Full wwPDB NMR Structure Validation Report (i)

Feb 16, 2022 – 08:25 AM EST

PDB ID	:	1M31
Title	:	Three-Dimensional Solution Structure of Apo-Mts1
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Deposited on	:	2002-06-26

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

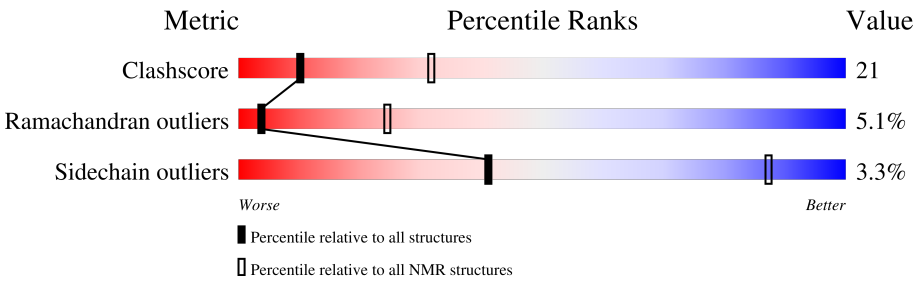
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	101	61% 32% • 6%
1	B	101	61% 32% • 6%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 8 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:96, B:2-B:96 (190)	0.91	7

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3264 atoms, of which 1626 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Placental calcium-binding protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1632	519	813	135	156	9	0
1	B	101	1632	519	813	135	156	9	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Placental calcium-binding protein

Chain A: 61% 32% • 6%

• Molecule 1: Placental calcium-binding protein

Chain B: 61% 32% • 6%

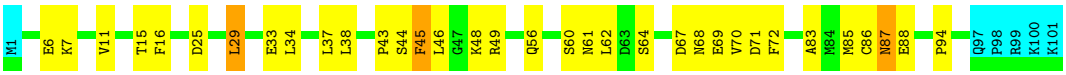
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

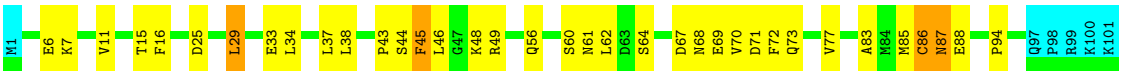
• Molecule 1: Placental calcium-binding protein

Chain A: 60% 31% • 6%



• Molecule 1: Placental calcium-binding protein

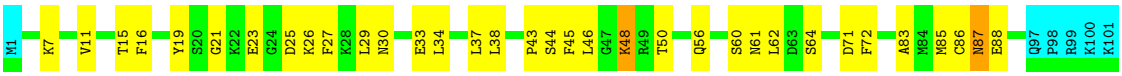
Chain B: 58% 32% • 6%



4.2.2 Score per residue for model 2

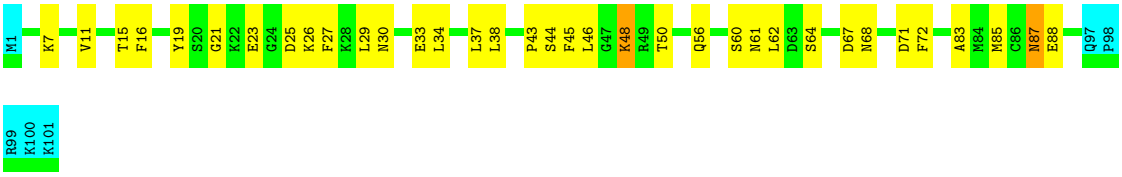
- Molecule 1: Placental calcium-binding protein

Chain A: 60% 32% • 6%



- Molecule 1: Placental calcium-binding protein

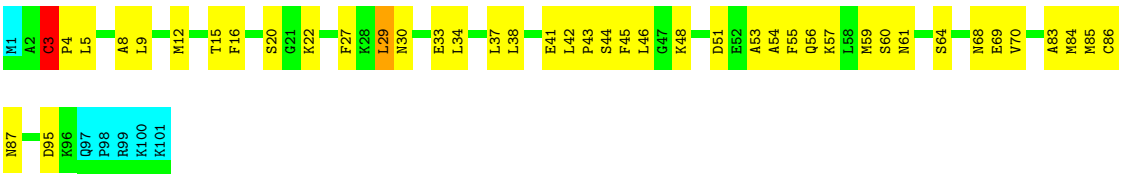
Chain B: 59% 33% • 6%



4.2.3 Score per residue for model 3

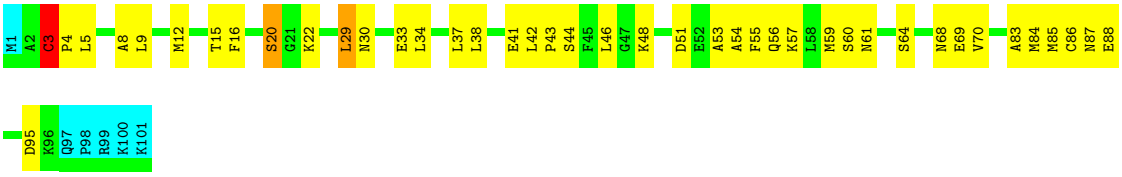
- Molecule 1: Placental calcium-binding protein

Chain A: 51% 41% •• 6%



- Molecule 1: Placental calcium-binding protein

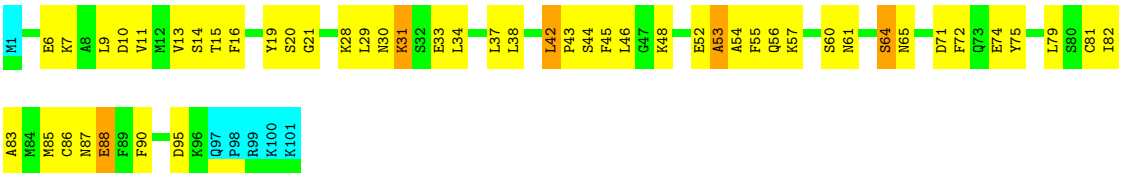
Chain B: 52% 39% •• 6%



4.2.4 Score per residue for model 4

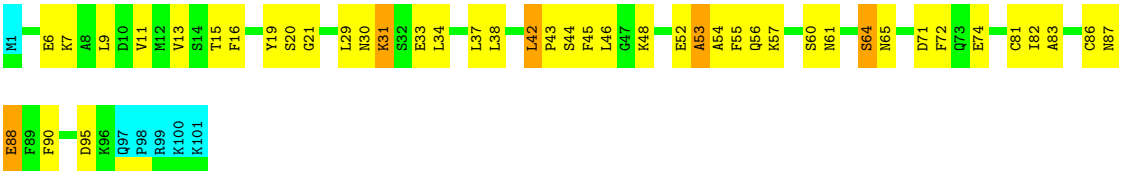
- Molecule 1: Placental calcium-binding protein

Chain A: 45% 45% 5% 6%



• Molecule 1: Placental calcium-binding protein

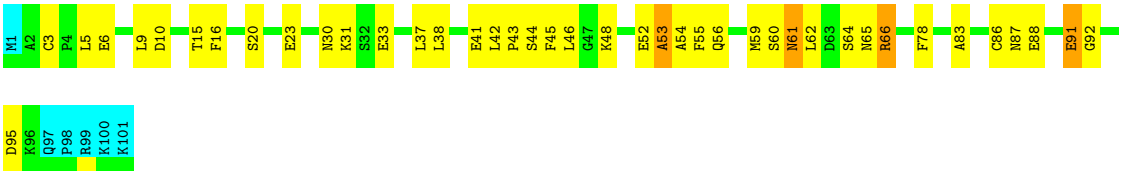
Chain B: 50% 39% 5% 6%



4.2.5 Score per residue for model 5

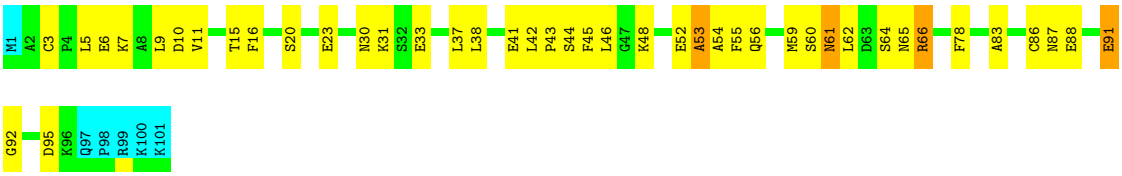
• Molecule 1: Placental calcium-binding protein

Chain A: 53% 37% • 6%



• Molecule 1: Placental calcium-binding protein

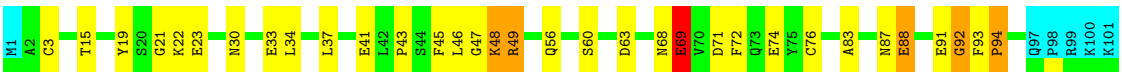
Chain B: 51% 39% • 6%



4.2.6 Score per residue for model 6

• Molecule 1: Placental calcium-binding protein

Chain A: 61% 27% 5% • 6%



• Molecule 1: Placental calcium-binding protein

Chain B: 57% 30% 6% • 6%

M1 A2 C3 P4 L5 E6 L9 T15 Y19 S20 G21 K22 E23 N30 K31 S32 E33 L34 L37 E41 L42 P43 L46 G47 K48 R49 Q56 S60 N61 L62 D63 N68 E69 V70 D71 F72 Q73 E74 Y75 C76 A83 N87 E88 E91 G92 F93 P94

Q97 P98 R99 K100 K101

4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Placental calcium-binding protein

Chain A: 52% 37% 5% 6%

M1 K7 V11 T15 F16 Y19 S20 G21 K22 E23 F27 K28 L29 N30 E33 E36 L37 L38 T39 R40 E41 L42 P43 S44 F45 L46 G47 K48 R49 T50 D51 E52 A53 Q56 M59 S60 N61 L62 D63 S64 N65 R66 D67 N68 D71 F72 Y75 L79

A83 N87 E88 Q97 P98 R99 K100 K101

- Molecule 1: Placental calcium-binding protein

Chain B: 50% 39% 5% 6%

M1 L5 E6 K7 A8 L9 D10 V11 T15 F16 Y19 S20 G21 K22 E23 F27 K28 L29 N30 E33 E36 L37 L38 T39 R40 E41 L42 P43 S44 F45 L46 G47 K48 R49 T50 D51 E52 A53 Q56 M59 S60 N61 L62 D63 S64 N65 R66 D67 N68 D71 F72

Y75 L79 A83 N87 E88 Q97 P98 R99 K100 K101

4.2.8 Score per residue for model 8

- Molecule 1: Placental calcium-binding protein

Chain A: 63% 29% •• 6%

M1 K7 V11 T15 Y19 S20 G21 N30 K31 S32 E33 L37 L38 E41 L42 P43 S44 F45 L46 G47 K48 R49 Q56 S60 N61 S64 E69 F72 Q73 E74 Y75 L79 A83 N87 Q97 P98 R99 K100 K101

- Molecule 1: Placental calcium-binding protein

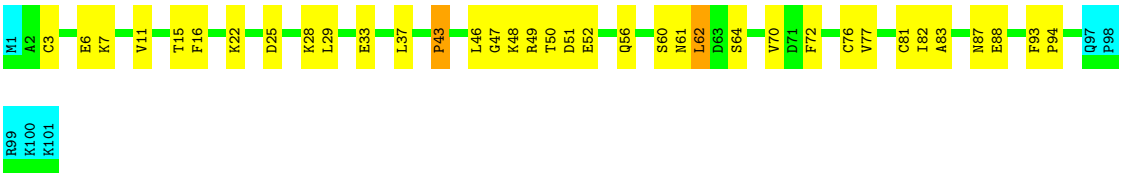
Chain B: 62% 30% •• 6%

M1 K7 D10 V11 S14 T15 Y19 S20 G21 N30 K31 S32 E33 L34 K35 E36 L37 L38 T39 R40 E41 L42 P43 S44 F45 L46 G47 K48 R49 Q56 S60 N61 S64 E69 F72 Q73 E74 A83 N87 Q97 P98 R99 K100 K101

4.2.9 Score per residue for model 9

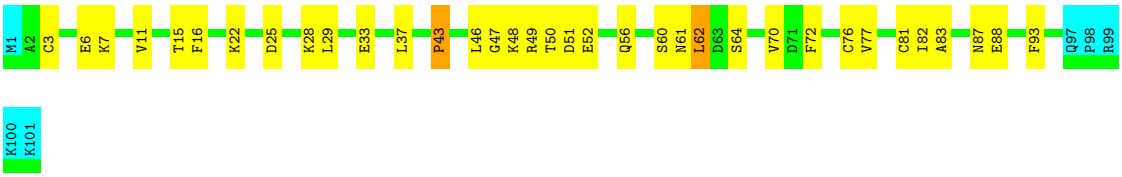
- Molecule 1: Placental calcium-binding protein

Chain A: 58% 34% • 6%



- Molecule 1: Placental calcium-binding protein

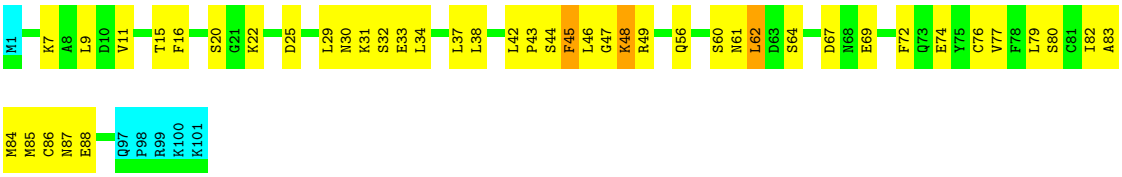
Chain B: 59% 33% • 6%



4.2.10 Score per residue for model 10

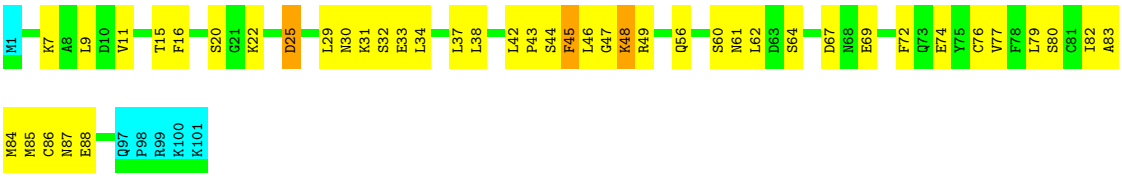
- Molecule 1: Placental calcium-binding protein

Chain A: 50% 41% • 6%



- Molecule 1: Placental calcium-binding protein

Chain B: 50% 41% • 6%



4.2.11 Score per residue for model 11

- Molecule 1: Placental calcium-binding protein

Chain A: 47% 40% 8% 6%

M1 A2 C3 P4 L5 E6 K7 A8 L9 D10 V11 M12 T15 F16 Y19 S20 G21 L29 N30 K31 S32 E33 L37 L38 T39 L42 P43 L46 G47 K48 R49 E52 A53 A54 F55 Q56 K57 L58 M59 S60 N61 S64 N65 V70 D71 F72 L79 S80 C81 I82

A83 N87 E88 E91 G92 F93 P94 D95 K96 Q97 P98 R99 K100 K101

- Molecule 1: Placental calcium-binding protein

Chain B: 49% 39% 7% 6%

M1 A2 C3 P4 L5 E6 K7 A8 L9 D10 V11 M12 T15 F16 Y19 S20 G21 L29 N30 E33 L37 L38 T39 L42 P43 L46 G47 K48 R49 E52 A53 A54 F55 Q56 K57 L58 M59 S60 N61 S64 N65 D71 F72 L79 S80 C81 I82 A83

N87 E88 E91 G92 F93 P94 D95 K96 Q97 P98 R99 K100 K101

4.2.12 Score per residue for model 12

- Molecule 1: Placental calcium-binding protein

Chain A: 50% 43% • 6%

M1 L5 E6 K7 A8 L9 D10 V11 T15 F16 Y19 S20 G21 K22 E23 G24 D25 K26 F27 K28 L29 N30 E33 L34 L37 L38 T39 R40 P43 S44 F45 L46 G47 K48 R49 Q56 S60 N61 L62 D63 S64 E69 V70 D71 E74 Y75 C76 V77 F78

C81 I82 A83 M84 M85 C86 N87 E88 P94 Q97 P98 R99 K100 K101

- Molecule 1: Placental calcium-binding protein

Chain B: 52% 40% • 6%

M1 L5 L9 T15 F16 Y19 S20 G21 K22 E23 G24 D25 K26 F27 K28 L29 N30 E33 L34 L37 L38 T39 R40 P43 S44 F45 L46 G47 K48 R49 Q56 S60 N61 L62 D63 S64 E69 V70 D71 E74 Y75 C76 V77 F78 C81 I82 A83 M84

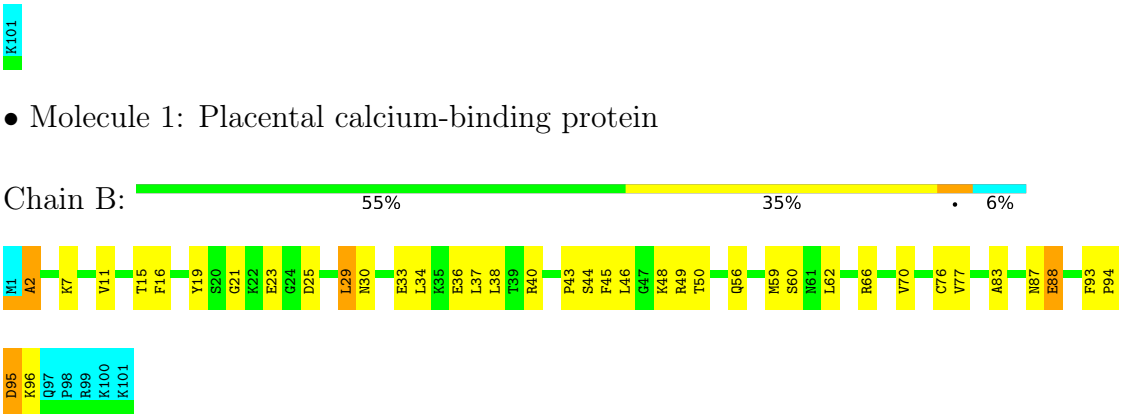
M85 C86 N87 E88 P94 Q97 P98 R99 K100 K101

4.2.13 Score per residue for model 13

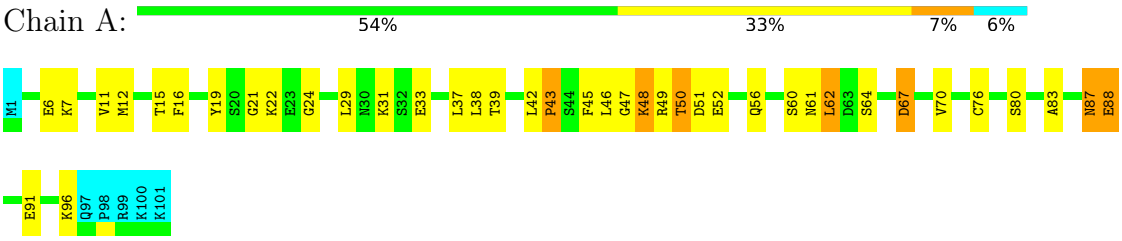
- Molecule 1: Placental calcium-binding protein

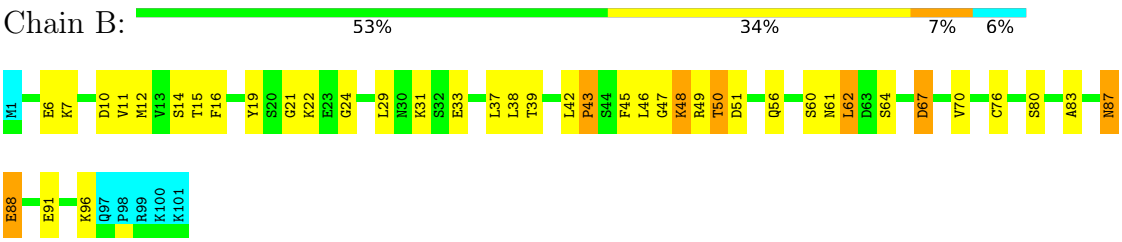
Chain A: 58% 34% • 6%

M1 A2 T15 F16 Y19 S20 G21 K22 E23 G24 D25 L29 N30 E33 L34 K35 E36 L37 L38 T39 R40 P43 S44 F45 L46 G47 K48 R49 T50 Q56 M59 S60 N61 L62 R66 C76 V77 A83 N87 E88 F93 P94 D95 K96 Q97 P98 R99 K100

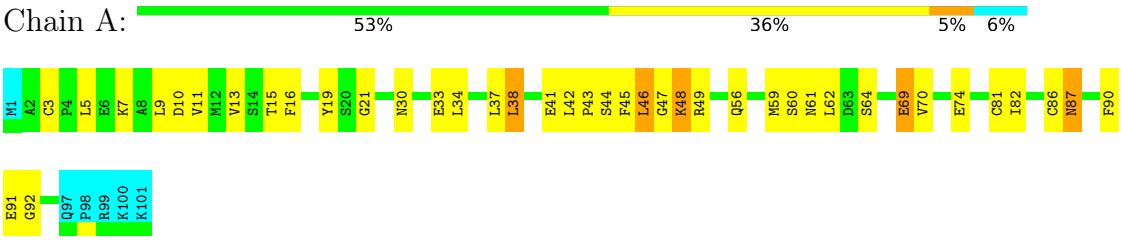


4.2.14 Score per residue for model 14





4.2.15 Score per residue for model 15



• Molecule 1: Placental calcium-binding protein

Chain B: 56% 33% 5% 6%

M1 A2 C3 D10 V13 S14 T15 F16 Y19 S20 G21 N30 K31 S32 E33 L34 L37 L38 E41 L42 P43 S44 F45 L46 G47 K48 R49 Q56 M59 S60 N61 L62 D63 S64 E69 V70 E74 C81 I82 C86 N87 F90 E91 G92 Q97 P98

R99 K100 K101

4.2.16 Score per residue for model 16

- Molecule 1: Placental calcium-binding protein

Chain A: 53% 35% 6% 6%

M1 K7 A8 L9 D10 V11 T15 F16 Y19 S20 G21 K22 F27 K28 L29 N30 K31 S32 E33 L34 L37 L38 P43 S44 F45 L46 G47 K48 D51 E52 A53 A54 F55 Q56 K57 S60 D63 E69 V70 D71 F72 Q73 E74 Y75 C76 C81 I82 A83 M84

M85 C86 N87 E88 Q97 P98 R99 K100 K101

- Molecule 1: Placental calcium-binding protein

Chain B: 53% 35% 6% 6%

M1 K7 A8 L9 D10 V11 T15 F16 Y19 S20 G21 K22 F27 K28 L29 N30 K31 S32 E33 L34 L37 L38 P43 S44 F45 L46 G47 K48 D51 E52 A53 A54 F55 Q56 K57 S60 D63 E69 V70 D71 F72 Q73 E74 Y75 C76 C81 I82 A83 M84

M85 C86 N87 E88 Q97 P98 R99 K100 K101

4.2.17 Score per residue for model 17

- Molecule 1: Placental calcium-binding protein

Chain A: 51% 42% • 6%

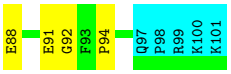
M1 A2 C3 P4 L5 A8 L9 T15 Y19 S20 G21 K22 D25 K26 L29 N30 K31 S32 E33 L34 L37 L38 T39 R40 E41 L42 P43 S44 F45 L46 G47 K48 Q56 M59 S60 N61 L62 D63 S64 N65 R66 D67 N68 E69 V70 E74 L79 I82

C86 N87 E88 E91 G92 F93 P94 D95 K96 Q97 P98 R99 K100 K101

- Molecule 1: Placental calcium-binding protein

Chain B: 54% 39% • 6%

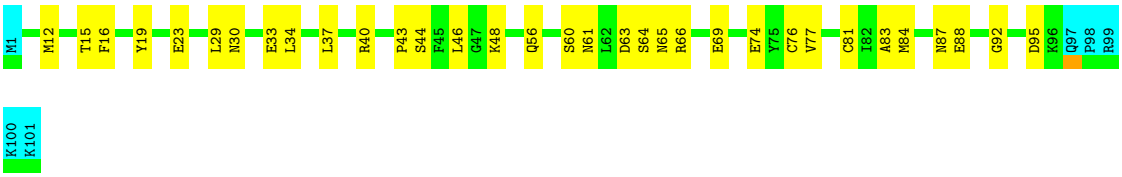
M1 A2 C3 P4 L5 A8 L9 T15 Y19 S20 G21 K22 D25 K26 F27 K28 L29 N30 E33 L34 L37 L38 T39 R40 P43 S44 F45 L46 G47 K48 Q56 S60 N61 L62 D63 S64 N65 R66 D67 N68 E69 V70 E74 L79 I82 C86 N87



4.2.18 Score per residue for model 18

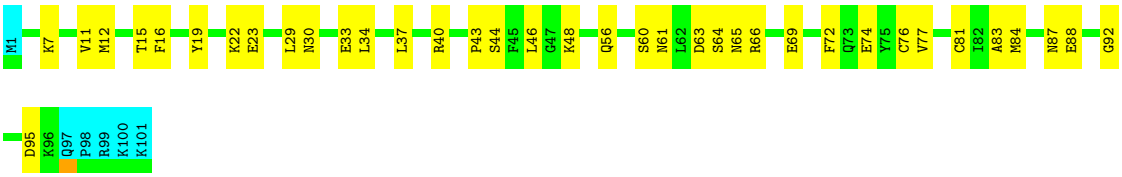
• Molecule 1: Placental calcium-binding protein

Chain A:



• Molecule 1: Placental calcium-binding protein

Chain B:



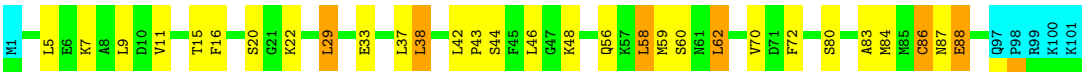
4.2.19 Score per residue for model 19

• Molecule 1: Placental calcium-binding protein

Chain A:

• Molecule 1: Placental calcium-binding protein

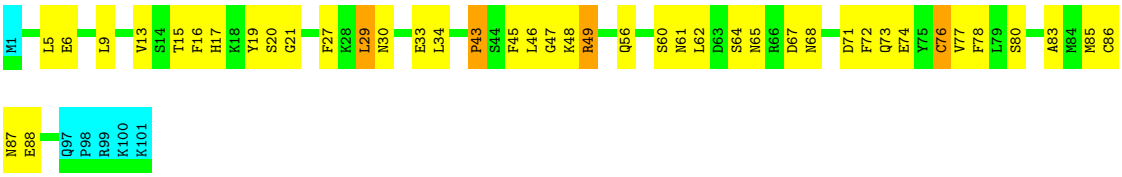
Chain B:



4.2.20 Score per residue for model 20

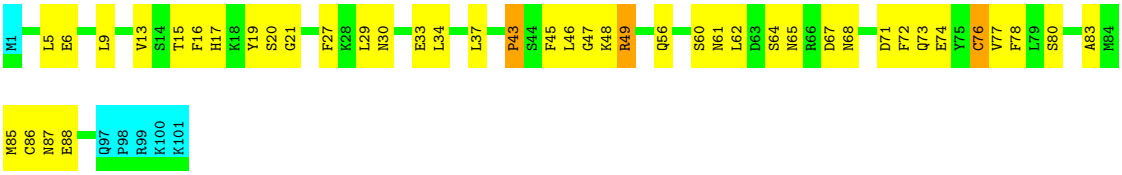
• Molecule 1: Placental calcium-binding protein

Chain A:



• Molecule 1: Placental calcium-binding protein

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Distance Geometry, Simulated Annealing.*

Of the 75 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

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	765	748	747	34±4
1	B	765	748	747	34±4
All	All	30600	29920	29880	1299

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ASN:ND2	1:B:13:VAL:HG21	0.75	1.97	15	1
1:A:62:LEU:HD12	1:A:62:LEU:O	0.72	1.84	14	4
1:A:13:VAL:HG21	1:B:87:ASN:ND2	0.69	2.02	15	1
1:B:62:LEU:HD12	1:B:62:LEU:O	0.68	1.87	14	4
1:A:38:LEU:C	1:A:38:LEU:HD13	0.67	2.10	1	3
1:B:38:LEU:HD13	1:B:38:LEU:C	0.66	2.11	1	3
1:B:37:LEU:HD23	1:B:37:LEU:O	0.66	1.90	10	2
1:A:9:LEU:C	1:A:9:LEU:HD13	0.66	2.11	4	2
1:B:9:LEU:C	1:B:9:LEU:HD13	0.65	2.11	4	2
1:B:31:LYS:NZ	1:B:78:PHE:CZ	0.64	2.66	5	1
1:A:37:LEU:HD23	1:A:37:LEU:O	0.63	1.93	10	2
1:A:87:ASN:HD22	1:A:87:ASN:H	0.63	1.34	14	1
1:B:38:LEU:HD11	1:B:46:LEU:CD1	0.62	2.24	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:87:ASN:HD22	1:B:87:ASN:H	0.62	1.34	14	1
1:B:19:TYR:CZ	1:B:40:ARG:NE	0.62	2.67	18	1
1:A:38:LEU:HD11	1:A:46:LEU:CD1	0.62	2.25	13	1
1:A:34:LEU:HD13	1:A:34:LEU:C	0.62	2.15	3	9
1:A:19:TYR:CZ	1:A:40:ARG:NE	0.62	2.67	18	1
1:B:83:ALA:O	1:B:87:ASN:N	0.61	2.33	11	18
1:B:87:ASN:HD22	1:B:87:ASN:N	0.61	1.94	14	1
1:A:83:ALA:O	1:A:87:ASN:N	0.61	2.33	11	18
1:A:58:LEU:C	1:A:58:LEU:HD12	0.61	2.16	19	1
1:B:56:GLN:O	1:B:60:SER:N	0.60	2.34	14	20
1:B:34:LEU:C	1:B:34:LEU:HD13	0.60	2.16	3	9
1:B:87:ASN:ND2	1:B:87:ASN:H	0.60	1.94	1	2
1:A:31:LYS:NZ	1:A:78:PHE:CZ	0.60	2.68	5	1
1:A:55:PHE:CE2	1:A:59:MET:SD	0.60	2.95	3	1
1:A:41:GLU:C	1:A:42:LEU:HD22	0.60	2.16	15	1
1:A:56:GLN:O	1:A:60:SER:N	0.60	2.35	2	20
1:B:41:GLU:C	1:B:42:LEU:HD22	0.60	2.16	15	1
1:A:22:LYS:NZ	1:A:40:ARG:NH1	0.60	2.50	17	2
1:A:87:ASN:ND2	1:A:87:ASN:H	0.59	1.96	1	2
1:B:55:PHE:CE2	1:B:59:MET:SD	0.59	2.95	3	1
1:A:87:ASN:HD22	1:A:87:ASN:N	0.59	1.94	14	1
1:B:58:LEU:C	1:B:58:LEU:HD12	0.59	2.17	19	1
1:A:29:LEU:O	1:A:70:VAL:HG23	0.59	1.97	9	2
1:A:44:SER:O	1:A:46:LEU:N	0.59	2.36	13	11
1:B:22:LYS:NZ	1:B:40:ARG:NH1	0.58	2.50	17	2
1:B:44:SER:O	1:B:46:LEU:N	0.58	2.36	13	11
1:A:52:GLU:O	1:A:54:ALA:N	0.58	2.37	11	4
1:A:38:LEU:O	1:A:42:LEU:N	0.57	2.37	10	10
1:B:38:LEU:O	1:B:42:LEU:N	0.57	2.37	10	10
1:A:87:ASN:ND2	1:B:72:PHE:CD1	0.57	2.71	9	1
1:A:30:ASN:O	1:A:33:GLU:N	0.57	2.38	11	15
1:A:12:MET:SD	1:B:12:MET:SD	0.56	3.03	3	4
1:B:52:GLU:O	1:B:54:ALA:N	0.56	2.37	11	4
1:A:79:LEU:HD21	1:B:9:LEU:HD21	0.56	1.75	10	1
1:B:30:ASN:O	1:B:33:GLU:N	0.56	2.38	11	16
1:B:46:LEU:C	1:B:48:LYS:H	0.56	2.04	4	19
1:B:76:CYS:SG	1:B:77:VAL:N	0.56	2.78	20	6
1:B:29:LEU:O	1:B:70:VAL:HG23	0.56	1.99	9	2
1:A:72:PHE:CE2	1:B:83:ALA:CB	0.56	2.88	19	3
1:A:62:LEU:HD12	1:A:62:LEU:C	0.55	2.21	9	3
1:A:22:LYS:NZ	1:A:40:ARG:HH12	0.55	2.00	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:19:TYR:CE1	1:B:40:ARG:NE	0.55	2.73	18	1
1:B:52:GLU:O	1:B:55:PHE:N	0.55	2.39	5	2
1:A:76:CYS:SG	1:A:77:VAL:N	0.55	2.80	20	6
1:A:19:TYR:CE1	1:A:40:ARG:NE	0.55	2.74	18	1
1:A:62:LEU:HD12	1:A:62:LEU:N	0.55	2.17	2	1
1:A:62:LEU:CD1	1:A:62:LEU:N	0.55	2.70	13	3
1:B:44:SER:O	1:B:48:LYS:N	0.55	2.40	12	12
1:B:62:LEU:HD12	1:B:62:LEU:N	0.55	2.17	2	1
1:A:8:ALA:HB1	1:B:8:ALA:HB1	0.55	1.77	3	3
1:B:62:LEU:CD1	1:B:62:LEU:N	0.55	2.70	13	3
1:A:33:GLU:O	1:A:37:LEU:N	0.55	2.34	9	19
1:A:44:SER:O	1:A:48:LYS:N	0.55	2.40	12	12
1:B:43:PRO:O	1:B:47:GLY:N	0.55	2.39	11	5
1:B:29:LEU:O	1:B:70:VAL:N	0.55	2.40	17	7
1:A:52:GLU:O	1:A:55:PHE:N	0.55	2.40	5	2
1:B:87:ASN:OD1	1:B:88:GLU:N	0.55	2.40	19	4
1:B:85:MET:SD	1:B:86:CYS:SG	0.55	3.05	12	1
1:A:46:LEU:C	1:A:48:LYS:H	0.54	2.04	4	19
1:A:22:LYS:HZ2	1:A:40:ARG:NH1	0.54	2.00	17	1
1:B:21:GLY:C	1:B:23:GLU:H	0.54	2.06	13	4
1:A:64:SER:O	1:A:65:ASN:C	0.54	2.45	7	1
1:A:85:MET:SD	1:A:86:CYS:SG	0.54	3.05	12	1
1:A:30:ASN:OD1	1:A:30:ASN:N	0.54	2.40	13	1
1:B:30:ASN:OD1	1:B:30:ASN:N	0.54	2.40	13	1
1:A:29:LEU:O	1:A:70:VAL:N	0.54	2.40	17	7
1:A:71:ASP:OD1	1:A:72:PHE:N	0.54	2.41	4	7
1:A:47:GLY:O	1:A:49:ARG:N	0.54	2.41	7	8
1:B:36:GLU:OE2	1:B:40:ARG:NH2	0.54	2.41	13	2
1:A:6:GLU:OE2	1:B:45:PHE:CD2	0.54	2.61	1	3
1:B:64:SER:O	1:B:65:ASN:C	0.54	2.45	7	1
1:B:22:LYS:NZ	1:B:40:ARG:HH12	0.54	1.99	12	1
1:A:45:PHE:CG	1:B:6:GLU:OE2	0.54	2.61	14	1
1:A:21:GLY:C	1:A:23:GLU:H	0.54	2.06	13	4
1:A:80:SER:O	1:A:84:MET:SD	0.54	2.66	10	2
1:B:33:GLU:O	1:B:37:LEU:N	0.54	2.34	9	20
1:B:47:GLY:O	1:B:49:ARG:N	0.54	2.41	7	8
1:A:62:LEU:N	1:A:62:LEU:CD1	0.54	2.71	2	1
1:B:71:ASP:OD1	1:B:72:PHE:N	0.53	2.41	4	7
1:B:80:SER:O	1:B:84:MET:SD	0.53	2.66	10	2
1:B:7:LYS:O	1:B:11:VAL:N	0.53	2.40	1	14
1:A:19:TYR:OH	1:A:40:ARG:NE	0.53	2.38	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ASN:OD1	1:A:88:GLU:N	0.53	2.41	19	3
1:A:62:LEU:O	1:A:68:ASN:ND2	0.53	2.42	7	1
1:B:27:PHE:CD2	1:B:27:PHE:O	0.53	2.62	16	3
1:A:43:PRO:O	1:A:47:GLY:N	0.53	2.39	11	4
1:B:62:LEU:N	1:B:62:LEU:HD12	0.53	2.18	13	3
1:B:91:GLU:OE1	1:B:91:GLU:N	0.53	2.41	14	1
1:A:83:ALA:CB	1:B:72:PHE:CE2	0.53	2.92	19	4
1:A:46:LEU:HD12	1:A:47:GLY:H	0.53	1.63	15	1
1:B:62:LEU:O	1:B:68:ASN:ND2	0.53	2.42	7	1
1:A:19:TYR:CE1	1:A:37:LEU:CD1	0.53	2.92	11	1
1:A:62:LEU:N	1:A:62:LEU:HD12	0.53	2.17	13	3
1:B:19:TYR:OH	1:B:40:ARG:NE	0.53	2.39	18	1
1:A:27:PHE:CD2	1:A:27:PHE:O	0.53	2.61	7	4
1:A:36:GLU:OE2	1:A:40:ARG:NH2	0.53	2.41	13	2
1:A:59:MET:O	1:A:62:LEU:N	0.53	2.41	5	2
1:A:7:LYS:O	1:A:11:VAL:N	0.53	2.40	1	13
1:B:62:LEU:N	1:B:62:LEU:CD1	0.53	2.71	2	1
1:B:59:MET:O	1:B:62:LEU:N	0.53	2.41	5	2
1:A:91:GLU:N	1:A:91:GLU:OE1	0.53	2.41	14	1
1:B:46:LEU:HD12	1:B:47:GLY:H	0.53	1.64	15	1
1:A:45:PHE:CD2	1:B:6:GLU:OE2	0.52	2.62	1	4
1:B:62:LEU:HD12	1:B:62:LEU:C	0.52	2.23	9	3
1:B:34:LEU:HD13	1:B:34:LEU:O	0.52	2.04	17	7
1:A:83:ALA:CB	1:B:72:PHE:CE1	0.52	2.92	8	2
1:B:44:SER:C	1:B:46:LEU:H	0.52	2.07	16	10
1:A:19:TYR:O	1:A:21:GLY:N	0.52	2.42	4	10
1:B:93:PHE:O	1:B:95:ASP:N	0.52	2.41	13	1
1:A:19:TYR:CE1	1:A:40:ARG:CZ	0.52	2.92	18	1
1:A:81:CYS:SG	1:A:82:ILE:N	0.52	2.83	4	5
1:A:45:PHE:O	1:A:45:PHE:CD2	0.52	2.62	8	1
1:A:44:SER:C	1:A:46:LEU:H	0.52	2.07	16	11
1:B:19:TYR:CE1	1:B:37:LEU:CD1	0.52	2.92	11	1
1:B:45:PHE:CD1	1:B:45:PHE:O	0.52	2.62	8	3
1:B:19:TYR:CE1	1:B:40:ARG:CZ	0.52	2.91	18	1
1:B:88:GLU:H	1:B:88:GLU:CD	0.52	2.08	6	1
1:B:19:TYR:O	1:B:21:GLY:N	0.52	2.43	4	10
1:B:50:THR:OG1	1:B:51:ASP:N	0.52	2.42	9	2
1:A:45:PHE:CD1	1:B:6:GLU:OE2	0.52	2.63	4	1
1:B:22:LYS:NZ	1:B:33:GLU:OE1	0.52	2.41	19	3
1:B:61:ASN:O	1:B:64:SER:N	0.51	2.39	3	10
1:B:81:CYS:SG	1:B:82:ILE:N	0.51	2.83	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:CD1	1:A:78:PHE:CG	0.51	2.94	12	1
1:B:88:GLU:N	1:B:88:GLU:OE1	0.51	2.43	9	2
1:A:74:GLU:OE1	1:A:74:GLU:N	0.51	2.44	4	1
1:B:34:LEU:CD1	1:B:78:PHE:CG	0.51	2.93	12	1
1:A:73:GLN:O	1:A:76:CYS:SG	0.51	2.69	20	1
1:A:85:MET:O	1:A:86:CYS:SG	0.51	2.69	1	5
1:A:50:THR:OG1	1:A:51:ASP:N	0.51	2.43	9	2
1:A:6:GLU:OE2	1:B:45:PHE:CG	0.51	2.64	14	1
1:B:85:MET:O	1:B:86:CYS:SG	0.51	2.68	20	5
1:B:91:GLU:OE2	1:B:92:GLY:N	0.51	2.43	5	1
1:A:72:PHE:CD1	1:B:87:ASN:ND2	0.51	2.78	9	1
1:A:22:LYS:NZ	1:A:33:GLU:OE1	0.51	2.41	19	2
1:A:42:LEU:O	1:A:46:LEU:HD11	0.51	2.05	15	1
1:B:19:TYR:C	1:B:21:GLY:N	0.51	2.64	4	13
1:A:6:GLU:OE2	1:B:45:PHE:CD1	0.51	2.64	4	1
1:B:27:PHE:CD1	1:B:27:PHE:O	0.51	2.64	12	2
1:A:22:LYS:NZ	1:A:33:GLU:OE2	0.51	2.44	3	1
1:B:5:LEU:O	1:B:9:LEU:N	0.51	2.39	20	8
1:A:91:GLU:OE2	1:A:92:GLY:N	0.51	2.44	5	1
1:B:75:TYR:CE2	1:B:79:LEU:HD11	0.51	2.41	7	1
1:B:38:LEU:HD21	1:B:82:ILE:HD11	0.51	1.81	11	1
1:A:93:PHE:O	1:A:95:ASP:N	0.51	2.41	13	1
1:A:61:ASN:O	1:A:64:SER:N	0.51	2.40	10	7
1:A:88:GLU:H	1:A:88:GLU:CD	0.50	2.08	6	1
1:B:42:LEU:HD22	1:B:42:LEU:N	0.50	2.21	15	1
1:A:23:GLU:OE1	1:A:30:ASN:ND2	0.50	2.45	18	1
1:A:87:ASN:O	1:A:88:GLU:CB	0.50	2.59	18	1
1:B:90:PHE:CD1	1:B:90:PHE:O	0.50	2.65	4	1
1:B:83:ALA:HB1	1:B:87:ASN:ND2	0.50	2.21	7	1
1:B:22:LYS:NZ	1:B:33:GLU:OE2	0.50	2.44	3	1
1:A:76:CYS:SG	1:B:76:CYS:SG	0.50	3.09	6	2
1:A:88:GLU:OE1	1:A:88:GLU:N	0.50	2.43	9	1
1:A:27:PHE:O	1:A:27:PHE:CD1	0.50	2.64	12	1
1:A:19:TYR:C	1:A:21:GLY:N	0.50	2.64	4	13
1:A:41:GLU:O	1:B:3:CYS:SG	0.50	2.69	5	3
1:A:83:ALA:HB1	1:A:87:ASN:ND2	0.50	2.22	7	1
1:B:16:PHE:CE2	1:B:29:LEU:HD11	0.50	2.42	7	2
1:A:42:LEU:HD22	1:A:42:LEU:N	0.50	2.21	15	1
1:B:87:ASN:O	1:B:88:GLU:CB	0.50	2.60	18	1
1:A:3:CYS:SG	1:B:41:GLU:O	0.50	2.70	15	3
1:A:47:GLY:C	1:A:49:ARG:H	0.50	2.09	8	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:PHE:O	1:A:90:PHE:CD1	0.50	2.64	4	1
1:B:47:GLY:C	1:B:49:ARG:H	0.50	2.09	8	7
1:B:87:ASN:ND2	1:B:88:GLU:H	0.50	2.05	14	1
1:A:34:LEU:HD13	1:A:34:LEU:O	0.50	2.06	17	6
1:A:3:CYS:O	1:A:5:LEU:N	0.50	2.45	17	2
1:B:3:CYS:O	1:B:5:LEU:N	0.50	2.45	17	2
1:B:23:GLU:OE1	1:B:30:ASN:ND2	0.49	2.45	18	1
1:B:74:GLU:N	1:B:74:GLU:OE1	0.49	2.44	4	1
1:A:86:CYS:SG	1:A:86:CYS:O	0.49	2.70	17	2
1:B:22:LYS:HZ1	1:B:40:ARG:NH1	0.49	2.06	17	2
1:A:5:LEU:O	1:A:9:LEU:N	0.49	2.40	20	6
1:B:86:CYS:SG	1:B:86:CYS:O	0.49	2.70	17	3
1:A:47:GLY:C	1:A:49:ARG:N	0.49	2.66	15	8
1:A:48:LYS:O	1:A:49:ARG:CB	0.49	2.61	20	4
1:B:46:LEU:HD12	1:B:47:GLY:N	0.49	2.23	15	1
1:B:73:GLN:O	1:B:76:CYS:SG	0.49	2.67	20	1
1:B:48:LYS:O	1:B:49:ARG:CB	0.49	2.61	20	4
1:A:9:LEU:HD21	1:B:79:LEU:HD21	0.49	1.82	10	1
1:A:3:CYS:O	1:A:3:CYS:SG	0.49	2.71	6	1
1:B:47:GLY:C	1:B:49:ARG:N	0.49	2.66	6	9
1:A:16:PHE:CE2	1:A:29:LEU:HD11	0.49	2.43	7	2
1:A:38:LEU:HD21	1:A:82:ILE:HD11	0.49	1.83	11	1
1:A:68:ASN:N	1:A:68:ASN:OD1	0.49	2.46	3	1
1:B:42:LEU:O	1:B:46:LEU:HD11	0.49	2.08	15	1
1:A:34:LEU:O	1:A:38:LEU:CB	0.49	2.61	13	4
1:A:71:ASP:OD1	1:A:74:GLU:N	0.48	2.42	12	1
1:B:21:GLY:O	1:B:23:GLU:N	0.48	2.46	2	3
1:A:21:GLY:O	1:A:23:GLU:N	0.48	2.46	2	3
1:A:3:CYS:N	1:A:4:PRO:CD	0.48	2.75	3	1
1:B:34:LEU:O	1:B:38:LEU:CB	0.48	2.61	13	3
1:A:46:LEU:HD12	1:A:47:GLY:N	0.48	2.24	15	1
1:A:61:ASN:O	1:A:64:SER:CB	0.48	2.62	18	13
1:B:93:PHE:CD1	1:B:93:PHE:N	0.48	2.82	13	2
1:A:52:GLU:O	1:A:53:ALA:C	0.48	2.52	5	2
1:B:51:ASP:O	1:B:52:GLU:C	0.48	2.52	16	1
1:B:61:ASN:O	1:B:64:SER:CB	0.48	2.62	3	13
1:A:21:GLY:O	1:A:24:GLY:O	0.48	2.31	14	1
1:A:87:ASN:CG	1:B:13:VAL:HG21	0.48	2.29	15	1
1:B:44:SER:C	1:B:46:LEU:N	0.48	2.67	2	14
1:A:87:ASN:ND2	1:A:88:GLU:H	0.48	2.07	14	1
1:A:51:ASP:O	1:A:52:GLU:C	0.48	2.52	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLU:O	1:A:37:LEU:CB	0.48	2.62	11	11
1:B:68:ASN:OD1	1:B:69:GLU:N	0.48	2.45	1	1
1:B:33:GLU:O	1:B:37:LEU:CB	0.48	2.62	11	9
1:B:38:LEU:C	1:B:38:LEU:CD1	0.48	2.82	1	3
1:B:52:GLU:O	1:B:53:ALA:C	0.48	2.52	5	2
1:A:44:SER:C	1:A:46:LEU:N	0.47	2.68	13	13
1:B:61:ASN:O	1:B:67:ASP:OD2	0.47	2.32	1	1
1:B:3:CYS:N	1:B:4:PRO:CD	0.47	2.77	3	1
1:A:68:ASN:O	1:A:69:GLU:O	0.47	2.32	6	1
1:A:69:GLU:O	1:A:74:GLU:OE1	0.47	2.32	18	8
1:A:9:LEU:C	1:A:9:LEU:CD1	0.47	2.83	11	3
1:A:75:TYR:CE2	1:A:79:LEU:HD11	0.47	2.44	7	3
1:B:9:LEU:C	1:B:9:LEU:CD1	0.47	2.83	11	2
1:A:37:LEU:O	1:A:41:GLU:OE1	0.47	2.32	5	1
1:A:45:PHE:CD1	1:A:45:PHE:O	0.47	2.68	10	2
1:B:94:PRO:O	1:B:95:ASP:O	0.47	2.32	11	2
1:B:3:CYS:SG	1:B:3:CYS:O	0.47	2.73	6	1
1:A:36:GLU:OE2	1:A:40:ARG:CZ	0.47	2.63	7	1
1:A:38:LEU:C	1:A:38:LEU:CD1	0.47	2.81	1	3
1:B:68:ASN:N	1:B:68:ASN:OD1	0.47	2.46	3	1
1:B:84:MET:SD	1:B:95:ASP:O	0.47	2.73	3	2
1:B:36:GLU:OE2	1:B:40:ARG:CZ	0.47	2.62	7	1
1:A:45:PHE:CD2	1:A:45:PHE:O	0.47	2.68	1	1
1:A:93:PHE:CD1	1:A:93:PHE:N	0.47	2.82	13	2
1:B:21:GLY:O	1:B:24:GLY:O	0.47	2.31	14	1
1:A:16:PHE:CZ	1:A:29:LEU:HD13	0.47	2.45	3	2
1:B:37:LEU:O	1:B:41:GLU:OE1	0.47	2.32	5	1
1:B:68:ASN:O	1:B:69:GLU:O	0.47	2.32	6	1
1:A:88:GLU:CG	1:A:91:GLU:O	0.47	2.63	17	1
1:B:87:ASN:ND2	1:B:87:ASN:N	0.47	2.63	1	1
1:B:69:GLU:O	1:B:74:GLU:OE1	0.47	2.32	18	8
1:A:61:ASN:O	1:A:67:ASP:OD2	0.47	2.33	1	1
1:A:19:TYR:C	1:A:21:GLY:H	0.47	2.13	6	11
1:A:68:ASN:OD1	1:A:69:GLU:N	0.46	2.47	1	1
1:A:44:SER:O	1:A:48:LYS:CA	0.46	2.63	12	8
1:A:84:MET:SD	1:A:95:ASP:O	0.46	2.73	3	2
1:B:52:GLU:O	1:B:56:GLN:N	0.46	2.42	9	1
1:A:94:PRO:O	1:A:95:ASP:O	0.46	2.32	11	2
1:B:88:GLU:CG	1:B:91:GLU:O	0.46	2.63	17	1
1:B:85:MET:SD	1:B:85:MET:O	0.46	2.73	2	1
1:B:31:LYS:N	1:B:31:LYS:CD	0.46	2.77	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:TYR:CE2	1:A:37:LEU:CD1	0.46	2.99	14	1
1:A:88:GLU:N	1:A:88:GLU:OE1	0.46	2.46	2	1
1:B:85:MET:SD	1:B:85:MET:C	0.46	2.93	2	1
1:B:87:ASN:N	1:B:87:ASN:ND2	0.46	2.63	14	1
1:B:45:PHE:CD2	1:B:45:PHE:O	0.46	2.68	1	1
1:A:27:PHE:CD1	1:B:88:GLU:OE2	0.46	2.68	3	1
1:B:16:PHE:CZ	1:B:29:LEU:HD13	0.46	2.45	3	2
1:A:19:TYR:CZ	1:A:37:LEU:CD1	0.46	2.99	11	2
1:B:38:LEU:HD21	1:B:82:ILE:CD1	0.46	2.41	11	1
1:B:31:LYS:CE	1:B:67:ASP:O	0.46	2.64	14	1
1:A:90:PHE:CD1	1:A:90:PHE:N	0.46	2.83	15	1
1:B:38:LEU:HD11	1:B:82:ILE:HD13	0.46	1.87	15	1
1:B:90:PHE:N	1:B:90:PHE:CD1	0.46	2.83	15	1
1:A:85:MET:C	1:A:85:MET:SD	0.46	2.94	2	1
1:B:19:TYR:CZ	1:B:37:LEU:HD12	0.46	2.46	11	2
1:B:19:TYR:CE2	1:B:37:LEU:CD1	0.46	2.98	14	1
1:A:83:ALA:O	1:A:87:ASN:ND2	0.46	2.43	1	2
1:B:38:LEU:HD13	1:B:38:LEU:O	0.46	2.10	2	3
1:A:25:ASP:OD1	1:A:26:LYS:N	0.46	2.49	17	2
1:A:31:LYS:N	1:A:31:LYS:CD	0.46	2.78	4	1
1:A:85:MET:SD	1:A:85:MET:O	0.46	2.74	2	1
1:B:91:GLU:C	1:B:93:PHE:H	0.46	2.14	11	1
1:A:91:GLU:C	1:A:93:PHE:H	0.46	2.14	11	1
1:A:15:THR:CG2	1:A:16:PHE:N	0.46	2.79	1	17
1:A:31:LYS:CE	1:A:67:ASP:O	0.46	2.64	14	1
1:A:46:LEU:C	1:A:48:LYS:N	0.45	2.69	4	5
1:B:46:LEU:C	1:B:48:LYS:N	0.45	2.69	4	6
1:B:55:PHE:CZ	1:B:59:MET:SD	0.45	3.09	3	1
1:B:20:SER:O	1:B:23:GLU:O	0.45	2.34	5	2
1:A:38:LEU:HD11	1:A:82:ILE:HD11	0.45	1.88	17	1
1:B:91:GLU:O	1:B:92:GLY:O	0.45	2.34	6	1
1:B:15:THR:CG2	1:B:16:PHE:N	0.45	2.80	1	17
1:B:54:ALA:O	1:B:57:LYS:N	0.45	2.50	3	2
1:B:16:PHE:CZ	1:B:29:LEU:HD23	0.45	2.47	1	1
1:B:44:SER:O	1:B:48:LYS:CA	0.45	2.64	12	8
1:A:20:SER:O	1:A:23:GLU:O	0.45	2.35	5	2
1:B:19:TYR:CZ	1:B:37:LEU:CD1	0.45	2.99	11	3
1:A:58:LEU:HD13	1:A:81:CYS:SG	0.45	2.52	11	1
1:B:22:LYS:H	1:B:22:LYS:CD	0.45	2.25	16	1
1:B:88:GLU:OE2	1:B:91:GLU:O	0.45	2.35	17	1
1:B:25:ASP:OD1	1:B:26:LYS:N	0.45	2.49	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:ASP:O	1:B:68:ASN:ND2	0.45	2.49	7	2
1:B:38:LEU:HD11	1:B:82:ILE:HD11	0.45	1.88	17	1
1:A:27:PHE:CE1	1:B:88:GLU:OE2	0.45	2.70	3	1
1:B:58:LEU:HD13	1:B:81:CYS:SG	0.45	2.52	11	1
1:A:87:ASN:N	1:A:87:ASN:ND2	0.45	2.64	14	1
1:A:13:VAL:HG21	1:B:87:ASN:CG	0.45	2.32	15	1
1:A:51:ASP:N	1:A:51:ASP:OD1	0.45	2.50	9	2
1:A:38:LEU:O	1:A:42:LEU:O	0.45	2.35	4	2
1:B:65:ASN:O	1:B:66:ARG:O	0.45	2.35	5	1
1:B:19:TYR:C	1:B:21:GLY:H	0.45	2.15	4	12
1:A:93:PHE:O	1:A:94:PRO:O	0.45	2.35	11	2
1:A:38:LEU:HD11	1:A:82:ILE:HD13	0.45	1.87	15	1
1:A:38:LEU:HD13	1:A:38:LEU:O	0.45	2.12	2	2
1:B:38:LEU:O	1:B:42:LEU:O	0.45	2.35	19	2
1:A:72:PHE:CE1	1:B:83:ALA:CB	0.45	2.99	8	1
1:A:9:LEU:HD13	1:A:9:LEU:O	0.45	2.12	11	1
1:A:95:ASP:OD2	1:B:27:PHE:O	0.45	2.35	17	1
1:A:54:ALA:HB1	1:A:85:MET:SD	0.44	2.53	16	1
1:A:87:ASN:OD1	1:A:88:GLU:OE2	0.44	2.35	2	1
1:A:55:PHE:CZ	1:A:59:MET:SD	0.44	3.10	3	1
1:B:51:ASP:O	1:B:53:ALA:N	0.44	2.50	16	2
1:A:91:GLU:O	1:A:92:GLY:O	0.44	2.34	6	1
1:A:19:TYR:CZ	1:A:37:LEU:HD12	0.44	2.47	11	2
1:A:64:SER:O	1:A:65:ASN:CG	0.44	2.55	11	1
1:B:64:SER:O	1:B:65:ASN:CG	0.44	2.55	11	1
1:B:67:ASP:OD1	1:B:68:ASN:N	0.44	2.51	20	1
1:B:59:MET:C	1:B:59:MET:SD	0.44	2.96	7	3
1:A:87:ASN:ND2	1:A:87:ASN:N	0.44	2.66	1	1
1:A:59:MET:SD	1:A:59:MET:C	0.44	2.96	7	4
1:B:93:PHE:O	1:B:94:PRO:O	0.44	2.35	11	2
1:A:51:ASP:O	1:A:53:ALA:N	0.44	2.50	16	2
1:A:41:GLU:C	1:A:42:LEU:HD12	0.44	2.33	8	1
1:B:87:ASN:OD1	1:B:88:GLU:OE2	0.44	2.36	2	1
1:A:67:ASP:OD1	1:A:68:ASN:N	0.44	2.51	20	1
1:B:41:GLU:C	1:B:42:LEU:HD12	0.44	2.33	8	1
1:A:38:LEU:HD21	1:A:82:ILE:CD1	0.44	2.43	11	1
1:B:62:LEU:O	1:B:67:ASP:OD2	0.44	2.36	1	1
1:A:87:ASN:N	1:A:87:ASN:OD1	0.44	2.51	5	1
1:B:9:LEU:HD13	1:B:9:LEU:O	0.44	2.13	11	1
1:B:22:LYS:HZ1	1:B:40:ARG:HH12	0.44	1.56	12	1
1:A:59:MET:O	1:A:62:LEU:CB	0.44	2.66	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:C	1:A:34:LEU:CD1	0.44	2.86	1	4
1:A:54:ALA:O	1:A:57:LYS:N	0.43	2.51	3	2
1:B:57:LYS:O	1:B:61:ASN:N	0.43	2.51	4	1
1:A:67:ASP:O	1:A:68:ASN:ND2	0.43	2.50	7	1
1:B:51:ASP:C	1:B:53:ALA:H	0.43	2.16	7	1
1:B:30:ASN:O	1:B:32:SER:N	0.43	2.51	10	2
1:B:34:LEU:O	1:B:38:LEU:N	0.43	2.48	13	2
1:B:59:MET:O	1:B:62:LEU:CB	0.43	2.66	15	1
1:A:88:GLU:OE2	1:A:91:GLU:O	0.43	2.35	17	1
1:A:65:ASN:O	1:A:66:ARG:O	0.43	2.36	5	1
1:B:87:ASN:N	1:B:87:ASN:OD1	0.43	2.51	5	1
1:B:63:ASP:O	1:B:63:ASP:OD1	0.43	2.37	12	4
1:A:51:ASP:C	1:A:53:ALA:H	0.43	2.16	7	1
1:A:30:ASN:O	1:A:32:SER:N	0.43	2.51	8	2
1:B:3:CYS:O	1:B:6:GLU:OE1	0.43	2.37	9	1
1:B:51:ASP:N	1:B:51:ASP:OD1	0.43	2.50	9	1
1:A:10:ASP:OD1	1:A:14:SER:OG	0.43	2.35	4	1
1:A:29:LEU:O	1:A:70:VAL:CG2	0.43	2.66	9	1
1:B:3:CYS:C	1:B:5:LEU:H	0.43	2.16	17	1
1:A:3:CYS:O	1:A:6:GLU:OE1	0.43	2.37	9	1
1:B:38:LEU:HD11	1:B:82:ILE:CD1	0.43	2.44	10	1
1:B:54:ALA:HB1	1:B:85:MET:SD	0.43	2.54	16	1
1:A:80:SER:OG	1:B:76:CYS:CB	0.43	2.67	20	1
1:B:83:ALA:O	1:B:87:ASN:ND2	0.43	2.44	1	2
1:B:71:ASP:OD1	1:B:74:GLU:N	0.43	2.42	12	1
1:A:62:LEU:O	1:A:67:ASP:OD2	0.43	2.36	1	1
1:B:61:ASN:O	1:B:64:SER:OG	0.43	2.35	5	1
1:A:3:CYS:C	1:A:5:LEU:H	0.43	2.16	17	1
1:B:56:GLN:O	1:B:60:SER:OG	0.43	2.34	19	2
1:A:91:GLU:OE2	1:A:92:GLY:CA	0.43	2.67	5	1
1:B:34:LEU:HD23	1:B:34:LEU:C	0.43	2.34	12	1
1:B:76:CYS:O	1:B:80:SER:N	0.43	2.41	14	1
1:B:29:LEU:O	1:B:69:GLU:OE2	0.43	2.37	16	1
1:A:41:GLU:OE2	1:B:3:CYS:SG	0.43	2.76	17	1
1:A:21:GLY:C	1:A:23:GLU:N	0.43	2.71	13	2
1:B:37:LEU:HD21	1:B:41:GLU:OE1	0.43	2.14	3	1
1:A:13:VAL:HG22	1:A:72:PHE:CE1	0.43	2.49	4	1
1:A:57:LYS:O	1:A:61:ASN:N	0.43	2.51	4	1
1:A:10:ASP:O	1:A:10:ASP:OD1	0.43	2.37	15	1
1:A:88:GLU:OE2	1:A:92:GLY:O	0.43	2.37	17	1
1:A:58:LEU:C	1:A:58:LEU:CD1	0.43	2.85	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:GLU:OE1	1:A:92:GLY:O	0.43	2.37	15	1
1:B:91:GLU:OE2	1:B:92:GLY:CA	0.42	2.67	5	1
1:A:34:LEU:C	1:A:34:LEU:HD23	0.42	2.34	12	1
1:B:10:ASP:O	1:B:10:ASP:OD1	0.42	2.37	15	1
1:B:66:ARG:O	1:B:67:ASP:C	0.42	2.57	17	1
1:B:88:GLU:OE2	1:B:92:GLY:O	0.42	2.38	17	1
1:A:76:CYS:SG	1:B:80:SER:OG	0.42	2.71	20	1
1:B:21:GLY:C	1:B:23:GLU:N	0.42	2.73	2	2
1:B:35:LYS:O	1:B:39:THR:HG23	0.42	2.14	8	1
1:A:62:LEU:C	1:A:62:LEU:CD1	0.42	2.87	9	1
1:B:31:LYS:O	1:B:34:LEU:N	0.42	2.52	10	1
1:B:77:VAL:O	1:B:81:CYS:SG	0.42	2.77	18	1
1:B:58:LEU:C	1:B:58:LEU:CD1	0.42	2.85	19	1
1:A:63:ASP:O	1:A:63:ASP:OD1	0.42	2.37	12	4
1:A:69:GLU:OE1	1:A:71:ASP:OD1	0.42	2.37	6	1
1:B:43:PRO:O	1:B:47:GLY:CA	0.42	2.67	9	2
1:A:22:LYS:H	1:A:22:LYS:CD	0.42	2.26	16	1
1:A:29:LEU:O	1:A:69:GLU:OE2	0.42	2.38	16	1
1:A:66:ARG:O	1:A:67:ASP:C	0.42	2.56	17	1
1:A:16:PHE:CE2	1:A:29:LEU:HD12	0.42	2.49	20	1
1:B:52:GLU:OE1	1:B:52:GLU:N	0.42	2.43	4	1
1:B:25:ASP:O	1:B:25:ASP:OD1	0.42	2.38	10	1
1:B:88:GLU:CD	1:B:88:GLU:N	0.42	2.73	6	1
1:A:52:GLU:O	1:A:56:GLN:N	0.42	2.41	14	2
1:A:64:SER:O	1:A:65:ASN:O	0.42	2.37	7	1
1:A:43:PRO:O	1:A:47:GLY:CA	0.42	2.68	9	2
1:A:31:LYS:O	1:A:34:LEU:N	0.42	2.52	10	1
1:B:9:LEU:CD1	1:B:9:LEU:C	0.42	2.88	16	1
1:A:58:LEU:HD12	1:A:58:LEU:O	0.42	2.15	19	1
1:A:25:ASP:N	1:A:25:ASP:OD1	0.42	2.53	1	1
1:B:69:GLU:OE1	1:B:71:ASP:OD1	0.42	2.38	6	1
1:A:47:GLY:O	1:A:48:LYS:C	0.42	2.58	16	2
1:A:71:ASP:OD1	1:A:71:ASP:N	0.42	2.52	12	1
1:B:65:ASN:O	1:B:66:ARG:C	0.42	2.58	18	1
1:A:86:CYS:O	1:A:86:CYS:SG	0.42	2.78	5	2
1:A:37:LEU:C	1:A:37:LEU:HD23	0.42	2.34	7	1
1:A:87:ASN:ND2	1:B:72:PHE:CE2	0.42	2.87	10	1
1:B:91:GLU:OE1	1:B:92:GLY:O	0.42	2.37	15	1
1:B:47:GLY:O	1:B:48:LYS:C	0.42	2.58	16	1
1:A:3:CYS:C	1:A:5:LEU:N	0.42	2.73	17	1
1:B:3:CYS:C	1:B:5:LEU:N	0.42	2.74	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:GLN:O	1:B:77:VAL:HG23	0.41	2.15	1	1
1:A:61:ASN:O	1:A:64:SER:OG	0.41	2.34	5	1
1:A:25:ASP:O	1:A:25:ASP:OD1	0.41	2.38	10	1
1:A:34:LEU:O	1:A:38:LEU:N	0.41	2.50	12	2
1:B:16:PHE:O	1:B:20:SER:OG	0.41	2.38	3	1
1:A:52:GLU:OE1	1:A:52:GLU:N	0.41	2.42	4	1
1:A:88:GLU:CD	1:A:88:GLU:N	0.41	2.72	6	1
1:B:64:SER:O	1:B:65:ASN:O	0.41	2.37	7	1
1:A:30:ASN:C	1:A:32:SER:N	0.41	2.72	10	1
1:A:38:LEU:HD11	1:A:82:ILE:CD1	0.41	2.45	10	1
1:B:30:ASN:O	1:B:31:LYS:C	0.41	2.58	16	2
1:A:61:ASN:ND2	1:A:78:PHE:CE1	0.41	2.89	20	1
1:B:37:LEU:C	1:B:37:LEU:HD23	0.41	2.34	7	1
1:A:65:ASN:O	1:A:66:ARG:C	0.41	2.58	18	1
1:A:76:CYS:CB	1:B:80:SER:OG	0.41	2.69	20	1
1:A:30:ASN:O	1:A:31:LYS:C	0.41	2.58	8	3
1:B:10:ASP:OD1	1:B:14:SER:OG	0.41	2.36	8	1
1:B:95:ASP:OD1	1:B:96:LYS:N	0.41	2.53	11	1
1:B:25:ASP:OD2	1:B:28:LYS:NZ	0.41	2.44	12	1
1:A:37:LEU:HD21	1:A:41:GLU:OE1	0.41	2.15	3	1
1:A:72:PHE:CE1	1:B:87:ASN:ND2	0.41	2.87	10	1
1:B:71:ASP:OD1	1:B:71:ASP:N	0.41	2.52	12	1
1:B:10:ASP:O	1:B:14:SER:N	0.41	2.39	14	1
1:B:13:VAL:CG1	1:B:17:HIS:NE2	0.41	2.84	20	1
1:A:69:GLU:N	1:A:69:GLU:CD	0.41	2.73	15	1
1:B:71:ASP:CB	1:B:74:GLU:OE1	0.41	2.69	20	1
1:B:30:ASN:C	1:B:32:SER:N	0.41	2.72	10	1
1:B:34:LEU:C	1:B:34:LEU:CD1	0.41	2.89	2	2
1:A:28:LYS:NZ	1:A:71:ASP:CG	0.41	2.74	4	1
1:B:31:LYS:O	1:B:62:LEU:CD2	0.41	2.69	6	1
1:B:13:VAL:HG22	1:B:72:PHE:CE1	0.41	2.50	4	1
1:B:38:LEU:N	1:B:38:LEU:CD2	0.41	2.84	4	1
1:A:23:GLU:OE1	1:A:33:GLU:OE2	0.41	2.39	7	1
1:B:25:ASP:OD1	1:B:25:ASP:N	0.41	2.52	13	1
1:A:16:PHE:CZ	1:A:29:LEU:HD23	0.41	2.51	1	1
1:A:55:PHE:CZ	1:A:85:MET:CE	0.41	3.04	4	1
1:A:25:ASP:OD2	1:A:28:LYS:NZ	0.41	2.44	12	1
1:B:69:GLU:CD	1:B:69:GLU:N	0.41	2.74	15	1
1:A:31:LYS:O	1:A:34:LEU:HB3	0.41	2.16	17	1
1:A:6:GLU:OE2	1:A:10:ASP:OD2	0.40	2.39	5	1
1:A:71:ASP:O	1:A:72:PHE:C	0.40	2.59	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:23:GLU:OE1	1:B:33:GLU:OE2	0.40	2.39	7	1
1:A:76:CYS:O	1:A:80:SER:N	0.40	2.41	14	1
1:A:77:VAL:O	1:A:81:CYS:SG	0.40	2.77	18	1
1:A:95:ASP:OD1	1:A:96:LYS:N	0.40	2.53	11	1
1:A:22:LYS:HZ1	1:A:40:ARG:HH12	0.40	1.59	12	1
1:A:13:VAL:CG1	1:A:17:HIS:NE2	0.40	2.84	20	1
1:A:71:ASP:CB	1:A:74:GLU:OE1	0.40	2.69	20	1
1:B:25:ASP:N	1:B:25:ASP:OD1	0.40	2.54	1	1
1:A:38:LEU:N	1:A:38:LEU:CD2	0.40	2.84	4	1
1:B:58:LEU:HD12	1:B:58:LEU:O	0.40	2.15	19	1
1:A:83:ALA:O	1:A:87:ASN:OD1	0.40	2.39	20	1
1:B:61:ASN:ND2	1:B:78:PHE:CE1	0.40	2.90	20	1
1:B:6:GLU:OE2	1:B:10:ASP:OD2	0.40	2.39	5	1
1:A:25:ASP:O	1:A:28:LYS:O	0.40	2.40	9	1
1:B:25:ASP:O	1:B:28:LYS:O	0.40	2.40	9	1
1:A:50:THR:O	1:A:52:GLU:N	0.40	2.49	19	1
1:A:25:ASP:OD1	1:A:25:ASP:N	0.40	2.53	13	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	95/101 (94%)	82±3 (86±4%)	8±3 (9±3%)	5±2 (5±2%)	4 24
1	B	95/101 (94%)	82±3 (86±3%)	9±3 (9±3%)	5±2 (5±2%)	4 24
All	All	3800/4040 (94%)	3266 (86%)	341 (9%)	193 (5%)	4 24

All 48 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	43	PRO	20
1	B	43	PRO	20
1	A	88	GLU	12
1	B	88	GLU	12

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Mol	Chain	Res	Type	Models (Total)
1	A	45	PHE	10
1	B	45	PHE	9
1	A	48	LYS	8
1	B	48	LYS	8
1	A	94	PRO	6
1	B	86	CYS	5
1	B	94	PRO	5
1	A	64	SER	4
1	B	64	SER	4
1	A	53	ALA	4
1	A	65	ASN	4
1	A	86	CYS	4
1	B	53	ALA	4
1	B	65	ASN	4
1	A	49	ARG	3
1	B	49	ARG	3
1	A	50	THR	3
1	B	50	THR	3
1	A	20	SER	2
1	B	20	SER	2
1	A	66	ARG	2
1	B	66	ARG	2
1	A	92	GLY	2
1	B	92	GLY	2
1	A	67	ASP	2
1	B	67	ASP	2
1	A	4	PRO	2
1	A	95	ASP	2
1	B	4	PRO	2
1	B	95	ASP	2
1	A	3	CYS	1
1	B	3	CYS	1
1	A	22	LYS	1
1	A	69	GLU	1
1	B	22	LYS	1
1	B	69	GLU	1
1	A	51	ASP	1
1	B	51	ASP	1
1	A	2	ALA	1
1	B	2	ALA	1
1	A	96	LYS	1
1	B	96	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	52	GLU	1
1	B	52	GLU	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	86/92 (93%)	83±1 (97±1%)	3±1 (3±1%)	41 87
1	B	86/92 (93%)	83±1 (97±1%)	3±1 (3±1%)	41 87
All	All	3440/3680 (93%)	3328 (97%)	112 (3%)	41 87

All 51 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	29	LEU	8
1	B	29	LEU	8
1	A	62	LEU	5
1	A	87	ASN	4
1	B	87	ASN	4
1	A	15	THR	4
1	B	15	THR	4
1	B	62	LEU	4
1	A	20	SER	3
1	A	69	GLU	3
1	B	20	SER	3
1	B	69	GLU	3
1	A	22	LYS	3
1	B	22	LYS	3
1	A	38	LEU	3
1	B	38	LEU	3
1	A	49	ARG	2
1	B	49	ARG	2
1	A	59	MET	2
1	B	59	MET	2
1	A	48	LYS	2
1	B	48	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	39	THR	2
1	A	79	LEU	2
1	B	39	THR	2
1	B	79	LEU	2
1	A	76	CYS	2
1	B	76	CYS	2
1	A	3	CYS	1
1	B	3	CYS	1
1	A	31	LYS	1
1	A	42	LEU	1
1	B	31	LYS	1
1	B	42	LEU	1
1	A	61	ASN	1
1	A	91	GLU	1
1	B	61	ASN	1
1	B	91	GLU	1
1	A	88	GLU	1
1	B	88	GLU	1
1	B	25	ASP	1
1	A	96	LYS	1
1	B	96	LYS	1
1	A	46	LEU	1
1	A	70	VAL	1
1	B	46	LEU	1
1	B	70	VAL	1
1	A	9	LEU	1
1	B	9	LEU	1
1	A	58	LEU	1
1	B	58	LEU	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