W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 09:00 PM BST

PDB ID : 2IEM
Title : Solution structure of an oxidized form (Cys51-Cys198) of E. coli Methionine Sulfoxide Reductase A (MsrA)
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Deposited on : 2006-09-19

The following versions of software and data (see references (i)) 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 is 59%.

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.
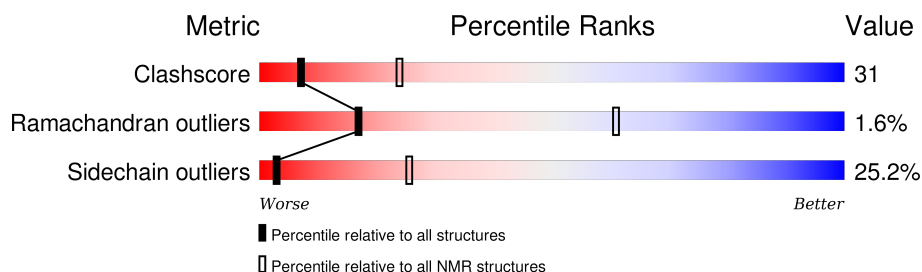
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	211	34% 39% 5% 23%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:21-A:121, A:133-A:194 (163)	0.41	3

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3176 atoms, of which 1543 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptide methionine sulfoxide reductase msrA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	211	3176	1031	1543	280	314	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	SER	CYS	ENGINEERED	UNP P0A744
A	206	SER	CYS	ENGINEERED	UNP P0A744

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: Peptide methionine sulfoxide reductase msrA
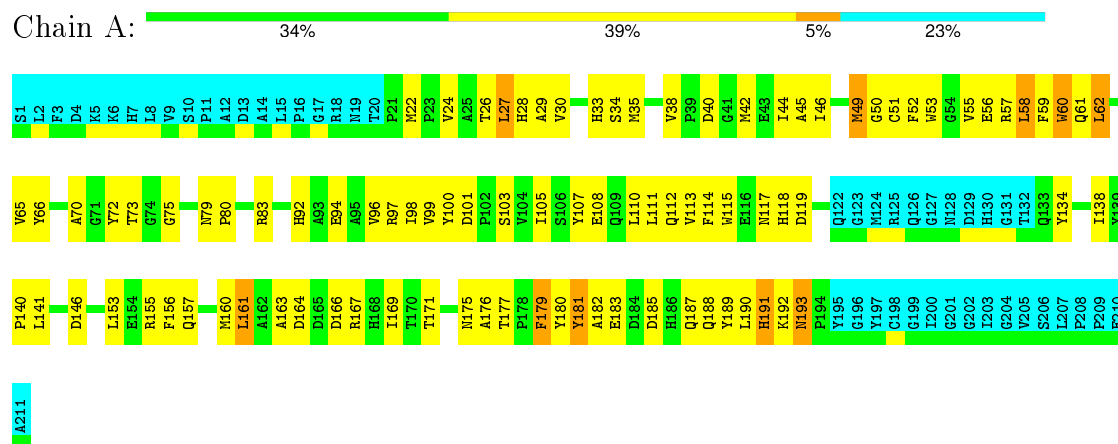
4.2   Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1   Score per residue for model 1

- Molecule 1: Peptide methionine sulfoxide reductase msrA
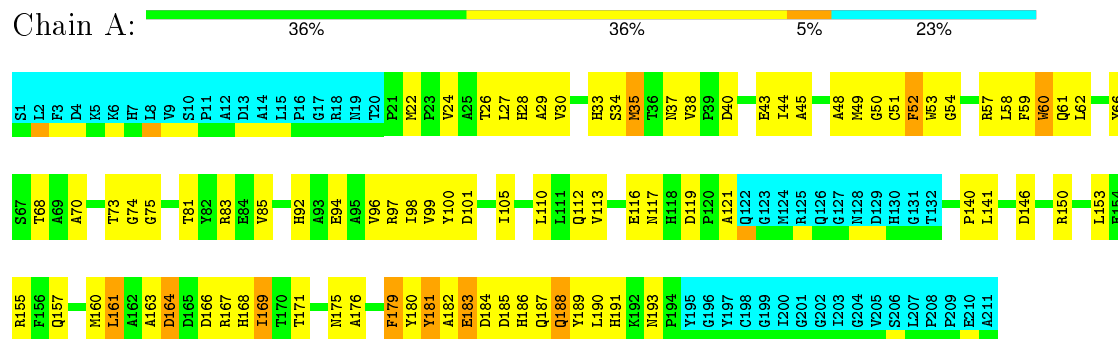
4.2.2 Score per residue for model 2

• Molecule 1: Peptide methionine sulfoxide reductase msrA

Chain A: 37% 32% 8% 23%

4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Peptide methionine sulfoxide reductase msrA

Chain A: 38% 32% 8% 23%

4.2.4 Score per residue for model 4

• Molecule 1: Peptide methionine sulfoxide reductase msrA

Chain A: 36% 32% 9% 23%

4.2.5 Score per residue for model 5

• Molecule 1: Peptide methionine sulfoxide reductase msrA
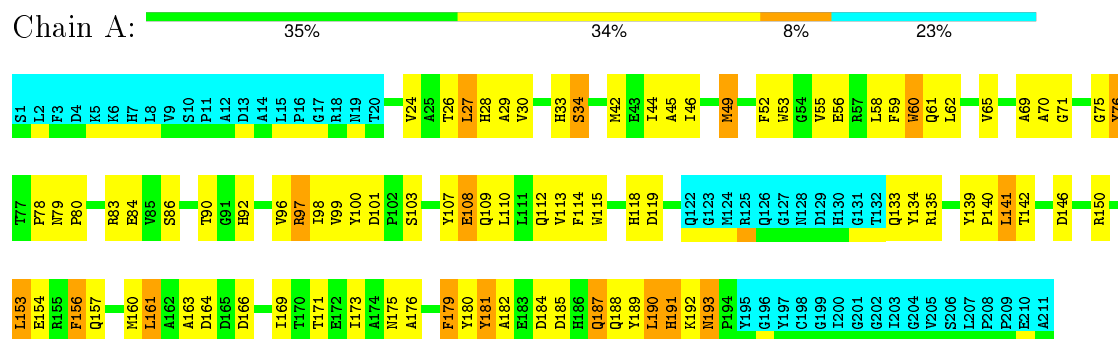
4.2.6 Score per residue for model 6

• Molecule 1: Peptide methionine sulfoxide reductase msrA
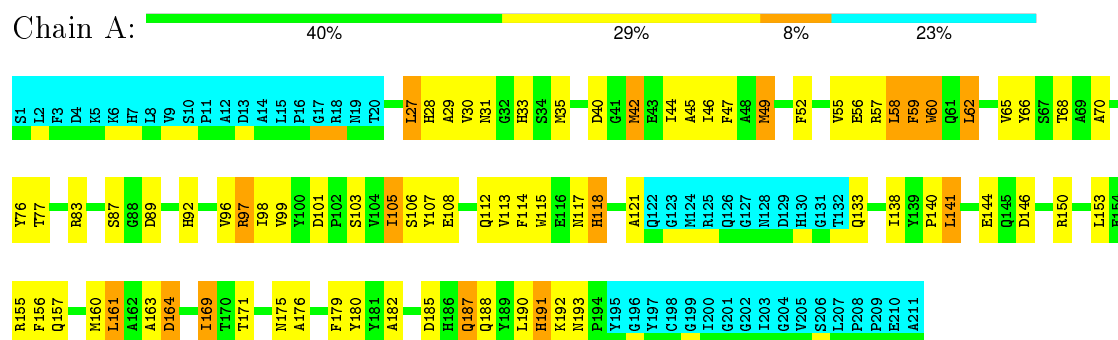
4.2.7 Score per residue for model 7

• Molecule 1: Peptide methionine sulfoxide reductase msrA
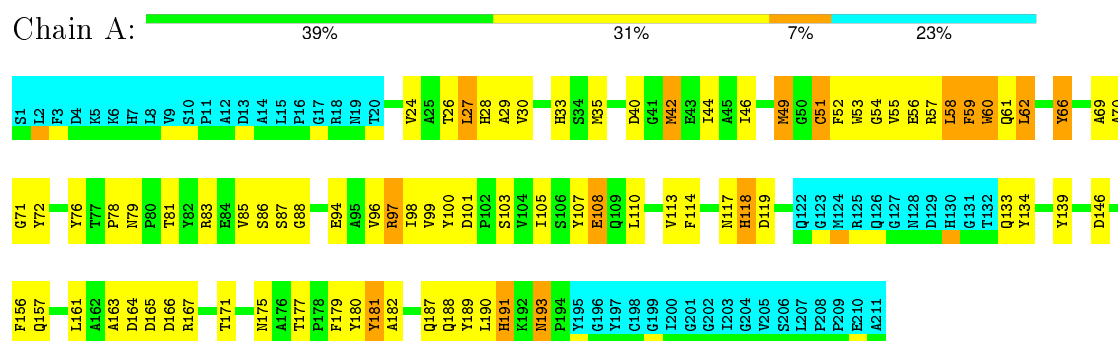
4.2.8 Score per residue for model 8

• Molecule 1: Peptide methionine sulfoxide reductase msrA
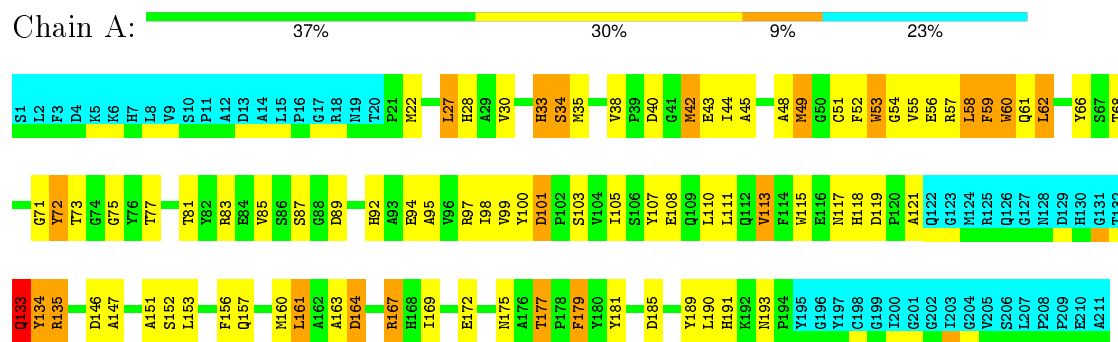
4.2.9 Score per residue for model 9

• Molecule 1: Peptide methionine sulfoxide reductase msrA
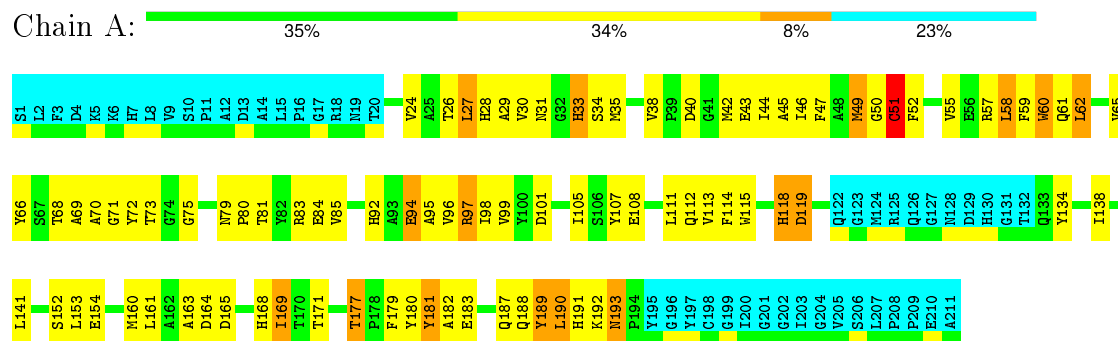
4.2.10 Score per residue for model 10

• Molecule 1: Peptide methionine sulfoxide reductase msrA
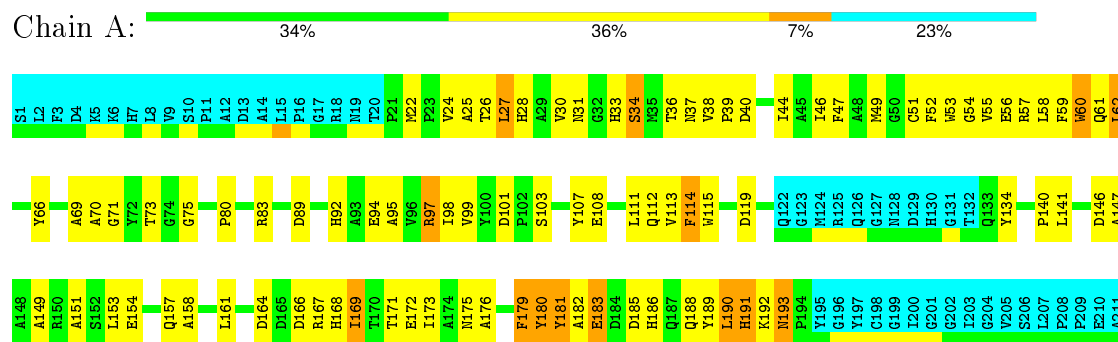
4.2.11 Score per residue for model 11

• Molecule 1: Peptide methionine sulfoxide reductase msrA
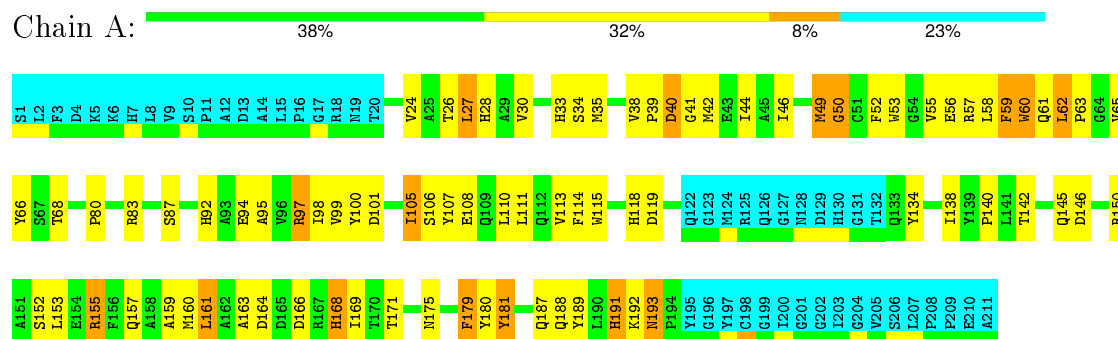
4.2.12 Score per residue for model 12

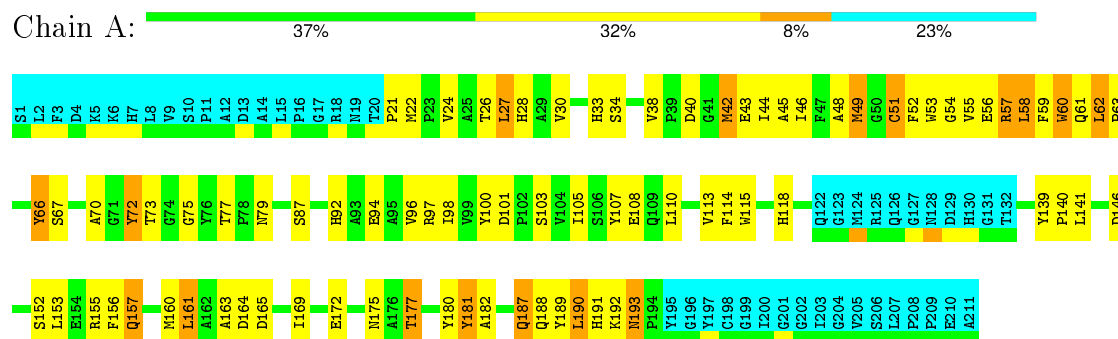• Molecule 1: Peptide methionine sulfoxide reductase msrA
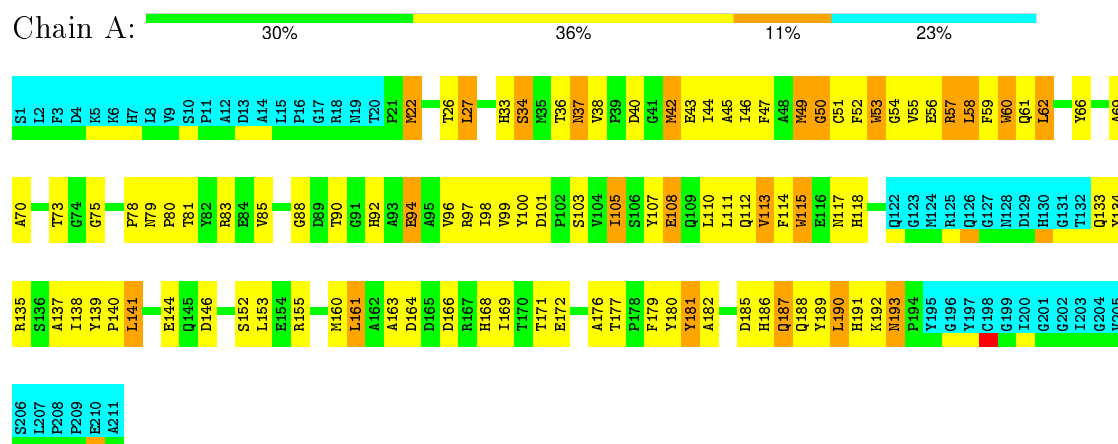
4.2.13 Score per residue for model 13

• Molecule 1: Peptide methionine sulfoxide reductase msrA
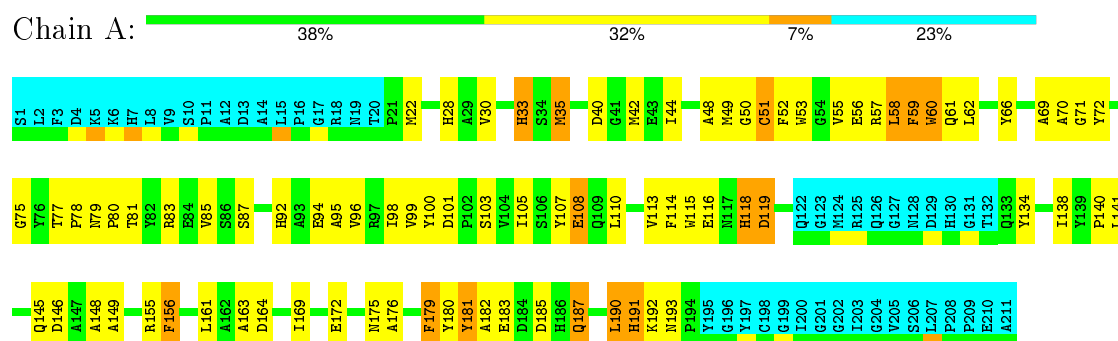
4.2.14 Score per residue for model 14

• Molecule 1: Peptide methionine sulfoxide reductase msrA
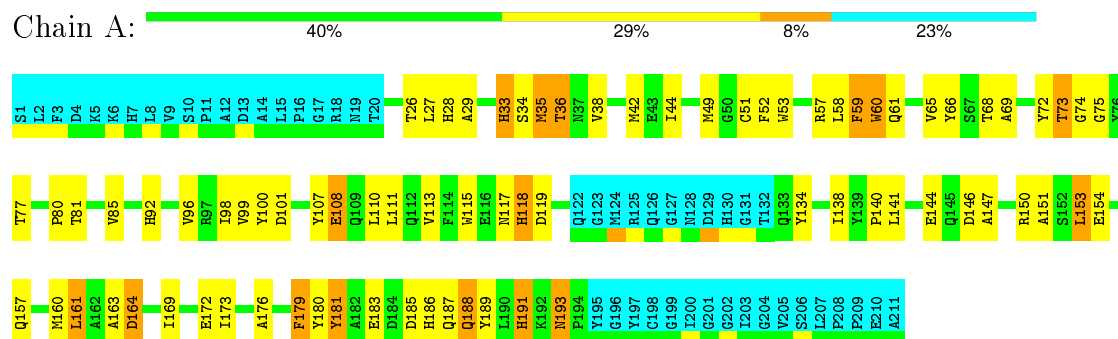
4.2.15 Score per residue for model 15

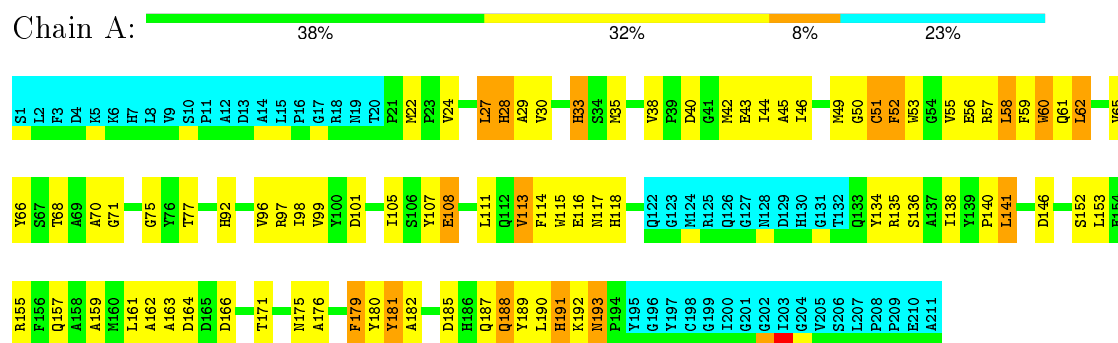• Molecule 1: Peptide methionine sulfoxide reductase msrA
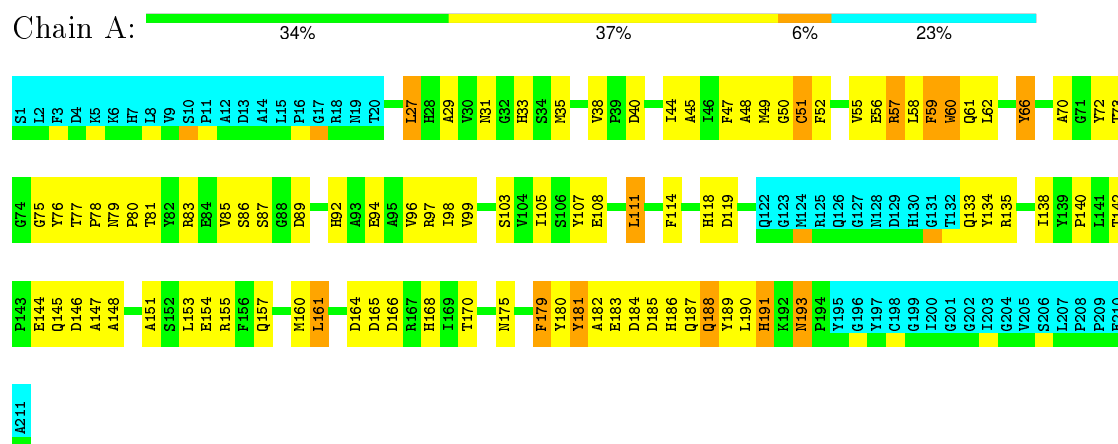
4.2.16 Score per residue for model 16

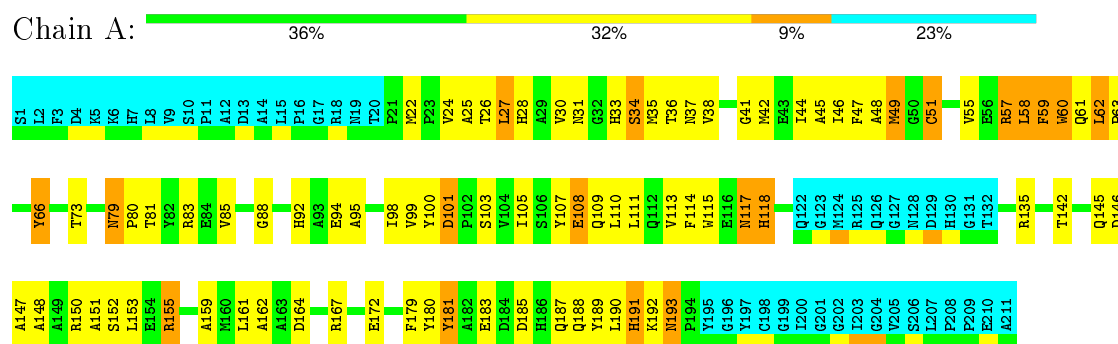• Molecule 1: Peptide methionine sulfoxide reductase msrA
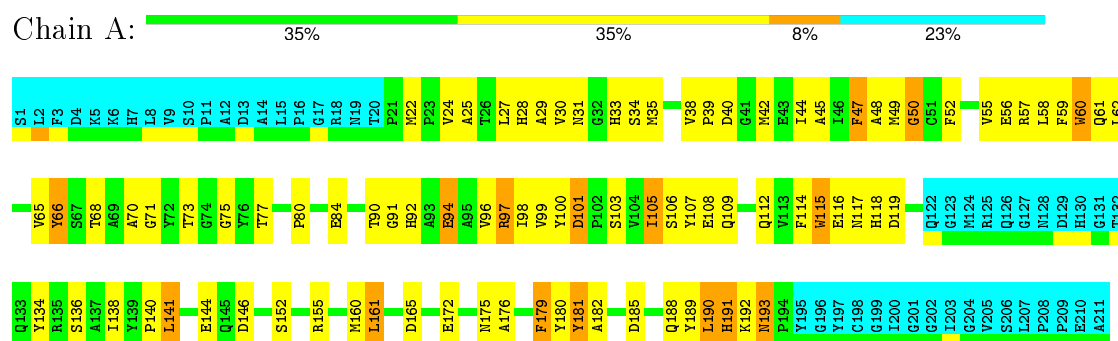
4.2.17 Score per residue for model 17

• Molecule 1: Peptide methionine sulfoxide reductase msrA

Chain A:

34%   35%   9%   23%
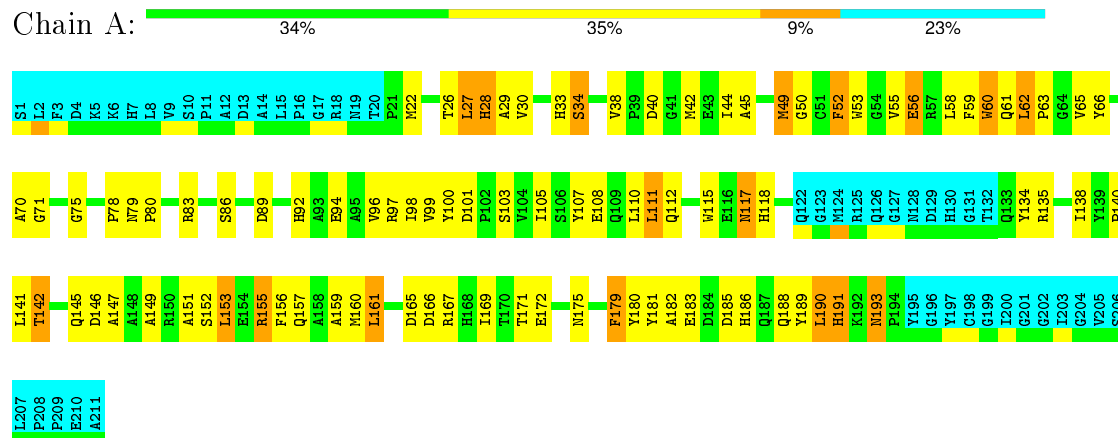
4.2.18 Score per residue for model 18

• Molecule 1: Peptide methionine sulfoxide reductase msrA

Chain A:

36%   32%   9%   23%
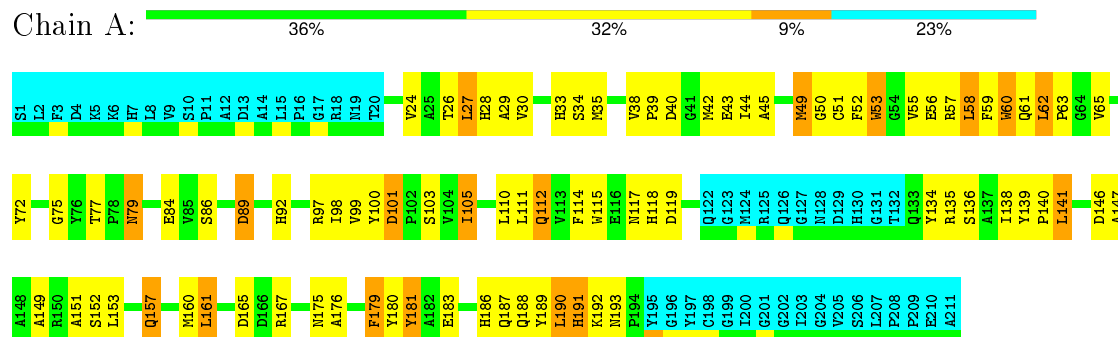
4.2.19 Score per residue for model 19

• Molecule 1: Peptide methionine sulfoxide reductase msrA

Chain A:

33%   36%   9%   23%
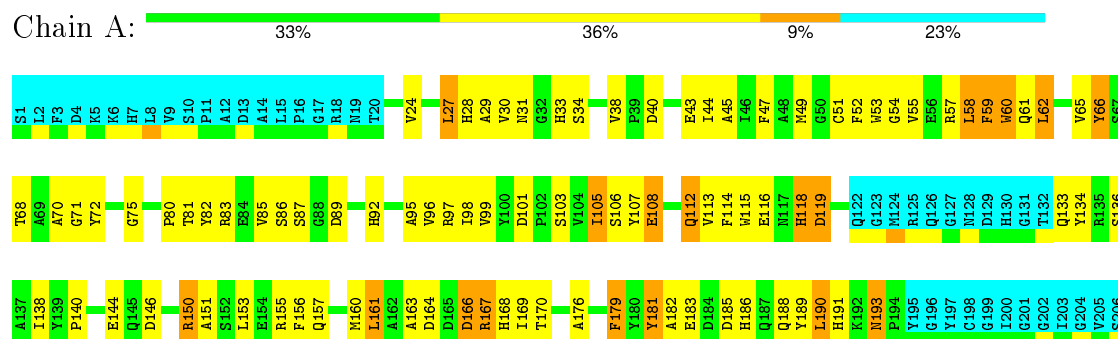
L207 P208 P209 E210 A211

4.2.20 Score per residue for model 20

• Molecule 1: Peptide methionine sulfoxide reductase msrA

Chain A:

35%   35%   8%   23%

S1 L2 F3 D4 K5 K6 H7 L8 V9 S10 P11 A12 D13 A14 L15 P16 G17 R18 N19 T20 P21 M22 P23 V24 A25 T26 L27 H28 A29 V30 N31 G32 H33 S34 M35 T36 N37 V38 M42 E43 I44 A45 I46 M49 F52 W53 G54 V55 E56 R57 L58 F59 W60 Q61 V65 Y66

S67 T68 A69 A70 G75 Y76 T77 R83 D89 H92 A93 E94 A95 V96 R97 I98 V99 Y100 D101 P102 S103 V104 I105 S106 Y107 E108 Q109 L110 L111 Q112 V113 F114 W115 H118 D119 Q122 G123 M124 R125 Q126 G127 N128 D129 H130 G131 T132 Q133 Y134 R135 S136 L141 D146

A147 R150 A151 S152 L153 E154 R155 F156 L161 A162 A163 D164 D165 D166 R167 H168 T171 N175 A176 T177 P178 F179 Y180 Y181 A182 E183 D184 D185 H186 Q187 Q188 Y189 L190 H191 K192 N193 P194 Y195 G196 Y197 C198 G199 I200 G201 G202 I203 G204 V205 S206 L207 P208 P209 E210 A211

5 Refinement protocol and experimental data overview ⓘ

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	
DYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6786
Number of chemical shift lists	1
Total number of shifts	1579
Number of shifts mapped to atoms	1579
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	59%

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.

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	1284	1206	1187	77±12
All	All	25680	24120	23743	1531

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:30:VAL:HG11	1:A:60:TRP:CE2	1.00	1.92	2	11
1:A:62:LEU:HD11	1:A:113:VAL:HG11	0.99	1.31	5	3
1:A:30:VAL:HG11	1:A:60:TRP:CD2	0.95	1.96	8	13
1:A:140:PRO:O	1:A:176:ALA:HB2	0.94	1.62	14	8
1:A:38:VAL:HG21	1:A:44:ILE:HD11	0.93	1.39	1	12
1:A:153:LEU:HD11	1:A:171:THR:CG2	0.93	1.93	10	1
1:A:47:PHE:CZ	1:A:98:ILE:HD13	0.92	1.99	16	1
1:A:62:LEU:HD11	1:A:113:VAL:HG21	0.90	1.43	4	6
1:A:182:ALA:HB1	1:A:186:HIS:NE2	0.90	1.80	12	1
1:A:182:ALA:HB1	1:A:186:HIS:CE1	0.88	2.03	12	1
1:A:73:THR:HG21	1:A:179:PHE:CZ	0.87	2.03	12	3
1:A:47:PHE:CE2	1:A:59:PHE:CZ	0.84	2.66	16	1
1:A:69:ALA:HB1	1:A:181:TYR:CE1	0.83	2.08	7	1
1:A:46:ILE:HG21	1:A:179:PHE:CE2	0.83	2.08	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:77:THR:HG21	1:A:84:GLU:OE2	0.82	1.73	18	1
1:A:153:LEU:HD11	1:A:171:THR:HG21	0.82	1.49	10	1
1:A:26:THR:C	1:A:27:LEU:HD13	0.81	1.96	4	7
1:A:81:THR:O	1:A:85:VAL:HG23	0.81	1.76	4	9
1:A:53:TRP:CH2	1:A:189:TYR:CD2	0.80	2.69	12	1
1:A:55:VAL:HA	1:A:58:LEU:HD23	0.80	1.53	8	5
1:A:44:ILE:O	1:A:141:LEU:HD12	0.80	1.74	9	1
1:A:51:CYS:O	1:A:55:VAL:HG23	0.80	1.75	9	4
1:A:53:TRP:CH2	1:A:189:TYR:CD1	0.80	2.69	8	2
1:A:53:TRP:CZ3	1:A:189:TYR:CE1	0.79	2.71	3	6
1:A:29:ALA:HB3	1:A:188:GLN:OE1	0.79	1.77	18	9
1:A:69:ALA:HB1	1:A:187:GLN:OE1	0.79	1.78	14	1
1:A:70:ALA:HB3	1:A:187:GLN:OE1	0.78	1.78	7	4
1:A:141:LEU:HD22	1:A:176:ALA:CB	0.78	2.09	16	3
1:A:29:ALA:HB1	1:A:191:HIS:CE1	0.78	2.13	6	4
1:A:59:PHE:CZ	1:A:98:ILE:HG23	0.77	2.13	20	1
1:A:138:ILE:HG22	1:A:140:PRO:HD3	0.77	1.54	17	11
1:A:97:ARG:C	1:A:98:ILE:HD12	0.77	2.00	7	5
1:A:62:LEU:CD1	1:A:113:VAL:HG11	0.76	2.10	5	2
1:A:53:TRP:CZ2	1:A:189:TYR:CD2	0.76	2.74	12	2
1:A:52:PHE:CZ	1:A:70:ALA:HB1	0.75	2.16	9	3
1:A:62:LEU:HD13	1:A:63:PRO:HD2	0.73	1.60	18	3
1:A:53:TRP:CZ2	1:A:189:TYR:CG	0.73	2.76	8	1
1:A:29:ALA:HB3	1:A:188:GLN:CD	0.73	2.03	1	2
1:A:46:ILE:CG2	1:A:179:PHE:CE2	0.73	2.72	4	3
1:A:153:LEU:HD23	1:A:153:LEU:N	0.72	1.98	17	1
1:A:59:PHE:CE2	1:A:98:ILE:HG23	0.72	2.20	20	1
1:A:29:ALA:HB3	1:A:188:GLN:HG3	0.72	1.61	3	1
1:A:70:ALA:HA	1:A:96:VAL:HG12	0.71	1.59	16	13
1:A:44:ILE:CG1	1:A:99:VAL:HG22	0.71	2.15	9	17
1:A:73:THR:HG21	1:A:179:PHE:CE2	0.71	2.19	12	2
1:A:30:VAL:HG22	1:A:191:HIS:ND1	0.71	1.99	5	3
1:A:47:PHE:CZ	1:A:59:PHE:CE1	0.71	2.78	16	1
1:A:190:LEU:HD23	1:A:193:ASN:O	0.71	1.85	16	1
1:A:52:PHE:CE1	1:A:96:VAL:CG1	0.71	2.74	9	1
1:A:105:ILE:HD11	1:A:110:LEU:CD1	0.71	2.15	18	1
1:A:55:VAL:HG12	1:A:59:PHE:CE2	0.71	2.21	11	7
1:A:153:LEU:C	1:A:153:LEU:HD23	0.71	2.07	14	7
1:A:100:TYR:CE2	1:A:110:LEU:CD1	0.71	2.74	11	11
1:A:105:ILE:HD13	1:A:106:SER:N	0.71	2.00	11	4
1:A:114:PHE:CE2	1:A:138:ILE:HD11	0.71	2.21	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TRP:HB3	1:A:190:LEU:HD23	0.70	1.62	18	5
1:A:53:TRP:CH2	1:A:189:TYR:CE2	0.70	2.79	12	2
1:A:30:VAL:HG22	1:A:191:HIS:CG	0.70	2.21	17	6
1:A:62:LEU:HD22	1:A:110:LEU:HD23	0.70	1.64	12	1
1:A:105:ILE:HD11	1:A:110:LEU:CD2	0.70	2.17	17	1
1:A:53:TRP:HE1	1:A:186:HIS:HD1	0.70	1.30	10	1
1:A:153:LEU:HD11	1:A:171:THR:HG23	0.69	1.63	20	3
1:A:59:PHE:CE2	1:A:98:ILE:HD11	0.69	2.21	13	8
1:A:59:PHE:CE2	1:A:98:ILE:CD1	0.69	2.75	6	3
1:A:59:PHE:CZ	1:A:98:ILE:CG2	0.69	2.75	20	1
1:A:52:PHE:CZ	1:A:53:TRP:CD1	0.69	2.80	7	1
1:A:169:ILE:HG13	1:A:171:THR:HG22	0.69	1.65	11	1
1:A:47:PHE:CE2	1:A:59:PHE:CE1	0.69	2.81	16	1
1:A:153:LEU:HD23	1:A:153:LEU:C	0.68	2.08	1	6
1:A:49:MET:HB3	1:A:55:VAL:HG21	0.68	1.66	18	6
1:A:59:PHE:CE2	1:A:98:ILE:HD13	0.68	2.23	6	2
1:A:49:MET:CB	1:A:55:VAL:HG21	0.67	2.19	11	6
1:A:53:TRP:CE3	1:A:189:TYR:CE1	0.67	2.83	3	2
1:A:107:TYR:CD1	1:A:108:GLU:N	0.67	2.63	16	16
1:A:58:LEU:O	1:A:58:LEU:HD12	0.67	1.88	12	4
1:A:147:ALA:O	1:A:151:ALA:HB2	0.67	1.90	18	7
1:A:98:ILE:HD12	1:A:98:ILE:N	0.66	2.06	16	3
1:A:100:TYR:CD1	1:A:105:ILE:HG23	0.66	2.26	4	7
1:A:97:ARG:NE	1:A:179:PHE:CD2	0.66	2.64	7	1
1:A:53:TRP:CH2	1:A:189:TYR:CE1	0.65	2.84	8	4
1:A:60:TRP:C	1:A:60:TRP:CD1	0.65	2.69	16	5
1:A:27:LEU:HD13	1:A:27:LEU:N	0.65	2.05	4	2
1:A:24:VAL:HG21	1:A:181:TYR:HB3	0.65	1.68	1	10
1:A:53:TRP:CE3	1:A:189:TYR:CD1	0.65	2.85	3	5
1:A:53:TRP:CD2	1:A:189:TYR:CD1	0.65	2.85	3	3
1:A:182:ALA:CB	1:A:186:HIS:CE1	0.65	2.79	12	1
1:A:142:THR:HG23	1:A:145:GLN:HB2	0.65	1.68	17	1
1:A:60:TRP:CZ2	1:A:61:GLN:NE2	0.65	2.64	9	2
1:A:115:TRP:CZ2	1:A:152:SER:CB	0.64	2.80	12	6
1:A:189:TYR:CE1	1:A:193:ASN:ND2	0.64	2.65	18	1
1:A:52:PHE:CD1	1:A:53:TRP:N	0.64	2.66	11	2
1:A:44:ILE:HG12	1:A:99:VAL:HG22	0.64	1.70	3	16
1:A:60:TRP:HA	1:A:65:VAL:HG11	0.64	1.70	6	2
1:A:73:THR:CB	1:A:179:PHE:CE1	0.64	2.81	4	2
1:A:52:PHE:CE1	1:A:96:VAL:HG13	0.64	2.26	9	1
1:A:71:GLY:HA2	1:A:182:ALA:HB2	0.63	1.70	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TRP:CH2	1:A:189:TYR:CZ	0.63	2.87	19	2
1:A:82:TYR:CE1	1:A:186:HIS:CE1	0.63	2.87	19	1
1:A:49:MET:HB2	1:A:55:VAL:HG21	0.63	1.68	11	4
1:A:141:LEU:HD22	1:A:176:ALA:HB3	0.63	1.71	3	3
1:A:68:THR:HG23	1:A:98:ILE:HG13	0.63	1.70	16	1
1:A:35:MET:SD	1:A:69:ALA:HB2	0.63	2.34	13	1
1:A:59:PHE:O	1:A:65:VAL:HG21	0.63	1.94	17	8
1:A:161:LEU:HD23	1:A:168:HIS:NE2	0.63	2.09	12	1
1:A:52:PHE:CZ	1:A:96:VAL:CG1	0.62	2.82	9	1
1:A:30:VAL:HG23	1:A:188:GLN:HG2	0.62	1.72	7	1
1:A:115:TRP:HZ3	1:A:171:THR:HG21	0.62	1.54	17	1
1:A:29:ALA:HB2	1:A:188:GLN:OE1	0.62	1.95	15	1
1:A:30:VAL:HG22	1:A:191:HIS:CD2	0.62	2.30	4	1
1:A:26:THR:HG22	1:A:27:LEU:HD13	0.62	1.71	9	7
1:A:115:TRP:CZ3	1:A:171:THR:HG21	0.62	2.30	17	1
1:A:60:TRP:CZ2	1:A:61:GLN:OE1	0.61	2.54	8	1
1:A:73:THR:OG1	1:A:179:PHE:CE1	0.61	2.54	4	2
1:A:38:VAL:HG22	1:A:99:VAL:HG11	0.61	1.72	12	2
1:A:49:MET:HB3	1:A:55:VAL:HG11	0.61	1.73	5	1
1:A:142:THR:HG23	1:A:145:GLN:CB	0.61	2.25	17	1
1:A:24:VAL:HG11	1:A:181:TYR:CE1	0.61	2.30	16	1
1:A:49:MET:SD	1:A:114:PHE:CE2	0.60	2.94	6	2
1:A:26:THR:HG22	1:A:27:LEU:CD1	0.60	2.26	12	6
1:A:153:LEU:HD23	1:A:154:GLU:N	0.60	2.11	5	2
1:A:73:THR:CG2	1:A:179:PHE:CZ	0.60	2.84	12	2
1:A:189:TYR:CE2	1:A:193:ASN:OD1	0.60	2.54	12	1
1:A:118:HIS:CE1	1:A:119:ASP:O	0.60	2.55	8	8
1:A:179:PHE:C	1:A:179:PHE:CD1	0.60	2.75	5	6
1:A:59:PHE:CE2	1:A:65:VAL:HG22	0.60	2.32	20	1
1:A:22:MET:HE1	1:A:81:THR:HG23	0.60	1.73	12	1
1:A:33:HIS:CG	1:A:34:SER:N	0.60	2.70	16	10
1:A:49:MET:SD	1:A:114:PHE:CZ	0.60	2.95	20	1
1:A:62:LEU:HD11	1:A:113:VAL:CG1	0.59	2.21	5	1
1:A:57:ARG:HD3	1:A:190:LEU:HD13	0.59	1.72	16	1
1:A:179:PHE:CZ	1:A:181:TYR:CE1	0.59	2.90	17	1
1:A:33:HIS:CD2	1:A:34:SER:O	0.59	2.56	4	4
1:A:60:TRP:C	1:A:60:TRP:CE3	0.59	2.76	10	10
1:A:153:LEU:N	1:A:153:LEU:CD2	0.59	2.66	17	1
1:A:58:LEU:HD12	1:A:58:LEU:C	0.59	2.18	12	1
1:A:28:HIS:CE1	1:A:188:GLN:OE1	0.58	2.55	16	2
1:A:59:PHE:CZ	1:A:98:ILE:HD13	0.58	2.32	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:TYR:CD1	1:A:134:TYR:O	0.58	2.57	14	7
1:A:134:TYR:O	1:A:134:TYR:CD1	0.58	2.57	5	5
1:A:73:THR:HG23	1:A:95:ALA:HB3	0.58	1.74	10	1
1:A:60:TRP:CE3	1:A:60:TRP:C	0.58	2.76	1	3
1:A:62:LEU:HD21	1:A:113:VAL:HG21	0.58	1.75	6	1
1:A:52:PHE:CD1	1:A:94:GLU:CG	0.58	2.87	9	1
1:A:53:TRP:CZ3	1:A:189:TYR:CD1	0.58	2.92	19	2
1:A:105:ILE:HD11	1:A:109:GLN:CG	0.58	2.29	16	1
1:A:169:ILE:HD12	1:A:171:THR:CG2	0.58	2.29	5	1
1:A:49:MET:HB2	1:A:55:VAL:HG11	0.57	1.75	17	2
1:A:52:PHE:CZ	1:A:96:VAL:HG12	0.57	2.34	9	1
1:A:72:TYR:N	1:A:72:TYR:CD1	0.57	2.73	2	2
1:A:44:ILE:HG13	1:A:99:VAL:HG22	0.57	1.76	9	5
1:A:105:ILE:C	1:A:105:ILE:HD13	0.57	2.19	18	1
1:A:30:VAL:HG11	1:A:60:TRP:CE3	0.57	2.34	8	3
1:A:179:PHE:CD1	1:A:179:PHE:C	0.57	2.78	14	3
1:A:49:MET:SD	1:A:114:PHE:CD2	0.57	2.97	6	1
1:A:168:HIS:CE1	1:A:169:ILE:O	0.57	2.57	11	1
1:A:53:TRP:CZ2	1:A:189:TYR:CD1	0.57	2.93	18	2
1:A:24:VAL:HG21	1:A:181:TYR:CB	0.57	2.29	20	7
1:A:24:VAL:HG21	1:A:181:TYR:CG	0.57	2.35	16	1
1:A:187:GLN:C	1:A:188:GLN:HG2	0.56	2.21	18	3
1:A:98:ILE:N	1:A:98:ILE:HD12	0.56	2.14	7	2
1:A:51:CYS:CB	1:A:55:VAL:HG23	0.56	2.31	10	2
1:A:47:PHE:CZ	1:A:98:ILE:CD1	0.56	2.83	16	1
1:A:107:TYR:CD1	1:A:107:TYR:C	0.56	2.79	19	1
1:A:118:HIS:C	1:A:118:HIS:CD2	0.56	2.78	7	3
1:A:111:LEU:O	1:A:115:TRP:CD1	0.56	2.58	10	3
1:A:58:LEU:O	1:A:62:LEU:HD23	0.56	2.01	2	2
1:A:169:ILE:HD12	1:A:171:THR:HG22	0.56	1.75	5	1
1:A:52:PHE:CE2	1:A:70:ALA:HB1	0.56	2.36	9	2
1:A:30:VAL:CG1	1:A:60:TRP:CD2	0.56	2.83	8	3
1:A:97:ARG:CZ	1:A:179:PHE:CD2	0.56	2.88	7	1
1:A:22:MET:CE	1:A:81:THR:HG23	0.56	2.30	12	1
1:A:62:LEU:HD23	1:A:65:VAL:HG23	0.56	1.77	3	2
1:A:58:LEU:HD22	1:A:117:ASN:CG	0.56	2.21	4	2
1:A:72:TYR:CZ	1:A:182:ALA:HB1	0.56	2.36	13	2
1:A:189:TYR:C	1:A:189:TYR:CD1	0.55	2.80	9	1
1:A:100:TYR:CD2	1:A:110:LEU:HD11	0.55	2.36	12	6
1:A:52:PHE:CD1	1:A:52:PHE:N	0.55	2.74	1	5
1:A:52:PHE:HZ	1:A:70:ALA:HB1	0.55	1.61	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:59:PHE:CD2	1:A:65:VAL:CG2	0.55	2.90	20	1
1:A:97:ARG:NE	1:A:179:PHE:CG	0.55	2.75	7	1
1:A:80:PRO:HG3	1:A:92:HIS:CD2	0.55	2.36	12	8
1:A:183:GLU:CB	1:A:186:HIS:CD2	0.55	2.89	15	2
1:A:107:TYR:C	1:A:107:TYR:CD1	0.55	2.80	16	4
1:A:59:PHE:CD1	1:A:98:ILE:HG21	0.55	2.37	19	1
1:A:179:PHE:O	1:A:179:PHE:CD1	0.55	2.60	18	2
1:A:140:PRO:C	1:A:141:LEU:HD22	0.55	2.22	1	2
1:A:153:LEU:CD1	1:A:171:THR:HG23	0.55	2.32	5	2
1:A:153:LEU:O	1:A:153:LEU:HD23	0.55	2.02	15	3
1:A:58:LEU:CD2	1:A:117:ASN:ND2	0.55	2.69	6	2
1:A:111:LEU:O	1:A:115:TRP:CD2	0.55	2.59	12	4
1:A:59:PHE:HD1	1:A:65:VAL:HG21	0.55	1.62	19	1
1:A:72:TYR:CZ	1:A:182:ALA:CB	0.55	2.90	13	2
1:A:191:HIS:CD2	1:A:192:LYS:N	0.55	2.75	16	3
1:A:30:VAL:HG21	1:A:60:TRP:CE2	0.55	2.37	13	2
1:A:57:ARG:HA	1:A:60:TRP:CE3	0.54	2.37	16	4
1:A:47:PHE:CD2	1:A:114:PHE:CE2	0.54	2.95	6	1
1:A:42:MET:SD	1:A:66:TYR:CG	0.54	3.00	2	5
1:A:30:VAL:HG11	1:A:60:TRP:CG	0.54	2.37	9	3
1:A:141:LEU:CD1	1:A:176:ALA:HB3	0.54	2.32	20	1
1:A:62:LEU:CD1	1:A:113:VAL:HG21	0.54	2.28	4	1
1:A:47:PHE:CD2	1:A:59:PHE:CZ	0.54	2.96	4	1
1:A:118:HIS:CE1	1:A:119:ASP:OD1	0.54	2.61	15	1
1:A:121:ALA:HB2	1:A:169:ILE:HG13	0.54	1.78	8	1
1:A:97:ARG:CB	1:A:179:PHE:CZ	0.54	2.89	6	2
1:A:105:ILE:HD11	1:A:110:LEU:HG	0.54	1.80	17	1
1:A:115:TRP:CZ2	1:A:153:LEU:HD21	0.54	2.37	17	1
1:A:139:TYR:N	1:A:139:TYR:CD1	0.54	2.75	18	1
1:A:111:LEU:HD23	1:A:112:GLN:N	0.54	2.17	17	1
1:A:59:PHE:CZ	1:A:114:PHE:CZ	0.54	2.96	10	1
1:A:57:ARG:O	1:A:61:GLN:CG	0.54	2.55	9	8
1:A:42:MET:CE	1:A:66:TYR:CG	0.53	2.91	20	1
1:A:121:ALA:HB1	1:A:168:HIS:O	0.53	2.04	1	1
1:A:28:HIS:CE1	1:A:188:GLN:CD	0.53	2.81	16	1
1:A:30:VAL:CG1	1:A:60:TRP:CE2	0.53	2.83	7	6
1:A:30:VAL:CG2	1:A:191:HIS:CD2	0.53	2.91	4	1
1:A:60:TRP:CG	1:A:61:GLN:N	0.53	2.75	10	13
1:A:30:VAL:HG11	1:A:60:TRP:CZ2	0.53	2.38	7	4
1:A:141:LEU:CD2	1:A:176:ALA:HB3	0.53	2.33	3	2
1:A:82:TYR:CD1	1:A:186:HIS:NE2	0.53	2.77	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:GLU:HB3	1:A:186:HIS:CD2	0.53	2.38	15	6
1:A:113:VAL:HG22	1:A:117:ASN:HD21	0.53	1.63	12	1
1:A:27:LEU:N	1:A:27:LEU:HD22	0.53	2.19	20	4
1:A:72:TYR:CE2	1:A:182:ALA:HA	0.53	2.39	13	2
1:A:46:ILE:HG22	1:A:139:TYR:CD2	0.53	2.38	7	3
1:A:100:TYR:CE2	1:A:110:LEU:HD11	0.53	2.39	11	5
1:A:141:LEU:HD12	1:A:176:ALA:HB3	0.53	1.81	20	1
1:A:153:LEU:HD23	1:A:153:LEU:O	0.53	2.03	19	4
1:A:52:PHE:N	1:A:52:PHE:CD1	0.53	2.77	17	5
1:A:28:HIS:CD2	1:A:68:THR:O	0.53	2.61	16	6
1:A:115:TRP:CZ2	1:A:152:SER:OG	0.53	2.58	8	1
1:A:98:ILE:CD1	1:A:98:ILE:N	0.53	2.71	16	2
1:A:73:THR:CG2	1:A:179:PHE:CE2	0.53	2.91	12	1
1:A:105:ILE:CD1	1:A:106:SER:O	0.53	2.57	19	2
1:A:69:ALA:HB3	1:A:97:ARG:HB3	0.53	1.80	20	1
1:A:115:TRP:CZ2	1:A:138:ILE:HD11	0.52	2.40	17	2
1:A:153:LEU:O	1:A:157:GLN:CB	0.52	2.57	17	1
1:A:72:TYR:CZ	1:A:182:ALA:HA	0.52	2.39	15	2
1:A:187:GLN:O	1:A:188:GLN:HG2	0.52	2.04	3	3
1:A:105:ILE:HD11	1:A:110:LEU:CG	0.52	2.34	17	1
1:A:27:LEU:HD22	1:A:27:LEU:N	0.52	2.19	7	7
1:A:52:PHE:CD1	1:A:94:GLU:HG3	0.52	2.39	9	1
1:A:105:ILE:CD1	1:A:109:GLN:CD	0.52	2.78	16	1
1:A:97:ARG:HB2	1:A:179:PHE:CZ	0.52	2.40	6	5
1:A:154:GLU:O	1:A:158:ALA:CB	0.52	2.57	10	1
1:A:59:PHE:CD2	1:A:98:ILE:HD11	0.52	2.40	9	1
1:A:59:PHE:CD2	1:A:98:ILE:CD1	0.52	2.92	9	2
1:A:28:HIS:CE1	1:A:188:GLN:HG2	0.52	2.40	17	9
1:A:69:ALA:HB3	1:A:97:ARG:HG2	0.52	1.82	5	1
1:A:111:LEU:O	1:A:115:TRP:CE2	0.52	2.63	12	1
1:A:42:MET:HE2	1:A:66:TYR:HB2	0.52	1.80	3	1
1:A:115:TRP:CZ2	1:A:152:SER:HB2	0.52	2.39	18	6
1:A:53:TRP:O	1:A:57:ARG:CB	0.52	2.58	20	1
1:A:30:VAL:CG2	1:A:191:HIS:CG	0.52	2.93	17	1
1:A:33:HIS:CD2	1:A:34:SER:N	0.52	2.78	18	2
1:A:45:ALA:N	1:A:98:ILE:O	0.51	2.43	20	15
1:A:68:THR:HG22	1:A:98:ILE:HG23	0.51	1.81	9	1
1:A:60:TRP:CD2	1:A:61:GLN:N	0.51	2.78	11	12
1:A:62:LEU:HD23	1:A:63:PRO:HD2	0.51	1.81	4	2
1:A:105:ILE:HD11	1:A:110:LEU:HD21	0.51	1.82	17	1
1:A:58:LEU:C	1:A:58:LEU:HD12	0.51	2.25	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ALA:HB1	1:A:94:GLU:O	0.51	2.06	15	5
1:A:60:TRP:C	1:A:60:TRP:CD2	0.51	2.84	1	10
1:A:60:TRP:CD1	1:A:60:TRP:C	0.51	2.84	15	2
1:A:193:ASN:ND2	1:A:193:ASN:N	0.51	2.58	12	2
1:A:28:HIS:NE2	1:A:188:GLN:NE2	0.51	2.59	11	4
1:A:65:VAL:HG13	1:A:98:ILE:HG23	0.51	1.83	9	1
1:A:59:PHE:CD2	1:A:98:ILE:HD13	0.51	2.41	19	1
1:A:29:ALA:CB	1:A:188:GLN:OE1	0.51	2.59	17	11
1:A:168:HIS:O	1:A:168:HIS:CD2	0.51	2.64	10	1
1:A:79:ASN:N	1:A:80:PRO:HD3	0.51	2.21	12	2
1:A:69:ALA:CB	1:A:181:TYR:CE1	0.51	2.90	7	1
1:A:105:ILE:HD11	1:A:110:LEU:HD11	0.51	1.81	18	1
1:A:69:ALA:CB	1:A:187:GLN:OE1	0.50	2.56	14	1
1:A:38:VAL:HG13	1:A:42:MET:HB3	0.50	1.83	16	3
1:A:163:ALA:O	1:A:164:ASP:CB	0.50	2.60	9	14
1:A:49:MET:SD	1:A:114:PHE:CE1	0.50	3.04	9	1
1:A:59:PHE:CE1	1:A:98:ILE:HG21	0.50	2.40	19	1
1:A:80:PRO:CG	1:A:92:HIS:CD2	0.50	2.93	9	2
1:A:152:SER:O	1:A:156:PHE:CB	0.50	2.60	17	1
1:A:81:THR:O	1:A:85:VAL:CG2	0.50	2.60	1	2
1:A:153:LEU:CD2	1:A:153:LEU:C	0.50	2.80	1	5
1:A:193:ASN:N	1:A:193:ASN:ND2	0.50	2.59	7	2
1:A:45:ALA:HB1	1:A:47:PHE:CE2	0.50	2.41	15	1
1:A:153:LEU:C	1:A:153:LEU:CD2	0.50	2.79	6	6
1:A:72:TYR:CE1	1:A:182:ALA:CB	0.50	2.94	13	2
1:A:114:PHE:CE2	1:A:138:ILE:CD1	0.50	2.94	9	1
1:A:59:PHE:O	1:A:65:VAL:CG2	0.50	2.60	5	4
1:A:47:PHE:CG	1:A:114:PHE:CZ	0.50	2.99	10	1
1:A:111:LEU:HB3	1:A:115:TRP:CZ2	0.50	2.42	3	5
1:A:96:VAL:HG23	1:A:98:ILE:HD11	0.50	1.82	7	1
1:A:58:LEU:HD12	1:A:58:LEU:O	0.50	2.06	6	1
1:A:170:THR:HG22	1:A:170:THR:O	0.50	2.06	19	1
1:A:160:MET:HG3	1:A:161:LEU:N	0.50	2.21	19	11
1:A:48:ALA:CB	1:A:94:GLU:O	0.50	2.60	8	4
1:A:53:TRP:CH2	1:A:189:TYR:CG	0.50	2.99	8	1
1:A:97:ARG:CZ	1:A:179:PHE:CG	0.50	2.95	7	1
1:A:73:THR:CB	1:A:179:PHE:CZ	0.50	2.95	4	1
1:A:188:GLN:CG	1:A:188:GLN:O	0.50	2.60	14	1
1:A:57:ARG:NH2	1:A:61:GLN:NE2	0.50	2.60	20	1
1:A:147:ALA:O	1:A:151:ALA:CB	0.50	2.59	18	5
1:A:56:GLU:O	1:A:60:TRP:CE3	0.50	2.65	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:PHE:CD2	1:A:98:ILE:HG12	0.49	2.42	19	3
1:A:118:HIS:CG	1:A:119:ASP:N	0.49	2.79	14	7
1:A:115:TRP:HB3	1:A:156:PHE:CZ	0.49	2.42	5	1
1:A:52:PHE:CG	1:A:94:GLU:OE1	0.49	2.65	11	1
1:A:179:PHE:CD1	1:A:179:PHE:O	0.49	2.64	17	1
1:A:60:TRP:CE3	1:A:60:TRP:O	0.49	2.66	20	5
1:A:60:TRP:CE2	1:A:61:GLN:HG2	0.49	2.43	9	11
1:A:59:PHE:CE2	1:A:98:ILE:HG12	0.49	2.42	20	1
1:A:71:GLY:N	1:A:97:ARG:NH2	0.49	2.60	7	1
1:A:54:GLY:HA2	1:A:190:LEU:HD23	0.49	1.84	7	1
1:A:72:TYR:CE1	1:A:85:VAL:HG11	0.49	2.42	9	2
1:A:97:ARG:CZ	1:A:99:VAL:HG21	0.49	2.38	6	1
1:A:73:THR:OG1	1:A:177:THR:CG2	0.49	2.60	8	2
1:A:153:LEU:HD13	1:A:173:ILE:HD11	0.49	1.84	14	2
1:A:76:TYR:C	1:A:76:TYR:CD1	0.49	2.85	5	1
1:A:97:ARG:HG3	1:A:179:PHE:CE1	0.49	2.43	6	1
1:A:69:ALA:O	1:A:96:VAL:HG13	0.49	2.07	14	1
1:A:52:PHE:CG	1:A:53:TRP:N	0.49	2.81	12	2
1:A:56:GLU:OE1	1:A:70:ALA:HB2	0.49	2.07	2	1
1:A:51:CYS:HB3	1:A:55:VAL:HG23	0.49	1.83	2	3
1:A:97:ARG:HD2	1:A:179:PHE:CD1	0.49	2.42	7	1
1:A:105:ILE:HD11	1:A:109:GLN:HG2	0.49	1.84	16	1
1:A:55:VAL:HG22	1:A:117:ASN:OD1	0.49	2.07	16	1
1:A:115:TRP:CH2	1:A:171:THR:HG21	0.49	2.42	5	1
1:A:52:PHE:O	1:A:56:GLU:CB	0.49	2.61	16	5
1:A:66:TYR:N	1:A:99:VAL:O	0.49	2.44	20	8
1:A:57:ARG:CZ	1:A:61:GLN:CD	0.49	2.80	10	1
1:A:42:MET:SD	1:A:66:TYR:CD1	0.49	3.06	2	2
1:A:155:ARG:O	1:A:159:ALA:CB	0.49	2.61	4	1
1:A:55:VAL:HG23	1:A:56:GLU:N	0.48	2.23	5	1
1:A:100:TYR:CE2	1:A:110:LEU:HD13	0.48	2.41	4	2
1:A:72:TYR:CE1	1:A:182:ALA:HB1	0.48	2.43	13	1
1:A:191:HIS:CD2	1:A:191:HIS:N	0.48	2.81	11	1
1:A:60:TRP:CH2	1:A:191:HIS:CB	0.48	2.95	16	1
1:A:55:VAL:HG12	1:A:59:PHE:CZ	0.48	2.43	17	2
1:A:75:GLY:HA3	1:A:92:HIS:CD2	0.48	2.44	15	7
1:A:54:GLY:O	1:A:58:LEU:CB	0.48	2.61	1	2
1:A:97:ARG:HD3	1:A:99:VAL:HG23	0.48	1.84	6	1
1:A:111:LEU:CB	1:A:115:TRP:CZ2	0.48	2.95	18	1
1:A:157:GLN:O	1:A:160:MET:CG	0.48	2.61	17	11
1:A:38:VAL:HG13	1:A:39:PRO:HD2	0.48	1.85	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TRP:CB	1:A:190:LEU:HD23	0.48	2.38	19	1
1:A:75:GLY:HA3	1:A:92:HIS:CG	0.48	2.43	12	13
1:A:52:PHE:CE1	1:A:70:ALA:HB1	0.48	2.43	10	1
1:A:107:TYR:CE1	1:A:148:ALA:CB	0.48	2.96	15	2
1:A:169:ILE:CG1	1:A:171:THR:HG22	0.48	2.37	11	1
1:A:58:LEU:HD22	1:A:117:ASN:HD22	0.48	1.68	8	1
1:A:161:LEU:HD22	1:A:165:ASP:O	0.48	2.09	16	1
1:A:51:CYS:O	1:A:55:VAL:CG2	0.48	2.57	9	1
1:A:42:MET:SD	1:A:101:ASP:CA	0.48	3.01	18	1
1:A:155:ARG:O	1:A:159:ALA:N	0.48	2.47	17	2
1:A:109:GLN:O	1:A:113:VAL:HG23	0.48	2.09	4	1
1:A:107:TYR:O	1:A:111:LEU:HD23	0.48	2.08	4	1
1:A:59:PHE:CD1	1:A:98:ILE:HG12	0.48	2.44	7	6
1:A:27:LEU:CB	1:A:33:HIS:C	0.48	2.82	3	3
1:A:57:ARG:O	1:A:61:GLN:CB	0.48	2.62	9	1
1:A:169:ILE:HG22	1:A:171:THR:HG23	0.48	1.85	9	1
1:A:187:GLN:C	1:A:188:GLN:CG	0.48	2.82	12	3
1:A:30:VAL:CG1	1:A:60:TRP:CZ2	0.48	2.97	2	3
1:A:62:LEU:CD2	1:A:105:ILE:HD13	0.48	2.39	4	1
1:A:97:ARG:CD	1:A:179:PHE:CD1	0.47	2.97	19	1
1:A:114:PHE:CE2	1:A:138:ILE:CG1	0.47	2.97	9	1
1:A:114:PHE:CZ	1:A:138:ILE:HG12	0.47	2.44	9	1
1:A:28:HIS:CE1	1:A:188:GLN:CG	0.47	2.97	19	4
1:A:107:TYR:CG	1:A:108:GLU:N	0.47	2.83	16	4
1:A:46:ILE:HD13	1:A:177:THR:O	0.47	2.09	20	1
1:A:66:TYR:CB	1:A:99:VAL:O	0.47	2.63	10	1
1:A:189:TYR:O	1:A:193:ASN:ND2	0.47	2.47	9	14
1:A:36:THR:HG23	1:A:37:ASN:N	0.47	2.25	10	3
1:A:80:PRO:HB3	1:A:92:HIS:CD2	0.47	2.44	11	4
1:A:115:TRP:HH2	1:A:171:THR:HG21	0.47	1.68	5	1
1:A:97:ARG:CZ	1:A:99:VAL:CG2	0.47	2.93	6	1
1:A:28:HIS:CE1	1:A:30:VAL:HB	0.47	2.44	20	14
1:A:46:ILE:O	1:A:47:PHE:CD1	0.47	2.68	12	2
1:A:114:PHE:O	1:A:118:HIS:N	0.47	2.47	16	10
1:A:54:GLY:O	1:A:57:ARG:CG	0.47	2.63	12	1
1:A:50:GLY:O	1:A:52:PHE:N	0.47	2.48	9	2
1:A:73:THR:HB	1:A:179:PHE:CD1	0.47	2.45	4	1
1:A:59:PHE:CG	1:A:98:ILE:HG12	0.47	2.44	11	14
1:A:24:VAL:HG11	1:A:181:TYR:CD1	0.47	2.45	2	2
1:A:60:TRP:CD2	1:A:60:TRP:C	0.47	2.88	7	3
1:A:52:PHE:CE2	1:A:53:TRP:CD1	0.47	3.03	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ALA:HB2	1:A:169:ILE:HG22	0.47	1.85	6	1
1:A:81:THR:O	1:A:85:VAL:N	0.47	2.47	12	1
1:A:60:TRP:CZ2	1:A:61:GLN:HG2	0.47	2.45	11	1
1:A:97:ARG:NE	1:A:179:PHE:CD1	0.47	2.83	3	1
1:A:100:TYR:CD1	1:A:100:TYR:C	0.47	2.88	8	4
1:A:55:VAL:HG12	1:A:59:PHE:CD2	0.47	2.45	13	3
1:A:36:THR:OG1	1:A:181:TYR:OH	0.47	2.33	14	1
1:A:38:VAL:CG2	1:A:44:ILE:HD11	0.47	2.40	11	1
1:A:118:HIS:CD2	1:A:136:SER:CB	0.47	2.98	18	1
1:A:24:VAL:CG2	1:A:182:ALA:O	0.47	2.63	7	1
1:A:105:ILE:HD13	1:A:106:SER:O	0.47	2.09	19	2
1:A:177:THR:HG22	1:A:179:PHE:CE1	0.47	2.44	9	1
1:A:30:VAL:CG1	1:A:60:TRP:CE3	0.47	2.98	8	3
1:A:97:ARG:HB2	1:A:179:PHE:CE1	0.47	2.45	8	1
1:A:51:CYS:O	1:A:55:VAL:N	0.46	2.42	9	2
1:A:189:TYR:CD1	1:A:189:TYR:C	0.46	2.88	14	2
1:A:58:LEU:HD11	1:A:113:VAL:CG1	0.46	2.40	20	2
1:A:55:VAL:CG1	1:A:59:PHE:CE2	0.46	2.97	11	3
1:A:111:LEU:HD21	1:A:138:ILE:HD13	0.46	1.88	15	1
1:A:56:GLU:HG3	1:A:57:ARG:N	0.46	2.26	12	1
1:A:180:TYR:O	1:A:181:TYR:C	0.46	2.54	11	4
1:A:118:HIS:HD1	1:A:119:ASP:N	0.46	2.08	16	1
1:A:94:GLU:N	1:A:94:GLU:OE1	0.46	2.48	16	1
1:A:59:PHE:CD2	1:A:65:VAL:HG21	0.46	2.45	20	1
1:A:44:ILE:HG23	1:A:97:ARG:CG	0.46	2.39	10	2
1:A:60:TRP:O	1:A:60:TRP:CE3	0.46	2.68	2	3
1:A:88:GLY:CA	1:A:133:GLN:OE1	0.46	2.63	7	1
1:A:57:ARG:HA	1:A:60:TRP:CZ3	0.46	2.46	15	2
1:A:183:GLU:O	1:A:186:HIS:N	0.46	2.49	1	1
1:A:42:MET:HE1	1:A:66:TYR:CD1	0.46	2.46	20	1
1:A:157:GLN:CD	1:A:169:ILE:HG21	0.46	2.31	10	1
1:A:115:TRP:CH2	1:A:153:LEU:HG	0.46	2.45	10	1
1:A:47:PHE:CD2	1:A:114:PHE:CZ	0.46	3.03	10	1
1:A:62:LEU:HD21	1:A:105:ILE:CD1	0.46	2.41	9	1
1:A:28:HIS:CD2	1:A:188:GLN:NE2	0.46	2.84	11	1
1:A:140:PRO:O	1:A:176:ALA:CB	0.46	2.59	10	1
1:A:166:ASP:O	1:A:168:HIS:N	0.46	2.48	19	2
1:A:35:MET:O	1:A:97:ARG:NH2	0.46	2.49	1	1
1:A:118:HIS:CD2	1:A:118:HIS:C	0.46	2.88	14	1
1:A:42:MET:SD	1:A:101:ASP:CB	0.46	3.04	18	1
1:A:76:TYR:N	1:A:76:TYR:CD1	0.46	2.83	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ARG:NH2	1:A:181:TYR:OH	0.46	2.49	1	1
1:A:57:ARG:NH2	1:A:61:GLN:OE1	0.46	2.49	10	1
1:A:31:ASN:ND2	1:A:66:TYR:O	0.46	2.49	19	2
1:A:39:PRO:HG3	1:A:66:TYR:CE2	0.46	2.46	16	1
1:A:53:TRP:CZ3	1:A:189:TYR:CZ	0.46	3.04	3	1
1:A:47:PHE:CZ	1:A:55:VAL:CG1	0.46	2.98	19	1
1:A:70:ALA:O	1:A:182:ALA:N	0.46	2.49	16	7
1:A:26:THR:O	1:A:35:MET:N	0.46	2.49	20	3
1:A:28:HIS:N	1:A:33:HIS:O	0.46	2.49	3	3
1:A:187:GLN:O	1:A:188:GLN:C	0.45	2.54	3	3
1:A:72:TYR:OH	1:A:182:ALA:HB1	0.45	2.11	13	2
1:A:76:TYR:CD1	1:A:76:TYR:N	0.45	2.85	15	1
1:A:46:ILE:HG21	1:A:179:PHE:CZ	0.45	2.45	4	1
1:A:57:ARG:NH1	1:A:61:GLN:OE1	0.45	2.50	11	1
1:A:28:HIS:NE2	1:A:68:THR:O	0.45	2.50	19	5
1:A:52:PHE:CZ	1:A:53:TRP:NE1	0.45	2.85	7	1
1:A:100:TYR:CD1	1:A:105:ILE:CG2	0.45	2.99	13	2
1:A:190:LEU:HD13	1:A:193:ASN:O	0.45	2.11	12	1
1:A:159:ALA:O	1:A:162:ALA:HB3	0.45	2.11	3	2
1:A:36:THR:CG2	1:A:37:ASN:N	0.45	2.80	12	3
1:A:49:MET:HG3	1:A:114:PHE:CE1	0.45	2.46	5	1
1:A:73:THR:OG1	1:A:74:GLY:N	0.45	2.50	14	2
1:A:108:GLU:HA	1:A:111:LEU:HD12	0.45	1.87	9	1
1:A:81:THR:OG1	1:A:84:GLU:CB	0.45	2.65	9	1
1:A:27:LEU:CD1	1:A:27:LEU:N	0.45	2.76	4	1
1:A:115:TRP:CE3	1:A:156:PHE:CE2	0.45	3.05	2	2
1:A:53:TRP:NE1	1:A:186:HIS:O	0.45	2.50	17	1
1:A:72:TYR:CD2	1:A:85:VAL:HG21	0.45	2.47	15	1
1:A:100:TYR:CZ	1:A:110:LEU:CD1	0.45	3.00	4	2
1:A:53:TRP:CE2	1:A:189:TYR:CD2	0.45	3.05	11	1
1:A:56:GLU:OE1	1:A:188:GLN:N	0.45	2.49	3	1
1:A:141:LEU:CD2	1:A:176:ALA:CB	0.45	2.95	3	1
1:A:52:PHE:CE1	1:A:53:TRP:CD1	0.45	3.04	18	1
1:A:118:HIS:NE2	1:A:136:SER:CB	0.45	2.79	3	1
1:A:175:ASN:O	1:A:177:THR:N	0.45	2.50	20	1
1:A:77:THR:O	1:A:92:HIS:NE2	0.45	2.49	14	6
1:A:47:PHE:CE1	1:A:138:ILE:HG23	0.45	2.47	15	1
1:A:115:TRP:HB3	1:A:156:PHE:CE2	0.45	2.47	13	1
1:A:107:TYR:CE2	1:A:148:ALA:HB2	0.45	2.46	4	1
1:A:44:ILE:CG2	1:A:97:ARG:CG	0.45	2.94	10	1
1:A:42:MET:SD	1:A:66:TYR:CD2	0.45	3.10	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLY:CA	1:A:179:PHE:CE2	0.45	3.00	13	1
1:A:118:HIS:NE2	1:A:119:ASP:O	0.45	2.50	19	1
1:A:153:LEU:HD21	1:A:169:ILE:HD11	0.44	1.89	1	1
1:A:101:ASP:N	1:A:101:ASP:OD1	0.44	2.51	8	1
1:A:28:HIS:CD2	1:A:67:SER:HB3	0.44	2.47	2	1
1:A:56:GLU:CD	1:A:70:ALA:HB2	0.44	2.32	2	1
1:A:113:VAL:O	1:A:117:ASN:N	0.44	2.50	3	2
1:A:57:ARG:HA	1:A:60:TRP:CE2	0.44	2.48	12	2
1:A:57:ARG:HE	1:A:190:LEU:HD12	0.44	1.73	19	1
1:A:179:PHE:CZ	1:A:181:TYR:HA	0.44	2.48	16	4
1:A:49:MET:CG	1:A:114:PHE:CE1	0.44	3.00	5	1
1:A:187:GLN:NE2	1:A:188:GLN:NE2	0.44	2.65	11	1
1:A:72:TYR:O	1:A:73:THR:CG2	0.44	2.66	15	1
1:A:161:LEU:HD23	1:A:168:HIS:CD2	0.44	2.47	12	1
1:A:153:LEU:HD12	1:A:173:ILE:HD11	0.44	1.90	10	1
1:A:72:TYR:C	1:A:73:THR:HG23	0.44	2.33	15	1
1:A:69:ALA:HB3	1:A:97:ARG:CG	0.44	2.43	9	1
1:A:65:VAL:HG11	1:A:68:THR:CG2	0.44	2.43	14	1
1:A:58:LEU:CD2	1:A:117:ASN:CG	0.44	2.86	3	1
1:A:47:PHE:CD2	1:A:114:PHE:CE1	0.44	3.05	10	1
1:A:47:PHE:HE1	1:A:138:ILE:HG23	0.44	1.72	15	1
1:A:141:LEU:HD13	1:A:141:LEU:O	0.44	2.12	5	1
1:A:86:SER:O	1:A:133:GLN:NE2	0.44	2.51	5	1
1:A:112:GLN:HA	1:A:115:TRP:CE3	0.44	2.47	12	3
1:A:30:VAL:HG21	1:A:60:TRP:CD1	0.44	2.48	9	1
1:A:49:MET:O	1:A:50:GLY:C	0.44	2.56	16	1
1:A:59:PHE:CD2	1:A:98:ILE:CG1	0.44	3.01	19	1
1:A:115:TRP:O	1:A:118:HIS:ND1	0.44	2.51	6	1
1:A:111:LEU:O	1:A:115:TRP:CG	0.44	2.71	12	1
1:A:168:HIS:NE2	1:A:169:ILE:O	0.44	2.50	9	1
1:A:118:HIS:ND1	1:A:119:ASP:O	0.44	2.50	16	1
1:A:138:ILE:HG21	1:A:149:ALA:HB1	0.44	1.90	18	1
1:A:59:PHE:CD2	1:A:65:VAL:CG1	0.43	3.00	20	1
1:A:35:MET:O	1:A:97:ARG:NH1	0.43	2.51	20	1
1:A:28:HIS:NE2	1:A:188:GLN:CD	0.43	2.71	16	1
1:A:45:ALA:HB3	1:A:98:ILE:HG22	0.43	1.88	20	1
1:A:105:ILE:CD1	1:A:109:GLN:HB2	0.43	2.43	20	1
1:A:142:THR:OG1	1:A:145:GLN:CG	0.43	2.66	11	2
1:A:160:MET:O	1:A:163:ALA:HB3	0.43	2.13	5	3
1:A:137:ALA:HB3	1:A:139:TYR:CE1	0.43	2.49	12	1
1:A:115:TRP:CE2	1:A:152:SER:HB2	0.43	2.48	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ARG:HB2	1:A:179:PHE:CE2	0.43	2.48	6	1
1:A:145:GLN:O	1:A:149:ALA:N	0.43	2.50	13	1
1:A:45:ALA:O	1:A:98:ILE:N	0.43	2.52	17	4
1:A:149:ALA:O	1:A:152:SER:OG	0.43	2.36	17	1
1:A:51:CYS:O	1:A:55:VAL:HG21	0.43	2.13	15	1
1:A:49:MET:HG3	1:A:114:PHE:CE2	0.43	2.48	2	1
1:A:114:PHE:C	1:A:114:PHE:CD1	0.43	2.91	13	2
1:A:88:GLY:CA	1:A:133:GLN:NE2	0.43	2.81	12	1
1:A:65:VAL:HG13	1:A:98:ILE:CG2	0.43	2.43	9	1
1:A:111:LEU:HB3	1:A:115:TRP:CE2	0.43	2.47	18	2
1:A:55:VAL:CG1	1:A:59:PHE:CZ	0.43	3.02	17	1
1:A:42:MET:CE	1:A:66:TYR:CD1	0.43	3.01	20	1
1:A:42:MET:HG2	1:A:99:VAL:CG1	0.43	2.43	3	1
1:A:71:GLY:HA3	1:A:179:PHE:CE2	0.43	2.49	5	2
1:A:97:ARG:CZ	1:A:179:PHE:CB	0.43	2.96	7	1
1:A:52:PHE:CD2	1:A:53:TRP:N	0.43	2.87	12	1
1:A:105:ILE:HD11	1:A:109:GLN:CD	0.43	2.34	16	1
1:A:153:LEU:CD1	1:A:173:ILE:HD11	0.43	2.44	10	1
1:A:72:TYR:CZ	1:A:182:ALA:CA	0.43	3.01	13	2
1:A:58:LEU:HD22	1:A:117:ASN:ND2	0.43	2.28	6	2
1:A:84:GLU:OE2	1:A:90:THR:CG2	0.43	2.67	5	1
1:A:54:GLY:O	1:A:58:LEU:N	0.43	2.51	19	2
1:A:97:ARG:HD3	1:A:179:PHE:CD1	0.43	2.49	19	1
1:A:110:LEU:O	1:A:114:PHE:CB	0.43	2.67	5	1
1:A:57:ARG:HA	1:A:60:TRP:CH2	0.43	2.49	15	1
1:A:107:TYR:CE1	1:A:108:GLU:HG3	0.43	2.49	5	1
1:A:179:PHE:CE1	1:A:181:TYR:N	0.43	2.87	16	2
1:A:147:ALA:O	1:A:151:ALA:N	0.42	2.52	17	1
1:A:182:ALA:O	1:A:183:GLU:C	0.42	2.58	10	4
1:A:46:ILE:HD12	1:A:176:ALA:HB1	0.42	1.89	3	2
1:A:79:ASN:OD1	1:A:79:ASN:N	0.42	2.52	4	1
1:A:118:HIS:C	1:A:118:HIS:ND1	0.42	2.71	19	1
1:A:31:ASN:CG	1:A:66:TYR:O	0.42	2.58	20	4
1:A:49:MET:SD	1:A:114:PHE:CD1	0.42	3.12	16	2
1:A:97:ARG:CZ	1:A:179:PHE:HB2	0.42	2.44	7	1
1:A:59:PHE:CD1	1:A:65:VAL:HG21	0.42	2.45	19	1
1:A:115:TRP:CZ3	1:A:156:PHE:CD2	0.42	3.07	20	1
1:A:42:MET:CG	1:A:99:VAL:CG1	0.42	2.97	13	1
1:A:57:ARG:HA	1:A:60:TRP:CD2	0.42	2.49	14	5
1:A:153:LEU:CD1	1:A:171:THR:CG2	0.42	2.83	10	1
1:A:152:SER:O	1:A:156:PHE:N	0.42	2.52	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ASN:N	1:A:80:PRO:CD	0.42	2.82	12	1
1:A:79:ASN:N	1:A:79:ASN:OD1	0.42	2.52	18	1
1:A:112:GLN:HG3	1:A:113:VAL:N	0.42	2.30	19	1
1:A:149:ALA:O	1:A:153:LEU:N	0.42	2.50	10	1
1:A:59:PHE:CE1	1:A:114:PHE:CE2	0.42	3.08	10	1
1:A:71:GLY:O	1:A:95:ALA:O	0.42	2.38	9	5
1:A:121:ALA:HB3	1:A:167:ARG:O	0.42	2.15	8	1
1:A:115:TRP:CE3	1:A:156:PHE:CZ	0.42	3.08	2	2
1:A:47:PHE:CB	1:A:114:PHE:CZ	0.42	3.02	10	1
1:A:69:ALA:O	1:A:179:PHE:CE2	0.42	2.73	10	1
1:A:142:THR:OG1	1:A:145:GLN:CD	0.42	2.58	11	3
1:A:72:TYR:CE2	1:A:94:GLU:OE2	0.42	2.72	8	1
1:A:182:ALA:O	1:A:187:GLN:NE2	0.42	2.49	2	2
1:A:114:PHE:CZ	1:A:138:ILE:CG1	0.42	3.03	9	1
1:A:107:TYR:HE2	1:A:148:ALA:HB2	0.42	1.73	4	1
1:A:115:TRP:HB3	1:A:156:PHE:CE1	0.42	2.50	19	1
1:A:44:ILE:HG13	1:A:99:VAL:HG13	0.42	1.91	15	1
1:A:78:PRO:O	1:A:79:ASN:CG	0.42	2.58	15	1
1:A:52:PHE:CD1	1:A:52:PHE:C	0.42	2.92	8	1
1:A:188:GLN:O	1:A:188:GLN:CG	0.42	2.67	1	1
1:A:97:ARG:CZ	1:A:181:TYR:OH	0.42	2.67	12	1
1:A:29:ALA:CB	1:A:188:GLN:HG3	0.42	2.45	14	1
1:A:105:ILE:HD13	1:A:106:SER:H	0.42	1.72	11	1
1:A:42:MET:HE2	1:A:101:ASP:OD1	0.42	2.15	11	1
1:A:95:ALA:CB	1:A:179:PHE:CZ	0.42	3.02	11	1
1:A:105:ILE:CD1	1:A:109:GLN:HG2	0.42	2.45	16	1
1:A:160:MET:C	1:A:160:MET:SD	0.42	2.98	16	1
1:A:53:TRP:CG	1:A:189:TYR:HB3	0.42	2.50	5	2
1:A:62:LEU:CD2	1:A:105:ILE:CD1	0.42	2.97	15	1
1:A:111:LEU:C	1:A:111:LEU:HD23	0.41	2.36	17	1
1:A:180:TYR:O	1:A:181:TYR:O	0.41	2.37	15	7
1:A:57:ARG:HG3	1:A:60:TRP:CZ2	0.41	2.50	6	1
1:A:55:VAL:O	1:A:58:LEU:N	0.41	2.53	12	1
1:A:97:ARG:NH1	1:A:181:TYR:OH	0.41	2.53	12	1
1:A:58:LEU:HD22	1:A:117:ASN:OD1	0.41	2.15	4	1
1:A:57:ARG:CG	1:A:60:TRP:CZ2	0.41	3.03	14	1
1:A:189:TYR:CZ	1:A:193:ASN:ND2	0.41	2.87	18	1
1:A:27:LEU:N	1:A:27:LEU:CD1	0.41	2.78	11	1
1:A:71:GLY:CA	1:A:180:TYR:O	0.41	2.67	17	1
1:A:183:GLU:HB2	1:A:186:HIS:CD2	0.41	2.51	15	1
1:A:60:TRP:CH2	1:A:61:GLN:OE1	0.41	2.74	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:TYR:O	1:A:76:TYR:CD1	0.41	2.74	6	1
1:A:24:VAL:HG11	1:A:181:TYR:CD2	0.41	2.51	4	1
1:A:42:MET:SD	1:A:101:ASP:OD1	0.41	2.79	18	1
1:A:105:ILE:C	1:A:105:ILE:CD1	0.41	2.86	18	1
1:A:53:TRP:CE2	1:A:189:TYR:HB3	0.41	2.51	17	1
1:A:42:MET:SD	1:A:100:TYR:O	0.41	2.79	20	1
1:A:169:ILE:HD13	1:A:169:ILE:N	0.41	2.31	10	1
1:A:55:VAL:CG2	1:A:56:GLU:N	0.41	2.83	5	1
1:A:85:VAL:HG12	1:A:133:GLN:HG2	0.41	1.90	19	1
1:A:59:PHE:CE1	1:A:114:PHE:CZ	0.41	3.09	10	1
1:A:29:ALA:CB	1:A:188:GLN:CD	0.41	2.82	1	1
1:A:56:GLU:OE2	1:A:70:ALA:N	0.41	2.53	13	1
1:A:41:GLY:O	1:A:101:ASP:OD1	0.41	2.38	11	2
1:A:94:GLU:O	1:A:94:GLU:OE1	0.41	2.39	16	1
1:A:78:PRO:O	1:A:79:ASN:C	0.41	2.58	12	5
1:A:49:MET:O	1:A:94:GLU:OE1	0.41	2.39	20	1
1:A:72:TYR:C	1:A:73:THR:CG2	0.41	2.89	15	1
1:A:94:GLU:N	1:A:133:GLN:O	0.41	2.54	8	1
1:A:33:HIS:O	1:A:34:SER:C	0.41	2.59	8	4
1:A:39:PRO:O	1:A:40:ASP:C	0.41	2.59	11	2
1:A:98:ILE:HG22	1:A:100:TYR:HD2	0.41	1.75	7	1
1:A:45:ALA:HB1	1:A:47:PHE:HE1	0.41	1.76	9	1
1:A:98:ILE:N	1:A:98:ILE:CD1	0.41	2.84	11	1
1:A:31:ASN:OD1	1:A:66:TYR:O	0.41	2.39	10	1
1:A:73:THR:HB	1:A:179:PHE:CE1	0.41	2.49	4	1
1:A:193:ASN:N	1:A:193:ASN:HD22	0.40	2.14	7	1
1:A:50:GLY:O	1:A:94:GLU:OE1	0.40	2.39	12	1
1:A:60:TRP:C	1:A:62:LEU:N	0.40	2.74	19	1
1:A:153:LEU:HD13	1:A:173:ILE:CD1	0.40	2.47	5	1
1:A:71:GLY:N	1:A:179:PHE:CE2	0.40	2.90	13	1
1:A:69:ALA:HB3	1:A:97:ARG:HD3	0.40	1.94	12	1
1:A:42:MET:SD	1:A:100:TYR:C	0.40	2.99	18	2
1:A:49:MET:O	1:A:94:GLU:OE2	0.40	2.40	4	1
1:A:46:ILE:HG23	1:A:179:PHE:CE1	0.40	2.52	11	1
1:A:112:GLN:OE1	1:A:112:GLN:O	0.40	2.38	19	1
1:A:150:ARG:HG3	1:A:151:ALA:N	0.40	2.31	19	1
1:A:53:TRP:CE2	1:A:189:TYR:CB	0.40	3.04	17	1
1:A:187:GLN:HA	1:A:187:GLN:NE2	0.40	2.30	15	1
1:A:80:PRO:HG3	1:A:92:HIS:CE1	0.40	2.51	5	1
1:A:115:TRP:CH2	1:A:156:PHE:HB2	0.40	2.51	6	1
1:A:190:LEU:O	1:A:193:ASN:O	0.40	2.39	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:GLU:HB3	1:A:90:THR:CG2	0.40	2.46	16	1
1:A:111:LEU:HB2	1:A:115:TRP:CZ2	0.40	2.52	18	1
1:A:49:MET:CE	1:A:117:ASN:HB3	0.40	2.46	17	1
1:A:105:ILE:HD11	1:A:109:GLN:HB3	0.40	1.94	4	1
1:A:95:ALA:CB	1:A:179:PHE:CE2	0.40	3.05	4	1
1:A:42:MET:SD	1:A:101:ASP:CG	0.40	2.99	16	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/211 (77%)	150±2 (92±1%)	11±3 (7±2%)	3±1 (2±1%)	17	61
All	All	3260/4220 (77%)	2992 (92%)	217 (7%)	51 (2%)	17	61

All 11 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	181	TYR	17
1	A	175	ASN	13
1	A	50	GLY	9
1	A	25	ALA	3
1	A	28	HIS	2
1	A	187	GLN	2
1	A	136	SER	1
1	A	51	CYS	1
1	A	34	SER	1
1	A	167	ARG	1
1	A	133	GLN	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/168 (79%)	99±3 (75±3%)	33±3 (25±3%)	3	25
All	All	2640/3360 (79%)	1975 (75%)	665 (25%)	3	25

All 91 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	60	TRP	20
1	A	161	LEU	20
1	A	191	HIS	20
1	A	49	MET	19
1	A	146	ASP	19
1	A	27	LEU	19
1	A	193	ASN	19
1	A	58	LEU	19
1	A	101	ASP	18
1	A	103	SER	15
1	A	40	ASP	15
1	A	185	ASP	15
1	A	190	LEU	15
1	A	83	ARG	15
1	A	62	LEU	14
1	A	179	PHE	13
1	A	155	ARG	13
1	A	35	MET	13
1	A	22	MET	11
1	A	141	LEU	10
1	A	118	HIS	10
1	A	169	ILE	10
1	A	166	ASP	10
1	A	51	CYS	10
1	A	192	LYS	10
1	A	167	ARG	9
1	A	59	PHE	9
1	A	42	MET	9
1	A	33	HIS	9
1	A	34	SER	9
1	A	43	GLU	9
1	A	172	GLU	9
1	A	87	SER	8

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Mol	Chain	Res	Type	Models (Total)
1	A	135	ARG	8
1	A	112	GLN	8
1	A	108	GLU	8
1	A	105	ILE	8
1	A	150	ARG	8
1	A	164	ASP	7
1	A	94	GLU	7
1	A	97	ARG	7
1	A	180	TYR	7
1	A	113	VAL	7
1	A	66	TYR	7
1	A	144	GLU	6
1	A	57	ARG	6
1	A	165	ASP	6
1	A	119	ASP	6
1	A	187	GLN	6
1	A	56	GLU	6
1	A	177	THR	6
1	A	117	ASN	5
1	A	183	GLU	5
1	A	72	TYR	5
1	A	116	GLU	5
1	A	89	ASP	5
1	A	86	SER	5
1	A	156	PHE	4
1	A	188	GLN	4
1	A	52	PHE	4
1	A	157	GLN	4
1	A	37	ASN	3
1	A	53	TRP	3
1	A	184	ASP	3
1	A	61	GLN	3
1	A	153	LEU	3
1	A	79	ASN	3
1	A	168	HIS	3
1	A	136	SER	2
1	A	73	THR	2
1	A	31	ASN	2
1	A	142	THR	2
1	A	115	TRP	2
1	A	171	THR	2
1	A	111	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	154	GLU	2
1	A	160	MET	1
1	A	114	PHE	1
1	A	189	TYR	1
1	A	68	THR	1
1	A	77	THR	1
1	A	134	TYR	1
1	A	98	ILE	1
1	A	76	TYR	1
1	A	109	GLN	1
1	A	90	THR	1
1	A	175	ASN	1
1	A	181	TYR	1
1	A	133	GLN	1
1	A	36	THR	1
1	A	47	PHE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 59% for the well-defined parts and 56% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6786

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1579
Number of shifts mapped to atoms	1579
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}\text{C}_\alpha$	192	-0.45 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	167	-0.53 ± 0.16	Should be applied
$^{13}\text{C}'$	184	-0.45 ± 0.08	None needed (< 0.5 ppm)
^{15}N	172	0.13 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 59%, i.e. 1146 atoms were assigned a chemical shift out of a possible 1935. 10 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	714/791 (90%)	269/314 (86%)	304/326 (93%)	141/151 (93%)
Sidechain	432/917 (47%)	211/539 (39%)	221/342 (65%)	0/36 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/227 (0%)	0/120 (0%)	0/97 (0%)	0/10 (0%)
Overall	1146/1935 (59%)	480/973 (49%)	525/765 (69%)	141/197 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 56%, i.e. 1392 atoms were assigned a chemical shift out of a possible 2472. 12 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	873/1023 (85%)	325/406 (80%)	376/422 (89%)	172/195 (88%)
Sidechain	519/1183 (44%)	245/697 (35%)	274/438 (63%)	0/48 (0%)
Aromatic	0/266 (0%)	0/141 (0%)	0/113 (0%)	0/12 (0%)
Overall	1392/2472 (56%)	570/1244 (46%)	650/973 (67%)	172/255 (67%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	183	GLU	H	11.40	11.34 – 5.34	5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: