Full wwPDB NMR Structure Validation Report (i)

Oct 16, 2021 – 11:49 PM EDT

PDB ID	:	1ORM
Title	:	NMR FOLD OF THE OUTER MEMBRANE PROTEIN OMPX IN DHPC MICELLES
Authors	:	Fernandez, C.; Adeishvili, K.; Wuthrich, K.
Deposited on	:	2003-03-14

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:

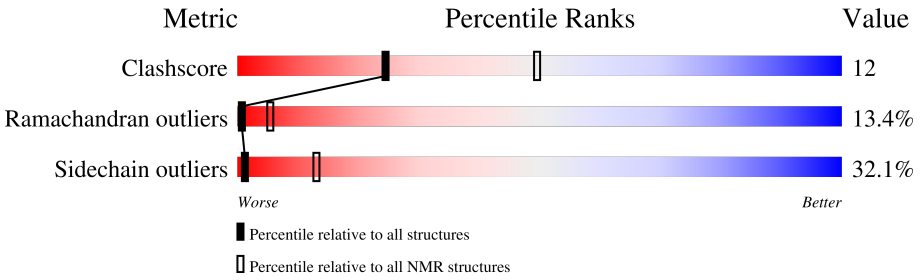
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	148	39% 48% • 11%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2-A:50, A:57-A:91, A:102-A:148 (131)	1.85	15

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 1 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2237 atoms, of which 1080 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Outer membrane protein X.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	148	2237	731	1080	190	233	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASN	HIS	engineered mutation	UNP P0A917

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: Outer membrane protein X

Chain A: 39% 48% • 11%

A1 T2 S3 Y9 S12 D13 G16 Q17 M18 N19 K20 M21 L26 K27 Y28 R29 E32 D33 N34 S35 P36 L37 G38 V39 I40 G41 S42 F43 E47 K48 S49 R50 T51 A52 S53 S54 G55 D56 Y57 N58 K59 N60 Q61 Y62 Y63 G64 I65 Y71 R72 I73 N74 D75 W76

A77 S78 I79 Y80 Y87 G88 K89 F90 Q91 T92 T93 E94 Y95 P96 T97 Y98 K99 N100 D101 T102 S103 D104 S108 L113 M118 E119 N120 L123 D124 F125 S126 Y127 E128 Q129 S130 R131 I132 R133 S134 V135 D136 V137 W140 I141 Y146 R147 F148

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: Outer membrane protein X

Chain A: 52% 32% • • 11%

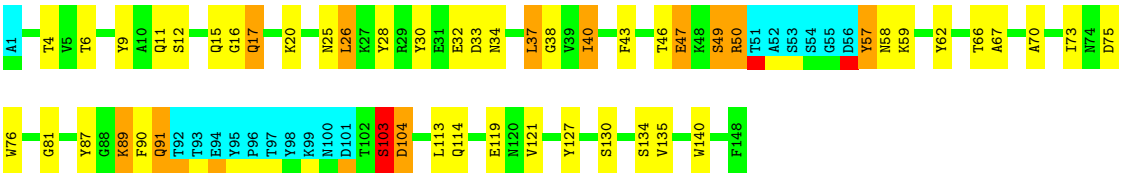
A1 T2 S3 T4 V5 S12 M18 N19 K20 M21 G22 N25 L26 K27 Y28 R29 E32 D33 N34 I40 G41 S42 K48 S49 R50 T51 A52 S53 S54 G55 D56 Y57 N60 I65 G68 Y71 R72 I73 N74 D75 W76 G81 V82 F90 Q91 T92 T93 E94

Y95 P96 T97 Y98 K99 N100 D101 D104 F107 L113 Q114 F115 M118 E119 N120 V121 A122 L123 Y127 E128 Q129 S130 R131 I132 R133 S134 W140 V144 G145 Y146 R147 F148

4.2.2 Score per residue for model 2

• Molecule 1: Outer membrane protein X

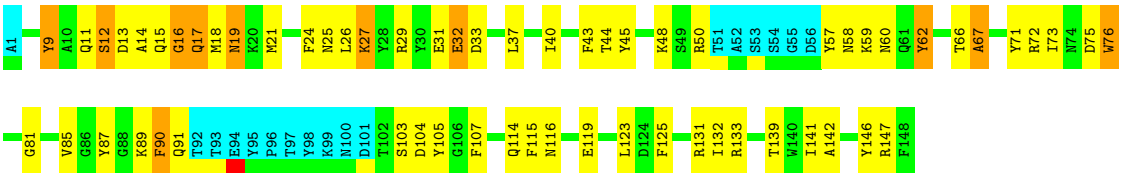
Chain A: 55% 26% 7% • 11%



4.2.3 Score per residue for model 3

- Molecule 1: Outer membrane protein X

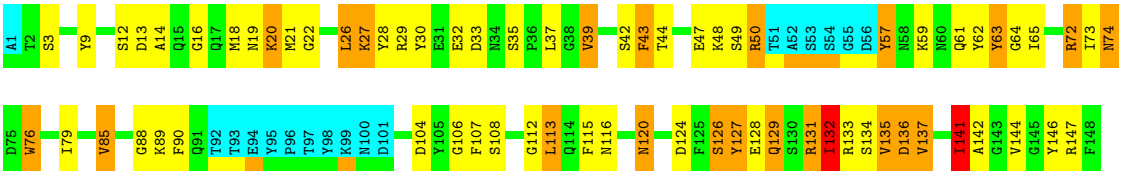
Chain A: 47% 34% 7% 11%



4.2.4 Score per residue for model 4

- Molecule 1: Outer membrane protein X

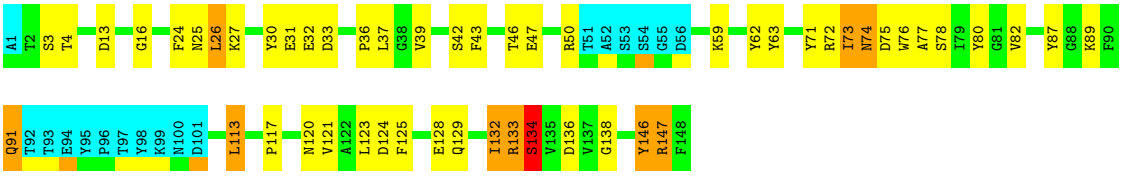
Chain A: 41% 32% 14% • 11%



4.2.5 Score per residue for model 5

- Molecule 1: Outer membrane protein X

Chain A: 53% 28% 6% • 11%



4.2.6 Score per residue for model 6

- Molecule 1: Outer membrane protein X

Chain A: 49% 30% 7% • 11%

A1 T2 S3 G8 Y9 A10 D13 G16 Q17 M18 N19 K20 M21 F24 N25 L26 K27 Y28 R29 D33 N34 S35 P36 L37 G38 V39 I40 G41 S42 F43 T44 K48 S49 R50 T51 A52 S53 S54 G55 D56 Y57 N58 K59 N60 G61 Y62 Y63 R72 W76 A77 S78 I79

Y80 Y87 Q91 T92 T93 E94 Y95 P96 T97 Y98 K99 N100 D101 F107 S108 Y109 G110 A111 G112 L113 N116 P117 M118 E119 A122 L123 Y127 E128 R131 I132 R133 S134 V135 D136 T139 Y146 R147 F148

4.2.7 Score per residue for model 7

- Molecule 1: Outer membrane protein X

Chain A: 51% 26% 9% • 11%

A1 T2 S3 T4 V5 D13 A14 M18 N19 K20 L26 N34 S35 P36 L37 K48 S49 R50 T51 A52 S53 S54 G55 D56 Y57 N58 K59 N60 Q61 Y62 Y63 Y71 R72 I73 N74 D75 W76 A77 S78 I79 V83 G84 V85 G86 Y87 G88 K89 F90 Q91 T92 T93 E94 Y95

P96 T97 Y98 K99 N100 D101 T102 S103 D104 Y105 G106 F107 L113 Q114 F115 E119 N120 V121 A122 L123 D124 F125 S126 I132 R133 S134 V135 D136 V137 G138 T139 W140 I141 R147 F148

4.2.8 Score per residue for model 8

- Molecule 1: Outer membrane protein X

Chain A: 49% 28% 9% • 11%

A1 T2 S3 T4 V5 T6 G7 G8 Y9 D13 A14 Q15 G16 Q17 G23 F24 N25 L26 K27 Y28 R29 Y30 E31 E32 D33 L37 S42 K48 S49 R50 T51 A52 S53 S54 G55 D56 K59 N60 Q61 Y62 I65 T66 Y71 R72 I73 N74 D75 W76 A77 S78 I79 Y80

Y87 G88 K89 T92 T93 E94 Y95 P96 T97 Y98 K99 N100 D101 T102 S103 D104 Y105 G106 F107 L113 Q114 M118 E119 N120 L123 D124 F125 S126 Y127 E128 R131 I132 R133 S134 T139 W140 I141 Y146 R147 F148

4.2.9 Score per residue for model 9

- Molecule 1: Outer membrane protein X

Chain A: 41% 36% 11% • 11%

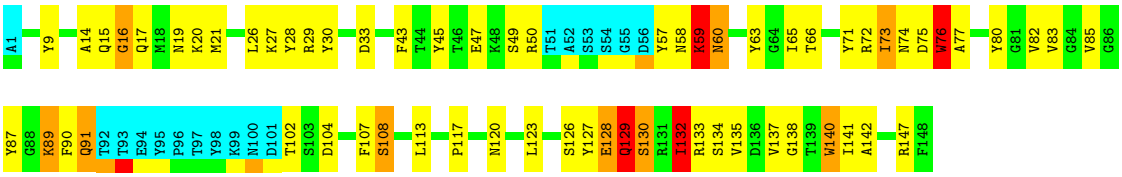
A1 T2 S3 T6 D13 A14 Q15 G16 Q17 M18 N19 K20 M21 N25 L26 K27 Y28 R29 Y30 E31 E32 D33 L37 S42 F43 T44 Y45 T46 E47 K48 S49 R50 T51 A52 S53 S54 G55 D56 Y57 N58 K59 Y62 Y63 Y71 R72 I73 N74 D75 W76 A77 S78 I79 Y80

V83 G84 V85 G86 Y87 G88 K89 F90 Q91 T92 T93 E94 Y95 P96 T97 Y98 K99 N100 D101 T102 Y109 G112 L113 Q114 F115 N116 P117 M118 E119 Y127 E128 Q129 S130 R131 I132 R133 S134 V135 D136 V137 G138 T139 W140 I141 V144 G145 Y146 R147 F148

4.2.10 Score per residue for model 10

- Molecule 1: Outer membrane protein X

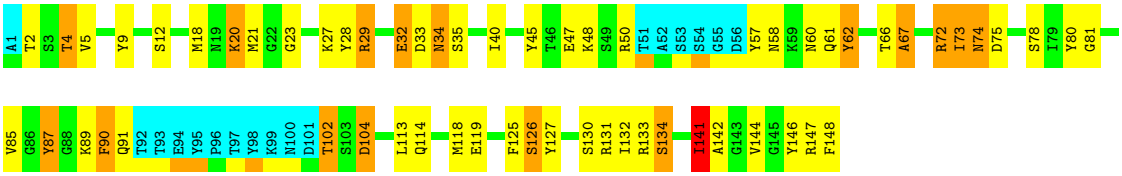
Chain A: 45% 34% 6% • 11%



4.2.11 Score per residue for model 11

- Molecule 1: Outer membrane protein X

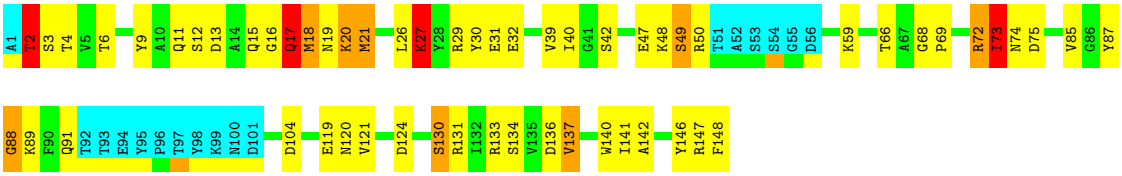
Chain A: 48% 29% 11% • 11%



4.2.12 Score per residue for model 12

- Molecule 1: Outer membrane protein X

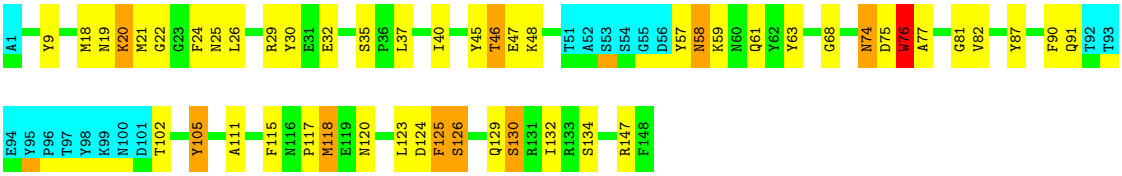
Chain A: 49% 31% 5% • 11%



4.2.13 Score per residue for model 13

- Molecule 1: Outer membrane protein X

Chain A: 55% 27% 6% • 11%



4.2.14 Score per residue for model 14

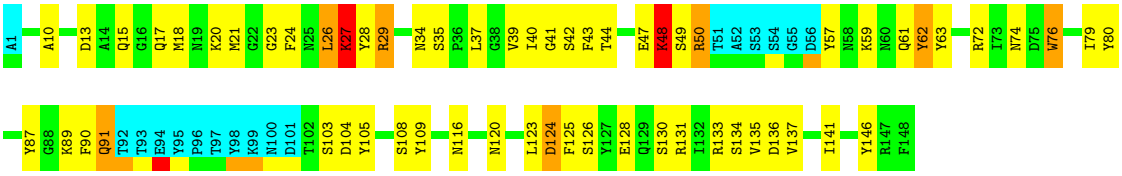
- Molecule 1: Outer membrane protein X

Chain A: 36% 36% 14% • 11%

4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Outer membrane protein X

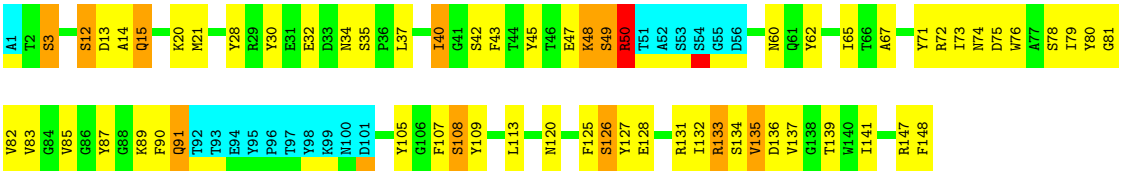
Chain A: 47% 35% 5% • 11%



4.2.16 Score per residue for model 16

- Molecule 1: Outer membrane protein X

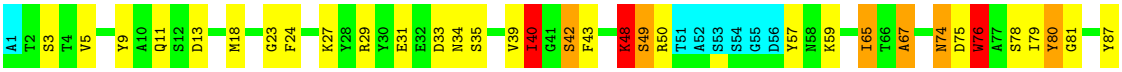
Chain A: 46% 34% 7% • 11%

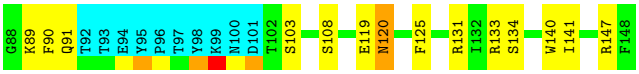


4.2.17 Score per residue for model 17

- Molecule 1: Outer membrane protein X

Chain A: 57% 25% 5% • 11%

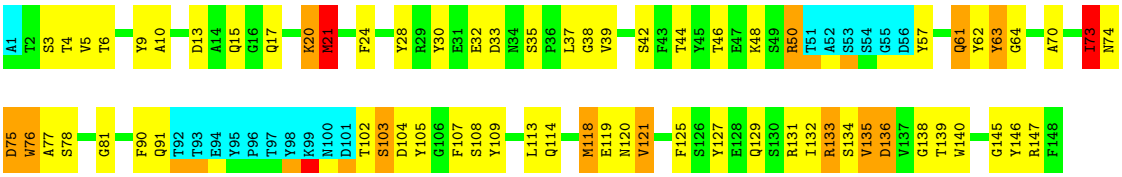




4.2.18 Score per residue for model 18

• Molecule 1: Outer membrane protein X

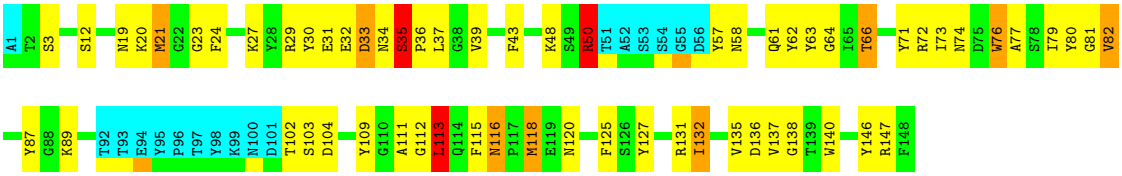
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Outer membrane protein X

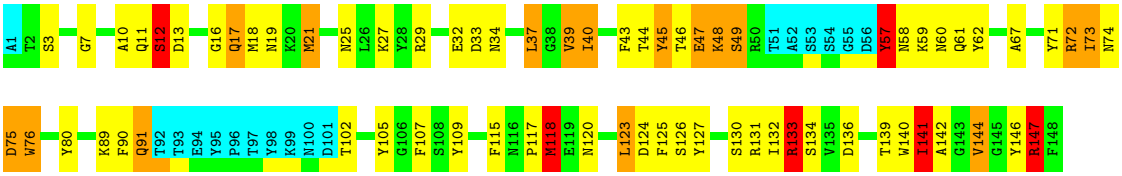
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Outer membrane protein X

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *TORSION ANGLE DYNAMICS (DYANA)*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	1.5

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	1030	968	957	24±8
All	All	20600	19360	19140	470

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ILE:HD12	1:A:68:GLY:O	0.84	1.72	1	1
1:A:7:GLY:O	1:A:141:ILE:HG22	0.79	1.77	8	1
1:A:78:SER:O	1:A:79:ILE:HG23	0.78	1.78	14	1
1:A:22:GLY:O	1:A:46:THR:HG23	0.78	1.79	13	1
1:A:82:VAL:HG22	1:A:109:TYR:CD2	0.74	2.18	16	1
1:A:113:LEU:HD13	1:A:113:LEU:N	0.73	1.98	5	1
1:A:67:ALA:HB1	1:A:81:GLY:O	0.72	1.83	17	1
1:A:37:LEU:HD12	1:A:70:ALA:HB1	0.71	1.62	18	1
1:A:26:LEU:HD23	1:A:27:LYS:N	0.71	2.00	3	1
1:A:29:ARG:NH1	1:A:39:VAL:HG12	0.70	2.01	12	1
1:A:73:ILE:HG23	1:A:73:ILE:O	0.69	1.87	7	4
1:A:37:LEU:C	1:A:37:LEU:HD22	0.69	2.07	20	1
1:A:122:ALA:HB1	1:A:143:GLY:O	0.68	1.88	14	1
1:A:135:VAL:O	1:A:135:VAL:HG13	0.68	1.88	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:TYR:CE2	1:A:90:PHE:CE2	0.68	2.81	10	1
1:A:132:ILE:HG23	1:A:133:ARG:N	0.68	2.02	4	1
1:A:102:THR:HG23	1:A:102:THR:O	0.66	1.91	18	3
1:A:79:ILE:HG23	1:A:79:ILE:O	0.66	1.90	8	1
1:A:121:VAL:O	1:A:122:ALA:HB2	0.66	1.91	14	1
1:A:40:ILE:HG23	1:A:40:ILE:O	0.66	1.91	17	2
1:A:4:THR:O	1:A:4:THR:HG22	0.65	1.90	2	1
1:A:37:LEU:HD13	1:A:70:ALA:O	0.65	1.92	2	1
1:A:65:ILE:HD13	1:A:85:VAL:O	0.65	1.90	4	1
1:A:132:ILE:HG23	1:A:132:ILE:O	0.65	1.90	9	2
1:A:44:THR:HG22	1:A:63:TYR:CE1	0.64	2.27	6	1
1:A:4:THR:HG22	1:A:147:ARG:HA	0.63	1.71	7	1
1:A:82:VAL:HG13	1:A:82:VAL:O	0.63	1.94	13	1
1:A:44:THR:HG23	1:A:44:THR:O	0.63	1.94	15	1
1:A:10:ALA:HB2	1:A:139:THR:HG23	0.63	1.71	20	1
1:A:141:ILE:C	1:A:141:ILE:HD12	0.62	2.15	7	1
1:A:9:TYR:O	1:A:141:ILE:HD13	0.62	1.93	3	1
1:A:29:ARG:HB3	1:A:40:ILE:HD13	0.62	1.70	3	1
1:A:4:THR:HG21	1:A:146:TYR:O	0.62	1.95	1	1
1:A:45:TYR:O	1:A:45:TYR:CD2	0.62	2.52	14	1
1:A:135:VAL:HG13	1:A:136:ASP:N	0.61	2.10	7	1
1:A:141:ILE:HG23	1:A:142:ALA:N	0.61	2.10	20	3
1:A:115:PHE:CD2	1:A:115:PHE:O	0.61	2.54	19	1
1:A:66:THR:O	1:A:67:ALA:HB3	0.61	1.95	3	1
1:A:76:TRP:O	1:A:77:ALA:HB3	0.61	1.94	10	3
1:A:42:SER:O	1:A:65:ILE:HG22	0.61	1.96	17	1
1:A:87:TYR:CD1	1:A:104:ASP:O	0.60	2.54	11	1
1:A:140:TRP:O	1:A:141:ILE:HD13	0.60	1.95	10	1
1:A:82:VAL:O	1:A:82:VAL:HG23	0.60	1.95	1	2
1:A:57:TYR:CD1	1:A:57:TYR:O	0.60	2.55	4	1
1:A:45:TYR:CD1	1:A:45:TYR:O	0.60	2.55	10	1
1:A:87:TYR:CE1	1:A:89:LYS:O	0.60	2.55	10	1
1:A:121:VAL:O	1:A:121:VAL:HG13	0.60	1.96	5	1
1:A:90:PHE:O	1:A:90:PHE:CD2	0.59	2.55	3	1
1:A:146:TYR:O	1:A:146:TYR:CD2	0.59	2.55	5	1
1:A:65:ILE:HG23	1:A:65:ILE:O	0.59	1.96	8	2
1:A:76:TRP:CE3	1:A:116:ASN:OD1	0.59	2.55	3	1
1:A:28:TYR:CD2	1:A:28:TYR:O	0.59	2.56	11	1
1:A:30:TYR:O	1:A:39:VAL:HG12	0.59	1.97	5	1
1:A:66:THR:O	1:A:67:ALA:HB2	0.59	1.96	11	1
1:A:85:VAL:O	1:A:85:VAL:HG12	0.58	1.98	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ILE:HD11	1:A:126:SER:HB3	0.58	1.74	14	1
1:A:105:TYR:CD1	1:A:105:TYR:O	0.58	2.57	8	2
1:A:112:GLY:O	1:A:113:LEU:HD23	0.58	1.99	9	1
1:A:7:GLY:HA2	1:A:26:LEU:HD22	0.58	1.75	14	1
1:A:40:ILE:HG22	1:A:68:GLY:CA	0.58	2.28	12	1
1:A:43:PHE:CD1	1:A:43:PHE:O	0.58	2.57	10	1
1:A:28:TYR:O	1:A:40:ILE:HG23	0.57	1.99	2	1
1:A:85:VAL:O	1:A:85:VAL:HG13	0.57	1.99	10	2
1:A:111:ALA:O	1:A:127:TYR:CD1	0.57	2.57	6	1
1:A:146:TYR:CD2	1:A:146:TYR:O	0.57	2.58	20	2
1:A:30:TYR:O	1:A:30:TYR:CD2	0.57	2.58	13	1
1:A:43:PHE:O	1:A:43:PHE:CD2	0.56	2.58	4	2
1:A:73:ILE:O	1:A:73:ILE:HD13	0.56	2.00	5	1
1:A:40:ILE:HD13	1:A:40:ILE:N	0.56	2.15	20	1
1:A:83:VAL:HG13	1:A:83:VAL:O	0.56	2.01	7	2
1:A:90:PHE:CE1	1:A:102:THR:OG1	0.56	2.55	9	1
1:A:90:PHE:O	1:A:90:PHE:CD1	0.56	2.59	1	1
1:A:62:TYR:CD2	1:A:87:TYR:O	0.56	2.59	3	1
1:A:80:TYR:O	1:A:80:TYR:CD2	0.56	2.59	17	1
1:A:28:TYR:CG	1:A:28:TYR:O	0.55	2.58	15	2
1:A:75:ASP:C	1:A:76:TRP:CG	0.55	2.80	17	2
1:A:62:TYR:CE2	1:A:63:TYR:CE2	0.55	2.95	15	1
1:A:123:LEU:HD12	1:A:123:LEU:O	0.55	2.01	14	1
1:A:25:ASN:O	1:A:26:LEU:HD22	0.54	2.01	8	1
1:A:68:GLY:N	1:A:69:PRO:CD	0.54	2.70	14	2
1:A:76:TRP:O	1:A:76:TRP:CG	0.54	2.61	20	1
1:A:72:ARG:O	1:A:73:ILE:HG22	0.54	2.03	12	2
1:A:66:THR:HG23	1:A:67:ALA:N	0.54	2.16	2	1
1:A:59:LYS:O	1:A:90:PHE:CG	0.54	2.60	10	1
1:A:39:VAL:HG22	1:A:39:VAL:O	0.54	2.01	4	2
1:A:39:VAL:HG22	1:A:68:GLY:HA2	0.54	1.80	14	1
1:A:140:TRP:CG	1:A:140:TRP:O	0.54	2.60	14	1
1:A:39:VAL:HG22	1:A:68:GLY:CA	0.54	2.32	14	1
1:A:57:TYR:CG	1:A:57:TYR:O	0.53	2.60	18	2
1:A:65:ILE:HD13	1:A:65:ILE:H	0.53	1.62	14	1
1:A:115:PHE:CE2	1:A:116:ASN:O	0.53	2.61	9	1
1:A:121:VAL:O	1:A:122:ALA:CB	0.53	2.57	14	1
1:A:134:SER:O	1:A:135:VAL:HG12	0.53	2.04	7	1
1:A:80:TYR:CD1	1:A:80:TYR:O	0.53	2.62	6	1
1:A:82:VAL:CG2	1:A:109:TYR:CD2	0.53	2.90	16	1
1:A:27:LYS:CB	1:A:41:GLY:O	0.53	2.56	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ILE:O	1:A:79:ILE:CG2	0.53	2.56	8	1
1:A:13:ASP:O	1:A:14:ALA:HB2	0.52	2.03	7	2
1:A:30:TYR:O	1:A:30:TYR:CG	0.52	2.61	13	2
1:A:5:VAL:O	1:A:5:VAL:HG13	0.52	2.04	8	2
1:A:40:ILE:CG1	1:A:40:ILE:O	0.52	2.58	14	1
1:A:73:ILE:HG21	1:A:77:ALA:H	0.52	1.63	14	1
1:A:127:TYR:O	1:A:127:TYR:CD2	0.52	2.63	11	1
1:A:39:VAL:O	1:A:39:VAL:HG13	0.52	2.04	6	2
1:A:137:VAL:HG12	1:A:138:GLY:H	0.52	1.65	19	2
1:A:45:TYR:CD1	1:A:45:TYR:C	0.52	2.83	10	1
1:A:28:TYR:O	1:A:28:TYR:CD2	0.52	2.63	15	1
1:A:23:GLY:O	1:A:24:PHE:CG	0.52	2.63	19	1
1:A:80:TYR:CD2	1:A:111:ALA:HB2	0.52	2.39	14	1
1:A:137:VAL:O	1:A:137:VAL:HG23	0.52	2.05	14	1
1:A:43:PHE:CG	1:A:43:PHE:O	0.52	2.62	20	1
1:A:105:TYR:O	1:A:105:TYR:CG	0.52	2.63	7	2
1:A:112:GLY:C	1:A:113:LEU:HD23	0.52	2.25	19	1
1:A:62:TYR:O	1:A:62:TYR:CD1	0.52	2.63	7	1
1:A:59:LYS:HD3	1:A:62:TYR:CE2	0.51	2.40	9	1
1:A:127:TYR:CG	1:A:127:TYR:O	0.51	2.63	2	1
1:A:45:TYR:O	1:A:45:TYR:CG	0.51	2.63	20	3
1:A:117:PRO:O	1:A:118:MET:CB	0.51	2.58	20	1
1:A:106:GLY:HA3	1:A:132:ILE:HD13	0.51	1.81	4	1
1:A:73:ILE:O	1:A:73:ILE:CG2	0.51	2.57	7	2
1:A:10:ALA:HB2	1:A:141:ILE:CG1	0.51	2.35	15	1
1:A:24:PHE:CD1	1:A:24:PHE:C	0.51	2.83	18	1
1:A:71:TYR:CD1	1:A:80:TYR:CE1	0.51	2.99	8	1
1:A:32:GLU:O	1:A:33:ASP:CB	0.51	2.58	3	1
1:A:90:PHE:O	1:A:90:PHE:CG	0.51	2.63	3	2
1:A:85:VAL:HG23	1:A:85:VAL:O	0.51	2.05	9	1
1:A:9:TYR:CB	1:A:141:ILE:HG21	0.51	2.36	8	1
1:A:33:ASP:O	1:A:34:ASN:CB	0.50	2.59	19	1
1:A:72:ARG:C	1:A:73:ILE:HD13	0.50	2.27	4	1
1:A:61:GLN:O	1:A:62:TYR:CG	0.50	2.64	6	1
1:A:90:PHE:CE1	1:A:102:THR:CB	0.50	2.94	9	1
1:A:9:TYR:CG	1:A:9:TYR:O	0.50	2.63	13	1
1:A:57:TYR:O	1:A:57:TYR:CD1	0.50	2.65	18	1
1:A:11:GLN:O	1:A:12:SER:CB	0.50	2.59	20	1
1:A:111:ALA:O	1:A:127:TYR:CE1	0.50	2.64	6	1
1:A:76:TRP:O	1:A:77:ALA:CB	0.50	2.60	10	3
1:A:76:TRP:O	1:A:76:TRP:CE3	0.50	2.65	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:TYR:O	1:A:71:TYR:CG	0.50	2.64	7	1
1:A:59:LYS:O	1:A:90:PHE:CB	0.50	2.60	10	1
1:A:114:GLN:O	1:A:115:PHE:CB	0.50	2.59	14	1
1:A:134:SER:O	1:A:135:VAL:HG22	0.50	2.06	2	1
1:A:121:VAL:CG1	1:A:145:GLY:O	0.50	2.60	14	1
1:A:10:ALA:O	1:A:21:MET:CB	0.50	2.60	18	1
1:A:146:TYR:O	1:A:146:TYR:CG	0.49	2.64	5	3
1:A:2:THR:O	1:A:3:SER:CB	0.49	2.60	14	1
1:A:129:GLN:O	1:A:130:SER:CB	0.49	2.60	10	1
1:A:137:VAL:HG22	1:A:138:GLY:H	0.49	1.67	10	1
1:A:20:LYS:O	1:A:21:MET:C	0.49	2.50	18	1
1:A:124:ASP:CG	1:A:141:ILE:CD1	0.49	2.81	7	1
1:A:13:ASP:HB3	1:A:137:VAL:HG11	0.49	1.83	9	1
1:A:130:SER:O	1:A:135:VAL:HG23	0.49	2.08	9	1
1:A:62:TYR:CE2	1:A:87:TYR:O	0.49	2.66	11	1
1:A:147:ARG:CG	1:A:147:ARG:O	0.49	2.60	11	1
1:A:59:LYS:CD	1:A:62:TYR:CD2	0.49	2.95	9	1
1:A:140:TRP:CE3	1:A:141:ILE:O	0.49	2.65	9	1
1:A:129:GLN:HB3	1:A:137:VAL:HG12	0.49	1.83	10	1
1:A:102:THR:O	1:A:102:THR:CG2	0.49	2.60	18	1
1:A:116:ASN:OD1	1:A:122:ALA:CB	0.49	2.60	6	1
1:A:57:TYR:O	1:A:58:ASN:CB	0.49	2.60	20	1
1:A:125:PHE:O	1:A:126:SER:CB	0.49	2.59	8	1
1:A:132:ILE:CG1	1:A:132:ILE:O	0.49	2.61	10	1
1:A:14:ALA:HB3	1:A:19:ASN:HB2	0.48	1.83	3	1
1:A:34:ASN:O	1:A:35:SER:CB	0.48	2.61	19	1
1:A:121:VAL:O	1:A:121:VAL:CG1	0.48	2.61	5	1
1:A:80:TYR:O	1:A:80:TYR:CG	0.48	2.66	8	2
1:A:137:VAL:O	1:A:137:VAL:CG2	0.48	2.61	14	1
1:A:29:ARG:N	1:A:40:ILE:HG21	0.48	2.22	15	1
1:A:139:THR:O	1:A:139:THR:HG23	0.48	2.08	6	3
1:A:132:ILE:CG2	1:A:133:ARG:N	0.48	2.72	4	1
1:A:73:ILE:C	1:A:73:ILE:CD1	0.48	2.81	7	3
1:A:17:GLN:O	1:A:18:MET:CB	0.48	2.62	12	1
1:A:59:LYS:O	1:A:60:ASN:CB	0.48	2.61	7	2
1:A:62:TYR:CE1	1:A:87:TYR:HB2	0.48	2.42	16	1
1:A:44:THR:O	1:A:44:THR:HG22	0.48	2.09	18	1
1:A:37:LEU:C	1:A:37:LEU:CD2	0.48	2.81	20	1
1:A:75:ASP:OD2	1:A:76:TRP:CD1	0.48	2.67	1	1
1:A:49:SER:O	1:A:50:ARG:CB	0.48	2.62	9	1
1:A:112:GLY:O	1:A:113:LEU:CB	0.48	2.62	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:THR:O	1:A:6:THR:HG23	0.48	2.09	12	2
1:A:134:SER:O	1:A:135:VAL:CB	0.48	2.62	7	1
1:A:79:ILE:CG2	1:A:80:TYR:N	0.48	2.77	9	1
1:A:115:PHE:N	1:A:123:LEU:CB	0.48	2.77	14	1
1:A:10:ALA:HB2	1:A:141:ILE:HG13	0.48	1.85	15	1
1:A:138:GLY:O	1:A:139:THR:HG23	0.48	2.09	18	1
1:A:5:VAL:O	1:A:5:VAL:HG12	0.48	2.09	7	2
1:A:124:ASP:O	1:A:125:PHE:CD2	0.48	2.67	15	1
1:A:44:THR:CG2	1:A:45:TYR:N	0.47	2.76	9	1
1:A:58:ASN:O	1:A:59:LYS:CB	0.47	2.62	10	1
1:A:26:LEU:O	1:A:27:LYS:C	0.47	2.52	15	1
1:A:66:THR:O	1:A:67:ALA:CB	0.47	2.62	3	2
1:A:4:THR:HG22	1:A:147:ARG:CA	0.47	2.38	7	1
1:A:6:THR:OG1	1:A:123:LEU:CD2	0.47	2.62	8	1
1:A:48:LYS:O	1:A:49:SER:CB	0.47	2.61	12	2
1:A:25:ASN:O	1:A:26:LEU:HD12	0.47	2.09	2	1
1:A:124:ASP:O	1:A:141:ILE:CG2	0.47	2.63	14	1
1:A:72:ARG:O	1:A:73:ILE:HG23	0.47	2.09	9	1
1:A:79:ILE:HD11	1:A:126:SER:CB	0.47	2.39	14	1
1:A:59:LYS:HD3	1:A:62:TYR:CD2	0.47	2.45	9	1
1:A:134:SER:C	1:A:135:VAL:HG23	0.47	2.30	10	1
1:A:44:THR:O	1:A:44:THR:CG2	0.47	2.61	15	1
1:A:49:SER:OG	1:A:58:ASN:CB	0.47	2.62	2	1
1:A:144:VAL:O	1:A:144:VAL:HG13	0.47	2.10	4	2
1:A:40:ILE:O	1:A:40:ILE:CG2	0.47	2.62	17	2
1:A:24:PHE:CD1	1:A:24:PHE:O	0.47	2.68	18	1
1:A:132:ILE:O	1:A:132:ILE:CD1	0.47	2.63	9	1
1:A:107:PHE:O	1:A:108:SER:CB	0.47	2.63	6	1
1:A:47:GLU:O	1:A:48:LYS:CB	0.47	2.62	14	3
1:A:128:GLU:O	1:A:129:GLN:CB	0.47	2.63	4	1
1:A:59:LYS:CD	1:A:62:TYR:CE2	0.47	2.98	9	1
1:A:146:TYR:O	1:A:147:ARG:CG	0.46	2.64	20	1
1:A:2:THR:CG2	1:A:3:SER:N	0.46	2.79	9	1
1:A:6:THR:HG23	1:A:25:ASN:ND2	0.46	2.24	9	1
1:A:66:THR:O	1:A:66:THR:HG23	0.46	2.09	8	1
1:A:128:GLU:O	1:A:129:GLN:CG	0.46	2.64	4	1
1:A:87:TYR:CD1	1:A:87:TYR:C	0.46	2.89	12	1
1:A:142:ALA:O	1:A:144:VAL:HG12	0.46	2.11	14	1
1:A:14:ALA:HB1	1:A:137:VAL:HG12	0.46	1.88	16	1
1:A:124:ASP:CG	1:A:141:ILE:HD13	0.46	2.31	7	1
1:A:22:GLY:O	1:A:45:TYR:CE2	0.46	2.69	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ILE:HG22	1:A:73:ILE:O	0.46	2.11	16	1
1:A:4:THR:O	1:A:4:THR:CG2	0.46	2.60	2	1
1:A:135:VAL:HG12	1:A:137:VAL:HG13	0.46	1.88	14	1
1:A:135:VAL:CG1	1:A:136:ASP:N	0.46	2.78	7	1
1:A:132:ILE:HG22	1:A:132:ILE:O	0.46	2.10	11	1
1:A:105:TYR:O	1:A:105:TYR:CD1	0.46	2.69	13	1
1:A:130:SER:O	1:A:131:ARG:CB	0.46	2.64	14	1
1:A:33:ASP:O	1:A:34:ASN:ND2	0.46	2.49	19	1
1:A:132:ILE:O	1:A:133:ARG:CB	0.46	2.62	16	5
1:A:36:PRO:C	1:A:37:LEU:HD13	0.46	2.31	7	1
1:A:37:LEU:CD2	1:A:37:LEU:C	0.45	2.84	7	1
1:A:28:TYR:O	1:A:28:TYR:CG	0.45	2.70	11	1
1:A:119:GLU:O	1:A:120:ASN:ND2	0.45	2.49	17	1
1:A:73:ILE:C	1:A:73:ILE:HD13	0.45	2.32	7	1
1:A:4:THR:HG22	1:A:5:VAL:H	0.45	1.70	18	1
1:A:132:ILE:HG23	1:A:133:ARG:H	0.45	1.70	4	1
1:A:24:PHE:O	1:A:24:PHE:CG	0.45	2.69	5	1
1:A:48:LYS:O	1:A:50:ARG:N	0.45	2.49	7	2
1:A:65:ILE:CG1	1:A:85:VAL:HG12	0.45	2.41	10	1
1:A:27:LYS:HD3	1:A:43:PHE:CE1	0.45	2.47	15	1
1:A:19:ASN:O	1:A:21:MET:N	0.45	2.50	12	1
1:A:40:ILE:HG22	1:A:68:GLY:HA3	0.45	1.86	12	1
1:A:23:GLY:O	1:A:24:PHE:CD2	0.45	2.70	15	1
1:A:79:ILE:O	1:A:80:TYR:CG	0.45	2.69	15	1
1:A:135:VAL:HG13	1:A:137:VAL:HG23	0.45	1.89	15	1
1:A:47:GLU:CG	1:A:48:LYS:N	0.45	2.80	20	1
1:A:130:SER:HB2	1:A:137:VAL:HG21	0.45	1.89	12	1
1:A:25:ASN:HB2	1:A:43:PHE:CE2	0.45	2.47	2	1
1:A:14:ALA:O	1:A:16:GLY:N	0.45	2.50	10	3
1:A:125:PHE:CD1	1:A:125:PHE:C	0.45	2.90	5	1
1:A:65:ILE:O	1:A:65:ILE:CG2	0.45	2.65	8	1
1:A:79:ILE:O	1:A:112:GLY:N	0.45	2.49	19	2
1:A:20:LYS:O	1:A:22:GLY:N	0.45	2.50	4	1
1:A:134:SER:O	1:A:136:ASP:N	0.45	2.50	6	3
1:A:133:ARG:O	1:A:134:SER:C	0.45	2.54	11	1
1:A:75:ASP:HB2	1:A:76:TRP:CD1	0.44	2.46	3	1
1:A:125:PHE:CB	1:A:141:ILE:O	0.44	2.66	16	1
1:A:6:THR:HG22	1:A:28:TYR:HA	0.44	1.88	18	1
1:A:89:LYS:O	1:A:90:PHE:CG	0.44	2.70	2	1
1:A:132:ILE:O	1:A:133:ARG:C	0.44	2.56	20	3
1:A:83:VAL:O	1:A:83:VAL:CG1	0.44	2.64	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:VAL:O	1:A:82:VAL:CG2	0.44	2.64	1	1
1:A:133:ARG:O	1:A:134:SER:CB	0.44	2.64	5	1
1:A:141:ILE:HG22	1:A:142:ALA:N	0.44	2.27	10	1
1:A:26:LEU:HD21	1:A:40:ILE:HD11	0.44	1.89	12	1
1:A:23:GLY:HA2	1:A:45:TYR:CD2	0.44	2.47	14	1
1:A:105:TYR:CD1	1:A:105:TYR:C	0.44	2.90	8	1
1:A:109:TYR:CD1	1:A:109:TYR:N	0.44	2.86	9	1
1:A:82:VAL:HG21	1:A:128:GLU:CB	0.44	2.43	10	1
1:A:73:ILE:O	1:A:74:ASN:CB	0.44	2.65	12	1
1:A:57:TYR:O	1:A:59:LYS:N	0.44	2.51	13	1
1:A:82:VAL:O	1:A:82:VAL:CG1	0.44	2.65	13	1
1:A:78:SER:O	1:A:79:ILE:CG2	0.44	2.60	14	1
1:A:50:ARG:HD2	1:A:57:TYR:CZ	0.44	2.48	15	1
1:A:129:GLN:O	1:A:137:VAL:HG23	0.44	2.12	4	1
1:A:62:TYR:CZ	1:A:87:TYR:O	0.44	2.71	11	1
1:A:80:TYR:C	1:A:80:TYR:CD1	0.44	2.91	11	1
1:A:40:ILE:O	1:A:40:ILE:CD1	0.44	2.65	17	1
1:A:43:PHE:CB	1:A:64:GLY:O	0.44	2.66	4	1
1:A:126:SER:OG	1:A:127:TYR:N	0.44	2.50	16	2
1:A:113:LEU:N	1:A:113:LEU:CD1	0.44	2.70	5	1
1:A:73:ILE:O	1:A:75:ASP:N	0.44	2.50	11	2
1:A:30:TYR:O	1:A:30:TYR:CD1	0.44	2.71	12	1
1:A:134:SER:O	1:A:135:VAL:C	0.44	2.56	4	2
1:A:132:ILE:O	1:A:132:ILE:CG2	0.44	2.61	9	1
1:A:130:SER:O	1:A:131:ARG:CG	0.44	2.65	14	1
1:A:19:ASN:CB	1:A:47:GLU:OE1	0.44	2.66	20	1
1:A:46:THR:O	1:A:47:GLU:CB	0.44	2.66	2	1
1:A:37:LEU:HD21	1:A:71:TYR:CD1	0.44	2.48	9	1
1:A:134:SER:O	1:A:135:VAL:CG2	0.44	2.66	2	1
1:A:134:SER:C	1:A:136:ASP:N	0.44	2.71	4	1
1:A:135:VAL:O	1:A:135:VAL:CG1	0.44	2.59	4	1
1:A:116:ASN:ND2	1:A:118:MET:O	0.44	2.51	6	1
1:A:139:THR:O	1:A:139:THR:CG2	0.43	2.66	3	1
1:A:5:VAL:O	1:A:5:VAL:CG1	0.43	2.66	8	1
1:A:105:TYR:C	1:A:105:TYR:CD1	0.43	2.90	3	1
1:A:105:TYR:O	1:A:105:TYR:CD2	0.43	2.71	7	1
1:A:89:LYS:O	1:A:90:PHE:CD1	0.43	2.71	2	1
1:A:58:ASN:O	1:A:59:LYS:CG	0.43	2.66	13	1
1:A:5:VAL:HG13	1:A:5:VAL:O	0.43	2.12	1	1
1:A:44:THR:HG22	1:A:63:TYR:CZ	0.43	2.48	6	1
1:A:82:VAL:HG21	1:A:128:GLU:HB2	0.43	1.89	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:VAL:HG23	1:A:40:ILE:N	0.43	2.28	14	1
1:A:65:ILE:HD13	1:A:65:ILE:N	0.43	2.28	14	1
1:A:21:MET:SD	1:A:21:MET:N	0.43	2.91	18	1
1:A:115:PHE:O	1:A:115:PHE:CG	0.43	2.71	19	1
1:A:141:ILE:CG2	1:A:142:ALA:N	0.43	2.79	20	3
1:A:140:TRP:CZ3	1:A:141:ILE:O	0.43	2.71	9	1
1:A:59:LYS:O	1:A:90:PHE:CD2	0.43	2.71	10	1
1:A:45:TYR:CD1	1:A:45:TYR:N	0.43	2.87	13	1
1:A:62:TYR:CE1	1:A:87:TYR:CB	0.43	3.01	16	1
1:A:43:PHE:CD1	1:A:43:PHE:N	0.43	2.86	19	1
1:A:134:SER:O	1:A:135:VAL:CG1	0.43	2.66	9	2
1:A:58:ASN:C	1:A:59:LYS:CG	0.43	2.86	10	1
1:A:8:GLY:O	1:A:10:ALA:N	0.43	2.52	6	1
1:A:87:TYR:CG	1:A:104:ASP:O	0.43	2.71	11	1
1:A:68:GLY:N	1:A:69:PRO:HD2	0.43	2.29	14	1
1:A:132:ILE:O	1:A:134:SER:N	0.43	2.52	1	1
1:A:4:THR:HG23	1:A:146:TYR:HA	0.43	1.90	5	1
1:A:123:LEU:O	1:A:123:LEU:HD12	0.43	2.13	5	1
1:A:115:PHE:CD2	1:A:116:ASN:O	0.43	2.72	9	1
1:A:25:ASN:HA	1:A:43:PHE:CD2	0.43	2.49	2	1
1:A:109:TYR:CZ	1:A:128:GLU:CD	0.43	2.93	6	1
1:A:124:ASP:OD1	1:A:141:ILE:CD1	0.43	2.67	7	1
1:A:140:TRP:O	1:A:140:TRP:CD1	0.43	2.71	14	1
1:A:87:TYR:CE1	1:A:88:GLY:O	0.42	2.72	12	1
1:A:27:LYS:CG	1:A:41:GLY:O	0.42	2.66	14	1
1:A:75:ASP:O	1:A:76:TRP:CD2	0.42	2.72	17	1
1:A:135:VAL:HG12	1:A:136:ASP:N	0.42	2.29	18	1
1:A:109:TYR:CD1	1:A:109:TYR:C	0.42	2.92	19	1
1:A:108:SER:CB	1:A:129:GLN:O	0.42	2.67	4	1
1:A:120:ASN:OD1	1:A:120:ASN:N	0.42	2.52	4	1
1:A:63:TYR:CE1	1:A:64:GLY:O	0.42	2.72	19	1
1:A:146:TYR:O	1:A:147:ARG:CB	0.42	2.68	20	1
1:A:125:PHE:CD1	1:A:125:PHE:O	0.42	2.72	5	1
1:A:49:SER:C	1:A:50:ARG:CG	0.42	2.88	16	1
1:A:57:TYR:O	1:A:91:GLN:N	0.42	2.53	20	1
1:A:43:PHE:CD1	1:A:43:PHE:C	0.42	2.92	2	1
1:A:66:THR:CB	1:A:82:VAL:HG21	0.42	2.44	19	1
1:A:141:ILE:C	1:A:141:ILE:CD1	0.42	2.88	7	1
1:A:80:TYR:CD1	1:A:80:TYR:C	0.42	2.93	16	1
1:A:135:VAL:O	1:A:136:ASP:CB	0.42	2.67	19	1
1:A:7:GLY:O	1:A:144:VAL:HG12	0.42	2.14	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:MET:O	1:A:20:LYS:N	0.42	2.53	4	1
1:A:144:VAL:O	1:A:144:VAL:CG1	0.42	2.67	4	1
1:A:61:GLN:O	1:A:62:TYR:CD2	0.42	2.73	8	1
1:A:63:TYR:CG	1:A:64:GLY:N	0.42	2.87	19	1
1:A:73:ILE:CG2	1:A:74:ASN:N	0.42	2.83	5	1
1:A:23:GLY:C	1:A:24:PHE:CG	0.42	2.93	19	1
1:A:71:TYR:O	1:A:72:ARG:CB	0.41	2.67	9	1
1:A:137:VAL:HG22	1:A:138:GLY:N	0.41	2.30	10	1
1:A:80:TYR:CD2	1:A:111:ALA:CB	0.41	3.02	19	1
1:A:26:LEU:N	1:A:42:SER:CB	0.41	2.83	4	1
1:A:121:VAL:HG23	1:A:145:GLY:O	0.41	2.15	18	1
1:A:32:GLU:O	1:A:33:ASP:CG	0.41	2.58	19	1
1:A:90:PHE:O	1:A:91:GLN:C	0.41	2.59	20	1
1:A:4:THR:O	1:A:146:TYR:O	0.41	2.38	11	1
1:A:49:SER:O	1:A:50:ARG:C	0.41	2.59	4	2
1:A:39:VAL:HG12	1:A:39:VAL:O	0.41	2.14	19	1
1:A:66:THR:HA	1:A:82:VAL:CG2	0.41	2.45	19	1
1:A:9:TYR:CD1	1:A:23:GLY:O	0.41	2.74	8	1
1:A:85:VAL:O	1:A:85:VAL:CG1	0.41	2.69	16	1
1:A:128:GLU:OE1	1:A:139:THR:HG21	0.41	2.16	16	1
1:A:6:THR:O	1:A:6:THR:CG2	0.41	2.68	18	1
1:A:87:TYR:CE2	1:A:90:PHE:CZ	0.41	3.08	10	1
1:A:20:LYS:C	1:A:21:MET:SD	0.41	2.99	18	1
1:A:90:PHE:CZ	1:A:102:THR:OG1	0.41	2.61	9	1
1:A:127:TYR:O	1:A:127:TYR:CG	0.41	2.74	6	1
1:A:83:VAL:HG22	1:A:107:PHE:CE1	0.41	2.50	16	1
1:A:71:TYR:O	1:A:80:TYR:CD1	0.41	2.74	20	1
1:A:66:THR:CG2	1:A:67:ALA:N	0.41	2.84	2	1
1:A:106:GLY:O	1:A:107:PHE:CD1	0.41	2.74	4	1
1:A:135:VAL:HG22	1:A:135:VAL:O	0.41	2.16	9	1
1:A:26:LEU:O	1:A:27:LYS:CB	0.41	2.69	12	1
1:A:72:ARG:O	1:A:73:ILE:O	0.41	2.39	12	1
1:A:116:ASN:CB	1:A:122:ALA:O	0.41	2.69	14	1
1:A:121:VAL:HG11	1:A:145:GLY:O	0.41	2.16	14	1
1:A:26:LEU:O	1:A:27:LYS:O	0.41	2.38	15	1
1:A:37:LEU:HD12	1:A:38:GLY:O	0.41	2.16	2	1
1:A:75:ASP:OD1	1:A:76:TRP:N	0.41	2.51	3	1
1:A:13:ASP:O	1:A:14:ALA:CB	0.41	2.69	7	1
1:A:125:PHE:CE1	1:A:141:ILE:HB	0.41	2.51	15	1
1:A:38:GLY:N	1:A:70:ALA:HB3	0.41	2.30	18	1
1:A:126:SER:O	1:A:139:THR:O	0.40	2.39	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:O	1:A:61:GLN:N	0.40	2.53	14	1
1:A:112:GLY:O	1:A:113:LEU:HD22	0.40	2.17	4	1
1:A:85:VAL:HG13	1:A:87:TYR:CE2	0.40	2.51	7	1
1:A:27:LYS:O	1:A:41:GLY:N	0.40	2.53	15	1
1:A:46:THR:O	1:A:61:GLN:O	0.40	2.40	18	1
1:A:40:ILE:HG22	1:A:68:GLY:HA2	0.40	1.93	12	1
1:A:20:LYS:O	1:A:20:LYS:CG	0.40	2.69	13	1
1:A:102:THR:O	1:A:102:THR:HG23	0.40	2.16	13	1
1:A:115:PHE:O	1:A:116:ASN:OD1	0.40	2.39	19	1
1:A:103:SER:O	1:A:104:ASP:CB	0.40	2.69	2	1
1:A:90:PHE:CD1	1:A:90:PHE:O	0.40	2.74	13	1
1:A:79:ILE:CG1	1:A:112:GLY:HA3	0.40	2.47	14	1
1:A:76:TRP:O	1:A:77:ALA:C	0.40	2.59	19	1
1:A:73:ILE:HD13	1:A:73:ILE:O	0.40	2.16	10	1
1:A:4:THR:O	1:A:146:TYR:N	0.40	2.46	11	1
1:A:44:THR:O	1:A:63:TYR:O	0.40	2.40	18	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	130/148 (88%)	78±5 (60±4%)	34±4 (26±3%)	17±5 (13±4%)	1 5
All	All	2600/2960 (88%)	1564 (60%)	688 (26%)	348 (13%)	1 5

All 110 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	50	ARG	14
1	A	120	ASN	13
1	A	74	ASN	12
1	A	76	TRP	11
1	A	49	SER	9
1	A	34	ASN	8

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Mol	Chain	Res	Type	Models (Total)
1	A	81	GLY	8
1	A	16	GLY	8
1	A	131	ARG	8
1	A	73	ILE	7
1	A	17	GLN	7
1	A	126	SER	7
1	A	32	GLU	6
1	A	33	ASP	6
1	A	39	VAL	6
1	A	118	MET	6
1	A	144	VAL	5
1	A	59	LYS	5
1	A	67	ALA	5
1	A	132	ILE	5
1	A	72	ARG	5
1	A	48	LYS	5
1	A	57	TYR	4
1	A	60	ASN	4
1	A	91	GLN	4
1	A	103	SER	4
1	A	19	ASN	4
1	A	21	MET	4
1	A	27	LYS	4
1	A	141	ILE	4
1	A	147	ARG	4
1	A	135	VAL	4
1	A	78	SER	4
1	A	3	SER	3
1	A	12	SER	3
1	A	18	MET	3
1	A	25	ASN	3
1	A	58	ASN	3
1	A	63	TYR	3
1	A	88	GLY	3
1	A	116	ASN	3
1	A	136	ASP	3
1	A	77	ALA	3
1	A	117	PRO	3
1	A	37	LEU	3
1	A	108	SER	3
1	A	2	THR	3
1	A	79	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	102	THR	3
1	A	40	ILE	3
1	A	121	VAL	2
1	A	90	PHE	2
1	A	62	TYR	2
1	A	129	GLN	2
1	A	36	PRO	2
1	A	134	SER	2
1	A	138	GLY	2
1	A	146	TYR	2
1	A	9	TYR	2
1	A	13	ASP	2
1	A	41	GLY	2
1	A	42	SER	2
1	A	61	GLN	2
1	A	111	ALA	2
1	A	14	ALA	2
1	A	140	TRP	2
1	A	28	TYR	2
1	A	65	ILE	2
1	A	89	LYS	2
1	A	128	GLU	2
1	A	113	LEU	2
1	A	15	GLN	2
1	A	130	SER	2
1	A	20	LYS	2
1	A	23	GLY	2
1	A	35	SER	2
1	A	104	ASP	2
1	A	22	GLY	1
1	A	6	THR	1
1	A	47	GLU	1
1	A	87	TYR	1
1	A	24	PHE	1
1	A	107	PHE	1
1	A	142	ALA	1
1	A	43	PHE	1
1	A	44	THR	1
1	A	127	TYR	1
1	A	26	LEU	1
1	A	109	TYR	1
1	A	139	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	114	GLN	1
1	A	30	TYR	1
1	A	83	VAL	1
1	A	4	THR	1
1	A	29	ARG	1
1	A	124	ASP	1
1	A	68	GLY	1
1	A	125	PHE	1
1	A	38	GLY	1
1	A	85	VAL	1
1	A	105	TYR	1
1	A	115	PHE	1
1	A	122	ALA	1
1	A	80	TYR	1
1	A	64	GLY	1
1	A	75	ASP	1
1	A	82	VAL	1
1	A	45	TYR	1
1	A	123	LEU	1
1	A	133	ARG	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	104/118 (88%)	71±4 (68±4%)	33±4 (32±4%)	1 13
All	All	2080/2360 (88%)	1413 (68%)	667 (32%)	1 13

All 95 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	20	LYS	14
1	A	21	MET	14
1	A	147	ARG	14
1	A	29	ARG	13
1	A	91	GLN	13

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Mol	Chain	Res	Type	Models (Total)
1	A	113	LEU	13
1	A	133	ARG	13
1	A	89	LYS	13
1	A	76	TRP	13
1	A	134	SER	12
1	A	140	TRP	12
1	A	26	LEU	11
1	A	27	LYS	11
1	A	48	LYS	11
1	A	104	ASP	11
1	A	37	LEU	11
1	A	13	ASP	11
1	A	72	ARG	11
1	A	3	SER	11
1	A	119	GLU	10
1	A	123	LEU	10
1	A	62	TYR	10
1	A	75	ASP	10
1	A	35	SER	10
1	A	12	SER	9
1	A	18	MET	9
1	A	32	GLU	9
1	A	118	MET	9
1	A	9	TYR	9
1	A	17	GLN	9
1	A	59	LYS	9
1	A	131	ARG	9
1	A	61	GLN	9
1	A	87	TYR	9
1	A	42	SER	8
1	A	73	ILE	8
1	A	15	GLN	8
1	A	50	ARG	8
1	A	125	PHE	8
1	A	146	TYR	8
1	A	47	GLU	8
1	A	71	TYR	7
1	A	130	SER	7
1	A	31	GLU	7
1	A	33	ASP	7
1	A	78	SER	7
1	A	57	TYR	6

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Mol	Chain	Res	Type	Models (Total)
1	A	60	ASN	6
1	A	107	PHE	6
1	A	115	PHE	6
1	A	127	TYR	6
1	A	40	ILE	6
1	A	49	SER	6
1	A	103	SER	6
1	A	114	GLN	6
1	A	63	TYR	6
1	A	74	ASN	6
1	A	126	SER	6
1	A	136	ASP	6
1	A	108	SER	6
1	A	128	GLU	5
1	A	129	GLN	5
1	A	148	PHE	5
1	A	11	GLN	5
1	A	28	TYR	5
1	A	79	ILE	5
1	A	124	ASP	5
1	A	141	ILE	5
1	A	19	ASN	4
1	A	65	ILE	4
1	A	30	TYR	4
1	A	43	PHE	4
1	A	90	PHE	4
1	A	132	ILE	4
1	A	24	PHE	4
1	A	109	TYR	4
1	A	105	TYR	4
1	A	121	VAL	3
1	A	44	THR	3
1	A	45	TYR	3
1	A	85	VAL	3
1	A	137	VAL	3
1	A	46	THR	3
1	A	80	TYR	3
1	A	58	ASN	3
1	A	120	ASN	3
1	A	66	THR	3
1	A	25	ASN	2
1	A	135	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	34	ASN	2
1	A	102	THR	2
1	A	2	THR	2
1	A	116	ASN	2
1	A	6	THR	1
1	A	4	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