Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2KC3
Title	:	NMR solution structure of complete receptor binding domain of human apolipoprotein E
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Deposited on	:	2008-12-15

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

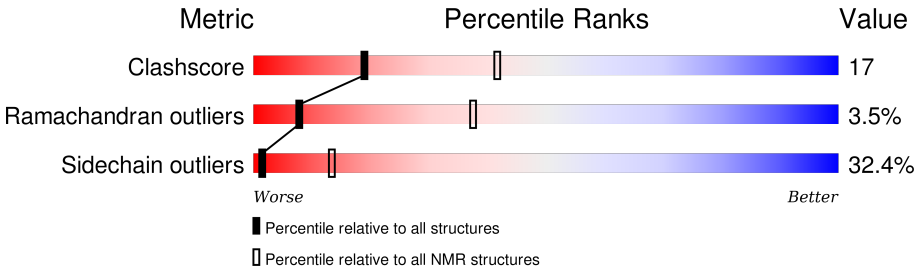
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	184	45% 40% • 10% •

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:18-A:181 (164)	0.52	9

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2981 atoms, of which 1494 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein E.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	183	2981	916	1494	278	288	5	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P02649

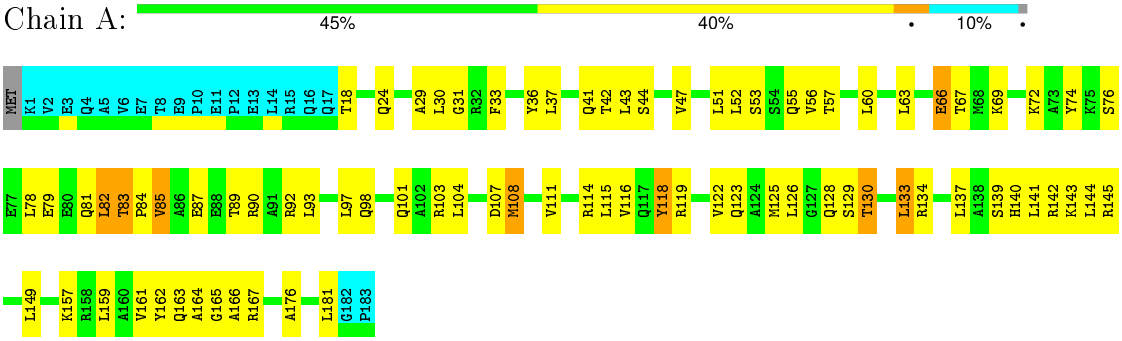
4 Residue-property plots

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: Apolipoprotein E

Chain A:



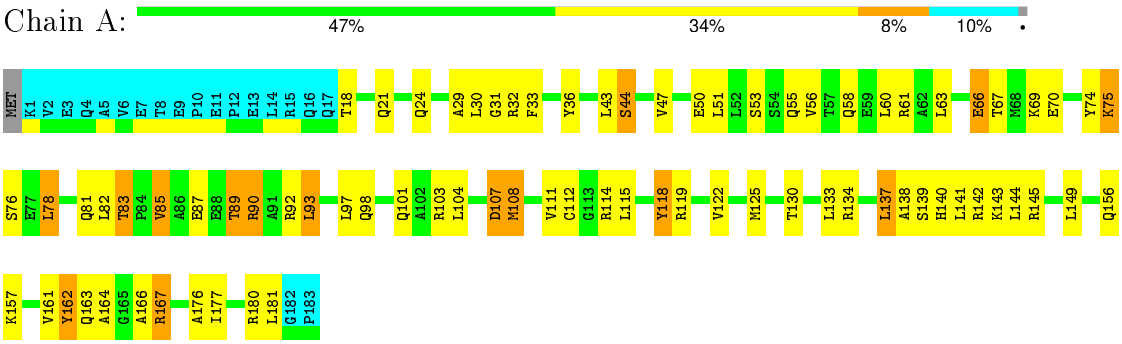
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Apolipoprotein E

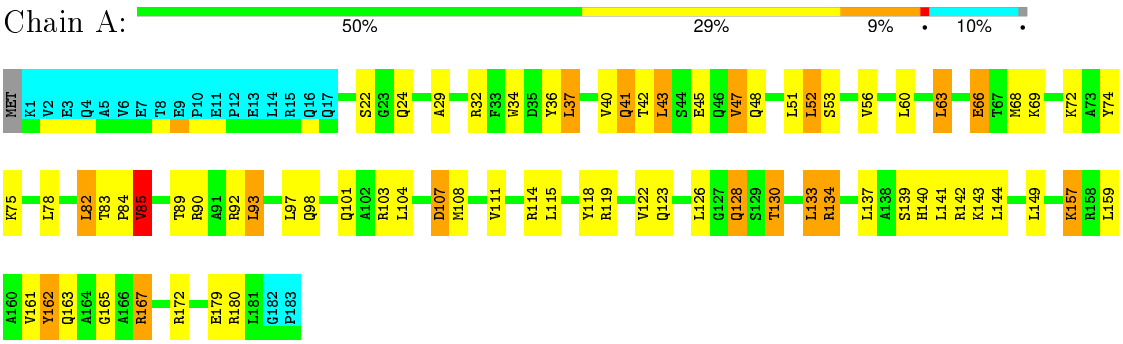
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein E

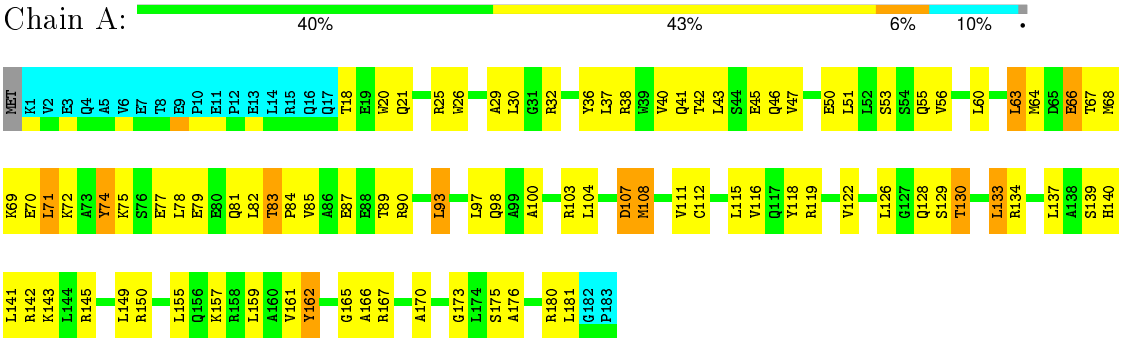
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Apolipoprotein E

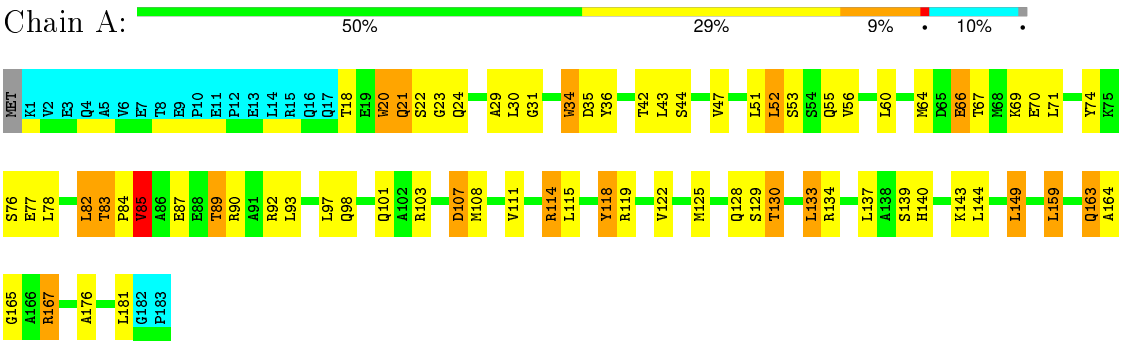
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Apolipoprotein E

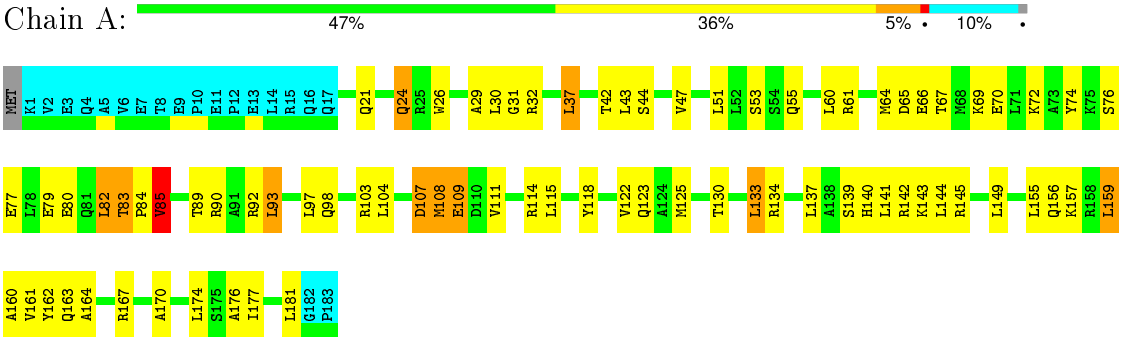
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Apolipoprotein E

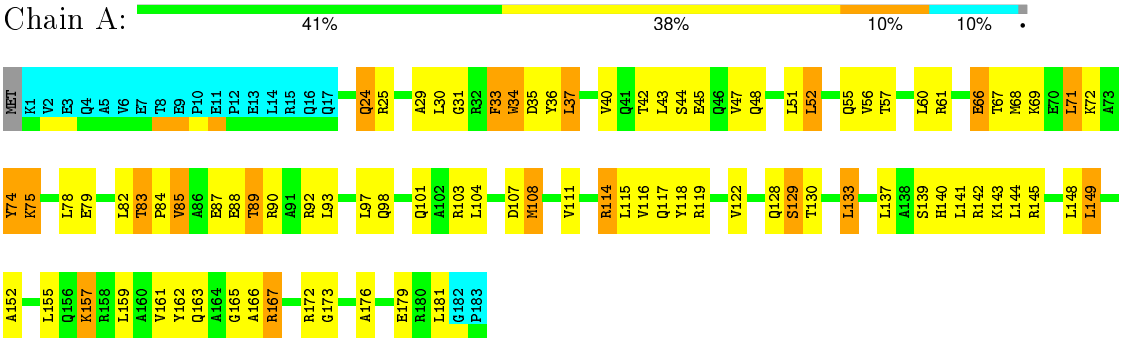
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Apolipoprotein E

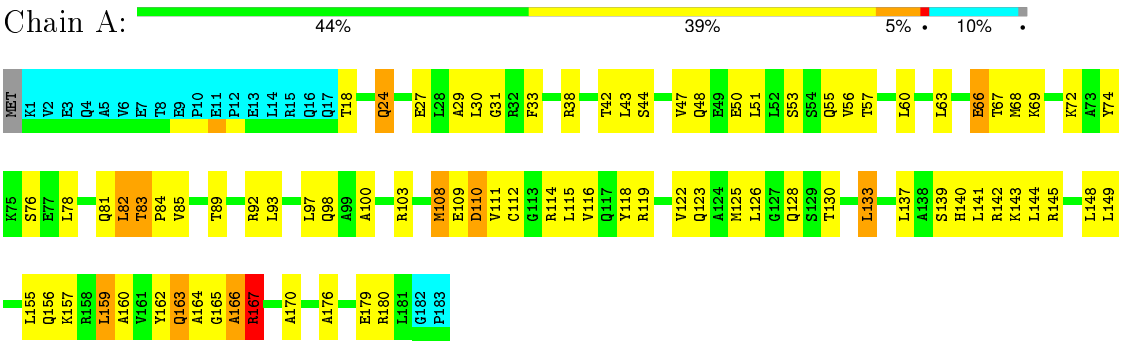
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Apolipoprotein E

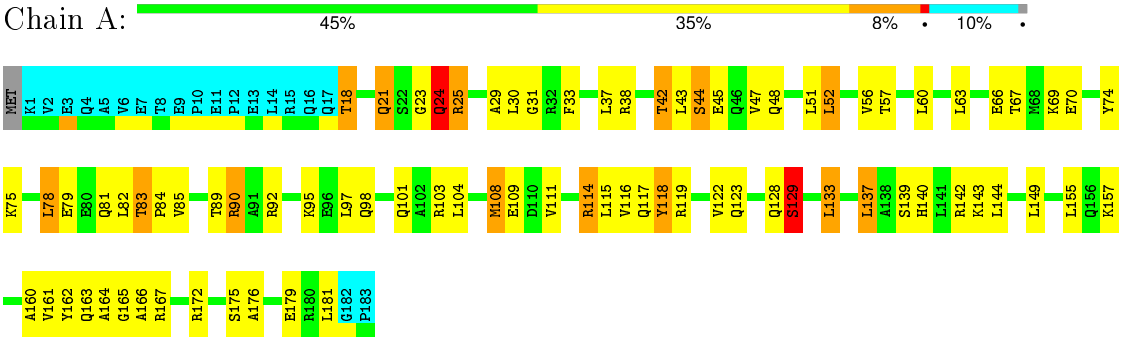
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Apolipoprotein E

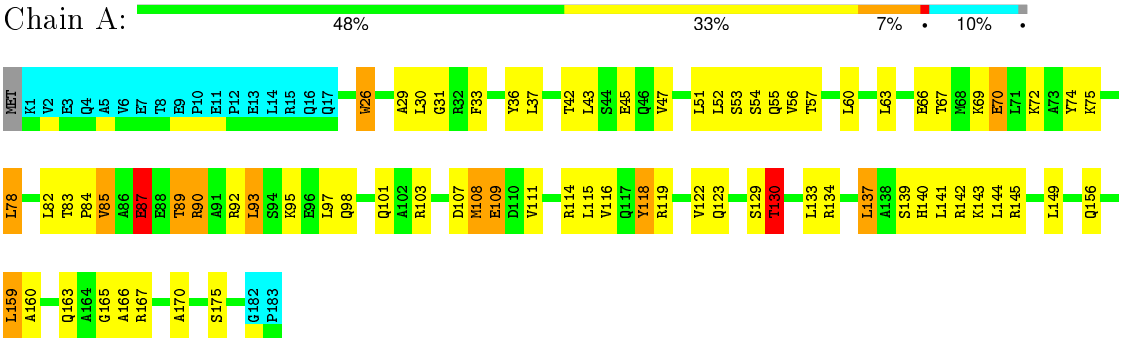
Chain A:



4.2.9 Score per residue for model 9 (medoid)

• Molecule 1: Apolipoprotein E

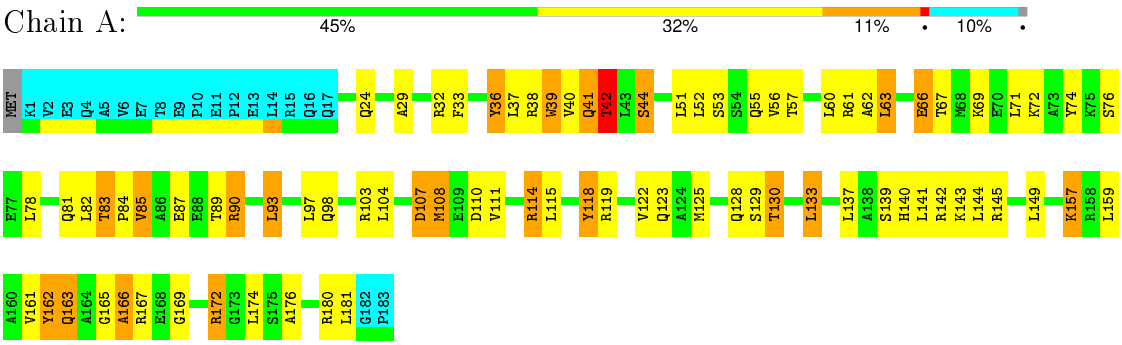
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Apolipoprotein E

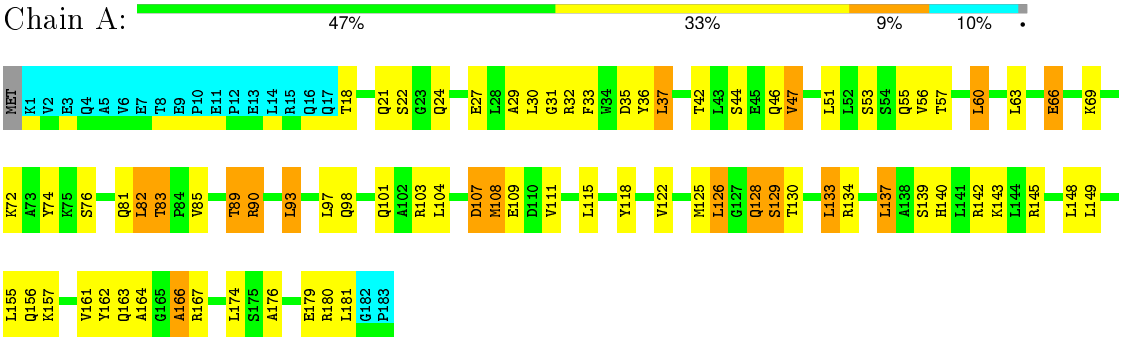
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Apolipoprotein E

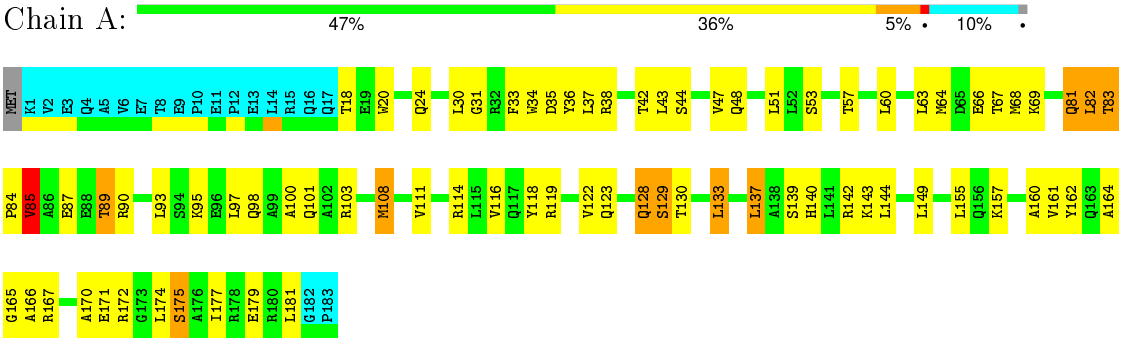
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Apolipoprotein E

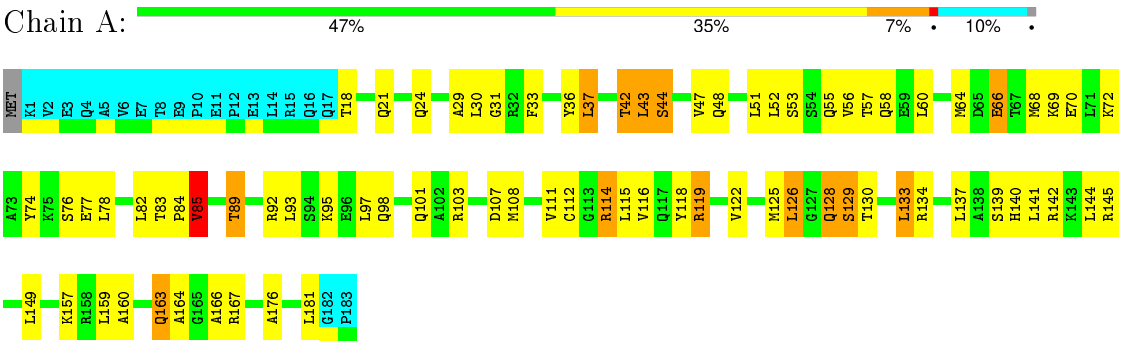
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Apolipoprotein E

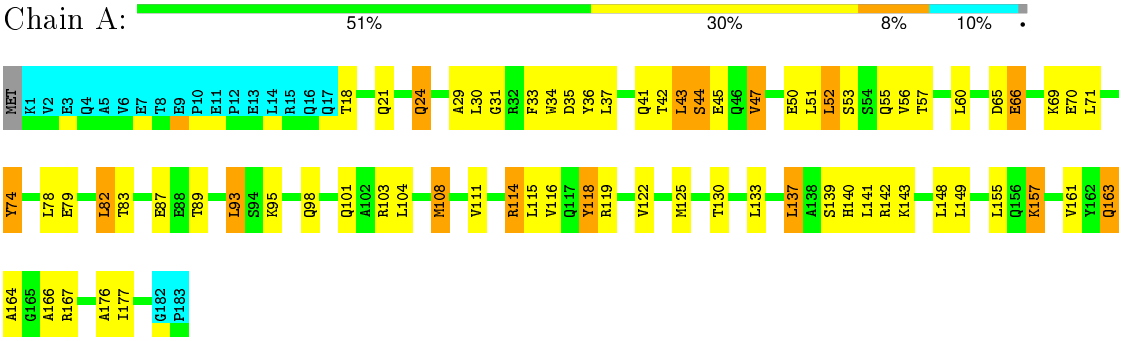
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Apolipoprotein E

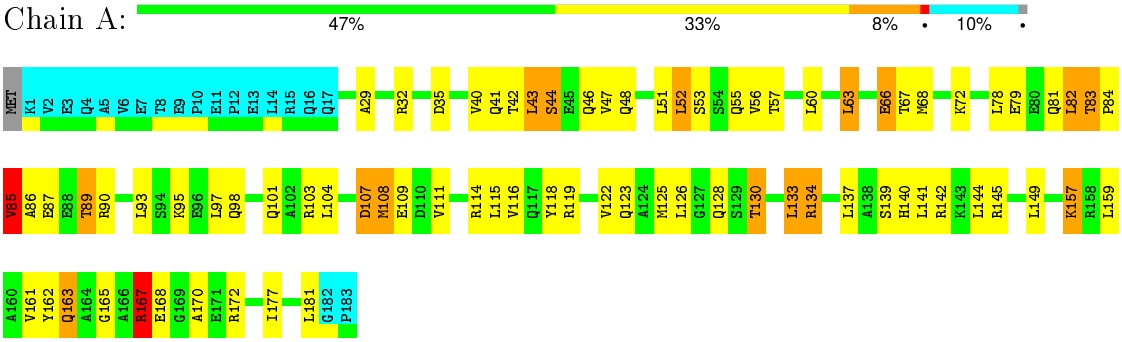
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Apolipoprotein E

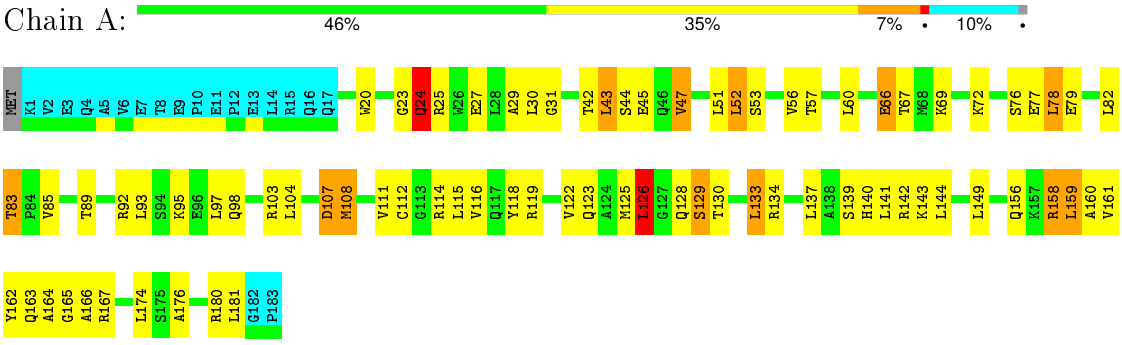
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Apolipoprotein E

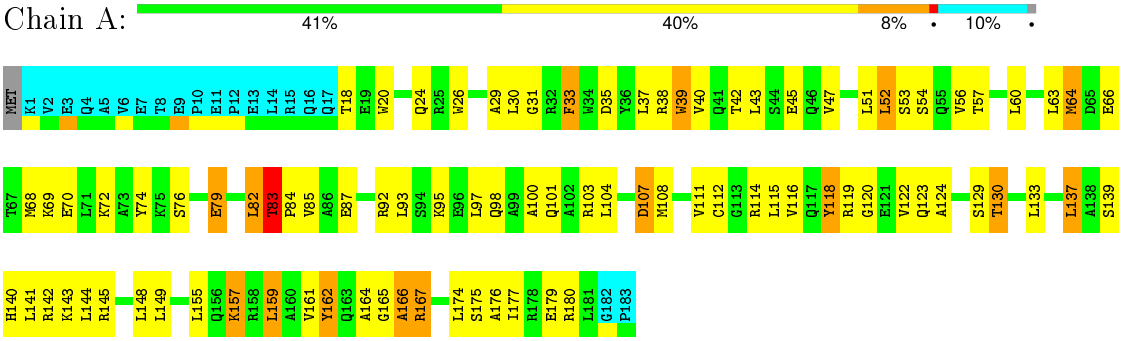
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Apolipoprotein E

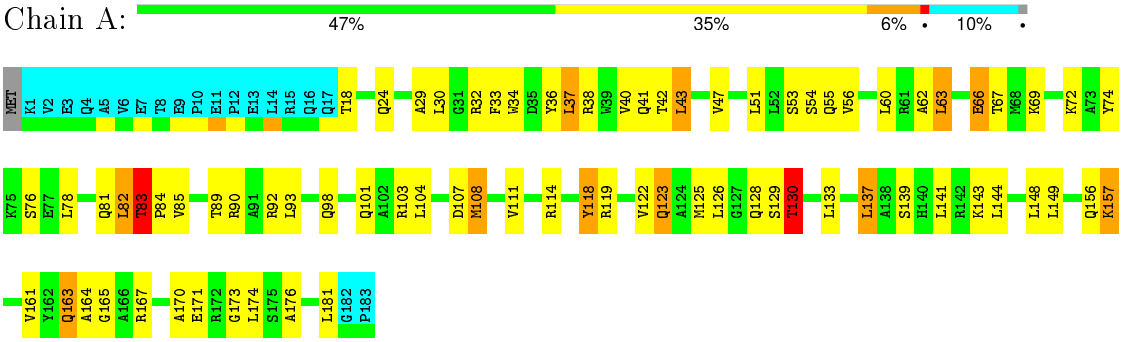
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Apolipoprotein E

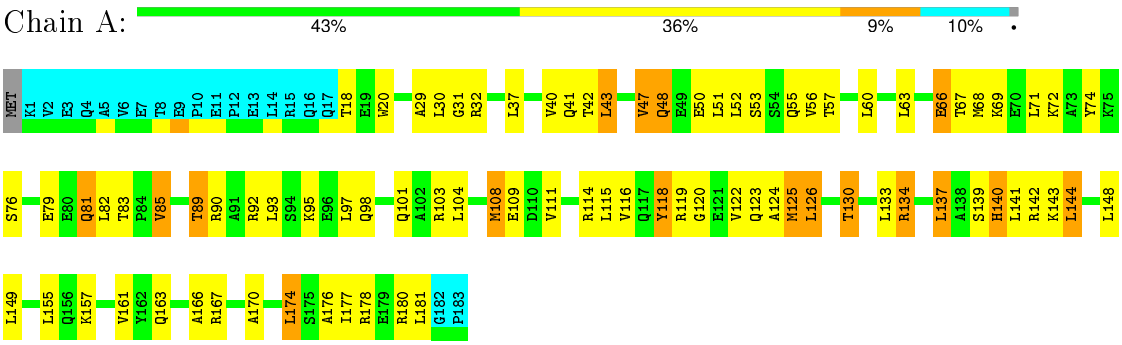
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Apolipoprotein E

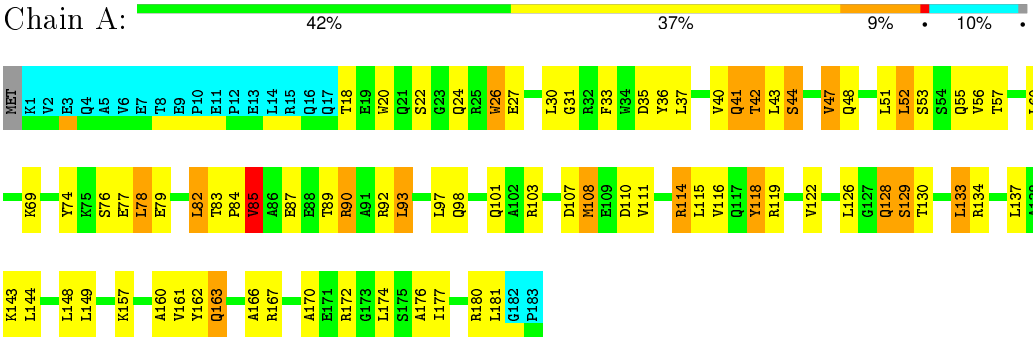
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Apolipoprotein E

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

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

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

Software name	Classification	Version
CYANA	geometry optimization	2.1
CNS	refinement	

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	1336	1349	1349	45±7
All	All	26720	26980	26980	903

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:ALA:HB3	1:A:170:ALA:HB2	0.98	1.34	7	1
1:A:43:LEU:HD13	1:A:47:VAL:HG11	0.92	1.42	15	3
1:A:82:LEU:HD11	1:A:176:ALA:HB2	0.90	1.42	7	2
1:A:141:LEU:HD12	1:A:144:LEU:HD12	0.89	1.45	17	7
1:A:83:THR:HG21	1:A:93:LEU:HD21	0.87	1.44	20	1
1:A:97:LEU:HD11	1:A:159:LEU:HD12	0.85	1.47	6	1
1:A:83:THR:HG22	1:A:93:LEU:HD21	0.83	1.48	11	1
1:A:122:VAL:HG21	1:A:133:LEU:HD13	0.82	1.50	2	11
1:A:82:LEU:HD21	1:A:176:ALA:HB2	0.77	1.56	5	1
1:A:83:THR:CG2	1:A:86:ALA:HB2	0.76	2.10	15	1
1:A:82:LEU:O	1:A:83:THR:O	0.76	2.04	1	1
1:A:81:GLN:HA	1:A:170:ALA:HB1	0.76	1.57	12	3
1:A:33:PHE:CD1	1:A:63:LEU:HD13	0.74	2.17	9	2
1:A:82:LEU:HD12	1:A:83:THR:OG1	0.72	1.84	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:HD21	1:A:115:LEU:HD22	0.71	1.61	20	5
1:A:104:LEU:HD13	1:A:152:ALA:HB2	0.71	1.63	6	1
1:A:93:LEU:HD11	1:A:162:TYR:CD1	0.71	2.20	1	4
1:A:29:ALA:HB3	1:A:70:GLU:OE2	0.71	1.85	3	3
1:A:107:ASP:O	1:A:111:VAL:HG23	0.71	1.85	10	15
1:A:118:TYR:CZ	1:A:137:LEU:HD12	0.71	2.21	19	7
1:A:60:LEU:HD11	1:A:115:LEU:HD12	0.70	1.62	15	14
1:A:84:PRO:HD3	1:A:164:ALA:HB3	0.69	1.64	12	4
1:A:140:HIS:CD2	1:A:141:LEU:N	0.69	2.61	14	2
1:A:36:TYR:O	1:A:40:VAL:HG23	0.68	1.88	10	3
1:A:125:MET:C	1:A:126:LEU:HD13	0.66	2.11	19	1
1:A:83:THR:CG2	1:A:161:VAL:HG12	0.66	2.21	18	1
1:A:166:ALA:HB3	1:A:170:ALA:CB	0.66	2.17	7	1
1:A:51:LEU:HD23	1:A:56:VAL:HG21	0.66	1.68	18	4
1:A:166:ALA:CB	1:A:170:ALA:HB2	0.66	2.18	7	1
1:A:82:LEU:HD22	1:A:176:ALA:HB1	0.66	1.67	14	1
1:A:41:GLN:O	1:A:42:THR:C	0.65	2.35	10	1
1:A:47:VAL:HG12	1:A:51:LEU:CD1	0.65	2.20	18	1
1:A:33:PHE:CD1	1:A:63:LEU:HD22	0.65	2.26	20	2
1:A:82:LEU:HD12	1:A:173:GLY:HA3	0.65	1.68	3	2
1:A:37:LEU:HD21	1:A:111:VAL:HG11	0.64	1.67	5	2
1:A:18:THR:HG21	1:A:164:ALA:HB2	0.64	1.67	4	2
1:A:82:LEU:HG	1:A:83:THR:HG22	0.64	1.69	13	2
1:A:97:LEU:HD13	1:A:179:GLU:OE2	0.64	1.93	17	3
1:A:37:LEU:HD13	1:A:60:LEU:HD21	0.64	1.68	10	1
1:A:157:LYS:O	1:A:161:VAL:HG23	0.64	1.92	2	14
1:A:29:ALA:HB2	1:A:70:GLU:OE2	0.63	1.93	17	4
1:A:118:TYR:O	1:A:122:VAL:HG23	0.63	1.93	19	19
1:A:56:VAL:CG2	1:A:115:LEU:HD13	0.63	2.23	14	13
1:A:115:LEU:HD21	1:A:141:LEU:HD22	0.63	1.70	3	5
1:A:79:GLU:HB2	1:A:177:ILE:HD12	0.63	1.70	20	1
1:A:33:PHE:CZ	1:A:148:LEU:HD21	0.62	2.29	6	1
1:A:114:ARG:HD2	1:A:144:LEU:HD11	0.62	1.69	10	12
1:A:78:LEU:HD13	1:A:163:GLN:HB2	0.62	1.70	6	1
1:A:37:LEU:HD23	1:A:60:LEU:HD21	0.62	1.70	5	1
1:A:85:VAL:HG11	1:A:89:THR:OG1	0.62	1.94	10	4
1:A:82:LEU:N	1:A:170:ALA:HB1	0.62	2.09	18	5
1:A:29:ALA:HB3	1:A:70:GLU:CD	0.62	2.14	3	2
1:A:67:THR:HG21	1:A:108:MET:HE1	0.62	1.70	3	13
1:A:40:VAL:HG13	1:A:50:GLU:OE2	0.62	1.95	3	1
1:A:78:LEU:HD13	1:A:163:GLN:HG3	0.62	1.70	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TRP:CZ2	1:A:159:LEU:HD11	0.62	2.28	17	3
1:A:82:LEU:O	1:A:170:ALA:HB2	0.62	1.93	15	1
1:A:82:LEU:HD11	1:A:175:SER:CB	0.61	2.25	12	1
1:A:82:LEU:HD13	1:A:176:ALA:HB2	0.61	1.69	1	2
1:A:78:LEU:HD22	1:A:163:GLN:HA	0.61	1.71	4	1
1:A:57:THR:HG21	1:A:116:VAL:HB	0.61	1.73	13	12
1:A:122:VAL:CG2	1:A:133:LEU:HD13	0.61	2.26	16	7
1:A:84:PRO:HA	1:A:166:ALA:HB2	0.61	1.71	12	3
1:A:75:LYS:HA	1:A:78:LEU:HD23	0.61	1.72	1	2
1:A:89:THR:O	1:A:93:LEU:HD12	0.61	1.95	6	9
1:A:83:THR:HG23	1:A:90:ARG:CD	0.61	2.25	15	1
1:A:116:VAL:HG23	1:A:119:ARG:CZ	0.61	2.26	13	1
1:A:115:LEU:HA	1:A:118:TYR:CE2	0.61	2.31	11	2
1:A:43:LEU:HD12	1:A:134:ARG:CD	0.61	2.25	2	1
1:A:60:LEU:HA	1:A:63:LEU:HD23	0.60	1.71	18	5
1:A:78:LEU:HD12	1:A:78:LEU:O	0.60	1.96	16	2
1:A:74:TYR:CE2	1:A:78:LEU:HD12	0.60	2.31	6	1
1:A:37:LEU:HD12	1:A:37:LEU:O	0.60	1.96	10	2
1:A:165:GLY:O	1:A:166:ALA:HB2	0.60	1.96	17	2
1:A:78:LEU:HD21	1:A:162:TYR:CE2	0.60	2.32	20	1
1:A:44:SER:O	1:A:47:VAL:HG22	0.60	1.96	1	3
1:A:37:LEU:O	1:A:40:VAL:HG22	0.60	1.97	18	2
1:A:60:LEU:HA	1:A:63:LEU:HD12	0.60	1.73	12	4
1:A:79:GLU:OE1	1:A:177:ILE:HD12	0.60	1.97	15	1
1:A:18:THR:CG2	1:A:164:ALA:HB2	0.60	2.27	11	5
1:A:85:VAL:HG11	1:A:89:THR:HB	0.60	1.71	1	3
1:A:82:LEU:HD21	1:A:90:ARG:NE	0.60	2.12	1	1
1:A:43:LEU:H	1:A:47:VAL:HG21	0.59	1.57	18	1
1:A:37:LEU:HD22	1:A:60:LEU:CD2	0.59	2.26	6	1
1:A:60:LEU:CD1	1:A:115:LEU:HD12	0.59	2.28	10	15
1:A:56:VAL:HG21	1:A:115:LEU:HD13	0.59	1.73	9	11
1:A:29:ALA:HB1	1:A:66:GLU:HB3	0.59	1.75	2	13
1:A:137:LEU:O	1:A:141:LEU:CB	0.59	2.50	19	2
1:A:83:THR:HG22	1:A:84:PRO:HD2	0.59	1.73	18	5
1:A:123:GLN:O	1:A:126:LEU:HD23	0.59	1.98	16	1
1:A:111:VAL:HA	1:A:144:LEU:HD13	0.59	1.73	10	12
1:A:115:LEU:HD21	1:A:141:LEU:CD2	0.59	2.27	2	5
1:A:33:PHE:CG	1:A:63:LEU:HD22	0.59	2.33	1	2
1:A:78:LEU:O	1:A:78:LEU:HD12	0.58	1.98	8	1
1:A:51:LEU:CD2	1:A:115:LEU:HD22	0.58	2.27	3	4
1:A:43:LEU:HA	1:A:47:VAL:HG21	0.58	1.73	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:THR:O	1:A:166:ALA:HB2	0.58	1.99	11	1
1:A:60:LEU:HD13	1:A:111:VAL:HG12	0.58	1.75	18	4
1:A:47:VAL:HG22	1:A:51:LEU:CD1	0.58	2.28	15	1
1:A:78:LEU:HD22	1:A:78:LEU:O	0.58	1.98	15	1
1:A:48:GLN:OE1	1:A:52:LEU:HD12	0.58	1.99	19	1
1:A:159:LEU:HD23	1:A:160:ALA:N	0.58	2.14	7	2
1:A:158:ARG:HE	1:A:159:LEU:N	0.58	1.96	16	1
1:A:89:THR:HG22	1:A:93:LEU:CD1	0.57	2.29	14	3
1:A:85:VAL:HG11	1:A:89:THR:CB	0.57	2.29	9	4
1:A:50:GLU:HB3	1:A:56:VAL:HG13	0.57	1.75	19	4
1:A:174:LEU:HD12	1:A:177:ILE:CG2	0.57	2.30	17	3
1:A:84:PRO:O	1:A:85:VAL:HG13	0.57	1.99	4	7
1:A:33:PHE:HA	1:A:63:LEU:HD22	0.57	1.76	11	2
1:A:93:LEU:HD11	1:A:162:TYR:CE1	0.57	2.34	5	3
1:A:33:PHE:HB3	1:A:63:LEU:HD13	0.57	1.76	1	2
1:A:130:THR:HA	1:A:133:LEU:HD21	0.57	1.77	18	4
1:A:114:ARG:HD2	1:A:144:LEU:HD12	0.57	1.75	19	2
1:A:78:LEU:HD21	1:A:162:TYR:CD2	0.57	2.34	20	1
1:A:165:GLY:O	1:A:170:ALA:HB2	0.56	2.00	12	1
1:A:51:LEU:HD22	1:A:137:LEU:HD13	0.56	1.76	13	2
1:A:93:LEU:O	1:A:93:LEU:HD12	0.56	2.00	11	3
1:A:93:LEU:HD13	1:A:161:VAL:HG11	0.56	1.77	19	2
1:A:52:LEU:O	1:A:52:LEU:HD12	0.56	2.00	8	4
1:A:116:VAL:HG23	1:A:119:ARG:NH1	0.56	2.15	13	1
1:A:82:LEU:HG	1:A:176:ALA:HB2	0.56	1.77	6	4
1:A:97:LEU:HD21	1:A:159:LEU:CD1	0.55	2.31	6	1
1:A:82:LEU:HD13	1:A:82:LEU:N	0.55	2.15	11	1
1:A:112:CYS:O	1:A:116:VAL:HG12	0.55	2.01	13	3
1:A:44:SER:O	1:A:47:VAL:HG12	0.55	2.02	15	2
1:A:60:LEU:HD11	1:A:115:LEU:CD1	0.55	2.32	11	11
1:A:52:LEU:HD12	1:A:52:LEU:O	0.55	2.01	15	5
1:A:81:GLN:C	1:A:82:LEU:HD13	0.55	2.22	11	1
1:A:104:LEU:HD13	1:A:152:ALA:CB	0.55	2.30	6	1
1:A:51:LEU:HD22	1:A:137:LEU:CD1	0.55	2.31	10	2
1:A:83:THR:HG23	1:A:90:ARG:HD3	0.55	1.78	15	1
1:A:30:LEU:HD12	1:A:30:LEU:C	0.54	2.23	4	2
1:A:97:LEU:HG	1:A:158:ARG:NE	0.54	2.16	16	1
1:A:51:LEU:C	1:A:51:LEU:HD12	0.54	2.23	10	8
1:A:63:LEU:O	1:A:67:THR:HG22	0.54	2.01	15	5
1:A:137:LEU:HA	1:A:140:HIS:NE2	0.54	2.17	19	1
1:A:118:TYR:CD1	1:A:118:TYR:C	0.54	2.80	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:GLY:O	1:A:166:ALA:HB3	0.54	2.03	12	1
1:A:82:LEU:HD11	1:A:176:ALA:HB3	0.54	1.78	18	1
1:A:140:HIS:CD2	1:A:140:HIS:C	0.54	2.81	14	1
1:A:78:LEU:HD21	1:A:163:GLN:HG3	0.54	1.78	13	1
1:A:97:LEU:O	1:A:97:LEU:HD23	0.53	2.02	16	7
1:A:111:VAL:HG22	1:A:144:LEU:HB3	0.53	1.78	15	4
1:A:82:LEU:HD11	1:A:175:SER:HB2	0.53	1.79	12	1
1:A:82:LEU:O	1:A:83:THR:HG22	0.53	2.03	1	1
1:A:78:LEU:HD13	1:A:163:GLN:HA	0.53	1.79	14	2
1:A:82:LEU:HD13	1:A:90:ARG:HD2	0.53	1.79	2	5
1:A:137:LEU:CD2	1:A:141:LEU:HD22	0.53	2.34	19	1
1:A:104:LEU:HD22	1:A:155:LEU:HD23	0.53	1.79	5	3
1:A:78:LEU:HD23	1:A:163:GLN:HB2	0.53	1.80	18	1
1:A:89:THR:HG23	1:A:92:ARG:NH2	0.53	2.19	8	1
1:A:126:LEU:HD13	1:A:126:LEU:N	0.52	2.20	19	1
1:A:33:PHE:CA	1:A:63:LEU:HD22	0.52	2.35	11	2
1:A:84:PRO:CA	1:A:166:ALA:HB2	0.52	2.35	3	3
1:A:43:LEU:HD12	1:A:134:ARG:HG2	0.52	1.81	19	2
1:A:114:ARG:CD	1:A:140:HIS:CD2	0.52	2.93	14	1
1:A:97:LEU:HD11	1:A:159:LEU:HD23	0.52	1.81	10	3
1:A:29:ALA:HB1	1:A:66:GLU:CG	0.52	2.35	3	1
1:A:29:ALA:HB2	1:A:70:GLU:HG3	0.52	1.82	13	2
1:A:18:THR:OG1	1:A:164:ALA:HB2	0.52	2.04	13	2
1:A:93:LEU:HD12	1:A:93:LEU:O	0.51	2.05	2	5
1:A:37:LEU:CD2	1:A:111:VAL:HG11	0.51	2.36	9	1
1:A:115:LEU:HD13	1:A:115:LEU:C	0.51	2.25	4	1
1:A:29:ALA:HB3	1:A:70:GLU:OE1	0.51	2.05	4	2
1:A:26:TRP:CE2	1:A:159:LEU:HD11	0.51	2.40	5	1
1:A:82:LEU:O	1:A:83:THR:CB	0.51	2.57	15	1
1:A:30:LEU:HD12	1:A:31:GLY:N	0.51	2.19	9	15
1:A:51:LEU:HD12	1:A:51:LEU:C	0.51	2.25	16	4
1:A:51:LEU:HD22	1:A:118:TYR:OH	0.51	2.06	19	4
1:A:18:THR:HG21	1:A:160:ALA:HB1	0.51	1.82	20	3
1:A:82:LEU:H	1:A:170:ALA:HB1	0.51	1.66	5	2
1:A:125:MET:O	1:A:126:LEU:C	0.51	2.48	16	2
1:A:156:GLN:HA	1:A:159:LEU:HD22	0.51	1.81	16	1
1:A:93:LEU:HD22	1:A:161:VAL:CG1	0.51	2.36	2	4
1:A:82:LEU:HD21	1:A:176:ALA:CB	0.51	2.33	5	1
1:A:82:LEU:HD11	1:A:176:ALA:H	0.51	1.64	4	1
1:A:137:LEU:HA	1:A:140:HIS:CD2	0.51	2.41	20	4
1:A:37:LEU:O	1:A:37:LEU:HD22	0.51	2.06	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:GLN:C	1:A:82:LEU:HG	0.51	2.26	15	1
1:A:26:TRP:CE2	1:A:74:TYR:HB2	0.51	2.40	20	1
1:A:43:LEU:HA	1:A:47:VAL:HG11	0.51	1.82	1	1
1:A:141:LEU:HA	1:A:144:LEU:HD12	0.50	1.83	10	3
1:A:51:LEU:HD13	1:A:137:LEU:CD1	0.50	2.36	20	4
1:A:137:LEU:O	1:A:137:LEU:HD23	0.50	2.05	16	4
1:A:60:LEU:HD22	1:A:111:VAL:HG11	0.50	1.81	14	4
1:A:37:LEU:HD12	1:A:145:ARG:CB	0.50	2.36	6	1
1:A:129:SER:O	1:A:130:THR:CB	0.50	2.60	13	5
1:A:60:LEU:HD13	1:A:112:CYS:HA	0.50	1.83	1	3
1:A:22:SER:O	1:A:23:GLY:C	0.50	2.48	4	1
1:A:18:THR:HG23	1:A:160:ALA:O	0.50	2.06	12	2
1:A:90:ARG:HA	1:A:93:LEU:HD23	0.50	1.83	5	6
1:A:97:LEU:HD23	1:A:97:LEU:O	0.50	2.07	5	9
1:A:43:LEU:HD12	1:A:134:ARG:HD2	0.50	1.84	2	1
1:A:137:LEU:HD23	1:A:137:LEU:O	0.50	2.06	7	4
1:A:43:LEU:N	1:A:47:VAL:HG21	0.50	2.21	18	1
1:A:82:LEU:HD22	1:A:176:ALA:HB2	0.49	1.82	1	1
1:A:83:THR:HB	1:A:161:VAL:HG12	0.49	1.84	20	2
1:A:83:THR:HG22	1:A:86:ALA:HB2	0.49	1.84	15	1
1:A:78:LEU:HD13	1:A:162:TYR:O	0.49	2.07	16	1
1:A:82:LEU:O	1:A:83:THR:CG2	0.49	2.61	1	1
1:A:41:GLN:O	1:A:43:LEU:HD23	0.49	2.08	14	1
1:A:37:LEU:HD12	1:A:145:ARG:HB2	0.49	1.84	6	1
1:A:156:GLN:O	1:A:160:ALA:HB2	0.49	2.07	16	4
1:A:82:LEU:HD13	1:A:176:ALA:CB	0.49	2.38	1	1
1:A:84:PRO:HD2	1:A:161:VAL:HG12	0.49	1.84	12	1
1:A:141:LEU:HD21	1:A:145:ARG:NH2	0.49	2.22	1	1
1:A:82:LEU:HD23	1:A:90:ARG:HD2	0.49	1.85	5	1
1:A:93:LEU:HD22	1:A:161:VAL:HG11	0.49	1.84	14	2
1:A:100:ALA:HB1	1:A:155:LEU:HB2	0.49	1.84	12	4
1:A:78:LEU:HD13	1:A:163:GLN:CB	0.49	2.37	2	2
1:A:47:VAL:HG12	1:A:51:LEU:HD11	0.49	1.83	18	1
1:A:140:HIS:ND1	1:A:141:LEU:N	0.49	2.61	20	3
1:A:82:LEU:HD13	1:A:90:ARG:CD	0.49	2.37	2	2
1:A:63:LEU:HD11	1:A:108:MET:HE2	0.48	1.85	3	3
1:A:82:LEU:HD11	1:A:176:ALA:N	0.48	2.22	4	1
1:A:78:LEU:HD21	1:A:163:GLN:CG	0.48	2.37	13	1
1:A:129:SER:HB2	1:A:133:LEU:HD23	0.48	1.84	8	1
1:A:63:LEU:HD12	1:A:64:MET:N	0.48	2.22	17	1
1:A:83:THR:HG23	1:A:162:TYR:HA	0.48	1.86	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:LEU:O	1:A:174:LEU:HD12	0.48	2.09	5	1
1:A:118:TYR:CZ	1:A:137:LEU:CD1	0.48	2.97	12	1
1:A:162:TYR:CE2	1:A:176:ALA:HB1	0.48	2.43	5	1
1:A:29:ALA:CB	1:A:70:GLU:OE1	0.48	2.61	4	2
1:A:83:THR:HG21	1:A:93:LEU:CD2	0.48	2.31	20	1
1:A:140:HIS:CG	1:A:141:LEU:N	0.48	2.82	13	4
1:A:108:MET:N	1:A:148:LEU:HD12	0.48	2.24	18	4
1:A:83:THR:HG21	1:A:90:ARG:HG3	0.48	1.85	11	1
1:A:78:LEU:HD13	1:A:163:GLN:CG	0.48	2.38	7	1
1:A:51:LEU:HD13	1:A:118:TYR:CE1	0.47	2.44	5	3
1:A:78:LEU:HD11	1:A:162:TYR:CD2	0.47	2.44	1	1
1:A:82:LEU:HD13	1:A:90:ARG:CZ	0.47	2.39	12	3
1:A:115:LEU:HA	1:A:118:TYR:CZ	0.47	2.44	5	2
1:A:114:ARG:CG	1:A:140:HIS:CE1	0.47	2.98	19	1
1:A:137:LEU:O	1:A:141:LEU:HB3	0.47	2.09	19	1
1:A:137:LEU:HA	1:A:140:HIS:CE1	0.47	2.44	14	1
1:A:81:GLN:CB	1:A:170:ALA:HB1	0.47	2.38	7	1
1:A:84:PRO:HG3	1:A:161:VAL:HG12	0.47	1.86	15	1
1:A:74:TYR:CD2	1:A:78:LEU:HD22	0.47	2.45	3	1
1:A:41:GLN:O	1:A:42:THR:CB	0.47	2.62	2	1
1:A:42:THR:C	1:A:43:LEU:HD23	0.47	2.29	2	1
1:A:33:PHE:CG	1:A:63:LEU:HD13	0.47	2.44	17	1
1:A:165:GLY:O	1:A:166:ALA:CB	0.47	2.62	17	2
1:A:166:ALA:O	1:A:167:ARG:CB	0.47	2.62	17	1
1:A:83:THR:HB	1:A:93:LEU:HD23	0.47	1.86	17	1
1:A:97:LEU:HD22	1:A:179:GLU:OE2	0.47	2.10	7	2
1:A:93:LEU:HD22	1:A:161:VAL:HG12	0.47	1.84	10	1
1:A:37:LEU:O	1:A:40:VAL:HG12	0.47	2.09	19	1
1:A:43:LEU:HD12	1:A:134:ARG:HD3	0.47	1.86	2	1
1:A:81:GLN:CB	1:A:165:GLY:HA3	0.47	2.40	18	1
1:A:86:ALA:HB3	1:A:167:ARG:HD2	0.47	1.85	15	1
1:A:78:LEU:HD23	1:A:79:GLU:N	0.47	2.25	20	1
1:A:126:LEU:N	1:A:126:LEU:HD22	0.47	2.25	19	1
1:A:34:TRP:HA	1:A:37:LEU:HD23	0.47	1.87	2	1
1:A:110:ASP:HB3	1:A:144:LEU:HD21	0.46	1.87	7	1
1:A:84:PRO:HB3	1:A:166:ALA:HB3	0.46	1.85	10	1
1:A:71:LEU:HD21	1:A:101:GLN:NE2	0.46	2.25	19	1
1:A:93:LEU:HD21	1:A:162:TYR:CD1	0.46	2.45	2	1
1:A:37:LEU:HD12	1:A:37:LEU:C	0.46	2.31	10	1
1:A:33:PHE:HE1	1:A:60:LEU:HD23	0.46	1.70	9	1
1:A:122:VAL:HG11	1:A:133:LEU:HD13	0.46	1.86	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:TYR:CE1	1:A:137:LEU:HD12	0.46	2.44	14	5
1:A:34:TRP:NE1	1:A:149:LEU:HD12	0.46	2.25	6	2
1:A:33:PHE:HZ	1:A:148:LEU:HD21	0.46	1.70	6	1
1:A:78:LEU:HD21	1:A:162:TYR:O	0.46	2.10	15	1
1:A:51:LEU:HD13	1:A:137:LEU:HD11	0.46	1.87	20	2
1:A:60:LEU:CD1	1:A:111:VAL:HG12	0.46	2.40	18	1
1:A:133:LEU:O	1:A:137:LEU:HB2	0.46	2.10	20	2
1:A:137:LEU:O	1:A:141:LEU:HB2	0.45	2.10	19	3
1:A:60:LEU:HD22	1:A:111:VAL:CG1	0.45	2.41	2	5
1:A:83:THR:OG1	1:A:93:LEU:HD13	0.45	2.11	7	1
1:A:90:ARG:HE	1:A:176:ALA:HB2	0.45	1.71	11	1
1:A:97:LEU:HA	1:A:158:ARG:HD2	0.45	1.88	16	1
1:A:74:TYR:CE1	1:A:78:LEU:HD12	0.45	2.46	14	1
1:A:43:LEU:CA	1:A:47:VAL:HG11	0.45	2.41	1	1
1:A:115:LEU:N	1:A:115:LEU:HD23	0.45	2.27	11	2
1:A:97:LEU:HG	1:A:158:ARG:HB2	0.45	1.88	16	1
1:A:82:LEU:HD12	1:A:83:THR:HG1	0.45	1.71	15	1
1:A:23:GLY:O	1:A:24:GLN:CB	0.45	2.64	8	2
1:A:56:VAL:HG21	1:A:115:LEU:HG	0.45	1.89	4	1
1:A:47:VAL:HG13	1:A:51:LEU:HD12	0.45	1.88	20	1
1:A:78:LEU:HD12	1:A:163:GLN:HA	0.45	1.88	20	1
1:A:37:LEU:HD23	1:A:111:VAL:HG11	0.45	1.89	8	1
1:A:122:VAL:HG13	1:A:133:LEU:HD22	0.45	1.89	19	1
1:A:174:LEU:HD23	1:A:177:ILE:CG2	0.45	2.42	19	1
1:A:82:LEU:C	1:A:83:THR:HG22	0.45	2.30	10	1
1:A:30:LEU:HD13	1:A:34:TRP:CZ3	0.45	2.47	18	1
1:A:78:LEU:HD22	1:A:163:GLN:HG2	0.45	1.88	7	1
1:A:86:ALA:HB3	1:A:167:ARG:CD	0.45	2.41	15	1
1:A:111:VAL:HG13	1:A:141:LEU:HD11	0.45	1.88	20	1
1:A:40:VAL:CG1	1:A:141:LEU:HD21	0.45	2.42	6	1
1:A:81:GLN:O	1:A:82:LEU:HG	0.45	2.12	15	1
1:A:97:LEU:C	1:A:97:LEU:HD23	0.44	2.32	16	1
1:A:79:GLU:O	1:A:176:ALA:HB1	0.44	2.11	17	1
1:A:93:LEU:HD11	1:A:162:TYR:HB2	0.44	1.89	3	1
1:A:83:THR:HG21	1:A:90:ARG:CG	0.44	2.43	11	1
1:A:51:LEU:HD13	1:A:118:TYR:HE1	0.44	1.72	5	1
1:A:37:LEU:HD13	1:A:60:LEU:CD2	0.44	2.42	10	1
1:A:82:LEU:HD13	1:A:176:ALA:N	0.44	2.27	13	1
1:A:137:LEU:CD2	1:A:137:LEU:C	0.44	2.85	19	1
1:A:141:LEU:HD21	1:A:145:ARG:HH22	0.44	1.72	1	1
1:A:83:THR:HG21	1:A:161:VAL:HG12	0.44	1.89	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD21	1:A:111:VAL:HG21	0.44	1.87	13	1
1:A:82:LEU:HD22	1:A:90:ARG:HD2	0.44	1.90	6	2
1:A:37:LEU:HD22	1:A:37:LEU:O	0.44	2.13	5	3
1:A:33:PHE:CE2	1:A:148:LEU:HD11	0.44	2.48	11	2
1:A:51:LEU:HD12	1:A:52:LEU:N	0.44	2.27	13	5
1:A:97:LEU:HD21	1:A:159:LEU:HD22	0.44	1.90	4	1
1:A:118:TYR:C	1:A:118:TYR:CD1	0.43	2.90	1	2
1:A:47:VAL:HG22	1:A:51:LEU:HD11	0.43	1.90	15	1
1:A:39:TRP:HE1	1:A:56:VAL:HG12	0.43	1.73	17	1
1:A:33:PHE:CZ	1:A:62:ALA:HB3	0.43	2.49	10	2
1:A:162:TYR:CE1	1:A:176:ALA:HB1	0.43	2.47	20	2
1:A:118:TYR:CZ	1:A:137:LEU:HD11	0.43	2.49	11	1
1:A:110:ASP:CB	1:A:144:LEU:HD21	0.43	2.43	7	1
1:A:107:ASP:HB2	1:A:148:LEU:HD12	0.43	1.89	20	1
1:A:120:GLY:O	1:A:124:ALA:HB2	0.43	2.14	17	2
1:A:108:MET:CG	1:A:109:GLU:N	0.43	2.81	9	6
1:A:41:GLN:O	1:A:43:LEU:HD12	0.43	2.13	18	1
1:A:84:PRO:N	1:A:166:ALA:HB2	0.43	2.29	8	2
1:A:18:THR:HG22	1:A:164:ALA:HB2	0.43	1.89	11	1
1:A:33:PHE:N	1:A:33:PHE:CD1	0.43	2.84	1	2
1:A:83:THR:HG22	1:A:93:LEU:CD2	0.43	2.34	11	1
1:A:82:LEU:HD21	1:A:90:ARG:HG3	0.43	1.90	9	1
1:A:37:LEU:CD2	1:A:148:LEU:HD13	0.42	2.44	17	1
1:A:37:LEU:HD13	1:A:145:ARG:HD3	0.42	1.89	5	1
1:A:83:THR:HG23	1:A:164:ALA:HB3	0.42	1.89	5	1
1:A:126:LEU:HD12	1:A:126:LEU:O	0.42	2.14	16	1
1:A:83:THR:CG2	1:A:164:ALA:HB3	0.42	2.44	5	1
1:A:79:GLU:OE2	1:A:177:ILE:HD13	0.42	2.14	14	2
1:A:133:LEU:O	1:A:137:LEU:CB	0.42	2.67	20	1
1:A:129:SER:C	1:A:133:LEU:HD23	0.42	2.34	8	1
1:A:21:GLN:NE2	1:A:81:GLN:HE22	0.42	2.12	8	1
1:A:126:LEU:HD22	1:A:126:LEU:N	0.42	2.29	13	1
1:A:83:THR:HG23	1:A:161:VAL:O	0.42	2.15	6	1
1:A:93:LEU:CD2	1:A:161:VAL:HG11	0.42	2.44	14	1
1:A:83:THR:HG23	1:A:90:ARG:HG3	0.42	1.90	4	1
1:A:82:LEU:HD12	1:A:176:ALA:HA	0.42	1.91	17	1
1:A:71:LEU:O	1:A:75:LYS:CB	0.42	2.68	3	2
1:A:81:GLN:O	1:A:82:LEU:O	0.42	2.36	15	1
1:A:84:PRO:C	1:A:85:VAL:HG22	0.42	2.34	4	2
1:A:78:LEU:HD21	1:A:163:GLN:NE2	0.42	2.30	9	1
1:A:56:VAL:HG23	1:A:57:THR:N	0.42	2.29	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD11	1:A:159:LEU:HD11	0.42	1.89	10	1
1:A:82:LEU:CD2	1:A:176:ALA:HB2	0.42	2.37	5	1
1:A:174:LEU:HD12	1:A:177:ILE:HG23	0.42	1.92	17	1
1:A:34:TRP:HE1	1:A:149:LEU:HD12	0.42	1.75	4	2
1:A:159:LEU:O	1:A:159:LEU:HD12	0.42	2.15	9	1
1:A:130:THR:HA	1:A:133:LEU:HD23	0.42	1.92	15	2
1:A:40:VAL:O	1:A:41:GLN:C	0.42	2.57	15	1
1:A:82:LEU:HD12	1:A:173:GLY:CA	0.41	2.42	3	1
1:A:93:LEU:CD2	1:A:161:VAL:HG21	0.41	2.45	14	1
1:A:33:PHE:CE1	1:A:148:LEU:HD11	0.41	2.50	6	1
1:A:104:LEU:HD22	1:A:155:LEU:CD2	0.41	2.45	11	1
1:A:122:VAL:HG23	1:A:123:GLN:N	0.41	2.30	18	1
1:A:166:ALA:O	1:A:167:ARG:C	0.41	2.58	7	1
1:A:20:TRP:O	1:A:21:GLN:C	0.41	2.59	4	1
1:A:82:LEU:HD21	1:A:90:ARG:HD2	0.41	1.93	9	1
1:A:40:VAL:HG12	1:A:47:VAL:HG23	0.41	1.92	2	1
1:A:81:GLN:O	1:A:170:ALA:HA	0.41	2.15	15	1
1:A:26:TRP:N	1:A:26:TRP:CD2	0.41	2.85	20	1
1:A:67:THR:HA	1:A:70:GLU:CG	0.41	2.46	9	1
1:A:82:LEU:HD12	1:A:180:ARG:HH21	0.41	1.75	11	1
1:A:63:LEU:C	1:A:63:LEU:HD12	0.41	2.35	2	1
1:A:43:LEU:HD13	1:A:138:ALA:CB	0.41	2.45	1	1
1:A:82:LEU:HD12	1:A:173:GLY:HA2	0.41	1.91	18	1
1:A:141:LEU:HD21	1:A:145:ARG:HH21	0.41	1.75	7	1
1:A:37:LEU:HD23	1:A:60:LEU:CD2	0.41	2.45	20	1
1:A:93:LEU:HD21	1:A:162:TYR:HB2	0.41	1.93	17	1
1:A:78:LEU:HD23	1:A:78:LEU:C	0.41	2.36	20	1
1:A:78:LEU:HD23	1:A:163:GLN:HB3	0.41	1.92	10	1
1:A:56:VAL:O	1:A:60:LEU:HD12	0.41	2.16	7	2
1:A:26:TRP:O	1:A:70:GLU:OE2	0.41	2.39	9	1
1:A:162:TYR:O	1:A:163:GLN:C	0.41	2.58	15	1
1:A:82:LEU:HD22	1:A:90:ARG:CD	0.41	2.46	8	1
1:A:60:LEU:HA	1:A:63:LEU:HD21	0.41	1.92	17	1
1:A:93:LEU:HD21	1:A:162:TYR:CB	0.41	2.46	17	1
1:A:108:MET:CA	1:A:148:LEU:HD12	0.41	2.46	6	1
1:A:60:LEU:O	1:A:64:MET:HG2	0.41	2.16	12	1
1:A:33:PHE:HE2	1:A:148:LEU:HD11	0.41	1.75	11	1
1:A:47:VAL:O	1:A:51:LEU:HG	0.41	2.16	11	1
1:A:37:LEU:HD12	1:A:145:ARG:CD	0.41	2.46	11	1
1:A:43:LEU:HD22	1:A:47:VAL:HG21	0.41	1.92	15	1
1:A:137:LEU:CD2	1:A:137:LEU:O	0.41	2.69	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HD12	1:A:169:GLY:CA	0.40	2.45	10	1
1:A:37:LEU:HD13	1:A:111:VAL:HG11	0.40	1.91	12	1
1:A:37:LEU:HD12	1:A:145:ARG:HD2	0.40	1.93	3	1
1:A:148:LEU:HD23	1:A:148:LEU:C	0.40	2.36	6	1
1:A:84:PRO:CD	1:A:161:VAL:HG12	0.40	2.46	12	1
1:A:111:VAL:HG13	1:A:145:ARG:HH22	0.40	1.74	9	1
1:A:75:LYS:NZ	1:A:177:ILE:HD12	0.40	2.31	1	1
1:A:71:LEU:C	1:A:71:LEU:HD13	0.40	2.37	4	1
1:A:118:TYR:OH	1:A:133:LEU:CD1	0.40	2.69	19	1
1:A:93:LEU:CD1	1:A:161:VAL:HG11	0.40	2.46	19	1
1:A:104:LEU:CD1	1:A:152:ALA:HB2	0.40	2.42	6	1
1:A:36:TYR:O	1:A:39:TRP:CD1	0.40	2.74	10	1
1:A:26:TRP:CE2	1:A:30:LEU:CD2	0.40	3.04	3	1
1:A:33:PHE:CB	1:A:63:LEU:HD22	0.40	2.45	1	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	164/184 (89%)	140±3 (85±2%)	19±3 (11±2%)	6±2 (4±1%)	8	37
All	All	3280/3680 (89%)	2794 (85%)	370 (11%)	116 (4%)	8	37

All 20 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	167	ARG	17
1	A	85	VAL	14
1	A	128	GLN	12
1	A	166	ALA	10
1	A	165	GLY	9
1	A	83	THR	8
1	A	126	LEU	8
1	A	87	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	24	GLN	7
1	A	130	THR	6
1	A	42	THR	4
1	A	41	GLN	3
1	A	44	SER	2
1	A	129	SER	2
1	A	172	ARG	2
1	A	21	GLN	1
1	A	25	ARG	1
1	A	82	LEU	1
1	A	164	ALA	1
1	A	43	LEU	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	138/156 (88%)	93±3 (68±2%)	45±3 (32±2%)	1 13
All	All	2760/3120 (88%)	1865 (68%)	895 (32%)	1 13

All 105 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	108	MET	20
1	A	66	GLU	20
1	A	103	ARG	20
1	A	139	SER	20
1	A	98	GLN	20
1	A	149	LEU	20
1	A	69	LYS	19
1	A	119	ARG	18
1	A	53	SER	18
1	A	142	ARG	18
1	A	143	LYS	18
1	A	42	THR	18
1	A	74	TYR	16

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Mol	Chain	Res	Type	Models (Total)
1	A	133	LEU	16
1	A	43	LEU	16
1	A	55	GLN	15
1	A	181	LEU	15
1	A	24	GLN	15
1	A	140	HIS	15
1	A	47	VAL	14
1	A	44	SER	14
1	A	72	LYS	14
1	A	101	GLN	14
1	A	92	ARG	13
1	A	163	GLN	13
1	A	130	THR	13
1	A	129	SER	13
1	A	76	SER	12
1	A	134	ARG	12
1	A	89	THR	12
1	A	85	VAL	11
1	A	83	THR	11
1	A	36	TYR	11
1	A	123	GLN	11
1	A	118	TYR	10
1	A	157	LYS	10
1	A	52	LEU	10
1	A	107	ASP	10
1	A	82	LEU	10
1	A	137	LEU	10
1	A	125	MET	10
1	A	114	ARG	10
1	A	68	MET	9
1	A	32	ARG	9
1	A	104	LEU	9
1	A	167	ARG	9
1	A	93	LEU	9
1	A	95	LYS	9
1	A	180	ARG	9
1	A	48	GLN	9
1	A	90	ARG	8
1	A	159	LEU	8
1	A	162	TYR	8
1	A	45	GLU	8
1	A	35	ASP	8

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Mol	Chain	Res	Type	Models (Total)
1	A	128	GLN	7
1	A	38	ARG	7
1	A	20	TRP	7
1	A	21	GLN	7
1	A	33	PHE	6
1	A	63	LEU	6
1	A	37	LEU	6
1	A	79	GLU	6
1	A	172	ARG	6
1	A	77	GLU	6
1	A	174	LEU	6
1	A	78	LEU	5
1	A	87	GLU	5
1	A	64	MET	5
1	A	175	SER	5
1	A	81	GLN	5
1	A	126	LEU	4
1	A	145	ARG	4
1	A	27	GLU	4
1	A	61	ARG	4
1	A	34	TRP	4
1	A	179	GLU	4
1	A	25	ARG	4
1	A	75	LYS	4
1	A	46	GLN	3
1	A	109	GLU	3
1	A	54	SER	3
1	A	156	GLN	3
1	A	22	SER	3
1	A	18	THR	3
1	A	110	ASP	3
1	A	71	LEU	3
1	A	41	GLN	3
1	A	117	GLN	2
1	A	39	TRP	2
1	A	155	LEU	2
1	A	26	TRP	2
1	A	58	GLN	2
1	A	171	GLU	2
1	A	65	ASP	2
1	A	168	GLU	1
1	A	144	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	70	GLU	1
1	A	80	GLU	1
1	A	60	LEU	1
1	A	158	ARG	1
1	A	88	GLU	1
1	A	67	THR	1
1	A	150	ARG	1
1	A	178	ARG	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided