A129 A130 W133 L134 Q135 F142 L143 N144 R145 K146 L147 V148 S149 G150 P151 S152 S153 G154

4.2.12 Score per residue for model 12

- Molecule 1: RWD domain containing protein 2

Chain A: 43% 35% 5% 17%

G1 S2 S3 G4 S5 S6 G7 M8 S9 A10 K13 E14 S15 L16 Q17 L21 E22 M23 F27 D40 V41 N42 A43 L44 T45 N46 I47 K48 R49 Y50 L51 E52 G53 T54 R55 E56 A57 L58 P59 I62 E63 F64 V65 Q69 E72 P73 K74 V75 D78 L79 Q80 V81

T82 M83 P84 H85 S86 Y87 P88 Y89 L90 A91 L92 Q93 L94 R97 Q106 L107 L108 L109 N110 K111 G112 L113 T114 S115 Y116 I117 G118 T119 C126 A129 A130 I131 Q132 W133 S140 Y141 F142 L143 N144 R145 K146 L147 V148 S149 G150 P151 S152 S153 G154

4.2.13 Score per residue for model 13

- Molecule 1: RWD domain containing protein 2

Chain A: 57% 23% • 17%

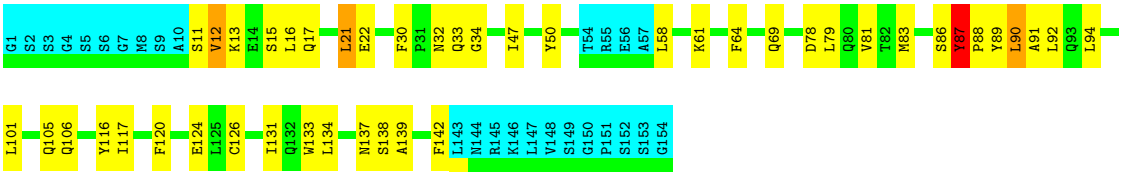
G1 S2 S3 G4 S5 S6 G7 M8 S9 A10 S11 V12 K13 E14 S15 L16 Q17 L18 Q19 L20 L21 E22 M23 E24 M25 F30 V36 I47 Y50 L51 T54 R55 E56 A57 L58 P59 P60 K61 I62 E63 F64 V65 I66 D78 L79 H85 S86 Y87 P88 Y89 L90 A91 L92

Q93 L94 D102 R103 H104 Q105 Q106 L107 L108 D121 L134 Q135 L143 N144 R145 K146 L147 V148 S149 G150 P151 S152 S153 G154

4.2.14 Score per residue for model 14

- Molecule 1: RWD domain containing protein 2

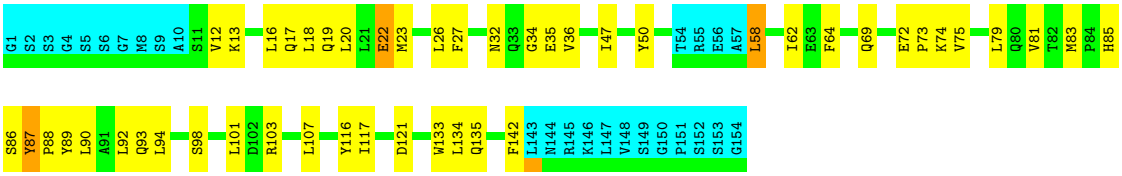
Chain A: 54% 27% • • 17%



4.2.15 Score per residue for model 15

- Molecule 1: RWD domain containing protein 2

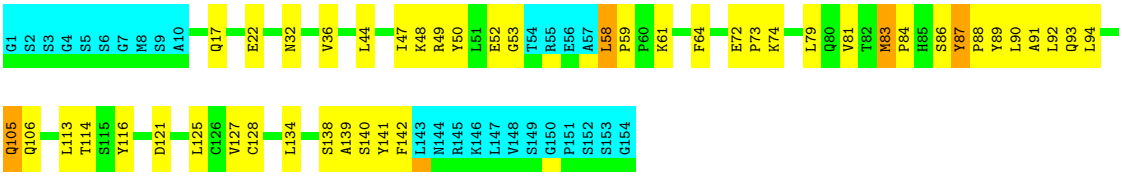
Chain A: 52% 29% • 17%



4.2.16 Score per residue for model 16

- Molecule 1: RWD domain containing protein 2

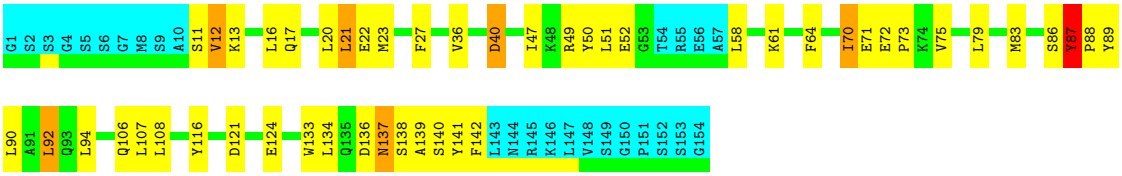
Chain A: 53% 27% • 17%



4.2.17 Score per residue for model 17

- Molecule 1: RWD domain containing protein 2

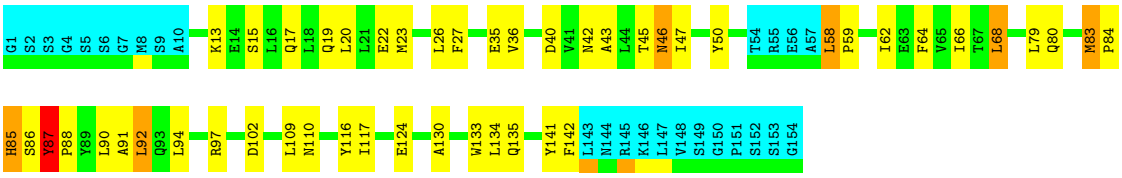
Chain A: 51% 27% • • 17%



4.2.18 Score per residue for model 18

- Molecule 1: RWD domain containing protein 2

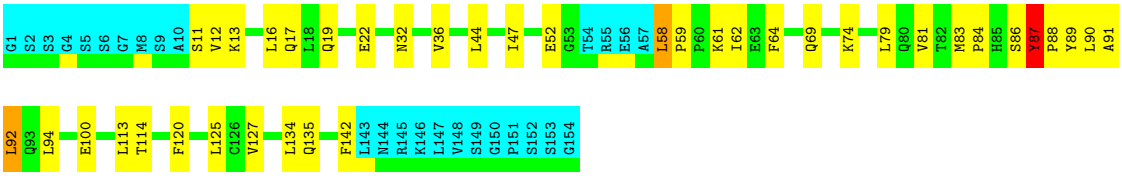
Chain A: 51% 27% • • 17%



4.2.19 Score per residue for model 19

- Molecule 1: RWD domain containing protein 2

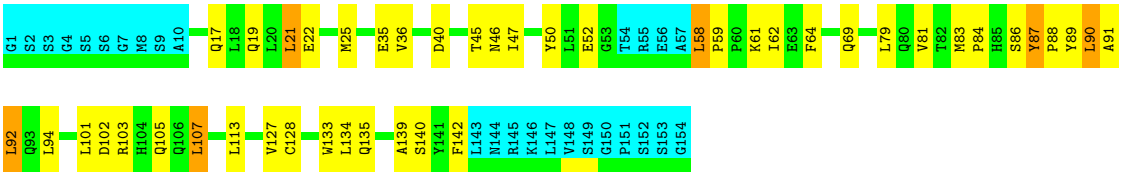
Chain A: 57% 24% •• 17%



4.2.20 Score per residue for model 20

- Molecule 1: RWD domain containing protein 2

Chain A: 54% 25% • 17%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function,structures with the lowest energy,structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	1029	1040	1038	42±6
All	All	20580	20800	20760	837

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:90:LEU:HD23	1:A:91:ALA:N	0.89	1.81	3	3
1:A:109:LEU:HD12	1:A:141:TYR:CD2	0.86	2.05	1	1
1:A:79:LEU:HD11	1:A:94:LEU:HD22	0.86	1.47	2	20
1:A:36:VAL:HG13	1:A:64:PHE:CD2	0.83	2.09	17	12
1:A:22:GLU:OE1	1:A:26:LEU:HD12	0.81	1.76	15	3
1:A:40:ASP:OD2	1:A:43:ALA:HB2	0.78	1.79	18	1
1:A:13:LYS:CG	1:A:51:LEU:HD23	0.76	2.10	12	2
1:A:115:SER:O	1:A:119:THR:HG23	0.76	1.80	1	3
1:A:21:LEU:HD12	1:A:21:LEU:C	0.74	2.02	10	16
1:A:58:LEU:HD13	1:A:59:PRO:HD2	0.74	1.57	8	15
1:A:13:LYS:HG2	1:A:51:LEU:HD23	0.74	1.56	12	1
1:A:84:PRO:CG	1:A:90:LEU:HD23	0.73	2.13	16	1
1:A:109:LEU:HD12	1:A:141:TYR:CE2	0.72	2.19	1	1
1:A:90:LEU:HD13	1:A:91:ALA:N	0.72	2.00	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:HD13	1:A:91:ALA:H	0.71	1.44	20	1
1:A:75:VAL:HG21	1:A:142:PHE:CZ	0.71	2.21	17	2
1:A:87:TYR:CD2	1:A:92:LEU:HD23	0.69	2.22	12	8
1:A:19:GLN:HB3	1:A:62:ILE:HD12	0.69	1.62	8	13
1:A:101:LEU:HD21	1:A:142:PHE:CE1	0.68	2.23	2	4
1:A:65:VAL:HG11	1:A:78:ASP:OD2	0.68	1.89	2	2
1:A:40:ASP:CG	1:A:43:ALA:HB2	0.67	2.10	12	3
1:A:64:PHE:O	1:A:81:VAL:HG12	0.67	1.90	8	2
1:A:90:LEU:HD12	1:A:90:LEU:C	0.67	2.10	18	4
1:A:30:PHE:CZ	1:A:66:ILE:HG21	0.66	2.26	13	2
1:A:87:TYR:C	1:A:87:TYR:CD1	0.65	2.70	15	20
1:A:21:LEU:HD12	1:A:22:GLU:N	0.65	2.07	4	7
1:A:12:VAL:HG12	1:A:16:LEU:CD1	0.64	2.22	17	2
1:A:58:LEU:HD13	1:A:59:PRO:CD	0.64	2.21	8	14
1:A:101:LEU:HD22	1:A:105:GLN:HB3	0.63	1.67	20	1
1:A:79:LEU:CD1	1:A:94:LEU:HD22	0.62	2.25	7	16
1:A:109:LEU:CD1	1:A:141:TYR:CD2	0.62	2.83	1	1
1:A:50:TYR:C	1:A:50:TYR:CD1	0.61	2.74	1	5
1:A:109:LEU:HD12	1:A:141:TYR:CE1	0.61	2.31	4	2
1:A:92:LEU:C	1:A:92:LEU:HD12	0.61	2.16	1	5
1:A:117:ILE:HD11	1:A:130:ALA:HB2	0.60	1.73	7	3
1:A:23:MET:O	1:A:27:PHE:CD2	0.60	2.55	12	5
1:A:85:HIS:CD2	1:A:85:HIS:N	0.60	2.69	4	14
1:A:117:ILE:HG23	1:A:126:CYS:HB3	0.59	1.74	12	5
1:A:90:LEU:HD22	1:A:91:ALA:N	0.59	2.12	14	1
1:A:22:GLU:HB3	1:A:125:LEU:HD13	0.59	1.75	16	3
1:A:30:PHE:CD1	1:A:35:GLU:OE1	0.58	2.56	1	2
1:A:107:LEU:C	1:A:107:LEU:HD12	0.58	2.18	7	2
1:A:83:MET:SD	1:A:87:TYR:CE1	0.58	2.97	19	1
1:A:12:VAL:HG12	1:A:16:LEU:HD12	0.58	1.75	17	3
1:A:20:LEU:HD21	1:A:44:LEU:O	0.57	1.99	4	1
1:A:30:PHE:CZ	1:A:66:ILE:CG2	0.57	2.87	13	1
1:A:21:LEU:CD1	1:A:25:MET:HE3	0.57	2.30	5	2
1:A:16:LEU:HD23	1:A:19:GLN:OE1	0.56	2.00	15	2
1:A:63:GLU:OE2	1:A:82:THR:HG23	0.56	1.99	4	1
1:A:87:TYR:CE2	1:A:92:LEU:HD23	0.56	2.35	6	9
1:A:67:THR:HG23	1:A:76:LYS:HG2	0.56	1.76	5	1
1:A:117:ILE:CD1	1:A:130:ALA:HB2	0.56	2.30	7	1
1:A:107:LEU:HD12	1:A:107:LEU:O	0.56	2.00	9	3
1:A:20:LEU:HD11	1:A:47:ILE:HG22	0.56	1.76	17	2
1:A:16:LEU:HD13	1:A:47:ILE:HG23	0.56	1.76	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:VAL:HG21	1:A:142:PHE:CE2	0.56	2.36	17	1
1:A:35:GLU:CD	1:A:35:GLU:N	0.56	2.59	10	1
1:A:26:LEU:HD22	1:A:66:ILE:CD1	0.55	2.31	18	1
1:A:68:LEU:N	1:A:68:LEU:CD2	0.55	2.69	6	3
1:A:22:GLU:OE1	1:A:125:LEU:HD22	0.55	2.01	11	1
1:A:83:MET:SD	1:A:87:TYR:CZ	0.55	3.00	19	2
1:A:21:LEU:C	1:A:21:LEU:CD1	0.55	2.76	10	10
1:A:90:LEU:HD22	1:A:90:LEU:C	0.55	2.22	14	1
1:A:90:LEU:HD22	1:A:91:ALA:C	0.55	2.22	14	1
1:A:16:LEU:HD22	1:A:47:ILE:HG12	0.55	1.79	10	1
1:A:90:LEU:HD12	1:A:91:ALA:N	0.55	2.15	13	2
1:A:17:GLN:CD	1:A:17:GLN:C	0.54	2.65	13	3
1:A:30:PHE:CE2	1:A:66:ILE:HD13	0.54	2.37	2	1
1:A:68:LEU:HD11	1:A:131:ILE:HG23	0.54	1.80	10	1
1:A:97:ARG:CB	1:A:106:GLN:NE2	0.54	2.71	3	3
1:A:73:PRO:O	1:A:75:VAL:HG22	0.53	2.03	15	1
1:A:92:LEU:HD12	1:A:93:GLN:N	0.53	2.18	5	4
1:A:65:VAL:HG13	1:A:79:LEU:O	0.53	2.04	2	1
1:A:116:TYR:CE1	1:A:133:TRP:CD1	0.53	2.97	5	3
1:A:86:SER:CB	1:A:90:LEU:HD12	0.53	2.34	14	1
1:A:64:PHE:CZ	1:A:81:VAL:HG11	0.52	2.39	15	6
1:A:90:LEU:C	1:A:90:LEU:CD1	0.52	2.77	4	4
1:A:116:TYR:CZ	1:A:133:TRP:CD1	0.52	2.98	5	2
1:A:116:TYR:CE2	1:A:133:TRP:CB	0.52	2.92	11	3
1:A:26:LEU:HD23	1:A:29:MET:CE	0.52	2.34	6	1
1:A:107:LEU:HD12	1:A:107:LEU:C	0.52	2.25	9	3
1:A:116:TYR:CE2	1:A:133:TRP:HB2	0.52	2.40	11	6
1:A:20:LEU:HD11	1:A:47:ILE:CG2	0.52	2.35	17	3
1:A:36:VAL:CG1	1:A:64:PHE:CD2	0.51	2.91	6	2
1:A:18:LEU:HD23	1:A:21:LEU:HD21	0.51	1.82	4	1
1:A:116:TYR:CE2	1:A:133:TRP:CG	0.51	2.98	11	3
1:A:116:TYR:CG	1:A:133:TRP:CD1	0.51	2.99	18	3
1:A:69:GLN:C	1:A:69:GLN:NE2	0.51	2.64	4	2
1:A:26:LEU:O	1:A:30:PHE:CD2	0.51	2.64	4	1
1:A:84:PRO:CB	1:A:90:LEU:HD23	0.51	2.35	16	1
1:A:101:LEU:HG	1:A:142:PHE:CZ	0.50	2.41	2	3
1:A:21:LEU:CD1	1:A:25:MET:CE	0.50	2.88	5	6
1:A:81:VAL:O	1:A:81:VAL:HG13	0.50	2.07	4	1
1:A:110:ASN:ND2	1:A:110:ASN:N	0.50	2.59	6	1
1:A:133:TRP:CE2	1:A:137:ASN:ND2	0.50	2.79	6	1
1:A:63:GLU:OE2	1:A:82:THR:CG2	0.50	2.60	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:VAL:O	1:A:81:VAL:CG1	0.50	2.60	4	4
1:A:90:LEU:HD23	1:A:91:ALA:C	0.50	2.27	11	2
1:A:11:SER:O	1:A:13:LYS:N	0.50	2.45	14	1
1:A:22:GLU:OE1	1:A:83:MET:CE	0.50	2.60	18	4
1:A:90:LEU:HD23	1:A:90:LEU:C	0.50	2.27	3	2
1:A:133:TRP:O	1:A:137:ASN:ND2	0.49	2.45	17	1
1:A:15:SER:O	1:A:19:GLN:NE2	0.49	2.45	5	2
1:A:17:GLN:NE2	1:A:17:GLN:O	0.49	2.45	7	3
1:A:88:PRO:CB	1:A:124:GLU:O	0.49	2.61	5	11
1:A:90:LEU:CD1	1:A:91:ALA:N	0.49	2.76	13	2
1:A:45:THR:O	1:A:47:ILE:N	0.49	2.46	18	3
1:A:40:ASP:N	1:A:40:ASP:OD1	0.49	2.45	18	3
1:A:105:GLN:NE2	1:A:141:TYR:O	0.49	2.45	2	2
1:A:32:ASN:O	1:A:34:GLY:N	0.49	2.45	14	2
1:A:50:TYR:CE2	1:A:58:LEU:CD2	0.49	2.95	15	1
1:A:22:GLU:OE1	1:A:23:MET:N	0.49	2.45	15	2
1:A:47:ILE:O	1:A:50:TYR:N	0.49	2.45	11	7
1:A:90:LEU:CD2	1:A:91:ALA:O	0.49	2.61	14	1
1:A:134:LEU:O	1:A:138:SER:N	0.48	2.46	17	4
1:A:33:GLN:N	1:A:33:GLN:OE1	0.48	2.46	4	1
1:A:13:LYS:HG2	1:A:50:TYR:CE2	0.48	2.43	17	2
1:A:42:ASN:O	1:A:46:ASN:ND2	0.48	2.45	12	4
1:A:26:LEU:HD22	1:A:66:ILE:HD11	0.48	1.85	3	1
1:A:85:HIS:CD2	1:A:85:HIS:H	0.48	2.27	13	4
1:A:21:LEU:HD12	1:A:25:MET:HE3	0.48	1.84	5	2
1:A:86:SER:CB	1:A:90:LEU:CB	0.48	2.91	16	1
1:A:36:VAL:HG13	1:A:64:PHE:HD2	0.48	1.63	17	4
1:A:87:TYR:N	1:A:90:LEU:CD1	0.48	2.77	14	1
1:A:116:TYR:CD2	1:A:133:TRP:CD1	0.48	3.01	11	4
1:A:98:SER:HB3	1:A:101:LEU:HD12	0.48	1.85	9	2
1:A:79:LEU:HD13	1:A:134:LEU:HD11	0.48	1.86	15	1
1:A:87:TYR:HA	1:A:88:PRO:C	0.48	2.30	9	20
1:A:38:LEU:HD23	1:A:64:PHE:HB3	0.48	1.85	4	1
1:A:14:GLU:O	1:A:17:GLN:N	0.47	2.47	4	4
1:A:117:ILE:HD11	1:A:130:ALA:CB	0.47	2.38	7	1
1:A:116:TYR:CD2	1:A:133:TRP:CG	0.47	3.02	11	2
1:A:90:LEU:CD2	1:A:91:ALA:N	0.47	2.69	3	1
1:A:58:LEU:HD12	1:A:85:HIS:CE1	0.47	2.45	3	1
1:A:133:TRP:CZ3	1:A:137:ASN:OD1	0.47	2.68	17	1
1:A:80:GLN:NE2	1:A:97:ARG:HH21	0.47	2.07	18	1
1:A:101:LEU:CG	1:A:142:PHE:CZ	0.47	2.98	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ILE:CD1	1:A:62:ILE:HD11	0.47	2.39	12	1
1:A:88:PRO:O	1:A:89:TYR:C	0.47	2.52	19	17
1:A:45:THR:HG22	1:A:49:ARG:HD3	0.47	1.85	12	1
1:A:84:PRO:HG3	1:A:90:LEU:HD21	0.47	1.85	18	1
1:A:83:MET:HE1	1:A:127:VAL:HG11	0.47	1.87	19	1
1:A:116:TYR:CD1	1:A:133:TRP:CD1	0.47	3.03	5	2
1:A:38:LEU:O	1:A:40:ASP:N	0.47	2.48	8	1
1:A:133:TRP:CE3	1:A:137:ASN:OD1	0.47	2.68	17	1
1:A:67:THR:HG21	1:A:76:LYS:HD2	0.47	1.87	1	1
1:A:50:TYR:CD1	1:A:50:TYR:O	0.47	2.68	15	1
1:A:64:PHE:CD1	1:A:64:PHE:N	0.47	2.82	16	6
1:A:110:ASN:O	1:A:112:GLY:N	0.47	2.49	12	1
1:A:18:LEU:CD1	1:A:18:LEU:N	0.47	2.78	15	1
1:A:22:GLU:OE2	1:A:83:MET:HE3	0.47	2.10	18	2
1:A:73:PRO:O	1:A:75:VAL:N	0.46	2.47	15	3
1:A:67:THR:HG23	1:A:76:LYS:HG3	0.46	1.87	8	1
1:A:86:SER:O	1:A:87:TYR:C	0.46	2.52	20	20
1:A:133:TRP:CD1	1:A:137:ASN:ND2	0.46	2.84	14	1
1:A:87:TYR:CD2	1:A:88:PRO:HA	0.46	2.46	17	19
1:A:104:HIS:HA	1:A:107:LEU:HD23	0.46	1.87	7	1
1:A:22:GLU:O	1:A:26:LEU:HD12	0.46	2.10	6	1
1:A:86:SER:CB	1:A:90:LEU:HB3	0.46	2.40	16	11
1:A:45:THR:O	1:A:46:ASN:C	0.46	2.54	12	7
1:A:134:LEU:O	1:A:137:ASN:N	0.46	2.49	7	4
1:A:19:GLN:NE2	1:A:84:PRO:O	0.46	2.49	19	2
1:A:37:LYS:CG	1:A:65:VAL:HB	0.46	2.41	11	1
1:A:50:TYR:O	1:A:53:GLY:N	0.46	2.48	3	3
1:A:18:LEU:HD12	1:A:18:LEU:N	0.46	2.25	10	1
1:A:79:LEU:CG	1:A:94:LEU:HD22	0.46	2.41	7	3
1:A:87:TYR:CG	1:A:88:PRO:HA	0.46	2.46	12	20
1:A:26:LEU:HD13	1:A:64:PHE:CZ	0.46	2.46	3	1
1:A:17:GLN:NE2	1:A:17:GLN:C	0.45	2.69	4	1
1:A:64:PHE:CE1	1:A:81:VAL:HG11	0.45	2.46	12	1
1:A:22:GLU:OE2	1:A:83:MET:CE	0.45	2.64	18	1
1:A:72:GLU:HA	1:A:73:PRO:C	0.45	2.32	9	7
1:A:11:SER:O	1:A:12:VAL:C	0.45	2.55	17	8
1:A:113:LEU:O	1:A:116:TYR:N	0.45	2.49	11	4
1:A:127:VAL:HG13	1:A:128:CYS:N	0.45	2.26	16	3
1:A:13:LYS:HB3	1:A:51:LEU:HD23	0.45	1.87	17	1
1:A:18:LEU:HA	1:A:21:LEU:HD23	0.45	1.89	1	1
1:A:107:LEU:HD12	1:A:108:LEU:N	0.45	2.25	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HB3	1:A:47:ILE:HG23	0.45	1.88	10	1
1:A:105:GLN:O	1:A:106:GLN:C	0.45	2.55	14	4
1:A:139:ALA:O	1:A:142:PHE:N	0.45	2.50	14	1
1:A:134:LEU:O	1:A:135:GLN:C	0.45	2.55	10	11
1:A:12:VAL:O	1:A:13:LYS:C	0.45	2.56	5	8
1:A:45:THR:O	1:A:48:LYS:N	0.45	2.50	4	2
1:A:120:PHE:CB	1:A:126:CYS:HG	0.45	2.25	14	1
1:A:86:SER:HB3	1:A:90:LEU:CB	0.45	2.42	16	11
1:A:70:ILE:O	1:A:71:GLU:C	0.45	2.54	5	3
1:A:16:LEU:HB3	1:A:47:ILE:HG21	0.45	1.88	4	1
1:A:90:LEU:C	1:A:90:LEU:HD23	0.45	2.32	5	1
1:A:22:GLU:OE1	1:A:22:GLU:C	0.45	2.55	10	2
1:A:18:LEU:N	1:A:18:LEU:HD12	0.45	2.27	15	1
1:A:116:TYR:CE2	1:A:133:TRP:CD1	0.44	3.04	5	3
1:A:49:ARG:N	1:A:49:ARG:HD2	0.44	2.26	12	1
1:A:62:ILE:HG22	1:A:62:ILE:O	0.44	2.11	5	1
1:A:64:PHE:HE2	1:A:66:ILE:HD11	0.44	1.72	8	1
1:A:87:TYR:HA	1:A:89:TYR:N	0.44	2.26	20	1
1:A:105:GLN:O	1:A:108:LEU:N	0.44	2.50	13	1
1:A:103:ARG:O	1:A:107:LEU:HD23	0.44	2.12	15	1
1:A:90:LEU:HG	1:A:91:ALA:N	0.44	2.28	16	1
1:A:113:LEU:O	1:A:114:THR:C	0.44	2.56	1	7
1:A:81:VAL:HG23	1:A:94:LEU:HD21	0.44	1.90	15	2
1:A:94:LEU:HD13	1:A:113:LEU:HD21	0.44	1.88	12	1
1:A:108:LEU:C	1:A:141:TYR:CE1	0.44	2.90	17	1
1:A:15:SER:CB	1:A:85:HIS:O	0.44	2.66	12	2
1:A:32:ASN:O	1:A:33:GLN:C	0.44	2.56	6	1
1:A:17:GLN:C	1:A:17:GLN:NE2	0.44	2.71	7	1
1:A:113:LEU:HB2	1:A:133:TRP:CZ3	0.44	2.47	12	3
1:A:84:PRO:HG3	1:A:90:LEU:HD12	0.44	1.89	20	1
1:A:139:ALA:O	1:A:140:SER:C	0.44	2.54	17	4
1:A:19:GLN:NE2	1:A:87:TYR:O	0.44	2.51	6	1
1:A:119:THR:O	1:A:120:PHE:C	0.44	2.56	9	1
1:A:58:LEU:CD1	1:A:85:HIS:CE1	0.43	3.01	3	2
1:A:50:TYR:CD1	1:A:50:TYR:C	0.43	2.91	6	3
1:A:46:ASN:O	1:A:49:ARG:N	0.43	2.51	7	1
1:A:139:ALA:O	1:A:141:TYR:N	0.43	2.51	16	2
1:A:23:MET:O	1:A:26:LEU:N	0.43	2.50	10	1
1:A:20:LEU:HD23	1:A:62:ILE:HD11	0.43	1.89	15	1
1:A:133:TRP:CD2	1:A:137:ASN:ND2	0.43	2.86	6	1
1:A:38:LEU:C	1:A:40:ASP:N	0.43	2.72	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LYS:CB	1:A:51:LEU:HD23	0.43	2.43	13	2
1:A:84:PRO:HG3	1:A:90:LEU:HD23	0.43	1.89	16	1
1:A:71:GLU:C	1:A:73:PRO:O	0.43	2.57	2	1
1:A:44:LEU:N	1:A:44:LEU:HD23	0.43	2.28	16	4
1:A:41:VAL:HG23	1:A:42:ASN:N	0.43	2.29	8	1
1:A:126:CYS:O	1:A:129:ALA:N	0.43	2.51	12	1
1:A:90:LEU:HD22	1:A:91:ALA:O	0.43	2.13	14	1
1:A:22:GLU:OE1	1:A:127:VAL:HG11	0.43	2.14	1	1
1:A:78:ASP:OD1	1:A:78:ASP:C	0.43	2.56	8	2
1:A:19:GLN:O	1:A:62:ILE:CD1	0.43	2.66	3	1
1:A:35:GLU:N	1:A:35:GLU:OE1	0.43	2.51	10	1
1:A:102:ASP:O	1:A:103:ARG:C	0.43	2.55	20	3
1:A:14:GLU:O	1:A:15:SER:C	0.43	2.57	5	5
1:A:63:GLU:CG	1:A:82:THR:HG23	0.43	2.43	2	1
1:A:21:LEU:HD11	1:A:25:MET:HE3	0.43	1.91	8	1
1:A:83:MET:HB3	1:A:87:TYR:CD1	0.43	2.48	9	1
1:A:86:SER:HB2	1:A:90:LEU:CD1	0.43	2.44	14	1
1:A:86:SER:HB2	1:A:90:LEU:HD12	0.43	1.90	14	1
1:A:106:GLN:O	1:A:107:LEU:C	0.42	2.57	17	2
1:A:38:LEU:O	1:A:39:GLU:C	0.42	2.58	2	1
1:A:90:LEU:HD23	1:A:91:ALA:CA	0.42	2.44	3	1
1:A:63:GLU:CD	1:A:82:THR:HG23	0.42	2.35	4	1
1:A:110:ASN:ND2	1:A:110:ASN:H	0.42	2.12	6	1
1:A:137:ASN:O	1:A:141:TYR:CD1	0.42	2.72	8	1
1:A:21:LEU:HD12	1:A:21:LEU:O	0.42	2.14	7	1
1:A:117:ILE:HG23	1:A:126:CYS:CB	0.42	2.44	12	1
1:A:15:SER:OG	1:A:16:LEU:N	0.42	2.52	14	1
1:A:81:VAL:CG1	1:A:81:VAL:O	0.42	2.67	14	1
1:A:47:ILE:O	1:A:49:ARG:N	0.42	2.52	11	2
1:A:50:TYR:CE2	1:A:58:LEU:HD22	0.42	2.49	15	1
1:A:19:GLN:O	1:A:22:GLU:CG	0.42	2.68	18	1
1:A:22:GLU:OE1	1:A:83:MET:HE2	0.42	2.15	5	1
1:A:104:HIS:O	1:A:105:GLN:C	0.42	2.58	8	2
1:A:80:GLN:NE2	1:A:97:ARG:NH2	0.42	2.68	18	1
1:A:30:PHE:CZ	1:A:131:ILE:HD13	0.42	2.50	14	2
1:A:97:ARG:CD	1:A:106:GLN:NE2	0.42	2.83	5	1
1:A:68:LEU:CD1	1:A:131:ILE:HG23	0.42	2.45	10	1
1:A:110:ASN:O	1:A:113:LEU:N	0.42	2.52	12	1
1:A:34:GLY:O	1:A:35:GLU:C	0.42	2.57	15	1
1:A:117:ILE:HG22	1:A:117:ILE:O	0.42	2.14	6	2
1:A:21:LEU:CD1	1:A:22:GLU:N	0.42	2.81	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:VAL:HG22	1:A:80:GLN:OE1	0.42	2.13	12	1
1:A:11:SER:C	1:A:13:LYS:N	0.42	2.73	14	1
1:A:23:MET:HA	1:A:23:MET:CE	0.41	2.45	3	2
1:A:69:GLN:O	1:A:69:GLN:CD	0.41	2.59	1	1
1:A:42:ASN:O	1:A:46:ASN:CG	0.41	2.59	2	1
1:A:18:LEU:HD12	1:A:18:LEU:H	0.41	1.75	11	1
1:A:49:ARG:O	1:A:52:GLU:CG	0.41	2.68	4	1
1:A:45:THR:C	1:A:47:ILE:N	0.41	2.73	18	1
1:A:47:ILE:O	1:A:48:LYS:C	0.41	2.59	3	1
1:A:134:LEU:O	1:A:138:SER:CB	0.41	2.69	14	1
1:A:97:ARG:HD3	1:A:106:GLN:NE2	0.41	2.30	5	1
1:A:35:GLU:OE1	1:A:35:GLU:CA	0.41	2.68	7	1
1:A:62:ILE:O	1:A:62:ILE:HG22	0.41	2.14	1	1
1:A:33:GLN:O	1:A:34:GLY:C	0.41	2.58	6	1
1:A:34:GLY:N	1:A:35:GLU:OE1	0.41	2.54	10	1
1:A:88:PRO:O	1:A:90:LEU:N	0.41	2.54	19	1
1:A:137:ASN:O	1:A:141:TYR:CE1	0.41	2.74	8	1
1:A:139:ALA:C	1:A:141:TYR:N	0.41	2.73	16	2
1:A:90:LEU:CD1	1:A:90:LEU:N	0.41	2.84	14	1
1:A:84:PRO:CG	1:A:90:LEU:HD21	0.41	2.45	18	1
1:A:120:PHE:CZ	1:A:129:ALA:CB	0.41	3.03	4	1
1:A:32:ASN:ND2	1:A:32:ASN:H	0.41	2.13	8	1
1:A:32:ASN:O	1:A:35:GLU:CG	0.41	2.69	15	1
1:A:21:LEU:CD1	1:A:25:MET:HE1	0.41	2.46	20	1
1:A:52:GLU:O	1:A:52:GLU:OE2	0.41	2.39	20	1
1:A:97:ARG:HB2	1:A:106:GLN:NE2	0.41	2.31	3	2
1:A:109:LEU:HA	1:A:141:TYR:CE2	0.41	2.51	12	1
1:A:110:ASN:C	1:A:112:GLY:N	0.41	2.72	12	1
1:A:90:LEU:CD1	1:A:90:LEU:H	0.41	2.29	14	1
1:A:117:ILE:HD11	1:A:130:ALA:CA	0.40	2.45	7	1
1:A:25:MET:HG3	1:A:26:LEU:N	0.40	2.32	10	2
1:A:129:ALA:O	1:A:130:ALA:C	0.40	2.59	11	1
1:A:24:GLU:CG	1:A:25:MET:N	0.40	2.83	13	1
1:A:86:SER:O	1:A:87:TYR:O	0.40	2.40	14	1
1:A:12:VAL:CG1	1:A:16:LEU:CD1	0.40	2.97	17	1
1:A:113:LEU:HD11	1:A:130:ALA:HB1	0.40	1.93	10	1
1:A:22:GLU:OE2	1:A:83:MET:SD	0.40	2.80	12	1
1:A:86:SER:CB	1:A:90:LEU:HB2	0.40	2.46	19	1
1:A:70:ILE:O	1:A:73:PRO:O	0.40	2.40	10	1
1:A:68:LEU:N	1:A:68:LEU:HD22	0.40	2.31	18	1
1:A:27:PHE:O	1:A:30:PHE:O	0.40	2.40	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:GLN:O	1:A:108:LEU:N	0.40	2.54	8	1
1:A:46:ASN:CB	1:A:59:PRO:HB3	0.40	2.47	10	1
1:A:83:MET:CE	1:A:127:VAL:HG11	0.40	2.46	11	1
1:A:87:TYR:CD1	1:A:88:PRO:N	0.40	2.90	11	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	128/154 (83%)	99±4 (77±3%)	26±4 (20±3%)	3±1 (3±1%)	8	44
All	All	2560/3080 (83%)	1976 (77%)	517 (20%)	67 (3%)	8	44

All 18 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	92	LEU	13
1	A	87	TYR	10
1	A	74	LYS	7
1	A	61	LYS	7
1	A	34	GLY	3
1	A	131	ILE	3
1	A	33	GLN	3
1	A	32	ASN	3
1	A	101	LEU	2
1	A	70	ILE	2
1	A	120	PHE	2
1	A	103	ARG	2
1	A	140	SER	2
1	A	46	ASN	2
1	A	48	LYS	2
1	A	12	VAL	2
1	A	39	GLU	1
1	A	111	LYS	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	117/136 (86%)	108±2 (92±2%)	9±2 (8±2%)	16	63
All	All	2340/2720 (86%)	2156 (92%)	184 (8%)	16	63

All 40 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	58	LEU	20
1	A	87	TYR	20
1	A	17	GLN	17
1	A	21	LEU	13
1	A	83	MET	13
1	A	69	GLN	12
1	A	85	HIS	12
1	A	121	ASP	7
1	A	52	GLU	6
1	A	78	ASP	6
1	A	23	MET	5
1	A	40	ASP	5
1	A	102	ASP	4
1	A	35	GLU	4
1	A	107	LEU	4
1	A	22	GLU	3
1	A	68	LEU	3
1	A	50	TYR	2
1	A	136	ASP	2
1	A	32	ASN	2
1	A	74	LYS	2
1	A	110	ASN	2
1	A	63	GLU	2
1	A	90	LEU	2
1	A	97	ARG	1
1	A	93	GLN	1
1	A	14	GLU	1
1	A	37	LYS	1
1	A	33	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	76	LYS	1
1	A	95	PHE	1
1	A	72	GLU	1
1	A	44	LEU	1
1	A	124	GLU	1
1	A	105	GLN	1
1	A	49	ARG	1
1	A	61	LYS	1
1	A	137	ASN	1
1	A	42	ASN	1
1	A	100	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

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