



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:17 pm GMT

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

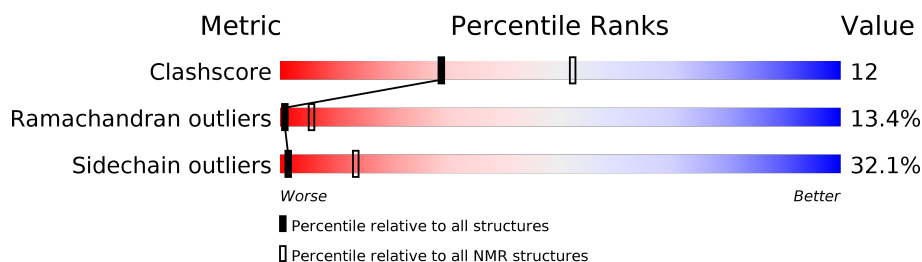
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	148	

2 Ensemble composition and analysis

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

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
1	A	148	Total	C	H	N	O	S	0
			2237	731	1080	190	233	3	

There is a discrepancy between the modelled and reference sequences:

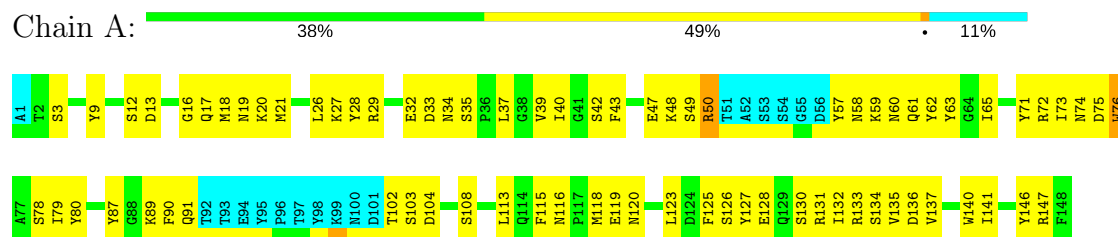
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASN	HIS	ENGINEERED	UNP P0A917

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

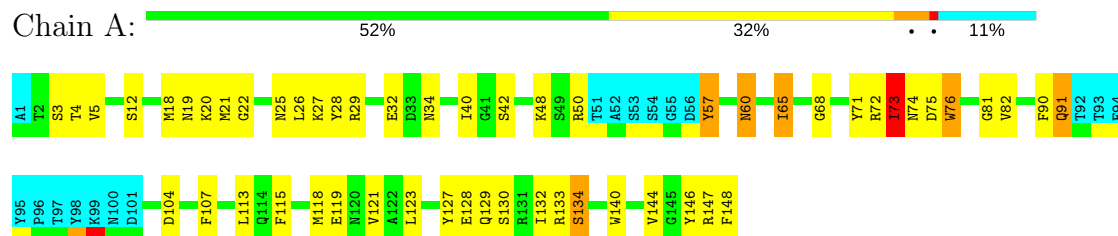


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

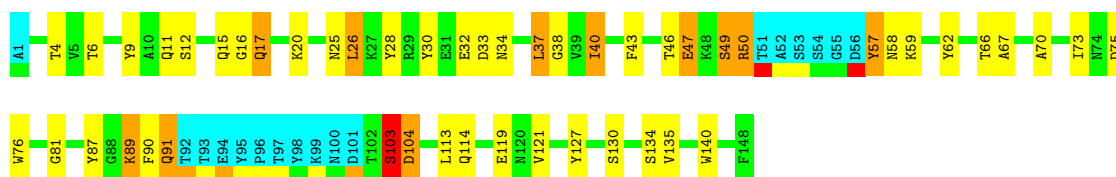
- Molecule 1: Outer membrane protein X



4.2.2 Score per residue for model 2

- Molecule 1: Outer membrane protein X

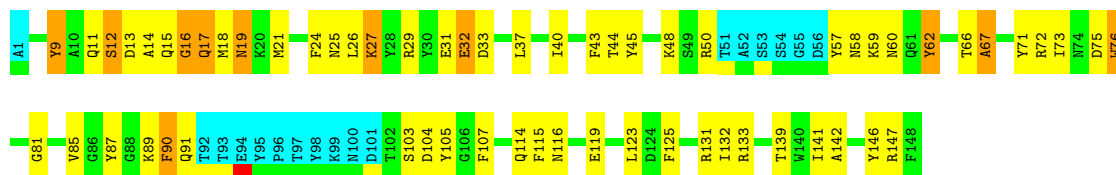




4.2.3 Score per residue for model 3

- Molecule 1: Outer membrane protein X

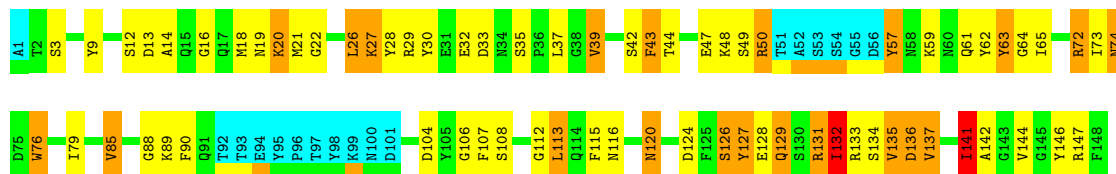
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Outer membrane protein X

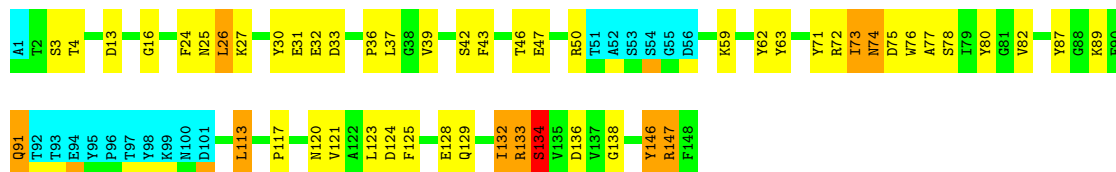
Chain A:



4.2.5 Score per residue for model 5

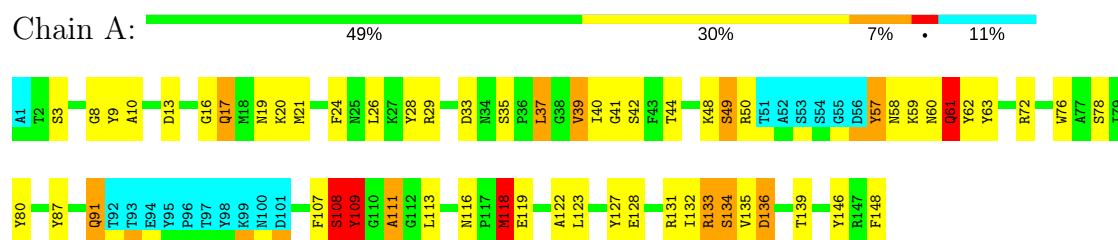
- Molecule 1: Outer membrane protein X

Chain A:



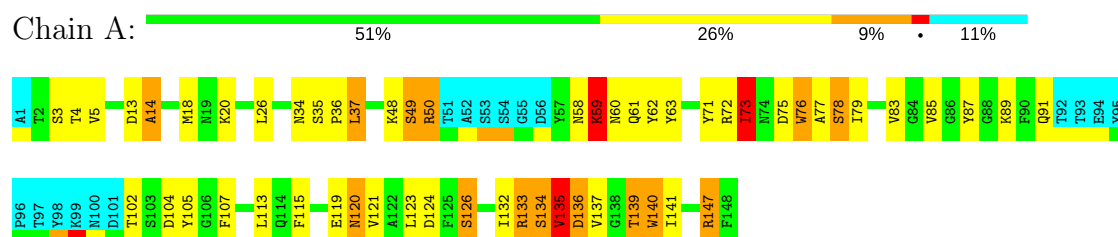
4.2.6 Score per residue for model 6

- Molecule 1: Outer membrane protein X



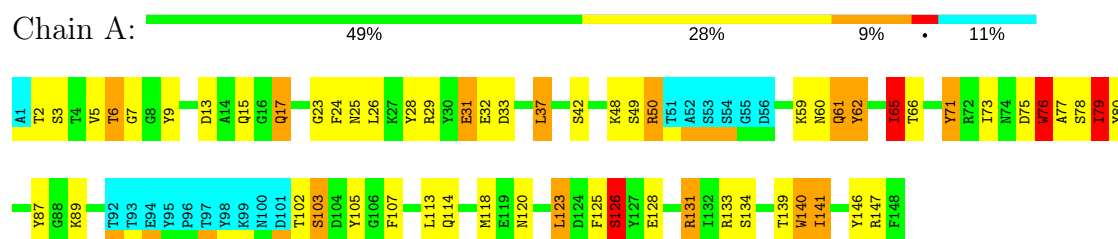
4.2.7 Score per residue for model 7

- Molecule 1: Outer membrane protein X



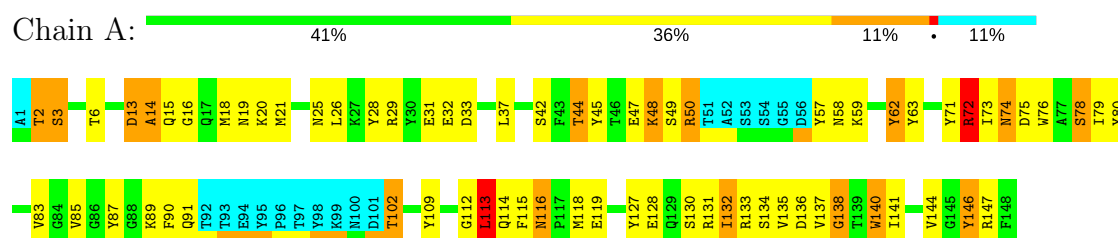
4.2.8 Score per residue for model 8

- Molecule 1: Outer membrane protein X



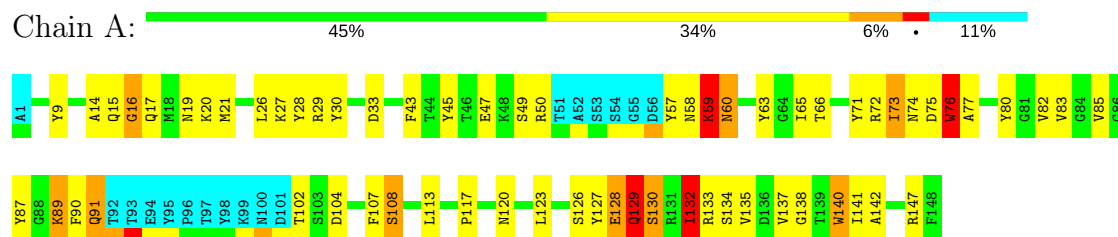
4.2.9 Score per residue for model 9

- Molecule 1: Outer membrane protein X



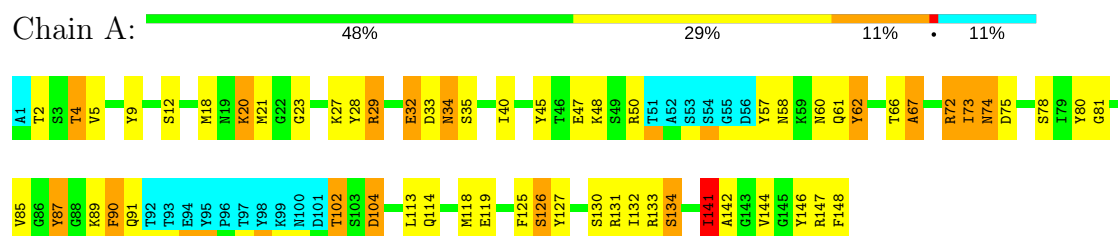
4.2.10 Score per residue for model 10

- Molecule 1: Outer membrane protein X



4.2.11 Score per residue for model 11

- Molecule 1: Outer membrane protein X



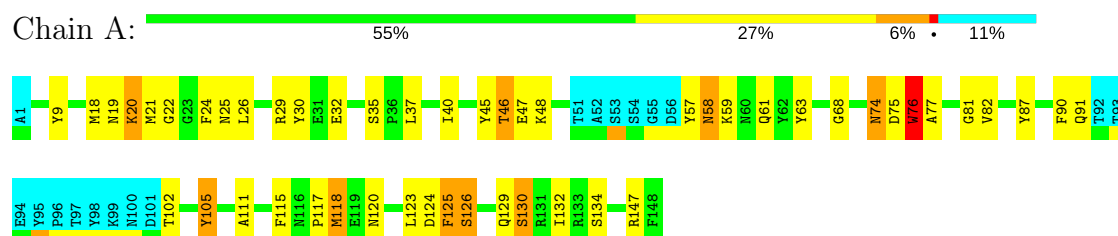
4.2.12 Score per residue for model 12

- Molecule 1: Outer membrane protein X



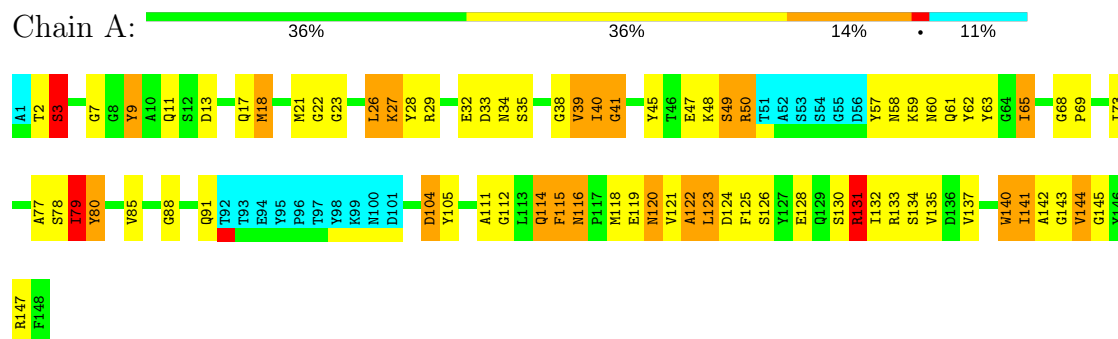
4.2.13 Score per residue for model 13

- Molecule 1: Outer membrane protein X



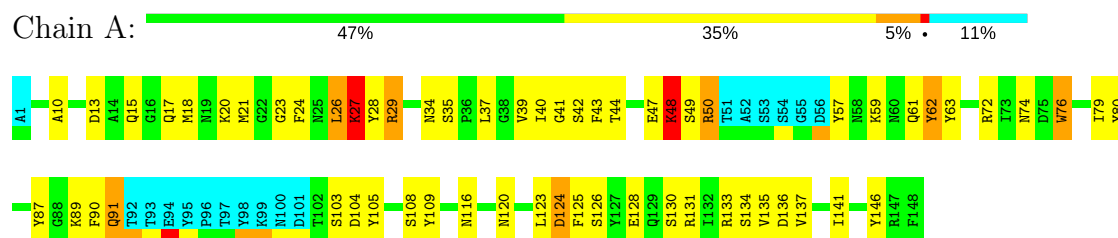
4.2.14 Score per residue for model 14

- Molecule 1: Outer membrane protein X



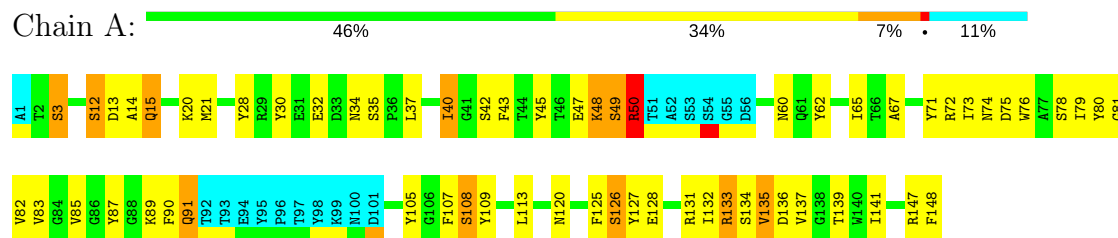
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Outer membrane protein X



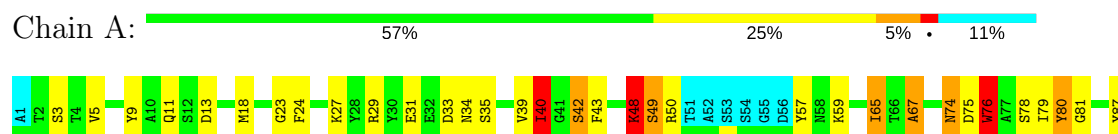
4.2.16 Score per residue for model 16

- Molecule 1: Outer membrane protein X



4.2.17 Score per residue for model 17

- Molecule 1: Outer membrane protein X

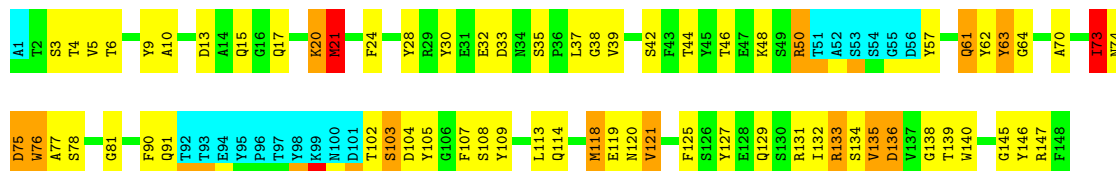




4.2.18 Score per residue for model 18

- Molecule 1: Outer membrane protein X

Chain A: 43% 36% 8% 11%



5 Refinement protocol and experimental data overview

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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:O	1:A:73:ILE:HG23	0.69	1.87	7	3
1:A:37:LEU:HD22	1:A:37:LEU:C	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:O	1:A:102:THR:HG23	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	1
1:A:4:THR:O	1:A:4:THR:HG22	0.65	1.90	2	1
1:A:65:ILE:HD13	1:A:85:VAL:O	0.65	1.90	4	1
1:A:37:LEU:HD13	1:A:70:ALA:O	0.65	1.92	2	1
1:A:132:ILE:O	1:A:132:ILE:HG23	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:115:PHE:CD2	1:A:115:PHE:O	0.61	2.54	19	1
1:A:141:ILE:HG23	1:A:142:ALA:N	0.61	2.10	20	3
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:45:TYR:CD1	1:A:45:TYR:O	0.60	2.55	10	1
1:A:57:TYR:O	1:A:57:TYR:CD1	0.60	2.55	4	1
1:A:82:VAL:HG23	1:A:82:VAL:O	0.60	1.95	1	2
1:A:87:TYR:CE1	1:A:89:LYS:O	0.60	2.55	10	1
1:A:121:VAL:HG13	1:A:121:VAL:O	0.60	1.96	5	1
1:A:90:PHE:CD2	1:A:90:PHE:O	0.59	2.55	3	1
1:A:146:TYR:CD2	1:A:146:TYR:O	0.59	2.55	5	3
1:A:65:ILE:O	1:A:65:ILE:HG23	0.59	1.96	8	1
1:A:76:TRP:CE3	1:A:116:ASN:OD1	0.59	2.55	3	1
1:A:40:ILE:O	1:A:40:ILE:HG23	0.59	1.98	13	1
1:A:28:TYR:O	1:A:28:TYR:CD2	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:VAL:O	1:A:85:VAL:HG12	0.58	1.98	16	1
1:A:79:ILE:HD11	1:A:126:SER:HB3	0.58	1.74	14	1
1:A:105:TYR:O	1:A:105:TYR:CD1	0.58	2.57	8	3
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:O	1:A:43:PHE:CD1	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:HG13	1:A:85:VAL:O	0.57	1.99	10	2
1:A:111:ALA:O	1:A:127:TYR:CD1	0.57	2.57	6	1
1:A:30:TYR:O	1:A:30:TYR:CD2	0.57	2.58	13	1
1:A:43:PHE:CD2	1:A:43:PHE:O	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:N	1:A:40:ILE:HD13	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: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:90:PHE:CD1	1:A:90:PHE:O	0.56	2.59	1	1
1:A:28:TYR:CG	1:A:28:TYR:O	0.55	2.58	15	1
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:O	1:A:123:LEU:HD12	0.55	2.01	14	2
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:CG	1:A:76:TRP:O	0.54	2.61	20	1
1:A:59:LYS:O	1:A:90:PHE:CG	0.54	2.60	10	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:39:VAL:HG22	1:A:39:VAL:O	0.54	2.01	4	2
1:A:140:TRP:O	1:A:140:TRP:CG	0.54	2.60	14	1
1:A:39:VAL:HG22	1:A:68:GLY:HA2	0.54	1.80	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	1
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:82:VAL:CG2	1:A:109:TYR:CD2	0.53	2.90	16	1
1:A:80:TYR:O	1:A:80:TYR:CD1	0.53	2.62	6	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:CG2	1:A:79:ILE:O	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	1
1:A:5:VAL:O	1:A:5:VAL:HG13	0.52	2.04	8	1
1:A:40:ILE:O	1:A:40:ILE:CG1	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:CD2	1:A:127:TYR:O	0.52	2.63	11	1
1:A:137:VAL:HG12	1:A:138:GLY:H	0.52	1.65	19	2
1:A:23:GLY:O	1:A:24:PHE:CG	0.52	2.63	19	1
1:A:45:TYR:CD1	1:A:45:TYR:C	0.52	2.83	10	1
1:A:28:TYR:CD2	1:A:28:TYR:O	0.52	2.63	15	1
1:A:39:VAL:HG13	1:A:39:VAL:O	0.52	2.04	6	1
1:A:43:PHE:O	1:A:43:PHE:CG	0.52	2.62	20	1
1:A:80:TYR:CD2	1:A:111:ALA:HB2	0.52	2.39	14	1
1:A:137:VAL:HG23	1:A:137:VAL:O	0.52	2.05	14	1
1:A:112:GLY:C	1:A:113:LEU:HD23	0.52	2.25	19	1
1:A:105:TYR:O	1:A:105:TYR:CG	0.52	2.63	7	2
1:A:62:TYR:CD1	1:A:62:TYR:O	0.52	2.63	7	1
1:A:59:LYS:HD3	1:A:62:TYR:CE2	0.51	2.40	9	1
1:A:45:TYR:O	1:A:45:TYR:CG	0.51	2.63	20	3
1:A:127:TYR:O	1:A:127:TYR:CG	0.51	2.63	2	1
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:CG2	1:A:73:ILE:O	0.51	2.57	7	1
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:CG	1:A:90:PHE:O	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:28:TYR:O	1:A:28:TYR:CG	0.50	2.64	1	2
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:57:TYR:CD1	1:A:57:TYR:O	0.50	2.65	18	1
1:A:9:TYR:O	1:A:9:TYR:CG	0.50	2.63	13	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:O	1:A:90:PHE:CB	0.50	2.60	10	1
1:A:76:TRP:O	1:A:76:TRP:CE3	0.50	2.65	1	1
1:A:114:GLN:O	1:A:115:PHE:CB	0.50	2.59	14	1
1:A:71:TYR:O	1:A:71:TYR:CG	0.50	2.64	7	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:CG	1:A:146:TYR:O	0.49	2.64	5	3
1:A:73:ILE:O	1:A:73:ILE:CG2	0.49	2.60	18	1
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:13:ASP:HB3	1:A:137:VAL:HG11	0.49	1.83	9	1
1:A:124:ASP:CG	1:A:141:ILE:CD1	0.49	2.81	7	1
1:A:147:ARG:O	1:A:147:ARG:CG	0.49	2.60	11	1
1:A:62:TYR:CE2	1:A:87:TYR:O	0.49	2.66	11	1
1:A:130:SER:O	1:A:135:VAL:HG23	0.49	2.08	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:140:TRP:CE3	1:A:141:ILE:O	0.49	2.65	9	1
1:A:59:LYS:CD	1:A:62:TYR:CD2	0.49	2.95	9	1
1:A:57:TYR:O	1:A:58:ASN:CB	0.49	2.60	20	1
1:A:116:ASN:OD1	1:A:122:ALA:CB	0.49	2.60	6	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:34:ASN:O	1:A:35:SER:CB	0.48	2.61	19	1
1:A:14:ALA:HB3	1:A:19:ASN:HB2	0.48	1.83	3	1
1:A:30:TYR:CG	1:A:30:TYR:O	0.48	2.66	12	1
1:A:121:VAL:CG1	1:A:121:VAL:O	0.48	2.61	5	1
1:A:80:TYR:CG	1:A:80:TYR:O	0.48	2.66	8	1
1:A:137:VAL:CG2	1:A:137:VAL:O	0.48	2.61	14	1
1:A:29:ARG:N	1:A:40:ILE:HG21	0.48	2.22	15	1
1:A:132:ILE:CG2	1:A:133:ARG:N	0.48	2.72	4	1
1:A:17:GLN:O	1:A:18:MET:CB	0.48	2.62	12	1
1:A:139:THR:O	1:A:139:THR:HG23	0.48	2.08	6	1
1:A:73:ILE:C	1:A:73:ILE:CD1	0.48	2.81	7	1
1:A:59:LYS:O	1:A:60:ASN:CB	0.48	2.61	7	2
1:A:37:LEU:CD2	1:A:37:LEU:C	0.48	2.81	20	2
1:A:62:TYR:CE1	1:A:87:TYR:HB2	0.48	2.42	16	1
1:A:44:THR:HG22	1:A:44:THR:O	0.48	2.09	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:THR:HG23	1:A:6:THR:O	0.48	2.09	12	1
1:A:75:ASP:OD2	1:A:76:TRP:CD1	0.48	2.67	1	1
1:A:112:GLY:O	1:A:113:LEU:CB	0.48	2.62	9	1
1:A:49:SER:O	1:A:50:ARG:CB	0.48	2.62	9	1
1:A:139:THR:HG23	1:A:139:THR:O	0.48	2.08	3	2
1:A:79:ILE:CG2	1:A:80:TYR:N	0.48	2.77	9	1
1:A:134:SER:O	1:A:135:VAL:CB	0.48	2.62	7	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:115:PHE:N	1:A:123:LEU:CB	0.48	2.77	14	1
1:A:124:ASP:O	1:A:125:PHE:CD2	0.48	2.67	15	1
1:A:5:VAL:O	1:A:5:VAL:HG12	0.48	2.09	7	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:44:THR:CG2	1:A:45:TYR:N	0.47	2.76	9	1
1:A:66:THR:O	1:A:67:ALA:CB	0.47	2.62	3	2
1:A:48:LYS:O	1:A:49:SER:CB	0.47	2.61	12	2
1:A:6:THR:OG1	1:A:123:LEU:CD2	0.47	2.62	8	1
1:A:4:THR:HG22	1:A:147:ARG:CA	0.47	2.38	7	1
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:134:SER:C	1:A:135:VAL:HG23	0.47	2.30	10	1
1:A:44:THR:CG2	1:A:44:THR:O	0.47	2.61	15	1
1:A:59:LYS:HD3	1:A:62:TYR:CD2	0.47	2.45	9	1
1:A:40:ILE:CG2	1:A:40:ILE:O	0.47	2.62	17	1
1:A:144:VAL:HG13	1:A:144:VAL:O	0.47	2.10	4	2
1:A:24:PHE:CD1	1:A:24:PHE:O	0.47	2.68	18	1
1:A:80:TYR:O	1:A:80:TYR:CG	0.47	2.67	6	1
1:A:49:SER:OG	1:A:58:ASN:CB	0.47	2.62	2	1
1:A:132:ILE:CD1	1:A:132:ILE:O	0.47	2.63	9	1
1:A:47:GLU:O	1:A:48:LYS:CB	0.47	2.62	14	3
1:A:107:PHE:O	1:A:108:SER:CB	0.47	2.63	6	1
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:73:ILE:HG23	1:A:73:ILE:O	0.46	2.10	11	1
1:A:146:TYR:O	1:A:147:ARG:CG	0.46	2.64	20	1
1:A:65:ILE:HG23	1:A:65:ILE:O	0.46	2.10	1	1
1:A:6:THR:HG23	1:A:25:ASN:ND2	0.46	2.24	9	1
1:A:2:THR:CG2	1:A:3:SER:N	0.46	2.79	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:THR:HG23	1:A:66:THR:O	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:5:VAL:HG12	1:A:5:VAL:O	0.46	2.10	17	1
1:A:73:ILE:O	1:A:73:ILE:HG22	0.46	2.11	16	1
1:A:22:GLY:O	1:A:45:TYR:CE2	0.46	2.69	14	1
1:A:124:ASP:CG	1:A:141:ILE:HD13	0.46	2.31	7	1
1:A:4:THR:CG2	1:A:4:THR:O	0.46	2.60	2	1
1:A:135:VAL:HG12	1:A:137:VAL:HG13	0.46	1.88	14	1
1:A:33:ASP:O	1:A:34:ASN:ND2	0.46	2.49	19	1
1:A:132:ILE:HG22	1:A:132:ILE:O	0.46	2.10	11	1
1:A:130:SER:O	1:A:131:ARG:CB	0.46	2.64	14	1
1:A:135:VAL:CG1	1:A:136:ASP:N	0.46	2.78	7	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:119:GLU:O	1:A:120:ASN:ND2	0.45	2.49	17	1
1:A:4:THR:HG22	1:A:5:VAL:H	0.45	1.70	18	1
1:A:73:ILE:HD13	1:A:73:ILE:C	0.45	2.32	7	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:132:ILE:HG23	1:A:133:ARG:H	0.45	1.70	4	1
1:A:24:PHE:CG	1:A:24:PHE:O	0.45	2.69	5	1
1:A:6:THR:O	1:A:6:THR:HG23	0.45	2.11	18	1
1:A:19:ASN:O	1:A:21:MET:N	0.45	2.50	12	1
1:A:135:VAL:HG13	1:A:137:VAL:HG23	0.45	1.89	15	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:47:GLU:CG	1:A:48:LYS:N	0.45	2.80	20	1
1:A:40:ILE:HG22	1:A:68:GLY:HA3	0.45	1.86	12	1
1:A:130:SER:HB2	1:A:137:VAL:HG21	0.45	1.89	12	1
1:A:79:ILE:O	1:A:112:GLY:N	0.45	2.49	19	2
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:25:ASN:HB2	1:A:43:PHE:CE2	0.45	2.47	2	1
1:A:133:ARG:O	1:A:134:SER:C	0.45	2.54	11	1
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	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:132:ILE:O	1:A:133:ARG:C	0.44	2.56	20	3
1:A:89:LYS:O	1:A:90:PHE:CG	0.44	2.70	2	1
1:A:83:VAL:CG1	1:A:83:VAL:O	0.44	2.64	7	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: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:23:GLY:HA2	1:A:45:TYR:CD2	0.44	2.47	14	1
1:A:82:VAL:HG21	1:A:128:GLU:CB	0.44	2.43	10	1
1:A:50:ARG:HD2	1:A:57:TYR:CZ	0.44	2.48	15	1
1:A:73:ILE:O	1:A:74:ASN:CB	0.44	2.65	12	1
1:A:105:TYR:CD1	1:A:105:TYR:C	0.44	2.90	8	1
1:A:57:TYR:O	1:A:59:LYS:N	0.44	2.51	13	1
1:A:82:VAL:CG1	1:A:82:VAL:O	0.44	2.65	13	1
1:A:109:TYR:N	1:A:109:TYR:CD1	0.44	2.86	9	1
1:A:78:SER:O	1:A:79:ILE:CG2	0.44	2.60	14	1
1:A:40:ILE:CD1	1:A:40:ILE:O	0.44	2.65	17	1
1:A:80:TYR:C	1:A:80:TYR:CD1	0.44	2.91	11	1
1:A:62:TYR:CZ	1:A:87:TYR:O	0.44	2.71	11	1
1:A:129:GLN:O	1:A:137:VAL:HG23	0.44	2.12	4	1
1:A:73:ILE:O	1:A:75:ASP:N	0.44	2.50	11	2
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:30:TYR:O	1:A:30:TYR:CD1	0.44	2.71	12	1
1:A:113:LEU:N	1:A:113:LEU:CD1	0.44	2.70	5	1
1:A:134:SER:O	1:A:135:VAL:C	0.44	2.56	4	2
1:A:19:ASN:CB	1:A:47:GLU:OE1	0.44	2.66	20	1
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: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:135:VAL:O	1:A:135:VAL:CG1	0.44	2.59	4	1
1:A:134:SER:C	1:A:136:ASP:N	0.44	2.71	4	1
1:A:116:ASN:ND2	1:A:118:MET:O	0.44	2.51	6	1
1:A:134:SER:O	1:A:135:VAL:CG2	0.44	2.66	2	1
1:A:139:THR:CG2	1:A:139:THR:O	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:115:PHE:CG	1:A:115:PHE:O	0.43	2.71	19	1
1:A:82:VAL:HG21	1:A:128:GLU:HB2	0.43	1.89	10	1
1:A:5:VAL:HG13	1:A:5:VAL:O	0.43	2.12	1	2
1:A:21:MET:N	1:A:21:MET:SD	0.43	2.91	18	1
1:A:44:THR:HG22	1:A:63:TYR:CZ	0.43	2.48	6	1
1:A:40:ILE:O	1:A:40:ILE:CG2	0.43	2.66	13	1
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:43:PHE:CD1	1:A:43:PHE:N	0.43	2.86	19	1
1:A:59:LYS:O	1:A:90:PHE:CD2	0.43	2.71	10	1
1:A:141:ILE:CG2	1:A:142:ALA:N	0.43	2.79	20	3
1:A:62:TYR:CE1	1:A:87:TYR:CB	0.43	3.01	16	1
1:A:45:TYR:N	1:A:45:TYR:CD1	0.43	2.87	13	1
1:A:140:TRP:CZ3	1:A:141:ILE:O	0.43	2.71	9	1
1:A:57:TYR:O	1:A:57:TYR:CG	0.43	2.71	14	1
1:A:58:ASN:C	1:A:59:LYS:CG	0.43	2.86	10	1
1:A:134:SER:O	1:A:135:VAL:CG1	0.43	2.66	9	2
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:115:PHE:CD2	1:A:116:ASN:O	0.43	2.72	9	1
1:A:39:VAL:O	1:A:39:VAL:HG13	0.43	2.12	18	1
1:A:109:TYR:CZ	1:A:128:GLU:CD	0.43	2.93	6	1
1:A:25:ASN:HA	1:A:43:PHE:CD2	0.43	2.49	2	1
1:A:140:TRP:O	1:A:140:TRP:CD1	0.43	2.71	14	1
1:A:124:ASP:OD1	1:A:141:ILE:CD1	0.43	2.67	7	1
1:A:109:TYR:C	1:A:109:TYR:CD1	0.42	2.92	19	1
1:A:75:ASP:O	1:A:76:TRP:CD2	0.42	2.72	17	1
1:A:87:TYR:CE1	1:A:88:GLY:O	0.42	2.72	12	1
1:A:135:VAL:HG12	1:A:136:ASP:N	0.42	2.29	18	1
1:A:27:LYS:CG	1:A:41:GLY:O	0.42	2.66	14	1
1:A:63:TYR:CE1	1:A:64:GLY:O	0.42	2.72	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:146:TYR:O	1:A:147:ARG:CB	0.42	2.68	20	1
1:A:125:PHE:O	1:A:125:PHE:CD1	0.42	2.72	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:TYR:O	1:A:91:GLN:N	0.42	2.53	20	1
1:A:49:SER:C	1:A:50:ARG:CG	0.42	2.88	16	1
1:A:66:THR:CB	1:A:82:VAL:HG21	0.42	2.44	19	1
1:A:73:ILE:CD1	1:A:73:ILE:C	0.42	2.87	18	2
1:A:43:PHE:CD1	1:A:43:PHE:C	0.42	2.92	2	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
1:A:80:TYR:CD1	1:A:80:TYR:C	0.42	2.93	16	1
1:A:141:ILE:C	1:A:141:ILE:CD1	0.42	2.88	7	1
1:A:18:MET:O	1:A:20:LYS:N	0.42	2.53	4	1
1:A:63:TYR:CG	1:A:64:GLY:N	0.42	2.87	19	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:23:GLY:C	1:A:24:PHE:CG	0.42	2.93	19	1
1:A:73:ILE:CG2	1:A:74:ASN:N	0.42	2.83	5	1
1:A:80:TYR:CD2	1:A:111:ALA:CB	0.41	3.02	19	1
1:A:137:VAL:HG22	1:A:138:GLY:N	0.41	2.30	10	1
1:A:102:THR:HG23	1:A:102:THR:O	0.41	2.15	20	1
1:A:71:TYR:O	1:A:72:ARG:CB	0.41	2.67	9	1
1:A:32:GLU:O	1:A:33:ASP:CG	0.41	2.58	19	1
1:A:26:LEU:N	1:A:42:SER:CB	0.41	2.83	4	1
1:A:90:PHE:O	1:A:91:GLN:C	0.41	2.59	20	1
1:A:121:VAL:HG23	1:A:145:GLY:O	0.41	2.15	18	1
1:A:4:THR:O	1:A:146:TYR:O	0.41	2.38	11	1
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:49:SER:O	1:A:50:ARG:C	0.41	2.59	4	2
1:A:128:GLU:OE1	1:A:139:THR:HG21	0.41	2.16	16	1
1:A:85:VAL:O	1:A:85:VAL:CG1	0.41	2.69	16	1
1:A:9:TYR:CD1	1:A:23:GLY:O	0.41	2.74	8	1
1:A:6:THR:CG2	1:A:6:THR:O	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:71:TYR:O	1:A:80:TYR:CD1	0.41	2.74	20	1
1:A:83:VAL:HG22	1:A:107:PHE:CE1	0.41	2.50	16	1
1:A:127:TYR:CG	1:A:127:TYR:O	0.41	2.74	6	1
1:A:26:LEU:O	1:A:27:LYS:O	0.41	2.38	15	1
1:A:106:GLY:O	1:A:107:PHE:CD1	0.41	2.74	4	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:THR:CG2	1:A:67:ALA:N	0.41	2.84	2	1
1:A:135:VAL:HG22	1:A:135:VAL:O	0.41	2.16	9	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:125:PHE:CE1	1:A:141:ILE:HB	0.41	2.51	15	1
1:A:75:ASP:OD1	1:A:76:TRP:N	0.41	2.51	3	1
1:A:38:GLY:N	1:A:70:ALA:HB3	0.41	2.30	18	1
1:A:37:LEU:HD12	1:A:38:GLY:O	0.41	2.16	2	1
1:A:13:ASP:O	1:A:14:ALA:CB	0.41	2.69	7	1
1:A:126:SER:O	1:A:139:THR:O	0.40	2.39	8	1
1:A:59:LYS:O	1:A:61:GLN:N	0.40	2.53	14	1
1:A:27:LYS:O	1:A:41:GLY:N	0.40	2.53	15	1
1:A:112:GLY:O	1:A:113:LEU:HD22	0.40	2.17	4	1
1:A:46:THR:O	1:A:61:GLN:O	0.40	2.40	18	1
1:A:85:VAL:HG13	1:A:87:TYR:CE2	0.40	2.51	7	1
1:A:115:PHE:O	1:A:116:ASN:OD1	0.40	2.39	19	1
1:A:40:ILE:HG22	1:A:68:GLY:HA2	0.40	1.93	12	1
1:A:20:LYS:CG	1:A:20:LYS:O	0.40	2.69	13	1
1:A:76:TRP:O	1:A:77:ALA:C	0.40	2.59	19	1
1:A:103:SER:O	1:A:104:ASP:CB	0.40	2.69	2	1
1:A:90:PHE:O	1:A:90:PHE:CD1	0.40	2.74	13	1
1:A:79:ILE:CG1	1:A:112:GLY:HA3	0.40	2.47	14	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 ⓘ

6.3.1 Protein backbone ⓘ

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	81	GLY	8
1	A	131	ARG	8
1	A	16	GLY	8
1	A	34	ASN	8
1	A	17	GLN	7
1	A	126	SER	7
1	A	73	ILE	7
1	A	32	GLU	6
1	A	39	VAL	6
1	A	33	ASP	6
1	A	118	MET	6
1	A	132	ILE	5
1	A	48	LYS	5
1	A	144	VAL	5
1	A	67	ALA	5
1	A	59	LYS	5
1	A	72	ARG	5
1	A	60	ASN	4
1	A	147	ARG	4
1	A	57	TYR	4
1	A	135	VAL	4
1	A	141	ILE	4
1	A	78	SER	4
1	A	103	SER	4
1	A	19	ASN	4
1	A	21	MET	4
1	A	27	LYS	4
1	A	91	GLN	4
1	A	116	ASN	3
1	A	58	ASN	3
1	A	88	GLY	3
1	A	18	MET	3
1	A	79	ILE	3
1	A	2	THR	3
1	A	3	SER	3
1	A	77	ALA	3
1	A	63	TYR	3
1	A	117	PRO	3

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Mol	Chain	Res	Type	Models (Total)
1	A	12	SER	3
1	A	102	THR	3
1	A	37	LEU	3
1	A	108	SER	3
1	A	40	ILE	3
1	A	136	ASP	3
1	A	25	ASN	3
1	A	129	GLN	2
1	A	65	ILE	2
1	A	20	LYS	2
1	A	146	TYR	2
1	A	128	GLU	2
1	A	28	TYR	2
1	A	130	SER	2
1	A	9	TYR	2
1	A	41	GLY	2
1	A	35	SER	2
1	A	36	PRO	2
1	A	61	GLN	2
1	A	104	ASP	2
1	A	134	SER	2
1	A	42	SER	2
1	A	111	ALA	2
1	A	62	TYR	2
1	A	13	ASP	2
1	A	121	VAL	2
1	A	113	LEU	2
1	A	90	PHE	2
1	A	14	ALA	2
1	A	15	GLN	2
1	A	140	TRP	2
1	A	23	GLY	2
1	A	138	GLY	2
1	A	89	LYS	2
1	A	45	TYR	1
1	A	43	PHE	1
1	A	127	TYR	1
1	A	24	PHE	1
1	A	105	TYR	1
1	A	29	ARG	1
1	A	82	VAL	1
1	A	75	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	26	LEU	1
1	A	142	ALA	1
1	A	44	THR	1
1	A	114	GLN	1
1	A	68	GLY	1
1	A	85	VAL	1
1	A	30	TYR	1
1	A	123	LEU	1
1	A	115	PHE	1
1	A	38	GLY	1
1	A	64	GLY	1
1	A	107	PHE	1
1	A	4	THR	1
1	A	133	ARG	1
1	A	124	ASP	1
1	A	47	GLU	1
1	A	109	TYR	1
1	A	22	GLY	1
1	A	83	VAL	1
1	A	6	THR	1
1	A	80	TYR	1
1	A	87	TYR	1
1	A	139	THR	1
1	A	125	PHE	1
1	A	122	ALA	1

6.3.2 Protein sidechains ⓘ

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	147	ARG	14
1	A	20	LYS	14
1	A	21	MET	14
1	A	29	ARG	13
1	A	76	TRP	13
1	A	133	ARG	13
1	A	113	LEU	13
1	A	91	GLN	13
1	A	89	LYS	13
1	A	134	SER	12
1	A	140	TRP	12
1	A	26	LEU	11
1	A	104	ASP	11
1	A	48	LYS	11
1	A	3	SER	11
1	A	72	ARG	11
1	A	37	LEU	11
1	A	27	LYS	11
1	A	13	ASP	11
1	A	75	ASP	10
1	A	35	SER	10
1	A	119	GLU	10
1	A	123	LEU	10
1	A	62	TYR	10
1	A	18	MET	9
1	A	131	ARG	9
1	A	32	GLU	9
1	A	59	LYS	9
1	A	9	TYR	9
1	A	12	SER	9
1	A	61	GLN	9
1	A	17	GLN	9
1	A	118	MET	9
1	A	87	TYR	9
1	A	146	TYR	8
1	A	42	SER	8
1	A	73	ILE	8
1	A	15	GLN	8
1	A	47	GLU	8
1	A	125	PHE	8
1	A	50	ARG	8
1	A	130	SER	7
1	A	78	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	31	GLU	7
1	A	71	TYR	7
1	A	33	ASP	7
1	A	49	SER	6
1	A	127	TYR	6
1	A	60	ASN	6
1	A	57	TYR	6
1	A	40	ILE	6
1	A	126	SER	6
1	A	115	PHE	6
1	A	103	SER	6
1	A	107	PHE	6
1	A	63	TYR	6
1	A	74	ASN	6
1	A	108	SER	6
1	A	114	GLN	6
1	A	136	ASP	6
1	A	129	GLN	5
1	A	128	GLU	5
1	A	79	ILE	5
1	A	28	TYR	5
1	A	124	ASP	5
1	A	141	ILE	5
1	A	148	PHE	5
1	A	11	GLN	5
1	A	43	PHE	4
1	A	24	PHE	4
1	A	65	ILE	4
1	A	105	TYR	4
1	A	132	ILE	4
1	A	30	TYR	4
1	A	90	PHE	4
1	A	19	ASN	4
1	A	109	TYR	4
1	A	45	TYR	3
1	A	58	ASN	3
1	A	44	THR	3
1	A	66	THR	3
1	A	85	VAL	3
1	A	121	VAL	3
1	A	137	VAL	3
1	A	120	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	46	THR	3
1	A	80	TYR	3
1	A	116	ASN	2
1	A	25	ASN	2
1	A	2	THR	2
1	A	135	VAL	2
1	A	34	ASN	2
1	A	102	THR	2
1	A	4	THR	1
1	A	6	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 carbohydrates 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

No chemical shift data were provided