



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:44 pm GMT

PDB ID : 1CMG
Title : NMR SOLUTION STRUCTURE OF CALCIUM-LOADED CALMODULIN
CARBOXY-TERMINAL DOMAIN
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Deposited on : 1995-07-19

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

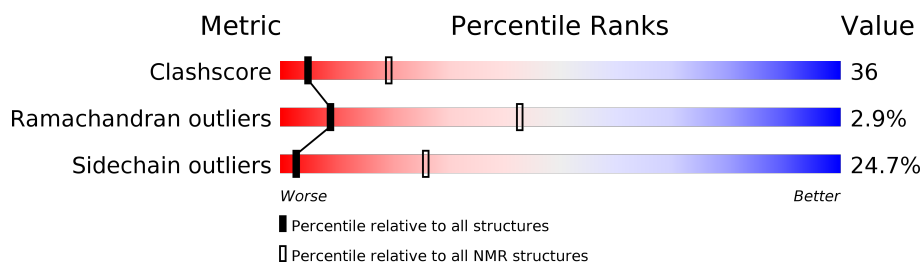
1 Overall quality at a glance

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	73	<div> <div></div> <div>23%</div> <div>56%</div> <div>8%</div> <div>12%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:83-A:146 (64)	0.56	12

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1131 atoms, of which 545 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CALMODULIN (VERTEBRATE).

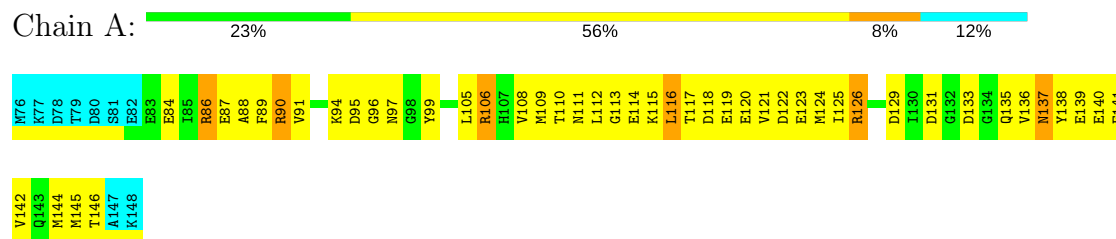
Mol	Chain	Residues	Atoms						Trace
1	A	73	Total	C	H	N	O	S	0
			1131	356	545	96	129	5	

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: CALMODULIN (VERTEBRATE)

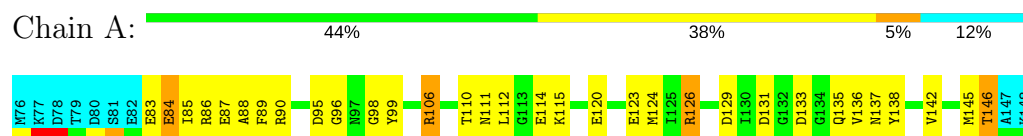


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

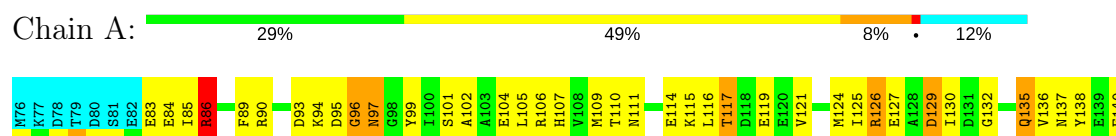
4.2.1 Score per residue for model 1

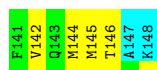
- Molecule 1: CALMODULIN (VERTEBRATE)



4.2.2 Score per residue for model 2

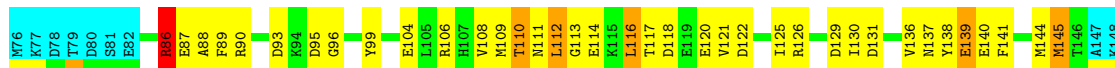
- Molecule 1: CALMODULIN (VERTEBRATE)





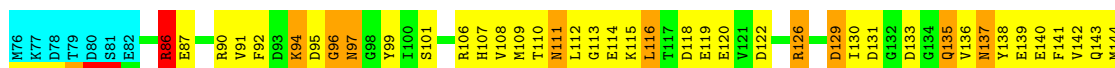
4.2.3 Score per residue for model 3

- Molecule 1: CALMODULIN (VERTEBRATE)



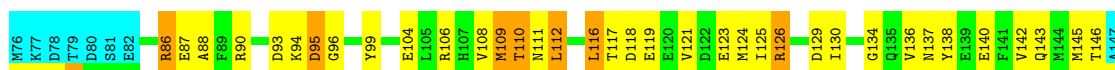
4.2.4 Score per residue for model 4

- Molecule 1: CALMODULIN (VERTEBRATE)



4.2.5 Score per residue for model 5

- Molecule 1: CALMODULIN (VERTEBRATE)



4.2.6 Score per residue for model 6

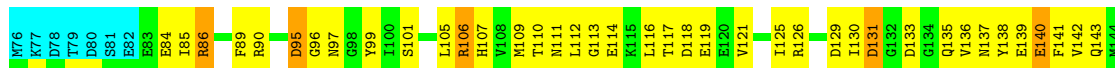
- Molecule 1: CALMODULIN (VERTEBRATE)





4.2.7 Score per residue for model 7

- Molecule 1: CALMODULIN (VERTEBRATE)



4.2.8 Score per residue for model 8

- Molecule 1: CALMODULIN (VERTEBRATE)



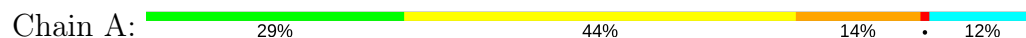
4.2.9 Score per residue for model 9

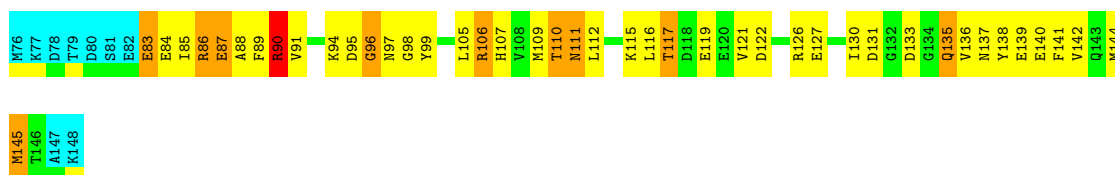
- Molecule 1: CALMODULIN (VERTEBRATE)



4.2.10 Score per residue for model 10

- Molecule 1: CALMODULIN (VERTEBRATE)





4.2.11 Score per residue for model 11

- Molecule 1: CALMODULIN (VERTEBRATE)

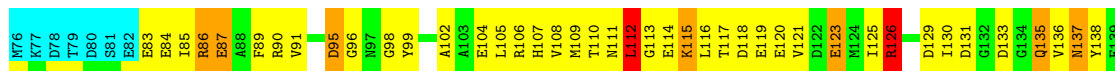
Chain A: 38% 38% 7% • 12%



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: CALMODULIN (VERTEBRATE)

Chain A: 23% 49% 12% • 12%



4.2.13 Score per residue for model 13

- Molecule 1: CALMODULIN (VERTEBRATE)

Chain A: 37% 38% 11% • 12%



4.2.14 Score per residue for model 14

- Molecule 1: CALMODULIN (VERTEBRATE)

Chain A: 25% 42% 21% 12%





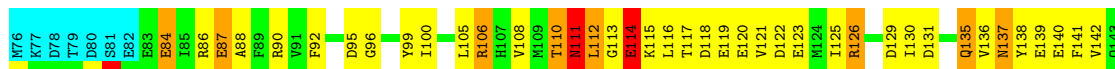
4.2.15 Score per residue for model 15

- Molecule 1: CALMODULIN (VERTEBRATE)



4.2.16 Score per residue for model 16

- Molecule 1: CALMODULIN (VERTEBRATE)



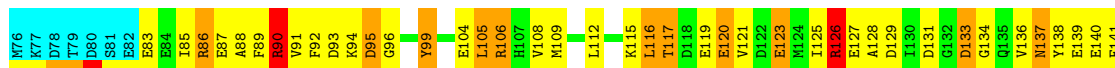
4.2.17 Score per residue for model 17

- Molecule 1: CALMODULIN (VERTEBRATE)



4.2.18 Score per residue for model 18

- Molecule 1: CALMODULIN (VERTEBRATE)



V142
Q143
M144
M145
T146
A147
K148

4.2.19 Score per residue for model 19

- Molecule 1: CALMODULIN (VERTEBRATE)

Chain A:  30% 37% 21% 12%

M76 K77 D78 T79 D80 S81 E82 E83 E84 I85 R86 E87 A88 F89 R90 Y91 F92 D95 G96 N97 Y98 Y99 S101 L105 R106 H107 V108 M109 T110 N111 L112 G113 E114 K115 L116 L117 D118 E119 E120 D121 V121 D122 E123 M124 I125 R126 D129 D133 G134 Q135 V136 N137 Y138 E139 V142 Q143

M144
M145
T146
A147
K148

4.2.20 Score per residue for model 20

- Molecule 1: CALMODULIN (VERTEBRATE)

Chain A:  27% 49% 10% 12%

M76 K77 D78 T79 D80 S81 E82 E83 E84 I85 R86 E87 A88 F89 R90 D93 K94 D95 G96 N97 Y98 Y99 E104 L105 R106 H107 V108 M109 T110 G113 E114 K115 L116 T117 D118 E119 E120 V121 D122 E123 M124 I125 R126 E127 D131 G132 D133 G134 Q135 V136 N137 Y138 V142 Q143 M144

M145
T146
A147
K148

5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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 [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	4.0±0.2
All	All	0	79

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	90	ARG	Sidechain	20
1	A	106	ARG	Sidechain	20
1	A	86	ARG	Sidechain	20
1	A	126	ARG	Sidechain	19

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	516	477	477	36±7
All	All	10320	9540	9540	722

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:HD22	1:A:109:MET:HE2	1.01	1.03	14	1
1:A:105:LEU:HD22	1:A:109:MET:CE	0.93	1.94	14	1
1:A:138:TYR:O	1:A:142:VAL:HG23	0.90	1.66	9	19
1:A:111:ASN:O	1:A:112:LEU:HD23	0.89	1.67	5	2
1:A:117:THR:O	1:A:121:VAL:HG23	0.86	1.71	17	13
1:A:114:GLU:HG3	1:A:116:LEU:HD23	0.86	1.48	16	1
1:A:92:PHE:CZ	1:A:108:VAL:HG11	0.83	2.07	18	1
1:A:125:ILE:HG21	1:A:134:GLY:O	0.83	1.72	14	5
1:A:107:HIS:CD2	1:A:108:VAL:HG23	0.83	2.09	17	1
1:A:107:HIS:NE2	1:A:108:VAL:HG23	0.80	1.91	17	1
1:A:105:LEU:O	1:A:105:LEU:HD23	0.80	1.77	11	2
1:A:117:THR:HG22	1:A:120:GLU:HG2	0.78	1.55	9	2
1:A:109:MET:HB3	1:A:116:LEU:HD13	0.77	1.57	9	4
1:A:116:LEU:HD21	1:A:124:MET:SD	0.77	2.20	11	2
1:A:110:THR:HG23	1:A:115:LYS:HA	0.76	1.56	10	1
1:A:129:ASP:OD1	1:A:136:VAL:HG22	0.76	1.80	12	2
1:A:105:LEU:HD23	1:A:121:VAL:HG13	0.76	1.56	19	2
1:A:111:ASN:C	1:A:112:LEU:HD23	0.75	2.00	16	1
1:A:112:LEU:HD12	1:A:112:LEU:O	0.75	1.81	10	1
1:A:117:THR:HG23	1:A:118:ASP:N	0.73	1.98	13	5
1:A:109:MET:HB2	1:A:116:LEU:HD12	0.72	1.59	5	1
1:A:105:LEU:CD2	1:A:109:MET:HE2	0.71	2.00	14	1
1:A:130:ILE:HD12	1:A:140:GLU:OE1	0.71	1.86	10	1
1:A:114:GLU:CG	1:A:116:LEU:HD23	0.70	2.14	16	1
1:A:106:ARG:HG2	1:A:121:VAL:HG21	0.70	1.62	18	1
1:A:102:ALA:HB1	1:A:121:VAL:HG11	0.69	1.65	15	4
1:A:85:ILE:HG12	1:A:146:THR:HG23	0.68	1.63	12	1
1:A:108:VAL:HG12	1:A:108:VAL:O	0.68	1.87	3	1
1:A:109:MET:HB3	1:A:116:LEU:HD22	0.67	1.67	8	1
1:A:116:LEU:C	1:A:116:LEU:HD12	0.66	2.11	19	1
1:A:99:TYR:CE1	1:A:137:ASN:CB	0.66	2.79	3	6
1:A:92:PHE:CE2	1:A:108:VAL:HG11	0.65	2.26	18	1
1:A:91:VAL:O	1:A:108:VAL:HG21	0.64	1.91	15	4
1:A:117:THR:HG22	1:A:120:GLU:CG	0.64	2.22	9	1
1:A:99:TYR:CD2	1:A:135:GLN:NE2	0.64	2.66	11	4
1:A:106:ARG:O	1:A:110:THR:HG22	0.63	1.93	13	3
1:A:99:TYR:CE2	1:A:135:GLN:NE2	0.63	2.67	12	4
1:A:87:GLU:O	1:A:91:VAL:HG23	0.62	1.94	12	3
1:A:85:ILE:HG21	1:A:142:VAL:HG22	0.61	1.71	14	4
1:A:99:TYR:CE1	1:A:137:ASN:HB3	0.60	2.31	15	6
1:A:146:THR:O	1:A:146:THR:HG22	0.60	1.95	19	2
1:A:92:PHE:CD1	1:A:105:LEU:HD12	0.60	2.32	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:THR:O	1:A:146:THR:CG2	0.60	2.49	19	1
1:A:107:HIS:O	1:A:110:THR:HG22	0.60	1.97	4	4
1:A:109:MET:CG	1:A:116:LEU:HD22	0.60	2.26	11	1
1:A:116:LEU:HD13	1:A:121:VAL:HG23	0.59	1.73	19	1
1:A:125:ILE:HG22	1:A:129:ASP:OD2	0.59	1.96	8	1
1:A:142:VAL:HG13	1:A:146:THR:OG1	0.59	1.97	12	1
1:A:92:PHE:CE2	1:A:108:VAL:CG1	0.59	2.84	18	1
1:A:106:ARG:HB2	1:A:121:VAL:HG21	0.59	1.74	9	1
1:A:105:LEU:CD2	1:A:109:MET:CG	0.59	2.80	18	2
1:A:116:LEU:HD12	1:A:117:THR:N	0.58	2.13	19	1
1:A:99:TYR:CD1	1:A:135:GLN:OE1	0.58	2.57	1	1
1:A:109:MET:HB3	1:A:116:LEU:HD11	0.58	1.75	6	1
1:A:111:ASN:HB3	1:A:112:LEU:HD23	0.58	1.74	14	1
1:A:136:VAL:HG12	1:A:137:ASN:N	0.57	2.13	2	20
1:A:137:ASN:ND2	1:A:140:GLU:CG	0.57	2.67	4	2
1:A:104:GLU:O	1:A:107:HIS:CE1	0.57	2.57	17	1
1:A:85:ILE:HG23	1:A:145:MET:CB	0.57	2.29	10	1
1:A:85:ILE:CG2	1:A:142:VAL:HG22	0.57	2.29	18	4
1:A:141:PHE:CZ	1:A:145:MET:SD	0.57	2.98	17	3
1:A:137:ASN:HB3	1:A:140:GLU:OE1	0.56	1.99	13	1
1:A:108:VAL:HG12	1:A:111:ASN:HB2	0.56	1.77	3	1
1:A:137:ASN:OD1	1:A:137:ASN:N	0.56	2.38	12	4
1:A:113:GLY:O	1:A:114:GLU:CB	0.56	2.52	16	4
1:A:137:ASN:OD1	1:A:140:GLU:CG	0.56	2.53	2	2
1:A:107:HIS:CG	1:A:108:VAL:N	0.56	2.72	17	1
1:A:99:TYR:CE2	1:A:137:ASN:HB3	0.56	2.35	20	1
1:A:106:ARG:HH12	1:A:110:THR:HG21	0.56	1.60	11	1
1:A:116:LEU:HD13	1:A:120:GLU:HG2	0.56	1.77	18	1
1:A:110:THR:HG23	1:A:115:LYS:CA	0.56	2.29	10	1
1:A:99:TYR:CE1	1:A:137:ASN:HB2	0.56	2.36	3	6
1:A:116:LEU:CD1	1:A:117:THR:N	0.56	2.69	19	1
1:A:117:THR:CG2	1:A:118:ASP:N	0.56	2.69	13	2
1:A:109:MET:CB	1:A:116:LEU:HD22	0.56	2.30	8	1
1:A:109:MET:HG3	1:A:116:LEU:HD22	0.56	1.78	11	1
1:A:84:GLU:O	1:A:88:ALA:HB2	0.56	2.01	15	2
1:A:110:THR:HG22	1:A:114:GLU:HA	0.55	1.77	19	1
1:A:94:LYS:NZ	1:A:107:HIS:CD2	0.55	2.74	10	1
1:A:142:VAL:C	1:A:146:THR:HG1	0.55	2.05	12	1
1:A:85:ILE:HG21	1:A:142:VAL:HG13	0.55	1.79	19	1
1:A:116:LEU:H	1:A:116:LEU:HD23	0.54	1.62	7	4
1:A:110:THR:O	1:A:112:LEU:N	0.54	2.41	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:PHE:CE1	1:A:137:ASN:C	0.54	2.81	18	14
1:A:141:PHE:CZ	1:A:145:MET:HG3	0.54	2.37	3	4
1:A:125:ILE:HG23	1:A:136:VAL:HG23	0.54	1.78	6	7
1:A:137:ASN:CB	1:A:140:GLU:OE1	0.54	2.55	13	1
1:A:109:MET:CB	1:A:116:LEU:HD12	0.54	2.33	5	1
1:A:105:LEU:O	1:A:109:MET:CG	0.54	2.56	2	3
1:A:137:ASN:ND2	1:A:140:GLU:HG2	0.54	2.18	4	2
1:A:109:MET:SD	1:A:116:LEU:HD12	0.54	2.43	10	1
1:A:124:MET:O	1:A:127:GLU:CG	0.53	2.57	6	2
1:A:136:VAL:CG1	1:A:137:ASN:N	0.53	2.71	2	19
1:A:84:GLU:O	1:A:88:ALA:CB	0.53	2.56	15	2
1:A:114:GLU:O	1:A:115:LYS:O	0.53	2.27	12	1
1:A:130:ILE:HD12	1:A:140:GLU:OE2	0.53	2.02	5	2
1:A:140:GLU:OE1	1:A:140:GLU:CA	0.53	2.55	4	2
1:A:105:LEU:CD2	1:A:105:LEU:O	0.53	2.57	6	1
1:A:105:LEU:CD2	1:A:109:MET:HG3	0.53	2.34	11	4
1:A:109:MET:O	1:A:113:GLY:CA	0.52	2.57	6	4
1:A:137:ASN:OD1	1:A:139:GLU:N	0.52	2.42	15	3
1:A:106:ARG:CG	1:A:121:VAL:HG21	0.52	2.33	18	1
1:A:99:TYR:CE1	1:A:135:GLN:OE1	0.52	2.63	1	1
1:A:141:PHE:CZ	1:A:145:MET:CG	0.52	2.92	14	2
1:A:116:LEU:HD12	1:A:121:VAL:HG22	0.52	1.79	17	1
1:A:110:THR:CB	1:A:114:GLU:O	0.52	2.57	1	1
1:A:137:ASN:N	1:A:137:ASN:OD1	0.52	2.42	20	4
1:A:111:ASN:O	1:A:113:GLY:N	0.52	2.42	16	1
1:A:105:LEU:CD2	1:A:109:MET:SD	0.52	2.98	10	1
1:A:116:LEU:HD23	1:A:116:LEU:N	0.52	2.19	8	1
1:A:110:THR:OG1	1:A:115:LYS:N	0.52	2.42	17	1
1:A:119:GLU:CG	1:A:120:GLU:N	0.51	2.74	4	1
1:A:88:ALA:CB	1:A:145:MET:SD	0.51	2.97	6	1
1:A:106:ARG:O	1:A:109:MET:CG	0.51	2.57	20	1
1:A:137:ASN:CA	1:A:140:GLU:OE1	0.51	2.59	13	1
1:A:99:TYR:CE1	1:A:137:ASN:ND2	0.51	2.78	12	1
1:A:111:ASN:HB3	1:A:112:LEU:HD12	0.51	1.82	7	1
1:A:109:MET:SD	1:A:116:LEU:CD1	0.51	2.98	10	1
1:A:115:LYS:O	1:A:116:LEU:O	0.51	2.28	19	1
1:A:95:ASP:O	1:A:97:ASN:N	0.51	2.43	6	9
1:A:99:TYR:CD2	1:A:136:VAL:O	0.51	2.63	20	1
1:A:117:THR:O	1:A:121:VAL:CG2	0.51	2.57	5	2
1:A:98:GLY:O	1:A:137:ASN:ND2	0.51	2.42	13	2
1:A:86:ARG:HA	1:A:138:TYR:CE1	0.51	2.40	20	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:TYR:CE2	1:A:137:ASN:HB2	0.51	2.40	5	1
1:A:111:ASN:O	1:A:112:LEU:CB	0.51	2.57	12	1
1:A:109:MET:HB3	1:A:116:LEU:HD21	0.50	1.83	14	2
1:A:130:ILE:CD1	1:A:140:GLU:OE2	0.50	2.59	5	1
1:A:92:PHE:CE2	1:A:108:VAL:HB	0.50	2.42	14	2
1:A:130:ILE:CG1	1:A:140:GLU:OE1	0.50	2.59	4	2
1:A:138:TYR:CE1	1:A:142:VAL:CG2	0.50	2.94	20	3
1:A:116:LEU:CD2	1:A:124:MET:SD	0.50	2.98	11	3
1:A:133:ASP:OD1	1:A:133:ASP:N	0.50	2.44	18	1
1:A:94:LYS:N	1:A:94:LYS:CD	0.50	2.74	4	1
1:A:110:THR:O	1:A:111:ASN:C	0.50	2.50	3	8
1:A:106:ARG:O	1:A:110:THR:CG2	0.50	2.59	6	1
1:A:108:VAL:O	1:A:108:VAL:CG1	0.50	2.59	3	1
1:A:109:MET:CB	1:A:116:LEU:CD2	0.50	2.90	8	1
1:A:108:VAL:O	1:A:108:VAL:HG12	0.50	2.07	5	1
1:A:129:ASP:OD1	1:A:130:ILE:N	0.50	2.45	13	1
1:A:106:ARG:O	1:A:110:THR:OG1	0.50	2.30	10	2
1:A:125:ILE:CG2	1:A:129:ASP:OD1	0.49	2.59	16	1
1:A:95:ASP:O	1:A:96:GLY:C	0.49	2.50	4	20
1:A:129:ASP:OD1	1:A:136:VAL:CG2	0.49	2.58	12	1
1:A:138:TYR:CZ	1:A:142:VAL:HG21	0.49	2.42	7	3
1:A:109:MET:HB3	1:A:116:LEU:CD1	0.49	2.38	6	1
1:A:87:GLU:HG3	1:A:88:ALA:N	0.49	2.23	5	3
1:A:86:ARG:NH1	1:A:138:TYR:CD2	0.49	2.81	9	1
1:A:101:SER:OG	1:A:102:ALA:N	0.49	2.46	14	1
1:A:141:PHE:CZ	1:A:145:MET:HG2	0.49	2.43	7	2
1:A:99:TYR:CD2	1:A:135:GLN:HG3	0.49	2.43	4	3
1:A:142:VAL:O	1:A:146:THR:HG22	0.49	2.08	11	3
1:A:108:VAL:HG12	1:A:111:ASN:CG	0.48	2.29	5	1
1:A:105:LEU:CD2	1:A:109:MET:HG2	0.48	2.38	18	2
1:A:102:ALA:CB	1:A:121:VAL:HG11	0.48	2.38	15	1
1:A:138:TYR:CZ	1:A:142:VAL:CG2	0.48	2.96	20	4
1:A:116:LEU:HD12	1:A:121:VAL:N	0.48	2.22	7	1
1:A:140:GLU:OE1	1:A:140:GLU:HA	0.48	2.09	4	2
1:A:137:ASN:CG	1:A:138:TYR:N	0.48	2.66	19	1
1:A:110:THR:HG21	1:A:115:LYS:HA	0.48	1.84	17	1
1:A:108:VAL:O	1:A:111:ASN:OD1	0.48	2.31	4	3
1:A:85:ILE:HD13	1:A:85:ILE:N	0.48	2.22	7	1
1:A:105:LEU:CD1	1:A:125:ILE:HG12	0.48	2.37	18	2
1:A:116:LEU:HD23	1:A:116:LEU:H	0.48	1.69	17	1
1:A:116:LEU:HD22	1:A:124:MET:SD	0.48	2.49	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:VAL:O	1:A:109:MET:C	0.47	2.53	17	2
1:A:109:MET:HB2	1:A:116:LEU:HD21	0.47	1.85	3	1
1:A:130:ILE:CG1	1:A:140:GLU:CD	0.47	2.82	16	2
1:A:99:TYR:CD2	1:A:137:ASN:HB3	0.47	2.44	20	1
1:A:93:ASP:OD1	1:A:104:GLU:OE2	0.47	2.32	3	2
1:A:137:ASN:OD1	1:A:140:GLU:HG3	0.47	2.09	7	2
1:A:92:PHE:CE1	1:A:108:VAL:HG11	0.47	2.45	4	1
1:A:89:PHE:CE1	1:A:137:ASN:O	0.47	2.67	10	3
1:A:116:LEU:CD1	1:A:121:VAL:HG22	0.47	2.38	17	1
1:A:93:ASP:OD1	1:A:99:TYR:O	0.47	2.33	6	3
1:A:105:LEU:HD21	1:A:124:MET:HB2	0.47	1.85	20	1
1:A:126:ARG:HG3	1:A:127:GLU:N	0.47	2.24	18	2
1:A:99:TYR:CZ	1:A:137:ASN:HB3	0.47	2.44	3	1
1:A:137:ASN:O	1:A:141:PHE:CB	0.47	2.63	10	3
1:A:112:LEU:CD1	1:A:112:LEU:O	0.47	2.58	10	1
1:A:111:ASN:OD1	1:A:112:LEU:N	0.47	2.47	1	1
1:A:114:GLU:O	1:A:116:LEU:HD23	0.47	2.10	14	1
1:A:137:ASN:N	1:A:140:GLU:OE1	0.47	2.48	13	1
1:A:94:LYS:HD3	1:A:107:HIS:CE1	0.47	2.45	20	1
1:A:99:TYR:HA	1:A:136:VAL:O	0.47	2.10	10	5
1:A:129:ASP:OD2	1:A:140:GLU:OE1	0.47	2.33	3	1
1:A:99:TYR:N	1:A:99:TYR:CD1	0.46	2.82	9	5
1:A:94:LYS:HD2	1:A:94:LYS:N	0.46	2.25	4	1
1:A:126:ARG:O	1:A:129:ASP:OD2	0.46	2.32	5	1
1:A:109:MET:CE	1:A:116:LEU:HD12	0.46	2.39	10	1
1:A:105:LEU:O	1:A:109:MET:HG3	0.46	2.10	8	2
1:A:130:ILE:HG13	1:A:140:GLU:OE1	0.46	2.11	4	2
1:A:123:GLU:O	1:A:126:ARG:HG2	0.46	2.10	12	1
1:A:106:ARG:O	1:A:109:MET:HG3	0.46	2.09	20	1
1:A:93:ASP:OD1	1:A:104:GLU:OE1	0.46	2.33	5	1
1:A:145:MET:SD	1:A:145:MET:O	0.46	2.74	3	2
1:A:125:ILE:O	1:A:129:ASP:OD1	0.46	2.34	7	1
1:A:98:GLY:O	1:A:137:ASN:OD1	0.46	2.32	10	1
1:A:123:GLU:O	1:A:126:ARG:HG3	0.46	2.11	15	2
1:A:137:ASN:C	1:A:137:ASN:OD1	0.46	2.53	3	2
1:A:142:VAL:O	1:A:146:THR:OG1	0.46	2.31	16	1
1:A:129:ASP:OD1	1:A:135:GLN:O	0.46	2.33	4	2
1:A:87:GLU:CG	1:A:88:ALA:N	0.46	2.78	5	2
1:A:87:GLU:OE2	1:A:88:ALA:N	0.46	2.49	16	1
1:A:92:PHE:CE1	1:A:108:VAL:CG1	0.46	2.99	16	1
1:A:105:LEU:HD21	1:A:109:MET:SD	0.46	2.50	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:HD22	1:A:109:MET:HG3	0.46	1.88	18	2
1:A:93:ASP:OD1	1:A:95:ASP:OD1	0.46	2.32	9	2
1:A:92:PHE:CZ	1:A:108:VAL:CG1	0.46	2.90	18	1
1:A:109:MET:CB	1:A:116:LEU:HD11	0.46	2.39	6	1
1:A:87:GLU:O	1:A:88:ALA:C	0.46	2.53	6	11
1:A:141:PHE:CD1	1:A:141:PHE:C	0.46	2.89	7	1
1:A:102:ALA:CA	1:A:121:VAL:HG11	0.46	2.41	11	2
1:A:106:ARG:HG2	1:A:121:VAL:CG2	0.46	2.38	18	1
1:A:99:TYR:CD2	1:A:135:GLN:CD	0.46	2.89	10	1
1:A:120:GLU:O	1:A:121:VAL:C	0.46	2.54	15	3
1:A:141:PHE:C	1:A:141:PHE:CD1	0.46	2.88	16	1
1:A:102:ALA:HA	1:A:121:VAL:HG11	0.46	1.88	13	1
1:A:141:PHE:CE2	1:A:145:MET:HG3	0.46	2.46	14	1
1:A:136:VAL:C	1:A:137:ASN:OD1	0.46	2.54	12	3
1:A:129:ASP:HB3	1:A:135:GLN:O	0.46	2.11	1	1
1:A:113:GLY:O	1:A:114:GLU:HB3	0.45	2.11	16	2
1:A:99:TYR:CD2	1:A:135:GLN:HB3	0.45	2.46	19	1
1:A:129:ASP:OD2	1:A:135:GLN:O	0.45	2.34	12	3
1:A:109:MET:O	1:A:113:GLY:C	0.45	2.55	14	2
1:A:116:LEU:HB2	1:A:120:GLU:CB	0.45	2.41	13	2
1:A:137:ASN:O	1:A:141:PHE:HB3	0.45	2.11	10	1
1:A:115:LYS:O	1:A:116:LEU:C	0.45	2.54	19	1
1:A:119:GLU:HG3	1:A:120:GLU:N	0.45	2.27	4	1
1:A:105:LEU:O	1:A:109:MET:HG2	0.45	2.12	2	2
1:A:137:ASN:OD1	1:A:140:GLU:HG2	0.45	2.10	2	1
1:A:95:ASP:OD2	1:A:104:GLU:OE2	0.45	2.34	18	2
1:A:130:ILE:HG12	1:A:140:GLU:CG	0.45	2.42	15	1
1:A:137:ASN:OD1	1:A:137:ASN:C	0.45	2.55	15	1
1:A:129:ASP:CG	1:A:130:ILE:N	0.45	2.69	3	1
1:A:116:LEU:HD11	1:A:121:VAL:HG22	0.45	1.88	8	2
1:A:124:MET:O	1:A:127:GLU:HG2	0.45	2.11	6	1
1:A:90:ARG:O	1:A:93:ASP:O	0.45	2.35	18	1
1:A:111:ASN:CG	1:A:112:LEU:N	0.45	2.69	19	2
1:A:129:ASP:O	1:A:129:ASP:OD1	0.45	2.34	17	2
1:A:99:TYR:CE2	1:A:135:GLN:HB3	0.45	2.46	19	1
1:A:85:ILE:N	1:A:85:ILE:HD13	0.45	2.26	14	1
1:A:111:ASN:O	1:A:112:LEU:HB3	0.45	2.12	12	1
1:A:90:ARG:O	1:A:91:VAL:C	0.45	2.55	17	7
1:A:129:ASP:OD1	1:A:129:ASP:C	0.45	2.55	5	1
1:A:110:THR:HA	1:A:114:GLU:O	0.45	2.12	1	2
1:A:111:ASN:C	1:A:112:LEU:CD2	0.45	2.81	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:HD12	1:A:125:ILE:HG12	0.44	1.88	18	2
1:A:119:GLU:O	1:A:123:GLU:HB2	0.44	2.12	20	1
1:A:113:GLY:O	1:A:114:GLU:CG	0.44	2.65	16	2
1:A:116:LEU:C	1:A:116:LEU:CD1	0.44	2.83	19	1
1:A:137:ASN:ND2	1:A:140:GLU:HG3	0.44	2.28	9	6
1:A:83:GLU:O	1:A:87:GLU:HG2	0.44	2.13	10	1
1:A:109:MET:O	1:A:113:GLY:O	0.44	2.35	9	1
1:A:117:THR:OG1	1:A:120:GLU:HB3	0.44	2.12	12	1
1:A:104:GLU:O	1:A:107:HIS:HB3	0.44	2.13	20	1
1:A:142:VAL:O	1:A:143:GLN:C	0.44	2.55	7	1
1:A:119:GLU:O	1:A:123:GLU:OE1	0.44	2.35	8	1
1:A:85:ILE:H	1:A:85:ILE:HD12	0.44	1.73	12	1
1:A:121:VAL:O	1:A:122:ASP:C	0.44	2.55	19	2
1:A:99:TYR:CZ	1:A:130:ILE:HD11	0.44	2.48	2	1
1:A:124:MET:O	1:A:127:GLU:HG3	0.44	2.12	9	1
1:A:117:THR:OG1	1:A:120:GLU:HG3	0.44	2.13	20	1
1:A:125:ILE:O	1:A:127:GLU:N	0.44	2.51	2	1
1:A:129:ASP:OD1	1:A:131:ASP:N	0.44	2.50	13	1
1:A:138:TYR:O	1:A:142:VAL:CG2	0.44	2.57	6	3
1:A:141:PHE:CD1	1:A:144:MET:CE	0.44	3.00	10	1
1:A:87:GLU:O	1:A:89:PHE:N	0.44	2.51	9	6
1:A:95:ASP:OD2	1:A:104:GLU:CD	0.43	2.57	12	1
1:A:141:PHE:O	1:A:145:MET:SD	0.43	2.76	7	1
1:A:141:PHE:O	1:A:145:MET:HB2	0.43	2.13	7	2
1:A:113:GLY:O	1:A:114:GLU:OE2	0.43	2.36	17	1
1:A:108:VAL:CG1	1:A:111:ASN:HB2	0.43	2.42	3	1
1:A:109:MET:SD	1:A:124:MET:SD	0.43	3.16	8	1
1:A:137:ASN:C	1:A:140:GLU:OE1	0.43	2.57	13	1
1:A:85:ILE:HD11	1:A:146:THR:OG1	0.43	2.12	19	1
1:A:110:THR:CB	1:A:115:LYS:HA	0.43	2.43	17	1
1:A:111:ASN:O	1:A:112:LEU:HG	0.43	2.13	16	1
1:A:116:LEU:HB2	1:A:120:GLU:HB2	0.43	1.90	16	3
1:A:120:GLU:OE2	1:A:124:MET:CE	0.43	2.66	11	1
1:A:86:ARG:NH1	1:A:138:TYR:CG	0.43	2.86	9	1
1:A:102:ALA:HB1	1:A:121:VAL:CG1	0.43	2.41	15	2
1:A:145:MET:O	1:A:145:MET:SD	0.43	2.77	14	1
1:A:92:PHE:CE1	1:A:108:VAL:HB	0.43	2.48	8	2
1:A:106:ARG:O	1:A:107:HIS:C	0.43	2.57	11	2
1:A:85:ILE:HG22	1:A:142:VAL:HG22	0.43	1.90	7	1
1:A:116:LEU:HG	1:A:120:GLU:CG	0.43	2.43	11	1
1:A:97:ASN:ND2	1:A:97:ASN:C	0.43	2.71	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ASN:O	1:A:112:LEU:C	0.43	2.55	16	1
1:A:114:GLU:O	1:A:116:LEU:N	0.43	2.51	14	1
1:A:117:THR:OG1	1:A:120:GLU:CB	0.43	2.67	12	1
1:A:125:ILE:HG23	1:A:136:VAL:CG2	0.43	2.43	6	2
1:A:130:ILE:HG12	1:A:140:GLU:CD	0.43	2.34	16	1
1:A:105:LEU:HD12	1:A:105:LEU:O	0.43	2.13	15	1
1:A:112:LEU:N	1:A:112:LEU:HD23	0.43	2.29	17	1
1:A:141:PHE:CE2	1:A:145:MET:SD	0.43	3.12	17	1
1:A:116:LEU:O	1:A:116:LEU:HG	0.43	2.14	16	1
1:A:120:GLU:OE2	1:A:124:MET:HE3	0.43	2.13	11	1
1:A:117:THR:CG2	1:A:120:GLU:HG2	0.43	2.38	9	1
1:A:113:GLY:O	1:A:116:LEU:HD23	0.43	2.14	15	1
1:A:111:ASN:OD1	1:A:112:LEU:CD1	0.43	2.67	1	1
1:A:146:THR:CG2	1:A:146:THR:O	0.43	2.66	2	1
1:A:99:TYR:CA	1:A:136:VAL:O	0.43	2.67	10	2
1:A:123:GLU:O	1:A:126:ARG:CG	0.43	2.66	18	2
1:A:99:TYR:CD1	1:A:99:TYR:N	0.42	2.87	6	2
1:A:113:GLY:C	1:A:114:GLU:CG	0.42	2.87	17	2
1:A:141:PHE:CE1	1:A:144:MET:HE3	0.42	2.49	10	1
1:A:139:GLU:O	1:A:143:GLN:OE1	0.42	2.37	11	1
1:A:83:GLU:O	1:A:84:GLU:C	0.42	2.57	1	1
1:A:109:MET:HE3	1:A:116:LEU:HD12	0.42	1.90	10	1
1:A:95:ASP:C	1:A:95:ASP:OD1	0.42	2.57	9	1
1:A:111:ASN:OD1	1:A:112:LEU:HD12	0.42	2.14	1	1
1:A:85:ILE:HG21	1:A:142:VAL:HA	0.42	1.90	13	1
1:A:94:LYS:HD3	1:A:107:HIS:NE2	0.42	2.30	20	1
1:A:101:SER:O	1:A:102:ALA:C	0.42	2.58	2	1
1:A:112:LEU:HD23	1:A:112:LEU:N	0.42	2.30	13	1
1:A:117:THR:OG1	1:A:120:GLU:HG2	0.41	2.15	8	1
1:A:99:TYR:HB3	1:A:136:VAL:O	0.41	2.15	10	4
1:A:106:ARG:NH1	1:A:110:THR:HG21	0.41	2.29	11	1
1:A:87:GLU:C	1:A:89:PHE:N	0.41	2.73	11	4
1:A:120:GLU:OE2	1:A:124:MET:HG2	0.41	2.15	6	1
1:A:129:ASP:C	1:A:129:ASP:OD1	0.41	2.58	7	1
1:A:111:ASN:ND2	1:A:112:LEU:HG	0.41	2.30	5	1
1:A:105:LEU:HD22	1:A:125:ILE:HG12	0.41	1.92	16	1
1:A:133:ASP:CG	1:A:135:GLN:OE1	0.41	2.58	4	1
1:A:117:THR:OG1	1:A:118:ASP:N	0.41	2.54	6	2
1:A:130:ILE:HG12	1:A:140:GLU:OE1	0.41	2.15	7	1
1:A:90:ARG:O	1:A:92:PHE:N	0.41	2.53	11	1
1:A:97:ASN:OD1	1:A:99:TYR:O	0.41	2.39	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:GLY:O	1:A:114:GLU:HB2	0.41	2.15	12	4
1:A:133:ASP:OD1	1:A:134:GLY:N	0.41	2.53	20	1
1:A:90:ARG:CB	1:A:90:ARG:CZ	0.41	2.98	10	1
1:A:127:GLU:HG3	1:A:128:ALA:N	0.41	2.30	9	1
1:A:128:ALA:O	1:A:129:ASP:C	0.41	2.58	18	1
1:A:93:ASP:OD1	1:A:95:ASP:CG	0.41	2.59	18	1
1:A:118:ASP:O	1:A:119:GLU:C	0.41	2.57	14	1
1:A:110:THR:HA	1:A:114:GLU:CA	0.41	2.45	20	1
1:A:99:TYR:CE2	1:A:137:ASN:ND2	0.41	2.89	5	1
1:A:105:LEU:CD2	1:A:125:ILE:HG12	0.41	2.46	15	1
1:A:95:ASP:C	1:A:97:ASN:N	0.41	2.74	6	1
1:A:109:MET:O	1:A:114:GLU:O	0.41	2.38	20	1
1:A:99:TYR:CB	1:A:136:VAL:O	0.41	2.69	10	1
1:A:105:LEU:C	1:A:105:LEU:HD23	0.41	2.36	11	1
1:A:105:LEU:O	1:A:109:MET:HB2	0.41	2.16	15	2
1:A:122:ASP:OD1	1:A:122:ASP:C	0.41	2.58	15	1
1:A:89:PHE:CD1	1:A:138:TYR:HA	0.41	2.51	17	2
1:A:105:LEU:HG	1:A:109:MET:CG	0.41	2.46	17	1
1:A:129:ASP:HB2	1:A:133:ASP:OD1	0.41	2.16	13	1
1:A:90:ARG:O	1:A:93:ASP:N	0.40	2.54	6	1
1:A:92:PHE:CB	1:A:100:ILE:HD13	0.40	2.45	16	1
1:A:85:ILE:HG13	1:A:146:THR:CG2	0.40	2.47	7	1
1:A:90:ARG:C	1:A:92:PHE:N	0.40	2.73	11	1
1:A:128:ALA:O	1:A:140:GLU:HB3	0.40	2.16	15	2
1:A:137:ASN:ND2	1:A:140:GLU:CD	0.40	2.75	8	1
1:A:113:GLY:O	1:A:114:GLU:C	0.40	2.57	7	1
1:A:104:GLU:OE1	1:A:104:GLU:HA	0.40	2.16	2	1
1:A:92:PHE:CD1	1:A:108:VAL:HB	0.40	2.51	15	1
1:A:109:MET:HB3	1:A:116:LEU:HG	0.40	1.93	18	1
1:A:130:ILE:HA	1:A:140:GLU:HG3	0.40	1.93	2	1
1:A:120:GLU:O	1:A:124:MET:CG	0.40	2.69	1	1
1:A:107:HIS:CG	1:A:108:VAL:H	0.40	2.33	17	1
1:A:126:ARG:HA	1:A:129:ASP:OD2	0.40	2.16	5	1
1:A:133:ASP:N	1:A:133:ASP:OD1	0.40	2.55	1	1
1:A:89:PHE:HA	1:A:141:PHE:CE1	0.40	2.51	17	1
1:A:106:ARG:HA	1:A:109:MET:HG2	0.40	1.93	20	1
1:A:141:PHE:CD1	1:A:141:PHE:O	0.40	2.75	16	1
1:A:120:GLU:O	1:A:124:MET:SD	0.40	2.80	11	1
1:A:112:LEU:C	1:A:112:LEU:HD12	0.40	2.37	15	1
1:A:123:GLU:O	1:A:127:GLU:HG3	0.40	2.17	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	64/73 (88%)	54±2 (85±4%)	8±3 (12±4%)	2±1 (3±2%)	9	43
All	All	1280/1460 (88%)	1085 (85%)	158 (12%)	37 (3%)	9	43

All 12 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	96	GLY	7
1	A	114	GLU	6
1	A	131	ASP	5
1	A	111	ASN	4
1	A	115	LYS	4
1	A	112	LEU	3
1	A	116	LEU	2
1	A	132	GLY	2
1	A	126	ARG	1
1	A	121	VAL	1
1	A	146	THR	1
1	A	98	GLY	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	55/63 (87%)	41±4 (75±6%)	14±4 (25±6%)	3	26
All	All	1100/1260 (87%)	828 (75%)	272 (25%)	3	26

All 38 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	145	MET	15
1	A	126	ARG	13
1	A	115	LYS	12
1	A	137	ASN	11
1	A	84	GLU	11
1	A	116	LEU	11
1	A	135	GLN	11
1	A	90	ARG	10
1	A	110	THR	10
1	A	119	GLU	10
1	A	144	MET	10
1	A	123	GLU	10
1	A	131	ASP	9
1	A	139	GLU	9
1	A	86	ARG	9
1	A	95	ASP	8
1	A	146	THR	8
1	A	94	LYS	8
1	A	122	ASP	8
1	A	112	LEU	8
1	A	106	ARG	7
1	A	111	ASN	6
1	A	118	ASP	6
1	A	83	GLU	6
1	A	129	ASP	5
1	A	133	ASP	5
1	A	101	SER	5
1	A	87	GLU	4
1	A	117	THR	4
1	A	109	MET	4
1	A	127	GLU	3
1	A	124	MET	3
1	A	105	LEU	3
1	A	140	GLU	2
1	A	97	ASN	2
1	A	99	TYR	2
1	A	114	GLU	2
1	A	120	GLU	2

6.3.3 RNA ⓘ

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